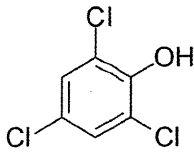
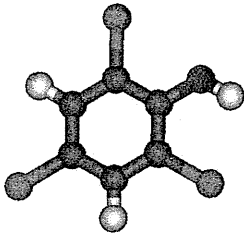
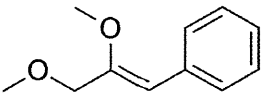
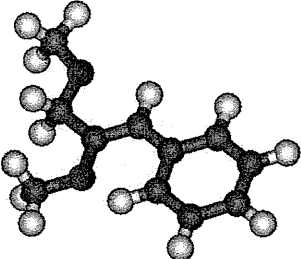
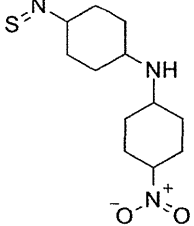
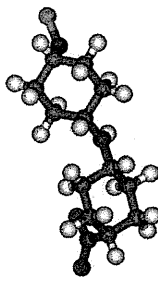
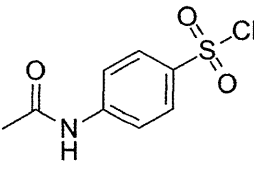
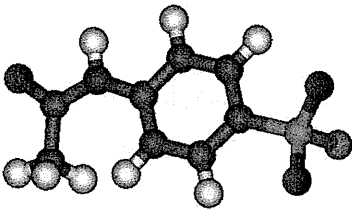
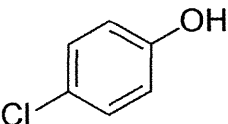
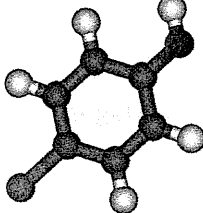
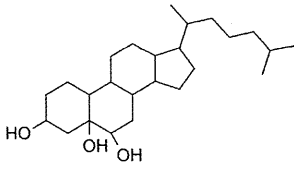
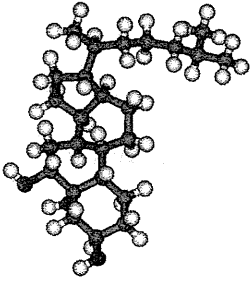
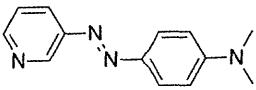
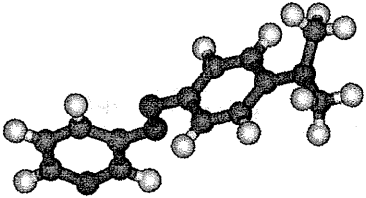
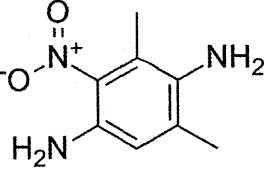
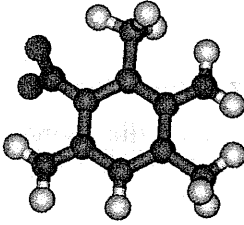
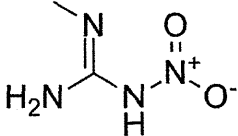
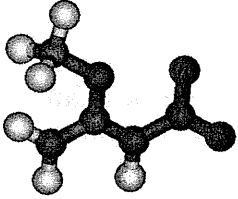
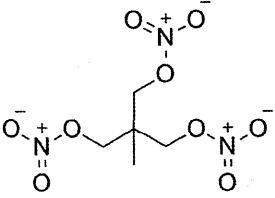
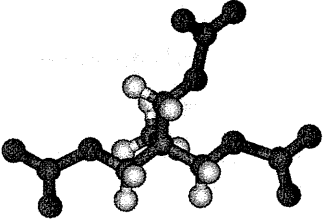
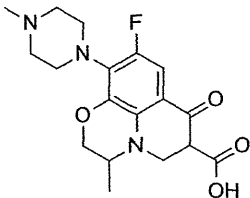
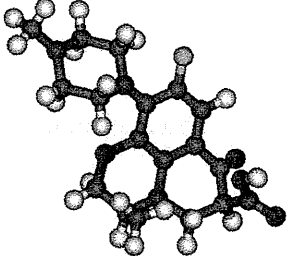
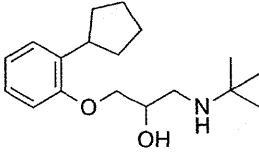
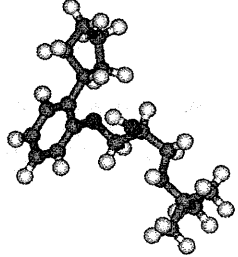
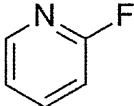
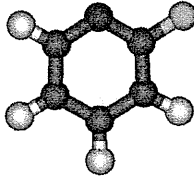
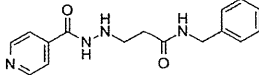
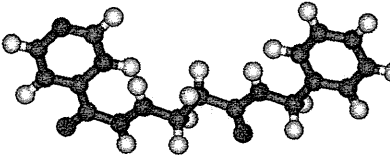
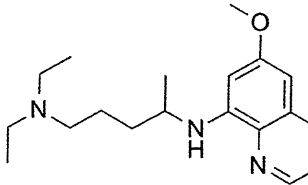
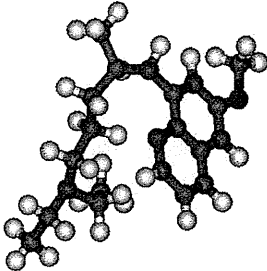
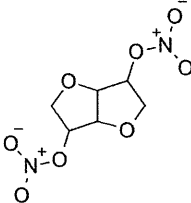
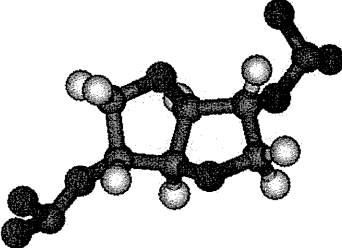
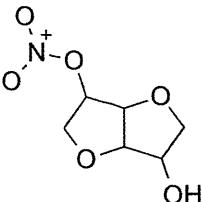
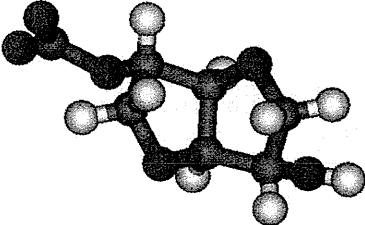
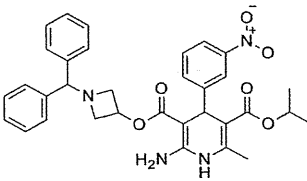
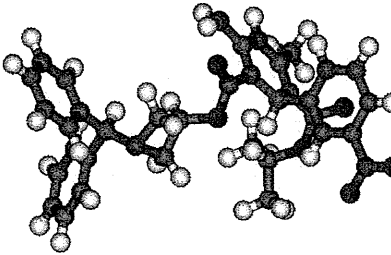
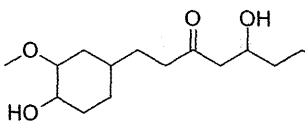
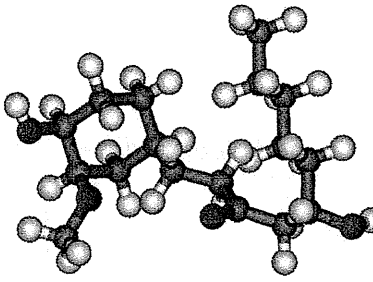
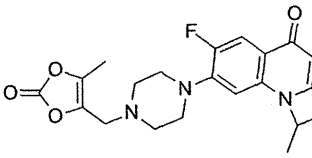
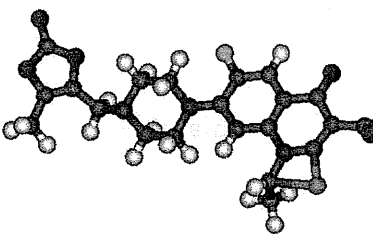
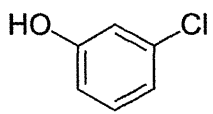
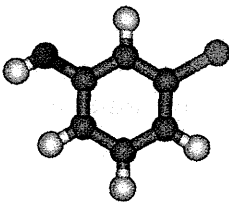
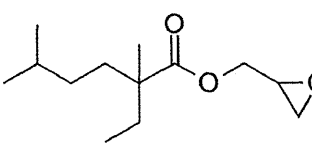
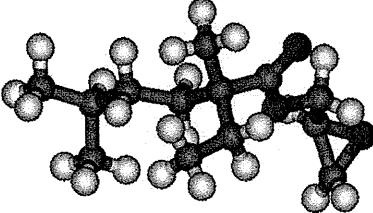
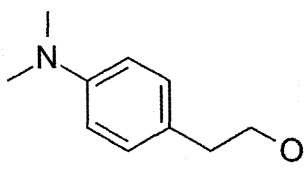
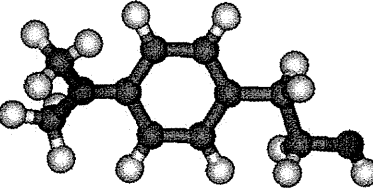
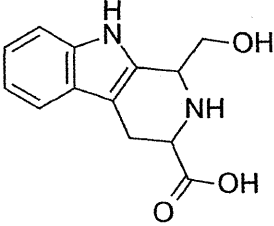
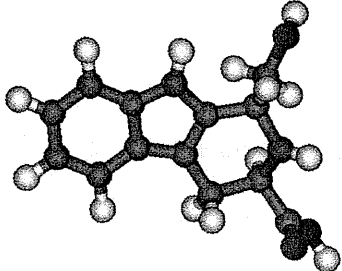
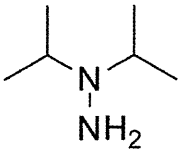
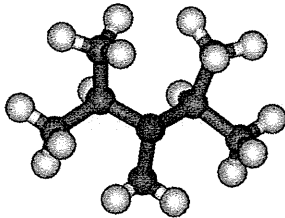
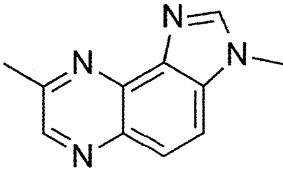
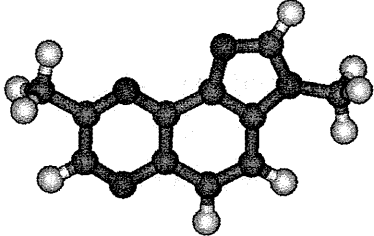
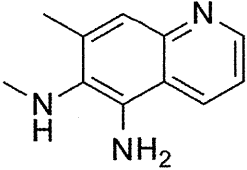
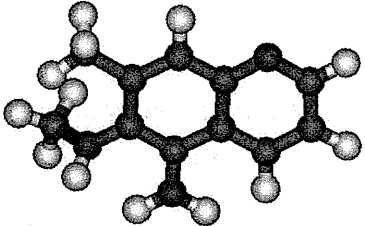
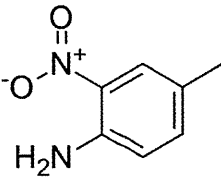
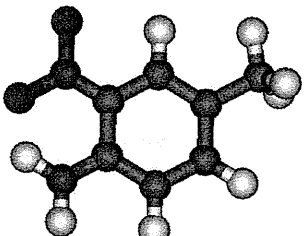
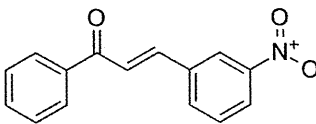
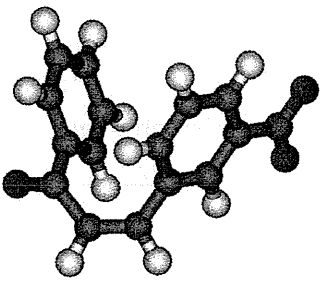
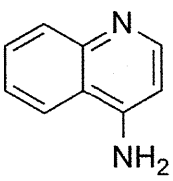
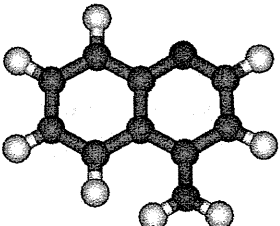


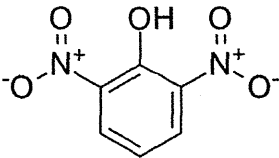
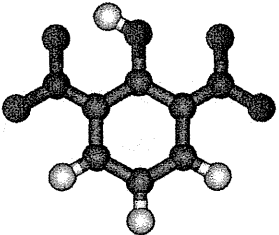
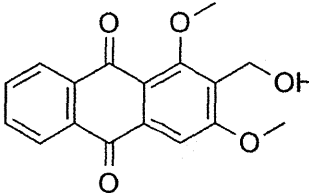
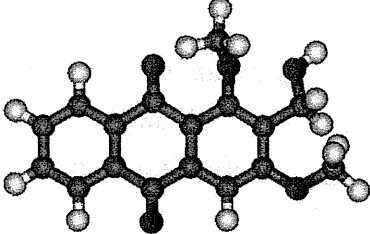
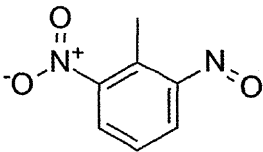
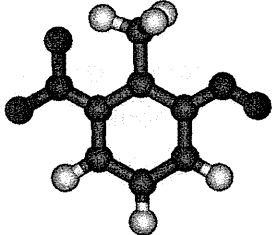
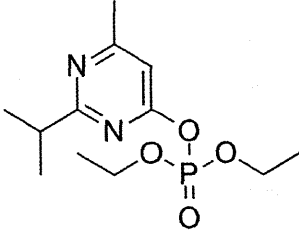
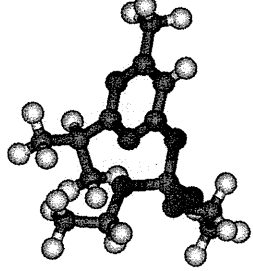
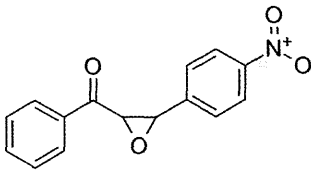
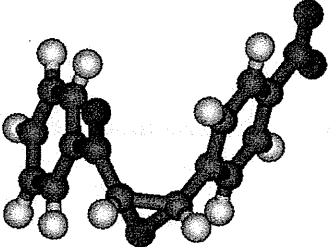
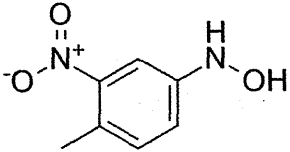
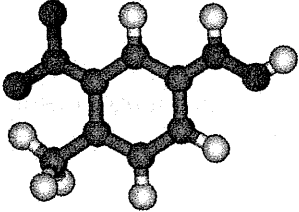
18	2,4,6-trichlorophenol		
19	z-2,3-dimethoxypropenylbenzene		
20	amoscanate		
21	4-(acetylamino)benzenesulfonyl chloride		
22	4-chlorophenol		
23	cholestane-3beta,5alpha,6beta-triol		

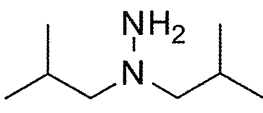
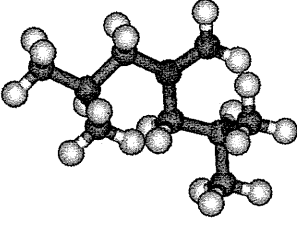
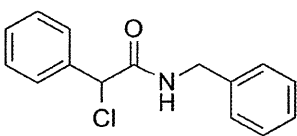
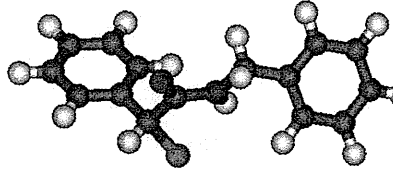
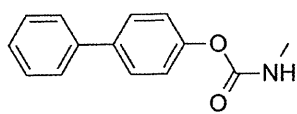
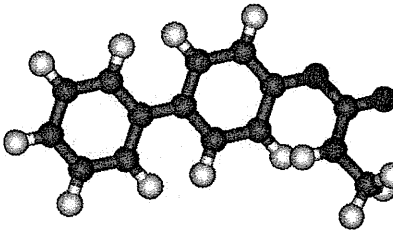
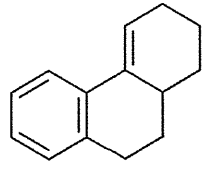

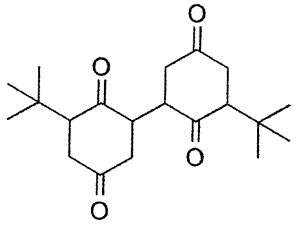
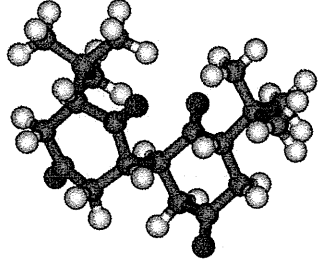
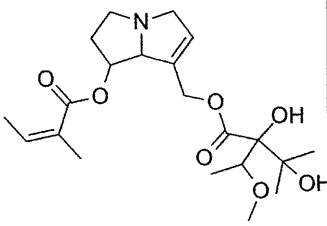
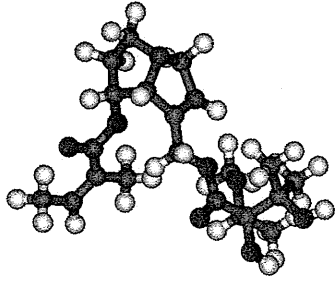
24	4'-(n,n-dimethylamino)-1'-phenylazo-3-pyridine		
25	4-amino-3-nitro-2,6-dimethylaniline		
26	n-methyl-n'-nitroguanidine		
27	trimethylolethane trinitrate		
28	dr3354		
29	(-)-penbutolol		

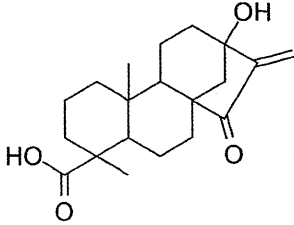
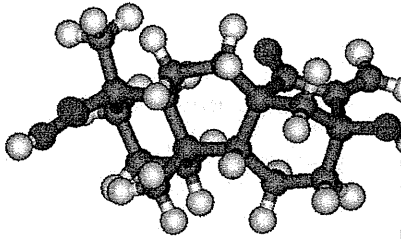
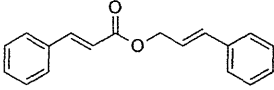
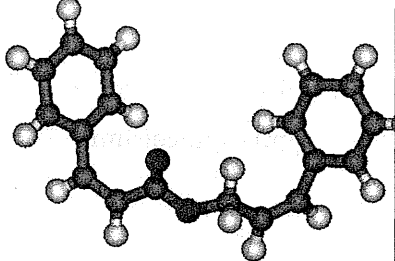
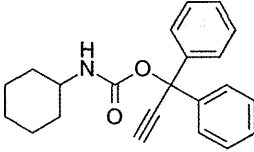
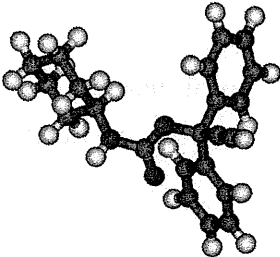
30	2-fluoropyridine		
31	nialamide		
32	pamaquine		
33	isodinit		
34	monisid		
35	azelnidipine		

36	gingerol		
37	prulifloxacin		
38	3-chlorophenol		
39	neodecanoic acid, 2,3-epoxypropyl ester		
40	4-(dimethylamino) benzeneethanol		
41	### tetrahydro-beta-carboline-3-carboxylic acid		

42	n,n-diisopropylhydrazine		
43	3,8-dimethyl-3h-imidazo[4,5-f]quinoxaline		
44	6,7-dimethylquinoline-5,6-diamine		
45	4-methyl-2-nitroaniline		
46	3-nitrochalcone		
47	4-aminoquinoline		

48	2,6-dinitrophenol		
49	2-(hydroxymethyl)-1,3-dimethoxyanthraquinone		
50	2-nitroso-6-nitrotoluene		
51	diazoxon		
52	4-nitrochalcone oxide		
53	4-hydroxylamino-2-nitrotoluene		

54	n,n-diisobutylhydrazine		
55	n-benzyl-2-chloro-2-phenylacetamide		
56	p-biphenyl n-methylcarbamate		
57	1,2,3,9,10,10a-hexahydrophenanthrene		
58	3,3'-di-tert-butylbiphenyldiquinone (2,5,2',5')		
59	lasiocarpine		

60	15-oxosteviol	 <p>Chemical structure of 15-oxosteviol, a complex steroid-like molecule with multiple fused rings, a hydroxyl group (OH), a carbonyl group (C=O), and a carboxylic acid group (HO-C=O).</p>	 <p>Ball-and-stick model of 15-oxosteviol, showing the spatial arrangement of atoms in the molecule.</p>
61	cinnamyl cinnamate	 <p>Chemical structure of cinnamyl cinnamate, consisting of two cinnamyl groups linked by an ester bond.</p>	 <p>Ball-and-stick model of cinnamyl cinnamate, showing the spatial arrangement of atoms in the molecule.</p>
62	1,1-diphenyl-2-propynyl-n-cyclohexyl carbamate	 <p>Chemical structure of 1,1-diphenyl-2-propynyl-n-cyclohexyl carbamate, featuring a cyclohexane ring, a carbamate group, and a propargyl group substituted with two phenyl rings.</p>	 <p>Ball-and-stick model of 1,1-diphenyl-2-propynyl-n-cyclohexyl carbamate, showing the spatial arrangement of atoms in the molecule.</p>

研究成果の刊行に関する一覧表

発表者氏名	論文タイトル名	発表誌名	巻	ページ	出版年
参考：コンピュータシミュレーションを含むもの					
栗原正明	コンピュータシミュレーションによる違法ドラッグの活性予測	<i>YAKUGAKU ZASSHI</i>	133	13-16	2013
Demizu, Y., Nagoya, S., Shirakawa, M., Kawamura, M., Yamagata, N., Sato, Y., Doi, M., Kurihara, M.	Development of stapled short helical peptides capable of inhibiting vitamin D receptor (VDR)-coactivator interactions	<i>Bioorg. Med. Chem. Lett.</i>	23	4292-4296	2013
N. Sakakibara, T. Hamasaki, M. Baba, Y. Demizu, M. Kurihara, K. Irie, M. Iwai, E. Asada, Y. Kato, T. Maruyama;	Synthesis and evaluation of novel 3-(3,5-dimethylbenzyl)-uracil analogs as potential anti-HIV-1 agents	<i>Bioorg. Med. Chem.,</i>	21	5900-5806	2013
I. Kato, M. Oba, M. Kurihara, Y. Takano, M. Tanaka	Synthesis of Cyclic α,α -Disubstituted Amino Acid Bearing a Pendent Chiral Center	<i>Peptide Science 2012</i>		129-130	2013
A. Imanishi, M. Oba, Y. Demizu, M. Kurihara, M. Doi, H. Takazaki, H. Suemune, M. Tanaka;	Synthesis of Chiral Five-membered Ring Amino Acids with an Azido Group, and Their Peptides	<i>Peptide Science 2012</i>		131-132	2013
N. Yamazaki, Y. Demizu, Y. Sato, M. Doi, M. Kurihara	Helical Foldamer Containing a Combination of Cyclopentane-1,2-diamine and 2,2-Dimethylmalonic Acid;	<i>J. Org. Chem.</i>	78	9991-9994	2013
M. Oba, N. Ishikawa, Y. Demizu, M. Kurihara, H. Suemune, M. Tanaka	Helical Oligomer with Changeable Chiral Acetal Moiety	<i>Eur. J. Org. Chem.</i>		7679-7682	2013
Y. Demizu, H. Yamashita, N. Yamazaki, Y. Sato, M. Doi, M. Tanaka, M. Kurihara;	Oligopeptides with equal amounts of l- and d-amino acids may prefer a helix screw sense	<i>J. Org. Chem.,</i>	78	12106-12113	2013

43	ISSSTY_v1a_7367_02May011_53	95-54-5	c1(N)c(N)cccc1	3
44	ISSSTY_v1a_7367_02May011_54	117-39-5	C1(O)C(=O)c2c(O)cc(O)cc2OC=1c1cc(O)c(O)cc1	3
45	ISSSTY_v1a_7367_02May011_55	1321-74-0	HC=Cc1c(C=CH)cccc1	1
46	ISSSTY_v1a_7367_02May011_56	509-14-8	C([N+](=O)[O-])([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]	3
47	ISSSTY_v1a_7367_02May011_57	111-30-8	HC(C(H)C(H)C=O)C=O	3
48	ISSSTY_v1a_7367_02May011_58	56-53-1	HC(H)C(H)C(c1ccc(O)cc1)=C(c1ccc(O)cc1)C(H)C(H)H	1
49	ISSSTY_v1a_7367_02May011_59	75-25-2	C(Br)(Br)Br	1
50	ISSSTY_v1a_7367_02May011_60	100-21-0	C(=O)(O)c1ccc(C(=O)O)cc1	1
51	ISSSTY_v1a_7367_02May011_61	67-68-5	HC(H)S(=O)C(H)H	1
52	ISSSTY_v1a_7367_02May011_62	94-59-7	HC(c1cc2c(cc1)OC(H)O2)C=CH	1
53	ISSSTY_v1a_7367_02May011_64	7722-84-1	OO	3
54	ISSSTY_v1a_7367_02May011_65	95-80-7	HC(H)c1c(N)cc(N)cc1	3
55	ISSSTY_v1a_7367_02May011_66	100-52-7	c1(C=O)cccc1	3
56	ISSSTY_v1a_7367_02May011_67	2642-98-0	c1(N)c2c(c3c(c4c(cccc4)cc3)c1)cccc2	3
57	ISSSTY_v1a_7367_02May011_68	930-55-2	HC1C(H)C(H)C(H)N1N=O	3
58	ISSSTY_v1a_7367_02May011_69	50-78-2	HC(H)C(=O)Oc1c(C(=O)O)cccc1	1
59	ISSSTY_v1a_7367_02May011_70	120-61-6	HC(H)OC(=O)c1ccc(C(=O)OC(H)H)cc1	1
60	ISSSTY_v1a_7367_02May011_71	5307-14-2	c1(N)c(N(=O)=O)cc(N)cc1	3
61	ISSSTY_v1a_7367_02May011_73	50-18-0	HC1C(H)C(H)NP(=O)(N(C(H)C(H)Cl)C(H)C(H)Cl)O1	3
62	ISSSTY_v1a_7367_02May011_74	56-57-5	c1([N+](=O)[O-])c2c(cccc2)[n+](c1)cc1	3
63	ISSSTY_v1a_7367_02May011_75	35796	C1(C=O)=CC=CO1	1
64	ISSSTY_v1a_7367_02May011_76	56-23-5	C(Cl)(Cl)(Cl)Cl	3
65	ISSSTY_v1a_7367_02May011_77	27639	HC(Cl)Cl	3
66	ISSSTY_v1a_7367_02May011_78	542-56-3	HC(H)C(C(H)H)C(H)ON=O	3
67	ISSSTY_v1a_7367_02May011_79	140-49-8	HC(H)C(=O)Nc1ccc(C(=O)C(H)Cl)cc1	3
68	ISSSTY_v1a_7367_02May011_81	94-75-7	HC(C(=O)O)Oc1c(Cl)cc(Cl)cc1	1
69	ISSSTY_v1a_7367_02May011_82	680-31-9	HC(H)N(C(H)H)P(=O)(N(C(H)H)C(H)H)N(C(H)H)C(H)H)	1
70	ISSSTY_v1a_7367_02May011_83	133-06-2	HC1C2C(=O)N(SC(Cl)(Cl)Cl)C(=O)C2C(H)C=C1	3
71	ISSSTY_v1a_7367_02May011_84	3252-43-5	C(N)C(Br)Br	3
72	ISSSTY_v1a_7367_02May011_85	106-50-3	c1(N)ccc(N)cc1	3
73	ISSSTY_v1a_7367_02May011_86	91-20-3	c12c(cccc1)cccc2	1
74	ISSSTY_v1a_7367_02May011_87	78-93-3	HC(H)C(=O)C(H)C(H)H	1
75	ISSSTY_v1a_7367_02May011_89	51-28-5	c1(O)c([N+](=O)[O-])cc([N+](=O)[O-])cc1	1
76	ISSSTY_v1a_7367_02May011_90	100-97-0	HC1N2C(H)N3C(H)N(C(H)N1C3H)C2H	1
77	ISSSTY_v1a_7367_02May011_91	120-80-9	c1(O)c(O)cccc1	1
78	ISSSTY_v1a_7367_02May011_92	123-86-4	HC(H)C(=O)OC(H)C(H)C(H)C(H)H	1
79	ISSSTY_v1a_7367_02May011_93	518-82-1	HC(H)c1cc2C(=O)c3c(C(=O)c2c(O)c1)c(O)cc(O)c3	3
80	ISSSTY_v1a_7367_02May011_94	64091-91-4	HC(H)N(C(H)C(H)C(H)C(=O)c1ccnc1)N=O	3
81	ISSSTY_v1a_7367_02May011_95	313-67-7	HC(H)Oc1c2c(c3c(c(C(=O)O)cc4c3OC(H)O4)c(N(=O)=O)c2)ccc1	3
82	ISSSTY_v1a_7367_02May011_96	123-91-1	HC1C(H)OC(H)C(H)O1	1
83	ISSSTY_v1a_7367_02May011_98	108-30-5	HC1C(=O)OC(=O)C1H	1
84	ISSSTY_v1a_7367_02May011_99	75-27-4	C(Cl)(Cl)Br	3

85	ISSSTY_v1a_7367_02May011_100	75-07-0	HC(H)C=O	1
86	ISSSTY_v1a_7367_02May011_101	57-41-0	C1(=O)C(c2ccccc2)(c2ccccc2)NC(=O)N1	1
87	ISSSTY_v1a_7367_02May011_103	122-04-3	C(=O)(Cl)c1ccc(N(=O)=O)cc1	3
88	ISSSTY_v1a_7367_02May011_104	106-89-8	HC(Cl)C1C(H)O1	3
89	ISSSTY_v1a_7367_02May011_105	108-95-2	c1(O)cccc1	1
90	ISSSTY_v1a_7367_02May011_106	78-84-2	HC(H)C(C(H)H)C=O	3
91	ISSSTY_v1a_7367_02May011_107	106-93-4	HC(Br)C(H)Br	3
92	ISSSTY_v1a_7367_02May011_108	61-57-4	HC1C(H)N(C2=NC=C(N(=O)=O)S2)C(=O)N1	3
93	ISSSTY_v1a_7367_02May011_109	124-04-9	HC(C(=O)O)C(H)C(H)C(H)C(=O)O	1
94	ISSSTY_v1a_7367_02May011_110	100-42-5	HC=Cc1cccc1	1
95	ISSSTY_v1a_7367_02May011_111	52315-07-8	HC(H)C1(C(H)H)C(C(=O)OC(c2cc(Oc3ccccc3)ccc2)C_N)C1C=C(Cl)Cl	1
96	ISSSTY_v1a_7367_02May011_112	97-53-0	HC(H)Oc1c(O)ccc(C(H)C=CH)c1	1
97	ISSSTY_v1a_7367_02May011_113	91-23-6	HC(H)Oc1c(N(=O)=O)cccc1	3
98	ISSSTY_v1a_7367_02May011_115	121-69-7	HC(H)N(c1cccc1)C(H)H	1
99	ISSSTY_v1a_7367_02May011_116	99-56-9	c1(N)c(N)cc(N(=O)=O)cc1	3
100	ISSSTY_v1a_7367_02May011_118	97-18-7	c1(Cl)c(O)c(Sc2c(O)c(Cl)cc(Cl)c2)cc(Cl)c1	1
101	ISSSTY_v1a_7367_02May011_119	136911	HC(C(H)OC(=O)C=CH)OC(=O)C=CH	1
102	ISSSTY_v1a_7367_02May011_121	1634-04-4	HC(H)C(C(H)H)(C(H)H)OC(H)H	1
103	ISSSTY_v1a_7367_02May011_122	148-24-3	c1(O)c2c(cccn2)ccc1	3
104	ISSSTY_v1a_7367_02May011_123	57-97-6	HC(H)c1c2c(c(C(H)H)c3c4c(ccc13)cccc4)cccc2	3
105	ISSSTY_v1a_7367_02May011_124	17026-81-2	HC(H)C(=O)Nc1cc(N)c(OC(H)C(H)H)cc1	3
106	ISSSTY_v1a_7367_02May011_125	107-06-2	HC(Cl)C(H)Cl	3
107	ISSSTY_v1a_7367_02May011_126	99-57-0	c1(O)c(N)cc(N(=O)=O)cc1	3
108	ISSSTY_v1a_7367_02May011_127	78-83-1	HC(H)C(C(H)H)C(H)O	1
109	ISSSTY_v1a_7367_02May011_128	6638-64-8	C1(=O)c2c(-c3c(cc(N(=O)=O)cc3)O1)cccc2	3
110	ISSSTY_v1a_7367_02May011_129	107-22-2	C(=O)C=O	3
111	ISSSTY_v1a_7367_02May011_130	139-13-9	HC(C(=O)O)N(C(H)C(=O)O)C(H)C(=O)O	1
112	ISSSTY_v1a_7367_02May011_131	28861	C(Cl)(Cl)=CCl	3
113	ISSSTY_v1a_7367_02May011_133	117-79-3	c12C(=O)c3c(C(=O)c1cc(N)cc2)cccc3	3
114	ISSSTY_v1a_7367_02May011_134	58-27-5	HC(H)C1C(=O)c2c(C(=O)C=1)cccc2	3
115	ISSSTY_v1a_7367_02May011_135	52-68-6	HC(H)OP(=O)(C(O)C(Cl)(Cl)Cl)OC(H)H	1
116	ISSSTY_v1a_7367_02May011_136	56-54-2	HC(H)Oc1cc2c([C@](O)[C@]3C(H)[C@@]4C(H)C(H)N3C(H)[C@]4C=CH)ccnc2cc1	1
117	ISSSTY_v1a_7367_02May011_138	443-48-1	HC(H)C1N(C(H)C(H)O)C(N(=O)=O)=CN=1	3
118	ISSSTY_v1a_7367_02May011_139	624-83-9	HC(H)N=C=O	1
119	ISSSTY_v1a_7367_02May011_140	88-99-3	C(=O)(O)c1c(C(=O)O)cccc1	1
120	ISSSTY_v1a_7367_02May011_141	88-74-4	c1(N)c(N(=O)=O)cccc1	1
121	ISSSTY_v1a_7367_02May011_142	1330-78-5	HC(H)c1ccc(OP(=O)(Oc2ccc(C(H)H)cc2)Oc2ccc(C(H)H)cc2)cc1	1
122	ISSSTY_v1a_7367_02May011_143	106-99-0	HC=CC=CH	3
123	ISSSTY_v1a_7367_02May011_145	106-88-7	HC(H)C(H)C1C(H)O1	3
124	ISSSTY_v1a_7367_02May011_146	70-25-7	HC(H)N(C(N)=NN(=O)=O)N=O	3
125	ISSSTY_v1a_7367_02May011_147	1817-73-8	c1(Br)c(N)c([N+](=O)[O-])cc([N+](=O)[O-])c1	3
126	ISSSTY_v1a_7367_02May011_148	127-00-4	HC(H)C(O)C(H)Cl	3

127	ISSSTY_v1a_7367_02May011_149	35407	HC(Br)C(Br)C(H)Cl	3
128	ISSSTY_v1a_7367_02May011_150	27336	C(=O)(O)c1ccc(Cl)cc1	1
129	ISSSTY_v1a_7367_02May011_151	80-43-3	HC(H)C(c1ccccc1)(C(H)H)OOC(c1ccccc1)(C(H)H)C(H)H	1
130	ISSSTY_v1a_7367_02May011_152	97-90-5	HC(H)C(C(=O)OC(H)C(H)OC(=O)C(C(H)H)=CH)=CH	1
131	ISSSTY_v1a_7367_02May011_153	57-63-6	HC(H)[C@@]12[C@](O)(C_C)C(H)C(H)[C@]1[C@@]1C(H)C(H)c3c(ccc(O)c3)[C@]1C(H)C2H	1
132	ISSSTY_v1a_7367_02May011_154	91-93-0	HC(H)Oc1c(N=C=O)ccc(-c2cc(OC(H)H)c(N=C=O)cc2)c1	3
133	ISSSTY_v1a_7367_02May011_155	42397-65-9	c1([N+](=O)[O-])c2c3c4c(c([N+](=O)[O-])ccc4ccc3cc1)cc2	3
134	ISSSTY_v1a_7367_02May011_156	29135	HC=CC(=O)O	1
135	ISSSTY_v1a_7367_02May011_157	59-50-7	HC(H)c1c(Cl)ccc(O)c1	1
136	ISSSTY_v1a_7367_02May011_158	88-72-2	HC(H)c1c(N(=O)=O)cccc1	1
137	ISSSTY_v1a_7367_02May011_159	1836-77-7	c1(Cl)c(Oc2ccc(N(=O)=O)cc2)c(Cl)cc(Cl)c1	3
138	ISSSTY_v1a_7367_02May011_160	13048-33-4	HC(C(H)C(H)C(H)C(H)OC(=O)C=CH)OC(=O)C=CH	1
139	ISSSTY_v1a_7367_02May011_161	101-80-4	c1(Oc2ccc(N)cc2)ccc(N)cc1	3
140	ISSSTY_v1a_7367_02May011_162	106-49-0	HC(H)c1ccc(N)cc1	1
141	ISSSTY_v1a_7367_02May011_163	78-96-6	HC(H)C(O)C(H)N	1
142	ISSSTY_v1a_7367_02May011_164	104-40-5	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)c1ccc(O)cc1	1
143	ISSSTY_v1a_7367_02May011_165	96-33-3	HC(H)OC(=O)C=CH	1
144	ISSSTY_v1a_7367_02May011_166	6623-66-1	C1(=O)c2c(-c3c(ccc(N(=O)=O)c3)O1)cccc2	3
145	ISSSTY_v1a_7367_02May011_168	1948-33-0	HC(H)C(c1c(O)ccc(O)c1)(C(H)H)C(H)H	1
146	ISSSTY_v1a_7367_02May011_169	62-23-7	C(=O)(O)c1ccc(N(=O)=O)cc1	3
147	ISSSTY_v1a_7367_02May011_170	924-42-5	HC=CC(=O)NC(H)O	1
148	ISSSTY_v1a_7367_02May011_171	78-88-6	HC(Cl)C(Cl)=CH	3
149	ISSSTY_v1a_7367_02May011_172	67-63-0	HC(H)C(O)C(H)H	1
150	ISSSTY_v1a_7367_02May011_174	91-59-8	c12c(cc(N)cc1)cccc2	3
151	ISSSTY_v1a_7367_02May011_177	95-49-8	HC(H)c1c(Cl)cccc1	1
152	ISSSTY_v1a_7367_02May011_178	67-20-9	HC1C(=O)NC(=O)N1N=CC1=CC=C(N(=O)=O)O1	3
153	ISSSTY_v1a_7367_02May011_180	124-48-1	C(Cl)(Br)Br	1
154	ISSSTY_v1a_7367_02May011_181	67-66-3	C(Cl)(Cl)Cl	1
155	ISSSTY_v1a_7367_02May011_182	29167	HC(Cl)C(=O)O	1
156	ISSSTY_v1a_7367_02May011_183	106-46-7	c1(Cl)ccc(Cl)cc1	1
157	ISSSTY_v1a_7367_02May011_185	51-79-6	HC(H)C(H)OC(N)=O	1
158	ISSSTY_v1a_7367_02May011_186	822-36-6	HC(H)C1=CN=CN1	1
159	ISSSTY_v1a_7367_02May011_187	33229-34-4	HC(O)C(H)N(c1cc(N(=O)=O)c(NC(H)C(H)O)cc1)C(H)C(H)O	3
160	ISSSTY_v1a_7367_02May011_188	100-47-0	C(N)c1cccc1	1
161	ISSSTY_v1a_7367_02May011_189	6358-31-2	HC(H)C(=O)C(C(=O)Nc1c(OC(H)H)cccc1)N=Nc1c(OC(H)H)cc(N(=O)=O)cc1	1
162	ISSSTY_v1a_7367_02May011_190	65-85-0	C(=O)(O)c1cccc1	1
163	ISSSTY_v1a_7367_02May011_191	102-01-2	HC(H)C(=O)C(H)C(=O)Nc1cccc1	1
164	ISSSTY_v1a_7367_02May011_192	544-63-8	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(=O)O	1
165	ISSSTY_v1a_7367_02May011_193	149-30-4	c12c(ccc1)NC(=S)S2	1
166	ISSSTY_v1a_7367_02May011_194	118-96-7	HC(H)c1c([N+](=O)[O-])cc([N+](=O)[O-])cc1N(=O)=O	3
167	ISSSTY_v1a_7367_02May011_196	88-73-3	c1(Cl)c(N(=O)=O)cccc1	3
168	ISSSTY_v1a_7367_02May011_197	621-64-7	HC(H)C(H)C(H)N(C(H)C(H)C(H)H)N=O	3

169	ISSSTY_v1a_7367_02May011_198	107-07-3	HC(Cl)C(H)O	3
170	ISSSTY_v1a_7367_02May011_200	95-46-5	HC(H)c1c(Br)cccc1	1
171	ISSSTY_v1a_7367_02May011_201	556-52-5	HC(O)C1C(H)O1	3
172	ISSSTY_v1a_7367_02May011_202	97-88-1	HC(H)C(C(=O)OC(H)C(H)C(H)C(H)H)=CH	1
173	ISSSTY_v1a_7367_02May011_204	91-17-8	HC1C(H)C(H)C(H)C2C(H)C(H)C(H)C(H)C12	1
174	ISSSTY_v1a_7367_02May011_205	123-30-8	c1(O)ccc(N)cc1	1
175	ISSSTY_v1a_7367_02May011_206	119-90-4	HC(H)Oc1c(N)ccc(-c2cc(OC(H)H)c(N)cc2)c1	3
176	ISSSTY_v1a_7367_02May011_208	77439-76-0	C1(=O)C(Cl)=C(C(Cl)Cl)C(O)O1	3
177	ISSSTY_v1a_7367_02May011_209	62-50-0	HC(H)C(H)OS(=O)(=O)C(H)H	3
178	ISSSTY_v1a_7367_02May011_210	18451	HC(H)C1C(=O)C2=C(C(=O)C=1N)[C@@](C(H)OC(N)=O)[C@@]1(OC(H)H)[C@]3[C@@](C(H)N2)N3	3
179	ISSSTY_v1a_7367_02May011_211	106-43-4	HC(H)c1ccc(Cl)cc1	1
180	ISSSTY_v1a_7367_02May011_212	62-44-2	HC(H)C(=O)Nc1ccc(OC(H)C(H)H)cc1	1
181	ISSSTY_v1a_7367_02May011_213	481-72-1	HC(O)c1cc2C(=O)c3c(C(=O)c2c(O)c1)c(O)ccc3	3
182	ISSSTY_v1a_7367_02May011_214	16219-75-3	HC(H)C=C1C(H)C2C(H)C1C=C2	1
183	ISSSTY_v1a_7367_02May011_215	96-45-7	HC1C(H)NC(=S)N1	3
184	ISSSTY_v1a_7367_02May011_216	481-42-5	HC(H)C1C(=O)c2c(C(=O)C=1)c(O)ccc2	3
185	ISSSTY_v1a_7367_02May011_217	100-02-7	c1(O)ccc(N(=O)=O)cc1	1
186	ISSSTY_v1a_7367_02May011_218	126-99-8	HC=C(Cl)C=CH	1
187	ISSSTY_v1a_7367_02May011_219	52-86-8	HC(C(=O)c1ccc(F)cc1)C(H)C(H)N1C(H)C(H)C(O)(c2ccc(Cl)cc2)C(H)C1H	1
188	ISSSTY_v1a_7367_02May011_220	111-40-0	HC(N)C(H)NC(H)C(H)N	1
189	ISSSTY_v1a_7367_02May011_221	115-29-7	HC1C2C3(Cl)C(Cl)C(Cl)C(Cl)(C(Cl)=C3Cl)C2C(H)OS(=O)O1	1
190	ISSSTY_v1a_7367_02May011_222	3333-52-6	HC(H)C(C(C_N)(C(H)H)C(H)H)(C_N)C(H)H	1
191	ISSSTY_v1a_7367_02May011_223	109-99-9	HC1C(H)C(H)C(H)O1	1
192	ISSSTY_v1a_7367_02May011_224	122021-01-6	HC(H)C(H)C(H)C(H)C(C(H)C(H)H)C(H)OC(=O)c1ccc(N(C(H)H)N=O)cc1	1
193	ISSSTY_v1a_7367_02May011_225	789-07-1	c12c3c4c(cc(N(=O)=O)cc4ccc3ccc1)cc2	3
194	ISSSTY_v1a_7367_02May011_226	97-00-7	c1(Cl)c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
195	ISSSTY_v1a_7367_02May011_227	96-29-7	HC(H)C(C(H)C(H)H)=NO	1
196	ISSSTY_v1a_7367_02May011_229	98-15-7	C(F)(F)(F)c1cc(Cl)ccc1	1
197	ISSSTY_v1a_7367_02May011_230	107-05-1	HC(Cl)C=CH	3
198	ISSSTY_v1a_7367_02May011_231	108-24-7	HC(H)C(=O)OC(=O)C(H)H	1
199	ISSSTY_v1a_7367_02May011_232	1477-55-0	HC(N)c1cc(C(H)N)ccc1	1
200	ISSSTY_v1a_7367_02May011_233	108-01-0	HC(H)N(C(H)H)C(H)C(H)O	1
201	ISSSTY_v1a_7367_02May011_235	84-79-7	HC(H)C(C(H)H)=CC(H)C1C(=O)C(=O)c2c(C=1O)cccc2	1
202	ISSSTY_v1a_7367_02May011_236	534-22-5	HC(H)C1=CC=CO1	1
203	ISSSTY_v1a_7367_02May011_237	115-11-7	HC(H)C(C(H)H)=CH	1
204	ISSSTY_v1a_7367_02May011_239	88-16-4	C(F)(F)(F)c1c(Cl)cccc1	1
205	ISSSTY_v1a_7367_02May011_240	90-30-2	c1(Nc2ccccc2)c2c(cccc2)ccc1	1
206	ISSSTY_v1a_7367_02May011_241	79-00-5	HC(Cl)C(Cl)Cl	3
207	ISSSTY_v1a_7367_02May011_243	60599-38-4	HC(H)C(=O)C(H)N(C(H)C(=O)C(H)H)N=O	3
208	ISSSTY_v1a_7367_02May011_244	1576-35-8	HC(H)c1ccc(S(=O)(=O)NN)cc1	3
209	ISSSTY_v1a_7367_02May011_245	105-60-2	HC1C(=O)NC(H)C(H)C(H)C1H	1
210	ISSSTY_v1a_7367_02May011_246	2475-45-8	c12C(=O)c3c(C(=O)c1c(N)ccc2N)c(N)ccc3N	3

211	ISSSTY_v1a_7367_02May011_247	91-22-5	c12c(cccc1)cccn2	3
212	ISSSTY_v1a_7367_02May011_248	107-21-1	HC(O)C(H)O	1
213	ISSSTY_v1a_7367_02May011_249	58-55-9	HC(H)N1C(=O)C2=C(N(C(H)H)C1=O)N=CN2	1
214	ISSSTY_v1a_7367_02May011_250	2784-94-3	HC(H)Nc1c(N(=O)=O)cc(N(C(H)C(H)O)C(H)C(H)O)cc1	3
215	ISSSTY_v1a_7367_02May011_251	150-76-5	HC(H)Oc1ccc(O)cc1	1
216	ISSSTY_v1a_7367_02May011_252	1506-02-1	HC(H)C1(C(H)H)c2c(C(C(H)H)(C(H)H)C(H)C1C(H)H)cc(C(=O)C(H)H)c(C(H)H)c2	1
217	ISSSTY_v1a_7367_02May011_253	130-15-4	C1(=O)c2c(C(=O)C=C1)cccc2	3
218	ISSSTY_v1a_7367_02May011_254	144-62-7	C(=O)(O)C(=O)O	1
219	ISSSTY_v1a_7367_02May011_255	108-46-3	c1(O)cc(O)ccc1	1
220	ISSSTY_v1a_7367_02May011_258	42397-64-8	c1([N+](=O)[O-])c2c3c4c(c([N+](=O)[O-])ccc4cc2)ccc3cc1	3
221	ISSSTY_v1a_7367_02May011_260	94-36-0	C(=O)(c1ccccc1)OOC(=O)c1ccccc1	1
222	ISSSTY_v1a_7367_02May011_261	135-88-6	c12c(cc(Nc3ccccc3)cc1)cccc2	1
223	ISSSTY_v1a_7367_02May011_262	87-62-7	HC(H)c1c(N)c(C(H)H)ccc1	1
224	ISSSTY_v1a_7367_02May011_263	598-55-0	HC(H)OC(N)=O	1
225	ISSSTY_v1a_7367_02May011_264	53609-64-6	HC(H)C(O)C(H)N(C(H)C(O)C(H)H)N=O	3
226	ISSSTY_v1a_7367_02May011_265	121-88-0	c1(N)c(O)cc(N(=O)=O)cc1	3
227	ISSSTY_v1a_7367_02May011_266	933-75-5	c1(Cl)c(Cl)c(O)c(Cl)cc1	1
228	ISSSTY_v1a_7367_02May011_267	83-38-5	c1(Cl)c(C=O)c(Cl)ccc1	1
229	ISSSTY_v1a_7367_02May011_270	99-99-0	HC(H)c1ccc(N(=O)=O)cc1	1
230	ISSSTY_v1a_7367_02May011_271	121-92-6	C(=O)(O)c1cc(N(=O)=O)ccc1	3
231	ISSSTY_v1a_7367_02May011_272	14371-10-9	c1(C=CC=O)ccccc1	1
232	ISSSTY_v1a_7367_02May011_273	59-87-0	C1(C=NNC(N)=O)=CC=C(N(=O)=O)O1	3
233	ISSSTY_v1a_7367_02May011_274	100-64-1	HC1C(=NO)C(H)C(H)C(H)C1H	1
234	ISSSTY_v1a_7367_02May011_275	108-21-4	HC(H)C(=O)OC(C(H)H)C(H)H	1
235	ISSSTY_v1a_7367_02May011_277	563-47-3	HC(H)C(C(H)Cl)=CH	1
236	ISSSTY_v1a_7367_02May011_278	20830-81-3	HC(H)C(=O)[C@@]1(O)C(H)c2c(O)c3C(=O)c4c(C(=O)c3c(O)c2[C@@](O)[C@@]2C(H)[C@](N)[C@](O)[C@](C(H)H)O2)C1H)c(O)C(H)H)ccc4	3
237	ISSSTY_v1a_7367_02May011_279	36405	c1(N)cc(N(=O)=O)ccc1	3
238	ISSSTY_v1a_7367_02May011_280	874-42-0	c1(Cl)c(C=O)ccc(Cl)c1	1
239	ISSSTY_v1a_7367_02May011_281	111-44-4	HC(Cl)C(H)OC(H)C(H)Cl	3
240	ISSSTY_v1a_7367_02May011_282	118-91-2	C(=O)(O)c1c(Cl)cccc1	1
241	ISSSTY_v1a_7367_02May011_284	75-00-3	HC(H)C(H)Cl	3
242	ISSSTY_v1a_7367_02May011_286	684-93-5	HC(H)N(C(N)=O)N=O	3
243	ISSSTY_v1a_7367_02May011_288	95-85-2	c1(O)c(N)cc(Cl)cc1	3
244	ISSSTY_v1a_7367_02May011_289	131-11-3	HC(H)OC(=O)c1c(C(=O)OC(H)H)cccc1	1
245	ISSSTY_v1a_7367_02May011_290	91-66-7	HC(H)C(H)N(c1ccccc1)C(H)C(H)H	1
246	ISSSTY_v1a_7367_02May011_291	96-48-0	HC1C(=O)OC(H)C1H	1
247	ISSSTY_v1a_7367_02May011_292	92-93-3	c1(-c2ccc(N(=O)=O)cc2)cccc1	3
248	ISSSTY_v1a_7367_02May011_293	29007	HC=CC(N)=O	1
249	ISSSTY_v1a_7367_02May011_294	389-08-2	HC(H)c1ccc2C(=O)C(C(=O)O)=CN(C(H)C(H)H)c2n1	3
250	ISSSTY_v1a_7367_02May011_295	104-76-7	HC(H)C(H)C(H)C(H)C(C(H)C(H)H)C(H)O	1
251	ISSSTY_v1a_7367_02May011_296	121-14-2	HC(H)c1c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
252	ISSSTY_v1a_7367_02May011_297	134682-95-4	HC(H)C(H)C(H)C(H)C(C(H)C(H)H)C(H)OC(=O)c1cc(N(=O)=O)c(N(C(H)H)C(H)H)cc1	3

253	ISSSTY_v1a_7367_02May011_298	892-21-7	c1(N(=O)=O)c2c3c(c4c(c3ccc2)cccc4)cc1	3
254	ISSSTY_v1a_7367_02May011_299	106-42-3	HC(H)c1ccc(C(H)H)cc1	1
255	ISSSTY_v1a_7367_02May011_300	100-61-8	HC(H)Nc1ccccc1	1
256	ISSSTY_v1a_7367_02May011_301	344-07-0	c1(Cl)c(F)c(F)c(F)c(F)c1F	1
257	ISSSTY_v1a_7367_02May011_302	604-75-1	c1(C2c3c(ccc(Cl)c3)NC(=O)C(O)N=2)ccccc1	1
258	ISSSTY_v1a_7367_02May011_303	532-27-4	HC(Cl)C(=O)c1ccccc1	1
259	ISSSTY_v1a_7367_02May011_305	110-80-5	HC(H)C(H)OC(H)C(H)O	1
260	ISSSTY_v1a_7367_02May011_306	16543-55-8	HC1C(H)C(H)C(c2cccnc2)N1N=O	3
261	ISSSTY_v1a_7367_02May011_307	119-36-8	HC(H)OC(=O)c1c(O)cccc1	1
262	ISSSTY_v1a_7367_02May011_308	79-43-6	C(=O)(O)C(Cl)Cl	3
263	ISSSTY_v1a_7367_02May011_309	30516-87-1	HC(H)C1C(=O)NC(=O)N([C@@]2C(H)[C@](N=N_N)[C@@](C(H)O)O2)C=1	3
264	ISSSTY_v1a_7367_02May011_310	4180-23-8	HC(H)C=Cc1ccc(OC(H)H)cc1	1
265	ISSSTY_v1a_7367_02May011_311	8003-22-3	C1(=O)c2c(C(=O)C1c1ccc3c(cccc3)n1)cccc2	3
266	ISSSTY_v1a_7367_02May011_312	99-61-6	c1(C=O)cc(N(=O)=O)ccc1	3
267	ISSSTY_v1a_7367_02May011_313	89-98-5	c1(Cl)c(C=O)cccc1	1
268	ISSSTY_v1a_7367_02May011_314	141-32-2	HC(H)C(H)C(H)C(H)OC(=O)C=CH	1
269	ISSSTY_v1a_7367_02May011_315	535-80-8	C(=O)(O)c1cc(Cl)ccc1	1
270	ISSSTY_v1a_7367_02May011_316	101-72-4	HC(H)C(C(H)H)Nc1ccc(Nc2ccccc2)cc1	1
271	ISSSTY_v1a_7367_02May011_317	17924-92-4	HC(H)[C@@]1C(H)C(H)C(H)C(=O)C(H)C(H)C(H)C=Cc2c(C(=O)O1)c(O)cc(O)c2	1
272	ISSSTY_v1a_7367_02May011_318	18420	HC(H)C(H)C1(c2ccccc2)C(=O)NC(=O)NC1=O	3
273	ISSSTY_v1a_7367_02May011_319	97-56-3	HC(H)c1c(N)ccc(N=Nc2c(C(H)H)cccc2)c1	3
274	ISSSTY_v1a_7367_02May011_320	625-48-9	HC(O)C(H)N(=O)=O	3
275	ISSSTY_v1a_7367_02May011_321	52645-53-1	HC(H)C1(C(H)H)[C@](C(=O)OC(H)c2cc(Oc3ccccc3)ccc2)[C@]1C=C(Cl)Cl	1
276	ISSSTY_v1a_7367_02May011_322	110-02-1	C1C=CSC=1	1
277	ISSSTY_v1a_7367_02May011_323	96-18-4	HC(Cl)C(Cl)C(H)Cl	3
278	ISSSTY_v1a_7367_02May011_324	552-89-6	c1(N(=O)=O)c(C=O)cccc1	1
279	ISSSTY_v1a_7367_02May011_325	36015	C(F)(F)(F)c1ccccc1	1
280	ISSSTY_v1a_7367_02May011_326	51264-14-3	HC(H)Oc1c(Nc2c3c(cccc3)nc3c2ccccc3)ccc(NS(=O)(=O)C(H)H)c1	3
281	ISSSTY_v1a_7367_02May011_327	75411-83-5	HC(H)C(O)C(H)N(C(H)H)N=O	3
282	ISSSTY_v1a_7367_02May011_328	609-31-4	HC(H)C(H)C(C(H)O)N(=O)=O	1
283	ISSSTY_v1a_7367_02May011_329	584-79-2	HC(H)C1=C(C(H)C=CH)C(=O)C(H)C1OC(=O)C1C(C(H)H)(C(H)H)C1C=C(C(H)H)C(H)H	3
284	ISSSTY_v1a_7367_02May011_330	19287-45-7	HB(H)B(H)H	3
285	ISSSTY_v1a_7367_02May011_331	134308-13-7	HC(H)c1ccc(C(=O)c2cc(O)c(O)c(N(=O)=O)c2)cc1	1
286	ISSSTY_v1a_7367_02May011_332	61499-28-3	HC(H)C(=O)C(H)N(C(H)C(O)C(H)H)N=O	3
287	ISSSTY_v1a_7367_02May011_333	68-22-4	HC(H)[C@@]12[C@](O)(C_c)C(H)C(H)[C@]1[C@@]1C(H)C(H)C3[C@@](C(H)C(H)C(=O)C=3)[C@]1C(H)C2H	1
288	ISSSTY_v1a_7367_02May011_334	117-80-6	C1(Cl)C(=O)c2c(C(=O)C=1Cl)cccc2	3
289	ISSSTY_v1a_7367_02May011_335	149-57-5	HC(H)C(H)C(H)C(H)C(C(=O)O)C(H)C(H)H	1
290	ISSSTY_v1a_7367_02May011_336	298-81-7	HC(H)Oc1c2c(C=CC(=O)O2)cc2c1OC=C2	3
291	ISSSTY_v1a_7367_02May011_337	122-14-5	HC(H)c1c(N(=O)=O)ccc(OP(=S)(OC(H)H)OC(H)H)c1	3
292	ISSSTY_v1a_7367_02May011_338	107-31-3	HC(H)OC=O	1
293	ISSSTY_v1a_7367_02May011_340	95-76-1	c1(Cl)c(Cl)cc(N)cc1	1
294	ISSSTY_v1a_7367_02May011_341	57-14-7	HC(H)N(N)C(H)H	3

295	ISSSTY_v1a_7367_02May011_342	1071-83-6	HC(C(=O)O)NC(H)P(=O)(O)O	1
296	ISSSTY_v1a_7367_02May011_343	60-80-0	HC(H)C1=CC(=O)N(c2ccccc2)N1C(H)H	1
297	ISSSTY_v1a_7367_02May011_344	60414-81-5	HC(H)C(=O)OC(C(H)H)C(H)N(C(H)C(C(H)H)OC(=O)C(H)H)N=O	3
298	ISSSTY_v1a_7367_02May011_346	96-69-5	HC(H)C(c1c(O)cc(C(H)H)c(Sc2c(C(H)H)cc(O)c(C(C(H)H)C(H)H)C(H)H)c2)c1)(C(H)H)C(H)H	1
299	ISSSTY_v1a_7367_02May011_347	102-06-7	c1(N=C(N)Nc2ccccc2)cccc1	1
300	ISSSTY_v1a_7367_02May011_348	3077-85-8	c12-c3c(ccc(N(=O)=O)c3)Nc1cccc2	3
301	ISSSTY_v1a_7367_02May011_349	108-05-4	HC(H)C(=O)OC=CH	1
302	ISSSTY_v1a_7367_02May011_350	302-17-0	C(Cl)(Cl)(Cl)C(O)O	3
303	ISSSTY_v1a_7367_02May011_351	1825-21-4	HC(H)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	3
304	ISSSTY_v1a_7367_02May011_352	108-10-1	HC(H)C(=O)C(H)C(C(H)H)C(H)H	1
305	ISSSTY_v1a_7367_02May011_353	89-25-8	HC(H)C1C(H)C(=O)N(c2ccccc2)N=1	1
306	ISSSTY_v1a_7367_02May011_354	84-66-2	HC(H)C(H)OC(=O)c1c(C(=O)OC(H)C(H)H)cccc1	1
307	ISSSTY_v1a_7367_02May011_355	140-88-5	HC(H)C(H)OC(=O)C=CH	1
308	ISSSTY_v1a_7367_02May011_356	55984-51-5	HC(H)C(=O)C(H)N(C(H)H)N=O	3
309	ISSSTY_v1a_7367_02May011_357	90-45-9	c12c(c(N)c3c(cccc3)n1)cccc2	3
310	ISSSTY_v1a_7367_02May011_358	83-72-7	C1(=O)C(=O)c2c(C(O)=C1)cccc2	1
311	ISSSTY_v1a_7367_02May011_360	1456-28-6	HC(H)C1C(H)N(N=O)C(H)C(C(H)H)O1	3
312	ISSSTY_v1a_7367_02May011_362	126222-34-2	HC(H)C(C(H)H)C(H)H)S(=O)(=O)C(H)[C@@](C(=O)N[C@@](C(=O)N[C@@](C(H)C1C(H)C(H)C(H)C1H)[C@@](O)[C@@](O)C1C(H)C(H)C(H)C1=CN=CN1)C(H)C1cccc1	1
313	ISSSTY_v1a_7367_02May011_363	103878-84-8	HC(N)C(H)NC(=O)c1ccc(Cl)cn1	1
314	ISSSTY_v1a_7367_02May011_364	4376-20-9	HC(H)C(H)C(H)C(H)C(C(H)C(H)H)C(H)OC(=O)c1c(C(=O)O)cccc1	1
315	ISSSTY_v1a_7367_02May011_365	75-65-0	HC(H)C(O)(C(H)H)C(H)H	1
316	ISSSTY_v1a_7367_02May011_366	29348	HC(H)C(c1ccc(O)cc1)(c1ccc(O)cc1)C(H)H	1
317	ISSSTY_v1a_7367_02May011_367	92-70-6	C(=O)(O)c1c(O)cc2c(cccc2)c1	1
318	ISSSTY_v1a_7367_02May011_368	108-39-4	HC(H)c1cc(O)ccc1	1
319	ISSSTY_v1a_7367_02May011_369	28652-72-4	HC(H)c1c(-c2ccccc2)cccc1	1
320	ISSSTY_v1a_7367_02May011_371	520-18-3	C1(O)C(=O)c2c(O)cc(O)cc2OC=1c1ccc(O)cc1	3
321	ISSSTY_v1a_7367_02May011_372	14901-07-6	HC(H)C1(C(H)H)C(C=CC(=O)C(H)H)=C(C(H)H)C(H)C(H)C1H	1
322	ISSSTY_v1a_7367_02May011_373	2835-95-2	HC(H)c1c(O)cc(N)cc1	3
323	ISSSTY_v1a_7367_02May011_375	60-33-3	HC(H)C(H)C(H)C(H)C(H)C(H)C=CC(H)C=CC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(=O)O	1
324	ISSSTY_v1a_7367_02May011_376	26471-62-5	HC(H)c1c(N=C=O)cc(N=C=O)cc1	3
325	ISSSTY_v1a_7367_02May011_377	2213-63-0	c12c(cccc1)nc(Cl)c(Cl)n2	1
326	ISSSTY_v1a_7367_02May011_379	74-83-9	HC(H)Br	3
327	ISSSTY_v1a_7367_02May011_380	120-57-0	HC1Oc2c(cc(C=O)cc2)O1	1
328	ISSSTY_v1a_7367_02May011_381	51-98-9	HC(H)[C@]12[C@@](C_c)(OC(=O)C(H)H)C(H)C(H)[C@]1[C@@]1C(H)C(H)C3[C@@](C(H)C(H)C(=O)C=3)[C@]1C(H)C2H	1
329	ISSSTY_v1a_7367_02May011_382	35311	HC1C(c2ccccc2)O1	3
330	ISSSTY_v1a_7367_02May011_384	2784-27-2	C1(=O)C(c2ccc(O)cc2)(c2ccccc2)NC(=O)N1	1
331	ISSSTY_v1a_7367_02May011_385	693-13-0	HC(H)C(C(H)H)N=C=NC(C(H)H)C(H)H	1
332	ISSSTY_v1a_7367_02May011_386	141-78-6	HC(H)C(=O)OC(H)C(H)H	1
333	ISSSTY_v1a_7367_02May011_387	112-55-0	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)S	1
334	ISSSTY_v1a_7367_02May011_388	97-63-2	HC(H)C(C(=O)OC(H)C(H)H)=CH	1
335	ISSSTY_v1a_7367_02May011_389	67730-11-4	HC(H)C1C2N(c3c(ccc(N)n3)N=2)C=CC=1	3
336	ISSSTY_v1a_7367_02May011_390	95-84-1	HC(H)c1cc(N)c(O)cc1	3

337	ISSSTY_v1a_7367_02May011_391	118-79-6	c1(Br)c(O)c(Br)cc(Br)c1	1
338	ISSSTY_v1a_7367_02May011_392	1122-58-3	HC(H)N(c1cc[n+][cc1])C(H)H	1
339	ISSSTY_v1a_7367_02May011_393	91-64-5	c12c(C=CC(=O)O1)cccc2	3
340	ISSSTY_v1a_7367_02May011_395	111-76-2	HC(H)C(H)C(H)C(H)OC(H)C(H)O	1
341	ISSSTY_v1a_7367_02May011_396	142-09-6	HC(H)C(C(=O)OC(H)C(H)C(H)C(H)C(H)H)=CH	1
342	ISSSTY_v1a_7367_02May011_398	491-70-3	C1(=O)c2c(O)cc(O)cc2OC(c2cc(O)c(O)cc2)=C1	1
343	ISSSTY_v1a_7367_02May011_399	603-34-9	c1(N(c2ccccc2)c2ccccc2)ccccc1	1
344	ISSSTY_v1a_7367_02May011_400	693-98-1	HC(H)C1=NC=CN1	1
345	ISSSTY_v1a_7367_02May011_401	54827-17-7	HC(H)c1c(N)c(C(H)H)cc(-c2cc(C(H)H)c(N)c(C(H)H)c2)c1	1
346	ISSSTY_v1a_7367_02May011_402	134-32-7	c1(N)c2c(cccc2)ccc1	3
347	ISSSTY_v1a_7367_02May011_403	5989-27-5	HC(H)C1C(H)C(H)[C@@](C(C(H)H)=CH)C(H)C=1	1
348	ISSSTY_v1a_7367_02May011_404	37151-16-9	HC(O)[C@]1[C@@](O)[C@@](O)[C@](N2c3c(c(N)nc(-c4ccc(N(=O)=O)cc4)n3)N=C2)O1	3
349	ISSSTY_v1a_7367_02May011_406	90-34-6	HC(H)C(C(H)C(H)C(H)N)Nc1c2c(cc(OC(H)H)c1)cccn2	3
350	ISSSTY_v1a_7367_02May011_407	91-94-1	c1(-c2cc(Cl)c(N)cc2)cc(Cl)c(N)cc1	3
351	ISSSTY_v1a_7367_02May011_408	109-06-8	HC(H)c1cccn1	1
352	ISSSTY_v1a_7367_02May011_410	100-19-6	HC(H)C(=O)c1ccc(N(=O)=O)cc1	3
353	ISSSTY_v1a_7367_02May011_411	108-03-2	HC(H)C(H)C(H)N(=O)=O	1
354	ISSSTY_v1a_7367_02May011_412	554-84-7	c1(O)cc(N(=O)=O)ccc1	3
355	ISSSTY_v1a_7367_02May011_413	552-16-9	C(=O)(O)c1c(N(=O)=O)cccc1	3
356	ISSSTY_v1a_7367_02May011_414	86-30-6	c1(N(c2ccccc2)N=O)ccccc1	3
357	ISSSTY_v1a_7367_02May011_415	69304-47-8	HC(O)[C@]1[C@@](O)C(H)[C@@](N2C(=O)NC(=O)C(C=CBr)=C2)O1	1
358	ISSSTY_v1a_7367_02May011_416	305-03-3	HC(c1ccc(N(C(H)C(H)Cl)C(H)C(H)Cl)cc1)C(H)C(H)C(=O)O	3
359	ISSSTY_v1a_7367_02May011_417	83-66-9	HC(H)C(c1c(OC(H)H)c([N+](=O)[O-])c(C(H)H)c([N+](=O)[O-])c1)(C(H)H)C(H)H	3
360	ISSSTY_v1a_7367_02May011_418	62-56-6	C(N)(N)=S	1
361	ISSSTY_v1a_7367_02May011_419	1319-77-3	HC(H)c1ccc(O)cc1	1
362	ISSSTY_v1a_7367_02May011_420	101-68-8	HC(c1ccc(N=C=O)cc1)c1ccc(N=C=O)cc1	1
363	ISSSTY_v1a_7367_02May011_421	36373	HC(H)c1cc(N(=O)=O)ccc1	1
364	ISSSTY_v1a_7367_02May011_422	111-41-1	HC(O)C(H)NC(H)C(H)N	3
365	ISSSTY_v1a_7367_02May011_423	110-86-1	c1cccn1	1
366	ISSSTY_v1a_7367_02May011_424	105650-23-5	HC(H)N1c2c(N=C1N)ncc(-c1ccccc1)c2	3
367	ISSSTY_v1a_7367_02May011_425	96-23-1	HC(Cl)C(O)C(H)Cl	3
368	ISSSTY_v1a_7367_02May011_426	112-57-2	HC(N)C(H)NC(H)C(H)NC(H)C(H)NC(H)C(H)N	3
369	ISSSTY_v1a_7367_02May011_427	38083-17-9	HC(H)C(C(=O)C(N1C=CN=C1)Oc1ccc(Cl)cc1)(C(H)H)C(H)H	1
370	ISSSTY_v1a_7367_02May011_428	128-37-0	HC(H)C(c1c(O)c(C(C(H)H)(C(H)H)C(H)H)cc(C(H)H)c1)(C(H)H)C(H)H	1
371	ISSSTY_v1a_7367_02May011_429	15687-27-1	HC(H)C(c1ccc(C(H)C(C(H)H)C(H)H)cc1)C(=O)O	1
372	ISSSTY_v1a_7367_02May011_430	2122-77-2	HC(O)C(H)Oc1c(Cl)cc(Cl)c(Cl)c1	1
373	ISSSTY_v1a_7367_02May011_431	75-77-4	HC(H)[Si](Cl)(C(H)H)C(H)H	1
374	ISSSTY_v1a_7367_02May011_433	75-78-5	HC(H)[Si](Cl)(Cl)C(H)H	1
375	ISSSTY_v1a_7367_02May011_434	78-67-1	HC(H)C(C_N)(C(H)H)N=NC(C_N)(C(H)H)C(H)H	1
376	ISSSTY_v1a_7367_02May011_435	67-21-0	HC(H)C(H)SC(H)C(H)C(N)C(=O)O	1
377	ISSSTY_v1a_7367_02May011_436	2524-03-0	HC(H)OP(=S)(Cl)OC(H)H	1
378	ISSSTY_v1a_7367_02May011_437	98-56-6	C(F)(F)(F)c1ccc(Cl)cc1	1

379	ISSSTY_v1a_7367_02May011_439	92-52-4	c1(-c2ccccc2)ccccc1	1
380	ISSSTY_v1a_7367_02May011_440	3096-52-4	c12C(=O)c3c(-c1ccc(N(=O)=O)c2)ccccc3	3
381	ISSSTY_v1a_7367_02May011_441	3290-92-4	HC(H)C(C(=O)OC(H)C(C(H)C(H)H)(C(H)OC(=O)C(C(H)H)=CH)C(H)OC(=O)C(C(H)H)=CH)=CH	1
382	ISSSTY_v1a_7367_02May011_442	25103-58-6	HC(H)C(S)(C(C(C(H)H)(C(H)H)C(C(H)H)C(H)H)(C(H)H)C(H)H)C(H)H	1
383	ISSSTY_v1a_7367_02May011_443	52-90-4	HC(S)C(N)C(=O)O	3
384	ISSSTY_v1a_7367_02May011_444	124-07-2	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(=O)O	1
385	ISSSTY_v1a_7367_02May011_445	140-29-4	HC(c1ccccc1)C_N	1
386	ISSSTY_v1a_7367_02May011_446	1116-54-7	HC(O)C(H)N(C(H)C(H)O)N=O	3
387	ISSSTY_v1a_7367_02May011_447	79-46-9	HC(H)C(C(H)H)N(=O)=O	3
388	ISSSTY_v1a_7367_02May011_448	75-35-4	HC=C(Cl)Cl	3
389	ISSSTY_v1a_7367_02May011_449	137-26-8	HC(H)N(C(=S)SSC(=S)N(C(H)H)C(H)H)C(H)H	3
390	ISSSTY_v1a_7367_02May011_450	485-47-2	C1(=O)C(O)(O)C(=O)c2c1ccccc2	1
391	ISSSTY_v1a_7367_02May011_451	6287-38-3	c1(Cl)c(Cl)cc(C=O)cc1	1
392	ISSSTY_v1a_7367_02May011_452	655-86-7	c1(N)c(N)c2c(cc1)nc1c(cccc1)n2	3
393	ISSSTY_v1a_7367_02May011_453	290-37-9	c1cnccn1	1
394	ISSSTY_v1a_7367_02May011_454	50782-69-9	HC(H)C(H)OP(=O)(C(H)H)SC(H)C(H)N(C(C(H)H)C(H)H)C(C(H)H)C(H)H	1
395	ISSSTY_v1a_7367_02May011_455	7390-81-0	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C1C(H)O1	1
396	ISSSTY_v1a_7367_02May011_456	105-36-2	HC(H)C(H)OC(=O)C(H)Br	3
397	ISSSTY_v1a_7367_02May011_458	117-08-8	C1(=O)c2c(C(=O)O1)c(Cl)c(Cl)c(Cl)c2Cl	1
398	ISSSTY_v1a_7367_02May011_459	23214-92-8	HC(H)[C@@]1[C@@](O)[C@@](N)C(H)[C@@]1O[C@]2c3c(O)c4C(=O)c5c(C(=O)c4c(O)c3C(H)[C@](O)(C(=O)C(H)O)C2H)cccc5OC(H)H)O1	3
399	ISSSTY_v1a_7367_02May011_460	110-83-8	HC1C(H)C(H)C(H)C=C1	1
400	ISSSTY_v1a_7367_02May011_461	1330-20-7	HC(H)c1cc(C(H)H)ccc1	1
401	ISSSTY_v1a_7367_02May011_462	597-25-1	HC(H)OP(=O)(N1C(H)C(H)OC(H)C1H)OC(H)H	1
402	ISSSTY_v1a_7367_02May011_463	10161-33-8	HC(H)[C@@]12[C@@](O)C(H)C(H)[C@]1[C@]1C(=C3C(C(H)C1H)=CC(=O)C(H)C3H)C=C2	1
403	ISSSTY_v1a_7367_02May011_465	542-75-6	HC(Cl)C=CCl	3
404	ISSSTY_v1a_7367_02May011_466	40297-54-9	HC(c1ccc(N(=O)=O)cc1)Nc1c2c(N(C3C(O)C(O)C(C(H)O)O3)C=N2)ncn1	3
405	ISSSTY_v1a_7367_02May011_467	10453-86-8	HC(H)C1(C(H)H)C(C(=O)OC(H)C2C=C(C(H)c3ccccc3)OC=2)C1C=C(C(H)H)C(H)H	1
406	ISSSTY_v1a_7367_02May011_469	136112-70-4	c1(-c2ccc([N+](=O)[O-])cc2)nc(N)c2c(N(c3ccc([N+](=O)[O-])cc3)C=N2)n1	3
407	ISSSTY_v1a_7367_02May011_471	84-75-3	HC(H)C(H)C(H)C(H)C(H)C(H)OC(=O)c1c(C(=O)OC(H)C(H)C(H)C(H)C(H)H)cccc1	1
408	ISSSTY_v1a_7367_02May011_472	35142-05-3	HC(H)Oc1c2c(c3c(c(C(=O)O)cc4c3OC(H)O4)cc2)ccc1	3
409	ISSSTY_v1a_7367_02May011_473	123-54-6	HC(H)C(=O)C(H)C(=O)C(H)H	3
410	ISSSTY_v1a_7367_02May011_476	589-18-4	HC(H)c1ccc(C(H)O)cc1	1
411	ISSSTY_v1a_7367_02May011_477	140-11-4	HC(H)C(=O)OC(H)c1ccccc1	1
412	ISSSTY_v1a_7367_02May011_480	688-74-4	HC(H)C(H)C(H)C(H)OB(OC(H)C(H)C(H)H)OC(H)C(H)C(H)C(H)H	1
413	ISSSTY_v1a_7367_02May011_482	119-61-9	c1(C(=O)c2ccccc2)ccccc1	1
414	ISSSTY_v1a_7367_02May011_483	21145-77-7	HC(H)C1(C(H)H)c2c(C(C(H)H)(C(H)H)C(H)C1C(H)H)cc(C(=O)C(H)H)c(C(H)H)c2	1
415	ISSSTY_v1a_7367_02May011_484	8024-37-1	HC(H)Oc1c(O)ccc(C=CC(=O)C(H)C(=O)C=Cc2cc(OC(H)H)c(O)cc2)c1	1
416	ISSSTY_v1a_7367_02May011_485	119-84-6	HC1c2c(cccc2)OC(=O)C1H	1
417	ISSSTY_v1a_7367_02May011_486	606-20-2	HC(H)c1c([N+](=O)[O-])cccc1[N+](=O)[O-]	3
418	ISSSTY_v1a_7367_02May011_487	108-90-7	c1(Cl)ccccc1	1
419	ISSSTY_v1a_7367_02May011_488	552-30-7	C1(=O)c2c(C(=O)O1)cc(C(=O)O)cc2	1
420	ISSSTY_v1a_7367_02May011_489	51-21-8	C1(=O)C(F)=CNC(=O)N1	1

421	ISSSTY_v1a_7367_02May011_490	625-86-5	HC(H)C1=CC=C(C(H)H)O1	1
422	ISSSTY_v1a_7367_02May011_492	5410-97-9	c12-c3c(cc(N(=O)=O)cc3)Oc1cccc2	3
423	ISSSTY_v1a_7367_02May011_494	396-01-0	c1(-c2c(N)nc3c(c(N)nc(N)n3)n2)cccc1	1
424	ISSSTY_v1a_7367_02May011_498	67-72-1	C(Cl)(Cl)(Cl)C(Cl)(Cl)Cl	1
425	ISSSTY_v1a_7367_02May011_499	628-34-2	HC(H)C(H)OC(H)C(H)Cl	3
426	ISSSTY_v1a_7367_02May011_500	421-70-5	C(F)(F)(I)C(F)(F)Br	3
427	ISSSTY_v1a_7367_02May011_502	822-06-0	HC(C(H)C(H)C(H)C(H)C(H)N=C=O)N=C=O	1
428	ISSSTY_v1a_7367_02May011_503	4337-65-9	HC(H)C(H)C(H)C(H)C(C(H)C(H)H)C(H)OC(=O)C(H)C(H)C(H)C(H)C(=O)O	1
429	ISSSTY_v1a_7367_02May011_504	63-25-2	HC(H)NC(=O)Oc1c2c(cccc2)ccc1	3
430	ISSSTY_v1a_7367_02May011_505	109-69-3	HC(H)C(H)C(H)C(H)Cl	1
431	ISSSTY_v1a_7367_02May011_506	15625-89-5	HC(H)C(H)C(C(H)OC(=O)C=CH)(C(H)OC(=O)C=CH)C(H)OC(=O)C=CH	3
432	ISSSTY_v1a_7367_02May011_508	77-47-4	C1(Cl)C(Cl)(Cl)C(Cl)=C(Cl)C=1Cl	1
433	ISSSTY_v1a_7367_02May011_509	524-42-5	C1(=O)C(=O)c2c(C=C1)cccc2	3
434	ISSSTY_v1a_7367_02May011_510	28376	c1(C2(c3ccc(O)cc3)c3c(C(=O)O2)cccc3)ccc(O)cc1	1
435	ISSSTY_v1a_7367_02May011_511	136112-71-5	C1(c2ccc([N+](=O)[O-])cc2)N(c2ccc([N+](=O)[O-])cc2)c2c(c(N)ncn2)N=1	3
436	ISSSTY_v1a_7367_02May011_512	108-88-3	HC(H)c1cccc1	1
437	ISSSTY_v1a_7367_02May011_513	108171-26-2	HC(H)C(H)C(Cl)C(Cl)C(Cl)C(H)C(Cl)C(Cl)C(Cl)C(H)H	1
438	ISSSTY_v1a_7367_02May011_514	21314-05-6	c1(N)c2c(N(c3ccc(N(=O)=O)cc3)C=N2)ncn1	3
439	ISSSTY_v1a_7367_02May011_516	934-32-7	c12c(cccc1)N=C(N)N2	1
440	ISSSTY_v1a_7367_02May011_517	103-23-1	HC(H)C(H)C(H)C(H)C(C(H)C(H)H)C(H)OC(=O)C(H)C(H)C(H)C(H)C(=O)OC(H)C(H)C(H)H)C(H)C(H)C(H)C(H)H	1
441	ISSSTY_v1a_7367_02May011_518	120-32-1	HC(c1c(O)ccc(Cl)c1)c1cccc1	1
442	ISSSTY_v1a_7367_02May011_520	102-71-6	HC(O)C(H)N(C(H)C(H)O)C(H)C(H)O	1
443	ISSSTY_v1a_7367_02May011_521	109875-50-5	c1(-c2ccc(N(=O)=O)cc2)nc(N)c2c(N=CN2)n1	3
444	ISSSTY_v1a_7367_02May011_522	125-33-7	HC(H)C(H)C1(c2cccc2)C(=O)NC(H)NC1=O	3
445	ISSSTY_v1a_7367_02May011_523	58-15-1	HC(H)C1=C(N(C(H)H)C(H)H)C(=O)N(c2cccc2)N1C(H)H	1
446	ISSSTY_v1a_7367_02May011_524	50-81-7	HC(O)C(O)C1C(=O)C(O)=C(O)O1	1
447	ISSSTY_v1a_7367_02May011_525	14191-22-1	c12-c3c(cc(N(=O)=O)cc3)Nc1cccc2	3
448	ISSSTY_v1a_7367_02May011_526	33457	HC(H)c1c(N=C=O)cccc1N=C=O	3
449	ISSSTY_v1a_7367_02May011_527	136-77-6	HC(H)C(H)C(H)C(H)C(H)C(H)c1c(O)cc(O)cc1	1
450	ISSSTY_v1a_7367_02May011_528	100-69-6	HC=Cc1ccccn1	1
451	ISSSTY_v1a_7367_02May011_529	140-67-0	HC(H)Oc1ccc(C(H)C=CH)cc1	1
452	ISSSTY_v1a_7367_02May011_530	136112-69-1	c1(Nc2ccc(N(=O)=O)cc2)c2c(N=CN2)ncn1	1
453	ISSSTY_v1a_7367_02May011_531	764-42-1	C(N)C=CC_N	1
454	ISSSTY_v1a_7367_02May011_532	1143-38-0	HC1c2c(C(=O)c3c(O)cccc13)c(O)ccc2	3
455	ISSSTY_v1a_7367_02May011_533	112-24-3	HC(N)C(H)NC(H)C(H)NC(H)C(H)N	3
456	ISSSTY_v1a_7367_02May011_534	83-79-4	HC(H)C([C@]1C(H)c2c3c(C(=O)[C@]4c5c(cc(OC(H)H)c(OC(H)H)c5)OC(H)[C@]4O3)ccc2O1)=CH	1
457	ISSSTY_v1a_7367_02May011_535	64-19-7	HC(H)C(=O)O	1
458	ISSSTY_v1a_7367_02May011_538	100-40-3	HC1C(H)C(C=CH)C(H)C=C1	1
459	ISSSTY_v1a_7367_02May011_539	27735	C(N)=O	1
460	ISSSTY_v1a_7367_02May011_540	54-31-9	HC(C1=CC=CO1)Nc1c(C(=O)O)cc(S(N)(=O)=O)c(Cl)c1	1
461	ISSSTY_v1a_7367_02May011_541	599-79-1	C(=O)(O)C1C(=O)C=CC(=N)Nc2ccc(S(=O)(=O)Nc3ccccn3)cc2)C=1	1
462	ISSSTY_v1a_7367_02May011_542	98-55-5	HC(H)C(O)(C(H)H)[C@@]1C(H)C(H)C(C(H)H)=CC1H	1