

Search Overview

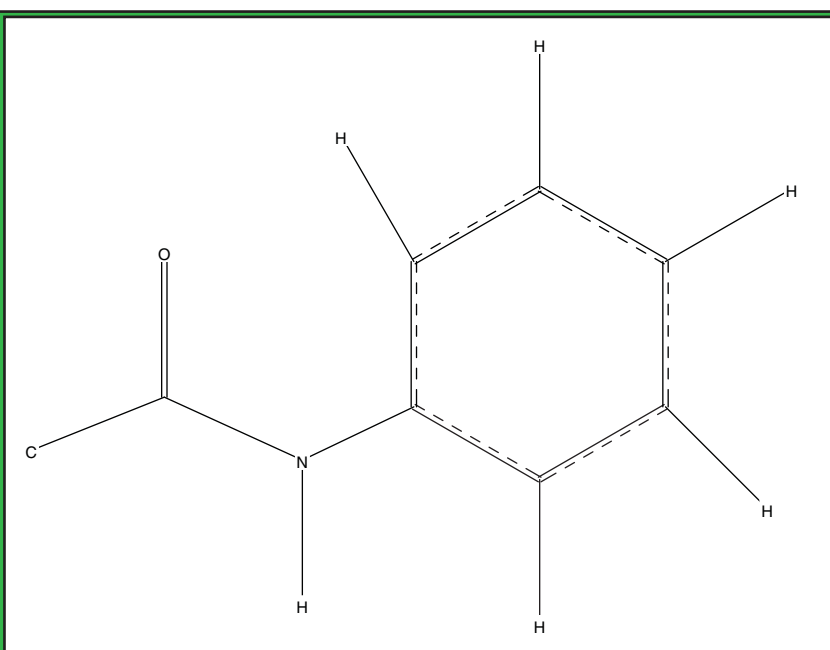
Search: search5
Date/Time done: Sat Feb 09 10:06:45 2013
Database(s): CSD version 5.34 updates (Nov 2012)
CSD version 5.34 (November 2012)
Restriction Info: No refcode restrictions applied
Filters: 3D coordinates determined No ions
No powder structures Only Organics
Percentage Completed: 100%
Number of Hits: 277

Single query used. Search found structures that:

match

Query 1

Query 1



Search: search5 (Sat Feb 09 10:06:45 2013): Hits 1-8

BEBKIE

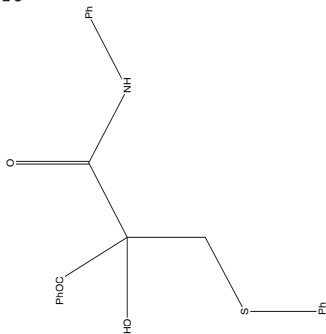
Reference: A. Russo, G. Guidi, G. Croco, A. Lattanzi (2012) *Chem.-Eur.J.*, 18, 1512

Formula: C₂₂H₁₉N₃O₃S₁

Compound Name: (R)-2-hydroxy-3-oxo-N,2-diphenyl-2-(phenylsulfanyl)propanamide

Space Group: P2₁2₁2₁ **Cell:** *a* 5.609(5) *b* 16.194(5) *c* 20.450(6)
Space Group No.: 19 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 8.39 **Temperature(K)**: 293 **Density(g/cm³)**: 1.350

Parameters
Fragment 1
HTOO (D) 2.401
CHO (A) 117.460



LOSJUZO1

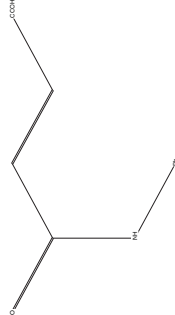
Reference: Shouwen Yan, Yantao Huang, Shaohua Wu, Yong Zhou, Ming Zhou (2012) *Acta Crystallogr. Sect.E: Struct. Rep. Online*, 68, 62738

Formula: C₁₀H₉N₃O₃

Compound Name: 3-(phenylamino)acrylic acid

Synonym: 4-Amino-4-oxobut-2-enoic acid
Space Group: P2₁/n **Cell:** *a* 7.246(6) *b* 10.659(4) *c* 11.779(1)
Space Group No.: 14 **α** 90.00 **β** 89.12(6) **γ** 90.00
R-Factor (%): 4.93 **Temperature(K)**: 298 **Density(g/cm³)**: 1.425

Parameters
Fragment 1
HTOO (D) 2.259
CHO (A) 119.960



RARDEV

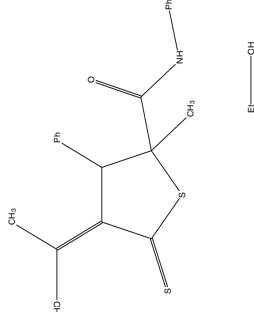
Reference: Feng Yu, Xiaoliang Hu, Xiaodong Gu, Jiarong Ye (2012) *Org.Lett.*, 14, 2038

Formula: C₂₀H₁₉N₃O₂S₂C₂H₅O₁

Compound Name: 4-(1-Hydroxyethylidene)-2-methyl-N,2-diphenyl-5-thioxotetrahydrothiophene-2-carboxamide ethanol solvate

Space Group: P2₁2₁2₁ **Cell:** *a* 8.639(6) *b* 14.148(1) *c* 17.959(1)
Space Group No.: 19 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 3.88 **Temperature(K)**: 293 **Density(g/cm³)**: 1.298

Parameters
Fragment 1
HTOO (D) 2.098
CHO (A) 83.172



ABIXUF

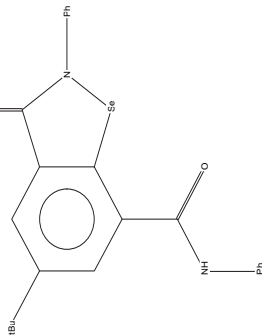
Reference: S.S.Zade, S.Pandit, S.K.Tipathi, H.B.Singh, G.Warnerbauer (2004) *Eur.J.Org.Chem.*, 3857

Formula: C₂₄H₂₂H₂O₂S₄

Compound Name: 5-t-Buyl-2-phenyl-7-(phenylcarbamoyl)benzocyclohexaenol-3(2H)-one

Space Group: P6₃ **Cell:** *a* 18.657(1) *b* 18.671(1) *c* 18.661(1)
Space Group No.: 15 **α** 90.00 **β** 145.28(6) **γ** 90.00
R-Factor (%): 3.49 **Temperature(K)**: 293 **Density(g/cm³)**: 1.417

Parameters
Fragment 1
HTOO (D) 2.251
CHO (A) 120.924



ACAKEU

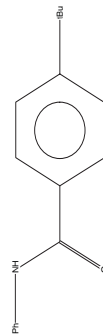
Reference: H.Adams, P.L.Bernad Junior, D.S.Eggleston, R.C.Haltiwanger, K.D.M.Harris, G.A.Hembury, C.A.Hunter, D.J.Livingstone, B.M.Kanuki, J.F.McCabe (2001) *Chem.Commun.*, 1336

Formula: C₁₇H₁₉N₃O₁

Compound Name: N-phenyl-4-t-butylbenzamide

Space Group: P6₃ **Cell:** *a* 12.655(1) *b* 9.291(1) *c* 25.584(5)
Space Group No.: 61 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 6.13 **Temperature(K)**: 296 **Density(g/cm³)**: 1.119

Parameters
Fragment 1
HTOO (D) 2.319
CHO (A) 117.834



ACANIL01

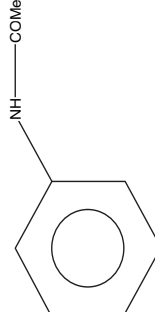
Reference: H.J.Wasserman, R.R.Ryann, S.P.Layne (1985) *Acta Crystallogr. Sect.C:Cryst.Struct.Commun.*, 41,783

Formula: C₉H₉N₃O₁

Compound Name: Acetanilide

Space Group: P6₃ **Cell:** *a* 19.509(11) *b* 9.384(8) *c* 7.778(10)
Space Group No.: 61 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 3.30 **Temperature(K)**: 113 **Density(g/cm³)**: 1.264

Parameters
Fragment 1
HTOO (D) 2.282
CHO (A) 118.019



ACANIL02

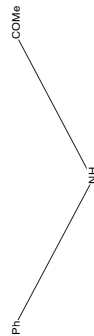
Reference: S.W.Johnson, J.E.Kent, M.Barthele, R.K.McMullan, M.Muller (1995) *J.Phys.Chem.*, 99, 16253

Formula: C₉H₉N₃O₁

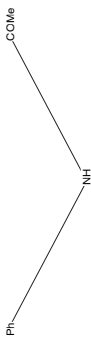
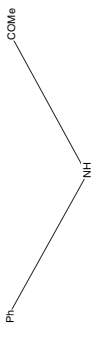
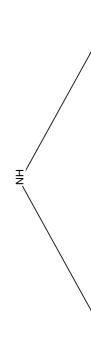
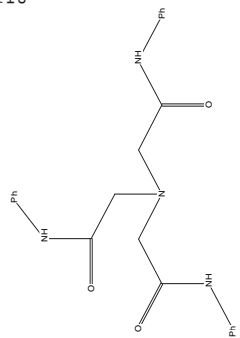
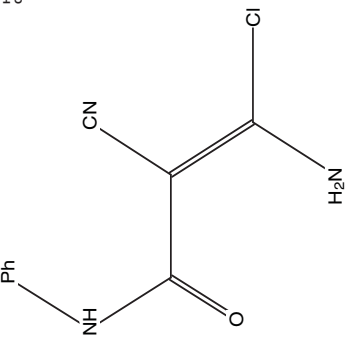
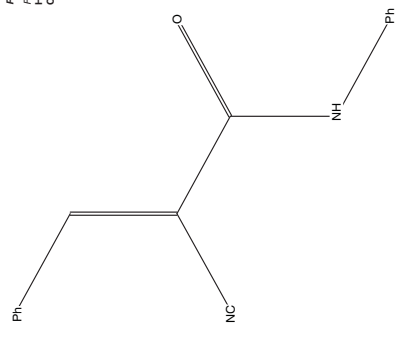
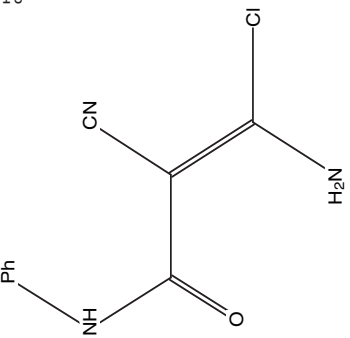
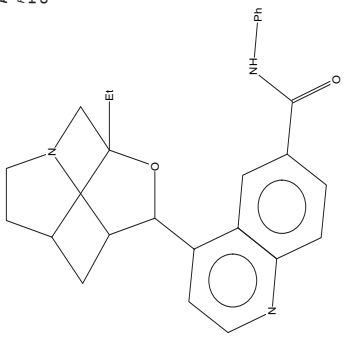
Compound Name: Acetanilide

Space Group: P6₃ **Cell:** *a* 19.468(3) *b* 9.332(1) *c* 7.735(1)
Space Group No.: 61 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 4.70 **Temperature(K)**: 15 **Density(g/cm³)**: 1.278

Parameters
Fragment 1
HTOO (D) 2.232
CHO (A) 114.866



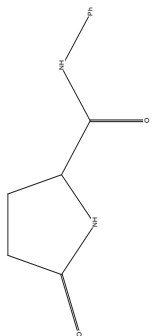
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| ACANIL03 | ACANIL04 | ACANIL05 | ACIBET | AQIKIV | ANOTHI | ACYACR | AXEDUD |
|---|--|--|--|--|---|--|---|
| <p>Reference: S.W.Johnson, J.Eckert, M.Barthele, R.K.McMullin, M.Muller (1999) <i>J.Phys.Chem.</i>, 99, 16253</p> <p>Formula: C₉H₉N₁O₁</p> <p>Compound Name: Acetanilide</p> <p>Space Group: P1 Space Group No.: 1 R-Factor (%): 7.60</p> <p>Cell: a 19.815(3) b 8.774(1) c 7.680(1) (Å, °) α 90.00 β 90.00 γ 90.00</p> <p>Temperature(K): 295 Density(g/cm³): 1.211</p> <p>Parameters Fragment 1 HTOO (D) 2.257 CHO (A) 113.966</p> | <p>Reference: C.J.Brown, D.E.C.Cornbridge (1984) <i>Acta Crystallogr.</i>, 7, 711</p> <p>Formula: C₉H₉N₁O₁</p> <p>Compound Name: Acetanilide</p> <p>Space Group: P1 Space Group No.: 1 R-Factor (%): 0.00</p> <p>Cell: a 18.610 b 8.153 c 7.979 (Å, °) α 90.00 β 90.00 γ 90.00</p> <p>Temperature(K): 295 Density(g/cm³): 1.208</p> <p>Parameters Fragment 1 HTOO (D) 2.233 CHO (A) 116.254</p> | <p>Reference: V.R.Hallwiler, T.S.Thakur, T.N.G.Rao, G.R.Dorainju (2011) <i>Crysil Growth Obs.</i>, 1, 110-116</p> <p>Formula: C₉H₉N₁O₁</p> <p>Compound Name: N-Phenylacetamide</p> <p>Space Group: P1 Space Group No.: 1 R-Factor (%): 2.50</p> <p>Cell: a 9.371(10) b 7.797(0) c 19.530(1) (Å, °) α 90.00 β 90.00 γ 90.00</p> <p>Temperature(K): 100 Density(g/cm³): 1.260</p> <p>Parameters Fragment 1 HTOO (D) 2.244 CHO (A) 114.471</p> | <p>Reference: J.M.Prowland, G.J.Ibanez, M.N.O'Meara, M.P.Li, M.Wassenaar (2001) <i>Acta Crystallogr. Sect.E:Struct.Rep. Online</i>, 57, 01001</p> <p>Formula: C₂₄H₂₄N₄O₂</p> <p>Compound Name: Nitridicacetamide</p> <p>Space Group: P-1 Space Group No.: 2 R-Factor (%): 6.70</p> <p>Cell: a 8.411(2) b 8.819(2) c 14.898(4) (Å, °) α 84.68(0) β 82.42(0) γ 68.44(0)</p> <p>Temperature(K): 91 Density(g/cm³): 1.350</p> <p>Parameters Fragment 1 HTOO (D) 2.410 CHO (A) 116.519</p> <p>Fragment 2 HTOO (D) 0.936 CHO (A) 118.829</p> | <p>Reference: H.D.Black, H.-D.Lodemann, R.Almann (1975) <i>Crysl.Struct.Communic.</i>, 4, 77</p> <p>Formula: C₁₀H₉Cl₁N₃O₁</p> <p>Compound Name: 3-Amino-3-chloro-2-oxo-acylic acid amide</p> <p>Space Group: P-1 Space Group No.: 2 R-Factor (%): 5.70</p> <p>Cell: a 7.817(4) b 10.015(5) c 7.124(4) (Å, °) α 100.15(8) β 107.28(8) γ 72.94(8)</p> <p>Temperature(K): 295 Density(g/cm³): 1.434</p> <p>Parameters Fragment 1 HTOO (D) 2.289 CHO (A) 118.780</p> | <p>Reference: Hengzhen Qi, Xinyao Li, Jiao Xu (2011) <i>Org.Biomol.Chem.</i>, 9, 2702</p> <p>Formula: C₁₆H₁₂N₂O₂</p> <p>Compound Name: 2-Cyano-N-(3-phenylacetyl)acrylamide</p> <p>Space Group: P21/c Space Group No.: 14 R-Factor (%): 4.53</p> <p>Cell: a 12.294(4) b 4.847(1) c 20.381(6) (Å, °) α 90.00 β 91.32(0) γ 90.00</p> <p>Temperature(K): 93 Density(g/cm³): 1.357</p> <p>Parameters Fragment 1 HTOO (D) 2.294 CHO (A) 118.564</p> | <p>Reference: H.D.Black, H.-D.Lodemann, R.Almann (1975) <i>Crysl.Struct.Communic.</i>, 4, 77</p> <p>Formula: C₁₀H₉Cl₁N₃O₁</p> <p>Compound Name: 3-Amino-3-chloro-2-oxo-acylic acid amide</p> <p>Space Group: P-1 Space Group No.: 2 R-Factor (%): 5.70</p> <p>Cell: a 7.817(4) b 10.015(5) c 7.124(4) (Å, °) α 100.15(8) β 107.28(8) γ 72.94(8)</p> <p>Temperature(K): 295 Density(g/cm³): 1.434</p> <p>Parameters Fragment 1 HTOO (D) 2.289 CHO (A) 118.780</p> | <p>Reference: Cheng-Kui Pih, Xiu-Chun Zhang, Min Shi (2011) <i>Eur.J.Org.Chem.</i>, 4, 473</p> <p>Formula: C₂₆H₂₇N₃O₂H₂O</p> <p>Compound Name: N-Phenyl-10,11-dihydro-3,β-epoxycyclohexan-6-carboxamide malonamide</p> <p>Space Group: P212121 Space Group No.: 19 R-Factor (%): 5.45</p> <p>Cell: a 9.551(1) b 12.757(1) c 18.091(3) (Å, °) α 90.00 β 90.00 γ 90.00</p> <p>Temperature(K): 293 Density(g/cm³): 1.259</p> <p>Parameters Fragment 1 HTOO (D) 2.210 CHO (A) 118.769</p> |
|  |  |  |  |  |  |  |  |

AZUZAX

Reference: Wei-Yan Qin, Bo-Liu, Jing Ma, Hui-Juan Wang (2011) *Acta Crystallogr., Sect.E: Struct.Rep.Online* **7**, 02763
Formula: C₁₁H₁₂N₂O₂
Compound Name: (S)-5-Oxo-N-phenylpyrrolidine-2-carboxamide
Synonym: 5-Oxo-N-phenylpyrrolidamide
Space Group: P2₁ **Cell:** *a* 4.918(3) *b* 9.95(7) *c* 10.382(7)
Space Group No.: 4 **α** 90.00 **β** 99.05(3) **γ** 90.00
R-Factor (%): 3.20 **Temperature(K)**: 296 **Density(g/cm³)**: 1.346

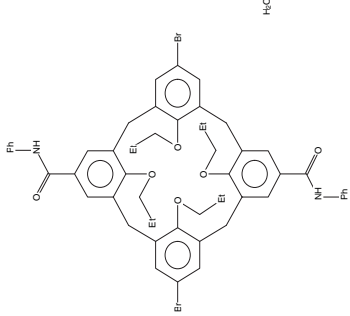
Parameters
Fragment 1
HTOO (D) 2.308
CHO (A) 119.288



BAGVIO

Reference: F.C.Krebs, M.Larsen, M.Jorgensen, P.F.Jensen, M.Balci, K.Schumacher (1998) *J.Org.Chem.* **63**, 872
Formula: C₂₄H₂₀Br₂N₂O₂·0.814(H₂O)
Compound Name: 1,1,2,3-Dibromo-5,7-bis(4-ethoxyphenyl)acetonyl-2,2,3,3-tetrahydropyridin-4(1H)-one hemihydrate
Space Group: P2₁/n **Cell:** *a* 16.025(0) *b* 20.138(0) *c* 20.820(2)
Space Group No.: 14 **α** 90.00 **β** 90.92(0) **γ** 90.00
R-Factor (%): 12.46 **Temperature(K)**: 100 **Density(g/cm³)**: 1.364

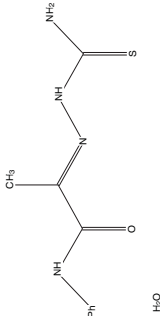
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Fragment 1
HTOO (D) 2.045
CHO (A) 121.485
Fragment 2
HTOO (D) 2.360
CHO (A) 117.100
Fragment 3
HTOO (D) 2.302
CHO (A) 119.574
Fragment 4
HTOO (D) 2.287
CHO (A) 120.167



BEINEM

Reference: V.Kh.Kravtsov, V.A.Brudskii, N.I.Belichuk, T.A.Nikol'skaya (1992) *Kristallografiya/Crystallogr.Rep.* **37**, 17
Formula: C₁₀H₁₂N₂O₁S₁·0.814(H₂O)
Compound Name: Thiosemicarbazone-(methyl)anilido hemihydrate
Space Group: P-1 **Cell:** *a* 11.895(5) *b* 14.395(6) *c* 7.349(4)
Space Group No.: 2 **α** 95.61(5) **β** 94.83(5) **γ** 96.89(5)
R-Factor (%): 6.40 **Temperature(K)**: 295 **Density(g/cm³)**: 1.332

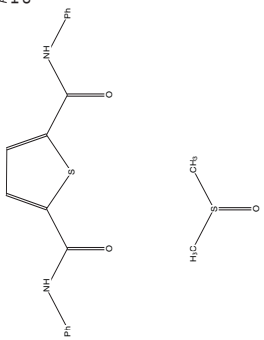
Parameters
Fragment 1
HTOO (D) 2.554
CHO (A) 113.294



BILXEA

Reference: P.A.Gallo, M.B.Humbous, M.E.Light, C.N.Warner (2004) *Collect.Czech.Chem.Commun.* **69**, 3301
Formula: C₁₈H₁₄H₂O₂S₂·2(C₂H₄O₁S₁)
Compound Name: N,N-Diphenylthiophene-2,5-dicarboxamide dimethylsulfoxide solvate
Space Group: P2₁/n **Cell:** *a* 6.658(8) *b* 28.225(8) *c* 8.551(10)
Space Group No.: 14 **α** 90.00 **β** 89.43(6) **γ** 90.00
R-Factor (%): 3.69 **Temperature(K)**: 120 **Density(g/cm³)**: 1.390

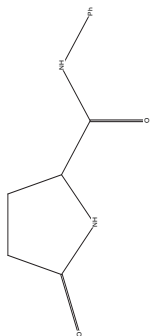
Parameters
Fragment 1
HTOO (D) 2.308
CHO (A) 116.951
Fragment 2
HTOO (D) 2.258
CHO (A) 119.243



BMPAC

Reference: M.van Poucke, A.T.H.Lunstra (1980) *Cryst.Struct.Comm.* **9**, 575
Formula: C₂₂H₁₉N₃O₄
Compound Name: 2-Benzoyl-2-(1,3-dimethyl-2,6-dioxo-7-purifyl)-acetamide
Space Group: C2/c **Cell:** *a* 23.618(7) *b* 9.293(1) *c* 19.082(4)
Space Group No.: 15 **α** 90.00 **β** 98.45(5) **γ** 90.00
R-Factor (%): 5.80 **Temperature(K)**: 295 **Density(g/cm³)**: 1.338

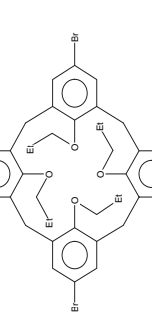
Parameters
Fragment 1
HTOO (D) 2.348
CHO (A) 120.163



BOXFAV

Reference: S.Haikema, R.J.Gaymans, G.J.van Hummel (1983) *Acta Crystallogr., Sect.C: Cryst.Struct.Comm.* **39**, 385
Formula: C₁₈H₂₀N₂O₂
Compound Name: N,N-Diphenylacetamide
Space Group: P6ca **Cell:** *a* 15.228(4) *b* 11.265(3) *c* 8.488(9)
Space Group No.: 61 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 4.20 **Temperature(K)**: 295 **Density(g/cm³)**: 1.209

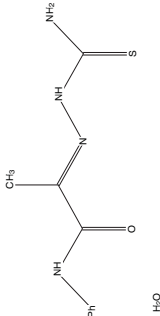
Parameters
Fragment 1
HTOO (D) 2.375
CHO (A) 113.922



BOZJEG

Reference: Guozhong Ye, W.P.Henry, Chunlong Chen, Aihua Zhou, C.U.Pitman Junior (2009) *Tetrahedron Lett.* **50**, 2135
Formula: C₂₁H₂₄N₂O₂·0.9(C₂H₄O₁S₁)
Compound Name: 2-(1,3-Dimethyltetrahydropyrimidin-2(1H)-ylidene)-N,N-diphenyl-N-phenylacetamide
Space Group: P2₁/c **Cell:** *a* 14.376(4) *b* 19.797(5) *c* 8.935(2)
Space Group No.: 14 **α** 90.90 **β** 93.65(6) **γ** 90.90
R-Factor (%): 4.35 **Temperature(K)**: 273 **Density(g/cm³)**: 1.261

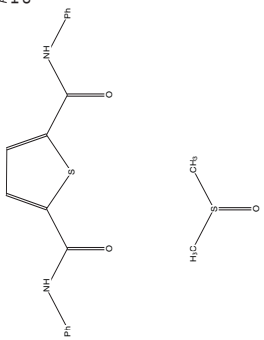
Parameters
Fragment 1
HTOO (D) 2.300
CHO (A) 124.162



BOZJEG

Reference: Guozhong Ye, W.P.Henry, Chunlong Chen, Aihua Zhou, C.U.Pitman Junior (2009) *Tetrahedron Lett.* **50**, 2135
Formula: C₂₁H₂₄N₂O₂·0.9(C₂H₄O₁S₁)
Compound Name: 2-(1,3-Dimethyltetrahydropyrimidin-2(1H)-ylidene)-N,N-diphenyl-N-phenylacetamide
Space Group: P2₁/n **Cell:** *a* 10.655(1) *b* 10.415(1) *c* 20.055(3)
Space Group No.: 14 **α** 90.90 **β** 94.25(6) **γ** 90.90
R-Factor (%): 9.18 **Temperature(K)**: 233 **Density(g/cm³)**: 1.373

Parameters
Fragment 1
HTOO (D) 2.315
CHO (A) 114.228



Search: search5 (Sat Feb 09 10:06:45 2013): Hits 25-32

BOZJIK

Reference: Guozhong Ye, W.P. Henry, Chunlong Chen, Aihua Zhou, C.U. Pittman Junior (2009) *Tetrahedron Lett.* **50**:2 125

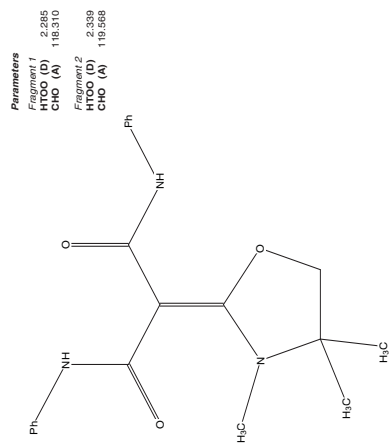
Formula: C₁₇H₂₃N₃O₃

Compound Name: N,N-Diphenyl-2,3,4,4-trimethyl-1,3-oxazolidin-2-ylidene)malonamide

Space Group: P2₁/n **a** 0.775(3) **b** 17.274(5) **c** 11.654(5)

Space Group No.: 14 **α** 90.00 **β** 108.24(6) **γ** 90.00

R-Factor (%): 5.43 **Temperature(K)**: 233 **Density(g/cm³)**: 1.285



BZANIL01

Reference: K.F. Bowers, C. Ghiswain, J.N. Low, J.M.S. Skelton, G. Wandell (2003) *Acta Crystallogr., Sect. C Cryst. Struct. Commun.* **59**, 97-10139

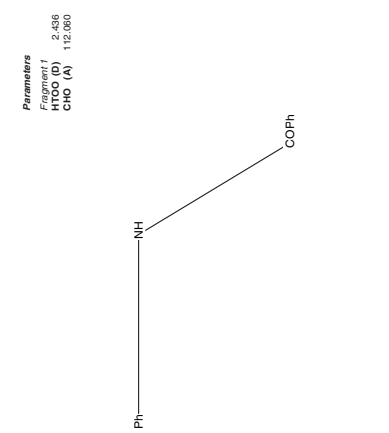
Formula: C₁₃H₁₁N₃O₃

Compound Name: N-Benzoyloxaline

Space Group: P-1 **a** 5.341(0) **b** 7.773(0) **c** 12.390(1)

Space Group No.: 2 **α** 72.74(0) **β** 79.39(0) **γ** 89.91(0)

R-Factor (%): 6.10 **Temperature(K)**: 120 **Density(g/cm³)**: 1.359



CACYOV

Reference: M.C. Elliott, E. Kuswilk, D.J. Wilcock (2001) *Tetrahedron*, **57**:10159

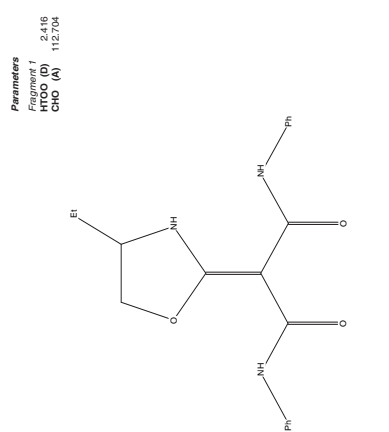
Formula: C₂₀H₂₁N₃O₃

Compound Name: (R)-2-[bis(Phenylcarbamoyl)methylamino]-4-ethyloxazolidine

Space Group: P-1 **a** 8.150(2) **b** 10.825(6) **c** 18.915(10)

Space Group No.: 2 **α** 78.48(1) **β** 80.17(3)

R-Factor (%): 5.36 **Temperature(K)**: 233 **Density(g/cm³)**: 1.341



CASPOC

Reference: Xie-Mei Li, Yong-Hong Wen, Miao-Jie Li, Wang-Feng Zhang (2005) *Acta Crystallogr., Sect. E Struct. Rep. Online*, **61**:023889

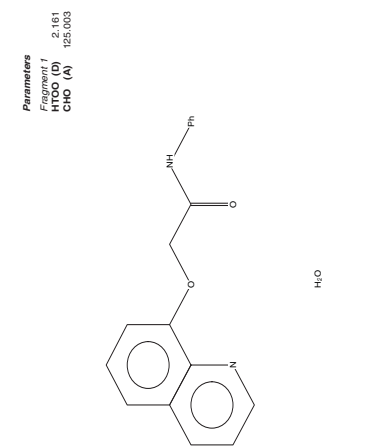
Formula: C₁₇H₁₄N₂O₂·0.5(H₂O)

Compound Name: N-Phenyl-2-(quinolin-8-yl)oxalacetamide hemihydrate

Space Group: C2/c **a** 11.093(5) **b** 12.844(6) **c** 19.584(6)

Space Group No.: 15 **α** 90.00 **β** 91.86(6) **γ** 90.00

R-Factor (%): 4.88 **Temperature(K)**: 293 **Density(g/cm³)**: 1.358



CAYQUP

Reference: Jun Wu, Mei-Feng Chen, Li-Hong Wang, Pei-Zhi Zhang (2005) *Acta Crystallogr., Sect. E Struct. Rep. Online* **61**:03728

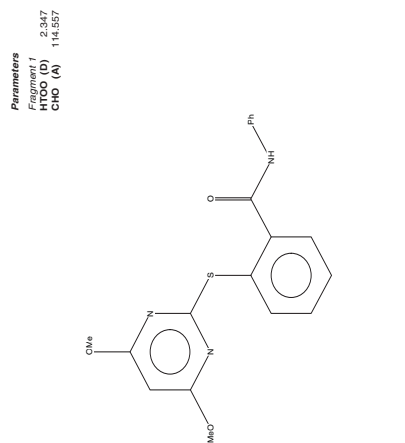
Formula: C₁₉H₁₇N₃O₃S₁

Compound Name: 2-(4,6-Dimethoxyoxypyrimidin-2-ylidene)-N-phenylbenzamide

Space Group: P6ca **a** 9.375(0) **b** 14.485(0) **c** 26.439(0)

Space Group No.: 61 **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 3.30 **Temperature(K)**: 295 **Density(g/cm³)**: 1.380



CIBPIM

Reference: G. Smith, C.H.L. Kennard, G.F. Kabbar (1983) *Aust.J.Chem.* **36**:2455

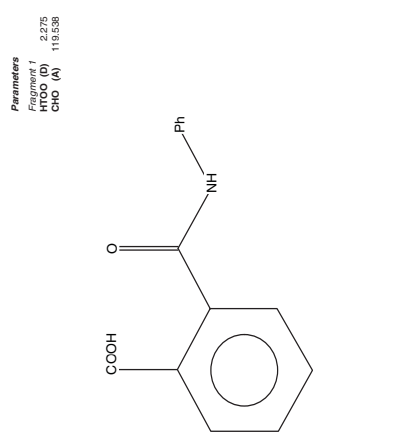
Formula: C₁₄H₁₁N₃O₃

Compound Name: 2-(Phenylcarbamoyl)benzoic acid

Space Group: P2₁/c **a** 10.372(3) **b** 9.564(4) **c** 23.622(6)

Space Group No.: 14 **α** 90.00 **β** 99.11(2) **γ** 90.00

R-Factor (%): 5.80 **Temperature(K)**: 295 **Density(g/cm³)**: 1.385



CIBPIM01

Reference: G. Bocelli, C. Rizzi, O. Chi (1989) *Z.Kristallogr.* **188**:301

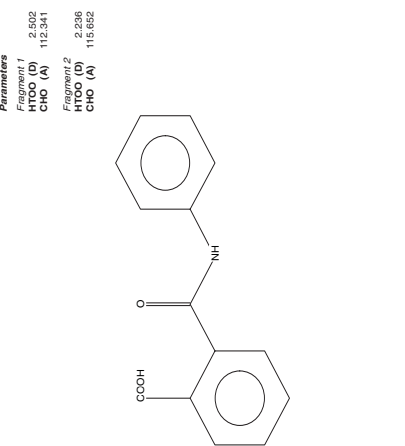
Formula: C₁₄H₁₁N₃O₃

Compound Name: 2-Carboxybenzamide

Space Group: P2₁/a **a** 23.622(3) **b** 9.561(2) **c** 10.372(2)

Space Group No.: 14 **α** 90.00 **β** 99.08(3) **γ** 90.00

R-Factor (%): 5.00 **Temperature(K)**: 295 **Density(g/cm³)**: 1.382



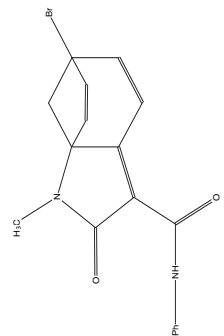
Search: search5 (Sat Feb 09 10:06:45 2013): Hits 33-40

CHSIV

Reference: G.Himbart, K.Diehl, G.Miass (1984) *Chem.Commun.*, 300
Formula: C₁₄H₁₄Br₂N₂O₂
Compound Name: 8-Bromo-2-methyl-4-phenylpyridin-2-aziridinylidene-2,1,0-benzocis-4,6,9-triazepin-5-one

Space Group: P-1
Space Group No.: 2
Cell: a 0.925(2) b 0.565(2) c 10.623(1)
 (A, °) α 71.20(1) β 81.28(1) γ 114.43(2)
Temperature(K): 295 **Density(g/cm³):** 1.527

Parameters
Fragment 1
 HTOO (D) 2.437
 CHO (A) 118.553

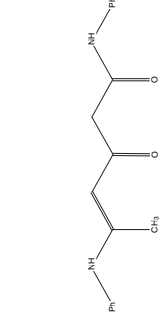


CIMCAC

Reference: P.Bland, A.Dieberg, R.Rogues, S.Castello, V.Nemati, J.Morales (1994) *Acta Crystallogr., Sect. C Cryst. Struct. Commun.*, 40, 1374
Formula: C₁₈H₁₈N₂O₂
Compound Name: 3-Oxo-5-phenylamino-hex-4-ene-antile

Space Group: P2₁/c
Space Group No.: 14
Cell: a 11.131(3) b 15.778(4) c 9.679(2)
 (A, °) α 90.00 β 112.43(2) γ 90.00
Temperature(K): 295 **Density(g/cm³):** 1.244

Parameters
Fragment 1
 HTOO (D) 0.251
 CHO (A) 117.512

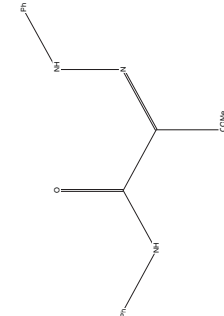


CIVYIP01

Reference: G.V.Gidunova, V.A.Talenko, O.A.Tambina, A.Gidunov (1984) *Zh.Strukt.Khim.(Russ.)*, 32, 55-53
Formula: C₁₈H₁₈N₂O₂
Compound Name: 2-(2-Phenylhydrazono)acetacetanilide

Space Group: P2₁/n
Space Group No.: 14
Cell: a 14.839(2) b 4.529(2) c 21.489(2)
 (A, °) α 90.00 β 104.57(2) γ 90.00
Temperature(K): 295 **Density(g/cm³):** 1.336

Parameters
Fragment 1
 HTOO (D) 0.238
 CHO (A) 115.742

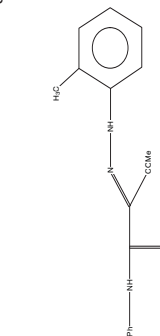


CIVZEM10

Reference: E.F.Paulus, W.Piaper (1989) *Z.Kristallogr.*, 171, 187
Formula: C₁₇H₁₇N₂O₂
Compound Name: N-Phenyl-2-(2-methyl-phenylhydrazono)-3-oxo-butyramido

Space Group: I2/c
Space Group No.: 15
Cell: a 20.982(3) b 11.623(1) c 26.881(4)
 (A, °) α 90.00 β 110.80(1) γ 90.00
Temperature(K): 295 **Density(g/cm³):** 1.282

Parameters
Fragment 1
 HTOO (D) 2.296
 CHO (A) 118.769

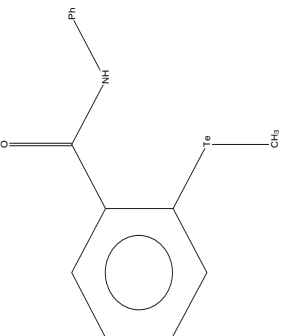


CIZOOR

Reference: R.W.Gable, M.J.Lewis, C.H.Schesser (1989) *Acta Crystallogr., Sect. C Cryst. Struct. Commun.*, 45, 2100
Formula: C₁₄H₁₃N₃O₁Te₁
Compound Name: 2-Methylfluoro-N-phenylbenzamide

Space Group: P6cc
Space Group No.: 61
Cell: a 9.714(2) b 16.742(2) c 16.540(2)
 (A, °) α 90.00 β 90.00 γ 90.00
Temperature(K): 295 **Density(g/cm³):** 1.673

Parameters
Fragment 1
 HTOO (D) 2.328
 CHO (A) 119.857

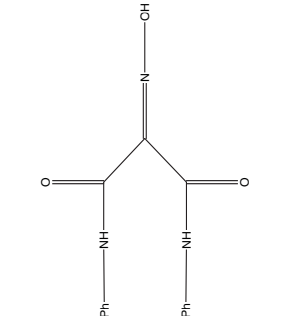


COXROW

Reference: V.D.Jidlov, E.Herdwick, F.P.Schmidbaben (2008) *Chem.-Eur.J.*, 14, 6098
Formula: C₁₈H₁₈N₂O₂
Compound Name: 2,2,8,8-tetraethylphenylcarbamoyl-3,4,6,7,8,9-hexahydro-2H-pyrimido(1,2-b)pyrimidine

Space Group: P-1
Space Group No.: 2
Cell: a 9.858(9) b 12.020(3) c 13.020(4)
 (A, °) α 81.99(2) β 69.12(2) γ 89.93(2)
Temperature(K): 295 **Density(g/cm³):** 1.359

Parameters
Fragment 1
 HTOO (D) 2.371
 CHO (A) 114.916

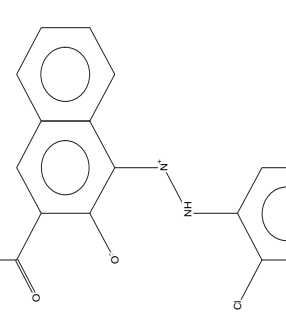


CPZPAN

Reference: A.Whittaker (1977) *Z.Kristallogr.-Krisallogrom., Kristalphys., Kristalchem.*, 146, 173
Formula: C₂₃H₁₅O₂N₃
Compound Name: 1-(2,5-Dichlorophenyl)isox-2-hydroxy-3-phenylamidoanaphthalene

Space Group: P2₁/c
Space Group No.: 14
Cell: a 10.329(6) b 9.051(3) c 21.981(15)
 (A, °) α 90.00 β 104.33(10) γ 90.00
Temperature(K): 15.30 **Density(g/cm³):** 1.458

Parameters
Fragment 1
 HTOO (D) 2.267
 CHO (A) 128.351



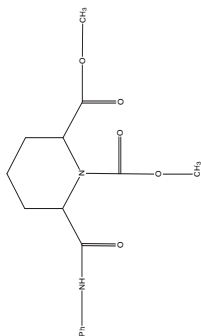
CUPVEO

Reference: K.Irie, K.Aoe, T.Tanaka, S.Saito (1985) *Chem. Commun.*, 653

Formula: C₁₆H₂₀N₂O₅
Compound Name: 1,2-bis(methoxycarbonyl)-6-phenylpiperidine

Synonym: Methyl N-methoxycarbonyl-6-phenylpiperidyl-ascorbate
Space Group: P2₁2₁2₁ *a* 9.808(0) *b* 17.284(0) *c* 9.710(0)
Space Group No.: 19 α 90.00 β 90.00 γ 90.00
R-Factor (%): 6.10 **Temperature(K):** 295 **Density(g/cm³):** 1.294

Parameters
Fragment 1
HTOO (D) 2.245
CHO (A) 123.132



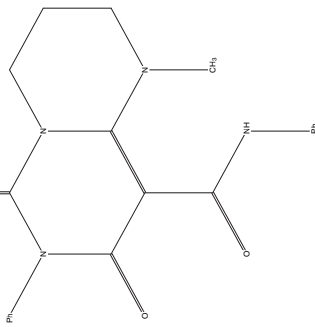
DABPIH

Reference: Guozheng Ye, S.Chatterjee, Min Li, Aihua Zhou, J. Org. Chem., 72, 5297 (2007)
 Cui, P. (2010) *Tetrahedron*, 66, 2519

Formula: C₂₁H₂₂N₄O₃
Compound Name: 1-Methyl-6,8-dioxo-N,7-diphenyl-1,3,4,6,7,8-hexahydro-2H-pyrimido[1,6-*b*]pyrimidine-9-carboxamide

Space Group: P2₁/n *a* 8.420(2) *b* 12.954(3) *c* 17.488(6)
Space Group No.: 14 α 90.00 β 100.43(0) γ 90.00
R-Factor (%): 3.99 **Temperature(K):** 273 **Density(g/cm³):** 1.339

Parameters
Fragment 1
HTOO (D) 2.271
CHO (A) 122.252



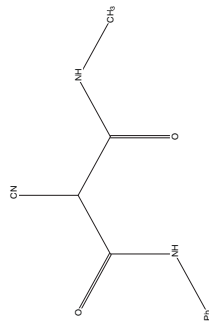
DIUGIN

Reference: A.Basheer, H.Yamatoka, S.C.Ammal, Z.Rappoport (2007) *J.Org.Chem.*, 72, 5297

Formula: C₁₁H₁₁N₃O₂
Compound Name: 2-Cyano-N-phenyl-N-methylacetamide

Space Group: P4₂ *a* 18.937(4) *b* 24.295(5) *c* 8.212(1)
Space Group No.: 45 α 90.00 β 90.00 γ 90.00
R-Factor (%): 4.05 **Temperature(K):** 100 **Density(g/cm³):** 1.338

Parameters
Fragment 1
HTOO (D) 2.232
CHO (A) 121.764



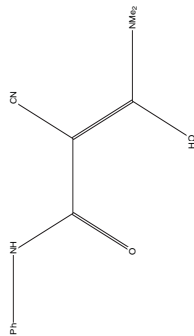
DIUHUA

Reference: A.Basheer, H.Yamatoka, S.C.Ammal, Z.Rappoport (2007) *J.Org.Chem.*, 72, 5297

Formula: C₁₅H₁₃N₃O₂
Compound Name: 2-Cyano-3-(dimethylamino)-3-hydroxy-N-phenylacrylamide

Space Group: P2₁/n *a* 15.757(4) *b* 10.505(2) *c* 8.586(1)
Space Group No.: 14 α 90.00 β 89.85(0) γ 90.00
R-Factor (%): 3.58 **Temperature(K):** 123 **Density(g/cm³):** 1.413

Parameters
Fragment 1
HTOO (D) 2.234
CHO (A) 118.600



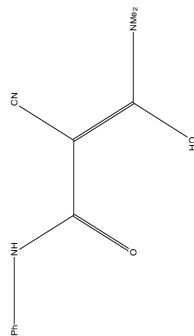
DIUHUA01

Reference: A.Basheer, H.Yamatoka, S.C.Ammal, Z.Rappoport (2007) *J.Org.Chem.*, 72, 5297

Formula: C₁₂H₁₃N₃O₂
Compound Name: 2-Cyano-3-(dimethylamino)-3-hydroxy-N-phenylacrylamide

Space Group: P2₁/n *a* 20.486(5) *b* 9.317(3) *c* 5.900(1)
Space Group No.: 14 α 90.00 β 93.76(0) γ 90.00
R-Factor (%): 7.16 **Temperature(K):** 293 **Density(g/cm³):** 1.366

Parameters
Fragment 1
HTOO (D) 2.177
CHO (A) 120.151



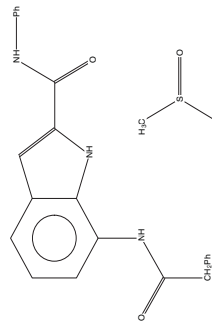
DISTJU

Reference: G.W.Bates, Triyanti, M.E.Light, M.Albrecht, P.A.Gale (2007) *J.Org.Chem.*, 72, 8321

Formula: C₂₃H₁₉N₃O₂S₂H₆O₁S₁
Compound Name: 7-[(Phenylseleno)(amino)-N-phenyl]-1H-indole-2-carboxamide

Space Group: P-1 *a* 9.988(0) *b* 10.374(0) *c* 11.598(0)
Space Group No.: 2 α 70.83(0) β 89.46(0) γ 87.13(0)
R-Factor (%): 5.00 **Temperature(K):** 120 **Density(g/cm³):** 1.338

Parameters
Fragment 1
HTOO (D) 2.392
CHO (A) 114.127



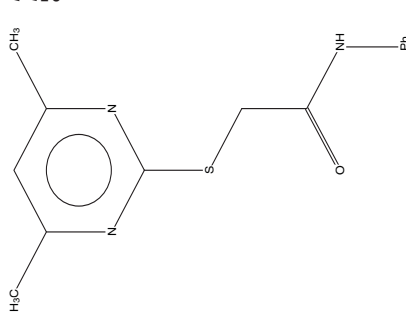
DIWXAJ

Reference: Li-Xin Gao, Guang-Jun Feng, Jin-Guo Feng, Dong-Liang, Wei Wang (2008) *Acta Crystallogr., Sect.E: Struct. Rep. Online* 64, 0760

Formula: C₁₄H₁₅N₃O₁S₁
Compound Name: 2-(4,6-dimethylpyrimidin-2-ylsulfanyl)-N-phenylacetamide

Space Group: P6₃ *a* 9.168(1) *b* 15.485(3) *c* 20.738(4)
Space Group No.: 61 α 90.00 β 90.00 γ 90.00
R-Factor (%): 4.03 **Temperature(K):** 571 **Density(g/cm³):** 1.230

Parameters
Fragment 1
HTOO (D) 2.304
CHO (A) 119.265



DIXCAP

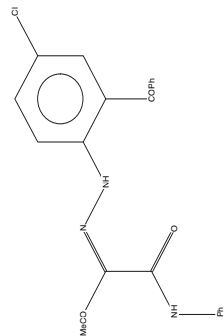
Reference: Z. Bahmani, H. Khavari (2008) *Z. Kristallogr. New Cryst. Struct.*, **223**, 43

Formula: C₂₁H₁₈Cl₁N₂O₃

Compound Name: 2-[(2-Benzyloxy-4-chlorophenyl)diazenyl]-3-oxo-N-phenylbutanamide

Space Group: P2₁/c
Space Group No.: 14
R-Factor (%): 6.35
Temperature(K): 120
Density(g/cm³): 1.387

Parameters
Fragment 1
HTOO (D): 2.309
CHO (A): 120.891



DIXDOD

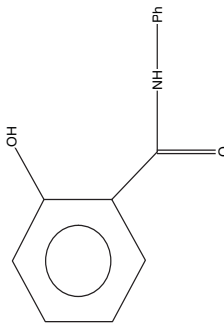
Reference: S. Kishino, T. Mitsuhashi, T. Iwamoto, K. Yamaguchi, M. Hissai (1980) *Acta Crystallogr. Sect. C: Cryst. Struct. Commun.*, **42**, 457

Formula: C₁₃H₁₁N₁O₂

Compound Name: Salicylanilide

Space Group: P2₁
Space Group No.: 6
R-Factor (%): 5.00
Temperature(K): 295
Density(g/cm³): 1.337

Parameters
Fragment 1
HTOO (D): 2.250
CHO (A): 123.059



DOBHEI

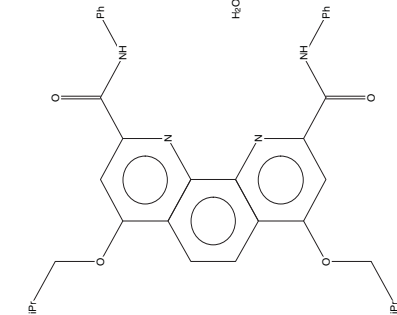
Reference: Hai-Yu Hu, Jun-Feng Xiang, Yong Yang, Qian-Feng Chen (2008) *Org. Lett.*, **10**, 1275

Formula: C₂₄H₂₄N₂O₂·0.8(H₂O)

Compound Name: 4,7-bis(2-methylpropoxy)-N,N'-diphenyl-1,10-phenanthroline-2,9-dicarboxamide hemihydrate

Space Group: P2₁
Space Group No.: 6
R-Factor (%): 6.53
Temperature(K): 113
Density(g/cm³): 1.303

Parameters
Fragment 1
HTOO (D): 2.378
CHO (A): 123.544



DOGPEV

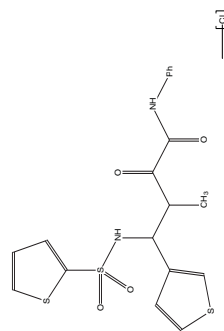
Reference: Gang Liu, H. Morimoto, S. Matsunaga, M. Shibasaki (2008) *Angew. Chem., Int. Ed.*, **47**, 6847

Formula: C₁₉H₁₈H₂O₂S₂C₁H₂Cl₂

Compound Name: (-)-(R)-4-(3-methyl-2-oxo-N-phenyl-4-(thiophen-3-yl)-4-(thiophen-2-sulfonamido)butanamide dichloromethane solvate

Space Group: P-1
Space Group No.: 2
R-Factor (%): 7.77
Temperature(K): 93
Density(g/cm³): 1.508

Parameters
Fragment 1
HTOO (D): 2.493
CHO (A): 112.424



DOGPIZ

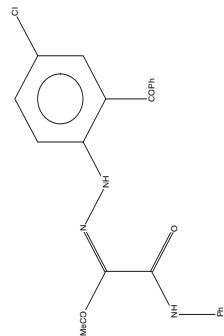
Reference: Gang Liu, H. Morimoto, S. Matsunaga, M. Shibasaki (2008) *Angew. Chem., Int. Ed.*, **47**, 6847

Formula: C₂₁H₂₂N₂O₄S₂

Compound Name: (-)-(R)-3-(4R)-2-hydroxy-3-methyl-N-(4-diphenyl-4-(thiophen-2-sulfonamido)butanamide

Space Group: P2₁/2₁/2₁
Space Group No.: 19
R-Factor (%): 5.06
Temperature(K): 93
Density(g/cm³): 1.444

Parameters
Fragment 1
HTOO (D): 2.297
CHO (A): 122.563



DOGPIZ

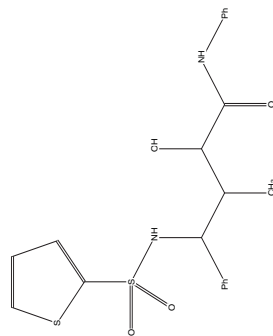
Reference: Gang Liu, H. Morimoto, S. Matsunaga, M. Shibasaki (2008) *Angew. Chem., Int. Ed.*, **47**, 6847

Formula: C₂₁H₂₂N₂O₄S₂

Compound Name: (-)-(R)-3-(4R)-2-hydroxy-3-methyl-N-(4-diphenyl-4-(thiophen-2-sulfonamido)butanamide

Space Group: P2₁/2₁/2₁
Space Group No.: 19
R-Factor (%): 5.06
Temperature(K): 93
Density(g/cm³): 1.444

Parameters
Fragment 1
HTOO (D): 2.297
CHO (A): 122.563



DUJUCJH

Reference: B.T. Gowda, S. Foni, B.S. Sureswathi, H. Fuess (2008) *Acta Crystallogr. Sect. E: Struct. Rep. Online*, **65**, 6364

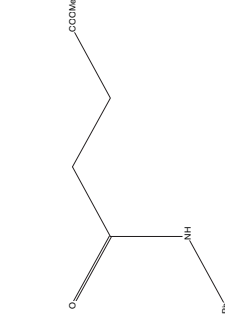
Formula: C₁₁H₁₃N₁O₃

Compound Name: Methyl 4-amino-4-oxobutanoate

Synonym: Methyl N-phenylsuccinamate

Space Group: P2₁
Space Group No.: 3
R-Factor (%): 4.87
Temperature(K): 299
Density(g/cm³): 1.304

Parameters
Fragment 1
HTOO (D): 2.305
CHO (A): 120.970



DUJFOE

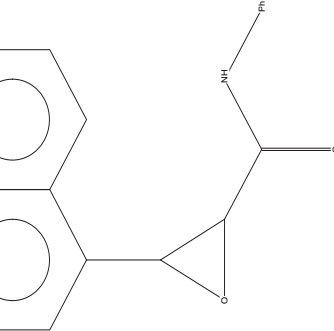
Reference: Lin-Mei Chen, Tai-Ran King (2009) *Acta Crystallogr. Sect. E: Struct. Rep. Online*, **65**, 6317

Formula: C₁₉H₁₅N₁O₂

Compound Name: 3-(1-Naphthyl)-N-phenylpropane-2-carboxamide

Space Group: P2₁/2₁/2₁
Space Group No.: 19
R-Factor (%): 3.20
Temperature(K): 290
Density(g/cm³): 1.245

Parameters
Fragment 1
HTOO (D): 2.301
CHO (A): 120.389



DOUBIO

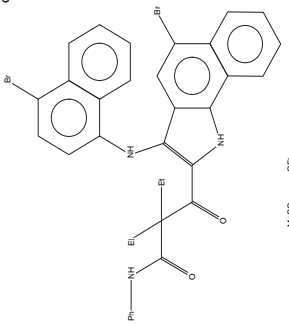
Reference: Gao-Feng Shi, Zhi-Mei Kong, Xiao-Ping Jiang, Ying Cheng (2008) *Synthesis*, **2883**

Formula: C₂₅H₂₅Br₂N₂O₂·0.5(C₂H₄O₂)

Compound Name: 5-Bromo-3-(4-bromonaphthalen-1-ylamino)-2-(2-ethyl-2-(phenylamino)acetyl)butan-1-yl-H-benzo[d]thiazole ethyl acetate solvate

Space Group: P-1
Space Group No.: 2
R-Factor (%): 5.98
Temperature(K): 113
Density(g/cm³): 1.526

Parameters
Fragment 1
HTOO (D): 2.433
CHO (A): 121.210

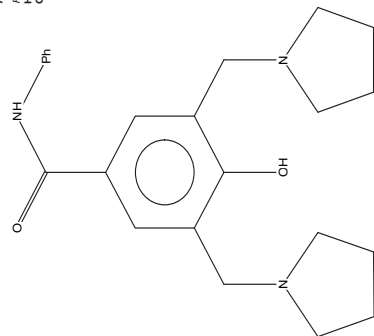


DUTTUH10

Reference: M.L.Glowka, R.L.Daigle, P.W.Coddling (1991) *J.Med.Chem.* 34:2078
Formula: C₂₂H₂₃N₃O₂
Compound Name: 2,6-bis(1-pyrrolidinylmethyl)-4-benzamidoephano

Space Group: P2₁/n
Space Group No.: 14
R-Factor (%): 3.40
Temperature(K): 295
Density(g/cm³): 1.197

Parameters
Fragment 1
HTOO (D) 2.284
CHO (A) 118.655

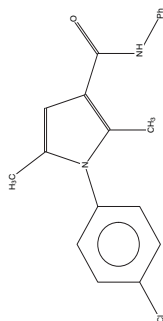


EJEFUV

Reference: Yeming Wang, Xie Bi, Dehua Li, Peiqi Luo, Yanyan Wang, Jun Yang, Qian Zhang, Qun Liu (2011) *Chem Commun.* 47:200
Formula: C₁₇H₁₇ClN₂O
Compound Name: 1-(4-chlorophenyl)-2,5-dimethyl-N-phenyl-1H-pyrrole-3-carboxamide

Space Group: P2₁/c
Space Group No.: 14
R-Factor (%): 6.96
Temperature(K): 293
Density(g/cm³): 1.263

Parameters
Fragment 1
HTOO (D) 0.291
CHO (A) 121.654

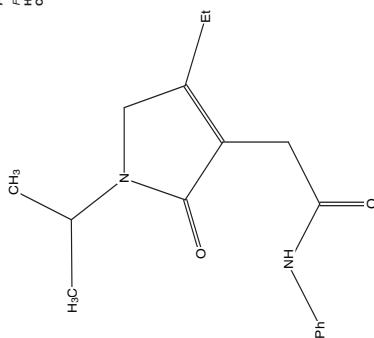


EPCMPO

Reference: G.Audaisio, W.Pozio, L.Zetta, P.Ferruti (1979) *J.Chem.Soc.,Perkin Trans.2* 1391
Formula: C₁₇H₂₂N₂O₂
Compound Name: 4-ethyl-1-isopropyl-3-(phenylcarbamoyl)-methyl-3-pyrrolin-2-one

Space Group: Pca
Space Group No.: 61
R-Factor (%): 4.80
Temperature(K): 295
Density(g/cm³): 1.174

Parameters
Fragment 1
HTOO (D) 2.155
CHO (A) 119.260

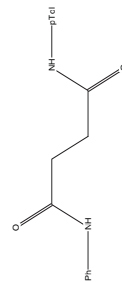


ERUDEB

Reference: B.S.Saraswathi, S.Foro, B.T.Gowda (2011) *Acta Crystallogr., Sect.E:Struct.Rep. Online* 67, o1485
Formula: C₁₇H₁₈N₂O₂H₂O
Compound Name: N-(4-methylphenyl)-N-phenylbutanediamide monohydrate
Synonym: N-(4-Methylphenyl)-N-phenylsuccinamide monohydrate

Space Group: P2₁/n
Space Group No.: 14
R-Factor (%): 11.73
Temperature(K): 293
Density(g/cm³): 1.271

Parameters
Fragment 1
HTOO (D) 0.937
CHO (A) 118.730



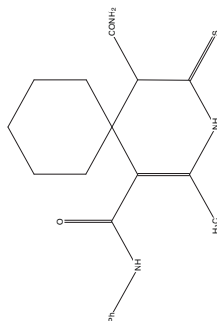
H₂O

EYOPEN

Reference: A.D.Dyachenko, S.M.Dasenko, V.D.Dyachenko, E.B.Rusanov (2003) *Khim.Get.Sost.,SSSR(Russ./Chem.Heterocycl.Comp.)* 372
Formula: C₁₉H₂₄N₂O₂S
Compound Name: 3-Carbonyl-6-methyl-2-thioxo-5-phenylcarbamoyl-1,2,3,4-tetrahydroindolizino[4,3-b]pyridinobenzene

Space Group: C2/c
Space Group No.: 15
R-Factor (%): 6.98
Temperature(K): 295
Density(g/cm³): 1.264

Parameters
Fragment 1
HTOO (D) 0.271
CHO (A) 121.651

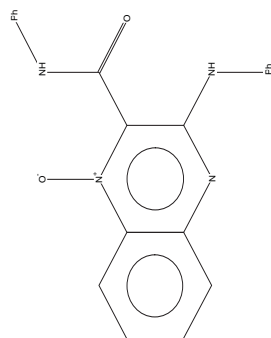


FAQIX

Reference: D.Moya Aguilagos, A.Linden, H.Haemganner (1999) *Helv.Chim.Acta* 82:238
Formula: C₂₁H₁₆N₂O₂
Compound Name: N-Phenyl-3-(phenylamino)quinoline-2-carboxamide 1-oxide

Space Group: Pna2₁
Space Group No.: 33
R-Factor (%): 3.86
Temperature(K): 173
Density(g/cm³): 1.424

Parameters
Fragment 1
HTOO (D) 2.227
CHO (A) 121.958

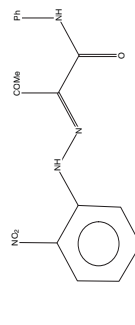
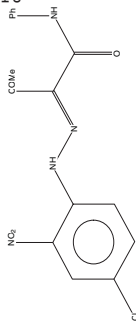


DUXXID

Reference: A.Whitaker (1998) *Acta Crystallogr., Sect.C:Cryst.Struct Commun.* 42:1586
Formula: 0.6(C₁₆H₁₃ClN₂O₂)·0.4(C₁₆H₁₃N₂O₂)
Compound Name: c-(4-Chloro-2-nitrophenyl)hydrazonoacetosuccinamide c-(2-nitrophenyl)hydrazonoacetosuccinamide

Space Group: P2₁/n
Space Group No.: 14
R-Factor (%): 6.50
Temperature(K): 295
Density(g/cm³): 1.453

Parameters
Fragment 1
HTOO (D) 0.264
CHO (A) 117.665

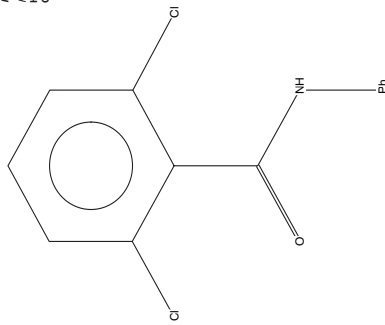


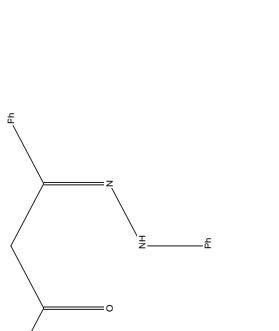
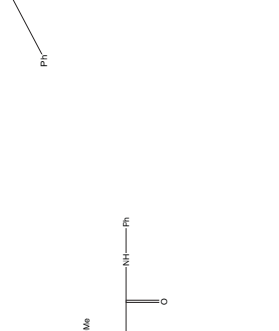
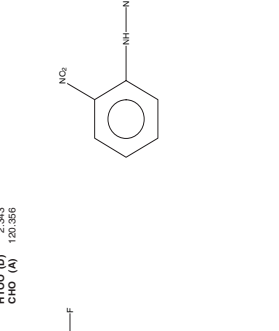
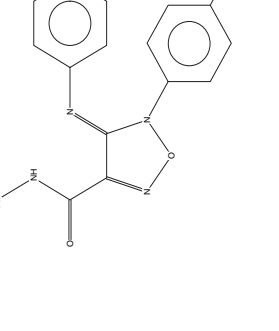
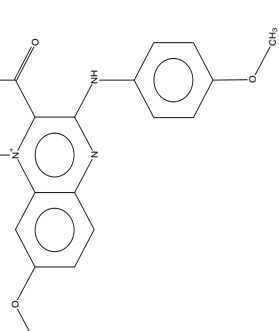

EVEJUL

Reference: Hui Liu, Ning Xu, Bo Yang, Wei Wang, Ping-fang Han (2011) *Acta Crystallogr., Sect.E:Struct.Rep. Online* 67, o1738
Formula: C₁₃H₉Cl₂N₂O
Compound Name: 2,6-Dichloro-N-phenylbenzamide

Space Group: P2₁/c
Space Group No.: 14
R-Factor (%): 6.73
Temperature(K): 293
Density(g/cm³): 1.389

Parameters
Fragment 1
HTOO (D) 2.400
CHO (A) 116.315

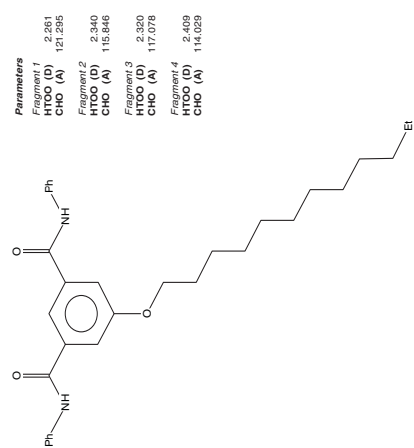


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|---------------|--|---|--|---|
| FAQOOD | <p>Reference: D.Moya Anglada, A.Lindén, H.Hemgärdner (1999) <i>Helv.Chim.Acta</i> 82,238</p> <p>Formula: C₂₁H₂₀N₂O₄</p> <p>Compound Name: 3-(4-Methoxyphenylamino)-7-methoxy-N-phenylquinoline-2-carboxamide 1-oxide</p> | <p>Space Group: P2₁/n</p> <p>Space Group No.: 14</p> <p>R-Factor (%): 4.48</p> <p>Temperature(K): 173</p> <p>Density(g/cm³): 1.390</p> | <p>Parameters</p> <p>Fragment 1</p> <p>HTOO (D): 2.333</p> <p>CHO (A): 119.098</p> |  |
| FAQREU | <p>Reference: D.Moya Anglada, A.Lindén, H.Hemgärdner (1999) <i>Helv.Chim.Acta</i> 82,238</p> <p>Formula: C₂₁H₁₈F₂N₂O₂</p> <p>Compound Name: 5-(4-Fluorophenyl)-4-(4-fluorophenylamino)-4,5-dihydro-N-phenyl-1,2,5-oxadiazole-3-carboxamide</p> | <p>Space Group: I2/a</p> <p>Space Group No.: 15</p> <p>R-Factor (%): 4.98</p> <p>Temperature(K): 173</p> <p>Density(g/cm³): 1.418</p> | <p>Parameters</p> <p>Fragment 1</p> <p>HTOO (A): 0.992</p> <p>CHO (A): 120.123</p> <p>Fragment 2</p> <p>HTOO (A): 2.943</p> <p>CHO (A): 120.358</p> |  |
| FOVNOT | <p>Reference: A.Witaker (1985) <i>Z.Kristallogr.</i> 171,17</p> <p>Formula: C₁₇H₁₇N₃O₂</p> <p>Compound Name: <i>o</i>-(2-Nitrobenzylidenehydrazono)-<i>o</i>-acetylacetanilide</p> <p>Synonym: C.I.Pigment Yellow 5</p> | <p>Space Group: P2₁/n</p> <p>Space Group No.: 14</p> <p>R-Factor (%): 6.60</p> <p>Temperature(K): 295</p> <p>Density(g/cm³): 1.425</p> | <p>Parameters</p> <p>Fragment 1</p> <p>HTOO (A): 2.321</p> <p>CHO (A): 114.719</p> |  |
| FULQEU | <p>Reference: G.M.de Lima, J.L.Wardell, S.M.S.V.Wardell (2010) <i>J.Chem.Cryst.</i> 40,213</p> <p>Formula: C₂₁H₁₉N₃O₁</p> <p>Compound Name: (E)-3,N-Diphenyl-3-(phenylhydrazono)propanamide</p> | <p>Space Group: P2₁/c</p> <p>Space Group No.: 14</p> <p>R-Factor (%): 8.82</p> <p>Temperature(K): 120</p> <p>Density(g/cm³): 1.266</p> | <p>Parameters</p> <p>Fragment 1</p> <p>HTOO (D): 2.365</p> <p>CHO (A): 116.930</p> |  |
| GASTAW | <p>Reference: S.P.Yong, M.C.Williams, S.G.Pyne, A.T.Ung, B.W.Skelton, A.H.White, P.Turner (2005) <i>Tetrahedron</i> 61,18120</p> <p>Formula: C₂₂H₂₂N₂O₂</p> <p>Compound Name: (S)-2-Benzy-1-oxo-N-phenyl-2-azaspiro(4.4)non-7-ene-7-carboxamide</p> | <p>Space Group: Pca2₁</p> <p>Space Group No.: 29</p> <p>R-Factor (%): 6.60</p> <p>Temperature(K): 150</p> <p>Density(g/cm³): 1.253</p> | <p>Parameters</p> <p>Fragment 1</p> <p>HTOO (D): 2.319</p> <p>CHO (A): 117.554</p> |  |
| GASVED | <p>Reference: S.P.Yong, M.C.Williams, S.G.Pyne, A.T.Ung, B.W.Skelton, A.H.White, P.Turner (2005) <i>Tetrahedron</i> 61,18120</p> <p>Formula: C₂₂H₂₂N₂O₂</p> <p>Compound Name: (R)-2-Benzy-1-oxo-N-phenyl-2-azaspiro(4.4)non-6-ene-6-carboxamide</p> | <p>Space Group: P-1</p> <p>Space Group No.: 2</p> <p>R-Factor (%): 5.50</p> <p>Temperature(K): 150</p> <p>Density(g/cm³): 1.320</p> | <p>Parameters</p> <p>Fragment 1</p> <p>HTOO (D): 2.279</p> <p>CHO (A): 118.024</p> |  |
| GASXED | <p>Reference: P.J.Campal, R.A.Mack, V.S.Georgiev (1989) <i>Acta Crystallogr. Sect.C:Cryst.Struct Commun.</i> 44,284</p> <p>Formula: C₁₇H₁₅N₃O₃</p> <p>Compound Name: 2,5-Dihydro-4-(4-methylphenylamino)-2-oxo-5-(N-phenyl)imidazobenzamide</p> | <p>Space Group: C2/c</p> <p>Space Group No.: 15</p> <p>R-Factor (%): 4.50</p> <p>Temperature(K): 295</p> <p>Density(g/cm³): 1.357</p> | <p>Parameters</p> <p>Fragment 1</p> <p>HTOO (D): 2.281</p> <p>CHO (A): 120.894</p> | |
| GECZOE | <p>Reference: Zhi-Qiang Hu, Hai-Yu Hu, Chuan-Feng Chen (2008) <i>J.Org.Chem.</i> 71,1131</p> <p>Formula: C₂₂H₂₂N₂O₂·2(C₆H₅O)</p> <p>Compound Name: 1,2-bis(4,7-Dibutoxy-9-phenylcarbamoyl)-1,10-phenanthroline-2,9-carboximidobiphenylene methanol solvate</p> | <p>Space Group: P-1</p> <p>Space Group No.: 2</p> <p>R-Factor (%): 7.42</p> <p>Temperature(K): 293</p> <p>Density(g/cm³): 1.220</p> | <p>Parameters</p> <p>Fragment 1</p> <p>HTOO (D): 2.292</p> <p>CHO (A): 120.073</p> <p>Fragment 2</p> <p>HTOO (D): 2.220</p> <p>CHO (A): 121.800</p> | |
| GECZOE | <p>Reference: Zhi-Qiang Hu, Hai-Yu Hu, Chuan-Feng Chen (2008) <i>J.Org.Chem.</i> 71,1131</p> <p>Formula: C₂₂H₂₂N₂O₂·2(C₆H₅O)</p> <p>Compound Name: 1,2-bis(4,7-Dibutoxy-9-phenylcarbamoyl)-1,10-phenanthroline-2,9-carboximidobiphenylene methanol solvate</p> | <p>Space Group: P-1</p> <p>Space Group No.: 2</p> <p>R-Factor (%): 7.42</p> <p>Temperature(K): 293</p> <p>Density(g/cm³): 1.220</p> | <p>Parameters</p> <p>Fragment 1</p> <p>HTOO (D): 2.292</p> <p>CHO (A): 120.073</p> <p>Fragment 2</p> <p>HTOO (D): 2.220</p> <p>CHO (A): 121.800</p> | |

| | | | | | | | | | |
|--|--|--|---|--|--|--|--|--|--|
| <p>HAFVOZ</p> <p>Reference: G.V.Gordunova, Z.Iezhkova, M.Yu.Antipin, Zh.Struk.Chim., 2009, 233, 115-4.</p> <p>Formula: C₂₇H₃₁N₃O₂(C₉H₇Cl)</p> <p>Compound Name: 1-(4-Diethylaminophenyl)hydrazo-3-phenylamido-1,2-naphthoquinone chlorobenzene solvate</p> <p>Space Group: C2/c</p> <p>Space Group No.: 15</p> <p>R-Factor (%): 4.30</p> <p>Temperature(K): 295</p> <p>Density(g/cm³): 1.288</p> <p>Parameters Fragment 1 HT00 (D) 2.289 CHO (A) 125.882</p> | <p>HAXRAA</p> <p>Reference: T.Watadani, S.Nunemura, Y.Takahashi, I.F.Hji (2005) Adv.Sci.X-Ray Struct.Anal.Chim., 21,1-131</p> <p>Formula: C₁₉H₁₁N₃O₅</p> <p>Compound Name: (2S,3S)-3-(Phenylcarbamoyl)-2,3-dihydroxypropanoic acid</p> <p>Synonym: (2S,3S)-tartaric acid</p> <p>Space Group: P212121</p> <p>Space Group No.: 19</p> <p>R-Factor (%): 5.88</p> <p>Temperature(K): 297</p> <p>Density(g/cm³): 1.510</p> <p>Parameters Fragment 1 HT00 (D) 2.252 CHO (A) 182.402</p> | <p>HALXEZ</p> <p>Reference: A.G.Larina, A.V.Shepkov, V.M.Bobkov, A.P.Mochalov, L.Guzhny, O.L.Sarova, A.N.Lyubalya (2011) Tomskgor. List., 52, 877</p> <p>Formula: C₂₄H₂₄N₂O₂</p> <p>Compound Name: 4-(Bicyclo[4.1.0]hept-7-ylidene)-2-(4-methylphenyl)-N,6,5-triphenyl-1,2-oxazolone-3-carboxamide</p> <p>Space Group: P-1</p> <p>Space Group No.: 2</p> <p>R-Factor (%): 4.26</p> <p>Temperature(K): 210</p> <p>Density(g/cm³): 1.197</p> <p>Parameters Fragment 1 HT00 (D) 2.936 CHO (A) 119.624</p> | <p>HAJTUI</p> <p>Reference: I.B.D.Wign, P.A.Gala, M.B.HusHouse, M.E.Light (2004) Org.Letters, 26,265</p> <p>Formula: C₂₉H₃₀N₄O₂C₁₀H₈O₁</p> <p>Compound Name: 5-(2-(5-Phenylcarbamoyl)-3,4-dimethyl-1H-pyridin-2-yl)-3,4-dimethyl-N-phenyl-1H-pyridin-2-carboxamide methanol solvate</p> <p>Space Group: P212121</p> <p>Space Group No.: 19</p> <p>R-Factor (%): 7.65</p> <p>Temperature(K): 120</p> <p>Density(g/cm³): 1.244</p> <p>Parameters Fragment 1 HT00 (D) 2.927 CHO (A) 120.556</p> | <p>HERSH</p> <p>Reference: C.P.Olmo, K.Bohmke, G.Stierfeld, H.Vahrenkamp (2008) Eur.J.Inorg.Chem., 3869</p> <p>Formula: (Cat)₂H₂Br₂N₄O₂h₂(5-Me₂C₄H₆O₂)</p> <p>Compound Name: catena-(μ₂-Hydrogen bis(3-(N-phenylcarbamoyl)-5-methylpyrazolyl)borato)squa(methanol)-potassium methanol solvate</p> <p>Space Group: P-1</p> <p>Space Group No.: 2</p> <p>R-Factor (%): 5.54</p> <p>Temperature(K): 293</p> <p>Density(g/cm³): 1.302</p> <p>Parameters Fragment 1 HT00 (D) 2.443 CHO (A) 112.550</p> | <p>HORVUV</p> <p>Reference: V.N.Nesterov (1988) Kristallografiya(Russ.)(Crystallogr.Rep.), 43,847</p> <p>Formula: C₂₂H₁₉N₃O₂</p> <p>Compound Name: 1-Ethyl-2-(3-phenylcarbamoyl-3-cyanoprop-2-enylidene)-1,2-dihydroquinoline</p> <p>Space Group: P21/c</p> <p>Space Group No.: 14</p> <p>R-Factor (%): 6.20</p> <p>Temperature(K): 295</p> <p>Density(g/cm³): 1.288</p> <p>Parameters Fragment 1 HT00 (D) 2.217 CHO (A) 122.431</p> | <p>HOBTEC</p> <p>Reference: A.R.Razi, M.Danish, M.N.Tahir, B.Nisar, G.Park (2009) Acta Crystallogr., Sect.E Struct.Rep. Online, 65,01042</p> <p>Formula: C₁₃H₁₀N₂O₄</p> <p>Compound Name: 2-Hydroxy-3-nitro-N-phenylbenzamide</p> <p>Space Group: P21/n</p> <p>Space Group No.: 14</p> <p>R-Factor (%): 4.84</p> <p>Temperature(K): 296</p> <p>Density(g/cm³): 1.454</p> <p>Parameters Fragment 1 HT00 (D) 2.330 CHO (A) 117.141</p> | <p>HERSH</p> <p>Reference: Ting-Ting Long, Meili-Yueh-Jean, Tai-Jung Liu (1994) Acta Crystallogr., Sect.C Cryst. Struct. Commun., 50,1359</p> <p>Formula: C₁₆H₁₃N₃O₁</p> <p>Compound Name: (1S,2S,5R,6S)-1-(4-Carbamiloxy)-1,5-dimethylcyclo[3.2.0]p₅o</p> <p>Space Group: P212121</p> <p>Space Group No.: 19</p> <p>R-Factor (%): 6.34</p> <p>Temperature(K): 295</p> <p>Density(g/cm³): 1.101</p> <p>Parameters Fragment 1 HT00 (D) 2.316 CHO (A) 114.483</p> | <p>HERSH</p> <p>Reference: Ting-Ting Long, Meili-Yueh-Jean, Tai-Jung Liu (1994) Acta Crystallogr., Sect.C Cryst. Struct. Commun., 50,1359</p> <p>Formula: C₁₆H₁₃N₃O₁</p> <p>Compound Name: (1S,2S,5R,6S)-1-(4-Carbamiloxy)-1,5-dimethylcyclo[3.2.0]p₅o</p> <p>Space Group: P212121</p> <p>Space Group No.: 19</p> <p>R-Factor (%): 6.34</p> <p>Temperature(K): 295</p> <p>Density(g/cm³): 1.101</p> <p>Parameters Fragment 1 HT00 (D) 2.278 CHO (A) 120.594</p> | <p>HERSH</p> <p>Reference: Ting-Ting Long, Meili-Yueh-Jean, Tai-Jung Liu (1994) Acta Crystallogr., Sect.C Cryst. Struct. Commun., 50,1359</p> <p>Formula: C₁₆H₁₃N₃O₁</p> <p>Compound Name: (1S,2S,5R,6S)-1-(4-Carbamiloxy)-1,5-dimethylcyclo[3.2.0]p₅o</p> <p>Space Group: P212121</p> <p>Space Group No.: 19</p> <p>R-Factor (%): 6.34</p> <p>Temperature(K): 295</p> <p>Density(g/cm³): 1.101</p> <p>Parameters Fragment 1 HT00 (D) 2.278 CHO (A) 120.594</p> |
|--|--|--|---|--|--|--|--|--|--|

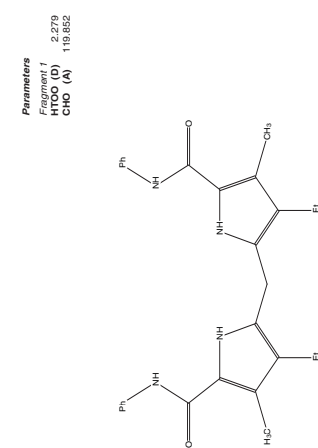
HURSOC

Reference: Ailing Fan, S.Vaiveerathi, J.J.Vitali (2003) *CrystEngComm*, 3,36
Formula: C₂₉H₄₀N₂O₃
Compound Name: 5-(Dodecoyl)-N,N'-diphenylisophthalamide
Space Group: P2₁/c *a* 17.75(6) *b* 4.526(4) *c* 24.620(8)
Space Group No.: 23 *α* 90.00 *β* 90.00 *γ* 90.00
R-Factor (%): 5.97 **Temperature(K):** 223 **Density(g/cm³):** 1.131



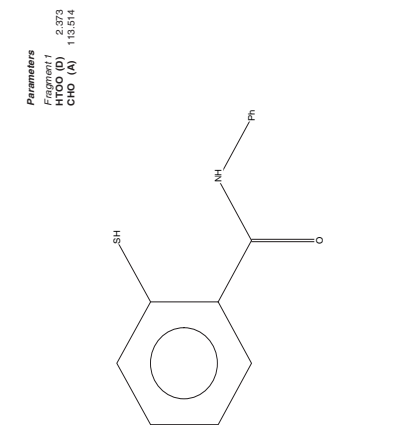
ILIVEE

Reference: LEID Vega, S.Cimolo, P.A.Gale, M.B.Hursthous, M.E.Light (2003) *Chem Commun.*, 1886
Formula: C₂₉H₃₂N₂O₂
Compound Name: 5-(5-methylnitrophenyl)-4-ethyl-3-methyl-1H-pyrole-2-carboxamide
Space Group: P2₁/c *a* 11.011(3) *b* 17.487(3) *c* 13.771(2)
Space Group No.: 14 *α* 90.00 *β* 95.63(1) *γ* 90.00
R-Factor (%): 6.46 **Temperature(K):** 120 **Density(g/cm³):** 1.180



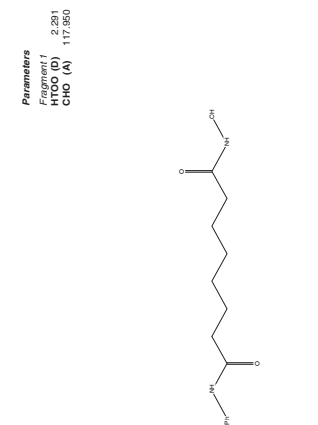
ICOPUN

Reference: Yumiao Han, Qun Luo, Xiang Hao, Xianchen Li, Jintao Li, Kun Wu, Shuang Lu, P.J.Slater (2011) *Dalton Trans.*, 40, 11519
Formula: C₁₃H₁₁N₂O₂S₁
Compound Name: N-Phenyl-2-sulfanybenzamide
Space Group: P2₁/2₁2₁ *a* 9.638(1) *b* 11.635(2) *c* 20.051(4)
Space Group No.: 19 *α* 90.00 *β* 90.00 *γ* 90.00
R-Factor (%): 3.55 **Temperature(K):** 173 **Density(g/cm³):** 1.355



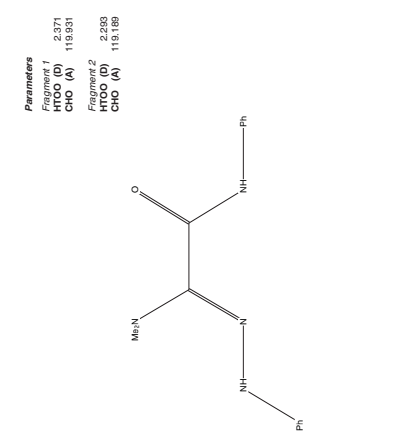
IQILAW

Reference: D.M.Griffin, B.Szoes, T.Keogh, X.Yu,Suponissav, E.Farkas, P.Bajfy, C.J.Mannion (2011) *J.Horg Biochem.*, 105,743
Formula: C₁₄H₂₆N₂O₃
Compound Name: N-Hydroxy-N'-phenyloctanediamide
Space Group: P2₁/n *a* 10.994(1) *b* 7.748(1) *c* 16.388(9)
Space Group No.: 14 *α* 90.00 *β* 98.82(0) *γ* 90.00
R-Factor (%): 4.85 **Temperature(K):** 100 **Density(g/cm³):** 1.271



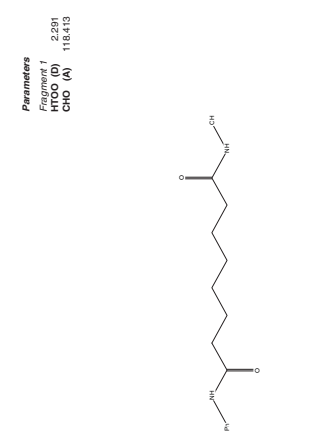
ICUZIQ

Reference: P.Frohberg, C.Wagner, R.Meier, W.Spi (2006) *Tetrahedron*, 62,1050
Formula: C₁₇H₁₈N₂O₁
Compound Name: (E)-2-(dimethylamino)-N-phenyl-2-(phenylhydrazono)acetamide (Z)-2-(dimethylamino)-N-phenyl-2-(phenylhydrazono)acetamide
Space Group: P2₁/c *a* 11.770(4) *b* 15.400(4) *c* 17.382(8)
Space Group No.: 14 *α* 90.00 *β* 102.13(3) *γ* 90.00
R-Factor (%): 4.74 **Temperature(K):** 293 **Density(g/cm³):** 1.219



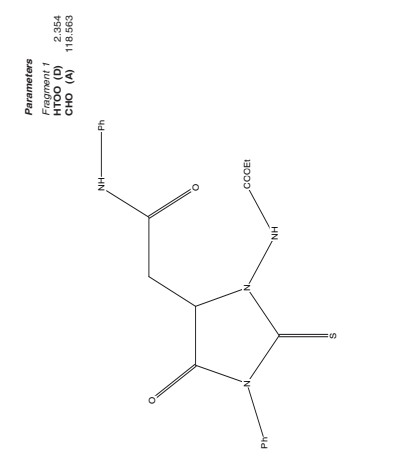
IQILAW01

Reference: C.Pulgauer, R.Barbas, A.Porelli, I.Valvoda, X.Vila, X.Ancos, M.Font-Bardia, R.Peters (2012) *CrystEngComm*, 14,382
Formula: C₁₄H₂₆N₂O₃
Compound Name: N-Hydroxy-N'-phenyloctanediamide
Space Group: P2₁/n *a* 10.983(7) *b* 7.853(4) *c* 16.433(6)
Space Group No.: 14 *α* 90.00 *β* 97.92(3) *γ* 90.00
R-Factor (%): 5.11 **Temperature(K):** 293 **Density(g/cm³):** 1.237



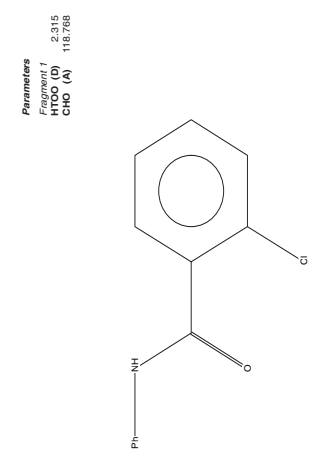
IFAYUH

Reference: S.Bouzroun, L.Hammal, B.Medjer-Kelli, F.Balagouna, M.Hamadine, S.Poulin (2007) *Symm Commun.*, 38,448
Formula: C₂₆H₂₆N₂O₄S₁
Compound Name: Ethyl (4-oxo-5-(2-oxo-2-phenylamino)ethyl)-3-phenyl-2-thioximidazolidin-1-ylacetamide
Space Group: P-1 *a* 7.964 *b* 9.148 *c* 14.145
Space Group No.: 2 *α* 94.53 *β* 90.47 *γ* 101.41
R-Factor (%): 5.65 **Temperature(K):** 293 **Density(g/cm³):** 1.361



IOOHIF

Reference: B.T.Gawda, K.Jothi, H.Paulus, H.Fuess (2003) *Z.Naturforsch., A:Phys.Sci.*, 58,225
Formula: C₁₃H₁₀Cl₁N₁O₁
Compound Name: 2-chloro-N-phenylbenzamide
Space Group: P43 *a* 8.795(4) *b* 8.795(4) *c* 15.115(6)
Space Group No.: 78 *α* 90.00 *β* 90.00 *γ* 90.00
R-Factor (%): 4.75 **Temperature(K):** 296 **Density(g/cm³):** 1.316

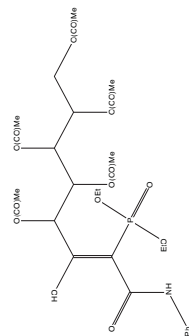


IQOOEL

Reference: H.Renke, R.Meisel, K.Peske (2010) *Private Communication*,
Formula: C₂₀H₂₄N₂O₁₅F₁₁
Compound Name: 4,5,6,7,8-penta-O-acetyl-2-deoxy-2-deoxyphosphono-D-galacto-3-
 octulosonic acid anilide

Space Group: P2₁2₁2₁ **a** 13.028(1) **b** 15.806(1) **c** 16.183(2)
Space Group No.: 19 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 8.16 **Temperature(K)**: 233 **Density(g/cm³)**: 1.315

Parameters
Fragment 1
HTOO (D) 2.458
CHO (A) 112.168

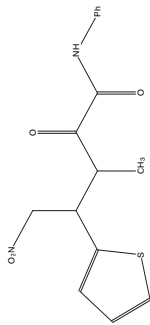


IOUZUQ

Reference: O.Bask, W.Raimondi, M.de M.S.Duque, D.Bonito,
 I.Costantino, J.Rodriguez (2010) *Org.Lett.*, 12,3246
Formula: C₁₆H₁₈N₂O₄S₁
Compound Name: 3-Methyl-5-nitro-2-oxo-N-phenyl-4-(2-thenyl)pentanamide

Space Group: P2₁ **a** 15.707(5) **b** 5.657(5) **c** 18.456(5)
Space Group No.: 4 **α** 90.00 **β** 105.53(6) **γ** 90.00
R-Factor (%): 9.97 **Temperature(K)**: 293 **Density(g/cm³)**: 1.351

Parameters
Fragment 1
HTOO (D) 2.371
CHO (A) 117.350

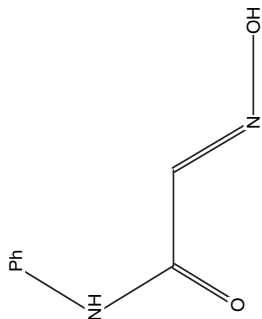


ISNACN10

Reference: J.L.Blanco, C.Miravettes, M.Forn-Alaba, J.P.Delcort,
 G.Guaman (1973) *Cryst.Struct.Comm.*, 2,319
Formula: C₉H₈N₂O₂
Compound Name: Isotonosacetanilide

Space Group: P2₁ **a** 8.672 **b** 17.710 **c** 8.186
Space Group No.: 8 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 7.60 **Temperature(K)**: 295 **Density(g/cm³)**: 1.389

Parameters
Fragment 1
HTOO (D) 2.335
CHO (A) 118.924

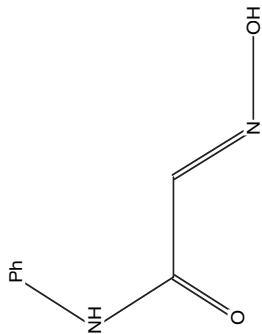


ISNACN11

Reference: Shaojie Liu, Mingliang Ma, Hongyu Zhou, Yan Li, Ling Han
 (2006) *Acta Crystallogr., Sect.E:Struct.Relat.Phys.Chem.*, 62,3116
Formula: C₉H₈N₂O₂
Compound Name: (E)-2-(Hydroxyimino)-N-phenylacetamide

Space Group: P2₁ **a** 8.655(1) **b** 9.147(1) **c** 17.676(2)
Space Group No.: 8 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 4.79 **Temperature(K)**: 293 **Density(g/cm³)**: 1.394

Parameters
Fragment 1
HTOO (D) 2.346
CHO (A) 121.222

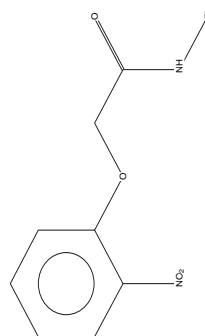


ISUTIZ

Reference: C.Giddewill, J.Ni, J.M.S.Skakke, J.L.Wardell (2004)
Acta Crystallogr., Sect.C:Cryst.Struct.Comm., 60,0230
Formula: C₁₁H₁₂N₂O₄
Compound Name: 2-Nitrophenoxycetanilide

Space Group: P2₁ **a** 8.586(5) **b** 6.613(5) **c** 22.022(5)
Space Group No.: 14 **α** 90.00 **β** 91.83(5) **γ** 90.00
R-Factor (%): 4.00 **Temperature(K)**: 120 **Density(g/cm³)**: 1.447

Parameters
Fragment 1
HTOO (D) 2.315
CHO (A) 120.641

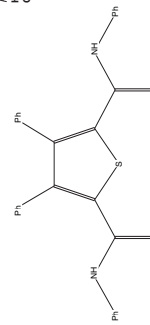


JALCUJ

Reference: S.J.Coles, P.A.Gale, M.B.Hughes, M.E.Light,
 C.N.Warner (2004) *Supramol.Chem.*, 16,469
Formula: C₂₀H₂₂N₂O₂S₁
Compound Name: 3,4-Diphenylthiophene-2,5-dicarboxylic acid diphenylamide

Space Group: P-1 **a** 8.478(5) **b** 9.748(5) **c** 26.135(5)
Space Group No.: 2 **α** 97.48(5) **β** 90.72(5) **γ** 92.98(5)
R-Factor (%): 4.14 **Temperature(K)**: 120 **Density(g/cm³)**: 1.319

Parameters
Fragment 1 2.337
HTOO (D) 120.129
CHO (A) 115.188
Fragment 2 2.385
HTOO (D) 115.188
Fragment 3 2.491
HTOO (D) 112.164
CHO (A) 112.164

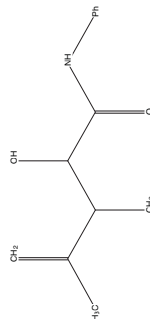


JAQYAC

Reference: D.A.Evans, J.Wu (2005) *J.Am.Chem.Soc.*, 127,8008
Formula: C₁₃H₁₇N₁O₂
Compound Name: (2S,3R)-2-Hydroxy-3,4-dimethyl-N-phenylpent-4-enamide

Space Group: P2₁/c **a** 12.503(2) **b** 11.806(2) **c** 8.403(1)
Space Group No.: 14 **α** 90.00 **β** 94.85(5) **γ** 90.00
R-Factor (%): 4.69 **Temperature(K)**: 193 **Density(g/cm³)**: 1.179

Parameters
Fragment 1 2.329
HTOO (D) 121.222
CHO (A) 121.222

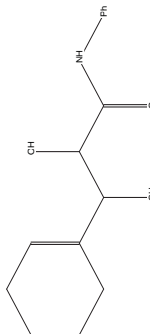


JAQYEG

Reference: D.A.Evans, J.Wu (2005) *J.Am.Chem.Soc.*, 127,8008
Formula: C₁₈H₂₁N₁O₂
Compound Name: (2S,3R)-3-Cyclohexenyl-2-hydroxy-N-phenylbutanamide

Space Group: P2₁ **a** 9.030(1) **b** 9.509(1) **c** 9.030(1)
Space Group No.: 4 **α** 90.00 **β** 112.32 **γ** 90.00
R-Factor (%): 5.89 **Temperature(K)**: 213 **Density(g/cm³)**: 1.201

Parameters
Fragment 1 2.356
HTOO (D) 121.222
CHO (A) 121.222

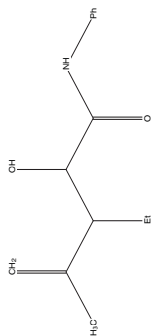


JAQYIK

Reference: D.A.Evans, J.Wu (2005) *J.Am.Chem.Soc.* 127,8006
Formula: C₁₄H₁₆N₂O₂
Compound Name: (2S,3R)-3-Ethyl-2-hydroxy-4-methyl-N-phenylpent-4-enamide

Space Group: P43
Space Group No.: 76
R-Factor (%): 3.83
Cell: *a* 9.071(1) *b* 9.071(1) *c* 32.245(8)
(Å, γ) α 90.00 β 90.00 γ 90.00
Temperature(K): 193 **Density(g/cm³):** 1.314

Parameters
Fragment 1
HTOO (D) 2.263
CHO (A) 121.174
Fragment 2
HTOO (D) 2.260
CHO (A) 122.038

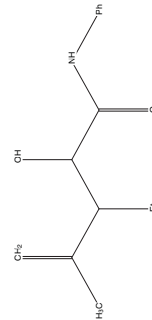


JAQYIK01

Reference: R.E.Marsh, D.A.Clemente (2007) *Inorg.Chim.Acta* 360, 4017
Formula: C₁₄H₁₆N₂O₂
Compound Name: (2S,3R)-3-ethyl-2-hydroxy-4-methyl-N-phenylpent-4-enamide

Space Group: Fd-3212
Space Group No.: 86
R-Factor (%): 0.00
Cell: *a* 8.071(1) *b* 8.071(1) *c* 32.245(8)
(Å, γ) α 90.00 β 90.00 γ 90.00
Temperature(K): 193 **Density(g/cm³):** 1.168

Parameters
Fragment 1
HTOO (D) 2.263
CHO (A) 121.966

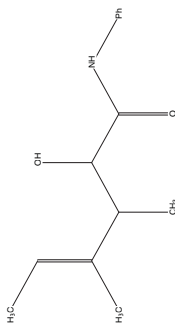


JAQYOO

Reference: D.A.Evans, J.Wu (2005) *J.Am.Chem.Soc.* 127,8006
Formula: C₁₄H₁₆N₂O₂
Compound Name: (2S,3R,E)-2-hydroxy-3,4-dimethyl-N-phenylhex-4-enamide

Space Group: P21
Space Group No.: 4
R-Factor (%): 3.48
Cell: *a* 8.413(1) *b* 9.704(1) *c* 8.675(1)
(Å, γ) α 90.00 β 110.05(0) γ 90.00
Temperature(K): 293 **Density(g/cm³):** 1.165

Parameters
Fragment 1
HTOO (D) 2.278
CHO (A) 120.897

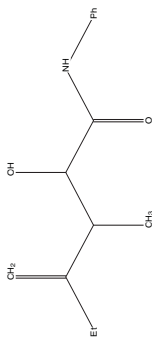


JATCUD

Reference: D.A.Evans, J.Wu (2005) *J.Am.Chem.Soc.* 127,8006
Formula: C₁₄H₁₆N₂O₂
Compound Name: (2S,3R)-2-hydroxy-3-methyl-4-methyl-N-phenylhexanamide

Space Group: P21212
Space Group No.: 18
R-Factor (%): 8.27
Cell: *a* 9.641(2) *b* 14.803(3) *c* 9.119(1)
(Å, γ) α 90.00 β 90.00 γ 90.00
Temperature(K): 193 **Density(g/cm³):** 1.183

Parameters
Fragment 1
HTOO (D) 2.281
CHO (A) 118.968

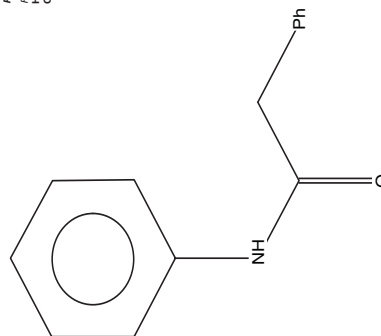


JODSAW

Reference: R.J.Lewis, P.Camilletti, A.J.Kelby, C.A.Marby, A.A.Slawn, D.J.Williams (1991) *J.Chem.Soc.Perkin Trans.2* 1825
Formula: C₁₄H₁₃N₃O₁
Compound Name: Phenylacetamide

Space Group: P21/n
Space Group No.: 14
R-Factor (%): 5.80
Cell: *a* 5.687(1) *b* 25.318(7) *c* 8.100(5)
(Å, γ) α 91.97(1) β 91.97(1) γ 90.00
Temperature(K): 295 **Density(g/cm³):** 1.204

Parameters
Fragment 1
HTOO (D) 2.416
CHO (A) 112.713

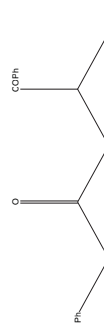


KAWPAA

Reference: R.L.Piggs, C.J.H.Moran, A.M.Z.Slewin, D.M.Smith, N.J.Westwood, W.S.D.Aisten, K.E.Shaun (2005) *Tetrahedron* 61, 11250
Formula: C₁₉H₁₆N₂O₄
Compound Name: Ethyl 2-benzyloxy-N-phenylsuccinamate

Space Group: P-1
Space Group No.: 2
R-Factor (%): 4.02
Cell: *a* 8.333(5) *b* 9.470(7) *c* 11.244(6)
(Å, γ) α 100.85(0) β 105.14(0) γ 100.85(1)
Temperature(K): 93 **Density(g/cm³):** 1.335

Parameters
Fragment 1
HTOO (D) 2.289
CHO (A) 121.274

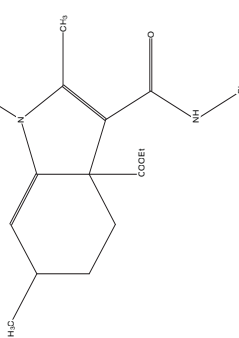


KESYEN

Reference: O.A.Altanasi, L.Da Crescenini, G.Fwi, P.Filippone, A.Golobic, S.Lilini, F.Mantellini (2008) *Synlett* 2735
Formula: C₂₁H₂₆N₂O₄
Compound Name: (R,R,S,S)-Ethyl 1-((aminocarbonyl)amino)-3-(aminocarbonyl)-2,6-dimethyl-5,6,6a,7a-tetrahydro-1H-benzobicyclo[3.2.1]octane

Space Group: P21/c
Space Group No.: 14
R-Factor (%): 4.50
Cell: *a* 13.638(6) *b* 12.886(6) *c* 11.997(0)
(Å, γ) α 90.00 β 90.00 γ 90.00
Temperature(K): 293 **Density(g/cm³):** 1.255

Parameters
Fragment 1
HTOO (D) 2.263
CHO (A) 118.395

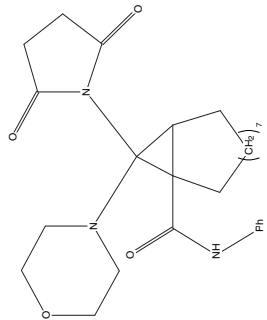


KATLUM

Reference: P.Ahmer, E.Vilgastar, G.Walmsheiser (1989) *Tetrahedron* 45,3189
Formula: C₂₇H₃₇N₃O₄
Compound Name: 1-(11,12-diphenyl-12-morpholino-N-phenyl)-12-succinimide-bicyclo[6.1.0]decan-7-carboxamide

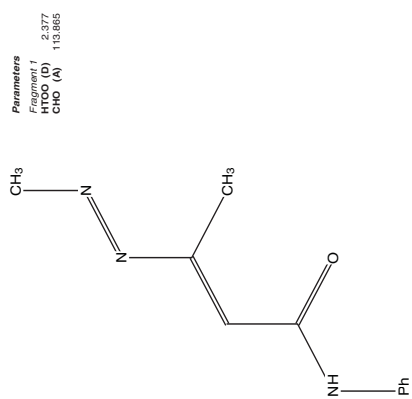
Space Group: P-1
Space Group No.: 2
R-Factor (%): 5.86
Cell: *a* 12.376(2) *b* 12.921(2) *c* 8.852(2)
(Å, γ) α 93.46(3) β 103.71(1) γ 84.77(3)
Temperature(K): 295 **Density(g/cm³):** 1.214

Parameters
Fragment 1
HTOO (D) 2.233
CHO (A) 117.793



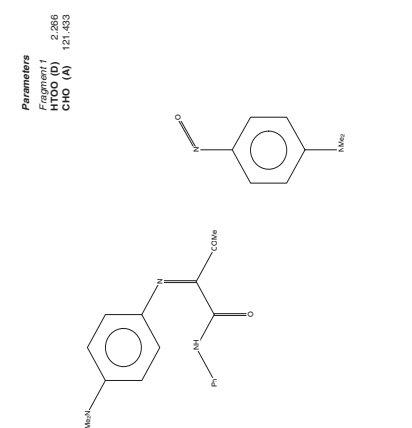
KOLSUZ

Reference: G.Ferguson, A.J.Lough, D.Mackay, G.Wentung (1991) *J.Chem.Soc., Perkin Trans. 1*, 3361
Formula: C₁₁H₁₃N₃O₁
Compound Name: (E)-1-Methyl-N-phenyl-2,2-diazapenta-2,4-diene-5-carboxamide
Space Group: P2₁/a c 8.654(3) b 15.666(2) c 11.639(2)
Space Group No.: 53 α 90.00 β 90.00 γ 90.00
R-Factor (%): 3.20 **Temperature(K):** 295 **Density(g/cm³):** 1.210



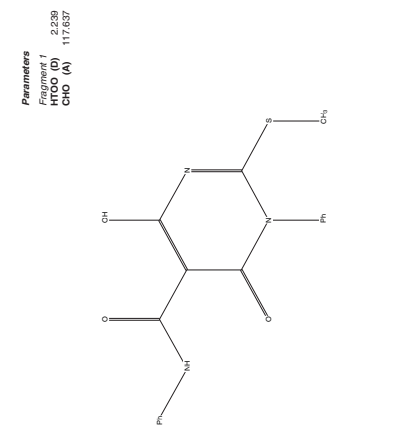
KUNPUE

Reference: K.Lawinski, W.Nitek, P.Miart (1993) *Acta Crystallogr., Sect.C:Cryst.Struct.Commun.*, 49, 188
Formula: C₁₉H₁₉N₃O₂C₉H₉N₃O₁
Compound Name: (2-{4-(Dimethylamino)phenyl}imino)-3-oxo-N-phenylbutanamide N,N-dimethyl-4-nitrosocaine
Space Group: P2₁2₁2₁ Cell: a 18.361(4) b 13.942(3) c 8.054(3)
Space Group No.: 19 α 90.00 β 90.00 γ 90.00
R-Factor (%): 3.50 **Temperature(K):** 295 **Density(g/cm³):** 1.249



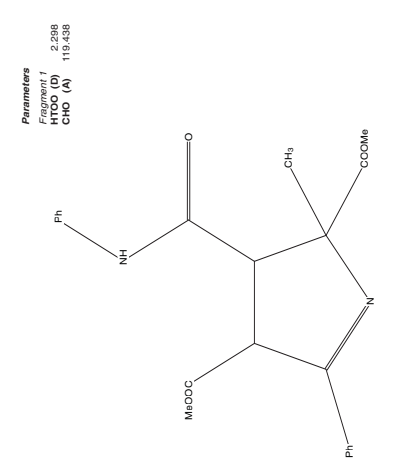
LAFZUN

Reference: R.Bosso, S.Marcaccio, P.Paoli, G.Pallagrin, R.Papino, T.Tarantola (1993) *J.Chem.Phys.*, 98, 472
Formula: C₁₁H₁₀N₂O₃S₁
Compound Name: N,N-Diphenyl-1,6-dihydro-4-hydroxy-2-methylthio-4-oxopyrimidine-5-carboxamide
Space Group: P2₁/n Cell: a 10.555(4) b 8.356(9) c 19.148(6)
Space Group No.: 14 α 90.00 β 90.00 γ 90.00
R-Factor (%): 5.70 **Temperature(K):** 295 **Density(g/cm³):** 1.330



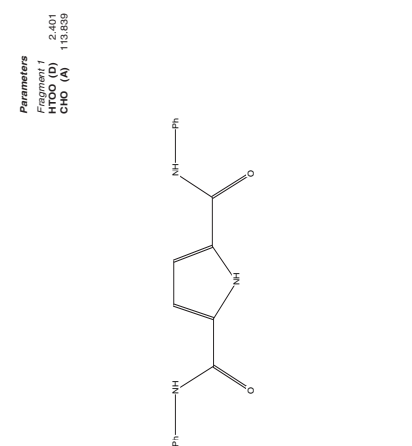
LAIKEN

Reference: S.Peddbhotla, J.J.Tripa (2004) *J.Am.Chem.Soc.*, 126, 12776
Formula: C₂₀H₂₂H₂O₅
Compound Name: Dimethyl 3-(phenylcarbamoyl)-3,4-dihydro-2-methyl-5-phenyl-2H-pyrole-2,4-dicarboxylate
Space Group: P-1 Cell: a 8.957(1) b 10.444(2) c 11.475(2)
Space Group No.: 2 α 99.06(3) β 104.61(9) γ 99.54(3)
R-Factor (%): 4.22 **Temperature(K):** 175 **Density(g/cm³):** 1.308



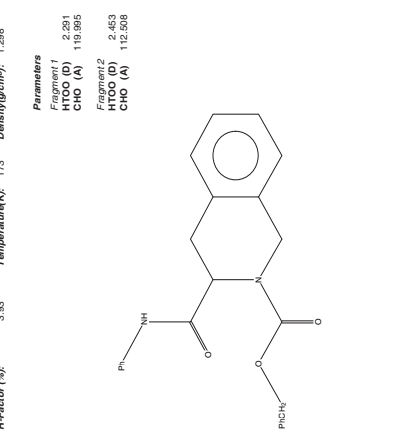
LANXAA

Reference: T.Zielinski, J.Jurczak (2005) *Tetrahedron*, 61, 4081
Formula: C₁₈H₁₅N₃O₂
Compound Name: N,N-diphenyl-1H-pyrole-2,5-dicarboxamide
Synonym: 1H-pyrole-2,5-dicarboxylic acid bis(phenylamide)
Space Group: Pnma Cell: a 7.654(0) b 35.244(3) c 5.192(0)
Space Group No.: 62 α 90.00 β 90.00 γ 90.00
R-Factor (%): 6.12 **Temperature(K):** 130 **Density(g/cm³):** 1.451



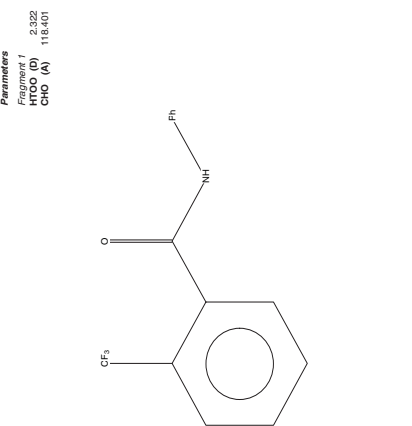
LAQKUL

Reference: T.Nacker, M.Chelone, T.Govender, H.G.Kruger, G.E.M.Maguire (2012) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, 68, s883
Formula: C₂₄H₂₆N₂O₃
Compound Name: (S)-Benzyl 3-phenylcarbamoyl-1,2,3,4-tetrahydroisoquinoline-2-carboxylate
Space Group: P2₁ Cell: a 13.034(0) b 10.808(0) c 14.043(0)
Space Group No.: 4 α 90.00 β 92.93(0) γ 90.00
R-Factor (%): 3.99 **Temperature(K):** 173 **Density(g/cm³):** 1.286



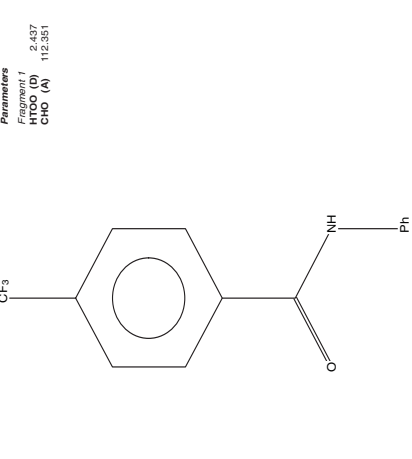
LASHEU

Reference: P.Panini, D.Chopra (2012) *CrystEngComm*, 14, 1972
Formula: C₁₄H₁₀F₃N₁O₁
Compound Name: N-Phenyl-2-(trifluoromethyl)benzamide
Space Group: P2₁/c Cell: a 9.991(10) b 16.421(5) c 15.645(6)
Space Group No.: 14 α 108.49(0) β 90.00
R-Factor (%): 5.51 **Temperature(K):** 120 **Density(g/cm³):** 1.447



LASHIY

Reference: P.Panini, D.Chopra (2012) *CrystEngComm*, 14, 1972
Formula: C₁₄H₁₀F₃N₁O₁
Compound Name: N-Phenyl-4-(trifluoromethyl)benzamide
Space Group: P-1 Cell: a 5.359(9) b 7.714(5) c 14.242(5)
Space Group No.: 2 α 77.10(0) β 81.61(0) γ 89.61(0)
R-Factor (%): 4.00 **Temperature(K):** 120 **Density(g/cm³):** 1.552



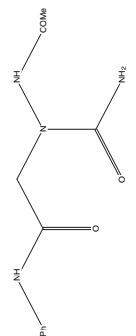
LERTAD

Reference: K.Peters, E.-M.Peters, A.Hatzheim, P.Koskitz (1999) *Z.Naturforsch. Neue Class.*, **54**, 2143-2147

Formula: C₁₁H₁₄N₂O₃
Compound Name: 1-Acetyl-2-phenylcarbamoylmethylamincarbamide

Space Group: P-1
Space Group No.: 2
R-Factor (%): 4.99
Parameters
Fragment 1
HTOO (D): 2.372
CHO (A): 118.728

Cell: a 5.858(10) b 7.115(10) c 15.515(1)
(Å, °) α 90.00 β 90.11(6) γ 107.83(10)
Temperature(K): 295 Density(g/cm³): 1.411



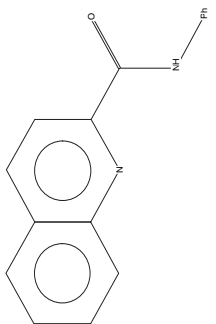
LUPAW

Reference: Lin-Hai-Jiang, Yi-Feng, Da-Bin-Qin, Huan-Xia-Zhang, Qian-Dai (2007) *Acta Crystallogr., Sect.E: Struct. Rep. Online*, **63**, 638-618

Formula: C₁₅H₁₂N₂O₄
Compound Name: N-Phenylquinoline-2-carboxamide

Space Group: Pna21
Space Group No.: 33
R-Factor (%): 4.12
Parameters
Fragment 1
HTOO (D): 2.263
CHO (A): 122.688

Cell: a 16.988(1) b 12.828(1) c 5.448(6)
(Å, °) α 90.00 β 90.00 γ 90.00
Temperature(K): 153 Density(g/cm³): 1.390



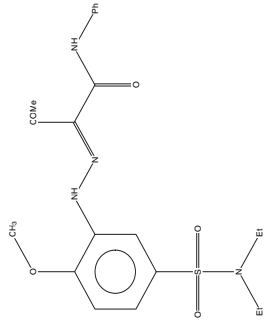
LIFUGJ

Reference: J.Fawcett, R.D.W. Kemmitt, D.R. Russell, O. Smirndag, Adam Crystallogr., Sect.C: Crystal Struct. Commun., **51**, 139

Formula: C₂₁H₂₄N₄O₄S₁
Compound Name: 2-(E)-(Diethylaminoalkoxy)-2-methoxyphenylhydrazono-3-oxo-N-phenylsulfamide

Space Group: P-1
Space Group No.: 2
R-Factor (%): 5.40
Parameters
Fragment 1
HTOO (D): 2.274
CHO (A): 122.072

Cell: a 12.261(20) b 9.02(11) c 11.482(4)
(Å, °) α 117.10(10) β 88.79(2) γ 97.88(1)
Temperature(K): 295 Density(g/cm³): 1.321



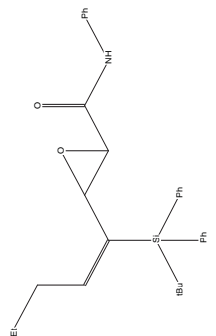
LIKLUN

Reference: D.A.Evans, Y.Aye (2007) *J.Am.Chem.Soc.*, **129**, 9606

Formula: C₂₅H₂₆N₂O₂Si₁
Compound Name: (E)-3-(E)-3-(1-(4-Butyldiphenylsilyl)pent-1-enyl)-N-phenylloxirane-2-carboxamide

Space Group: P6ca
Space Group No.: 61
R-Factor (%): 7.81
Parameters
Fragment 1
HTOO (D): 2.307
CHO (A): 123.264

Cell: a 0.608(1) b 21.075(4) c 26.118(5)
(Å, °) α 90.00 β 90.00 γ 90.00
Temperature(K): 299 Density(g/cm³): 1.192



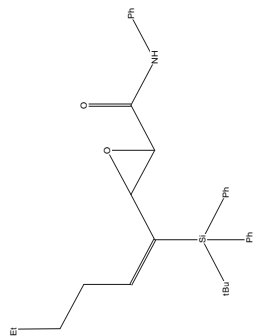
LIKMAU

Reference: D.A.Evans, Y.Aye (2007) *J.Am.Chem.Soc.*, **129**, 9606

Formula: C₃₁H₃₂N₂O₂Si₁
Compound Name: (E)-3-(E)-3-(1-(4-Butyldiphenylsilyl)hex-1-enyl)-N-phenylloxirane-2-carboxamide

Space Group: P6ca
Space Group No.: 61
R-Factor (%): 6.99
Parameters
Fragment 1
HTOO (D): 2.320
CHO (A): 120.475

Cell: a 9.660(1) b 21.302(4) c 26.248(4)
(Å, °) α 90.00 β 90.00 γ 90.00
Temperature(K): 193 Density(g/cm³): 1.190



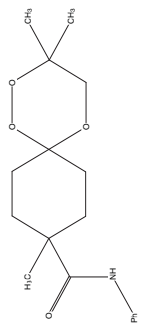
LIMWOD

Reference: S.A.-L.Laurent, J.Boissier, F.Coslekan, H.Gomezika, A.Robert, B.Meunier (2008) *Eur.J.Org.Chem.*, **895**

Formula: C₁₉H₂₅N₃O₄
Compound Name: cis-3,3,3-Trimethyl-N-phenyl-1,2,5-hioxepiridine-5-oxo-2-carboxamide

Space Group: P6ca
Space Group No.: 61
R-Factor (%): 5.30
Parameters
Fragment 1
HTOO (D): 2.374
CHO (A): 113.715

Cell: a 12.532(3) b 9.207(3) c 23.188(8)
(Å, °) α 90.00 β 90.00 γ 90.00
Temperature(K): 173 Density(g/cm³): 1.258



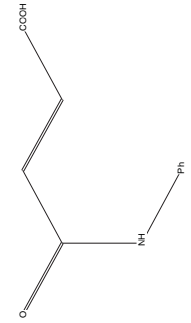
LOSUJZ

Reference: Kong, Min-Lo, S.W.Ng (2009) *Acta Crystallogr., Sect.E: Struct. Rep. Online*, **65**, 01101

Formula: C₁₀H₈N₂O₂
Compound Name: N-Phenylmaleamic acid
Synonym: 4-Amino-4-oxo-2-butenedioic acid

Space Group: P21/c
Space Group No.: 14
R-Factor (%): 6.80
Parameters
Fragment 1
HTOO (D): 2.269
CHO (A): 120.892

Cell: a 12.751(6) b 10.985(10) c 14.192(6)
(Å, °) α 90.00 β 116.30(10) γ 90.00
Temperature(K): 100 Density(g/cm³): 1.479



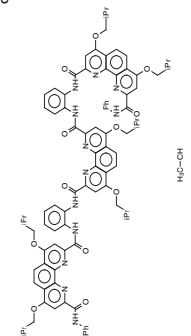
LUFJAY

Reference: Hai-Yu-Hu, Wei-Xun, Shi-Qiang-Hu, Jun-Feng-Xiang, Chuan-Feng-Chen, Sheng-Gui-He (2009) *J.Org.Chem.*, **74**, 4849

Formula: C₃₀H₃₀N₂O₁₂C₁H₁O₁
Compound Name: N,N'-bis-(6,7-Dihydroxy-1,10-phenanthroline-2,9-ylidene)bis(carbamoyl)imino-dibenzamide (methanol solvate)

Space Group: P-1
Space Group No.: 2
R-Factor (%): 11.30
Parameters
Fragment 1
HTOO (D): 2.925
CHO (A): 120.446

Cell: a 13.471(3) b 17.872(4) c 18.784(4)
(Å, °) α 103.82(3) β 91.95(3) γ 110.35(3)
Temperature(K): 293 Density(g/cm³): 1.273



LUFJEC

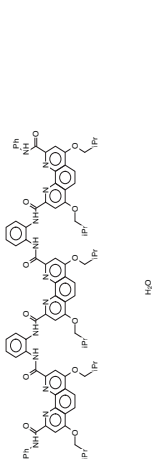
Reference: Hai-Yu Hu, Wei Xue, Zhi-Qiang Hu, Jun-Feng Xiang, Chuan-Feng Chen, Sheng-Gui He (2009) *J.Org.Chem.*, 74,4949

Formula: $C_{26}H_{26}N_2O_{12}$

Compound Name: N⁶,N⁷-(4,7-Diisobutoxy-1,10-phenanthroline-2,9-diyl)bis(carbonyl)imino-2,1-phenylenebis(6,7-diisobutoxy-N-phenyl-1,10-phenanthroline-2,9-dicarboxamide) monohydrate

Space Group: P-1
 Space Group No.: 2
 R-Factor (%): 16.66

Parameters
 Fragment 1
 HTOO (D) 2.283
 CHO (A) 121.177
 Fragment 2
 HTOO (D) 2.331
 CHO (A) 118.294



LUFJIG

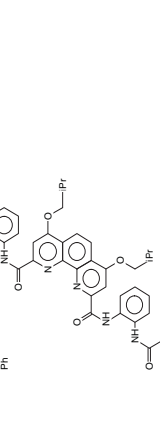
Reference: Hai-Yu Hu, Wei Xue, Zhi-Qiang Hu, Jun-Feng Xiang, Chuan-Feng Chen, Sheng-Gui He (2009) *J.Org.Chem.*, 74,4949

Formula: $C_{26}H_{26}N_2O_{12} \cdot 2(C_2H_5O_2)$

Compound Name: N⁶,N⁷-(4,7-Diisobutoxy-9-(diethylcarbamoyl)-1,10-phenanthroline-2,9-diyl)carbamoyl(aminophenyl)-N-(2-((4,7-diisobutoxy-9-(1-phenylethyl)carbamoyl)-1,10-phenanthroline-2,9-dicarboxamide)ethanol solvate

Space Group: P-1
 Space Group No.: 2
 R-Factor (%): 13.43

Parameters
 Fragment 1
 HTOO (D) 2.266
 CHO (A) 119.452



LUFJOM

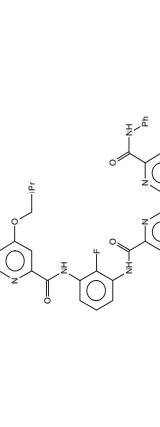
Reference: Hai-Yu Hu, Wei Xue, Zhi-Qiang Hu, Jun-Feng Xiang, Chuan-Feng Chen, Sheng-Gui He (2009) *J.Org.Chem.*, 74,4949

Formula: $C_{26}H_{26}N_2O_{12} \cdot 2(C_2H_5O_2)$

Compound Name: N⁶,N⁷-(2-Ethoxy-1,2-phenylenebis(4,7-diisobutoxy-9-(diethylcarbamoyl)-1,10-phenanthroline-2,9-dicarboxamide)) dichloromethane solvate

Space Group: C2/c
 Space Group No.: 15
 R-Factor (%): 6.32

Parameters
 Fragment 1
 HTOO (D) 2.088
 CHO (A) 118.173



LUFJUS

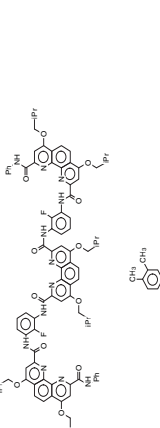
Reference: Hai-Yu Hu, Wei Xue, Zhi-Qiang Hu, Jun-Feng Xiang, Chuan-Feng Chen, Sheng-Gui He (2009) *J.Org.Chem.*, 74,4949

Formula: $C_{26}H_{26}N_2O_{12} \cdot 2(C_2H_5O_2)$

Compound Name: N⁶,N⁷-(4,7-Diisobutoxy-1,10-phenanthroline-2,9-diyl)bis(carbonyl)imino(2-fluoro-3-(phenylene))bis(4,7-diisobutoxy-N-phenyl-1,10-phenanthroline-2,9-dicarboxamide)

Space Group: C2/c
 Space Group No.: 15
 R-Factor (%): 6.89

Parameters
 Fragment 1
 HTOO (D) 2.304
 CHO (A) 118.453



LUHDUO

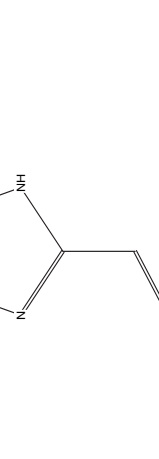
Reference: A Pichula-Siec, J Rzymowska, L Maszur, E Mandyk, M Pichula, Z Raczynska (2009) *Eur.J.Med.Chem.*, 44,3788

Formula: $C_{13}H_{14}N_4O_5$

Compound Name: 3-(2-Ethylthiazolyl)-1H-1,2,4-triazol-5-yl)-N-phenylacylamide

Space Group: Pn21
 Space Group No.: 33
 R-Factor (%): 5.90

Parameters
 Fragment 1
 HTOO (D) 2.313
 CHO (A) 120.898



LUSXAY

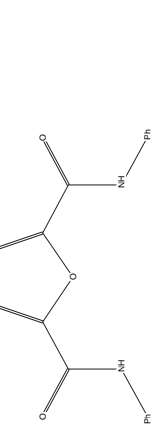
Reference: S Camelo, P A Gale, M B Huisthouse, M E Lipth, C N Warner (2003) *Tetrahedron Lett.*, 44,1367

Formula: $C_{20}H_{22}N_2O_5 \cdot C_2H_5N$

Compound Name: 3,4-Diphenyl-2,5-bis(4-phenylcarbamoyl)uran acetonitrile solvate

Space Group: P21/n
 Space Group No.: 14
 R-Factor (%): 4.35

Parameters
 Fragment 1
 HTOO (D) 2.324
 CHO (A) 118.967
 Fragment 2
 HTOO (D) 2.484
 CHO (A) 112.081



LUVCAF

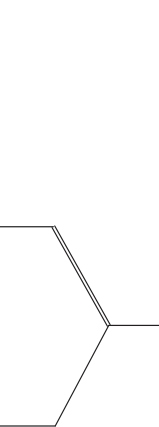
Reference: T Blach, B Gresh, T Sliemers, E Handweck (2003) *J.Org.Chem.*, 68,1107

Formula: $C_{17}H_{13}N_3O$

Compound Name: N-Phenylcyclohexene-1-carboxamide

Space Group: Pca21
 Space Group No.: 29
 R-Factor (%): 4.43

Parameters
 Fragment 1
 HTOO (D) 2.297
 CHO (A) 120.441



MAJPOE

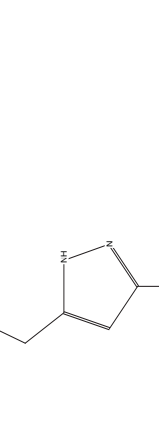
Reference: E.A. Smith, C. Potter, Z.C. Kennedy, A.J. Puchaly, A.M. Acevedo-Jake, S.D. Hasey, C.R. Metz, W.T. Pennington, D.G. VanBever, C.F. Ebeam (2010) *J.Heterocyclic.Chem.*, 47,147

Formula: $C_{17}H_{14}O_1N_5$

Compound Name: 2-(5-(4-Chlorophenyl)-1H-imidazol-5-yl)-N-phenylacetamide

Space Group: P21/c
 Space Group No.: 14
 R-Factor (%): 6.13

Parameters
 Fragment 1
 HTOO (D) 2.348
 CHO (A) 117.107

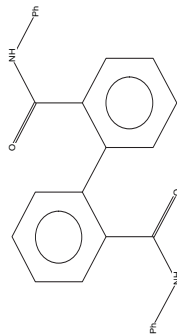


MANDIP

Reference: S. Gowami, A.K. Adak, R. Mukherjee, S. Jana, S. Dey, J.F. Gallagher (2005) *Tetrahedron* **61**, 4289
Formula: C₂₀H₂₀N₂O₂
Compound Name: Biphenyl-2,2'-dicarboxylic acid bis(phenylamides)

Space Group: P43212 **a** 10.782(0) **b** 10.782(0) **c** 36.522(4)
Space Group No.: 58 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 6.82 **Temperature(K):** 294 **Density(g/cm³):** 1.249

Parameters
Fragment 1
HTOO (D) 2.387
CHO (A) 117.377
Fragment 2
HTOO (D) 2.328
CHO (A) 116.901

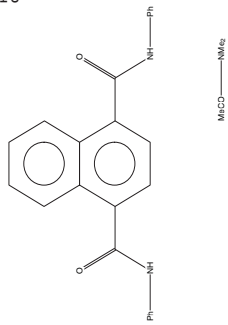


MENCAK

Reference: Ming-Qi Li, Lin-Hai Jing (2009) *Acta Crystallogr., Sect. E: Struct. Rep. Online* **62**, 23977
Formula: C₂₄H₁₈N₂O₂·2(C₈H₈N₂O)
Compound Name: N,N'-Diphenylmethylidene-1,4-dioxasolane dimethylacetamide solvate

Space Group: P21/c **a** 12.307(0) **b** 20.124(0) **c** 12.121(0)
Space Group No.: 14 **α** 90.00 **β** 108.17(0) **γ** 90.00
R-Factor (%): 4.36 **Temperature(K):** 153 **Density(g/cm³):** 1.259

Parameters
Fragment 1
HTOO (D) 2.292
CHO (A) 119.884
Fragment 2
HTOO (D) 2.292
CHO (A) 120.133

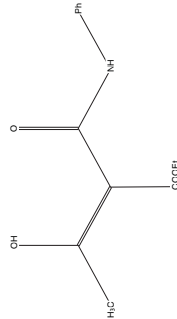


MEPTQD

Reference: J.K. Mukhopadhyay, S. Shinnak, Z. Flappoport (2000) *J.Org.Chem.* **65**, 6566
Formula: C₁₃H₁₂N₂O₂
Compound Name: ethyl 2-aminocarbonyl-3-hydroxybut-2-enoate

Space Group: P21/n **a** 14.548(5) **b** 14.137(3) **c** 8.516(1)
Space Group No.: 14 **α** 90.00 **β** 88.85(2) **γ** 90.00
R-Factor (%): 6.70 **Temperature(K):** 295 **Density(g/cm³):** 1.310

Parameters
Fragment 1
HTOO (D) 2.253
CHO (A) 113.669

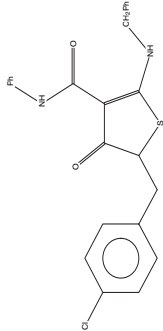


MERBIV

Reference: Yan, L.I., Fushun Liang, Xie Bi, Qun Liu (2006) *J.Org.Chem.* **71**, 8006
Formula: C₂₆H₂₁O₂
Compound Name: 2-(Benzylamino)-5-(4-chlorobenzyl)-4-oxo-N-phenyl-4,5-dihydrothiophene-3-carboxamide

Space Group: P-1 **a** 6.656(5) **b** 8.686(5) **c** 20.105(5)
Space Group No.: 2 **α** 95.74(0) **β** 94.71(0) **γ** 109.10(0)
R-Factor (%): 7.90 **Temperature(K):** 293 **Density(g/cm³):** 1.375

Parameters
Fragment 1
HTOO (D) 2.905
CHO (A) 117.359

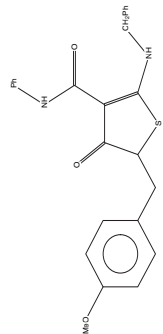


MERBOB

Reference: Yan, L.I., Fushun Liang, Xie Bi, Qun Liu (2006) *J.Org.Chem.* **71**, 8006
Formula: C₂₆H₂₂N₂O₃S₁
Compound Name: 2-(Benzylamino)-5-(4-methoxybenzyl)-4-oxo-N-phenyl-4,5-dihydrothiophene-3-carboxamide

Space Group: P21/n **a** 12.398(5) **b** 6.627(5) **c** 27.073(5)
Space Group No.: 14 **α** 90.00 **β** 94.63(6) **γ** 90.00
R-Factor (%): 8.04 **Temperature(K):** 293 **Density(g/cm³):** 1.332

Parameters
Fragment 1
HTOO (D) 2.283
CHO (A) 121.788



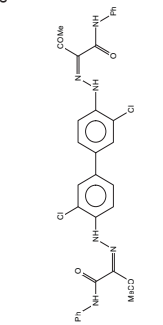
MEWGAW

Reference: M.J. Barrow, R.M. Christie, A.J. Lough, J.E. Monteith, P.N. Standing (2000) *Dyes Pigm.* **46**, 153
Formula: C₂₂H₁₆Cl₂N₂O₄
Compound Name: 2,2'-(3,3'-Dichloro-1,1'-biphenyl-4,4'-diyl)bis(acetate)(3-oxo-N-phenylacetamide)

Synonym: C.I. Pigment yellow

Space Group: P21/n **a** 17.850(6) **b** 7.370(10) **c** 24.005(8)
Space Group No.: 14 **α** 90.00 **β** 110.57(3) **γ** 90.00
R-Factor (%): 4.80 **Temperature(K):** 295 **Density(g/cm³):** 1.414

Parameters
Fragment 1
HTOO (D) 2.331
CHO (A) 116.046
Fragment 2
HTOO (D) 2.250
CHO (A) 125.948

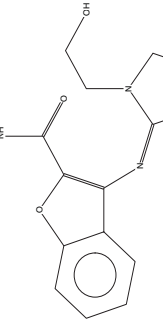


MOCWOR

Reference: Yang-Gan Hu, Ming-Guo Liu, Meng-Wu Ding (2008) *Helv.Chim.Acta* **91**, 882
Formula: C₂₆H₁₉N₃O₄
Compound Name: 3-[(2E)-3-(2-hydroxyethyl)oxazolidin-2-ylideneamino]-N-phenyl-2-benzofuranacetamide

Space Group: P21/c **a** 13.905(1) **b** 10.057(1) **c** 13.521(1)
Space Group No.: 14 **α** 90.90 **β** 111.12(6) **γ** 90.90
R-Factor (%): 6.21 **Temperature(K):** 292 **Density(g/cm³):** 1.374

Parameters
Fragment 1
HTOO (D) 2.487
CHO (A) 112.458



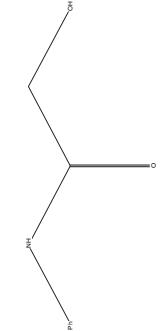
MORVAR

Reference: M.R. Hauser, L. Zhakarov, K.M. Dossan, Tongjeli Li (2008) *Cryst.Growth Des.* **8**, 4128
Formula: C₉H₉N₃O₂
Compound Name: 2-Hydroxy-N-phenylacetamide

Synonym: Glycylamide

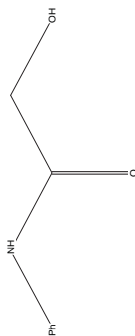
Space Group: P21/n **a** 5.761(10) **b** 12.283(30) **c** 10.389(10)
Space Group No.: 14 **α** 90.00 **β** 94.48(0) **γ** 90.00
R-Factor (%): 3.77 **Temperature(K):** 153 **Density(g/cm³):** 1.383

Parameters
Fragment 1
HTOO (D) 2.952
CHO (A) 123.577



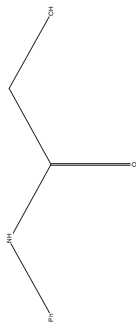
MORVAR01

Reference: M.R.Hauser, L.Zhalarov, K.M.Dovese, Tongliu L (2008) *Cryst Growth Des.*, 8,4128
Formula: C₉H₉N₃O₂
Compound Name: Glycolamide
Synonym: Pica
Space Group: *a* 14.167(3) *b* 5.634(1) *c* 18.694(6)
Space Group No.: 61 *α* 90.00 *β* 90.00 *γ* 90.00
R-Factor (%): 3.89 **Temperature(K):** 153 **Density(g/cm³):** 1.346
Parameters
Fragment 1
HTOO (D) 2.298
CHO (A) 121.601



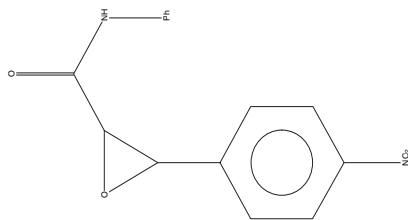
MORVAR02

Reference: G.J.Puipatuo, J.Janczak (2009) *J.Mol.Struct.*, 832,1
Formula: C₉H₉N₃O₂
Compound Name: N-Phenyl-2-hydroxyacetamide
Space Group: *a* 5.720(1) *b* 12.394(3) *c* 10.489(2)
Space Group No.: 14 *α* 90.00 *β* 94.02(3) *γ* 90.00
R-Factor (%): 3.72 **Temperature(K):** 295 **Density(g/cm³):** 1.351
Parameters
Fragment 1
HTOO (D) 2.289
CHO (A) 121.835



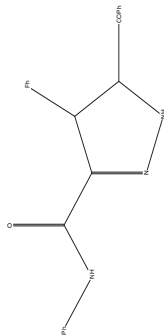
MUBKEA

Reference: Long He (2009) *Acta Crystallogr., Sect.E: Struct.Rep.Chem.* 65,02032
Formula: C₁₃H₁₂N₂O₄
Compound Name: 3-(4-Nitrophenyl)-N-phenyl-2-oximinocarbamide
Space Group: *a* 5.580(0) *b* 5.195(0) *c* 21.503(5)
Space Group No.: 4 *α* 90.00 *β* 95.11(6) *γ* 90.00
R-Factor (%): 3.91 **Temperature(K):** 293 **Density(g/cm³):** 1.421
Parameters
Fragment 1
HTOO (D) 2.456
CHO (A) 112.550



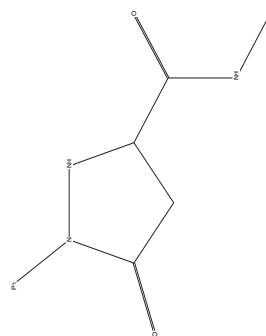
MUCCAP

Reference: Long He (2009) *Acta Crystallogr., Sect.E: Struct.Rep.Chem.* 65,02281
Formula: C₂₀H₁₉N₃O₂
Compound Name: 5-Benzoyl-N,4-diphenyl-4,5-dihydro-1H-pyrazole-3-carboxamide
Space Group: *a* 5.691(3) *b* 10.717(5) *c* 20.267(7)
Space Group No.: 14 *α* 90.00 *β* 92.75(6) *γ* 90.00
R-Factor (%): 3.37 **Temperature(K):** 295 **Density(g/cm³):** 1.341
Parameters
Fragment 1
HTOO (D) 2.314
CHO (A) 121.146



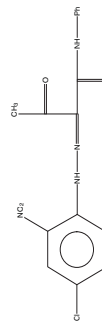
NAHFAP

Reference: R.Melgar-Fernandez, R.Gonzalez-Olvera, J.Vargas-Capozzi, R.Perez-Izabara, E.Juanes (2010) *ARKIVOC*, 11, 55-8
Formula: C₁₄H₁₆N₂O₂
Compound Name: (S)-5-cyclo-N,1-diphenylpyrazoline-3-carboxamide
Space Group: *a* 8.777(1) *b* 6.109(1) *c* 13.596(6)
Space Group No.: 4 *α* 90.00 *β* 101.76(3) *γ* 90.00
R-Factor (%): 4.12 **Temperature(K):** 293 **Density(g/cm³):** 1.309
Parameters
Fragment 1
HTOO (D) 2.308
CHO (A) 121.570



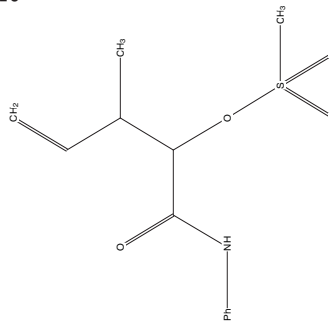
NCFAA01

Reference: A.Whitaker (1983) *Z.Kristallogr., Kristallphys., Kristallchem.*, 183,139
Formula: C₁₃H₁₃Cl₂N₂O₄
Compound Name: *trans*-(Acetyl)acetanilide-*trans*-4'-chloro-2'-nitrobenzene
Synonym: C.I.Pigment Yellow 6
Space Group: *a* 7.482(1) *b* 19.568(2) *c* 11.175(1)
Space Group No.: 14 *α* 90.00 *β* 105.96(1) *γ* 90.00
R-Factor (%): 5.30 **Temperature(K):** 295 **Density(g/cm³):** 1.327
Parameters
Fragment 1
HTOO (D) 2.964
CHO (A) 116.044



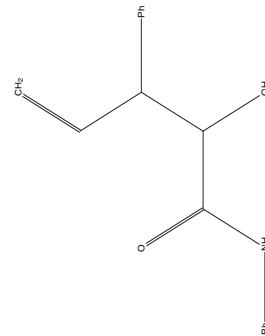
NEISAX

Reference: D.A.Evans, J.Wu, Y.Aye (2006) *Org.Lett.*, 8,2071
Formula: C₁₃H₁₇N₃O₄S₂
Compound Name: (2S,3S)-2-((methylsulfonyl)oxy)-3-methyl-N-phenylpent-4-enamide
Space Group: *a* 5.335(0) *b* 15.737(2) *c* 17.134(3)
Space Group No.: 19 *α* 90.00 *β* 90.00 *γ* 90.00
R-Factor (%): 3.94 **Temperature(K):** 193 **Density(g/cm³):** 1.308
Parameters
Fragment 1
HTOO (D) 2.531
CHO (A) 118.651



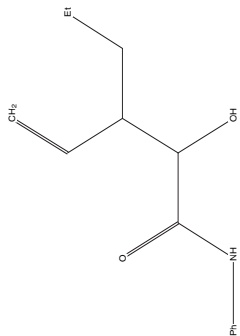
NEISEB

Reference: D.A.Evans, J.Wu, Y.Aye (2006) *Org.Lett.*, 8,2071
Formula: C₁₇H₁₇N₃O₂
Compound Name: (2S,3R)-2-hydroxy-N,3-diphenylpent-4-enamide
Space Group: *a* 8.410(1) *b* 8.837(1) *c* 20.288(4)
Space Group No.: 19 *α* 90.00 *β* 90.00 *γ* 90.00
R-Factor (%): 8.54 **Temperature(K):** 273 **Density(g/cm³):** 1.205
Parameters
Fragment 1
HTOO (D) 2.352
CHO (A) 122.103



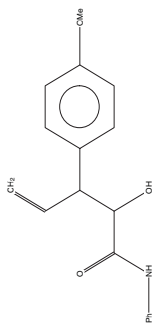
NEJSIF

Reference: D.A.Evans, J.Wu, Y.Aye (2006) *Org.Lett.*, **8**, 2071
Formula: C₁₄H₁₈N₂O₂
Compound Name: (S,S)-2-hydroxy-N-phenyl-3-propylpent-4-enamide
Space Group: P2₁ *a* 8.528(2) *b* 9.314(2) *c* 17.357(4)
Space Group No.: 4 *α* 90.00 *β* 97.88(0) *γ* 90.00
R-Factor (%): 4.73 **Temperature(K):** 193 **Density(g/cm³):** 1.135
Parameters
Fragment 1
HTOO (D) 2.315
CHO (A) 120.731



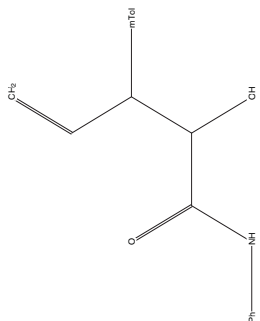
NEJSOL

Reference: D.A.Evans, J.Wu, Y.Aye (2006) *Org.Lett.*, **8**, 2071
Formula: C₁₄H₁₈N₂O₂
Compound Name: (S,S)-2-hydroxy-N-phenyl-3-methylpent-4-enamide
Space Group: P2₁2₁2₁ *a* 8.488(1) *b* 10.348(1) *c* 18.041(0)
Space Group No.: 19 *α* 90.00 *β* 90.00 *γ* 90.00
R-Factor (%): 8.67 **Temperature(K):** 183 **Density(g/cm³):** 1.249
Parameters
Fragment 1
HTOO (D) 2.297
CHO (A) 121.215



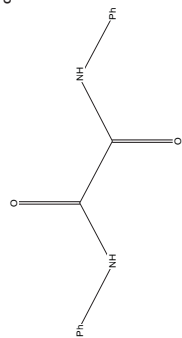
NEJSUR

Reference: D.A.Evans, J.Wu, Y.Aye (2006) *Org.Lett.*, **8**, 2071
Formula: C₁₄H₁₈N₂O₂
Compound Name: (S,S)-2-hydroxy-N-phenyl-3-methylpent-4-enamide
Space Group: P2₁2₁2₁ *a* 8.611(1) *b* 9.746(1) *c* 18.880(0)
Space Group No.: 19 *α* 90.00 *β* 90.00 *γ* 90.00
R-Factor (%): 7.23 **Temperature(K):** 193 **Density(g/cm³):** 1.181
Parameters
Fragment 1
HTOO (D) 2.323
CHO (A) 119.618



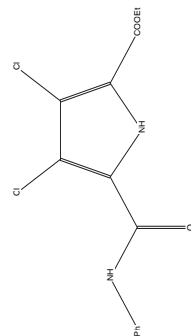
NIPTUC

Reference: B.Piotrowski, M.Gdaniec, M.J.Milewska, T.Polomski (2007) *CrystrEngComm*, **7**, 938
Formula: C₁₄H₁₂N₂O₂·2(C₉H₇F₃O)
Compound Name: N,N-Diphenylethanediamide bis(2,3,4,5,6-pentafluorophenol)
Space Group: P2₁/c *a* 9.958(0) *b* 5.837(0) *c* 21.257(1)
Space Group No.: 14 *α* 90.00 *β* 94.83(0) *γ* 90.00
R-Factor (%): 4.65 **Temperature(K):** 130 **Density(g/cm³):** 1.686
Parameters
Fragment 1
HTOO (D) 2.321
CHO (A) 119.487



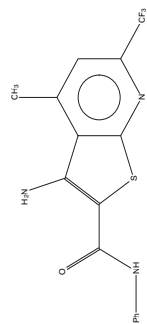
NIPYAN

Reference: M.ELIGHI, K.Nawakhan, P.A.Gale (2007) *Private Communication*.
Formula: C₁₁H₁₂Cl₂N₂O₃
Compound Name: Ethyl 3,4-dichloro-5-(phenylcarbamoyl)-1H-pyrrole-2-carboxylate
Space Group: P2₁/n *a* 9.726(0) *b* 4.909(0) *c* 29.937(0)
Space Group No.: 14 *α* 90.00 *β* 98.84(0) *γ* 90.00
R-Factor (%): 10.45 **Temperature(K):** 120 **Density(g/cm³):** 1.539
Parameters
Fragment 1
HTOO (D) 2.389
CHO (A) 117.033



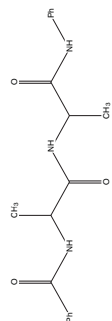
NUMKIP

Reference: K.G.Nishin, V.N.Nesarov, V.P.Ksaiy, A.M.Shestopalov, V.V.Semenov (1998) *Izv.Akad.Nauk SSSR Ser.Khim.(Russ.Chem.Bull.)*, 701
Formula: C₁₆H₁₂F₃N₃O₁S₁
Compound Name: 3-Amino-4-methyl-6-vinylcarbamoylthieno[2,3-b]pyridine-2-carboxamide
Space Group: C2/c *a* 12.084(6) *b* 8.592(2) *c* 30.030(10)
Space Group No.: 15 *α* 90.00 *β* 92.52(3) *γ* 90.00
R-Factor (%): 3.30 **Temperature(K):** 295 **Density(g/cm³):** 1.501
Parameters
Fragment 1
HTOO (D) 2.319
CHO (A) 120.311



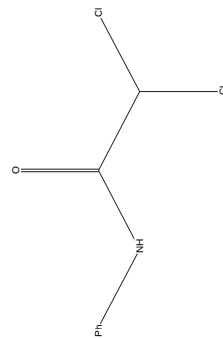
NUSDOU

Reference: M.Chill (1988) *Z.Kristallogr.-New.Cryst.Struct.*, **213**, 127
Formula: C₁₃H₁₂N₂O₂
Compound Name: N-Benzoyl-L-alanyl-L-alaninamide
Synonym: Asyclic peptide (2 residues): ALA-ALA
Space Group: P2₁2₁2₁ *a* 9.458(10) *b* 20.651(10) *c* 9.035(6)
Space Group No.: 19 *α* 90.00 *β* 90.00 *γ* 90.00
R-Factor (%): 5.05 **Temperature(K):** 295 **Density(g/cm³):** 1.279
Parameters
Fragment 1
HTOO (D) 2.377
CHO (A) 118.763



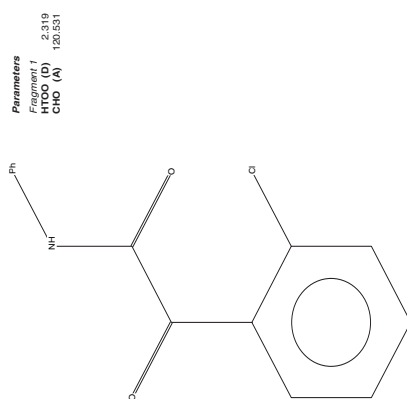
NUZBUF01

Reference: B.T.Gawda, H.Paulus, H.Fuess (2001) *Z.Naturforsch.-A.Phys.Sci.*, **56**, 386
Formula: C₉H₇Cl₂N₂O₁
Compound Name: N-Phenyl-2,2-dichloroacetamide
Space Group: P2₁/c *a* 8.788(3) *b* 11.138(4) *c* 9.521(3)
Space Group No.: 14 *α* 90.00 *β* 97.47(2) *γ* 90.00
R-Factor (%): 3.60 **Temperature(K):** 298 **Density(g/cm³):** 1.487
Parameters
Fragment 1
HTOO (D) 2.431
CHO (A) 113.440



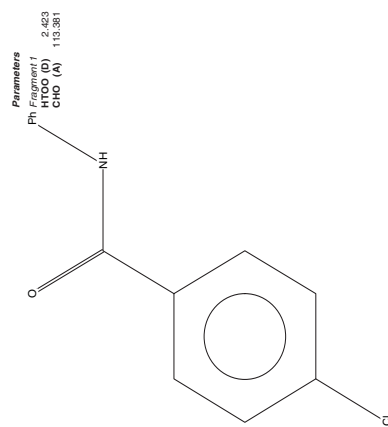
OBOYEL

Reference: Jing Dai, Jin-Long Wu (2011). *Acta Crystallogr., Sect. E: Struct. Rep. Online* **67**, 03152
Formula: C₁₄H₁₀Cl₁N₁O₂
Compound Name: 2-(2-Chlorophenyl)-2-oxo-N-phenylacetamide
Space Group: P2₁/c *a* 11.954(1) *b* 10.545(0) *c* 10.294(1)
Space Group No.: 14 *α* 90.00 *β* 100.85(1) *γ* 90.00
R-Factor (%): 3.40 **Temperature(K):** 293 **Density(g/cm³):** 1.438
Parameters
 Fragment 1 HT00 (D) 2.319
 Fragment 1 CHO (A) 120.531



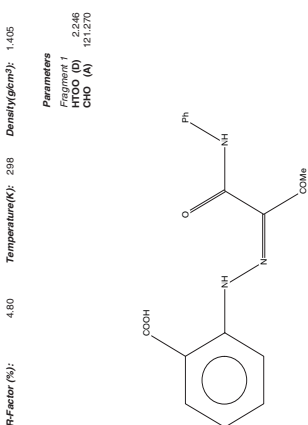
OBUCEV

Reference: V.Z.Rodrigues, L.Kucowa, B.T.Gowda, J.Kozak (2011). *Acta Crystallogr., Sect. E: Struct. Rep. Online* **67**, 023171
Formula: C₁₃H₁₀Cl₁N₁O₁
Compound Name: 4-Chloro-N-phenylbenzamide
Space Group: P-1 *a* 6.395(0) *b* 7.765(0) *c* 13.755(0)
Space Group No.: 2 *α* 105.88(0) *β* 100.85(0) *γ* 90.00(0)
R-Factor (%): 4.01 **Temperature(K):** 298 **Density(g/cm³):** 1.413
Parameters
 Fragment 1 HT00 (D) 2.423
 Fragment 1 CHO (A) 113.381



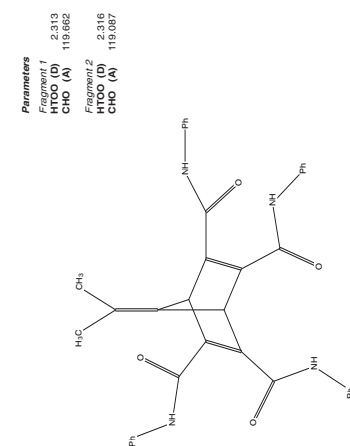
OCAVOF

Reference: Jintong Dong, Gailing Zheng, Meiyu Guo, Chuan Wu, Jianping Ren (2011). *Acta Crystallogr., Sect. E: Struct. Rep. Online* **67**, 02408
Formula: C₁₇H₁₂N₂O₄
Compound Name: 2-(2-(2-Carboxyphenyl)hydrazinylidene)-3-oxo-N-phenylbutanamide
Synonym: 2-(2-(2-Carboxyphenyl)hydrazinylidene)-3-oxo-N-phenylbutanamide
Space Group: P2₁/n *a* 15.55(1) *b* 5.893(0) *c* 10.775(1)
Space Group No.: 14 *α* 90.00 *β* 89.25(0) *γ* 90.00
R-Factor (%): 4.80 **Temperature(K):** 298 **Density(g/cm³):** 1.405
Parameters
 Fragment 1 HT00 (D) 2.246
 Fragment 1 CHO (A) 121.270



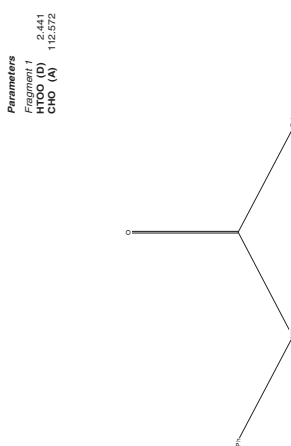
OJSEB

Reference: T.Winkler, R.Hogee, P.G.Jones, I.D.K. (2003). *Acta Crystallogr., Sect. E: Struct. Rep. Online* **59**, 0494
Formula: C₂₈H₂₂N₄O₄
Compound Name: 7-Isopropylidene-N,N,N',N''-tetraphenylmorphane-2,5-diene-2,3,5,6-tetra-carboxamide
Space Group: C2/c *a* 26.842(1) *b* 7.802(0) *c* 14.865(1)
Space Group No.: 15 *α* 90.00 *β* 104.71(0) *γ* 90.00
R-Factor (%): 4.27 **Temperature(K):** 143 **Density(g/cm³):** 1.343
Parameters
 Fragment 1 HT00 (D) 2.913
 Fragment 1 CHO (A) 119.862
 Fragment 2 HT00 (D) 2.916
 Fragment 2 CHO (A) 119.097



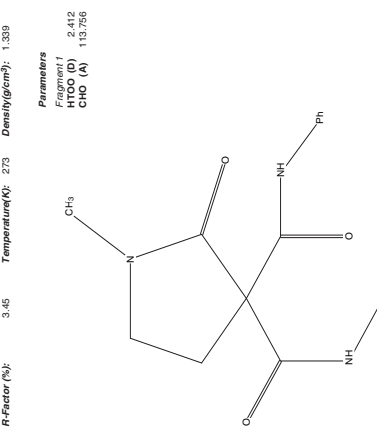
OJUUEJ

Reference: J.F.Gallagher, P.O'Neill (2009). *Private Communication*.
Formula: C₁₄H₁₃N₁O₁
Compound Name: 4-Methyl-N-phenylbenzamide
Space Group: P2₁/n *a* 5.364(0) *b* 30.794(1) *c* 6.898(0)
Space Group No.: 14 *α* 90.00 *β* 107.67(0) *γ* 90.00
R-Factor (%): 5.32 **Temperature(K):** 123 **Density(g/cm³):** 1.293
Parameters
 Fragment 1 HT00 (D) 2.441
 Fragment 1 CHO (A) 112.572



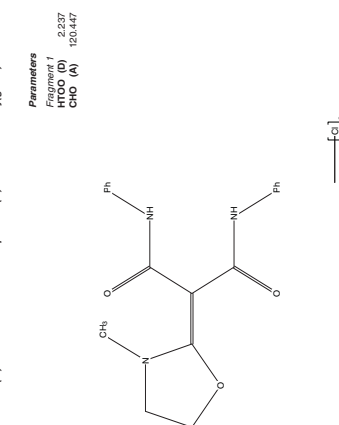
OLEQUS

Reference: Yingqian Song, W.P.Henry, H.I.De Silva, Guozhong Ye, C.U.Primas Janior (2011). *Tetrahedron Lett.* **52**, 853
Formula: C₁₃H₁₃N₃O₃
Compound Name: 1-Methyl-2-oxo-N,N-diphenylpyrrolidine-3,3-dicarboxamide
Synonym: *o,o*-bis(N-Phenylamido)-*l*-actam
Space Group: P-1 *a* 8.543(0) *b* 10.076(0) *c* 11.724(0)
Space Group No.: 2 *α* 114.7(0) *β* 91.04(0) *γ* 111.33(0)
R-Factor (%): 3.45 **Temperature(K):** 273 **Density(g/cm³):** 1.320
Parameters
 Fragment 1 HT00 (D) 2.415
 Fragment 1 CHO (A) 113.725



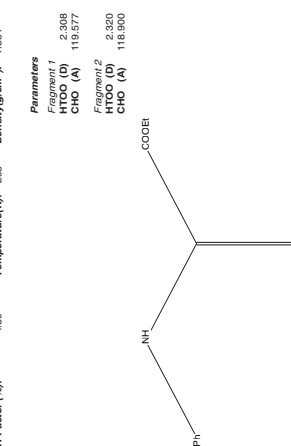
OLERAZ

Reference: Yingqian Song, W.P.Henry, H.I.De Silva, Guozhong Ye, C.U.Primas Janior (2011). *Tetrahedron Lett.* **52**, 853
Formula: C₁₃H₁₃N₃O₃·C₂H₄Cl₂
Compound Name: 2-(3-Methyloxolan-2-ylidene)-N,N-diphenylacetamide
Synonym: dichloromethane adduct
Space Group: C2/c *a* 23.876(7) *b* 7.80(3) *c* 20.976(7)
Space Group No.: 15 *α* 90.00 *β* 95.60(0) *γ* 90.00
R-Factor (%): 3.93 **Temperature(K):** 100 **Density(g/cm³):** 1.356
Parameters
 Fragment 1 HT00 (D) 2.237
 Fragment 1 CHO (A) 120.447



OLIZUE

Reference: E.V.Garcia-Baez, C.Z.Gomez-Castro, H.Hopff, F.J.Martinez-Martinez, I.I.Padilla-Martinez (2003). *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.* **59**, c541
Formula: C₁₀H₁₁N₁O₃
Compound Name: Ethyl N-phenylacetate
Space Group: P-1 *a* 7.803(0) *b* 10.642(0) *c* 13.243(0)
Space Group No.: 2 *α* 103.49(0) *β* 96.05(0) *γ* 110.17(0)
R-Factor (%): 4.39 **Temperature(K):** 295 **Density(g/cm³):** 1.351
Parameters
 Fragment 1 HT00 (D) 2.308
 Fragment 1 CHO (A) 119.577
 Fragment 2 HT00 (D) 2.320
 Fragment 2 CHO (A) 118.900

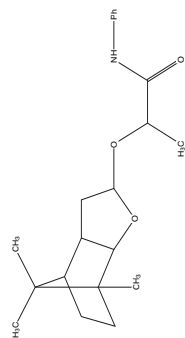


PABFII

Reference: K. Merelino, U. Gresser, G. Haberbauer, C.R. Noe (2002) *Private Communication*.
Formula: C₁₇H₂₃N₃O₃
Compound Name: N-Phenyl-2-(1,10,10-trimethyl-3-oxatrisicyclo[5.2.1]dec-4-yl-oxo)propionamide

Space Group: P43212
Space Group No.: 96
R-Factor (%): 4.89
Cell: a 15.184(2) b 15.184(2) c 17.107(2)
 α 90.00 β 90.00 γ 90.00
Temperature(K): 295
Density(g/cm³): 1.157

Parameters
Fragment 1
HTOO (D) 2.313
CHO (A) 121.739

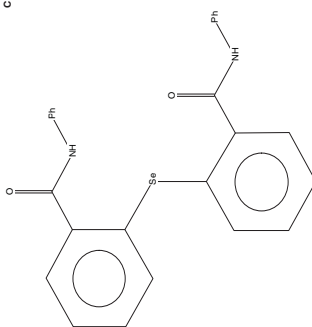


PACFEG

Reference: B.K. Sarma, D. Mirama, M. Minoura, G. Mugish (2010) *J. Am. Chem. Soc.* 132, 5384
Formula: C₁₆H₁₆N₂O₂ S₁
Compound Name: 2,2'-Spiro[9.9]bis(N-phenylacetamide)

Space Group: C2/c
Space Group No.: 15
R-Factor (%): 3.65
Cell: a 24.636(5) b 5.158(6) c 17.486(2)
 α 90.00 β 103.22(6) γ 90.00
Temperature(K): 273
Density(g/cm³): 1.534

Parameters
Fragment 1
HTOO (D) 2.378
CHO (A) 113.946

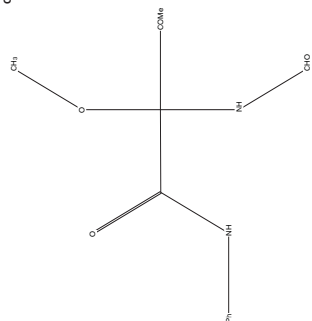


PADFOP

Reference: I. Matsuda, T. Ueda, N. Murakami, S. I. Nagai, J. Sakurai, Y. Kuroki, K. Hatano (1992) *Chem. Commun.* 828
Formula: C₁₂H₁₄N₂O₄
Compound Name: 2-(N-Fermandio)-2-methoxy-3-oxobutanamide

Space Group: P2₁/n
Space Group No.: 14
R-Factor (%): 4.80
Cell: a 8.244(1) b 6.975(1) c 17.691(2)
 α 90.00 β 103.38(1) γ 90.00
Temperature(K): 295
Density(g/cm³): 1.286

Parameters
Fragment 1
HTOO (D) 2.271
CHO (A) 120.050

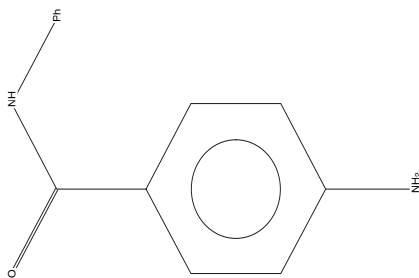


PADTIX

Reference: N.E.C. Duke, P. W. Coddling (1992) *J. Mex. Chem.* 35, 1806
Formula: C₁₃H₁₂N₂O₁
Compound Name: 4-Amino-N-phenylbenzamide

Space Group: Cc
Space Group No.: 9
R-Factor (%): 3.00
Cell: a 6.815(4) b 30.822(2) c 9.930(7)
 α 90.00 β 148.74(2) γ 90.00
Temperature(K): 295
Density(g/cm³): 1.315

Parameters
Fragment 1
HTOO (D) 2.490
CHO (A) 113.543

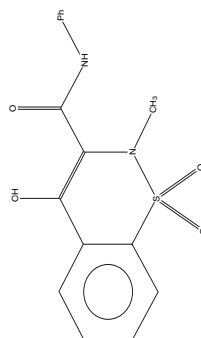


PAMNAE

Reference: F. Aman, W. A. Siddiqui, A. Ashraf, H.L. Siddiqui, M. Parvez (2012) *Acta Crystallogr. Sect. E Struct. Rep. Online* 68, 01780
Formula: C₁₈H₁₄N₂O₄S₁
Compound Name: 4-hydroxy-2-methyl-1,1-dioxo-N-phenyl-5H-1,2-benzothiazine-3-carboxamide

Space Group: P2₁/c
Space Group No.: 14
R-Factor (%): 4.80
Cell: a 10.505(2) b 7.449(3) c 15.235(4)
 α 90.00 β 103.60(1) γ 90.00
Temperature(K): 173
Density(g/cm³): 1.460

Parameters
Fragment 1
HTOO (D) 2.361
CHO (A) 115.646

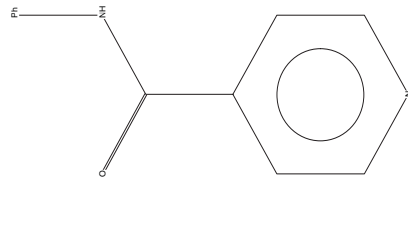


PEDDIM01

Reference: K.C. Mondal, P.S. Mukherjee (2007) *Synth. React. Inorg. Met.-Org. Nano-Met. Chem.* 37, 735
Formula: C₁₂H₁₀N₂O₁
Compound Name: N-Phenylacetamide

Space Group: P-1
Space Group No.: 2
R-Factor (%): 4.25
Cell: a 5.341(10) b 7.657(10) c 12.156(10)
 α 79.93(6) β 79.93(6) γ 89.97(10)
Temperature(K): 150
Density(g/cm³): 1.404

Parameters
Fragment 1
HTOO (D) 2.392
CHO (A) 113.725

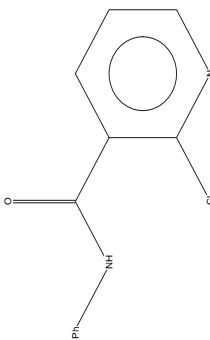


PELKUN

Reference: S. Ojiri, C. Gillevell, J.N. Low, A.G. de Oliveira, M.V.N. de Souza, T.R.A. Vasconcelos, S.M.S.V. Wariishi, J.L. Wariishi (2008) *Acta Crystallogr. Sect. B Struct. Sci.* 62, 651
Formula: C₁₂H₈Cl₁N₂O₁
Compound Name: N-Phenyl-2-chloroacetamide

Space Group: Pccn
Space Group No.: 56
R-Factor (%): 5.94
Cell: a 13.230(9) b 21.074(1) c 7.690(1)
 α 90.00 β 90.00 γ 90.00
Temperature(K): 120
Density(g/cm³): 1.442

Parameters
Fragment 1
HTOO (D) 2.283
CHO (A) 121.295

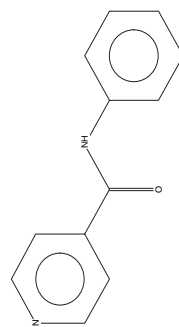


PEDDIM

Reference: D.K. Kumar, D.A. Jose, P. Dasidari, A. Das (2004) *Lingmul.* 20, 0413
Formula: C₁₂H₁₀N₂O₁
Compound Name: N-phenylacetamide

Space Group: P-1
Space Group No.: 2
R-Factor (%): 4.52
Cell: a 5.341(10) b 7.825(1) c 12.186(1)
 α 74.34(6) β 79.17(6) γ 89.91(6)
Temperature(K): 293
Density(g/cm³): 1.389

Parameters
Fragment 1
HTOO (D) 2.424
CHO (A) 112.506

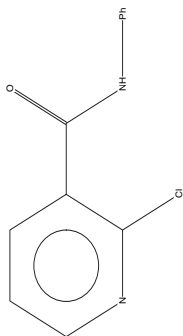


PELKUN01

Reference: S.Durdjevic, D.Leigh, A.Dawson, S.Parsons, A.Collins (2007) *Private Communication*,
Formula: C₁₂H₉ClN₂O₂
Compound Name: 2-Chloro-N-phenylnicotinamide

Space Group: Pcm
Space Group No.: 58
R-Factor (%): 3.88
Cell: a 13.245(0) b 11.045(1) c 7.703(0)
(A,°): α 90.00 β 90.00 γ 90.00
Temperature(K): 150
Density(g/cm³): 1.438

Parameters
Fragment 1
HTOO (D) 2.272
CHO (A) 121.310

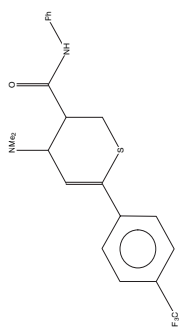


PINSAG

Reference: M.Pink, S.Ruggiani, U.Dietrich (1994) *Z.Kristallogr.* 209,33
Formula: C₁₇H₁₇F₃N₂O₃S₂
Compound Name: 6-(4-(2-fluorophenyl)phenyl)-4-dimethylamino-3,4-dihydro-2H-bipyran-3-carboxamide

Space Group: P-1
Space Group No.: 2
R-Factor (%): 3.50
Cell: a 8.617(2) b 10.045(3) c 20.651(4)
(A,°): α 76.08(2) β 80.78(1) γ 76.35(1)

Parameters
Fragment 1
HTOO (D) 2.249
CHO (A) 115.089
Fragment 2
HTOO (D) 2.242
CHO (A) 116.566

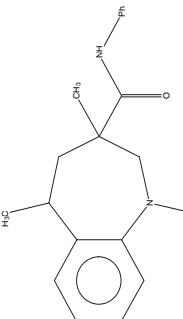


POGGUN

Reference: V.Lellier-Lima, P.Uric, J.Hiet, S.Srinandini, L.Toupet (1994) *J.Chem.Phys.* 100,1693
Formula: C₂₀H₂₄N₂O₂
Compound Name: N-Phenyl-1,3,5-trimethyl-2,3,4,5-tetrahydro-1H-1,2,4-triazepine-3-carboxamide

Space Group: P4
Space Group No.: 61
R-Factor (%): 5.30
Cell: a 10.067(3) b 14.577(4) c 23.554(4)
(A,°): α 90.00 β 90.00 γ 90.00
Temperature(K): 295
Density(g/cm³): 1.130

Parameters
Fragment 1
HTOO (D) 2.323
CHO (A) 118.247

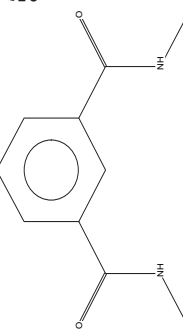


PULHUZ

Reference: J.F.Malone, C.M.Murray, G.M.Dolan, R.Docherty, A.J.Lavery (1997) *Chem.Mater.* 9,2683
Formula: C₂₀H₁₆N₂O₂
Compound Name: N,N-Diphenylisophthalamide

Space Group: Cc
Space Group No.: 9
R-Factor (%): 11.91
Cell: a 11.657(2) b 11.825(2) c 20.211(2)
(A,°): α 90.00 β 102.88(1) γ 80.00
Temperature(K): 295
Density(g/cm³): 1.328

Parameters
Fragment 1
HTOO (D) 2.337
CHO (A) 116.446
Fragment 2
HTOO (D) 2.463
CHO (A) 112.306
Fragment 3
HTOO (D) 2.459
CHO (A) 114.000

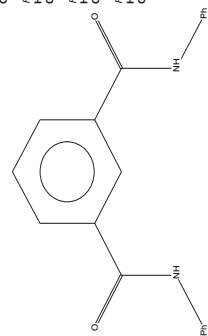


PULHUZ01

Reference: P.Nirmalanagapp, K.Taishiro, Y.Maeda, O.Rangsanman (2002) *J.Phys.Chem.B* 106,6842
Formula: C₂₀H₁₆N₂O₂
Compound Name: N,N-Diphenylisophthalamide

Space Group: P1
Space Group No.: 1
R-Factor (%): 9.50
Cell: a 8.363(0) b 8.370(0) c 23.347(1)
(A,°): α 98.90(0) β 101.59(0) γ 90.00(0)
Temperature(K): 298
Density(g/cm³): 1.327

Parameters
Fragment 1
HTOO (D) 2.410
CHO (A) 114.553
Fragment 2
HTOO (D) 2.398
CHO (A) 114.871
Fragment 3
HTOO (D) 2.441
CHO (A) 112.262
Fragment 4
HTOO (D) 2.411
CHO (A) 114.053
Fragment 5
HTOO (D) 2.412
CHO (A) 114.057

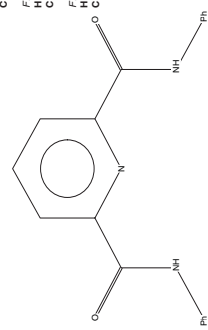


PULUJAH

Reference: J.F.Malone, C.M.Murray, G.M.Dolan, R.Docherty, A.J.Lavery (1997) *Chem.Mater.* 9,2683
Formula: C₁₇H₁₅N₃O₂
Compound Name: Pyridine-2,6-dicarboxylic acid bis(phenylamide)

Space Group: Cc
Space Group No.: 9
R-Factor (%): 4.44
Cell: a 12.024(2) b 12.021(2) c 21.932(9)
(A,°): α 90.00 β 103.17(1) γ 90.00
Temperature(K): 295
Density(g/cm³): 1.366

Parameters
Fragment 1
HTOO (D) 2.372
CHO (A) 115.321
Fragment 2
HTOO (D) 2.327
CHO (A) 118.194
Fragment 3
HTOO (D) 2.324
CHO (A) 117.779
Fragment 4
HTOO (D) 2.352
CHO (A) 117.098

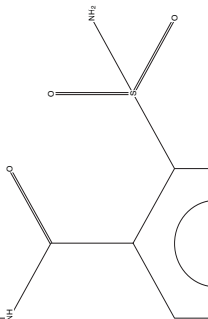


PUMFOD

Reference: W.A.Siddiqui, S.Ahmad, H.L.Siddiqui, T.Husain, M.Patvez (2010) *J.Chem.Cryst.* 40,116
Formula: C₁₃H₁₂N₂O₃S₁
Compound Name: N-Phenyl-5-sulfamoylbenzamide

Space Group: P21/c
Space Group No.: 14
R-Factor (%): 4.90
Cell: a 10.277(6) b 7.501(2) c 16.261(10)
(A,°): α 90.00 β 96.37(2) γ 90.00
Temperature(K): 173
Density(g/cm³): 1.473

Parameters
Fragment 1
HTOO (D) 2.324
CHO (A) 119.436

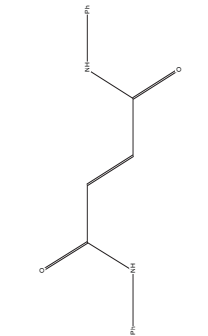


QAKCOW

Reference: B.T.Gawda, S.Foro, K.Shakumala, H.Fuess (2011) *Acta Crystallogr., Sect.E:Struct.Rep. Online* 67,0117
Formula: C₁₈H₁₄N₂O₂
Compound Name: N,N-Diphenylbut-2-enediamide

Space Group: P212121
Space Group No.: 19
R-Factor (%): 4.33
Cell: a 6.604(1) b 13.958(2) c 15.474(2)
(A,°): α 90.00 β 90.00 γ 90.00
Temperature(K): 299
Density(g/cm³): 1.296

Parameters
Fragment 1
HTOO (D) 2.255
CHO (A) 121.353

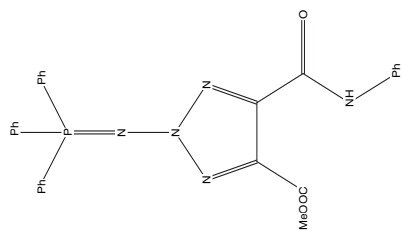


QAQBAM

Reference: Yingqian Miao, I. Muley, W.H. Wilson (2005) *J. Chem. Cryst.*, 35:265
Formula: C₂₀H₂₄N₄O₃P
Compound Name: Methyl 5-(phenylamino)carbamoyl-2-(triphenylphosphanylideneamino)-1,2,3-triazole-4-carboxylate

Space Group: P21/n
Space Group No.: 14
R-Factor (%): 5.21
Temperature(K): 302
Density(g/cm³): 1.321

Parameters
Fragment 1
 HTOO (D) 2.275
 CHO (A) 118.024
Fragment 2
 HTOO (D) 2.318
 CHO (A) 116.798
Fragment 3
 HTOO (D) 2.331
 CHO (A) 120.779

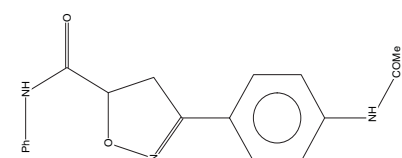


QAVYAO

Reference: J.D. Tozer, M.R. Tremblay, J.Ye-Kuhaluoma, J. Ogo, P. Wemwani Junior, K.D. Janda (2005) *J. Org. Chem.*, 70:7810
Formula: C₁₉H₁₇N₃O₃
Compound Name: (R)-3-(4-Acetylamino)phenyl-4,5-dihydroisoxazole-5-carboxylic acid phenylethyle

Space Group: P21
Space Group No.: 4
R-Factor (%): 4.34
Temperature(K): 298
Density(g/cm³): 1.374

Parameters
Fragment 1
 HTOO (D) 2.371
 CHO (A) 115.885
Fragment 2
 HTOO (D) 2.400
 CHO (A) 113.724

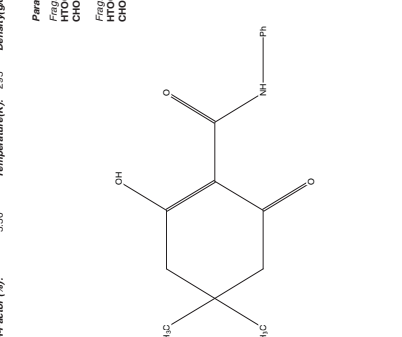


QECEU

Reference: J.K. Mukhopadhyaya, S. Sliemak, Z. Rappoport (2000) *J. Am. Chem. Soc.*, 122:1325
Formula: C₁₇H₁₇N₃O₃
Compound Name: 1-(6-phenylamino-*c*-hydroxyethylamino)-2-hydroxy-4,4-dimethylpiperidine

Space Group: P21/c
Space Group No.: 14
R-Factor (%): 5.50
Temperature(K): 295
Density(g/cm³): 1.259

Parameters
Fragment 1
 HTOO (D) 2.300
 CHO (A) 116.856
Fragment 2
 HTOO (D) 2.274
 CHO (A) 120.102

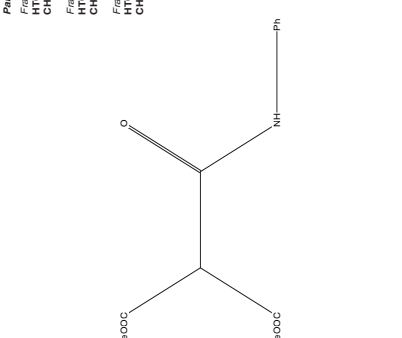


QECCQI

Reference: J.K. Mukhopadhyaya, S. Sliemak, Z. Rappoport (2000) *J. Am. Chem. Soc.*, 122:1325
Formula: C₁₉H₁₃N₃O₃
Compound Name: Methyl 2-methoxycarbonyl-3-oxo-3-phenylaminopropanoate

Space Group: P21/c
Space Group No.: 14
R-Factor (%): 5.80
Temperature(K): 295
Density(g/cm³): 1.294

Parameters
Fragment 1
 HTOO (D) 2.360
 CHO (A) 114.842
Fragment 2
 HTOO (D) 2.289
 CHO (A) 120.738
Fragment 3
 HTOO (D) 2.274
 CHO (A) 121.351

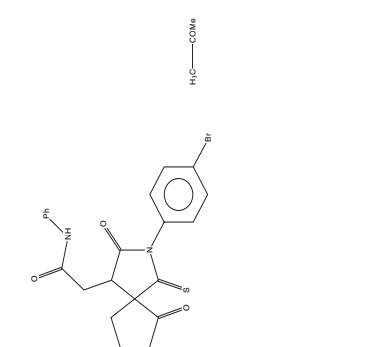


QISREQ

Reference: A. Budzowski, M. P. Ilek, K. Stadnicka (2007) *Monatsh. Chem.*, 138:1257
Formula: C₂₂H₁₉BrN₂O₃S₂Hg O₁
Compound Name: (4*R*,5*R*,6*S*)-2-(4-bromophenyl)-3-(6-oxo-*N*-phenyl-1*H*-thioxo-2-oxo-1*H*-pyridin-4-ylideneamino)acetic acid

Space Group: C2/c
Space Group No.: 15
R-Factor (%): 5.50
Temperature(K): 293
Density(g/cm³): 1.445

Parameters
Fragment 1
 HTOO (D) 2.342
 CHO (A) 119.282

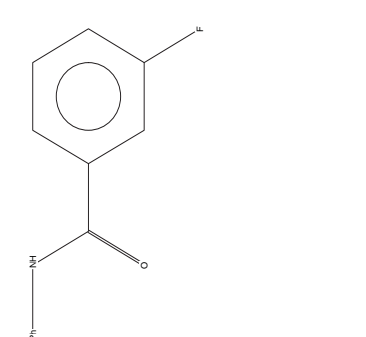


QITSW01

Reference: P. O'Neill, J.F. Gallagher, A. J. Lough (2008) *Private Communication*,
Formula: C₁₃H₁₀F₂N₂O₂
Compound Name: 3-Fluoro-*N*-phenylbenzamide

Space Group: P21/c
Space Group No.: 14
R-Factor (%): 5.28
Temperature(K): 150
Density(g/cm³): 1.442

Parameters
Fragment 1
 HTOO (D) 2.425
 CHO (A) 112.512

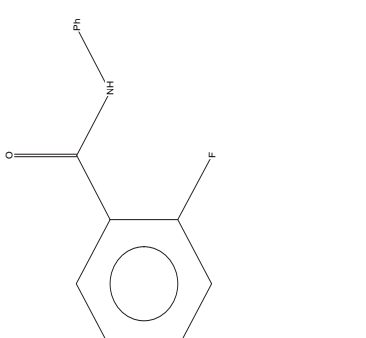


QITTE

Reference: D. Chopra, T.N.G. Row (2008) *CrytEngComm*, 10:54
Formula: C₁₃H₁₀F₁N₁O₁
Compound Name: 2-Fluoro-*N*-phenylbenzamide

Space Group: P21
Space Group No.: 4
R-Factor (%): 6.35
Temperature(K): 290
Density(g/cm³): 1.388

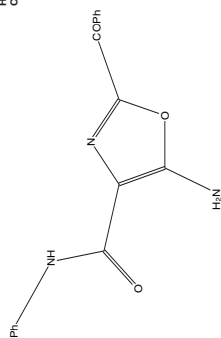
Parameters
Fragment 1
 HTOO (D) 2.344
 CHO (A) 115.243



QIWWAV

Reference: V.P. Kalya, E.B. Danilova, V.V. Semenov, A.A. Yakovlev, *Izv. Akad. Nauk SSSR Ser. Khim. (Russ./Russ. Chem. Bull.)*, 1773
Formula: C₁₇H₁₃N₃O₃
Compound Name: 5-Amino-2-benzoyl-N-phenyl-1,3-oxazol-4-carboxamide
Space Group: Pca21
Space Group No.: 29
Cell: a 12.095(4) b 32.744(11) c 7.452(3)
 α 90.00 β 90.00 γ 90.00
R-Factor (%): 5.15 **Temperature(K):** 120 **Density(g/cm³):** 1.414

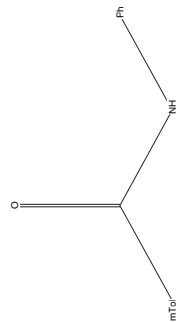
Parameters
Fragment 1
HTOO (D) 2.413
CHO (A) 115.857
Fragment 2
HTOO (D) 2.048
CHO (A) 118.630



QIXNAN

Reference: B.T. Gowda, S. Foro, B.P. Sowmya, H. Fues (2008) *Acta Crystallogr., Sect. E: Struct. Rep. Online* 84:1770
Formula: C₁₄H₁₃N₃O₃
Compound Name: 3-Methyl-N-phenylbenzamide
Space Group: P2₁/c
Space Group No.: 14
Cell: a 16.917(2) b 15.551(1) c 8.525(1)
 α 90.00 β 93.35(1) γ 90.00
R-Factor (%): 8.19 **Temperature(K):** 295 **Density(g/cm³):** 1.239

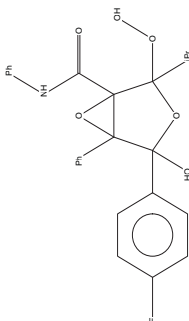
Parameters
Fragment 1
HTOO (D) 2.464
CHO (A) 112.953



QOQFLE

Reference: M. Ashfaq, M.N. Tahir, L.U. Khan, M.S. Iqbal, M.N. Arshad (2008) *Acta Crystallogr., Sect. E: Struct. Rep. Online* 84:1548
Formula: C₂₆H₂₄F₂N₂O₄
Compound Name: (R,R,2S,4S,5S)-4-(4-Fluorophenyl)-2-hydroperoxy-4-hydroxy-2-isopropyl-N,5-diphenyl-3,6-dioxabicyclo[3.1.0]hexane-1-carboxamide
Space Group: P2₁/n
Space Group No.: 14
Cell: a 11.745(9) b 17.450(1) c 17.089(9)
 α 90.00 β 94.44(1) γ 90.00
R-Factor (%): 4.91 **Temperature(K):** 295 **Density(g/cm³):** 1.314

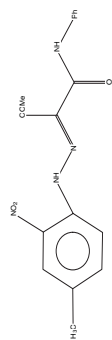
Parameters
Fragment 1
HTOO (D) 2.098
CHO (A) 118.504



QOQAZG02

Reference: C.J. Brown, H.R. Yadav (1984) *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.* 40:564
Formula: C₁₇H₁₆N₂O₄
Compound Name: (±)-Methyl-2-nitrophenyl(hydrazono)acetosulfonamide
Space Group: P2₁/a
Space Group No.: 14
Cell: a 15.034(11) b 20.581(13) c 7.526(10)
 α 90.00 β 90.00 γ 90.00
R-Factor (%): 4.40 **Temperature(K):** 295 **Density(g/cm³):** 1.403

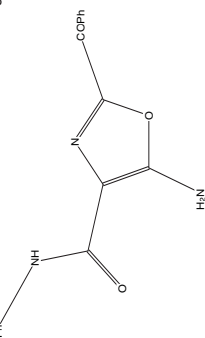
Parameters
Fragment 1
HTOO (D) 2.269
CHO (A) 116.815



QOQAZG03

Reference: E.F. Paulus (1984) *Z. Kristallogr.*, 187:65
Formula: C₁₇H₁₆N₂O₄
Compound Name: N-Phenyl-2-(4-methyl-2-nitrophenyl(hydrazono))-3-oxo-butyramide
Synonym: C.I. Pigment Yellow 111:860
Space Group: P2₁/n
Space Group No.: 14
Cell: a 7.659(1) b 20.375(2) c 19.446(1)
 α 90.00 β 98.18(1) γ 90.00
R-Factor (%): 4.16 **Temperature(K):** 295 **Density(g/cm³):** 1.413

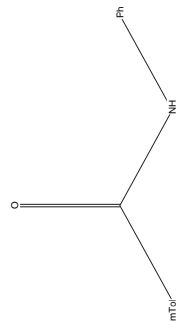
Parameters
Fragment 1
HTOO (D) 2.338
CHO (A) 120.953



QOQAZG21

Reference: A. Whittaker (1984) *Z. Kristallogr.*, 186:177
Formula: C₁₇H₁₆N₂O₄
Compound Name: (±)-1-Hydroxyethylidene-acetanilide-α-azo-(4'-methyl-2'-nitrobenzene)
Space Group: P2₁/c
Space Group No.: 14
Cell: a 7.587(42) b 20.382(53) c 12.033(46)
 α 90.00 β 120.68(28) γ 90.00
R-Factor (%): 8.00 **Temperature(K):** 295 **Density(g/cm³):** 1.414

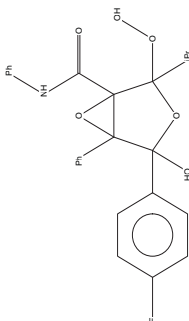
Parameters
Fragment 1
HTOO (D) 2.497
CHO (A) 116.927



QOQAZG31

Reference: A. Whittaker (1985) *Z. Kristallogr.*, 170:213
Formula: C₁₇H₁₆N₂O₄
Compound Name: (1-N-Acetyl-N-phenylacetamido)-methyl(ene)-azo-4-methyl-2-nitrobenzene
Synonym: C.I. Pigment Yellow 1 and C.I. Pigment Yellow 5
Space Group: P2₁/n
Space Group No.: 14
Cell: a 7.567(1) b 20.420(3) c 10.345(1)
 α 90.00 β 99.29(1) γ 90.00
R-Factor (%): 7.70 **Temperature(K):** 295 **Density(g/cm³):** 1.433

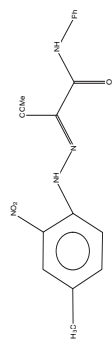
Parameters
Fragment 1
HTOO (D) 2.295
CHO (A) 116.103



QOQCOY10

Reference: C.J. Brown, H.R. Yadav (1984) *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.* 40:85
Formula: C₁₅H₁₄N₂O₃
Compound Name: (±)-Methyl-2-nitrophenyl(hydrazono)acetanilide
Space Group: P2₁/a
Space Group No.: 14
Cell: a 23.344(15) b 5.905(8) c 12.164(12)
 α 90.00 β 121.07(10) γ 90.00
R-Factor (%): 4.50 **Temperature(K):** 295 **Density(g/cm³):** 1.390

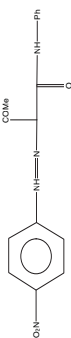
Parameters
Fragment 1
HTOO (D) 2.234
CHO (A) 118.072



QQOELA03

Reference: A. Whittaker, N. Walker (1965), *Z. Kristallogr.*, 171, 7
Formula: C₁₄H₁₆N₂O₄
Compound Name: *o*-(4-Nitrobenzenyl)hydrazono)-*o*-acetylacetamide
Synonym: C.I. Pigment Yellow 4
Space Group: P-1 *a* 7.691(2) *b* 10.247(2) *c* 11.195(2)
Space Group No.: 2 *α* 109.00(2) *β* 73.80(2) *γ* 112.21(2)
R-Factor (%): 5.40 **Temperature(K):** 295 **Density(g/cm³):** 1.430

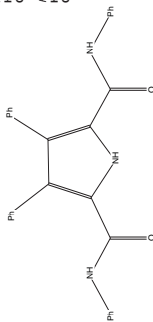
Parameters
Fragment 1
HTOO (D) 2.235
HTOO (A) 118.595
CHO (A)



RALZIN

Reference: P. A. Gale, S. Cambio, C. F. Chipman, M. E. Light, M. J. Hultineau (2007), *Tetrahedron Lett.*, 48, 2095
Formula: C₁₀H₈N₂O₂
Compound Name: N,N'-diphenyl-3,4-diphenylmale-2,5-dicarboximide
Space Group: P-1 *a* 8.146(5) *b* 6.145(5) *c* 27.453(5)
Space Group No.: 2 *α* 91.44(8) *β* 89.82(6) *γ* 73.53(3)
R-Factor (%): 6.22 **Temperature(K):** 150 **Density(g/cm³):** 1.283

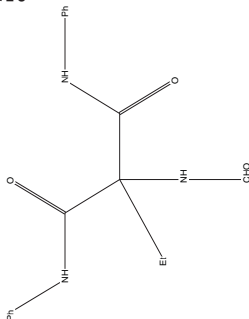
Parameters
Fragment 1
HTOO (D) 2.381
HTOO (A) 117.647
CHO (A)
Fragment 2
HTOO (D) 2.313
HTOO (A) 119.865
CHO (A)
Fragment 3
HTOO (D) 2.389
HTOO (A) 120.458
CHO (A)
Fragment 4
HTOO (D) 2.345
HTOO (A) 121.108
CHO (A)



REBPOF

Reference: L. Hoch, M. Huskova, J. Schmitz, G. Schmalkenburg, M. Kubackow (2012), *Synthesis*, 44, 1307
Formula: C₁₈H₁₆N₂O₂
Compound Name: 2-Ethyl-2-formylidene-N,N'-diphenylmalonamide
Space Group: P-1 *a* 8.514(10) *b* 15.195(10) *c* 18.051(10)
Space Group No.: 2 *α* 93.43(6) *β* 89.30(6) *γ* 114.48(6)
R-Factor (%): 4.36 **Temperature(K):** 123 **Density(g/cm³):** 1.306

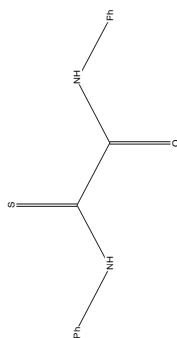
Parameters
Fragment 1
HTOO (D) 2.252
HTOO (A) 121.604
CHO (A)
Fragment 2
HTOO (D) 2.272
HTOO (A) 119.536
CHO (A)



RERGUQ

Reference: V. B. Rybakov, E. V. Babayev, Y. V. Dimiykh (2001), *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 57, 0414
Formula: C₁₄H₁₂H₂O₂S₁
Compound Name: N,N'-Diphenylthiooxamide
Space Group: P2₁/c *a* 4.026(5) *b* 14.463(8) *c* 20.726(12)
Space Group No.: 14 *α* 80.00 *β* 80.27(2) *γ* 80.00
R-Factor (%): 4.70 **Temperature(K):** 293 **Density(g/cm³):** 1.390

Parameters
Fragment 1
HTOO (D) 2.439
HTOO (A) 119.490
CHO (A)



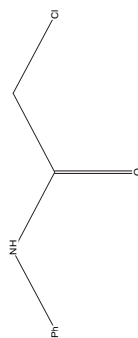
RERGUQ

RERGUQ

RIYWIG

Reference: B. T. Gowda, J. Kozlsek, M. Tokarik, H. Fuess (2008), *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 64, 0887
Formula: C₉H₈Cl₁N₁O₁
Compound Name: 2-Chloro-N-phenylacetamide
Space Group: C₂ *a* 5.062(1) *b* 18.361(6) *c* 9.115(2)
Space Group No.: 9 *α* 90.00 *β* 102.13(9) *γ* 90.00
R-Factor (%): 3.91 **Temperature(K):** 297 **Density(g/cm³):** 1.300

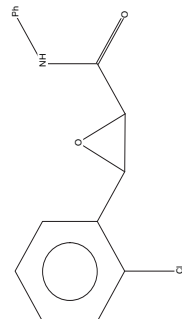
Parameters
Fragment 1
HTOO (D) 2.337
HTOO (A) 117.843
CHO (A)



RUGSOC

Reference: Lan-Mei Chen, Tai-Ran Kung (2009), *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 65, 03126
Formula: C₁₂H₁₂Cl₁N₁O₂
Compound Name: (R)-3-(3-(2-Chlorophenyl)-N-phenylacetamide-2-carboxamide
Space Group: P2₁2₁2₁ *a* 6.661(10) *b* 10.034(10) *c* 20.243(10)
Space Group No.: 19 *α* 90.00 *β* 90.00 *γ* 90.00
R-Factor (%): 3.06 **Temperature(K):** 295 **Density(g/cm³):** 1.344

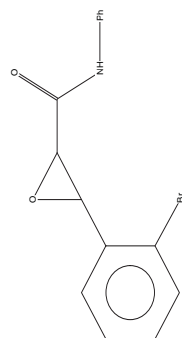
Parameters
Fragment 1
HTOO (D) 2.303
HTOO (A) 120.429
CHO (A)



RUUMAL

Reference: Long He, Hong-Mei Oh, Lan-Mei Chen (2009), *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 65, 02899
Formula: C₁₅H₁₂Br₁N₁O₂
Compound Name: 3-(2-Bromophenyl)-N-phenylacetamide-2-carboxamide
Space Group: P2₁2₁2₁ *a* 6.717(10) *b* 10.037(10) *c* 20.428(10)
Space Group No.: 19 *α* 90.00 *β* 90.00 *γ* 90.00
R-Factor (%): 2.81 **Temperature(K):** 295 **Density(g/cm³):** 1.534

Parameters
Fragment 1
HTOO (D) 2.308
HTOO (A) 120.258
CHO (A)

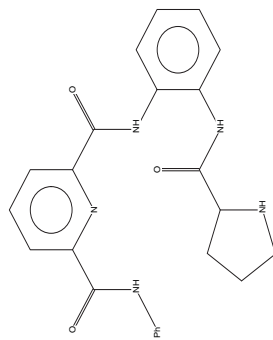


RULJAK

Reference: K.Misai, S.A.Hyatt, D.Turner, C.M.Haddad, J.R.Parquette (2009) *Chem Commun*, 3561
Formula: C₁₈H₂₃N₃O₃
Compound Name: N-Phenyl-N-(2-(L-prolylamino)phenyl)-2,6-pyridinedicarboxamide

Space Group: P2₁
Space Group No.: 4
R-Factor (%): 3.65
Temperature(K): 150
Density(g/cm³): 1.326

Parameters
Fragment 1
HTOO (D): 2.290
CHO (A): 120.053

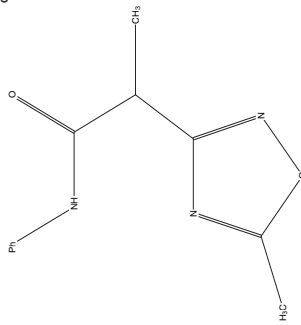


RULKIS

Reference: S.A.Hewitts, J.A.Murphy, Jian Lin, D.E.Hibbs, M.B.Hustubai (1997) *J.Chem.Soc.Paper Trans*, 1, 1559
Formula: C₁₂H₁₃N₃O₂
Compound Name: 2-(5-Methyl-1,2,4-oxadiazol-3-yl)propanamide

Space Group: P2₁/a
Space Group No.: 14
R-Factor (%): 4.88
Temperature(K): 295
Density(g/cm³): 1.275

Parameters
Fragment 1
HTOO (D): 2.278
CHO (A): 120.760

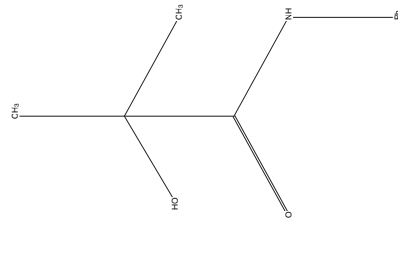


SABSAR

Reference: O.Miemo, B.M.Saitoyo, L.E.Moniell, T.Kobayashi, S.Sasagaki, J.Tanimiz (2010) *Tetrahedron Lett*, 51, 6728
Formula: C₁₀H₁₃N₃O₂
Compound Name: 2-Hydroxy-2-methyl-N-phenylpropanamide

Space Group: P2₁/c
Space Group No.: 14
R-Factor (%): 4.51
Temperature(K): 294
Density(g/cm³): 1.203

Parameters
Fragment 1
HTOO (D): 2.273
CHO (A): 121.011

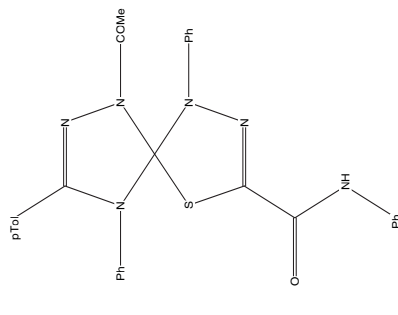


SEKWAH

Reference: A.A.Nidia, A.M.Mahrum, A.S.Shawall (2005) *Phosphorus,Sulfur,Silicon,Relat Elem*, 160,2111
Formula: C₃₁H₂₆N₄O₂S₁
Compound Name: 1,6-Diphenyl-7-(p-toyl)-3-(N-phenylcarbonyl)-9-acetyl-1,2,6,8,9-penta-aza-4-thia-spiro[4.4]nonane

Space Group: P-1
Space Group No.: 2
R-Factor (%): 4.70
Temperature(K): 298
Density(g/cm³): 1.313

Parameters
Fragment 1
HTOO (D): 2.904
CHO (A): 121.841

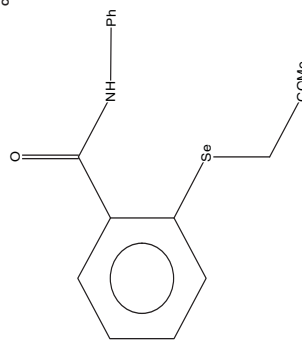


SENGUN

Reference: L.Dupont, O.Didberg, P.Jacquemin (1990) *Acta Crystallogr, Sect C,Cryst Struct Commun*, 46,484
Formula: C₁₈H₁₅N₃O₂S₄
Compound Name: 2-(Acetonylseleno)-benzanilide

Space Group: P2₁/n
Space Group No.: 14
R-Factor (%): 5.60
Temperature(K): 295
Density(g/cm³): 1.530

Parameters
Fragment 1
HTOO (D): 2.245
CHO (A): 112.448

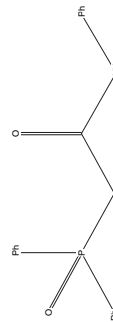


SISLEM

Reference: O.I.Alyashin, E.V.Sharova, L.L.Gilnets, K.A.Lyssenko, D.G.Golovanov, T.A.Mastyukova, G.A.Ptylova, I.G.Taranav, G.V.Mysasovskiy (2008) *Izv.Akad.Nauk SSSR, Ser: Khim, (Russ./Russ.Chem.Bull)*, 1, 1387
Formula: C₂₀H₁₈N₂O₂P₁
Compound Name: 2-(Diphenylphosphonyl)-N-phenylacetamide

Space Group: C₂
Space Group No.: 9
R-Factor (%): 3.35
Temperature(K): 173
Density(g/cm³): 1.306

Parameters
Fragment 1
HTOO (D): 2.205
CHO (A): 120.768

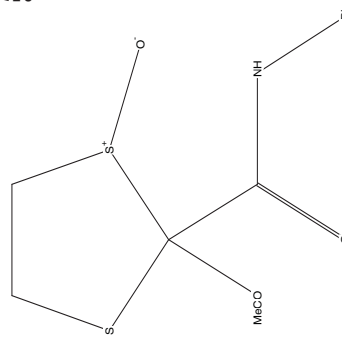


SITSYI

Reference: F.Cermola, A.Giarrugna, M.R.Iessa, G.Palumbo, R.Purcuro, M.Rubino, A.Tuzi (2007) *J.Org.Chem*, 72,10075
Formula: C₁₂H₁₃N₃O₂S₂
Compound Name: trans-2-Acetyl-2-(phenylcarbonyl)-1,3-dithiolan-1-ium-1-olate

Space Group: P2₁/c
Space Group No.: 14
R-Factor (%): 4.45
Temperature(K): 298
Density(g/cm³): 1.446

Parameters
Fragment 1
HTOO (D): 2.453
CHO (A): 112.640



SOBCAO

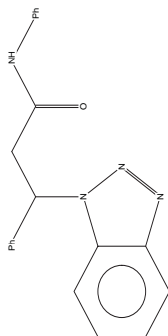
Reference: Xiaoxia Wang, Zhifang Li, Xiangming Zhu, Hui Xiao, Xueli Zou, Lidan Kong, Xiaoliang Li (2008) *Tetrahedron* **64**, 6510

Formula: C₁₇ H₁₆ N₄ O₁

Compound Name: 3-(1H-Benzotriazol-1-yl)-N,N,3-diphenylpropanamide

Space Group: P-1
Space Group No.: 2
R-Factor (%) : 4.19
Temperature(K): 296
Density(g/cm³): 1.297

Parameters
Fragment 1
HTOO (D) 2.291
CHO (A) 120.102



SOBDUJ

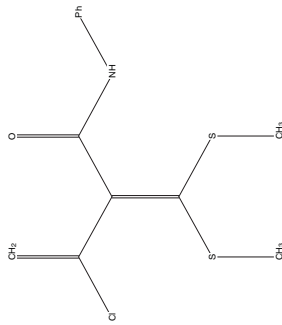
Reference: Yang Yang, Dexuan Xiang, Xiaoliang Zhao, Yongliu Liang, Jie Huang, Dawen Dong (2008) *Tetrahedron* **64**, 4359

Formula: C₁₃ H₁₄ Cl₁ N₁ O₂

Compound Name: 2-(bis(4-methylphenyl)amino)-3-chloro-N-phenylbut-3-enamide

Space Group: Pn21
Space Group No.: 53
R-Factor (%) : 4.77
Temperature(K): 293
Density(g/cm³): 1.341

Parameters
Fragment 1
HTOO (D) 2.388
CHO (A) 115.220



SOFLLA

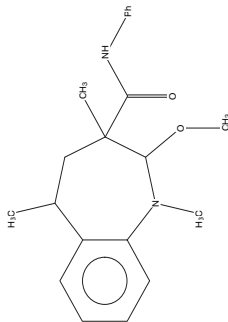
Reference: C. Nisole, P. Uric, J. Huet, L. Toupet (1991) *J. Chem. Res.* **204**, 1914

Formula: C₁₇ H₁₆ N₂ O₂

Compound Name: N-Phenyl-2-(2-methoxy-3,5-tetrahydro-1H-1,4-benzazepin-3-carboxamide)

Space Group: Cc
Space Group No.: 9
R-Factor (%) : 3.10
Temperature(K): 295
Density(g/cm³): 1.209

Parameters
Fragment 1
HTOO (D) 0.937
CHO (A) 113.035



SOGVUF

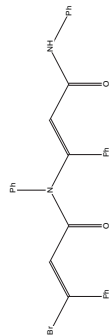
Reference: M. Cichanowicz-Rukowska, P. Sarda, B. Stec, A. Koliata (1991) *J. Crystallogr. Spectrosc. Res.* **21**, 1363

Formula: C₂₀ H₂₃ Br₁ N₂ O₂

Compound Name: β-(N-Phenyl)-N-(β-bromocinnamoyl)amino)cinnamamide

Space Group: P212121
Space Group No.: 19
R-Factor (%) : 6.70
Temperature(K): 295
Density(g/cm³): 1.363

Parameters
Fragment 1
HTOO (D) 2.203
CHO (A) 120.709
Fragment 2
HTOO (D) 2.199
CHO (A) 119.711



SOOBEG

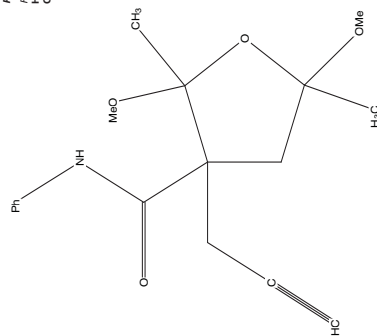
Reference: Jia Meng, Yu-Long Zhao, Chuan-Qing Ren, You Li, Zhu Li, Qun Liu (2009) *Chem.-Eur. J.* **15**, 1830

Formula: C₁₈ H₂₃ N₁ O₄

Compound Name: 2,5-Dimethoxy-2,5-dimethyl-N-phenyl-3-(4-oxo-2-yn-1-yl)tetrahydrofuran-3-carboxamide

Space Group: P21c
Space Group No.: 14
R-Factor (%) : 7.10
Temperature(K): 293
Density(g/cm³): 1.205

Parameters
Fragment 1
HTOO (D) 2.238
CHO (A) 121.944



SUHNIS

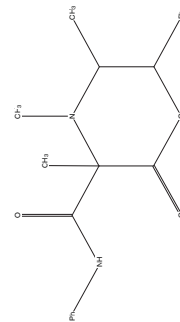
Reference: J.H. Woil, U.J. Woil, B. Nubar (1993) *Liebigs Ann.* **329**

Formula: C₂₀ H₂₂ N₂ O₃

Compound Name: (R)-4S,5S,8R)-3,4,5-Timethyl-N,6-diphenyl-2-oxomorpholine-3-carboxamide

Space Group: P212121
Space Group No.: 19
R-Factor (%) : 3.90
Temperature(K): 295
Density(g/cm³): 1.188

Parameters
Fragment 1
HTOO (D) 2.289
CHO (A) 119.730



SUQDIS

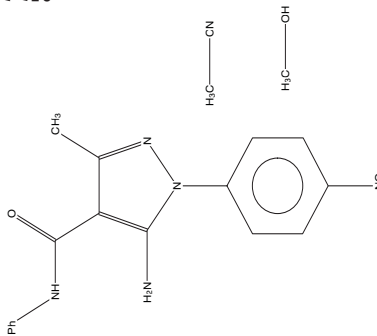
Reference: N.O. Haloran, J.P. James, C.A. Downey, P.O. Mailey, T.D. Itt, S. Bernard (2008) *Helveticas* **75**, 2681

Formula: C₁₇ H₁₅ N₃ O₃

Compound Name: 5-Amino-3-methyl-1-(4-mitrophenyl)-N-phenyl-1H-pyrazole-4-carboxamide acetone/methanol solvate

Space Group: P21/n
Space Group No.: 14
R-Factor (%) : 6.53
Temperature(K): 100
Density(g/cm³): 1.443

Parameters
Fragment 1
HTOO (D) 2.237
CHO (A) 121.053



SUOFOA

Reference: J.O.Luay, X.Formosa, W.Skranc, J.D.Wallis (2005) *Org.Biomol.Chem.*, 3,3273

Formula: C₁₈H₁₂O₄ N₂ O₂

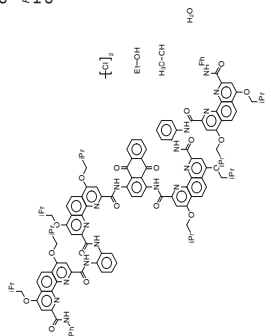
Compound Name: 8-Methoxy-N-phenyl-1-naphthamide

Space Group: P-1

Space Group No.: 2

R-Factor (%): 14.30

Parameters
 Fragment 1
 HTOO (D) 2.228
 CHO (A) 121.653
 Fragment 2
 HTOO (D) 2.370
 CHO (A) 115.291



SUOFUG

Reference: J.O.Luay, X.Formosa, W.Skranc, J.D.Wallis (2005) *Org.Biomol.Chem.*, 3,3273

Formula: C₁₈H₁₂O₄ N₂ O₂

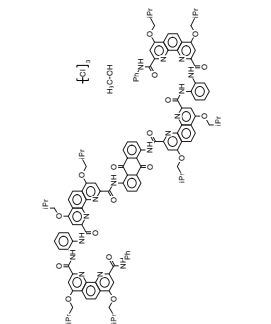
Compound Name: 8-Methoxy-N-phenyl-1-naphthamide

Space Group: P-1

Space Group No.: 2

R-Factor (%): 14.30

Parameters
 Fragment 1
 HTOO (D) 2.228
 CHO (A) 121.653
 Fragment 2
 HTOO (D) 2.370
 CHO (A) 115.291



TATNOS

Reference: S.Green, A.D.Wroblewski, J.Aube (2009) *Org.Lett.*, 7,2167

Formula: C₂₇H₃₄N₂O₇

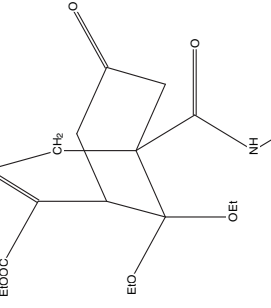
Compound Name: Ethyl 3-(3,4-dihydroxy-3,7-dioxo-5-phenylcarbamoyl)hexanoate

Space Group: P2₁/n

Space Group No.: 14

R-Factor (%): 3.53

Parameters
 Fragment 1
 HTOO (D) 2.289
 CHO (A) 113.932



TAWRIT

Reference: J.O.Luay, X.Formosa, W.Skranc, J.D.Wallis (2005) *Org.Biomol.Chem.*, 3,3273

Formula: C₁₈H₁₅N₃O₂

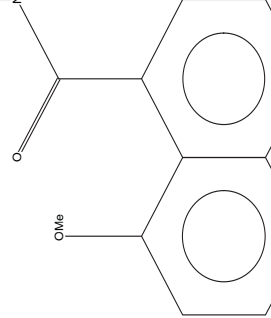
Compound Name: 8-Methoxy-N-phenyl-1-naphthamide

Space Group: P-1

Space Group No.: 2

R-Factor (%): 6.45

Parameters
 Fragment 1
 HTOO (D) 2.325
 CHO (A) 118.720
 Fragment 2
 HTOO (D) 2.345
 CHO (A) 115.314



TAWROZ

Reference: J.O.Luay, X.Formosa, W.Skranc, J.D.Wallis (2005) *Org.Biomol.Chem.*, 3,3273

Formula: C₁₈H₁₅N₃O₂

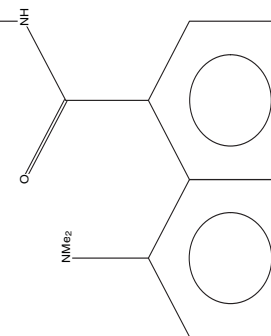
Compound Name: 8-(Dimethylamino)-N-phenyl-1-naphthamide

Space Group: P2₁/c

Space Group No.: 14

R-Factor (%): 4.49

Parameters
 Fragment 1
 HTOO (D) 2.341
 CHO (A) 118.574



TEBMOD

Reference: R.A.Layfield, S.M.Humphrey (2005) *Organometallics*, 24, 6063

Formula: C₂₆H₂₆Mg₂N₄O₆·4(C₆H₆O)

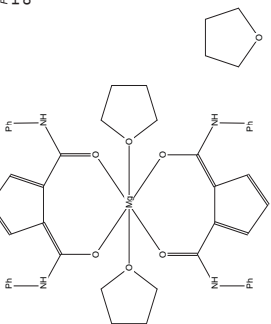
Compound Name: trans-bis(2-bis(phenylcarbamoyl)cyclopentadienyl)-bis(tetrahydrofuran)-magnesium tetrahydrofuran solvate

Space Group: P2₁2₁2₁

Space Group No.: 19

R-Factor (%): 7.78

Parameters
 Fragment 1
 HTOO (D) 2.268
 CHO (A) 118.971
 Fragment 2
 HTOO (D) 2.281
 CHO (A) 117.987



TEFJOD

Reference: M.M.Kravchenko, L.G.Vorontsova, M.G.Kumila, I.V.Zavarzin, V.N.Yarovenko (1996) *Izv.Akad.Nauk SSSR, Ser.Khim. (Russ.Chem.Bull.)*, 485

Formula: C₁₂H₁₆N₂O₂S

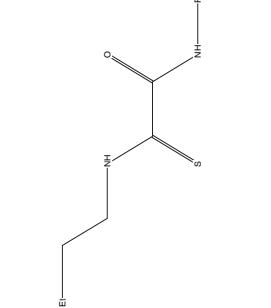
Compound Name: N-Bis(4-phenylphenyl)thioamide

Space Group: P12₁/n

Space Group No.: 14

R-Factor (%): 7.00

Parameters
 Fragment 1
 HTOO (D) 2.281
 CHO (A) 115.010



TEFZAG

Reference: F.F.Fleming, Zhiyu Zhang, Guodong Wei, O.W.Steward (2006) *J.Org.Chem.*, 71, 1430

Formula: C₁₆H₂₀N₂O₂

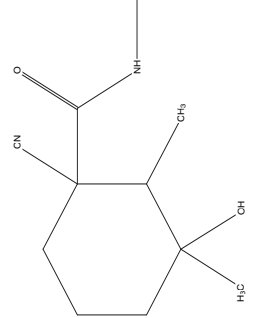
Compound Name: (1R,2R,3S)-1-Cyano-3-hydroxy-2,3-dimethyl-4-phenylpyrrolidinecarboxamide

Space Group: P2₁/c

Space Group No.: 14

R-Factor (%): 4.47

Parameters
 Fragment 1
 HTOO (D) 2.307
 CHO (A) 118.417
 Fragment 2
 HTOO (D) 2.346
 CHO (A) 119.251



TEGLEW

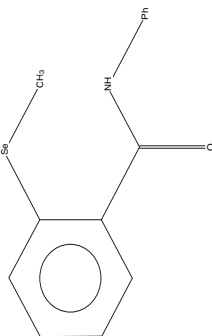
Reference: Mia C.Fong, R.W.Gable, C.H.Schesser (1996) *Acta Crystallogr., Sect.C:Cryst.Struct Commun.* **52**, 1886

Formula: C₁₄H₁₃N₃O₁S₄

Compound Name: 2-Methylseleno-N-phenylbenzamide

Space Group: P2₁ **Cell:** a 6.771(2) b 16.626(2) c 16.620(1)
Space Group No.: 51 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 0.00 **Temperature(K)**: 295 **Density(g/cm³)**: 1.493

Parameters
Fragment 1
HTOO (D): 2.272
HTOO (I): 120.099
CHO (A): 121.019



TITSUL

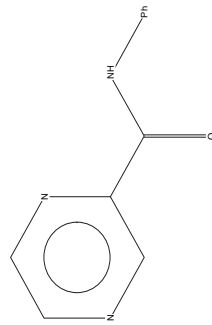
Reference: S.M.S.V. Wedell, M.V.N. de Souza, T.F.A. Vasconcelos, *Acta Crystallogr., Sect.B:Struct.Sci.* **64**, 64

Formula: C₁₁H₉N₃O₁

Compound Name: N-Phenylpyridine-2-carboxamide

Space Group: P-1 **Cell:** a 5.972(0) b 7.527(0) c 11.020(0)
Space Group No.: 2 **α** 83.30(0) **β** 85.38(0) **γ** 69.01(0)
R-Factor (%): 4.67 **Temperature(K)**: 120 **Density(g/cm³)**: 1.440

Parameters
Fragment 1
HTOO (D): 2.277
HTOO (I): 121.019
CHO (A): 121.019



TOMVAT

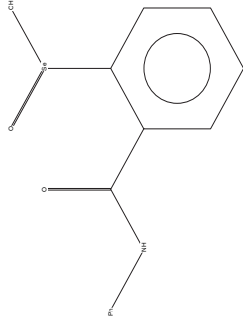
Reference: B.K.Sarma, G.Magesh (2008) *Chem-Eur.J.* **14**, 10603

Formula: C₁₇H₁₇N₃O₃S₄

Compound Name: 2-(Phenylcarbamoyl)benzenesulfonamide

Space Group: Pn2₁ **Cell:** a 19.062(4) b 14.125(3) c 4.588(0)
Space Group No.: 33 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 3.70 **Temperature(K)**: 295 **Density(g/cm³)**: 1.662

Parameters
Fragment 1
HTOO (D): 2.259
HTOO (I): 119.657
CHO (A): 119.657



TOPQAR

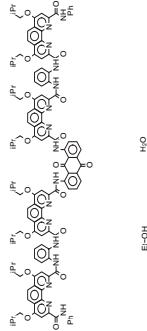
Reference: Hai-Yu Hu, Jun-Feng Xiang, Jing Cao, Chuan-Feng Chen (2009) *Org.Lett.* **10**, 3535

Formula: C₁₂₆H₁₂₆N₁₆O₁₆(C₂H₄O₂)₂(H₂O)₁

Compound Name: N,N'-bis[2-(2,4-diphenylaminoacetonyl)-4,7-dichlorophenyl]-10-phenanthroline-2-yl-carbamoyl-phenylamino-phenylamino-1,10-phenanthroline-2-yl-carbamoyl-1,8-naphthoquinonediimine ethanol solvate anhydride

Space Group: P-1 **Cell:** a 16.055(4) b 20.086(5) c 22.642(6)
Space Group No.: 2 **α** 84.27(3) **β** 70.17(2) **γ** 67.43(3)
R-Factor (%): 15.33 **Temperature(K)**: 173 **Density(g/cm³)**: 1.288

Parameters
Fragment 1
HTOO (D): 2.265
HTOO (I): 121.101
Fragment 2
HTOO (D): 2.259
HTOO (I): 121.337
CHO (A): 121.337



Et-OH HO

TOTMIY

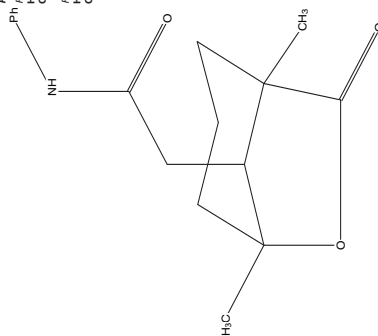
Reference: A.G.Schultz, S.J.Kirincich (1998) *J.Org.Chem.* **63**, 5426

Formula: C₁₇H₂₁N₃O₃

Compound Name: (1S,5R,6R)-1,5-Dimethyl-6-(N-phenylcarbamoylmethyl)-6-oxabicyclo[3.2.1]octan-7-one

Space Group: P2₁ **Cell:** a 7.331(1) b 22.379(2) c 9.718(1)
Space Group No.: 4 **α** 90.00 **β** 98.52(1) **γ** 90.00
R-Factor (%): 4.29 **Temperature(K)**: 295 **Density(g/cm³)**: 1.205

Parameters
Fragment 1
HTOO (D): 2.324
HTOO (I): 115.694
Fragment 2
HTOO (D): 2.369
HTOO (I): 114.907
CHO (A): 114.907



TOWBAI

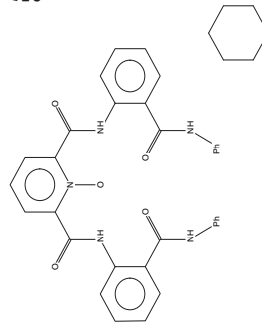
Reference: Y.Hamuro, S.J.Geb, A.D.Hamilton (1998) *J.Am.Chem.Soc.* **118**, 7529

Formula: C₂₃H₂₅N₅O₃(C₆H₅)₂

Compound Name: 2,6-Bis[2-(Phenylcarbamoyl)phenyl]carbamoylpyridine N-oxide cyclotriazane solvate

Space Group: P-1 **Cell:** a 9.267(2) b 12.707(3) c 13.273(3)
Space Group No.: 2 **α** 89.56(5) **β** 89.36(6) **γ** 81.44(5)
R-Factor (%): 6.79 **Temperature(K)**: 295 **Density(g/cm³)**: 1.321

Parameters
Fragment 1
HTOO (D): 2.260
HTOO (I): 119.634
Fragment 2
HTOO (D): 2.262
HTOO (I): 121.046
CHO (A): 121.046



TUCHOO

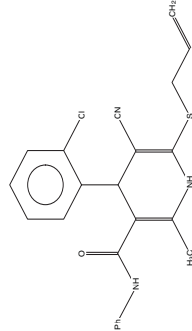
Reference: V.D.Dyachenko, S.G.Kivokolyeko, V.N.Nesterov, V.P.Livnev (1996) *Khim.Gets.Sostav,SSSR(Russ./Chem.Heterocycl.Comp.)*, 1243

Formula: C₂₄H₂₀O₁N₅O₁S₁

Compound Name: 2-Allylthio-4-(2-chlorophenyl)-3-cyano-6-methyl-5-phenylcarbamoyl-1,4-dihydropyridine

Space Group: P2₁/n **Cell:** a 10.176(2) b 11.462(3) c 19.542(5)
Space Group No.: 14 **α** 90.00 **β** 91.07 **γ** 90.00
R-Factor (%): 4.90 **Temperature(K)**: 295 **Density(g/cm³)**: 1.230

Parameters
Fragment 1
HTOO (D): 2.339
HTOO (I): 120.059
CHO (A): 120.059

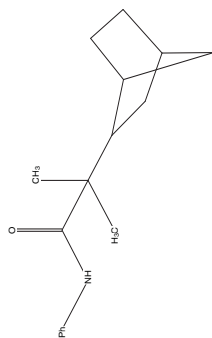


UMIWLJ

Reference: Y.Nahimoto, H.Ueda, Y.Iinamoto, M.Yasuda, A.Baba (2010) *Org.Lett.* 12,2390
Formula: C₁₇H₂₃N₃O
Compound Name: 2-(Bicyclo[2.2.1]hept-2-yl)-2-methyl-N-phenylpropanamide

Space Group: P2₁/a
Space Group No.: 14
R-Factor (%): 6.90
Temperature(K): 123
Density(g/cm³): 1.136

Parameters
Fragment 1
HTOO (D) 2.441
CHO (A) 115.940

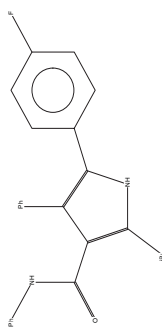


UPEFIF

Reference: T.J.Donohoe, N.J.Rice, J.F.Bower, C.K.A.Callens (2010) *Org.Lett.* 12,4994
Formula: C₁₉H₂₂F₂N₂O
Compound Name: 5-(4-Fluorophenyl)-2-isopropyl-N-(4-chlorophenyl)-1H-pyrrole-3-carboxamide

Space Group: P2₁/n
Space Group No.: 14
R-Factor (%): 4.10
Temperature(K): 150
Density(g/cm³): 1.253

Parameters
Fragment 1
HTOO (D) 2.438
CHO (A) 114.647

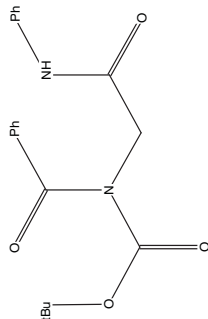


VAHCAI

Reference: W.Gruzicki, M.Gruzicka, H.Bradaczek (1987) *Leitg.Am.* 483
Formula: C₂₀H₂₂N₂O₄
Compound Name: N-Benzoyl-N-(t-butylisocyanonyl)glycynamide

Space Group: P2₁/n
Space Group No.: 14
R-Factor (%): 3.60
Temperature(K): 295
Density(g/cm³): 1.246

Parameters
Fragment 1
HTOO (D) 2.244
CHO (A) 122.463

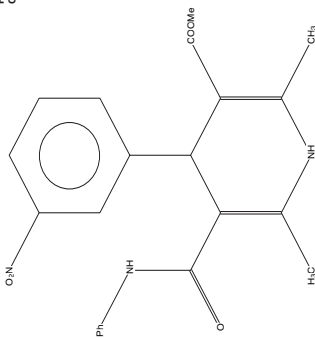


VIYNOH

Reference: S.Naveen, S.M.Ammalwar, J.S.Prasad, D.Minnar, A.Molina, A.Shan (2008) *J.Chem.Cryst.* 38,315
Formula: C₂₂H₂₁N₃O₃
Compound Name: methyl 2,6-dimethyl-5-(phenylcarbamoyl)-4-(p-tolophenyl)-1,4-dihydropyridine-3-carboxylate

Space Group: P2₁/c
Space Group No.: 14
R-Factor (%): 7.19
Temperature(K): 293
Density(g/cm³): 1.335

Parameters
Fragment 1
HTOO (D) 8.437
CHO (A) 112.457

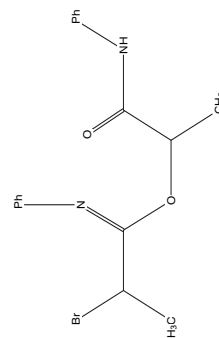


VOKCED

Reference: F.D'Angeli, P.Marchetti, G.Gaviccioni, V.Berlindas, F.Marian (1991) *Tetrahedron-Asymm.* 2,1111
Formula: C₁₈H₁₉BrN₂O₂
Compound Name: (S,S)-N-Phenyl-5-bromo-2-methyl-4-phenylpiperidine-3-oxohexanamide

Space Group: P2₁2₁2₁
Space Group No.: 19
R-Factor (%): 4.30
Temperature(K): 295
Density(g/cm³): 1.355

Parameters
Fragment 1
HTOO (D) 2.340
CHO (A) 117.797

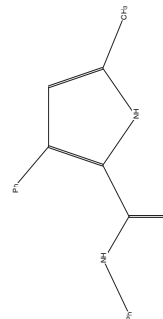


VUGDEG

Reference: E.M.Camp, G.D.Fallon, W.R.Jackson, Y.Nilsson (1992) *Aust.J.Chem.* 45,1167
Formula: C₁₈H₁₈N₂O₂
Compound Name: 5-Methyl-N-(3-phenylpyrrolid-2-yl)carboxamide

Space Group: P2₁/n
Space Group No.: 14
R-Factor (%): 5.10
Temperature(K): 295
Density(g/cm³): 1.248

Parameters
Fragment 1
HTOO (D) 2.388
CHO (A) 115.324

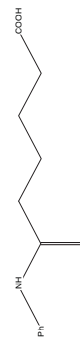


VUNYEI1

Reference: N.Fieder, W.Jones (1984) *Acta Crystallogr., Sect.C,Cryst.Struct.Comm.* 50,B16
Formula: C₁₂H₁₅N₃O₃
Compound Name: 6-Oxo-6-(phenylamino)hexanoic acid

Space Group: Pcab
Space Group No.: 61
R-Factor (%): 7.80
Temperature(K): 295
Density(g/cm³): 1.243

Parameters
Fragment 1
HTOO (D) 2.233
CHO (A) 113.863



WADZUY

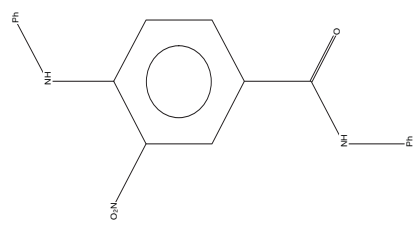
Reference: Guhua Chen, Jian Yan (2010) *Acta Crystallogr. Sect. E: Struct. Rep. Online* 66, 03286

Formula: C₁₉H₁₅N₃O₃

Compound Name: 4-Amino-3-nitro-N-phenylbenzamide

Space Group: P-1
Space Group No.: 2
R-Factor (%): 5.75

Parameters
Fragment 1
HTOO (D): 2.261
CHO (A): 120.859



WAGROM

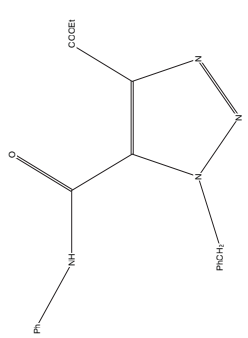
Reference: A.R. Kamitzky, Yuming Zhang, S.K. Singh, P.J. Steel (2003) *ARKIVOC* 4, 47-115

Formula: C₁₉H₁₈N₄O₃

Compound Name: Ethyl 5-aminotetrahydro-1-benzyl-1H-1,2,3-triazole-4-carboxylate

Space Group: P2₁/c
Space Group No.: 14
R-Factor (%): 3.85

Parameters
Fragment 1
HTOO (D): 2.278
CHO (A): 119.322



WAMBES

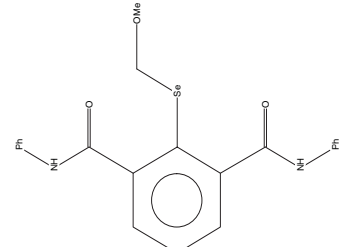
Reference: S.S. Zidek, S. Panahi, H.B. Singh, R.B. Suroj, R.J. Butcher (2005) *J. Org. Chem.* 70, 6893

Formula: C₂₆H₂₆N₂O₂Se₂

Compound Name: 4-(4-butylphenyl)-2,6-bis(phenylcarbamoyl)phenylselenine (methylomethyl)selenium

Space Group: P-1
Space Group No.: 2
R-Factor (%): 3.79

Parameters
Fragment 1
HTOO (D): 2.388
CHO (A): 117.523



WAPWEQ

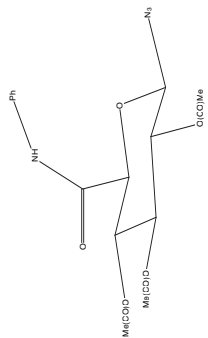
Reference: M. Toim, C.O'Brien, G.M. Fitzpatrick, H. Müller-Bunz, W.K. Glaser, P.V. Murphy (2005) *J. Org. Chem.* 70, 4086

Formula: C₁₈H₂₀N₄O₈

Compound Name: 2,3,4-Tri-O-acetyl-1-azido-1-deoxy-alpha-D-glucopyranuronic acid phenylamide

Space Group: P2₁2₁2₁
Space Group No.: 19
R-Factor (%): 2.54

Parameters
Fragment 1
HTOO (D): 2.949
CHO (A): 83.327



WARKUW

Reference: Bin Li, Zong-Xuan Shen, Yong Zhang, Du-Chun Zhang (2005) *Jiegou Huaxue (Chin. J. Struct. Chem.)* 24, 739

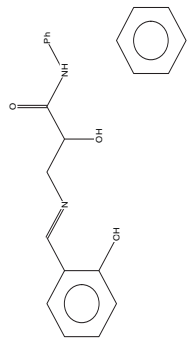
Formula: C₁₈H₁₆N₂O₃·0.5(C₆H₆)

Compound Name: N-Phenyl-(S)-hydroxy-3-(2-hydroxybenzyl)amino propanamide bitartrate salt

Space Group: P2₁
Space Group No.: 4
R-Factor (%): 6.24

Parameters
Fragment 1
HTOO (D): 2.288
CHO (A): 119.735

Fragment 2
HTOO (D): 2.344
CHO (A): 120.370



WERTIX

Reference: M.W. Glenn, M. LeCombe, J.B. Love, A.J. Blake, L.F. Lindoy, R. Luckey, K. Gao, B. Amboldi, C. Wilson, M. Schroder (2005) *New J. Chem.* 30, 1755

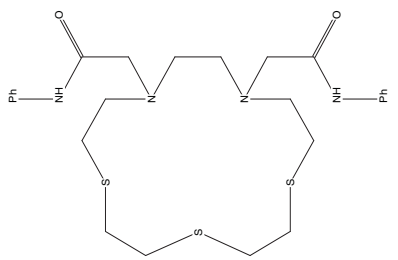
Formula: C₂₆H₂₆N₂O₂S₂

Compound Name: 10,13-bis(phenylcarbamoyl)imethyl-1,4,7-trithia 10,15-diazacyclodecane

Space Group: P2₁/n
Space Group No.: 14
R-Factor (%): 3.66

Parameters
Fragment 1
HTOO (D): 2.302
CHO (A): 123.251

Fragment 2
HTOO (D): 2.292
CHO (A): 121.382



WIGUEC

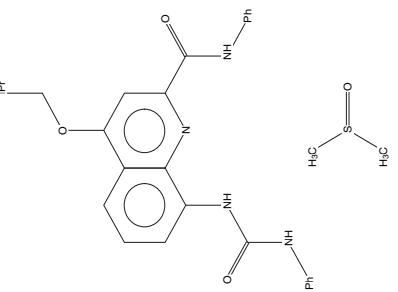
Reference: M. Albrecht, Triyanti, S. Schiffer, O. Oestika, G. Raabe, T. Wieland, L. Russo, K. Rissanen (2007) *Eur. J. Org. Chem.* 2850

Formula: C₂₇H₂₆N₂O₃·H₂O·S₂

Compound Name: 4-isobutoxy-8-(phenylamido)quinoline-2-carboxylic acid phenyl amide dimethylsulfoxide solvate

Space Group: P-1
Space Group No.: 2
R-Factor (%): 5.71

Parameters
Fragment 1
HTOO (D): 2.284
CHO (A): 121.111



WIGJG

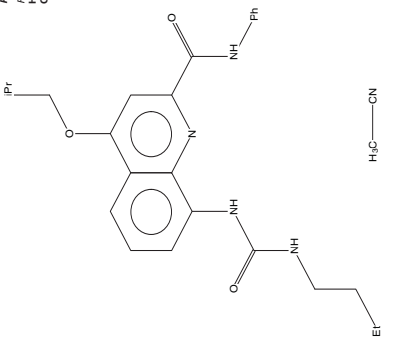
Reference: M. Albrecht, Triyanti, S. Schiffer, O. Oestika, G. Raabe, T. Wieland, L. Russo, K. Rissanen (2007) *Eur. J. Org. Chem.* 2850

Formula: C₂₅H₂₀N₂O₃·H₂O·H₂

Compound Name: 8-(3-methylureido)-4-isobutoxyquinoline-2-carboxylic acid phenyl amide acetamide solvate

Space Group: P2₁/n
Space Group No.: 14
R-Factor (%): 9.51

Parameters
Fragment 1
HTOO (D): 2.262
CHO (A): 121.259

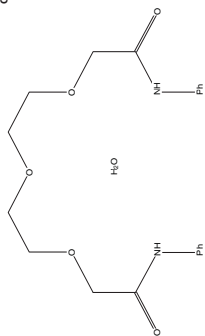


WIVROI

Reference: S.Meyer, R.Luis, B.Wetz, Y.Agnus, A.Varnik, M.Gross (2000) *New J.Chem.*, 24,371
Formula: C₂₀H₂₄N₂O₄2(H₂O)
Compound Name: N,N'-Diphenyl-3,5,9-trioxadecane-1,11-diamide monohydrate

Space Group: P2₁/c
Space Group No.: 14
R-Factor (%): 3.40
Temperature(K): 173
Density(g/cm³): 1.297

Parameters
Fragment 1
HTOO (D): 2.985
CHO (A): 120.748
Fragment 2
HTOO (D): 2.348
CHO (A): 114.042

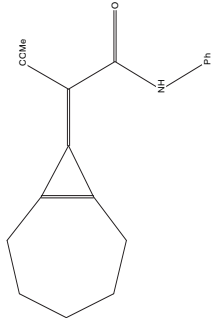


WOSXIL

Reference: H.Ingtinger, A.Altmeurer, T.Sommerfeld, T.Stojank (2000) *Eur.J.Org.Chem.*, 469
Formula: C₁₉H₁₉N₃O₂
Compound Name: 2-(Bicyclo[6.1.0]non-1(7)-en-8-ylidene)-3-oxo-butanamide

Space Group: P-1
Space Group No.: 2
R-Factor (%): 7.60
Temperature(K): 295
Density(g/cm³): 1.256

Parameters
Fragment 1
HTOO (D): 2.225
CHO (A): 121.454

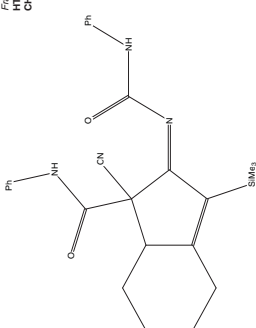


WUNPAX

Reference: HuiJun Zhang, Tianhao Meng, Si Demersemant, C.Branau, Zhenfeng Xi (2009) *Org.Lett.*, 11,1468
Formula: C₂₇H₂₉N₃O₂Si
Compound Name: 1-Cyano-N-phenyl-2-(phenylcarbamoyl)imino-3-(trimethylsilyloxy)-4,5,6,7,7a-hexahydro-1H-indole-1-carboxamide

Space Group: P-1
Space Group No.: 2
R-Factor (%): 7.60
Temperature(K): 173
Density(g/cm³): 1.215

Parameters
Fragment 1
HTOO (D): 2.933
CHO (A): 83.1628
Fragment 2
HTOO (D): 2.328
CHO (A): 119.693

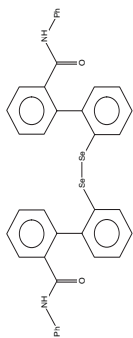


XAGGAN

Reference: M.-R.Spieler, A.Mohaine, L.Christians (2000) *Z.Kristallogr.-New Crystal Struct.*, 215,121
Formula: C₂₈H₂₈H₂O₂Se₂
Compound Name: Diphenyl-2-biphenyl-2'-carboxamide diselenide

Space Group: P2₁/2₁/2₁
Space Group No.: 18
R-Factor (%): 4.20
Temperature(K): 295
Density(g/cm³): 1.470

Parameters
Fragment 1
HTOO (D): 2.298
CHO (A): 119.684

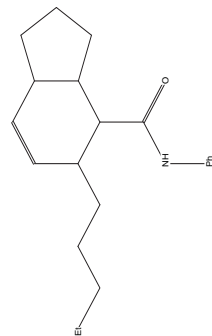


XANDUL

Reference: S.Kallio, J.Makikallio, T.Hess, I.Mullikainen (2000) *Z.Kristallogr.-New Crystal Struct.*, 215,585
Formula: C₂₁H₂₃N₃O
Compound Name: 5-(1-phenyl)-N-phenyl-2,3,3bc,4,5,7bc-hexahydro-1H-indene-4-carboxamide

Space Group: P6₃/c
Space Group No.: 81
R-Factor (%): 9.15
Temperature(K): 295
Density(g/cm³): 1.099

Parameters
Fragment 1
HTOO (D): 2.334
CHO (A): 117.792

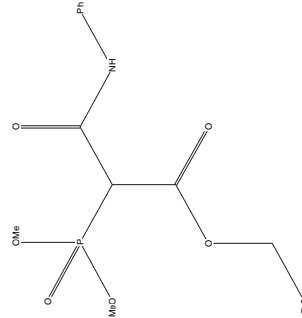


XIPNIU

Reference: Jinhua Song, H.Yamaoka, Z.Rappoport (2007) *J.Org.Chem.*, 72,7605
Formula: C₁₃H₁₅F₃N₃O₆P₁
Compound Name: 2,2,2-Trifluoroethyl 2-(dimethoxyphosphino)-2-(N-phenylcarbamoyl)acetate

Space Group: P2₁/c
Space Group No.: 14
R-Factor (%): 9.79
Temperature(K): 295
Density(g/cm³): 1.430

Parameters
Fragment 1
HTOO (D): 2.469
CHO (A): 112.873

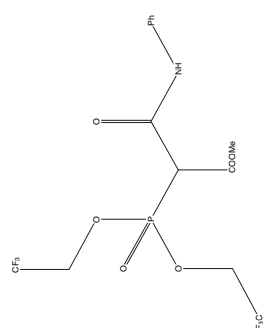


XIPPEP

Reference: Jinhua Song, H.Yamaoka, Z.Rappoport (2007) *J.Org.Chem.*, 72,7605
Formula: C₁₇H₁₇F₃N₃O₆P₁
Compound Name: Methyl 2-(tert-butyl(2,2,2-trifluoroethoxy)phosphino)-2-(N-phenylcarbamoyl)acetate

Space Group: P2₁/c
Space Group No.: 14
R-Factor (%): 10.92
Temperature(K): 295
Density(g/cm³): 1.456

Parameters
Fragment 1
HTOO (D): 2.344
CHO (A): 117.940

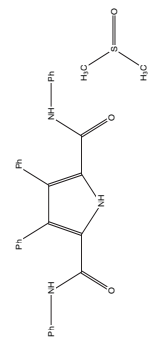


XOKDIK

Reference: P.A.Gale, S.Cimolo, G.J.Tizzard, C.P.Chauhan, M.E.Light, S.J.Cleese, M.B.Hunthouse (2001) *J.Org.Chem.*, 66,7849
Formula: C₃₀H₂₈N₂O₂H₂O₂Si
Compound Name: N,N'-Diphenyl-3,4-diphenyl-1H-pyrrole-2,5-dicarboxamide diethylsulfate sesquater

Space Group: P2₁/n
Space Group No.: 14
R-Factor (%): 6.16
Temperature(K): 120
Density(g/cm³): 1.308

Parameters
Fragment 1
HTOO (D): 2.299
CHO (A): 120.191
Fragment 2
HTOO (D): 2.324
CHO (A): 120.160

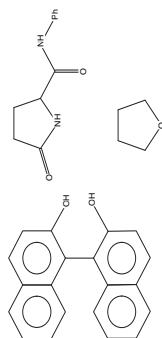


XONROH

Reference: Hailiang Du, Baojun Jiang, Jie Yang, Wang, Jie Sun, Jiebin Wang, *Killing Drug (2007) Termination Lett.* 43,3273
Formula: C₂₀H₁₄O₂C₁₁H₁₂N₂O₂C₄H₈O₁
Compound Name: (R)-1-(9-(2-naphthyl)(S)-5-oxopyrrolidine-2-carboxamide tetrahydrofuran solvate

Space Group: P2₁ **a** 11.049(0) **b** 8.866(0) **c** 14.950(1)
Space Group No.: 4 **Cell:** α 90.00 β 94.54(0) γ 90.00
R-Factor (%): 5.88 **Temperature(K)**: 293 **Density(g/cm³)**: 1.260

Parameters
Fragment 1
HTOO (D) 9.270
CHO (A) 118.201

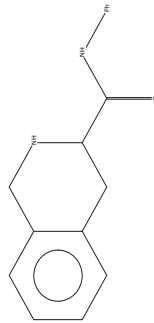


XUNBUE

Reference: D.Basaveiah, U.Das, S.Roy (2009) *J.Chem.Sci.(Bangalore)*121, 1003
Formula: C₁₆H₁₆N₂O₂
Compound Name: N-Phenyl-1,2,3,4-tetrahydroisoquinoline-3-carboxamide
Synonym: 3(S)-Anilinoacetyl-1,2,3,4-tetrahydroisoquinoline

Space Group: P2₁2₁2₁ **Cell:** **a** 6.627(0) **b** 8.233(0) **c** 27.680(0)
Space Group No.: 19 **Cell:** α 90.00 β 90.00 γ 90.00
R-Factor (%): 3.99 **Temperature(K)**: 298 **Density(g/cm³)**: 1.262

Parameters
Fragment 1
HTOO (D) 2.298
CHO (A) 121.321

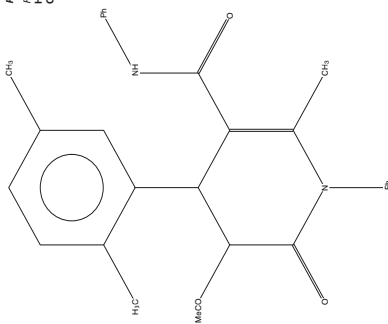


YAPBC

Reference: T.Singupala, K.S.Gayen, P.Pandit, D.K.Mali (2012) *Chem.-Educ.* 181,1506
Formula: C₂₄H₂₄N₂O₂
Compound Name: 5-Acetyl-4-(2,5-dimethylphenyl)-2-methyl-6-oxo-N,1-diphenyl-1,4,5,6-tetrahydroindole-3-carboxamide

Space Group: P2₁/c **Cell:** **a** 12.579(7) **b** 18.955(1) **c** 11.381(6)
Space Group No.: 14 **Cell:** α 90.00 β 104.50(0) γ 90.00
R-Factor (%): 4.53 **Temperature(K)**: 295 **Density(g/cm³)**: 1.152

Parameters
Fragment 1
HTOO (D) 9.330
CHO (A) 120.383

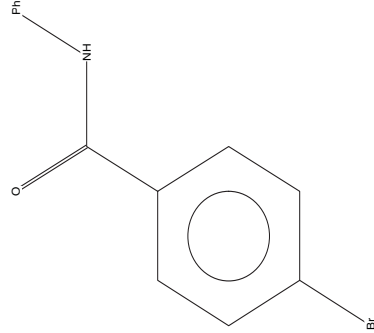


YAYJUF

Reference: H.-K.Fun, S.Chenragnemma, W.Sipat, P.Puanwara, Chinnak (2012) *Acta Crystallogr., Sect.E: Struct.Rep.Chem.* 68, 01889
Formula: C₁₃H₁₀Br₂N₁O₁
Compound Name: 4-Bromo-N-phenylbenzamide

Space Group: P-1 **a** 5.355(9) **b** 7.633(0) **c** 13.996(0)
Space Group No.: 2 **Cell:** α 105.76(0) β 100.69(0) γ 90.08(0)
R-Factor (%): 3.23 **Temperature(K)**: 100 **Density(g/cm³)**: 1.697

Parameters
Fragment 1
HTOO (D) 9.417
CHO (A) 113.682

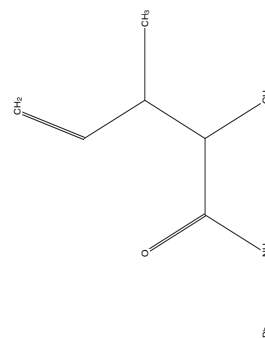


YEGCAP

Reference: D.A.Evans, J.Wu, Y.Ayi (2006) *Org.Lett.* 8,2071
Formula: C₁₂H₁₅N₁O₂
Compound Name: (2S,3R)-2-hydroxy-3-methyl-N-phenylpent-4-enamide

Space Group: C2/c **Cell:** **a** 24.869(14) **b** 11.616(7) **c** 8.095(6)
Space Group No.: 15 **Cell:** α 90.00 β 103.55(1) γ 90.00
R-Factor (%): 3.55 **Temperature(K)**: 193 **Density(g/cm³)**: 1.160

Parameters
Fragment 1
HTOO (D) 9.213
CHO (A) 118.769

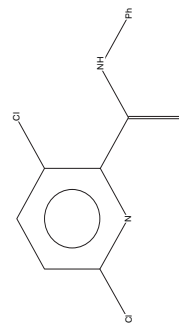


YIQWIF

Reference: Xian-Hong Yin, Kai Zhao, Yu Feng, Jie Zhu (2007) *Acta Crystallogr., Sect.E: Struct.Rep.Chem.* 63,04617
Formula: C₁₂H₈C₂N₂O₁
Compound Name: 3-(2-Chloro-N-phenylpicolinamide

Space Group: P2₁/c **Cell:** **a** 6.840(1) **b** 12.263(1) **c** 14.156(2)
Space Group No.: 14 **Cell:** α 90.00 β 101.04(0) γ 90.00
R-Factor (%): 3.71 **Temperature(K)**: 298 **Density(g/cm³)**: 1.522

Parameters
Fragment 1
HTOO (D) 2.308
CHO (A) 120.991



YISYAB

Reference: Hai-Yu Hu, Jun-Feng Xiang, Yong Yang, Chuan-Feng Chen (2008) *Org.Lett.* 10,69
Formula: C₂₄H₂₀N₁₀O₁₀(C₃H₆O)₂
Compound Name: N,N'-bis(2,2-Dimethoxy-1,1-bis(methoxy)-1-phenylethane-6-(5-yl)-3-oxo-1,2-(4,7-di-phenyl)-4,7-di-isobutoxy-1,10-phenanthroline-2,9-dicarboxamide) propa-2-n dichloromethane solvate

Space Group: P-1 **Cell:** **a** 18.177(3) **b** 18.428(3) **c** 22.747(5)
Space Group No.: 2 **Cell:** α 85.31(1) β 77.27(0) γ 70.02(1)
R-Factor (%): 11.70 **Temperature(K)**: 113 **Density(g/cm³)**: 1.198

Parameters
Fragment 1
HTOO (D) 2.260
CHO (A) 121.099

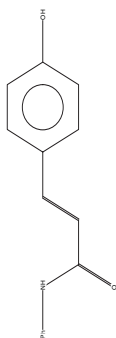


Search: search5 (Sat Feb 09 10:06:45 2013): Hits 273-277

YOXXAL

Reference: K. Okamoto, N. Hamada, T. Saji, T. Okamura, N. Uryama, H. Yamamoto (2009) *Chem. Lett.*, 38:156
Formula: C₁₃H₁₃N₂O₂
Compound Name: (E)-3-(4-hydroxyphenyl)-N-phenylacrylamide
Space Group: P2₁/n **a** 6.151(4) **b** 14.145(7) **c** 18.451(7)
Space Group No.: 14 **α** 90.00 **β** 90.82(4) **γ** 90.00
R-Factor (%): 3.82 **Temperature(K)**: 200 **Density(g/cm³)**: 1.305

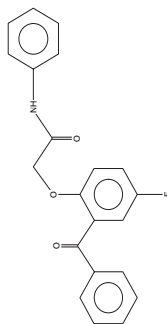
Parameters
Fragment 1
HTOO (D) 2.311
HTOO (A) 119.930
CHO (A)



YUKNAT

Reference: P. G. Witt, R. C. Behlert, N. Carmichael, D. Chiron, N. Doud, N. G. F. Jones, S. J. Leach, S. J. Leach, S. J. Leach, R. B. Lambert, D. C. Orr, S. J. P. Parker, D. M. Pym, S. L. Salfes, R. Shotton, G. G. Wangantien (1995) *J. Med. Chem.*, 38:1857
Formula: C₂₁H₁₈F₂N₂O₃
Compound Name: 2-(2-benzoyl-4-fluorophenoxy)-N-phenylacetamide
Space Group: P2₁/n **a** 14.508 **b** 5.156 **c** 23.123
Space Group No.: 14 **α** 90.00 **β** 91.18 **γ** 90.00
R-Factor (%): 0.00 **Temperature(K)**: 295 **Density(g/cm³)**: 1.342

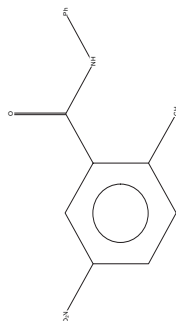
Parameters
Fragment 1
HTOO (D) 2.244
HTOO (A) 121.742
CHO (A)



YUQMAZ

Reference: A. R. Raza, B. Nisar, M. N. Tahir (2010) *Acta Crystallogr. Sect. E: Struct. Rep. Online*, 66:1632
Formula: C₁₃H₁₀N₂O₄
Compound Name: 2-Hydroxy-5-nitro-N-phenylbenzamide
Space Group: Pc **a** 8.951(10) **b** 4.765(10) **c** 19.527(10)
Space Group No.: 7 **α** 90.00 **β** 97.82(6) **γ** 90.00
R-Factor (%): 2.87 **Temperature(K)**: 298 **Density(g/cm³)**: 1.482

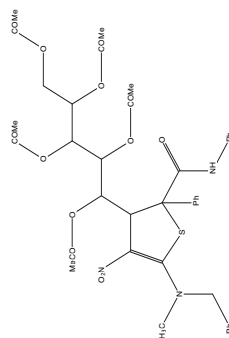
Parameters
Fragment 1
HTOO (D) 2.284
HTOO (A) 120.717
CHO (A)



ZUFWEC

Reference: M. Aviles, R. Babiano, A. Cubanillas, P. Chiriac, M. J. Dianez, M. D. Estrada, J. L. Jimenez, A. Lopez-Castro, J. C. Palacios, S. P. Garrido (1995) *Chem. Commun.*, 2213
Formula: C₂₆H₃₃N₃O₁₃S₁
Compound Name: 5-Benzyl(methylamino)-4-nitro-2-phenyl-2-(N-phenylcarbamoyl)-3-(pentan-2-oxo-1-(1-oxo-D-xylosyl)-2,3-dihydrothiophene)
Space Group: P2₁2₁2₁ **a** 8.998(1) **b** 12.599(7) **c** 36.649(4)
Space Group No.: 19 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 5.10 **Temperature(K)**: 295 **Density(g/cm³)**: 1.289

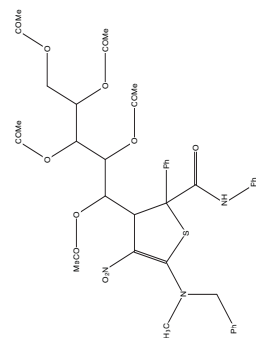
Parameters
Fragment 1
HTOO (D) 2.122
HTOO (A) 122.459
CHO (A)

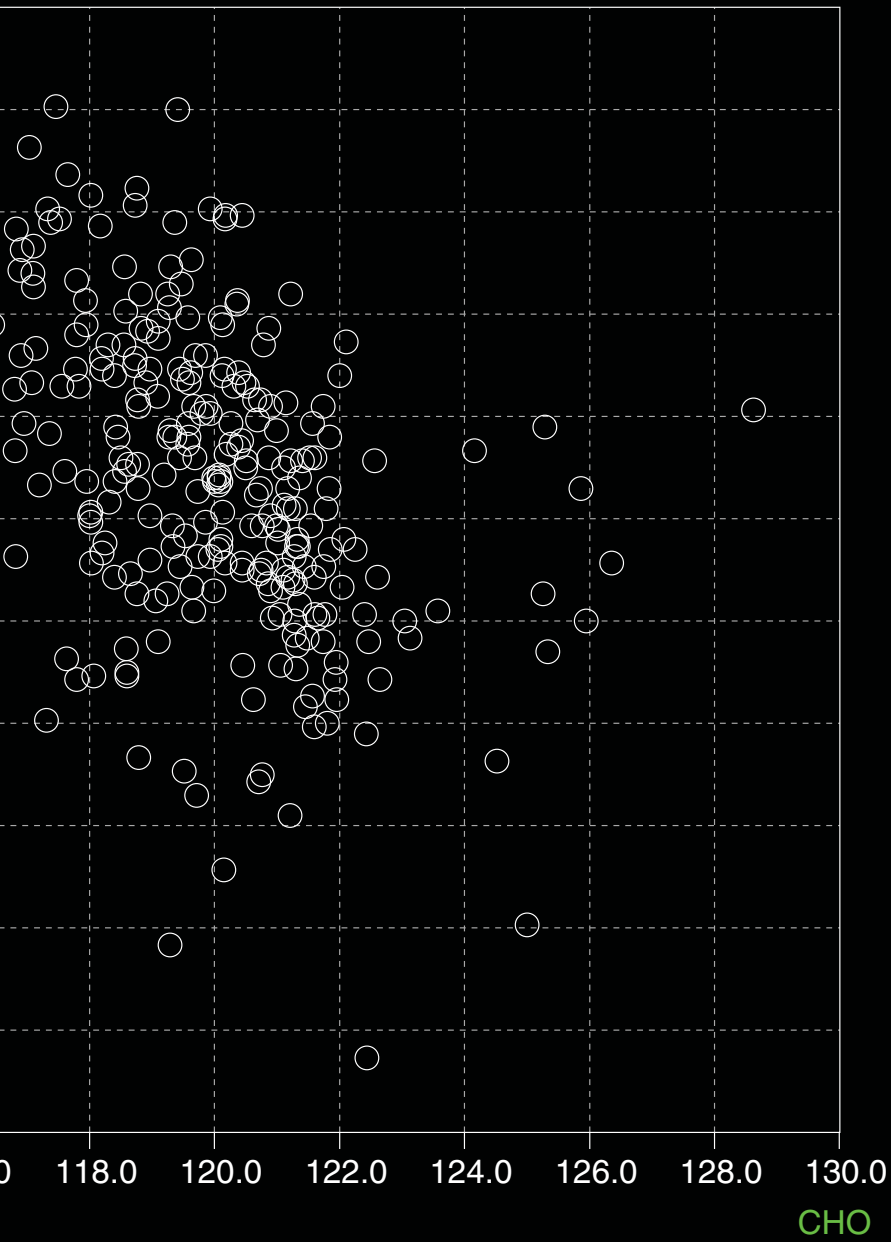


ZUFWAY

Reference: M. Aviles, R. Babiano, A. Cubanillas, P. Chiriac, M. J. Dianez, S. P. Garrido (1995) *Chem. Commun.*, 2213
Formula: C₂₆H₃₃N₃O₁₃S₁
Compound Name: 5-Benzyl(methylamino)-4-nitro-2-phenyl-2-(N-phenylcarbamoyl)-3-(pentan-2-oxo-1-(1-oxo-D-xylosyl)-2,3-dihydrothiophene)
Space Group: P2₁ **a** 10.303(1) **b** 10.303(1) **c** 33.750(2)
Space Group No.: 145 **α** 90.00 **β** 90.00 **γ** 120.00
R-Factor (%): 4.80 **Temperature(K)**: 295 **Density(g/cm³)**: 1.294

Parameters
Fragment 1
HTOO (D) 2.332
HTOO (A) 112.176
CHO (A)





Plot Data

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Obs.=313

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X-axis

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Mean SE=0.147

Sample SD=2.604

Y-axis

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Max.=2.401

Range=0.279

Mean=2.299

Mean SE=0.003

Sample SD=0.049

Search Overview

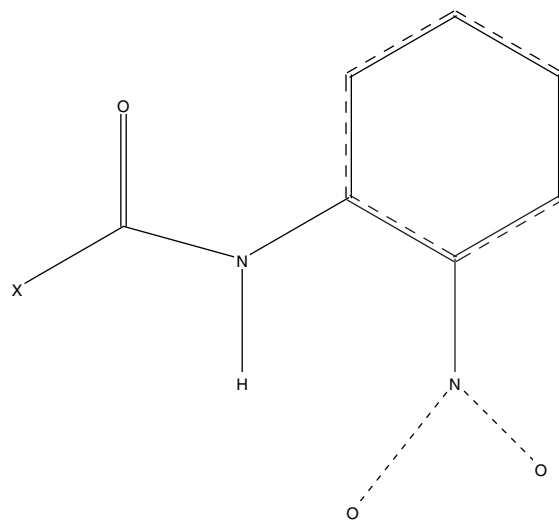
Search: search2
Date/Time done: Thu Jan 24 14:09:51 2013
Database(s): CSD version 5.34 updates (Nov 2012)
CSD version 5.34 (November 2012)
Restriction Info: No refcode restrictions applied
Filters: None
Percentage Completed: 100%
Number of Hits: 66

Single query used. Search found structures that:

match

Query 1

Query 1



Search: search2 (Thu Jan 24 14:09:51 2013): Hits 1-4

LEGLOA

Reference: B.-H.Zou, Z.Fang, H.Zhong, G.Kai, P.Wei (2012)
Acta Crystallogr., Sect.E:Struct.Rep.Online ,68,o2547

Formula: C₁₃ H₉ Cl₁ N₂ O₄

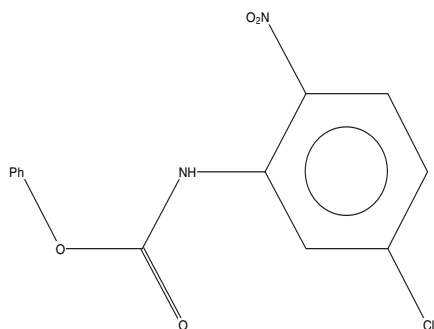
Compound Name: Phenyl (5-chloro-2-nitrophenyl)carbamate

Space Group: P21/c **Cell:** a 8.476(1) b 5.927(1) c 24.996(5)
Space Group No.: 14 **(Å,°)** α 90.00 β 94.77(3) γ 90.00

R-Factor (%): 4.55 **Temperature(K):** 293 **Density(g/cm³):** 1.553

Parameters

Fragment 1
NHTOO (D) 1.944
NHO (A) 134.877



QEDLOC

Reference: F.Zhang, Z.Fang, B.-H.Zou, G.Kai (2012)
Acta Crystallogr., Sect.E:Struct.Rep.Online ,68,o2771

Formula: C₁₁ H₁₃ Cl₁ N₂ O₃

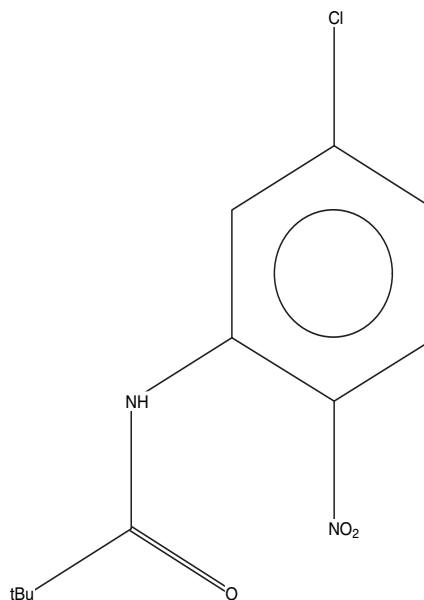
Compound Name: N-(5-Chloro-2-nitrophenyl)-2,2-dimethylpropanamide

Space Group: Pnma **Cell:** a 10.401(2) b 7.028(1) c 17.106(3)
Space Group No.: 62 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 6.36 **Temperature(K):** 293 **Density(g/cm³):** 1.364

Parameters

Fragment 1
NHTOO (D) 1.945
NHO (A) 134.757



VAXKUC

Reference: M.C.Davis, T.J.Groshens (2012) *Tetrahedron Lett.* ,53, 4154

Formula: C₂₁ H₃₁ N₅ O₁₀

Compound Name: Tri-*t*-butyl (2,4-dinitrobenzene-1,3,5-triyl)triscarbamate

Space Group: P6ca **Cell:** a 14.009(0) b 9.116(0) c 42.326(1)
Space Group No.: 61 **(Å,°)** α 90.00 β 90.00 γ 90.00

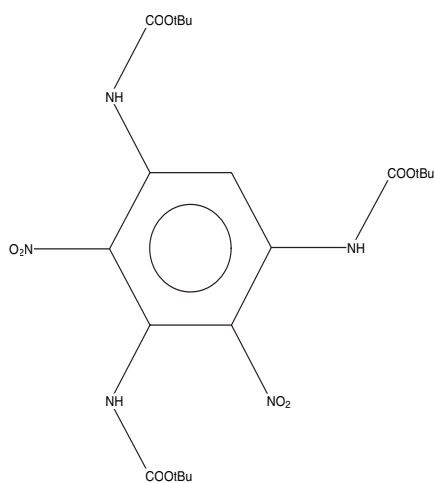
R-Factor (%): 4.45 **Temperature(K):** 296 **Density(g/cm³):** 1.262

Parameters

Fragment 1
NHTOO (D) 2.021
NHO (A) 129.648

Fragment 2
NHTOO (D) 1.990
NHO (A) 129.615

Fragment 3
NHTOO (D) 1.973
NHO (A) 133.686



VAXLAJ

Reference: M.C.Davis, T.J.Groshens (2012) *Tetrahedron Lett.* ,53, 4154

Formula: C₁₁ H₁₃ N₃ O₆

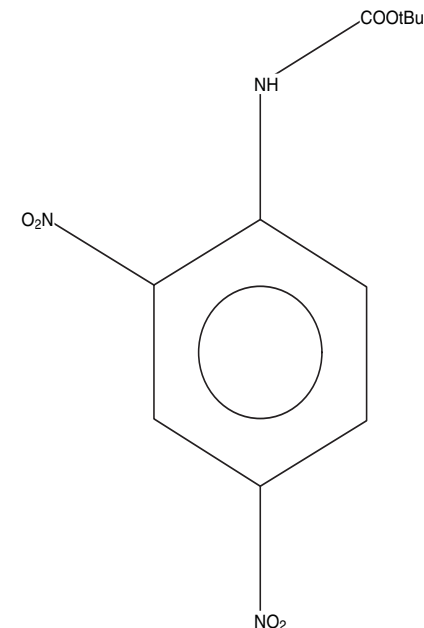
Compound Name: *t*-Butyl (2,4-dinitrophenyl)carbamate

Space Group: P21/c **Cell:** a 13.441(0) b 6.001(0) c 16.969(0)
Space Group No.: 14 **(Å,°)** α 90.00 β 107.93(0) γ 90.00

R-Factor (%): 3.42 **Temperature(K):** 296 **Density(g/cm³):** 1.445

Parameters

Fragment 1
NHTOO (D) 1.951
NHO (A) 134.682



Search: search2 (Thu Jan 24 14:09:51 2013): Hits 5-8

AVOJUR02

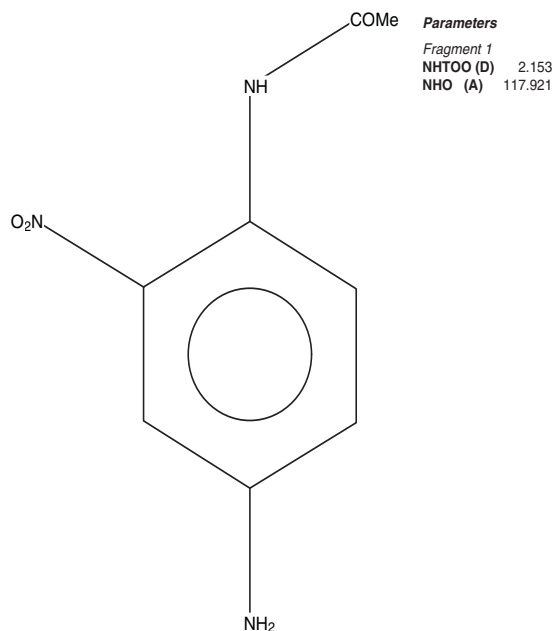
Reference: E.Pindelska, L.Dobrzycki, K.Wozniak, W.Kolodziejcki (2011) *Cryst.Growth Des.*, 11,2074

Formula: C₈ H₉ N₃ O₃

Compound Name: N-(4-Amino-2-nitrophenyl)acetamide

Space Group: P21/n **Cell:** a 12.702(1) b 3.818(0) c 17.365(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 91.63(0) γ 90.00

R-Factor (%): 4.48 **Temperature(K):** 100 **Density(g/cm³):** 1.540



AVOKIG

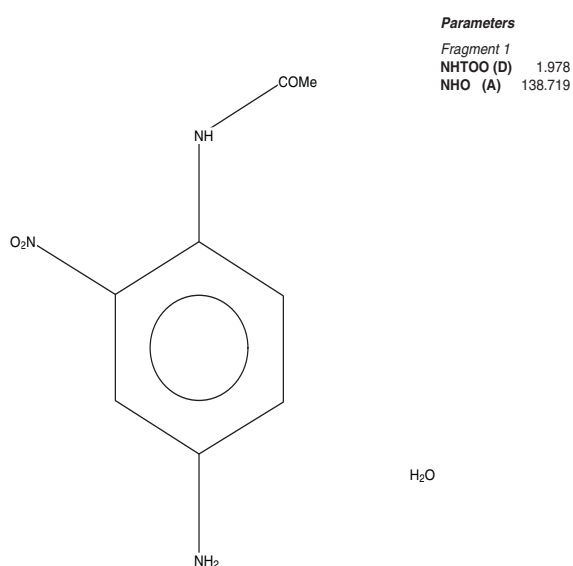
Reference: E.Pindelska, L.Dobrzycki, K.Wozniak, W.Kolodziejcki (2011) *Cryst.Growth Des.*, 11,2074

Formula: C₈ H₉ N₃ O₃·H₂O

Compound Name: N-(4-Amino-2-nitrophenyl)acetamide monohydrate

Space Group: C2/c **Cell:** a 22.656(1) b 11.727(0) c 7.326(0)
Space Group No.: 15 **(Å, °)** α 90.00 β 102.93(0) γ 90.00

R-Factor (%): 3.19 **Temperature(K):** 100 **Density(g/cm³):** 1.493



AYUPUF

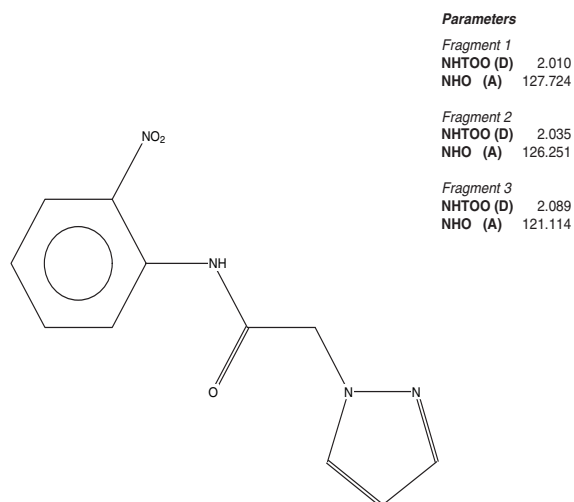
Reference: C.Zalaru, M.R.Caira, M.Iovu, E.Cristea (2004) *J.Chem.Cryst.*, 34,317

Formula: C₁₁ H₁₀ N₄ O₃

Compound Name: 2-(Pyrazol-1-yl)-2'-nitroacetanilide

Space Group: Pn **Cell:** a 4.694(0) b 22.389(0) c 15.748(0)
Space Group No.: 7 **(Å, °)** α 90.00 β 96.81(0) γ 90.00

R-Factor (%): 6.57 **Temperature(K):** 173 **Density(g/cm³):** 1.493



AYUQAM

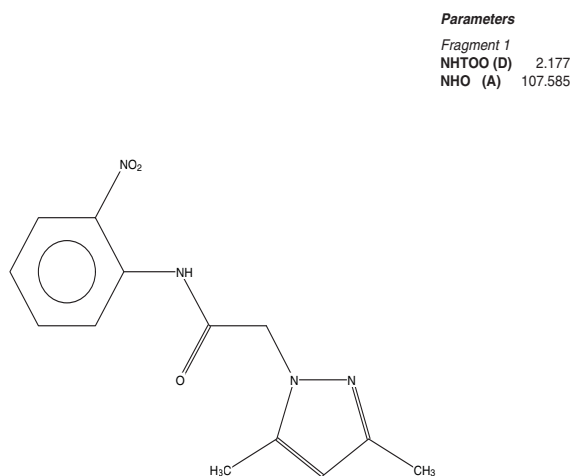
Reference: C.Zalaru, M.R.Caira, M.Iovu, E.Cristea (2004) *J.Chem.Cryst.*, 34,317

Formula: C₁₃ H₁₄ N₄ O₃

Compound Name: 2-(3,5-Dimethylpyrazol-1-yl)-2'-nitroacetanilide

Space Group: P-1 **Cell:** a 4.728(0) b 11.688(0) c 12.036(0)
Space Group No.: 2 **(Å, °)** α 87.69(0) β 85.05(0) γ 85.98(0)

R-Factor (%): 4.58 **Temperature(K):** 173 **Density(g/cm³):** 1.379



Search: search2 (Thu Jan 24 14:09:51 2013): Hits 9-12

AYUQEQ

Reference: C.Zalaru, M.R.Caira, M.Iovu, E.Cristea (2004)
J.Chem.Cryst. ,34,317

Formula: C₁₃ H₁₃ I₁ N₄ O₃

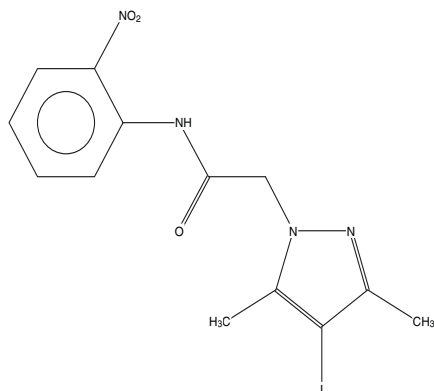
Compound Name: 2-(3,5-Dimethyl-4-iodo-pyrazol-1-yl)-2'-nitroacetanilide

Space Group: I2/a **Cell:** *a* 24.108(5) *b* 4.732(0) *c* 25.337(5)
Space Group No.: 15 (**Å, °**) α 90.00 β 96.09(3) γ 90.00

R-Factor (%): 2.94 **Temperature(K):** 193 **Density(g/cm³):** 1.850

Parameters

Fragment 1
NHTOO (D) 2.206
NHO (A) 110.618



BAYXIJ

Reference: Zhenming Yin, Ling Jiang, Jiaqi He, Jin-Pei Cheng (2003)
Chem.Commun. ,2326

Formula: C₉ H₇ N₃ O₇

Compound Name: methyl (2,4-dinitrophenyl)amidocarboxylate

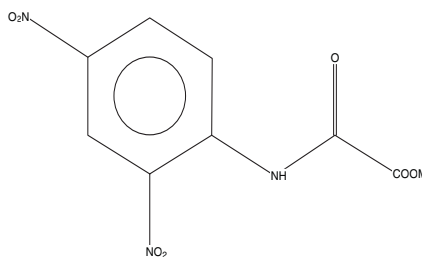
Synonym: N-oxaly 2,4-dinitroanilide

Space Group: P21/c **Cell:** *a* 12.810(3) *b* 4.645(2) *c* 18.340(5)
Space Group No.: 14 (**Å, °**) α 90.00 β 99.33(1) γ 90.00

R-Factor (%): 4.96 **Temperature(K):** 293 **Density(g/cm³):** 1.660

Parameters

Fragment 1
NHTOO (D) 1.892
NHO (A) 134.702



BOSVIO

Reference: L.A.Chetkina, Z.P.Povet'eva, V.K.Bel'skii, A.M.Andrievskii, A.N.Poplavskii, K.M.Dyumaev (1982)
Dokl.Akad.Nauk SSSR(Russ.)(Proc.Nat.Acad.Sci.USSR) ,266,1191

Formula: C₁₃ H₅ N₅ O₉

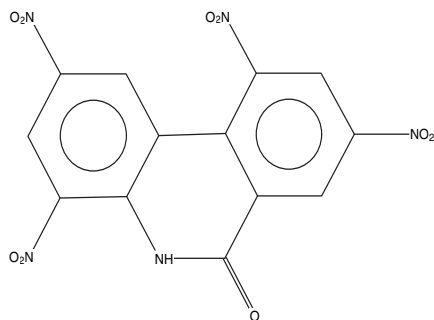
Compound Name: 2,4,8,10-Tetranitro-phenanthridine

Space Group: P212121 **Cell:** *a* 31.872(14) *b* 5.223(3) *c* 8.255(4)
Space Group No.: 19 (**Å, °**) α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.10 **Temperature(K):** 295 **Density(g/cm³):** 1.814

Parameters

Fragment 1
NHTOO (D) 1.853
NHO (A) 132.823



CIVVEI10

Reference: A.M.Andrievskii, A.N.Poplavskii, K.M.Dyumaev, L.A.Chetkina, V.K.Bel'skii, Yu.S.Bogachev, S.S.Berestova (1987)
Khim.Get.Soedin.,SSSR(Russ.)(Chem.Heterocycl.Comp.) ,314

Formula: C₁₅ H₈ N₄ O₉

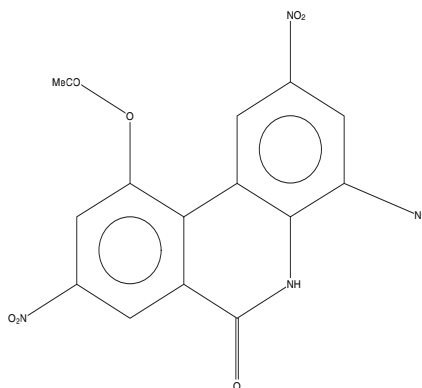
Compound Name: 10-Acetoxy-2,4,8-trinitro-6(5H)-phenanthridinone

Space Group: P212121 **Cell:** *a* 5.768(0) *b* 12.300(2) *c* 21.531(3)
Space Group No.: 19 (**Å, °**) α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.80 **Temperature(K):** 295 **Density(g/cm³):** 1.688

Parameters

Fragment 1
NHTOO (D) 2.096
NHO (A) 129.650



Search: search2 (Thu Jan 24 14:09:51 2013): Hits 13-16

CUZZUS

Reference: L.Cronin, D.A.Adams, D.J.Nightingale, J.H.Clark (2000)
Acta Crystallogr., Sect.C:Cryst.Struct.Commun., **56**,244

Formula: C₁₄ H₇ Cl₁ N₄ O₅

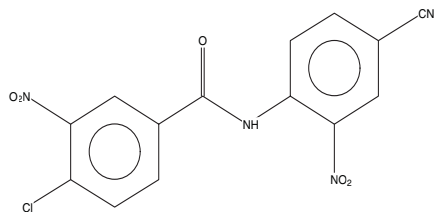
Compound Name: 4-Chloro-N-(4-cyano-2-nitrophenyl)-3-nitrobenzamide

Space Group: P-1 **Cell:** *a* 7.804(13) *b* 12.931(6) *c* 7.490(40)
Space Group No.: 2 **Cell:** *α* 91.59(16) *β* 112.90(20) *γ* 88.12(6)

R-Factor (%): 4.60 **Temperature(K):** 295 **Density(g/cm³):** 1.655

Parameters

Fragment 1
NHTOO (D) 2.067
NHO (A) 124.779



DATDOS

Reference: Hong-Jun Zang, Ming-Lin Guo (2005)
Acta Crystallogr., Sect.E:Struct.Rep.Online, **61**,o2772

Formula: C₁₁ H₁₁ N₂ O₇ P₁

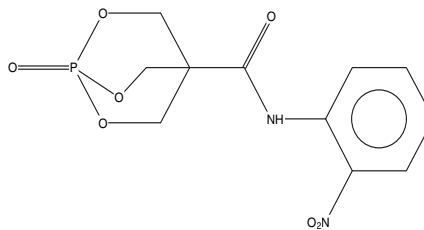
Compound Name: N-(2-Nitrophenyl)-1-oxo-2,6,7-trioxa-1-phosphabicyclo(2.2.2)octane-4-carboxamide

Space Group: P21/c **Cell:** *a* 8.238(1) *b* 12.269(2) *c* 12.937(2)
Space Group No.: 14 **Cell:** *α* 90.00 *β* 105.08(0) *γ* 90.00

R-Factor (%): 4.10 **Temperature(K):** 293 **Density(g/cm³):** 1.653

Parameters

Fragment 1
NHTOO (D) 1.965
NHO (A) 137.849



DIXDUJ

Reference: S.Kashino, T.Matsushita, T.Iwamoto, K.Yamaguchi,
M.Haisa (1986) *Acta Crystallogr., Sect.C:Cryst.Struct.Commun.*, **42**,457

Formula: C₈ H₈ N₂ O₃

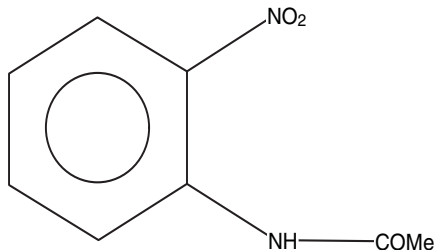
Compound Name: o-Nitroacetanilide

Space Group: P21/n **Cell:** *a* 15.507(3) *b* 4.958(0) *c* 10.924(2)
Space Group No.: 14 **Cell:** *α* 90.00 *β* 97.68(1) *γ* 90.00

R-Factor (%): 5.20 **Temperature(K):** 295 **Density(g/cm³):** 1.438

Parameters

Fragment 1
NHTOO (D) 2.010
NHO (A) 132.915



FAGDAU

Reference: D.Craig, J.W.Harvey, A.G.O'Brien, A.J.P.White (2010)
Chem. Commun., **46**,6932

Formula: C₁₉ H₁₉ N₃ O₅ S₁

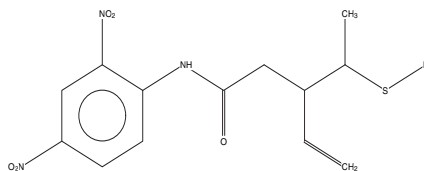
Compound Name: syn-N-(2,4-Dinitrophenyl)-3-(1-(phenylsulfanyl)ethyl)pent-4-enamide

Space Group: P-1 **Cell:** *a* 7.033(0) *b* 11.687(0) *c* 12.997(0)
Space Group No.: 2 **Cell:** *α* 69.17(0) *β* 78.71(0) *γ* 82.73(0)

R-Factor (%): 5.56 **Temperature(K):** 173 **Density(g/cm³):** 1.364

Parameters

Fragment 1
NHTOO (D) 1.958
NHO (A) 133.753



Search: search2 (Thu Jan 24 14:09:51 2013): Hits 17-20

FENPET

Reference: N.V.Novozhilova, N.S.Magomedova, G.L.Tudorovskaya, V.K.Bel'skii (1986) *Zh.Strukt.Khim.(Russ.)(J.Struct.Chem.)*, **27**,175-5

Formula: C₂₀H₁₂N₆O₁₀

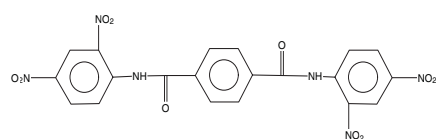
Compound Name: 2,4,2',4'-Tetranitro-N,N'-diphenylterephthalamide

Space Group: P1121/n **Cell:** *a* 19.183(10) *b* 10.285(8) *c* 5.239(2)
Space Group No.: 14 **(Å,°)** α 90.00 β 90.00 γ 102.55(5)

R-Factor (%): 4.70 **Temperature(K):** 295 **Density(g/cm³):** 1.634

Parameters

Fragment 1
NHTOO (D) 1.916
NHO (A) 137.040



FENPIX

Reference: N.V.Novozhilova, N.S.Magomedova, G.L.Tudorovskaya, V.K.Bel'skii (1986) *Zh.Strukt.Khim.(Russ.)(J.Struct.Chem.)*, **27**,169-5

Formula: C₁₃H₈N₄O₇

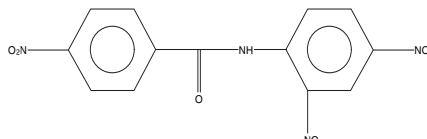
Compound Name: 2',4'-Trinitrobenzanilide

Space Group: P1121/n **Cell:** *a* 7.039(1) *b* 9.374(2) *c* 20.784(4)
Space Group No.: 14 **(Å,°)** α 90.00 β 90.00 γ 92.02(1)

R-Factor (%): 3.60 **Temperature(K):** 295 **Density(g/cm³):** 1.610

Parameters

Fragment 1
NHTOO (D) 1.880
NHO (A) 137.841



FENPIX01

Reference: Yue Sun, Guofeng Wang, Wei Guo (2009) *Tetrahedron*, **65**,3480

Formula: C₁₃H₈N₄O₇

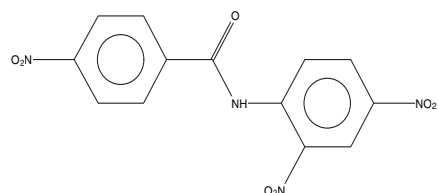
Compound Name: N-(2,4-Dinitrophenyl)-4-nitrobenzamide

Space Group: P21/n **Cell:** *a* 7.039(3) *b* 20.787(6) *c* 9.423(3)
Space Group No.: 14 **(Å,°)** α 90.00 β 92.08(5) γ 90.00

R-Factor (%): 3.96 **Temperature(K):** 293 **Density(g/cm³):** 1.602

Parameters

Fragment 1
NHTOO (D) 1.948
NHO (A) 135.112



FOBMEP

Reference: M.V.N.de Souza, T.R.A.Vasconcelos, S.M.S.V.Wardell, J.L.Wardell, J.N.Low, C.Glidewell (2005) *Acta Crystallogr., Sect.C:Cryst.Struct.Commun.*, **61**,o204

Formula: C₁₂H₈Cl₁N₃O₃

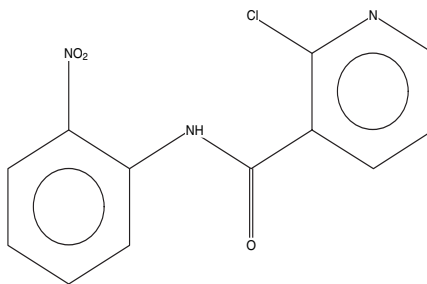
Compound Name: 2-Chloro-N-(2-nitrophenyl)nicotinamide

Space Group: P21/c **Cell:** *a* 6.996(0) *b* 22.424(0) *c* 7.209(0)
Space Group No.: 14 **(Å,°)** α 90.00 β 93.09(0) γ 90.00

R-Factor (%): 3.81 **Temperature(K):** 120 **Density(g/cm³):** 1.633

Parameters

Fragment 1
NHTOO (D) 2.009
NHO (A) 127.862



Search: search2 (Thu Jan 24 14:09:51 2013): Hits 21-24

FUSZEY

Reference: L.A.Chetkina, O.V.Semidetko, V.A.Shuvaeva, A.N.Poplavskii, V.K.Bel'skii, A.M.Andrievskii (1987) *Zh.Strukt.Khim.(Russ.)(J.Struct.Chem.)*, **28**,177-5

Formula: C₁₃H₈N₂O₃

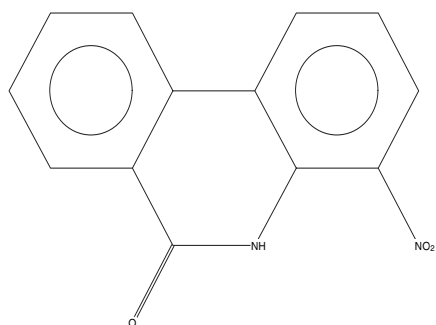
Compound Name: 4-Nitro-6(5H)-phenanthridinone

Space Group: P-1 **Cell:** a 6.975(4) b 7.704(8) c 10.850(9)
Space Group No.: 2 **(Å,°)** α 106.12(6) β 107.02(5) γ 72.32(6)

R-Factor (%): 4.40 **Temperature(K):** 295 **Density(g/cm³):** 1.535

Parameters

Fragment 1
NHTOO (D) 2.041
NHO (A) 133.865



HIJBAD

Reference: M.Kubicki, T.W.Kindopp, M.V.Cappareli, P.W.Codding (1996) *Acta Crystallogr.,Sect.B:Struct.Sci.* **52**,487

Formula: C₈H₄N₄O₆

Compound Name: 5,7-Dinitro-1,4-dihydro-2,3-quinoxalinedione

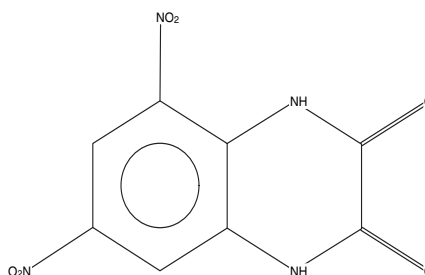
Space Group: P212121 **Cell:** a 6.977(0) b 13.083(1) c 20.401(1)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.50 **Temperature(K):** 295 **Density(g/cm³):** 1.799

Parameters

Fragment 1
NHTOO (D) 2.060
NHO (A) 125.463

Fragment 2
NHTOO (D) 2.058
NHO (A) 130.847



ICULUN

Reference: Xiaorong He, J.G.Stowell, K.R.Morris, R.R.Pfeiffer, Hui Li, G.P.Stahly, S.R.Byrn (2001) *Cryst.Growth Des.*, **1**,305

Formula: C₉H₇F₃N₂O₃

Compound Name: N-(2-Nitro-4-(trifluoromethyl)phenyl)acetamide

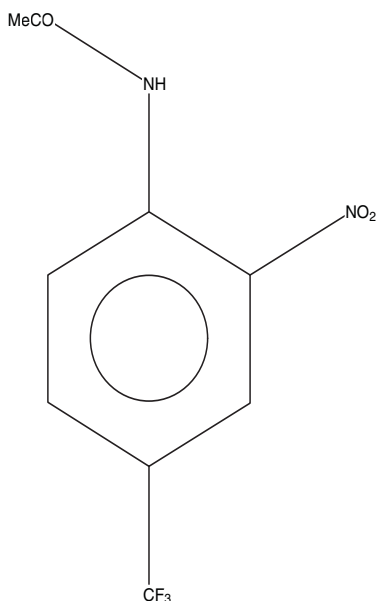
Synonym: 2-Nitro-4-(trifluoromethyl)acetanilide

Space Group: P21/c **Cell:** a 10.769(1) b 4.964(0) c 19.739(2)
Space Group No.: 14 **(Å,°)** α 90.00 β 92.11(0) γ 90.00

R-Factor (%): 5.70 **Temperature(K):** 293 **Density(g/cm³):** 1.563

Parameters

Fragment 1
NHTOO (D) 1.999
NHO (A) 133.734



INODIY

Reference: C.Glidewell, J.N.Low, J.M.S.Skackle, J.L.Wardell (2004) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.*, **60**,o120

Formula: C₁₄H₁₀N₂O₅

Compound Name: 2-(2-Nitrophenylaminocarbonyl)benzoic acid

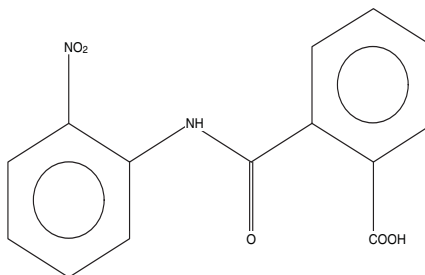
Synonym: N-(2-Nitrophenyl)benzamide-2-carboxylic acid

Space Group: Pbca **Cell:** a 7.276(0) b 14.888(0) c 23.041(0)
Space Group No.: 61 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.90 **Temperature(K):** 120 **Density(g/cm³):** 1.523

Parameters

Fragment 1
NHTOO (D) 2.142
NHO (A) 122.663



Search: search2 (Thu Jan 24 14:09:51 2013): Hits 25-28

JIPJAT

Reference: A.M.Andrievskii, O.V.Chelysheva, A.N.Poplavskii, V.V.Nikonov, L.A.Chetkina, V.K.Bel'skii, V.E.Zavodnik, A.A.Perov, N.A.Andronova, K.M.Dyumaev (1990) *Khim.Get.Soedin., SSSR(Russ.)(Chem.Heterocycl.Compnd.)*, 789

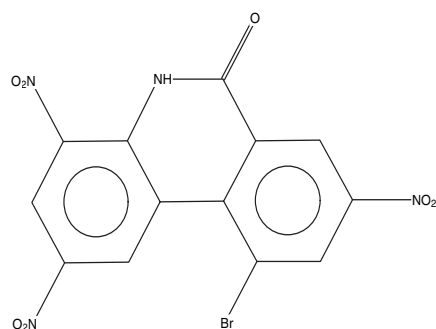
Formula: C₁₃ H₅ Br₁ N₄ O₇

Compound Name: 10-Bromo-2,4,8-trinitro-6(5H)-phenanthridinone

Space Group: R-3 **Cell:** a 28.057(5) b 28.057(5) c 9.116(2)
Space Group No.: 148 **(Å, °)** α 90.00 β 90.00 γ 120.00

R-Factor (%): 4.00 **Temperature(K):** 295 **Density(g/cm³):** 1.968

Parameters
 Fragment 1
 NHTOO (D) 1.926
 NHO (A) 131.569



JIPJAT10

Reference: O.V.Chelysheva, L.A.Chetkina, V.K.Bel'skii, V.E.Zavodnik, A.N.Sobolev, A.N.Poplavskii, V.V.Nikonov, A.M.Andrievskii (1990) *Kristallografiya(Russ.)(Crystallogr.Rep.)*, 35,874

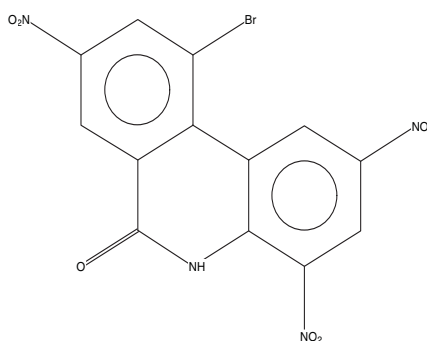
Formula: C₁₃ H₅ Br₁ N₄ O₇

Compound Name: 10-Bromo-2,4,8-trinitro-6(5H)-phenanthridinone

Space Group: R-3 **Cell:** a 28.057(5) b 28.057(5) c 9.116(2)
Space Group No.: 148 **(Å, °)** α 90.00 β 90.00 γ 120.00

R-Factor (%): 4.00 **Temperature(K):** 295 **Density(g/cm³):** 1.968

Parameters
 Fragment 1
 NHTOO (D) 1.926
 NHO (A) 131.569



JIPJEX

Reference: A.M.Andrievskii, O.V.Chelysheva, A.N.Poplavskii, V.V.Nikonov, L.A.Chetkina, V.K.Bel'skii, V.E.Zavodnik, A.A.Perov, N.A.Andronova, K.M.Dyumaev (1990) *Khim.Get.Soedin., SSSR(Russ.)(Chem.Heterocycl.Compnd.)*, 789

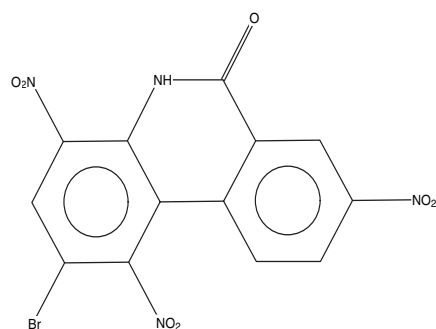
Formula: C₁₃ H₅ Br₁ N₄ O₇

Compound Name: 2-Bromo-1,4,8-trinitro-6(5H)-phenanthridinone

Space Group: Pb21a **Cell:** a 14.665(3) b 14.858(3) c 6.426(1)
Space Group No.: 29 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.10 **Temperature(K):** 295 **Density(g/cm³):** 1.941

Parameters
 Fragment 1
 NHTOO (D) 1.901
 NHO (A) 134.581



JIPJEX10

Reference: O.V.Chelysheva, L.A.Chetkina, V.K.Bel'skii, V.E.Zavodnik, A.N.Sobolev, A.N.Poplavskii, V.V.Nikonov, A.M.Andrievskii (1990) *Kristallografiya(Russ.)(Crystallogr.Rep.)*, 35,874

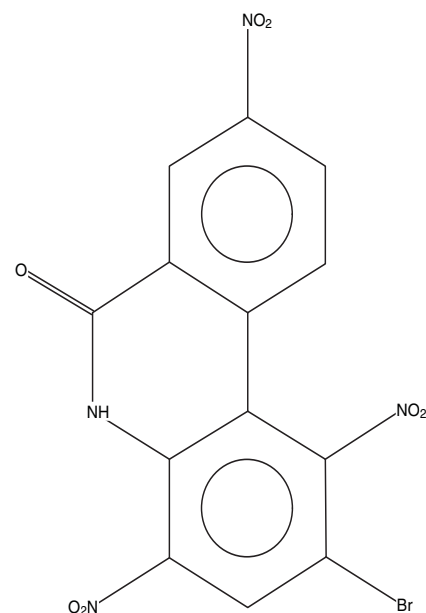
Formula: C₁₃ H₅ Br₁ N₄ O₇

Compound Name: 2-Bromo-1,4,8-trinitro-6(5H)-phenanthridinone

Space Group: Pb21a **Cell:** a 14.665(3) b 14.858(3) c 6.426(1)
Space Group No.: 29 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.10 **Temperature(K):** 295 **Density(g/cm³):** 1.941

Parameters
 Fragment 1
 NHTOO (D) 1.901
 NHO (A) 134.581



Search: search2 (Thu Jan 24 14:09:51 2013): Hits 29-32

KEJGIP

Reference: D.Dudis, R.Gilardi (1990)
Acta Crystallogr., Sect. C: Cryst. Struct. Commun. , **46**,648

Formula: C₉ H₈ N₄ O₈

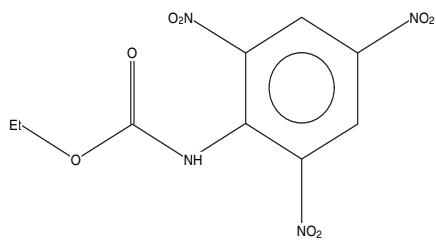
Compound Name: Ethyl (2,4,6-trinitrophenyl)carbamate

Space Group: P21 **Cell:** *a* 4.978(2) *b* 6.974(2) *c* 17.991(6)
Space Group No.: 4 **(Å, °)** *α* 90.00 *β* 94.69(3) *γ* 90.00

R-Factor (%): 5.80 **Temperature(K):** 295 **Density(g/cm³):** 1.602

Parameters

Fragment 1
NHTOO (D) 2.475
NHO (A) 93.955



LAPYUY

Reference: U.Chaithanya, S.Foro, B.T.Gowda (2012)
Acta Crystallogr., Sect. E: Struct. Rep. Online , **68**,0819

Formula: C₁₁ H₁₂ N₂ O₅

Compound Name: 4-((4-Methyl-2-nitrophenyl)amino)-4-oxobutanoic acid

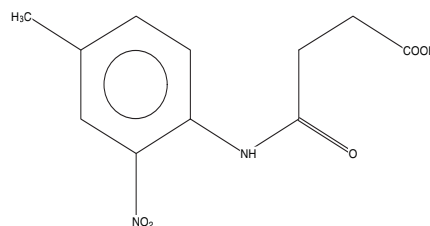
Synonym: N-(4-Methyl-2-nitrophenyl)succinamic acid

Space Group: P-1 **Cell:** *a* 4.853(0) *b* 11.015(2) *c* 11.787(2)
Space Group No.: 2 **(Å, °)** *α* 69.59(1) *β* 78.77(1) *γ* 83.62(2)

R-Factor (%): 4.59 **Temperature(K):** 293 **Density(g/cm³):** 1.448

Parameters

Fragment 1
NHTOO (D) 2.117
NHO (A) 120.887



LESFOF

Reference: A.S.Batsanov, G.Sanford, J.Trmcic (2006)
Private Communication ,

Formula: C₈ H₇ N₃ O₅

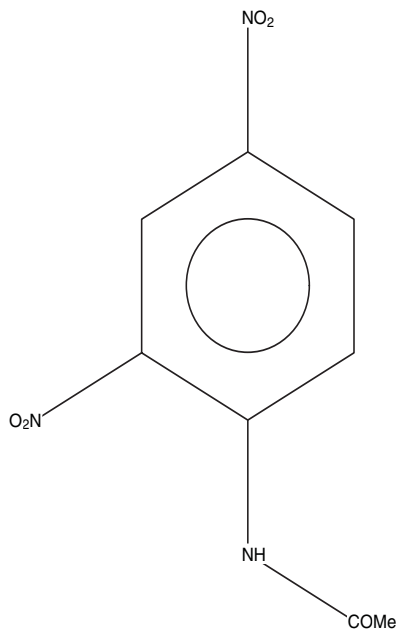
Compound Name: 2,4-Dinitroacetanilide

Space Group: P21/n **Cell:** *a* 6.081(0) *b* 15.715(0) *c* 9.781(0)
Space Group No.: 14 **(Å, °)** *α* 90.00 *β* 92.02(0) *γ* 90.00

R-Factor (%): 3.76 **Temperature(K):** 120 **Density(g/cm³):** 1.601

Parameters

Fragment 1
NHTOO (D) 1.875
NHO (A) 139.261



LESFOF01

Reference: A.S.Batsanov, G.Sanford, J.Trmcic (2006)
Private Communication ,

Formula: C₈ H₇ N₃ O₅

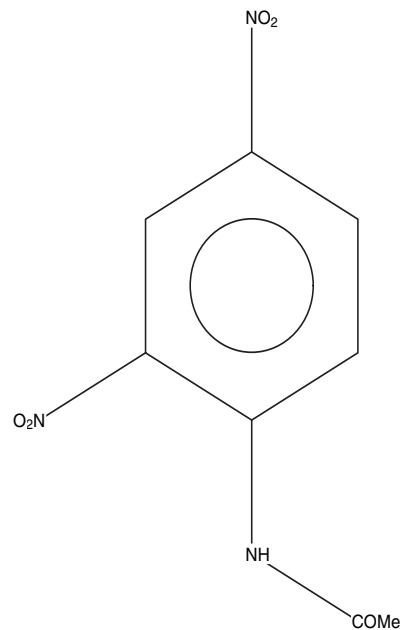
Compound Name: 2,4-Dinitroacetanilide

Space Group: P21/n **Cell:** *a* 10.692(1) *b* 4.668(0) *c* 18.570(1)
Space Group No.: 14 **(Å, °)** *α* 90.00 *β* 96.81(0) *γ* 90.00

R-Factor (%): 3.70 **Temperature(K):** 120 **Density(g/cm³):** 1.625

Parameters

Fragment 1
NHTOO (D) 1.903
NHO (A) 134.488



Search: search2 (Thu Jan 24 14:09:51 2013): Hits 33-36

MNIAAN01

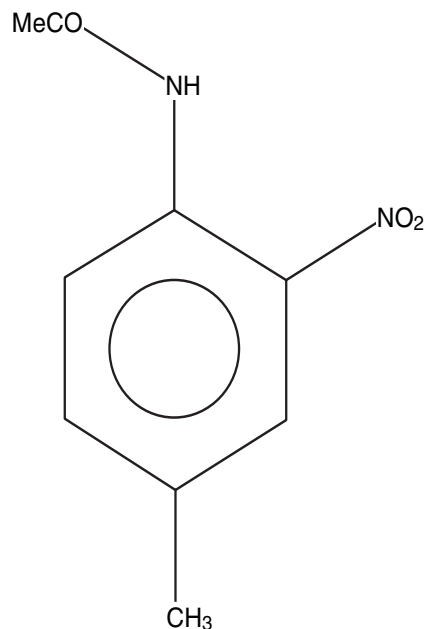
Reference: J.C.Moore, A.Yeadon, R.A.Palmer (1983)
J.Crystallogr.Spectrosc.Res. ,13,279

Formula: C₉ H₁₀ N₂ O₃

Compound Name: 4-Methyl-2-nitroacetanilide

Space Group: P-1 **Cell:** a 17.956(2) b 12.908(2) c 4.039(1)
Space Group No.: 2 **(Å,°)** α 93.13(2) β 83.71(2) γ 90.77(2)

R-Factor (%): 6.50 **Temperature(K):** 295 **Density(g/cm³):** 1.388



Parameters
Fragment 1
NHTOO (D) 1.949
NHO (A) 130.296
Fragment 2
NHTOO (D) 1.976
NHO (A) 131.326

MNIAAN02

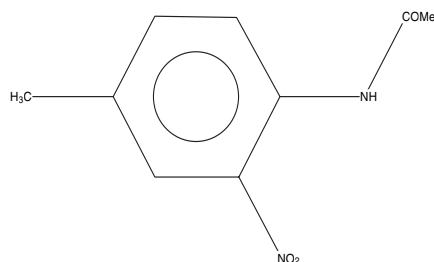
Reference: J.C.Moore, A.Yeadon, R.A.Palmer (1984)
J.Crystallogr.Spectrosc.Res. ,14,283

Formula: C₉ H₁₀ N₂ O₃

Compound Name: 4-Methyl-2-nitroacetanilide

Space Group: P21/c **Cell:** a 10.158(2) b 11.635(2) c 8.041(2)
Space Group No.: 14 **(Å,°)** α 90.00 β 94.55(2) γ 90.00

R-Factor (%): 8.00 **Temperature(K):** 295 **Density(g/cm³):** 1.362



Parameters
Fragment 1
NHTOO (D) 1.977
NHO (A) 140.802

MNIAAN12

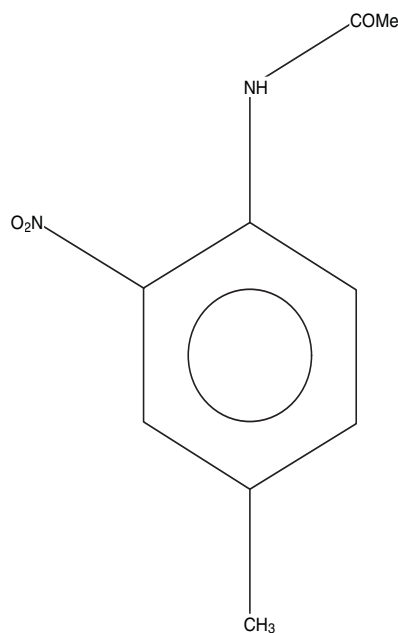
Reference: A.S.Batsanov, R.K.Harris, Phong Ghi (2011)
Private Communication ,

Formula: C₉ H₁₀ N₂ O₃

Compound Name: 4-Methyl-2-nitroacetanilide

Space Group: P-1 **Cell:** a 3.929(0) b 12.858(1) c 17.834(2)
Space Group No.: 2 **(Å,°)** α 89.21(1) β 84.13(1) γ 86.95(1)

R-Factor (%): 4.94 **Temperature(K):** 120 **Density(g/cm³):** 1.441



Parameters
Fragment 1
NHTOO (D) 2.041
NHO (A) 126.447
Fragment 2
NHTOO (D) 1.986
NHO (A) 129.635

MUBHEX

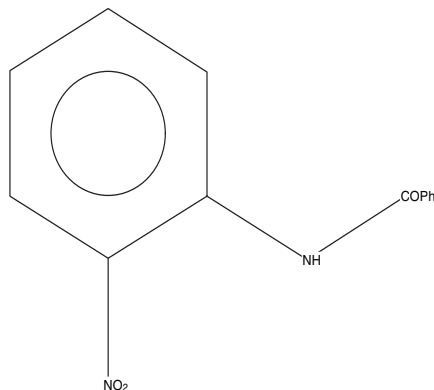
Reference: A.Saeed, J.Simpson (2009)
Acta Crystallogr.,Sect.E:Struct.Rep.Online ,65,o1845

Formula: C₁₃ H₁₀ N₂ O₃

Compound Name: N-(2-Nitrophenyl)benzamide

Space Group: P21/n **Cell:** a 7.206(0) b 7.425(0) c 20.603(1)
Space Group No.: 14 **(Å,°)** α 90.00 β 93.56(0) γ 90.00

R-Factor (%): 4.12 **Temperature(K):** 89 **Density(g/cm³):** 1.462



Parameters
Fragment 1
NHTOO (D) 1.927
NHO (A) 135.670

Search: search2 (Thu Jan 24 14:09:51 2013): Hits 37-40

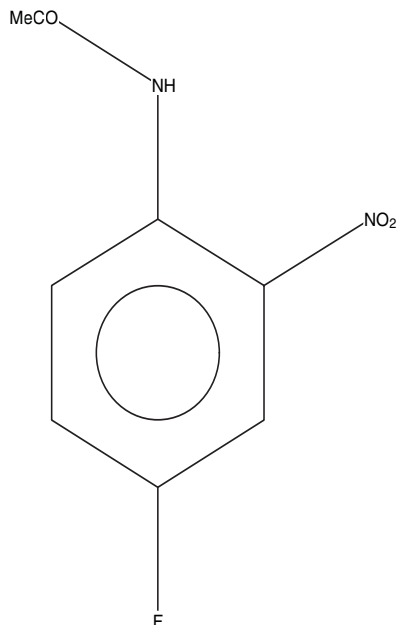
NELQIE

Reference: Jianying Qi, Zhongyuan Zhou, Dongsheng Liu, A.S.C.Chan (2001) *Acta Crystallogr., Sect. E: Struct. Rep. Online*, **57**, o675

Formula: C₈ H₇ F₁ N₂ O₃

Compound Name: 4-Fluoro-2-nitroacetanilide

Space Group: P2₁/c **Cell:** a 3.976(0) b 22.489(4) c 9.742(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 99.25(0) γ 90.00
R-Factor (%): 5.00 **Temperature(K):** 294 **Density(g/cm³):** 1.531



Parameters
 Fragment 1
 NHTOO (D) 2.466
 NHO (A) 100.182

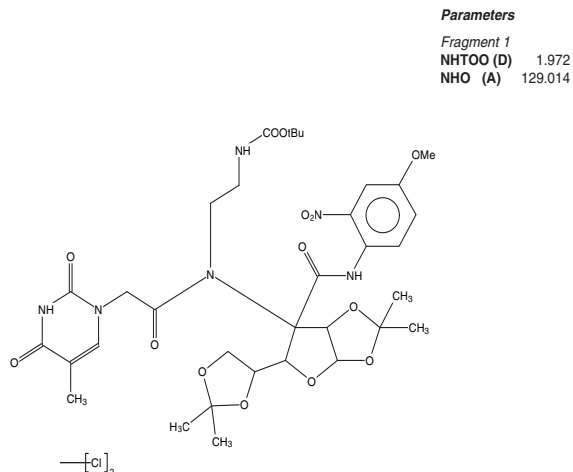
NIXHEH

Reference: I.Schlemminger (2001) *Thesis*,

Formula: C₃₄ H₄₆ N₆ O₁₄·2(C₁ H₂ Cl₂)

Compound Name: N-(7-(2,2-Dimethyl-1,3-dioxol-4-yl)-3,3-dimethyl-6-(4'-methoxy-2'-nitrophenylaminocarbonyl)-2,4,8-trioxabicyclo(3.3.0)octan-6-yl)-N-(1-thyminylacetyl)-2-(t-butoxycarbonylamino)ethylamine dichloromethane solvate

Space Group: P1 **Cell:** a 8.388(0) b 10.301(0) c 13.113(1)
Space Group No.: 1 **(Å, °)** α 92.48(0) β 97.67(0) γ 91.17(0)
R-Factor (%): 4.36 **Temperature(K):** 193 **Density(g/cm³):** 1.381



Parameters
 Fragment 1
 NHTOO (D) 1.972
 NHO (A) 129.014

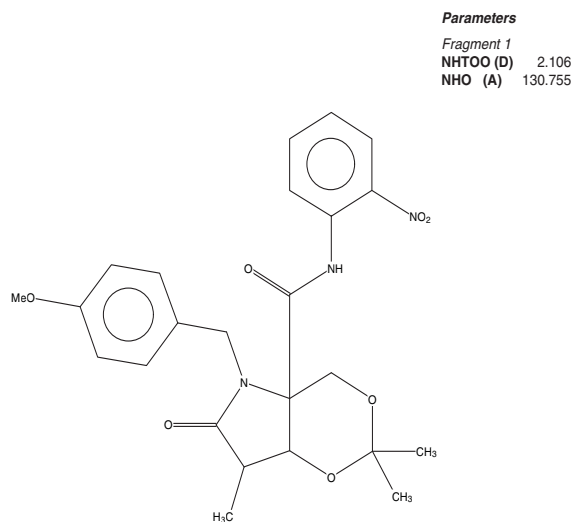
NOCWIM

Reference: C.B.Gilley, Y.Kobayashi (2008) *J.Org.Chem.*, **73**, 4198

Formula: C₂₄ H₂₇ N₃ O₇

Compound Name: (4aR,7R,7aS)-5-(4-Methoxybenzyl)hexahydro-2,2,7-trimethyl-N-(2-nitrophenyl)-6-oxo-(1,3)dioxino(5,4-b)pyrrole-4a-carboxamide

Space Group: C2 **Cell:** a 20.540(1) b 7.979(0) c 14.115(1)
Space Group No.: 5 **(Å, °)** α 90.00 β 105.38(0) γ 90.00
R-Factor (%): 4.90 **Temperature(K):** 100 **Density(g/cm³):** 1.398



Parameters
 Fragment 1
 NHTOO (D) 2.106
 NHO (A) 130.755

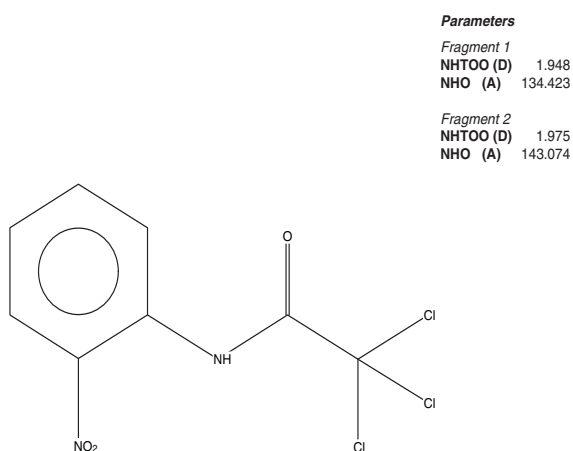
NOQJIM

Reference: Shi-qi Dou, H.Fuess, A.Weiss, B.T.Gowda, V.G.Krishnan (1997) *Z.Kristallogr.*, **212**, 532

Formula: C₈ H₅ Cl₃ N₂ O₃

Compound Name: N-(2-Nitrophenyl)-2,2,2-trichloroacetamide

Space Group: P-1 **Cell:** a 6.809(3) b 12.717(6) c 13.240(6)
Space Group No.: 2 **(Å, °)** α 98.67(2) β 96.14(2) γ 101.47(2)
R-Factor (%): 3.86 **Temperature(K):** 295 **Density(g/cm³):** 1.713



Parameters
 Fragment 1
 NHTOO (D) 1.948
 NHO (A) 134.423
 Fragment 2
 NHTOO (D) 1.975
 NHO (A) 143.074

Search: search2 (Thu Jan 24 14:09:51 2013): Hits 41-44

NUQFIP

Reference: Ting Sun, Gong-Chun Li, Jing Li, Feng-Ling Yang (2010)
Acta Crystallogr., Sect. E: Struct. Rep. Online, **66**, o1113

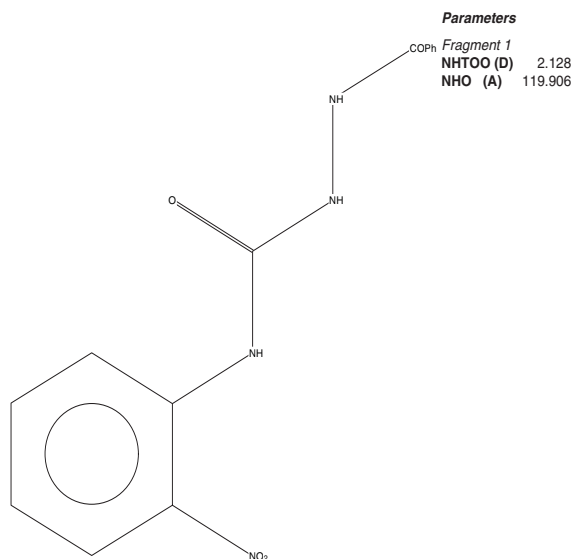
Formula: C₁₄ H₁₂ N₄ O₄

Compound Name: 1-Benzoyl-4-(2-nitrophenyl)semicarbazide

Synonym: 2-Benzoyl-N-(2-nitrophenyl)hydrazinecarboxamide

Space Group: P₂/c **Cell:** *a* 4.655(2) *b* 15.020(7) *c* 10.005(5)
Space Group No.: 7 **Cell:** *α* 90.00 *β* 97.95(0) *γ* 90.00

R-Factor (%): 2.80 **Temperature(K):** 113 **Density(g/cm³):** 1.439



OCAHAD

Reference: De-Cai Wang, Liang-Cheng Huang, Zhu-Yun Liu, Ping Wei, Ping-Kai Ou-yang (2011)
Acta Crystallogr., Sect. E: Struct. Rep. Online, **67**, o3332

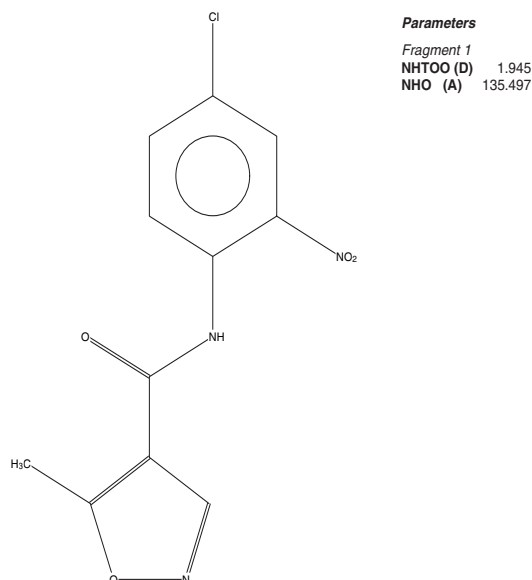
Formula: C₁₁ H₈ Cl₁ N₃ O₄

Compound Name: N-(4-Chloro-2-nitrophenyl)-5-methyl-1,2-oxazole-4-carboxamide

Synonym: N-(4-Chloro-2-nitrophenyl)-5-methylisoxazole-4-carboxamide

Space Group: P2₁/c **Cell:** *a* 5.387(1) *b* 23.537(5) *c* 9.460(1)
Space Group No.: 14 **Cell:** *α* 90.00 *β* 99.86(3) *γ* 90.00

R-Factor (%): 4.19 **Temperature(K):** 293 **Density(g/cm³):** 1.583



PAHCAD

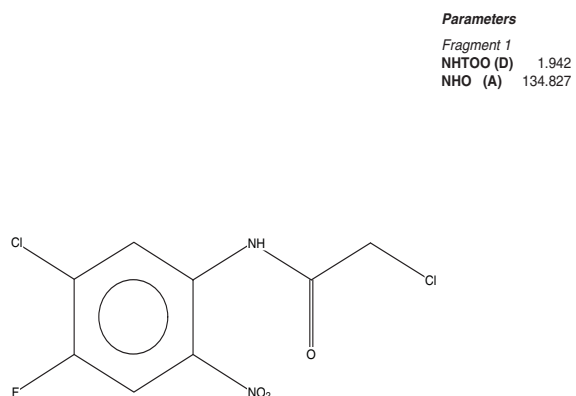
Reference: Ying Zhang, Tian-Yang Feng (2004)
Acta Crystallogr., Sect. E: Struct. Rep. Online, **60**, o1717

Formula: C₈ H₅ Cl₂ F₁ N₂ O₃

Compound Name: 2-Chloro-N-(5-chloro-4-fluoro-2-nitrophenyl)acetamide

Space Group: P2₁/n **Cell:** *a* 11.193(3) *b* 6.449(1) *c* 14.427(4)
Space Group No.: 14 **Cell:** *α* 90.00 *β* 93.14(0) *γ* 90.00

R-Factor (%): 3.48 **Temperature(K):** 293 **Density(g/cm³):** 1.706



QEBWUP

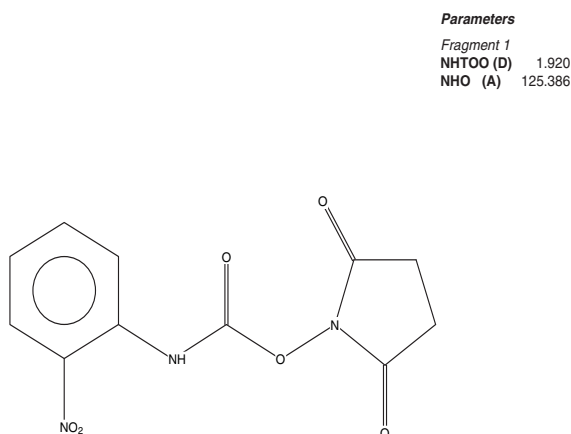
Reference: G. Guichard, V. Semetey, C. Didierjean, A. Aubry, J.-P. Briand, M. Rodriguez (1999) *J. Org. Chem.*, **64**, 8702

Formula: C₁₁ H₉ N₃ O₆

Compound Name: O-Succinimidyl-(2-nitrophenyl)carbamate

Space Group: P2₁/c **Cell:** *a* 12.530(1) *b* 10.077(2) *c* 9.572(2)
Space Group No.: 14 **Cell:** *α* 90.00 *β* 94.50(1) *γ* 90.00

R-Factor (%): 3.68 **Temperature(K):** 295 **Density(g/cm³):** 1.539



Search: search2 (Thu Jan 24 14:09:51 2013): Hits 45-48

QITLLE

Reference: A.S.Batsanov, J.P.Knowles, A.P.Lightfoot, G.Maw, C.E.Thirsk, S.J.R.Twiddle, A.Whiting (2007) *Org.Lett.* ,9,5565

Formula: C₁₉ H₂₉ N₃ O₇ Si₁

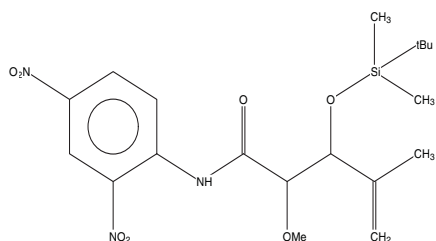
Compound Name: N-(2,4-Dinitrophenyl)-3-(t-butyl(dimethyl)siloxy)-2-methoxy-4-methylpent-4-enamide

Space Group: P21 **Cell:** a 13.183(1) b 6.613(0) c 13.797(1)
Space Group No.: 4 **(Å,°)** α 90.00 β 109.32(1) γ 90.00

R-Factor (%): 3.69 **Temperature(K):** 120 **Density(g/cm³):** 1.286

Parameters

Fragment 1
NHTOO (D) 1.969
NHO (A) 133.817



REZPES

Reference: B.T.Gowda, S.Foro, H.Fuess (2007) *Acta Crystallogr., Sect.E:Struct.Rep.Online* ,63,o1975

Formula: C₈ H₇ Cl₁ N₂ O₃

Compound Name: 2-Chloro-N-(2-nitrophenyl)acetamide

Space Group: Pc **Cell:** a 16.386(2) b 3.939(0) c 28.566(3)
Space Group No.: 7 **(Å,°)** α 90.00 β 90.27(0) γ 90.00

R-Factor (%): 5.33 **Temperature(K):** 303 **Density(g/cm³):** 1.546

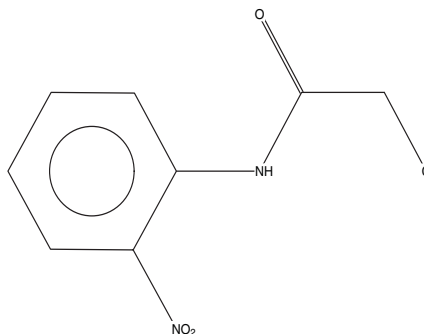
Parameters

Fragment 1
NHTOO (D) 1.949
NHO (A) 134.614

Fragment 2
NHTOO (D) 1.963
NHO (A) 134.271

Fragment 3
NHTOO (D) 1.966
NHO (A) 134.272

Fragment 4
NHTOO (D) 1.959
NHO (A) 134.735



RIBQID

Reference: Cheol-Min Park, Tetsuro Oie, A.M.Petros, Haichao Zhang, P.M.Nimmer, R.F.Henry, S.W.Elmore (2006) *J.Am.Chem.Soc.* ,128, 16206

Formula: C₁₄ H₁₄ N₄ O₅ S₁

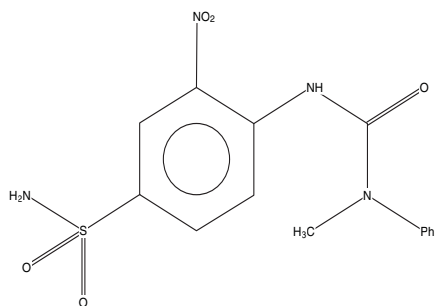
Compound Name: syn,anti-4-(3-Methyl-3-phenylureido)-3-nitrobenzenesulfonamide

Space Group: P21/c **Cell:** a 15.677(5) b 13.127(4) c 8.019(2)
Space Group No.: 14 **(Å,°)** α 90.00 β 95.39(0) γ 90.00

R-Factor (%): 8.58 **Temperature(K):** 293 **Density(g/cm³):** 1.416

Parameters

Fragment 1
NHTOO (D) 1.825
NHO (A) 141.420



RIBQID01

Reference: Cheol-Min Park, Tetsuro Oie, A.M.Petros, Haichao Zhang, P.M.Nimmer, R.F.Henry, S.W.Elmore (2006) *J.Am.Chem.Soc.* ,128, 16206

Formula: C₁₄ H₁₄ N₄ O₅ S₁

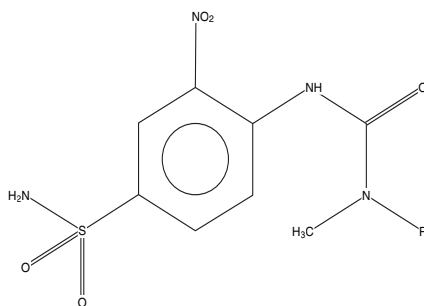
Compound Name: syn,anti-4-(3-Methyl-3-phenylureido)-3-nitrobenzenesulfonamide

Space Group: P21/c **Cell:** a 15.722(1) b 13.153(0) c 8.024(0)
Space Group No.: 14 **(Å,°)** α 90.00 β 95.40(0) γ 90.00

R-Factor (%): 12.07 **Temperature(K):** 295 **Density(g/cm³):** 1.409

Parameters

Fragment 1
NHTOO (D) 1.821
NHO (A) 136.368



Search: search2 (Thu Jan 24 14:09:51 2013): Hits 49-52

SOBGIA

Reference: D.Didier, B.Tylleman, N.Lambert, C.M.L.V.Velde, F.Blockhuys, A.Collas, S.Sergeyev (2008) *Tetrahedron* ,64,6252

Formula: C₁₆ H₁₆ N₄ O₅

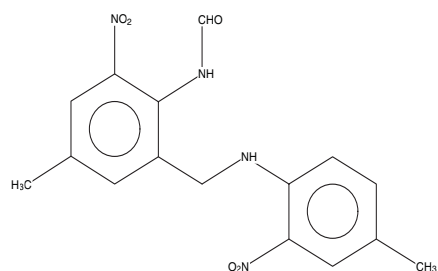
Compound Name: N-(4-Methyl-2-(((4-methyl-2-nitrophenyl)amino)methyl)-6-nitrophenyl)formamide

Space Group: P2₁/c **Cell:** a 13.101(5) b 14.951(4) c 8.316(3)
Space Group No.: 14 **(Å, °)** α 90.00 β 94.28(3) γ 90.00

R-Factor (%): 3.94 **Temperature(K):** 290 **Density(g/cm³):** 1.408

Parameters

Fragment 1
 NHTOO (D) 2.223
 NHO (A) 121.459



SUYNEF

Reference: I.I.Padilla-Martinez, F.J.Martinez-Martinez, E.V.Garcia-Baez, J.M.Torres-Valencia, S.Rojas-Lima, H.Hopfl (2001) *J.Chem.Soc.,Perkin Trans.2* ,1817

Formula: C₁₃ H₁₀ N₄ O₅, C₃ H₇ N₁ O₁

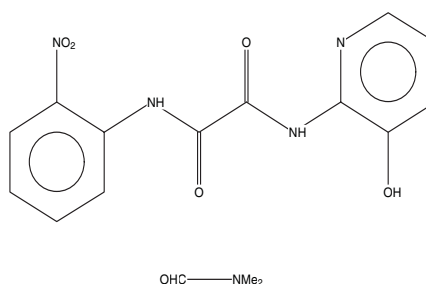
Compound Name: N-(3-Hydroxy-2-pyridyl)-N'-(2-nitrophenyl)oxamide dimethylformamide solvate

Space Group: P2₁/c **Cell:** a 7.219(0) b 14.699(0) c 16.693(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 91.33(0) γ 90.00

R-Factor (%): 4.90 **Temperature(K):** 293 **Density(g/cm³):** 1.408

Parameters

Fragment 1
 NHTOO (D) 1.780
 NHO (A) 135.084



TAFCUY

Reference: O.V.Semidetko, L.A.Chetkina, V.K.Bel'skii, A.M.Andrievskii, A.N.Poplavskii, K.M.Dyumaev (1989) *Kristallografiya(Russ.)(Crystallogr.Rep.)* ,34,106

Formula: C₁₃ H₅ N₅ O₉, 2(C₂ H₄ O₂)

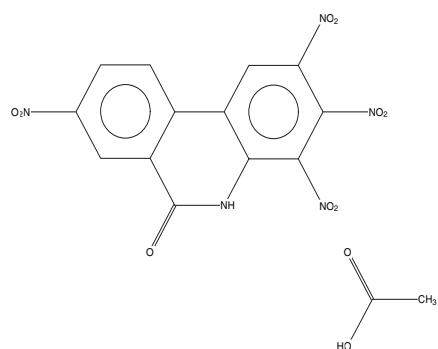
Compound Name: 2,3,4,8-Tetrinitro-6(5H)-phenanthridinone acetic acid solvate

Space Group: P-1 **Cell:** a 9.299(3) b 14.704(6) c 8.454(2)
Space Group No.: 2 **(Å, °)** α 85.05(2) β 112.82(8) γ 96.81(2)

R-Factor (%): 4.50 **Temperature(K):** 295 **Density(g/cm³):** 1.556

Parameters

Fragment 1
 NHTOO (D) 2.615
 NHO (A) 114.528



TAFDAF

Reference: O.V.Semidetko, L.A.Chetkina, V.K.Bel'skii, A.M.Andrievskii, A.N.Poplavskii, K.M.Dyumaev (1989) *Kristallografiya(Russ.)(Crystallogr.Rep.)* ,34,106

Formula: C₁₃ H₆ N₄ O₇, C₆ H₁₈ N₃ O₁ P₁

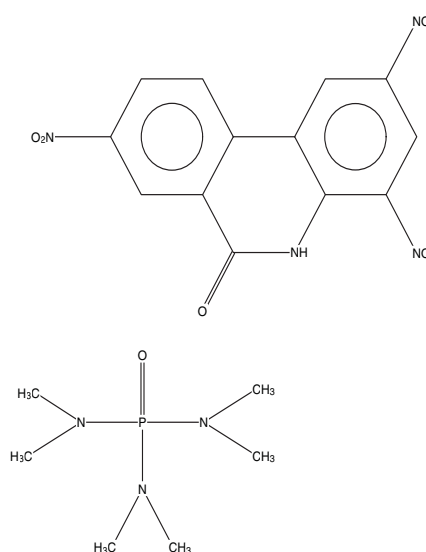
Compound Name: 2,4,8-Trinitro-6(5H)-phenanthridinone hexamethylphosphoramide

Space Group: Pcab **Cell:** a 11.759(3) b 15.614(4) c 25.939(8)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.10 **Temperature(K):** 295 **Density(g/cm³):** 1.421

Parameters

Fragment 1
 NHTOO (D) 2.414
 NHO (A) 105.307



Search: search2 (Thu Jan 24 14:09:51 2013): Hits 53-56

TITWAV

Reference: S.M.S.V.Wardell, M.V.N.de Souza, T.R.A.Vasconcelos, M.de L.Ferreira, J.L.Wardell, J.N.Low, C.Glidewell (2008) *Acta Crystallogr., Sect. B: Struct. Sci.* **64**,84

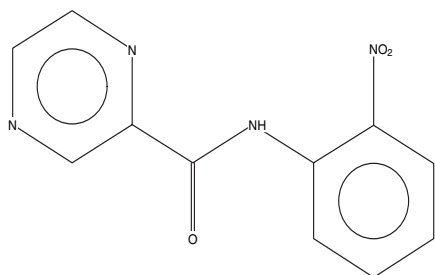
Formula: C₁₁H₈N₄O₃

Compound Name: N-(2-Nitrophenyl)pyrazine-2-carboxamide

Space Group: P2₁/n **Cell:** a 3.660(0) b 21.712(1) c 13.116(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 91.28(0) γ 90.00

R-Factor (%): 6.01 **Temperature(K):** 120 **Density(g/cm³):** 1.557

Parameters
 Fragment 1
 NHTOO (D) 1.939
 NHO (A) 136.694



TUMTIE

Reference: G.Rusek, K.Krajewski, T.Lis (1995) *Pol.J.Chem.* **69**,389

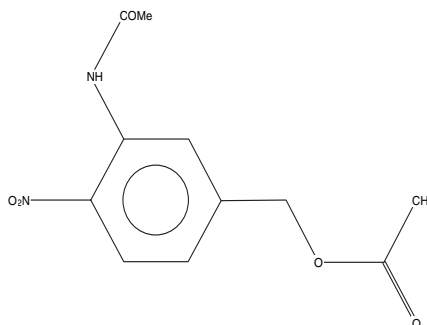
Formula: C₁₁H₁₂N₂O₅

Compound Name: 3-Acetamido-4-nitrobenzyl acetate

Space Group: P-1 **Cell:** a 7.228(5) b 8.148(5) c 10.462(7)
Space Group No.: 2 **(Å, °)** α 81.32(6) β 88.65(6) γ 70.58(5)

R-Factor (%): 4.00 **Temperature(K):** 295 **Density(g/cm³):** 1.459

Parameters
 Fragment 1
 NHTOO (D) 1.973
 NHO (A) 133.674



TUYMEF

Reference: G.Rusek, I.Bryndal, B.Picur, T.Lis, I.Brzostowska (2001) *J.Mol.Struct.* **597**,241

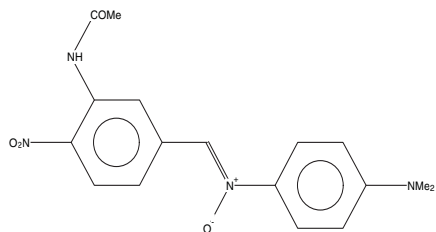
Formula: C₁₇H₁₈N₄O₄

Compound Name: N-(p-Dimethylaminophenyl)-α-(3-acetamido-4-nitrophenyl)nitrene

Space Group: P-1 **Cell:** a 6.813(4) b 8.646(5) c 14.644(6)
Space Group No.: 2 **(Å, °)** α 75.45(4) β 78.56(4) γ 89.10(4)

R-Factor (%): 7.73 **Temperature(K):** 299 **Density(g/cm³):** 1.390

Parameters
 Fragment 1
 NHTOO (D) 1.928
 NHO (A) 137.519



TUYMIJ

Reference: G.Rusek, I.Bryndal, B.Picur, T.Lis, I.Brzostowska (2001) *J.Mol.Struct.* **597**,241

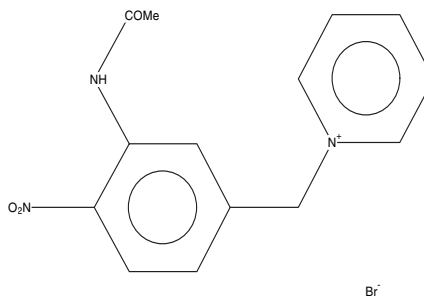
Formula: C₁₄H₁₄N₃O₃¹⁺·Br₁¹⁻

Compound Name: 3-Acetamido-4-nitrobenzylpyridinium bromide

Space Group: C2/c **Cell:** a 24.870(20) b 6.919(5) c 20.034(15)
Space Group No.: 15 **(Å, °)** α 90.00 β 124.28(7) γ 90.00

R-Factor (%): 5.55 **Temperature(K):** 120 **Density(g/cm³):** 1.642

Parameters
 Fragment 1
 NHTOO (D) 1.927
 NHO (A) 136.278



Search: search2 (Thu Jan 24 14:09:51 2013): Hits 57-60

VEGMOJ

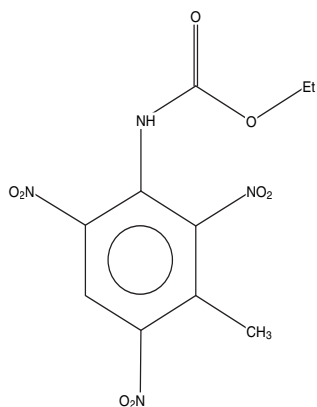
Reference: C.George, D.S.Dudis (1990)
Acta Crystallogr., Sect.C:Cryst.Struct.Commun. ,46,650

Formula: C₁₀H₁₀N₄O₈C₂H₆O₁S₁

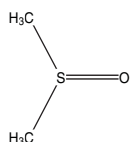
Compound Name: Ethyl (3-methyl-2,4,6-trinitrophenyl)carbamate dimethylsulfoxide solvate

Space Group: P-1 **Cell:** a 8.516(2) b 9.688(2) c 11.895(3)
Space Group No.: 2 **(Å, °)** α 73.43(2) β 80.78(2) γ 72.07(2)

R-Factor (%): 5.00 **Temperature(K):** 295 **Density(g/cm³):** 1.461



Parameters
Fragment 1
NHTOO (D) 2.921
NHO (A) 109.932



WAWMAJ

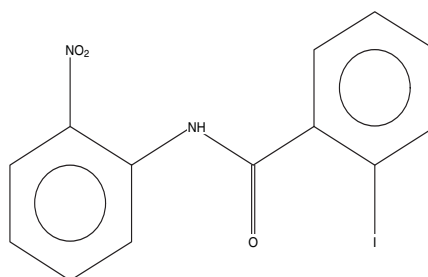
Reference: J.L.Wardell, J.M.S.Skakle, J.N.Low, C.Glidewell (2005)
Acta Crystallogr., Sect.C:Cryst.Struct.Commun. ,61,0634

Formula: C₁₃H₉I₁N₂O₃

Compound Name: N-(2-Nitrophenyl)-2-iodobenzamide

Space Group: P-1 **Cell:** a 7.277(0) b 7.621(0) c 11.682(0)
Space Group No.: 2 **(Å, °)** α 100.25(0) β 107.78(0) γ 92.53(0)

R-Factor (%): 1.84 **Temperature(K):** 120 **Density(g/cm³):** 2.025



Parameters
Fragment 1
NHTOO (D) 2.106
NHO (A) 119.196

WENVUG

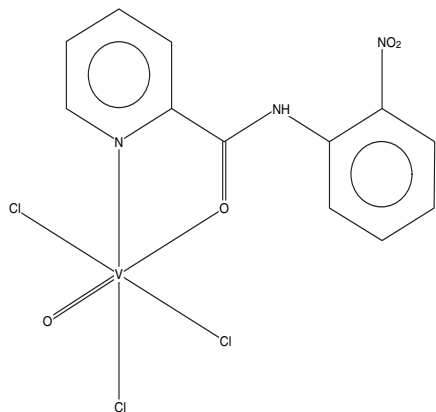
Reference: T.A.Kabanos, A.D.Keramidas, A.Papaioannou, A.Terzis (1994) *Inorg.Chem.* ,33,845

Formula: C₁₂H₉Cl₃N₃O₄V₁

Compound Name: (N-(2-Nitrophenyl)pyridine-2-carboxamide-O,N)-oxo-mer-trichloro-vanadium(IV)

Space Group: P2₁/n **Cell:** a 7.827(1) b 15.740(2) c 12.854(2)
Space Group No.: 14 **(Å, °)** α 90.00 β 101.50(1) γ 90.00

R-Factor (%): 2.68 **Temperature(K):** 295 **Density(g/cm³):** 1.783



Parameters
Fragment 1
NHTOO (D) 1.937
NHO (A) 140.323

WENWAN

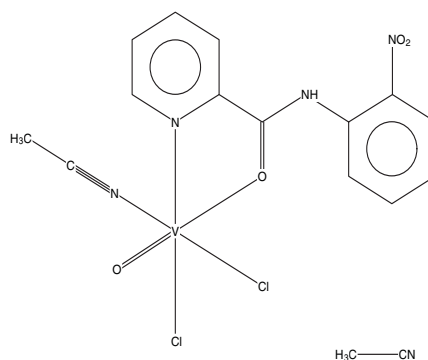
Reference: T.A.Kabanos, A.D.Keramidas, A.Papaioannou, A.Terzis (1994) *Inorg.Chem.* ,33,845

Formula: C₁₄H₁₂Cl₂N₄O₄V₁.0.5(C₂H₃N₁)

Compound Name: Acetonitrile-(N-(2-nitrophenyl)pyridine-2-carboxamide-O,N)-oxo-mer-trichloro-vanadium(IV) acetonitrile solvate

Space Group: P2₁/n **Cell:** a 11.032(0) b 12.097(0) c 14.136(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 100.48(1) γ 90.00

R-Factor (%): 2.82 **Temperature(K):** 295 **Density(g/cm³):** 1.585



Parameters
Fragment 1
NHTOO (D) 2.163
NHO (A) 123.143

Search: search2 (Thu Jan 24 14:09:51 2013): Hits 61-64

WEPKOS

Reference: Shu-Sheng Zhang, Li-Li Xu, Jin Zou, Sai Bi, Yong-Hong Wen (2006) *Acta Crystallogr., Sect. E: Struct. Rep. Online* ,62, o4478

Formula: C₈ H₆ Cl₂ N₂ O₃

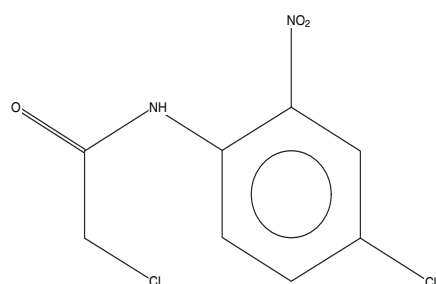
Compound Name: 2-Chloro-N-(4-chloro-2-nitrophenyl)acetamide

Space Group: P21/c **Cell:** a 5.265(1) b 19.641(6) c 9.577(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 96.47(0) γ 90.00

R-Factor (%): 4.29 **Temperature(K):** 293 **Density(g/cm³):** 1.681

Parameters

Fragment 1
 NHTOO (D) 1.984
 NHO (A) 131.092



YAYCEI

Reference: W.Sripet, S.Chantrapomma, P.Ruanwas, H.-K.Fun (2012) *Acta Crystallogr., Sect. E: Struct. Rep. Online* ,68, o1234

Formula: C₁₄ H₁₁ Br₁ N₂ O₄

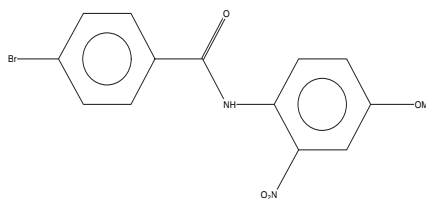
Compound Name: 4-Bromo-N-(4-methoxy-2-nitrophenyl)benzamide

Space Group: P-1 **Cell:** a 6.122(0) b 7.652(0) c 14.350(0)
Space Group No.: 2 **(Å, °)** α 89.20(0) β 84.80(0) γ 77.98(0)

R-Factor (%): 2.56 **Temperature(K):** 100 **Density(g/cm³):** 1.781

Parameters

Fragment 1
 NHTOO (D) 1.993
 NHO (A) 132.341



YICFAS

Reference: H.S.Yathirajan, S.Bindya, M.A.Ashok, B.Narayana, M.Bolte (2007) *Acta Crystallogr., Sect. E: Struct. Rep. Online* ,63, o2202

Formula: C₁₁ H₁₄ N₂ O₄

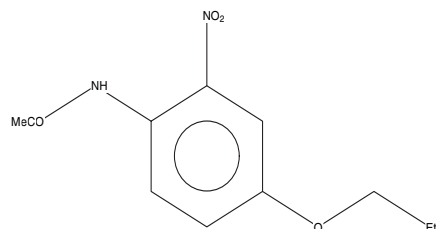
Compound Name: N-(2-Nitro-4-propoxyphenyl)acetamide

Space Group: P21/c **Cell:** a 16.906(1) b 4.006(0) c 18.099(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 111.49(0) γ 90.00

R-Factor (%): 3.85 **Temperature(K):** 173 **Density(g/cm³):** 1.388

Parameters

Fragment 1
 NHTOO (D) 1.959
 NHO (A) 132.476



YIVNUN

Reference: L.Aguilar-Castro, M.Tlahuexti, L.H.Mendoza-Huizar, A.R.Tapia-Benavides, H.Tlahuext (2008) *ARKIVOC* ,9,210-5

Formula: C₁₅ H₁₅ N₃ O₆ S₁

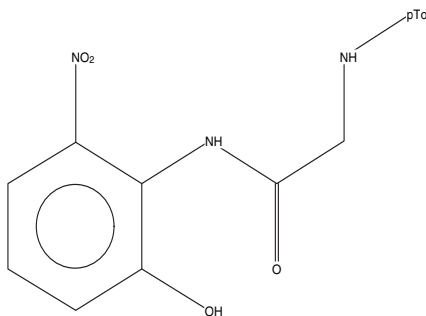
Compound Name: N-(2-Hydroxy-6-nitrophenyl)-2-((4-methylbenzenesulfonyl)amino)acetamide

Space Group: P21/n **Cell:** a 16.427(7) b 5.240(2) c 19.632(8)
Space Group No.: 14 **(Å, °)** α 90.00 β 97.98(0) γ 90.00

R-Factor (%): 4.67 **Temperature(K):** 293 **Density(g/cm³):** 1.450

Parameters

Fragment 1
 NHTOO (D) 2.112
 NHO (A) 120.531



Search: search2 (Thu Jan 24 14:09:51 2013): Hits 65-66

YOPREA

Reference: H.R.Pfaendler, F.Weisner (1995) *Heterocycles*, **40**,717

Formula: C₈ H₄ N₂ O₅

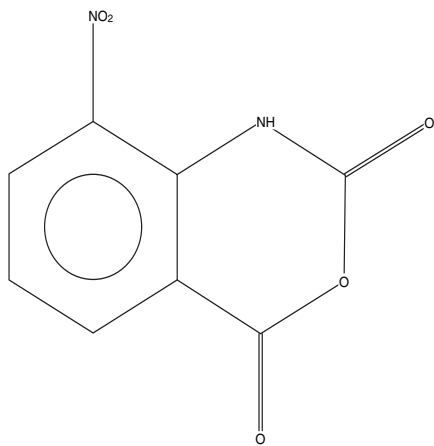
Compound Name: 3-Nitroisatoic anhydride

Space Group: P212121 **Cell:** *a* 5.066(2) *b* 11.499(2) *c* 13.894(4)
Space Group No.: 19 **(Å,°)** *α* 90.00 *β* 90.00 *γ* 90.00

R-Factor (%): 6.04 **Temperature(K):** 295 **Density(g/cm³):** 1.708

Parameters

Fragment 1
NHTOO (D) 1.989
NHO (A) 126.937



ZILROB

Reference: J.F.W.Keana, S.M.Kher, Sui Xiong Cai, C.M.Dinsmore, A.G.Glenn, J.Guastella, Jin-Cheng Huang, V.Ilyin, Yixin Lu, P.L.Mouser, R.L.Woodward, E.Weber (1995) *J.Med.Chem.*, **38**,4367

Formula: C₈ H₃ Cl₂ N₃ O₄ · C₂ H₆ O₁ S₁

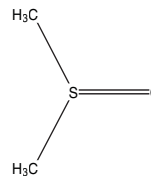
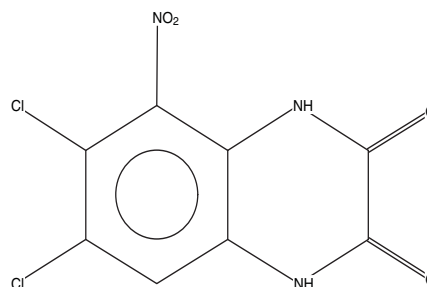
Compound Name: 6,7-Dichloro-1,4-dihydro-5-nitroquinoxaline-2,3-dione dimethylsulfoxide solvate

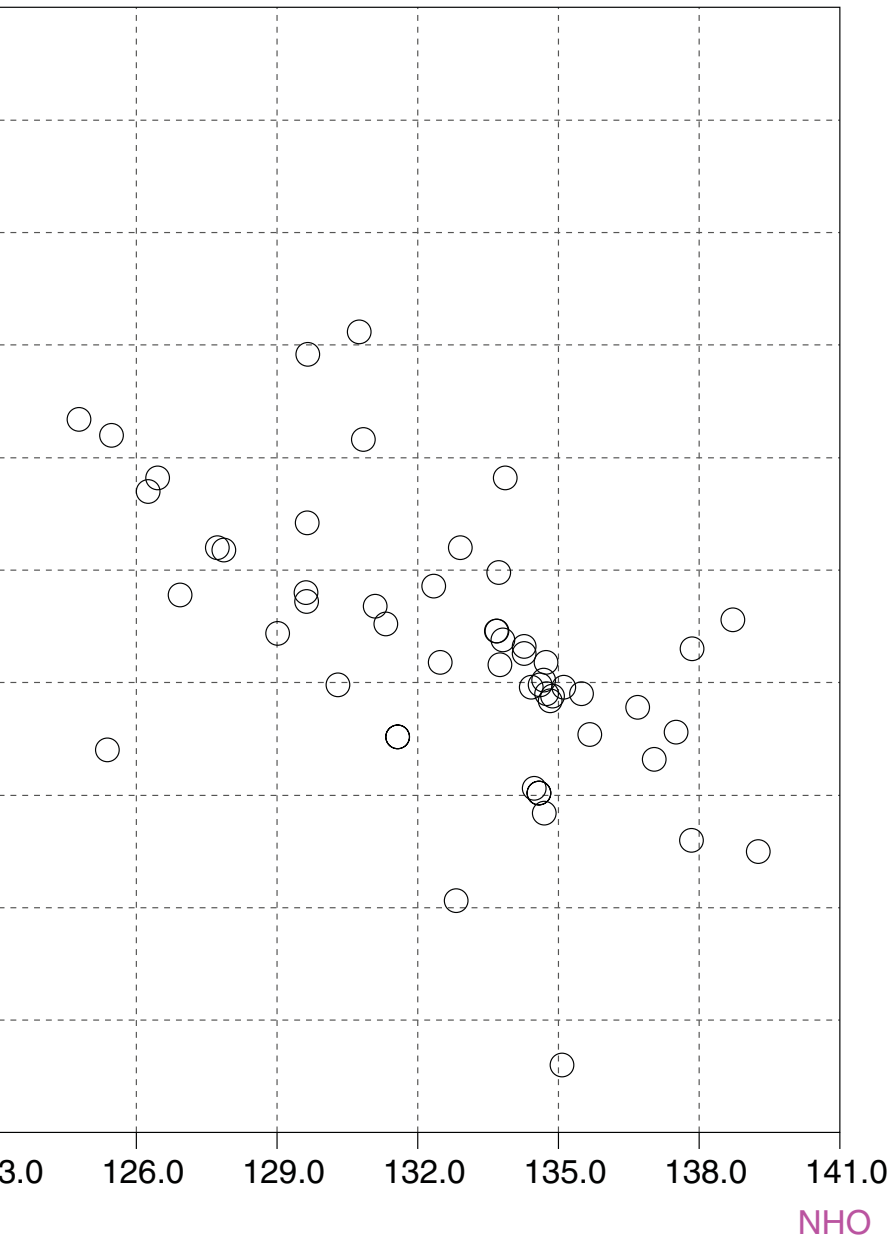
Space Group: P21/n **Cell:** *a* 10.349(3) *b* 6.504(1) *c* 21.131(4)
Space Group No.: 14 **(Å,°)** *α* 90.00 *β* 99.89(2) *γ* 90.00

R-Factor (%): 4.20 **Temperature(K):** 295 **Density(g/cm³):** 1.679

Parameters

Fragment 1
NHTOO (D) 2.765
NHO (A) 116.274





Plot Data

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Mean SE=0.677

Sample SD=5.327

Y-axis

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Max.=2.223

Range=0.443

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Mean SE=0.010

Sample SD=0.081

Search Overview

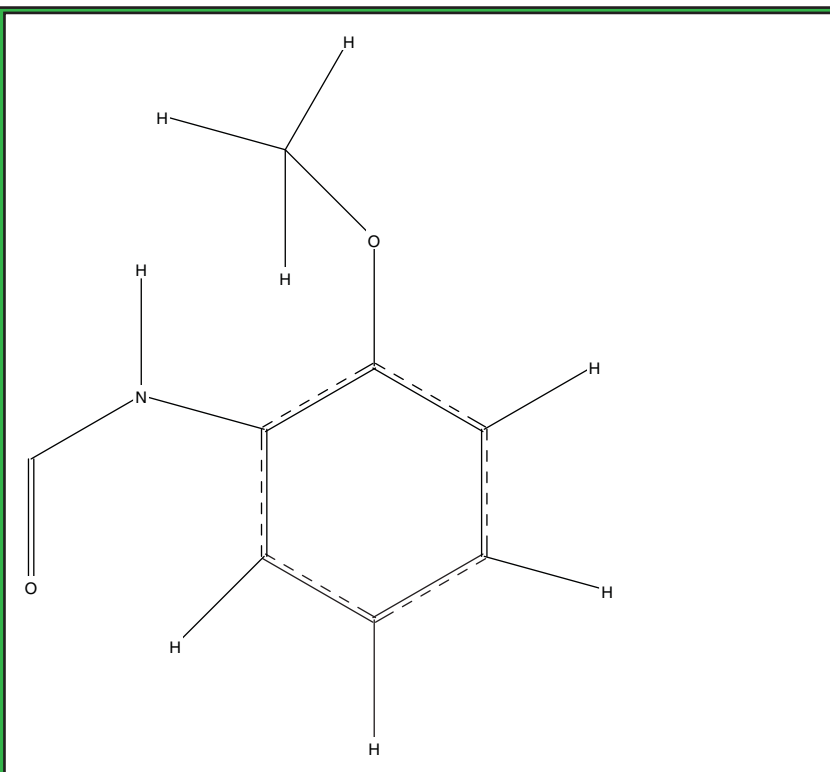
Search: search3
Date/Time done: Sat Feb 09 18:08:57 2013
Database(s): CSD version 5.34 updates (Nov 2012)
CSD version 5.34 (November 2012)
Restriction Info: No refcode restrictions applied
Filters: 3D coordinates determined Not polymeric
No ions No powder structures
Only Organics
Percentage Completed: 100%
Number of Hits: 50

Single query used. Search found structures that:

match

Query 1

Query 1



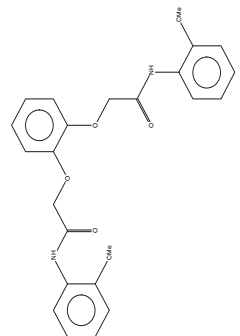
XEHCOE

Reference: A. Ducrot, P. Verwilt, L. Scarpantoni, S. Goulet, C. L. Chabaud, S. L. C. Chabaud, N. D. McClellan (2012) *Synthetic Chem.*, **24**, 482

Formula: C₂₁H₂₄N₂O₆
Compound Name: 2,2-(1,2-Phenylenediis(oxy)bis(N-(2-methoxyphenyl)acetamide)

Space Group: P2₁/c
Space Group No.: 14
R-Factor (%): 3.99

Parameters
Fragment 1
NHO (A) 107.229
NHOM (D) 2.1221



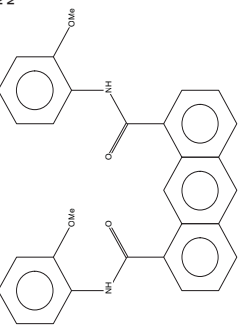
AFUJUV

Reference: En. Gao, Rui. He, Huan-Xia Zhang, Da-bin Qin (2007) *Acta Crystallogr., Sect. E: Struct. Rep. Online* **83**, 63916

Formula: C₂₀H₂₄N₂O₄
Compound Name: N,N'-bis(2-Methoxyphenyl)anthracene-1,8-dicarboxamide

Space Group: P2₁/c
Space Group No.: 14
R-Factor (%): 3.99

Parameters
Fragment 1
NHO (A) 108.979
NHOM (D) 2.205



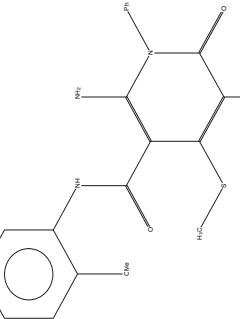
BAFPUV

Reference: V.D. Dyachenko, O.S. Bulyukova, A.D. Dyachenko, S. Shilkin (2011) *Zh. Obshch. Khim. (Russ. J. Gen. Chem.)*, **81**, 887

Formula: C₂₁H₁₈N₂O₄S₁
Compound Name: (rac)-2-Amino-5-cyano-N-(2-methoxyphenyl)-4-(methylsulfonyl)-5-oxo-1-phenyl-1,6-dihydro-pyridine-3-carboxamide

Space Group: Pca2₁
Space Group No.: 29
R-Factor (%): 4.58

Parameters
Fragment 1
NHO (A) 106.159
NHOM (D) 2.224



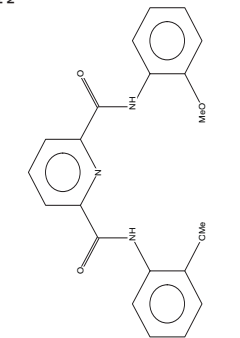
CABWUY

Reference: Qi Yun Yang, Zhong Yuan Zhou, Jian Ying Qi (2001) *Acta Crystallogr., Sect. E: Struct. Rep. Online* **57**(6) 161

Formula: C₂₁H₁₉N₃O₄
Compound Name: N,N'-bis(2-Methoxyphenyl)pyridine-2,6-dicarboxamide

Space Group: P2₁2₁2₁
Space Group No.: 19
R-Factor (%): 4.10

Parameters
Fragment 1
NHO (A) 105.282
NHOM (D) 2.216



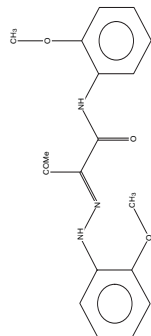
CEWUGU

Reference: E.F. Prullus, W. Reper, D. Wagner (1983) *Z. Kristallogr.*, **165**, 137

Formula: C₁₈H₁₉N₃O₄
Compound Name: N-(2-Methoxyphenyl)-2-(2-methoxyphenylhydrazono)-5-oxo-3-pyrazinone

Space Group: P2₁/n
Space Group No.: 14
R-Factor (%): 3.40

Parameters
Fragment 1
NHO (A) 99.438
NHOM (D) 2.232



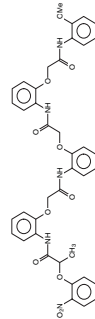
EFIFOP

Reference: M. Akazome, Y. Ishii, T. Niimi, K. Ogura (2008) *Tetrahedron Lett.*, **49**, 4430

Formula: C₂₉H₂₉N₅O₁₁
Compound Name: (R)-N-(2-(2-(2-(2-Methoxyphenylcarbamoyl)methoxy)nitrophenyl)propionamide

Space Group: P2₁2₁2₁
Space Group No.: 19
R-Factor (%): 4.95

Parameters
Fragment 1
NHO (A) 93.909
NHOM (D) 2.334



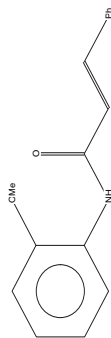
EHAIVAK

Reference: M.N. Nissa, D. Veinuragan, S.S.S. Raju, H.-K. Kim, V. Kasiath, G. Gopalakrishnan (2002) *Cryst. Res. Technol.*, **37**, 125

Formula: C₁₈H₁₅N₃O₂
Compound Name: 2-Methoxy-cinnamamide

Space Group: I41/a
Space Group No.: 88
R-Factor (%): 6.07

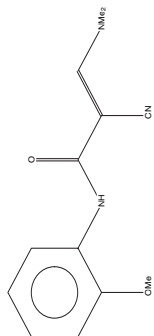
Parameters
Fragment 1
NHO (A) 108.404
NHOM (D) 2.198



EJEJAE

Reference: M. Yagawa, P. G. Anandian, D. Velumagan, K. Sekar, *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, **39**, 0394
Formula: C₁₃H₁₅N₃O₂
Compound Name: 2-Cyano-5-(dimethylamino)-N-(2-methoxyphenyl)acrylamide
Space Group: P2₁/c **a** 7.514(0) **b** 12.758(0) **c** 13.938(0)
Space Group No.: 14 **α** 90.00 **β** 92.80(0) **γ** 90.00
R-Factor (%): 4.79 **Temperature(K)**: 293 **Density(g/cm³)**: 1.221

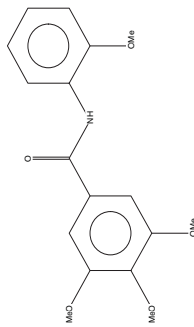
Parameters
Fragment 1
NHO (A) 105.101
NHOM (D) 2.1223



FOWXIZ

Reference: A. Saeed, L. F. Fakie, (2009) *Acta Crystallogr., Sect. E: Struct. Rep. Online*, **85**, 01948
Formula: C₁₇H₁₉N₃O₃
Compound Name: 3,4,5-Trimethoxy-N-(2-methoxyphenyl)isoaxamide
Space Group: Pca2₁ **a** 7.406(2) **b** 25.625(6) **c** 8.851(5)
Space Group No.: 29 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 5.09 **Temperature(K)**: 120 **Density(g/cm³)**: 1.305

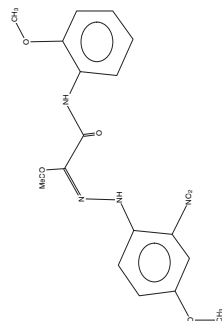
Parameters
Fragment 1
NHO (A) 96.301
NHOM (D) 2.442



FUCTOM

Reference: A. Whitaker, (1987) *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, **43**, 2141
Formula: C₁₁H₁₅N₃O₃
Compound Name: 2-(4-Methoxy-2-nitrophenyl)hydrazono)-N-(2-methoxyphenyl)-3-oxobutanamide
Synonym: α-(4-Methoxy-2-nitrophenyl)hydrazono)-ε-aceto-2-methoxycetamide
Space Group: P2₁/c **a** 7.285(0) **b** 8.032(0) **c** 27.550(1)
Space Group No.: 14 **α** 90.00 **β** 94.30(0) **γ** 90.00
R-Factor (%): 9.50 **Temperature(K)**: 295 **Density(g/cm³)**: 1.433

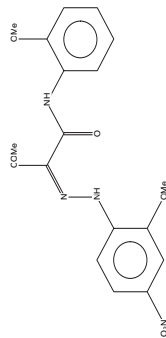
Parameters
Fragment 1
NHO (A) 104.188
NHOM (D) 2.150



FUCTUS

Reference: A. Whitaker, N.P.C. Walker, (1987) *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, **43**, 2137
Formula: C₁₈H₁₉N₃O₅
Compound Name: 2-(2-Methoxy-4-nitrophenyl)hydrazono)-N-(β-methoxyphenyl)-3-oxobutanamide
Synonym: α-(2-Methoxy-4-nitrophenyl)hydrazono)-ε-aceto-2-methoxycetamide
Space Group: P-1 **a** 10.729(2) **b** 11.676(2) **c** 7.658(1)
Space Group No.: 2 **α** 103.43(1) **β** 110.28(1) **γ** 88.08(1)
R-Factor (%): 7.20 **Temperature(K)**: 295 **Density(g/cm³)**: 1.437

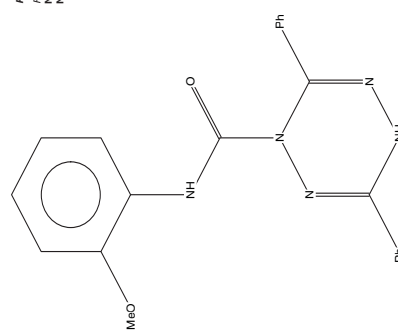
Parameters
Fragment 1
NHO (A) 105.384
NHOM (D) 2.261



GEJZIF

Reference: Guo-Yu Bao, Wei-Xiao Hu, (2008) *Cryst. Res. Technol.*, **41**, 103
Formula: C₂₂H₁₉N₃O₂
Compound Name: N-(2-Methoxyphenyl)-3-(6-diphenyl-1,4-dihydro-1,2,4,5-tetrazin-1-yl)acetamide
Space Group: P2₁2₁2₁ **a** 10.048(1) **b** 13.395(2) **c** 14.607(2)
Space Group No.: 19 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 5.16 **Temperature(K)**: 298 **Density(g/cm³)**: 1.252

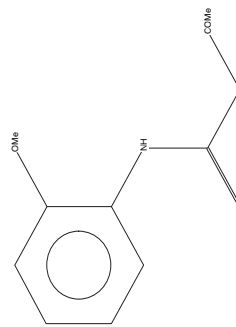
Parameters
Fragment 1
NHO (A) 109.141
NHOM (D) 2.137



GOYKUA

Reference: P. Gill, V. Bantolash, V. Ferraris, G. G. III, (2000) *J. Am. Chem. Soc.*, **122**, 10405
Formula: C₁₁H₁₃N₃O₃
Compound Name: o-Acetoacetonamide
Space Group: P2₁/a **a** 6.727(2) **b** 21.286(3) **c** 7.980(1)
Space Group No.: 14 **α** 90.00 **β** 113.70(2) **γ** 90.00
R-Factor (%): 4.20 **Temperature(K)**: 295 **Density(g/cm³)**: 1.314

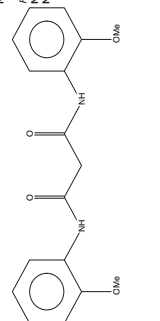
Parameters
Fragment 1
NHO (A) 108.464
NHOM (D) 2.229



GUXM0B

Reference: A. Daubinet, P.T. Kaye, (2002) *Synth. Commun.*, **32**, 2307
Formula: C₁₇H₁₉N₃O₄
Compound Name: N,N-Bis(2-Methoxyphenyl)malonamide
Space Group: P2₁/n **a** 8.567(0) **b** 15.330(0) **c** 23.518(1)
Space Group No.: 14 **α** 90.00 **β** 99.12(0) **γ** 90.00
R-Factor (%): 4.24 **Temperature(K)**: 173 **Density(g/cm³)**: 1.369

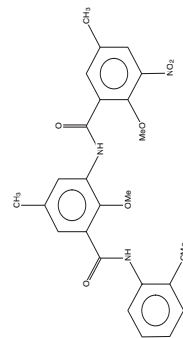
Parameters
Fragment 1
NHO (A) 105.488
NHOM (D) 2.168
Fragment 2
NHO (A) 107.739
NHOM (D) 2.133
Fragment 3
NHO (A) 94.508
NHOM (D) 2.373
Fragment 4
NHO (A) 92.333
NHOM (D) 2.453



HEXSOY

Reference: Hai-Ping Yi, Jiang Wu, Kui-Ling Ding, Xi-Kui Jiang, Zhan-Ting Li, (2007) *J. Org. Chem.*, **72**, 870
Formula: C₂₅H₂₅N₃O₇
Compound Name: N-(β-N-(2-Methoxyphenyl)carbamoyl)-5-methyl-2-methoxyphenyl)-2-methoxy-5-methyl-3-oxobutanamide
Space Group: P2₁/n **a** 14.767(1) **b** 7.371(0) **c** 21.722(3)
Space Group No.: 14 **α** 90.00 **β** 103.97(0) **γ** 90.00
R-Factor (%): 4.79 **Temperature(K)**: 293 **Density(g/cm³)**: 1.348

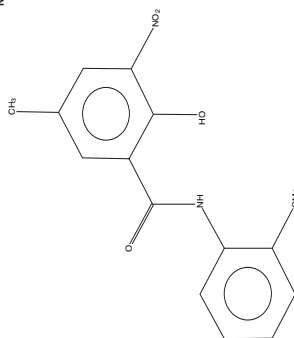
Parameters
Fragment 1
NHO (A) 104.577
NHOM (D) 2.261



HEXXUE

Reference: Hui-Ping Yi, Jiang Wu, Kui-Ling Ding, Xi-Kui Jiang, Zhen-Ting Lu (2007) *J. Org. Chem.*, 72,670
Formula: C₁₅H₁₄N₂O₅
Compound Name: N-(2-Methoxyphenyl)-2-hydroxy-5-methyl-3-nitrobenzamide
Space Group: P21/n **a** 6.951(6) **b** 24.545(2) **c** 5.656(6)
Space Group No.: 14 **α** 90.00 **β** 110.64(6) **γ** 90.00
R-Factor (%): 4.82 **Temperature(K):** 293 **Density(g/cm³):** 1.438

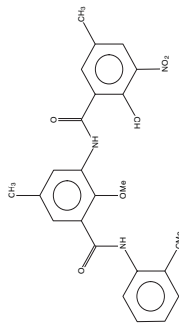
Parameters
Fragment 1
NHO (A) 109.285
NHOM (D) 2.158



HEXYAL

Reference: Hui-Ping Yi, Jiang Wu, Kui-Ling Ding, Xi-Kui Jiang, Zhen-Ting Lu (2007) *J. Org. Chem.*, 72,670
Formula: C₂₄H₂₄N₂O₇
Compound Name: N-(2-Methoxyphenyl)-2-(hydroxy-5-methyl-3-nitrobenzamide)
Space Group: P21/n **a** 8.020(1) **b** 24.590(5) **c** 11.300(2)
Space Group No.: 14 **α** 90.00 **β** 90.10(0) **γ** 90.00
R-Factor (%): 5.16 **Temperature(K):** 293 **Density(g/cm³):** 1.388

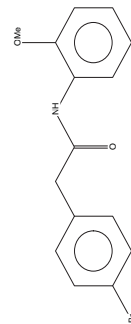
Parameters
Fragment 1
NHO (A) 16.898
NHOM (D) 2.087



HUFHAS

Reference: Zhu-Ping Xiao, Yu-Zhu Ouyang, Shi-Dong Qin, Tian Xie, Jia Yang (2010) *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 66,487
Formula: C₁₅H₁₄BrN₂O₂
Compound Name: 2-(4-Bromophenyl)-N-(2-methoxyphenyl)acetamide
Space Group: P-1 **a** 4.851(4) **b** 13.851(10) **c** 19.256(10)
Space Group No.: 2 **α** 74.8(3) **β** 87.47(6) **γ** 85.18(3)
R-Factor (%): 5.33 **Temperature(K):** 296 **Density(g/cm³):** 1.540

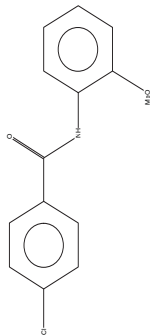
Parameters
Fragment 1
NHO (A) 96.108
NHOM (D) 2.450



HUGLAX

Reference: A. Saied, R.A. Khena, J. Simpson (2010) *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 66,0214
Formula: C₁₄H₁₂O₁N₂
Compound Name: 4-Chloro-N-(2-methoxyphenyl)benzamide
Space Group: P-1 **a** 7.651(6) **b** 8.924(6) **c** 8.972(6)
Space Group No.: 2 **α** 66.68(6) **β** 89.34(6) **γ** 69.54(6)
R-Factor (%): 3.94 **Temperature(K):** 89 **Density(g/cm³):** 1.459

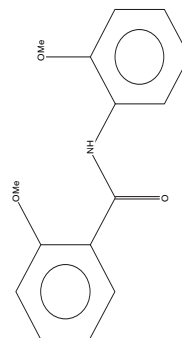
Parameters
Fragment 1
NHO (A) 109.541
NHOM (D) 2.166



ICULEX

Reference: R.D. Parra, Huangang Zeng, Jin Zhi, Cheng Zhang, Xiao Cheng Zeng, Bing Gong (2001) *Chem.-Eur. J.*, 7,4352
Formula: C₁₅H₁₅N₂O₃
Compound Name: N-(2-Methoxyphenyl)-2-methoxybenzamide
Space Group: P21/n **a** 8.366(6) **b** 7.442(6) **c** 20.891(2)
Space Group No.: 14 **α** 90.00 **β** 90.47(6) **γ** 90.00
R-Factor (%): 3.71 **Temperature(K):** 293 **Density(g/cm³):** 1.314

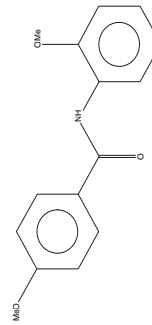
Parameters
Fragment 1
NHO (A) 105.264
NHOM (D) 2.180



ICULOH

Reference: R.D. Parra, Huangang Zeng, Jin Zhi, Cheng Zhang, Xiao Cheng Zeng, Bing Gong (2001) *Chem.-Eur. J.*, 7,4352
Formula: C₁₅H₁₅N₂O₃
Compound Name: N-(2-Methoxyphenyl)-4-methoxybenzamide
Space Group: P21/c **a** 5.388(6) **b** 13.184(4) **c** 18.248(1)
Space Group No.: 14 **α** 90.00 **β** 87.27(6) **γ** 90.00
R-Factor (%): 4.11 **Temperature(K):** 293 **Density(g/cm³):** 1.330

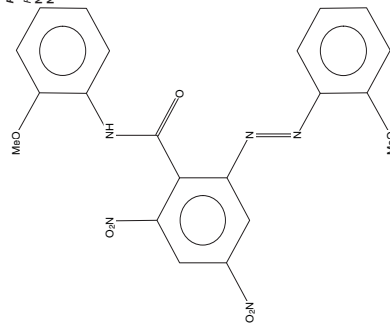
Parameters
Fragment 1
NHO (A) 98.792
NHOM (D) 2.370



IHETAQ

Reference: V.V. Chernyshev, A.V. Yatsenko, A.M. Kovshinov, A.A. Shevlev (2002) *J. Appl. Crystallogr.*, 35,689
Formula: C₂₁H₁₇N₃O₇
Compound Name: N-(2-methoxyphenyl)-2-(methoxyphenyl)diazo-4,6-dinitrobenzamide
Space Group: P212121 **a** 22.788(8) **b** 13.016(6) **c** 6.920(3)
Space Group No.: 19 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 5.00 **Temperature(K):** 295 **Density(g/cm³):** 1.461

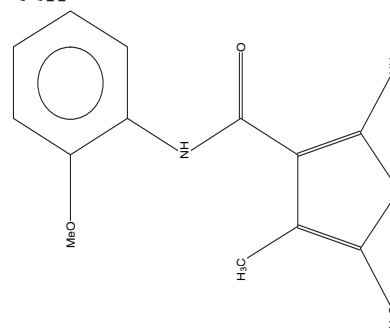
Parameters
Fragment 1
NHO (A) 103.583
NHOM (D) 2.505



KODXEH

Reference: K.C. Kumar, M.K. Kollu, P. Pillaraja, J. Saravanan, M.V. Kulkarni (2008) *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 64, 61311
Formula: C₁₄H₁₅N₂O₂S₁
Compound Name: 2-Amino-N-(2-methoxyphenyl)-4,5-dimethylthiophene-3-carboxamide
Space Group: P21/n **a** 8.606(2) **b** 7.519(1) **c** 21.297(5)
Space Group No.: 14 **α** 90.00 **β** 100.80(6) **γ** 90.00
R-Factor (%): 5.34 **Temperature(K):** 291 **Density(g/cm³):** 1.355

Parameters
Fragment 1
NHO (A) 109.348
NHOM (D) 2.149



LIVZOG

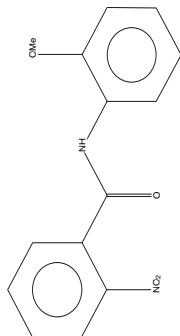
Reference: A.S. Saeed, S. Hussain, M. Bolte (2008). *Acta Crystallogr., Sect. E: Struct. Rep. Online*, **64**, 0603

Formula: C₁₄H₁₂N₂O₄

Compound Name: N-(2-methoxyphenyl)-2-nitrobenzamide

Space Group: P2₁/c **a** 7.657(1) **b** 6.927(0) **c** 16.503(1)
Space Group No.: 19 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 4.43 **Temperature(K)**: 173 **Density(g/cm³)**: 1.444

Parameters
Fragment 1
NHO (A) 109.373
NHOM (D) 2.241



LUDXAJ

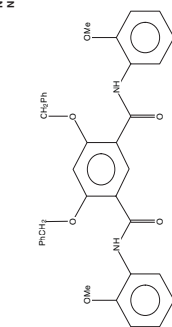
Reference: Bing Gong, Huaqiang Zeng, Jin Zhu, Lihua Yan, Qiang Zhong, T. Saponari, Xiao Cheng Zeng (2002). *Proc. Natl. Acad. Sci. USA*, **99**, 11583

Formula: C₂₂H₂₂N₂O₄

Compound Name: N,N'-bis(2-methoxyphenyl)-4,6-dimethylpyridazine-1,3-dicarboxamide

Space Group: P-1 **a** 10.891(3) **b** 11.717(3) **c** 11.842(3)
Space Group No.: 2 **α** 74.87(0) **β** 82.82(0) **γ** 83.71(0)
R-Factor (%): 8.05 **Temperature(K)**: 153 **Density(g/cm³)**: 1.355

Parameters
Fragment 1
NHO (A) 107.599
NHOM (D) 2.184
Fragment 2
NHO (A) 109.448
NHOM (D) 2.156



MINSAN

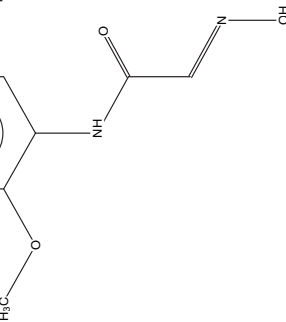
Reference: F. Flina, J. L. Bracco, C. Merletti, X. Solana, Acta Crystallogr., Sect. B: Struct. Crystallogr. Chem., **32**, 2480

Formula: C₉H₁₀N₂O₃

Compound Name: 2-Methoxy-isothreos-acetonilide

Space Group: P2₁2₁2₁ **a** 16.384(6) **b** 24.615(10) **c** 4.669(2)
Space Group No.: 19 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 4.50 **Temperature(K)**: 295 **Density(g/cm³)**: 1.370

Parameters
Fragment 1
NHO (A) 104.390
NHOM (D) 2.167
Fragment 2
NHO (A) 109.655
NHOM (D) 2.157



NELQEB

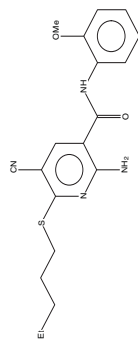
Reference: V.D. Dyachenko, R.P. Trachnev, A.N. Chernoga (2005). *Khim. Geterosicl., SSSR(Russ./Chem. Heterocycl. Comp.)*, **589**

Formula: C₁₉H₂₂N₂O₂S₁

Compound Name: 6-Amino-3-oxano-5-(o-methoxyphenylcarbamoyl)-2-pentylthiopyridine

Space Group: P2₁/c **a** 15.882(5) **b** 6.977(2) **c** 20.616(8)
Space Group No.: 14 **α** 90.00 **β** 105.84(6) **γ** 90.00
R-Factor (%): 6.80 **Temperature(K)**: 295 **Density(g/cm³)**: 1.265

Parameters
Fragment 1
NHO (A) 117.750
NHOM (D) 2.075



OLOCAT

Reference: Chia-Hsien Chang, R.M. Christie, G.M. Rosair (2003). *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, **59**, o556

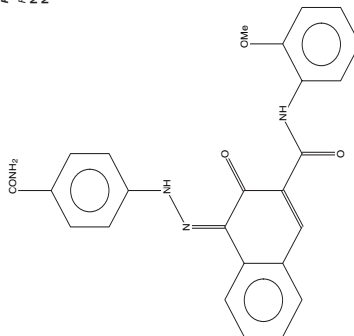
Formula: C₂₅H₂₀N₂O₄

Compound Name: 4-[(4-(Aminoisobutyl)phenyl)hydrazono]N-(6-methoxyphenyl)-3-oxo-3,4-dihydroquinazolin-2-carboxamide

Synonym: C.I. Pigment Red 286

Space Group: P2₁/n **a** 7.254(1) **b** 24.115(3) **c** 11.565(2)
Space Group No.: 14 **α** 90.00 **β** 94.22(1) **γ** 90.00
R-Factor (%): 4.18 **Temperature(K)**: 160 **Density(g/cm³)**: 1.450

Parameters
Fragment 1
NHO (A) 108.890
NHOM (D) 2.154



PEMCUI

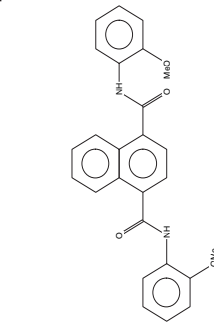
Reference: Lin-Hai Jing, Da-Bin Qin, Shao-Jin Gu, Huan-Xia Zhang, Gang Lei (2008). *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, **62**, o561

Formula: C₂₆H₂₂N₂O₄

Compound Name: N,N'-bis(2-methoxyphenyl)isophthalene-1,4-dicarboxamide

Space Group: Cc **a** 34.719(0) **b** 6.046(0) **c** 10.004(0)
Space Group No.: 9 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 2.91 **Temperature(K)**: 153 **Density(g/cm³)**: 1.352

Parameters
Fragment 1
NHO (A) 88.571
NHOM (D) 2.510



QIWXUQ

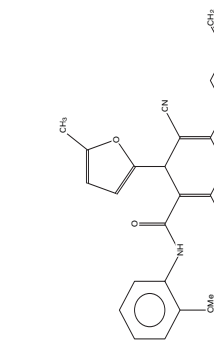
Reference: V.D. Dyachenko, A.N. Chernoga (2008). *Khim. Geterosicl., SSSR(Russ./Chem. Heterocycl. Comp.)*, **51**

Formula: C₂₃H₂₂N₂O₃S₁

Compound Name: 2-Allylthio-6-methyl-4-(6-methyl-2-huryl)-5-(2-methoxyphenylcarbamoyl)-3-oxano-1,4-dihydropyridine

Space Group: P2₁/n **a** 13.355(4) **b** 8.307(2) **c** 21.927(8)
Space Group No.: 14 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 6.81 **Temperature(K)**: 295 **Density(g/cm³)**: 1.146

Parameters
Fragment 1
NHO (A) 106.129
NHOM (D) 2.362

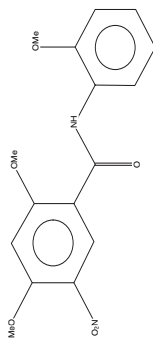


QIZMAN

Reference: Jin Zhu, R.D.Perra, Huiqiang Zeng, J. Am. Chem. Soc., **122**, 4219 (2000)

Formula: C₁₄H₁₆N₂O₆
Compound Name: N-(2-methoxyphenyl)-2,3-dimethoxy-4-nitrobenzamide
Space Group: P-1 **a** 7.186(0) **b** 8.334(0) **c** 13.215(0)
Space Group No.: 2 **α** 73.43(1) **β** 84.69(1) **γ** 88.50(1)
R-Factor (%): 3.86 **Temperature(K)**: 295 **Density(g/cm³)**: 1.465

Parameters
Fragment 1
NHO (A) 110.577
NHOM (D) 2.147

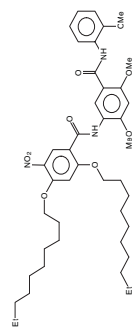


QIZMER

Reference: Jin Zhu, R.D.Perra, Huiqiang Zeng, J. Am. Chem. Soc., **122**, 4219 (2000)

Formula: C₂₃H₃₄N₂O₈
Compound Name: 1-(6-((6-nitro-2,4-bis(dicyclohexylamino)oxy)methyl)amino)-2,4-dimethoxyphenyl)-2-(6-methoxyphenyl)ethanone
Space Group: P-1 **a** 8.283(0) **b** 12.481(0) **c** 18.410(0)
Space Group No.: 2 **α** 84.11(1) **β** 84.97(1) **γ** 78.71(1)
R-Factor (%): 7.57 **Temperature(K)**: 100 **Density(g/cm³)**: 1.221

Parameters
Fragment 1
NHO (A) 109.897
NHOM (D) 2.162



QOQPUH

Reference: Wei-Hua Jiang, Wei-Sheng Liu, Kai-Bai Yu (2001) Acta Crystallogr., Sect.E: Struct. Rep. Chem. **37**, 0402

Formula: C₂₀H₂₄N₂O₆
Compound Name: N,N-bis(2-Methoxyphenyl)-3,6-dioxoethanildamide
Space Group: P2₁/c **a** 7.427(1) **b** 15.805(2) **c** 8.265(1)
Space Group No.: 14 **α** 90.00 **β** 88.98(1) **γ** 90.00
R-Factor (%): 3.71 **Temperature(K)**: 295 **Density(g/cm³)**: 1.324

Parameters
Fragment 1
NHO (A) 109.461
NHOM (D) 2.181

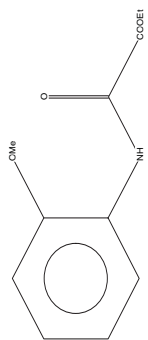


SAKOAW

Reference: F.J.Martinez-Martinez, I.Fradilla-Martinez, M.A.Brito, Acta Crystallogr., Sect.E: Struct. Rep. Chem. **57**, 0402 (2001)

Formula: C₁₁H₁₃N₁O₄
Compound Name: Ethyl N-(2-methoxyphenyl)oxalamate
Space Group: P-1 **a** 8.217(0) **b** 11.320(0) **c** 12.385(0)
Space Group No.: 2 **α** 80.25(0) **β** 81.84(0) **γ** 81.67(0)
R-Factor (%): 4.30 **Temperature(K)**: 295 **Density(g/cm³)**: 1.332

Parameters
Fragment 1
NHO (A) 107.189
NHOM (D) 2.147
Fragment 2
NHO (A) 110.455
NHOM (D) 2.208

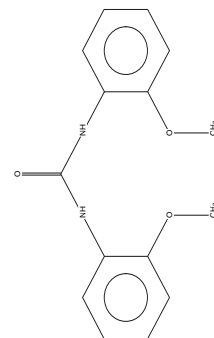


SILTUC

Reference: M.C.Erler, Z.Ubanczyk-Lipkowska, M.Zib-Ebrahimi, T.W.Panunto (1990). J. Am. Chem. Soc., **112**, 8415

Formula: C₁₅H₁₆N₂O₅
Compound Name: 1,3-bis(c-Methoxyphenyl)urea
Space Group: P2₁2₁2₁ **a** 11.030(3) **b** 12.551(3) **c** 4.754(8)
Space Group No.: 18 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 4.20 **Temperature(K)**: 295 **Density(g/cm³)**: 1.374

Parameters
Fragment 1
NHO (A) 98.489
NHOM (D) 2.435

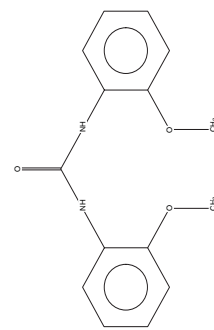


SILTUC01

Reference: M.C.Erler, Z.Ubanczyk-Lipkowska, M.Zib-Ebrahimi, T.W.Panunto (1990). J. Am. Chem. Soc., **112**, 8415

Formula: C₁₅H₁₆N₂O₅
Compound Name: 1,3-bis(o-Methoxyphenyl)urea
Space Group: P4₂/n **a** 11.828(1) **b** 11.828(1) **c** 8.833(9)
Space Group No.: 86 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 4.50 **Temperature(K)**: 295 **Density(g/cm³)**: 1.315

Parameters
Fragment 1
NHO (A) 108.296
NHOM (D) 2.185

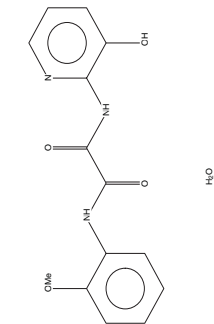


SUNYJ

Reference: I.J.Padilla-Martinez, F.J.Martinez-Martinez, E.V.Garcia-Baez, J.M.Torres-Valecia, S.Rojas-Lima, H.Hopf (2001) J.Chem.Soc., Perkin Trans.2, 1817

Formula: C₁₄H₁₄N₂O₄H₂O
Compound Name: N-(2-Hydroxy-2-pyridyl)-N'-(2-methoxyphenyl)oxamide monohydrate
Space Group: P2₁/c **a** 12.825(9) **b** 15.110(3) **c** 7.241(1)
Space Group No.: 14 **α** 90.00 **β** 101.02(5) **γ** 90.00
R-Factor (%): 3.99 **Temperature(K)**: 293 **Density(g/cm³)**: 1.452

Parameters
Fragment 1
NHO (A) 100.801
NHOM (D) 2.288

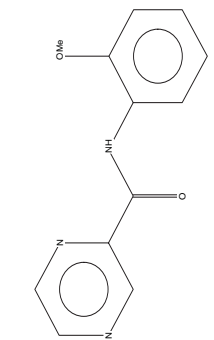


TITVOI

Reference: S.M.S.V.Wardell, M.V.N.de Souza, T.R.A.Vasconcelos, M.de L.Ferreira, J.J.Wardell, J.N.Low, C.Glatwell (2008) Acta Crystallogr., Sect.B: Struct.Sci., **64**, 34

Formula: C₁₂H₁₁N₃O₂
Compound Name: N-(2-Methoxyphenyl)pyrimazine-2-carboxamide
Space Group: P6₃ **a** 14.107(0) **b** 20.751(0) **c** 7.452(0)
Space Group No.: 61 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 3.83 **Temperature(K)**: 120 **Density(g/cm³)**: 1.390

Parameters
Fragment 1
NHO (A) 107.284
NHOM (D) 2.188



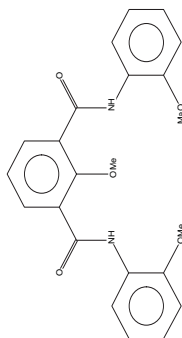
UDEDEN

Reference: Jing Wu, Feng Fang, Wen-Ya Liu, Jun-Li Hou, Chuang Li, J. Org. Chem. **72**, 2837 (2007)

Formula: C₂₄H₂₂N₂O₅
Compound Name: N,N'-bis(2-methoxyphenyl)-2-methoxyisophthalamide

Space Group: Pbc_a **a** 13.728(1) **b** 16.890(1) **c** 17.643(1)
Space Group No.: 61 α 90.00 β 90.00 γ 90.00
R-Factor (%): 4.59 **Temperature(K)**: 293 **Density(g/cm³)**: 1.319

Parameters
Fragment 1
NHO (A) 109.850
NHOM (D) 2.163
Fragment 2
NHO (A) 109.972
NHOM (D) 2.151



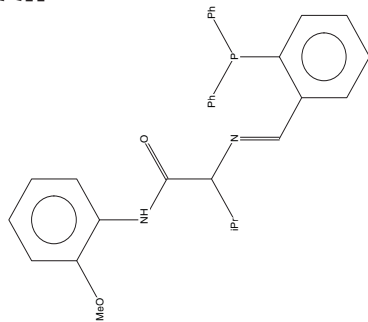
VUOQAM

Reference: A. Baccari, M. Baldrati, P. Palagatti, C. Felzani (2009) J. Organomet. Chem. **884**, 2581

Formula: C₂₁H₁₃N₂O₂P
Compound Name: N²-(2-(Diphenyl(phosphino)benzylidene)-N-(2-methoxyphenyl)vinylamide

Space Group: P2₁2₁2₁ **a** 26.112(8) **b** 15.256(6) **c** 7.002(2)
Space Group No.: 19 α 90.00 β 90.00 γ 90.00
R-Factor (%): 4.12 **Temperature(K)**: 293 **Density(g/cm³)**: 1.176

Parameters
Fragment 1
NHO (A) 109.935
NHOM (D) 2.181



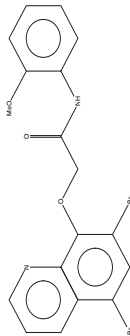
WAFQEN

Reference: Yang-Hong Wen, Hong-Qing Qin, Hui-Ling Wen (2010) Acta Crystallogr. Sect. E Struct. Rep. Online **86**, 03294

Formula: C₁₈H₁₄B₂N₂O₃
Compound Name: 2-((5,7-Dibromoquinolin-8-yl)oxy)-N-(2-methoxyphenyl)acetamide

Space Group: P2₁/n **a** 6.757(1) **b** 8.793(1) **c** 29.372(5)
Space Group No.: 14 α 90.00 β 88.04(6) γ 90.00
R-Factor (%): 4.38 **Temperature(K)**: 293 **Density(g/cm³)**: 1.829

Parameters
Fragment 1
NHO (A) 103.792
NHOM (D) 2.245



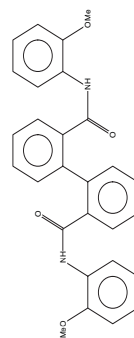
WOGYEX

Reference: Gui-Yu Wang, Di-Li, Dai-Bin Qin, Jie-Wei Luo, Li-Hui Guo (2008) Acta Crystallogr. Sect. E Struct. Rep. Online **64**, 2104

Formula: C₂₄H₂₂N₂O₄
Compound Name: N,N'-bis(2-methoxyphenyl)biphenyl-2,2'-dicarboxamide

Space Group: C₂ **a** 18.184(4) **b** 16.304(3) **c** 8.000(1)
Space Group No.: 9 α 90.00 β 108.90(3) γ 90.00
R-Factor (%): 3.85 **Temperature(K)**: 113 **Density(g/cm³)**: 1.340

Parameters
Fragment 1
NHO (A) 108.115
NHOM (D) 2.239



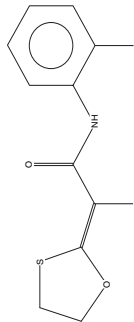
XUKFIT

Reference: Yan-Li, Qian Zhang, Xin Cheng, Qun-Li, Xiaohong Xu (2009) Synthesis **824**

Formula: C₁₇H₁₅N₃O₃S
Compound Name: (Z)-N-(2-Methoxyphenyl)-2-(1-(3-oxoindolin-2-ylidene)-3-oxobutanamide

Space Group: C2/c **a** 15.640(5) **b** 8.245(5) **c** 23.035(5)
Space Group No.: 15 α 90.00 β 106.46(6) γ 90.00
R-Factor (%): 4.10 **Temperature(K)**: 293 **Density(g/cm³)**: 1.307

Parameters
Fragment 1
NHO (A) 107.379
NHOM (D) 2.200



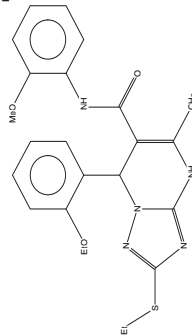
YELYAQ

Reference: V.A. Chabanov, E.A. Muravova, S.M. Desenko, V.I. Musatov, L.V. Knyazova, S.V. Shakhina, O.V. Shekhin, C.O. Kappe (2008) J. Comb. Chem. **8**, 427

Formula: C₂₄H₂₇N₃O₃S
Compound Name: 7-(2-Ethoxyphenyl)-2-ethylsulfonyl-5-methyl-4,7-dihydro-(1,2,4)triazol(1,5-b)pyrimidine-5-carboxylic acid 2-methoxyphenylamide

Space Group: P-1 **a** 11.810(1) **b** 12.827(1) **c** 17.070(1)
Space Group No.: 2 α 74.50(3) β 78.57(6) γ 86.38(0)
R-Factor (%): 7.63 **Temperature(K)**: 293 **Density(g/cm³)**: 1.326

Parameters
Fragment 1
NHO (A) 110.625
NHOM (D) 2.151
Fragment 2
NHO (A) 105.652
NHOM (D) 2.181



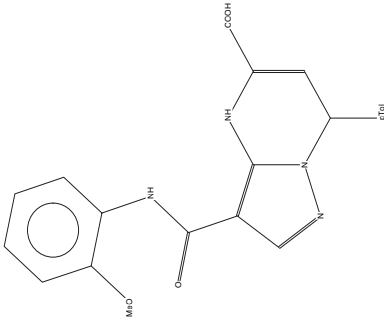
VATNAH

Reference: Y. I. Sakhno, S.V. Shakhina, O.V. Shekhin, V.I. Musatov, M. Michienno, S.M. Desenko, V.A. Chabanov (2010) Mol. Diversity **14**, 323

Formula: C₂₂H₂₂N₄O₄
Compound Name: 3-((2-Methoxyphenyl)carbamoyl)-7-(4-methylphenyl)-1,4-dihydro-1,2,4-triazolo[5,4-b]pyrimidine-5-carboxylic acid

Space Group: P2₁/c **a** 22.486(6) **b** 5.838(1) **c** 15.354(3)
Space Group No.: 14 α 90.00 β 94.21(2) γ 90.00
R-Factor (%): 6.81 **Temperature(K)**: 293 **Density(g/cm³)**: 1.336

Parameters
Fragment 1
NHO (A) 108.848
NHOM (D) 2.180



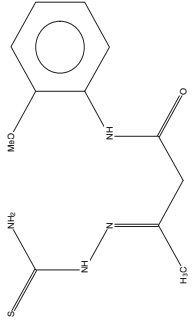
XIGZOC

Reference: J.S. Casas, M.V. Castano, E.E. Castellano, J. Elfrano, M.S. Garcia-Tasende, A. Gato, A. Sanchez, L.M. SanJuan, J. Sordo (2002) J. Org. Chem. **41**, 1500

Formula: C₁₉H₁₆N₂O₂S
Compound Name: o-Acetoacetaldehyde thiosemicarbazone

Space Group: C2/c **a** 23.950(7) **b** 8.878(1) **c** 13.778(6)
Space Group No.: 15 α 90.00 β 109.43(2) γ 90.00
R-Factor (%): 5.32 **Temperature(K)**: 293 **Density(g/cm³)**: 1.379

Parameters
Fragment 1
NHO (A) 107.565
NHOM (D) 2.240



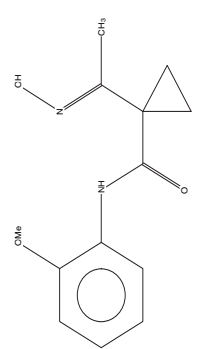
YOKAWA

Reference: Jun-Ling Wang, Shuang-Ming Meng, Ming-Zhong Tian, Feng (2009) Acta Crystallogr, Sect E: Struct, Rep, Online **65**, 01818

Formula: C₁₃H₁₆N₂O₃
Compound Name: 1-(1-(hydroxymino)ethyl)-N-(2-methoxyphenyl)cyclopropanecarboxamide
Synonym: 1-(N-hydroxyethanimidoyl)-N-(2-methoxyphenyl)cyclopropanecarboxamide

Space Group: P2₁c **Cell:** **a** 16.005(6) **b** 5.483(2) **c** 14.250(6)
Space Group No.: 14 **(A, γ)** **α** 90.00 **β** 100.05(6) **γ** 90.00
R-Factor (%): 7.32 **Temperature(K)**: 293 **Density(g/cm³)**: 1.335

Parameters
Fragment 1
NHO (A) 105.441
NHOM (D) 2.207



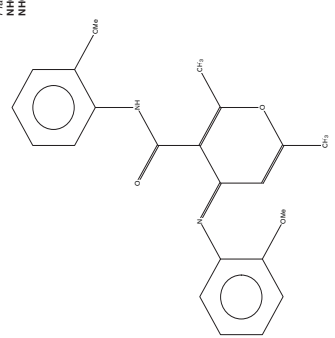
YUDHEL

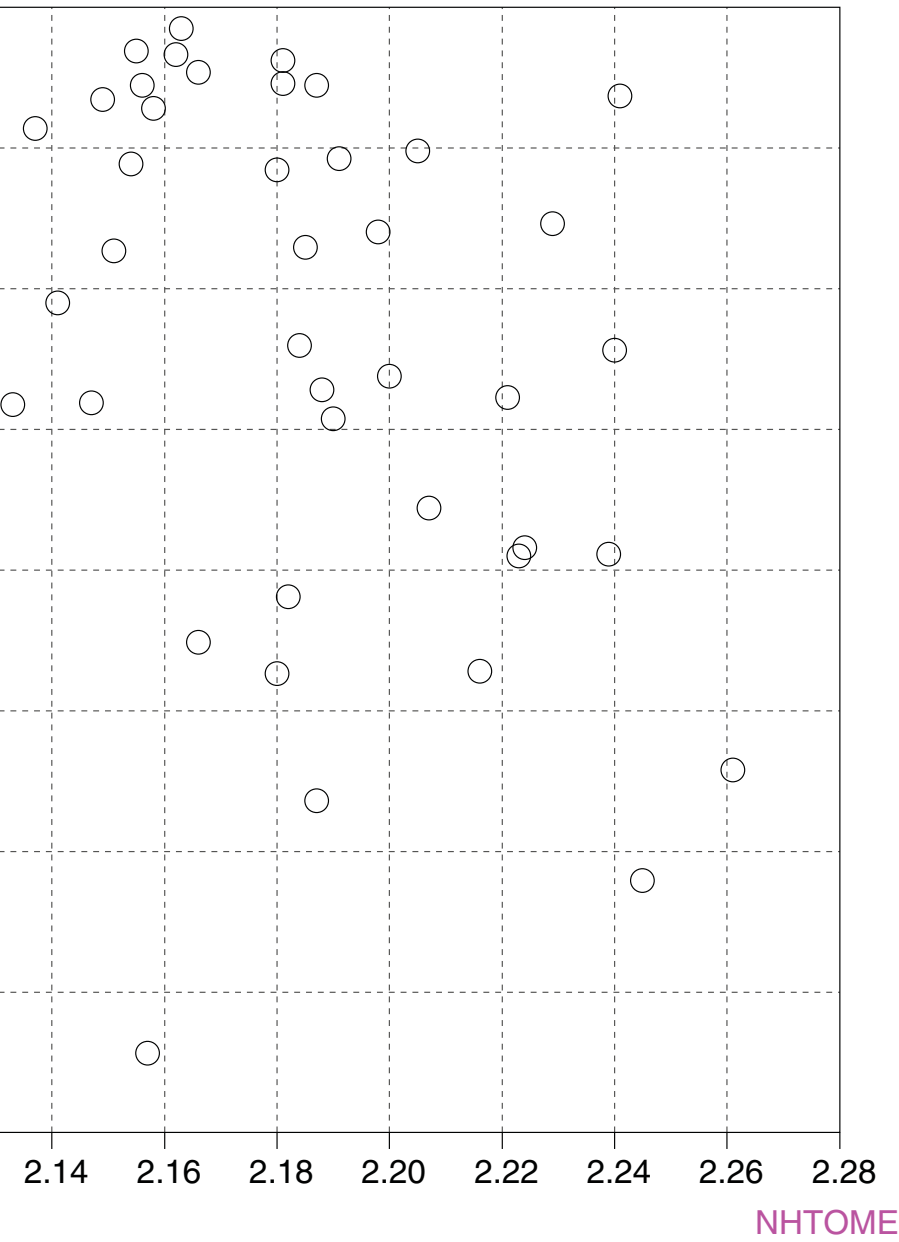
Reference: Yan Wang, Xin-Xin, Yongju Liang, Yiguo Liu, Hailing Du, Dawen Dong (2009) Adv.Synth.Catal. **351** 2217

Formula: C₂₂H₂₂N₂O₄
Compound Name: N-(2-Methoxyphenyl)-4-(2-methoxyphenyl)pyrimido[2,6-dimethyl]-4H-pyrimidin-3-carboxamide

Space Group: P-1 **Cell:** **a** 10.334(3) **b** 10.420(3) **c** 11.131(3)
Space Group No.: 2 **(A, γ)** **α** 64.78(6) **β** 71.97(6) **γ** 65.83(6)
R-Factor (%): 5.80 **Temperature(K)**: 293 **Density(g/cm³)**: 1.288

Parameters
Fragment 1
NHO (A) 109.803
NHOM (D) 2.155





Plot Data

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Test=1

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Obs.=43

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X-axis

Min.=2.081

Max.=2.261

Range=0.180

Mean=2.183

Mean SE=0.006

Sample SD=0.037

Y-axis

Min.=102.565

Max.=109.850

Range=7.285

Mean=107.462

Mean SE=0.293

Sample SD=1.922

Search Overview

Search: search3
Date/Time done: Fri Nov 02 22:22:39 2012
Database(s): CSD version 5.33 (November 2011)
CSD version 5.33 updates (Nov 2011)
Restriction Info: No refcode restrictions applied
Filters: 3D coordinates determined R factor <= 0.1
Not disordered No errors
Not polymeric No ions
No powder structures Only Organics
Percentage Completed: 100%
Number of Hits: 81

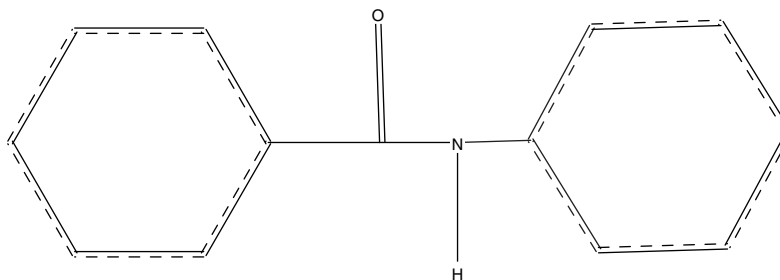
Summary of queries used. Search found structures that:

match

Query 1

Query 2

Query 1



Query 2

Disorder **exclude**
Errors **exclude**
Powder structures **exclude**
Temperature **range 80 - 120 K**

Search: search3 (Fri Nov 02 22:22:39 2012): Hits 1-4

BEBMEB

Reference: C.Glidewell, J.N.Low, J.M.S.Skakle, J.L.Wardell (2003)
Acta Crystallogr., Sect.C: Cryst. Struct. Commun., **59**,o636

Formula: C₁₃H₈I₂N₂O₃

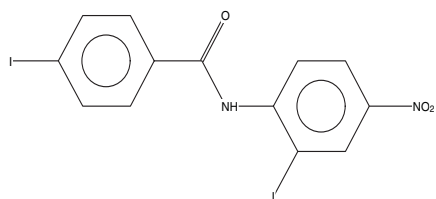
Compound Name: N-(2-Iodo-4-nitrophenyl)-4-iodobenzamide

Space Group: P2₁/c **Cell:** a 15.619(0) b 4.725(0) c 19.767(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 104.08(0) γ 90.00

R-Factor (%): 3.40 **Temperature(K):** 120 **Density(g/cm³):** 2.319

Parameters

Fragment 1
DIST1 (D) 1.500
DIST2 (D) 1.362
DIST3 (D) 1.407
DIST4 (D) 1.228



DIWRAD

Reference: A.Saeed, S.Hussain, U.Florke (2008)
Acta Crystallogr., Sect.E: Struct. Rep. Online, **64**,o705

Formula: C₁₃H₈Cl₁N₃O₅

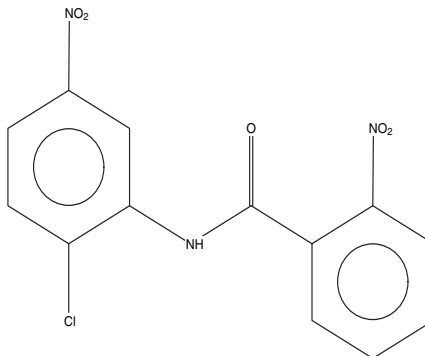
Compound Name: N-(2-Chloro-5-nitrophenyl)-2-nitrobenzamide

Space Group: Pbc_a **Cell:** a 7.805(0) b 13.862(1) c 24.101(3)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.27 **Temperature(K):** 120 **Density(g/cm³):** 1.639

Parameters

Fragment 1
DIST1 (D) 1.512
DIST2 (D) 1.362
DIST3 (D) 1.403
DIST4 (D) 1.216



DUCTOL

Reference: S.Saeed, N.Rashid, R.Hussain, P.G.Jones (2009)
Acta Crystallogr., Sect.E: Struct. Rep. Online, **65**,o2140

Formula: C₂₇H₂₂N₂O₂

Compound Name: N,N'-(Methylenedi-4,1-phenylene)dibenzamide

Synonym: N,N'-(Methylenedi-p-phenylene)dibenzamide

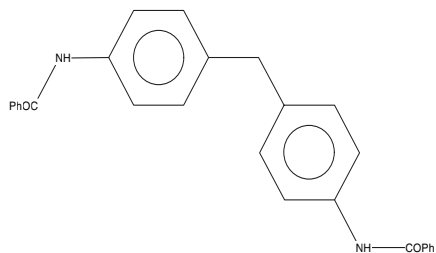
Space Group: P-1 **Cell:** a 5.730(0) b 9.601(1) c 20.045(2)
Space Group No.: 2 **(Å, °)** α 88.52(0) β 82.29(0) γ 75.67(1)

R-Factor (%): 3.77 **Temperature(K):** 100 **Density(g/cm³):** 1.275

Parameters

Fragment 1
DIST1 (D) 1.502
DIST2 (D) 1.346
DIST3 (D) 1.423
DIST4 (D) 1.231

Fragment 2
DIST1 (D) 1.502
DIST2 (D) 1.349
DIST3 (D) 1.419
DIST4 (D) 1.233



FOWXIZ

Reference: A.Saeed, U.Florke (2009)
Acta Crystallogr., Sect.E: Struct. Rep. Online, **65**,o1948

Formula: C₁₇H₁₉N₁O₅

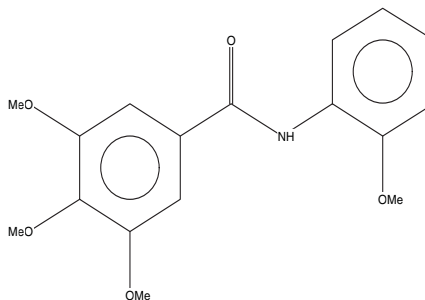
Compound Name: 3,4,5-Trimethoxy-N-(2-methoxyphenyl)benzamide

Space Group: Pca2₁ **Cell:** a 7.409(2) b 22.522(6) c 9.681(3)
Space Group No.: 29 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.09 **Temperature(K):** 120 **Density(g/cm³):** 1.305

Parameters

Fragment 1
DIST1 (D) 1.499
DIST2 (D) 1.371
DIST3 (D) 1.420
DIST4 (D) 1.224



Search: search3 (Fri Nov 02 22:22:39 2012): Hits 5-8

GISYOX01

Reference: A.Saeed, M.Arshad, J.Simpson (2010)
Acta Crystallogr., Sect.E: Struct. Rep. Online ,66,o2808

Formula: C₁₃H₁₀Cl₁N₁O₁

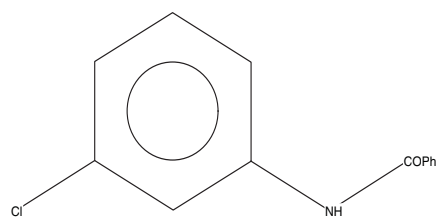
Compound Name: N-(3-Chlorophenyl)benzamide

Space Group: P21/c **Cell:** a 12.560(1) b 10.278(1) c 9.079(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 109.42(0) γ 90.00

R-Factor (%): 4.05 **Temperature(K):** 90 **Density(g/cm³):** 1.392

Parameters

Fragment 1
DIST1 (D) 1.499
DIST2 (D) 1.355
DIST3 (D) 1.417
DIST4 (D) 1.232



GOLWAG

Reference: B.T.Gowda, S.Foro, B.P.Sowmya, H.Fuess (2009)
Acta Crystallogr., Sect.E: Struct. Rep. Online ,65,o444

Formula: C₁₅H₁₄Cl₁N₁O₁

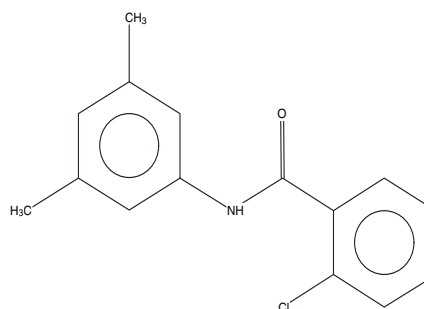
Compound Name: 2-Chloro-N-(3,5-dimethylphenyl)benzamide

Space Group: Pna21 **Cell:** a 9.187(0) b 13.971(0) c 10.271(0)
Space Group No.: 33 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.09 **Temperature(K):** 100 **Density(g/cm³):** 1.309

Parameters

Fragment 1
DIST1 (D) 1.501
DIST2 (D) 1.345
DIST3 (D) 1.432
DIST4 (D) 1.234



HUDXEK

Reference: A.Saeed, R.A.Khera, M.Siddiq, J.Simpson (2010)
Acta Crystallogr., Sect.E: Struct. Rep. Online ,66,o19

Formula: C₁₅H₁₅N₁O₁

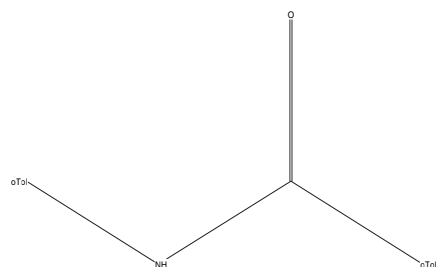
Compound Name: 2-Methyl-N-o-tolylbenzamide

Space Group: P21/n **Cell:** a 4.934(0) b 23.639(2) c 10.023(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 91.18(0) γ 90.00

R-Factor (%): 5.50 **Temperature(K):** 89 **Density(g/cm³):** 1.280

Parameters

Fragment 1
DIST1 (D) 1.501
DIST2 (D) 1.355
DIST3 (D) 1.427
DIST4 (D) 1.242



HUGLAX

Reference: A.Saeed, R.A.Khera, J.Simpson (2010)
Acta Crystallogr., Sect.E: Struct. Rep. Online ,66,o214

Formula: C₁₄H₁₂Cl₁N₁O₂

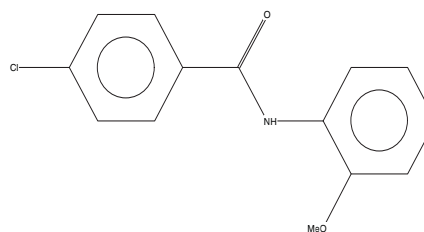
Compound Name: 4-Chloro-N-(2-methoxyphenyl)benzamide

Space Group: P-1 **Cell:** a 7.694(0) b 9.234(0) c 9.872(0)
Space Group No.: 2 **(Å, °)** α 66.68(0) β 89.94(0) γ 69.54(0)

R-Factor (%): 3.94 **Temperature(K):** 89 **Density(g/cm³):** 1.459

Parameters

Fragment 1
DIST1 (D) 1.498
DIST2 (D) 1.361
DIST3 (D) 1.404
DIST4 (D) 1.229



Search: search3 (Fri Nov 02 22:22:39 2012): Hits 9-12

INODIY

Reference: C.Glidewell, J.N.Low, J.M.S.Skakle, J.L.Wardell (2004)
Acta Crystallogr., Sect. C: Cryst. Struct. Commun., **60**, o120

Formula: C₁₄ H₁₀ N₂ O₅

Compound Name: 2-(2-Nitrophenylaminocarbonyl)benzoic acid

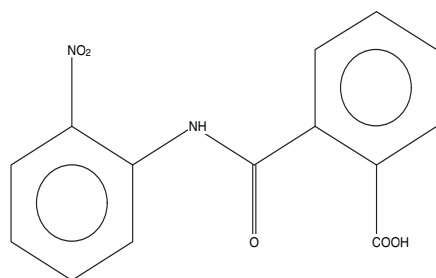
Synonym: N-(2-Nitrophenyl)benzamide-2-carboxylic acid

Space Group: Pbc_a **Cell:** *a* 7.276(0) *b* 14.888(0) *c* 23.041(0)
Space Group No.: 61 (**Å, °**) α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.90 **Temperature(K)**: 120 **Density(g/cm³)**: 1.523

Parameters

Fragment 1
DIST1 (D) 1.505
DIST2 (D) 1.363
DIST3 (D) 1.416
DIST4 (D) 1.222



INODUK

Reference: C.Glidewell, J.N.Low, J.M.S.Skakle, J.L.Wardell (2004)
Acta Crystallogr., Sect. C: Cryst. Struct. Commun., **60**, o120

Formula: C₁₄ H₁₀ N₂ O₅

Compound Name: 2-(4-Nitrophenylaminocarbonyl)benzoic acid

Synonym: N-(4-Nitrophenyl)benzamide-2-carboxylic acid

Space Group: P2₁/n **Cell:** *a* 10.210(1) *b* 9.375(0) *c* 27.409(2)
Space Group No.: 14 (**Å, °**) α 90.00 β 100.58(0) γ 90.00

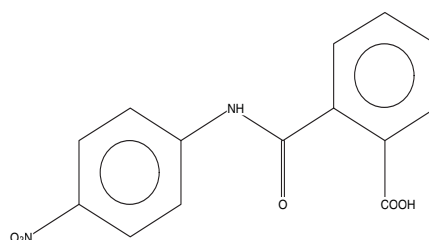
R-Factor (%): 6.90 **Temperature(K)**: 120 **Density(g/cm³)**: 1.474

Parameters

Fragment 1
DIST1 (D) 1.500
DIST2 (D) 1.348
DIST3 (D) 1.398
DIST4 (D) 1.232

Fragment 2

DIST1 (D) 1.499
DIST2 (D) 1.354
DIST3 (D) 1.404
DIST4 (D) 1.228



INODUK01

Reference: C.Glidewell, J.N.Low, J.M.S.Skakle, J.L.Wardell (2004)
Acta Crystallogr., Sect. C: Cryst. Struct. Commun., **60**, o120

Formula: C₁₄ H₁₀ N₂ O₅

Compound Name: 2-(4-Nitrophenylaminocarbonyl)benzoic acid

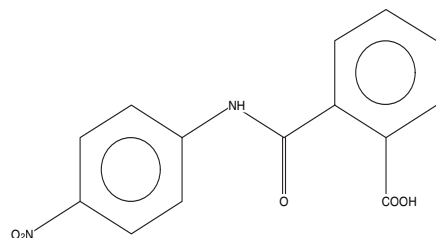
Synonym: N-(4-Nitrophenyl)benzamide-2-carboxylic acid

Space Group: P2₁12₁ **Cell:** *a* 3.919(0) *b* 12.690(0) *c* 27.703(1)
Space Group No.: 19 (**Å, °**) α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.50 **Temperature(K)**: 120 **Density(g/cm³)**: 1.380

Parameters

Fragment 1
DIST1 (D) 1.523
DIST2 (D) 1.349
DIST3 (D) 1.407
DIST4 (D) 1.222



JAVWIN01

Reference: D.Chopra, T.N.G.Row (2005) *Cryst. Growth Des.*, **5**, 1679

Formula: C₁₃ H₉ F₂ N₁ O₁

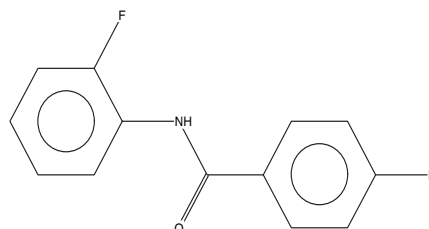
Compound Name: 4-Fluoro-N-(2-fluorophenyl)benzamide

Space Group: P2₁ **Cell:** *a* 4.962(1) *b* 5.486(1) *c* 19.174(5)
Space Group No.: 4 (**Å, °**) α 90.00 β 91.76(0) γ 90.00

R-Factor (%): 4.43 **Temperature(K)**: 100 **Density(g/cm³)**: 1.485

Parameters

Fragment 1
DIST1 (D) 1.496
DIST2 (D) 1.352
DIST3 (D) 1.408
DIST4 (D) 1.236



Search: search3 (Fri Nov 02 22:22:39 2012): Hits 13-16

LEPNEA

Reference: J.L.Wardell, J.N.Low, J.M.S.Skakle, C.Glidewell (2006)
Acta Crystallogr., Sect. B: Struct. Sci., **62**,931

Formula: C₁₃ H₉ I₁ N₂ O₃

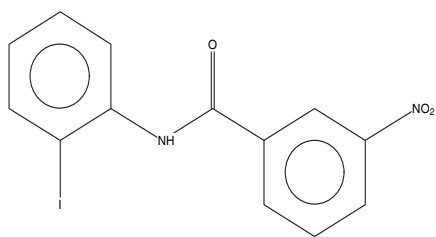
Compound Name: N-(2-Iodophenyl)-3-nitrobenzamide

Space Group: P21/c **Cell:** *a* 13.180(0) *b* 7.510(0) *c* 13.885(0)
Space Group No.: 14 **Cell:** (Å, °) α 90.00 β 111.16(0) γ 90.00

R-Factor (%): 2.52 **Temperature(K):** 120 **Density(g/cm³):** 1.908

Parameters

Fragment 1
DIST1 (D) 1.504
DIST2 (D) 1.348
DIST3 (D) 1.424
DIST4 (D) 1.229



LEPNIE

Reference: J.L.Wardell, J.N.Low, J.M.S.Skakle, C.Glidewell (2006)
Acta Crystallogr., Sect. B: Struct. Sci., **62**,931

Formula: C₁₃ H₉ I₁ N₂ O₃

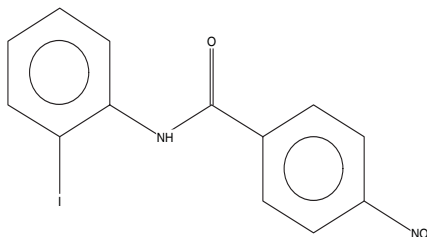
Compound Name: N-(2-Iodophenyl)-4-nitrobenzamide

Space Group: Pc **Cell:** *a* 10.053(0) *b* 4.870(1) *c* 13.572(0)
Space Group No.: 7 **Cell:** (Å, °) α 90.00 β 109.95(0) γ 90.00

R-Factor (%): 1.90 **Temperature(K):** 120 **Density(g/cm³):** 1.957

Parameters

Fragment 1
DIST1 (D) 1.501
DIST2 (D) 1.356
DIST3 (D) 1.409
DIST4 (D) 1.233



LEPNOK

Reference: J.L.Wardell, J.N.Low, J.M.S.Skakle, C.Glidewell (2006)
Acta Crystallogr., Sect. B: Struct. Sci., **62**,931

Formula: C₁₃ H₉ I₁ N₂ O₃

Compound Name: N-(3-Iodophenyl)-2-nitrobenzamide

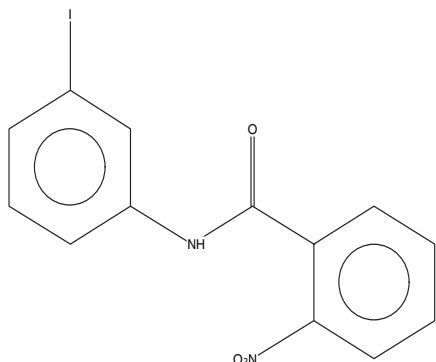
Space Group: P21 **Cell:** *a* 11.055(0) *b* 8.952(0) *c* 12.892(0)
Space Group No.: 4 **Cell:** (Å, °) α 90.00 β 96.39(0) γ 90.00

R-Factor (%): 2.02 **Temperature(K):** 120 **Density(g/cm³):** 1.928

Parameters

Fragment 1
DIST1 (D) 1.515
DIST2 (D) 1.348
DIST3 (D) 1.414
DIST4 (D) 1.225

Fragment 2
DIST1 (D) 1.507
DIST2 (D) 1.340
DIST3 (D) 1.418
DIST4 (D) 1.238



LEPNUQ

Reference: J.L.Wardell, J.N.Low, J.M.S.Skakle, C.Glidewell (2006)
Acta Crystallogr., Sect. B: Struct. Sci., **62**,931

Formula: C₁₃ H₉ I₁ N₂ O₃

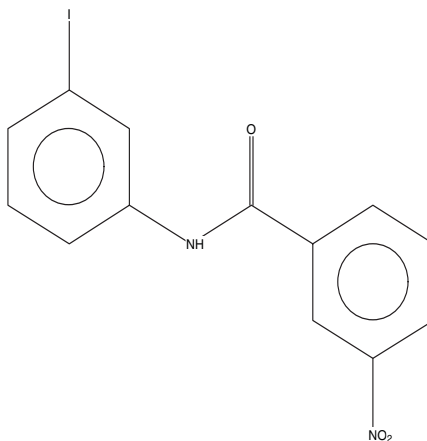
Compound Name: N-(3-Iodophenyl)-3-nitrobenzamide

Space Group: Cc **Cell:** *a* 13.849(0) *b* 10.050(0) *c* 9.420(0)
Space Group No.: 9 **Cell:** (Å, °) α 90.00 β 105.24(0) γ 90.00

R-Factor (%): 1.80 **Temperature(K):** 120 **Density(g/cm³):** 1.933

Parameters

Fragment 1
DIST1 (D) 1.500
DIST2 (D) 1.353
DIST3 (D) 1.415
DIST4 (D) 1.237



Search: search3 (Fri Nov 02 22:22:39 2012): Hits 17-20

LEPPAY

Reference: J.L.Wardell, J.N.Low, J.M.S.Skakle, C.Glidewell (2006)
Acta Crystallogr., Sect. B: Struct. Sci., **62**, 931

Formula: C₁₃ H₉ I₁ N₂ O₃

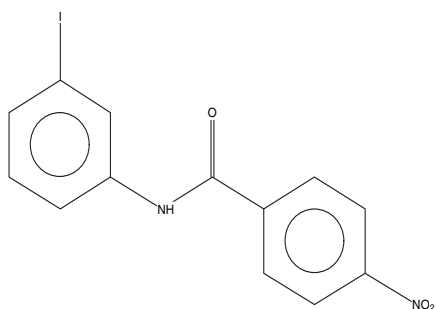
Compound Name: N-(3-Iodophenyl)-4-nitrobenzamide

Space Group: P2₁/n **Cell:** *a* 7.480(0) *b* 14.089(0) *c* 11.814(0)
Space Group No.: 14 **Cell:** (Å, °) *α* 90.00 *β* 93.26(0) *γ* 90.00

R-Factor (%): 8.38 **Temperature(K):** 120 **Density(g/cm³):** 1.967

Parameters

Fragment 1
DIST1 (D) 1.500
DIST2 (D) 1.369
DIST3 (D) 1.406
DIST4 (D) 1.228



LEPPEC

Reference: J.L.Wardell, J.N.Low, J.M.S.Skakle, C.Glidewell (2006)
Acta Crystallogr., Sect. B: Struct. Sci., **62**, 931

Formula: C₁₃ H₉ I₁ N₂ O₃

Compound Name: N-(4-Iodophenyl)-4-nitrobenzamide

Space Group: P-1 **Cell:** *a* 5.105(0) *b* 15.302(0) *c* 16.481(0)
Space Group No.: 2 **Cell:** (Å, °) *α* 95.36(0) *β* 95.50(0) *γ* 91.15(0)

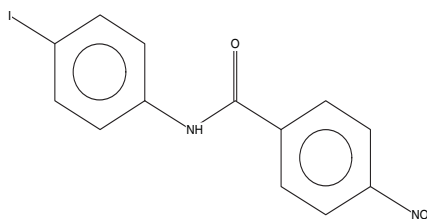
R-Factor (%): 2.88 **Temperature(K):** 120 **Density(g/cm³):** 1.917

Parameters

Fragment 1
DIST1 (D) 1.498
DIST2 (D) 1.356
DIST3 (D) 1.417
DIST4 (D) 1.233

Fragment 2

DIST1 (D) 1.496
DIST2 (D) 1.359
DIST3 (D) 1.417
DIST4 (D) 1.235



MAZWIU

Reference: C.Glidewell, J.N.Low, J.M.S.Skakle, J.L.Wardell (2006)
Acta Crystallogr., Sect. C: Cryst. Struct. Commun., **62**, o5

Formula: C₁₄ H₁₀ N₂ O₅

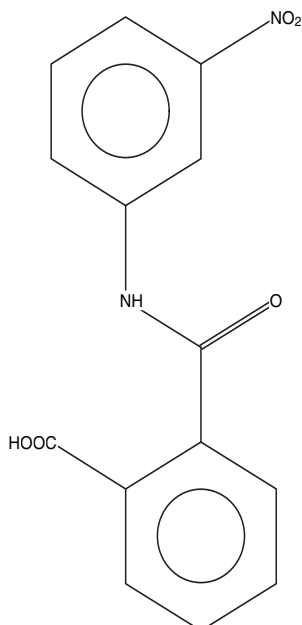
Compound Name: 2-(3-Nitrophenylaminocarbonyl)benzoic acid

Space Group: P2₁ **Cell:** *a* 4.051(0) *b* 12.076(3) *c* 12.771(3)
Space Group No.: 4 **Cell:** (Å, °) *α* 90.00 *β* 90.29(1) *γ* 90.00

R-Factor (%): 6.71 **Temperature(K):** 120 **Density(g/cm³):** 1.522

Parameters

Fragment 1
DIST1 (D) 1.522
DIST2 (D) 1.355
DIST3 (D) 1.399
DIST4 (D) 1.231



MODSOO

Reference: A.Saeed, R.A.Khera, M.Batool, U.Shaheen, U.Florke (2008) *Acta Crystallogr., Sect. E: Struct. Rep. Online*, **64**, o1625

Formula: C₁₆ H₁₆ Cl₁ N₁ O₄

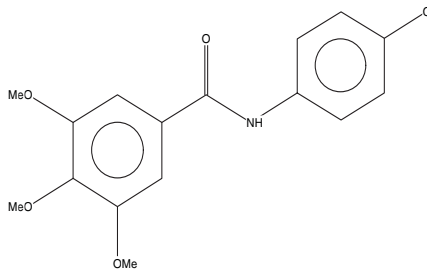
Compound Name: N-(4-Chlorophenyl)-3,4,5-trimethoxybenzamide

Space Group: Cc **Cell:** *a* 9.487(2) *b* 25.666(6) *c* 6.978(1)
Space Group No.: 9 **Cell:** (Å, °) *α* 90.00 *β* 112.34(0) *γ* 90.00

R-Factor (%): 4.50 **Temperature(K):** 120 **Density(g/cm³):** 1.360

Parameters

Fragment 1
DIST1 (D) 1.495
DIST2 (D) 1.356
DIST3 (D) 1.423
DIST4 (D) 1.224



Search: search3 (Fri Nov 02 22:22:39 2012): Hits 21-24

MUBHEX

Reference: A.Saeed, J.Simpson (2009) *Acta Crystallogr., Sect.E: Struct. Rep. Online* ,65,o1845

Formula: C₁₃H₁₀N₂O₃

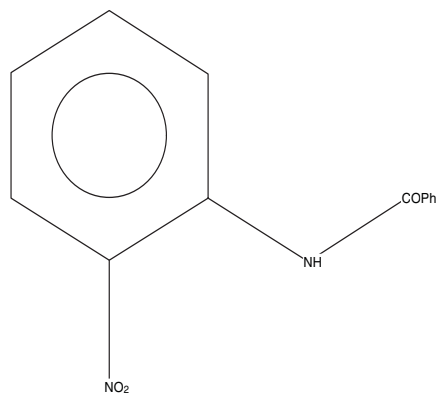
Compound Name: N-(2-Nitrophenyl)benzamide

Space Group: P21/n **Cell:** a 7.206(0) b 7.425(0) c 20.603(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 93.56(0) γ 90.00

R-Factor (%): 4.12 **Temperature(K):** 89 **Density(g/cm³):** 1.462

Parameters

Fragment 1
DIST1 (D) 1.498
DIST2 (D) 1.374
DIST3 (D) 1.401
DIST4 (D) 1.225



NORHUY

Reference: A.Saeed, R.A.Khera, M.Arfaan, J.Simpson, R.G.Stanley (2009) *Acta Crystallogr., Sect.E: Struct. Rep. Online* ,65,o802

Formula: C₁₄H₁₂F₁N₁O₂

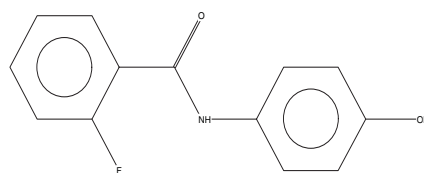
Compound Name: 2-Fluoro-N-(4-methoxyphenyl)benzamide

Space Group: P212121 **Cell:** a 5.290(0) b 6.644(0) c 31.782(1)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.45 **Temperature(K):** 89 **Density(g/cm³):** 1.458

Parameters

Fragment 1
DIST1 (D) 1.506
DIST2 (D) 1.352
DIST3 (D) 1.418
DIST4 (D) 1.232



PUFLEI

Reference: A.Saeed, R.A.Khera, H.Rafique, J.Simpson, R.G.Stanley (2009) *Acta Crystallogr., Sect.E: Struct. Rep. Online* ,65,o2527

Formula: C₁₄H₁₁Cl₂N₁O₁

Compound Name: 2,4-Dichloro-N-(4-methylphenyl)benzamide

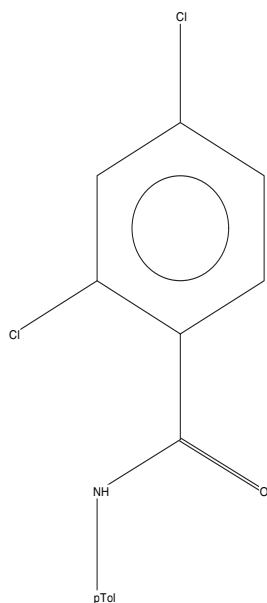
Synonym: 2,4-Dichloro-N-p-tolylbenzamide

Space Group: P21/c **Cell:** a 9.088(1) b 9.825(2) c 14.167(3)
Space Group No.: 14 **(Å, °)** α 90.00 β 94.21(0) γ 90.00

R-Factor (%): 4.11 **Temperature(K):** 89 **Density(g/cm³):** 1.475

Parameters

Fragment 1
DIST1 (D) 1.506
DIST2 (D) 1.351
DIST3 (D) 1.424
DIST4 (D) 1.234



RUFHAC

Reference: D.Guo, G.S.Nichol, J.P.Cain, S.H.Yalkowsky (2009) *Acta Crystallogr., Sect.E: Struct. Rep. Online* ,65,o2644

Formula: C₁₄H₅F₆N₁O₃

Compound Name: 2-(N-(2,4-Difluorophenyl)carbamoyl)-3,4,5,6-tetrafluorobenzoic acid

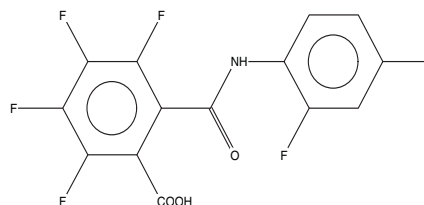
Space Group: P-1 **Cell:** a 7.529(0) b 7.680(0) c 24.197(1)
Space Group No.: 2 **(Å, °)** α 89.81(0) β 82.75(0) γ 68.71(0)

R-Factor (%): 6.65 **Temperature(K):** 100 **Density(g/cm³):** 1.795

Parameters

Fragment 1
DIST1 (D) 1.516
DIST2 (D) 1.349
DIST3 (D) 1.414
DIST4 (D) 1.231

Fragment 2
DIST1 (D) 1.503
DIST2 (D) 1.341
DIST3 (D) 1.406
DIST4 (D) 1.240



Search: search3 (Fri Nov 02 22:22:39 2012): Hits 25-28

TAWRIT01

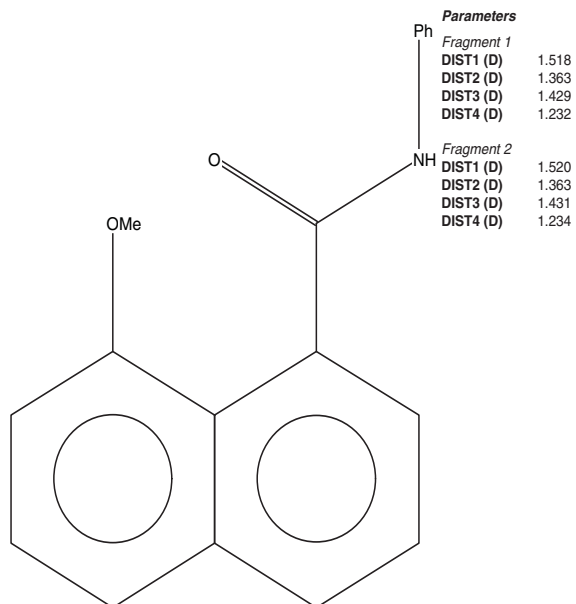
Reference: J.O'Leary, X.Formosa, W.Skranc, J.D.Wallis (2005)
Org.Biomol.Chem., 3,3273

Formula: C₁₈ H₁₅ N₁ O₂

Compound Name: 8-Methoxy-N-phenyl-1-naphthamide

Space Group: P-1 **Cell:** a 10.153(3) b 11.463(4) c 13.179(7)
Space Group No.: 2 **(Å, °)** α 77.35(2) β 84.61(4) γ 70.15(2)

R-Factor (%): 4.03 **Temperature(K):** 100 **Density(g/cm³):** 1.309



TAWRIT02

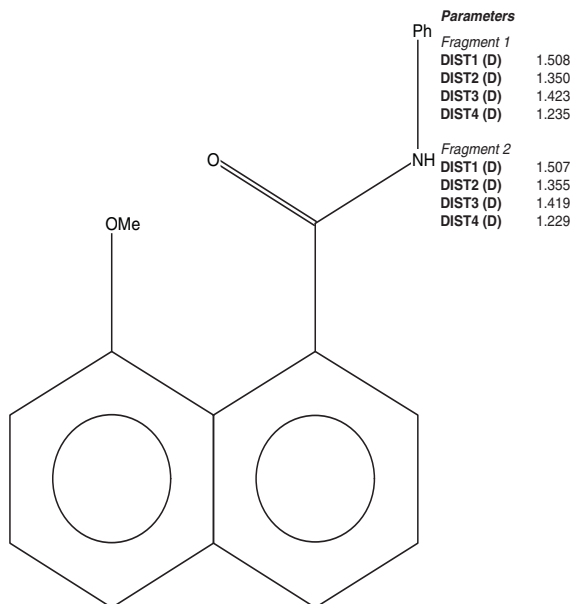
Reference: J.O'Leary, X.Formosa, W.Skranc, J.D.Wallis (2005)
Org.Biomol.Chem., 3,3273

Formula: C₁₈ H₁₅ N₁ O₂

Compound Name: 8-Methoxy-N-phenyl-1-naphthamide

Space Group: P21/n **Cell:** a 10.000(0) b 13.128(0) c 21.647(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.70(0) γ 90.00

R-Factor (%): 3.70 **Temperature(K):** 100 **Density(g/cm³):** 1.303



TAWROZ

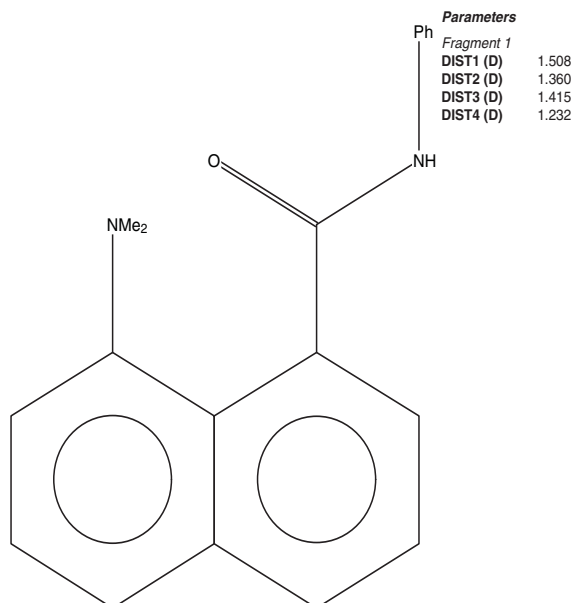
Reference: J.O'Leary, X.Formosa, W.Skranc, J.D.Wallis (2005)
Org.Biomol.Chem., 3,3273

Formula: C₁₉ H₁₈ N₂ O₁

Compound Name: 8-(Dimethylamino)-N-phenyl-1-naphthamide

Space Group: P21/c **Cell:** a 9.377(0) b 9.706(0) c 16.795(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 91.36(0) γ 90.00

R-Factor (%): 4.49 **Temperature(K):** 120 **Density(g/cm³):** 1.262



VACCOT

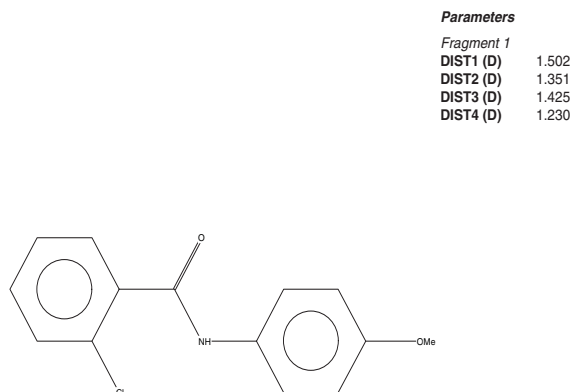
Reference: A.Saeed, J.Simpson (2010)
Acta Crystallogr., Sect.E:Struct.Rep.Online, 66,o2963

Formula: C₁₄ H₁₂ Cl₁ N₁ O₂

Compound Name: 2-Chloro-N-(4-methoxyphenyl)benzamide

Space Group: P21/n **Cell:** a 13.182(1) b 5.082(0) c 18.448(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 99.56(0) γ 90.00

R-Factor (%): 4.06 **Temperature(K):** 90 **Density(g/cm³):** 1.426



Search: search3 (Fri Nov 02 22:22:39 2012): Hits 29-32

WADCEL

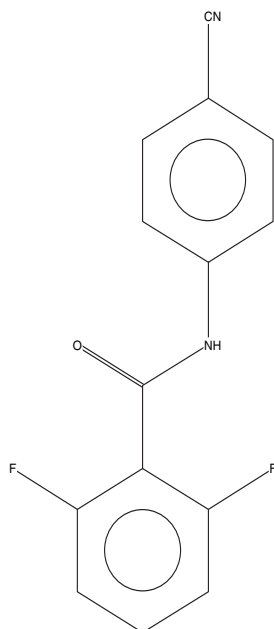
Reference: H.-K.Fun, J.H.Goh, J.Gowda, A.M.Khader, B.Kalluraya (2010) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **66**,o3192

Formula: C₁₄H₈F₂N₂O₁

Compound Name: N-(4-Cyanophenyl)-2,6-difluorobenzamide

Space Group: P2₁/c **Cell:** *a* 9.338(1) *b* 5.079(0) *c* 24.500(3)
Space Group No.: 14 **(Å, °)** *α* 90.00 *β* 100.20(0) *γ* 90.00

R-Factor (%): 4.26 **Temperature(K):** 100 **Density(g/cm³):** 1.500



Parameters

Fragment 1
DIST1 (D) 1.501
DIST2 (D) 1.357
DIST3 (D) 1.409
DIST4 (D) 1.225

WAWMAJ

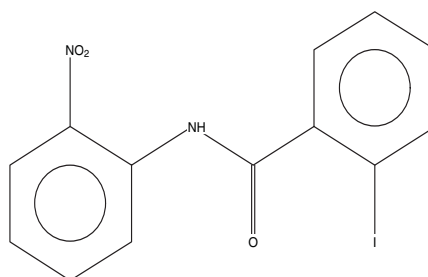
Reference: J.L.Wardell, J.M.S.Skakle, J.N.Low, C.Glidewell (2005) *Acta Crystallogr., Sect.C:Cryst.Struct.Commun.*, **61**,o634

Formula: C₁₃H₉I₁N₂O₃

Compound Name: N-(2-Nitrophenyl)-2-iodobenzamide

Space Group: P-1 **Cell:** *a* 7.277(0) *b* 7.621(0) *c* 11.682(0)
Space Group No.: 2 **(Å, °)** *α* 100.25(0) *β* 107.78(0) *γ* 92.53(0)

R-Factor (%): 1.84 **Temperature(K):** 120 **Density(g/cm³):** 2.025



Parameters

Fragment 1
DIST1 (D) 1.504
DIST2 (D) 1.379
DIST3 (D) 1.405
DIST4 (D) 1.219

WAWMEN

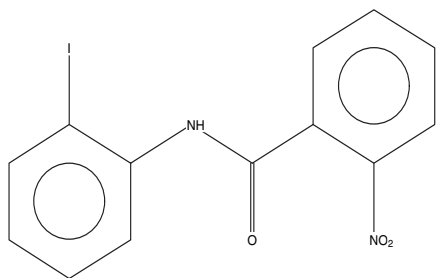
Reference: J.L.Wardell, J.M.S.Skakle, J.N.Low, C.Glidewell (2005) *Acta Crystallogr., Sect.C:Cryst.Struct.Commun.*, **61**,o634

Formula: C₁₃H₉I₁N₂O₃

Compound Name: N-(2-Iodophenyl)-2-nitrobenzamide

Space Group: P2₁12₁ **Cell:** *a* 8.891(0) *b* 9.747(0) *c* 15.011(0)
Space Group No.: 19 **(Å, °)** *α* 90.00 *β* 90.00 *γ* 90.00

R-Factor (%): 1.65 **Temperature(K):** 120 **Density(g/cm³):** 1.880



Parameters

Fragment 1
DIST1 (D) 1.504
DIST2 (D) 1.346
DIST3 (D) 1.419
DIST4 (D) 1.234

WOMWUR

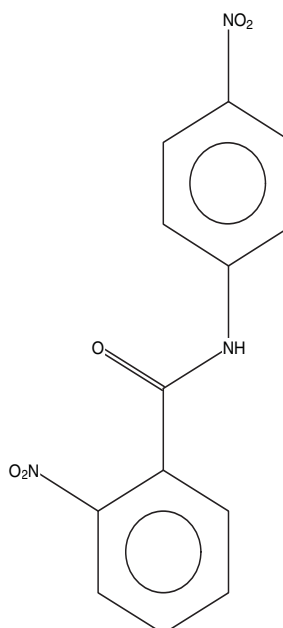
Reference: A.Saeed, S.Hussain, U.Florke (2008) *Turk.J.Chem.*, **32**, 481

Formula: C₁₃H₉N₃O₅

Compound Name: 2-Nitro-N-(4-nitrophenyl)benzamide

Space Group: P2₁12₁ **Cell:** *a* 8.944(1) *b* 9.715(1) *c* 13.802(1)
Space Group No.: 19 **(Å, °)** *α* 90.00 *β* 90.00 *γ* 90.00

R-Factor (%): 3.20 **Temperature(K):** 120 **Density(g/cm³):** 1.591



Parameters

Fragment 1
DIST1 (D) 1.512
DIST2 (D) 1.361
DIST3 (D) 1.409
DIST4 (D) 1.213

Search: search3 (Fri Nov 02 22:22:39 2012): Hits 33-35

YEGJID01

Reference: B.T.Gowda, S.Foro, B.P.Sowmya, H.Fuess (2008)
Acta Crystallogr., Sect.E:Struct.Rep.Online ,64,o383

Formula: C₁₄ H₁₃ N₁ O₁

Compound Name: 2-Methyl-N-phenylbenzamide

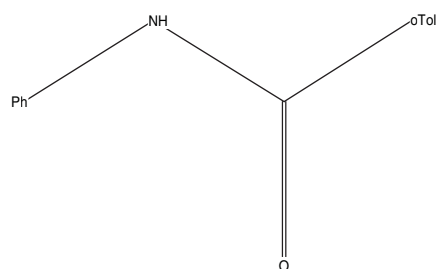
Space Group: Pbc_a **Cell:** *a* 14.404(1) *b* 8.682(0) *c* 18.710(1)
Space Group No.: 61 (*Å*, °) α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.78 **Temperature(K):** 100 **Density(g/cm³):** 1.199

Parameters

Fragment 1

DIST1 (D) 1.492
DIST2 (D) 1.352
DIST3 (D) 1.418
DIST4 (D) 1.237



YODMOU

Reference: B.T.Gowda, S.Foro, B.P.Sowmya, H.Fuess (2008)
Acta Crystallogr., Sect.E:Struct.Rep.Online ,64,o1605

Formula: C₁₆ H₁₇ N₁ O₁

Compound Name: N-(2,6-Dimethylphenyl)-2-methylbenzamide

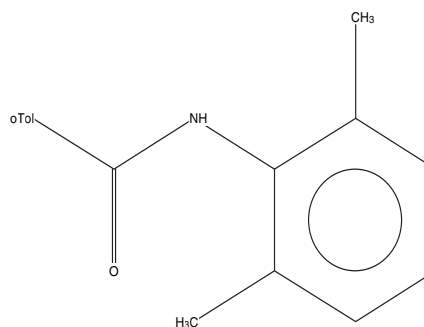
Space Group: Pbc_a **Cell:** *a* 11.687(1) *b* 10.019(0) *c* 22.108(2)
Space Group No.: 61 (*Å*, °) α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.65 **Temperature(K):** 100 **Density(g/cm³):** 1.228

Parameters

Fragment 1

DIST1 (D) 1.501
DIST2 (D) 1.350
DIST3 (D) 1.436
DIST4 (D) 1.232



YOVNED

Reference: A.Saeed, R.A.Khera, J.Simpson, R.G.Stanley (2009)
Acta Crystallogr., Sect.E:Struct.Rep.Online ,65,o1642

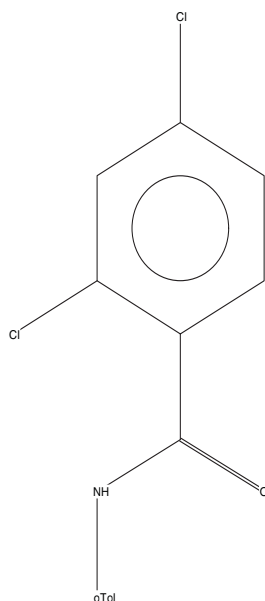
Formula: C₁₄ H₁₁ Cl₂ N₁ O₁

Compound Name: 2,4-Dichloro-N-(2-methylphenyl)benzamide

Synonym: 2,4-Dichloro-N-o-tolylbenzamide

Space Group: Cc **Cell:** *a* 22.517(4) *b* 6.041(0) *c* 9.633(1)
Space Group No.: 9 (*Å*, °) α 90.00 β 104.84(0) γ 90.00

R-Factor (%): 5.70 **Temperature(K):** 92 **Density(g/cm³):** 1.469



Parameters

Fragment 1

DIST1 (D) 1.505
DIST2 (D) 1.346
DIST3 (D) 1.431
DIST4 (D) 1.241