

# Search Overview

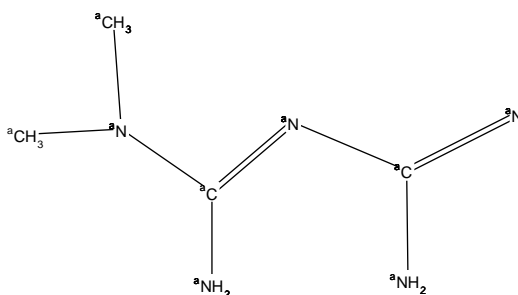
**Search:** search12  
**Date/Time done:** Mon Feb 13 20:05:08 2023  
**Database(s):** CSD version 5.43 updates (Mar 2022)  
CSD version 5.43 (November 2021)  
CSD version 5.43 updates (Jun 2022)  
CSD version 5.43 updates (Sep 2022)  
CSD version 5.43 updates (Nov 2022)  
**Restriction Info:** No refcode restrictions applied  
**Filters:** None  
**Percentage Completed:** 100%  
**Number of Hits:** 17

*Single query used. Search found structures that:*

match

**Query 2**

**Query 2**



# Search: search12 (Mon Feb 13 20:05:08 2023): Hits 1-4

## MAXJAA

**Reference:** Jingjing Sun, Lina Jia, Mengwei Wang, Yu Liu, Min Li, Dandan Han, Junbo Gong (2022) *Cryst.Growth Des.* ,22,1005

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>1</sub> O<sub>3</sub> S<sub>2</sub><sup>1-</sup>·C<sub>4</sub> H<sub>12</sub> N<sub>5</sub><sup>1+</sup>·C<sub>3</sub> H<sub>6</sub> O<sub>1</sub>

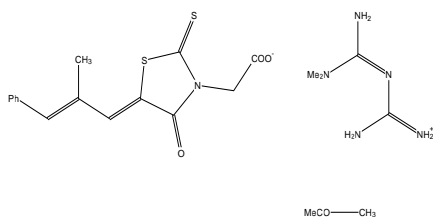
**Compound Name:** amino[[amino(dimethylamino)methylidene]amino]methaniminium [5-(2-methyl-3-phenylprop-2-en-1-ylidene)-4-oxo-2-sulfanylidene-1,3-thiazolidin-3-yl]acetate acetone solvate

**Synonym:** metformin epalrestat acetone solvate

**Space Group:** P-1 **Cell:** a 7.588(0) b 9.321(0) c 19.335(0)  
**Space Group No.:** 2 **(Å, °)** α 96.17(0) β 97.92(0) γ 108.14(0)

**R-Factor (%):** 3.25 **Temperature(K):** 123 **Density(g/cm<sup>3</sup>):** 1.324

**Parameters**  
 Fragment 1  
**TOR1 (T)** -156.076



## DEXBUF

**Reference:** J.B.Nanubolu, B.Sridhar, K.Ravikumar, K.D.Sawant, T.A.Naik, L.N.Patkar, S.Chelukuvada, B.Sreedhar (2013) *CrystEngComm* ,15,4448

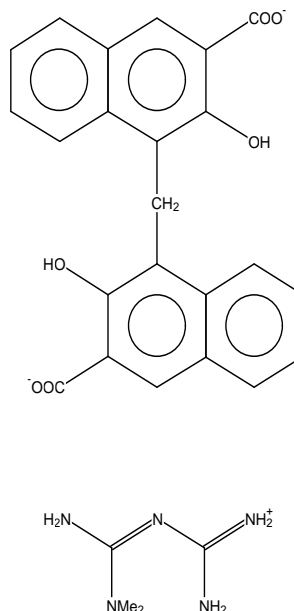
**Formula:** C<sub>23</sub> H<sub>14</sub> O<sub>6</sub><sup>2-</sup>·2(C<sub>4</sub> H<sub>12</sub> N<sub>5</sub><sup>1+</sup>)

**Compound Name:** bis(Metformin) embonic acid

**Space Group:** P-1 **Cell:** a 7.468(0) b 13.802(1) c 16.286(1)  
**Space Group No.:** 2 **(Å, °)** α 73.33(0) β 83.17(0) γ 82.67(0)

**R-Factor (%):** 3.63 **Temperature(K):** 294 **Density(g/cm<sup>3</sup>):** 1.352

**Parameters**  
 Fragment 1  
**TOR1 (T)** 147.696  
 Fragment 2  
**TOR1 (T)** 170.170



## DEXBUF01

**Reference:** J.B.Nanubolu, B.Sridhar, K.Ravikumar, K.D.Sawant, T.A.Naik, L.N.Patkar, S.Chelukuvada, B.Sreedhar (2013) *CrystEngComm* ,15,4448

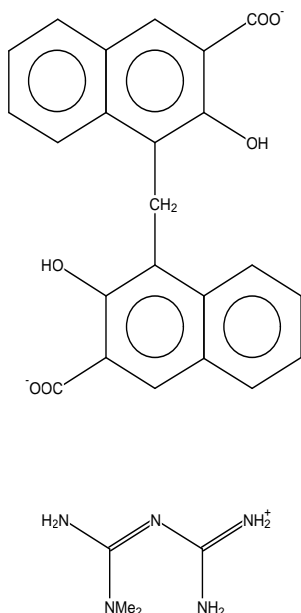
**Formula:** C<sub>23</sub> H<sub>14</sub> O<sub>6</sub><sup>2-</sup>·2(C<sub>4</sub> H<sub>12</sub> N<sub>5</sub><sup>1+</sup>)

**Compound Name:** bis(Metformin) embonic acid

**Space Group:** P2<sub>1</sub>/c **Cell:** a 17.810(0) b 7.928(0) c 25.802(0)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 119.50(0) γ 90.00

**R-Factor (%):** 4.39 **Temperature(K):** 294 **Density(g/cm<sup>3</sup>):** 1.355

**Parameters**  
 Fragment 1  
**TOR1 (T)** -146.972  
 Fragment 2  
**TOR1 (T)** -153.477



## EQUITIV

**Reference:** R.Olar, M.Badea, M.N.Greuc, C.-M.Balotescu, D.Marinescu, E.-E.Iorgulescu, V.Lazar, C.Bleotu (2010) *Analele Univ. Bucuresti Chim.* ,19,13

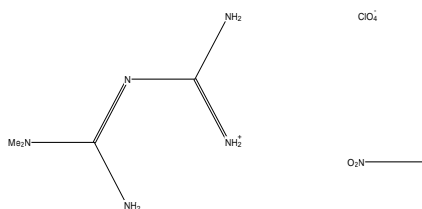
**Formula:** 2(C<sub>4</sub> H<sub>12</sub> N<sub>5</sub><sup>1+</sup>)·Cl<sub>1</sub> O<sub>4</sub><sup>1-</sup>·N<sub>1</sub> O<sub>3</sub><sup>1-</sup>

**Compound Name:** bis(amino((amino(dimethylamino)methylene)amino)methaniminium) nitrate perchlorate

**Space Group:** C2/c **Cell:** a 7.147(6) b 25.460(20) c 10.951(9)  
**Space Group No.:** 15 **(Å, °)** α 90.00 β 98.24(1) γ 90.00

**R-Factor (%):** 6.82 **Temperature(K):** 297 **Density(g/cm<sup>3</sup>):** 1.421

**Parameters**  
 Fragment 1  
**TOR1 (T)** 25.785



# Search: search12 (Mon Feb 13 20:05:08 2023): Hits 5-8

## EWISAH

**Reference:** J.A.Polito-Lucas, J.A.Nunez-Avila, S.Bernes, A.Perez-Benitez (2021) *IUCrData*, **6**,x210634

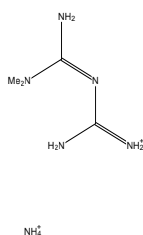
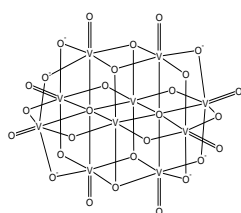
**Formula:** O<sub>28</sub> V<sub>10</sub><sup>6-</sup>·2(C<sub>4</sub> H<sub>12</sub> N<sub>5</sub><sup>1+</sup>)·4(H<sub>4</sub> N<sub>1</sub><sup>1+</sup>)·6(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** tetrakis(ammonium) bis(metforminium) icosakis(μ-oxo)-octa-oxo-deca-vanadium hexahydrate

**Space Group:** P-1 **Cell:** **a** 9.796(0) **b** 10.101(0) **c** 13.097(0)  
**Space Group No.:** 2 **(Å, °)** **α** 81.08(0) **β** 70.91(0) **γ** 63.32(0)

**R-Factor (%):** 2.54 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 2.121

**Parameters**  
 Fragment 1  
**TOR1 (T)** -154.277



H<sub>2</sub>O

## JUMXOH

**Reference:** Xufei Bian, Lan Jiang, Jing Zhou, Xiaoshu Guan, Jingyu Wang, Peng Xiang, Junyi Pan, Xiangnan Hu (2020) *Molecules*, **25**,1343

**Formula:** C<sub>18</sub> H<sub>18</sub> N<sub>3</sub> O<sub>3</sub> S<sub>1</sub><sup>1-</sup>·C<sub>4</sub> H<sub>12</sub> N<sub>5</sub><sup>1+</sup>

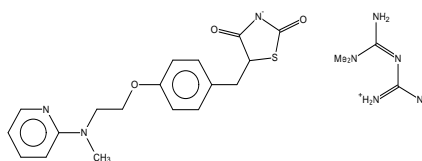
**Compound Name:** amino([amino(dimethylamino)methylidene]amino)methaniminium 5-[[4-(2-[methyl(pyridin-2-yl)amino]ethoxy)phenyl)methyl]-2,4-dioxo-1,3-thiazolidin-3-ide

**Synonym:** metformin rosigitazone

**Space Group:** P-1 **Cell:** **a** 6.948(0) **b** 11.315(0) **c** 17.241(0)  
**Space Group No.:** 2 **(Å, °)** **α** 72.38(0) **β** 82.37(0) **γ** 74.15(0)

**R-Factor (%):** 5.23 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.302

**Parameters**  
 Fragment 1  
**TOR1 (T)** 24.784



## NAKWAB

**Reference:** N.K.Manjunatha, Mahesha, B.H.Gayathri, N.K.Lokanath, M.T.Swamy, S.Chandra Nayaka, B.P.Siddaraju, N.Ragini, M.AL-Ghorbani, B.R.Kannika, S.Madan Kumar (2020) *Chem. Data Collect.*, **30**,100577

**Formula:** C<sub>4</sub> H<sub>12</sub> N<sub>5</sub><sup>1+</sup>·C<sub>6</sub> H<sub>2</sub> N<sub>3</sub> O<sub>7</sub><sup>1-</sup>

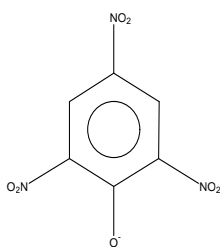
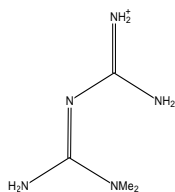
**Compound Name:** 2-(amino(iminio)methyl)-1,1-dimethylguanidine 2,4,6-trinitrophenolate

**Synonym:** metformin picrate

**Space Group:** P21/c **Cell:** **a** 11.476(1) **b** 5.644(0) **c** 24.213(3)  
**Space Group No.:** 14 **(Å, °)** **α** 90.00 **β** 94.29(0) **γ** 90.00

**R-Factor (%):** 5.83 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.522

**Parameters**  
 Fragment 1  
**TOR1 (T)** -18.142



## NICCEJ

**Reference:** J.Satyanarayana Reddy, N.Ravikumar, G.Gaddamanugu, K.N.Naresh, S.S.Rajan, K.Anand Solomon (2013) *J.Mol.Struct.*, **1039**, 137

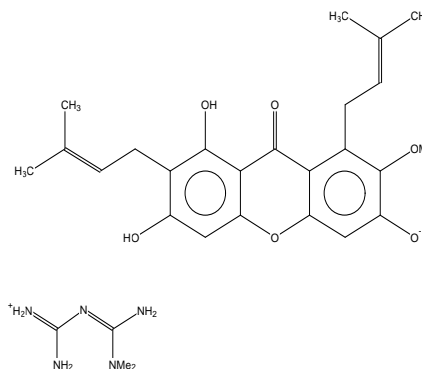
**Formula:** C<sub>24</sub> H<sub>25</sub> O<sub>6</sub><sup>1-</sup>·C<sub>4</sub> H<sub>12</sub> N<sub>5</sub><sup>1+</sup>

**Compound Name:** Amino(amino(dimethylamino)methylene)amino)methaniminium 6,8-dihydroxy-2-methoxy-1,7-bis(3-methylbut-2-en-1-yl)-9-oxo-9H-xanthen-3-olate

**Space Group:** P21/n **Cell:** **a** 12.053(5) **b** 11.729(5) **c** 20.653(5)  
**Space Group No.:** 14 **(Å, °)** **α** 90.00 **β** 101.45(0) **γ** 90.00

**R-Factor (%):** 4.51 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.253

**Parameters**  
 Fragment 1  
**TOR1 (T)** 155.712



# Search: search12 (Mon Feb 13 20:05:08 2023): Hits 9-12

## NUPXED

**Reference:** J.Dong, B.Liu, B.Yang (2015)  
*Acta Crystallogr., Sect.E:Cryst.Commun.*, **71**,o747

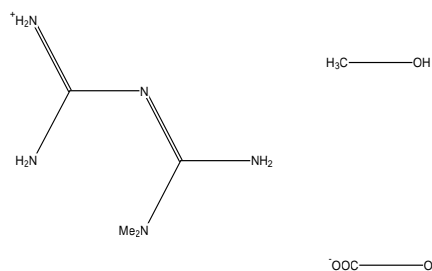
**Formula:**  $2(C_4 H_{12} N_5^{1+}), 2(C_1 H_4 O_1), C_1 O_3^{2-}$

**Compound Name:** bis(amino((amino(dimethylamino)methylene)amino)methaniminium) carbonate methanol solvate

**Space Group:** C2/c    **Cell:**    **a** 13.573(1)    **b** 10.563(0)    **c** 13.982(1)  
**Space Group No.:** 15    **(Å, °)**     $\alpha$  90.00     $\beta$  90.39(0)     $\gamma$  90.00

**R-Factor (%):** 8.26    **Temperature(K):** 298    **Density(g/cm<sup>3</sup>):** 1.274

**Parameters**  
**Fragment 1**  
**TOR1 (T)** 17.196



## OJOSUC

**Reference:** R.Olar, M.Badea, D.Marinescu, C.-M.Chifiriuc, C.Bleotu, M.N.Grecu, E.E.Iorgulescu, M.Bucur, V.Lazar, A.Finaru (2010)  
*Eur.J.Med.Chem.*, **45**,2868

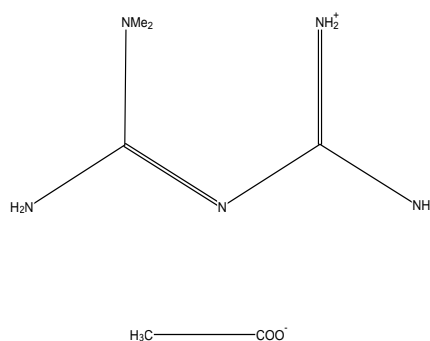
**Formula:**  $C_4 H_{12} N_5^{1+}, C_2 H_3 O_2^{1-}$

**Compound Name:** N,N-dimethylbiguanidinium acetate

**Space Group:** P21/n    **Cell:**    **a** 9.993(1)    **b** 8.894(0)    **c** 10.703(1)  
**Space Group No.:** 14    **(Å, °)**     $\alpha$  90.00     $\beta$  91.14(0)     $\gamma$  90.00

**R-Factor (%):** 6.56    **Temperature(K):** 297    **Density(g/cm<sup>3</sup>):** 1.321

**Parameters**  
**Fragment 1**  
**TOR1 (T)** -160.747



## OJOSUC01

**Reference:** Xiaodan Wei, Yuhua Fan, Caifeng Bi, Xingchen Yan, Xia Zhang, Xin Li (2014) *Bull.Korean Chem.Soc.* **35**,3495

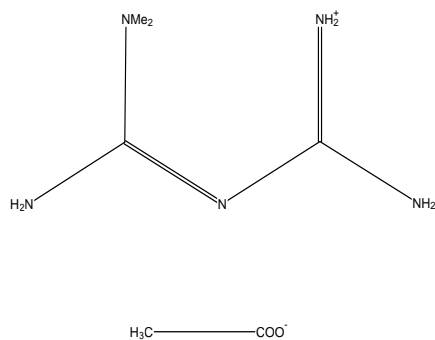
**Formula:**  $C_4 H_{12} N_5^{1+}, C_2 H_3 O_2^{1-}$

**Compound Name:** N,N-dimethylbiguanidinium acetate

**Space Group:** P21/n    **Cell:**    **a** 10.001(0)    **b** 8.906(0)    **c** 10.703(0)  
**Space Group No.:** 14    **(Å, °)**     $\alpha$  90.00     $\beta$  91.31(0)     $\gamma$  90.00

**R-Factor (%):** 4.26    **Temperature(K):** 298    **Density(g/cm<sup>3</sup>):** 1.319

**Parameters**  
**Fragment 1**  
**TOR1 (T)** -160.899



## QILBOF

**Reference:** E.Sanchez-Lara, S.Trevino, B.L.Sanchez-Gaytan, E.Sanchez-Mora, M.E.Castro, F.Melendez-Bustamante, M.A.Mendez-Rojas, E.Gonzalez-Vergara (2018) *Frontiers in Chemistry*, **6**,402

**Formula:**  $O_{28} V_{10}^{6+}, 6(C_4 H_{12} N_5^{1+}), 6(H_2 O_1)$

**Compound Name:** hexakis(amino[[amino(dimethylamino)methylidene]amino)methaniminium) icosakis(μ-oxido)-octaoxo-deca-vanadium(v) hexahydrate

**Synonym:** hexakis(metforminium) icosakis(μ-oxido)-octaoxo-deca-vanadium(v) hexahydrate

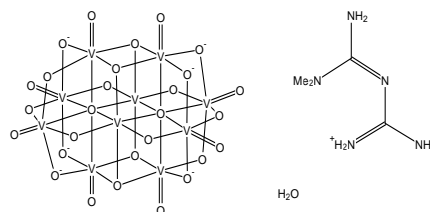
**Space Group:** P-1    **Cell:**    **a** 11.562(0)    **b** 13.279(0)    **c** 13.769(0)  
**Space Group No.:** 2    **(Å, °)**     $\alpha$  96.01(0)     $\beta$  107.35(0)     $\gamma$  115.56(0)

**R-Factor (%):** 5.09    **Temperature(K):** 293    **Density(g/cm<sup>3</sup>):** 1.750

**Parameters**  
**Fragment 1**  
**TOR1 (T)** -162.291

**Fragment 2**  
**TOR1 (T)** 150.600

**Fragment 3**  
**TOR1 (T)** 156.245



# Search: search12 (Mon Feb 13 20:05:08 2023): Hits 13-16

## ROLFUW

**Reference:** L.Jia, S.Wu, J.Gong (2019)  
*Acta Crystallogr., Sect.C: Cryst. Struct. Chem.*, **75**,1250

**Formula:** C<sub>12</sub> H<sub>17</sub> N<sub>2</sub> O<sub>3</sub> S<sub>1</sub><sup>1-</sup>·C<sub>4</sub> H<sub>12</sub> N<sub>5</sub><sup>1+</sup>

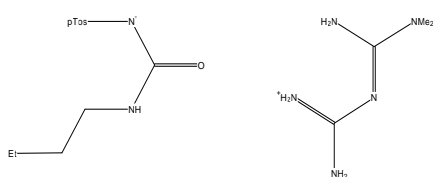
**Compound Name:** amino[[amino(dimethylamino)methylidene]amino]methaniminium (butylcarbamoyl)(4-methylbenzene-1-sulfonyl)azanide

**Synonym:** metformin tolbutamide

**Space Group:** P21/n **Cell:** a 7.985(1) b 28.569(6) c 8.826(1)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 91.61(3) γ 90.00

**R-Factor (%):** 5.79 **Temperature(K):** 113 **Density(g/cm<sup>3</sup>):** 1.318

**Parameters**  
**Fragment 1**  
**TOR1 (T)** -15.057



## UKODUW

**Reference:** Wenquan Feng (2020)  
*CSD Communication(Private Communication)*,

**Formula:** C<sub>14</sub> H<sub>10</sub> Cl<sub>2</sub> N<sub>1</sub> O<sub>2</sub><sup>1-</sup>·C<sub>4</sub> H<sub>12</sub> N<sub>5</sub><sup>1+</sup>

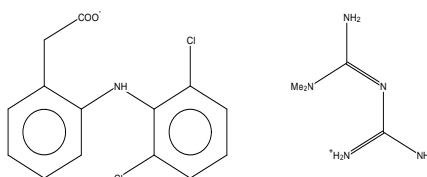
**Compound Name:** amino[[amino(dimethylamino)methylidene]amino]methaniminium [2-(2,6-dichloroanilino)phenyl]acetate

**Synonym:** diclofenac metformin

**Space Group:** P21/c **Cell:** a 8.876(0) b 10.182(1) c 22.402(2)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 94.21(0) γ 90.00

**R-Factor (%):** 5.54 **Temperature(K):** 296 **Density(g/cm<sup>3</sup>):** 1.399

**Parameters**  
**Fragment 1**  
**TOR1 (T)** -158.821



## WIBSIJ

**Reference:** P.Lemoine, A.Tomas, B.Viossat, N.-H.Dung (1994)  
*Acta Crystallogr., Sect.C: Cryst. Struct. Commun.*, **50**,1437

**Formula:** C<sub>4</sub> H<sub>13</sub> N<sub>5</sub><sup>2+</sup>·Cl<sub>4</sub> Cu<sub>1</sub><sup>2-</sup>

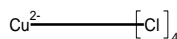
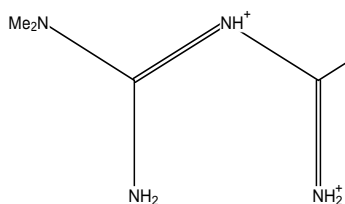
**Compound Name:** 1,3-Diamino-1-dimethylamino-3-iminio-2-azoniapropane tetrachloro-copper(ii)

**Synonym:** N,N-Dimethylimidodicarbonimidic diamide tetrachloro-copper(ii), Metformine tetrachloro-copper(ii)

**Space Group:** P21/a **Cell:** a 11.128(5) b 7.926(3) c 14.735(8)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 108.10(5) γ 90.00

**R-Factor (%):** 4.60 **Temperature(K):** 295 **Density(g/cm<sup>3</sup>):** 1.810

**Parameters**  
**Fragment 1**  
**TOR1 (T)** -154.307



## DELKAK

**Reference:** L.F.Diniz, P.S.Carvalho, J.E.Goncalves, R.Diniz, C.Fernandes (2022) *New J.Chem.*, **46**,13725

**Formula:** C<sub>4</sub> H<sub>12</sub> N<sub>5</sub><sup>1+</sup>·C<sub>3</sub> H<sub>3</sub> O<sub>4</sub><sup>1-</sup>

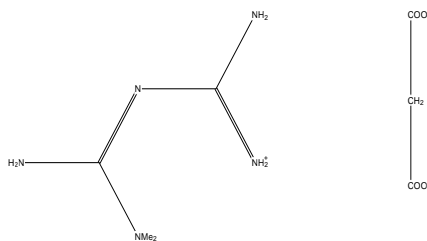
**Compound Name:** amino[[amino(dimethylamino)methylidene]amino]methaniminium carboxyacetate

**Synonym:** Metformin malonate

**Space Group:** P21/c **Cell:** a 12.538(0) b 5.006(0) c 17.612(0)  
**Space Group No.:** 14 **(Å, °)** α 90.00 β 91.97(0) γ 90.00

**R-Factor (%):** 3.89 **Temperature(K):** 293 **Density(g/cm<sup>3</sup>):** 1.402

**Parameters**  
**Fragment 1**  
**TOR1 (T)** 33.221



# Search: search12 (Mon Feb 13 20:05:08 2023): Hit 17

YEJVOC

**Reference:** Lan Jiang, Xiangnan Hu, Linhong Cai (2022) *Molecules*, 27,3472

**Formula:** C<sub>4</sub> H<sub>12</sub> N<sub>5</sub><sup>1+</sup>, C<sub>6</sub> H<sub>5</sub> O<sub>5</sub> S<sub>1</sub><sup>1-</sup>

**Compound Name:** amino[[amino(dimethylamino)methylidene]amino]methaniminium 2,5-dihydroxybenzene-1-sulfonate

**Synonym:** metformin 2,5-dihydroxybenzenesulfonic acid

**Space Group:** C2/c    **Cell:**    **a** 10.876(0)    **b** 10.904(0)    **c** 24.643(0)  
**Space Group No.:** 15    (**Å, °**)    **α** 90.00    **β** 93.86(0)    **γ** 90.00

**R-Factor (%):** 4.24    **Temperature(K):** 293    **Density(g/cm<sup>3</sup>):** 1.455

## Parameters

**Fragment 1**  
**TOR1 (T)** -27.003

