3,241	ISSSTY_v1a_7367_02May011_4062	29611-03-8	HC(H)Oc1c2C3=C(C(=O)Oc2c2c(c1)O[C@@]1[C@]2C=CO1)[C@@](O)C(H)C3H	3
3,242	ISSSTY_v1a_7367_02May011_4063	42464-80-2	HC(H)C(=O)Nc1c2c(ccc1)nccc2	1
3,243	ISSSTY_v1a_7367_02May011_4064	612-22-6	HC(H)C(H)c1c(N(=O)=O)cccc1	1
3,244	ISSSTY_v1a_7367_02May011_4065	100-12-9	HC(H)C(H)c1ccc(N(=O)=O)cc1	1
3,245	ISSSTY_v1a_7367_02May011_4066	66-56-8	c1(O)c([N+](=O)[O-])c([N+](=O)[O-])ccc1	3
3,246	ISSSTY_v1a_7367_02May011_4067	329-71-5	c1([N+](=O)[O-])c(O)cc([N+](=O)[O-])cc1	3
3,247	ISSSTY_v1a_7367_02May011_4068	573-56-8	c1([N+](=O)[O-])c(O)c([N+](=O)[O-])ccc1	1
3,248	ISSSTY_v1a_7367_02May011_4069	577-71-9	c1([N+](=O)[O-])c([N+](=O)[O-])cc(O)cc1	3
3,249	ISSSTY_v1a_7367_02May011_4070	606-22-4	c1([N+](=O)[O-])c(N)c([N+](=O)[O-])ccc1	3
3,250	ISSSTY_v1a_7367_02May011_4071	122587-22-8	HC(H)OC(=O)C1=C(Cl)C(Cl)=C(N(=O)=O)O1	3
3,251	ISSSTY_v1a_7367_02May011_4072	6884-87-3	HC(H)C(=O)Nc1ccc(S(=O)(=O)NC(H)H)cc1	1
3,252	ISSSTY_v1a_7367_02May011_4073	586-78-7	c1(Br)ccc(N(=O)=O)cc1	3
3,253	ISSSTY_v1a_7367_02May011_4074	89-59-8	HC(H)c1c(N(=O)=O)cc(Cl)cc1	1
3,254	ISSSTY_v1a_7367_02May011_4075	83-41-0	HC(H)c1c(C(H)H)c(N(=O)=O)ccc1	1
3,255	ISSSTY_v1a_7367_02May011_4076	81-20-9	HC(H)c1c(N(=O)=O)c(C(H)H)ccc1	1
3,256	ISSSTY_v1a_7367_02May011_4077	36501	HC(H)c1cc(C(H)H)cc(N(=O)=O)c1	1
3,257	ISSSTY_v1a_7367_02May011_4078	89-58-7	HC(H)c1c(N(=O)=O)cc(C(H)H)cc1	3
3,258	ISSSTY_v1a_7367_02May011_4079	616-72-8	HC(H)c1c([N+](=O)[O-])cc([N+](=O)[O-])c(C(H)H)c1	3
3,259	ISSSTY_v1a_7367_02May011_4080	96-99-1	C(=O)(O)c1cc(N(=O)=O)c(Cl)cc1	3
3,260	ISSSTY_v1a_7367_02May011_4081	528-45-0	C(=O)(O)c1cc([N+](=O)[O-])c([N+](=O)[O-])cc1	3
3,261	ISSSTY_v1a_7367_02May011_4082	99-34-3	C(=O)(O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1	3
3,262	ISSSTY_v1a_7367_02May011_4083	80-82-0	c1(S(=O)(=O)O)c(N(=O)=O)cccc1	1
3,263	ISSSTY_v1a_7367_02May011_4084	98-47-5	c1(S(=O)(=O)O)cc(N(=O)=O)ccc1	1
3,264	ISSSTY_v1a_7367_02May011_4085	138-42-1	c1(S(=O)(=O)O)ccc(N(=O)=O)cc1	1
3,265	ISSSTY_v1a_7367_02May011_4086	74367-78-5	HC(Cl)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1	3
3,266	ISSSTY_v1a_7367_02May011_4087	100-16-3	c1(NN)ccc(N(=O)=O)cc1	3
3,267	ISSSTY_v1a_7367_02May011_4088	119-26-6	c1(NN)c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
3,268	ISSSTY_v1a_7367_02May011_4089	1594-56-5	c1(SC_N)c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
3,269	ISSSTY_v1a_7367_02May011_4090	130638	HC(c1ccccc1)C(H)N=C=S	3
3,270	ISSSTY_v1a_7367_02May011_4091	92557-61-4	HC(H)N1c2c(C(C(H)[C@@]3(O)[C@@]4(O)[C@]([C@@](O)C(H)O4)OC3=O)=C1)cccc2	3

3,271	ISSSTY_v1a_7367_02May011_4092	14698-29-4	HC(H)C(H)N1c2c(C(=O)C(C(=O)O)=C1)cc1c(c2)OC(H)O1	3
3,272	ISSSTY_v1a_7367_02May011_4093	1192-62-7	HC(H)C(=O)C1=CC=CO1	3
3,273	ISSSTY_v1a_7367_02May011_4094	1204-60-0	c1(-c2cc(C=O)ccc2)ccccc1	1
3,274	ISSSTY_v1a_7367_02May011_4095	479-79-8	c12C(=O)c3c4c(ccc3-c1cccc2)cccc4	1
3,275	ISSSTY_v1a_7367_02May011_4096	86853-97-6	c12C(=O)c3c(c4c(cccc4)cc3)-c1c1c(cccc1)cc2	3
3,276	ISSSTY_v1a_7367_02May011_4097	92130-56-8	HC(H)c1c2c(c3c(c1)nccc3)N=CN2C(H)H	1
3,277	ISSSTY_v1a_7367_02May011_4098	13909-09-6	HC(H)C1C(H)C(H)C(NC(=O)N(C(H)C(H)Cl)N=O)C(H)C1H	3
3,278	ISSSTY_v1a_7367_02May011_4099	67019-20-9	HC(H)C(H)C(=O)NC1=C2C(C=CC=C2)=NS1	1
3,279	ISSSTY_v1a_7367_02May011_4100	6313-44-6	c12C(=O)c3c(C(N(=O)=O)c1cccc2)cccc3	1
3,280	ISSSTY_v1a_7367_02May011_4101	39653-72-0	C(_N)C1c2c3c(cccc3ccc2)C=1	3
3,281	ISSSTY_v1a_7367_02May011_4102	28434-86-8	c1(N)c(Cl)cc(Oc2cc(Cl)c(N)cc2)cc1	3
3,282	ISSSTY_v1a_7367_02May011_4103	613-50-3	c12c(cc(N(=O)=O)cc1)cccn2	3
3,283	ISSSTY_v1a_7367_02May011_4104	1421-85-8	c12-c3c(C4C(c1cc1c5c(ccc1c2)cccc5)O4)cccc3	3
3,284	ISSSTY_v1a_7367_02May011_4105	78-76-2	HC(H)C(H)C(Br)C(H)H	3
3,285	ISSSTY_v1a_7367_02May011_4106	111119-29-0	HC(H)OC(H)C(O)C(H)N1C(Cl)=NC(N(=O)=O)=C1	3
3,286	ISSSTY_v1a_7367_02May011_4107	1498903	HC(H)Oc1c(O)c2C(=O)c3c(C(=O)c2cc1)cccc3	1
3,287	ISSSTY_v1a_7367_02May011_4108	83312-51-0	HC(H)c1cc2C(=O)c3c(C(=O)c2cc1)ccc(O)c3	3
3,288	ISSSTY_v1a_7367_02May011_4109	2589-39-1	HC(H)c1c(O)c2C(=O)c3c(C(=O)c2c(O)c1)cccc3	3
3,289	ISSSTY_v1a_7367_02May011_4110	79560-36-4	HC(H)OC(H)c1c(O)c2C(=O)c3c(C(=O)c2cc1O)cccc3	3
3,290	ISSSTY_v1a_7367_02May011_4111	477-83-8	HC(H)Oc1c2C(=O)c3c(C(=O)c2cc(O)c1C(H)O)cccc3	3
3,291	ISSSTY_v1a_7367_02May011_4112	61434-48-8	HC(H)Oc1c2C(=O)c3c(C(=O)c2cc(OC(H)H)c1C(H)O)cccc3	1
3,292	ISSSTY_v1a_7367_02May011_4113	94574-56-8	HC(H)C(=O)OC(H)c1c(O)c2C(=O)c3c(C(=O)c2cc1O)cccc3	3
3,293	ISSSTY_v1a_7367_02May011_4114	3736-59-2	c12C(=O)c3c(C(=O)c1c(O)c(C(=O)c(O)c2)cccc3	1
3,294	ISSSTY_v1a_7367_02May011_4115	477-84-9	HC(H)Oc1c2C(=O)c3c(C(=O)c2cc(O)c1C=O)cccc3	1
3,295	ISSSTY_v1a_7367_02May011_4116	478-06-8	c12C(=O)c3c(C(=O)c1c(O)c(C(=O)O)c(O)c2)cccc3	1
3,296	ISSSTY_v1a_7367_02May011_4117	73-03-0	HC(O)[C@]1C(H)[C@@](O)[C@](N2c3c(c(N)ncn3)N=C2)O1	3
3,297	ISSSTY_v1a_7367_02May011_4118	132832-26-9	c1(O)c(O)c2c3c4c(c5c6c(ccc5c3ccc2cc1)cccc6)O4	3
3,298	ISSSTY_v1a_7367_02May011_4119	514-78-3	HC(H)C1(C(H)H)C(C=CC(C(H)H)=CC=CC(C(H)H)=CC=CC=C(C(H)H)C=CC=C(C(H)H)C=CC2C(C(H)HX C(H)H)C(H)C(H)C(=O)C=2C(H)H)=C(C(H)HC(=O)C(H)C1H	1
3,299	ISSSTY_v1a_7367_02May011_4121	23031-38-1	HC(H)C1(C(H)H)C(C(=O)OC(H)C2=CC=C(C(H)C_C)O2)C1C=C(C(H)H)C(H)H	3
3,300	ISSSTY_v1a_7367_02May011_4122	20562-02-1	HC(H)[C##]12C(C(H)[C#]O[C#]3[C#X]O[C##]3[C#]O[C#]4[C#]O[C##]O[C##]O[C##]O[C##]C(H)HO4][C##]O[C##]O[C##]O[C##]O[C##]C(H)HO4[C##]O[C##X[C##]O[H)O3]C(H)C1H0=CC(H)=CC(H)[C#]3[C##X(C(H)HX(C(H)C(H)[C##]	1

3,301	ISSSTY_v1a_7367_02May011_4123	80-78-4	HC(H)[C@@]12C(C(H)[C@@](O)C(H)C1H=CC(H)[C@]1[C@]3[C@@](C(H)H)C(H)C(H)[C@@]21)[C@]1[C@](C(H)H)[C@]2C(H)C(H)[C@](C(H)H)C(H)N2[C@]1C3H	1
3,302	ISSSTY_v1a_7367_02May011_4124	20562-03-2	HC(H)[C@@]12C(C(H)C@XO[C@@])C@XO[C@@]XO[C@@]XO(C@@)XO(C@H)C@H04)C@@)C@XO(C@@)[C@@]XO[C@@]XO[C@@]XO[C@](C@XC@H)H04)(C@@)X(C@H00)X3)C(H)C1H=CC(H)[C@]1[C@]3[C@@]X(C@HH)X0C@H)C@H[C@@]2	1
3,303	ISSSTY_v1a_7367_02May011_4126	114480-41-0	HC(H)c1c2c(c3c(c1)nccc3)N=C(NC(=O)C(H)H)N2C(H)H	3
3,304	ISSSTY_v1a_7367_02May011_4127	86831-65-4	HC(H)C(H)N(C(H)C(H)H)N([O-])N=O	3
3,305	ISSSTY_v1a_7367_02May011_4128	108529-37-9	HC(H)C(=O)NC1N(C(H)H)c2c(c3c(cc2)nccc3)N=1	3
3,306	ISSSTY_v1a_7367_02May011_4132	766-94-9	HC=COc1ccccc1	3
3,307	ISSSTY_v1a_7367_02May011_4133	869-01-2	HC(H)C(H)C(H)C(H)N(C(N)=O)N=O	3
3,308	ISSSTY_v1a_7367_02May011_4134	124617-83-0	HC(H)C(=O)ON(C(=O)c1ccccc1)OC(H)C(H)H	3
3,309	ISSSTY_v1a_7367_02May011_4136	124617-85-2	HC(H)C(=O)OC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)ONC(=O)c1ccccc1	3
3,310	ISSSTY_v1a_7367_02May011_4150	150445-96-8	HC(c1c([N+](=O)[O-])cccc1)ON=CC1N(C(H)c2ccccc2)c2c(cc([N+](=O)[O-])cc2)N=1	3
3,311	ISSSTY_v1a_7367_02May011_4151	150445-97-9	HC(c1cc([N+](=O)[O-])ccc1)ON=CC1N(C(H)c2ccc(Cl)cc2)c2c(cc([N+](=O)[O-])cc2)N=1	1
3,312	ISSSTY_v1a_7367_02May011_4152	150445-98-0	HC(c1c(Cl)cc(Cl)cc1)N1c2c(cc([N+](=O)[O-])cc2)N=C1C=NOC(H)c1c([N+](=O)[O-])cccc1	3
3,313	ISSSTY_v1a_7367_02May011_4153	150445-99-1	HC(c1cc([N+](=O)[O-])ccc1)ON=CC1N(C(H)c2ccc(F)cc2)c2c(cc([N+](=O)[O-])cc2)N=1	1
3,314	ISSSTY_v1a_7367_02May011_4154	150446-00-7	HC(H)C1=C(C=NOC(H)c2cc([N+](=O)[O-])ccc2)c2c(ccc([N+](=O)[O-])c2)N1C(H)c1ccccc1	3
3,315	ISSSTY_v1a_7367_02May011_4155	150446-02-9	HC(H)C1=C(C=NOC(H)c2ccc(Cl)cc2)c2c(ccc(N(=O)=O)c2)N1C(H)c1ccccc1	1
3,316	ISSSTY_v1a_7367_02May011_4156	150446-04-1	HC(H)C1=C(C(H)N2C=CN=C2)c2c(ccc(N(=O)=O)c2)N1C(H)c1ccccc1	3
3,317	ISSSTY_v1a_7367_02May011_4157	1086-00-6	HC(Cl)c1c2c3c4c(ccc3cc1)cccc4cc2	3
3,318	ISSSTY_v1a_7367_02May011_4158	132297-89-3	HC(H)Oc1cc2c(cc1)nc1c(c3c4c(cccc14)ccc3)c2	3
3,319	ISSSTY_v1a_7367_02May011_4159	94223-87-7	HC(H)c1cc2c(cc1)nc1c(c3c4c(cccc14)ccc3)c2	1
3,320	ISSSTY_v1a_7367_02May011_4160	94223-88-8	HC(H)c1cc2c(cc1)nc1c(c3c4c(cccc14)ccc3)c2	3
3,321	ISSSTY_v1a_7367_02May011_4161	958-09-8	HC(O)[C@]1[C@@](O)C(H)[C@](N2c3c(c(N)ncn3)N=C2)O1	1
3,322	ISSSTY_v1a_7367_02May011_4162	2371-42-8	HC(H)C1(O)C2(C(H)H)C(C(H)H)(C(H)H)C(C(H)C2H)C1H	1
3,323	ISSSTY_v1a_7367_02May011_4164	54406-48-3	HC(H)C1(C(H)H)C(C(=O)OC(C(C(H)H)=CC(H)C(H)H)C_C)C1C=C(C(H)H)C(H)H	1
3,324	ISSSTY_v1a_7367_02May011_4166	130933-91-4	c12c3c(c4c(c5c([C@](O)[C@@](O)[C@@]6[C@@]5O6)cc4)cc3ccc1)C=C2	3
3,325	ISSSTY_v1a_7367_02May011_4172	1635-63-8	HC(H)NP1(NC(H)H)N=P(NC(H)H)(NC(H)H)N=P(NC(H)H)(NC(H)H)N=1	1
3,326	ISSSTY_v1a_7367_02May011_4173	6607-30-3	HC(H)P1(C(H)H)N=P(C(H)H)(C(H)H)N=P(C(H)H)(C(H)H)N=1	1
3,327	ISSSTY_v1a_7367_02May011_4174	69322-61-8	C(=O)(O)c1ccc(ON2P(Oc3ccc(C(=O)O)cc3)N(Oc3ccc(C(=O)O)cc3)P(Oc3ccc(C(=O)O)cc3)N=P2(Oc2ccc(C(=O)O)cc2)Oc2ccc(C(=O)O)cc2)cc1	1
3,328	ISSSTY_v1a_7367_02May011_4175	6379-69-7	HC(H)[C@]12[C@@]3(C(H)H)[C@]4(C(H)O4)[C@@](C(H)[C@@]3OC(=O)C=CC(H)H)O[C@]1C=C(C(H)H)C(=O)C2H	1
3,329	ISSSTY_v1a_7367_02May011_4176	7083-63-8	HC1c2c(-c3c(N)cccc13)cccc2	3
3,330	ISSSTY_v1a_7367_02May011_4177	3366-65-2	c12c(c3c(cc(N)cc3)cc1)cccc2	3

3,331	ISSSTY_v1a_7367_02May011_4178	590-88-5	HC(H)C(N)C(H)C(H)N	1
3,332	ISSSTY_v1a_7367_02May011_4179	3385-21-5	HC1C(H)C(H)[C@]([N+](H)H)C(H)[C@]1[N+](H)H	1
3,333	ISSSTY_v1a_7367_02May011_4181	1892-54-2	c12c(c3c(ccc(N)c3)cc1)cccc2	3
3,334	ISSSTY_v1a_7367_02May011_4182	2479-46-1	c1(Oc2ccc(N)cc2)cc(Oc2ccc(N)cc2)ccc1	3
3,335	ISSSTY_v1a_7367_02May011_4183	109-01-3	HC(H)N1C(H)C(H)NC(H)C1H	1
3,336	ISSSTY_v1a_7367_02May011_4184	50-24-8	HC(H)[C@@]12[C@@](O)(C(=O)C(H)O)C(H)C(H)[C@]1[C@@]1C(H)C(H)C3[C@@]C(H)H)(C=CC(=O)C=3)[C@]1[C@@](O)C2H	1
3,337	ISSSTY_v1a_7367_02May011_4185	80-70-6	HC(H)N(C(=N)N(C(H)H)C(H)H)C(H)H	1
3,338	ISSSTY_v1a_7367_02May011_4186	106-58-1	HC(H)N1C(H)C(H)N(C(H)H)C(H)C1H	1
3,339	ISSSTY_v1a_7367_02May011_4187	1732-23-6	c12c3c4c(cc(N)cc4ccc3ccc1)cc2	3
3,340	ISSSTY_v1a_7367_02May011_4188	143922-95-6	HC(H)c1c(N(=O)=O)cccc1N=O	1
3,341	ISSSTY_v1a_7367_02May011_4189	280-57-9	HC1C(H)N2C(H)C(H)N1C(H)C2H	1
3,342	ISSSTY_v1a_7367_02May011_4190	143922-96-7	HC(H)c1c(N)cccc1[N-][N+](=O)c1c(C(H)H)c(N)ccc1	3
3,343	ISSSTY_v1a_7367_02May011_4191	2449-49-2	HC(H)C(c1ccccc1)N(C(H)H)C(H)H	1
3,344	ISSSTY_v1a_7367_02May011_4192	143922-98-9	HC(H)C(=O)c1c(C(H)H)c([N+](=O)[N-]c2c(C(H)H)c(C(=O)C(H)H)ccc2)ccc1N	1
3,345	ISSSTY_v1a_7367_02May011_4193	143922-99-0	HC(H)C(=O)c1c(C(H)H)c(N=Nc2c(C(H)H)c(C(=O)C(H)H)ccc2)ccc1N	1
3,346	ISSSTY_v1a_7367_02May011_4194	116539-70-9	HC(H)C(H)C(H)C(H)N(C(H)C(O)C1C=CC(=O)C(=[N+]=[N-])C=1)N=O	3
3,347	ISSSTY_v1a_7367_02May011_4197	2693-46-1	c1(N)c2c3c(c4c(c3ccc2)cccc4)cc1	3
3,348	ISSSTY_v1a_7367_02May011_4198	3060-89-7	HC(H)N(C(=O)Nc1ccc(Br)cc1)OC(H)H	1
3,349	ISSSTY_v1a_7367_02May011_4199	18691-97-9	HC(H)N(C1=Nc2c(cccc2)S1)C(=O)NC(H)H	1
3,350	ISSSTY_v1a_7367_02May011_4200	55520-40-6	HC(c1ccc(O)cc1)[C@](N)C(=O)O	1
3,351	ISSSTY_v1a_7367_02May011_4201	3062-57-5	c12-c3c(c([N+](=O)[O-])ccc3)Nc1ccc([N+](=O)[O-])c2	3
3,352	ISSSTY_v1a_7367_02May011_4202	3244-54-0	c12-c3c(ccc([N+](=O)[O-])c3)Nc1ccc([N+](=O)[O-])c2	3
3,353	ISSSTY_v1a_7367_02May011_4203	153654-33-2	c12-c3c(cc(O)c(N(=O)=O)c3)Nc1cccc2	3
3,354	ISSSTY_v1a_7367_02May011_4204	153654-34-3	c12-c3c(c([N+](=O)[O-])c(O)c([N+](=O)[O-])c3)Nc1cccc2	3
3,355	ISSSTY_v1a_7367_02May011_4205	153654-32-1	c12-c3c(c([N+](=O)[O-])c(O)c([N+](=O)[O-])c3)Nc1ccc([N+](=O)[O-])c2	3
3,356	ISSSTY_v1a_7367_02May011_4206	505-23-7	HC1C(H)C(H)SC(H)S1	3
3,357	ISSSTY_v1a_7367_02May011_4207	60692-90-2	c12-c3c4c(ccc3C3C(c1cccc2)O3)cccc4	3
3,358	ISSSTY_v1a_7367_02May011_4208	71382-54-2	c12-c3c4c(ccc3C3C(c1cccc2)N3)cccc4	3
3,359	ISSSTY_v1a_7367_02May011_4209	121-61-9	HC(H)C(=O)Nc1ccc(S(N)(=O)=O)cc1	1
3,360	ISSSTY_v1a_7367_02May011_4210	1709-52-0	HC(H)NS(=O)(=O)c1ccc(N)cc1	1

3,361	ISSSTY_v1a_7367_02May011_4211	1709-39-3	HC(H)C(H)N(C(H)C(H)H)S(=O)(=O)c1ccc(N)cc1	1
3,362	ISSSTY_v1a_7367_02May011_4213	19077-98-6	HC(H)C(=O)Nc1ccc(S(=O)(=O)Nc2ccccn2)cc1	1
3,363	ISSSTY_v1a_7367_02May011_4214	1028-11-1	c1(S(=O)(=O)N(c2ccccn2)N(=O)=O)ccccc1	1
3,364	ISSSTY_v1a_7367_02May011_4218	26676-89-1	HC(C1c2c(cccc2)NC=1)[C@]1(O)C2(O)C(C(O)C(H)O2)OC1=O	1
3,365	ISSSTY_v1a_7367_02May011_4219	13963-57-0	?	3
3,366	ISSSTY_v1a_7367_02May011_4221	1794-45-2	c1(Cl)c(C=CC=O)cccc1	3
3,367	ISSSTY_v1a_7367_02May011_4223	2435-76-9	C1(=O)C(=[N+]=[N-])C=NC(=O)N1	3
3,368	ISSSTY_v1a_7367_02May011_4224	1484-12-4	HC(H)N1c2c(-c3c1cccc3)cccc2	3
3,369	ISSSTY_v1a_7367_02May011_4225	117760-92-6	c1(N(=O)=O)c2c(c3c(c4c(cccc4)cc3)c1)[C@](O)[C@@](O)C=C2	3
3,370	ISSSTY_v1a_7367_02May011_4226	683-51-2	HC(H)C(Cl)=C=O	3
3,371	ISSSTY_v1a_7367_02May011_4227	1995932	HC(H)C(=C(Cl)C=O)C(H)H	3
3,372	ISSSTY_v1a_7367_02May011_4229	158366-45-1	HC(H)C(=O)C1=CC=CN1N(=O)=O	3
3,373	ISSSTY_v1a_7367_02May011_4230	158366-46-2	HC(H)C(=O)C1=C([N+](=O)[O-])C=C([N+](=O)[O-])N1[N+](=O)[O-]	3
3,374	ISSSTY_v1a_7367_02May011_4232	57491-68-6	HC(Sc1c(N)cccc1)Sc1c(N)cccc1	3
3,375	ISSSTY_v1a_7367_02May011_4234	27093-62-5	HC(H)N1c2c(-c3c4c(ccc13)cccc4)c1c(cccc1)cc2	3
3,376	ISSSTY_v1a_7367_02May011_4240	111070-55-4	C1(C=NN2C=CC=N2)=CC=C(N(=O)=O)O1	3
3,377	ISSSTY_v1a_7367_02May011_4241	111070-57-6	c1(C2C=C(c3ccccc3)N(N=CC3=CC=C(N(=O)=O)O3)C(=O)C=2)ccccc1	3
3,378	ISSSTY_v1a_7367_02May011_4242	17241-59-7	HC(O)c1cc2C(=O)c3c(C(=O)c2cc1)cccc3	1
3,379	ISSSTY_v1a_7367_02May011_4243	2319-96-2	HC(H)c1c2c(c3c(cc4c(cccc4)c3)c1)cccc2	3
3,380	ISSSTY_v1a_7367_02May011_4244	316-14-3	HC(H)c1c2c(c3c(cccc3)c1)cc1c(cccc1)c2	3
3,381	ISSSTY_v1a_7367_02May011_4245	26946-33-8	HC(c1c([N+](=O)[O-])cc(N)cc1)c1c([N+](=O)[O-])cc(N)cc1	3
3,382	ISSSTY_v1a_7367_02May011_4246	2381-15-9	HC(H)c1cc2c(cc3c(c4c(cccc4)cc3)c2)cc1	3
3,383	ISSSTY_v1a_7367_02May011_4247	6344-63-4	HC1c2c(-c3c1c(N)ccc3)cccc2	3
3,384	ISSSTY_v1a_7367_02May011_4248	6344-66-7	HC1c2c(-c3c1ccc(N)c3)cccc2	3
3,385	ISSSTY_v1a_7367_02May011_4250	4176-53-8	c1(N)c2c(c3c(cccc3)cc2)ccc1	3
3,386	ISSSTY_v1a_7367_02May011_4253	947-73-9	c1(N)c2c(c3c(cccc3)c1)cccc2	3
3,387	ISSSTY_v1a_7367_02May011_4255	17075-03-5	c12c3c4c(c(N)cc3ccc1)cccc4cc2	3
3,388	ISSSTY_v1a_7367_02May011_4256	13177-25-8	c1(N)c2c3c(c4c2c(ccc4)cc1)cccc3	3
3,389	ISSSTY_v1a_7367_02May011_4257	13177-26-9	c12c3c(c4c(c3cc(N)c1)cccc4)ccc2	3
3,390	ISSSTY_v1a_7367_02May011_4258	13177-27-0	c1(N)c2c(c3c4c(cccc24)ccc3)ccc1	3

3,391	ISSSTY_v1a_7367_02May011_4260	5869-25-0	c12c3c(c4c(c3ccc1)cc(N)cc4)ccc2	3
3,392	ISSSTY_v1a_7367_02May011_4261	773168	HC(H)C(H)OC(H)C1C(H)O1	3
3,393	ISSSTY_v1a_7367_02May011_4262	106264-79-3	HC(H)c1c(N)c(SC(H)H)cc(SC(H)H)c1N	3
3,394	ISSSTY_v1a_7367_02May011_4268	124390-37-0	HC(H)c1c2c3c(c(N(=O)=O)cc2c2c(cccc2)c1)cccc3	3
3,395	ISSSTY_v1a_7367_02May011_4274	42576-02-3	HC(H)OC(=O)c1c(N(=O)=O)ccc(Oc2c(Cl)cc(Cl)cc2)c1	3
3,396	ISSSTY_v1a_7367_02May011_4275	96918-17-1	c12c3c4c(c5c(C=C(N(=O)=O)O5)cc4ccc3ccc1)cc2	3
3,397	ISSSTY_v1a_7367_02May011_4276	591-12-8	HC(H)C1=CC(H)C(=O)O1	1
3,398	ISSSTY_v1a_7367_02May011_4282	99-73-0	HC(Br)C(=O)c1ccc(Br)cc1	1
3,399	ISSSTY_v1a_7367_02May011_4283	566-76-7	HC(H)[C@@]12C(=O)[C@](O)C(H)[C@@]1[C@]1C(H)C(H)c3c(ccc(O)c3)[C@@]1C(H)C2H	1
3,400	ISSSTY_v1a_7367_02May011_4284	106-24-1	HC(H)C(C(H)H)=CC(H)C(H)C(C(H)H)=CC(H)O	1
3,401	ISSSTY_v1a_7367_02May011_4285	28921-94-0	HC(H)C=C[C@@]1[C@@](O)C=CC(=O)O1	1
3,402	ISSSTY_v1a_7367_02May011_4286	52559-52-1	HC(H)C(H)c1c(NC(=O)C(H)O)c(C(H)C(H)H)ccc1	3
3,403	ISSSTY_v1a_7367_02May011_4287	6967-29-9	HC(H)C(H)c1c(NC(=O)C(H)Cl)c(C(H)C(H)H)ccc1	3
3,404	ISSSTY_v1a_7367_02May011_4288	99766-47-9	HC(H)C(H)c1c(N=O)c(C(H)C(H)H)ccc1	3
3,405	ISSSTY_v1a_7367_02May011_4289	56681-55-1	HC(H)C(H)c1c(N(C(=O)C(H)O)C(H)OC(H)H)c(C(H)C(H)H)ccc1	1
3,406	ISSSTY_v1a_7367_02May011_4291	1595627	HC(H)c1c(O)c2C(=O)c3c(C(=O)c2cc1)cccc3	3
3,407	ISSSTY_v1a_7367_02May011_4302	6639-36-7	c12-c3c(ccc(N(=O)=O)c3)Sc1cccc2	3
3,408	ISSSTY_v1a_7367_02May011_4309	57775-29-8	HC(H)C(C(H)H)NC(H)C(O)C(H)Oc1c2-c3c(cccc3)Nc2ccc1	1
3,409	ISSSTY_v1a_7367_02May011_4317	42200-33-9	HC(H)C(C(H)H)(C(H)H)NC(H)C(O)C(H)Oc1c2c(C(H)[C@@](O)[C@@](O)C2H)ccc1	1
3,410	ISSSTY_v1a_7367_02May011_4318	52898-98-3	HC(H)C1C2C(C(C(H)OC(=O)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)H)=CC=2)=CC(C(C(H)H)=CH)C(H)C=1	3
3,411	ISSSTY_v1a_7367_02May011_4320	85-33-6	HC(H)C(c1cc2c(c(C(H)H)cc1)ccc2C=O)=CH	3
3,412	ISSSTY_v1a_7367_02May011_4321	113393-59-2	HC(H)C(c1cc2c(c(C(H)H)cc1)ccc2C(H)O)=CH	3
3,413	ISSSTY_v1a_7367_02May011_4322	28164-57-0	HC(H)c1c(C2C(=O)c3c(C(=O)C=2)c(O)cc(C(H)H)c3)c(O)c2C(=O)C=CC(=O)c2c1	1
3,414	ISSSTY_v1a_7367_02May011_4324	253-53-2	c12c(ccnc1)cnnc2	1
3,415	ISSSTY_v1a_7367_02May011_4325	61166-05-0	HC(H)N1c2c(-c3c1ccc(N(=O)=O)c3)cccc2	3
3,416	ISSSTY_v1a_7367_02May011_4326	162022-86-8	c12c(ccnc1)cnn(=O)c2	3
3,417	ISSSTY_v1a_7367_02May011_4327	162022-87-9	c12c(ccn(=O)c1)cnnc2	3
3,418	ISSSTY_v1a_7367_02May011_4328	162022-88-0	c1(NN)c2c(cncc2)cnn1	3
3,419	ISSSTY_v1a_7367_02May011_4329	18028-55-2	HC(H)c1c2-c3c(cccc3)Nc2c(C(H)H)cc1	3
3,420	ISSSTY_v1a_7367_02May011_4330	133591-38-5	HC(H)c1c2-c3c(ccc(N(=O)=O)c3)Nc2c(C(H)H)cc1	3

3,421	ISSSTY_v1a_7367_02May011_4331	162022-91-5	HC(H)Oc1c2c(ccnc2)cnn1	1
3,422	ISSSTY_v1a_7367_02May011_4332	162022-92-6	c1(Cl)c2c(cncc2)cnn1	1
3,423	ISSSTY_v1a_7367_02May011_4333	253-73-6	c12c(cccn1)cnnc2	1
3,424	ISSSTY_v1a_7367_02May011_4334	19866-61-6	c12c(cccn1)cn(=O)nc2	1
3,425	ISSSTY_v1a_7367_02May011_4335	19866-62-7	c12c(cccn1)cnn(=O)c2	1
3,426	ISSSTY_v1a_7367_02May011_4336	23590-73-0	c1(NN)c2c(cccn2)cnn1	3
3,427	ISSSTY_v1a_7367_02May011_4337	56525-92-9	HC(H)Oc1c2c(cnn1)nccc2	1
3,428	ISSSTY_v1a_7367_02May011_4338	56525-94-1	HC(H)Oc1c2c(cccn2)cnn1	1
3,429	ISSSTY_v1a_7367_02May011_4340	18636-89-0	c12c(cccc1)cnn(=O)c2	1
3,430	ISSSTY_v1a_7367_02May011_4341	24953-56-8	HC(H)Oc1c2c(cccc2)cnn1	1
3,431	ISSSTY_v1a_7367_02May011_4342	130005-62-8	HC(H)c1c2-c3c(ccc(O)c3)Nc2c(C(H)H)cc1N	3
3,432	ISSSTY_v1a_7367_02May011_4343	129117-54-0	HC(H)c1c2-c3c(ccc(OC(H)H)c3)Nc2c(C(H)H)cc1N	3
3,433	ISSSTY_v1a_7367_02May011_4344	61166-04-9	HC(H)N1c2c(-c3c1ccc(N)c3)cccc2	3
3,434	ISSSTY_v1a_7367_02May011_4346	18028-56-3	HC(H)c1c2-c3c(ccc(C(H)H)c3)Nc2c(C(H)H)cc1	3
3,435	ISSSTY_v1a_7367_02May011_4349	24777-14-8	HC(H)OC1C(=O)C=CC(=C2NC(c3ccccc3)=C(c3ccccc3)N2)C=1	3
3,436	ISSSTY_v1a_7367_02May011_4354	32912	c1(O)c(C=O)cccc1	1
3,437	ISSSTY_v1a_7367_02May011_4356	92439-25-3	HC(H)c1c(O)c2C(=O)c3c(C(=O)c2cc1O)c(O)ccc3	3
3,438	ISSSTY_v1a_7367_02May011_4357	63390-12-5	c1(-c2cc(Cl)c(N)c(Cl)c2)cc(Cl)c(N)cc1	3
3,439	ISSSTY_v1a_7367_02May011_4358	121111-61-3	HC(H)c1ccc(C2=C(c3ccc(C(H)H)cc3)N=C(c3cc(OC(H)H)c(OC(H)H)cc3)N2)cc1	3
3,440	ISSSTY_v1a_7367_02May011_4359	7044-99-7	HC(H)Oc1ccc(C2=C(c3ccc(OC(H)H)cc3)N=C(c3ccccc3)N2)cc1	3
3,441	ISSSTY_v1a_7367_02May011_4360	121111-59-9	HC(H)c1c(C2=NC(c3ccc(C(H)H)cc3)=C(c3ccc(C(H)H)cc3)N2)ccc(C(H)H)c1	3
3,442	ISSSTY_v1a_7367_02May011_4361	37393-11-6	HC(O)c1c(O)c2C(=O)c3c(C(=O)c2cc1O[C@]1[C@](O)[C@@](O)[C@](O)[C@@](C(H)O[C@@]2[C@](O)[C@@](O)[C@](O)C(H)O2)O1)cccc3	3
3,443	ISSSTY_v1a_7367_02May011_4362	1728-95-6	HC(H)Oc1ccc(C2=NC(c3ccccc3)=C(c3ccccc3)N2)cc1	3
3,444	ISSSTY_v1a_7367_02May011_4363	19200-30-7	HC(H)C(H)N(C(=S)S[C@@]1[C@](O)[C@@](O)[C@](O)[C@@](C(H)O)O1)C(H)C(H)H	1
3,445	ISSSTY_v1a_7367_02May011_4365	98499-59-3	HC(H)SC(H)Nc1ccccc1	3
3,446	ISSSTY_v1a_7367_02May011_4367	194590-84-6	HC(H)C(=O)Nc1c(N2N=C3C(C(Cl)=C(N)C=C3Br)=N2)cc(OC(H)H)c(N(C(H)C(H)OC(H)H)C(H)C(H)OC(H)H)c1	3
3,447	ISSSTY_v1a_7367_02May011_4369	201-06-9	c12c(c3c4c(C=Cc4ccc3)c1)cccc2	3
3,448	ISSSTY_v1a_7367_02May011_4370	21247-98-3	HC(O)c1c2c(c3c4c5c(ccc14)cccc5cc3)cccc2	3
3,449	ISSSTY_v1a_7367_02May011_4371	568-75-2	HC(H)c1c2c(c(C(H)O)c3c1c1c(cccc1)cc3)cccc2	3
3,450	ISSSTY_v1a_7367_02May011_4373	519-23-3	HC(H)c1c2-c3c(cccc3)Nc2c(C(H)H)c2c1cncc2	3

3,451	ISSSTY_v1a_7367_02May011_4376	55256-58-1	HC(H)Oc1c2C(=O)c3c(OC(H)H)c4c(cc3Oc2ccc1Cl)OC1C4C=CO1	3
3,452	ISSSTY_v1a_7367_02May011_4378	55256-57-0	HC(H)C(O)(C(H)H)C(H)C(H)c1c2c(C(=O)c3c(O)c4c(cc3O2)O[C@@]2[C@]4C=CO2)c(O)cc1	3
3,453	ISSSTY_v1a_7367_02May011_4380	55256-55-8	HC(H)C(O)(C(H)H)C(H)C(H)c1c2c(C(=O)c3c(OC(H)H)c4c(cc3O2)O[C@@]2[C@]4C=CO2)c(O)cc1	3
3,454	ISSSTY_v1a_7367_02May011_4381	55256-53-6	HC(H)C(O)(C(H)H)C(H)C(H)c1c2c(C(=O)c3c(O)c4[C@@]5(O)C=CO[C@@]5Oc4cc3O2)c(O)cc1	3
3,455	ISSSTY_v1a_7367_02May011_4385	58775-50-1	HC(H)C(C(H)H)=CC(H)c1c2c(C(=O)c3c(O)c4[C@@]5(O)C=CO[C@@]5Oc4cc3O2)c(O)cc1	3
3,456	ISSSTY_v1a_7367_02May011_4388	52819-96-2	HC(H)Oc1c2C3=C(C(=O)C(H)[C@]3O)C(=O)Oc2c2c(c1)O[C@@]1[C@]2C=CO1	3
3,457	ISSSTY_v1a_7367_02May011_4390	299257	HC(H)C(=O)Nc1ccc(C(H)c2ccc(NC(=O)C(H)H)cc2)cc1	1
3,458	ISSSTY_v1a_7367_02May011_4391	1030-27-9	HC(H)N(c1ccc(C=CC(=O)c2ccccc2)cc1)C(H)H	1
3,459	ISSSTY_v1a_7367_02May011_4394	21794-55-8	HC(H)C(=O)C1(O)C(H)c2c(O)c3C(=O)c4c(C(=O)c3c(O)c2C(O)C1H)c(OC(H)H)ccc4	3
3,460	ISSSTY_v1a_7367_02May011_4396	52744-22-6	HC(H)C(=O)[C@]1(O)C(H)c2c(O)c3C(=O)c4c(C(=O)c3c(O)c2[C@@](O)C1H)c(O)ccc4	3
3,461	ISSSTY_v1a_7367_02May011_4397	16234-96-1	HC(H)C(H)[C@]1(O)C(H)[C@](O)c2c(O)c3C(=O)c4c(C(=O)c3cc2[C@@]1C(=O)OC(H)H)cccc4O	3
3,462	ISSSTY_v1a_7367_02May011_4399	1608-51-1	c1(C(=O)C=Cc2ccc(F)cc2)ccccc1	1
3,463	ISSSTY_v1a_7367_02May011_4400	159416-83-8	HC(H)c1c(-c2c(O)c3c(c(OC(H)H)cc(C(H)H)c3)c(O)c2)c(OC(H)H)c2c(c(O)ccc2O)c1	1
3,464	ISSSTY_v1a_7367_02May011_4402	100-33-4	HC(C(H)C(H)C(H)C(H)Oc1ccc(C(=N)N)cc1)Oc1ccc(C(=N)N)cc1	1
3,465	ISSSTY_v1a_7367_02May011_4404	4816-14-2	C(=N)(N)c1cc2c(C=C(c3ccc(C(=N)N)cc3)S2)cc1	1
3,466	ISSSTY_v1a_7367_02May011_4405	64431-93-2	HC1C(H)N=C(c2cc3c(C=C(c4ccc(C5=NC(H)C(H)N5)cc4)N3)cc2)N1	1
3,467	ISSSTY_v1a_7367_02May011_4406	73819-63-3	C12C(C=C(C(=N)N)C=C1)=NC(=C(N)N)C=2	1
3,468	ISSSTY_v1a_7367_02May011_4408	3009-50-5	HC(H)N(c1ccc(N=Nc2ccc(OC(H)H)cc2)cc1)C(H)H	3
3,469	ISSSTY_v1a_7367_02May011_4409	101821-43-6	C12C(=C(N)C(=C(N)N)N=1)C=CC(C(=N)N)=C2	1
3,470	ISSSTY_v1a_7367_02May011_4412	162022-85-7	c12c(ccnc1)cn(=O)nc2	1
3,471	ISSSTY_v1a_7367_02May011_4413	162022-89-1	c1(NN)c2c(ccnc2)cnn1	3
3,472	ISSSTY_v1a_7367_02May011_4414	20426-12-4	c1(C(=O)C=Cc2ccc(O)cc2)ccccc1	1
3,473	ISSSTY_v1a_7367_02May011_4416	51856-71-4	HC(H)c1c([N+](=O)[O-])cc([N+](=O)[O-])cc1[N-][N+](=O)c1cc([N+](=O)[O-])c(C(H)H)c([N+](=O)[O-])c1	3
3,474	ISSSTY_v1a_7367_02May011_4418	162022-90-4	HC(H)Oc1c2c(cncc2)cnn1	1
3,475	ISSSTY_v1a_7367_02May011_4420	383514	HC(H)C(c1c(O)c(C(C(H)H)(C(H)H)C(H)H)cc(C=Cc2cc(C(C(H)H)(C(H)H)C(H)H)c(O)c(C(C(H)H)(C(H)H)C(H)H)c2)c1)(C(H)H)C(H)H	1
3,476	ISSSTY_v1a_7367_02May011_4421	809-73-4	HC(H)C(C1C(=O)C(C(C(H)H)(C(H)H)C(H)H)=CC(=CC=C2C=C(C(C(H)H)(C(H)H)C(H)H)C(=O)C(C(H)H)(C(H)H)C(H)H)=C2)C=1)(C(H)H)C(H)H	1
3,477	ISSSTY_v1a_7367_02May011_4422	13154-57-9	HC(H)C(C1C(=O)C(C(C(H)H)(C(H)H)C(H)H)=CC(C(H)H)(OOC(C(H)H)(C(H)H)C(H)H)C=1)(C(H)H)C(H)H	1
3,478	ISSSTY_v1a_7367_02May011_4423	63019-39-6	c12c(c3c(c4c(ccc(O)c4)cc3)cc1)cccc2	3
3,479	ISSSTY_v1a_7367_02May011_4424	63019-40-9	c12c(c3c(c4c(O)cccc4cc3)cc1)cccc2	3
3,480	ISSSTY_v1a_7367_02May011_4425	84498-34-0	c12c(c3c(c4c(cc3O)cccc4)cc1)cccc2	1

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3,481	ISSSTY_v1a_7367_02May011_4426	162022-93-7	c1(Cl)c2c(ccnc2)cnn1	1
3,482	ISSSTY_v1a_7367_02May011_4428	20970-16-5	c1(NN)c2c(cnn1)nccc2	3
3,483	ISSSTY_v1a_7367_02May011_4430	5784-45-2	c1(Cl)c2c(cccc2)cnn1	1
3,484	ISSSTY_v1a_7367_02May011_4431	23590-59-2	c1(Cl)c2c(cccn2)cnn1	3
3,485	ISSSTY_v1a_7367_02May011_4432	23590-58-1	c1(Cl)c2c(cnn1)nccc2	1
3,486	ISSSTY_v1a_7367_02May011_4433	7467-29-0	HC(H)c1c(N)cc(N)c(N=Nc2c(C(H)H)cccc2)c1	3
3,487	ISSSTY_v1a_7367_02May011_4434	84434-45-7	HC(H)c1c(N)c(N=Nc2c(C(H)H)cccc2)ccc1N	3
3,488	ISSSTY_v1a_7367_02May011_4435	84434-42-4	HC(H)c1c(N)c(N=Nc2ccccc2)ccc1N	3
3,489	ISSSTY_v1a_7367_02May011_4436	70634-28-5	HC(H)C(c1c(N(=O)=O)ccc(-c2ccccc2)c1)(C(H)H)C(H)H	1
3,490	ISSSTY_v1a_7367_02May011_4437	279242-17-0	HC(H)C(c1ccc(-c2ccc(N=O)cc2)cc1)(C(H)H)C(H)H	3
3,491	ISSSTY_v1a_7367_02May011_4438	59282-34-7	HC(H)C(c1c(O)c(N(=O)=O)cc(OC(H)H)c1)(C(H)H)C(H)H	1
3,492	ISSSTY_v1a_7367_02May011_4439	2940-63-8	HC(H)C(C1C(=O)C(=O)C=C(OC(H)H)C=1)(C(H)H)C(H)H	1
3,493	ISSSTY_v1a_7367_02May011_4440	962-58-3	HC(H)c1cc(OP(=O)(OC(H)C(H)H)OC(H)C(H)H)nc(C(C(H)H)C(H)H)n1	3
3,494	ISSSTY_v1a_7367_02May011_4441	2255-17-6	HC(H)c1c(N(=O)=O)ccc(OP(=O)(OC(H)H)OC(H)H)c1	3
3,495	ISSSTY_v1a_7367_02May011_4442	105553-32-0	HC(H)C(=O)C(C(=O)N(c1ccccc1)N(C(H)H)N=O)=NO	3
3,496	ISSSTY_v1a_7367_02May011_4444	32306-29-9	HC(H)C(H)OP(=O)(OC1C=C(c2ccccc2)ON=1)OC(H)C(H)H	1
3,497	ISSSTY_v1a_7367_02May011_4445	311-45-5	HC(H)C(H)OP(=O)(Oc1ccc(N(=O)=O)cc1)OC(H)C(H)H	3
3,498	ISSSTY_v1a_7367_02May011_4446	83-75-0	HC(H)C(H)OC(=O)O[C@](c1c2c(ccc(OC(H)H)c2)ncc1)[C@@]1C(H)[C@]2C(H)C(H)H)N1C(H)[C@]2C=CH	1
3,499	ISSSTY_v1a_7367_02May011_4448	41069-00-5	c1(C(=O)[C@@]2[C@](c3ccccc3)O2)ccc(N(=O)=O)cc1	3
3,500	ISSSTY_v1a_7367_02May011_4449	90811-87-3	c1(C(=O)C=Cc2ccc(Oc3ccccc3)cc2)ccccc1	1
3,501	ISSSTY_v1a_7367_02May011_4450	2453-44-3	c1(C(=O)C=Cc2ccccc2)ccc(-c2ccccc2)cc1	1
3,502	ISSSTY_v1a_7367_02May011_4451	952-97-6	c1(Sc2ccccc2)ccc(N(=O)=O)cc1	3
3,503	ISSSTY_v1a_7367_02May011_4452	86-87-3	HC(c1c2c(cccc2)ccc1)C(=O)O	1
3,504	ISSSTY_v1a_7367_02May011_4453	82414-03-7	HC(H)c1c(N(=O)=O)cc(N=O)cc1	1
3,505	ISSSTY_v1a_7367_02May011_4454	128531-59-9	HC(H)C(H)N(C(=S)SSC(H)[C@@](C(=O)NC(H)C(=O)O)NC(=O)C(H)C(H)[C@](N)C(=O)O)C(H)C(H)H	1
3,506	ISSSTY_v1a_7367_02May011_4455	188970-78-7	c12-c3c4c(c(N(=O)=O)cc3Nc1ccc1c2cccc1)cccc4	3
3,507	ISSSTY_v1a_7367_02May011_4456	188970-86-7	c12-c3c4c(c(N(=O)=O)cc3Nc1ccc1c2cccc1)ccc(O)c4	3
3,508	ISSSTY_v1a_7367_02May011_4457	188970-88-9	c12-c3c4c(c(N(=O)=O)cc3Nc1ccc1c2cc(O)cc1)cccc4	3
3,509	ISSSTY_v1a_7367_02May011_4458	188970-81-2	c12-c3c4c(c(N(=O)=O)cc3Nc1ccc1c2cccc1)cc(O)cc4	3
3,510	ISSSTY_v1a_7367_02May011_4459	188970-84-5	c12-c3c4c(c(N(=O)=O)cc3Nc1ccc1c(O)cccc21)cccc4	3

3,511	ISSSTY_v1a_7367_02May011_4460	138805-29-5	HC(H)c1c(N=Nc2c(C(H)H)ccc(N)c2)cc(N)cc1	3
3,512	ISSSTY_v1a_7367_02May011_4462	59863-59-1	HC1C(Cl)C(Cl)C(H)N1N=O	3
3,513	ISSSTY_v1a_7367_02May011_4463	73018-98-1	HC(O)C(O)C(H)N=N_N	3
3,514	ISSSTY_v1a_7367_02May011_4465	4273-73-8	HC(H)C1C(H)H)C(C=CC(C(H)H)=CC=CC(C(H)H)=CC=CC=C(C(H)H)C=CC=C(C(=O)OC(H)H)C(H)H)=C(C(H)H)C(H)C(H)C1H	1
3,515	ISSSTY_v1a_7367_02May011_4468	96614-59-4	HC(C(=O)N[C@](C(=O)NC(H)C(=O)O)C(H)SC(Cl)=CCl)C(H)[C@](N)C(=O)O	3
3,516	ISSSTY_v1a_7367_02May011_4469	619-90-9	HC(H)C(=O)OC(H)c1ccc(N(=O)=O)cc1	3
3,517	ISSSTY_v1a_7367_02May011_4470	35300-54-0	HC(H)C(H)C(H)C(=O)OC(H)c1ccc(N(=O)=O)cc1	3
3,518	ISSSTY_v1a_7367_02May011_4471	4457-41-4	HC(c1ccc(N(=O)=O)cc1)OC(=O)c1ccccc1	3
3,519	ISSSTY_v1a_7367_02May011_4472	55-80-1	HC(H)c1cc(N=Nc2ccc(N(C(H)H)C(H)H)cc2)ccc1	3
3,520	ISSSTY_v1a_7367_02May011_4473	60259-80-5	c1(N(=O)=O)ccc(CNN=Nc2ccc(C)cc2)cc1	3
3,521	ISSSTY_v1a_7367_02May011_4474	17564-64-6	HC(Cl)N1C(=O)c2c(C1=O)cccc2	3
3,522	ISSSTY_v1a_7367_02May011_4475	54455-37-7	HC(Cl)N1C(=O)c2c(C1=O)cc(N(=O)=O)cc2	3
3,523	ISSSTY_v1a_7367_02May011_4476	394039	HC(H)C(C(H)H)N=C(NC(C(H)H)C(H)H)OC(H)c1ccc(N(=O)=O)cc1	3
3,524	ISSSTY_v1a_7367_02May011_4477	309459	HC(H)C(=O)Oc1cc2c(C(C(H)Br)=CC(=O)O2)cc1	1
3,525	ISSSTY_v1a_7367_02May011_4478	35231-44-8	HC(H)Oc1cc2c(C(C(H)Br)=CC(=O)O2)cc1	1
3,526	ISSSTY_v1a_7367_02May011_4479	491-64-5	HC(H)Oc1cc2C(=O)c3c(O)cc(O)cc3Oc2cc1	3
3,527	ISSSTY_v1a_7367_02May011_4480	5000-65-7	HC(H)Oc1cc(C(=O)C(H)Br)ccc1	1
3,528	ISSSTY_v1a_7367_02May011_4481	4436-24-2	HC(c1ccccc1)C1C(H)O1	3
3,529	ISSSTY_v1a_7367_02May011_4482	18458-01-0	HC(H)c1ccc(C(H)C2C(H)O2)cc1	3
3,530	ISSSTY_v1a_7367_02May011_4483	4106-66-5	c12-c3c(cc(N)cc3)Oc1cccc2	3
3,531	ISSSTY_v1a_7367_02May011_4492	36519-91-2	HC(c1ccc(Cl)cc1)C1C(H)O1	3
3,532	ISSSTY_v1a_7367_02May011_4494	389104-54-5	HC(H)C(c1c2c(ccc1N)cccc2)C(H)H	3
3,533	ISSSTY_v1a_7367_02May011_4499	129018-59-3	HC(H)N1c2c(N=C1N(=O)=O)ncc(-c1ccccc1)c2	3
3,534	ISSSTY_v1a_7367_02May011_4500	135577-57-0	HC(H)N1c2c(N=C1N=N_N)ncc(-c1ccccc1)c2	3
3,535	ISSSTY_v1a_7367_02May011_4502	66452-61-7	HC(H)C(C(H)H)Sc1c(N)ccc(C(H)c2cc(SC(C(H)H)C(H)H)c(N)cc2)c1	3
3,536	ISSSTY_v1a_7367_02May011_4503	548-42-5	HC(H)C1C(H)N(C(H)H)[C@@]2C(H)C3c4c(cccc4[C@]2C=1)NC=3	3
3,537	ISSSTY_v1a_7367_02May011_4504	6756-41-8	HC(H)c1ccc(NN=C2c3c(C=CC2=O)cccc3)cc1	1
3,538	ISSSTY_v1a_7367_02May011_4506	529-49-7	c12C(=O)c3c(O)cc(O)cc3Oc1ccc(O)c2	3
3,539	ISSSTY_v1a_7367_02May011_4508	111017-06-2	HC(H)Oc1c(OC(H)H)c2c3c(C(H)C(H)N(C=O)c3cc3c2cccc3)c1	3
3,540	ISSSTY_v1a_7367_02May011_4509	62826-28-2	HC(H)Oc1c(C(H)C2C(H)O2)cccc1	3

3,541	ISSSTY_v1a_7367_02May011_4510	499-75-2	HC(H)c1c(O)cc(C(C(H)H)C(H)H)cc1	1
3,542	ISSSTY_v1a_7367_02May011_4511	53940-49-1	HC(H)Oc1c(O)ccc(C(H)C2C(H)O2)c1	3
3,543	ISSSTY_v1a_7367_02May011_4512	91-63-4	HC(H)c1ccc2c(cccc2)n1	3
3,544	ISSSTY_v1a_7367_02May011_4514	10102-44-0	N(=O)=O	3
3,545	ISSSTY_v1a_7367_02May011_4515	27602-80-8	HC(H)Oc1c(OC(H)H)cc(C(H)C2C(H)O2)cc1	3
3,546	ISSSTY_v1a_7367_02May011_4517	548-04-9	HC(H)c1c2c3c(C(=O)c4c5c(c6c7c(C(=O)c8c(c7c35)c2c(C(H)H)cc8O)c(O)cc6O)c(O)cc4O)c(O)c1	1
3,547	ISSSTY_v1a_7367_02May011_4518	4637-56-3	C1(=NO)c2c(cccc2)N(O)C=C1	3
3,548	ISSSTY_v1a_7367_02May011_4519	18463-85-9	HC(H)N(c1ccc(N=Nc2cc3c(cc2)N=CS3)cc1)C(H)H	3
3,549	ISSSTY_v1a_7367_02May011_4520	23703-14-2	HC(c1ccc(-c2ccccc2)cc1)C1C(H)O1	3
3,550	ISSSTY_v1a_7367_02May011_4522	2403-27-2	c1(C(=O)C=Cc2ccccc2)ccc(Br)cc1	1
3,551	ISSSTY_v1a_7367_02May011_4524	142382-12-5	HC(C(=O)C(H)C(H)c1ccc(C(=O)O)cc1)C(H)C_N	3
3,552	ISSSTY_v1a_7367_02May011_4525	59-92-7	HC(c1cc(O)c(O)cc1)C(N)C(=O)O	3
3,553	ISSSTY_v1a_7367_02May011_4526	7220-81-7	HC(H)Oc1c2C3=C(C(=O)C(H)C3H)C(=O)Oc2c2c(c1)OC1C2C(H)C(H)O1	3
3,554	ISSSTY_v1a_7367_02May011_4528	71382-44-0	c12-c3c(C4C(c1cc1c(cccc1)c2)N4)cccc3	3
3,555	ISSSTY_v1a_7367_02May011_4529	1126-76-7	HC(c1ccccc1)C(H)C1C(H)O1	3
3,556	ISSSTY_v1a_7367_02May011_4531	86853-91-0	C12C(c3c4C(=Cc5c4c(ccc5)cc3)C=1)=CC(=O)C=C2	3
3,557	ISSSTY_v1a_7367_02May011_4533	202-98-2	HC1c2c3c4c(c5c(cc14)cccc5)ccc3ccc2	3
3,558	ISSSTY_v1a_7367_02May011_4534	389104-53-4	HC(H)C(H)c1c2c(ccc1N)cccc2	3
3,559	ISSSTY_v1a_7367_02May011_4538	687-48-9	HC(H)C(H)OC(=O)N(C(H)H)C(H)H	3
3,560	ISSSTY_v1a_7367_02May011_4539	56438-59-6	HC(H)Oc1ccc(C(H)C(H)C2C(H)O2)cc1	3
3,561	ISSSTY_v1a_7367_02May011_4540	132742-05-3	HC1c2c(N(=O)=O)c3c4c5c(ccc4c2C=CC1H)cccc5cc3	1
3,562	ISSSTY_v1a_7367_02May011_4541	124489-20-9	HC(H)N1c2c(N=C1NO)ncc(-c1ccccc1)c2	3
3,563	ISSSTY_v1a_7367_02May011_4542	111990-50-2	HC(c1c2c(cccc2)ccc1)C(H)C1C(H)O1	3
3,564	ISSSTY_v1a_7367_02May011_4543	758-17-8	HC(H)N(N)C=O	1
3,565	ISSSTY_v1a_7367_02May011_4544	122587-20-6	HC(H)C(=O)C1=C(Cl)C(Cl)=C(N(=O)=O)O1	3
3,566	ISSSTY_v1a_7367_02May011_4545	162050-09-1	HC(Br)C(=O)C1=C(Cl)C(Cl)=C(N(=O)=O)O1	3
3,567	ISSSTY_v1a_7367_02May011_4546	19057-60-4	HC(H)[C##]12C(C(H)[C##])[C#]O[C##]H(C#)O[C#]C(C#)C(C#)[O](C#)CC(H)H04[C##]O[C#]O[C##][C#)C(O)C(O)[C##][O][C#]CH(H)O4[C##]C(H)O)O3C0H(C1H=CC(H)[C#])[C#]3[C#]C(H)H(C(H)C(H)[C##]21	1
3,568	ISSSTY_v1a_7367_02May011_4547	19083-00-2	HC(H)[C##]12C(C(H)[C##])[C#]O[C##]H(C#)O[C#]C(C#)C(C#)[O](C#)CC(H)H04[C##]O[C#]O[C##][C#]C(O)C(O)[C##][C(H)O)O4[C##]C(H)O)O3C0H(C1H=CC(H)[C#])[C#]3[C#]C(H)HH(C(H)[C##]2	1
3,569	ISSSTY_v1a_7367_02May011_4548	54522-52-0	HC(H)[C##]12C(C(H)O(C(H)[C##])3C(O[C##]H(C#)O[C#]C(C##)[O][C#]C(H)H(H)O)[C##](C#)O[C#]C(C##)[C#]O[C#]C(C##)[O][C#]C(C##)[O][C#]C(H)H04[C##]C(H)O)O3C0H(C1H=CC(H)[C#])[C#]3[C#]C(H)HH(C(H)C(H)[C##]21)C	1
3,570	ISSSTY_v1a_7367_02May011_4549	161696-98-6	HC(H)c1c2c(ccc1NC(H)H)nccn2	3

3,571	ISSSTY_v1a_7367_02May011_4550	54522-53-1	HC(H)(C##)12C(CH)(C##)(C##)3C(O(O(C##)4(C#)(O)(C#)(O)(C##)(O)(C#)(C(H)H)O4)(C##)(O)(C##)4(C#)(O)(C##)(O)(C#)(O)(C##)(C(H)O)O4)(C##)(O(H)O)3(C(H)(H)=CC(H)(C#)1(C#)](C#)(O(H)H)(C(H)O(H))(C##)21)(	1
3,572	ISSSTY_v1a_7367_02May011_4551	161697-00-3	HC(H)c1c2c(ccc1NC(H)H)nc(C(H)H)c(C(H)H)n2	3
3,573	ISSSTY_v1a_7367_02May011_4552	161697-01-4	HC(H)c1c2c(ccc1NC(H)H)nc(C(H)C(H)H)c(C(H)C(H)H)n2	3
3,574	ISSSTY_v1a_7367_02May011_4553	161697-03-6	HC(H)c1c2c(ccc1N)nc(C(H)H)c(C(H)H)n2	3
3,575	ISSSTY_v1a_7367_02May011_4554	161697-04-7	HC(H)c1c2c(ccc1N(C(H)H)C(H)H)nc(C(H)H)c(C(H)H)n2	3
3,576	ISSSTY_v1a_7367_02May011_4555	7576-88-7	HC(H)c1c(C(H)H)nc2c(cc(N)cc2)n1	3
3,577	ISSSTY_v1a_7367_02May011_4556	31125-05-0	HC(H)C(=O)c1ccc(N=O)cc1	3
3,578	ISSSTY_v1a_7367_02May011_4557	509-93-3	HC(H)[C@]12C(=O)C=C[C@]1[C@@](C(H)H)C(H)C(H)[C@]1C(=CH)C(=O)O[C@]21	1
3,579	ISSSTY_v1a_7367_02May011_4558	10147-37-2	HC(H)C(C(H)H)S(=O)(=O)Cl	3
3,580	ISSSTY_v1a_7367_02May011_4559	52101-49-2	HC(H)C(=O)C1=C(c2ccccc2)C(c2ccccc2)=C(N(=O)=O)O1	3
3,581	ISSSTY_v1a_7367_02May011_4560	93261-88-2	HC(Br)C(=O)C1=C(c2ccccc2)C(c2ccccc2)=C(N(=O)=O)O1	3
3,582	ISSSTY_v1a_7367_02May011_4561	67019-22-1	HC(H)C(C(=O)NC1=C2C(C=CC=C2)=NS1)C(H)H	1
3,583	ISSSTY_v1a_7367_02May011_4562	67019-24-3	HC(H)C(C(H)H)C(H)C(=O)NC1=C2C(C=CC=C2)=NS1	1
3,584	ISSSTY_v1a_7367_02May011_4563	67019-26-5	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(=O)NC1=C2C(C=CC=C2)=NS1	1
3,585	ISSSTY_v1a_7367_02May011_4564	67019-28-7	C12C(=C(NC(=O)c3ccccc3)SN=1)C=CC=C2	3
3,586	ISSSTY_v1a_7367_02May011_4565	67019-29-8	C12C(=C(NC(=O)Nc3ccccc3)SN=1)C=CC=C2	1
3,587	ISSSTY_v1a_7367_02May011_4566	99523-60-1	HC(H)C1C=CC2C(=C(NC(=O)C(H)C(H)H)SN=2)C=1	1
3,588	ISSSTY_v1a_7367_02May011_4567	91991-21-8	HC(H)C(H)C(H)C(=O)NC1=C2C(C=CC(Cl)=C2)=NS1	1
3,589	ISSSTY_v1a_7367_02May011_4568	91991-22-9	HC(H)C(H)C(H)C(H)C(=O)NC1=C2C(C=CC(Cl)=C2)=NS1	1
3,590	ISSSTY_v1a_7367_02May011_4569	91991-23-0	HC(H)C(C(H)H)C(H)C(=O)NC1=C2C(C=CC(Cl)=C2)=NS1	1
3,591	ISSSTY_v1a_7367_02May011_4570	98447-34-8	HC(H)C(H)C(H)C(=O)NC1=C2C(C=C(Cl)C=C2)=NS1	1
3,592	ISSSTY_v1a_7367_02May011_4571	87619-82-7	HC([C@](N)C(=O)O)SC(Cl)=C(Cl)C(Cl)=C(Cl)Cl	3
3,593	ISSSTY_v1a_7367_02May011_4572	98025-31-1	HC([C@](N)C(=O)O)SC(Cl)=C(Cl)Cl	3
3,594	ISSSTY_v1a_7367_02May011_4573	20589-85-9	C(Cl)(C(Cl)Cl)=CCl	3
3,595	ISSSTY_v1a_7367_02May011_4575	132832-27-0	c12c(c3c(c4c(c5c3cccc5)cccc4)cc1)[C@@]1[C@]([C@@](O)[C@]2O)O1	3
3,596	ISSSTY_v1a_7367_02May011_4576	76024-59-4	c12c(c3c(c4c1[C@](O)[C@@](O)[C@@]1[C@@]4O1)cccc3)cccc2	3
3,597	ISSSTY_v1a_7367_02May011_4577	132769-75-6	c12c(c3c4c(c5c6c(c(O)c(O)c5cc4)O6)ccc3cc1)cccc2	3
3,598	ISSSTY_v1a_7367_02May011_4578	127-90-2	HC(C(Cl)(Cl)Cl)C(Cl)OC(Cl)C(H)C(Cl)(Cl)Cl	3
3,599	ISSSTY_v1a_7367_02May011_4579	1447-88-7	HC(H)Oc1c(O)c2C(=O)C=C(c3ccc(O)cc3)Oc2cc1O	1
3,600	ISSSTY_v1a_7367_02May011_4580	123442-39-7	HC(H)Oc1c(OC(H)H)cc2C(=O)C(O)=C(c3ccc(O)cc3)Oc2c1	1

3,601	ISSSTY_v1a_7367_02May011_4583	122341-55-3	HC(H)C(H)N(C(H)C(O)C1C=CC(=[N+]=[N-])C(=O)C=1)N=O	3
3,602	ISSSTY_v1a_7367_02May011_4584	76144-81-5	HC(H)[N+](C(H)H)(C(H)H)NC(H)C(H)C(=O)[O-]	1
3,603	ISSSTY_v1a_7367_02May011_4585	63-91-2	HC(c1ccccc1)C(N)C(=O)O	1
3,604	ISSSTY_v1a_7367_02May011_4586	24385-10-2	HC(H)Oc1c2C(=O)c3c(C(=O)c2ccc1)c(O)c1c(c3O)[C@@](O)C(H)[C@@](O)(C(=O)C(H)O)C1H	3
3,605	ISSSTY_v1a_7367_02May011_4587	18774-09-9	HC(H)C1(OO)c2c(-c3c1ccccc3)cccc2	3
3,606	ISSSTY_v1a_7367_02May011_4588	96918-27-3	c12c3c4c(c5c(cc4ccc3ccc1)OC(N(=O)=O)=C5)cc2	3
3,607	ISSSTY_v1a_7367_02May011_4589	533-30-2	c12c(cc(N)cc1)SC=N2	3
3,608	ISSSTY_v1a_7367_02May011_4591	86674-50-2	c1(N(=O)=O)c2c3c4c([C@@](O)[C@](O)c3cc1)cccc4cc2	3
3,609	ISSSTY_v1a_7367_02May011_4592	56183-12-1	c12c3c4c([C@](O)[C@@](O)c3ccc1)cccc4cc2	1
3,610	ISSSTY_v1a_7367_02May011_4593	16156-54-0	HC(H)C(H)C(C(H)H)OS(=O)(=O)C(H)H	3
3,611	ISSSTY_v1a_7367_02May011_4594	102822-04-8	c12C(=O)C(=O)c3c4c(c(N(=O)=O)cc3)ccc(c14)ccc2	3
3,612	ISSSTY_v1a_7367_02May011_4595	102791-32-2	c12C(=O)C(=O)c3c4c(ccc(c14)ccc2N(=O)=O)ccc3	3
3,613	ISSSTY_v1a_7367_02May011_4596	6217-22-7	c12C(=O)C(=O)c3c4c(ccc(c14)ccc2)ccc3	1
3,614	ISSSTY_v1a_7367_02May011_4598	94764-55-3	c12-c3c(cc(N(=O)=O)cc3)Sc1cccc2	3
3,615	ISSSTY_v1a_7367_02May011_4599	23702-49-0	C1(=O)c2c3c4c(ccc3ccc2)cccc4O1	1
3,616	ISSSTY_v1a_7367_02May011_4600	137-17-7	HC(H)c1c(C(H)H)cc(N)c(C(H)H)c1	3
3,617	ISSSTY_v1a_7367_02May011_4603	18024-11-8	HC(H)c1c2-c3c(cccc3)N(C(H)H)c2c(C(H)H)cc1	3
3,618	ISSSTY_v1a_7367_02May011_4604	188107-70-2	HC(H)N1c2c(-c3c1cc(N(=O)=O)cc3)cccc2	3
3,619	ISSSTY_v1a_7367_02May011_4605	188107-71-3	HC(H)c1c2-c3c(cccc3)N(C(H)H)c2c(C(H)H)cc1N(=O)=O	3
3,620	ISSSTY_v1a_7367_02May011_4606	94-41-7	c1(C(=O)C=Cc2ccccc2)ccccc1	1
3,621	ISSSTY_v1a_7367_02May011_4607	7570-86-7	c1(C(=O)C2C(c3ccccc3)O2)ccccc1	3
3,622	ISSSTY_v1a_7367_02May011_4608	111249-52-6	HC(H)c1c2-c3c(cccc3)Nc2c(C(H)H)cc1N	3
3,623	ISSSTY_v1a_7367_02May011_4609	102059-18-7	HC(H)C(=O)Nc1ccc(C=CC(=O)c2ccccc2)cc1	3
3,624	ISSSTY_v1a_7367_02May011_4610	19337-19-0	HC(H)C(=O)Nc1ccc(C(=O)C=Cc2ccccc2)cc1	1
3,625	ISSSTY_v1a_7367_02May011_4611	82389-36-4	HC(H)C(=O)Nc1ccc([C@]2[C@@](C(=O)c3ccccc3)O2)cc1	3
3,626	ISSSTY_v1a_7367_02May011_4612	82389-38-6	HC(H)C(=O)Nc1ccc(C(=O)[C@]2[C@@](c3ccccc3)O2)cc1	3
3,627	ISSSTY_v1a_7367_02May011_4613	215245-16-2	HC(H)C(=O)Nc1c(N2N=C3C(C(Cl)=C(N)C=C3Br)=N2)cc(OC(H)H)c(N(C(H)C(H)H)C(H)C(H)C_N)c1	3
3,628	ISSSTY_v1a_7367_02May011_4614	76002-91-0	HC(H)C(c1ccc(OC(H)C2C(H)O2)cc1)(c1ccc(OC(H)C(O)C(H)O)cc1)C(H)H	3
3,629	ISSSTY_v1a_7367_02May011_4615	1774-66-9	c1(C(=O)C=Cc2ccc(Br)cc2)ccccc1	1
3,630	ISSSTY_v1a_7367_02May011_4616	484-47-9	c1(C2=C(c3ccccc3)N=C(c3ccccc3)N2)ccccc1	3

3,631	ISSSTY_v1a_7367_02May011_4617	120-66-1	HC(H)c1c(NC(=O)C(H)H)cccc1	1
3,632	ISSSTY_v1a_7367_02May011_4618	1728-96-7	HC(H)Oc1ccc(C2=C(c3ccc(OC(H)H)cc3)N=C(c3ccc(OC(H)H)cc3)N2)cc1	3
3,633	ISSSTY_v1a_7367_02May011_4619	27730-00-3	c1(C(=O)C=Cc2ccc(Br=O)cc2)ccccc1	1
3,634	ISSSTY_v1a_7367_02May011_4620	32157-71-4	c1(C(=O)[C@@]2[C@](c3ccccc3)O2)ccc(Br)cc1	1
3,635	ISSSTY_v1a_7367_02May011_4621	70786-65-1	HC(H)c1c(N(O)C(=O)C(H)H)cccc1	3
3,636	ISSSTY_v1a_7367_02May011_4622	112077-92-6	HC(H)c1c(N(C(=O)C(H)H)OC(=O)C(H)H)cccc1	1
3,637	ISSSTY_v1a_7367_02May011_4623	399-10-0	c1(C(=O)C=Cc2ccccc2)ccc(F)cc1	1
3,638	ISSSTY_v1a_7367_02May011_4624	362-05-0	HC(H)[C@]12C(H)C(H)[C@@]3c4c(C(H)C(H)[C@]3[C@@]1C(H)C(H)[C@]2O)cc(O)c(O)c4	1
3,639	ISSSTY_v1a_7367_02May011_4625	5976-61-4	HC(H)[C@]12C(H)C(H)[C@@]3c4c(c(O)c(O)cc4)C(H)C(H)[C@]3[C@@]1C(H)C(H)[C@]2O	1
3,640	ISSSTY_v1a_7367_02May011_4626	73936-27-3	c1(C(=O)[C@@]2[C@](c3ccccc3)O2)ccc(F)cc1	3
3,641	ISSSTY_v1a_7367_02May011_4627	101821-44-7	C12C(C=C(Br)C=C1)=NC(=C(N)N)C=2	1
3,642	ISSSTY_v1a_7367_02May011_4628	63-75-2	HC(H)N1C(H)C(C(=O)OC(H)H)=CC(H)C1H	3
3,643	ISSSTY_v1a_7367_02May011_4629	2657-25-2	c1(C(=O)C=Cc2ccccc2)ccc(O)cc1	1
3,644	ISSSTY_v1a_7367_02May011_4630	959-33-1	HC(H)Oc1ccc(C=CC(=O)c2ccccc2)cc1	1
3,645	ISSSTY_v1a_7367_02May011_4631	275795-16-9	HC(H)C(c1c(N=O)ccc(-c2ccccc2)c1)(C(H)H)C(H)H	3
3,646	ISSSTY_v1a_7367_02May011_4632	279242-11-4	HC(H)C(c1ccc(-c2ccc(N(=O)=O)cc2)cc1)(C(H)H)C(H)H	1
3,647	ISSSTY_v1a_7367_02May011_4633	959-23-9	HC(H)Oc1ccc(C(=O)C=Cc2ccccc2)cc1	1
3,648	ISSSTY_v1a_7367_02May011_4634	18873-03-5	HC(H)Oc1ccc(C(=O)C2C(c3ccccc3)O2)cc1	1
3,649	ISSSTY_v1a_7367_02May011_4635	27730-03-6	c1(C(=O)C2C(c3ccc(N(=O)=O)cc3)O2)ccccc1	1
3,650	ISSSTY_v1a_7367_02May011_4636	109143-18-2	HC(H)Oc1c2c(c(N(C(H)C(H)Cl)C(H)C(H)Cl)cc1)OC(N(=O)=O)=C2	3
3,651	ISSSTY_v1a_7367_02May011_4637	33942-93-7	HC(H)c1cc2c(cc1)nc1c3c(ccc1c2)cccc3	3
3,652	ISSSTY_v1a_7367_02May011_4638	7230-71-9	Cc1ccc2cc3ccc4ccccc4c3nc2c1	3
3,653	ISSSTY_v1a_7367_02May011_4639	13911-90-5	HC(H)c1c2c(ccc1)nc1c3c(ccc1c2)cccc3	3
3,654	ISSSTY_v1a_7367_02May011_4640	10567-95-0	HC(H)c1c2c(c3c(c(C(H)H)c4c(cccc4)n3)c1)cccc2	3
3,655	ISSSTY_v1a_7367_02May011_4641	86711-50-4	c1(C(=O)C2C(c3ccc(Oc4ccccc4)cc3)O2)ccccc1	1
3,656	ISSSTY_v1a_7367_02May011_4643	3340-94-1	HC(H)c1c2c(c3c(cccc3)cc2)nc2c1cccc2	3
3,657	ISSSTY_v1a_7367_02May011_4644	2403-28-3	c1(C(=O)C=Cc2ccc(-c3ccccc3)cc2)ccccc1	1
3,658	ISSSTY_v1a_7367_02May011_4645	51787-42-9	HC(H)c1c2c(c(C(H)H)c3c(c4c(cccc4)cc3)n2)cc(C(H)H)c1	3
3,659	ISSSTY_v1a_7367_02May011_4646	58430-01-6	HC(H)c1c2c(c3c(cccc3)cc2)nc2c1cc(C(H)H)c(C(H)H)c2	3
3,660	ISSSTY_v1a_7367_02May011_4647	32740-01-5	HC(H)c1c2c(c(C(H)H)c3c(c4c(cccc4)cc3)n2)ccc1	3

3,661	ISSSTY_v1a_7367_02May011_4648	82389-34-2	c1(C(=O)C2C(c3ccc(-c4ccccc4)cc3)O2)ccccc1	1
3,662	ISSSTY_v1a_7367_02May011_4649	82389-37-5	c1(C(=O)C2C(c3ccccc3)O2)ccc(-c2ccccc2)cc1	1
3,663	ISSSTY_v1a_7367_02May011_4651	95860-07-4	HC(H)c1c(NO)cc(N(=O)=O)cc1	1
3,664	ISSSTY_v1a_7367_02May011_4653	43192-03-6	HC(H)c1c(N(=O)=O)cc(NO)cc1	1
3,665	ISSSTY_v1a_7367_02May011_4654	13379-35-6	HC(H)Oc1cc2C(=O)c3c(O)cc(OC(H)H)cc3Oc2cc1	3
3,666	ISSSTY_v1a_7367_02May011_4655	67151-57-9	HC(H)c1c([N-][N+](=O)c2c(C(H)H)ccc([N+](=O)[O-])c2)cc(N(=O)=O)cc1	1
3,667	ISSSTY_v1a_7367_02May011_4656	5679-89-0	HC(H)c1c(N(=O)=O)cc([N-][N+](=O)c2cc([N+](=O)[O-])c(C(H)H)cc2)cc1	1
3,668	ISSSTY_v1a_7367_02May011_4658	5042-54-6	HC(H)c1c(N)cc(N)c(N=Nc2ccccc2)c1	3
3,669	ISSSTY_v1a_7367_02May011_4659	389104-60-3	HC(H)C(H)c1c(N)ccc(-c2ccccc2)c1	3
3,670	ISSSTY_v1a_7367_02May011_4660	127502-69-6	HC(H)C(c1c(N)ccc(-c2ccccc2)c1)C(H)H	3
3,671	ISSSTY_v1a_7367_02May011_4661	54810-82-1	HC(H)c1c(N)c(C(H)H)cc(-c2ccccc2)c1	3
3,672	ISSSTY_v1a_7367_02May011_4662	314084-63-4	HC(H)C(H)c1c(N)c(C(H)C(H)H)cc(-c2ccccc2)c1	1
3,673	ISSSTY_v1a_7367_02May011_4664	389104-62-5	HC(H)C(c1c(N)c(C(C(H)H)C(H)H)cc(-c2ccccc2)c1)C(H)H	1
3,674	ISSSTY_v1a_7367_02May011_4665	313-80-4	c12c3c4c(ccc3ccc1)ccnc4cc2	3
3,675	ISSSTY_v1a_7367_02May011_4666	125701-97-5	HC(H)c1c(C2=NC(c3ccc(OC(H)H)cc3)=C(c3ccc(OC(H)H)cc3)N2)ccc(C(H)H)c1	3
3,676	ISSSTY_v1a_7367_02May011_4668	105360-93-8	C12c3c4c(C=C1)cccc4ccc3NC(=O)C=2	3
3,677	ISSSTY_v1a_7367_02May011_4669	668-17-7	HC(H)C(H)[C@]1(O)C(H)[C@](OC2C(H)C(N(C(H)H)C(H)H)C(O)C(C(H)H)O2)c2c(O)c3C(=O)c4c(C(=O)c3cc2[C@@]1C(=O)OC(H)H)c(O)ccc4O	3
3,678	ISSSTY_v1a_7367_02May011_4670	5598-15-2	HC(H)C(H)OP(=O)(Oc1c(Cl)cc(Cl)c(Cl)n1)OC(H)C(H)H	1
3,679	ISSSTY_v1a_7367_02May011_4672	2012-00-2	HC(H)C(H)OP(=O)(c1ccccc1)Oc1ccc(N(=O)=O)cc1	3
3,680	ISSSTY_v1a_7367_02May011_4673	54738-93-1	c1(N(=O)=O)c2c(cc3c(cccc3)c2)ccc1	3
3,681	ISSSTY_v1a_7367_02May011_4674	31120-85-1	HC(H)C(H)OP(=O)(NC(C(H)H)C(H)H)Oc1c(C(=O)OC(C(H)H)C(H)H)cccc1	3
3,682	ISSSTY_v1a_7367_02May011_4675	27729-95-9	HC(H)Oc1ccc([C@@]2[C@](C(=O)c3ccccc3)O2)cc1	3
3,683	ISSSTY_v1a_7367_02May011_4676	51868-46-3	HC(H)C(=O)Nc1c(N=Nc2c(Br)cc([N+](=O)[O-])cc2[N+](=O)[O-])cc(OC(H)H)c(N(C(H)C=CH)C(H)C=CH)c1	3
3,684	ISSSTY_v1a_7367_02May011_4677	13301-61-6	HC(H)C(H)N(c1ccc(N=Nc2c(Cl)cc(N(=O)=O)cc2Cl)cc1)C(H)C(H)C_N	3
3,685	ISSSTY_v1a_7367_02May011_4678	932-97-8	C1(=O)C=CC(=[N+]=[N-])C=C1	3
3,686	ISSSTY_v1a_7367_02May011_4679	6375-47-9	HC(H)C(=O)Nc1cc(N)c(OC(H)H)cc1	3
3,687	ISSSTY_v1a_7367_02May011_4680	17420-30-3	C(_N)c1c(N)ccc(N(=O)=O)c1	3
3,688	ISSSTY_v1a_7367_02May011_4683	6214-18-2	HC(H)C(C(H)H)C(H)OS(=O)(=O)c1ccccc1	3
3,689	ISSSTY_v1a_7367_02May011_4685	109143-20-6	HC(H)Oc1c2c(c(N(C(H)C(H)Cl)C(H)C(H)Cl)cc1)C=C(N(=O)=O)O2	3
3,690	ISSSTY_v1a_7367_02May011_4686	109143-16-0	HC(Cl)C(H)N(c1cc2c(cc1)OC(N(=O)=O)=C2)C(H)C(H)Cl	3

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3,691	ISSSTY_v1a_7367_02May011_4687	605-32-3	c12C(=O)c3c(C(=O)c1cc(O)cc2)cccc3	3
3,692	ISSSTY_v1a_7367_02May011_4688	109143-19-3	HC(H)Oc1c(N(C(H)C(H)Cl)C(H)C(H)Cl)c2c(cc1)OC(N(=O)=O)=C2	3
3,693	ISSSTY_v1a_7367_02May011_4689	109143-17-1	HC(Cl)C(H)N(c1cc2c(C=C(N(=O)=O)O2)cc1)C(H)C(H)Cl	3
3,694	ISSSTY_v1a_7367_02May011_4690	152-84-1	HC([C@]1[C@@](O)[C@](O)[C@@](O)[C@](Oc2c(O)c3C(=O)c4c(C(=O)c3cc2)cccc4)O1)O[C@@]1[C@](O)[C@@](O)[C@](O)C(H)O1	1
3,695	ISSSTY_v1a_7367_02May011_4691	29706-59-0	HC(O)c1c(O)c2C(=O)c3c(C(=O)c2cc1O[C@]1[C@](O)[C@@](O)[C@](O)[C@@](C(H)O[C@@]2[C@](O)[C@@](O)[C@](O)C(H)O2)O1)cccc3	3
3,696	ISSSTY_v1a_7367_02May011_4692	3131-23-5	HC(H)C12C(=O)C(H)C(H)[C@]1C1C(H)C(H)c3c(O)c(O)ccc3[C@]1C(H)C2H	1
3,697	ISSSTY_v1a_7367_02May011_4693	362-06-1	HC(H)[C@@]12C(=O)C(H)C(H)[C@]1[C@@]1C(H)C(H)c3c(cc(O)c(O)c3)[C@]1C(H)C2H	1
3,698	ISSSTY_v1a_7367_02May011_4694	72076-98-3	c12c3c4c(c5c(cc4Sc3ccc1)cccc5)cc2	3
3,699	ISSSTY_v1a_7367_02May011_4695	142022-84-2	c12c3c4c(c5c(cc4S(=O)(=O)c3ccc1)cccc5)cc2	3
3,700	ISSSTY_v1a_7367_02May011_4696	63348-71-0	HC(H)c1c([N+](=O)[O-])c(S(=O)(=O)O)c([N+](=O)[O-])cc1	1
3,701	ISSSTY_v1a_7367_02May011_4697	52146-86-8	HC(H)c1c([N+](=O)[O-])cc([N+](=O)[O-])c(S(=O)(=O)O)c1	1
3,702	ISSSTY_v1a_7367_02May011_4698	99346-47-1	c1(O)c2c3c4c(c5c([C@@](O)[C@](O)C=C5)cc4cc2)ccc3cc1	3
3,703	ISSSTY_v1a_7367_02May011_4702	138261-41-3	HC(c1ccc(Cl)nc1)N1C(NN(=O)=O)=NC(H)C1H	3
3,704	ISSSTY_v1a_7367_02May011_4704	98046-73-2	HC1C(N=O)=CC2=C(N3C(C=CC=C3)=N2)N1	3
3,705	ISSSTY_v1a_7367_02May011_4705	482-35-9	HC(O)[C@]1[C@@](O)[C@](O)[C@@](O)[C@](OC2C(=O)c3c(O)cc(O)cc3OC=2c2cc(O)c(O)cc2)O1	3
3,706	ISSSTY_v1a_7367_02May011_4707	96287-03-5	HC(H)C1C2N(c3c(c(C(H)H)c(N)cn3)N=2)C=CC=1	3
3,707	ISSSTY_v1a_7367_02May011_4708	10265-92-6	HC(H)OP(N)(=O)SC(H)H	3
3,708	ISSSTY_v1a_7367_02May011_4710	27758-60-7	HC(H)c1ccc(N(N)c2ccc(C(H)H)cc2)cc1	3
3,709	ISSSTY_v1a_7367_02May011_4711	16596-38-6	HC(H)C(C(H)H)C(H)N(N)C(H)C(C(H)H)C(H)H	3
3,710	ISSSTY_v1a_7367_02May011_4713	644-21-3	HC(H)C(H)N(N)c1ccccc1	3
3,711	ISSSTY_v1a_7367_02May011_4717	1576-87-0	HC(H)C(H)C=CC=O	3
3,712	ISSSTY_v1a_7367_02May011_4719	188970-77-6	c12-c3c4c(c([N+](=O)[O-])cc3Nc1cc([N+](=O)[O-])c1c2cccc1)cccc4	3
3,713	ISSSTY_v1a_7367_02May011_4720	89784-39-4	HC(H)C(=O)N[C@](C(=O)O)C(H)SC(Cl)=C(Cl)C(Cl)=C(Cl)Cl	3
3,714	ISSSTY_v1a_7367_02May011_4721	481-73-2	HC(O)c1cc2C(=O)c3c(C(=O)c2c(O)c1)c(O)cc(O)c3	3
3,715	ISSSTY_v1a_7367_02May011_4722	138805-30-8	HC(H)c1c([N-][N+](=O)c2c(C(H)H)ccc(N)c2)cc(N)cc1	3
3,716	ISSSTY_v1a_7367_02May011_4723	188970-83-4	c12-c3c4c(c(N(=O)=O)cc3Nc1ccc1c2cccc1)c(O)ccc4	3
3,717	ISSSTY_v1a_7367_02May011_4735	626-43-7	c1(Cl)cc(Cl)cc(N)c1	1
3,718	ISSSTY_v1a_7367_02May011_4737	634-67-3	c1(Cl)c(Cl)c(Cl)c(N)cc1	1
3,719	ISSSTY_v1a_7367_02May011_4738	3333-66-2	HC(H)c1c2c(c3c(c(Cl)c4c(cccc4)n3)c1C(H)H)cccc2	3
3,720	ISSSTY_v1a_7367_02May011_4739	634-91-3	c1(Cl)c(Cl)c(Cl)cc(N)c1	1

3,721	ISSSTY_v1a_7367_02May011_4741	17722-52-0	HC(C(=O)Nc1ccc(Cl)cc1)C(H)C(=O)O	1
3,722	ISSSTY_v1a_7367_02May011_4742	17722-71-3	HC(C(=O)Nc1cc(Cl)c(Cl)cc1)C(H)C(N)=O	1
3,723	ISSSTY_v1a_7367_02May011_4743	53219-95-7	HC(C(=O)Nc1cc(Cl)cc(Cl)c1)C(H)C(=O)O	1
3,724	ISSSTY_v1a_7367_02May011_4744	112368-25-9	HC(C(=O)Nc1c(Cl)c(Cl)c(Cl)cc1)C(H)C(N)=O	1
3,725	ISSSTY_v1a_7367_02May011_4746	112368-26-0	HC(C(=O)Nc1cc(Cl)c(Cl)c(Cl)c1)C(H)C(N)=O	1
3,726	ISSSTY_v1a_7367_02May011_4747	6943-00-6	HC1C(=O)N(c2ccc(Cl)cc2)C(=O)C1H	1
3,727	ISSSTY_v1a_7367_02May011_4749	15386-58-0	HC1C(=O)N(c2cc(Cl)c(Cl)cc2)C(=O)C1H	1
3,728	ISSSTY_v1a_7367_02May011_4750	24096-53-5	HC1C(=O)N(c2cc(Cl)cc(Cl)c2)C(=O)C1H	1
3,729	ISSSTY_v1a_7367_02May011_4751	112368-27-1	HC1C(=O)N(c2c(Cl)c(Cl)c(Cl)cc2)C(=O)C1H	1
3,730	ISSSTY_v1a_7367_02May011_4752	27746-63-0	HC1C(=O)N(c2cc(Cl)c(Cl)c(Cl)c2)C(=O)C1H	1
3,731	ISSSTY_v1a_7367_02May011_4754	1068-57-1	HC(H)C(=O)NN	3
3,732	ISSSTY_v1a_7367_02May011_4755	19315-64-1	HC(H)C(=O)N(O)c1ccc(OC(H)C(H)H)cc1	3
3,733	ISSSTY_v1a_7367_02May011_4758	14634-93-6	HC(H)C(H)N(c1ccccc1)C([S-])=S[Zn++]S=C([S-])N(c1ccccc1)C(H)C(H)H	1
3,734	ISSSTY_v1a_7367_02May011_4759	95-33-0	HC1C(H)C(H)C(H)C(H)C1NSC1=Nc2c(cccc2)S1	1
3,735	ISSSTY_v1a_7367_02May011_4760	102-77-2	HC1C(H)N(SC2=Nc3c(cccc3)S2)C(H)C(H)O1	1
3,736	ISSSTY_v1a_7367_02May011_4761	26780-96-1	HC(H)C1c2c(cccc2)NC(C(H)H)(C(H)H)C=1	1
3,737	ISSSTY_v1a_7367_02May011_4762	61788-44-1	HC=Cc1c(O)ccc(C=CH)c1	1
3,738	ISSSTY_v1a_7367_02May011_4764	85-60-9	HC(H)C(c1c(O)cc(C(H)H)c(C(c2c(C(H)H)cc(O)c(C(C(H)H)(C(H)H)C(H)H)c2)C(H)C(H)C(H)H)c1)(C(H)H)C(H)H	1
3,739	ISSSTY_v1a_7367_02May011_4765	843-55-0	HC1C(c2ccc(O)cc2)(c2ccc(O)cc2)C(H)C(H)C(H)C1H	1
3,740	ISSSTY_v1a_7367_02May011_4766	119-47-1	HC(H)C(c1c(O)c(C(H)c2c(O)c(C(C(H)H)(C(H)H)C(H)H)cc(C(H)H)c2)cc(C(H)H)c1)(C(H)H)C(H)H	1
3,741	ISSSTY_v1a_7367_02May011_4767	91-53-2	HC(H)C1c2c(ccc(OC(H)C(H)H)c2)NC(C(H)H)(C(H)H)C=1	1
3,742	ISSSTY_v1a_7367_02May011_4768	548-39-0	C1(=O)c2c3c(C=C1)cccc3ccc2	3
3,743	ISSSTY_v1a_7367_02May011_4769	66291-31-4	HC(H)c1c(C(H)H)c2c3c(ccc2cc1)cccc3	1
3,744	ISSSTY_v1a_7367_02May011_4770	15254-64-5	HC(H)c1c2c3c(ccc2cc(C(H)H)c1)cccc3	3
3,745	ISSSTY_v1a_7367_02May011_4771	16664-45-2	HC(H)c1c2c(c3c(cccc3)cc2)cc(C(H)H)c1	3
3,746	ISSSTY_v1a_7367_02May011_4772	22349-59-3	HC(H)c1c2c(c3c(cccc3)cc2)c(C(H)H)cc1	3
3,747	ISSSTY_v1a_7367_02May011_4773	1070-13-9	HC(H)C(H)C(H)C(C=O)=CH	3
3,748	ISSSTY_v1a_7367_02May011_4774	922-63-4	HC(H)C(H)C(C=O)=CH	3
3,749	ISSSTY_v1a_7367_02May011_4775	94500-54-6	HC(Cl)c1c2c3c4c(ccc3cc3c2cccc3)cccc4c1	3
3,750	ISSSTY_v1a_7367_02May011_4778	94500-44-4	HC(Cl)c1c2c3c4c(c5c(cc4ccc3ccc2)cccc5)c1	3

3,751	ISSSTY_v1a_7367_02May011_4782	1107-26-2	HC(H)C1(C(H)H)C(C=CC(C(H)H)=CC=CC(C(H)H)=CC=CC=C(C(H)H)C=CC=C(C(H)H)C=O)=C(C(H)H)C(H)C(H)C1H	1
3,752	ISSSTY_v1a_7367_02May011_4785	7269-58-1	HC(O)[C@]1[C@@](O)[C@@](O)[C@](N2c3c(c(NO)nc(N)n3)N=C2)O1	3
3,753	ISSSTY_v1a_7367_02May011_4792	27762-78-3	HC(H)C(H)OC(C(=O)C(O)O)C(H)H	3
3,754	ISSSTY_v1a_7367_02May011_4793	6149-34-4	c1(Nc2ccc(N)cc2)ccc(N(=O)=O)cc1	3
3,755	ISSSTY_v1a_7367_02May011_4794	60516-11-2	HC(H)C(=O)Nc1ccc(Nc2ccc(N(=O)=O)cc2)cc1	3
3,756	ISSSTY_v1a_7367_02May011_4795	620-89-3	HC(H)c1ccc(Nc2ccc(N(=O)=O)cc2)cc1	3
3,757	ISSSTY_v1a_7367_02May011_4797	962-32-3	c12-c3c(C4C(c1cc1c(cccc1)c2)O4)cccc3	3
3,758	ISSSTY_v1a_7367_02May011_4798	138835-35-5	c12c(c3c4c5c(c(N(=O)=O)ccc5ccc4n1)cc3)cccc2	3
3,759	ISSSTY_v1a_7367_02May011_4799	138835-36-6	c12c(c3c4c5c(c(N(=O)=O)ccc5cc3)ccc4n1)cccc2	3
3,760	ISSSTY_v1a_7367_02May011_4800	138835-33-3	c12c(c3c4c5c(c([N+](=O)[O-])ccc5ccc4[n+]1[O-])cc3)cccc2	3
3,761	ISSSTY_v1a_7367_02May011_4801	138835-34-4	c12c(c3c4c5c(c([N+](=O)[O-])ccc5cc3)ccc4[n+]1[O-])cccc2	3
3,762	ISSSTY_v1a_7367_02May011_4802	125974-01-8	HC(Cl)C1=C(Cl)C(=O)OC1H	3
3,763	ISSSTY_v1a_7367_02May011_4804	93673-37-1	c12c3c(c4c(c5c([C@](O)[C@@](O)C=C5)cc4)cc3ccc1)C=C2	3
3,764	ISSSTY_v1a_7367_02May011_4806	24279-91-2	HC(H)C1C(=O)C(N2C(H)C2H)=C(C(C(H)OC(N)=O)OC(H)H)C(=O)C=1N1C(H)C1H	1
3,765	ISSSTY_v1a_7367_02May011_4807	488-41-5	HC(Br)C(O)C(O)C(O)C(O)C(H)Br	3
3,766	ISSSTY_v1a_7367_02May011_4809	3697-30-1	HC(H)C(H)c1c2c(c3c(cccc3)cc2)cc2c1cccc2	3
3,767	ISSSTY_v1a_7367_02May011_4814	71708-92-4	HC(H)C(=O)N(O)c1ccc(Oc2ccccc2)cc1	3
3,768	ISSSTY_v1a_7367_02May011_4816	2417-77-8	HC(Br)c1c2c(cc3c1cccc3)cccc2	3
3,769	ISSSTY_v1a_7367_02May011_4818	114924-37-7	HC(H)[C@@]12[C@](C=O)(C(C=O)=C3[C@](O)(C(H)C(C(H)H)C(H)H)C3H)[C@]1O)C2H	3
3,770	ISSSTY_v1a_7367_02May011_4819	114838-69-6	HC(H)[C@]12[C@@](C=O)(C(C=O)=C3[C@@](O)(C(H)C(C(H)H)C(H)H)C3H)[C@]1OC(=O)C(H)H)C2H	3
3,771	ISSSTY_v1a_7367_02May011_4820	108893-58-9	HC(H)[C@@]12[C@](C=O)(C(C=O)=C3[C@@](O)(C(H)C(C(H)H)C(H)H)C3H)[C@]1O)C2H	3
3,772	ISSSTY_v1a_7367_02May011_4823	114882-46-1	c1(N=O)c2c3c4c(c5c(cc4ccc3cc1)cccc5)cc2	3
3,773	ISSSTY_v1a_7367_02May011_4824	120388-69-4	c1(N=O)c2c3c4c(c5c(cc4cc2)cccc5)ccc3cc1	3
3,774	ISSSTY_v1a_7367_02May011_4825	120812-47-7	HC1c2c(c3c4c5c(c(N(=O)=O)ccc25)ccc4ccc3)C(H)C(H)C1H	3
3,775	ISSSTY_v1a_7367_02May011_4826	215226-71-4	HC(H)C(=C(Cl)C(=O)O)C=O	3
3,776	ISSSTY_v1a_7367_02May011_4827	215226-73-6	HC(Cl)C(=C(Cl)C(=O)O)C(Cl)Cl	3
3,777	ISSSTY_v1a_7367_02May011_4828	215226-72-5	HC(Cl)C(C(Cl)Cl)=CC(=O)O	3
3,778	ISSSTY_v1a_7367_02May011_4829	491-35-0	HC(H)c1c2c(cccc2)ncc1	3
3,779	ISSSTY_v1a_7367_02May011_4833	97931-39-0	HC1c2c3c4c(c(N(=O)=O)c5c(c4ccc3ccc2)cccc5)C1H	3
3,780	ISSSTY_v1a_7367_02May011_4834	67587-52-4	HC1C(H)N(N=O)C(H)C(O)O1	3

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3,781	ISSSTY_v1a_7367_02May011_4835	88598-56-5	HC1c2c(c3c4c5c(c(N(=O)=O)ccc5ccc4c2)cc3)C(H)C(H)C1H	3
3,782	ISSSTY_v1a_7367_02May011_4836	88598-57-6	HC1c2c(c3c4c5c(c(N(=O)=O)ccc5cc3)ccc4c2)C(H)C(H)C1H	3
3,783	ISSSTY_v1a_7367_02May011_4837	107-20-0	HC(Cl)C=O	3
3,784	ISSSTY_v1a_7367_02May011_4839	95840-05-4	[C@]1(O)[C@@](O)[C@@]2[C@](C=C1)O2	3
3,785	ISSSTY_v1a_7367_02May011_4840	121153-48-8	[C@]1(O)[C@@](O)[C@]2[C@@](C=C1)O2	3
3,786	ISSSTY_v1a_7367_02May011_4841	121153-49-9	[C@@]1(O)[C@](O)[C@@]2[C@](C=C1)O2	3
3,787	ISSSTY_v1a_7367_02May011_4843	120209-97-4	c12c(cc(N)cc1)nc1c(cc(N)cc1)n2	3
3,788	ISSSTY_v1a_7367_02May011_4850	93673-33-7	HC1c2c(C3=C4C(=C5C=CC=C1C35)O4)c1c(cccc1)cc2	3
3,789	ISSSTY_v1a_7367_02May011_4851	577-19-5	c1(Br)c(N(=O)=O)cccc1	3
3,790	ISSSTY_v1a_7367_02May011_4852	585-79-5	c1(Br)cc(N(=O)=O)ccc1	3
3,791	ISSSTY_v1a_7367_02May011_4853	96910-71-3	HC(H)[C@@]12[C@@](C=O)(C(C=O)=C[C@@]3(O)C(H)C(C(H)H)(C(H)H)C(H)[C@@]13)C2H	3
3,792	ISSSTY_v1a_7367_02May011_4855	2213-00-5	HC(H)C1(C(H)H)C(H)[C@@]2C3(C(=O)OC(H)H)[C@](C=O)(C(C=O)=C[C@@]2C1H)C3H	3
3,793	ISSSTY_v1a_7367_02May011_4857	109883-99-0	HC(H)C1(C(H)H)C(H)C2(O)C(C34C(C(C=O)=C2)(C(O)OC3=O)C4H)C1H	3
3,794	ISSSTY_v1a_7367_02May011_4858	603-02-1	HC(H)c1c([N+](=O)[O-])c(C(H)H)c([N+](=O)[O-])cc1	3
3,795	ISSSTY_v1a_7367_02May011_4860	610-28-6	C(=O)(O)c1c([N+](=O)[O-])ccc([N+](=O)[O-])c1	3
3,796	ISSSTY_v1a_7367_02May011_4861	96910-73-5	HC(H)C1(C(H)H)C(H)[C@]2(O)C=C(C(=O)C(C=O)=C[C@](C(H)H)[C@]2C1H	3
3,797	ISSSTY_v1a_7367_02May011_4867	99-33-2	C(=O)(Cl)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1	3
3,798	ISSSTY_v1a_7367_02May011_4872	96910-70-2	HC(H)[C@]12[C@@](C=O)(C(C(H)O)=C[C@@]3C(H)C(C(H)H)(C(H)H)C(H)[C@@]13)C2H	3
3,799	ISSSTY_v1a_7367_02May011_4874	30074	c12C(=O)c3c(-c4c1c(ccc4)ccc2)cccc3	3
3,800	ISSSTY_v1a_7367_02May011_4875	90-44-8	HC1c2c(C(=O)c3c1cccc3)cccc2	3
3,801	ISSSTY_v1a_7367_02May011_4877	104671-59-2	HC(H)C(=O)NOC(=O)NC(H)H	3
3,802	ISSSTY_v1a_7367_02May011_4878	106807-80-1	HC(H)C(=O)N(O)C(=O)NC(H)H	3
3,803	ISSSTY_v1a_7367_02May011_4881	51594-55-9	HC(Cl)[C@@]1C(H)O1	3
3,804	ISSSTY_v1a_7367_02May011_4882	67843-74-7	HC(Cl)[C@]1C(H)O1	3
3,805	ISSSTY_v1a_7367_02May011_4883	57044-25-4	HC(O)[C@]1C(H)O1	3
3,806	ISSSTY_v1a_7367_02May011_4884	60456-23-7	HC(O)[C@]1C(H)O1	3
3,807	ISSSTY_v1a_7367_02May011_4886	113826-06-5	HC(H)c1ccc(S(=O)(=O)OC(H)[C@@]2C(H)O2)cc1	3
3,808	ISSSTY_v1a_7367_02May011_4887	70987-78-9	HC(H)c1ccc(S(=O)(=O)OC(H)[C@]2C(H)O2)cc1	3
3,809	ISSSTY_v1a_7367_02May011_4888	129286-36-8	c1(F)c2c3c(c4c(c5c(cccc5)cc4)c3ccc2)cc1	3
3,810	ISSSTY_v1a_7367_02May011_4889	129286-37-9	c12c3c(c4c(c5c(cc(F)cc5)cc4)c3ccc1)ccc2	3

3,811	ISSSTY_v1a_7367_02May011_4890	28361-96-8	HC(Cl)C(H)SC(H)C(N)C(=O)O	3
3,812	ISSSTY_v1a_7367_02May011_4892	101043-65-6	c1(N(=O)=O)c2c3c4c(c(N=O)ccc4cc2)ccc3cc1	3
3,813	ISSSTY_v1a_7367_02May011_4893	105500-28-5	c12c(c3c([C@@](O)[C@](O)[C@@]4[C@@]3O4)cc1)cc1c3c(ccc1n2)cccc3	3
3,814	ISSSTY_v1a_7367_02May011_4894	105467-73-0	c12c(c3c([C@@](O)[C@](O)[C@]4[C@]3O4)cc1)cc1c3c(ccc1n2)cccc3	3
3,815	ISSSTY_v1a_7367_02May011_4895	118745-11-2	c1(C=Cc2ccc(N(O)C=O)cc2)ccccc1	3
3,816	ISSSTY_v1a_7367_02May011_4896	78281-06-8	c1(-c2ccc(NC(=O)O)cc2)ccccc1	3
3,817	ISSSTY_v1a_7367_02May011_4897	1707-31-9	c12c(cc(N(O)C=O)cc1)cccc2	3
3,818	ISSSTY_v1a_7367_02May011_4899	118745-12-3	HC(H)C(H)C(=O)N(O)c1ccc(C=Cc2ccccc2)cc1	3
3,819	ISSSTY_v1a_7367_02May011_4902	5329-87-3	HC1c2c(-c3c(cc(N(=O)=O)cc3)C1H)cccc2	3
3,820	ISSSTY_v1a_7367_02May011_4903	10549-22-1	HC1c2c3-c4c(C(H)C(H)c3cc(N(=O)=O)c2)cccc4C1H	3
3,821	ISSSTY_v1a_7367_02May011_4904	117929-14-3	HC1c2c3c4c(cc(N(=O)=O)cc4ccc3ccc2)C1H	3
3,822	ISSSTY_v1a_7367_02May011_4905	149127-56-0	HC(H)C(C(H)H)(N=NC(H)H)OO	3
3,823	ISSSTY_v1a_7367_02May011_4906	69533-68-2	HC1c2c(-c3c(cc([N+](=O)[O-])cc3)C1H)ccc([N+](=O)[O-])c2	3
3,824	ISSSTY_v1a_7367_02May011_4907	17573-23-8	HC1c2c(c3c4c5c(ccc4c2)cccc5cc3)C=CC1H	3
3,825	ISSSTY_v1a_7367_02May011_4908	117929-13-2	HC1c2c3-c4c(C(H)C(H)c3cc([N+](=O)[O-])c2)cc([N+](=O)[O-])cc4C1H	3
3,826	ISSSTY_v1a_7367_02May011_4909	117929-12-1	HC1c2c3c4c(cc([N+](=O)[O-])cc4ccc3cc([N+](=O)[O-])c2)C1H	3
3,827	ISSSTY_v1a_7367_02May011_4910	119-27-7	HC(H)Oc1c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
3,828	ISSSTY_v1a_7367_02May011_4911	2363-23-7	HC(H)Sc1c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
3,829	ISSSTY_v1a_7367_02May011_4912	581437	c1(Oc2ccc(Oc3ccc(N)cc3)cc2)ccc(N)cc1	3
3,830	ISSSTY_v1a_7367_02May011_4913	23815-63-6	HC([C@](N)C(=O)O)Sc1c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
3,831	ISSSTY_v1a_7367_02May011_4920	151378-31-3	c12C34c5c(c6c(cccc6)cc5)-c1ccccc2C(O)C(O)C3O4	3
3,832	ISSSTY_v1a_7367_02May011_4921	132335-15-0	c12-c3c(c4c(cccc4)cc3)C3C(c1cccc2)N3	3
3,833	ISSSTY_v1a_7367_02May011_4922	84850-16-8	c12c(c3c(c4c5c(c6c(c14)cccc6)cccc5)cccc3)O2	3
3,834	ISSSTY_v1a_7367_02May011_4923	132335-20-7	c12-c3c4c(c5c(c3C3C(c1cccc2)N3)cccc5)cccc4	3
3,835	ISSSTY_v1a_7367_02May011_4927	623-10-9	HC(H)c1ccc(NO)cc1	3
3,836	ISSSTY_v1a_7367_02May011_4929	2498-77-3	HC(H)c1c2c3c(cc4c(cccc4)c3)ccc2ccc1	3
3,837	ISSSTY_v1a_7367_02May011_4930	2498-76-2	HC(H)c1cc2c3c(cc4c(cccc4)c3)ccc2cc1	3
3,838	ISSSTY_v1a_7367_02May011_4931	2498-75-1	HC(H)c1cc2c(c3c(cc4c(cccc4)c3)cc2)cc1	3
3,839	ISSSTY_v1a_7367_02May011_4932	316-49-4	HC(H)c1c2c(c3c(cccc3)c1)cc1c(cccc1)c2	3
3,840	ISSSTY_v1a_7367_02May011_4933	2381-31-9	HC(H)c1c2c(cc3c4c(ccc3c2)cccc4)ccc1	3

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