

Search Overview

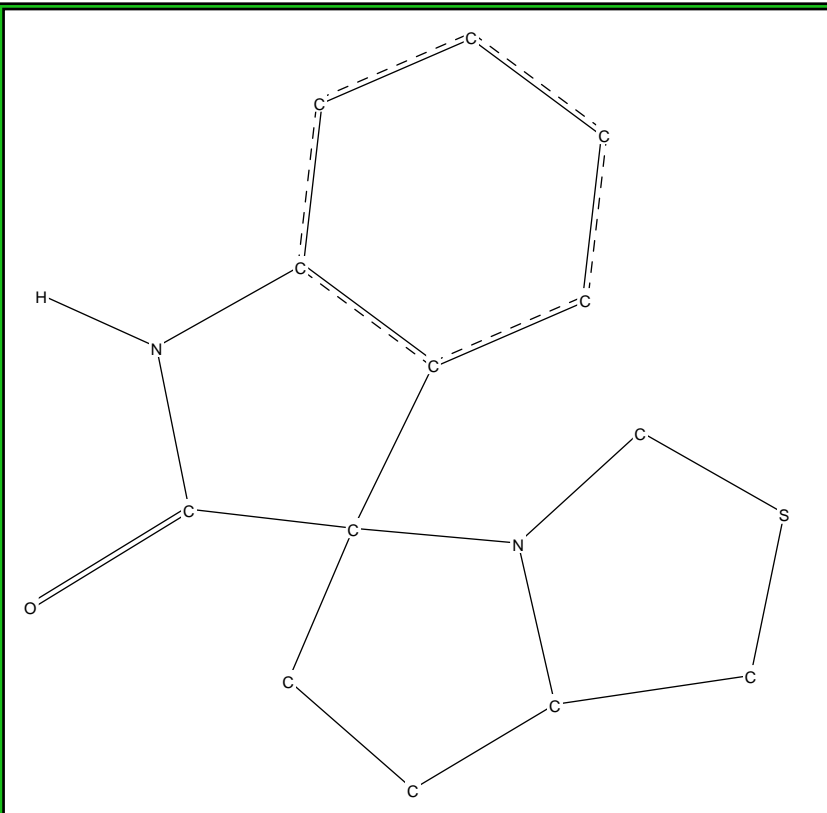
Search: search4
Date/Time done: Sat Dec 29 17:01:03 2018
Database(s): CSD version 5.39 updates (Nov 2017)
CSD version 5.39 (November 2017)
CSD version 5.39 (November 2017)
CSD version 5.39 updates (Feb 2018)
CSD version 5.39 updates (May 2018)
CSD version 5.39 updates (Aug 2018)
Restriction Info: No refcode restrictions applied
Filters: None
Percentage Completed: 100%
Number of Hits: 23

Single query used. Search found structures that:

match

Query 2

Query 2



AJIKEL

Reference:

C.Mhiri, S.Boudriga, M.Askri, M.Knorr, D.Sriram, P.Yogeeswari, F.Nana, C.Golz, C.Strohmam (2015) *Bioorg.Med.Chem.Lett.* ,**25**,4308

Formula:

C₂₆ H₁₈ Br₂ N₂ O₃ S₁

Compound Name:

5''-bromo-7''-(4-bromophenyl)-7',7a'-dihydro-1'H-dispiro[1-benzofuran-3,6'-pyrrolol[1,2-c][1,3]thiazole-5',3''-indole]-2,2''(1''H)-dione

Space Group:

P-1

Cell:

a 8.831(0) **b** 11.282(0) **c** 13.473(0)
α 68.87(0) **β** 72.34(0) **γ** 88.47(0)

Space Group No.:

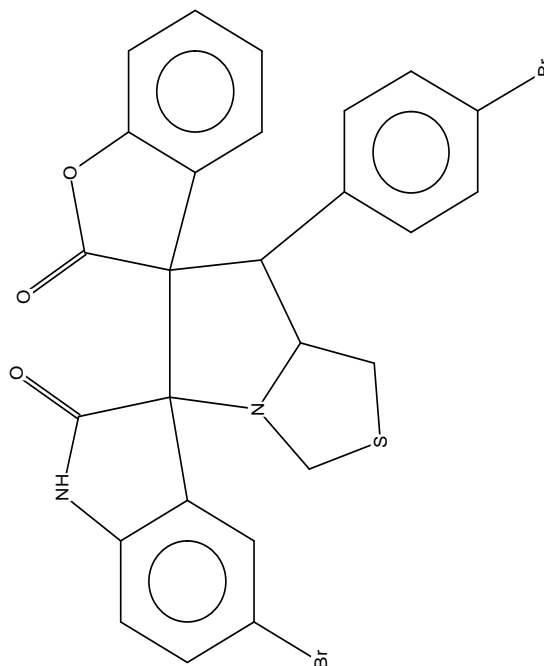
2

R-Factor (%): 3.40

Temperature(K): 173 **Density(g/cm³)**: 1.673

Parameters

Fragment 1
ANG1 (Å) 88.242



ALAREL

Reference:

S.U.Maheswari, K.Balamurugan, S.Perumal, P.Yogeeswari, D.Sriram (2010) *Bioorg.Med.Chem.Lett.* ,**20**,7278

Formula:

C₂₈ H₂₂ N₂ O₄ S₁

Compound Name:

7''-(4-Methoxyphenyl)-7',7a'-dihydro-1'H-dispiro[indene-2,6'-pyrrolol[1,2-c][1,3]thiazole-5',3''-indole]-1,2'',3''(1''H)-trione

Space Group:

P21/c

Cell:

a 9.596(1) **b** 10.279(1) **c** 24.202(4)
α 90.00 **β** 93.00(1) **γ** 90.00

Space Group No.:

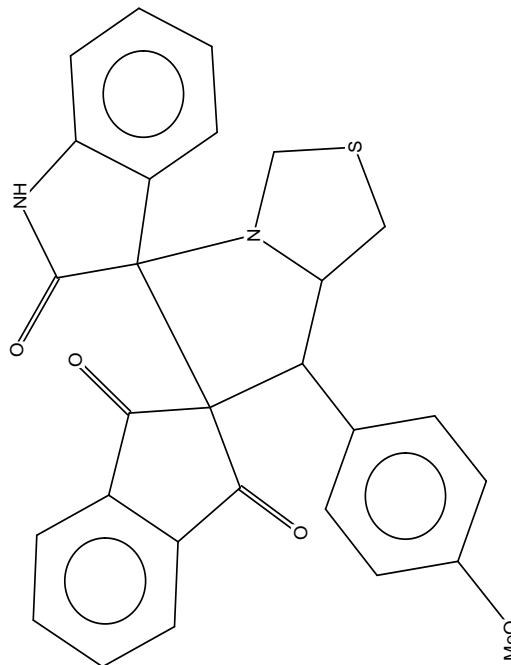
14

R-Factor (%): 5.29

Temperature(K): 293 **Density(g/cm³)**: 1.345

Parameters

Fragment 1
ANG1 (Å) 80.655



ALARIP

Reference: S.U.Maheswari, K.Balamurugan, S.Perumal, P.Yogeeswari, D.Sriram (2010) *Bioorg.Med.Chem.Lett.* ,**20**,7278

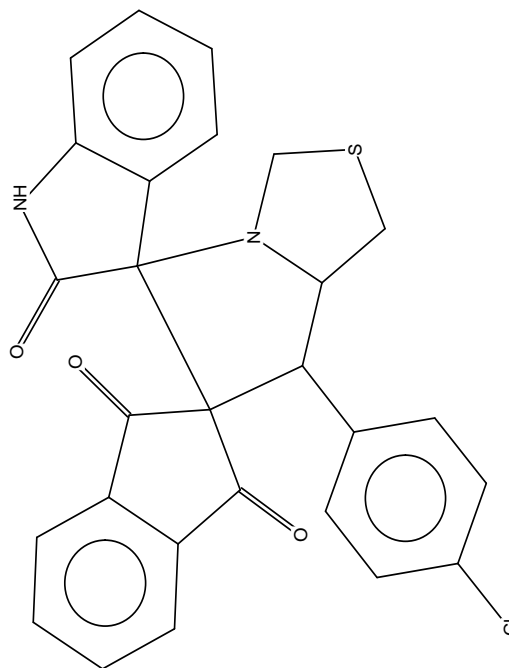
Formula: C₂₇ H₁₉ Cl₁ N₂ O₃ S₁

Compound Name: 7-(4-Chlorophenyl)-7',7a-dihydro-1'H-dispiro[indene-2,6'-pyrrolo[1,2-c][1,3]thiazole-5,3'-indole]-1,2',3'(1'H)-trione

Space Group: P2₁/c
Space Group No.: 14
R-Factor (%): 5.84
Cell: a 9.691(1) b 10.491(1) c 22.510(3)
(Å,°) α 90.00 β 93.46(1) γ 90.00
Temperature(K): 293 **Density(g/cm³):** 1.416

Parameters

Fragment 1
ANG1 (A) 81.939



BUGRAX

Reference: S.V.Karthikeyan, B.D.Bala, V.P.A.Raja, S.Perumal, P.Yogeeswari, D.Sriram (2010) *Bioorg.Med.Chem.Lett.* ,**20**,350

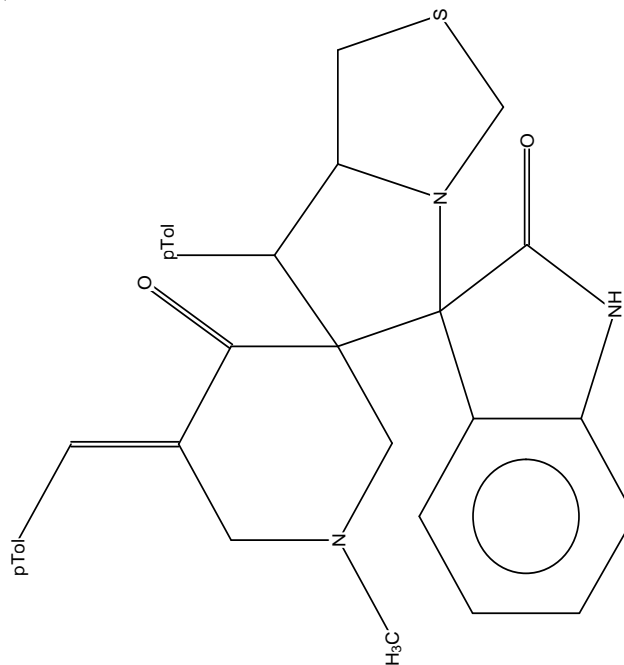
Formula: C₃₃ H₃₃ N₃ O₂ S₁

Compound Name: 1'-Methyl-5''-(4-methylbenzylidene)-7''-(4-methylphenyl)-7',7a-dihydro-1'H,4''H-dispiro[indole-3,5'-pyrrolo[1,2-c][1,3]thiazole-6,3''-piperidine]-2,4''(1H)-dione

Space Group: C2/c
Space Group No.: 15
R-Factor (%): 4.60
Cell: a 13.736 b 13.038 c 31.967
(Å,°) α 90.00 β 97.82 γ 90.00
Temperature(K): 293 **Density(g/cm³):** 1.255

Parameters

Fragment 1
ANG1 (A) 84.430



BUGREB

Reference: S.V.Karthikeyan, B.D.Bala, V.P.A.Raja, S.Perumal, P.Yogeeswari, D.Sriram (2010) *Bioorg.Med.Chem.Lett.* , **20**,350

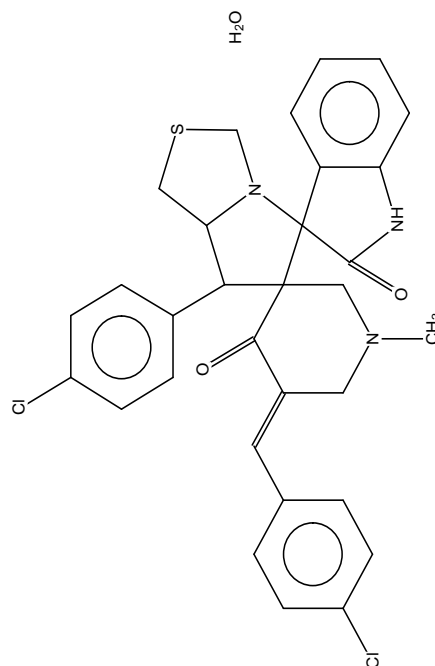
Formula: C₃₁ H₂₇ Cl₂ N₃ O₂ S₁ H₂ O₁

Compound Name: 5'-[(4-Chlorobenzylidene)-7-(4-chlorophenyl)-1'-methyl-7',7a'-dihydro-1'H,4''H-dispiro[indole-3,5'-pyrrolo[1,2-c][1,3]thiazole-6',3'-piperidine]-2,4''(1H)-dione monohydrate

Space Group: P2₁/c
Space Group No.: 14
R-Factor (%): 5.67
Cell: a 11.136(5) b 16.186(5) c 16.566(5)
 α 90.00 β 95.14(0) γ 90.00
Temperature(K): 293 **Density(g/cm³):** 1.328

Parameters

Fragment 1
ANG1 (A) 86.125



EMOKIC

Reference: R.S.Kumar, A.I.Almansour, N.Arumugam, S.M.Soliman, R.R.Kumar, H.A.Ghabbour (2016) *J.Mol.Struct.* , **1121**,93

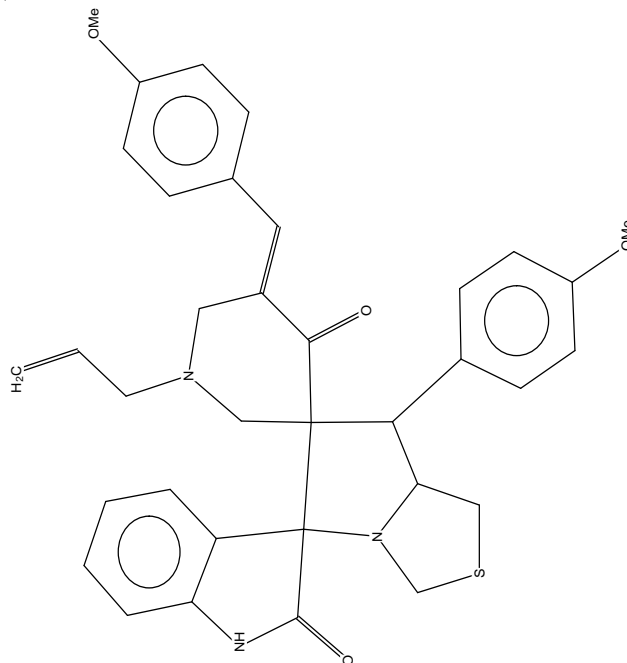
Formula: C₃₅ H₃₅ N₃ O₄ S₁

Compound Name: 1''-allyl-5''-(4-methoxybenzylidene)-7''-(4-methoxyphenyl)-7',7a''-dihydro-1'H,4''H-dispiro[indole-3,5'-pyrrolo[1,2-c][1,3]thiazole-6',3'-piperidine]-2,4''(1H)-dione

Space Group: P2₁/c
Space Group No.: 14
R-Factor (%): 5.27
Cell: a 11.618(0) b 12.247(0) c 21.706(0)
 α 90.00 β 103.02(0) γ 90.00
Temperature(K): 100 **Density(g/cm³):** 1.311

Parameters

Fragment 1
ANG1 (A) 82.528



EMONEA

Reference: P.Prasanna, K.Balamurugan, S.Perumal, P.Yogeeswari, D.Sriram (2010) *Eur.J.Med.Chem.* ,**45**,5653

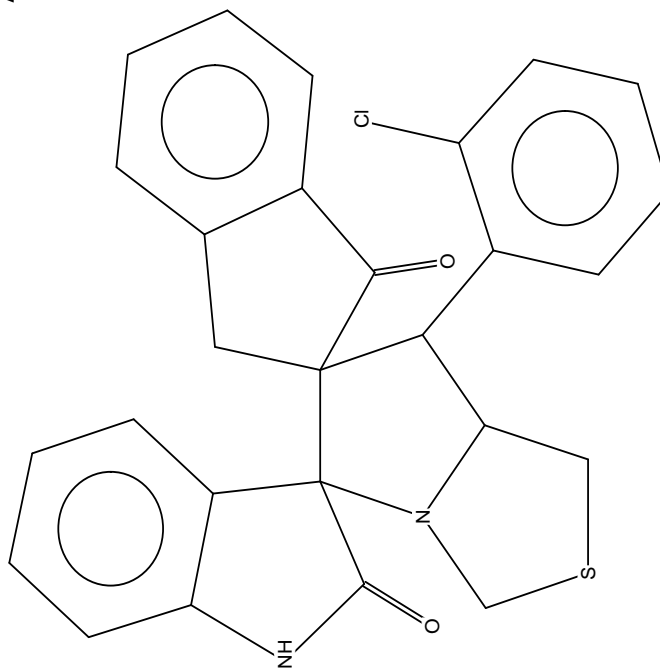
Formula: C₂₇ H₂₁ Cl₁ N₂ O₂ S₁

Compound Name: 7'-(2-Chlorophenyl)-7',7a'-dihydro-1'H-dispiro[indene-2,6'-pyrrolo[1,2-c][1,3]thiazole-5',3''-indole]-1,2'-(1''H,3H)-dione

Space Group: Pbc_a **Cell:** **a** 17.148(1) **b** 14.681(0) **c** 18.777(1)
Space Group No.: 61 **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 3.78 **Temperature(K):** 273 **Density(g/cm³):** 1.329

Parameters

Fragment 1
ANG1 (A) 87.232



FOGXUV

Reference: S.Salvanayagam, J.Paul, D.Velmurugan, K.Ravikumar, R.R.Durga, R.Raghunathan (2005) *Acta Crystallogr., Sect.E:Struct.Rep.Online* ,**61**,o1585

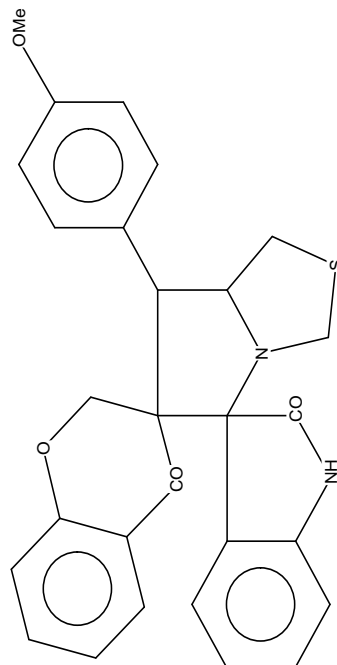
Formula: C₂₈ H₂₄ N₂ O₄ S₁

Compound Name: 7'-(4-Methoxyphenyl)-chroman-3-spiro-6'-hexahydro-1H-pyrrolo(1,2-c)thiazole-5'-spiro-3''-1''H-indole-4,2''(3''H)-dione

Space Group: P2₁/c **Cell:** **a** 9.556(0) **b** 16.104(1) **c** 15.263(1)
Space Group No.: 14 **α** 90.00 **β** 91.21(1) **γ** 90.00
R-Factor (%): 4.70 **Temperature(K):** 273 **Density(g/cm³):** 1.371

Parameters

Fragment 1
ANG1 (A) 84.068



FOWLAG

Reference: S.Haddad, S.Boudriga, F.Porzio, A.Soldera, M.Askri, D.Sriram, P.Yogeeswari, M.Knorr, Y.Rousselin, M.M.Kubicki (2014) *RSC Advances*, **4**,59462

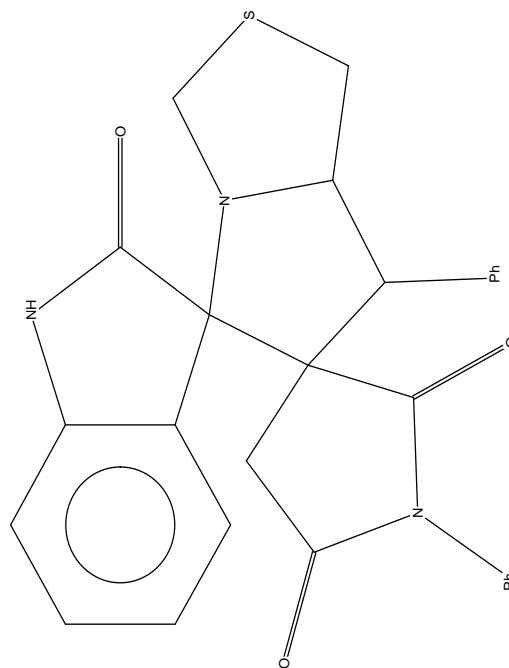
Formula: C₂₈ H₂₃ N₃ O₃ S₁

Compound Name: 1''',7''-diphenyl-7',7a'-dihydro-1'H,2''H,5''H-dispiro[indole-3,5'-pyrrolo[1,2-c][1,3]thiazole-6',3''-pyrrolidine]2,2'',5''(1H)-trione

Space Group: P-1
Space Group No.: 2
R-Factor (%): 3.36
Temperature(K): 115
Density(g/cm³): 1.378

Parameters

Fragment 1
ANG1 (A) 78.746



GITDOD

Reference: S.Sundaramoorthy, D.Gayathri, D.Velmurugan, M.Poornachandran, K.Ravikumar (2008) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **64**,o488

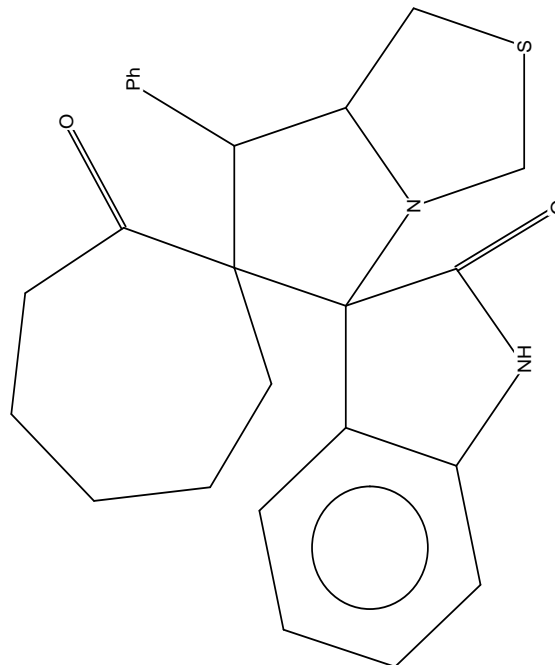
Formula: C₂₅ H₂₆ N₂ O₂ S₁

Compound Name: 1'-Phenyl-6'-thiacycloheptane-1-spiro-2'-perhydropyrrolizine-3'-spiro-3''-indoline-2,2''-dione

Space Group: P-1
Space Group No.: 2
R-Factor (%): 6.23
Temperature(K): 293
Density(g/cm³): 1.337

Parameters

Fragment 1
ANG1 (A) 77.600



GUCHET

Reference: Jie Li, Jing Wang, Zhou Xu, Songlei Zhu (2014)
ACS Comb. Sci., **16**, 506

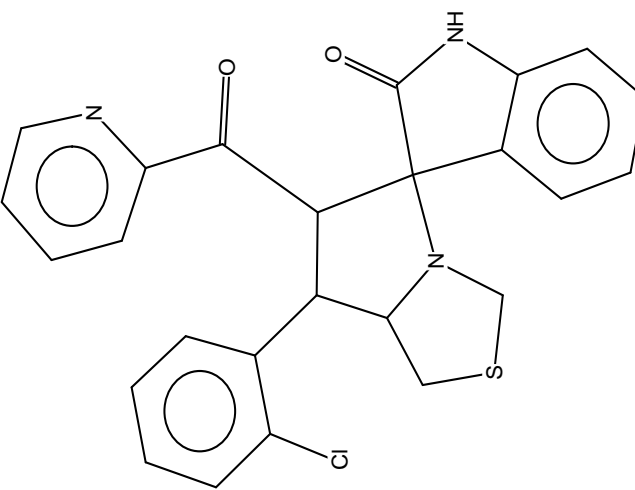
Formula: C₂₅ H₂₀ Cl₁ N₃ O₂ S₁, C₂ H₆ O₁

Compound Name: 7-(2-Chlorophenyl)-6-(pyridin-2-ylcarbonyl)-1',6',7',7a'-tetrahydrospiro[indole-3,5'-pyrrolo[1,2-c][1,3]thiazol]-2(1H)-one ethanol solvate

Space Group: P2₁/n **Cell:** **a** 11.552(0) **b** 16.654(0) **c** 13.774(0)

Space Group No.: 14 **α** 90.00 **β** 106.45(0) **γ** 90.00

R-Factor (%): 7.74 **Temperature(K):** 293 **Density(g/cm³):** 1.328



Parameters
Fragment 1
ANG1 (A) 79.942

Et—OH

JAWTOT

Reference: Mani Anusha Rani, S.V.Kumar, K.Malathi, M.Muthu, A.I.Almansour, R.S.Kumar, R.R.Kumar (2017) ACS Comb. Sci., **19**, 308

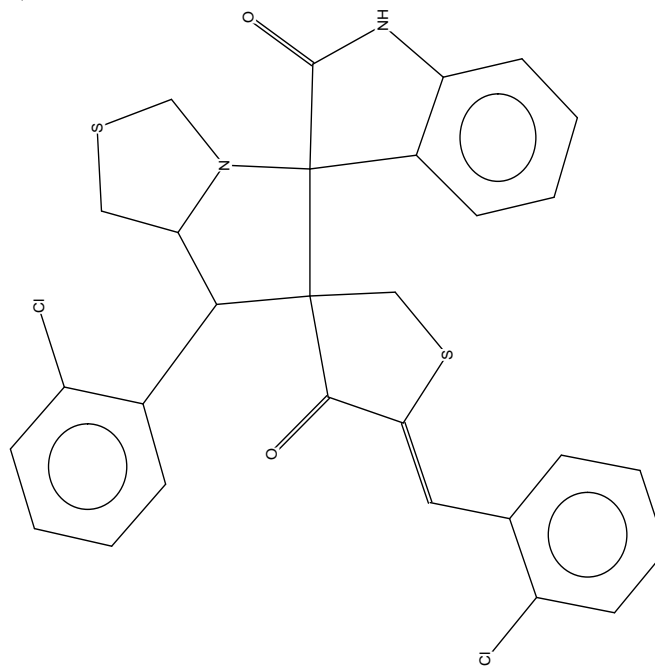
Formula: C₂₉ H₂₂ Cl₂ N₂ O₂ S₂

Compound Name: (Z)-5''-(2-Chlorobenzylidene)-7-(2-chlorophenyl)-7',7a'-dihydro-1'H,2''H,3''H-dispiro[indoline-3,5'-pyrrolo[1,2-c]thiazole-6,3''-thiophene]-2,4''-dione

Space Group: P2₁/c **Cell:** **a** 10.409(0) **b** 11.041(0) **c** 23.459(1)

Space Group No.: 14 **α** 90.00 **β** 93.02(0) **γ** 90.00

R-Factor (%): 5.14 **Temperature(K):** 293 **Density(g/cm³):** 1.395



Parameters
Fragment 1
ANG1 (A) 87.247

MUDLAA

Reference: S.Kanchithalaivan, Mani Anusha Rani, R.R.Kumar (2014) *Synth. Commun.* **44**,3122

Formula: C₃₈ H₄₆ N₂ O₃ S₁

Compound Name: 3-hydroxy-10,13-dimethyl-7-(4-methylphenyl)-1,3,4,5,6,7,7a,8,9,10,11,12,13,14,15-hexadecahydro-1H-dispiro[cyclopenta[a]phenanthrene-16,6'-pyrrolo[1,2-c][1,3]thiazole-5',3''-indole]-2',17'(1''H,2H)-dione

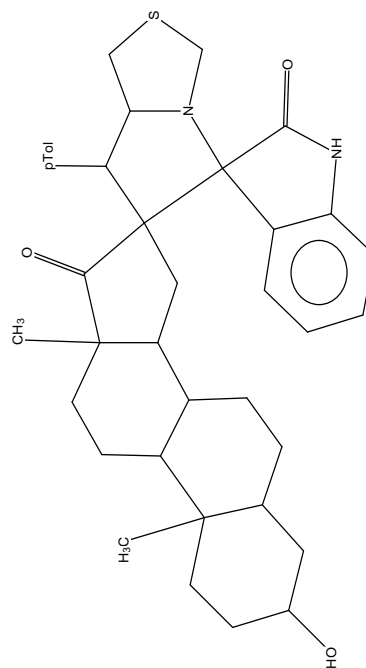
Synonym: (16R,5'R,7'R,7a'R)-spiro[5':3']oxindole-spiro[6:16]-7-(4-methylphenyl)-tetrahydro-1H-pyrrolo[1,2-c][1,3]thiazolo-trans-dehydroandrosterone

Space Group: C2
Space Group No.: 5
Cell: **a** 22.689(0) **b** 12.825(0) **c** 11.431(0)
(Å, °) **α** 90.00 **β** 99.73(0) **γ** 90.00

R-Factor (%): 4.99 **Temperature(K):** 293 **Density(g/cm³):** 1.238

Parameters

Fragment 1
ANG1 (A) 89.712



NUHHIJ

Reference: S.Suhitha, T.Srinivasan, R.Prasanna, K.Gunasekaran, R.Raghunathan, D.Velmurugan (2013) *Int.J.Chem Tech. Res.* **5**,2793

Formula: C₃₀ H₃₄ N₂ O₇ S₁

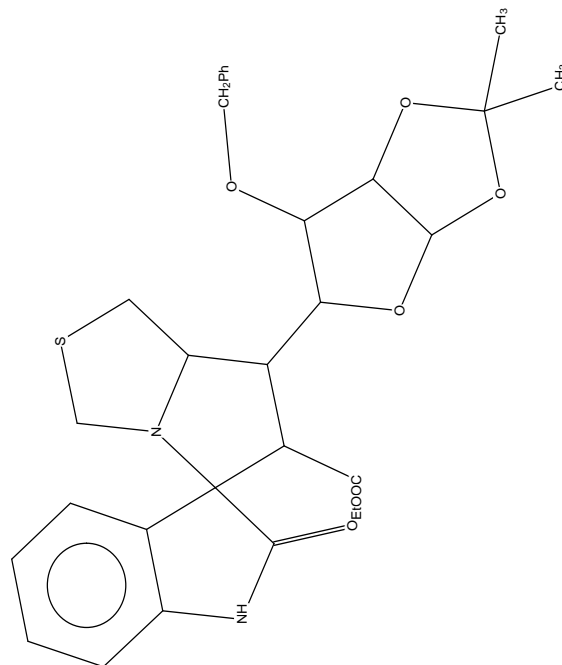
Compound Name: ethyl 7-(6-(benzyl(oxy)-2,2-dimethyltetrahydrofuro[2,3-c][1,3]dioxol-5-yl)-2-oxo-1,1,2,6,7,7a-hexahydrospiro[indole-3,5'-pyrrolo[1,2-c][1,3]thiazole]-6'-carboxylate

Space Group: P212121
Space Group No.: 19
Cell: **a** 9.378(0) **b** 12.622(0) **c** 23.992(1)
(Å, °) **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 4.56 **Temperature(K):** 293 **Density(g/cm³):** 1.325

Parameters

Fragment 1
ANG1 (A) 87.785



QEXMEM

Reference: D.Gayathri, S.Kalyani, D.Velmurugan, K.Ravikumar, M.Poornachandran (2007) *Acta Crystallogr., Sect.E: Struct. Rep. Online*, **63**,o852

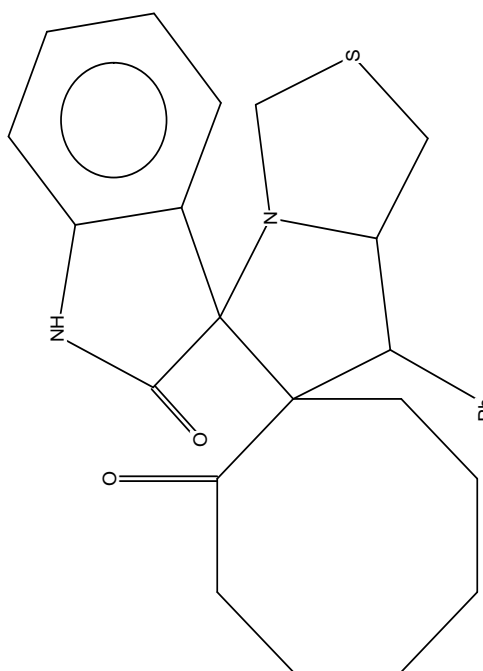
Formula: C₂₆ H₂₈ N₂ O₂ S₁

Compound Name: 7-Phenyl-cyclooctane-1-spiro-6'-2-thiapyrrolizidine-5'-spiro-3''-indole-2, 2''(3H)-dione

Space Group: P-1 **Cell:** **a** 9.090(0) **b** 10.501(0) **c** 12.751(0)
Space Group No.: 2 **α** 79.87(0) **β** 71.50(0) **γ** 68.57(0)
R-Factor (%): 4.65 **Temperature(K)**: 293 **Density(g/cm³)**: 1.340

Parameters

Fragment 1
ANG1 (Å) 78.252



QUBVEQ

Reference: M.P.Savithri, M.Suresh, R.Raghunathan, R.Raja, A.SubbiahPandi (2015) *Acta Crystallogr., Sect.E: Cryst. Commun.*, **71**, o148

Formula: C₂₃ H₂₀ N₂ O₄ S₂

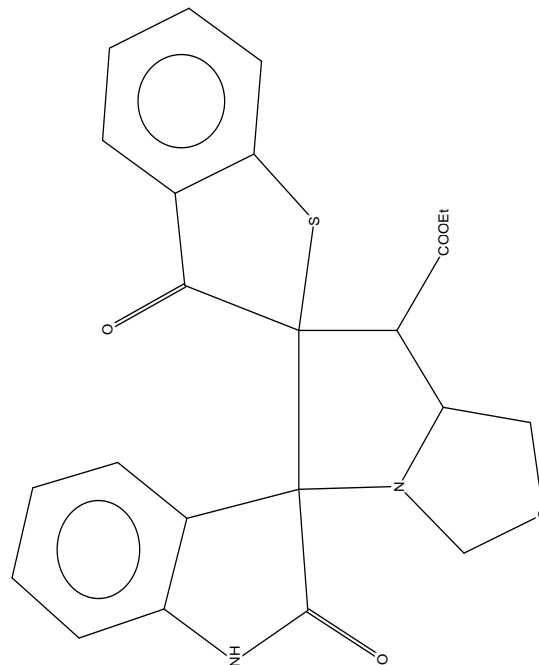
Compound Name: Ethyl 2'',3-dioxo-1'',2'',7'',7a'-tetrahydro-1'H,3'H-dispiro[1-benzothiophene-2,6'-pyrrolo[1,2-c][1,3]thiazole-5',3''-indole]-7'-carboxylate

Synonym: Ethyl 2'',3-dioxo-7'',7a'-dihydro-1'H,3'H,3'H-dispiro[benzo[b]thiophene-2,6'-pyrrolo[1,2-c]thiazole-5',3''-indoline]-7'-carboxylate

Space Group: P21/c **Cell:** **a** 11.889(0) **b** 10.218(0) **c** 17.504(0)
Space Group No.: 14 **α** 90.00 **β** 97.99(0) **γ** 90.00
R-Factor (%): 3.19 **Temperature(K)**: 293 **Density(g/cm³)**: 1.427

Parameters

Fragment 1
ANG1 (Å) 81.985



RAGMUK

Reference: G.Lofly, M.M.Said, E.I.S.H.El Ashry, E.I.S.H.El Tamany, A.Al-Dhfyhan, Y.M.A.Aziz, A.Barakat (2017) *Bioorg.Med.Chem.* ,**25**,1514

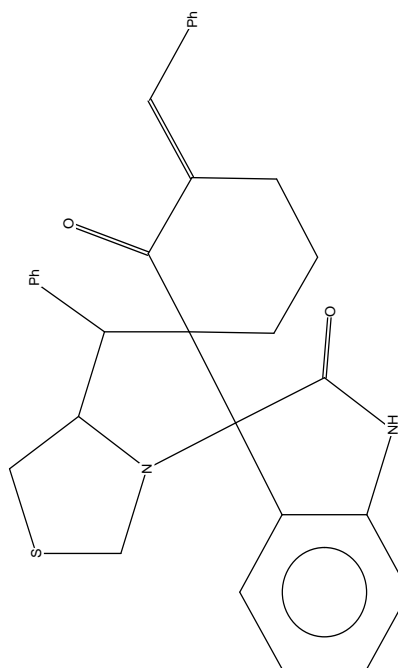
Formula: C₃₁ H₂₈ N₂ O₂ S₁

Compound Name: (1R,5R)-3-benzylidene-7-phenyl-7',7a'-dihydro-1'H,2H-dispiro[cyclohexane-1,6'-pyrrolo[1,2-c][1,3]thiazole-5',3'-indole]-2,2'-(1''H)-dione

Space Group: P-1
Space Group No.: 2
R-Factor (%): 5.59
Cell: (Å, °) a 7.772(0) b 10.508(0) c 15.496(0)
 α 97.10(0) β 100.91(0) γ 97.84(0)
Temperature(K): 100
Density(g/cm³): 1.345

Parameters

Fragment 1
ANG1 (Å) 83.636



RAGNAR

Reference: G.Lofly, M.M.Said, E.I.S.H.El Ashry, E.I.S.H.El Tamany, A.Al-Dhfyhan, Y.M.A.Aziz, A.Barakat (2017) *Bioorg.Med.Chem.* ,**25**,1514

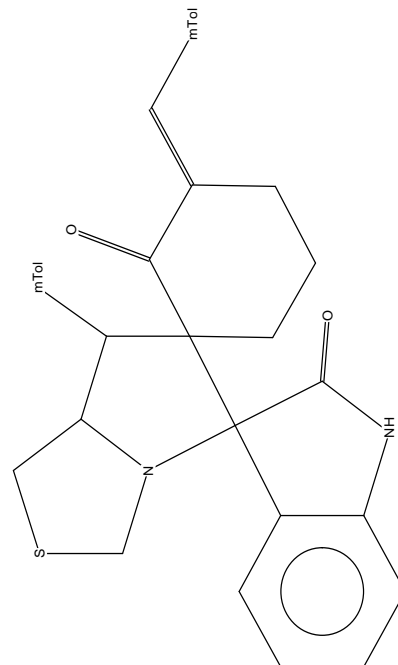
Formula: C₃₃ H₃₂ N₂ O₂ S₁

Compound Name: (1R,5R)-3-(3-methylbenzylidene)-7-(3-methylphenyl)-7',7a'-dihydro-1'H,2H-dispiro[cyclohexane-1,6'-pyrrolo[1,2-c][1,3]thiazole-5',3'-indole]-2,2'-(1''H)-dione

Space Group: P-1
Space Group No.: 2
R-Factor (%): 10.79
Cell: (Å, °) a 7.662(1) b 10.634(3) c 16.593(4)
 α 93.93(0) β 98.07(0) γ 91.40(0)
Temperature(K): 100
Density(g/cm³): 1.296

Parameters

Fragment 1
ANG1 (Å) 82.989



RAHBIO

Reference: G.Lofly, M.M.Said, E.I.S.H.El Ashry, E.I.S.H.El Tamany, A.Al-Dhfyar, Y.M.A.Aziz, A.Barakat (2017) *Bioorg.Med.Chem.* , **25**,1514

Formula: C₂₇ H₂₄ N₂ O₂ S₃

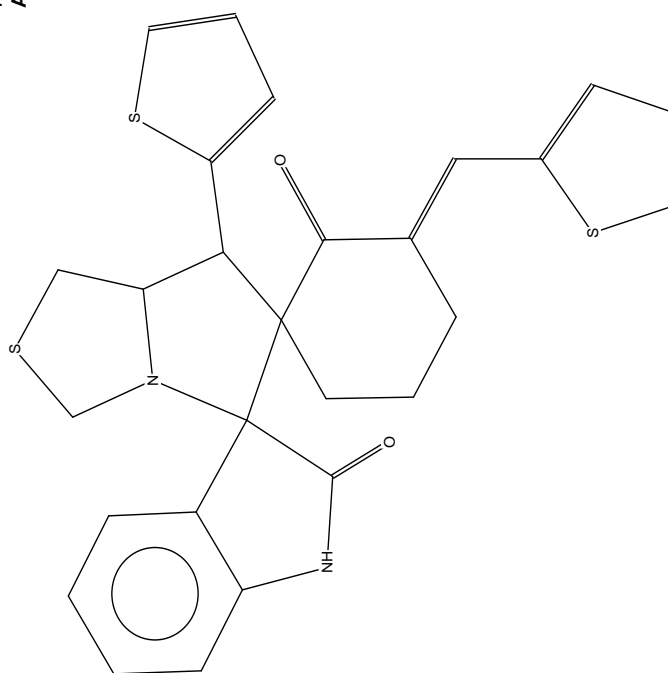
Compound Name: (1R,5'R,E)-7-(2-thienyl)-3-(2-thienylmethylene)-7,7a-dihydro-1'H,2'H-dispiro[cyclohexane-1,6'-pyrrolo[1,2-c][1,3]thiazole-5',3'-indole]-2,2'-(1''H)-dione

Space Group: P-1 **Cell:** **a** 7.828(1) **b** 10.445(1) **c** 15.031(2)
Space Group No.: 2 **α** 96.63(0) **β** 100.78(0) **γ** 99.81(0)

R-Factor (%): 8.27 **Temperature(K):** 100 **Density(g/cm³):** 1.425

Parameters

Fragment 1
ANG1 (A) 83.594



SUWNEE

Reference: R.Prasanna, S.Purushothaman, R.Raghunathan (2010) *Tetrahedron Lett.* , **51**,4538

Formula: C₂₇ H₃₄ N₂ O₈ S₁ H₂ O₁

Compound Name: Ethyl 2-oxo-7-(2,2,7,7-tetramethyltetrahydro-3aH-bis[1,3]dioxolo[4,5-b:4',5'-d]pyran-5-yl)-1,2,6',7',7a-hexahydrospiro[indole-3,5'-pyrrolo[1,2-c][1,3]thiazole]-6'-carboxylate monohydrate

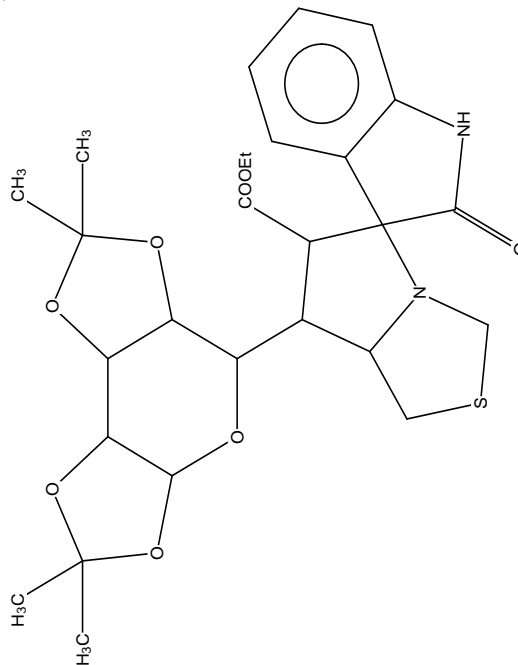
Synonym: 1,2,3,4-disopropylidene-5-C[spiro[2',3']oxindolo-3'-ethoxycarbonyl-thiapyrrolizidine]-D-galactopyranose monohydrate

Space Group: P212121 **Cell:** **a** 9.098(2) **b** 9.853(3) **c** 30.855(8)
Space Group No.: 19 **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 6.38 **Temperature(K):** 293 **Density(g/cm³):** 1.356

Parameters

Fragment 1
ANG1 (A) 84.475



H₂O

TEJRUW

Reference:

A.Subbiahpanidi, D.Velmurugan, K.Ravikumar, E.Ramesh, R.Raghunathan (2006) *Acta Crystallogr., Sect.E:Struct.Rep. Online* **62**, o2259

Formula:

C₃₇ H₃₂ N₂ O₂ S₁

Compound Name:

3-Benzylidene-3',7'-diphenylcyclohexanespiro-6'-(perhydro-2-thiapyrrolizine)-5'-spiro-3''-(1H-indole)-2,2''-dione

Space Group:

P2₁/c

Cell: a 10.031(0) b 20.860(1) c 14.131(0)

Space Group No.:

14

α 90.00 β 100.97(0) γ 90.00

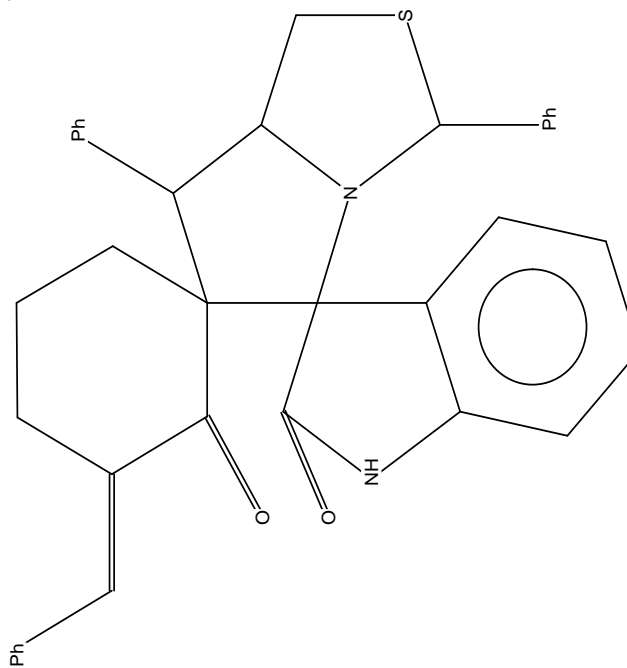
R-Factor (%):

5.14

Temperature(K): 293 Density(g/cm³): 1.301

Parameters

Fragment 1
ANG1 (Å) 81.015



XEVGIQ

Reference:

A.Kumar, G.Gupta, S.Srivastava, A.K.Bishnoi, R.Saxena, R.Kant, R.S.Khanna, P.R.Maulik, A.Dwivedi (2013) *RSC Advances* **3**, 4731

Formula:

C₃₂ H₂₅ Cl₁ N₂ O₂ S₁

Compound Name:

6'-Benzoyl-7'-(4-chlorophenyl)-3'-phenyl-1',6',7',7a'-tetrahydrospiro[indole-3,5'-pyrrolo[1,2-c][1,3]thiazol]-2(1H)-one

Space Group:

P2₁/c

Cell: a 10.428(5) b 16.883(5) c 17.610(5)

Space Group No.:

14

α 90.00 β 119.48(1) γ 90.00

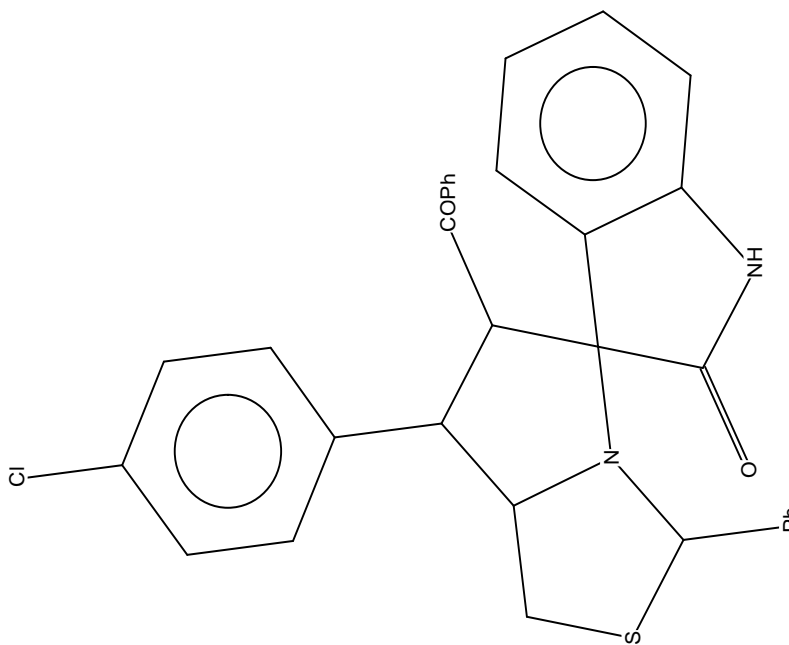
R-Factor (%):

7.04

Temperature(K): 293 Density(g/cm³): 1.322

Parameters

Fragment 1
ANG1 (Å) 81.438



XIJQUE

Reference: A.A.Shvets, Yu.V.Nelyubina, K.A.Lyssenko, S.V.Kurbatov (2012) *Izv.Akad.Nauk SSSR, Ser. Khim.* (Russ.) (*Russ. Chem. Bull.*), 1642

Formula: C₂₅ H₂₀ N₄ O₃ S₃

Compound Name: 3''-(2-Furylmethyl)-7''-(pyridin-3-yl)-2''-thioxo-7',7a'-dihydro-1'H,4''H-dispiro[indole-3,5'-pyrrolo[1,2-c][1,3]thiazole-6',5''-[1,3]thiazolidine]-2,4''(1H)-dione

Space Group: P2₁/c **Cell:** **a** 12.960(0) **b** 17.871(1) **c** 10.060(0)
Space Group No.: 14 **α** 90.00 **β** 95.04(0) **γ** 90.00
R-Factor (%): 4.84 **Temperature(K):** 120 **Density(g/cm³):** 1.490

Parameters

Fragment 1
ANG1 (Å) 88.254

