

4,441	ISSSTY_v1a_7367_02May011_5895	80-44-4	HC(H)C(H)C(H)C(H)OS(=O)(=O)c1ccccc1	3
4,442	ISSSTY_v1a_7367_02May011_5896	515-46-8	HC(H)C(H)OS(=O)(=O)c1ccccc1	3
4,443	ISSSTY_v1a_7367_02May011_5897	80-18-2	HC(H)OS(=O)(=O)c1ccccc1	3
4,444	ISSSTY_v1a_7367_02May011_5898	16156-53-9	HC(H)C(C(H)H)C(H)OS(=O)(=O)C(H)H	3
4,445	ISSSTY_v1a_7367_02May011_5899	1912-32-9	HC(H)C(H)C(H)C(H)OS(=O)(=O)C(H)H	3
4,446	ISSSTY_v1a_7367_02May011_5900	1912-31-8	HC(H)C(H)C(H)OS(=O)(=O)C(H)H	3
4,447	ISSSTY_v1a_7367_02May011_5901	80-42-2	HC(H)C(H)C(H)OS(=O)(=O)c1ccccc1	3
4,448	ISSSTY_v1a_7367_02May011_5902	303-33-3	HC(H)[C@](C@@)(O)(C(=O)OC(H)C1[C@@]2[C@@](O)C(H)C(H)N2C(H)C=1)C(C(H)H)C(H)H)OC(H)H	3
4,449	ISSSTY_v1a_7367_02May011_5906	75965-74-1	HC(H)Oc1cc2c(c3c(cc2)OC(N(=O)=O)=C3)cc1	3
4,450	ISSSTY_v1a_7367_02May011_5912	765-34-4	HC1C(C=O)O1	3
4,451	ISSSTY_v1a_7367_02May011_5914	53478-38-9	HC(H)S(=O)(=O)Nc1ccc(Nc2c3c(cccc3)nc3c2cccc3)cc1	3
4,452	ISSSTY_v1a_7367_02May011_5917	217-59-4	c12c(c3c(c4c1cccc4)cccc3)cccc2	3
4,453	ISSSTY_v1a_7367_02May011_5918	7332-00-5	HC(H)C(H)C(H)C(H)N=N_N	3
4,454	ISSSTY_v1a_7367_02May011_5919	6926-45-0	HC(H)C(H)C(H)C(H)C(H)C(H)N=N_N	3
4,455	ISSSTY_v1a_7367_02May011_5920	2148-31-4	HC(H)C(=O)N[C@](C(=O)O)C(H)SC(Cl)=CCl	3
4,456	ISSSTY_v1a_7367_02May011_5921	111348-61-9	HC(H)C(=O)N[C@](C(=O)O)C(H)SC(Cl)=C(Cl)Cl	3
4,457	ISSSTY_v1a_7367_02May011_5922	93780-95-1	c12c(c3c([C@@](O)[C@](O)[C@@]4[C@@]3O4)cc1)nc1c3c(ccc1c2)cccc3	3
4,458	ISSSTY_v1a_7367_02May011_5923	93781-00-1	c12c(c3c([C@](O)[C@@](O)[C@@]4[C@@]3O4)cc1)nc1c3c(ccc1c2)cccc3	3
4,459	ISSSTY_v1a_7367_02May011_5924	93780-98-4	c12c(c3c([C@@](O)[C@](O)[C@]4[C@]3O4)cc1)nc1c3c(ccc1c2)cccc3	3
4,460	ISSSTY_v1a_7367_02May011_5925	93780-96-2	c12c(c3c([C@](O)[C@@](O)[C@]4[C@]3O4)cc1)nc1c3c(ccc1c2)cccc3	3
4,461	ISSSTY_v1a_7367_02May011_5926	99152-10-0	HC(H)C(=O)N[C@@](C(=O)N(C(H)C(=O)O)N=O)C(C(H)H)C(H)H	3
4,462	ISSSTY_v1a_7367_02May011_5928	40568-90-9	HC(H)c1c2c3c4c(c5c(cc4ccc3cc1)cccc5)cc2	3
4,463	ISSSTY_v1a_7367_02May011_5930	16757-82-7	HC(H)c1cc2c3c4c(c5c(cc4ccc3c1)cccc5)cc2	3
4,464	ISSSTY_v1a_7367_02May011_5932	16757-81-6	HC(H)c1c2c3c4c(c5c(cc4cc2)cccc5)ccc3cc1	3
4,465	ISSSTY_v1a_7367_02May011_5933	16757-83-8	HC(H)c1c2c3c4c(c5c(cc4c1)cccc5)ccc3ccc2	3
4,466	ISSSTY_v1a_7367_02May011_5934	63041-77-0	HC(H)c1c2c(c3c4c5c(ccc4c2)cccc5cc3)ccc1	3
4,467	ISSSTY_v1a_7367_02May011_5935	63041-76-9	HC(H)c1cc2c(c3c4c5c(ccc4c2)cccc5cc3)cc1	3
4,468	ISSSTY_v1a_7367_02May011_5936	70644-19-8	HC(H)c1cc2c3c4c5c(ccc4cc2cc1)cccc5cc3	3
4,469	ISSSTY_v1a_7367_02May011_5937	63104-32-5	HC(H)c1c2c3c4c5c(ccc4cc2ccc1)cccc5cc3	3
4,470	ISSSTY_v1a_7367_02May011_5938	16757-80-5	HC(H)c1c2c3c4c(ccc3cc3c2cccc3)cccc4c1	3

4,471	ISSSTY_v1a_7367_02May011_5939	4514-19-6	HC(H)c1c2c3c4c(c5c(cc4ccc3ccc2)cccc5)c1	3
4,472	ISSSTY_v1a_7367_02May011_5940	24143-08-6	HC(H)C(=O)NC1C=NC(C2=CC=C(N(=O)=O)O2)=NO1	3
4,473	ISSSTY_v1a_7367_02May011_5945	94500-46-6	HC(Cl)c1c2c3c4c(c5c(cc4c1)cccc5)ccc3ccc2	3
4,474	ISSSTY_v1a_7367_02May011_5947	29852-26-4	HC(Cl)c1c2c3c(c4c(cccc4)c2)ccc2c3c(ccc2)c1	3
4,475	ISSSTY_v1a_7367_02May011_5951	86803-19-2	HC(Cl)c1c2c3c4c5c(ccc4cc2ccc1)cccc5cc3	3
4,476	ISSSTY_v1a_7367_02May011_5952	78411-56-0	HC(H)c1cnc2c3c(ccc2n1)N(C(H)H)C(N)=N3	3
4,477	ISSSTY_v1a_7367_02May011_5957	303-34-4	HC(H)C(O)[C@](O)(C(=O)OC(H)C1[C@@]2[C@@](OC(=O)C(C(H)H)=CC(H)H)C(H)C(H)N2C(H)C=1)[C@@](C(H)H)OC(H)H)C(H)H	3
4,478	ISSSTY_v1a_7367_02May011_5961	41267-76-9	HC(H)C1c2c(c3c4c(C(H)C(H)C(H)N4C(H)C(H)C3H)c2)OC(=O)C=1	3
4,479	ISSSTY_v1a_7367_02May011_5965	58336-35-9	HC1c2c3c(c4c(C=CC(=O)O4)c2)C(H)C(H)C(H)N3C(H)C1H	3
4,480	ISSSTY_v1a_7367_02May011_5966	3365-85-3	c1(-c2ccc(-c3ccc(N)cc3)cc2)ccc(N)cc1	3
4,481	ISSSTY_v1a_7367_02May011_5967	53693-66-6	HC(H)C(H)N(c1c(-c2cccc2)c(-c2cccc2)ccc1N(C(H)C(H)H)C(H)C(H)H)C(H)C(H)H	3
4,482	ISSSTY_v1a_7367_02May011_5976	99520-64-6	c12C3C4c5c6c(ccc5C5C(C=4c1cccc2)O5)cccc6C=3	3
4,483	ISSSTY_v1a_7367_02May011_5977	7696-62-0	HC(H)C(H)C(H)C(H)Oc1ccc(N=O)cc1	3
4,484	ISSSTY_v1a_7367_02May011_5978	100690-33-3	HC(H)C(H)C(H)C(H)C(H)Oc1ccc(N=O)cc1	3
4,485	ISSSTY_v1a_7367_02May011_5979	1517-05-1	HC(O)C(H)N=N_N	3
4,486	ISSSTY_v1a_7367_02May011_5980	138245-74-6	HC(O)[C@](O)[C@@](O)[C@@](O)[C@](O)C(H)N=N_N	3
4,487	ISSSTY_v1a_7367_02May011_5983	67019-41-4	C1(=NC(=O)c2ccc([N+](=O)[O-])cc2)c2c(ccc2)N(C(=O)c2ccc([N+](=O)[O-])cc2)S1	3
4,488	ISSSTY_v1a_7367_02May011_5987	99523-84-9	HC(H)c1cc2C(=NC(=O)c3cc([N+](=O)[O-])ccc3)SN(C(=O)c3cc([N+](=O)[O-])ccc3)c2cc1	3
4,489	ISSSTY_v1a_7367_02May011_5988	99523-85-0	HC(H)c1cc2C(=NC(=O)c3ccc([N+](=O)[O-])cc3)SN(C(=O)c3ccc([N+](=O)[O-])cc3)c2cc1	3
4,490	ISSSTY_v1a_7367_02May011_5990	91991-31-0	HC(C(=O)N1c2c(C(=NC(=O)C(H)C(H)C(H)Cl)S1)cc(Cl)cc2)C(H)C(H)Cl	3
4,491	ISSSTY_v1a_7367_02May011_5991	91991-42-3	C1(=NC(=O)c2ccc([N+](=O)[O-])cc2)c2c(ccc(Cl)c2)N(C(=O)c2ccc([N+](=O)[O-])cc2)S1	3
4,492	ISSSTY_v1a_7367_02May011_5992	106532-60-9	HC(H)C(=O)N1c2c(C(=NC(=O)C(H)H)S1)cc(N(=O)=O)cc2	3
4,493	ISSSTY_v1a_7367_02May011_5993	106532-61-0	HC(H)C(H)C(=O)N1c2c(C(=NC(=O)C(H)C(H)H)S1)cc(N(=O)=O)cc2	3
4,494	ISSSTY_v1a_7367_02May011_5994	106532-63-2	HC(H)C(H)C(H)C(=O)N1c2c(C(=NC(=O)C(H)C(H)C(H)H)S1)cc(N(=O)=O)cc2	3
4,495	ISSSTY_v1a_7367_02May011_5995	106532-64-3	HC(H)C(C(=O)N1c2c(C(=NC(=O)C(H)H)C(H)H)S1)cc(N(=O)=O)cc2)C(H)H	3
4,496	ISSSTY_v1a_7367_02May011_5996	106532-66-5	HC(H)C(H)C(H)C(H)C(=O)N1c2c(C(=NC(=O)C(H)C(H)C(H)C(H)H)S1)cc(N(=O)=O)cc2	3
4,497	ISSSTY_v1a_7367_02May011_5997	106532-67-6	HC(H)C(C(H)H)C(H)C(=O)N1c2c(C(=NC(=O)C(H)C(H)C(H)C(H)H)S1)cc(N(=O)=O)cc2	3
4,498	ISSSTY_v1a_7367_02May011_5998	106532-68-7	HC(H)C(H)C(H)C(H)C(H)C(=O)N1c2c(C(=NC(=O)C(H)C(H)C(H)C(H)C(H)H)S1)cc(N(=O)=O)cc2	3
4,499	ISSSTY_v1a_7367_02May011_5999	106532-69-8	HC(H)C(H)C(H)C(H)C(H)C(H)C(=O)N1c2c(C(=NC(=O)C(H)C(H)C(H)C(H)C(H)C(H)H)S1)cc(N(=O)=O)cc2	3
4,500	ISSSTY_v1a_7367_02May011_6000	106532-70-1	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(=O)N1c2c(C(=NC(=O)C(H)C(H)C(H)C(H)C(H)C(H)C(H)H)S1)cc(N(=O)=O)cc2	3

4,501	ISSSTY_v1a_7367_02May011_6001	106532-62-1	HC(C(=O)N1c2c(C(=NC(=O)C(H)C(H)Cl)S1)cc(N(=O)=O)cc2)C(H)Cl	3
4,502	ISSSTY_v1a_7367_02May011_6002	106532-65-4	HC(C(=O)N1c2c(C(=NC(=O)C(H)C(H)C(H)Cl)S1)cc(N(=O)=O)cc2)C(H)C(H)Cl	3
4,503	ISSSTY_v1a_7367_02May011_6003	106532-71-2	C1(=NC(=O)c2cccc2)c2c(ccc(N(=O)=O)c2)N(C(=O)c2cccc2)S1	3
4,504	ISSSTY_v1a_7367_02May011_6004	106532-72-3	C1(=NC(=O)c2c(Cl)cccc2)c2c(ccc(N(=O)=O)c2)N(C(=O)c2c(Cl)cccc2)S1	3
4,505	ISSSTY_v1a_7367_02May011_6005	106532-73-4	C1(=NC(=O)c2cc(Cl)cccc2)c2c(ccc(N(=O)=O)c2)N(C(=O)c2cc(Cl)cccc2)S1	3
4,506	ISSSTY_v1a_7367_02May011_6006	106532-74-5	C1(=NC(=O)c2ccc(Cl)cc2)c2c(ccc(N(=O)=O)c2)N(C(=O)c2ccc(Cl)cc2)S1	3
4,507	ISSSTY_v1a_7367_02May011_6007	106532-75-6	C1(=NC(=O)c2cc(Cl)c(Cl)cc2)c2c(ccc(N(=O)=O)c2)N(C(=O)c2cc(Cl)c(Cl)cc2)S1	3
4,508	ISSSTY_v1a_7367_02May011_6008	106532-76-7	C1(=NC(=O)c2c([N+](=O)[O-])cccc2)c2c(ccc([N+](=O)[O-])c2)N(C(=O)c2c(N(=O)=O)cccc2)S1	3
4,509	ISSSTY_v1a_7367_02May011_6009	106532-77-8	C1(=NC(=O)c2cc([N+](=O)[O-])cccc2)c2c(ccc([N+](=O)[O-])c2)N(C(=O)c2cc([N+](=O)[O-])cccc2)S1	3
4,510	ISSSTY_v1a_7367_02May011_6010	106532-78-9	C1(=NC(=O)c2ccc([N+](=O)[O-])cc2)c2c(ccc([N+](=O)[O-])c2)N(C(=O)c2ccc([N+](=O)[O-])cc2)S1	3
4,511	ISSSTY_v1a_7367_02May011_6011	99601-31-7	HC(H)c1cnc2c(c3c(cc2)N(C(H)C(H)H)C(N)=N3)n1	3
4,512	ISSSTY_v1a_7367_02May011_6012	99601-30-6	HC(H)c1cnc2c3c(ccc2n1)N(C(H)C(H)H)C(N)=N3	3
4,513	ISSSTY_v1a_7367_02May011_6013	100-65-2	c1(NO)cccc1	3
4,514	ISSSTY_v1a_7367_02May011_6015	89837-94-5	HC(H)C(=O)C(H)N(C(H)OC(=O)C(H)H)N=O	3
4,515	ISSSTY_v1a_7367_02May011_6016	112725-15-2	HC(H)C(=O)C(N(C(H)H)N=O)OC(=O)C(H)H	3
4,516	ISSSTY_v1a_7367_02May011_6017	31464-26-3	HC(H)N(c1ccc(N=Nc2cccc2)cc1)C(H)C(H)C_N	3
4,517	ISSSTY_v1a_7367_02May011_6018	92911-19-8	HC(H)Nc1ccc(N=Nc2cc3c(cc2)N=CS3)cc1	3
4,518	ISSSTY_v1a_7367_02May011_6020	39720-27-9	HC(H)C(=O)Oc1ccc(C(H)Cl)cc1	3
4,519	ISSSTY_v1a_7367_02May011_6027	80556-89-4	HC(C(=O)O)N(C(H)C(H)O)N=O	3
4,520	ISSSTY_v1a_7367_02May011_6036	4450-68-4	HC(H)c1ccc(S(=O)(=O)OC(H)c2ccc(N(=O)=O)cc2)cc1	3
4,521	ISSSTY_v1a_7367_02May011_6039	61734-86-9	HC(H)C(H)C(H)C(H)C(H)N(C(H)C(H)C(H)C(H)O)N=O	3
4,522	ISSSTY_v1a_7367_02May011_6040	34424-65-2	HC(H)C(O)C=CC=O	3
4,523	ISSSTY_v1a_7367_02May011_6041	105453-63-2	c12c(c3c(C=C[C@](O)[C@@]3O)cc1)cc1c(c3c(cccc3)cc1)c2	3
4,524	ISSSTY_v1a_7367_02May011_6043	105453-65-4	c12c(c3c([C@](O)[C@@](O)C=C3)cc1)cc1c(c3c(cccc3)cc1)c2	3
4,525	ISSSTY_v1a_7367_02May011_6044	105453-64-3	c12c(c3c([C@](O)[C@@](O)C=C3)cc1)cc1c(c3c(cccc3)cc1)c2	3
4,526	ISSSTY_v1a_7367_02May011_6045	105453-66-5	c12-c3c([C@](O)[C@@](O)c1cc1c4c(ccc1c2)cccc4)cccc3	3
4,527	ISSSTY_v1a_7367_02May011_6046	105453-67-6	c12-c3c([C@](O)[C@@](O)c1cc1c4c(ccc1c2)cccc4)cccc3	3
4,528	ISSSTY_v1a_7367_02May011_6048	14953-62-9	c1(C2=C(N(=O)=O)N=CN2)cccc1	3
4,529	ISSSTY_v1a_7367_02May011_6049	14953-63-0	HC(H)N1C(N(=O)=O)=C(c2cccc2)N=C1	3
4,530	ISSSTY_v1a_7367_02May011_6050	111380-09-7	HC(H)N1C(c2cccc2)=C(N=O)N=C1	3

4,531	ISSSTY_v1a_7367_02May011_6051	106232-36-4	c1(C2=C(N=O)N=CN2)cccc1	3
4,532	ISSSTY_v1a_7367_02May011_6052	111380-08-6	HC(H)N1C(N=O)=C(c2cccc2)N=C1	3
4,533	ISSSTY_v1a_7367_02May011_6053	97055-38-4	HC(H)OC1C(C(Cl)Cl)=C(Cl)C(=O)O1	3
4,534	ISSSTY_v1a_7367_02May011_6057	111955-16-9	HC(H)c1ccc(NC2[C@@](O)[C@](O)[C@](O)C(H)O2)cc1	3
4,535	ISSSTY_v1a_7367_02May011_6058	3054-60-2	HC(H)c1ccc(NC2[C@](O)[C@@](O)[C@](O)C(H)O2)cc1	3
4,536	ISSSTY_v1a_7367_02May011_6059	111955-22-7	HC(C1c2c(cccc2)NC=1)C(H)NC1[C@](O)[C@@](O)[C@](O)C(H)O1	3
4,537	ISSSTY_v1a_7367_02May011_6060	111955-14-7	HC1[C@@](O)[C@@](O)[C@@](O)C(N(c2ccc(N(=O)=O)cc2)N=O)O1	3
4,538	ISSSTY_v1a_7367_02May011_6061	111955-18-1	HC1[C@@](O)[C@](O)[C@@](O)C(N(c2ccc(N(=O)=O)cc2)N=O)O1	3
4,539	ISSSTY_v1a_7367_02May011_6062	111955-21-6	HC1[C@@](O)[C@](O)[C@](O)C(N(c2ccc(N(=O)=O)cc2)N=O)O1	3
4,540	ISSSTY_v1a_7367_02May011_6063	111955-15-8	HC1[C@](O)[C@](O)[C@@](O)C(N(c2ccc(N(=O)=O)cc2)N=O)O1	3
4,541	ISSSTY_v1a_7367_02May011_6064	125369-76-8	HC(H)c1ccc(C(C_N)=CC=Cc2c(N(=O)=O)cccc2)cc1	3
4,542	ISSSTY_v1a_7367_02May011_6065	125369-77-9	HC(H)Oc1c(C=CC=C(c2ccc(Br)cc2)C_N)cccc1	3
4,543	ISSSTY_v1a_7367_02May011_6068	116208-67-4	c1(F)c2c3c(c4c(c3ccc2)cc2c(cccc2)c4)cc1	3
4,544	ISSSTY_v1a_7367_02May011_6069	113600-17-2	c12c3c(c4c(c3ccc1)cc1c(c(F)ccc1)c4)ccc2	3
4,545	ISSSTY_v1a_7367_02May011_6070	113600-15-0	c12c3c(c4c(c3ccc1)cc1c(cc(F)cc1)c4)ccc2	3
4,546	ISSSTY_v1a_7367_02May011_6071	112575-92-5	c12C3c4c(-c1cc1c(ccc1)c2)cccc4C(O)C(O)C=3	3
4,547	ISSSTY_v1a_7367_02May011_6072	112309-61-2	HC(H)C1=C(Cl)C(=O)OC1O	3
4,548	ISSSTY_v1a_7367_02May011_6073	88169-60-2	HC(H)OC(=O)[C@@](N)C(H)SC(H)C(H)Cl	3
4,549	ISSSTY_v1a_7367_02May011_6074	58337-49-8	HC(H)C(=O)N[C@](C(=O)O)C(H)SC(H)C(H)Cl	3
4,550	ISSSTY_v1a_7367_02May011_6075	75607-61-3	HC(C(=O)N(C(=O)[C@@](N)C(H)SC(H)C(H)Cl)C(H)C(=O)O)C(H)[C@](N)C(=O)O	3
4,551	ISSSTY_v1a_7367_02May011_6076	112575-91-4	C1(=O)C(=O)c2c3C(c4c(-c3ccc2)cc2c(cccc2)c4)=C1	3
4,552	ISSSTY_v1a_7367_02May011_6077	100310-95-0	c12c3c(c4c(c3ccc1)cc1c(C(O)C(O)C=C1)c4)ccc2	3
4,553	ISSSTY_v1a_7367_02May011_6078	106428-28-8	HC(H)[C@]1(C(=O)O)C(H)C(H)C(H)[C@]2(C(H)H)C3[C@@]4(C(=O)C(=CH)[C@](O)C(H)C3H)C4H)C(H)C(H)C12	3
4,554	ISSSTY_v1a_7367_02May011_6079	6957-71-7	HC1c2c(-c3c1cc(NC=O)cc3)cccc2	3
4,555	ISSSTY_v1a_7367_02May011_6080	3671-71-4	HC1c2c(-c3c1cc(N(O)C(=O)c1cccc1)cc3)cccc2	3
4,556	ISSSTY_v1a_7367_02May011_6082	61064-66-2	HC1c2c(-c3c1cc(NCl)cc3)cccc2	3
4,557	ISSSTY_v1a_7367_02May011_6084	7151-65-7	HC(H)C(=O)N(Cl)c1cc2c(-c3c(cccc3)C2H)cc1	3
4,558	ISSSTY_v1a_7367_02May011_6087	125974-06-3	HC(Cl)C1C(O)OC(=O)C=1	3
4,559	ISSSTY_v1a_7367_02May011_6088	125973-99-1	HC(Cl)C1C(H)OC(=O)C=1	3
4,560	ISSSTY_v1a_7367_02May011_6089	92433-40-4	HC(H)C(=O)Nc1c(Cl)cc2-c3c(C(H)c2c1)cccc3	3

4,561	ISSSTY_v1a_7367_02May011_6091	60129-60-4	HC(H)C1(C(=O)O)C(H)C(H)C(H)C2(C(H)H)C3C4(C(H)C(=CH)C(OC5C(O)C(O)C(O)C(C(H)O)O5)(C(H)C3H)C4H)C(H)C12	3
4,562	ISSSTY_v1a_7367_02May011_6092	107759-11-5	HC(H)C(H)OC(=O)N(C(c1ccnc1)C(H)C(H)C=O)N=O	3
4,563	ISSSTY_v1a_7367_02May011_6093	2085-88-3	HC(H)C1(c2ccccc2)C(H)O1	3
4,564	ISSSTY_v1a_7367_02May011_6095	1669-70-1	HC(H)C1(c2ccc(Cl)cc2)C(H)O1	3
4,565	ISSSTY_v1a_7367_02May011_6096	104953-00-6	HC(H)C1C(c2ccc(C_N)cc2)O1	3
4,566	ISSSTY_v1a_7367_02May011_6097	75590-19-1	HC(H)C1(c2ccc(N(=O)=O)cc2)C(H)O1	3
4,567	ISSSTY_v1a_7367_02May011_6099	98600-98-7	HC(H)c1c2c(c3c([C@](O)[C@@](O)C=C3)c1)cc1c(cccc1)c2	3
4,568	ISSSTY_v1a_7367_02May011_6100	64371-62-6	HC(H)C1(c2ccc(-c3ccccc3)cc2)C(H)O1	3
4,569	ISSSTY_v1a_7367_02May011_6101	98601-00-4	HC(H)c1c2c(c3c(cccc3)c1)cc1c([C@](O)[C@@](O)C=C1)c2	3
4,570	ISSSTY_v1a_7367_02May011_6102	98601-01-5	HC(H)c1c2c(c3c(cccc3)c1)cc1c(C=C[C@](O)[C@@]1O)c2	3
4,571	ISSSTY_v1a_7367_02May011_6103	78996-87-9	HC(H)c1c2c(c3c(c(O)ccc3)c1)cc1c(cccc1)c2	3
4,572	ISSSTY_v1a_7367_02May011_6104	98601-02-6	HC(H)c1c2c(c3c(c(O)ccc3)c1)cc1c(C=C(O)C(H)C1O)c2	3
4,573	ISSSTY_v1a_7367_02May011_6105	304-28-9	HC(H)C(=O)Nc1cc2c(-c3c(cc(NC(=O)C(H)H)cc3)C2H)cc1	3
4,574	ISSSTY_v1a_7367_02May011_6109	68395-77-7	HC(H)c1cc(C(H)H)cc(NO)c1	3
4,575	ISSSTY_v1a_7367_02May011_6110	39638-32-9	HC(H)C(Cl)(C(H)H)OC(Cl)(C(H)H)C(H)H	3
4,576	ISSSTY_v1a_7367_02May011_6112	81943-37-5	HC(H)C(=O)OC(H)N(c1cccc1)N=O	3
4,577	ISSSTY_v1a_7367_02May011_6114	430227	HC(H)c1ccc(N(C(H)C(H)O)C(H)C(H)O)cc1	3
4,578	ISSSTY_v1a_7367_02May011_6115	3671-78-1	HC1c2c(-c3c1cc(NC(=O)c1cccc1)cc3)cccc2	3
4,579	ISSSTY_v1a_7367_02May011_6120	99240-66-1	HC(H)C(=O)N(c1cc2c(-c3c(cccc3)C2H)cc1)C(H)C(H)H	3
4,580	ISSSTY_v1a_7367_02May011_6121	24225-71-6	HC(H)C(=O)N(c1cc2c(-c3c(cccc3)C2H)cc1)Nc1cc2c(-c3c(cccc3)C2H)cc1	3
4,581	ISSSTY_v1a_7367_02May011_6122	13177-32-7	c12c3c(c4c(c3ccc1)cc(N(=O)=O)cc4)ccc2	3
4,582	ISSSTY_v1a_7367_02May011_6123	81316-80-5	c1(N(=O)=O)c2c3c(c4c(c3ccc2)cc2c(cccc2)c4)cc1	3
4,583	ISSSTY_v1a_7367_02May011_6124	13177-28-1	c1(N(=O)=O)c2c3c(c4c2c(ccc4)cc1)cccc3	3
4,584	ISSSTY_v1a_7367_02May011_6125	10353-98-7	c1(N(=O)=O)c2c3c(C=O2)cccc3cc1	3
4,585	ISSSTY_v1a_7367_02May011_6126	10353-99-8	c1(N(=O)=O)c2c3c(C=Cc3ccc2)cc1	3
4,586	ISSSTY_v1a_7367_02May011_6127	13177-31-6	c1(N(=O)=O)c2c(c3c4c(cccc24)ccc3)ccc1	3
4,587	ISSSTY_v1a_7367_02May011_6128	3807-77-0	HC1c2c3c(c(N(=O)=O)ccc3ccc2)C1H	3
4,588	ISSSTY_v1a_7367_02May011_6129	75476-80-1	HC1c2c(C=C1)ccc(N(=O)=O)c2	3
4,589	ISSSTY_v1a_7367_02May011_6130	13132-28-0	C1(N(=O)=O)c2c3c(cccc3ccc2)C=1	3
4,590	ISSSTY_v1a_7367_02May011_6142	550-60-7	c1(O)c(N(=O)=O)c2c(cccc2)cc1	3

4,591	ISSSTY_v1a_7367_02May011_6144	496-14-0	HC1c2c(C(H)O1)cccc2	3
4,592	ISSSTY_v1a_7367_02May011_6145	542-88-1	HC(Cl)OC(H)Cl	3
4,593	ISSSTY_v1a_7367_02May011_6146	6281-23-8	C(=O)(O)C=CC1=CC=C(N(=O)=O)O1	3
4,594	ISSSTY_v1a_7367_02May011_6147	1874-24-4	HC(H)OC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4,595	ISSSTY_v1a_7367_02May011_6148	16339-05-2	HC(H)C(H)C(H)C(H)C(H)N(C(H)C(H)C(H)C(H)H)N=O	3
4,596	ISSSTY_v1a_7367_02May011_6149	1874-12-0	HC(H)C(H)OC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4,597	ISSSTY_v1a_7367_02May011_6150	90147-18-5	HC(H)C(H)C(H)OC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4,598	ISSSTY_v1a_7367_02May011_6151	90147-21-0	HC(H)C(C(H)H)OC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4,599	ISSSTY_v1a_7367_02May011_6152	90147-19-6	HC(H)C(H)C(H)C(H)OC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4,600	ISSSTY_v1a_7367_02May011_6153	91134-58-6	HC(H)C(C(H)H)C(H)OC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4,601	ISSSTY_v1a_7367_02May011_6154	97461-38-6	HC(H)C(H)C(C(H)H)OC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4,602	ISSSTY_v1a_7367_02May011_6155	97461-39-7	HC(H)C(C(H)H)(C(H)H)OC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4,603	ISSSTY_v1a_7367_02May011_6156	91642-47-6	HC(H)C(H)C(H)C(H)C(H)OC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4,604	ISSSTY_v1a_7367_02May011_6157	14308-65-7	HC(H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4,605	ISSSTY_v1a_7367_02May011_6158	6755-13-1	HC(H)N(C(=O)C=CC1=CC=C(N(=O)=O)O1)C(H)H	3
4,606	ISSSTY_v1a_7367_02May011_6159	6755-16-4	HC(H)C(H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4,607	ISSSTY_v1a_7367_02May011_6160	90147-31-2	HC(H)C(H)C(H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4,608	ISSSTY_v1a_7367_02May011_6161	91182-09-1	HC(H)C(H)C(H)C(H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4,609	ISSSTY_v1a_7367_02May011_6162	39965-42-9	HC(H)C(C(H)H)(C(H)H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4,610	ISSSTY_v1a_7367_02May011_6163	89811-25-6	HC(H)C(C(H)H)C(H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4,611	ISSSTY_v1a_7367_02May011_6164	97461-40-0	HC(H)C(H)C(C(H)H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4,612	ISSSTY_v1a_7367_02May011_6165	97461-41-1	HC(H)C(C(H)H)(C(H)H)C(H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4,613	ISSSTY_v1a_7367_02May011_6166	97461-42-2	HC(H)C(H)C(H)C(H)C(H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4,614	ISSSTY_v1a_7367_02May011_6167	68162-37-8	HC(H)OC(=O)C(=CC1=CC=C([N+](=O)[O-])O1)[N+](=O)[O-]	3
4,615	ISSSTY_v1a_7367_02May011_6170	836-37-3	HC(H)OC(=O)C(C_N)=CC1=CC=C(N(=O)=O)O1	3
4,616	ISSSTY_v1a_7367_02May011_6173	97461-43-3	HC(H)C(C(=O)OC(H)H)=CC1=CC=C(N(=O)=O)O1	3
4,617	ISSSTY_v1a_7367_02May011_6174	69527-46-4	C(_N)C(C_N)=CC1=CC=C(N(=O)=O)O1	3
4,618	ISSSTY_v1a_7367_02May011_6175	122349-91-1	HC(H)c1c2c(cc(N)c(C(H)H)c2)nc(C(H)H)c1	3
4,619	ISSSTY_v1a_7367_02May011_6176	830-07-9	C1(C=C[N+](=O)[O-])=CC=C([N+](=O)[O-])O1	3
4,620	ISSSTY_v1a_7367_02May011_6178	75995-58-3	HC(H)C(Br)C(=O)NC(H)c1cccc1	3

4,621	ISSSTY_v1a_7367_02May011_6179	131432-91-2	HC(H)[C@@](Br)C(=O)NC(H)c1cccc1	3
4,622	ISSSTY_v1a_7367_02May011_6180	131432-92-3	HC(H)[C@](Br)C(=O)NC(H)c1cccc1	3
4,623	ISSSTY_v1a_7367_02May011_6181	51938-21-7	HC(H)C(H)C(H)C(H)N(C(H)C(H)C(=O)OC(H)H)N=O	3
4,624	ISSSTY_v1a_7367_02May011_6182	142713-63-1	HC(H)C(Br)C(=O)NC(H)c1ccc(OC(H)H)cc1	3
4,625	ISSSTY_v1a_7367_02May011_6183	142713-64-2	HC(H)C(Br)C(=O)NC(H)c1cc(OC(H)H)c(O)cc1	3
4,626	ISSSTY_v1a_7367_02May011_6184	142713-65-3	HC(H)C(Br)C(=O)NC(H)c1cc(OC(H)H)c(OC(H)H)cc1	3
4,627	ISSSTY_v1a_7367_02May011_6189	535-11-5	HC(H)C(H)OC(=O)C(Br)C(H)H	3
4,628	ISSSTY_v1a_7367_02May011_6190	119613-62-6	HC(H)C(H)c1c2c(c3c(cccc3)c1)ccc1c2[C@@]2[C@]([C@](O)[C@@]1O)O2	3
4,629	ISSSTY_v1a_7367_02May011_6192	51938-14-8	HC(H)C(H)C(H)C(H)N(C(H)C(H)O)N=O	3
4,630	ISSSTY_v1a_7367_02May011_6193	80984-66-3	c12-c3c4C5C(c1cccc2C1C(c3ccc4)N1)N5	3
4,631	ISSSTY_v1a_7367_02May011_6194	55400-88-9	c12c(c3c4c5c(c6c(cc5cc3)O6)ccc4c1)O2	3
4,632	ISSSTY_v1a_7367_02May011_6195	80984-67-4	c12-c3c(C4C(c1cc1-c5c(C6C(c1c2)N6)cccc5)N4)cccc3	3
4,633	ISSSTY_v1a_7367_02May011_6196	55400-87-8	c12c(c3c(c4c1cc1c(C5C(=C6C=CC=CC16)O5)c4)cccc3)O2	3
4,634	ISSSTY_v1a_7367_02May011_6197	10227-50-6	HC1C(H)N(C2=NC=CS2)C(=O)N1	3
4,635	ISSSTY_v1a_7367_02May011_6198	95741-47-2	HC(H)c1c2c3c4c(c5c(c4cc2ccc1)cccc5)ccc3	3
4,636	ISSSTY_v1a_7367_02May011_6199	61734-89-2	HC(H)C(=O)C(H)C(H)N(C(H)C(H)C(H)C(H)H)N=O	3
4,637	ISSSTY_v1a_7367_02May011_6201	51938-15-9	HC(H)C(=O)C(H)N(C(H)C(H)C(H)C(H)H)N=O	3
4,638	ISSSTY_v1a_7367_02May011_6202	98033-25-1	HC(H)C1N(C(H)H)c2c(c3c4c(ccc(O)c4)ccc3cc2)N=1	3
4,639	ISSSTY_v1a_7367_02May011_6205	97851-14-4	c1(-c2cc([N+](=O)[O-])c(O)cc2)cc([N+](=O)[O-])ccc1	3
4,640	ISSSTY_v1a_7367_02May011_6209	4097-53-4	c1(-c2cc([N+](=O)[O-])c(O)c([N+](=O)[O-])c2)cccc1	3
4,641	ISSSTY_v1a_7367_02May011_6210	39482-21-8	HC(H)[Si](C(H)H)(C(H)H)C(H)N(C(N)=O)N=O	3
4,642	ISSSTY_v1a_7367_02May011_6211	5737-13-3	c12C(=O)c3c4c(ccc(c14)ccc2)ccc3	3
4,643	ISSSTY_v1a_7367_02May011_6212	98090-89-2	HC(H)c1c2c3c4c(C(H)c3cc1)cccc4cc2	3
4,644	ISSSTY_v1a_7367_02May011_6213	98096-09-4	HC(H)c1c2c3c(C(=O)c4c3c(ccc4)cc2)cc1	3
4,645	ISSSTY_v1a_7367_02May011_6215	19246-18-5	HC(C(=O)O)NC(=O)[C@@](N)C(H)S	3
4,646	ISSSTY_v1a_7367_02May011_6216	226-36-8	c12c(c3c(cc4c5c(ccc4n3)cccc5)cc1)cccc2	3
4,647	ISSSTY_v1a_7367_02May011_6217	61203-01-8	HC(H)C(=O)C(Br)=CH	3
4,648	ISSSTY_v1a_7367_02May011_6219	6325-54-8	HC(Cl)c1c2c(c3c(cccc3)cc2)cc2c1cccc2	3
4,649	ISSSTY_v1a_7367_02May011_6220	5166-35-8	HC(H)C(C(Cl)C(H)H)=CH	3
4,650	ISSSTY_v1a_7367_02May011_6222	19996-03-3	HC(Cl)c1c2c(c(Cl)c3c1cccc3)cccc2	3

4,651	ISSSTY_v1a_7367_02May011_6223	25148-26-9	HC(H)c1c2c(c(C(H)Cl)c3c1cccc3)cccc2	3
4,652	ISSSTY_v1a_7367_02May011_6225	113163-21-6	c12c(c3c([C@](O)[C@@](O)C=C3)cc1)nccc2	3
4,653	ISSSTY_v1a_7367_02May011_6226	28622-66-4	c12c(c3c(C(O)C(O)C=C3)cc1)cccc2	3
4,654	ISSSTY_v1a_7367_02May011_6230	113216-90-3	C1(O)C(=O)C2=C(C3=C4C(C=CC=13)=CC=CN4)O2	3
4,655	ISSSTY_v1a_7367_02May011_6231	113163-22-7	c12c(c3c(C(O)C(O)C4C3O4)cc1)nccc2	3
4,656	ISSSTY_v1a_7367_02May011_6233	115794-66-6	HC(H)OC(=O)[C@]1[C@@](c2ccccc2)O1	3
4,657	ISSSTY_v1a_7367_02May011_6234	119143-43-0	HC1c2c(c3c(cc2)nccc3)C2C(C1H)O2	3
4,658	ISSSTY_v1a_7367_02May011_6236	115794-67-7	HC(H)OC(=O)[C@@]1[C@](c2ccccc2)O1	3
4,659	ISSSTY_v1a_7367_02May011_6237	113163-24-9	HC1c2c(c3c(cccn3)cc2)C2C(C1H)O2	3
4,660	ISSSTY_v1a_7367_02May011_6239	115794-68-8	HC(H)OC(=O)[C@]1[C@](c2ccccc2)O1	3
4,661	ISSSTY_v1a_7367_02May011_6242	112380-30-0	HC(H)C(H)C(H)C(H)N(C(C=O)=NO)N=O	3
4,662	ISSSTY_v1a_7367_02May011_6243	38134-58-6	HC(C(=O)N[C@](C(=O)NC(H)C(=O)O)C(H)SC(=O)NC(H)C(H)Cl)C(H)[C@](N)C(=O)O	3
4,663	ISSSTY_v1a_7367_02May011_6245	53330-03-3	HC(Cl)C(H)NC(=O)OC(=O)[C@@](N)C(H)S	3
4,664	ISSSTY_v1a_7367_02May011_6248	689-98-5	HC(Cl)C(H)N	3
4,665	ISSSTY_v1a_7367_02May011_6249	74339-99-4	c12c(c3c4c(c5c(c4c4c(cccc4)c3)ccc(O)c5)c1)cccc2	3
4,666	ISSSTY_v1a_7367_02May011_6250	93285-74-6	HC1C2c3c4c(c5c(cc4c4c(cccc4)c3)cccc5)C=2C(H)C(H)C1H	3
4,667	ISSSTY_v1a_7367_02May011_6251	15299-08-8	HC(H)c1cc2c(c3c4c(c5c(cc24)cccc5)cc2c3cccc2)cc1	3
4,668	ISSSTY_v1a_7367_02May011_6252	60032-80-6	HC1c2c(c3c4c(c5c(cc4c4c3cccc4)cccc5)c2)C(H)C(H)C1H	3
4,669	ISSSTY_v1a_7367_02May011_6253	138-89-6	HC(H)N(c1ccc(N=O)cc1)C(H)H	3
4,670	ISSSTY_v1a_7367_02May011_6256	144730-01-8	HC1C(=O)c2c(c3c(c(C(F)(F)F)c2)c2c(cccc2)cc3)C1H	3
4,671	ISSSTY_v1a_7367_02May011_6257	151109-62-5	HC1C(=O)c2c(c3c(c(C(F)(F)F)c2)c2c([C@](O)[C@@](O)C=C2)cc3)C1H	3
4,672	ISSSTY_v1a_7367_02May011_6258	120-22-9	HC(H)C(H)N(c1ccc(N=O)cc1)C(H)C(H)H	3
4,673	ISSSTY_v1a_7367_02May011_6262	531-82-8	HC(H)C(=O)NC1=NC(C2=CC=C(N(=O)=O)O2)=CS1	3
4,674	ISSSTY_v1a_7367_02May011_6263	122-69-0	HC(C=Cc1cccc1)OC(=O)C=Cc1cccc1	3
4,675	ISSSTY_v1a_7367_02May011_6264	86-57-7	c1(N(=O)=O)c2c(cccc2)ccc1	3
4,676	ISSSTY_v1a_7367_02May011_6265	4437-51-8	HC(H)C(H)C(=O)C(=O)C(H)C(H)H	3
4,677	ISSSTY_v1a_7367_02May011_6266	765-87-7	HC1C(=O)C(=O)C(H)C(H)C1H	3
4,678	ISSSTY_v1a_7367_02May011_6271	100490-36-6	HC1C(H)C(N)C(H)N1c1c(F)cc2C(=O)C(C(=O)O)=CN(c3c(F)cc(F)cc3)c2n1	3
4,679	ISSSTY_v1a_7367_02May011_6272	35282-68-9	HC(H)N(c1ccc(N=Nc2c(C(H)O)cccc2)cc1)C(H)H	3
4,680	ISSSTY_v1a_7367_02May011_6277	6051-98-5	c12C(=O)c3c(c4c(cccc4)cc3)-c1cccc2	3

4,681	ISSSTY_v1a_7367_02May011_6278	149996-82-7	HC(H)C(H)N(C=O)N=O	3
4,682	ISSSTY_v1a_7367_02May011_6279	7417-67-6	HC(H)C(=O)N(C(H)H)N=O	3
4,683	ISSSTY_v1a_7367_02May011_6280	67809-14-7	HC(H)N(C=O)N=O	3
4,684	ISSSTY_v1a_7367_02May011_6281	70951-83-6	c12c(c3c(c4c([C@@]5[C@]([C@](O)[C@@]4O)O5)cc3)cc1)cccc2	3
4,685	ISSSTY_v1a_7367_02May011_6282	83830-70-0	c12c(c3c(c4c(C5C(C(O)C4O)O5)cc3)cc1)cccc2	3
4,686	ISSSTY_v1a_7367_02May011_6283	90421-79-7	HC1C(C(H)OC2c3c(cccc3)SN=2)O1	3
4,687	ISSSTY_v1a_7367_02May011_6284	60768-66-3	c12c(C=NS1)cc(N(=O)=O)cc2	3
4,688	ISSSTY_v1a_7367_02May011_6285	89641-97-4	c1(N(=O)=O)c2c(C=NS2)ccc1	3
4,689	ISSSTY_v1a_7367_02May011_6287	53473-85-1	c12c(C=NS1)cc(N)cc2	3
4,690	ISSSTY_v1a_7367_02May011_6288	89795-79-9	c1(N)c2c(C=NS2)ccc1	3
4,691	ISSSTY_v1a_7367_02May011_6289	76919-33-0	HC1C(C(H)Oc2cc3c(cc2)SN=C3)O1	3
4,692	ISSSTY_v1a_7367_02May011_6290	148193-29-7	HC1C(C(H)Oc2c3c(C=NS3)ccc2)O1	3
4,693	ISSSTY_v1a_7367_02May011_6291	30747-87-6	C1(Cl)c2c(ccc(N(=O)=O)c2)SN=1	3
4,694	ISSSTY_v1a_7367_02May011_6292	19331-27-2	C1(Cl)c2c(cc(N(=O)=O)cc2)SN=1	3
4,695	ISSSTY_v1a_7367_02May011_6293	720-69-4	c1(C2=CC=C(N(=O)=O)O2)nc(N)nc(N)n1	3
4,696	ISSSTY_v1a_7367_02May011_6294	41533-75-9	C1(Cl)c2c(c(N(=O)=O)ccc2)SN=1	3
4,697	ISSSTY_v1a_7367_02May011_6295	148193-30-0	C1(Cl)c2c(ccc(N)c2)SN=1	3
4,698	ISSSTY_v1a_7367_02May011_6296	148193-31-1	C1(Cl)c2c(c(N)ccc2)SN=1	3
4,699	ISSSTY_v1a_7367_02May011_6297	64099-26-9	HC(H)OC1c2c(ccc(N(=O)=O)c2)SN=1	3
4,700	ISSSTY_v1a_7367_02May011_6298	148193-32-2	HC(H)OC1c2c(cc(N(=O)=O)cc2)SN=1	3
4,701	ISSSTY_v1a_7367_02May011_6299	64099-25-8	HC(H)OC1c2c(c(N(=O)=O)ccc2)SN=1	3
4,702	ISSSTY_v1a_7367_02May011_6300	64099-28-1	HC(H)OC1c2c(ccc(N)c2)SN=1	3
4,703	ISSSTY_v1a_7367_02May011_6301	148193-33-3	HC(H)OC1c2c(cc(N)cc2)SN=1	3
4,704	ISSSTY_v1a_7367_02May011_6302	64099-27-0	HC(H)OC1c2c(c(N)ccc2)SN=1	3
4,705	ISSSTY_v1a_7367_02May011_6303	148193-34-4	HC(H)OC1c2c(ccc(OC(H)C3C(H)O3)c2)SN=1	3
4,706	ISSSTY_v1a_7367_02May011_6304	148193-35-5	HC(H)OC1c2c(cc(OC(H)C3C(H)O3)cc2)SN=1	3
4,707	ISSSTY_v1a_7367_02May011_6305	148193-36-6	HC(H)OC1c2c(c(OC(H)C3C(H)O3)ccc2)SN=1	3
4,708	ISSSTY_v1a_7367_02May011_6306	4337-51-3	C1(=O)c2c(cc(N(=O)=O)cc2)SN1	3
4,709	ISSSTY_v1a_7367_02May011_6307	817-99-2	HC(C(N)=O)NC(=O)C=[N+]=[N-]	3
4,710	ISSSTY_v1a_7367_02May011_6308	148193-38-8	HC1C(C(H)N2C(=O)c3c(cc(OC(H)C4C(H)O4)cc3)S2)O1	3

4,711	ISSSTY_v1a_7367_02May011_6309	110021-94-8	HC(H)S(=O)(=O)Nc1ccc(Nc2c3c(ccc(N=N_N)c3)nc3c2cccc3)cc1	3
4,712	ISSSTY_v1a_7367_02May011_6310	64894-90-2	HC(H)S(=O)(=O)Nc1ccc(Nc2c3c(cc(N=N_N)cc3)nc3c2cccc3)cc1	3
4,713	ISSSTY_v1a_7367_02May011_6312	110004-65-4	HC(H)S(=O)(=O)Nc1ccc(Nc2c3c(cc(N=N_N)cc3)nc3c2ccc(N=N_N)c3)cc1	3
4,714	ISSSTY_v1a_7367_02May011_6314	145531-23-3	HC(C(H)C(H)N)S(=O)(=O)Nc1ccc(Nc2c3c(cc(N=N_N)cc3)nc3c2ccc(N=N_N)c3)cc1	3
4,715	ISSSTY_v1a_7367_02May011_6315	145531-24-4	HC(H)Oc1c(Nc2c3c(ccc(N=N_N)c3)nc3c2cccc3)ccc(NS(=O)(=O)C(H)H)c1	3
4,716	ISSSTY_v1a_7367_02May011_6316	999-29-1	HC(H)C(H)OC(=O)C(H)NC(=O)C=[N+]=[N-]	3
4,717	ISSSTY_v1a_7367_02May011_6317	80266-02-0	HC(H)Oc1c(Nc2c3c(cc(N=N_N)cc3)nc3c2cccc3)ccc(NS(=O)(=O)C(H)H)c1	3
4,718	ISSSTY_v1a_7367_02May011_6318	110004-69-8	HC(H)c1c2c(c(Nc3c(OC(H)H)cc(NS(=O)(=O)C(H)H)cc3)c3c(cc(N=N_N)cc3)n2)ccc1	3
4,719	ISSSTY_v1a_7367_02May011_6319	64894-89-9	C(=O)(O)c1ccc(Nc2c3c(cc(N=N_N)cc3)nc3c2cccc3)cc1	3
4,720	ISSSTY_v1a_7367_02May011_6320	89873-24-5	c12c(c(Nc3ccc(N=N_N)cc3)c3c(cccc3)n1)cccc2	3
4,721	ISSSTY_v1a_7367_02May011_6321	14618-80-5	HC(c1cccc1)OC(H)[C@@]1C(H)O1	3
4,722	ISSSTY_v1a_7367_02May011_6322	16495-13-9	HC(c1cccc1)OC(H)[C@]1C(H)O1	3
4,723	ISSSTY_v1a_7367_02May011_6323	820-75-7	HC(C(=O)NN)NC(=O)C=[N+]=[N-]	3
4,724	ISSSTY_v1a_7367_02May011_6324	56715-28-7	HC1[C@](C(H)Oc2c3c(cccc3)ccc2)O1	3
4,725	ISSSTY_v1a_7367_02May011_6325	61249-00-1	HC1[C@@](C(H)Oc2c3c(cccc3)ccc2)O1	3
4,726	ISSSTY_v1a_7367_02May011_6326	115314-17-5	HC1[C@](C(H)OS(=O)(=O)c2cc(N(=O)=O)ccc2)O1	3
4,727	ISSSTY_v1a_7367_02May011_6327	115314-14-2	HC1[C@@](C(H)OS(=O)(=O)c2cc(N(=O)=O)ccc2)O1	3
4,728	ISSSTY_v1a_7367_02May011_6328	106268-95-5	HC1[C@@](C(H)OC(=O)c2ccc(N(=O)=O)cc2)O1	3
4,729	ISSSTY_v1a_7367_02May011_6329	115459-65-9	HC1[C@@](C(H)OC(=O)c2ccc(N(=O)=O)cc2)O1	3
4,730	ISSSTY_v1a_7367_02May011_6330	125279-81-4	HC1[C@](C(H)Oc2ccc(N(=O)=O)cc2)O1	3
4,731	ISSSTY_v1a_7367_02May011_6331	125279-82-5	HC1[C@@](C(H)Oc2ccc(N(=O)=O)cc2)O1	3
4,732	ISSSTY_v1a_7367_02May011_6332	92180-79-5	HC(H)c1c(C(H)H)nc2c(c3c(cc2)N(C(H)H)C(N)=N3)n1	3
4,733	ISSSTY_v1a_7367_02May011_6333	108354-48-9	HC(H)c1c2c(c3c(c1)nccn3)N=C(N)N2C(H)H	3
4,734	ISSSTY_v1a_7367_02May011_6334	97389-17-8	HC(H)c1c2c(c3c(c1)nc(C(H)H)cn3)N=C(N)N2C(H)H	3
4,735	ISSSTY_v1a_7367_02May011_6335	146177-57-3	HC(H)c1c2c(c3c(c1)N(C(H)H)C(N)=N3)nccn2	3
4,736	ISSSTY_v1a_7367_02May011_6336	103139-94-2	HC(H)c1c2c(c3c(c1)N(C(H)H)C(N)=N3)nc(C(H)H)cn2	3
4,737	ISSSTY_v1a_7367_02May011_6337	115609-71-7	HC(H)c1c2c(c3c(c1)N(C(H)H)C(N)=N3)ncc(C(H)H)n2	3
4,738	ISSSTY_v1a_7367_02May011_6338	146177-59-5	HC(H)c1c2c(c3c(c1C(H)H)N(C(H)H)C(N)=N3)nccn2	3
4,739	ISSSTY_v1a_7367_02May011_6339	95896-78-9	HC(H)c1c2c(c3c(c1)ncc(C(H)H)n3)N=C(N)N2C(H)H	3
4,740	ISSSTY_v1a_7367_02May011_6340	132898-07-8	HC(H)c1c2c(c3c(c1)nc(C(H)H)c(C(H)H)n3)N=C(N)N2C(H)H	3

4,741	ISSSTY_v1a_7367_02May011_6341	146177-58-4	HC(H)c1c2c(c3c(c1)N(C(H)H)C(N)=N3)nc(C(H)H)c(C(H)H)n2	3
4,742	ISSSTY_v1a_7367_02May011_6342	146177-60-8	HC(H)c1c2c(c3c(c1C(H)H)N(C(H)H)C(N)=N3)nc(C(H)H)cn2	3
4,743	ISSSTY_v1a_7367_02May011_6343	146177-61-9	HC(H)c1c2c(c3c(c1C(H)H)N(C(H)H)C(N)=N3)ncc(C(H)H)n2	3
4,744	ISSSTY_v1a_7367_02May011_6344	88193-04-8	HC(H)c1c2c(c3-c4c5c(c(C(H)H)cc4Nc3c1)cccc5)cccc2	3
4,745	ISSSTY_v1a_7367_02May011_6345	146177-64-2	HC(H)c1c2c(c3c(c1)N(C(H)H)C(N)=N3)nc(-c1cccc1)cn2	3
4,746	ISSSTY_v1a_7367_02May011_6346	146177-62-0	HC(H)c1c2c(c3c(c1C(H)H)N(C(H)H)C(N)=N3)nc(C(H)H)c(C(H)H)n2	3
4,747	ISSSTY_v1a_7367_02May011_6348	146177-65-3	HC(H)c1c2c(c3c(c1)N(C(H)H)C(N)=N3)ncc(-c1cccc1)n2	3
4,748	ISSSTY_v1a_7367_02May011_6349	101021-43-6	HC(H)c1cc2c(c3-c4c5c(ccc4Nc3cc2)cccc5)cc1	3
4,749	ISSSTY_v1a_7367_02May011_6350	145763-35-5	HC(H)C(C(=O)C12C(=O)N[C@](O)(C(H)C(H)O)[C@@]1O2)=CC=CC(C(H)H)=CC(C(H)H)=CC1C(=O)OC(H)C=1	3
4,750	ISSSTY_v1a_7367_02May011_6352	111901-42-9	HC(H)c1c2c(c3c([C@](O)[C@@](O)[C@@]4[C@@]3O4)c1)ccc1c2cccc1	3
4,751	ISSSTY_v1a_7367_02May011_6353	111901-40-7	HC(H)c1c2c(c3c(cccc3)c1)ccc1c2[C@@]2[C@]([C@](O)[C@@]1O)O2	3
4,752	ISSSTY_v1a_7367_02May011_6358	6850-22-2	HC(H)N1C=C2C(C=C(N(=O)=O)C=C2)=N1	3
4,753	ISSSTY_v1a_7367_02May011_6359	13436-58-3	HC(H)N1C=C2C(C(N(=O)=O)=O)=CC=C2)=N1	3
4,754	ISSSTY_v1a_7367_02May011_6360	6146-52-7	c12c(C=CN1)cc(N(=O)=O)cc2	3
4,755	ISSSTY_v1a_7367_02May011_6361	114460-38-7	HC(H)N1c2c3c4c(ccc(O)c4)ccc3ccc2C=C1	3
4,756	ISSSTY_v1a_7367_02May011_6362	5709-68-2	HC(H)N1c2c(cccc2)N=C1N(=O)=O	3
4,757	ISSSTY_v1a_7367_02May011_6363	7597-18-4	c12c(C=NN1)ccc(N(=O)=O)c2	3
4,758	ISSSTY_v1a_7367_02May011_6364	114460-39-8	HC(H)C1N(C(H)H)c2c3c4c(ccc(O)c4)ccc3ccc2N=1	3
4,759	ISSSTY_v1a_7367_02May011_6365	114460-40-1	HC(H)c1c2c(c3c(ccc(O)c3)cc2)c2c(c1)NC(C(H)H)=N2	3
4,760	ISSSTY_v1a_7367_02May011_6366	114460-41-2	HC(H)C(H)C1=Nc2c3c4c(ccc(O)c4)ccc3ccc2N1	3
4,761	ISSSTY_v1a_7367_02May011_6367	149922-82-7	C12C(c3c4C(=Cc5c4c(ccc5)cc3)C=1)=CC(Cl)C=C2	3
4,762	ISSSTY_v1a_7367_02May011_6368	10387-13-0	HC(Cl)c1c2c(c(C(H)Cl)c3c1cccc3)cccc2	3
4,763	ISSSTY_v1a_7367_02May011_6369	19727-83-4	HC1c2c(cc(N(=O)=O)cc2)NC1H	3
4,764	ISSSTY_v1a_7367_02May011_6370	32692-19-6	HC1c2c(ccc(N(=O)=O)c2)NC1H	3
4,765	ISSSTY_v1a_7367_02May011_6371	5709-67-1	c12c(cccc1)N=C(N(=O)=O)N2	3
4,766	ISSSTY_v1a_7367_02May011_6372	2942-42-9	c1(N(=O)=O)c2c(C=NN2)ccc1	3
4,767	ISSSTY_v1a_7367_02May011_6377	5381-79-3	HC(H)N1c2c(ccc(N(=O)=O)c2)N=C1	3
4,768	ISSSTY_v1a_7367_02May011_6378	136911-37-0	HC(H)N1C(H)C(H)N=N1	3
4,769	ISSSTY_v1a_7367_02May011_6379	17886-23-6	HC(H)C(H)N1C(H)C(H)N=N1	3
4,770	ISSSTY_v1a_7367_02May011_6380	17886-25-8	HC(c1cccc1)N1C(H)C(H)N=N1	3

4,771	ISSSTY_v1a_7367_02May011_6381	3585-32-8	HC(H)N=NNC(H)H	3
4,772	ISSSTY_v1a_7367_02May011_6382	63980-20-1	HC(H)C(H)N=NNC(H)C(H)H	3
4,773	ISSSTY_v1a_7367_02May011_6383	29814-12-8	HC(H)C(C(H)H)OC(=O)C(Cl)=C(Cl)C=O	3
4,774	ISSSTY_v1a_7367_02May011_6384	115044-41-2	HC(H)C1=CNC2c(c3c(cc2)N(C(H)H)C(N=O)=N3)N1	3
4,775	ISSSTY_v1a_7367_02May011_6385	108283-47-2	HC(H)C(C(H)H)(C(H)H)OC(=O)[C@@](N)C(H)N=N_N	3
4,776	ISSSTY_v1a_7367_02May011_6386	91897-48-2	HC(H)N1C(H)C(C(H)O)=C[C@@]2c3c4C(C(H)[C@]12)=CN(C(H)C=CH)c4ccc3	3
4,777	ISSSTY_v1a_7367_02May011_6387	87633-43-0	HC(H)N1c2c3C(C(H)[C@@]4C(c3ccc2)=C[C@@](C(H)OC(H)H)C(H)N4C(H)H)=C1	3
4,778	ISSSTY_v1a_7367_02May011_6388	18523-47-2	HC(C(=O)O)C(H)N=N_N	3
4,779	ISSSTY_v1a_7367_02May011_6389	569-26-6	HC(H)[C@]1C(H)[C@@]2c3c4C(C(H)[C@]2N(C(H)H)C1H)=CNc4ccc3	3
4,780	ISSSTY_v1a_7367_02May011_6390	129134-96-9	HC(H)[C@]1C(H)C2c3c4C(C(H)[C@]2N(C(H)H)C1H)=CN(C1C(H)C(H)C(H)C1H)c4ccc3	3
4,781	ISSSTY_v1a_7367_02May011_6392	98931-06-7	HC(H)C(H)C(H)N1c2c3C(C(H)[C@@]4C(c3ccc2)C(H)[C@@](C(H)H)C(H)N4C_N)=C1	3
4,782	ISSSTY_v1a_7367_02May011_6393	108283-49-4	HC(H)C(C(H)H)(C(H)H)OC(=O)N([C@](C(=O)O)C(H)H)N=N_N	3
4,783	ISSSTY_v1a_7367_02May011_6394	98931-07-8	HC(H)[C@]1C(H)C2c3c4C(C(H)[C@]2N(C_N)C1H)=CN(C(H)C=CH)c4ccc3	3
4,784	ISSSTY_v1a_7367_02May011_6395	52517-34-7	HC(H)N1C(H)[C@](C(H)Br)C(H)C2c3c4C(C(H)[C@]12)=CNc4ccc3	3
4,785	ISSSTY_v1a_7367_02May011_6396	108283-48-3	HC(H)C(C(H)H)(C(H)H)OC(=O)[C@](C(H)H)N(C(=O)OC(C(H)H)(C(H)H)C(H)H)N=N_N	3
4,786	ISSSTY_v1a_7367_02May011_6398	149127-58-2	HC(H)C(C(H)H)(N=NC(H)C(H)C(H)H)OO	3
4,787	ISSSTY_v1a_7367_02May011_6399	117135-59-8	HC(H)C(C(H)H)(N=NC(H)C(H)C(H)C(H)H)OO	3
4,788	ISSSTY_v1a_7367_02May011_6400	142628-08-8	HC([C@](N)C(=O)O)SC(F)(F)C(Cl)Br	3
4,789	ISSSTY_v1a_7367_02May011_6401	126637-65-8	HC([C@](N)C(=O)O)SC(F)(F)C(Br)Br	3
4,790	ISSSTY_v1a_7367_02May011_6402	153342-07-5	HC([C@](N)C(=O)O)SC(F)(F)C(F)Br	3
4,791	ISSSTY_v1a_7367_02May011_6409	153260-28-7	HC(H)C1(C(H)H)C2=C(c3c(C1H)nccc3)N=C(N)S2	3
4,792	ISSSTY_v1a_7367_02May011_6411	488-11-9	C(=O)(O)C(Br)=C(Br)C=O	3
4,793	ISSSTY_v1a_7367_02May011_6412	149418-41-7	HC1C(Br)=C(Br)C(=O)O1	3
4,794	ISSSTY_v1a_7367_02May011_6413	26049-69-4	HC(H)N(C(H)H)NC1=NC(C2=CC=C(N(=O)=O)O2)=CS1	3
4,795	ISSSTY_v1a_7367_02May011_6414	191-26-4	c12c3c4c5c6c(cc4ccc3ccc1)cccc6ccc5c2	3
4,796	ISSSTY_v1a_7367_02May011_6415	155014-05-4	c1(N)c2c(ccc1)ncc(F)c2	3
4,797	ISSSTY_v1a_7367_02May011_6416	155014-06-5	HC(H)C(=O)Nc1c2c(cc(F)cn2)ccc1	3
4,798	ISSSTY_v1a_7367_02May011_6417	147293-13-8	HC(H)N1c2c(c3c(cccn3)cc2)N=C1N	3
4,799	ISSSTY_v1a_7367_02May011_6418	147293-14-9	HC(H)N1c2c(c3c(ccnc3)cc2)N=C1N	3
4,800	ISSSTY_v1a_7367_02May011_6419	147293-15-0	HC(H)N1c2c(c3c(cc2)cncc3)N=C1N	3

4,801	ISSSTY_v1a_7367_02May011_6425	505-57-7	HC(H)C(H)C(H)C=CC=O	3
4,802	ISSSTY_v1a_7367_02May011_6426	20930-10-3	HC(H)C_CC(c1ccccc1)(c1ccccc1)OC(=O)NC1C(H)C(H)C(H)C(H)C1H	3
4,803	ISSSTY_v1a_7367_02May011_6427	10087-89-5	HC1C(H)C(H)C(H)C(H)C1NC(=O)OC(c1ccccc1)(c1ccccc1)C_C	3
4,804	ISSSTY_v1a_7367_02May011_6428	330-54-1	HC(H)N(C(=O)Nc1cc(Cl)c(Cl)cc1)C(H)H	3
4,805	ISSSTY_v1a_7367_02May011_6429	185-75-1	HC1C2(C(H)C(H)C(H)OC2H)O1	3
4,806	ISSSTY_v1a_7367_02May011_6433	215-62-3	c12c(c3c(c4c1cc1c(cccc1)n4)cccc3)cccc2	3
4,807	ISSSTY_v1a_7367_02May011_6434	1146-04-9	HC(H)C1C2(C(O)(C(H)H)C(=O)C3C=1C(O)C(C(H)H)(C(H)H)C=3)C(H)C2H	3
4,808	ISSSTY_v1a_7367_02May011_6435	1149-99-1	HC(H)C1C2(C(O)(C(H)H)C(=O)C3C=1C(O)C(C(H)H)(C(H)O)C=3)C(H)C2H	3
4,809	ISSSTY_v1a_7367_02May011_6436	224-53-3	c12c(c3c(cc4c(c5c(cccc5)cc4)n3)cc1)cccc2	3
4,810	ISSSTY_v1a_7367_02May011_6437	54897-63-1	HC(H)C(H)N(C(H)C(H)C(H)C(=O)O)N=O	3
4,811	ISSSTY_v1a_7367_02May011_6438	142762-84-3	HC(H)OC(=O)[C@@]1C(H)S[C@@]2C(Cl)=C(Cl)C(=O)N12	3
4,812	ISSSTY_v1a_7367_02May011_6439	152612-74-3	HC(H)OC(=O)[C@@]1C(H)S[C@@]2C(Cl)=C(Cl)C(=O)N12	3
4,813	ISSSTY_v1a_7367_02May011_6440	152612-73-2	HC(H)OC(=O)C1C(H)SC2C(Cl)=C(Cl)C(=O)N12	3
4,814	ISSSTY_v1a_7367_02May011_6441	54897-62-0	HC(H)C(H)N(C(H)C(H)C(H)C(H)O)N=O	3
4,815	ISSSTY_v1a_7367_02May011_6443	4559-64-2	c1(N)c(N)cc2c(c1)nc1c(cc(Cl)cc1)n2	3
4,816	ISSSTY_v1a_7367_02May011_6444	13147-25-6	HC(H)C(H)N(C(H)C(H)O)N=O	3
4,817	ISSSTY_v1a_7367_02May011_6445	5836-85-1	HC(H)Oc1c2c(c3c(C=O)C(H)C3H)c1)ccc1c2cccc1	3
4,818	ISSSTY_v1a_7367_02May011_6447	125239-64-7	HC(H)Oc1c(N)cc2c(c1)nc1c(cc(OC(H)H)c(N)c1)n2	3
4,819	ISSSTY_v1a_7367_02May011_6450	125239-65-8	HC(H)Oc1c(N)cc2c(c1)nc1c(ccc(N)c1)n2	3
4,820	ISSSTY_v1a_7367_02May011_6451	159714-85-9	HC(H)C(H)c1c2c3c(c4c(c2cc2c1cccc2)cccc4)O3	3
4,821	ISSSTY_v1a_7367_02May011_6452	159714-86-0	HC(H)C(H)c1c2c3c(c4c(c2cc2c1cccc2)cccc4)N3	3
4,822	ISSSTY_v1a_7367_02May011_6453	146683-80-9	HC(H)c1c2c(c3c(c4c2cc2c(cccc2)c4)O3)ccc1	3
4,823	ISSSTY_v1a_7367_02May011_6454	159714-84-8	HC(H)c1c2c(c3c(c4c2cc2c(cccc2)c4)N3)ccc1	3
4,824	ISSSTY_v1a_7367_02May011_6455	71382-46-2	HC(H)c1c2c(c(C(H)H)c3c4c(c5c(c13)cccc5)N4)cccc2	3
4,825	ISSSTY_v1a_7367_02May011_6456	39834-38-3	HC(H)c1c2-c3c(C4C(c2c(C(H)H)c2c1cccc2)O4)cccc3	3
4,826	ISSSTY_v1a_7367_02May011_6457	109527-10-8	HC(H)C(=O)O[C@@]1C(H)OC(Nc2ccc(N(=O)=O)cc2)[C@](OC(=O)C(H)H)[C@]1OC(=O)C(H)H	3
4,827	ISSSTY_v1a_7367_02May011_6459	111858-64-1	HC1[C@@](O)[C@@](O)[C@](O)C(N(c2ccc(C(=O)O)cc2)N=O)O1	3
4,828	ISSSTY_v1a_7367_02May011_6460	111858-68-5	HC(H)c1ccc(N(C(H)C2(O)[C@@](O)[C@](O)[C@](O)C(H)O2)N=O)cc1	3
4,829	ISSSTY_v1a_7367_02May011_6461	145667-72-7	HC(Br)[C@](Br)C(H)Cl	3
4,830	ISSSTY_v1a_7367_02May011_6462	145667-73-8	HC(Br)[C@@](Br)C(H)Cl	3

4,831	ISSSTY_v1a_7367_02May011_6463	111858-66-3	HC(C1c2c(cccc2)NC=1)C(H)N(C1[C@](O)[C@@](O)[C@](O)C(H)O1)N=O	3
4,832	ISSSTY_v1a_7367_02May011_6466	163401-68-1	HC(H)C(H)C(H)C(Cl)C(=O)S	3
4,833	ISSSTY_v1a_7367_02May011_6467	125157-97-3	HC(H)C1c2c(c(C(H)H)ccc2)N(C(H)H)C2C=1c1c(cccc1)N=2	3
4,834	ISSSTY_v1a_7367_02May011_6468	55738-54-0	HC(H)N(C(H)H)C=NC1=NN=C(C=CC2=CC=C(N(=O)=O)O2)O1	3
4,835	ISSSTY_v1a_7367_02May011_6469	1516-74-1	c12c(cccc1)N=C(N=N_N)N2	3
4,836	ISSSTY_v1a_7367_02May011_6470	1516-73-0	HC(H)N1c2c(cccc2)N=C1N=N_N	3
4,837	ISSSTY_v1a_7367_02May011_6473	126420-92-6	HC(c1ccc(F)cc1)N1C2c3c(-c4c(cccc4)C12)cccc3	3
4,838	ISSSTY_v1a_7367_02May011_6474	126370-96-5	HC(c1ccc(Cl)cc1)N1C2c3c(-c4c(cccc4)C12)cccc3	3
4,839	ISSSTY_v1a_7367_02May011_6475	126420-93-7	HC(c1ccc(Br)cc1)N1C2c3c(-c4c(cccc4)C12)cccc3	3
4,840	ISSSTY_v1a_7367_02May011_6476	126370-97-6	HC(c1c(C(F)(F)F)ccc1)N1C2c3c(-c4c(cccc4)C12)cccc3	3
4,841	ISSSTY_v1a_7367_02May011_6477	126420-94-8	HC(H)c1ccc(C(H)N2C3c4c(-c5c(cccc5)C23)cccc4)cc1	3
4,842	ISSSTY_v1a_7367_02May011_6478	126370-98-7	HC(H)Oc1cc(C(H)N2C3c4c(-c5c(cccc5)C23)cccc4)ccc1	3
4,843	ISSSTY_v1a_7367_02May011_6479	160543-14-6	HC(H)c1c2c(c3c([C@](O)[C@@](O)C=C3)cc2)nc2c1cc(C(H)O)cc2	3
4,844	ISSSTY_v1a_7367_02May011_6480	126370-99-8	HC(H)Oc1ccc(C(H)N2C3c4c(-c5c(cccc5)C23)cccc4)cc1	3
4,845	ISSSTY_v1a_7367_02May011_6481	160543-15-7	HC(H)c1cc2c(C(H)O)c3c(c4c([C@](O)[C@@](O)C=C4)cc3)nc2cc1	3
4,846	ISSSTY_v1a_7367_02May011_6483	126420-95-9	HC(H)c1c(C(H)N2C3c4c(-c5c(cccc5)C23)cccc4)c(C(H)H)cc(C(H)H)c1	3
4,847	ISSSTY_v1a_7367_02May011_6484	160637-28-5	HC(H)c1c2c(c3c([C@](O)[C@@](O)C=C3)cc2)nc2c1cc(C(H)H)cc2	3
4,848	ISSSTY_v1a_7367_02May011_6486	126371-00-4	HC(c1ccc(N(=O)=O)cc1)N1C2c3c(-c4c(cccc4)C12)cccc3	3
4,849	ISSSTY_v1a_7367_02May011_6487	160543-00-0	HC(H)c1cc2c(C(H)O)c3c(c4c(cccc4)cc3)nc2cc1	3
4,850	ISSSTY_v1a_7367_02May011_6488	160543-02-2	HC(H)c1c2c(c3c(cccc3)cc2)nc2c1cc(C(H)O)cc2	3
4,851	ISSSTY_v1a_7367_02May011_6489	160543-04-4	HC(O)c1c2c(c3c(cccc3)cc2)nc2c1cc(C(H)O)cc2	3
4,852	ISSSTY_v1a_7367_02May011_6490	160637-30-9	HC(H)c1c2c(c3c([C@](O)[C@@](O)C=C3)cc2)nc2c1ccc(C(H)H)c2	3
4,853	ISSSTY_v1a_7367_02May011_6491	160637-29-6	HC(H)c1c2c(c3c(cccc3)cc2)nc2c1[C@](O)[C@@](O)C(C(H)H)=C2	3
4,854	ISSSTY_v1a_7367_02May011_6493	160543-08-8	HC(H)c1c2c(c3c(cccc3)cc2)nc2c1ccc(C(H)O)c2	3
4,855	ISSSTY_v1a_7367_02May011_6496	394-70-7	c1(F)c2c(cccc2)ncc1	3
4,856	ISSSTY_v1a_7367_02May011_6498	57-74-9	HC1C2C3(Cl)C(Cl)(Cl)C(Cl)(C(Cl)=C3Cl)C2C(Cl)C1Cl	3
4,857	ISSSTY_v1a_7367_02May011_6499	95741-57-4	HC(H)c1cc2c3c(c4c(c3ccc2)cc2c(cccc2)c4)c1	3
4,858	ISSSTY_v1a_7367_02May011_6500	95741-56-3	HC(H)c1c2c(c(C(H)H)c3c4c5c(c13)cccc5ccc4)cccc2	3
4,859	ISSSTY_v1a_7367_02May011_6501	32818-80-7	HC(H)N(C(H)O)N(=O)=O	3
4,860	ISSSTY_v1a_7367_02May011_6502	36239-01-7	HC(H)C(=O)OC(H)N(C(H)H)N(=O)=O	3

4,861	ISSSTY_v1a_7367_02May011_6503	157996-62-8	c12c(c(N)c3c(ccc([N+](=O)[O-])c3)n1)cc([N+](=O)[O-])cc2	3
4,862	ISSSTY_v1a_7367_02May011_6504	790-60-3	c12c(c3c(c4c1cc1c(ccc1)c4)cccc3)O2	3
4,863	ISSSTY_v1a_7367_02May011_6505	1193-54-0	C1(=O)C(CI)=C(CI)C(=O)N1	3
4,864	ISSSTY_v1a_7367_02May011_6506	170660-62-5	HC1C(=C(CI)CI)C(=O)NC1=O	3
4,865	ISSSTY_v1a_7367_02May011_6507	170660-63-6	C1(=O)C(=C(CI)CI)C(CI)C(=O)N1	3
4,866	ISSSTY_v1a_7367_02May011_6509	28342-33-8	HC(H)N1C(=O)c2c(-c3c1c1c(cc4c(c1)OC(H)O4)cc3)ccc(OC(H)H)c2OC(H)H	3
4,867	ISSSTY_v1a_7367_02May011_6510	816-57-9	HC(H)C(H)C(H)N(C(N)=O)N=O	3
4,868	ISSSTY_v1a_7367_02May011_6512	7132-67-4	c12c(c(N)c3c(ccc(O)c3)n1)cccc2	3
4,869	ISSSTY_v1a_7367_02May011_6513	15444-20-9	HC(H)Oc1c2-c3c(C(=O)c4c2c(cc1OC(H)H)ccn4)cccc3	3
4,870	ISSSTY_v1a_7367_02May011_6514	70403-81-5	HC(H)Oc1c2-c3c(C(=O)c4c2c(cc1OC(H)H)ccn4)cc(OC(H)H)cc3	3
4,871	ISSSTY_v1a_7367_02May011_6515	88741-67-7	HC(H)Oc1c(O)c2C(=O)c3c(-c4c2c(ccn4)c1)cc(OC(H)H)cc3	3
4,872	ISSSTY_v1a_7367_02May011_6516	88741-68-8	HC(H)Oc1c2C(=O)c3c(-c4c2c(cc1OC(H)H)ccn4)cc(OC(H)H)cc3	3
4,873	ISSSTY_v1a_7367_02May011_6522	72100-19-7	c12c(c3c(c4c1cc1c(c(O)c(O)cc1)c4)cccc3)cccc2	3
4,874	ISSSTY_v1a_7367_02May011_6523	132172-57-7	c1(O)c(O)c2c(c3c(c4c2cc2c(ccc2)c4)cccc3)cc1	3
4,875	ISSSTY_v1a_7367_02May011_6524	132172-58-8	c1(O)c(O)c2c(c3c(c4c2cccc4)cc2c(ccc2)c3)cc1	3
4,876	ISSSTY_v1a_7367_02May011_6525	88488-97-5	c12c(c3c(c4c1cc1c(ccc1)c4)ccc(O)c3)cccc2	3
4,877	ISSSTY_v1a_7367_02May011_6526	113058-38-1	c12c(c3c(c4c1cc1c(ccc1)c4)cc(O)cc3)cccc2	3
4,878	ISSSTY_v1a_7367_02May011_6528	113058-39-2	c1(O)c2c(c3c(c4c2cccc4)cc2c(ccc2)c3)ccc1	3
4,879	ISSSTY_v1a_7367_02May011_6529	39081-15-7	c12c(c3c(c4c1cc1c(c(O)ccc1)c4)cccc3)cccc2	3
4,880	ISSSTY_v1a_7367_02May011_6530	39147-43-8	c12c(c3c(c4c1cc1c(cc(O)cc1)c4)cccc3)cccc2	3
4,881	ISSSTY_v1a_7367_02May011_6531	132172-56-6	c12c(c3c(c4c1C=CC=CO4)cccc3)cc1c(ccc1)c2	3
4,882	ISSSTY_v1a_7367_02May011_6532	117022-35-2	HC(H)c1c2c(c3c(c4c(C(O)C(O)C5C4O5)cc3)c(C(H)H)c2)ccc1	3
4,883	ISSSTY_v1a_7367_02May011_6533	129176-04-1	HC(Br)[C@]1[C@](Cl)O1	3
4,884	ISSSTY_v1a_7367_02May011_6534	129176-05-2	HC(Br)C1C(Cl)O1	3
4,885	ISSSTY_v1a_7367_02May011_6535	90745-27-0	HC(H)c1c2c(N(=O)=O)cccc2ccc1	3
4,886	ISSSTY_v1a_7367_02May011_6536	54755-21-4	HC(H)c1cc2c(N(=O)=O)cccc2cc1	3
4,887	ISSSTY_v1a_7367_02May011_6537	13615-38-8	HC(H)c1cc2c(N(=O)=O)cccc2cc1	3
4,888	ISSSTY_v1a_7367_02May011_6538	91137-27-8	HC(H)c1c2c(c(N(=O)=O)ccc2)ccc1	3
4,889	ISSSTY_v1a_7367_02May011_6539	1951-56-0	HC(H)C(C(H)H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4,890	ISSSTY_v1a_7367_02May011_6540	54755-20-3	HC(H)c1cc2c(c(N(=O)=O)ccc2)cc1	3

4,891	ISSSTY_v1a_7367_02May011_6541	880-93-3	HC(H)c1c2c(c(N(=O)=O)cc1)cccc2	3
4,892	ISSSTY_v1a_7367_02May011_6543	105752-67-8	HC(H)c1c2c(cc(N(=O)=O)cc2)ccc1	3
4,893	ISSSTY_v1a_7367_02May011_6544	63017-87-8	HC(H)c1c2c(ccc1N(=O)=O)cccc2	3
4,894	ISSSTY_v1a_7367_02May011_6545	41037-13-2	HC(H)c1c2c(cc(N(=O)=O)c1)cccc2	3
4,895	ISSSTY_v1a_7367_02May011_6546	116530-07-5	HC(H)c1c2c(ccc(N(=O)=O)c2)ccc1	3
4,896	ISSSTY_v1a_7367_02May011_6547	91137-28-9	HC(H)c1cc2c(ccc(N(=O)=O)c2)cc1	3
4,897	ISSSTY_v1a_7367_02May011_6548	54357-08-3	HC(H)c1cc2c(cc(N(=O)=O)cc2)cc1	3
4,898	ISSSTY_v1a_7367_02May011_6552	19655-56-2	HC(H)C(H)c1c2c(cccn2)ccc1	3
4,899	ISSSTY_v1a_7367_02May011_6553	134109-03-8	c12c(c(Cl)c3c(c4c([C@](O)[C@@](O)C=C4)cc3)c1)cccc2	3
4,900	ISSSTY_v1a_7367_02May011_6554	35509-27-4	C(N)c1c2c(cccn2)ccc1	3
4,901	ISSSTY_v1a_7367_02May011_6558	60657-25-2	c12c3c4c(c5c(C=C[C@](O)[C@]5O)cc4ccc3ccc1)cc2	3
4,902	ISSSTY_v1a_7367_02May011_6561	32795-84-9	c12c(c(Br)c3c(c4c(cccc4)cc3)c1)cccc2	3
4,903	ISSSTY_v1a_7367_02May011_6563	94339-56-7	HC1c2c(c3c4c5c(ccc4c2)cccc5cc3)C=CC1O	3
4,904	ISSSTY_v1a_7367_02May011_6564	94339-55-6	HC1C(O)c2c(c3c4c5c(ccc4c2)cccc5cc3)C=C1	3
4,905	ISSSTY_v1a_7367_02May011_6565	199536-62-4	HC(Br)C1=C(Br)C(=O)OC1H	3
4,906	ISSSTY_v1a_7367_02May011_6567	199536-64-6	HC(Br)C1=C(Br)C(=O)OC1O	3
4,907	ISSSTY_v1a_7367_02May011_6568	199536-79-3	HC1C(C(Br)Br)=C(Br)C(=O)O1	3
4,908	ISSSTY_v1a_7367_02May011_6569	199536-82-8	HC1C(C(Br)Br)=C(Cl)C(=O)O1	3
4,909	ISSSTY_v1a_7367_02May011_6570	199536-84-0	HC(Cl)C1=C(Br)C(=O)OC1H	3
4,910	ISSSTY_v1a_7367_02May011_6571	199536-65-7	HC(Br)C1=C(Cl)C(=O)OC1H	3
4,911	ISSSTY_v1a_7367_02May011_6573	230-46-6	c12c(c3c(cccn3)cc1)ccn2	3
4,912	ISSSTY_v1a_7367_02May011_6574	191861-16-2	c1(F)c2c(c3c(cccn3)c1)ccn2	3
4,913	ISSSTY_v1a_7367_02May011_6575	191861-17-3	c12c(c3c(cccn3)cc1)cc(F)cn2	3
4,914	ISSSTY_v1a_7367_02May011_6577	191861-19-5	c1(F)c2c(c3c(cccn3)c1)nccc2	3
4,915	ISSSTY_v1a_7367_02May011_6579	163275-58-9	c1(F)c2c(c3c(cccc3)c1)nccc2	3
4,916	ISSSTY_v1a_7367_02May011_6580	163275-59-0	c1(F)c2c(c3c(cccn3)c1)cccc2	3
4,917	ISSSTY_v1a_7367_02May011_6581	163275-60-3	c1(F)c2c(c3c(cccn3)cc2)ccc1	3
4,918	ISSSTY_v1a_7367_02May011_6582	163275-61-4	c12c(c3c(ccc(F)c3)cc1)nccc2	3
4,919	ISSSTY_v1a_7367_02May011_6584	163275-64-7	c12c(c3c(c(F)ccc3F)cc1)nccc2	3
4,920	ISSSTY_v1a_7367_02May011_6585	163275-65-8	c12c(c3c(cccc3)cc1)cc(F)cn2	3

4,921	ISSSTY_v1a_7367_02May011_6586	163275-66-9	c12c(c3c(c(F)ccc3)cc1)cccn2	3
4,922	ISSSTY_v1a_7367_02May011_6587	163275-67-0	c1(F)c2c3c(ccc2ccc1)nccc3	3
4,923	ISSSTY_v1a_7367_02May011_6588	163275-68-1	c12c(c3c(c(F)ccc3F)cc1)cccn2	3
4,924	ISSSTY_v1a_7367_02May011_6589	88492-34-6	HC(C(O)C(H)N1c2c(c(N)ncn2)N=C1)N=N_N	3
4,925	ISSSTY_v1a_7367_02May011_6590	87009-12-9	C1(=O)C=CNC(=O)N1	3
4,926	ISSSTY_v1a_7367_02May011_6591	133762-80-8	HC(H)C1C(=O)NC(=O)N(C(H)C(O)C(H)N=N_N)C=1	3
4,927	ISSSTY_v1a_7367_02May011_6593	66927-03-5	HC([C@@](O)[C@](O)[C@](O)[C@@](O)C=O)N=N_N	3
4,928	ISSSTY_v1a_7367_02May011_6594	20847-05-6	HC([C@@](O)[C@@](O)[C@](O)[C@@](O)C=O)N=N_N	3
4,929	ISSSTY_v1a_7367_02May011_6595	2381-39-7	HC(H)c1c2c(c3c4c5c(ccc14)cccc5cc3)cccc2	3
4,930	ISSSTY_v1a_7367_02May011_6596	117333-21-8	HC(C1c2c(cccc2)N(N=O)C=1)C(O)C(=O)O	3
4,931	ISSSTY_v1a_7367_02May011_6598	7068-83-9	HC(H)C(H)C(H)C(H)N(C(H)H)N=O	3
4,932	ISSSTY_v1a_7367_02May011_6599	13088-34-1	C(Cl)(Cl)=C1C=CC(=O)O1	3
4,933	ISSSTY_v1a_7367_02May011_6600	112654-68-9	C1(=O)C(Cl)=CC(=C(Cl)Cl)O1	3
4,934	ISSSTY_v1a_7367_02May011_6601	31555-54-1	C1(=O)C(Cl)=C(Cl)C(=C(Cl)Cl)O1	3
4,935	ISSSTY_v1a_7367_02May011_6602	101328-96-5	C1(=O)C(Cl)(Cl)C(=O)C=C1	3
4,936	ISSSTY_v1a_7367_02May011_6603	61445-55-4	HC(H)N(C(H)C(H)C(H)C(=O)O)N=O	3
4,937	ISSSTY_v1a_7367_02May011_6604	88552-47-0	C1(=O)C(Cl)(Cl)C(=O)C(Cl)=C1	3
4,938	ISSSTY_v1a_7367_02May011_6609	202345-21-9	HC(H)c1c(NO)nc2c(-c3c(cccc3)N2)c1	3
4,939	ISSSTY_v1a_7367_02May011_6610	23045-12-7	HC(H)c1cc2c(N)c3c(cccc3)nc2cc1	3
4,940	ISSSTY_v1a_7367_02May011_6611	194479-75-9	HC(H)c1cc2c(N)c3c(ccc(C(H)H)c3)nc2cc1	3
4,941	ISSSTY_v1a_7367_02May011_6612	23250-39-7	c12c(c(N)c3c(ccc(Cl)c3)n1)cccc2	3
4,942	ISSSTY_v1a_7367_02May011_6613	157996-59-3	c12c(c(N)c3c(ccc(Br)c3)n1)cccc2	3
4,943	ISSSTY_v1a_7367_02May011_6614	194479-79-3	c12c(c(N)c3c(ccc(I)c3)n1)cccc2	3
4,944	ISSSTY_v1a_7367_02May011_6616	55090-44-3	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)N(C(H)H)N=O	3
4,945	ISSSTY_v1a_7367_02May011_6619	97170-07-5	HC(H)c1c2c(c3c(cccc3)c1)ccc1c2[C@]2[C@@]([C@@](O)[C@@]1O)O2	3
4,946	ISSSTY_v1a_7367_02May011_6621	7258-52-8	HC1c2c(c3c4c(ccc3cc2)cccc4)C(H)C1H	3
4,947	ISSSTY_v1a_7367_02May011_6622	183249-37-8	HC1c2c(c3c4c(ccc3cc2)cccc4)C=C1	3
4,948	ISSSTY_v1a_7367_02May011_6624	212-54-4	HC1c2c(-c3c1c1c4c(ccc1cc3)cccc4)cccc2	3
4,949	ISSSTY_v1a_7367_02May011_6628	611-35-8	c1(Cl)c2c(cccc2)ncc1	3
4,950	ISSSTY_v1a_7367_02May011_6630	635-27-8	c1(Cl)c2c(ccc1)nccc2	3

4,951	ISSSTY_v1a_7367_02May011_6631	612-57-7	c12c(cc(Cl)cc1)cccn2	3
4,952	ISSSTY_v1a_7367_02May011_6633	622-79-7	HC(c1ccccc1)N=N_N	3
4,953	ISSSTY_v1a_7367_02May011_6635	51938-16-0	HC(H)N(C(H)C(H)C(H)C(H)O)N=O	3
4,954	ISSSTY_v1a_7367_02May011_6636	173216-43-8	HC(H)[C@@](c1ccccc1)C(H)C(H)N=N_N	3
4,955	ISSSTY_v1a_7367_02May011_6637	173216-44-9	HC(C(H)C(c1ccccc1)c1ccccc1)N=N_N	3
4,956	ISSSTY_v1a_7367_02May011_6638	134625-72-2	HC([C@](O)c1ccccc1)N=N_N	3
4,957	ISSSTY_v1a_7367_02May011_6639	124817-06-7	HC([C@@](O)c1ccccc1)N=N_N	3
4,958	ISSSTY_v1a_7367_02May011_6640	173216-45-0	HC(c1ccccc1)[C@](C(H)N=N_N)C(H)O	3
4,959	ISSSTY_v1a_7367_02May011_6641	173216-46-1	HC(c1ccccc1)[C@@](C(H)N=N_N)C(H)O	3
4,960	ISSSTY_v1a_7367_02May011_6642	84506-41-2	HC(H)[C@@](C(=O)OC(H)H)C(H)N=N_N	3
4,961	ISSSTY_v1a_7367_02May011_6643	107747-84-2	HC(H)[C@](C(=O)OC(H)H)C(H)N=N_N	3
4,962	ISSSTY_v1a_7367_02May011_6644	121745-57-1	HC(O)[C@](O)[C@@](c1ccccc1)N=N_N	3
4,963	ISSSTY_v1a_7367_02May011_6645	116911-14-9	HC(O)[C@@](O)[C@](c1ccccc1)N=N_N	3
4,964	ISSSTY_v1a_7367_02May011_6646	6367-36-8	HC(H)C(C(H)H)(C(H)H)OC(=O)C(H)N=N_N	3
4,965	ISSSTY_v1a_7367_02May011_6647	134874-62-7	c1([N+](=O)[O-])c2c3c(c4c(c5c3c(ccc5)cc2)cccc4)c([N+](=O)[O-])c1	3
4,966	ISSSTY_v1a_7367_02May011_6648	120014-85-9	HC1c2c3c4c5c(c(N(=O)=O)ccc5ccc4cc2C(O)C(H)C1H)cc3	3
4,967	ISSSTY_v1a_7367_02May011_6649	134998-76-8	HC1c2c(c3c4c5c(c(N=O)ccc5cc3)ccc4c2)C(H)C(H)C1H	3
4,968	ISSSTY_v1a_7367_02May011_6650	67616-44-8	HC(C(H)O)SN=O	3
4,969	ISSSTY_v1a_7367_02May011_6652	115-02-6	HC(C(N)C(=O)O)OC(=O)C=[N+]=[N-]	3
4,970	ISSSTY_v1a_7367_02May011_6653	21638-36-8	HC(H)C1C(H)N(N=CC2=CC=C(N(=O)=O)O2)C(=O)N1	3
4,971	ISSSTY_v1a_7367_02May011_6654	89930-59-6	HC(H)C1C(H)N(C(H)H)[C@@]2C(H)C3c4c(cccc4[C@]2C=1)N(C(H)C(H)C(H)H)C=3	3
4,972	ISSSTY_v1a_7367_02May011_6655	53757-29-2	HC(H)C1=NC(C2=CC=C(N(=O)=O)O2)=CS1	3
4,973	ISSSTY_v1a_7367_02May011_6656	101328-75-0	HC(H)C1C(H)N(C(H)H)[C@@]2C(H)C3c4c(cccc4[C@]2C=1)N(C(H)C(H)C(H)C(H)H)C=3	3
4,974	ISSSTY_v1a_7367_02May011_6657	82617-23-0	HC1C(OC(N)=O)O1	3
4,975	ISSSTY_v1a_7367_02May011_6658	239-35-0	c12-c3c(c4c(cccc4)cc3)Sc1cccc2	3
4,976	ISSSTY_v1a_7367_02May011_6662	92078-92-7	HC(H)NN=O	3
4,977	ISSSTY_v1a_7367_02May011_6665	333-27-7	HC(H)OS(=O)(=O)C(F)(F)F	3
4,978	ISSSTY_v1a_7367_02May011_6670	184582-64-7	HC(H)C(=O)NSc1c2c(ccc(O)c2)nc2c1cc(O)cc2	3
4,979	ISSSTY_v1a_7367_02May011_6671	29700-20-7	HC(O)C1=CC=C(c2c3c(-c4c(cccc4)N3)ccn2)O1	3
4,980	ISSSTY_v1a_7367_02May011_6673	66267-19-4	c12c(c3c([C@@](O)[C@](O)C=C3)cc1)cc1c(c3c(cccc3)cc1)c2	3

4,981	ISSSTY_v1a_7367_02May011_6676	28657-80-9	HC(H)C(H)N1c2c(C(=O)C(C(=O)O)=N1)cc1c(c2)OC(H)O1	3
4,982	ISSSTY_v1a_7367_02May011_6677	70458-92-3	HC(H)C(H)N1c2c(C(=O)C(C(=O)O)=C1)cc(F)c(N1C(H)C(H)N(C(H)H)C(H)C1H)c2	3
4,983	ISSSTY_v1a_7367_02May011_6678	125369-79-1	C(N)C(c1c(Cl)cccc1)=CC=Cc1cccc1	3
4,984	ISSSTY_v1a_7367_02May011_6679	155144-64-2	HC(H)c1cc(-c2c(F)cc3c(c2)N(C2C(H)C2H)C2=CC(=O)N(O)C(=O)N32)cc(C(H)H)n1	3
4,985	ISSSTY_v1a_7367_02May011_6680	115550-35-1	HC(H)N1C(H)C(H)N(c2c3c4c(C(=O)C(C(=O)O)=CN4N(C(H)H)C(H)O3)cc2F)C(H)C1H	3
4,986	ISSSTY_v1a_7367_02May011_6681	103978-08-1	HC(H)C(H)N1c2c(C(=O)C(C(=O)O)=C1)cc(F)c(-c1ccc(O)cc1)c2F	3
4,987	ISSSTY_v1a_7367_02May011_6682	93106-60-6	HC(H)C(H)N1C(H)C(H)N(c2c(F)cc3C(=O)C(C(=O)O)=CN(C4C(H)C4H)c3c2)C(H)C1H	3
4,988	ISSSTY_v1a_7367_02May011_6685	42286-46-4	c12C(=O)C(=O)c3c4c(c5c(cccc5)c3)ccc(c14)ccc2	3
4,989	ISSSTY_v1a_7367_02May011_6686	34522-72-0	c1(F)c2c(cc(F)c1)nccc2	3
4,990	ISSSTY_v1a_7367_02May011_6694	139347-89-0	HC(H)c1c2c(c3c(c4c(C(O)C(O)C5C4O5)cc3)c1C(H)H)cccc2	3
4,991	ISSSTY_v1a_7367_02May011_6695	139627-44-4	HC(H)c1c2c(c3c(c4c(C(O)C(O)C5C4O5)cc3)c(C(H)H)c2)ccc1	3
4,992	ISSSTY_v1a_7367_02May011_6696	91540-29-3	HC(H)C(H)C(H)C(H)C(H)N1C2c3c(-c4c(cccc4)C12)cccc3	3
4,993	ISSSTY_v1a_7367_02May011_6697	139493-54-2	HC(H)c1c2c(c3c(ccc(C(H)H)c3)c1)ccc1c2[C@@]2[C@]([C@](O)[C@@]1O)O2	3
4,994	ISSSTY_v1a_7367_02May011_6698	81593-13-7	HC(H)C(H)OP(=O)(N1C2c3c(-c4c(cccc4)C12)cccc3)OC(H)C(H)H	3
4,995	ISSSTY_v1a_7367_02May011_6699	106686-67-3	HC(c1cccc1)S(=O)(=O)N1C2c3c(-c4c(cccc4)C12)cccc3	3
4,996	ISSSTY_v1a_7367_02May011_6702	8004-87-3	HC(H)N(c1ccc([C+](c2ccc(N(C(H)H)C(H)H)cc2)c2ccc(NC(H)H)cc2)cc1)C(H)H	3
4,997	ISSSTY_v1a_7367_02May011_6703	128753-82-2	HC(H)C12C(OC(H)H)(c3c(cccc3)O1)OO2	3
4,998	ISSSTY_v1a_7367_02May011_6704	128753-83-3	HC(H)C12c3c(cccc3)OC1OO2	3
4,999	ISSSTY_v1a_7367_02May011_6705	772-43-0	C(N)(C1=CC=C(N(=O)=O)O1)=NO	3
5,000	ISSSTY_v1a_7367_02May011_6706	128753-86-6	HC(H)C12C(C(H)H)(c3c(c(C(=O)C(H)H)ccc3)O1)OO2	3
5,001	ISSSTY_v1a_7367_02May011_6707	128753-87-7	HC(H)C12C(C(H)H)(c3c(cccc3OC(H)H)O1)OO2	3
5,002	ISSSTY_v1a_7367_02May011_6708	128753-88-8	HC(H)C12C(C(H)H)(c3c(c(OC(H)H)ccc3)O1)OO2	3
5,003	ISSSTY_v1a_7367_02May011_6709	128753-90-2	HC(H)C12C(C(H)H)(c3c(cc(OC(=O)C(H)H)cc3)O1)OO2	3
5,004	ISSSTY_v1a_7367_02May011_6711	128753-91-3	HC(H)C12C(C(H)H)(c3c(ccc(OC(=O)C(H)H)c3)O1)OO2	3
5,005	ISSSTY_v1a_7367_02May011_6714	128753-95-7	HC(H)C12c3c(cccc3)OC1(C(H)OC(H)H)OO2	3
5,006	ISSSTY_v1a_7367_02May011_6715	128753-96-8	HC(H)C12c3c(cccc3)OC1(C(H)OC(=O)C(H)H)OO2	3
5,007	ISSSTY_v1a_7367_02May011_6716	128753-99-1	HC(H)C12c3c(cccc3)OC1(C(H)OC(=O)Nc1ccc(Cl)cc1)OO2	3
5,008	ISSSTY_v1a_7367_02May011_6717	129812-24-4	HC(H)C12C(C(H)H)(c3c(cc4c(C(C(H)H)=CC(=O)O4)c3)O1)OO2	3
5,009	ISSSTY_v1a_7367_02May011_6718	129833-00-7	HC(H)C12C(C(H)H)(c3c(c4c(C(C(H)H)=CC(=O)O4)cc3)O1)OO2	3
5,010	ISSSTY_v1a_7367_02May011_6719	2578-75-8	HC(H)C(=O)NC1=NN=C(C2=CC=C(N(=O)=O)O2)S1	3

5,011	ISSSTY_v1a_7367_02May011_6720	129812-26-6	HC(H)C12C(C(H)H)(c3c4C(C(H)H)=CC(=O)Oc4ccc3O1)OO2	3
5,012	ISSSTY_v1a_7367_02May011_6725	710-25-8	C(N)(=O)C=CC1=CC=C(N(=O)=O)O1	3
5,013	ISSSTY_v1a_7367_02May011_6726	3675-13-6	C(=O)C=CC=O	3
5,014	ISSSTY_v1a_7367_02May011_6729	53757-28-1	C1(C2=CC=C(N(=O)=O)O2)=CSC=N1	3
5,015	ISSSTY_v1a_7367_02May011_6732	220042-15-9	C1(C2C(=O)C=C(Nc3ccc(N(=O)=O)cc3)C(=O)C=2)=NN=C(NC(=O)c2cccc2)S1	3
5,016	ISSSTY_v1a_7367_02May011_6734	128350-00-5	HC(H)C(C(c1cccc1)C(c1cc(Cl)c(Cl)cc1)C_N)C=C(c1cc(Cl)c(Cl)cc1)C_N	3
5,017	ISSSTY_v1a_7367_02May011_6735	1390-65-4	HC(H)c1c2C(=O)c3c(C(=O)c2cc(O)c1C(=O)O)c(O)c(O)c(C1C(O)C(O)C(O)C(C(H)O)O1)c3O	3
5,018	ISSSTY_v1a_7367_02May011_6736	3741-15-9	c1(N(=O)=O)c2c(cccc2)ncc1	3
5,019	ISSSTY_v1a_7367_02May011_6738	125847-46-3	c12-c3c(c4c([C@@](O)[C@](O)C=C4)cc3)Sc1cccc2	3
5,020	ISSSTY_v1a_7367_02May011_6742	96563-10-9	HC(H)C1c2c(-c3c1cc(F)cc3)ccc(F)c2	3
5,021	ISSSTY_v1a_7367_02May011_6743	2523-37-7	HC(H)C1c2c(-c3c1cccc3)cccc2	3
5,022	ISSSTY_v1a_7367_02May011_6744	96563-11-0	HC(H)C1c2c(-c3c1cc(F)cc3)cccc2	3
5,023	ISSSTY_v1a_7367_02May011_6745	504-78-9	HC1C(H)[N+](H)C(H)S1	3
5,024	ISSSTY_v1a_7367_02May011_6746	102234-07-1	HC1C2(C(=O)N(C(H)C(H)N3C(H)C3H)C(=O)N2)C(H)C(H)C(H)C1H	3
5,025	ISSSTY_v1a_7367_02May011_6749	923-32-0	HC(C(N)C(=O)O)SSC(H)C(N)C(=O)O	3
5,026	ISSSTY_v1a_7367_02May011_6750	70-54-2	HC(N)C(H)C(H)C(H)C(N)C(=O)O	3
5,027	ISSSTY_v1a_7367_02May011_6752	609-36-9	HC1C(H)C(H)C(C(=O)O)N1	3
5,028	ISSSTY_v1a_7367_02May011_6753	80-68-2	HC(H)C(O)C(N)C(=O)O	3
5,029	ISSSTY_v1a_7367_02May011_6758	141691-42-1	HC(H)N1c2c(ccc(C_N)c2)N=C1N	3
5,030	ISSSTY_v1a_7367_02May011_6759	139953-95-0	HC(H)C(H)C(H)OC=CC=CC=CC=CC=CC(H)C(H)H	3
5,031	ISSSTY_v1a_7367_02May011_6760	225366-91-6	c1(F)c(F)c2c(cc1)nccc2	3
5,032	ISSSTY_v1a_7367_02May011_6761	1234799	HC(H)C1C(C(O)=C2C(=O)C(=O)N(C(H)c3ccnc3)C2c2ccc(Cl)cc2)=C(C(H)H)NC=1C(=O)OC(H)C(H)H	3
5,033	ISSSTY_v1a_7367_02May011_6762	139953-97-2	HC(H)C(H)C=CC=CC=CC=CC=COC(H)C(O)C(H)H	3
5,034	ISSSTY_v1a_7367_02May011_6763	145241-76-5	c1(F)c(F)c2c(ccn2)cc1	3
5,035	ISSSTY_v1a_7367_02May011_6764	139953-98-3	HC(H)C(H)C=CC=CC=CC=CC=COC(H)C(O)c1cccc1	3
5,036	ISSSTY_v1a_7367_02May011_6765	139259-93-1	HC(H)C(c1ccc(C(H)ON(C(=O)c2cccc2)OC(=O)C(H)H)cc1)(C(H)H)C(H)H	3
5,037	ISSSTY_v1a_7367_02May011_6766	220168-39-8	HC(c1cccc1)ON(C(=O)c1cccc1)OC(=O)c1cccc1	3
5,038	ISSSTY_v1a_7367_02May011_6768	145241-75-4	c1(F)c2c(cc(F)c1)cccn2	3
5,039	ISSSTY_v1a_7367_02May011_6769	1234712	c1(F)c(F)c(F)c(F)c2c1cccn2	3
5,040	ISSSTY_v1a_7367_02May011_6770	220168-56-9	HC(H)C(c1ccc(C(=O)ON(C(=O)c2cccc2)OC(H)c2cccc2)cc1)(C(H)H)C(H)H	3