

# Search Overview

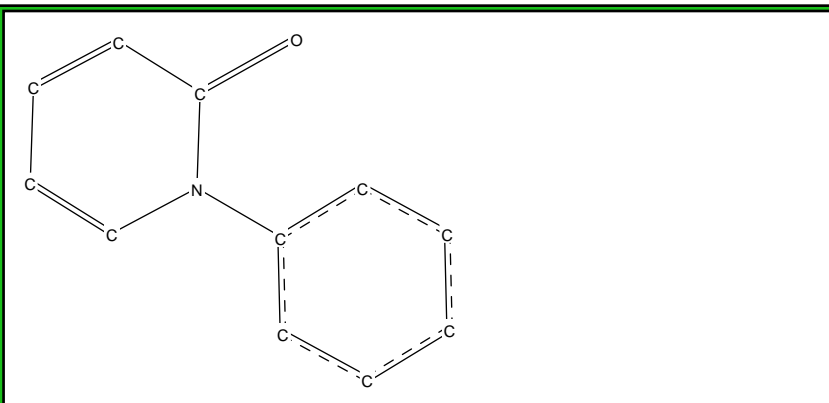
**Search:** search4  
**Date/Time done:** Sun May 19 12:50:34 2019  
**Database(s):** CSD version 5.40 updates (Feb 2019)  
CSD version 5.40 (November 2018)  
**Restriction Info:** No refcode restrictions applied  
**Filters:** None  
**Percentage Completed:** 100%  
**Number of Hits:** 40

**Single query used. Search found structures that:**

match

**Query 1**

**Query 1**



# Search: search4 (Sun May 19 12:50:34 2019): Hits 1-4

## AQIKIV

**Reference:** V.P.Tkachova, N.Yu.Gorobets, R.P.Tkachov, O.D.Dyachenko, E.B.Rusanov, V.D.Dyachenko (2010) *ARKIVOC*, **11**, 254-11

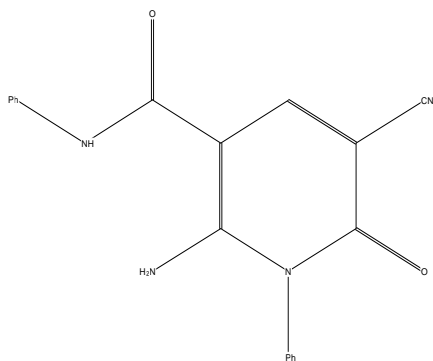
**Formula:** C<sub>19</sub>H<sub>14</sub>N<sub>4</sub>O<sub>2</sub>

**Compound Name:** 2-Amino-5-cyano-6-oxo-N,1-diphenyl-1,6-dihydropyridine-3-carboxamide

**Space Group:** P21 **Cell:** a 9.216(1) b 8.239(1) c 10.873(1)  
**Space Group No.:** 4 **(Å, °)** α 90.00 β 93.05(0) γ 90.00

**R-Factor (%):** 4.20 **Temperature(K):** 296 **Density(g/cm<sup>3</sup>):** 1.331

**Parameters**  
 Fragment 1  
**ANG1 (Å)** 73.016



## AZANOE

**Reference:** G.H.Elgemeie, P.G.Jones (2004) *Acta Crystallogr., Sect.E:Struct.Rep.Online* **60**,o2107

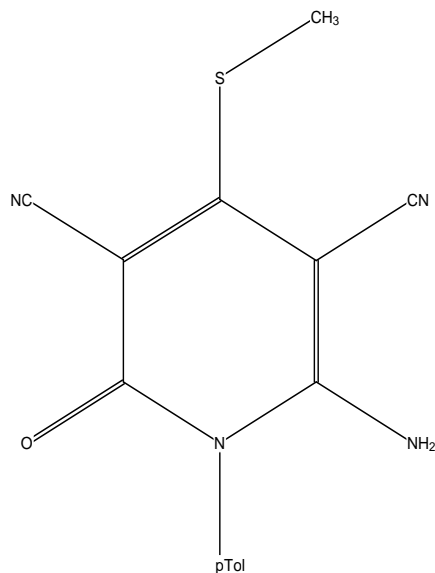
**Formula:** C<sub>15</sub>H<sub>12</sub>N<sub>4</sub>O<sub>1</sub>S<sub>1</sub>

**Compound Name:** 6-Amino-4-(methylsulfanyl)-2-oxo-1-tolyl-1,2-dihydropyridine-3,5-dicarbonitrile

**Space Group:** P21/n **Cell:** a 8.560(0) b 9.611(0) c 17.932(0)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 100.36(0) γ 90.00

**R-Factor (%):** 3.28 **Temperature(K):** 173 **Density(g/cm<sup>3</sup>):** 1.356

**Parameters**  
 Fragment 1  
**ANG1 (Å)** 85.557



## BAFPUV

**Reference:** V.D.Dyachenko, O.S.Butyukova, A.D.Dyachenko, O.V.Shishkin (2011) *Zh.Obshch.Khim.(Russ.)(Russ.J.Gen.Chem.)*, **81**, 857

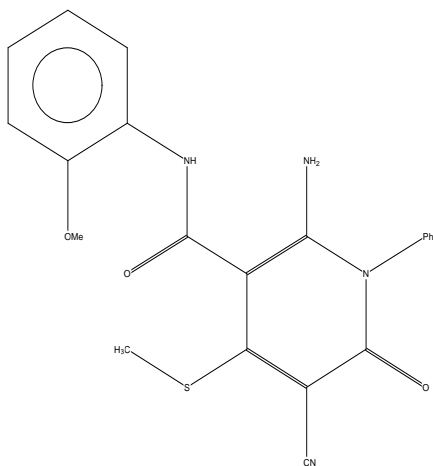
**Formula:** C<sub>21</sub>H<sub>18</sub>N<sub>4</sub>O<sub>3</sub>S<sub>1</sub>

**Compound Name:** (rac)-2-Amino-5-cyano-N-(2-methoxyphenyl)-4-(methylsulfanyl)-6-oxo-1-phenyl-1,6-dihydropyridine-3-carboxamide

**Space Group:** Pca21 **Cell:** a 35.753(1) b 5.464(0) c 9.937(0)  
**Space Group No.:** 29 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 4.58 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.391

**Parameters**  
 Fragment 1  
**ANG1 (Å)** 84.616



## BAFQAC

**Reference:** V.D.Dyachenko, O.S.Butyukova, A.D.Dyachenko, O.V.Shishkin (2011) *Zh.Obshch.Khim.(Russ.)(Russ.J.Gen.Chem.)*, **81**, 857

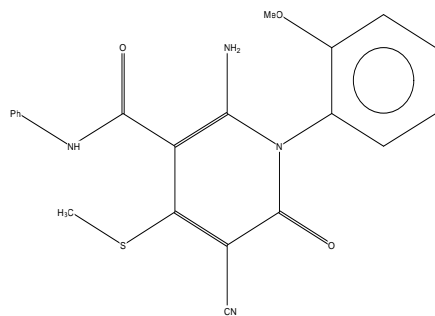
**Formula:** C<sub>21</sub>H<sub>18</sub>N<sub>4</sub>O<sub>3</sub>S<sub>1</sub>

**Compound Name:** 2-Amino-5-cyano-1-(2-methoxyphenyl)-4-(methylsulfanyl)-6-oxo-N-phenyl-1,6-dihydropyridine-3-carboxamide

**Space Group:** P21/c **Cell:** a 9.189(1) b 16.664(3) c 13.221(3)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 98.78(1) γ 90.00

**R-Factor (%):** 5.68 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.349

**Parameters**  
 Fragment 1  
**ANG1 (Å)** 80.908



# Search: search4 (Sun May 19 12:50:34 2019): Hits 5-8

## BAMTOB

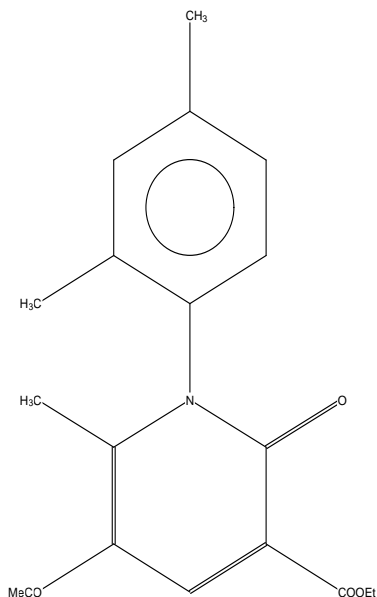
**Reference:** S.S.Hayotsyan, A.H.Hasratyan, S.G.Konkova, A.Kh.Khachatryan, A.E.Badasyan, A.G.Ayvazyan, G.A.Panosyan, M.S.Sargsyan (2014) *Chemistry of Heterocyclic Compounds*, **50**,1126

**Formula:** C<sub>19</sub>H<sub>21</sub>N<sub>1</sub>O<sub>4</sub>

**Compound Name:** ethyl 5-acetyl-1-(2,4-dimethylphenyl)-6-methyl-2-oxo-1,2-dihydropyridine-3-carboxylate

**Space Group:** P-1 **Cell:** a 8.847(1) b 10.083(2) c 11.343(2)  
**Space Group No.:** 2 **(Å, °)** α 111.01(3) β 96.31(3) γ 107.42(3)

**R-Factor (%):** 5.43 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.244



**Parameters**  
 Fragment 1  
**ANG1 (Å)** 85.446

## DACNIG

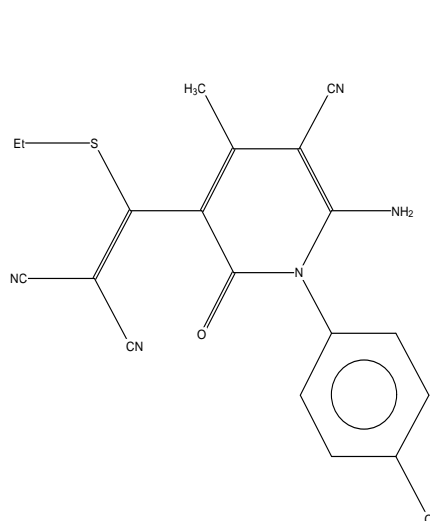
**Reference:** Xiuyun Yang, Yanyan Cheng, Fei Zhao, Yunhui Li, Yuanli Ding, Yongjiu Liang, Fengjiao Gan, Dewen Dong (2011) *Tetrahedron*, **67**,8343

**Formula:** C<sub>19</sub>H<sub>14</sub>Cl<sub>1</sub>N<sub>5</sub>O<sub>1</sub>S<sub>1</sub>

**Compound Name:** ((6-Amino-1-(4-chlorophenyl)-5-cyano-4-methyl-2-oxo-1,2-dihydropyridin-3-yl)(ethylsulfanyl)methylene)malononitrile

**Space Group:** Pbcu **Cell:** a 16.362(1) b 10.661(1) c 22.235(2)  
**Space Group No.:** 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 4.47 **Temperature(K):** 298 **Density(g/cm<sup>3</sup>):** 1.356



**Parameters**  
 Fragment 1  
**ANG1 (Å)** 76.040

## DITSOQ

**Reference:** K.Keshav, A.J.Elias (2013) *Inorg.Chem.Commun.*, **35**,346

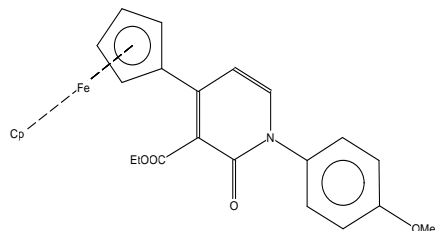
**Formula:** C<sub>25</sub>H<sub>23</sub>Fe<sub>1</sub>N<sub>1</sub>O<sub>4</sub>

**Compound Name:** (2-(Ethoxycarbonyl)-4-(4-ethylphenyl)-3-oxocyclohexa-1,5-dien-1-yl) ferrocene

**Space Group:** P-1 **Cell:** a 7.249(1) b 10.326(1) c 15.293(2)  
**Space Group No.:** 2 **(Å, °)** α 97.17(0) β 103.27(0) γ 102.86(0)

**R-Factor (%):** 4.09 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.423

**Parameters**  
 Fragment 1  
**ANG1 (Å)** 62.153



## DOCKIP

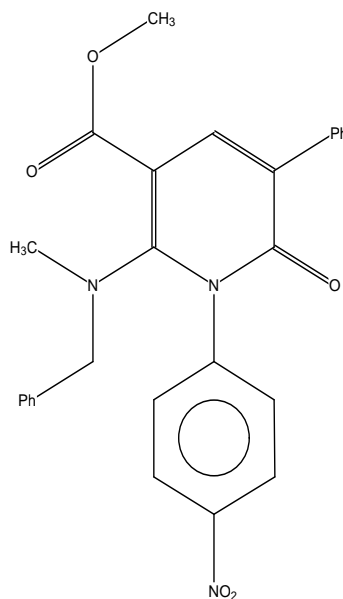
**Reference:** M.J.Arevalo, M.Avalos, R.Babiano, P.Cintas, M.B.Hursthouse, J.L.Jimenez, M.E.Light, I.Lopez, J.C.Palacios (2000) *Tetrahedron*, **56**,1247

**Formula:** C<sub>27</sub>H<sub>23</sub>N<sub>3</sub>O<sub>5</sub>

**Compound Name:** 6-(Benzyl(methyl)amino)-5-methoxycarbonyl-1-(4-nitrophenyl)-3-phenylpyridin-2-one

**Space Group:** P-1 **Cell:** a 10.097(0) b 10.387(0) c 13.135(0)  
**Space Group No.:** 2 **(Å, °)** α 99.62(0) β 101.52(0) γ 116.23(0)

**R-Factor (%):** 4.39 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.346



**Parameters**  
 Fragment 1  
**ANG1 (Å)** 71.977

# Search: search4 (Sun May 19 12:50:34 2019): Hits 9-12

## EBATIK

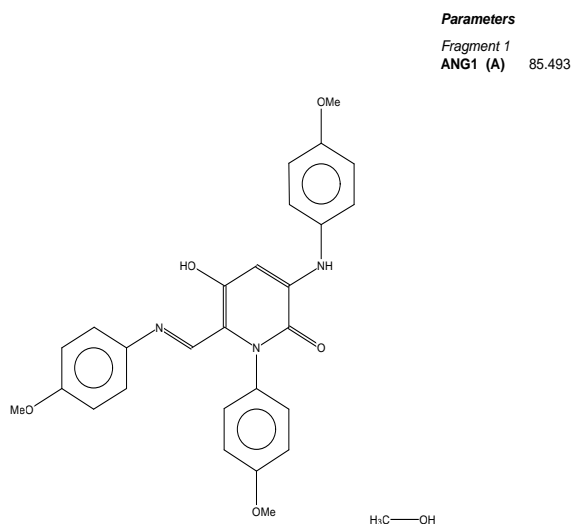
**Reference:** M.Kozul, Z.Stiplosek, Z.Orhanovic, K.Jakopic, A.Nagl, A.Hergold-Brundic (1999) *J.Heterocycl.Chem.* ,**36**,493

**Formula:** C<sub>27</sub> H<sub>25</sub> N<sub>3</sub> O<sub>5</sub>.0.5(C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>)

**Compound Name:** 5-Hydroxy-3-(4-methoxyphenylamino)-6-(4-methoxyphenylimino)methyl-N-(4-methoxyphenyl)-2-pyridone methanol solvate

**Space Group:** C2/c    **Cell:**    *a* 16.046(5)    *b* 8.755(3)    *c* 36.790(9)  
**Space Group No.:** 15    **(Å,°)**    α 90.00    β 97.42(2)    γ 90.00

**R-Factor (%):** 7.14    **Temperature(K):** 295    **Density(g/cm<sup>3</sup>):** 1.264



## FEQJET

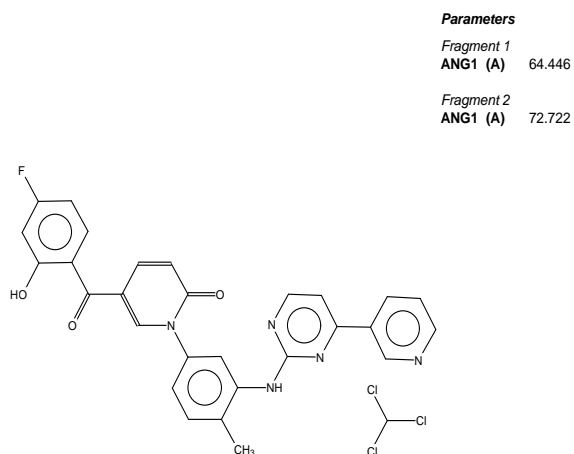
**Reference:** P.Manchanda, B.Parshad, A.Kumar, R.Tiwari, A.Shirazi, K.Parang, S.Sharma (2017) *Arch.Pharm.Chem.Life Sci.* ,**350**,e1600390

**Formula:** C<sub>28</sub> H<sub>20</sub> F<sub>1</sub> N<sub>5</sub> O<sub>3</sub>.x(C<sub>1</sub> H<sub>1</sub> Cl<sub>3</sub>)

**Compound Name:** 5-(4-fluoro-2-hydroxybenzoyl)-1-(4-methyl-3-((4-pyridin-3-yl)pyrimidin-2-yl)amino)phenylpyridin-2(1H)-one chloroform solvate

**Space Group:** P21    **Cell:**    *a* 10.417(5)    *b* 21.881(5)    *c* 14.589(5)  
**Space Group No.:** 4    **(Å,°)**    α 90.00    β 104.23(0)    γ 90.00

**R-Factor (%):** 11.36    **Temperature(K):** 173    **Density(g/cm<sup>3</sup>):** 1.263



## HANDIL

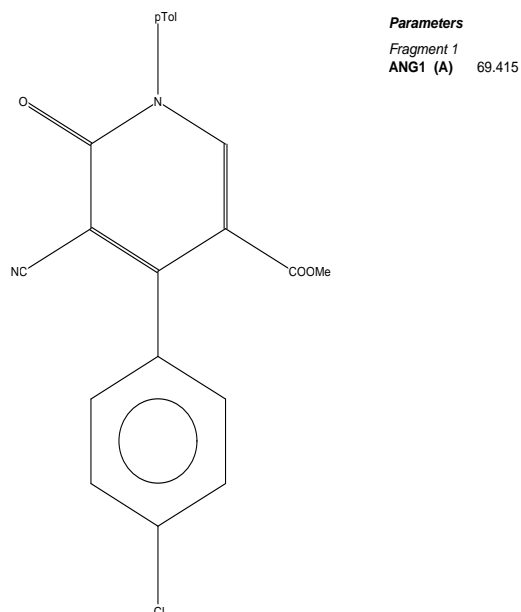
**Reference:** Jing Sun, Yan Sun, Er-Yan Xia, Chao-Guo Yan (2011) *ACS Comb. Sci.* ,**13**,436

**Formula:** C<sub>21</sub> H<sub>15</sub> Cl<sub>1</sub> N<sub>2</sub> O<sub>3</sub>

**Compound Name:** Methyl 4-(4-chlorophenyl)-5-cyano-1-(4-methylphenyl)-6-oxo-1,6-dihydropyridine-3-carboxylate

**Space Group:** P21/c    **Cell:**    *a* 11.362(3)    *b* 13.771(3)    *c* 11.908(3)  
**Space Group No.:** 14    **(Å,°)**    α 90.00    β 95.54(0)    γ 90.00

**R-Factor (%):** 4.19    **Temperature(K):** 296    **Density(g/cm<sup>3</sup>):** 1.357



## HURMUD

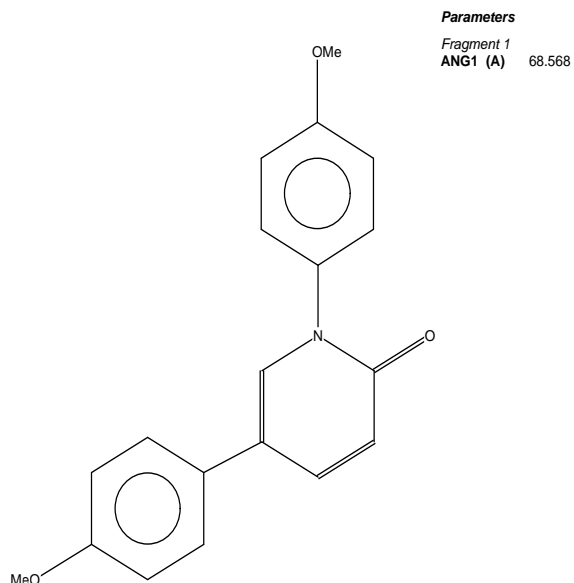
**Reference:** J.S.Siddle, A.S.Batsanov, S.T.Caldwell, G.Cooke, M.R.Bryce (2010) *Tetrahedron* ,**66**,6138

**Formula:** C<sub>19</sub> H<sub>17</sub> N<sub>1</sub> O<sub>3</sub>

**Compound Name:** 1,5-bis(4-methoxyphenyl)pyridin-2(1H)-one

**Space Group:** P21/c    **Cell:**    *a* 10.647(0)    *b* 12.516(0)    *c* 11.497(0)  
**Space Group No.:** 14    **(Å,°)**    α 90.00    β 93.90(0)    γ 90.00

**R-Factor (%):** 4.91    **Temperature(K):** 120    **Density(g/cm<sup>3</sup>):** 1.336



# Search: search4 (Sun May 19 12:50:34 2019): Hits 13-16

## IDOMAR

**Reference:** F.Ren, G.Li, Q.Zhang, J.Yao, X.Zhang (2013)  
*Acta Crystallogr., Sect.E:Struct.Rep. Online*, **69**,o732

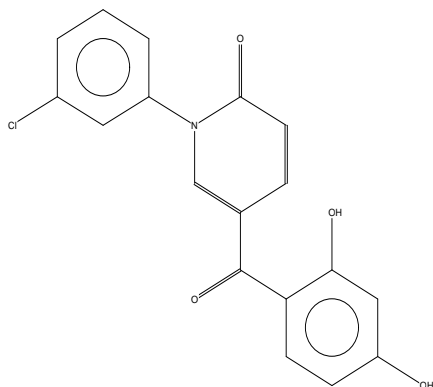
**Formula:** C<sub>18</sub> H<sub>12</sub> Cl<sub>1</sub> N<sub>1</sub> O<sub>4</sub>

**Compound Name:** 1-(3-Chlorophenyl)-5-(2,4-dihydroxybenzoyl)pyridin-2(1H)-one

**Space Group:** P-1 **Cell:** a 6.689(3) b 9.009(4) c 13.257(6)  
**Space Group No.:** 2 **(Å,°)** α 87.19(0) β 87.72(0) γ 82.67(0)

**R-Factor (%):** 7.80 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.435

**Parameters**  
Fragment 1  
ANG1 (Å) 85.808



## IQOREM

**Reference:** H.Reinke, I.O.Martinez, K.Peseke (2010)  
*CSD Communication(Private Communication)*,

**Formula:** C<sub>30</sub> H<sub>33</sub> N<sub>1</sub> O<sub>7</sub>

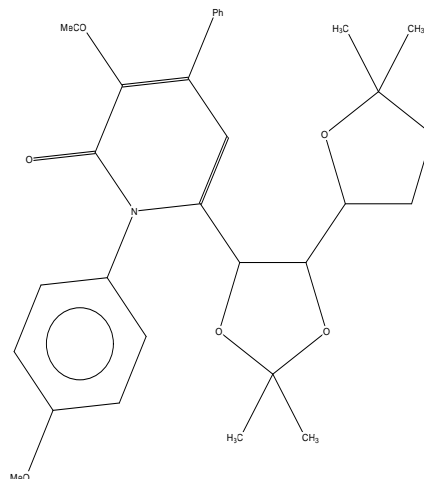
**Compound Name:** 3-Acetyl-1,2-dihydro-1-(4-methoxyphenyl)-6-(methyl 2-O-benzyl-4,6-O-benzylidene-3-deoxy-α-D-altropyranosid-3-ylmethyl)-4-phenylpyridin-2-one

**Synonym:** 3-Acetyl-1-(4-methoxyphenyl)-4-phenyl-6-(2,2,2',2'-tetramethyl-4,4'-bi-1,3-dioxol-5-yl)pyridin-2(1H)-one

**Space Group:** P21 **Cell:** a 12.165(0) b 9.001(0) c 12.224(0)  
**Space Group No.:** 4 **(Å,°)** α 90.00 β 90.34(0) γ 90.00

**R-Factor (%):** 3.84 **Temperature(K):** 173 **Density(g/cm<sup>3</sup>):** 1.289

**Parameters**  
Fragment 1  
ANG1 (Å) 86.707



## LIHKAP

**Reference:** Wei Pan, Dewen Dong, Kewei Wang, Jie Zhang,  
Rigenhada Wu, Dexuan Xiang, Qun Liu (2007) *Org.Lett.*, **9**,2421

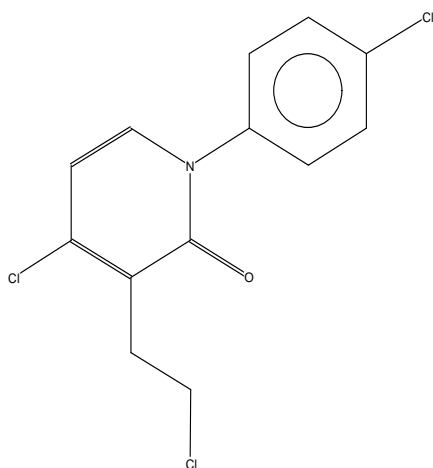
**Formula:** C<sub>13</sub> H<sub>10</sub> Cl<sub>3</sub> N<sub>1</sub> O<sub>1</sub>

**Compound Name:** 4-Chloro-3-(2-chloroethyl)-1-(4-chlorophenyl)pyridin-2(1H)-one

**Space Group:** P21/n **Cell:** a 11.077(0) b 7.208(0) c 17.355(0)  
**Space Group No.:** 14 **(Å,°)** α 90.00 β 105.98(0) γ 90.00

**R-Factor (%):** 4.18 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.509

**Parameters**  
Fragment 1  
ANG1 (Å) 51.687



## MAYWUF

**Reference:** H.Schirok, C.Alonso-Alija, J.Benet-Buchholz, A.H.Goller,  
R.Grosser, M.Michels, H.Paulsen (2005) *J.Org.Chem.*, **70**,9463

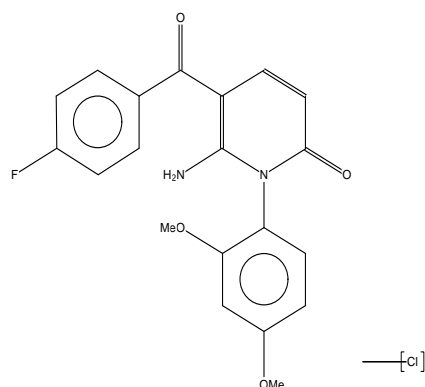
**Formula:** C<sub>20</sub> H<sub>17</sub> F<sub>1</sub> N<sub>2</sub> O<sub>4</sub> C<sub>1</sub> H<sub>1</sub> Cl<sub>3</sub>

**Compound Name:** (S)-6-Amino-5-(4-fluorobenzoyl)-1-(2,4-dimethoxyphenyl)-2(1H)-pyridone chloroform solvate

**Space Group:** P21 **Cell:** a 11.610(0) b 7.543(0) c 12.852(0)  
**Space Group No.:** 4 **(Å,°)** α 90.00 β 104.62(0) γ 90.00

**R-Factor (%):** 5.48 **Temperature(K):** 90 **Density(g/cm<sup>3</sup>):** 1.487

**Parameters**  
Fragment 1  
ANG1 (Å) 83.936



# Search: search4 (Sun May 19 12:50:34 2019): Hits 17-20

## MOMTIT

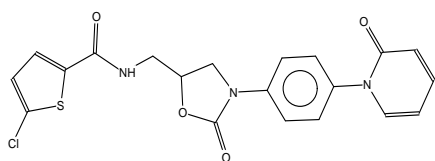
**Reference:** Wei Liu, Jing Yuan, Shi-Jun Zhang, Wei-Ren Xu, Chang-Jiang Huang, Li-Da Tang (2014) *Jiegou Huaxue(Chin. J.Chin.J.Struct.Chem.)*, **33**,1091

**Formula:** C<sub>20</sub> H<sub>16</sub> Cl<sub>1</sub> N<sub>3</sub> O<sub>4</sub> S<sub>1</sub>

**Compound Name:** 5-chloro-N-((2-oxo-3-(4-(2-oxopyridin-1(2H)-yl)phenyl)-1,3-oxazolidin-5-yl)methyl)thiophene-2-carboxamide

**Space Group:** P21 **Cell:** a 5.790(1) b 13.086(3) c 12.889(3)  
**Space Group No.:** 4 **(Å,°)** α 90.00 β 100.86(3) γ 90.00

**R-Factor (%):** 3.22 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.489



**Parameters**  
 Fragment 1  
 ANG1 (A) 56.071

## NAQXEL

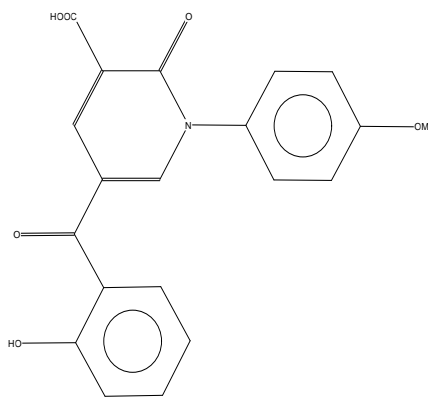
**Reference:** R.S.G.R.Seixas, G.C.Ribeiro, S.Guieu, A.M.S.Silva (2016) *Chem. Sel.*, **1**,318

**Formula:** C<sub>20</sub> H<sub>15</sub> N<sub>1</sub> O<sub>6</sub>

**Compound Name:** 5-(2-hydroxybenzoyl)-1-(4-methoxyphenyl)-2-oxo-1,2-dihydropyridine-3-carboxylic acid

**Space Group:** P21/c **Cell:** a 8.359(0) b 8.092(0) c 24.902(1)  
**Space Group No.:** 14 **(Å,°)** α 90.00 β 95.45(0) γ 90.00

**R-Factor (%):** 3.42 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.447



**Parameters**  
 Fragment 1  
 ANG1 (A) 61.777

## NEDWUO

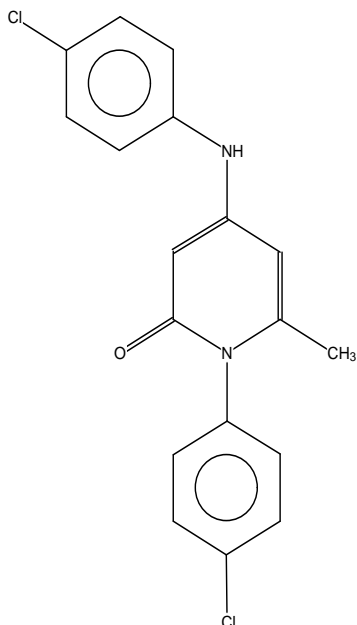
**Reference:** V.Bertolasi, P.Gilli, V.Ferretti, G.Gilli (1998) *Acta Crystallogr.,Sect.B:Struct.Sci.*, **54**,50

**Formula:** C<sub>18</sub> H<sub>14</sub> Cl<sub>2</sub> N<sub>2</sub> O<sub>1</sub>

**Compound Name:** 1-(4-Chlorophenyl)-4-(4-chlorophenylamino)-6-methyl-2-pyridone

**Space Group:** Pbca **Cell:** a 14.244(2) b 9.645(1) c 23.711(3)  
**Space Group No.:** 61 **(Å,°)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 4.10 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.408



**Parameters**  
 Fragment 1  
 ANG1 (A) 76.625

## NESBAO

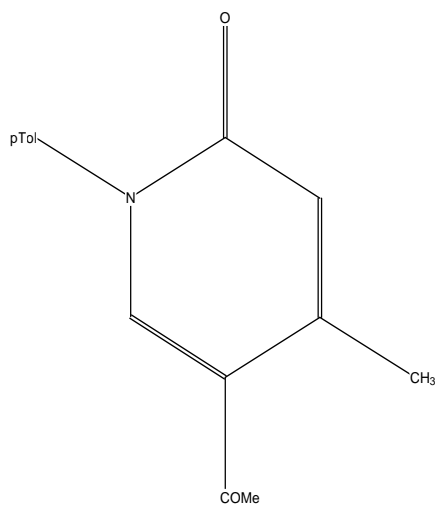
**Reference:** G.A.Cartwright, R.O.Gould, H.McNab (1997) *Chem.Commun.*, 1293

**Formula:** C<sub>15</sub> H<sub>15</sub> N<sub>1</sub> O<sub>2</sub>

**Compound Name:** 5-Acetyl-N-p-tolyl-4-methyl-2-pyridone

**Space Group:** P212121 **Cell:** a 5.557(4) b 9.645(4) c 24.272(10)  
**Space Group No.:** 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 2.60 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.232



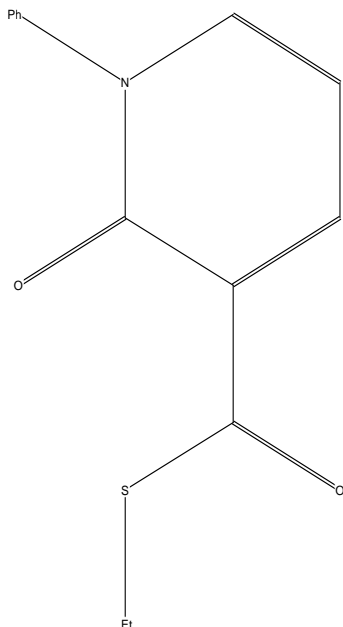
**Parameters**  
 Fragment 1  
 ANG1 (A) 81.481

# Search: search4 (Sun May 19 12:50:34 2019): Hits 21-24

## NOLBIA

**Reference:** Jun Liu, Deqiang Liang, Mang Wang, Qun Liu (2008) *Synthesis*, 3633  
**Formula:** C<sub>14</sub> H<sub>13</sub> N<sub>1</sub> O<sub>2</sub> S<sub>1</sub>  
**Compound Name:** S-Ethyl 2-oxo-1-phenyl-1,2-dihydro-3-pyridinecarbothioate

**Space Group:** P21 **Cell:** a 5.643(1) b 12.163(3) c 9.504(2)  
**Space Group No.:** 4 **(Å, °)** α 90.00 β 90.00 γ 90.00  
**R-Factor (%):** 4.28 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.320

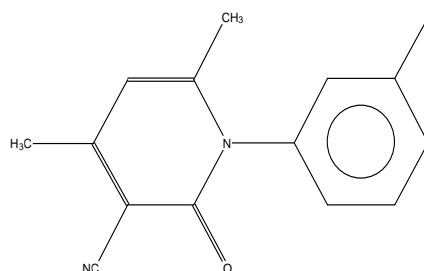


**Parameters**  
**Fragment 1**  
**ANG1 (Å)** 65.502

## PAVQIO

**Reference:** M.S.Al-Said, M.M.Ghorab, H.A.Ghabbour, S.Arshad, H.-K.Fun (2012) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, 68,01679  
**Formula:** C<sub>16</sub> H<sub>16</sub> N<sub>2</sub> O<sub>1</sub>  
**Compound Name:** 1-(3-Ethylphenyl)-4,6-dimethyl-2-oxo-1,2-dihydropyridine-3-carbonitrile

**Space Group:** P21/c **Cell:** a 8.383(0) b 7.185(0) c 23.526(0)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 93.20(0) γ 90.00  
**R-Factor (%):** 4.74 **Temperature(K):** 296 **Density(g/cm<sup>3</sup>):** 1.184

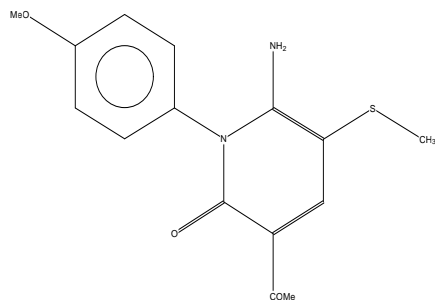


**Parameters**  
**Fragment 1**  
**ANG1 (Å)** 85.331

## POSZEE

**Reference:** Qian Zhang, Xu Liu, Xiaoqing Xin, Rui Zhang, Yongjiu Liang, Dewen Dong (2014) *Chem.Commun.*, 50,15378  
**Formula:** C<sub>15</sub> H<sub>16</sub> N<sub>2</sub> O<sub>3</sub> S<sub>1</sub>  
**Compound Name:** 3-Acetyl-6-amino-1-(4-methoxyphenyl)-5-(methylthio)pyridin-2(1H)-one

**Space Group:** Pccn **Cell:** a 18.861(1) b 9.284(0) c 16.581(1)  
**Space Group No.:** 56 **(Å, °)** α 90.00 β 90.00 γ 90.00  
**R-Factor (%):** 4.58 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.393

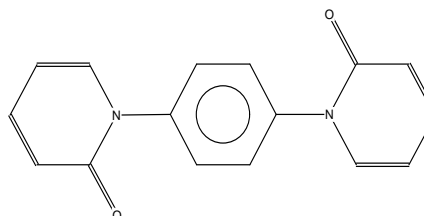


**Parameters**  
**Fragment 1**  
**ANG1 (Å)** 86.203

## QERTEN

**Reference:** Chenguang Li, P.D.Robinson, D.J.Dyer (2006) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, 62,05045  
**Formula:** C<sub>16</sub> H<sub>12</sub> N<sub>2</sub> O<sub>2</sub>  
**Compound Name:** 1-(4-(2-Oxopyridin-1(2H)-yl)phenyl)pyridin-2(1H)-one

**Space Group:** P-1 **Cell:** a 5.891(1) b 6.703(1) c 8.871(1)  
**Space Group No.:** 2 **(Å, °)** α 76.50(3) β 71.33(3) γ 67.44(3)  
**R-Factor (%):** 4.00 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.444



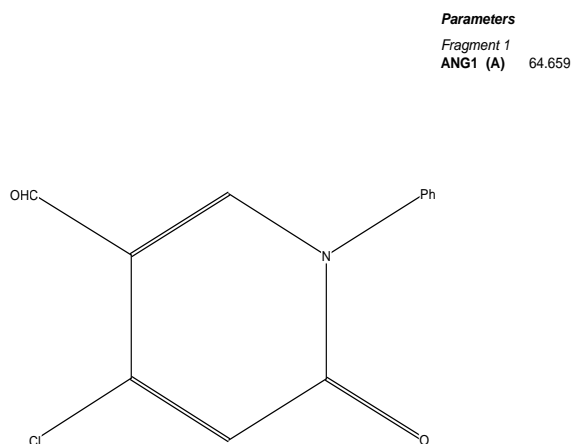
**Parameters**  
**Fragment 1**  
**ANG1 (Å)** 55.947

# Search: search4 (Sun May 19 12:50:34 2019): Hits 25-28

## QIWFIM

**Reference:** Dexuan Xiang, Kewei Wang, Yongjiu Liang, Guangyuan Zhou, Dewen Dong (2008) *Org.Lett.* ,10,345  
**Formula:** C<sub>12</sub>H<sub>8</sub>Cl<sub>1</sub>N<sub>1</sub>O<sub>2</sub>  
**Compound Name:** 4-Chloro-6-oxo-1-phenyl-1,6-dihydropyridine-3-carbaldehyde

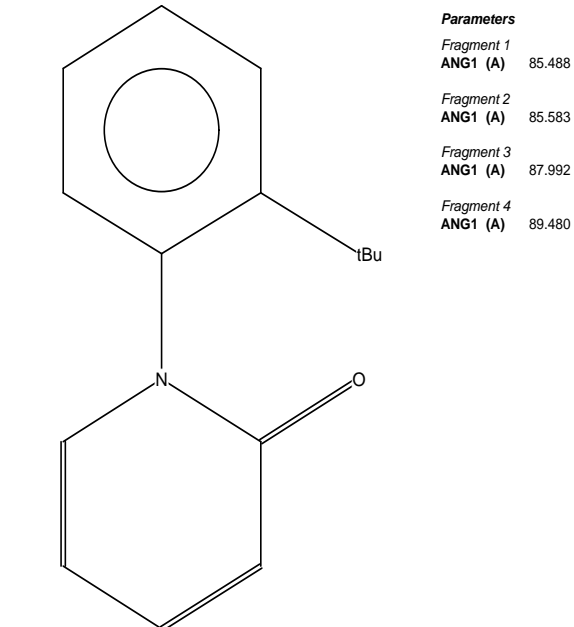
**Space Group:** P21/c **Cell:** a 11.067(5) b 12.890(5) c 7.536(5)  
**Space Group No.:** 14 **Cell:** (Å, °) α 90.00 β 103.02(0) γ 90.00  
**R-Factor (%):** 3.23 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.482



## SAPTUA

**Reference:** E. Kumarasamy, J.L.Jesuraj, J.N.Omlid, A.Ugrinov, J.Sivaguru (2011) *J.Am.Chem.Soc.* ,133,17106  
**Formula:** C<sub>15</sub>H<sub>17</sub>N<sub>1</sub>O<sub>1</sub>  
**Compound Name:** (M)-(-)-1-(2-t-Butylphenyl)pyridin-2(1H)-one

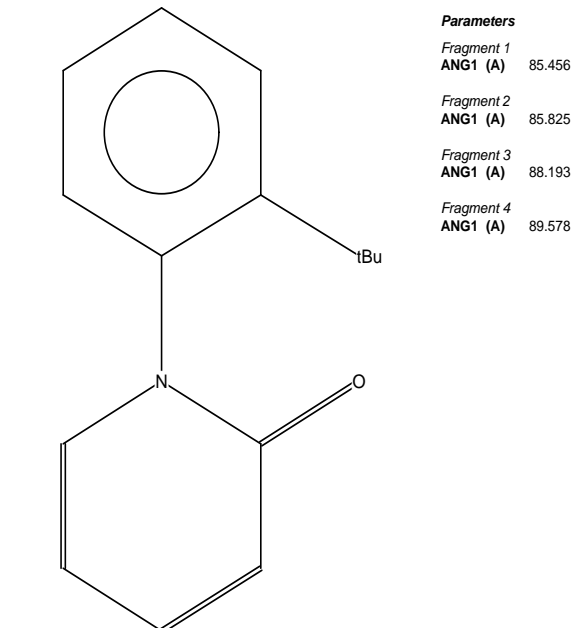
**Space Group:** P21 **Cell:** a 15.318(0) b 11.433(0) c 16.002(0)  
**Space Group No.:** 4 **Cell:** (Å, °) α 90.00 β 117.60(0) γ 90.00  
**R-Factor (%):** 4.19 **Temperature(K):** 100 **Density(g/cm<sup>3</sup>):** 1.216



## SAPVAI

**Reference:** E.Kumarasamy, J.L.Jesuraj, J.N.Omlid, A.Ugrinov, J.Sivaguru (2011) *J.Am.Chem.Soc.* ,133,17106  
**Formula:** C<sub>15</sub>H<sub>17</sub>N<sub>1</sub>O<sub>1</sub>  
**Compound Name:** (P)-(+)-1-(2-t-Butylphenyl)pyridin-2(1H)-one

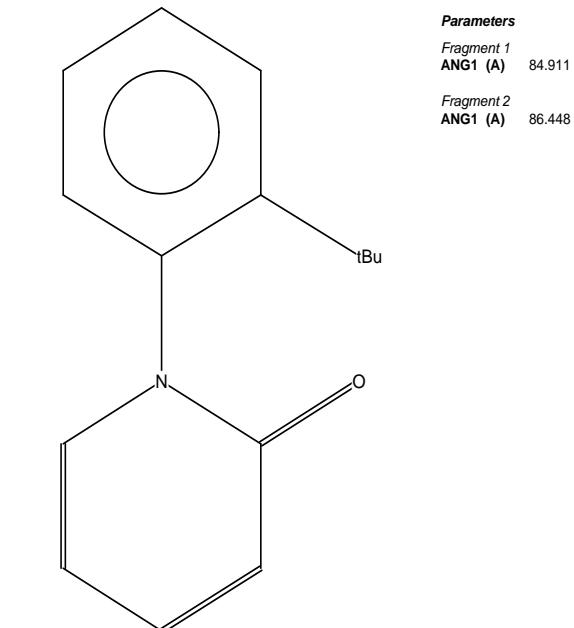
**Space Group:** P21 **Cell:** a 15.322(0) b 11.427(0) c 16.041(0)  
**Space Group No.:** 4 **Cell:** (Å, °) α 90.00 β 117.82(0) γ 90.00  
**R-Factor (%):** 6.87 **Temperature(K):** 100 **Density(g/cm<sup>3</sup>):** 1.216



## SAPVAI01

**Reference:** E.Kumarasamy, J.L.Jesuraj, J.N.Omlid, A.Ugrinov, J.Sivaguru (2011) *J.Am.Chem.Soc.* ,133,17106  
**Formula:** C<sub>15</sub>H<sub>17</sub>N<sub>1</sub>O<sub>1</sub>  
**Compound Name:** (P)-(+)-1-(2-t-Butylphenyl)pyridin-2(1H)-one

**Space Group:** P212121 **Cell:** a 6.875(0) b 12.488(0) c 30.403(0)  
**Space Group No.:** 19 **Cell:** (Å, °) α 90.00 β 90.00 γ 90.00  
**R-Factor (%):** 2.61 **Temperature(K):** 100 **Density(g/cm<sup>3</sup>):** 1.157





# Search: search4 (Sun May 19 12:50:34 2019): Hits 29-32

## SAPVIQ

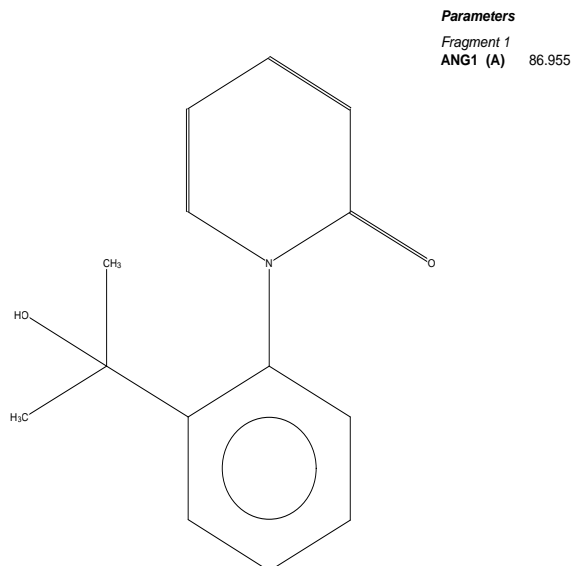
**Reference:** E.Kumarasamy, J.L.Jesuraj, J.N.Omid, A.Ugrinov, J.Sivaguru (2011) *J.Am.Chem.Soc.* ,133,17106

**Formula:** C<sub>14</sub> H<sub>15</sub> N<sub>1</sub> O<sub>2</sub>

**Compound Name:** 1-(2-(2-Hydroxypropan-2-yl)phenyl)pyridin-2(1H)-one

**Space Group:** Pbc<sub>a</sub> **Cell:** a 8.577(0) b 15.017(0) c 18.426(0)  
**Space Group No.:** 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 3.69 **Temperature(K):** 100 **Density(g/cm<sup>3</sup>):** 1.283



## SAPVOW

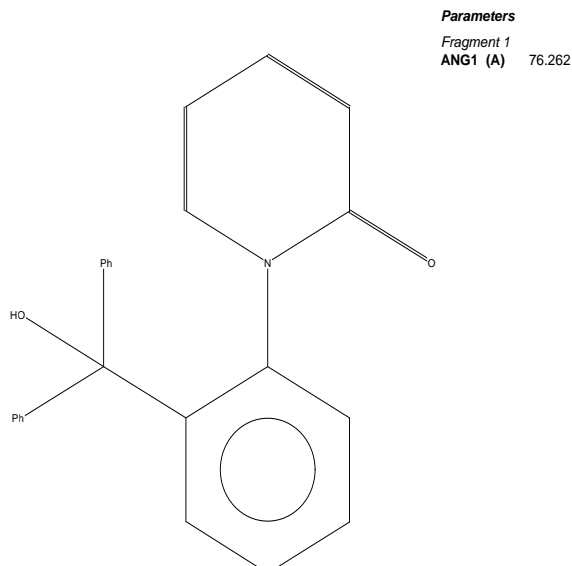
**Reference:** E.Kumarasamy, J.L.Jesuraj, J.N.Omid, A.Ugrinov, J.Sivaguru (2011) *J.Am.Chem.Soc.* ,133,17106

**Formula:** C<sub>24</sub> H<sub>19</sub> N<sub>1</sub> O<sub>2</sub>

**Compound Name:** 1-(2-(Hydroxy(diphenyl)methyl)phenyl)pyridin-2(1H)-one

**Space Group:** P2<sub>1</sub>/n **Cell:** a 17.601(10) b 6.388(4) c 18.243(10)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 114.99(0) γ 90.00

**R-Factor (%):** 4.68 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.263



## TEMKIH

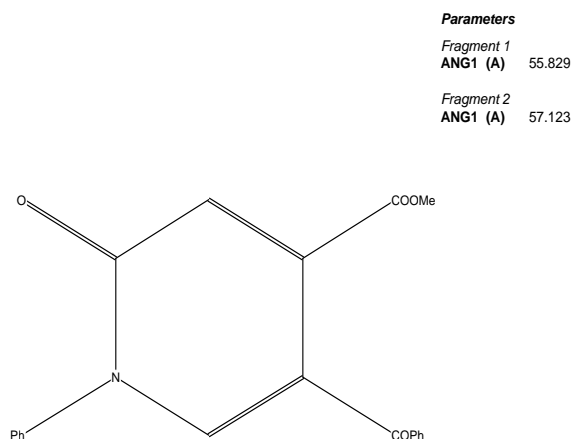
**Reference:** Yushang Shao, Wenjun Yao, Jun Liu, Kai Zhu, Yanzhong Li (2012) *Synthesis* ,44,3301

**Formula:** C<sub>20</sub> H<sub>15</sub> N<sub>1</sub> O<sub>4</sub>

**Compound Name:** Methyl 5-benzoyl-2-oxo-1-phenyl-1,2-dihydropyridine-4-carboxylate

**Space Group:** Pna2<sub>1</sub> **Cell:** a 20.251(1) b 10.933(0) c 14.994(1)  
**Space Group No.:** 33 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 6.71 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.334



## USOTIH

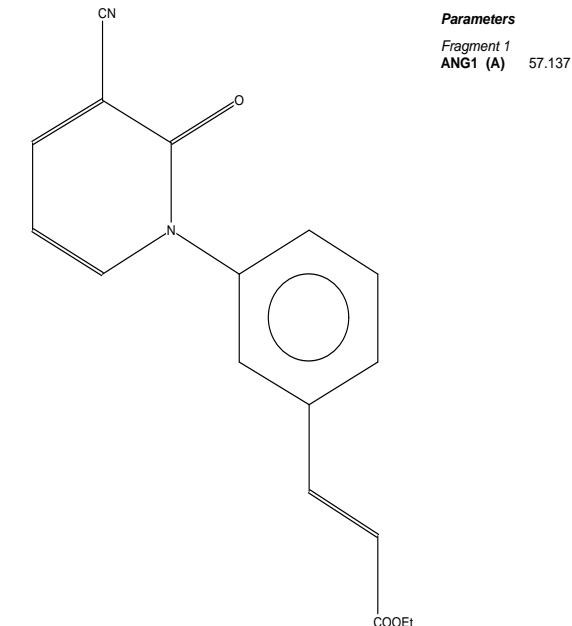
**Reference:** M.Hebert, P.Petiot, E.Benoit, J.Dansereau, T.Ahmad, A.Le Roch, X.Ottenwaelde, A.Gagnon (2016) *J.Org.Chem.* ,81,5401

**Formula:** C<sub>17</sub> H<sub>14</sub> N<sub>2</sub> O<sub>3</sub>

**Compound Name:** ethyl 3-(3-(3-cyano-2-oxopyridin-1(2H)-yl)phenyl)acrylate

**Space Group:** P-1 **Cell:** a 7.015(0) b 7.074(0) c 15.121(0)  
**Space Group No.:** 2 **(Å, °)** α 83.64(0) β 80.15(0) γ 73.30(0)

**R-Factor (%):** 4.72 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.383



# Search: search4 (Sun May 19 12:50:34 2019): Hits 33-36

## VATBOJ

**Reference:** Li Xing, B.Devadas, R.V.Devraj, S.R.Selness, Huey Shieh, J.K.Walker, M.Mao, D.Messing, B.Samas, J.Z.Yang, G.D.Anderson, E.G.Webb, J.B.Monahan (2012) *ChemMedChem* **7**,273

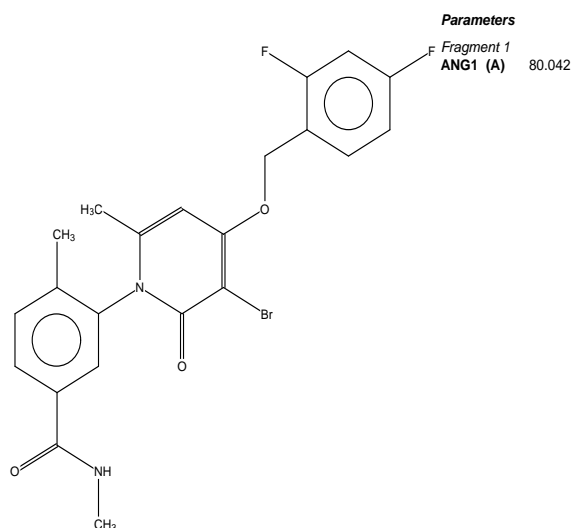
**Formula:** C<sub>22</sub>H<sub>19</sub>BrF<sub>2</sub>N<sub>2</sub>O<sub>3</sub>

**Compound Name:** 3-(3-Bromo-4-((2,4-difluorobenzyl)oxy)-6-methyl-2-oxopyridin-1(2H)-yl)-N,4-dimethylbenzamide

**Synonym:** PDB Chemical Component code: I45

**Space Group:** P21 **Cell:** a 11.227(1) b 7.432(1) c 12.747(2)  
**Space Group No.:** 4 **Cell:** (Å, °) α 90.00 β 101.64(0) γ 90.00

**R-Factor (%):** 4.82 **Temperature(K):** 301 **Density(g/cm<sup>3</sup>):** 1.522



## VIDNOM

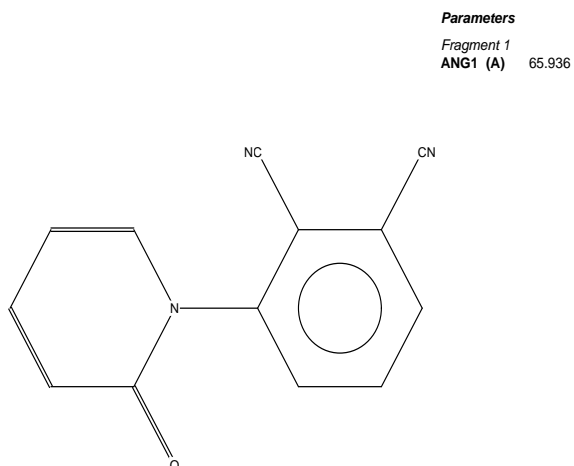
**Reference:** Jin-Ping Xue, Hua-Li Zhu, Nai-Sheng Chen, Jin-Ling Huang (2007) *Acta Crystallogr., Sect. E: Struct. Rep. Online* **63**, o2434

**Formula:** C<sub>13</sub>H<sub>7</sub>N<sub>3</sub>O<sub>1</sub>

**Compound Name:** 3-(2-Oxo-2H-pyridin-1-yl)phthalonitrile

**Space Group:** P21/n **Cell:** a 8.132(6) b 11.739(6) c 11.224(6)  
**Space Group No.:** 14 **Cell:** (Å, °) α 90.00 β 97.21(3) γ 90.00

**R-Factor (%):** 3.96 **Temperature(K):** 173 **Density(g/cm<sup>3</sup>):** 1.382



## VISLUF

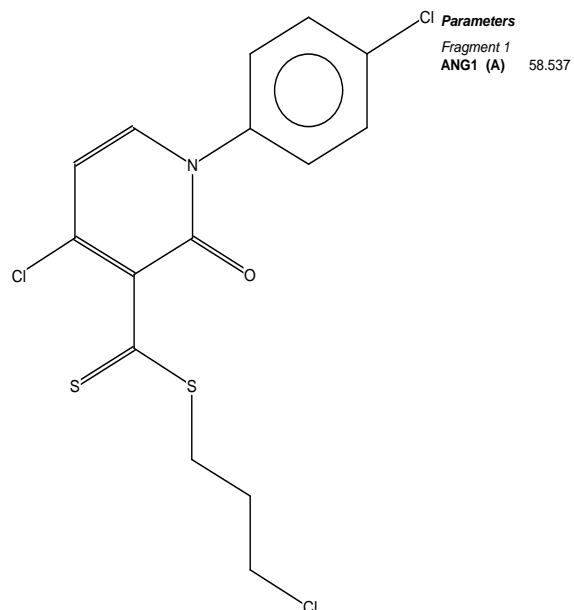
**Reference:** Li Chen, Yu-Long Zhao, Qun Liu, Chao Cheng, Cheng-Ri Piao (2007) *J. Org. Chem.* **72**,9259

**Formula:** C<sub>15</sub>H<sub>12</sub>Cl<sub>3</sub>N<sub>1</sub>O<sub>1</sub>S<sub>2</sub>

**Compound Name:** 3-Chloropropyl 4-chloro-1-(4-chlorophenyl)-2-oxo-1,2-dihydropyridine-3-carbodithioate

**Space Group:** P21/c **Cell:** a 8.775(0) b 22.221(2) c 8.826(0)  
**Space Group No.:** 14 **Cell:** (Å, °) α 90.00 β 97.23(0) γ 90.00

**R-Factor (%):** 3.83 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.528



## WEDCEP

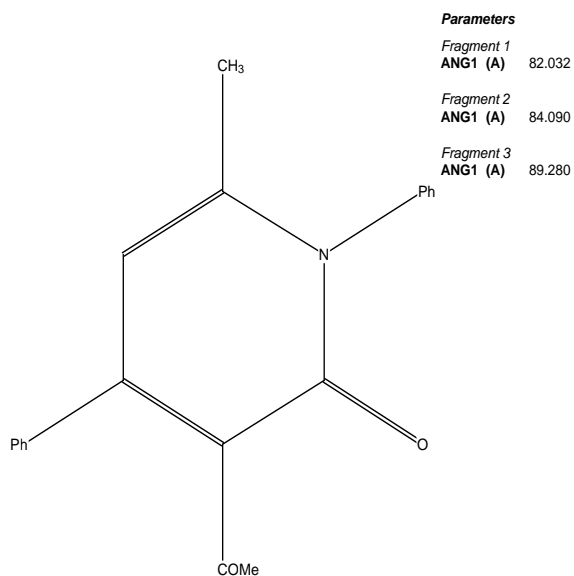
**Reference:** C.Allais, O.Basle, J.-M.Grassot, M.Fontaine, S.Anguille, J.Rodriguez, T.Constantieux (2012) *Adv. Synth. Catal.* **354**,2084

**Formula:** C<sub>20</sub>H<sub>17</sub>N<sub>1</sub>O<sub>2</sub>

**Compound Name:** 3-Acetyl-6-methyl-1,4-diphenylpyridin-2(1H)-one

**Space Group:** P-1 **Cell:** a 7.413(0) b 16.092(0) c 21.111(0)  
**Space Group No.:** 2 **Cell:** (Å, °) α 102.31(0) β 98.76(0) γ 91.70(0)

**R-Factor (%):** 7.62 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.246



# Search: search4 (Sun May 19 12:50:34 2019): Hits 37-40

## XIQGAF

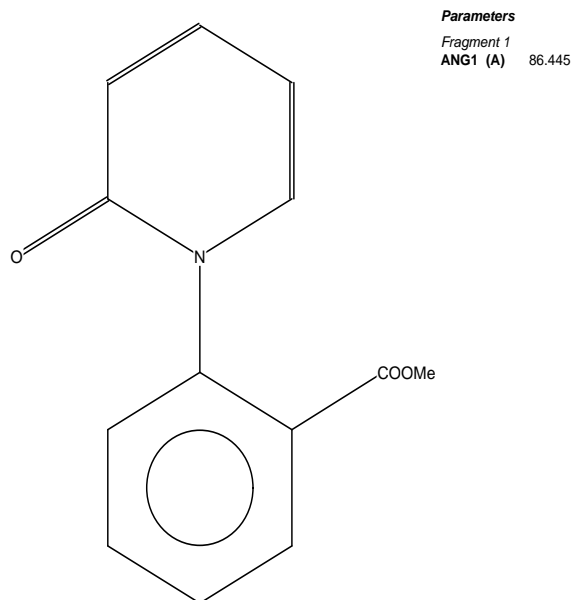
**Reference:** D.K.Rayabarapu, K.K.Majumdar, T.Sambaiah, Chein-Hong Cheng (2001) *J.Org.Chem.*, **66**,3646

**Formula:** C<sub>13</sub>H<sub>11</sub>N<sub>1</sub>O<sub>3</sub>

**Compound Name:** methyl 2-(2-oxo-1,2-dihydro-1-pyridyl)benzoate

**Space Group:** P21/c **Cell:** a 9.362(1) b 12.970(1) c 9.287(1)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 91.07(0) γ 90.00

**R-Factor (%):** 4.82 **Temperature(K):** 294 **Density(g/cm<sup>3</sup>):** 1.351



## XIQGEJ

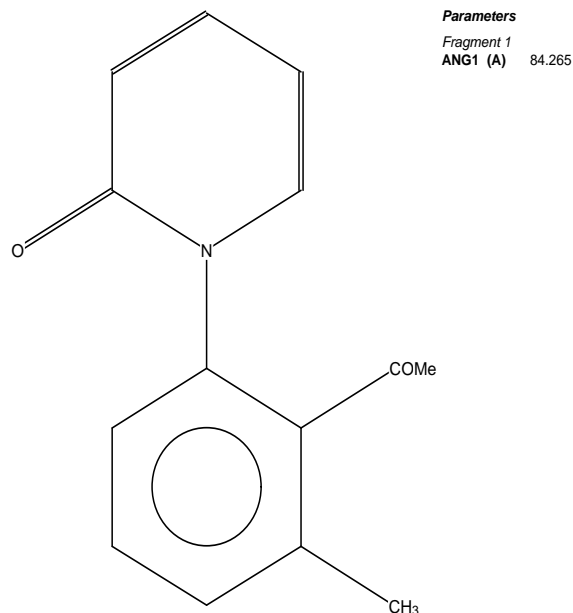
**Reference:** D.K.Rayabarapu, K.K.Majumdar, T.Sambaiah, Chein-Hong Cheng (2001) *J.Org.Chem.*, **66**,3646

**Formula:** C<sub>14</sub>H<sub>13</sub>N<sub>1</sub>O<sub>2</sub>

**Compound Name:** 1-(2-acetyl-3-methylphenyl)-1,2-dihydro-2-pyridone

**Space Group:** P21/c **Cell:** a 8.171(0) b 7.945(0) c 19.026(2)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 102.40(0) γ 90.00

**R-Factor (%):** 5.27 **Temperature(K):** 294 **Density(g/cm<sup>3</sup>):** 1.251



## YAPBUO

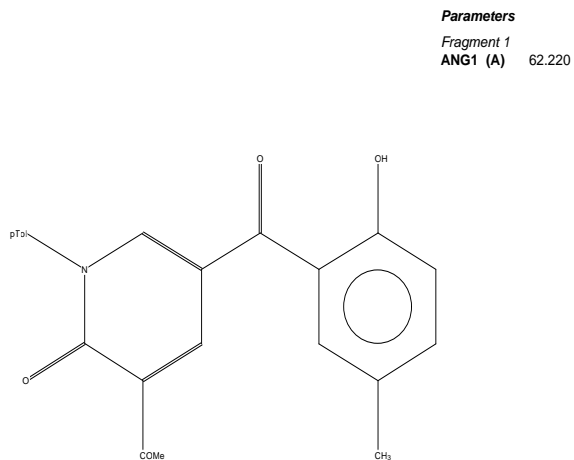
**Reference:** T.Sengupta, K.S.Gayen, P.Pandit, D.K.Maiti (2012) *Chem.-Eur.J.*, **18**,1905

**Formula:** C<sub>22</sub>H<sub>19</sub>N<sub>1</sub>O<sub>4</sub>

**Compound Name:** 3-Acetyl-5-(2-hydroxy-5-methylbenzoyl)-1-(4-methylphenyl)pyridin-2(1H)-one

**Space Group:** Pbc<sub>a</sub> **Cell:** a 20.885(6) b 7.102(1) c 24.625(7)  
**Space Group No.:** 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

**R-Factor (%):** 4.52 **Temperature(K):** 296 **Density(g/cm<sup>3</sup>):** 1.314



## ZESVIF

**Reference:** Qing-Hu Teng, Xiang-Jun Peng, Zu-Yu Mo, Yan-Li Xu, Hai-Tao Tang, Heng-Shan Wang, Hong-Bin Sun, Ying-Ming Pan (2018) *Green Chemistry*, **20**,2007

**Formula:** C<sub>24</sub>H<sub>19</sub>N<sub>1</sub>O<sub>1</sub>

**Compound Name:** 1-(4-methylphenyl)-4,6-diphenylpyridin-2(1H)-one

**Space Group:** P-1 **Cell:** a 9.462(0) b 9.753(0) c 10.539(0)  
**Space Group No.:** 2 **(Å, °)** α 68.19(0) β 78.20(0) γ 88.78(0)

**R-Factor (%):** 4.21 **Temperature(K):** 150 **Density(g/cm<sup>3</sup>):** 1.270

