

2143	ISSSTY_v1a_7367_02May011_2670	155164-62-8	C1(=O)C(CI)=C(CI)C=NN1S(=O)(=O)c1c(CI)cc(CI)cc1	1
2144	ISSSTY_v1a_7367_02May011_2671	155164-64-0	HC(H)C(H)C(=O)N1C(=O)C(CI)=C(CI)C=N1	1
2145	ISSSTY_v1a_7367_02May011_2672	155164-61-7	C1(=O)C(CI)=C(CI)C=NN1S(=O)(=O)c1ccc(N(=O)=O)cc1	3
2146	ISSSTY_v1a_7367_02May011_2673	155164-66-2	C1(=O)C(CI)=C(CI)C=NN1C(=O)c1cccc1	1
2147	ISSSTY_v1a_7367_02May011_2674	155164-60-6	C1(=O)C(CI)=C(CI)C=NN1S(=O)(=O)c1ccc(CI)cc1	1
2148	ISSSTY_v1a_7367_02May011_2675	1918-00-9	HC(H)Oc1c(C(=O)O)c(CI)ccc1C1	1
2149	ISSSTY_v1a_7367_02May011_2677	155164-59-3	HC(H)Oc1ccc(S(=O)(=O)N2C(=O)C(CI)=C(CI)C=N2)cc1	1
2150	ISSSTY_v1a_7367_02May011_2678	135086-97-4	C1(=O)C2C(c3c(cccc3)N=2)=NNN1N	3
2151	ISSSTY_v1a_7367_02May011_2679	610-39-9	HC(H)c1cc([N+](=O)[O-])c([N+](=O)[O-])cc1	3
2152	ISSSTY_v1a_7367_02May011_2680	7440-66-6	[Zn]	1
2153	ISSSTY_v1a_7367_02May011_2683	1918-13-4	C(N)(=S)c1c(CI)cccc1C1	3
2154	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
2155	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@@](C(H)O)O4)(C(H)[C@@](C(H)H)C3=O)C=1C(H)C2H	3
2156	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
2157	ISSSTY_v1a_7367_02May011_2690	72869-86-4	HC(H)C(C(=O)OC(H)C(H)OC(=O)NC(H)C(C(H)H)(C(H)H)C(H)C(C(H)H)C(H)C(H)NC(=O)OC(H)C(H)OC(=O)C(C(H)H)=CH)=CH	1
2158	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
2159	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
2160	ISSSTY_v1a_7367_02May011_2693	62613-82-5	HC1C(=O)N(C(H)C(N)=O)C(H)C1O	1
2161	ISSSTY_v1a_7367_02May011_2694	88-69-7	HC(H)C(c1c(O)cccc1)C(H)H	1
2162	ISSSTY_v1a_7367_02May011_2695	120-23-0	HC(C(=O)O)Oc1cc2c(cccc2)cc1	1
2163	ISSSTY_v1a_7367_02May011_2697	35470	c1(N)c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
2164	ISSSTY_v1a_7367_02May011_2698	25003-82-1	c12c(c3c(cc4c(ccnc4)c3)cc1)cccc2	3
2165	ISSSTY_v1a_7367_02May011_2699	110520-17-7	c12c(c3c(c4c1cc1c(ccnc1)c4)cccc3)cccc2	3
2166	ISSSTY_v1a_7367_02May011_2700	24496-65-9	c12c3c4c(c5c(cc4ccc3ccc1)cccc5)cn2	3
2167	ISSSTY_v1a_7367_02May011_2701	24903-48-8	c12c(c3c(cc4c5c(ccc4c3)cccc5)cc1)cncc2	3
2168	ISSSTY_v1a_7367_02May011_2702	218-08-6	c12c(c3c(c4c(cccc4)cc3)cc1)cccc2	3
2169	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
2170	ISSSTY_v1a_7367_02May011_2704	156-43-4	HC(H)C(H)Oc1ccc(N)cc1	3
2171	ISSSTY_v1a_7367_02May011_2705	194-03-6	c12c3c4c(ccc3ccc1)cccc4cn2	3
2172	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
2173	ISSSTY_v1a_7367_02May011_2707	86412-49-9	HC(H)C(=O)N(O)c1cc(Cl)c(CI)cc1	1
2174	ISSSTY_v1a_7367_02May011_2708	18296-44-1	HC(H)C(=O)OC(H)C1c2[C@@]([C@@]3(C(H)O)3)[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
2175	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)c2cc(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
2176	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
2177	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
2178	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
2179	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
2180	ISSSTY_v1a_7367_02May011_2715	7664-38-2	O=P(O)(O)O	1
2181	ISSSTY_v1a_7367_02May011_2716	6915-15-7	HC(C(=O)O)C(O)C(=O)O	1
2182	ISSSTY_v1a_7367_02May011_2717	50-21-5	HC(H)C(O)C(=O)O	1
2183	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
2184	ISSSTY_v1a_7367_02May011_2719	613-47-8	c12c(cc(NO)cc1)cccc2	3







2311	ISSSTY_v1a_7367_02May011_2870	17528-53-9	HC(C(=O)O)Oc1ccc(N(C(H)C(H)Cl)C(H)C(H)Cl)cc1	3
2312	ISSSTY_v1a_7367_02May011_2871	39932-99-5	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
2313	ISSSTY_v1a_7367_02May011_2872	78448-08-5	c12-c3c4c(ccc(O)c4)ccc3Nc1ccc1c2cccc1	3
2314	ISSSTY_v1a_7367_02May011_2873	7297-53-2	c1(C=Cc2cc(Cl)ccc2)ccc(N(=O)=O)cc1	3
2315	ISSSTY_v1a_7367_02May011_2875	61949-77-7	HC(H)C1(C(H)H)[C@](C(=O)OC(H)c2cc(Oc3cccc3)ccc2)[C@@]1C=C(Cl)Cl	1
2316	ISSSTY_v1a_7367_02May011_2876	61949-76-6	HC(H)C1(C(H)H)[C@](C(=O)OC(H)c2cc(Oc3cccc3)ccc2)[C@]1C=C(Cl)Cl	1
2317	ISSSTY_v1a_7367_02May011_2878	585-86-4	HC(O)C(O)C(O)C(C(O)C(H)O)OC1C(O)C(O)C(O)C(C(H)O)O1	1
2318	ISSSTY_v1a_7367_02May011_2879	88381-44-6	HC1C(C(=O)O)N(N=O)C(H)S1	1
2319	ISSSTY_v1a_7367_02May011_2880	143603-81-0	HC(H)c1ccc(C=NC2c3c(cccc3)NC=2C(=O)OC(H)C(H)H)cc1	1
2320	ISSSTY_v1a_7367_02May011_2881	143603-72-9	HC(H)C(H)OC(=O)C1=C(N=Cc2ccc(N(=O)=O)cc2)c2c(cccc2)N1	3
2321	ISSSTY_v1a_7367_02May011_2882	18969	HC(c1ccccc1)NC(=O)C(H)C(H)NNC(=O)c1ccncc1	3
2322	ISSSTY_v1a_7367_02May011_2883	150-60-7	HC(c1ccccc1)SSC(H)c1ccccc1	3
2323	ISSSTY_v1a_7367_02May011_2884	159394-73-7	C(N)c1ccc(C=Cc2ccc(N(=O)=O)cc2)cc1	3
2324	ISSSTY_v1a_7367_02May011_2885	92134-96-8	HC1C(H)N(N=O)C(C(O)C(O)C(O)C(O)C(H)O)S1	3
2325	ISSSTY_v1a_7367_02May011_2886	158729-18-1	c1(S(=O)(=O)Oc2c(Cl)cc(Cl)cc2)c2c(cccn2)ccc1	3
2326	ISSSTY_v1a_7367_02May011_2887	98809-36-0	HC(H)c1ccc(NS(=O)(=O)c2c3c(cccn3)ccc2)cc1	1
2327	ISSSTY_v1a_7367_02May011_2888	736-31-2	c1(C=Cc2ccc([N+](=O)[O-])cc2)ccc([N+](=O)[O-])cc1	3
2328	ISSSTY_v1a_7367_02May011_2890	158729-25-0	c1(S(=O)(=O)Nc2cc(N(=O)=O)ccc2)c2c(cccn2)ccc1	1
2329	ISSSTY_v1a_7367_02May011_2891	158729-27-2	c1(S(=O)(=O)Nc2c(Cl)cc(Cl)cc2)c2c(cccn2)ccc1	1
2330	ISSSTY_v1a_7367_02May011_2892	92134-94-6	HC1C(H)N(N=O)C(C(O)C(O)C(O)C(H)O)S1	1
2331	ISSSTY_v1a_7367_02May011_2893	158729-29-4	c1(S(=O)(=O)Nc2cc(Cl)cc(Cl)c2)c2c(cccn2)ccc1	1
2332	ISSSTY_v1a_7367_02May011_2895	86-59-9	C(=O)Oc1c2c(cccn2)ccc1	1
2333	ISSSTY_v1a_7367_02May011_2896	6456-78-6	C(=O)Oc1c2c(cc(Cl)c1)cccn2	3
2334	ISSSTY_v1a_7367_02May011_2897	64507-38-6	C(=O)Oc1c2c(cc(Br)c1)cccn2	1
2335	ISSSTY_v1a_7367_02May011_2898	68140-48-7	HC(H)C(=O)c1c(C(H)H)cc2C(C(H)H)(C(H)H)C(C(H)H)C(C(H)H)C(H)H)c2c1	1
2336	ISSSTY_v1a_7367_02May011_2899	55706-57-5	HC(H)c1cc(C(=O)O)c2c(cccn2)c1	1
2337	ISSSTY_v1a_7367_02May011_2900	25635-22-7	HC(H)C(H)OC(=O)c1c2c(cccn2)ccc1	1
2338	ISSSTY_v1a_7367_02May011_2901	7297-52-1	c1(C=Cc2ccc(N(=O)=O)cc2)ccc(N)cc1	3
2339	ISSSTY_v1a_7367_02May011_2902	134959-55-0	HC(c1ccccc1)OC(=O)c1c2c(cccn2)ccc1	1
2340	ISSSTY_v1a_7367_02May011_2903	134959-56-1	HC(c1ccc(Cl)cc1)OC(=O)c1c2c(cccn2)ccc1	1
2341	ISSSTY_v1a_7367_02May011_2904	134959-57-2	HC(c1c(Cl)cc(Cl)cc1)OC(=O)c1c2c(cccn2)ccc1	1
2342	ISSSTY_v1a_7367_02May011_2905	38707-70-9	c12c(c(C=O)ccc1)nccc2	3
2343	ISSSTY_v1a_7367_02May011_2906	89060-18-4	c12c(c(C=Nc3cccc3)ccc1)nccc2	3
2344	ISSSTY_v1a_7367_02May011_2907	134959-60-7	HC(H)c1cc(C(=O)O)c(N=Cc2c3c(cccn3)ccc2)cc1	1
2345	ISSSTY_v1a_7367_02May011_2908	491-92-9	HC(H)C(H)N(C(H)C(H)H)C(H)C(H)C(C(H)H)Nc1c2c(cc(OC(H)H)c1)cccn2	3
2346	ISSSTY_v1a_7367_02May011_2909	1929-73-3	HC(H)C(H)C(H)C(H)OC(H)C(H)OC(=O)C(H)Oc1c(Cl)cc(Cl)cc1	1
2347	ISSSTY_v1a_7367_02May011_2910	95-63-6	HC(H)c1c(C(H)H)cc(C(H)H)cc1	1
2348	ISSSTY_v1a_7367_02May011_2911	67274-52-6	HC(H)C(=O)N(O)c1ccc(N(=O)=O)cc1	3
2349	ISSSTY_v1a_7367_02May011_2912	84-24-2	HC(H)C(H)C(H)C(H)C(H)c1c(C(=O)O)c(O)cc2c1Oc1c(C(=O)O2)c(C(H)C(=O)C(H)C(H)C(H)C(H)H)cc(O)c1	1
2350	ISSSTY_v1a_7367_02May011_2913	18296	HC(H)[C@@]12[C@@](O)C(C(=O)C(H)O)[C@](C(H)H)C(H)[C@]1[C@@]1[C@@](F)([C@@]3C(H)H)C(C(H)C(H)H)CC(=O)C=C3[C@@](O)C2H	1
2351	ISSSTY_v1a_7367_02May011_2914	50-47-5	HC(H)NC(H)C(H)C(H)N1c2c(C(H)C(H)c3c1cccc3)cccc2	1
2352	ISSSTY_v1a_7367_02May011_2917	87-33-2	HC1[C@@](ON(=O)=O)[C@@]2[C@]([C@](ON(=O)=O)C(H)O2)O1	1













2563	ISSSTY_v1a_7367_02May011_3176	75996-85-9	HC(H)C(H)OC(=O)C(H)C1=C(C(=O)O)c2c(cccc2)N1C(H)H	1
2564	ISSSTY_v1a_7367_02May011_3177	51630-58-1	HC(H)C(C(H)H)C(c1ccc(Cl)cc1)C(=O)OC(c1cc(Oc2ccccc2)ccc1)C_N	1
2565	ISSSTY_v1a_7367_02May011_3178	110963-29-6	C1(N)c2c(cccc2)NC=1C(=O)NN	3
2566	ISSSTY_v1a_7367_02May011_3179	61-54-1	HC(C1c2c(cccc2)NC=1)C(H)N	1
2567	ISSSTY_v1a_7367_02May011_3180	112653-29-9	HC(O)C1(O)C(H)C(NC(C(H)O)C(H)O)C(O)C(O)C1O	1
2568	ISSSTY_v1a_7367_02May011_3181	107-01-7	HC(H)C=CC(H)H	1
2569	ISSSTY_v1a_7367_02May011_3182	131119-02-3	HC(H)N1c2c(-c3c1c(C(=O)OC(H)C(H)Cl)n(=O)nn3)cccc2	3
2570	ISSSTY_v1a_7367_02May011_3183	77-85-0	HC(H)C(C(H)O)(C(H)O)C(H)O	1
2571	ISSSTY_v1a_7367_02May011_3185	133-37-9	C(=O)(O)C(O)C(O)C(=O)O	1
2572	ISSSTY_v1a_7367_02May011_3186	108-59-8	HC(H)OC(=O)C(H)C(=O)OC(H)H	1
2573	ISSSTY_v1a_7367_02May011_3187	629-11-8	HC(O)C(H)C(H)C(H)C(H)C(H)O	1
2574	ISSSTY_v1a_7367_02May011_3188	13195-64-7	HC(H)C(C(H)H)OC(=O)C(H)C(=O)OC(C(H)H)C(H)H	1
2575	ISSSTY_v1a_7367_02May011_3189	16830-15-2	<small>HC(H)C(C(H)H)OC(=O)C(H)C(=O)OC(C(H)H)C(H)H</small>	1
2576	ISSSTY_v1a_7367_02May011_3190	423-39-2	C(F)(F)(I)C(F)(F)C(F)(F)C(F)(F)F	1
2577	ISSSTY_v1a_7367_02May011_3191	303-98-0	<small>HC(H)C(C(H)H)OC(=O)C(H)C(=O)OC(C(H)H)C(H)H</small>	1
2578	ISSSTY_v1a_7367_02May011_3192	14047-09-7	c1(Cl)c(Cl)cc(N=Nc2cc(Cl)c(Cl)cc2)cc1	1
2579	ISSSTY_v1a_7367_02May011_3193	24245-99-6	C12C(C=C(N(=O)=O)C=C1)=CSN=2	3
2580	ISSSTY_v1a_7367_02May011_3194	7785-26-4	HC(H)C1(C(H)H)[C@@]2C(C(H)H)=CC(H)[C@]1C2H	1
2581	ISSSTY_v1a_7367_02May011_3195	4205-90-7	HC1C(H)N=C(Nc2c(Cl)cccc2Cl)N1	1
2582	ISSSTY_v1a_7367_02May011_3196	54-80-8	HC(H)C(C(H)H)NC(H)C(O)c1cc2c(cccc2)cc1	1
2583	ISSSTY_v1a_7367_02May011_3197	135086-93-0	C1(=O)C2C(c3c(cccc3)N=2)=NNN1N=Cc1ccc(Cl)cc1	3
2584	ISSSTY_v1a_7367_02May011_3198	703-83-3	HC(H)C(H)NC1=C2C(C=CC=C2)=NS1	1
2585	ISSSTY_v1a_7367_02May011_3199	555-66-8	HC(H)C(H)C(H)C(H)C(H)C=CC(=O)C(H)C(H)c1cc(OC(H)H)c(O)cc1	3
2586	ISSSTY_v1a_7367_02May011_3200	37517-30-9	HC(H)C(=O)c1c(OC(H)C(O)C(H)NC(C(H)H)C(H)H)ccc(NC(=O)C(H)C(H)C(H)H)c1	1
2587	ISSSTY_v1a_7367_02May011_3201	844-26-8	c1(Cl)c(O)c(S(=O)c2c(O)c(Cl)cc(Cl)c2)cc(Cl)c1	3
2588	ISSSTY_v1a_7367_02May011_3202	294-93-9	HC1C(H)OC(H)C(H)OC(H)C(H)OC(H)C(H)O1	1
2589	ISSSTY_v1a_7367_02May011_3203	72-69-5	HC(H)NC(H)C(H)C=C1c2c(C(H)C(H)c3c1cccc3)cccc2	1
2590	ISSSTY_v1a_7367_02May011_3204	54-92-2	HC(H)C(C(H)H)NNC(=O)c1ccncc1	1
2591	ISSSTY_v1a_7367_02May011_3206	135086-92-9	C1(=O)C2C(c3c(cccc3)N=2)=NNN1N=Cc1cccc1	3
2592	ISSSTY_v1a_7367_02May011_3207	108-43-0	c1(Cl)cc(O)ccc1	3
2593	ISSSTY_v1a_7367_02May011_3208	135086-91-8	C1(=O)C2C(c3c(cccc3)N=2)=NNN1N=Cc1ccc(N(=O)=O)cc1	3
2594	ISSSTY_v1a_7367_02May011_3209	135086-96-3	HC(H)C(=O)Nc1ccc(C=NN2C(=O)C3C(c4c(cccc4)N=3)=NN2)cc1	3
2595	ISSSTY_v1a_7367_02May011_3210	150114-71-9	C(=O)(O)c1c(Cl)c(N)cc(Cl)n1	1
2596	ISSSTY_v1a_7367_02May011_3211	139953-78-9	HC(H)OC(=O)c1ccc(C=NN2C(=O)C3C(c4c(cccc4)N=3)=NN2)cc1	3
2597	ISSSTY_v1a_7367_02May011_3212	68268-44-0	HC(H)C(C(H)H)C(H)N(C1=C2C(C=CC=C2)=NS1)C(=O)C(H)C(H)Cl	1
2598	ISSSTY_v1a_7367_02May011_3213	135086-94-1	HC(H)Oc1ccc(C=NN2C(=O)C3C(c4c(cccc4)N=3)=NN2)cc1	3
2599	ISSSTY_v1a_7367_02May011_3215	13684-56-5	HC(H)C(H)OC(=O)Nc1cc(OC(=O)Nc2ccccc2)ccc1	1
2600	ISSSTY_v1a_7367_02May011_3217	10125-76-5	O=Nc2ccc(c1ccccc1)cc2	3
2601	ISSSTY_v1a_7367_02May011_3218	99685-96-8	<small>C/21+2C_18+C1_C_16+C_14/C_12/C_27+C1C+2C=30c_23c_28c_31c_11c4c_10c3c3c7c6c3c5c4c_31c_22c_20c5c6c/19c_17c7c_15c8c_13c/24c8c_10c_25c_11c_29C_26.C_12/C1c_13c_14c_15c_16c_17C/18=C_19.C/2</small>	1
2602	ISSSTY_v1a_7367_02May011_3219	2467-03-0	Oc1cccc1Cc2ccc(O)cc2	1
2603	ISSSTY_v1a_7367_02May011_3220	620-92-8	HC(c1ccc(O)cc1)c1ccc(O)cc1	1
2604	ISSSTY_v1a_7367_02May011_3221	301-02-0	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C=CC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(N)=O	1



2647	ISSSTY_v1a_7367_02May011_3283	12789-03-6	HC1C2C3(CI)C(CI)(CI)C(CI)(C(CI)=C3CI)C2C(CI)C1CI	3
2648	ISSSTY_v1a_7367_02May011_3284	963-89-3	HC(H)c1c2c(c3c(cccc3)cc2)nc2c1cc(C(H)H)cc2	3
2649	ISSSTY_v1a_7367_02May011_3287	606-31-5	c1([N+](=O)[O-])c(C=O)c([N+](=O)[O-])ccc1	3
2650	ISSSTY_v1a_7367_02May011_3288	50935-04-1	HC(H)C(=O)[C@@]1(O)C(H)c2c(O)c3C(=O)c4c(C(=O)c3c(O)c2[C@@]1(OC2C(H)C(N)C(O)C(C(H)H)O2)C1H)c(O)ccc4	3
2651	ISSSTY_v1a_7367_02May011_3289	37841-91-1	HC(H)[C@]12[C@@](C=O)(C(C=O)=C[C@@]3C(H)C(C(H)H)(C(H)H)C(H)[C@@]13)C2H	3
2652	ISSSTY_v1a_7367_02May011_3290	2212-99-9	HC(H)C1(C(H)H)C(H)[C@@]2[C@]34[C@](C(C=O)=C[C@@]2C1H)(C(O)OC3=O)C4H	3
2653	ISSSTY_v1a_7367_02May011_3291	119525-97-2	HC(H)C1(C(H)H)C(H)[C@@]2C34C(C(=O)=C[C@@]2(O)[C@]1OC(=O)C=CC(H)C(H)C(H)H)([C@@](O)OC3=O)C4H	3
2654	ISSSTY_v1a_7367_02May011_3292	2402-77-9	c1(CI)c(CI)cccn1	3
2655	ISSSTY_v1a_7367_02May011_3293	147-94-4	HC(O)[C@]1[C@@](O)[C@](O)[C@](N2C(=O)N=C(N)C=C2)O1	1
2656	ISSSTY_v1a_7367_02May011_3294	2402-78-0	c1(CI)cccc(CI)n1	1
2657	ISSSTY_v1a_7367_02May011_3297	146795-34-8	C(=O)(C1C=C(N(=O)=O)SC=1)Nc1cccc1	3
2658	ISSSTY_v1a_7367_02May011_3298	77314-23-9	HC(H)N1c2c(c3c(cc2)nccc3)N=C1NO	3
2659	ISSSTY_v1a_7367_02May011_3299	143924-52-1	c12c(c3c4c5c(C(O)c4c1)cccc5cc3)cccc2	3
2660	ISSSTY_v1a_7367_02May011_3300	98-87-3	c1(C(CI)CI)cccc1	3
2661	ISSSTY_v1a_7367_02May011_3301	3068-88-0	HC(H)C1C(H)C(=O)O1	3
2662	ISSSTY_v1a_7367_02May011_3302	2508-20-5	HC1c2c(-c3c1cc(N=O)cc3)cccc2	3
2663	ISSSTY_v1a_7367_02May011_3303	120302-30-9	HC(C1c2c(cc(N(=O)=O)cc2)NC=1)C(H)O	3
2664	ISSSTY_v1a_7367_02May011_3304	105579-74-6	C1(=O)c2c3c([C@]4c5c(C(=O)[C@@]6[C@@]4O6)c(O)ccc5[C@@]3[C@@]3[C@@]1O3)ccc2O	3
2665	ISSSTY_v1a_7367_02May011_3305	607-59-0	HC(H)N(c1ccc(N=Nc2c3c(cccc3)ccc2)cc1)C(H)H	3
2666	ISSSTY_v1a_7367_02May011_3306	613-65-0	HC(H)N(c1ccc(N=Nc2cc3c(cccc3)cc2)cc1)C(H)H	3
2667	ISSSTY_v1a_7367_02May011_3307	134-58-7	C12C(C(=O)N=C(N)N=1)=NNN2	1
2668	ISSSTY_v1a_7367_02May011_3308	2422-79-9	HC(H)c1c2c3c(ccc2cc2c1cccc2)cccc3	3
2669	ISSSTY_v1a_7367_02May011_3309	78448-09-6	c12-c3c4c(c(O)ccc4)ccc3Nc1ccc1c2cccc1	3
2670	ISSSTY_v1a_7367_02May011_3310	139-59-3	c1(Oc2cccc2)ccc(N)cc1	3
2671	ISSSTY_v1a_7367_02May011_3312	10102-43-9	N=O	3
2672	ISSSTY_v1a_7367_02May011_3316	52671-42-8	c1(Oc2cccc2)ccc(N=O)cc1	3
2673	ISSSTY_v1a_7367_02May011_3317	188107-72-4	HC(H)c1c2-c3c(ccc(C(H)H)c3)Nc2c(C(H)H)cc1N(=O)=O	3
2674	ISSSTY_v1a_7367_02May011_3318	218-02-0	c12c(c3c(c4c(cccc4)cc3)cc1)ccnc2	3
2675	ISSSTY_v1a_7367_02May011_3319	78-85-3	HC(H)C(C=O)=CH	3
2676	ISSSTY_v1a_7367_02May011_3322	102-32-9	HC(c1cc(O)c(O)cc1)C(=O)O	3
2677	ISSSTY_v1a_7367_02May011_3323	128714-76-1	c1([N+](=O)[O-])c2c3c4c(c([N+](=O)[O-])c5c(c4ccc3cc1)cccc5)cc2	3
2678	ISSSTY_v1a_7367_02May011_3324	24463-15-8	HC(O)c1c2c3c4c(ccc3cc1)cccc4cc2	3
2679	ISSSTY_v1a_7367_02May011_3325	1124-33-0	c1([N+](=O)[O-])cc[n+](O)cc1	3
2680	ISSSTY_v1a_7367_02May011_3326	27729-98-2	c1(C(=O)[C@]2[C@@](c3ccc(F)cc3)O2)cccc1	1
2681	ISSSTY_v1a_7367_02May011_3327	6795-23-9	HC(H)Oc1c2C3=C(C(=O)C(H)C3H)C(=O)Oc2c2C3(O)C=COC3Oc2c1	3
2682	ISSSTY_v1a_7367_02May011_3328	25843-45-2	HC(H)[N-][N+](=O)C(H)H	3
2683	ISSSTY_v1a_7367_02May011_3331	33419-42-0	HC(H)[C@]1OC(H)[C@@]2[C@@]([C@](O)[C@@]([C@]1OC)3c4c([C@@]5c5cc(OC(H)H)c(O)c(OC(H)H)c5)[C@]5C(=O)OC(H)[C@@]35)cc3c4)OC(H)O3)O2)O1	1
2684	ISSSTY_v1a_7367_02May011_3335	142438-59-3	HC(H)C12C(C(=O)OC(H)H)(C(=O)OC1C(C(H)H)C(H)H)O2	3
2685	ISSSTY_v1a_7367_02May011_3336	60971-98-4	HC(H)C1(O)C(C(H)H)=C(C(=O)OC(H)H)C(=O)O1	1
2686	ISSSTY_v1a_7367_02May011_3343	628-05-7	HC(H)C(H)C(H)C(H)C(H)N(=O)=O	1
2687	ISSSTY_v1a_7367_02May011_3344	100593-23-5	c1(N(=O)=O)c2c3c4c(c(N=O)ccc4ccc3cc1)cc2	3
2688	ISSSTY_v1a_7367_02May011_3345	85060-01-1	HC(H)C([O-])C(C(H)H)[N+](=O)[O-]	1

2689	ISSSTY_v1a_7367_02May011_3346	5447-99-4	HC(H)C(H)C(C(O)C(H)H)N(=O)=O	1
2690	ISSSTY_v1a_7367_02May011_3347	142457-04-3	HC(H)C12C(C(=O)OC(H)H)(C(=O)NC1(O)C(C(H)H)C(H)H)O2	3
2691	ISSSTY_v1a_7367_02May011_3348	371-40-4	c1(F)ccc(N)cc1	3
2692	ISSSTY_v1a_7367_02May011_3350	15403-45-9	HC(H)OC(=O)c1c(N)ccc(-c2cc(C(=O)OC(H)H)c(N)cc2)c1	3
2693	ISSSTY_v1a_7367_02May011_3351	4309-66-4	c1(C=Cc2ccc(N)cc2)ccccc1	3
2694	ISSSTY_v1a_7367_02May011_3353	26761-45-5	HC(H)C(C(=O)OC(H)C1C(H)O1)(C(H)C(H)H)C(H)C(H)C(C(H)H)C(H)H	3
2695	ISSSTY_v1a_7367_02May011_3354	5493-45-8	HC1C(H)C(H)C(H)C(C(=O)OC(H)C2C(H)O2)C1C(=O)OC(H)C1C(H)O1	3
2696	ISSSTY_v1a_7367_02May011_3355	930-37-0	HC(H)OC(H)C1C(H)O1	3
2697	ISSSTY_v1a_7367_02May011_3356	4016-14-2	HC(H)C(C(H)H)OC(H)C1C(H)O1	3
2698	ISSSTY_v1a_7367_02May011_3357	7665-72-7	HC(H)C(C(H)H)(C(H)H)OC(H)C1C(H)O1	3
2699	ISSSTY_v1a_7367_02May011_3359	2210-79-9	HC(H)c1c(OC(H)C2C(H)O2)ccccc1	3
2700	ISSSTY_v1a_7367_02May011_3360	2425-79-8	HC(C(H)C(H)C(H)OC(H)C1C(H)O1)OC(H)C1C(H)O1	3
2701	ISSSTY_v1a_7367_02May011_3361	17557-23-2	HC(H)C(C(H)H)(C(H)OC(H)C1C(H)O1)C(H)OC(H)C1C(H)O1	3
2702	ISSSTY_v1a_7367_02May011_3362	4584-57-0	HC(H)Nc1ccc(C=Cc2ccc(N(=O)=O)cc2)cc1C(H)H	3
2703	ISSSTY_v1a_7367_02May011_3363	59229-75-3	HC(H)c1c(N)cc(N(=O)=O)cc1N	3
2704	ISSSTY_v1a_7367_02May011_3365	133740-20-2	HC(H)C1=Cc2c(C(=O)O1)c(O)c1c(c2OC(H)H)cc(OC(H)H)cc1O	3
2705	ISSSTY_v1a_7367_02May011_3366	93-52-7	HC(Br)C(Br)c1ccccc1	3
2706	ISSSTY_v1a_7367_02May011_3367	71461-13-7	HC1C(=O)NC(H)C(H)C(H)C(N2C(=O)[C@@]3c4c(ccc(c4)[C@]1NC(H)C(H)C(H)NC(H)C(H)C(H)C2H)O[C@@]3c1ccc(O)cc1	3
2707	ISSSTY_v1a_7367_02May011_3369	476-66-4	C1(=O)c2c3-c4c(C(=O)Oc3c(O)c(O)c2)cc(O)c(O)c4O1	1
2708	ISSSTY_v1a_7367_02May011_3371	420-12-2	HC1C(H)S1	3
2709	ISSSTY_v1a_7367_02May011_3372	2902-96-7	HC(H)C(C(H)O)N(=O)=O	1
2710	ISSSTY_v1a_7367_02May011_3373	68302-57-8	HC(H)C(c1cc2C(=O)c3c(nc(N)c(C(=O)O)c3)Oc2cc1)C(H)H	1
2711	ISSSTY_v1a_7367_02May011_3374	13608-87-2	HC(H)C(=O)c1c(Cl)c(Cl)c(Cl)cc1	3
2712	ISSSTY_v1a_7367_02May011_3375	6270-16-2	HC(H)C(O)C(C(H)H)N(=O)=O	3
2713	ISSSTY_v1a_7367_02May011_3376	5275-46-7	HC(H)C(C(H)H)(N=O)N(=O)=O	3
2714	ISSSTY_v1a_7367_02May011_3377	82-86-0	c12C(=O)C(=O)c3c1c(ccc3)ccc2	3
2715	ISSSTY_v1a_7367_02May011_3378	122-57-6	HC(H)C(=O)C=Cc1ccccc1	3
2716	ISSSTY_v1a_7367_02May011_3379	518-34-3	HC(H)N1C(H)C(H)c2c3c(c(OC(H)H)c(OC(H)H)c2)Oc2c(OC(H)H)cc4c([C@@]1C(H)c5ccc(cc5)O)c5c(OC(H)H)ccc(C(H)[C@@]13)c5)N(C(H)H)C(H)C4H)c2	3
2717	ISSSTY_v1a_7367_02May011_3382	80-08-0	c1(S(=O)(=O)c2ccc(N)cc2)ccc(N)cc1	1
2718	ISSSTY_v1a_7367_02May011_3384	115664-49-8	c1(N(=O)=O)c2c3c(c4c5c(C6C(c(c25)cc1)O6)ccc4)ccccc3	3
2719	ISSSTY_v1a_7367_02May011_3385	114454-59-0	c1(N(=O)=O)c2c3c(c4c5c([C@](O)[C@@](O)(c(c25)cc1)ccc4)ccccc3	3
2720	ISSSTY_v1a_7367_02May011_3386	115664-50-1	c1(O)c2c3c(c4c(c5c(N(=O)=O)ccc(c35)cc2)ccccc4)cc1	3
2721	ISSSTY_v1a_7367_02May011_3387	21626-89-1	HC1c2c(C(=O)N3C(H)c4c(C(=O)N13)ccccc4)ccccc2	1
2722	ISSSTY_v1a_7367_02May011_3388	72-55-9	c1(C(c2ccc(Cl)cc2)=C(Cl)Cl)ccc(Cl)cc1	1
2723	ISSSTY_v1a_7367_02May011_3389	61422-45-5	HC(H)C(H)C(H)C(H)C(H)C(H)NC(=O)N1C(=O)NC(=O)C(F)=C1	1
2724	ISSSTY_v1a_7367_02May011_3390	17902-23-7	HC1C(H)C(H)C(N2C(=O)NC(=O)C(F)=C2)O1	1
2725	ISSSTY_v1a_7367_02May011_3391	832-69-9	HC(H)c1c2c(c3c(ccccc3)cc2)ccc1	3
2726	ISSSTY_v1a_7367_02May011_3392	1576-67-6	HC(H)c1cc2c3c(ccc(C(H)H)c3)ccc2cc1	3
2727	ISSSTY_v1a_7367_02May011_3393	1785-51-9	C1(=O)c2c3c4c(C(=O)C=Cc4cc2)ccc3C=C1	3
2728	ISSSTY_v1a_7367_02May011_3394	2304-85-0	C1(=O)c2c3c4c(C(=O)C=Cc4ccc3C=C1)cc2	3
2729	ISSSTY_v1a_7367_02May011_3395	37962-27-9	C(=O)(C=CC1=CC=C([N+](=O)[O-])O1)NN=CC1=CC=C([N+](=O)[O-])O1	3
2730	ISSSTY_v1a_7367_02May011_3396	494-03-1	HC(Cl)C(H)N(c1cc2c(cccc2)cc1)C(H)C(H)Cl	3

2731	ISSSTY_v1a_7367_02May011_3397	149-91-7	C(=O)(O)c1cc(O)c(O)c(O)c1	1
2732	ISSSTY_v1a_7367_02May011_3399	3132-64-7	HC(Br)C1C(H)O1	3
2733	ISSSTY_v1a_7367_02May011_3400	3083-25-8	HC(C(Cl)(Cl)Cl)C1C(H)O1	3
2734	ISSSTY_v1a_7367_02May011_3401	475-75-2	HC1Oc2c3-c4c(C(=O)c5c3c(cc2O1)ccn5)cccc4	3
2735	ISSSTY_v1a_7367_02May011_3402	129-15-7	HC(H)c1c(N(=O)=O)c2C(=O)c3c(C(=O)c2cc1)cccc3	3
2736	ISSSTY_v1a_7367_02May011_3403	117-05-5	c12C(=O)c3c(C(=O)c1c(NC(=O)c1cccc1)ccc2)cccc3Cl	3
2737	ISSSTY_v1a_7367_02May011_3405	3586-69-4	c12c(cc3c(cc(N(=O)=O)cc3)c1)cccc2	3
2738	ISSSTY_v1a_7367_02May011_3406	353-59-3	C(F)(F)(Cl)Br	3
2739	ISSSTY_v1a_7367_02May011_3407	83-95-4	HC(H)Oc1c(OC(H)H)c2c(c(OC(H)H)c3c(n2)OC=C3)cc1	3
2740	ISSSTY_v1a_7367_02May011_3408	106-90-1	HC1C(C(H)OC(=O)C=CH)O1	3
2741	ISSSTY_v1a_7367_02May011_3409	872-05-9	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C=CH	1
2742	ISSSTY_v1a_7367_02May011_3410	2437-56-1	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C=CH	1
2743	ISSSTY_v1a_7367_02May011_3411	821-95-4	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C=CH	1
2744	ISSSTY_v1a_7367_02May011_3412	13360-61-7	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=CH	1
2745	ISSSTY_v1a_7367_02May011_3413	123-77-3	C(N)(=O)N=NC(N)=O	3
2746	ISSSTY_v1a_7367_02May011_3414	132929-89-6	HC1c2c3c4c5c(c(N(=O)=O)ccc5ccc4cc2C=CC1H)cc3	3
2747	ISSSTY_v1a_7367_02May011_3416	84-56-0	c12c(c3c(cc4c(cccc4)c3)cc1)nccc2	3
2748	ISSSTY_v1a_7367_02May011_3417	366-18-7	c1(-c2ccccn2)ccccn1	3
2749	ISSSTY_v1a_7367_02May011_3418	99217-04-6	HC(H)C(=O)Oc1c2c3c4c(ccc3c(N(=O)=O)c1)cccc4cc2	3
2750	ISSSTY_v1a_7367_02May011_3419	128-08-5	HC1C(=O)N(Br)C(=O)C1H	3
2751	ISSSTY_v1a_7367_02May011_3420	581-47-5	c1(-c2ccccn2)ccncc1	3
2752	ISSSTY_v1a_7367_02May011_3421	4238-71-5	HC(c1cccc1)N1C=CN=C1	3
2753	ISSSTY_v1a_7367_02May011_3422	1148-79-4	c1(-c2cccc(-c3ccccn3)n2)ccccn1	3
2754	ISSSTY_v1a_7367_02May011_3424	110-13-4	HC(H)C(=O)C(H)C(H)C(=O)C(H)H	1
2755	ISSSTY_v1a_7367_02May011_3425	224-42-0	c12c(c3c(cccc3)cc1)cc1c3c(ccc1n2)cccc3	3
2756	ISSSTY_v1a_7367_02May011_3426	97-99-4	HC1C(H)C(H)C(C(H)O)O1	1
2757	ISSSTY_v1a_7367_02May011_3427	1333-38-6	HC(H)C1C=CC(=O)O1	1
2758	ISSSTY_v1a_7367_02May011_3428	109-08-0	HC(H)c1cnccn1	1
2759	ISSSTY_v1a_7367_02May011_3429	5910-89-4	HC(H)c1c(C(H)H)ncn1	1
2760	ISSSTY_v1a_7367_02May011_3430	123-32-0	HC(H)c1cnc(C(H)H)cn1	1
2761	ISSSTY_v1a_7367_02May011_3431	13925-00-3	HC(H)C(H)c1cnccn1	1
2762	ISSSTY_v1a_7367_02May011_3432	14667-55-1	HC(H)c1c(C(H)H)nc(C(H)H)cn1	1
2763	ISSSTY_v1a_7367_02May011_3433	109-97-7	C1C=CNC=1	1
2764	ISSSTY_v1a_7367_02May011_3434	96-54-8	HC(H)N1C=CC=C1	1
2765	ISSSTY_v1a_7367_02May011_3435	554-14-3	HC(H)C1=CC=CS1	1
2766	ISSSTY_v1a_7367_02May011_3436	616-44-4	HC(H)C1C=CSC=1	1
2767	ISSSTY_v1a_7367_02May011_3437	67-71-0	HC(H)S(=O)(=O)C(H)H	1
2768	ISSSTY_v1a_7367_02May011_3438	624-92-0	HC(H)SSC(H)H	1
2769	ISSSTY_v1a_7367_02May011_3439	80-71-7	HC(H)C1=C(O)C(=O)C(H)C1H	1
2770	ISSSTY_v1a_7367_02May011_3440	108-31-6	C1(=O)C=CC(=O)O1	1
2771	ISSSTY_v1a_7367_02May011_3441	104-87-0	HC(H)c1ccc(C=O)cc1	1
2772	ISSSTY_v1a_7367_02May011_3442	32994	HC(H)Oc1c(O)cccc1	1





2815	ISSSTY_v1a_7367_02May011_3494	86-73-7	HC1c2c(-c3c1cccc3)cccc2	1
2816	ISSSTY_v1a_7367_02May011_3495	157989-11-2	HC(H)C(C(H)F)NC(H)C(O)C(H)Oc1c2-c3c(cccc3)Nc2ccc1	3
2817	ISSSTY_v1a_7367_02May011_3498	6271-79-0	c1(-c2cc([N+](=O)[O-])c(N)cc2)cc([N+](=O)[O-])c(N)cc1	3
2818	ISSSTY_v1a_7367_02May011_3499	61841-39-2	c1(-c2cc(N(=O)=O)c(N)cc2)ccc(N)cc1	3
2819	ISSSTY_v1a_7367_02May011_3500	2243-78-9	c1(-c2cc(N(=O)=O)c(N)cc2)ccc(N)cc1	3
2820	ISSSTY_v1a_7367_02May011_3501	611-23-4	HC(H)c1c(N=O)cccc1	3
2821	ISSSTY_v1a_7367_02May011_3502	105802-11-7	HC(H)c1c(N(=O)=O)c2c(c3c1c1c(cccc1)cc3)cccc2	3
2822	ISSSTY_v1a_7367_02May011_3505	33956-49-9	HC(H)C=CC=CC(H)C(H)C(H)C(H)C(H)C(H)O	1
2823	ISSSTY_v1a_7367_02May011_3506	584-48-5	c1(Br)c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
2824	ISSSTY_v1a_7367_02May011_3509	31272-21-6	HC(H)C1C(C(=O)c2c(F)cccc2)=C(N)N(C(H)H)N=1	3
2825	ISSSTY_v1a_7367_02May011_3510	95331-48-9	HC(H)C(=O)N(O)c1c2c3c4c(ccc3cc1)cccc4cc2	3
2826	ISSSTY_v1a_7367_02May011_3513	50438-75-0	HC(H)N(c1ccc(C(H)C(H)O)cc1)C(H)H	3
2827	ISSSTY_v1a_7367_02May011_3517	581-46-4	c1(-c2cccnc2)cccnc1	3
2828	ISSSTY_v1a_7367_02May011_3518	100333-37-7	c12c3c(c4c(c5c(C(O)C(O)C=C5)cc4)c3ccc1)ccc2	3
2829	ISSSTY_v1a_7367_02May011_3519	2381-40-0	HC(H)c1c2c(c3c(cccc3)cc2)nc2c1ccc(C(H)H)c2	3
2830	ISSSTY_v1a_7367_02May011_3520	7570-37-8	HC(H)Oc1ccc(C=Cc2ccc(N)cc2)cc1	3
2831	ISSSTY_v1a_7367_02May011_3521	97136-66-8	HC(H)c1ccc(C=Cc2ccc(N)cc2)cc1	3
2832	ISSSTY_v1a_7367_02May011_3522	79305-82-1	c1(C=Cc2cc(N)ccc2)ccc(N)cc1	3
2833	ISSSTY_v1a_7367_02May011_3523	93535-04-7	c1(C=Cc2cc(Cl)ccc2)ccc(N)cc1	3
2834	ISSSTY_v1a_7367_02May011_3524	108618-28-6	C(N)c1cc(C=Cc2ccc(N)cc2)ccc1	3
2835	ISSSTY_v1a_7367_02May011_3525	108618-29-7	C(N)c1ccc(C=Cc2ccc(N)cc2)cc1	3
2836	ISSSTY_v1a_7367_02May011_3526	56-38-2	HC(H)C(H)OP(=S)(Oc1ccc(N(=O)=O)cc1)OC(H)C(H)H	3
2837	ISSSTY_v1a_7367_02May011_3527	115664-55-6	c1(N(=O)=O)c2c3c(c4c(c3c(O)cc2)cccc4)cc1	3
2838	ISSSTY_v1a_7367_02May011_3528	2531-84-2	HC(H)c1cc2c(c3c(cccc3)cc2)cc1	3
2839	ISSSTY_v1a_7367_02May011_3529	700-02-7	C12C=C(N)N(O)C=N1)N=CN=2	3
2840	ISSSTY_v1a_7367_02May011_3530	10184-51-7	HC(H)N1C2=C(C(=N)N(O)C=N2)N=C1	3
2841	ISSSTY_v1a_7367_02May011_3531	7269-60-5	HC(H)N1c2c(c(NO)ncn2)N=C1	3
2842	ISSSTY_v1a_7367_02May011_3532	4261-14-7	HC(c1cccc1)N1c2c(c(N)ncn2)N=C1	3
2843	ISSSTY_v1a_7367_02May011_3533	50474-48-1	HC(c1cccc1)N1c2c(c(NO)ncn2)N=C1	3
2844	ISSSTY_v1a_7367_02May011_3534	122365-34-8	c1(N)c2c(N(C(c3cccc3)c3cccc3)C=N2)ncn1	3
2845	ISSSTY_v1a_7367_02May011_3535	122365-35-9	C1(=N)C2=C(N(C(c3cccc3)c3cccc3)C=N2)N=CN1O	3
2846	ISSSTY_v1a_7367_02May011_3536	122365-36-0	c1(C(c2cccc2)(c2cccc2)N2C3=C(C(=N)N(O)C=N3)N=C2)cccc1	3
2847	ISSSTY_v1a_7367_02May011_3537	518-83-2	c12C(=O)c3c(C(=O)c1c(O)cc(O)c2)cccc3	3
2848	ISSSTY_v1a_7367_02May011_3539	789-47-9	c12c(c3c(c4c(cc(N)cc4)cc3)cc1)cccc2	3
2849	ISSSTY_v1a_7367_02May011_3541	92279-99-7	HC(H)Oc1c2c(c(NC(H)C(H)C(H)NC(H)C(H)Cl)c3c(cccc3)n2)ccc1	3
2850	ISSSTY_v1a_7367_02May011_3544	151258-40-1	c12C3c4c(c5c(cccc5)cc4)-c1cccc2C(O)C(O)C=3	3
2851	ISSSTY_v1a_7367_02May011_3547	50-30-6	C(=O)(O)c1c(Cl)cccc1Cl	1
2852	ISSSTY_v1a_7367_02May011_3548	6334-18-5	c1(Cl)c(Cl)c(C=O)ccc1	1
2853	ISSSTY_v1a_7367_02May011_3549	51-36-5	C(=O)(O)c1cc(Cl)cc(Cl)c1	1
2854	ISSSTY_v1a_7367_02May011_3550	539-21-9	c1(NN=C(N)N)ccc(N=NC(N)=S)cc1	3
2855	ISSSTY_v1a_7367_02May011_3552	1711-06-4	HC(H)c1cc(C(=O)Cl)ccc1	3
2856	ISSSTY_v1a_7367_02May011_3553	88-95-9	C(=O)(Cl)c1c(C(=O)Cl)cccc1	3

2857	ISSSTY_v1a_7367_02May011_3554	103-80-0	HC(c1ccccc1)C(=O)Cl	3
2858	ISSSTY_v1a_7367_02May011_3555	63885-23-4	HC(H)C(H)N=C(N)N(N=O)N(=O)=O	3
2859	ISSSTY_v1a_7367_02May011_3556	50-79-3	C(=O)(O)c1c(Cl)ccc(Cl)c1	1
2860	ISSSTY_v1a_7367_02May011_3557	14088-71-2	HC1C(H)C1C(O)(c1ccc(Cl)cc1)c1ccc(Cl)cc1	1
2861	ISSSTY_v1a_7367_02May011_3561	1758-33-4	HC(H)[C@]1[C@](C(H)H)O1	3
2862	ISSSTY_v1a_7367_02May011_3562	21490-63-1	HC(H)[C@@]1[C@](C(H)H)O1	3
2863	ISSSTY_v1a_7367_02May011_3563	507-70-0	HC(H)C12C(C(H)H)(C(H)H)C(C(H)C1H)C(H)C2O	1
2864	ISSSTY_v1a_7367_02May011_3564	89-83-8	HC(H)c1cc(O)c(C(C(H)H)C(H)H)cc1	1
2865	ISSSTY_v1a_7367_02May011_3565	23511-78-6	HC(Br)C(H)C(Br)Br	3
2866	ISSSTY_v1a_7367_02May011_3566	22755-15-3	HC(H)C(=O)Nc1c2c3c4c(ccc3cc1)cccc4cc2	3
2867	ISSSTY_v1a_7367_02May011_3568	700481	HC(H)C(H)C(H)C(H)N(C(H)C(H)C(H)C(H)O)N=O	3
2868	ISSSTY_v1a_7367_02May011_3574	51481-10-8	HC(H)[C@@]12[C@@]3(C(H)O3)[C@@]([C@@](O)C1H)O[C@@]1[C@]2(C(H)O)[C@@](O)C(=O)C(C(H)H)=C1	1
2869	ISSSTY_v1a_7367_02May011_3577	524-15-2	HC(H)Oc1c2c(c(OC(H)H)c3c(n2)OC=C3)ccc1	3
2870	ISSSTY_v1a_7367_02May011_3578	60827-45-4	HC(Cl)[C@@](O)C(H)O	3
2871	ISSSTY_v1a_7367_02May011_3580	57090-45-6	HC(Cl)[C@](O)C(H)O	3
2872	ISSSTY_v1a_7367_02May011_3581	2461-42-9	HC1C(C(H)Oc2c3c(cccc3)ccc2)O1	3
2873	ISSSTY_v1a_7367_02May011_3583	14861-17-7	c1(Oc2ccc(N)cc2)c(Cl)cc(Cl)cc1	3
2874	ISSSTY_v1a_7367_02May011_3584	59683-60-2	HC(H)Oc1c(N)ccc(Oc2c(Cl)cc(Cl)cc2)c1	3
2875	ISSSTY_v1a_7367_02May011_3585	109621-20-7	HC(H)C(=O)N[C@@](C(=O)OC(H)H)C(H)SC(H)C(Br)C(H)H	3
2876	ISSSTY_v1a_7367_02May011_3586	155379-81-0	HC(H)C(c1c(N)c(N=O)=O)cc(Nc1)C(H)H	1
2877	ISSSTY_v1a_7367_02May011_3587	114899-77-3	HC(H)c1c2c(c3c1OC(=O)C(H)H)[C@@]1[C@@]4C5c6c(O)c(OC(H)H)c(C(H)H)cc6C(H)C(C)O)N4[C@]3C(H)OC(=O)C3c4c(C(H)H)N3)cc(O)c(OC(H)H)c4)C(H)S1)N5C(H)H)OC(H)O2	3
2878	ISSSTY_v1a_7367_02May011_3589	132059-53-1	C1(=O)C(Br)=C(C(Br)Br)C(O)O1	3
2879	ISSSTY_v1a_7367_02May011_3590	611-09-6	C1(=O)C(=O)c2c(ccc(N(=O)=O)c2)N1	3
2880	ISSSTY_v1a_7367_02May011_3591	132059-52-0	C1(=O)C(Cl)=C(C(Br)Br)C(O)O1	3
2881	ISSSTY_v1a_7367_02May011_3592	73198-02-4	HC1C2c3c(cccc3)NC=2C(C(H)O)NC1C(=O)O	1
2882	ISSSTY_v1a_7367_02May011_3594	126572-78-9	HC(O)C(=C(Cl)C(=O)O)C(Cl)Cl	3
2883	ISSSTY_v1a_7367_02May011_3595	115340-67-5	C(=O)(O)C(Cl)=C(C=O)C(Cl)Cl	3
2884	ISSSTY_v1a_7367_02May011_3596	105596-42-7	c1(N(=O)=O)c2c3c4c(C5C(c3cc1)O5)cccc4cc2	3
2885	ISSSTY_v1a_7367_02May011_3597	105596-43-8	c1(N(=O)=O)c2c3c4c(C5C2O5)cccc4ccc3cc1	3
2886	ISSSTY_v1a_7367_02May011_3598	922-65-6	HC=CC(O)C=CH	3
2887	ISSSTY_v1a_7367_02May011_3599	446-86-6	HC(H)N1C(Sc2c3c(N=CN3)ncn2)=C(N(=O)=O)N=C1	3
2888	ISSSTY_v1a_7367_02May011_3600	132742-02-0	HC1c2c(c(N(=O)=O)O)c3c4c5c(ccc24)cccc5cc3)C=CC1H	3
2889	ISSSTY_v1a_7367_02May011_3603	4836-66-2	HC(O)c1c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
2890	ISSSTY_v1a_7367_02May011_3604	2835-98-5	HC(H)c1cc(O)c(N)cc1	3
2891	ISSSTY_v1a_7367_02May011_3605	23282-20-4	HC(H)[C@@]12[C@@]3(C(H)O3)[C@@]([C@@](O)[C@]1O)O[C@@]1[C@]2(C(H)O)[C@@](O)C(=O)C(C(H)H)=C1	1
2892	ISSSTY_v1a_7367_02May011_3606	106-95-6	HC(Br)C=CH	3
2893	ISSSTY_v1a_7367_02May011_3607	92-55-7	HC(H)C(=O)OC(C1=CC=C(N(=O)=O)O1)OC(=O)C(H)H	3
2894	ISSSTY_v1a_7367_02May011_3608	92758-43-5	c1(N)c2c3c4c(c5c(cc4ccc3cc1)cccc5)cc2	3
2895	ISSSTY_v1a_7367_02May011_3609	88598-59-8	c1(N(=O)=O)c2c3c4c(c5c([C@](O)[C@@](O)C=C5)cc4ccc3cc1)cc2	3
2896	ISSSTY_v1a_7367_02May011_3610	88598-60-1	c1(N(=O)=O)c2c3c4c(c5c(C=C[C@](O)[C@@]5O)cc4ccc3cc1)cc2	3
2897	ISSSTY_v1a_7367_02May011_3619	54364-62-4	HC(H)C(=O)OC(H)C(H)C(H)C(H)C(H)C(H)C(H)C=CC=CC(H)C(H)H	1
2898	ISSSTY_v1a_7367_02May011_3620	517-82-8	HC(H)C(H)C1C(O)=C(O)C2C(=C(O)C(=O)C(=O)C=2O)C=1O	3



2941	ISSSTY_v1a_7367_02May011_3675	7481-89-2	HC1C(H)[C@@](C(H)O)O[C@@]1N1C(=O)N=C(N)C=C1	1
2942	ISSSTY_v1a_7367_02May011_3677	110-57-6	HC(C)C=CC(H)Cl	3
2943	ISSSTY_v1a_7367_02May011_3678	17418-58-5	c12C(=O)c3c(C(=O)c1c(N)c(Oc1cccc1)cc2O)cccc3	3
2944	ISSSTY_v1a_7367_02May011_3680	96-31-1	HC(H)NC(=O)NC(H)H	1
2945	ISSSTY_v1a_7367_02May011_3681	23255-69-8	HC(H)C12C3(C(H)O3)C([C@](O)[C@@]1OC(=O)C(H)H)OC1C2(C(H)O)[C@](O)(C(=O)C(C(H)H)=C1	1
2946	ISSSTY_v1a_7367_02May011_3684	122-60-1	HC1C(C(H)Oc2cccc2)O1	3
2947	ISSSTY_v1a_7367_02May011_3685	66-97-7	c12c(C=CC(=O)O1)cc1c(c2)OC=C1	1
2948	ISSSTY_v1a_7367_02May011_3686	3414-62-8	HC(O)[C@]1[C@@](O)[C@@](O)[C@@](N2c3c(c(NO)ncn3)N=C2)O1	3
2949	ISSSTY_v1a_7367_02May011_3688	5926-90-9	HC(H)C(H)C(H)C(H)C(H)C(H)OC(H)C1C(H)O1	3
2950	ISSSTY_v1a_7367_02May011_3689	542-78-9	HC(C=O)C=O	3
2951	ISSSTY_v1a_7367_02May011_3690	2186-24-5	HC(H)c1ccc(OC(H)C2C(H)O2)cc1	3
2952	ISSSTY_v1a_7367_02May011_3691	56856-83-8	HC(H)C(=O)OC(H)N(C(H)H)N=O	3
2953	ISSSTY_v1a_7367_02May011_3692	621-90-9	HC(H)Nc1ccc(N=Nc2cccc2)cc1	3
2954	ISSSTY_v1a_7367_02May011_3696	121-33-5	HC(H)Oc1c(O)ccc(C=O)c1	1
2955	ISSSTY_v1a_7367_02May011_3697	641-90-7	HC(H)c1cc2C(=O)c3c(C(=O)c2c(O)c1)c(O)c(O)c(O)c3	3
2956	ISSSTY_v1a_7367_02May011_3698	52748-31-9	C1C2C(C=COC=1)O2	1
2957	ISSSTY_v1a_7367_02May011_3699	58917-91-2	c12c3c4c(c5c([C@](O)[C@@](O)[C@@]6[C@@]5O6)cc4ccc3ccc1)cc2	3
2958	ISSSTY_v1a_7367_02May011_3700	31087	c12c(c3c(cccc3)cc1)cccn2	3
2959	ISSSTY_v1a_7367_02May011_3701	22603-58-3	HC(H)c1c([N+](=O)[O-])c(N)c([N+](=O)[O-])cc1[N+](=O)[O-]	3
2960	ISSSTY_v1a_7367_02May011_3702	28995-89-3	c1([N+](=O)[O-])c2c([N+](=O)[O-])cc([N+](=O)[O-])cc2cc([N+](=O)[O-])c1	3
2961	ISSSTY_v1a_7367_02May011_3703	606-35-9	HC(H)Oc1c([N+](=O)[O-])cc([N+](=O)[O-])cc1N(=O)=O	3
2962	ISSSTY_v1a_7367_02May011_3704	131-73-7	c1([N+](=O)[O-])c(Nc2c([N+](=O)[O-])cc([N+](=O)[O-])cc2[N+](=O)[O-])c([N+](=O)[O-])cc([N+](=O)[O-])c1	3
2963	ISSSTY_v1a_7367_02May011_3705	68743-68-0	HC(H)C(H)OC(=O)N(C(H)C(H)C(H)C(=O)c1ccnc1)N=O	3
2964	ISSSTY_v1a_7367_02May011_3706	98911-07-0	HC(H)C(=O)N(O)c1ccc(Oc2ccc(Cl)cc2)cc1	3
2965	ISSSTY_v1a_7367_02May011_3707	71711-58-5	HC(H)c1c2c(c3c(c(N)c4c(cccc4)n3)c1C(H)H)cccc2	3
2966	ISSSTY_v1a_7367_02May011_3709	2798-25-6	HC(H)Oc1cc(O)c2C(=O)c3c(c(O)ccc3O)Oc2c1	3
2967	ISSSTY_v1a_7367_02May011_3710	5557-27-7	HC(H)Oc1c2C(=O)c3c(c(OC(H)H)ccc3O)Oc2cc(OC(H)H)c1	3
2968	ISSSTY_v1a_7367_02May011_3712	642-83-1	HC(H)C(=O)OC1C(=O)OC2C(OC(=O)C(H)H)C(=O)OC12	1
2969	ISSSTY_v1a_7367_02May011_3713	21362-69-6	HC(H)[C@@]12C(H)C(H)[C@@]3[C@@]4(C(H)H)C(H)[C@@]5C(H)C(H)[C@@]4C(H)C(H)[C@@]3[C@@]1C(H)C(H)[C@@]2OC1(OC(H)H)C(H)C(H)C(H)C1H)S5	1
2970	ISSSTY_v1a_7367_02May011_3714	59-14-3	HC(O)C1C(O)C(H)C(N2C(=O)NC(=O)C(Br)=C2)O1	1
2971	ISSSTY_v1a_7367_02May011_3715	1528-74-1	c1(-c2ccc([N+](=O)[O-])cc2)ccc([N+](=O)[O-])cc1	3
2972	ISSSTY_v1a_7367_02May011_3717	1165-39-5	HC(H)Oc1c2C3=C(C(=O)Oc2c2c(c1)OC1C2C=CO1)C(=O)OC(H)C3H	3
2973	ISSSTY_v1a_7367_02May011_3719	394-69-4	c1(F)c2c(ccc1)nccc2	3
2974	ISSSTY_v1a_7367_02May011_3720	394-68-3	c1(F)c2c(cccn2)ccc1	3
2975	ISSSTY_v1a_7367_02May011_3721	55-98-1	HC(H)S(=O)(=O)OC(H)C(H)C(H)C(H)OS(=O)(=O)C(H)H	3
2976	ISSSTY_v1a_7367_02May011_3722	67694-87-5	c12c(c3c([C@@](O)[C@](O)[C@@]4[C@@]3O4)cc1)cccc2	3
2977	ISSSTY_v1a_7367_02May011_3723	67737-62-6	c12c(c3c([C@](O)[C@@](O)[C@@]4[C@@]3O4)cc1)cccc2	3
2978	ISSSTY_v1a_7367_02May011_3724	1169-60-4	HC(H)OC(=O)c1c2c(c3c(c(OC(H)H)ccc3)cc2N(=O)=O)c2c(c1)OC(H)O2	3
2979	ISSSTY_v1a_7367_02May011_3725	35142-06-4	HC(H)OC(=O)c1c2c(c3c(c(OC(H)H)ccc3)cc2)c2c(c1)OC(H)O2	3
2980	ISSSTY_v1a_7367_02May011_3727	611-34-7	c1(N)c2c(ccc1)nccc2	3
2981	ISSSTY_v1a_7367_02May011_3728	578-66-5	c1(N)c2c(cccn2)ccc1	3
2982	ISSSTY_v1a_7367_02May011_3729	79-24-3	HC(H)C(H)N(=O)=O	1