

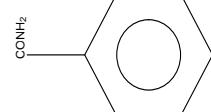
EMINUJ

Reference:

A.Bulut, O.Z.Yesil, N.Dagci, H.Icibulak, H.Omerz, S.B.7727
2(C₁₀H₁₄N₂O₁)^{1/2}C₆O₃⁻²⁻
Dinicotinimide squarate

Compound Name:

P21/c
Space Group No.: 14
Cell:
(*A*,*a*)
 α : 90.00
 β : 108.82(1)
 γ : 90.00
R-Factor (%): 4.00
Temperature(K): 293
Density(g/cm³): 1.548



Reference:

M.A.Soleimani, F.A.Maunert, T.C.W.Mak, W.W.K.Wu, P.T.Toussaint (2005) *J. Infrared, Spectrosc. Crys. Struct. Commun.*, **134**, 15-19

Formula:

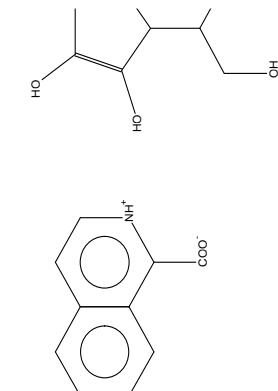
C₁₀H₁₄N₂O₂C₆H₅O₈

Compound Name:

1,5-diquinolinium-6,8-dicarboxylic acid Lasalocid acid

Space Group:

P21212
Space Group No.: 18
Cell:
(*A*,*a*)
 α : 90.00
 β : 90.00
 γ : 90.00
R-Factor (%): 4.22
Temperature(K): 293
Density(g/cm³): 1.1



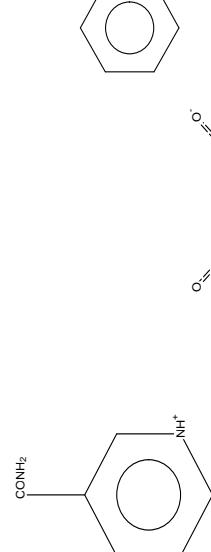
ERAVAU

Reference:

A.Bulut, O.Z.Yesil, N.Dagci, H.Icibulak, H.Omerz, S.B.7727
2(C₁₀H₁₄N₂O₁)^{1/2}C₆O₃⁻²⁻
Dinicotinimide squarate

Compound Name:

P21/c
Space Group No.: 14
Cell:
(*A*,*a*)
 α : 90.00
 β : 108.82(1)
 γ : 90.00
R-Factor (%): 4.00
Temperature(K): 293
Density(g/cm³): 1.548



Reference:

M.A.Soleimani, F.A.Maunert, T.C.W.Mak, W.W.K.Wu, P.T.Toussaint (2005) *J. Infrared, Spectrosc. Crys. Struct. Commun.*, **134**, 15-19

Formula:

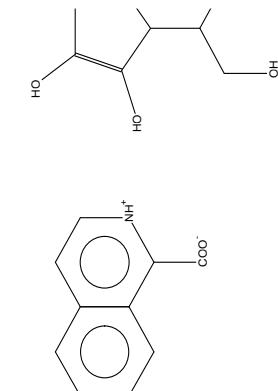
C₁₀H₁₄N₂O₂C₆H₅O₈

Compound Name:

1,5-diquinolinium-6,8-dicarboxylic acid Lasalocid acid

Space Group:

P21212
Space Group No.: 18
Cell:
(*A*,*a*)
 α : 90.00
 β : 90.00
 γ : 90.00
R-Factor (%): 4.22
Temperature(K): 293
Density(g/cm³): 1.1



FAjSOY

Reference:

F.H.Herbststein, D.Ashkenazi, M.Kaltori, M.Kapton, S.S.42,575
Dithia[4.3.3]propylene diisulfide monohydrate

Compound Name:

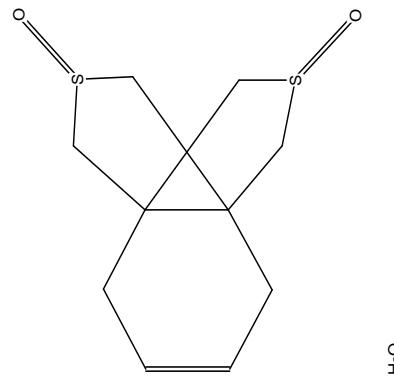
Dithia[4.3.3]propylene diisulfide monohydrate

Formula:

C₁₀H₁₄O₂S₂H₂O₁

Space Group:

P212121
Space Group No.: 19
Cell:
(*A*,*a*)
 α : 90.00
 β : 90.00
 γ : 90.00
R-Factor (%): 4.80
Temperature(K): 295
Density(g/cm³): 1.443



GEBMJ

Reference:

K.Fridenvang, L.Gronborg, B.Jensen (1988) *Acta Crystallogr., Sect.C/Crys. Struct. Commun.*, **44**, 841
Methoxytrichloro picate hemihydrate

Compound Name:

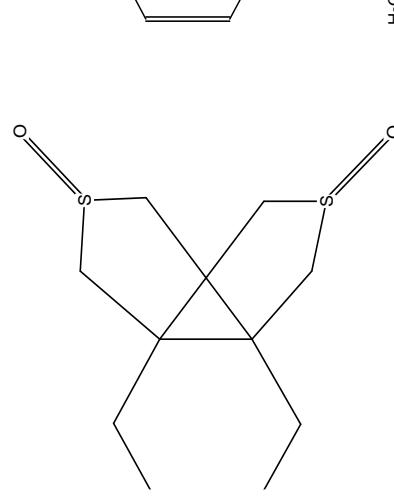
1,3,5-tris(4-methoxy-1-methylphenyl)benzene 2,5-dimethylhex-3-yn-2,5-diol

Formula:

C₂₄H₂₄O₅C₆H₅O₂

Space Group:

P21n
Space Group No.: 13
Cell:
(*A*,*a*)
 α : 90.00
 β : 106.74(2)
 γ : 90.00
R-Factor (%): 4.40
Temperature(K): 295
Density(g/cm³): 1.125



GATCAG

Reference:

Hong-Yan Chen, Tong-Li Zhang, Jian-Guo Zhang (2005) *Juguo HuaXueZhi/Chinese J. Struct.Chem.*, **24**, 473
(S)-(+)Mandelic acid

Compound Name:

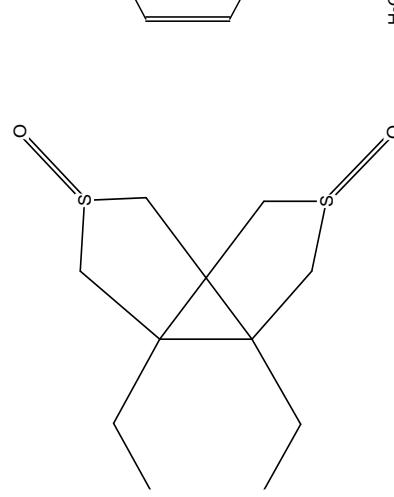
semicarbazide nitrophthalimidone dihydrate

Formula:

C₁₀H₁₂N₂O₄·2H₂O

Space Group:

P-1
Space Group No.: 2
Cell:
(*A*,*a*)
 α : 67.46(5)
 β : 77.36(9)
 γ : 76.94
R-Factor (%): 3.94
Temperature(K): 293
Density(g/cm³): 1.1



COOH

Reference:

A.O.Pati, W.T.Bennington, I.C.Paul, D.V.Cuthill, G.E.Dikarya (1987) *J. Am. Chem. Soc.*, **109**, 1529

Compound Name:

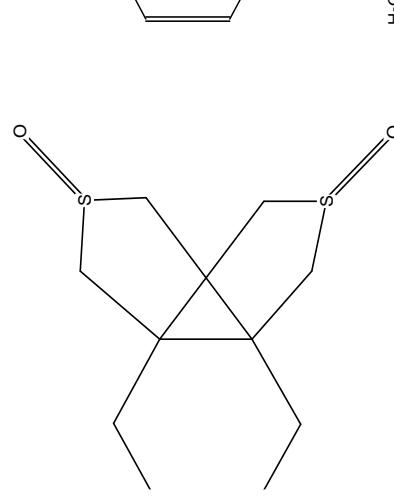
(S)-(+)Mandelic acid

Formula:

C₉H₈O₃

Space Group:

P-1
Space Group No.: 2
Cell:
(*A*,*a*)
 α : 70.27(1)
 β : 90.00
 γ : 95.18(2)



HO

Reference:

F.H.Herbststein, D.Ashkenazi, M.Kaltori, M.Kapton, S.S.42,575
Dithia[4.3.3]propylene diisulfide monohydrate

Compound Name:

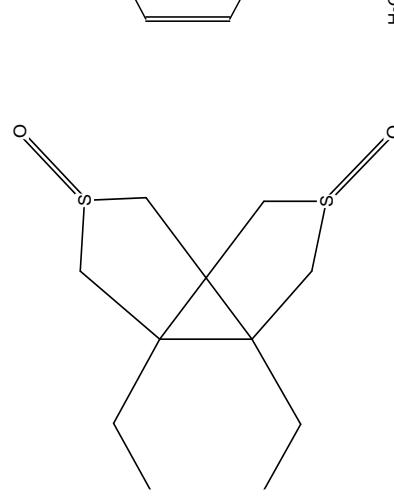
Dithia[4.3.3]propylene diisulfide monohydrate

Formula:

C₁₀H₁₄O₂S₂H₂O₁

Space Group:

P212121
Space Group No.: 19
Cell:
(*A*,*a*)
 α : 90.00
 β : 90.00
 γ : 90.00
R-Factor (%): 4.80
Temperature(K): 295
Density(g/cm³): 1.443



Ph

Reference:

F.H.Herbststein, D.Ashkenazi, M.Kaltori, M.Kapton, S.S.42,575
Dithia[4.3.3]propylene diisulfide monohydrate

Compound Name:

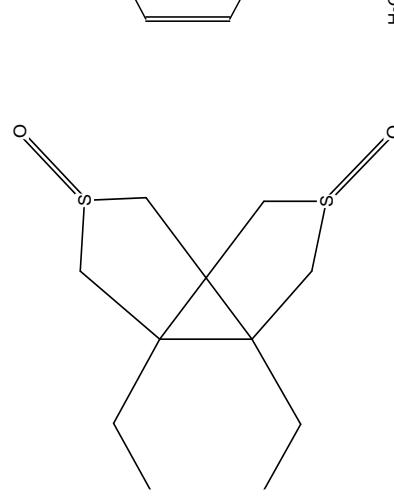
Dithia[4.3.3]propylene diisulfide monohydrate

Formula:

C₁₀H₁₄O₂S₂H₂O₁

Space Group:

P212121
Space Group No.: 19
Cell:
(*A*,*a*)
 α : 90.00
 β : 90.00
 γ : 90.00
R-Factor (%): 4.80
Temperature(K): 295
Density(g/cm³): 1.443

H₂NOC

Reference:

K.Fridenvang, L.Gronborg, B.Jensen (1988) *Acta Crystallogr., Sect.C/Crys. Struct. Commun.*, **44**, 841
Methoxytrichloro picate hemihydrate

Compound Name:

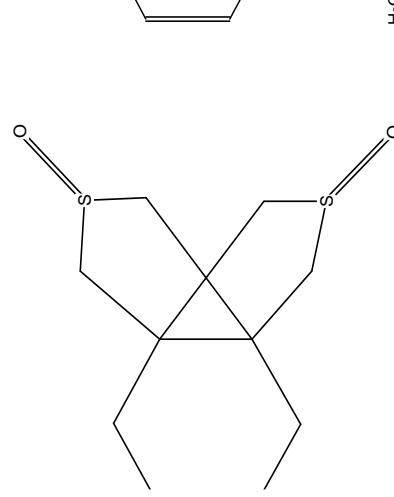
1,3,5-tris(4-methoxy-1-methylphenyl)benzene 2,5-dimethylhex-3-yn-2,5-diol

Formula:

C₂₄H₂₄O₅C₆H₅O₂

Space Group:

P21n
Space Group No.: 13
Cell:
(*A*,*a*)
 α : 90.00
 β : 106.74(2)
 γ : 90.00
R-Factor (%): 4.40
Temperature(K): 295
Density(g/cm³): 1.125

H₂O

Reference:

K.Fridenvang, L.Gronborg, B.Jensen (1988) *Acta Crystallogr., Sect.C/Crys. Struct. Commun.*, **44**, 841
Methoxytrichloro picate hemihydrate

Compound Name:

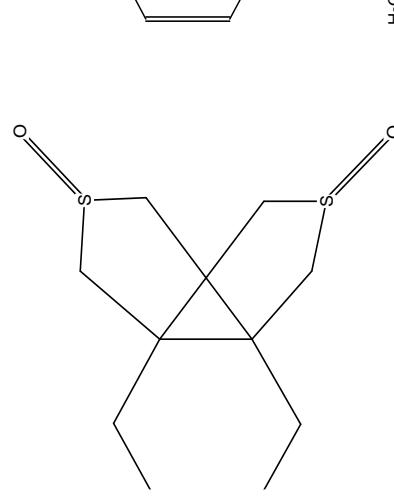
1,3,5-tris(4-methoxy-1-methylphenyl)benzene 2,5-dimethylhex-3-yn-2,5-diol

Formula:

C₂₄H₂₄O₅C₆H₅O₂

Space Group:

P21n
Space Group No.: 13
Cell:
(*A*,*a*)
 α : 90.00
 β : 106.74(2)
 γ : 90.00
R-Factor (%): 4.40
Temperature(K): 295
Density(g/cm³): 1.125

H₂O

Reference:

K.Fridenvang, L.Gronborg, B.Jensen (1988) *Acta Crystallogr., Sect.C/Crys. Struct. Commun.*, **44**, 841
Methoxytrichloro picate hemihydrate

Compound Name:

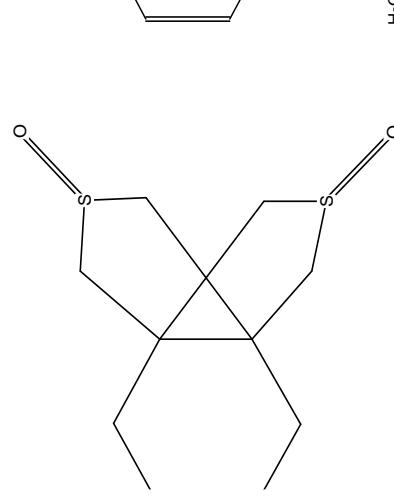
1,3,5-tris(4-methoxy-1-methylphenyl)benzene 2,5-dimethylhex-3-yn-2,5-diol

Formula:

C₂₄H₂₄O₅C₆H₅O₂

Space Group:

P21n
Space Group No.: 13
Cell:
(*A*,*a*)
 α : 90.00
 β : 106.74(2)
 γ : 90.00
R-Factor (%): 4.40
Temperature(K): 295
Density(g/cm³): 1.125

H₂O

Reference:

K.Fridenvang, L.Gronborg, B.Jensen (1988) *Acta Crystallogr., Sect.C/Crys. Struct. Commun.*, **44**, 841
Methoxytrichloro picate hemihydrate

Compound Name:

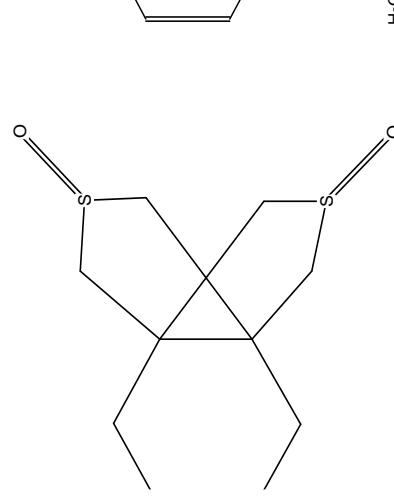
1,3,5-tris(4-methoxy-1-methylphenyl)benzene 2,5-dimethylhex-3-yn-2,5-diol

Formula:

C₂₄H₂₄O₅C₆H₅O₂

Space Group:

P21n
Space Group No.: 13
Cell:
(*A*,*a*)
 α : 90.00
 β : 106.74(2)
 γ : 90.00
R-Factor (%): 4.40
Temperature(K): 295
Density(g/cm³): 1.125

H₂O

Reference:

K.Fridenvang, L.Gronborg, B.Jensen (1988) *Acta Crystallogr., Sect.C/Crys. Struct. Commun.*, **44**, 841
Methoxytrichloro picate hemihydrate

Compound Name:

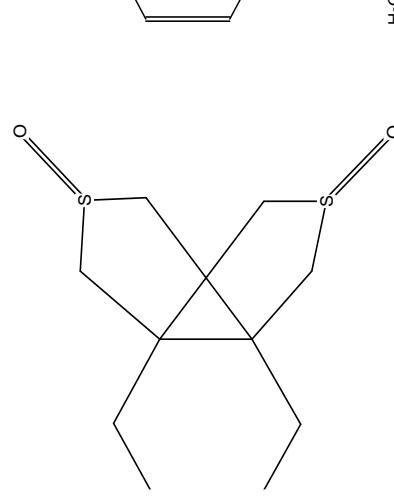
1,3,5-tris(4-methoxy-1-methylphenyl)benzene 2,5-dimethylhex-3-yn-2,5-diol

Formula:

C₂₄H₂₄O₅C₆H₅O₂

Space Group:

P21n
Space Group No.: 13
Cell:
(*A*,*a*)
 α : 90.00
 β : 106.74(2)
 γ : 90.00
R-Factor (%): 4.40
Temperature(K): 295
Density(g/cm³): 1.125

H₂O

Reference:

K.Fridenvang, L.Gronborg, B.Jensen (1988) *Acta Crystallogr., Sect.C/Crys. Struct. Commun.*, **44**, 841
Methoxytrichloro picate hemihydrate

Compound Name:

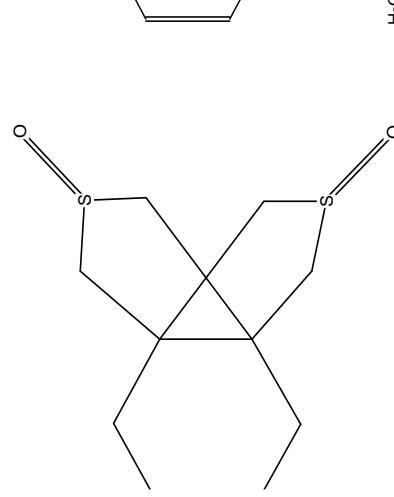
1,3,5-tris(4-methoxy-1-methylphenyl)benzene 2,5-dimethylhex-3-yn-2,5-diol

Formula:

C₂₄H₂₄O₅C₆H₅O₂

Space Group:

P21n
Space Group No.: 13
Cell:
(*A*,*a*)
 α : 90.00
 β : 106.74(2)
 γ : 90.00
R-Factor (%): 4.40
Temperature(K): 295
Density(g/cm³): 1.125

H₂O

Reference:

K.Fridenvang, L.Gronborg, B.Jensen (1988) *Acta Crystallogr., Sect.C/Crys. Struct. Commun.*, **44**, 841
Methoxytrichloro picate hemihydrate

Compound Name:

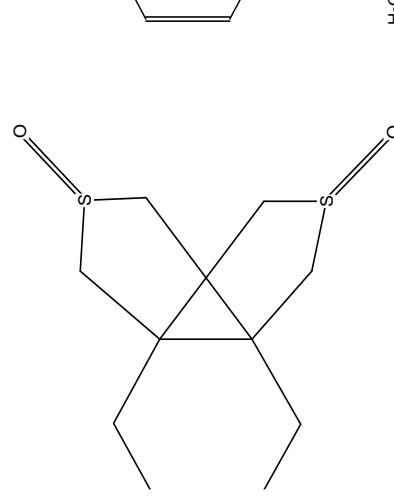
1,3,5-tris(4-methoxy-1-methylphenyl)benzene 2,5-dimethylhex-3-yn-2,5-diol

Formula:

C₂₄H₂₄O₅C₆H₅O₂

Space Group:

P21n
Space Group No.: 13
Cell:
(*A*,*a*)
 α : 90.00
 β : 106.74(2)
 γ : 90.00
R-Factor (%): 4.40
Temperature(K): 295
Density(g/cm³): 1.125

H₂O

Reference:

K.Fridenvang, L.Gronborg, B.Jensen (1988) *Acta Crystallogr., Sect.C/Crys. Struct. Commun.*, **44**, 841
Methoxytrichloro picate hemihydrate

Compound Name:

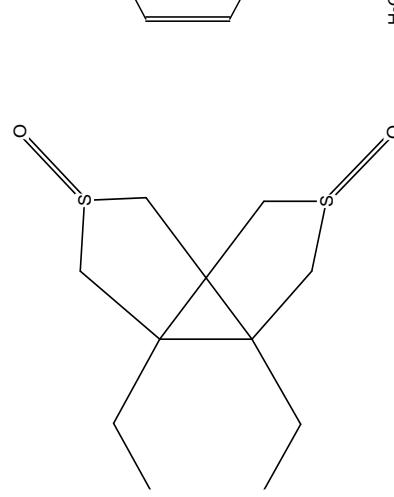
1,3,5-tris(4-methoxy-1-methylphenyl)benzene 2,5-dimethylhex-3-yn-2,5-diol

Formula:

C₂₄H₂₄O₅C₆H₅O₂

Space Group:

P21n
Space Group No.: 13
Cell:
(*A*,*a*)
 α : 90.00
 β : 106.74(2)
 γ : 90.00
R-Factor (%): 4.40
Temperature(K): 295
Density(g/cm³): 1.125

H₂O

Reference:

K.Fridenvang, L.Gronborg, B.Jensen (1988) *Acta Crystallogr., Sect.C/Crys. Struct. Commun.*, **44**, 841
Methoxytrichloro picate hemihydrate

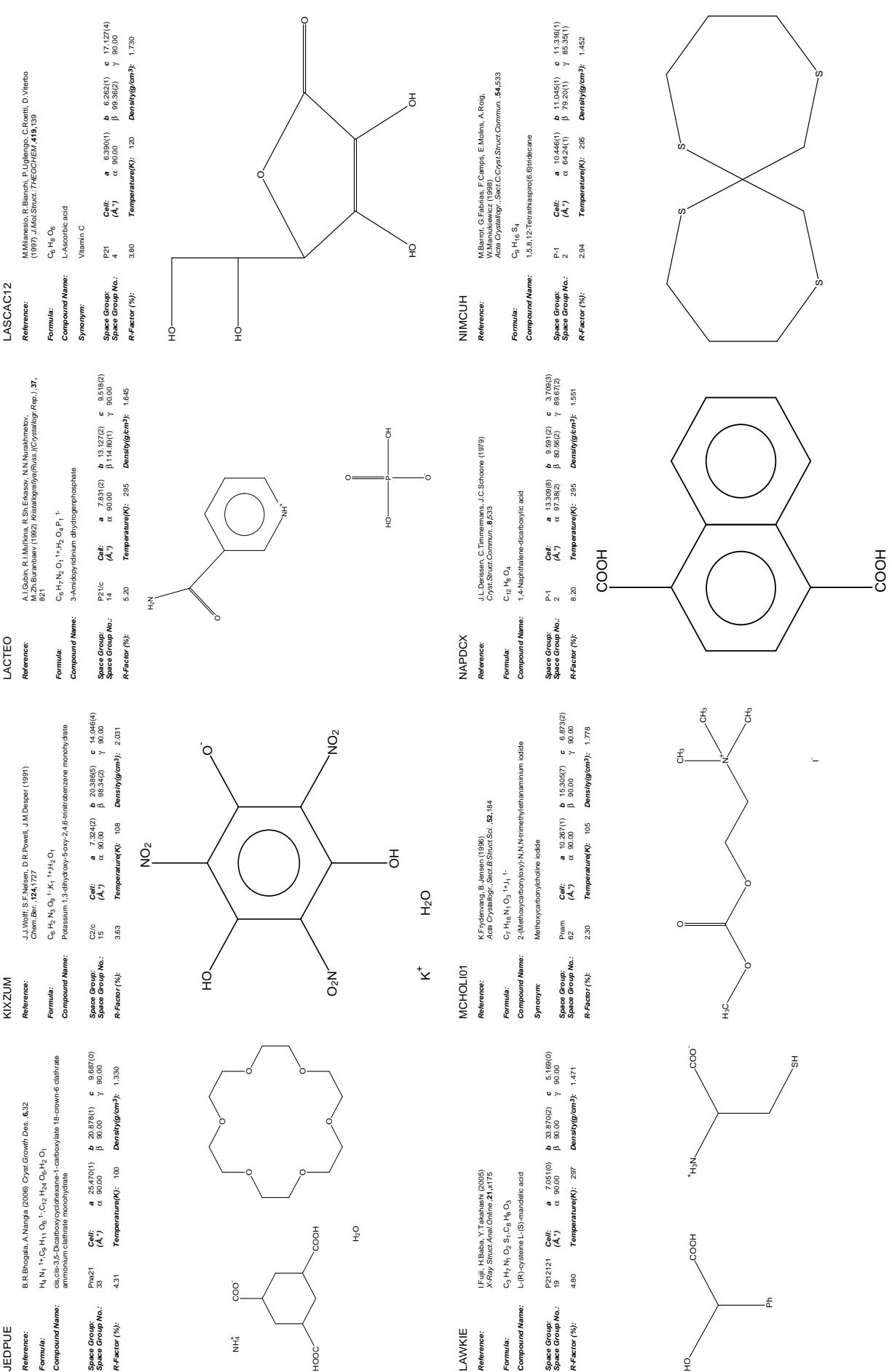
Compound Name:

1,3,5-tris(4-methoxy-1-methylphenyl)benzene 2,5-dimethylhex-3-yn-2,5-diol

Formula:

C₂₄H₂₄O₅C₆H₅O₂

GIKZAB	M.Kaitoff (1987) <i>Tetrahedron</i> , 43 , 1503 Reference: S.L. Wall, E.S. Meadows, L.J. Barbour, G.W. Gokel (1989) <i>J Am Chem Soc</i> , 121 , 5613 Formula: $2C_6H_5N_1O_1^+ \cdot C_8H_2O_2^-$ Compound Name: 1,6-dis(2-chlorophenyl)-1,6-diolefinic diacid (2-pyridone) diacetate	
GOXWAR	M.C.Walne, R.J.Foltynowicz, G.A.Stephenson, P.E.Fawcett, J.G.Rowell, S.R.Byrn (2003) <i>Private Communication</i> , C ₂₂ H ₃₄ N ₂ O ₄ Reference: S.L. Wall, E.S. Meadows, L.J. Barbour, G.W. Gokel (1989) <i>J Am Chem Soc</i> , 121 , 5613 Formula: N,N-bis[1-phenyl-3-(ethylidene)-7,16-diazabicyclo[2.4.4]octane-2,4-diene-1,6-diol bis(Z'-pyridone)] diacetate	
GU-XUA	P21/c Cell: a 17.01(9) b 11.942(6) c 8.73(4) A_v: α 90.00 β 101.50(2) γ 90.00 Space Group No.: 4 R-Factor (%): 6.00 Temperature(K): 295 Density(g/cm³): 1.289	
HEZNIEF	M.C.Walne, R.J.Foltynowicz, G.A.Stephenson, P.E.Fawcett, J.G.Rowell, S.R.Byrn (2003) <i>Private Communication</i> , C ₂₈ H ₄₁ N ₁ O ₄ C ₁ H ₄ O ₁ ·2H ₂ O ₁ Reference: S.A.Bourne, M.R.Cairns, L.R.Nassimbeni, I.Shabalala (1994) <i>J Pharm Sci</i> , 83 , 187 Formula: C ₁₃ H ₁₃ N ₁ O ₅ S ₂ C ₄ H ₆ O ₂ Compound Name: 4-Succinylaminon-N-2-thiacyclo[4.2.2]octan-2-ylbenzenesulfonamide 1-butanol clathrate	
HEZNOP	S.A.Bourne, M.R.Cairns, L.R.Nassimbeni, I.Shabalala (1994) <i>J Pharm Sci</i> , 83 , 187 Reference: Hong Liang, Xing-Hui Yi, Kun Bei Yu (2003) <i>Hecheng-Huaxue(Zhong) [Chem Smith.Chem]</i> , 11 , 128 Formula: C ₁₀ H ₁₁ N ₂ O ₁ ⁺ ·C ₆ H ₅ N ₃ O ₂ ⁻ Compound Name: Pyridinium-3-carboxamide picrate	
IPOZO	Yue-Ping Fang, Meng-Hua Zeng, Rong-Ying Zeng, Hong Liang, Xing-Hui Yi, Kun Bei Yu (2003) <i>Hecheng-Huaxue(Zhong) [Chem Smith.Chem]</i> , 11 , 128 Reference: E.C.Taylor, J.L.Pont, D.Van Engen, J.C.Wamer (1986) <i>J Org Chem</i> , 51 , 5093 Formula: C ₁₀ H ₁₁ N ₂ O ₁ ⁺ ·C ₆ H ₅ N ₃ O ₂ ⁻ Compound Name: 2-Carboxymethyl-8-methylethyl-7,8-dihydro-3H-1,3,7-triazine (3,2-d)(1,2,4)triazine	
JEDPEO	E.C.Taylor, J.L.Pont, D.Van Engen, J.C.Wamer (1986) <i>J Org Chem</i> , 51 , 5093 Reference: H ₄ N ₁ O ₁ ⁺ ·C ₆ H ₅ N ₃ O ₂ ⁻ Formula: C ₁₀ H ₁₁ N ₂ O ₁ ⁺ ·C ₆ H ₅ N ₃ O ₂ ⁻ Compound Name: di-cis,5-Diancyanoethyl-1-cationate 1,8-crown-6 dihydroxydiammonium clathrate	
KPOZD	P21/c Cell: a 7.781 b 7.781 c 8.138(2) A_v: α 90.00 β 90.00 γ 90.00 Space Group No.: 14 R-Factor (%): 4.32 Temperature(K): 295 Density(g/cm³): 1.505 R-Factor (%): 5.30 Temperature(K): 295 Density(g/cm³): 1.505	
LKZAB	S.A.Bourne, M.R.Cairns, L.R.Nassimbeni, I.Shabalala (1994) <i>J Pharm Sci</i> , 83 , 187 Reference: S.A.Bourne, M.R.Cairns, L.R.Nassimbeni, I.Shabalala (1994) <i>J Pharm Sci</i> , 83 , 187 Formula: C ₁₃ H ₁₃ N ₁ O ₅ S ₂ C ₄ H ₆ O ₂ Compound Name: 4-Succinylaminon-N-2-thiacyclo[4.2.2]octan-2-ylbenzenesulfonamide 1,4-dioxane clathrate	
LU-ZWY	P21/c Cell: a 12.77(1) b 14.15(6) c 98.93(2) A_v: α 94.48(3) β 100.92(3) γ 98.93(2) Space Group No.: 2 R-Factor (%): 5.40 Temperature(K): 295 Density(g/cm³): 1.505	
MX-ZWY	P21/c Cell: a 14.08(2) b 14.08(2) c 11.45(8) A_v: α 90.00 β 90.00 γ 120.00 Space Group No.: 14 R-Factor (%): 7.80 Temperature(K): 295 Density(g/cm³): 1.357	



NOXKAM	D.Braga, F.Greponi, D.Walther, K.Heubach, A.Schmidt, (1997) <i>Organometalates</i> , 16,4910 C ₆ H ₁₁ N, O ₂	OFUHUS Reference: Ning Shan, A.D.Bond, W.Jones (2002) <i>Tetrahedron Lett.</i> , 43(3) 191 Formula: C ₁₂ H ₁₄ N ₂ O ₄ C ₆ H ₅ N ₂ Compound Name: 1,1,4,4-Tetramethylbut-2-yn-4-diol	PIKLEA Reference: A.Ota, Y.Kawashima, H.Oishi, T.Ishida (1993) <i>Chem.Pharm.Bull.</i> , 41,1661 Formula: C ₁₈ H ₂₂ N ₂ O ₂ S, C ₆ H ₅ O ₃ Compound Name: (R)-(+)-2-(5-Methoxy-2-(<i>p</i> -methyl-2-(3,4-(methylenedioxy)-2-methylpropoxy)phenyl)-2-methyl-1,4-dioxane-3-carboxylic acid mandelate	QIJZOY Reference: L.A.Filip, M.R.Caires, S.J.Farias, M.T.Boglia (2001) <i>Acta Cryst.(Sect.C, Cryst.Commun.)</i> , 57,435 Formula: C ₁₈ H ₁₄ N ₂ O ₅ S, S Compound Name: 5-(4-(4-(Pivaloyl-2-aminotetrahydrofuryl)phenyl)-2-(3,4-(methylenedioxy)-2-methylpropoxy)phenyl)-2-methyl-1,4-dioxane-3-carboxylic acid mandelate					
Space Group: Space Group No.: R-Factor (%):	P-1 2 3.74	Cell: (<i>A</i> , <i>c</i>) <i>a</i> 856(2) <i>α</i> 91.90(3) <i>b</i> 8.836(2) <i>β</i> 112.3(3) <i>c</i> 9.424(3)	Space Group: Space Group No.: R-Factor (%):	P21/n (<i>A</i> , <i>c</i>) <i>a</i> 11.791(0) <i>α</i> 90.00 <i>b</i> 17.758(0) <i>γ</i> 90.00	Cell: (<i>A</i> , <i>c</i>) <i>a</i> 11.791(0) <i>α</i> 90.00 <i>b</i> 17.758(0) <i>γ</i> 90.00	Symmetry: Space Group: Space Group No.: R-Factor (%):	<i>c</i> 27.80(0) <i>γ</i> 90.00	Symmetry: Space Group: Space Group No.: R-Factor (%):	<i>c</i> 27.80(0) <i>γ</i> 90.00
Temperature(K): Density(g/cm ³):	180 1.089	Temperature(K): Density(g/cm ³):	180 1.436	Temperature(K): Density(g/cm ³):	180 0.90(3) <i>α</i> 90.00 <i>β</i> 94.40(2) <i>γ</i> 90.00	Temperature(K): Density(g/cm ³):	180 1.368	Temperature(K): Density(g/cm ³):	180 1.368
Space Group: Space Group No.: R-Factor (%):	P-1 2 4.35	Cell: (<i>A</i> , <i>c</i>) <i>a</i> 9.564(3) <i>α</i> 90.00 <i>b</i> 31.07(9) <i>γ</i> 90.00	Space Group: Space Group No.: R-Factor (%):	P21 (<i>A</i> , <i>c</i>) <i>a</i> 9.564(3) <i>α</i> 90.00 <i>b</i> 31.07(9) <i>γ</i> 90.00	Cell: (<i>A</i> , <i>c</i>) <i>a</i> 9.564(3) <i>α</i> 90.00 <i>b</i> 31.07(9) <i>γ</i> 90.00	Symmetry: Space Group: Space Group No.: R-Factor (%):	<i>c</i> 5.643(1) <i>γ</i> 90.00	Symmetry: Space Group: Space Group No.: R-Factor (%):	<i>c</i> 5.643(1) <i>γ</i> 90.00
Temperature(K): Density(g/cm ³):	255 1.497	Temperature(K): Density(g/cm ³):	255 1.368	Temperature(K): Density(g/cm ³):	255 1.368	Temperature(K): Density(g/cm ³):	255 1.368	Temperature(K): Density(g/cm ³):	255 1.368
Space Group: Space Group No.: R-Factor (%):	P-1 2 4.35	Cell: (<i>A</i> , <i>c</i>) <i>a</i> 9.564(3) <i>α</i> 90.00 <i>b</i> 31.07(9) <i>γ</i> 90.00	Space Group: Space Group No.: R-Factor (%):	P21 (<i>A</i> , <i>c</i>) <i>a</i> 9.564(3) <i>α</i> 90.00 <i>b</i> 31.07(9) <i>γ</i> 90.00	Cell: (<i>A</i> , <i>c</i>) <i>a</i> 9.564(3) <i>α</i> 90.00 <i>b</i> 31.07(9) <i>γ</i> 90.00	Symmetry: Space Group: Space Group No.: R-Factor (%):	<i>c</i> 5.643(1) <i>γ</i> 90.00	Symmetry: Space Group: Space Group No.: R-Factor (%):	<i>c</i> 5.643(1) <i>γ</i> 90.00
Temperature(K): Density(g/cm ³):	295 1.497	Temperature(K): Density(g/cm ³):	295 1.368	Temperature(K): Density(g/cm ³):	295 1.368	Temperature(K): Density(g/cm ³):	295 1.368	Temperature(K): Density(g/cm ³):	295 1.368

SLFNMB01	G.P.Bennetti, F.Giordano, A.La Manna, G.Giuseppetti, C.Tarini (1982) <i>Crys Struct Commun.</i> , 11 ,821 Reference: G.P.Bennetti, F.Giordano, A.La Manna, G.Giuseppetti, C.Tarini (1982) <i>Crys Struct Commun.</i> , 11 ,821 Formula: C ₁₀ H ₁₁ N ₃ O ₃ S ₁ Compound Name: 3-Sulfanilamido-5-methylisoxazole Synonym: Sulfanethioxazole Space Group: C2/c Cell: a: 16.062(2) \AA ; b: 5.479(1) \AA ; c: 25.757(3) \AA Space Group No.: 15 R-Factor (%): 3.20 Temperature(K): 295 Density(g/cm³): 1.493 R-Factor (%): 1.493		SLFNMB02 Reference: C.Tarini (1982) <i>Crys Struct Commun.</i> , 11 ,821 Formula: C ₁₀ H ₁₁ N ₃ O ₃ S ₁ Compound Name: 3-Sulfanilamido-5-methylisoxazole Synonym: Sulfanethioxazole Space Group: C2/c Cell: a: 16.062(2) \AA ; b: 5.479(1) \AA ; c: 25.757(3) \AA Space Group No.: 15 R-Factor (%): 3.20 Temperature(K): 295 Density(g/cm³): 1.493 R-Factor (%): 1.493	
SLFNMB03	J.Rambaud, R.Roures, S.Aberola, F.Sabon (1980) Reference: J.Rambaud, R.Roures, S.Aberola, F.Sabon (1980) Formula: C ₁₀ H ₁₁ N ₃ O ₃ S ₁ Compound Name: 3-Sulfanilamido-5-methylisoxazole Synonym: Sulfanethioxazole Space Group: C2/c Cell: a: 16.046(5) \AA ; b: 5.470(2) \AA ; c: 25.747(1) \AA Space Group No.: 15 R-Factor (%): 4.70 Temperature(K): 295 Density(g/cm³): 1.497 R-Factor (%): 1.497		SLFNMB03 Reference: J.Rambaud, R.Roures, S.Aberola, F.Sabon (1980) Formula: C ₁₀ H ₁₁ N ₃ O ₃ S ₁ Compound Name: 3-Sulfanilamido-5-methylisoxazole Synonym: Sulfanethioxazole Space Group: C2/c Cell: a: 16.046(5) \AA ; b: 5.470(2) \AA ; c: 25.747(1) \AA Space Group No.: 15 R-Factor (%): 4.70 Temperature(K): 295 Density(g/cm³): 1.497 R-Factor (%): 1.497	
SLFNMB04	L.Maury, J.Rambaud, B.Pauvert, Y.Lassere, G.Berge, M.Audran (1985) <i>Can.J.Chem.</i> , 63 ,3012 Reference: L.Maury, J.Rambaud, B.Pauvert, Y.Lassere, G.Berge, M.Audran (1985) <i>Can.J.Chem.</i> , 63 ,3012 Formula: C ₁₀ H ₁₁ N ₃ O ₃ S ₁ Compound Name: N-(5-Methyl-3-isoxazolyl)-N-sulfanilamide Synonym: Sulfanethioxazole Space Group: C2/c Cell: a: 16.046(5) \AA ; b: 5.470(2) \AA ; c: 25.747(1) \AA Space Group No.: 15 R-Factor (%): 4.08 Temperature(K): 295 Density(g/cm³): 1.413 R-Factor (%): 1.413		SLFNMB04 Reference: L.Maury, J.Rambaud, B.Pauvert, Y.Lassere, G.Berge, M.Audran (1985) <i>Can.J.Chem.</i> , 63 ,3012 Formula: C ₁₀ H ₁₁ N ₃ O ₃ S ₁ Compound Name: N-(5-Methyl-3-isoxazolyl)-N-sulfanilamide Synonym: Sulfanethioxazole Space Group: C2/c Cell: a: 16.046(5) \AA ; b: 5.470(2) \AA ; c: 25.747(1) \AA Space Group No.: 15 R-Factor (%): 4.08 Temperature(K): 295 Density(g/cm³): 1.413 R-Factor (%): 1.413	
TAFBUX	A.I.Gorbun, N.N.Nurukhmetov, M.Zh.Burabbaev, R.I.Mukhina, R.Sh.Ermasov (1989) Reference: A.I.Gorbun, N.N.Nurukhmetov, M.Zh.Burabbaev, R.I.Mukhina, R.Sh.Ermasov (1989) Formula: C ₆ H ₇ N ₂ O ₁ +•Cl ⁻¹⁻ Compound Name: 1-Hydro-3-carbamoyl-pyridine chloride Synonym: 1-hydroxy-3-carbamoylpyridine chloride Space Group: C2/c Cell: a: 12.055 \AA ; b: 24.476(1) \AA ; c: 17.422(0) \AA Space Group No.: 15 R-Factor (%): 3.70 Temperature(K): 295 Density(g/cm³): 1.491 R-Factor (%): 1.491	<chem>CN(C=O)C1=CC=C(C=C1)[NH+]Cl</chem>	TAFBUX Reference: A.I.Gorbun, N.N.Nurukhmetov, M.Zh.Burabbaev, R.I.Mukhina, R.Sh.Ermasov (1989) Reference: A.I.Gorbun, N.N.Nurukhmetov, M.Zh.Burabbaev, R.I.Mukhina, R.Sh.Ermasov (1989) Formula: C ₆ H ₇ N ₂ O ₁ +•Cl ⁻¹⁻ Compound Name: 1-Hydro-3-carbamoyl-pyridine chloride Synonym: 1-hydroxy-3-carbamoylpyridine chloride Space Group: C2/c Cell: a: 12.055 \AA ; b: 24.476(1) \AA ; c: 17.422(0) \AA Space Group No.: 15 R-Factor (%): 3.70 Temperature(K): 295 Density(g/cm³): 1.491 R-Factor (%): 1.491	<chem>CN(C=O)C1=CC=C(C=C1)[NH+]Cl</chem>
SMZTMP	G.Giuseppetti, C.Tadini, G.P.Bettinelli, F.Giordano, A.la Manna (1980) <i>Farmaco Ed.Sc.</i> , 35 ,138 Reference: G.Giuseppetti, C.Tadini, G.P.Bettinelli, F.Giordano, A.la Manna (1980) <i>Farmaco Ed.Sc.</i> , 35 ,138 Formula: C ₁₄ H ₁₈ N ₃ O ₃ S ₁ Compound Name: 3-Sulfanilamido-5-methylisoxazole Synonym: Sulfanethioxazole Space Group: P1 Cell: a: 11.640(3) \AA ; b: 16.761(3) \AA ; c: 12.422(2) \AA Space Group No.: 14 R-Factor (%): 5.40 Temperature(K): 295 Density(g/cm³): 1.463 R-Factor (%): 1.463		SMZTMP Reference: G.Giuseppetti, C.Tadini, G.P.Bettinelli, F.Giordano, A.la Manna (1980) <i>Farmaco Ed.Sc.</i> , 35 ,138 Reference: G.Giuseppetti, C.Tadini, G.P.Bettinelli, F.Giordano, A.la Manna (1980) <i>Farmaco Ed.Sc.</i> , 35 ,138 Formula: C ₁₄ H ₁₈ N ₃ O ₃ S ₁ Compound Name: 3-Sulfanilamido-5-methylisoxazole Synonym: Sulfanethioxazole Space Group: P1 Cell: a: 11.640(3) \AA ; b: 16.761(3) \AA ; c: 12.422(2) \AA Space Group No.: 14 R-Factor (%): 5.40 Temperature(K): 295 Density(g/cm³): 1.463 R-Factor (%): 1.463	
SLFNMB05	C.P.Price, A.G.Greissak, A.J.Matzger (2005) Reference: J Am Chem Soc., 127 ,3512 Formula: C ₁₀ H ₁₁ N ₃ O ₃ S ₁ Compound Name: 3-(4-Aminobenzesulfonyl)amido-5-methylisoxazole Synonym: Sulfanethioxazole Space Group: P21/n Cell: a: 11.640(3) \AA ; b: 9.708(0) \AA ; c: 15.419(4) \AA Space Group No.: 14 R-Factor (%): 9.14 Temperature(K): 153 Density(g/cm³): 1.438 R-Factor (%): 1.438		SLFNMB05 Reference: C.P.Price, A.G.Greissak, A.J.Matzger (2005) Reference: J Am Chem Soc., 127 ,3512 Formula: C ₁₀ H ₁₁ N ₃ O ₃ S ₁ Compound Name: 3-(4-Aminobenzesulfonyl)amido-5-methylisoxazole Synonym: Sulfanethioxazole Space Group: P21/n Cell: a: 11.640(3) \AA ; b: 9.708(0) \AA ; c: 15.419(4) \AA Space Group No.: 14 R-Factor (%): 9.14 Temperature(K): 153 Density(g/cm³): 1.438 R-Factor (%): 1.438	
SLFNMB06	C.P.Price, A.G.Greissak, A.J.Matzger (2005) Reference: J Am Chem Soc., 127 ,3512 Formula: C ₁₀ H ₁₁ N ₃ O ₃ S ₁ Compound Name: 3-(4-Aminobenzesulfonyl)amido-5-methylisoxazole Synonym: Sulfanethioxazole Space Group: P21/n Cell: a: 11.640(3) \AA ; b: 9.708(0) \AA ; c: 15.419(4) \AA Space Group No.: 14 R-Factor (%): 9.14 Temperature(K): 153 Density(g/cm³): 1.438 R-Factor (%): 1.438		SLFNMB06 Reference: C.P.Price, A.G.Greissak, A.J.Matzger (2005) Reference: J Am Chem Soc., 127 ,3512 Formula: C ₁₀ H ₁₁ N ₃ O ₃ S ₁ Compound Name: 3-(4-Aminobenzesulfonyl)amido-5-methylisoxazole Synonym: Sulfanethioxazole Space Group: P21/n Cell: a: 11.640(3) \AA ; b: 9.708(0) \AA ; c: 15.419(4) \AA Space Group No.: 14 R-Factor (%): 9.14 Temperature(K): 153 Density(g/cm³): 1.438 R-Factor (%): 1.438	
SLFNMB07				

VAXLIP

Reference: A.I.Gubin, R.I.Murikova, R.Shi.Eriksova, N.N.Nurukhimova, R.I.Murikova (1988) Kristallografiya(Russ.),Crystallogr.(Rep.) 33:504

Formula: $C_8H_7N_1O_1$ • N_1O_1

Compound Name: Nicotinamide hydroxamate

Space Group: P21/c
Space Group No.: 14
Temperature(K): 4.80
R-Factor (%): 1.2558

Cell: $a = 6.723(2)$ $b = 12.556(4)$ $c = 3.941(3)$
 $\alpha = 96.00^\circ$ $\beta = 98.90(1)^\circ$ $\gamma = 96.00^\circ$

Compound Name: VAZCOP

Reference: J.Hantung K.Daniel, P.Schmidt, S.Laug, I.Svoboda, H.Fuess (2005) Acta Crystallogr.-Sect E Struct Rep. Online 61:3974

Formula: $C_{18}H_{10}O_2N_2S_4$

Compound Name: 1,2-dist(4-phenoxyphenyl)-1,3-thiazo(2-yl)imidafuran

Space Group: C2/c
Space Group No.: 15
Temperature(K): 3.94
R-Factor (%): 1.2558

Cell: $a = 20.23(3)$ $b = 9.998(3)$ $c = 37.594(3)$
 $\alpha = 96.90^\circ$ $\beta = 91.53(1)^\circ$ $\gamma = 90.00^\circ$

Reference: A.I.Gubin, R.I.Murikova, R.Shi.Eriksova, N.N.Nurukhimova, M.Zh.Burannayev (1991) Kristallografiya(Russ.),Crystallogr.(Rep.) 36: 1567

Formula: $C_6H_7N_2O_1I_1$

Compound Name: (2-Hydroxy-5-methylphenyl)phosphine oxide

Space Group: P21/n
Space Group No.: 14
Temperature(K): 1.304
R-Factor (%): 1.2524

Cell: $a = 10.720(2)$ $b = 9.899(2)$ $c = 15.287(3)$
 $\alpha = 96.00^\circ$ $\beta = 92.46(2)^\circ$ $\gamma = 96.00^\circ$

Reference: F.Belanger-Gariépy, M.Danguienne, F.Louisell, A.L.Beauchamp (2000) Acta Crystallogr., Sect C,Cryst. Commun. 56: 4338

Formula: $C_9H_{17}O_2P_1$

Compound Name: (2-Hydroxy-5-methylphenyl)phosphine oxide

Space Group: P21/n
Space Group No.: 14
Temperature(K): 2.073
R-Factor (%): 2.073

Cell: $a = 10.720(2)$ $b = 9.899(2)$ $c = 15.287(3)$
 $\alpha = 96.00^\circ$ $\beta = 92.46(2)^\circ$ $\gamma = 96.00^\circ$

Reference: Ning Shan, E.Batchelder, N.Jones (2002) *Acta Crystallogr.*, **48**: 271

Formula: $C_{12}H_8O_2C_{12}H_8N_2$

Compound Name: Naphthalene-1,4-dicarboxylic acid bis(4,7-phenanthroline)

Space Group: P21/c
Space Group No.: 14
Temperature(K): 5.00
R-Factor (%): 1.421

Cell: $a = 7.381(0)$ $b = 12.104(0)$ $c = 30.180(1)$
 $\alpha = 96.00^\circ$ $\beta = 90.07(0)^\circ$ $\gamma = 90.00^\circ$

Reference: P.Hahn, T.Lüger, F.E.Hahn, S.J.Bentig, C.Orvg (2000) *Z.Kristallogr.-Rev.*, **215**: 237

Formula: $C_{19}H_{17}O_2P_1$

Compound Name: (2-Hydroxy-5-methylphenyl)phosphine oxide

Space Group: P21/n
Space Group No.: 14
Temperature(K): 1.30
R-Factor (%): 1.2541

Cell: $a = 9.366(2)$ $b = 11.693(1)$ $c = 14.554(0)$
 $\alpha = 90.00^\circ$ $\beta = 99.78(0)^\circ$ $\gamma = 96.00^\circ$

Reference: VOBWIT01

Formula: $C_8H_7N_1O_1$ • N_1O_1

Compound Name: Nicotinamide hydroxamate

Space Group: P21/n
Space Group No.: 14
Temperature(K): 7.39
R-Factor (%): 1.2541

Cell: $a = 10.720(2)$ $b = 9.899(2)$ $c = 15.287(3)$
 $\alpha = 96.00^\circ$ $\beta = 92.46(2)^\circ$ $\gamma = 96.00^\circ$

Reference: VOBWIT

Formula: $C_6H_7N_2O_1I_1$

Compound Name: (2-Hydroxy-5-methylphenyl)phosphine oxide

Space Group: P21/n
Space Group No.: 14
Temperature(K): 2.073
R-Factor (%): 1.2524

Cell: $a = 10.720(2)$ $b = 9.899(2)$ $c = 15.287(3)$
 $\alpha = 96.00^\circ$ $\beta = 92.46(2)^\circ$ $\gamma = 96.00^\circ$