

Supplementary Information for:

An optimized intermolecular force field for hydrogen bonded organic molecular crystals using atomic multipole electrostatics

Edward O. Pyzer-Knapp, Hugh P. G. Thompson and Graeme M. Day

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1. Original W99 force field parameters
2. Revised parameters in eV
3. Chemical diagrams and Cambridge Structural Database reference codes for the parameterization set of crystal structures
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Original W99 force field parameters

Atom type definitions are:

H1: hydrogen in G-H group	N1: nitrogen with triple bond
H2: hydrogen in alcoholic group	N2: nitrogen with no bonded hydrogen (except triple bond)
H3: hydrogen in carboxyl group	N3: nitrogen with one bonded hydrogen
H4: hydrogen in N-H group	N4: nitrogen with two or more bonded hydrogens
C4: carbon bonded to four other atoms	O1: oxygen bonded to one other atom
C3: carbon bonded to three other atoms	O2: oxygen bonded to two other atoms
C2: carbon bonded to two other atoms	

Refer to equation (2) for functional form. All interactions between atoms of two different types are determined by the combining rules (equations 3-5). In the revised force fields W99rev631, W99rev6311, W99rev631P and W99rev6311P, all interactions between a hydrogen and the acceptor atom of a hydrogen bond are replaced by the parameters in Table 2.

In eV and Å

Atom type	A (eV)	B (Å ⁻¹)	C (eV Å ⁶)
H1	131.42	3.56	2.885
H2	3.74	3.56	0
H3	1.20	3.56	0
H4	7.93	3.56	0
C4	1363.64	3.60	10.140
C3	2802.12	3.60	17.637
C2	1069.96	3.60	14.874
N1	998.59	3.48	14.588
N2	1060.98	3.48	14.491
N3	1989.27	3.48	24.631
N4	4201.08	3.48	58.349
O2	2949.92	3.96	13.327
O1	2498.23	3.96	13.067

In kJ/mol and Å

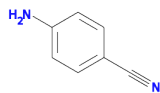
Atom type	A (eV)	B (Å ⁻¹)	C (eV Å ⁶)
H1	12680	3.56	278.37
H2	361.3	3.56	0
H3	115.7	3.56	0
H4	764.9	3.56	0
C4	131571	3.60	978.36
C3	270363	3.60	1701.73
C2	103235	3.60	1435.09
N1	96349	3.48	1407.57
N2	102369	3.48	1398.15
N3	191935	3.48	2376.55
N4	405341	3.48	5629.82
O2	284623	3.96	1285.87
O1	241042	3.96	1260.73

Re-optimised parameters, in eV (parameters in kJ/mol given in Table 2 of the main text).

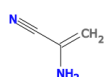
Acceptor atom	W99	W99rev631	W99rev6311	W99rev631P	W99rev6311P
donor atom: H2					
O1	96.7	101	129	126	154
O2	105.1	77	105	114	131
N1	61.1	131	149	162	187
N2	63	124	166	138	150
N3	86.3	115	163	132	144
N4	125.4	125.4	125.4	125.4	125.4
donor atom: H3					
O1	54.7	58	127	104	138
O2	59.5	89	133	116	129
N1	34.6	102	70	133	92
N2	35.7	118	118	142	186
N3	48.8	48.8	48.8	48.8	48.8
N4	71	71	71	71	71
donor atom: H4					
O1	140.7	48	56	118	143
O2	152.9	116	112	149	140
N1	89	96	141	144	192
N2	91.7	80	77	129	151
N3	125.6	43	34	58	51
N4	182.5	196	198	212	197

Crystal structure (CSD) reference codes and molecular diagrams of the training set

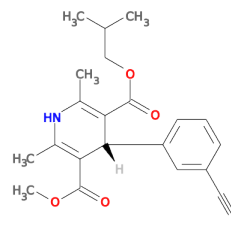
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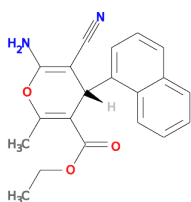
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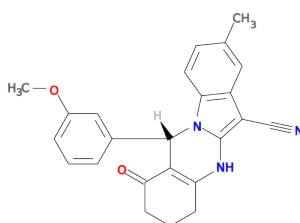
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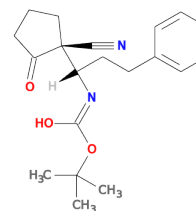
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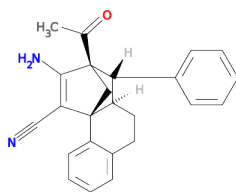
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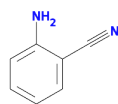
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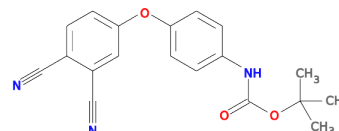
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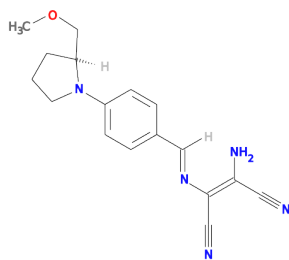
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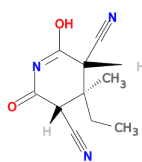
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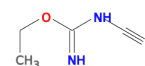
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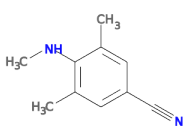
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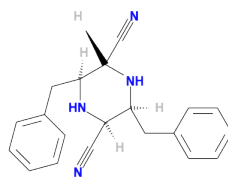
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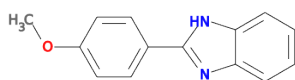


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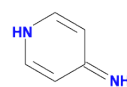
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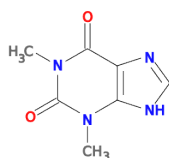
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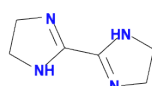
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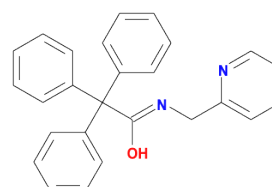
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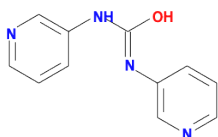
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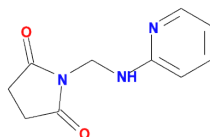
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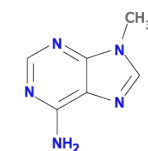
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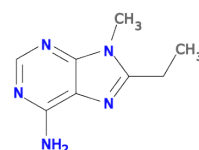
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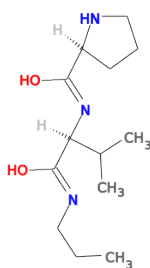


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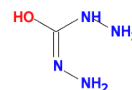
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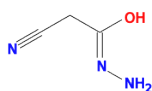
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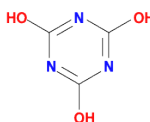
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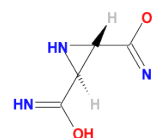
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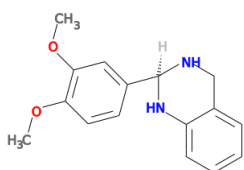
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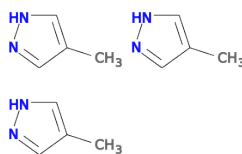
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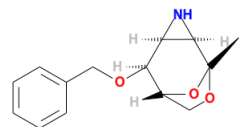
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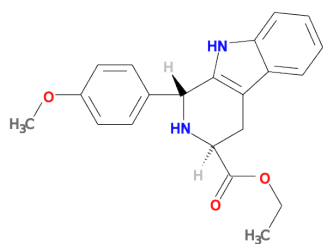
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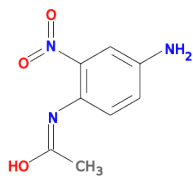


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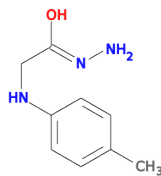


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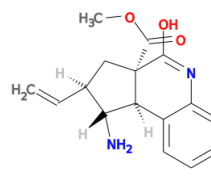
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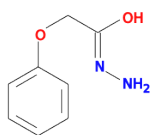
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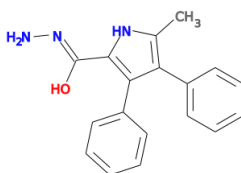
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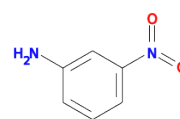
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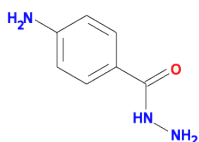
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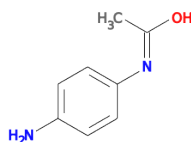
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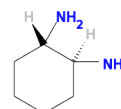
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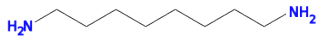
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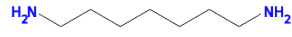
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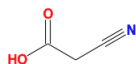


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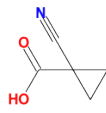


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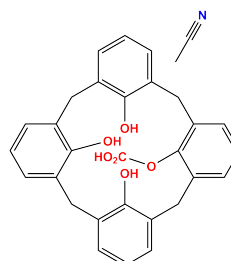
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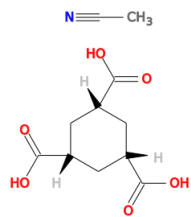
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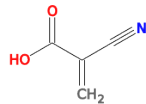
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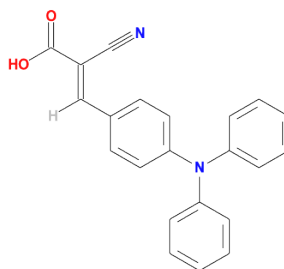
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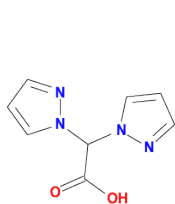


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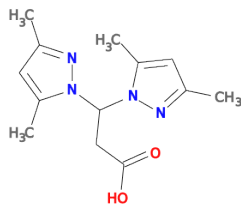


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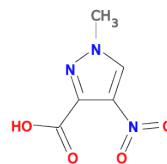
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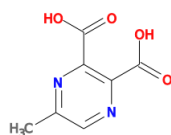
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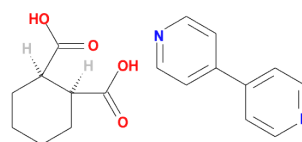
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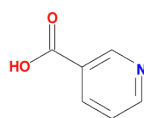
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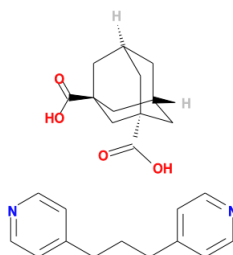
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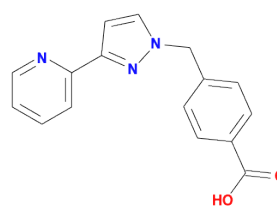
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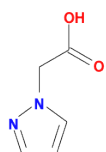
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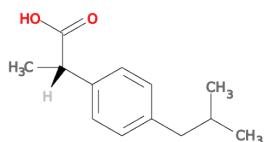


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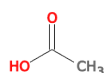


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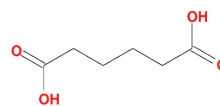
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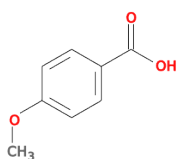
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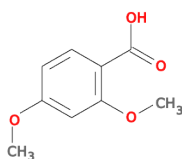
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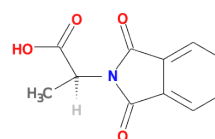
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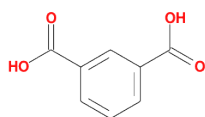
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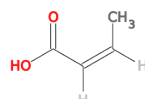
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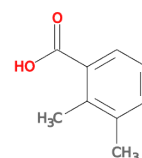
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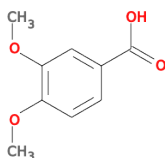
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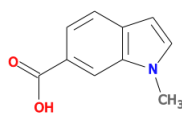
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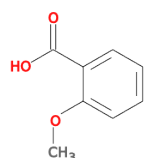
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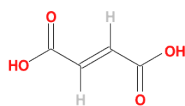
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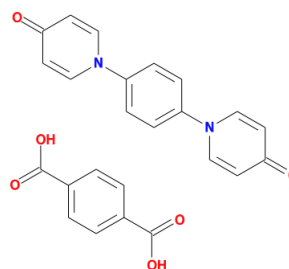
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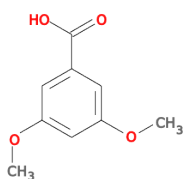
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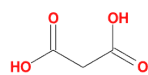
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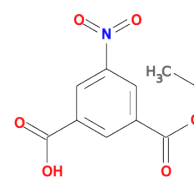
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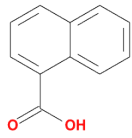
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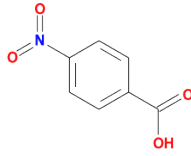
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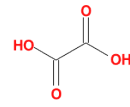
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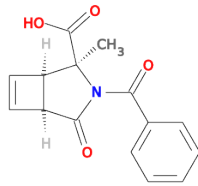
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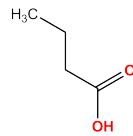
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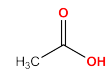
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SACDIL

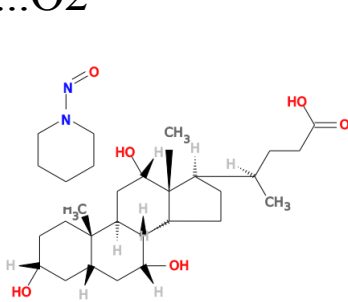


SUBRAC01

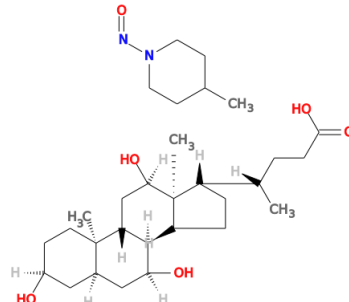


SUCACB03

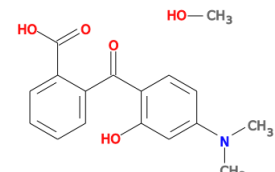
H3...O2



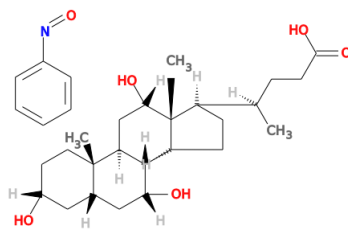
JOQHEC



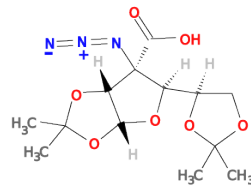
JOQHIG



OGES EZ

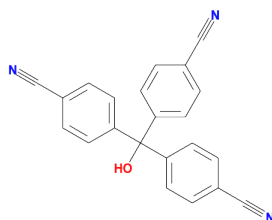


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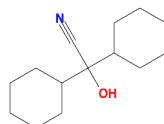


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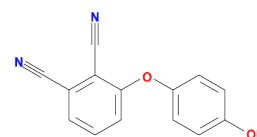
H2...N1



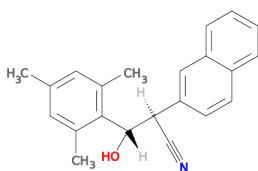
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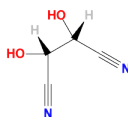
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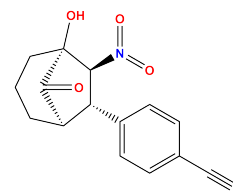
AHITOB



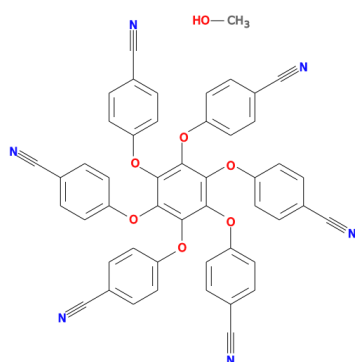
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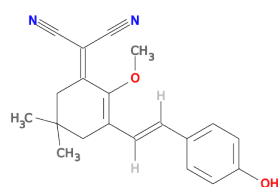
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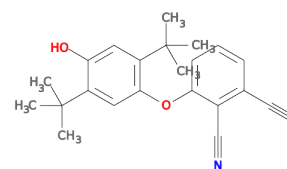
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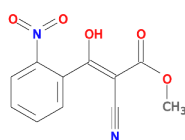
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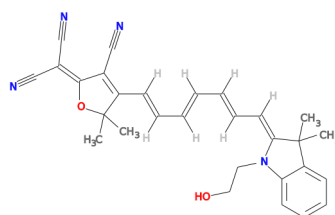
PAKBEK



POYDOX

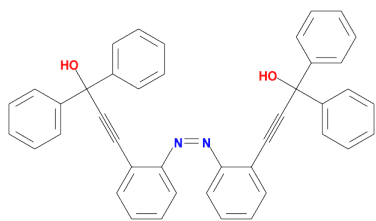


SEMYOZ

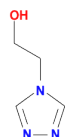


YAHGIZ

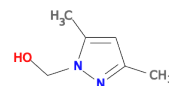
H2...N2



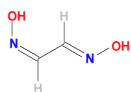
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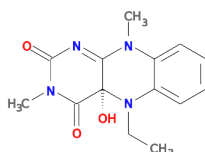
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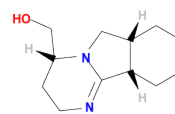
FIWFOH



GLOXIM11

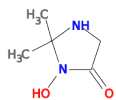


HAMSIZ

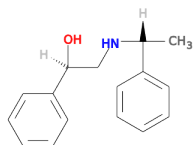


MATPEC

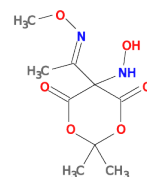
H2...N3



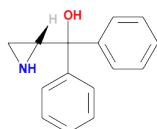
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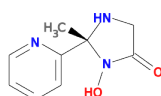
ENIYEF



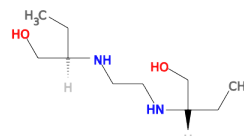
HANLEP



HOKCEP02



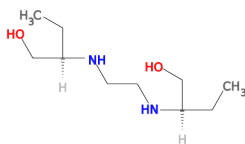
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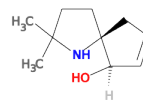
NERPOQ



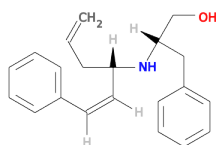
PETYOD



VIKMAE

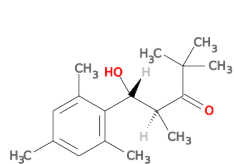


XOLPEU

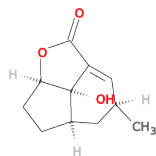


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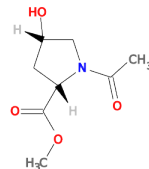
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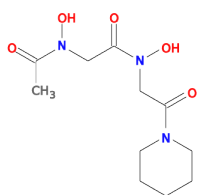
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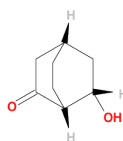
EBOVUN



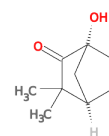
EMITEA



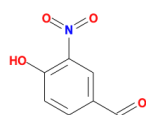
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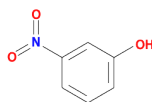
KEGHAG



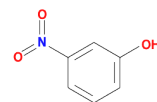
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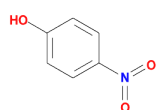
MIXXUN



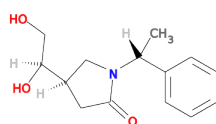
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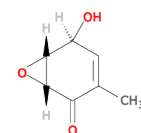
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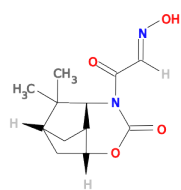
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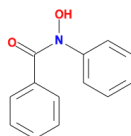
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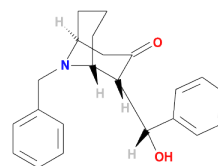
SEWHUY



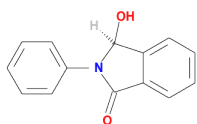
XAQTUF



XETNOA

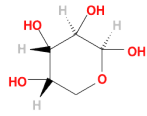


ZAPNIP

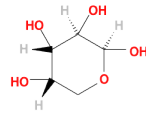


ZZZAWJ13

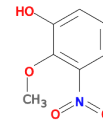
H2...O2



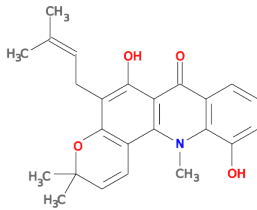
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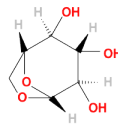
ABINOS02



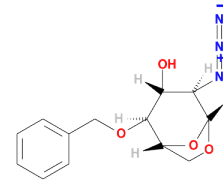
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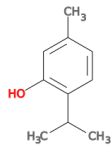
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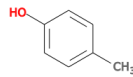
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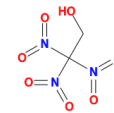
AHUZUZ



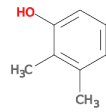
IPMEPL



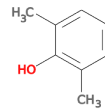
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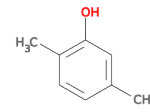
DIKXEB



DIMPHE12



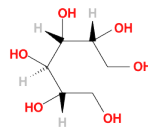
DMEPOL10



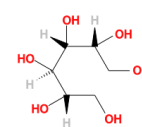
DMPHOL11



ETANOL



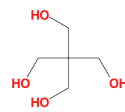
GLUCIT01



GLUCIT02



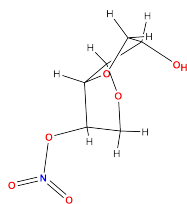
METHOL02



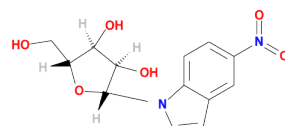
PERYTO10



PHENOL03

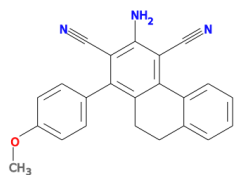


PIMKOO

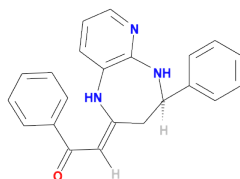


VIJFOK

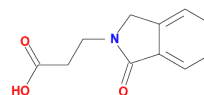
Validation set structures



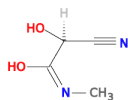
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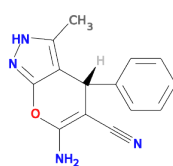
BAJYOB



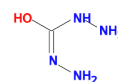
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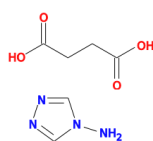
BOLZIL



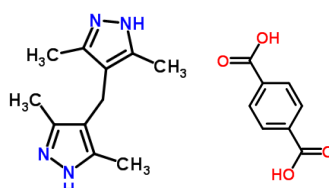
BOYZUL



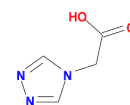
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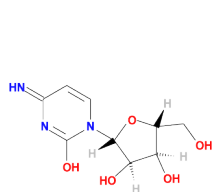
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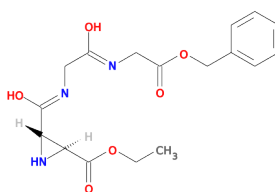
CUMRAE



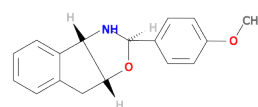
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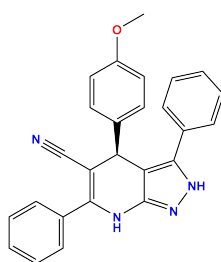
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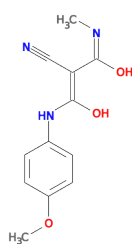
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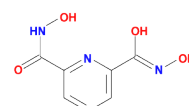
DEXSIJ



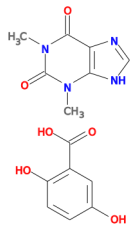
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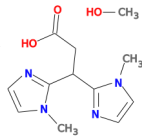
DIJGUZ



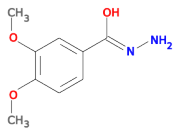
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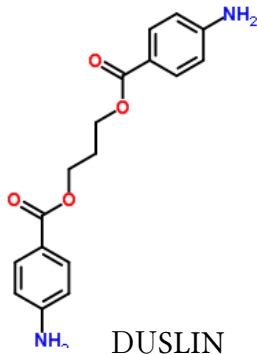
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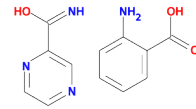
FINMEV



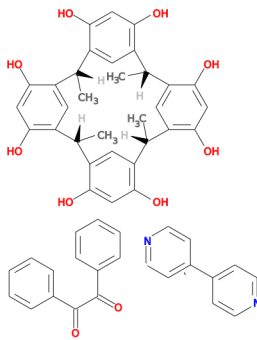
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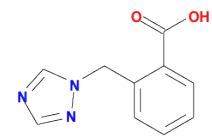
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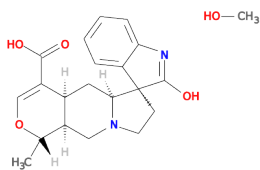
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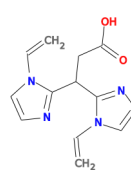
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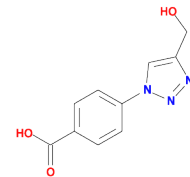
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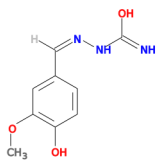
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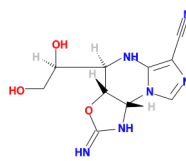
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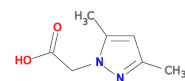
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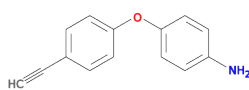
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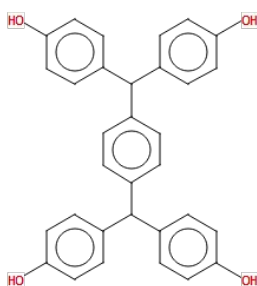
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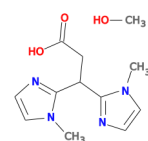
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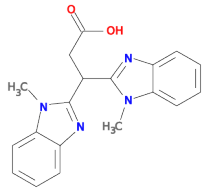
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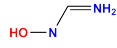
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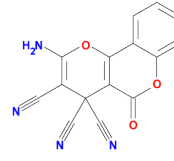
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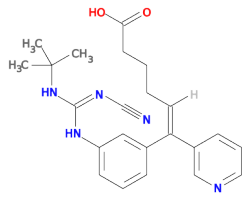
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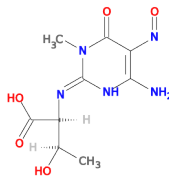
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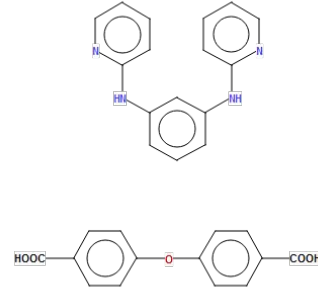
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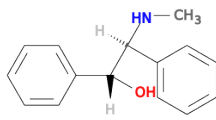
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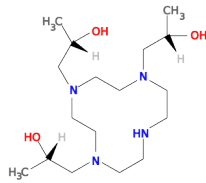
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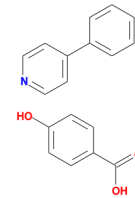
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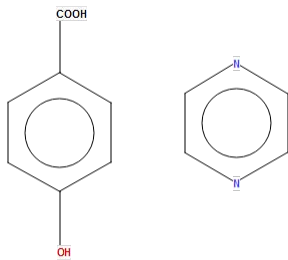
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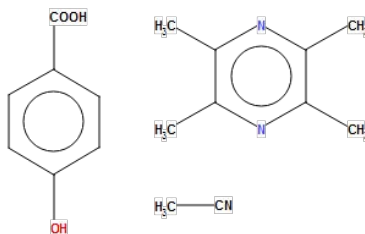
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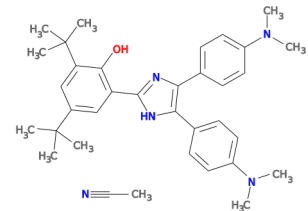
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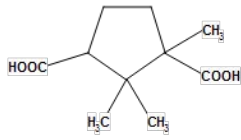
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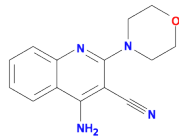
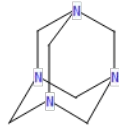
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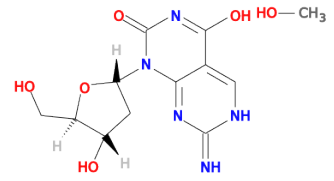
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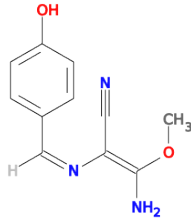
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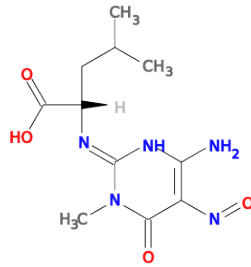
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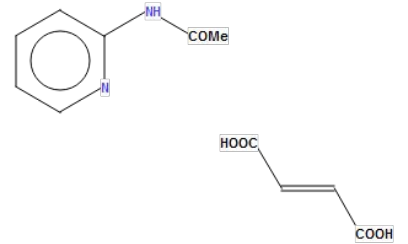
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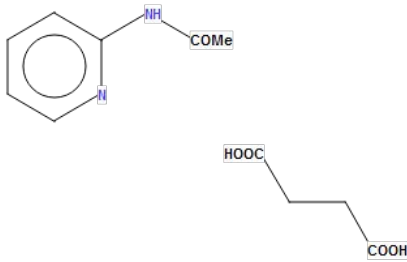
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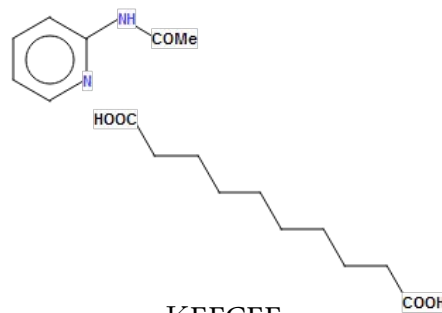
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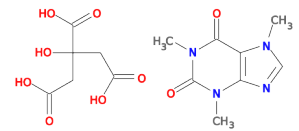
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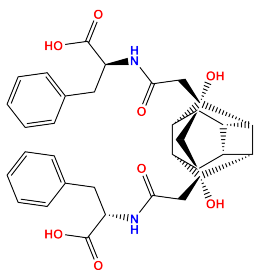
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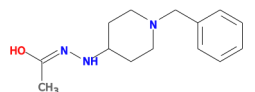
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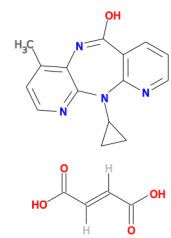
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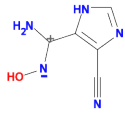
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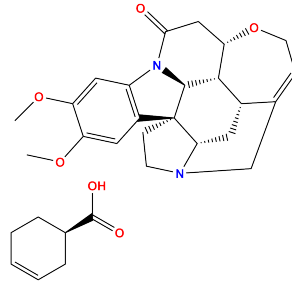
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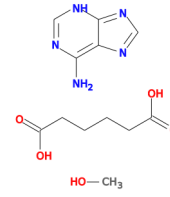
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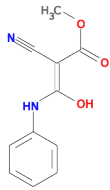
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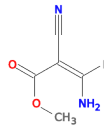
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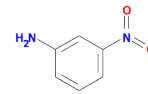
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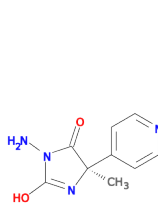
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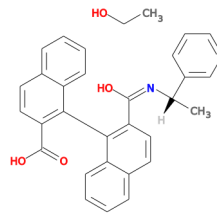
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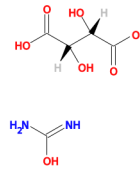
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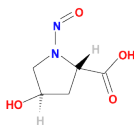
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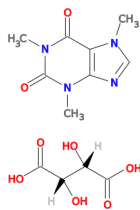
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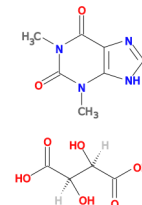
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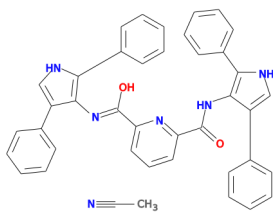
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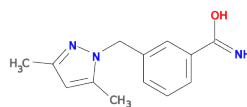
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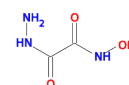
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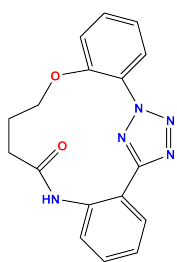
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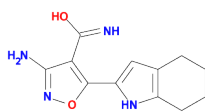
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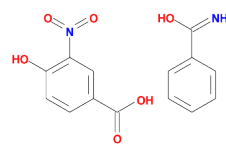
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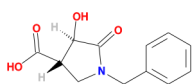
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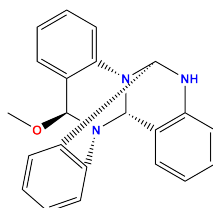
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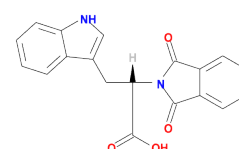
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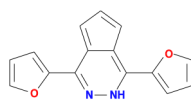
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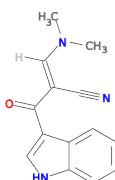
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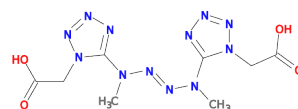
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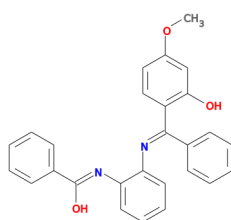
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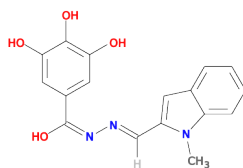
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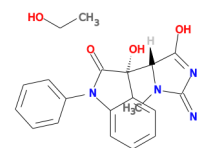
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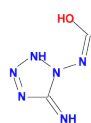
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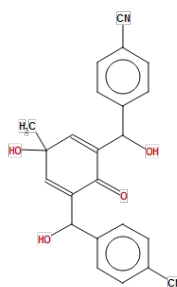
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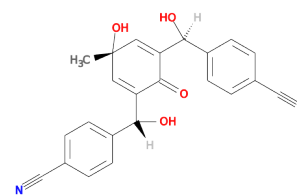
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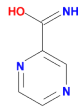
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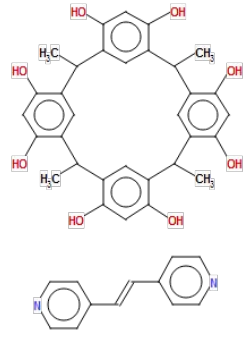
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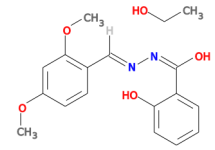
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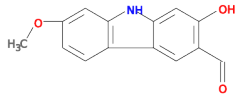
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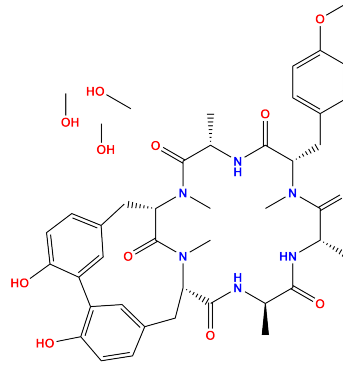
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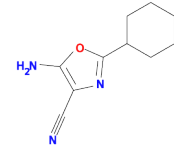
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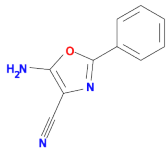
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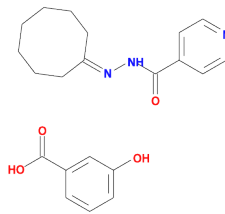
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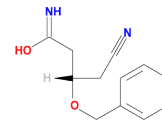
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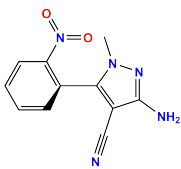
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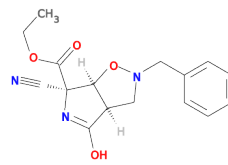
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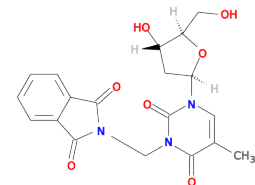
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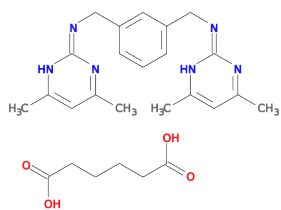
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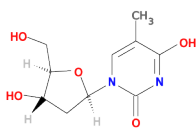
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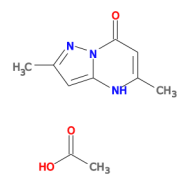
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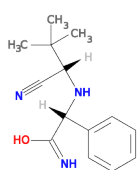
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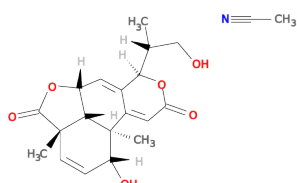
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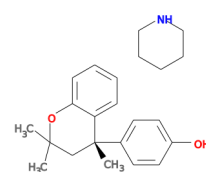
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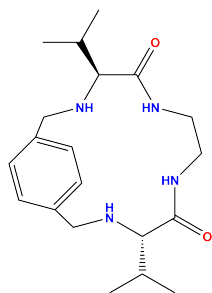
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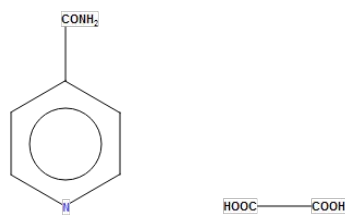
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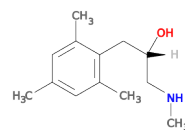
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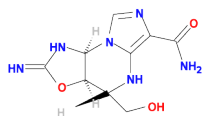
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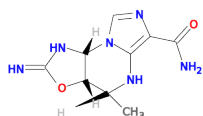
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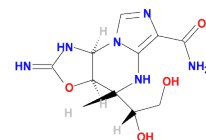
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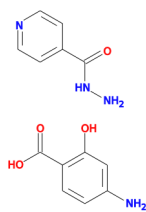
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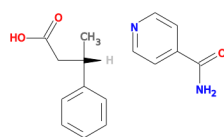
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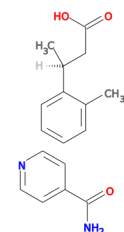
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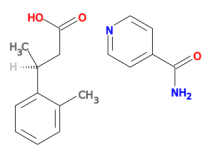
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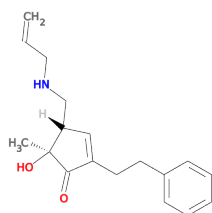
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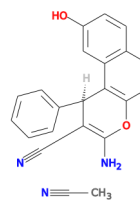
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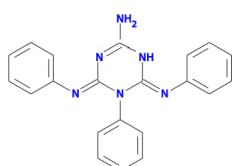
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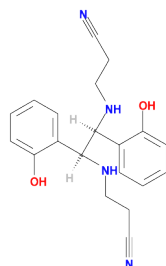
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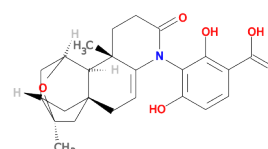
VALSOR



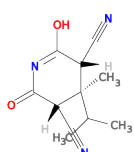
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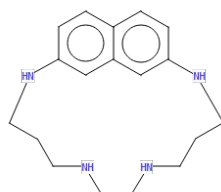
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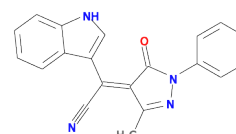
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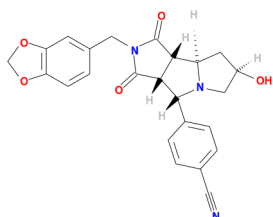
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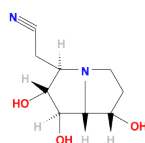
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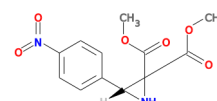
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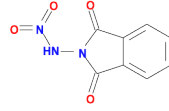
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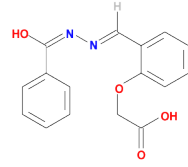
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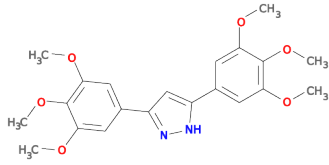
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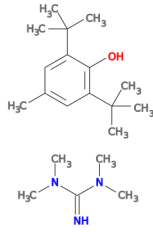
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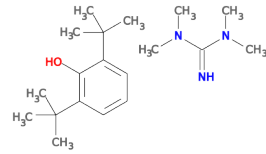
XEBWAE



YESWUP



YUQYUF



YUQYOZ

Sublimation enthalpy data used in parameterization and validation

compound	CSD reference code	ΔH_{subl} (kJ/mol)	T (K)	source
acetanilide	ACANIL02	80.6	313.5	Chickos
acetic acid	ACETAC03	67.95	298	Otero-de-la-Roza
adipic acid	ADIPAC12	133.6	298	Chickos
1,6-anhydro- β -D-Glucopyranose	AHGLPY13	125.1	365	NIST
imidazole	IMAZOL06	81.37	298	Otero-de-la-Roza
3-aminopyridine	AMIPYR	80.7	298	NIST
4-aminopyridine	AMPYRE01	87.1	298	NIST
p-methoxybenzoic acid	ANISIC03	111.6	298	NIST
thymol	IPMEPL	95.73	298	NIST
2,4-dimethoxybenzoic acid	ISUQUI	123.4	298	NIST
theophylline	BAPLOT01	135	298	NIST
isophthalic acid	BENZDC01	142	298	NIST
benzamide	BZAMID02	102	298	NIST
caprolactam	CAPLAC	89.8	298	NIST
p-cresol	CRESOL01	73.1	298	NIST
crotonic acid	CROTAC	72.2	298	NIST
cianoacetamide	CYANAC	99.7	336.5	NIST
cyanuric acid	CYURAC12	133	298	NIST
2,3-dimethylphenol	DIMPHE12	84	298	NIST
2,2-dimethylpropanamide	DIXTAF	89	298	NIST
2,3-dimethylbenzoic acid	DMBZAC01	104.6	298	NIST
2,6-dimethylphenol	DMEPOL10	75.6	298	NIST
2,6-dimethoxybenzoic acid	DMOXBA01	121.7	298	NIST
2,5-dimethylphenol	DMPHOL11	84.6	298	NIST
3,4-dimethoxybenzoic acid	DMXBZA01	129.8	298	NIST
formic acid	FORMAC02	60.5	274.5	NIST
formamide	FORMAM02	71.77	298	Otero-de-la-Roza
o-methoxybenzoic acid	FUFBOX01	110.7	298	NIST
fumaric acid	FUMAAC01	123.6	298	NIST
D-glucitol	GLUCIT01	186	298	NIST
glutarimide	GLUTIM	94.1	298	NIST
3,5-dimethoxybenzoic acid	HEKMOZ	127.1	298	NIST
isobutyramide	IBURAM	86	298	NIST
N-acetyl-L-	JEXNAB	133.1	298	NIST

valinamide				
maleic acid	MALIAC12	105.4	318.5	NIST
malonic acid	MALNAC09	111.4	298	NIST
9-methyl-adenine	MEADEN02	121.3	396	NIST
N-methyluracil	METURA01	121.7	385.5	NIST
				NIST Averaged value (2 data points)
methylurea	MEUREA	96.3	298	
m-nitroaniline	MNIANL02	96.5	298	NIST
				NIST Averaged value (2 data points)
m-nitrophenol	MNPHOL17	95.7	298	
				NIST Averaged value (8 data points)
4-nitroaniline	NANILI02	101	298	
				NIST Averaged value (2 data points)
1-naphthoic acid	NAPOAC01	112	298	
4-nitrobenzoic acid	NBZOAC05	119.7	298	NIST
				NIST Averaged value (3 data points)
nicotinic acid	NICOAC02	117.5	298	
4-nitrophenol	NITPOL03	92.4	298	NIST
oxalic acid	OXALAC04	93.63	298	NIST
oxalic acid	OXALAC06	93.7	298	NIST
pentaerythritol	PERYTO10	163	298	NIST
phenol	PHENOL03	65.3	280.5	NIST
2-pyridone	PYRIDO04	86.6	298	NIST
				NIST Averaged value (7 data points)
pyrazole	PYRZOL02	70	298	
suberic acid	SUBRAC01	147.8	298	NIST
succinic acid	SUCACB03	123.1	298	NIST
terephthalic acid	TEPHTH03	146.6	298	NIST
2,4,6-trinitroaniline	TNIOAN	125.3	298	NIST
				NIST Averaged value (6 data points)
1,2,4-triazole	TRAZOL02	83	298	
urea	UREAXX12	93.79	298	Otero-de-la-Roza
1,1-dimethylurea	WIFKEB01	93.5	298	NIST

NIST = NIST chemistry webbook, <http://webbook.nist.gov/chemistry/>

Chikos = J. S. Chikos and W. E. Acree, *Journal of Physical and Chemical Reference Data*, 2002, 31, 537-698

Otero-de-la-Roza = A. Otero-eRoza and E. R. Johnson, *the journal of chemical physics*, 2012, 137, 054103