

2,101	ISSSTY_v1a_7367_02May011_2605	67910-07-0	HC(H)C(C(H)H)C(H)C(=O)OC(H)C1C2C(C(O)=CC=2)=COC=1	3
2,102	ISSSTY_v1a_7367_02May011_2608	1121-55-7	HC=Cc1cccnc1	1
2,103	ISSSTY_v1a_7367_02May011_2609	83463-62-1	C(N)C(Cl)Br	3
2,104	ISSSTY_v1a_7367_02May011_2610	138580-44-6	HC(H)c1c2-c3c(ccccc3)Nc2c2C(=O)C=CC(=O)c2n1	3
2,105	ISSSTY_v1a_7367_02May011_2611	138580-46-8	HC(H)C1C(=O)c2c(C(=O)C=1)nc(C(H)H)c1-c3c(ccccc3)Nc21	3
2,106	ISSSTY_v1a_7367_02May011_2612	5694-00-8	HC1C(C(N)=O)O1	3
2,107	ISSSTY_v1a_7367_02May011_2614	138580-48-0	HC(H)c1c2-c3c(ccccc3)Nc2c2C(=O)C(N3C(H)C(H)N(C(H)H)C(H)C3H)=CC(=O)c2n1	3
2,108	ISSSTY_v1a_7367_02May011_2615	87406-72-2	HC1C(C(H)N(C(=O)C=CH)C(H)C2C(H)O2)O1	3
2,109	ISSSTY_v1a_7367_02May011_2616	73-24-5	c1(N)c2c(N=CN2)ncn1	3
2,110	ISSSTY_v1a_7367_02May011_2617	1845-30-3	HC(H)C1(C(H)H)[C@]2C(C(H)H)=C[C@@](O)[C@@]1C2H	1
2,111	ISSSTY_v1a_7367_02May011_2618	65071-98-9	HC(H)C(=O)OC(H)C(H)O	1
2,112	ISSSTY_v1a_7367_02May011_2619	57471-01-9	HC(H)C(=O)c1c(OC(H)C(O)C(H)NC(C(H)H)(C(H)H)C(H)H)ccc(N(C(C(H)H)(C(H)H)C(H)H)C(N)=O)c1	1
2,113	ISSSTY_v1a_7367_02May011_2620	2541-69-7	HC(H)c1c2c(c3c(ccccc3)cc2)cc2c1cccc2	3
2,114	ISSSTY_v1a_7367_02May011_2621	24305-27-9	HC(C1=CN=CN1)[C@](C(=O)N1C(H)C(H)C(H)[C@@]1C(N)=O)NC(=O)[C@]1C(H)C(H)C(=O)N1	1
2,115	ISSSTY_v1a_7367_02May011_2622	1456-55-9	HC(H)[C@]12C(=O)N3[C@@](C(=O)N1C(H)H)([C@](O)[C@@]1(O)c4c(c(OC(H)H)c(OC(H)H)c(Cl)c4)N(C(H)H)[C@@]31)SS2	1
2,116	ISSSTY_v1a_7367_02May011_2624	24424-99-5	HC(H)C(C(H)H)(C(H)H)OC(=O)OC(=O)OC(C(H)H)(C(H)H)C(H)H	1
2,117	ISSSTY_v1a_7367_02May011_2626	1928-38-7	HC(H)OC(=O)C(H)Oc1c(Cl)cc(Cl)cc1	1
2,118	ISSSTY_v1a_7367_02May011_2627	101901-07-9	HC(H)C(H)c1c2c(C3=C(C(C(H)C(=O)OC(H)C(H)H)OC(H)C3H)N2)ccc1O	3
2,119	ISSSTY_v1a_7367_02May011_2628	101901-08-0	HC(H)C(H)OC(=O)C(H)C1C2=C(c3c(c(C(O)C(H)H)ccc3)N2)C(H)C(H)O1	1
2,120	ISSSTY_v1a_7367_02May011_2629	41340-36-7	HC(H)C(H)c1c2c(C(C(H)C(H)O)=CN2)ccc1	1
2,121	ISSSTY_v1a_7367_02May011_2630	115066-03-0	HC(H)C1(C(H)C(H)H)C2=C(c3c(c(C(H)C(H)H)ccc3)N2)C(H)C(H)O1	1
2,122	ISSSTY_v1a_7367_02May011_2631	41340-19-6	HC(H)c1c2c(C3=C(C(C(H)C(=O)OC(H)C(H)H)OC(H)C3H)N2)ccc1	1
2,123	ISSSTY_v1a_7367_02May011_2632	135086-99-6	C1(N)c2c(cccc2)NC=1C(=O)NN=Cc1cccc1	1
2,124	ISSSTY_v1a_7367_02May011_2633	21096	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(=O)O	1
2,125	ISSSTY_v1a_7367_02May011_2634	959-98-8	HC1[C@@]2C3(Cl)C(Cl)(Cl)[C@](Cl)(C(Cl)=C3Cl)[C@@]2C(H)OS(=O)O1	1
2,126	ISSSTY_v1a_7367_02May011_2635	2517-43-3	HC(H)C(C(H)C(H)O)OC(H)H	1
2,127	ISSSTY_v1a_7367_02May011_2637	92134-93-5	HC1C(H)N(N=O)C(C(H)O)S1	3
2,128	ISSSTY_v1a_7367_02May011_2638	92134-95-7	HC(H)C(O)C(O)C(O)C(O)C1N(N=O)C(H)C(H)S1	1
2,129	ISSSTY_v1a_7367_02May011_2639	75-37-6	HC(H)C(F)F	1
2,130	ISSSTY_v1a_7367_02May011_2640	92134-97-9	HC1C(C(=O)O)N(N=O)C(C(O)C(O)C(O)C(O)C(H)O)S1	1

2,131	ISSSTY_v1a_7367_02May011_2641	526-73-8	HC(H)c1c(C(H)H)c(C(H)H)ccc1	3
2,132	ISSSTY_v1a_7367_02May011_2642	108-67-8	HC(H)c1cc(C(H)H)cc(C(H)H)c1	1
2,133	ISSSTY_v1a_7367_02May011_2643	76-14-2	C(F)(F)(Cl)C(F)(F)Cl	1
2,134	ISSSTY_v1a_7367_02May011_2644	84736-60-7	c1(N(=O)=O)ccc(N(O)C=O)cc1	3
2,135	ISSSTY_v1a_7367_02May011_2645	125-46-2	HC(H)C(=O)c1c2c(C3(C(H)H)C(=O)C(C(=O)C(H)H)C(=O)C=C3O2)c(O)c(C(H)H)c1O	1
2,136	ISSSTY_v1a_7367_02May011_2646	90689-60-4	HC(H)c1c2C(=O)Oc3c(C(C(H)H)c(C(=O)O)c(O)c3C(H)OC(=O)C(H)H)Oc2c(C=O)c(O)c1	3
2,137	ISSSTY_v1a_7367_02May011_2647	122-88-3	HC(C(=O)O)Oc1ccc(Cl)cc1	1
2,138	ISSSTY_v1a_7367_02May011_2648	27113-22-0	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(=O)C(H)C(H)c1cc(OC(H)H)c(O)cc1	1
2,139	ISSSTY_v1a_7367_02May011_2650	33089-61-1	HC(H)c1c(N=CN(C(H)H)C=Nc2c(C(H)H)cc(C(H)H)cc2)ccc(C(H)H)c1	1
2,140	ISSSTY_v1a_7367_02May011_2652	4435-53-4	HC(H)C(=O)OC(H)C(H)C(C(H)H)OC(H)H	1
2,141	ISSSTY_v1a_7367_02May011_2653	4189-44-0	C(=N)(N)S(=O)[O-]	3
2,142	ISSSTY_v1a_7367_02May011_2654	84-60-6	c12C(=O)c3c(C(=O)c1cc(O)cc2)ccc(O)c3	1
2,143	ISSSTY_v1a_7367_02May011_2655	577-33-3	c1(O)c(O)c2c(c(O)c3c(cccc3)c2)cc1	3
2,144	ISSSTY_v1a_7367_02May011_2656	13593-03-8	HC(H)C(H)OP(=S)(Oc1cnc2c(cccc2)n1)OC(H)C(H)H	1
2,145	ISSSTY_v1a_7367_02May011_2657	81-61-8	c12C(=O)c3c(C(=O)c1c(O)c(O)cc2)c(O)ccc3O	3
2,146	ISSSTY_v1a_7367_02May011_2658	28932-22-1	C1(=O)c2c(C(=O)C3C(O)=CC=C(O)C13)c(O)ccc2O	3
2,147	ISSSTY_v1a_7367_02May011_2659	68641-49-6	HC1C(H)N(P(=O)(Cl)N2C(=O)OC(H)C2H)C(=O)O1	3
2,148	ISSSTY_v1a_7367_02May011_2660	116-85-8	c12C(=O)c3c(C(=O)c1c(O)ccc2N)cccc3	3
2,149	ISSSTY_v1a_7367_02May011_2662	68884-32-2	HC(c1c2c(cccc2)ccc1)C1C(H)O1	3
2,150	ISSSTY_v1a_7367_02May011_2663	7774-68-7	HC(Cl)C(Cl)C(H)OC(H)C(Cl)C(H)Cl	3
2,151	ISSSTY_v1a_7367_02May011_2666	155164-54-8	HC(H)C(H)S(=O)(=O)N1C(=O)C(Cl)=C(Cl)C=N1	3
2,152	ISSSTY_v1a_7367_02May011_2667	100986-86-5	HC(H)[C@]1C(H)Oc2c3c(C(=O)C(C(=O)O)=CN13)cc(F)c2N1C(H)C(H)N(C(H)H)C(H)C1H	1
2,153	ISSSTY_v1a_7367_02May011_2669	155164-57-1	C1(=O)C(Cl)=C(Cl)C=NN1S(=O)(=O)c1cccc1	1
2,154	ISSSTY_v1a_7367_02May011_2670	155164-62-8	C1(=O)C(Cl)=C(Cl)C=NN1S(=O)(=O)c1c(Cl)cc(Cl)cc1	1
2,155	ISSSTY_v1a_7367_02May011_2671	155164-64-0	HC(H)C(H)C(=O)N1C(=O)C(Cl)=C(Cl)C=N1	1
2,156	ISSSTY_v1a_7367_02May011_2672	155164-61-7	C1(=O)C(Cl)=C(Cl)C=NN1S(=O)(=O)c1ccc(N(=O)=O)cc1	3
2,157	ISSSTY_v1a_7367_02May011_2673	155164-66-2	C1(=O)C(Cl)=C(Cl)C=NN1C(=O)c1cccc1	1
2,158	ISSSTY_v1a_7367_02May011_2674	155164-60-6	C1(=O)C(Cl)=C(Cl)C=NN1S(=O)(=O)c1ccc(Cl)cc1	1
2,159	ISSSTY_v1a_7367_02May011_2675	1918-00-9	HC(H)Oc1c(C(=O)O)c(Cl)ccc1Cl	1
2,160	ISSSTY_v1a_7367_02May011_2677	155164-59-3	HC(H)Oc1ccc(S(=O)(=O)N2C(=O)C(Cl)=C(Cl)C=N2)cc1	1

2,161	ISSSTY_v1a_7367_02May011_2678	135086-97-4	C1(=O)C2C(c3c(cccc3)N=2)=NNN1N	3
2,162	ISSSTY_v1a_7367_02May011_2679	610-39-9	HC(H)c1cc([N+](=O)[O-])c([N+](=O)[O-])cc1	3
2,163	ISSSTY_v1a_7367_02May011_2680	7440-66-6	[Zn]	1
2,164	ISSSTY_v1a_7367_02May011_2683	1918-13-4	C(N)(=S)c1c(Cl)cccc1Cl	3
2,165	ISSSTY_v1a_7367_02May011_2687	38363-40-5	HC(H)C(C(H)H)(C(H)H)NC(H)[C@@](O)C(H)Oc1c(C2C(H)C(H)C(H)C2H)cccc1	3
2,166	ISSSTY_v1a_7367_02May011_2688	87625-62-5	HC(H)c1c2([C@](O)(C(H)H)[C@@]3C(OC4[C@](O)[C@@](O)[C@@](O)(C(H)O)O4)(C(H)[C@@](C(H)H)C3=O)C=1)(C(H)C2H)	3
2,167	ISSSTY_v1a_7367_02May011_2689	109-16-0	HC(H)C(C(=O)OC(H)C(H)OC(H)C(H)OC(H)C(H)OC(=O)C(C(H)H)=CH)=CH	1
2,168	ISSSTY_v1a_7367_02May011_2690	72869-86-4	HC(H)C(C(=O)OC(H)C(H)OC(=O)NC(H)C(H)H)(C(H)H)C(H)C(H)C(H)C(H)NC(=O)OC(H)C(H)OC(=O)C(C(H)H)=CH)=CH	1
2,169	ISSSTY_v1a_7367_02May011_2691	1565-94-2	HC(H)C(c1ccc(OC(H)C(O)C(H)OC(=O)C(C(H)H)=CH)cc1)(c1ccc(OC(H)C(O)C(H)OC(=O)C(C(H)H)=CH)cc1)C(H)H	1
2,170	ISSSTY_v1a_7367_02May011_2692	86780-90-7	HC(H)C1=C(C(=O)OC(H)H)C(c2c(N(=O)=O)cccc2)C(C(=O)OC(H)C(=O)C(H)H)=C(C(H)H)N1	1
2,171	ISSSTY_v1a_7367_02May011_2693	62613-82-5	HC1C(=O)N(C(H)C(N)=O)C(H)C1O	1
2,172	ISSSTY_v1a_7367_02May011_2694	88-69-7	HC(H)C(c1c(O)cccc1)C(H)H	1
2,173	ISSSTY_v1a_7367_02May011_2695	120-23-0	HC(C(=O)O)Oc1cc2c(cccc2)cc1	1
2,174	ISSSTY_v1a_7367_02May011_2697	35470	c1(N)c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
2,175	ISSSTY_v1a_7367_02May011_2698	25003-82-1	c12c(c3c(cc4c(ccnc4)c3)cc1)cccc2	3
2,176	ISSSTY_v1a_7367_02May011_2699	110520-17-7	c12c(c3c(c4c1cc1c(ccnc1)c4)cccc3)cccc2	3
2,177	ISSSTY_v1a_7367_02May011_2700	24496-65-9	c12c3c4c(c5c(cc4ccc3ccc1)cccc5)cn2	3
2,178	ISSSTY_v1a_7367_02May011_2701	24903-48-8	c12c(c3c(cc4c5c(ccc4c3)cccc5)cc1)cncc2	3
2,179	ISSSTY_v1a_7367_02May011_2702	218-08-6	c12c(c3c(c4c(cccc4)cc3)cc1)cccn2	3
2,180	ISSSTY_v1a_7367_02May011_2703	89-82-7	HC(H)C(=C1C(=O)C(H)[C@](C(H)H)C(H)C1H)C(H)H	1
2,181	ISSSTY_v1a_7367_02May011_2704	156-43-4	HC(H)C(H)Oc1ccc(N)cc1	3
2,182	ISSSTY_v1a_7367_02May011_2705	194-03-6	c12c3c4c(ccc3ccc1)cccc4cn2	3
2,183	ISSSTY_v1a_7367_02May011_2706	56211-40-6	HC(H)c1cc(Nc2c(S(=O)(=O)NC(=O)NC(C(H)H)C(H)H)cncc2)ccc1	1
2,184	ISSSTY_v1a_7367_02May011_2707	86412-49-9	HC(H)C(=O)N(O)c1cc(Cl)c(Cl)cc1	1
2,185	ISSSTY_v1a_7367_02May011_2708	18296-44-1	HC(H)C(=O)OC(H)C1C2[C@@]([C@]3(C(H)O3)[C@@](OC(=O)C(H)C(C(H)H)C(H)H)C=2)[C@](OC(=O)C(H)C(C(H)H)C(H)H)OC=1	3
2,186	ISSSTY_v1a_7367_02May011_2709	118-82-1	HC(H)C(c1c(O)c(C(C(H)H)(C(H)H)C(H)H)cc(C(H)e2cc(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
2,187	ISSSTY_v1a_7367_02May011_2710	70140-81-7	HC(H)C(H)OP(=S)(OC(H)C(C(H)H)C(H)H)SC(H)Cl	1
2,188	ISSSTY_v1a_7367_02May011_2712	70140-82-8	HC(H)C(C(H)H)C(H)OP(=S)(OC(H)C(C(H)H)C(H)H)SC(H)Cl	1
2,189	ISSSTY_v1a_7367_02May011_2713	50-48-6	HC(H)N(C(H)H)C(H)C(H)C=C1c2c(C(H)C(H)c3c1cccc3)cccc2	1
2,190	ISSSTY_v1a_7367_02May011_2714	50-49-7	HC(H)N(C(H)H)C(H)C(H)C(H)N1c2c(C(H)C(H)c3c1cccc3)cccc2	1

2,191	ISSSTY_v1a_7367_02May011_2715	7664-38-2	O=P(O)(O)O	1
2,192	ISSSTY_v1a_7367_02May011_2716	6915-15-7	HC(C(=O)O)C(O)C(=O)O	1
2,193	ISSSTY_v1a_7367_02May011_2717	50-21-5	HC(H)C(O)C(=O)O	1
2,194	ISSSTY_v1a_7367_02May011_2718	25973-55-1	HC(H)C(c1c(O)c(N2N=C3C(C=CC=C3)=N2)cc(C(C(H)H)(C(H)H)C(H)C(H)H)c1)(C(H)H)C(H)C(H)H	1
2,195	ISSSTY_v1a_7367_02May011_2719	613-47-8	c12c(cc(NO)cc1)cccc2	3
2,196	ISSSTY_v1a_7367_02May011_2720	141-04-8	HC(H)C(C(H)H)C(H)OC(=O)C(H)C(H)C(H)C(H)C(=O)OC(H)C(C(H)H)C(H)H	1
2,197	ISSSTY_v1a_7367_02May011_2721	90-46-0	c12c(C(O)c3c(cccc3)O1)cccc2	3
2,198	ISSSTY_v1a_7367_02May011_2722	495-48-7	c1([N-][N+](=O)c2cccc2)cccc1	3
2,199	ISSSTY_v1a_7367_02May011_2725	139953-76-7	C1(=O)C2C(c3c(cccc3)N=2)=NNN1NC=C1C=CC(=O)C=C1	3
2,200	ISSSTY_v1a_7367_02May011_2726	102-60-3	HC(H)C(O)C(H)N(C(H)C(H)N(C(H)C(O)C(H)H)C(H)C(O)C(H)H)C(H)C(O)C(H)H	1
2,201	ISSSTY_v1a_7367_02May011_2728	147151-61-9	HC(H)[C@]12C(H)C(H)[C@@]3[C@]4(C(H)H)C(H)C(H)[C@]5OC(=O)C=C6c6cc(N(C(H)C(H)C(O)C(H)C(O)cccc)C(H)[C@@]4C(H)C(H)[C@]3[C@@]1C(H)C(H)C(=O)N2	3
2,202	ISSSTY_v1a_7367_02May011_2729	133502-50-8	HC(H)N(c1ccc(Cc2ccc(N(C(H)H)C(H)H)cc2)=C2C=CC(=N)C=C2)cc1)C(H)H	1
2,203	ISSSTY_v1a_7367_02May011_2730	139953-77-8	C1(=O)C2C(c3c(cccc3)N=2)=NNN1N=Cc1ccc(C(=O)O)cc1	3
2,204	ISSSTY_v1a_7367_02May011_2731	2675-77-6	HC(H)Oc1c(Cl)cc(OC(H)H)c(Cl)c1	1
2,205	ISSSTY_v1a_7367_02May011_2732	109-43-3	HC(H)C(H)C(H)C(H)OC(=O)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(=O)OC(H)C(H)C(H)C(H)H	1
2,206	ISSSTY_v1a_7367_02May011_2733	79-36-7	C(=O)(Cl)C(Cl)Cl	3
2,207	ISSSTY_v1a_7367_02May011_2734	9004-53-9	HC(O)[C@]1[C@@](O)[C@](O)[C@@](O)C(O)[C@]2[C@@](C(H)O)OC(O)[C@]3[C@@](C(H)O)O[C@](O)[C@](O)[C@@]3O)[C@](O)[C@@]2O)O1	1
2,208	ISSSTY_v1a_7367_02May011_2735	519-73-3	c1(C(c2cccc2)c2cccc2)cccc1	1
2,209	ISSSTY_v1a_7367_02May011_2736	91828-72-7	c1(N(=O)=O)c2c(c3c(c4c([C@](O)[C@@](O)C=C4)cc3)c1)cccc2	3
2,210	ISSSTY_v1a_7367_02May011_2737	709-98-8	HC(H)C(H)C(=O)Nc1cc(Cl)c(Cl)cc1	1
2,211	ISSSTY_v1a_7367_02May011_2738	4130-42-1	HC(H)C(c1c(O)c(C(C(H)H)(C(H)H)C(H)H)cc(C(H)C(H)H)c1)(C(H)H)C(H)H	1
2,212	ISSSTY_v1a_7367_02May011_2739	53950-62-2	c1(Cl)c(Cl)cc(N(O)C=O)cc1	1
2,213	ISSSTY_v1a_7367_02May011_2740	91678	HC(H)C(H)C(=O)N(O)c1cc(Cl)c(Cl)cc1	1
2,214	ISSSTY_v1a_7367_02May011_2741	21232-47-3	c1(Cl)c(Cl)cc([N-][N+](=O)c2cc(Cl)c(Cl)cc2)cc1	1
2,215	ISSSTY_v1a_7367_02May011_2743	115664-59-0	c1(N(=O)=O)c2c3c(c4c(c3ccc2)ccc(O)c4)cc1	3
2,216	ISSSTY_v1a_7367_02May011_2745	100-43-6	HC=Cc1ccncc1	1
2,217	ISSSTY_v1a_7367_02May011_2746	525-66-6	HC(H)C(C(H)H)NC(H)C(O)C(H)Oc1c2c(cccc2)ccc1	1
2,218	ISSSTY_v1a_7367_02May011_2747	105-76-0	HC(H)C(H)C(H)C(H)OC(=O)C=CC(=O)OC(H)C(H)C(H)C(H)H	1
2,219	ISSSTY_v1a_7367_02May011_2748	693-57-2	HC(C(=O)[O-])C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)[N+](H)H	1
2,220	ISSSTY_v1a_7367_02May011_2750	72-33-3	HC(H)[C@]12[C@](O)(C_C)C(H)C(H)[C@]1[C@@]1C(H)C(H)c3c(ccc(OC(H)H)c3)[C@]1C(H)C2H	1

2,221	ISSSTY_v1a_7367_02May011_2752	114656-95-0	HC(H)c1c2-c3c(ccccc3)Nc2c2C(=O)C(OC(H)H)=CC(=O)c2n1	3
2,222	ISSSTY_v1a_7367_02May011_2753	26741-53-7	HC(H)C(c1c(O[P@]2OC(H)[C@]3(C(H)O[P@@])Oc4c(C(C(H)H)(C(H)H)C(H)H)cc4)OC3H)C(H)O2)ccc(C(C(H)H)(C(H)H)C(H)H)c1X(C(H)H)C(H)H	1
2,223	ISSSTY_v1a_7367_02May011_2754	113698-23-0	HC(H)c1c2-c3c(ccccc3)Nc2c2C(=O)C=C(N3C(H)C3H)C(=O)c2n1	3
2,224	ISSSTY_v1a_7367_02May011_2755	618-87-1	c1(N)cc([N+](=O)[O-])cc([N+](=O)[O-])c1	3
2,225	ISSSTY_v1a_7367_02May011_2756	534-52-1	HC(H)c1c(O)c([N+](=O)[O-])cc([N+](=O)[O-])c1	1
2,226	ISSSTY_v1a_7367_02May011_2757	4648-33-3	HC(H)Oc1ccc(C=Cc2ccc(N(=O)=O)cc2)cc1	3
2,227	ISSSTY_v1a_7367_02May011_2758	68053-32-7	HC(H)[C@]12[C@@](C=O)(C=O)=C3C(H)C(C(H)H)(C(H)H)C(H)[C@]3[C@]1O)C2H	3
2,228	ISSSTY_v1a_7367_02May011_2759	479-45-8	HC(H)N(c1c([N+](=O)[O-])cc([N+](=O)[O-])cc1[N+](=O)[O-])[N+](=O)[O-]	3
2,229	ISSSTY_v1a_7367_02May011_2760	626-60-8	c1(Cl)cccnc1	1
2,230	ISSSTY_v1a_7367_02May011_2761	158729-32-9	c1(S(=O)(=O)NO)c2c(cccn2)ccc1	1
2,231	ISSSTY_v1a_7367_02May011_2763	2400-17-1	HC(H)NC1=C2C(C=CC=C2)=NS1	1
2,232	ISSSTY_v1a_7367_02May011_2764	372-47-4	c1(F)cccnc1	1
2,233	ISSSTY_v1a_7367_02May011_2765	51357-79-0	C12C(=C(N)SN=1)C=C(Cl)C=C2	3
2,234	ISSSTY_v1a_7367_02May011_2766	708-42-9	HC(H)C(H)C(H)NC1=C2C(C=CC=C2)=NS1	1
2,235	ISSSTY_v1a_7367_02May011_2767	16110-09-1	c1(Cl)ccc(Cl)cn1	1
2,236	ISSSTY_v1a_7367_02May011_2768	2457-47-8	c1(Cl)cc(Cl)cnc1	1
2,237	ISSSTY_v1a_7367_02May011_2769	2589-58-4	HC(H)C(H)C(C(H)H)NC1=C2C(C=CC=C2)=NS1	1
2,238	ISSSTY_v1a_7367_02May011_2770	1513-65-1	c1(F)cccc(F)n1	1
2,239	ISSSTY_v1a_7367_02May011_2771	108-99-6	HC(H)c1cccnc1	1
2,240	ISSSTY_v1a_7367_02May011_2772	182963	C12C(=C(N)SN=1)C=CC=C2	3
2,241	ISSSTY_v1a_7367_02May011_2773	149862-55-5	HC(H)C(H)C(H)C(H)NC1=C2C(C=CC=C2)=NS1	1
2,242	ISSSTY_v1a_7367_02May011_2774	108-89-4	HC(H)c1ccncc1	1
2,243	ISSSTY_v1a_7367_02May011_2775	34250-70-9	HC(H)C(=O)NC1=C2C(C=CC=C2)=NS1	3
2,244	ISSSTY_v1a_7367_02May011_2776	109-09-1	c1(Cl)ccccn1	3
2,245	ISSSTY_v1a_7367_02May011_2777	372-48-5	c1(F)ccccn1	3
2,246	ISSSTY_v1a_7367_02May011_2779	78448-07-4	c12-c3c4c(cc(O)cc4)ccc3Nc1ccc1c2cccc1	3
2,247	ISSSTY_v1a_7367_02May011_2780	149862-57-7	HC(H)C(C(H)H)C(H)C(H)NC1=C2C(C=CC=C2)=NS1	1
2,248	ISSSTY_v1a_7367_02May011_2781	272-16-2	c12c(C=NS1)cccc2	1
2,249	ISSSTY_v1a_7367_02May011_2782	99523-57-6	HC(H)C1C=CC2C(=C(NC(=O)C(H)Cl)SN=2)C=1	3
2,250	ISSSTY_v1a_7367_02May011_2783	99523-58-7	HC(H)C1C=CC2C(=C(NC(=O)C(Cl)Cl)SN=2)C=1	3

2,251	ISSSTY_v1a_7367_02May011_2784	96-49-1	HC1C(H)OC(=O)O1	1
2,252	ISSSTY_v1a_7367_02May011_2785	621-95-4	HC(c1ccc(N)cc1)C(H)c1ccc(N)cc1	3
2,253	ISSSTY_v1a_7367_02May011_2786	67019-30-1	HC(H)C(=O)N(C1=C2C(C=CC=C2)=NS1)C(H)H	1
2,254	ISSSTY_v1a_7367_02May011_2787	90421-84-4	HC1C(C(H)N2C(=O)c3c(cccc3)S2)O1	1
2,255	ISSSTY_v1a_7367_02May011_2788	148193-37-7	C1(=O)c2c(cc(N)cc2)SN1	1
2,256	ISSSTY_v1a_7367_02May011_2789	68268-20-2	HC(H)C(H)C(H)N(C1=C2C(C=CC=C2)=NS1)C(=O)C(H)C(H)Cl	3
2,257	ISSSTY_v1a_7367_02May011_2790	113698-18-3	HC(H)c1c2C3=C(C(H)C(H)C(H)C3H)Nc2c2C(=O)C=C(OC(H)H)C(=O)c2n1	3
2,258	ISSSTY_v1a_7367_02May011_2791	126983-60-6	HC(H)OC1C(=O)c2c(C(=O)C=1)c1c(-c3c(ccnc3)N1)cn2	3
2,259	ISSSTY_v1a_7367_02May011_2792	607-35-2	c1(N(=O)=O)c2c(cccn2)ccc1	3
2,260	ISSSTY_v1a_7367_02May011_2793	2634-33-5	C1(=O)c2c(cccc2)SN1	1
2,261	ISSSTY_v1a_7367_02May011_2794	13171-00-1	HC(H)C(=O)c1c2c(C(C(H)H)(C(H)H)C(H)C2H)cc(C(C(H)H)(C(H)H)C(H)H)c1	1
2,262	ISSSTY_v1a_7367_02May011_2795	33704-61-9	HC(H)C1(C(H)H)C2C(=O)C(H)C(H)C(H)C=2C(C(H)H)(C(H)H)C1C(H)H	1
2,263	ISSSTY_v1a_7367_02May011_2796	15323-35-0	HC(H)C1(C(H)H)c2c(C(C(H)H)(C(H)H)C1C(H)H)cc(C(=O)C(H)H)c(C(H)H)c2	1
2,264	ISSSTY_v1a_7367_02May011_2797	108612-45-9	HC(H)N(C1=NC=CC(=O)N1)C1C(H)C(H)N(C2N(C(H)c3ccc(F)cc3)c3c(cccc3)N=2)C(H)C1H	1
2,265	ISSSTY_v1a_7367_02May011_2798	67019-32-3	HC(H)C(=O)NC1=C2C(C(Cl)=CC(Cl)=C2)=NS1	1
2,266	ISSSTY_v1a_7367_02May011_2799	75-71-8	C(F)(F)(Cl)Cl	1
2,267	ISSSTY_v1a_7367_02May011_2800	143603-79-6	HC(H)C(=O)Nc1ccc(C=NC2c3c(cccc3)NC=2C(=O)OC(H)C(H)H)cc1	3
2,268	ISSSTY_v1a_7367_02May011_2801	98982-99-1	HC(H)[N+](C(O-)](C(H)H)C(H)C(H)N(c1cccn1)C(H)c1ccc(OC(H)H)cc1	1
2,269	ISSSTY_v1a_7367_02May011_2802	5836-29-3	HC1c2c(C(C3C(=O)c4c(cccc4)OC=3O)C(H)C1H)cccc2	1
2,270	ISSSTY_v1a_7367_02May011_2803	158729-15-8	c1(S(=O)(=O)Oc2c(N(=O)=O)cccc2)c2c(cccn2)ccc1	3
2,271	ISSSTY_v1a_7367_02May011_2804	106-23-0	HC(H)C(C(H)H)=CC(H)C(H)[C@@](C(H)H)C(H)C=O	1
2,272	ISSSTY_v1a_7367_02May011_2805	158729-16-9	c1(S(=O)(=O)Oc2cc(N(=O)=O)ccc2)c2c(cccn2)ccc1	3
2,273	ISSSTY_v1a_7367_02May011_2806	158729-19-2	c1(S(=O)(=O)Oc2cc(Cl)c(Cl)cc2)c2c(cccn2)ccc1	3
2,274	ISSSTY_v1a_7367_02May011_2807	158729-21-6	HC(H)c1cc(NS(=O)(=O)c2c3c(cccn3)ccc2)ccc1	1
2,275	ISSSTY_v1a_7367_02May011_2808	158729-22-7	c1(S(=O)(=O)Nc2c(Cl)cccc2)c2c(cccn2)ccc1	1
2,276	ISSSTY_v1a_7367_02May011_2809	158729-17-0	HC(H)c1cc(N(=O)=O)c(OS(=O)(=O)c2c3c(cccn3)ccc2)cc1	3
2,277	ISSSTY_v1a_7367_02May011_2810	7235-40-7	HC(H)C1(C(H)H)C(C(=O)C(C(H)H)=CC(=O)C(C(H)H)C=CC(=O)C(C(H)H)C=CC(=O)C(C(H)H)C(H)C(H)C(H)C1H)	1
2,278	ISSSTY_v1a_7367_02May011_2811	1947-37-1	HC(H)SC(H)C(H)C(C(=O)N)C(C(=O)N)C(C(N)=O)C(H)c1cccc1)C(H)C(=O)N)C(=O)C(C(H)C1c2c(cccc2)NC=1)NC(=O)OC(H)c1cccc1	1
2,279	ISSSTY_v1a_7367_02May011_2812	158729-26-1	HC(H)N(c1ccc(NS(=O)(=O)c2c3c(cccn3)ccc2)cc1)C(H)H	3
2,280	ISSSTY_v1a_7367_02May011_2814	24246-00-2	C1(N(=O)=O)C2C(C=CC=1)=CSN=2	3

2,311	ISSSTY_v1a_7367_02May011_2855	113359-04-9	HC(H)ON=C(O)N=C(N)SN=1)C(=O)N[C@]1C(=O)N2C(C(=O)[O-])=C(C(H)N3c4cccn[n+])4C=C3)C(H)S[C@@]12	1
2,312	ISSSTY_v1a_7367_02May011_2856	105149-00-6	HC(H)C(=O)[C@]1(O)C(=O)C(H)H[C@]2(C(H)H)C(H)C(H)[C@@]3[C@]4(C(H)H)C(C(Cl)=C[C@]3[C@@]2C(H)C1H)=CC(=O)OC4H	1
2,313	ISSSTY_v1a_7367_02May011_2858	136-85-6	HC(H)C1C=CC2C(C=1)=NNN=2	1
2,314	ISSSTY_v1a_7367_02May011_2860	115664-58-9	c1(N(=O)=O)c2c3c(c4c(c3ccc2)cc(O)cc4)cc1	3
2,315	ISSSTY_v1a_7367_02May011_2861	22769-68-2	HC(H)OC(=O)NC1=Nc2c(cc(O)cc2)N1	1
2,316	ISSSTY_v1a_7367_02May011_2862	366-29-0	HC(H)N(c1ccc(-c2ccc(N(C(H)H)C(H)H)cc2)cc1)C(H)H	3
2,317	ISSSTY_v1a_7367_02May011_2863	24085-06-1	HC(H)C(=O)c1cc(C(H)OC(=O)C(H)H)c(OC(=O)C(H)H)cc1	3
2,318	ISSSTY_v1a_7367_02May011_2864	80214-83-1	HC(H)Oc1cc(C=Cc2ccc(N(=O)=O)cc2)ccc1	3
2,319	ISSSTY_v1a_7367_02May011_2865	14064-58-5	c1(C=Cc2ccc(N(=O)=O)cc2)ccc(Cl)cc1	3
2,320	ISSSTY_v1a_7367_02May011_2866	14064-55-2	c1(C=Cc2cc([N+](=O)[O-])ccc2)ccc([N+](=O)[O-])cc1	3
2,321	ISSSTY_v1a_7367_02May011_2868	51042-51-4	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(N)=O	1
2,322	ISSSTY_v1a_7367_02May011_2869	124-26-5	HC(C(=O)O)Oc1ccc(N(C(H)C(H)Cl)C(H)C(H)Cl)cc1	3
2,323	ISSSTY_v1a_7367_02May011_2870	17528-53-9	HC(H)[C@]12C(H)C(H)[C@@]3[C@]4(C(H)H)C(H)C(H)[C@](O)C(H)[C@@]4C(H)C(H)[C@]3[C@@]1C(H)C(H)C(=O)N2	1
2,324	ISSSTY_v1a_7367_02May011_2871	39932-99-5	c12-c3c4c(ccc(O)c4)ccc3Nc1ccc1c2cccc1	3
2,325	ISSSTY_v1a_7367_02May011_2872	78448-08-5	c1(C=Cc2cc(Cl)ccc2)ccc(N(=O)=O)cc1	3
2,326	ISSSTY_v1a_7367_02May011_2873	7297-53-2	HC(H)C1(C(H)H)[C@](C(=O)OC(H)c2cc(Oc3ccccc3)ccc2)[C@@]1C=C(Cl)Cl	1
2,327	ISSSTY_v1a_7367_02May011_2875	61949-77-7	HC(H)C1(C(H)H)[C@](C(=O)OC(H)c2cc(Oc3ccccc3)ccc2)[C@]1C=C(Cl)Cl	1
2,328	ISSSTY_v1a_7367_02May011_2876	61949-76-6	HC(O)C(O)C(O)C(C(O)C(H)O)OC1C(O)C(O)C(O)C(C(H)O)O1	1
2,329	ISSSTY_v1a_7367_02May011_2878	585-86-4	HC1C(C(=O)O)N(N=O)C(H)S1	1
2,330	ISSSTY_v1a_7367_02May011_2879	88381-44-6	HC(H)c1ccc(C=NC2c3c(cccc3)NC=2C(=O)OC(H)C(H)H)cc1	1
2,331	ISSSTY_v1a_7367_02May011_2880	143603-81-0	HC(H)C(H)OC(=O)C1=C(N=Cc2ccc(N(=O)=O)cc2)c2c(cccc2)N1	3
2,332	ISSSTY_v1a_7367_02May011_2881	143603-72-9	HC(c1ccccc1)NC(=O)C(H)C(H)NNC(=O)c1ccncc1	3
2,333	ISSSTY_v1a_7367_02May011_2882	18969	HC(c1ccccc1)SSC(H)c1ccccc1	3
2,334	ISSSTY_v1a_7367_02May011_2883	150-60-7	C(N)c1ccc(C=Cc2ccc(N(=O)=O)cc2)cc1	3
2,335	ISSSTY_v1a_7367_02May011_2884	159394-73-7	HC1C(H)N(N=O)C(C(O)C(O)C(O)C(H)O)S1	3
2,336	ISSSTY_v1a_7367_02May011_2885	92134-96-8	c1(S(=O)(=O)Oc2c(Cl)cc(Cl)cc2)c2c(ccn2)ccc1	3
2,337	ISSSTY_v1a_7367_02May011_2886	158729-18-1	HC(H)c1ccc(NS(=O)(=O)c2c3c(cccn3)ccc2)cc1	1
2,338	ISSSTY_v1a_7367_02May011_2887	98809-36-0	c1(C=Cc2ccc([N+](=O)[O-])cc2)ccc([N+](=O)[O-])cc1	3
2,339	ISSSTY_v1a_7367_02May011_2888	736-31-2	c1(S(=O)(=O)Nc2cc(N(=O)=O)ccc2)c2c(cccn2)ccc1	1
2,340	ISSSTY_v1a_7367_02May011_2890	158729-25-0		1

2,401	ISSSTY_v1a_7367_02May011_2963	102791-33-3	C1(=O)c2c3c4c(c(N(=O)=O)ccc4O1)ccc3ccc2	3
2,402	ISSSTY_v1a_7367_02May011_2964	56355-17-0	HC(H)C(c1ccc(OC2=NC=CS2)cc1)C(=O)O	1
2,403	ISSSTY_v1a_7367_02May011_2965	155164-67-3	HC(H)c1ccc(C(=O)N2C(=O)C(Cl)=C(Cl)C=N2)cc1	1
2,404	ISSSTY_v1a_7367_02May011_2966	498-02-2	HC(H)C(=O)c1cc(OC(H)H)c(O)cc1	1
2,405	ISSSTY_v1a_7367_02May011_2967	2478-38-8	HC(H)C(=O)c1cc(OC(H)H)c(O)c(OC(H)H)c1	1
2,406	ISSSTY_v1a_7367_02May011_2968	155164-65-1	HC(H)C(H)C(H)C(H)C(=O)N1C(=O)C(Cl)=C(Cl)C=N1	1
2,407	ISSSTY_v1a_7367_02May011_2971	102791-34-4	C1(=O)c2c3c4c(c(N(=O)=O)ccc4ccc3ccc2)O1	3
2,408	ISSSTY_v1a_7367_02May011_2972	5397-37-5	HC1c2c(-c3c1ccc(N(=O)=O)c3)cccc2	3
2,409	ISSSTY_v1a_7367_02May011_2973	155164-68-4	HC(H)Oc1ccc(C(=O)N2C(=O)C(Cl)=C(Cl)C=N2)cc1	1
2,410	ISSSTY_v1a_7367_02May011_2975	21725-46-2	HC(H)C(C,N)(C(H)H)Nc1nc(Cl)nc(NC(H)C(H)H)n1	1
2,411	ISSSTY_v1a_7367_02May011_2976	114656-96-1	HC(H)c1c2-c3c(cccc3)Nc2c2C(=O)C(N3C(H)C3H)=CC(=O)c2n1	3
2,412	ISSSTY_v1a_7367_02May011_2977	13345-21-6	c1(O)c2c3c4c(c5c(cc4cc2)cccc5)ccc3cc1	3
2,413	ISSSTY_v1a_7367_02May011_2979	114607-46-4	C1(c2cc(NC(=O)C(=O)O)ccc2)N=NNN=1	1
2,414	ISSSTY_v1a_7367_02May011_2980	43210-67-9	HC(H)OC(=O)NC1=Nc2c(cc(Sc3ccccc3)cc2)N1	1
2,415	ISSSTY_v1a_7367_02May011_2984	143603-80-9	HC(H)C(H)OC(=O)C1=C(NC=C2C=CC(=O)C=C2)c2c(cccc2)N1	3
2,416	ISSSTY_v1a_7367_02May011_2986	155164-58-2	HC(H)c1ccc(S(=O)(=O)N2C(=O)C(Cl)=C(Cl)C=N2)cc1	1
2,417	ISSSTY_v1a_7367_02May011_2987	171866-15-2	HC(H)C1C(O)C(O)C(I)C(OC2c3c(O)c4C(=O)c5c(C(=O)c4c(O)c3C(H)C(O)C(H)O)C2H)cccc5)O1	3
2,418	ISSSTY_v1a_7367_02May011_2988	74550-97-3	HC1C(=O)N(C(H)N2C(H)C(H)OC(H)C2H)C(=O)C(H)N1C(H)C(H)N1C(H)C(=O)N(C(H)N2C(H)C(H)OC(H)C2H)C(=O)C1H	3
2,419	ISSSTY_v1a_7367_02May011_2989	93-18-5	HC(H)C(H)Oc1cc2c(cccc2)cc1	1
2,420	ISSSTY_v1a_7367_02May011_2990	1120-21-4	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)H	1
2,421	ISSSTY_v1a_7367_02May011_2994	16045-92-4	HC(C(=O)O)C(Cl)C(=O)O	1
2,422	ISSSTY_v1a_7367_02May011_2995	534-07-6	HC(Cl)C(=O)C(H)Cl	3
2,423	ISSSTY_v1a_7367_02May011_2996	89-57-6	C(=O)(O)c1c(O)ccc(N)c1	1
2,424	ISSSTY_v1a_7367_02May011_2997	74940-61-7	HC(H)OP(=O)(C(C(Cl)(Cl)Cl)OC(=O)C(H)Cl)OC(H)H	1
2,425	ISSSTY_v1a_7367_02May011_2998	17024-17-8	c1(N(=O)=O)c2c(c3c(cccc3)cc2)ccc1	3
2,426	ISSSTY_v1a_7367_02May011_2999	159092-66-7	c1([N+](=O)[O-])c2c(c3c([N+](=O)[O-])cccc3cc2)ccc1	3
2,427	ISSSTY_v1a_7367_02May011_3000	159092-68-9	c1([N+](=O)[O-])c2c(c3c(cc2[N+](=O)[O-])cccc3)ccc1	3
2,428	ISSSTY_v1a_7367_02May011_3001	159092-69-0	c12c(c3c(cc([N+](=O)[O-])cc3)cc1)cc([N+](=O)[O-])cc2	3
2,429	ISSSTY_v1a_7367_02May011_3002	159092-70-3	c1([N+](=O)[O-])c2c(c3c(cc([N+](=O)[O-])cc3)c1)cccc2	3
2,430	ISSSTY_v1a_7367_02May011_3003	159092-72-5	c1([N+](=O)[O-])c2c3c(ccc([N+](=O)[O-])c3)ccc2ccc1	3

2,461	ISSSTY_v1a_7367_02May011_3047	121-00-6	HC(H)C(c1c(O)ccc(OC(H)H)c1)(C(H)H)C(H)H	1
2,462	ISSSTY_v1a_7367_02May011_3048	135673-14-2	HC(H)C(=O)Nc1ccc(Oc2ccc(N=O)cc2)cc1	3
2,463	ISSSTY_v1a_7367_02May011_3049	172374-57-1	HC(H)C(=O)Nc1ccc(Oc2ccc(NO)cc2)cc1	3
2,464	ISSSTY_v1a_7367_02May011_3050	54779-53-2	HC(H)c1c2-c3c(ccc(N)c3)Nc2c(C(H)H)c2c1cncc2	3
2,465	ISSSTY_v1a_7367_02May011_3051	421492	HC(c1ccccc1)SC(H)C(N)C(=O)O	1
2,466	ISSSTY_v1a_7367_02May011_3052	115767-74-3	HC(H)C(H)C(c1ccc(C(C(H)H)C(H)H)cc1)=C(c1ccc(OC(H)C(H)N(C(H)H)C(H)H)cc1)c1ccc(OP(=O)(O)O)cc1	1
2,467	ISSSTY_v1a_7367_02May011_3053	42924-53-8	HC(H)C(=O)C(H)C(H)c1cc2c(cc(OC(H)H)cc2)cc1	1
2,468	ISSSTY_v1a_7367_02May011_3054	630-20-6	HC(Cl)C(Cl)(Cl)Cl	3
2,469	ISSSTY_v1a_7367_02May011_3056	116-29-0	c1(Cl)c(Cl)cc(Cl)c(S(=O)(=O)c2ccc(Cl)cc2)c1	1
2,470	ISSSTY_v1a_7367_02May011_3057	33069-62-4	HC(H)C(C(H)C(H)C(H)C(H)C(H)C(=O)OC(H)C(H)N1C(H)C(H)N(C(H)C(H)C(H)N2c3c(ccc(C(F)F)F)c3)Sc3c2cccc3)C(H)C1H	1
2,471	ISSSTY_v1a_7367_02May011_3058	2746-81-8	HC(H)C(H)C(H)C(H)C(H)C(=O)OC(H)C(H)N1C(H)C(H)N(C(H)C(H)C(H)N2c3c(ccc(C(F)F)F)c3)Sc3c2cccc3)C(H)C1H	1
2,472	ISSSTY_v1a_7367_02May011_3059	1635-61-6	c1(N(=O)=O)c(N)cc(Cl)cc1	3
2,473	ISSSTY_v1a_7367_02May011_3061	67464-46-4	c12-c3c(C4C(c1ccccc2)N4)ccccc3	3
2,474	ISSSTY_v1a_7367_02May011_3063	2648-51-3	C(Cl)(Cl)=CC=O	3
2,475	ISSSTY_v1a_7367_02May011_3064	91626-52-7	HC(H)S(=O)(=O)N1C(=O)C(Cl)=C(Cl)C=N1	3
2,476	ISSSTY_v1a_7367_02May011_3065	155164-55-9	HC(H)C(H)C(H)S(=O)(=O)N1C(=O)C(Cl)=C(Cl)C=N1	3
2,477	ISSSTY_v1a_7367_02May011_3067	155164-63-9	HC(H)C(=O)N1C(=O)C(Cl)=C(Cl)C=N1	1
2,478	ISSSTY_v1a_7367_02May011_3068	73341-53-4	HC(H)C1C2N(c3c(ccc(NO)n3)N=2)C=CC=1	3
2,479	ISSSTY_v1a_7367_02May011_3069	997-55-7	HC(H)C(=O)N[C@](C(=O)O)C(H)C(=O)O	1
2,480	ISSSTY_v1a_7367_02May011_3070	155164-69-5	C1(=O)C(Cl)=C(Cl)C=NN1C(=O)c1ccc(N(=O)=O)cc1	3
2,481	ISSSTY_v1a_7367_02May011_3071	128505-52-2	HC(H)C(=O)N[C@](C(=O)O)C(H)SC(=S)N(SC(H)C(H)H)SC(H)C(H)H	1
2,482	ISSSTY_v1a_7367_02May011_3072	25265-77-4	HC(H)C(C(H)H)(C(H)OC(=O)C(C(H)H)C(H)H)C(O)C(C(H)H)C(H)H	1
2,483	ISSSTY_v1a_7367_02May011_3073	106-98-9	HC(H)C(H)C=CH	1
2,484	ISSSTY_v1a_7367_02May011_3074	107-25-5	HC(H)OC=CH	1
2,485	ISSSTY_v1a_7367_02May011_3075	132742-01-9	HC1c2c3c4c5c(c(N(=O)=O)ccc5cc3)ccc4cc2C=CC1H	3
2,486	ISSSTY_v1a_7367_02May011_3076	132742-03-1	HC1c2c(c3c4c5c(c(N(=O)=O)ccc5ccc4c2)cc3)C=CC1H	3
2,487	ISSSTY_v1a_7367_02May011_3077	5581-32-8	HC(H)C(c1ccc(OC(H)C(O)C(H)O)cc1)(c1ccc(OC(H)C(O)C(H)O)cc1)C(H)H	1
2,488	ISSSTY_v1a_7367_02May011_3079	22316-47-8	HC(H)N1c2c(cc(Cl)cc2)N(c2ccccc2)C(=O)C(H)C1=O	1
2,489	ISSSTY_v1a_7367_02May011_3080	70585-50-1	C(=O)(O)c1c2c(cc(I)c1)cccn2	1
2,490	ISSSTY_v1a_7367_02May011_3081	35001-52-6	HC(H)C(c1cc(NC(=O)C(=O)Nc2c(C(H)C(H)H)cccc2)c(OC(H)C(H)H)cc1)(C(H)H)C(H)H	1

2,521	ISSSTY_v1a_7367_02May011_3114	148317-76-4	HC(C(H)N1C(=O)c2c(C3C(=O)c4c(C1=3)cccc4)cccc2)NC(H)C(H)O	1
2,522	ISSSTY_v1a_7367_02May011_3116	56980-96-2	HC(H)C(=O)c1c(OC(H)C(O)C(H)NC(C(H)H)(C(H)H)C(H)H)ccc(NC(N)=O)c1	3
2,523	ISSSTY_v1a_7367_02May011_3117	57470-96-9	HC(H)C(=O)c1c(OC(H)C(O)C(H)NC(C(H)H)(C(H)H)C(H)H)ccc(NC(=O)NC(H)C(H)H)c1	1
2,524	ISSSTY_v1a_7367_02May011_3118	22181-94-8	HC(H)C(H)OC(=O)C(H)NC(=O)C(H)C(H)C(H)C(H)Sc1c2c(N=CN2)ncn1	1
2,525	ISSSTY_v1a_7367_02May011_3119	17796-82-6	HC1C(H)C(H)C(H)C(H)C1SN1C(=O)c2c(C1=O)cccc2	1
2,526	ISSSTY_v1a_7367_02May011_3120	2837-89-0	C(F)(F)(F)C(F)Cl	1
2,527	ISSSTY_v1a_7367_02May011_3121	622-96-8	HC(H)c1ccc(C(H)C(H)H)cc1	1
2,528	ISSSTY_v1a_7367_02May011_3122	119169-78-7	HC(H)[C@@]12C(C(=O)O)C(H)C1H)=CC(H)[C@]1[C@@]3[C@@](C(H)H)(C(H)H)[C@@]21)[C@@](C(=O)NC(C(H)H)(C(H)H)C(H)H)C3H	1
2,529	ISSSTY_v1a_7367_02May011_3123	104789-46-0	HC(Cl)C(H)NC(=O)Sc1c2c(N=CN2)ncn1	3
2,530	ISSSTY_v1a_7367_02May011_3124	159394-71-5	C(N)c1cc(C=Cc2ccc(N(=O)=O)cc2)ccc1	3
2,531	ISSSTY_v1a_7367_02May011_3125	1668-19-5	HC(H)N(C(H)H)C(H)C(H)C=C1c2c(C(H)O)c3c1cccc3)cccc2	1
2,532	ISSSTY_v1a_7367_02May011_3126	159394-72-6	C(N)c1cc(C=Cc2ccc(N(=O)=O)cc2)ccc1	3
2,533	ISSSTY_v1a_7367_02May011_3127	1214-39-7	HC(c1cccc1)Nc1c2c(N=CN2)ncn1	1
2,534	ISSSTY_v1a_7367_02May011_3129	7803-51-2	P	1
2,535	ISSSTY_v1a_7367_02May011_3130	690-39-1	HC(C(F)(F)F)C(F)(F)F	1
2,536	ISSSTY_v1a_7367_02May011_3131	107097-80-3	HC(H)C(H)C(H)C(H)C(H)N(C(=O)C(C(H)C(H)C(=O)O)NC(=O)c1cc(Cl)c(Cl)cc1)C(H)C(H)C(H)OC(H)H	1
2,537	ISSSTY_v1a_7367_02May011_3133	71628-96-1	HC(H)C12c3c(c4C(=O)c5c(C(=O)c4c(O)c3)c(O)c3c(C)[C@](O)(C(H)H)C(H)[C@@]3OC(H)H)c5)OC[C@@](O)[C@@](N(C(H)H)C(H)H)[C@@]1O)O2	3
2,538	ISSSTY_v1a_7367_02May011_3134	159092-67-8	c1([N+](=O)[O-])c2c(c3c(ccc([N+](=O)[O-])c3)cc2)ccc1	3
2,539	ISSSTY_v1a_7367_02May011_3135	2314-61-6	C1(c2cccc2)=CSC(=S)S1	1
2,540	ISSSTY_v1a_7367_02May011_3136	95-93-2	HC(H)c1c(C(H)H)cc(C(H)H)c(C(H)H)c1	1
2,541	ISSSTY_v1a_7367_02May011_3137	2062-78-4	HC(C(H)C(H)C(c1ccc(F)cc1)c1ccc(F)cc1)N1C(H)C(H)C(N2c3c(cccc3)NC2=O)C(H)C1H	1
2,542	ISSSTY_v1a_7367_02May011_3138	5786-21-0	HC(H)N1C(H)C(H)N(C2=C3C(C=CC=C3)=Nc3c(cc(Cl)cc3)N2)C(H)C1H	1
2,543	ISSSTY_v1a_7367_02May011_3139	90509-02-7	HC(H)OC(=O)NC1=Nc2c(cc(OS(=O)(=O)c3ccc(F)cc3)cc2)N1	1
2,544	ISSSTY_v1a_7367_02May011_3140	100527-20-6	c12c(c3c(ccc([N+](=O)[O-])c3)cc1)cc([N+](=O)[O-])cc2	3
2,545	ISSSTY_v1a_7367_02May011_3141	159092-71-4	c1([N+](=O)[O-])c2c(c3c(cccc3)c1)ccc([N+](=O)[O-])c2	3
2,546	ISSSTY_v1a_7367_02May011_3142	159092-73-6	c1([N+](=O)[O-])c2c(c3c(cccc3)c1)cc([N+](=O)[O-])cc2	3
2,547	ISSSTY_v1a_7367_02May011_3143	159092-75-8	c1([N+](=O)[O-])c2c(c3c(cccc3)c1)c([N+](=O)[O-])ccc2	3
2,548	ISSSTY_v1a_7367_02May011_3144	159092-76-9	c1([N+](=O)[O-])c2c(c3c(c([N+](=O)[O-])ccc3)c1)c([N+](=O)[O-])ccc2	3
2,549	ISSSTY_v1a_7367_02May011_3145	159092-74-7	c1([N+](=O)[O-])c2c3c(c([N+](=O)[O-])cc2ccc1)cccc3	3
2,550	ISSSTY_v1a_7367_02May011_3146	159092-80-5	c1([N+](=O)[O-])c2c3c(c([N+](=O)[O-])cc2ccc1)cc([N+](=O)[O-])cc3	3

