

2983	ISSSTY_v1a_7367_02May011_3732	99333-90-1	c12c3c4c(c(O)c(N(=O)=O)cc4ccc3ccc1)cc2	3
2984	ISSSTY_v1a_7367_02May011_3733	134785-76-5	HC(H)OC(=O)NC1=Nc2c(cc(C(c3ccc(F)cc3)=NO)cc2)N1	3
2985	ISSSTY_v1a_7367_02May011_3735	215-58-7	c12c(c3c(c4c1cc1c(cccc1)c4)cccc3)cccc2	3
2986	ISSSTY_v1a_7367_02May011_3736	1720513	c12c(cc(N=O)cc1)cccc2	3
2987	ISSSTY_v1a_7367_02May011_3737	87185-24-8	c1([N+](=O)[O-])c2c(cc([N+](=O)[O-])c([N+](=O)[O-])c2)ccc1	3
2988	ISSSTY_v1a_7367_02May011_3738	87-56-9	C(=O)(O)C(CI)=C(CI)C=O	3
2989	ISSSTY_v1a_7367_02May011_3739	108342-09-2	HC(C(N)C(=O)O)N=N_N	3
2990	ISSSTY_v1a_7367_02May011_3740	14691-88-4	HC(H)C1(C(H)H)C(H)C([N+](H)H)C(H)C(C(H)H)(C(H)H)N1O	3
2991	ISSSTY_v1a_7367_02May011_3741	117929-15-4	c12c3c4c(cc([N+](=O)[O-])cc4ccc3cc([N+](=O)[O-])c1)cc2	3
2992	ISSSTY_v1a_7367_02May011_3742	779-03-3	c12c(c(N)c3c(cccc3)c1)cccc2	3
2993	ISSSTY_v1a_7367_02May011_3746	6358-53-8	HC(H)Oc1c(NN=C2c3c(C=CC2=O)cccc3)cc(OC(H)H)cc1	3
2994	ISSSTY_v1a_7367_02May011_3747	156243-39-9	HC(H)c1c2c(cc3c1N(C(H)H)C(N)=N3)ncc(C(H)H)n2	3
2995	ISSSTY_v1a_7367_02May011_3748	153954-29-1	HC(H)c1cnc2c(c3c(c(C(H)O)c2)N(C(H)H)C(N)=N3)n1	3
2996	ISSSTY_v1a_7367_02May011_3749	120314-14-9	HC(C1c2c(cccc2)N(N=O)C=1)C(H)O	3
2997	ISSSTY_v1a_7367_02May011_3755	33813-20-6	HC1C(H)N2C(=N1)SSC2=S	1
2998	ISSSTY_v1a_7367_02May011_3758	585-08-0	c12-c3c([C@]4[C@@](c1cccc2)O4)cccc3	3
2999	ISSSTY_v1a_7367_02May011_3760	71382-50-8	c12c(c3c4c5c(C6C(c4c1)N6)cccc5cc3)cccc2	3
3000	ISSSTY_v1a_7367_02May011_3761	2373-51-5	HC(H)SC(H)CI	3
3001	ISSSTY_v1a_7367_02May011_3763	573-12-6	C1(=O)C(=O)c2c(c3c(cccc3)cc2)C=C1	3
3002	ISSSTY_v1a_7367_02May011_3766	64920-32-7	c12c(c3c(c4c(C=C[C@@](O)[C@]4O)cc3)cc1)cccc2	3
3003	ISSSTY_v1a_7367_02May011_3767	96383-86-7	c12c(c3c(c4c([C@@](O)[C@](O)C=C4)cc3)cc1)cc(O)cc2	3
3004	ISSSTY_v1a_7367_02May011_3769	2980-32-7	c12C(=O)c3c(c(O)ccc3O)Oc1cc(O)cc2O	3
3005	ISSSTY_v1a_7367_02May011_3770	37597-20-9	HC(H)Oc1c(OC(H)H)cc2c(C(H)C(H)N(N=O)C2H)c1	3
3006	ISSSTY_v1a_7367_02May011_3771	37850-99-0	HC(H)C(=O)c1c2C(=O)c3c(C(=O)c2c(O)cc1O)c(O)cc(O)c3	1
3007	ISSSTY_v1a_7367_02May011_3775	612-62-4	c12c(ccc(Cl)n1)cccc2	1
3008	ISSSTY_v1a_7367_02May011_3777	132059-51-9	C1(=O)C(CI)=C(C(CI)Br)C(O)O1	3
3009	ISSSTY_v1a_7367_02May011_3778	3722-54-1	HC(H)Oc1c2C(=O)c3c(ccc(OC(H)H)c3)Oc2cc(OC(H)H)c1	3
3010	ISSSTY_v1a_7367_02May011_3779	60-35-5	HC(H)C(N)=O	1
3011	ISSSTY_v1a_7367_02May011_3780	28166-06-5	c1(F)c([N+](=O)[O-])cc(N=N_N)cc1	3
3012	ISSSTY_v1a_7367_02May011_3782	1516-21-8	HC(H)Oc1ccc(N=O)cc1	3
3013	ISSSTY_v1a_7367_02May011_3785	86827-66-9	HC(H)c1c2c3c(C(=O)C(=O)C=C3)ccc2c2c(cccc2)c1	3
3014	ISSSTY_v1a_7367_02May011_3786	111238-10-9	HC(H)c1c2c3c(C(=O)C(=O)C=C3)ccc2cc2c1cccc2	3
3015	ISSSTY_v1a_7367_02May011_3787	71989-02-1	HC(H)c1c2c(c3c(C(=O)C(=O)C=C3)cc2)cc2c1cccc2	3
3016	ISSSTY_v1a_7367_02May011_3788	55022-75-8	[C@@]12[C@@](C3[C@@]4[C@](C1N=N3)O4)O2	1
3017	ISSSTY_v1a_7367_02May011_3789	52748-34-2	C(=O)C1C=COC=C1	1
3018	ISSSTY_v1a_7367_02May011_3790	4245-77-6	HC(H)C(H)N(C(N)=NN(=O)=O)N=O	3
3019	ISSSTY_v1a_7367_02May011_3791	56183-24-5	c12-c3c(c4c(cccc4)cc3)[C@@](O)[C@](O)c1cccc2	1
3020	ISSSTY_v1a_7367_02May011_3792	54083-22-6	HC(H)C([C@@]1(O)C(H)c2c(O)c3C(=O)c4c(C(=O)c3c(O)c2[C@@](OC2C(H)C(N)C(O)C(C(H)H)O2)C1H)c(OC(H)H)ccc4)=NNC(=O)c1cccc1	3
3021	ISSSTY_v1a_7367_02May011_3793	56420-45-2	HC(H)[C@@]1[C@](O)[C@@](N)C(H)[C@](O)[C@]2c3c(O)c4C(=O)c5c(C(=O)c4c(O)c3C(H)[C@](O)(C(=O)C(H)O)C2H)cccc5OC(H)H)O1	3
3022	ISSSTY_v1a_7367_02May011_3794	63710-10-1	HC(H)C(H)[C@]1(O)C(H)[C@@](OC2C(H)C(N)C(H)C(H)C(OC3C(H)C(O)C(OC4C(H)C(O)C(C(H)H)O4)C(C(H)H)O3)C(C(H)H)O2)2c(O)c3C(=O)c4c(C(=O)c3cc2[C@@]1C(=O)OC(H)H)c(O)ccc4O	3
3023	ISSSTY_v1a_7367_02May011_3795	3930-19-6	HC(H)C1C(=C2C(=O)C(OC(H)H)=C(OC(H)H)C=C2)C(N)=C(c2ccc3C(=O)C(OC(H)H)=C(N)C(=O)c3n2)NC=1C(=O)O	3
3024	ISSSTY_v1a_7367_02May011_3799	129-66-8	C(=O)(O)c1c([N+](=O)[O-])cc([N+](=O)[O-])cc1[N+](=O)[O-]	3

3025	ISSSTY_v1a_7367_02May011_3800	195-68-6	c12c(c3c4c(C=CS4)ccc3cc1)cccc2	3
3026	ISSSTY_v1a_7367_02May011_3801	2226-96-2	HC(H)C1(C(H)H)C(H)C(O)C(H)C(C(H)H)(C(H)H)N1O	3
3027	ISSSTY_v1a_7367_02May011_3802	619-24-9	C(N)c1cc(N(=O)=O)ccc1	3
3028	ISSSTY_v1a_7367_02May011_3803	610-67-3	HC(H)C(H)Oc1c(N(=O)=O)cccc1	3
3029	ISSSTY_v1a_7367_02May011_3804	3740-52-1	HC(c1c(N(=O)=O)cccc1)C(=O)O	3
3030	ISSSTY_v1a_7367_02May011_3805	104-03-0	HC(c1ccc(N(=O)=O)cc1)C(=O)O	3
3031	ISSSTY_v1a_7367_02May011_3809	87-68-3	C(Cl)(C(Cl)=C(Cl)Cl)=C(Cl)Cl	3
3032	ISSSTY_v1a_7367_02May011_3811	106671-91-4	c1(C2=C(N=O)N3C(=N2)SC=C3)ccc(Cl)cc1	3
3033	ISSSTY_v1a_7367_02May011_3812	106671-90-3	c1(C2=C(N=O)N3C(=N2)SC=C3)ccc(N(=O)=O)cc1	3
3034	ISSSTY_v1a_7367_02May011_3813	106636-46-8	HC(H)C1=CN2C(N=O)=C(c3ccc(N(=O)=O)cc3)N=C2S1	3
3035	ISSSTY_v1a_7367_02May011_3814	106671-89-0	c1(C2=C(N(=O)=O)N3C(=N2)SC=C3)ccc(Cl)cc1	3
3036	ISSSTY_v1a_7367_02May011_3815	16311-38-9	c1(C2=C([N+](=O)[O-])N3C(=N2)SC=C3)ccc([N+](=O)[O-])cc1	3
3037	ISSSTY_v1a_7367_02May011_3816	95152-79-7	HC(H)C1=CN2C([N+](=O)[O-])=C(c3ccc([N+](=O)[O-])cc3)N=C2S1	3
3038	ISSSTY_v1a_7367_02May011_3817	106636-50-4	HC(H)c1ccc(C2=C(N(=O)=O)N3C(=N2)SC(H)C3H)cc1	3
3039	ISSSTY_v1a_7367_02May011_3818	106636-49-1	HC1C(H)N2C(N(=O)=O)=C(c3ccc(Cl)cc3)N=C2S1	3
3040	ISSSTY_v1a_7367_02May011_3819	106636-48-0	HC1C(H)N2C([N+](=O)[O-])=C(c3ccc([N+](=O)[O-])cc3)N=C2S1	3
3041	ISSSTY_v1a_7367_02May011_3820	6098-44-8	HC(H)C(=O)N(c1cc2c(-c3c(cccc3)C2H)cc1)OC(=O)C(H)H	3
3042	ISSSTY_v1a_7367_02May011_3826	30039-44-2	HC(H)C(H)C(=O)OC(H)c1ccc(N(=O)=O)cc1	3
3043	ISSSTY_v1a_7367_02May011_3827	84761-86-4	c12-c3c(Cl)cccc3Oc1cccc2	1
3044	ISSSTY_v1a_7367_02May011_3828	100-11-8	HC(Br)c1ccc(N(=O)=O)cc1	3
3045	ISSSTY_v1a_7367_02May011_3830	150446-03-0	HC(H)C1=C(C=NOC(H)c2cccc2)c2c(ccc([N+](=O)[O-])c2)N1C(H)c1cc([N+](=O)[O-])ccc1	3
3046	ISSSTY_v1a_7367_02May011_3831	51230-49-0	c12-c3c(ccc(Cl)c3)Oc1cccc2	3
3047	ISSSTY_v1a_7367_02May011_3833	25074-67-3	c12-c3c(ccc(Cl)c3)Oc1cccc2	3
3048	ISSSTY_v1a_7367_02May011_3834	150446-01-8	HC(H)C1=C(C=NOC(H)c2c(Cl)cc(Cl)cc2)c2c(ccc(N(=O)=O)c2)N1C(H)c1ccc(Cl)cc1	1
3049	ISSSTY_v1a_7367_02May011_3835	74992-96-4	c12-c3c(c(Cl)ccc3)Oc1cccc2	1
3050	ISSSTY_v1a_7367_02May011_3836	71424-66-3	HC(H)c1c2c(C(=CH)C(H)C(H)C3C(C(H)H)(C(H)H)C23)c2C(=O)[C@@](C(H)H)C(H)c2c1O	1
3051	ISSSTY_v1a_7367_02May011_3837	207-09-0	c12c3c(c4c(c3ccc1)cc1c(cccc1)n4)ccc2	1
3052	ISSSTY_v1a_7367_02May011_3838	103630-34-8	HC(H)C1C(=O)C2=C(C(=O)[C@](C(H)H)C2H)C2C(=CH)C(H)C(H)C(C(C(H)H)=CH)[C@@]2C=1	1
3053	ISSSTY_v1a_7367_02May011_3839	55610-00-9	HC1Oc2c3c4c(C(=O)Nc4cc4c3cccc4)cc2O1	3
3054	ISSSTY_v1a_7367_02May011_3841	103667-52-3	HC(H)C1C(=O)C2=C(C(=O)[C@@](C(H)H)C2H)C2C(=CH)C(H)C(H)C(C(C(H)H)=CH)[C@@]2C=1	1
3055	ISSSTY_v1a_7367_02May011_3842	38965-71-8	HC1Oc2c3c(c(C(=O)O)cc2O1)c(N(=O)=O)cc1c(O)cccc31	3
3056	ISSSTY_v1a_7367_02May011_3844	103630-35-9	HC(H)[C@@]1(O)C(=O)C2=C(C(=O)C(C(H)H)=C[C@]3C(C(C(H)H)=CH)C(H)C(H)C(=CH)C23)C1H	1
3057	ISSSTY_v1a_7367_02May011_3847	103667-53-4	HC(H)[C@]1(O)C(=O)C2=C(C(=O)C(C(H)H)=C[C@]3C(C(C(H)H)=CH)C(H)C(H)C(=CH)C23)C1H	1
3058	ISSSTY_v1a_7367_02May011_3852	2562-38-1	HC1C(H)C(H)C(H)C1N(=O)=O	3
3059	ISSSTY_v1a_7367_02May011_3853	29916-56-1	HC1[C-](N(=O)=O)C(H)C(H)C1H	3
3060	ISSSTY_v1a_7367_02May011_3854	17683-09-9	HC(H)c1ccc(NN=NC(H)c2cccc2)cc1	3
3061	ISSSTY_v1a_7367_02May011_3855	24463-19-2	HC(Cl)c1c2c(cc3c1cccc3)cccc2	3
3062	ISSSTY_v1a_7367_02May011_3856	22788-18-7	HC(C(=O)O)C(H)OP(N)(=O)N(C(H)C(H)Cl)C(H)C(H)Cl	3
3063	ISSSTY_v1a_7367_02May011_3857	10159-53-2	HC(Cl)C(H)N(C(H)C(H)Cl)P(N)(=O)O	3
3064	ISSSTY_v1a_7367_02May011_3858	27046-19-1	HC1C(=O)NP(=O)(N(C(H)C(H)Cl)C(H)C(H)Cl)OC1H	3
3065	ISSSTY_v1a_7367_02May011_3859	57470-04-9	c1(Cl)ccc(N(O)C=O)cc1	3
3066	ISSSTY_v1a_7367_02May011_3860	1503-91-9	HC(H)C(=O)N(O)c1ccc(Cl)cc1	1

3067	ISSSTY_v1a_7367_02May011_3861	68299-98-9	HC(O)C(=O)N(O)c1ccc(Cl)cc1	1
3068	ISSSTY_v1a_7367_02May011_3862	14385-22-9	HC(H)C(C(=O)N(O)c1ccc(Cl)cc1)C(H)H	3
3069	ISSSTY_v1a_7367_02May011_3863	81576-12-7	HC(C(=O)N(O)c1ccc(Cl)cc1)C(H)C(=O)O	3
3070	ISSSTY_v1a_7367_02May011_3864	31335-69-0	c1(NC(=O)O)ccccc1	1
3071	ISSSTY_v1a_7367_02May011_3865	96018-73-4	c1(Br)ccc(N(O)C=O)cc1	3
3072	ISSSTY_v1a_7367_02May011_3866	96018-75-6	c1(Cl)cc(N(O)C=O)ccc1	1
3073	ISSSTY_v1a_7367_02May011_3867	73747-07-6	HC(H)c1ccc(N(O)C=O)cc1	3
3074	ISSSTY_v1a_7367_02May011_3868	27451-21-4	HC(H)c1ccc(N(O)C(=O)C(H)H)cc1	1
3075	ISSSTY_v1a_7367_02May011_3869	1795-83-1	HC(H)C(=O)N(O)c1ccccc1	1
3076	ISSSTY_v1a_7367_02May011_3870	135-68-2	c1(-c2ccc(N)cc2)ccc(Cl)cc1	3
3077	ISSSTY_v1a_7367_02May011_3871	1211-40-1	c1(-c2ccc(N(=O)=O)cc2)ccc(N)cc1	3
3078	ISSSTY_v1a_7367_02May011_3872	13024-49-2	HC(c1ccc(N)cc1)C(H)c1ccccc1	3
3079	ISSSTY_v1a_7367_02May011_3873	1204-41-7	HC(H)c1c(-c2ccc(N)cc2)cccc1	3
3080	ISSSTY_v1a_7367_02May011_3876	133960-21-1	HC(H)C(=O)ONC1=C(c2ccccc2)C(c2ccccc2)=C(C(=O)OC(H)H)O1	1
3081	ISSSTY_v1a_7367_02May011_3877	111205-70-0	HC(H)OC(=O)C1=C(c2ccccc2)C(c2ccccc2)=C(NO)O1	1
3082	ISSSTY_v1a_7367_02May011_3878	133960-22-2	HC(H)C(=O)N(O)C1=C(c2ccccc2)C(c2ccccc2)=C(C(=O)OC(H)H)O1	1
3083	ISSSTY_v1a_7367_02May011_3879	134170-56-2	HC(H)C(=O)N(C1=C(c2ccccc2)C(c2ccccc2)=C(C(=O)OC(H)H)O1)OC(=O)C(H)H	1
3084	ISSSTY_v1a_7367_02May011_3880	121-87-9	c1(N)c(Cl)cc(N(=O)=O)cc1	3
3085	ISSSTY_v1a_7367_02May011_3882	135325-62-1	HC(Br)c1c2c3c(c4c2c(ccc4)cc1)cccc3	3
3086	ISSSTY_v1a_7367_02May011_3883	1476-11-5	HC(Cl)C=CC(H)Cl	3
3087	ISSSTY_v1a_7367_02May011_3884	88746-58-1	HC(Br)c1cc2c3c(c4c(c3ccc2)cccc4)c1	3
3088	ISSSTY_v1a_7367_02May011_3886	135294-98-3	HC(Br)c1c2c3c(c4c(c3ccc2)cccc4)cc1	3
3089	ISSSTY_v1a_7367_02May011_3888	77061-07-5	HC(Br)c1c2c(c3c4c(cccc24)ccc3)ccc1	3
3090	ISSSTY_v1a_7367_02May011_3890	126831-76-3	HC(Br)c1cc2c(c3c4c(cccc24)ccc3)cc1	3
3091	ISSSTY_v1a_7367_02May011_3892	71721-78-3	c1(Cl)c(Cl)cc2c(c1)Oc1c(cc(N(=O)=O)cc1)O2	3
3092	ISSSTY_v1a_7367_02May011_3893	71712-70-4	c12c(cc(Cl)c(N(=O)=O)c1)Oc1c(cc(Cl)c(Cl)c1)O2	3
3093	ISSSTY_v1a_7367_02May011_3894	142741-09-1	c12-c3c(c([N+])(=O)[O-])cc([N+](=O)[O-])c3)Nc1cnc([N+](=O)[O-])c2	3
3094	ISSSTY_v1a_7367_02May011_3895	101126-67-4	c1(Cl)c(N(=O)=O)c(Cl)c2c(c1)Oc1c(cc(Cl)c(Cl)c1)O2	1
3095	ISSSTY_v1a_7367_02May011_3896	101126-65-2	c1(Cl)c(Cl)c2c(c(Cl)c1N(=O)=O)Oc1c(cc(Cl)c(Cl)c1)O2	3
3096	ISSSTY_v1a_7367_02May011_3897	97055-37-3	C(=O)(O)C(Cl)=C(C(Cl)Cl)C(Cl)Cl	3
3097	ISSSTY_v1a_7367_02May011_3899	24930-41-4	c12c(c3c4c5c(ccc4n1)cccc5cc3)cccc2	3
3098	ISSSTY_v1a_7367_02May011_3900	129665-16-3	c12c(c3c4c5c(ccc4n1=O)cccc5cc3)cccc2	3
3099	ISSSTY_v1a_7367_02May011_3901	89925-00-8	HC(H)C1(C(N)=O)C(H)O1	3
3100	ISSSTY_v1a_7367_02May011_3905	78468-34-5	HC(O)c1c(N)cc(N(=O)=O)cc1	3
3101	ISSSTY_v1a_7367_02May011_3906	22996-17-4	HC(O)c1c(N(=O)=O)cc(N)cc1	3
3102	ISSSTY_v1a_7367_02May011_3911	14692-41-2	HC(H)N1c2c(c3c(cc2)nccc3)N=C1	3
3103	ISSSTY_v1a_7367_02May011_3912	92116-66-0	HC(H)c1cnc2c(c3c(cc2)N(C(H)H)C=N3)n1	1
3104	ISSSTY_v1a_7367_02May011_3913	303-45-7	HC(H)c1c(-c2c(O)c3c(c(C(C(H)H)C(H)H)c(O)c(O)c3C=O)cc2C(H)H)c(O)c2c(c(C(C(H)H)C(H)H)c(O)c(O)c2C=O)c1	1
3105	ISSSTY_v1a_7367_02May011_3914	14204-98-9	HC(H)Nc1c(N)c2c(cc1)nccc2	1
3106	ISSSTY_v1a_7367_02May011_3915	83407-42-5	HC(H)c1c(NC(H)H)c(N)c2c(c1)nccc2	1
3107	ISSSTY_v1a_7367_02May011_3916	92116-67-1	HC(H)c1cnc2c(c(N)c(NC(H)H)cc2)n1	1
3108	ISSSTY_v1a_7367_02May011_3917	27321-96-6	HC(H)C12C(C(H)C(OC(H)C(H)O)C(H)C1H)=CC(H)C1C3C(C(H)H)C(H)C(H)C21)C(C(C(H)H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C3H	1

3109	ISSSTY_v1a_7367_02May011_3919	109875-47-0	HC(O)[C@]1[C@@](O)[C@@](O)[C@](N2c3c(c(N)nc(-c4cc(N(=O)=O)ccc4)n3)N=C2)O1	3
3110	ISSSTY_v1a_7367_02May011_3920	23788-22-9	c1(O)ccc(ON2P(Oc3ccc(O)cc3)N(Oc3ccc(O)cc3)P(Oc3ccc(O)cc3)N=P2(Oc2ccc(O)cc2)Oc2ccc(O)cc2)cc1	1
3111	ISSSTY_v1a_7367_02May011_3922	51410-45-8	HC(H)Oc1ccc(C(H)C2C(H)O2)cc1	3
3112	ISSSTY_v1a_7367_02May011_3924	124617-84-1	HC(H)C(=O)OC(H)C(H)C(H)C(H)ONC(=O)c1cccc1	3
3113	ISSSTY_v1a_7367_02May011_3925	31383-81-0	HC(H)OC(=O)c1c(N)ccc(C(H)c2cc(C(=O)OC(H)H)c(N)cc2)c1	3
3114	ISSSTY_v1a_7367_02May011_3926	124617-86-3	HC(H)C(=O)ON(C(=O)c1cccc1)OC(H)c1cccc1	3
3115	ISSSTY_v1a_7367_02May011_3927	7330-46-3	HC(c1cc(C(=O)O)c(N)cc1)c1cc(C(=O)O)c(N)cc1	1
3116	ISSSTY_v1a_7367_02May011_3928	15403-44-8	HC(H)C(H)OC(=O)c1c(N)ccc(C(H)c2cc(C(=O)OC(H)C(H)H)c(N)cc2)c1	1
3117	ISSSTY_v1a_7367_02May011_3929	70883-13-5	HC(H)C(H)Sc1c(N)ccc(C(H)c2cc(SC(H)C(H)H)c(N)cc2)c1	3
3118	ISSSTY_v1a_7367_02May011_3931	135105-89-4	HC(H)Oc1c2c(cc(OC(H)H)c1)O[C@]1[C@@]2C=CO1	3
3119	ISSSTY_v1a_7367_02May011_3932	130933-92-5	c12c3c(c4c(c5c(C6C(C=C5)O6)cc4)cc3ccc1)C=C2	3
3120	ISSSTY_v1a_7367_02May011_3933	508-71-4	HC(H)C12C34C(H)C(H)C(H)C(C(H)H)(C(=O)O3)C4C(H)C(=O)C1C(H)C(C(H)H)(C=CH)C(H)C2H	1
3121	ISSSTY_v1a_7367_02May011_3934	610-48-0	HC(H)c1c2c(cc3c(cccc3)c2)ccc1	1
3122	ISSSTY_v1a_7367_02May011_3935	5806-00-8	HC(H)c1c([N-][N+](=O)c2c(C(H)H)c([N+](=O)[O-])ccc2)cccc1N(=O)=O	1
3123	ISSSTY_v1a_7367_02May011_3936	143922-97-8	HC(H)c1c(N)cccc1N=Nc1c(C(H)H)c(N)ccc1	3
3124	ISSSTY_v1a_7367_02May011_3937	27532-75-8	HC(H)c1c2c(cc3c1cc(C(H)H)cc3)cccc2	3
3125	ISSSTY_v1a_7367_02May011_3938	781-43-1	HC(H)c1c2c(c(C(H)H)c3c1cccc3)cccc2	3
3126	ISSSTY_v1a_7367_02May011_3939	28434-01-7	HC(H)C1(C(H)H)C(C(=O)OC(H)C2C=C(C(H)c3cccc3)OC=2)C1C=C(C(H)H)C(H)H	1
3127	ISSSTY_v1a_7367_02May011_3940	63018-94-0	HC(H)c1c2c(c(C(H)H)c3c1cc(C(H)H)cc3)cccc2	3
3128	ISSSTY_v1a_7367_02May011_3941	66552-77-0	HC(H)c1c2c(c(C(H)H)c3c1cc(C(H)H)c(C(H)H)c3)cccc2	3
3129	ISSSTY_v1a_7367_02May011_3942	481-39-0	C1(=O)c2c(C(=O)C=C1)c(O)ccc2	3
3130	ISSSTY_v1a_7367_02May011_3943	26148-68-5	c12-c3c(cccc3)Nc1nc(N)cc2	3
3131	ISSSTY_v1a_7367_02May011_3944	91259-16-4	c1(N(=O)=O)c2c3c(c4c5c(ccc(c25)cc1)ccc4)cccc3	3
3132	ISSSTY_v1a_7367_02May011_3946	838-88-0	HC(H)c1c(N)ccc(C(H)c2cc(C(H)H)c(N)cc2)c1	1
3133	ISSSTY_v1a_7367_02May011_3947	54-91-1	HC(C(=O)N1C(H)C(H)N(C(=O)C(H)C(H)Br)C(H)C1H)C(H)Br	3
3134	ISSSTY_v1a_7367_02May011_3948	54954-12-0	HC(O)[C@]1[C@@](O)[C@](O)[C@@](O)[C@](Oc2c3C(=O)c4c(O)cc(O)cc4Oc3c(O)cc2)O1	3
3135	ISSSTY_v1a_7367_02May011_3949	23445-00-3	HC(H)Oc1cc(O)c2C(=O)c3c(c(O)ccc3O[C@@]3[C@](O)[C@@](O)[C@](O)[C@@](C(H)O)O3)Oc2c1	3
3136	ISSSTY_v1a_7367_02May011_3950	574-25-4	HC(O)[C@]1[C@@](O)[C@@](O)[C@@](N2C3=C(C(=S)N=CN3)N=C2)O1	3
3137	ISSSTY_v1a_7367_02May011_3952	104-78-9	HC(H)C(H)N(C(H)C(H)H)C(H)C(H)C(H)N	1
3138	ISSSTY_v1a_7367_02May011_3953	965-52-6	C(=O)(c1ccc(O)cc1)NN=CC1=CC=C(N(=O)=O)O1	3
3139	ISSSTY_v1a_7367_02May011_3956	89-62-3	HC(H)c1cc(N(=O)=O)c(N)cc1	1
3140	ISSSTY_v1a_7367_02May011_3957	128-13-2	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@](O)[C@@]3[C@@]1C(H)C(H)[C@@]2[C@](C(H)H)C(H)C(H)C(=O)O	3
3141	ISSSTY_v1a_7367_02May011_3958	75888-03-8	HC1C(H)C(H)N(N=CC2=CC=C(N(=O)=O)O2)C(=O)N1	3
3142	ISSSTY_v1a_7367_02May011_3959	97509-29-0	c12c(c(N(=O)=O)c3c(C=C[C@@](O)[C@](O)3O)c1)cccc2	1
3143	ISSSTY_v1a_7367_02May011_3960	97509-27-8	c12c(c(N(=O)=O)c3c([C@@](O)[C@](O)C=C3)c1)cccc2	3
3144	ISSSTY_v1a_7367_02May011_3961	58-19-5	HC(H)[C@]12C(H)C(H)[C@@]3[C@@]4(C(H)H)C(H)[C@@](C(H)H)C(=O)C(H)[C@@]4C(H)C(H)[C@]3[C@@]1C(H)C(H)[C@]2O	1
3145	ISSSTY_v1a_7367_02May011_3962	299-75-2	HC(H)S(=O)(=O)OC(H)C(O)C(O)C(H)OS(=O)(=O)C(H)H	3
3146	ISSSTY_v1a_7367_02May011_3964	6264-66-0	c1(N)c(N)cc(Oc2ccc(N)cc2)cc1	3
3147	ISSSTY_v1a_7367_02May011_3965	947-72-8	c1(Cl)c2c(c3c(cccc3)c1)cccc2	3
3148	ISSSTY_v1a_7367_02May011_3966	4985-70-0	c1(Cl)c2c(cc3c(cccc3)c2)ccc1	1
3149	ISSSTY_v1a_7367_02May011_3967	17135-78-3	c12c(cc3c(cc(Cl)cc3)c1)cccc2	3
3150	ISSSTY_v1a_7367_02May011_3968	40277-05-2	HC1C(H)C(O)NP(=O)(N(C(H)C(H)Cl)C(H)C(H)Cl)O1	3

3151	ISSSTY_v1a_7367_02May011_3970	103-76-4	HC(O)C(H)N1C(H)C(H)NC(H)C1H	1
3152	ISSSTY_v1a_7367_02May011_3971	109-02-4	HC(H)N1C(H)C(H)OC(H)C1H	1
3153	ISSSTY_v1a_7367_02May011_3973	81407-76-3	HC(H)C1(C(H)H)[C@]2[C@@]3[C@](O)(C(=O)C(C=CC(H)H)=CC3=O)O1)C2H	3
3154	ISSSTY_v1a_7367_02May011_3974	16238-56-5	HC(H)c1c2c(c(C(H)Br)c3c1c1c(cccc1)cc3)cccc2	3
3155	ISSSTY_v1a_7367_02May011_3975	103-83-3	HC(H)N(C(H)H)C(H)c1cccc1	1
3156	ISSSTY_v1a_7367_02May011_3976	99803-60-8	HC(H)c1c(N=O)ccc(OP(=S)(OC(H)H)OC(H)H)c1	3
3157	ISSSTY_v1a_7367_02May011_3977	13306-69-9	HC(H)c1c(N)ccc(OP(=S)(OC(H)H)OC(H)H)c1	3
3158	ISSSTY_v1a_7367_02May011_3978	96018-74-5	c1(F)ccc(N(O)C=O)cc1	3
3159	ISSSTY_v1a_7367_02May011_3979	500873	HC(H)N1C(=O)c2c3c(c(OC(H)H)ccc3C1=O)ccc2	1
3160	ISSSTY_v1a_7367_02May011_3981	142382-11-4	HC(C(=O)C=Cc1ccc(C(=O)O)cc1)C(H)C_N	1
3161	ISSSTY_v1a_7367_02May011_3982	67274-48-0	HC(H)C(=O)N(O)c1ccc(Br)cc1	1
3162	ISSSTY_v1a_7367_02May011_3984	619-15-8	HC(H)c1c([N+](=O)[O-])ccc([N+](=O)[O-])c1	3
3163	ISSSTY_v1a_7367_02May011_3985	99675-03-3	HC(H)C(C(H)H)NP(=S)(Oc1c(C(=O)OC(C(H)H)C(H)H)cccc1)OC(H)H	1
3164	ISSSTY_v1a_7367_02May011_3986	14992-81-5	C(Cl)(c1c(Cl)c(Cl)ccc1)=C(Cl)Cl	1
3165	ISSSTY_v1a_7367_02May011_3988	90301-92-1	C(Cl)(c1c(Cl)c(Cl)c(Cl)cc1)=C(Cl)Cl	1
3166	ISSSTY_v1a_7367_02May011_3989	29086-38-2	C(Cl)(c1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl)=CCl	1
3167	ISSSTY_v1a_7367_02May011_3990	39179-91-4	HC(H)c1ccc(NC(H)C(H)Cl)cc1	3
3168	ISSSTY_v1a_7367_02May011_3991	29086-39-3	C(Cl)(c1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl)=CCl	1
3169	ISSSTY_v1a_7367_02May011_3992	29082-75-5	c1(Cl)c(Cl)c(Cl)c(Cl)c(Cl)c1C=C(Cl)Cl	1
3170	ISSSTY_v1a_7367_02May011_3994	29082-74-4	C(Cl)(c1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl)=C(Cl)Cl	1
3171	ISSSTY_v1a_7367_02May011_3995	2687-41-4	HC(H)C(=O)Nc1ccc(Oc2ccc(N)cc2)cc1	3
3172	ISSSTY_v1a_7367_02May011_3996	3070-86-8	HC(H)C(=O)Nc1ccc(Oc2ccc(NC(=O)C(H)H)cc2)cc1	1
3173	ISSSTY_v1a_7367_02May011_3997	24367-94-0	HC(H)C(=O)Nc1ccc(C(H)c2ccc(N)cc2)cc1	1
3174	ISSSTY_v1a_7367_02May011_3998	565-20-8	HC(H)C(=O)Nc1ccc(S(=O)(=O)c2ccc(N)cc2)cc1	1
3175	ISSSTY_v1a_7367_02May011_3999	77-46-3	HC(H)C(=O)Nc1ccc(S(=O)(=O)c2ccc(NC(=O)C(H)H)cc2)cc1	1
3176	ISSSTY_v1a_7367_02May011_4000	94208-87-4	HC(H)c1cc(C(H)H)cc(NN=C2c3c(C=CC2=O)cccc3)c1	1
3177	ISSSTY_v1a_7367_02May011_4001	27969-93-3	HC(H)c1c(NN=C2c3c(C=CC2=O)cccc3)c(C(H)H)ccc1	1
3178	ISSSTY_v1a_7367_02May011_4002	85-82-5	HC(H)c1c(NN=C2c3c(C=CC2=O)cccc3)cc(C(H)H)cc1	1
3179	ISSSTY_v1a_7367_02May011_4003	31969-03-6	HC(H)c1c(C(H)H)c(NN=C2c3c(C=CC2=O)cccc3)ccc1	1
3180	ISSSTY_v1a_7367_02May011_4004	16568-02-8	HC(H)C=NN(C(H)H)C=O	1
3181	ISSSTY_v1a_7367_02May011_4006	578-54-1	HC(H)C(H)c1c(N)cccc1	1
3182	ISSSTY_v1a_7367_02May011_4007	81340-58-1	c1(N(=O)=O)c2c3c(c4c5c(ccc(c25)cc1)ccc4)cccc3	3
3183	ISSSTY_v1a_7367_02May011_4008	84-88-8	c1(S(=O)(=O)O)c2c(c(O)cc1)ncccc2	3
3184	ISSSTY_v1a_7367_02May011_4009	773-76-2	c1(Cl)c(O)c2c(c(Cl)c1)cccn2	1
3185	ISSSTY_v1a_7367_02May011_4010	119-65-3	c12c(cccc1)ccnc2	1
3186	ISSSTY_v1a_7367_02May011_4012	130-95-0	c12c(c(C(O)C3CC4C(C=C)CN3CC4)ccn1)cc(OC)cc2	1
3187	ISSSTY_v1a_7367_02May011_4016	396-30-5	c12c(cc(F)cc1)cccn2	3
3188	ISSSTY_v1a_7367_02May011_4018	746-53-2	c12C(=O)c3c(c([N+](=O)[O-])cc([N+](=O)[O-])c3)-c1c([N+](=O)[O-])cc([N+](=O)[O-])c2	3
3189	ISSSTY_v1a_7367_02May011_4019	108043-88-5	HC(H)N1c2c(c3c(cc2)NC(=O)C=C3)N=C1N	3
3190	ISSSTY_v1a_7367_02May011_4020	113202-71-4	c1(N=O)c2c(c3c(c4c(cccc4)cc3)c1)cccc2	3
3191	ISSSTY_v1a_7367_02May011_4021	16683-64-0	c12c(c3c4c(C=C3)cccc4c1)cc1c(cccc1)c2	3
3192	ISSSTY_v1a_7367_02May011_4022	17987-99-4	C(=O)([O-])C1=C[N+](=O)c2c(cccc2)N1O	3

3193	ISSSTY_v1a_7367_02May011_4023	118174-26-8	HC(H)C(C(H)H)(C(H)H)OC(=O)N=NC=C1C=[N+](O-)]c2c(cccc2)N1O	3
3194	ISSSTY_v1a_7367_02May011_4024	6795-27-3	HC(H)C(=O)N=NC=C1C=[N+](O-)]c2c(cccc2)N1O	3
3195	ISSSTY_v1a_7367_02May011_4025	23696-28-8	HC(H)c1c(C(=O)NC(H)C(H)O)[n+](O-)]c2c(cccc2)[n+]1O-]	3
3196	ISSSTY_v1a_7367_02May011_4027	4003-94-5	c1(N(=O)=O)c(C=Cc2ccccc2)cccc1	3
3197	ISSSTY_v1a_7367_02May011_4028	614-48-2	c1(C(=O)C=Cc2cc(N(=O)=O)ccc2)cccc1	1
3198	ISSSTY_v1a_7367_02May011_4029	7473-93-0	c1(C(=O)C=Cc2c(N(=O)=O)cccc2)cccc1	1
3199	ISSSTY_v1a_7367_02May011_4030	25870-67-1	c1(C(=O)C=Cc2ccc([N+](=O)[O-])cc2)ccc([N+](=O)[O-])cc1	3
3200	ISSSTY_v1a_7367_02May011_4032	96839-34-8	HC(O)c1c([N+](=O)[O-])cccc1[N+](=O)[O-]	1
3201	ISSSTY_v1a_7367_02May011_4034	102000-59-9	C(=O)(O)c1c(N)cccc1N	3
3202	ISSSTY_v1a_7367_02May011_4035	5623-11-0	HC(H)C(=O)Nc1c(C(=O)O)c(N)ccc1	3
3203	ISSSTY_v1a_7367_02May011_4036	100-13-0	HC=Cc1ccc(N(=O)=O)cc1	3
3204	ISSSTY_v1a_7367_02May011_4037	98451-51-5	HC(O)c1c(N)cccc1N(=O)=O	1
3205	ISSSTY_v1a_7367_02May011_4038	580-22-3	c12c(ccc(N)n1)cccc2	3
3206	ISSSTY_v1a_7367_02May011_4039	161696-99-7	HC(H)c1c2c(ccc1NC(H)H)nc(C(H)H)cn2	3
3207	ISSSTY_v1a_7367_02May011_4040	580-17-6	c12c(cc(N)cn1)cccc2	3
3208	ISSSTY_v1a_7367_02May011_4041	156243-44-6	HC(H)c1c2c(ccc1NC(H)H)ncc(C(H)H)n2	3
3209	ISSSTY_v1a_7367_02May011_4042	161697-02-5	HC(H)c1c2c(ccc1NC(H)H)ncc(-c1cccc1)n2	3
3210	ISSSTY_v1a_7367_02May011_4043	578-68-7	c1(N)c2c(cccc2)ncc1	1
3211	ISSSTY_v1a_7367_02May011_4044	117760-93-7	c1(N)c2c(c3c(c4c([C@](O)[C@@](O)C=C4)cc3)c1)cccc2	3
3212	ISSSTY_v1a_7367_02May011_4045	580-15-4	c12c(cc(N)cc1)cccn2	1
3213	ISSSTY_v1a_7367_02May011_4046	55557-02-3	HC(H)OC(=O)C1C(H)N(N=O)C(H)C(H)C=1	3
3214	ISSSTY_v1a_7367_02May011_4047	580-19-8	c12c(cc(N)cc1)cccc2	3
3215	ISSSTY_v1a_7367_02May011_4048	105052-38-8	c12c3c(C=C(N(=O)=O)Oc3ccc1)ccc2	3
3216	ISSSTY_v1a_7367_02May011_4050	98046-75-4	c12c(cc(N(=O)=O)cn1)N=C1C=CC=CN21	3
3217	ISSSTY_v1a_7367_02May011_4051	98046-72-1	HC(H)C1C2=C(N3C(C(C(H)H)=CC=C3)=N2)NC(H)C=1N=O	3
3218	ISSSTY_v1a_7367_02May011_4052	98046-74-3	HC(H)C1C2N(c3c(c(C(H)H)c(N(=O)=O)cn3)N=2)C=CC=1	3
3219	ISSSTY_v1a_7367_02May011_4054	22433-76-7	HC(H)C(=O)Nc1cc2c(cc1)nccc2	3
3220	ISSSTY_v1a_7367_02May011_4055	36164-42-8	HC(H)C(=O)Nc1cc2c(cccn2)cc1	3
3221	ISSSTY_v1a_7367_02May011_4057	50502-17-5	HC(H)C(=O)Nc1ccc2c(cccc2)n1	1
3222	ISSSTY_v1a_7367_02May011_4058	555-84-0	HC1C(H)N(N=CC2=CC=C(N(=O)=O)O2)C(=O)N1	3
3223	ISSSTY_v1a_7367_02May011_4059	5417-50-5	HC(H)C(=O)Nc1cc2c(cccc2)nc1	1
3224	ISSSTY_v1a_7367_02May011_4061	32433-28-6	HC(H)C(=O)Nc1c2c(cccc2)ncc1	1
3225	ISSSTY_v1a_7367_02May011_4062	29611-03-8	HC(H)Oc1c2C3=C(C(=O)Oc2c2c(c1)O[C@@]1[C@]2C=CO1)[C@@](O)C(H)C3H	3
3226	ISSSTY_v1a_7367_02May011_4063	42464-80-2	HC(H)C(=O)Nc1c2c(ccc1)nccc2	1
3227	ISSSTY_v1a_7367_02May011_4064	612-22-6	HC(H)C(H)c1c(N(=O)=O)cccc1	1
3228	ISSSTY_v1a_7367_02May011_4065	100-12-9	HC(H)C(H)c1ccc(N(=O)=O)cc1	1
3229	ISSSTY_v1a_7367_02May011_4066	66-56-8	c1(O)c([N+](=O)[O-])c([N+](=O)[O-])ccc1	3
3230	ISSSTY_v1a_7367_02May011_4067	329-71-5	c1([N+](=O)[O-])c(O)cc([N+](=O)[O-])cc1	3
3231	ISSSTY_v1a_7367_02May011_4068	573-56-8	c1([N+](=O)[O-])c(O)c([N+](=O)[O-])ccc1	1
3232	ISSSTY_v1a_7367_02May011_4069	577-71-9	c1([N+](=O)[O-])c([N+](=O)[O-])cc(O)cc1	3
3233	ISSSTY_v1a_7367_02May011_4070	606-22-4	c1([N+](=O)[O-])c(N)c([N+](=O)[O-])ccc1	3
3234	ISSSTY_v1a_7367_02May011_4071	122587-22-8	HC(H)OC(=O)C1=C(CI)C(CI)=C(N(=O)=O)O1	3

3235	ISSSTY_v1a_7367_02May011_4072	6884-87-3	HC(H)C(=O)Nc1ccc(S(=O)(=O)NC(H)H)cc1	1
3236	ISSSTY_v1a_7367_02May011_4073	586-78-7	c1(Br)ccc(N(=O)=O)cc1	3
3237	ISSSTY_v1a_7367_02May011_4074	89-59-8	HC(H)c1c(N(=O)=O)cc(Cl)cc1	1
3238	ISSSTY_v1a_7367_02May011_4075	83-41-0	HC(H)c1c(C(H)H)c(N(=O)=O)ccc1	1
3239	ISSSTY_v1a_7367_02May011_4076	81-20-9	HC(H)c1c(N(=O)=O)c(C(H)H)ccc1	1
3240	ISSSTY_v1a_7367_02May011_4077	36501	HC(H)c1cc(C(H)H)cc(N(=O)=O)c1	1
3241	ISSSTY_v1a_7367_02May011_4078	89-58-7	HC(H)c1c(N(=O)=O)cc(C(H)H)cc1	3
3242	ISSSTY_v1a_7367_02May011_4079	616-72-8	HC(H)c1c([N+](=O)[O-])cc([N+](=O)[O-])c(C(H)H)c1	3
3243	ISSSTY_v1a_7367_02May011_4080	96-99-1	C(=O)(O)c1cc(N(=O)=O)c(Cl)cc1	3
3244	ISSSTY_v1a_7367_02May011_4081	528-45-0	C(=O)(O)c1cc([N+](=O)[O-])c([N+](=O)[O-])cc1	3
3245	ISSSTY_v1a_7367_02May011_4082	99-34-3	C(=O)(O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1	3
3246	ISSSTY_v1a_7367_02May011_4083	80-82-0	c1(S(=O)(=O)O)c(N(=O)=O)cccc1	1
3247	ISSSTY_v1a_7367_02May011_4084	98-47-5	c1(S(=O)(=O)O)cc(N(=O)=O)ccc1	1
3248	ISSSTY_v1a_7367_02May011_4085	138-42-1	c1(S(=O)(=O)O)ccc(N(=O)=O)cc1	1
3249	ISSSTY_v1a_7367_02May011_4086	74367-78-5	HC(Cl)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1	3
3250	ISSSTY_v1a_7367_02May011_4087	100-16-3	c1(NN)ccc(N(=O)=O)cc1	3
3251	ISSSTY_v1a_7367_02May011_4088	119-26-6	c1(NN)c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
3252	ISSSTY_v1a_7367_02May011_4089	1594-56-5	c1(SC_N)c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
3253	ISSSTY_v1a_7367_02May011_4090	130638	HC(c1cccc1)C(H)N=C=S	3
3254	ISSSTY_v1a_7367_02May011_4091	92557-61-4	HC(H)N1c2c(C(C(H)[C@@]3(O)[C@@]4(O)[C@]([C@@](O)C(H)O4)OC3=O)=C1)cccc2	3
3255	ISSSTY_v1a_7367_02May011_4092	14698-29-4	HC(H)C(H)N1c2c(C(=O)C(C(=O)O)=C1)cc1c(c2)OC(H)O1	3
3256	ISSSTY_v1a_7367_02May011_4093	1192-62-7	HC(H)C(=O)C1=CC=CO1	3
3257	ISSSTY_v1a_7367_02May011_4094	1204-60-0	c1(-c2cc(C=O)ccc2)cccc1	1
3258	ISSSTY_v1a_7367_02May011_4095	479-79-8	c12C(=O)c3c4c(ccc3-c1cccc2)cccc4	1
3259	ISSSTY_v1a_7367_02May011_4096	86853-97-6	c12C(=O)c3c(c4c(cccc4)cc3)-c1c1c(cccc1)cc2	3
3260	ISSSTY_v1a_7367_02May011_4097	92130-56-8	HC(H)c1c2c(c3c(c1)nccc3)N=CN2C(H)H	1
3261	ISSSTY_v1a_7367_02May011_4098	13909-09-6	HC(H)C1C(H)C(H)C(NC(=O)N(C(H)C(H)Cl)N=O)C(H)C1H	3
3262	ISSSTY_v1a_7367_02May011_4099	67019-20-9	HC(H)C(H)C(=O)NC1=C2C(C=CC=C2)=NS1	1
3263	ISSSTY_v1a_7367_02May011_4100	6313-44-6	c12C(=O)c3c(C(N(=O)=O)c1cccc2)cccc3	1
3264	ISSSTY_v1a_7367_02May011_4101	39653-72-0	C(N)C1c2c3c(cccc3ccc2)C=1	3
3265	ISSSTY_v1a_7367_02May011_4102	28434-86-8	c1(N)c(Cl)cc(OC2cc(Cl)c(N)cc2)cc1	3
3266	ISSSTY_v1a_7367_02May011_4103	613-50-3	c12c(cc(N(=O)=O)cc1)cccn2	3
3267	ISSSTY_v1a_7367_02May011_4104	1421-85-8	c12-c3c(C4C(c1cc1c5c(ccc1c2)cccc5)O4)cccc3	3
3268	ISSSTY_v1a_7367_02May011_4105	78-76-2	HC(H)C(H)C(Br)C(H)H	3
3269	ISSSTY_v1a_7367_02May011_4106	111119-29-0	HC(H)OC(H)C(O)C(H)N1C(Cl)=NC(N(=O)=O)=C1	3
3270	ISSSTY_v1a_7367_02May011_4107	1498903	HC(H)Oc1c(O)c2C(=O)c3c(C(=O)c2cc1)cccc3	1
3271	ISSSTY_v1a_7367_02May011_4108	83312-51-0	HC(H)c1cc2C(=O)c3c(C(=O)c2cc1)ccc(O)c3	3
3272	ISSSTY_v1a_7367_02May011_4109	2589-39-1	HC(H)c1c(O)c2C(=O)c3c(C(=O)c2c(O)c1)cccc3	3
3273	ISSSTY_v1a_7367_02May011_4110	79560-36-4	HC(H)OC(H)c1c(O)c2C(=O)c3c(C(=O)c2cc1O)cccc3	3
3274	ISSSTY_v1a_7367_02May011_4111	477-83-8	HC(H)Oc1c2C(=O)c3c(C(=O)c2cc(O)c1C(H)O)cccc3	3
3275	ISSSTY_v1a_7367_02May011_4112	61434-48-8	HC(H)Oc1c2C(=O)c3c(C(=O)c2cc(OC(H)H)c1C(H)O)cccc3	1
3276	ISSSTY_v1a_7367_02May011_4113	94574-56-8	HC(H)C(=O)OC(H)c1c(O)c2C(=O)c3c(C(=O)c2cc1O)cccc3	3

[illegible]

3319	ISSSTY_v1a_7367_02May011_4185	80-70-6	HC(H)N(C(=N)N(C(H)H)C(H)H)C(H)H	1
3320	ISSSTY_v1a_7367_02May011_4186	106-58-1	HC(H)N1C(H)C(H)N(C(H)H)C(H)C1H	1
3321	ISSSTY_v1a_7367_02May011_4187	1732-23-6	c12c3c4c(cc(N)cc4ccc3ccc1)cc2	3
3322	ISSSTY_v1a_7367_02May011_4188	143922-95-6	HC(H)c1c(N(=O)=O)cccc1N=O	1
3323	ISSSTY_v1a_7367_02May011_4189	280-57-9	HC1C(H)N2C(H)C(H)N1C(H)C2H	1
3324	ISSSTY_v1a_7367_02May011_4190	143922-96-7	HC(H)c1c(N)cccc1[N-][N+](=O)c1c(C(H)H)c(N)ccc1	3
3325	ISSSTY_v1a_7367_02May011_4191	2449-49-2	HC(H)C(c1cccc1)N(C(H)H)C(H)H	1
3326	ISSSTY_v1a_7367_02May011_4192	143922-98-9	HC(H)C(=O)c1c(C(H)H)c([N+](=O)[N-]c2c(C(H)H)c(C(=O)C(H)H)ccc2)ccc1N	1
3327	ISSSTY_v1a_7367_02May011_4193	143922-99-0	HC(H)C(=O)c1c(C(H)H)c(N=Nc2c(C(H)H)c(C(=O)C(H)H)ccc2)ccc1N	1
3328	ISSSTY_v1a_7367_02May011_4194	116539-70-9	HC(H)C(H)C(H)C(H)N(C(H)C(O)C1C=CC(=O)C(=[N+]=[N-])C=1)N=O	3
3329	ISSSTY_v1a_7367_02May011_4197	2693-46-1	c1(N)c2c3c(c4c(c3ccc2)cccc4)cc1	3
3330	ISSSTY_v1a_7367_02May011_4198	3060-89-7	HC(H)N(C(=O)Nc1ccc(Br)cc1)OC(H)H	1
3331	ISSSTY_v1a_7367_02May011_4199	18691-97-9	HC(H)N(C1=Nc2c(cccc2)S1)C(=O)NC(H)H	1
3332	ISSSTY_v1a_7367_02May011_4200	55520-40-6	HC(c1ccc(O)cc1)[C@](N)C(=O)O	1
3333	ISSSTY_v1a_7367_02May011_4201	3062-57-5	c12-c3c(c([N+](=O)[O-])ccc3)Nc1ccc([N+](=O)[O-])c2	3
3334	ISSSTY_v1a_7367_02May011_4202	3244-54-0	c12-c3c(ccc([N+](=O)[O-])c3)Nc1ccc([N+](=O)[O-])c2	3
3335	ISSSTY_v1a_7367_02May011_4203	153654-33-2	c12-c3c(cc(O)c(N(=O)=O)c3)Nc1cccc2	3
3336	ISSSTY_v1a_7367_02May011_4204	153654-34-3	c12-c3c(c([N+](=O)[O-])c(O)c([N+](=O)[O-])c3)Nc1cccc2	3
3337	ISSSTY_v1a_7367_02May011_4205	153654-32-1	c12-c3c(c([N+](=O)[O-])c(O)c([N+](=O)[O-])c3)Nc1ccc([N+](=O)[O-])c2	3
3338	ISSSTY_v1a_7367_02May011_4206	505-23-7	HC1C(H)C(H)SC(H)S1	3
3339	ISSSTY_v1a_7367_02May011_4207	60692-90-2	c12-c3c4c(ccc3C3C(c1cccc2)O3)cccc4	3
3340	ISSSTY_v1a_7367_02May011_4208	71382-54-2	c12-c3c4c(ccc3C3C(c1cccc2)N3)cccc4	3
3341	ISSSTY_v1a_7367_02May011_4209	121-61-9	HC(H)C(=O)Nc1ccc(S(N)(=O)=O)cc1	1
3342	ISSSTY_v1a_7367_02May011_4210	1709-52-0	HC(H)NS(=O)(=O)c1ccc(N)cc1	1
3343	ISSSTY_v1a_7367_02May011_4211	1709-39-3	HC(H)C(H)N(C(H)C(H)H)S(=O)(=O)c1ccc(N)cc1	1
3344	ISSSTY_v1a_7367_02May011_4213	19077-98-6	HC(H)C(=O)Nc1ccc(S(=O)(=O)Nc2cccn2)cc1	1
3345	ISSSTY_v1a_7367_02May011_4214	1028-11-1	c1(S(=O)(=O)N(c2cccn2)N(=O)=O)cccc1	1
3346	ISSSTY_v1a_7367_02May011_4218	26676-89-1	HC(C1c2c(cccc2)NC=1)[C@]1(O)C2(O)C(C(O)C(H)O2)OC1=O	1
3347	ISSSTY_v1a_7367_02May011_4219	13963-57-0	?	3
3348	ISSSTY_v1a_7367_02May011_4221	1794-45-2	c1(Cl)c(C=CC=O)cccc1	3
3349	ISSSTY_v1a_7367_02May011_4223	2435-76-9	C1(=O)C(=[N+]=[N-])C=NC(=O)N1	3
3350	ISSSTY_v1a_7367_02May011_4224	1484-12-4	HC(H)N1c2c(-c3c1cccc3)cccc2	3
3351	ISSSTY_v1a_7367_02May011_4225	117760-92-6	c1(N(=O)=O)c2c(c3c(c4c(cccc4)cc3)c1)[C@](O)[C@@](O)C=C2	3
3352	ISSSTY_v1a_7367_02May011_4226	683-51-2	HC(H)C(Cl)=C=O	3
3353	ISSSTY_v1a_7367_02May011_4227	1995932	HC(H)C(=C(Cl)C=O)C(H)H	3
3354	ISSSTY_v1a_7367_02May011_4229	158366-45-1	HC(H)C(=O)C1=CC=CN1N(=O)=O	3
3355	ISSSTY_v1a_7367_02May011_4230	158366-46-2	HC(H)C(=O)C1=C([N+](=O)[O-])C=C([N+](=O)[O-])N1[N+](=O)[O-]	3
3356	ISSSTY_v1a_7367_02May011_4232	57491-68-6	HC(Sc1c(N)cccc1)Sc1c(N)cccc1	3
3357	ISSSTY_v1a_7367_02May011_4234	27093-62-5	HC(H)N1c2c(-c3c4c(ccc13)cccc4)c1c(cccc1)cc2	3
3358	ISSSTY_v1a_7367_02May011_4240	111070-55-4	C1(C=NN2C=CC=N2)=CC=C(N(=O)=O)O1	3
3359	ISSSTY_v1a_7367_02May011_4241	111070-57-6	c1(C2C=C(c3ccccc3)N(N=CC3=CC=C(N(=O)=O)O3)C(=O)C=2)cccc1	3
3360	ISSSTY_v1a_7367_02May011_4242	17241-59-7	HC(O)c1cc2C(=O)c3c(C(=O)c2cc1)cccc3	1

3403	ISSSTY_v1a_7367_02May011_4331	162022-91-5	HC(H)Oc1c2c(ccnc2)cnn1	1
3404	ISSSTY_v1a_7367_02May011_4332	162022-92-6	c1(Cl)c2c(cnc2)cnn1	1
3405	ISSSTY_v1a_7367_02May011_4333	253-73-6	c12c(cccn1)cnn2	1
3406	ISSSTY_v1a_7367_02May011_4334	19866-61-6	c12c(cccn1)cn(=O)nc2	1
3407	ISSSTY_v1a_7367_02May011_4335	19866-62-7	c12c(cccn1)cnn(=O)c2	1
3408	ISSSTY_v1a_7367_02May011_4336	23590-73-0	c1(NN)c2c(cccn2)cnn1	3
3409	ISSSTY_v1a_7367_02May011_4337	56525-92-9	HC(H)Oc1c2c(cnn1)nc2	1
3410	ISSSTY_v1a_7367_02May011_4338	56525-94-1	HC(H)Oc1c2c(cccn2)cnn1	1
3411	ISSSTY_v1a_7367_02May011_4340	18636-89-0	c12c(cccn1)cnn(=O)c2	1
3412	ISSSTY_v1a_7367_02May011_4341	24953-56-8	HC(H)Oc1c2c(cccn2)cnn1	1
3413	ISSSTY_v1a_7367_02May011_4342	130005-62-8	HC(H)c1c2-c3c(ccc(O)c3)Nc2c(C(H)H)cc1N	3
3414	ISSSTY_v1a_7367_02May011_4343	129117-54-0	HC(H)c1c2-c3c(ccc(OC(H)H)c3)Nc2c(C(H)H)cc1N	3
3415	ISSSTY_v1a_7367_02May011_4344	61166-04-9	HC(H)N1c2c(-c3c1ccc(N)c3)cccc2	3
3416	ISSSTY_v1a_7367_02May011_4346	18028-56-3	HC(H)c1c2-c3c(ccc(C(H)H)c3)Nc2c(C(H)H)cc1	3
3417	ISSSTY_v1a_7367_02May011_4349	24777-14-8	HC(H)OC1C(=O)C=CC(=C2NC(c3cccc3)=C(c3cccc3)N2)C=1	3
3418	ISSSTY_v1a_7367_02May011_4354	32912	c1(O)c(C=O)cccc1	1
3419	ISSSTY_v1a_7367_02May011_4356	92439-25-3	HC(H)c1c(O)c2C(=O)c3c(C(=O)c2cc1O)c(O)ccc3	3
3420	ISSSTY_v1a_7367_02May011_4357	63390-12-5	c1(-c2cc(Cl)c(N)c(Cl)c2)cc(Cl)c(N)cc1	3
3421	ISSSTY_v1a_7367_02May011_4358	121111-61-3	HC(H)c1ccc(C2=C(c3ccc(C(H)H)cc3)N=C(c3cc(OC(H)H)c(OC(H)H)cc3)N2)cc1	3
3422	ISSSTY_v1a_7367_02May011_4359	7044-99-7	HC(H)Oc1ccc(C2=C(c3ccc(OC(H)H)cc3)N=C(c3cccc3)N2)cc1	3
3423	ISSSTY_v1a_7367_02May011_4360	121111-59-9	HC(H)c1c(C2=NC(c3ccc(C(H)H)cc3)=C(c3ccc(C(H)H)cc3)N2)ccc(C(H)H)c1	3
3424	ISSSTY_v1a_7367_02May011_4361	37393-11-6	HC(O)c1c(O)c2C(=O)c3c(C(=O)c2cc1O)[C@H]1[C@H](O)[C@@H](O)[C@H](O)[C@@H](C(H)O)[C@@H]2[C@H](O)[C@@H](O)[C@H](O)O1)cccc3	3
3425	ISSSTY_v1a_7367_02May011_4362	1728-95-6	HC(H)Oc1ccc(C2=NC(c3cccc3)=C(c3cccc3)N2)cc1	3
3426	ISSSTY_v1a_7367_02May011_4363	19200-30-7	HC(H)C(H)N(C=S)S[C@@H]1[C@H](O)[C@@H](O)[C@H](O)[C@@H](C(H)O)O1)C(H)C(H)H	1
3427	ISSSTY_v1a_7367_02May011_4365	98499-59-3	HC(H)SC(H)Nc1cccc1	3
3428	ISSSTY_v1a_7367_02May011_4367	194590-84-6	HC(H)C(=O)Nc1c(N2N=C3C(C(Cl)=C(N)C=C3Br)=N2)cc(OC(H)H)c(N(C(H)C(H)OC(H)H)C(H)C(H)OC(H)H)c1	3
3429	ISSSTY_v1a_7367_02May011_4369	201-06-9	c12c(c3c4c(C=Cc4ccc3)c1)cccc2	3
3430	ISSSTY_v1a_7367_02May011_4370	21247-98-3	HC(O)c1c2c(c3c4c5c(ccc14)cccc5cc3)cccc2	3
3431	ISSSTY_v1a_7367_02May011_4371	568-75-2	HC(H)c1c2c(c(C(H)O)c3c1c1c(cccc1)cc3)cccc2	3
3432	ISSSTY_v1a_7367_02May011_4373	519-23-3	HC(H)c1c2-c3c(cccc3)Nc2c(C(H)H)c2c1cncc2	3
3433	ISSSTY_v1a_7367_02May011_4376	55256-58-1	HC(H)Oc1c2C(=O)c3c(OC(H)H)c4c(cc3Oc2ccc1Cl)OC1C4C=CO1	3
3434	ISSSTY_v1a_7367_02May011_4378	55256-57-0	HC(H)C(O)(C(H)H)C(H)C(H)c1c2c(C(=O)c3c(O)c4c(cc3O2)O[C@@H]2[C@H]4C=CO2)c(O)cc1	3
3435	ISSSTY_v1a_7367_02May011_4380	55256-55-8	HC(H)C(O)(C(H)H)C(H)C(H)c1c2c(C(=O)c3c(OC(H)H)c4c(cc3O2)O[C@@H]2[C@H]4C=CO2)c(O)cc1	3
3436	ISSSTY_v1a_7367_02May011_4381	55256-53-6	HC(H)C(O)(C(H)H)C(H)C(H)c1c2c(C(=O)c3c(O)c4[C@@H]5(O)C=CO[C@@H]5Oc4cc3O2)c(O)cc1	3
3437	ISSSTY_v1a_7367_02May011_4385	58775-50-1	HC(H)C(C(H)H)=CC(H)c1c2c(C(=O)c3c(O)c4[C@@H]5(O)C=CO[C@@H]5Oc4cc3O2)c(O)cc1	3
3438	ISSSTY_v1a_7367_02May011_4388	52819-96-2	HC(H)Oc1c2C3=C(C(=O)C(H)[C@H]3O)C(=O)Oc2c2c(c1)O[C@@H]1[C@H]2C=CO1	3
3439	ISSSTY_v1a_7367_02May011_4390	299257	HC(H)C(=O)Nc1ccc(C(H)c2ccc(NC(=O)C(H)H)cc2)cc1	1
3440	ISSSTY_v1a_7367_02May011_4391	1030-27-9	HC(H)N(c1ccc(C=CC(=O)c2cccc2)cc1)C(H)H	1
3441	ISSSTY_v1a_7367_02May011_4394	21794-55-8	HC(H)C(=O)C1(O)C(H)C2c(O)c3C(=O)c4c(C(=O)c3c(O)c2C(O)C1H)c(OC(H)H)ccc4	3
3442	ISSSTY_v1a_7367_02May011_4396	52744-22-6	HC(H)C(=O)[C@@H]1(O)C(H)c2c(O)c3C(=O)c4c(C(=O)c3c(O)c2[C@@H](O)C1H)c(O)ccc4	3
3443	ISSSTY_v1a_7367_02May011_4397	16234-96-1	HC(H)C(H)[C@H]1(O)C(H)[C@H](O)c2c(O)c3C(=O)c4c(C(=O)c3cc2[C@@H]1C(=O)OC(H)H)cccc4O	3
3444	ISSSTY_v1a_7367_02May011_4399	1608-51-1	c1(C(=O)C=Cc2ccc(F)cc2)cccc1	1

3445	ISSSTY_v1a_7367_02May011_4400	159416-83-8	HC(H)c1c(-c2c(O)c3c(c(OC(H)H)cc(C(H)H)c3)c(O)c2)c(OC(H)H)c2c(c(O)ccc2O)c1	1
3446	ISSSTY_v1a_7367_02May011_4402	100-33-4	HC(C(H)C(H)C(H)C(H)Oc1ccc(C(=N)N)cc1)Oc1ccc(C(=N)N)cc1	1
3447	ISSSTY_v1a_7367_02May011_4404	4816-14-2	C(=N)(N)c1cc2c(C=C(c3ccc(C(=N)N)cc3)S2)cc1	1
3448	ISSSTY_v1a_7367_02May011_4405	64431-93-2	HC1C(H)N=C(c2cc3c(C=C(c4ccc(C5=NC(H)C(H)N5)cc4)N3)cc2)N1	1
3449	ISSSTY_v1a_7367_02May011_4406	73819-63-3	C12C(C=C(C(=N)N)C=C1)=NC(=C(N)N)C=2	1
3450	ISSSTY_v1a_7367_02May011_4408	3009-50-5	HC(H)N(c1ccc(N=Nc2ccc(OC(H)H)cc2)cc1)C(H)H	3
3451	ISSSTY_v1a_7367_02May011_4409	101821-43-6	C12C(=C(N)C(=C(N)N)N=1)C=CC(C(=N)N)=C2	1
3452	ISSSTY_v1a_7367_02May011_4412	162022-85-7	c12c(ccnc1)cn(=O)nc2	1
3453	ISSSTY_v1a_7367_02May011_4413	162022-89-1	c1(NN)c2c(ccnc2)cnn1	3
3454	ISSSTY_v1a_7367_02May011_4414	20426-12-4	c1(C(=O)C=Cc2ccc(O)cc2)ccccc1	1
3455	ISSSTY_v1a_7367_02May011_4416	51856-71-4	HC(H)c1c([N+](=O)[O-])cc([N+](=O)[O-])cc1[N-][N+](=O)c1cc([N+](=O)[O-])c(C(H)H)c([N+](=O)[O-])c1	3
3456	ISSSTY_v1a_7367_02May011_4418	162022-90-4	HC(H)Oc1c2c(cncc2)cnn1	1
3457	ISSSTY_v1a_7367_02May011_4420	383514	HC(H)C(c1c(O)c(C(C(H)H)C(H)H)C(H)H)cc(C=Cc2cc(C(C(H)H)C(H)H)C(H)H)c(O)c(C(C(H)H)C(H)H)C(H)H)c2c1)C(H)H)C(H)H	1
3458	ISSSTY_v1a_7367_02May011_4421	809-73-4	HC(H)C(C1C(=O)C(C(C(H)H)C(H)H)C(H)H)C(C(H)H)C(H)H)C(=O)C(C(C(H)H)C(H)H)C(H)H)C(H)H)C2)C=1)C(H)H)C(H)H	1
3459	ISSSTY_v1a_7367_02May011_4422	13154-57-9	HC(H)C(C1C(=O)C(C(C(H)H)C(H)H)C(H)H)C(C(H)H)C(H)H)C(=O)C(C(C(H)H)C(H)H)C(H)H)C(H)H)C2)C=1)C(H)H)C(H)H	1
3460	ISSSTY_v1a_7367_02May011_4423	63019-39-6	c12c(c3c(c4c(ccc(O)c4)cc3)cc1)cccc2	3
3461	ISSSTY_v1a_7367_02May011_4424	63019-40-9	c12c(c3c(c4c(O)cccc4cc3)cc1)cccc2	3
3462	ISSSTY_v1a_7367_02May011_4425	84498-34-0	c12c(c3c(c4c(cc3O)cccc4)cc1)cccc2	1
3463	ISSSTY_v1a_7367_02May011_4426	162022-93-7	c1(Cl)c2c(ccnc2)cnn1	1
3464	ISSSTY_v1a_7367_02May011_4428	20970-16-5	c1(NN)c2c(cnn1)ncccc2	3
3465	ISSSTY_v1a_7367_02May011_4430	5784-45-2	c1(Cl)c2c(cccc2)cnn1	1
3466	ISSSTY_v1a_7367_02May011_4431	23590-59-2	c1(Cl)c2c(cccn2)cnn1	3
3467	ISSSTY_v1a_7367_02May011_4432	23590-58-1	c1(Cl)c2c(cnn1)ncccc2	1
3468	ISSSTY_v1a_7367_02May011_4433	7467-29-0	HC(H)c1c(N)cc(N)c(N=Nc2c(C(H)H)cccc2)c1	3
3469	ISSSTY_v1a_7367_02May011_4434	84434-45-7	HC(H)c1c(N)c(N=Nc2c(C(H)H)cccc2)ccc1N	3
3470	ISSSTY_v1a_7367_02May011_4435	84434-42-4	HC(H)c1c(N)c(N=Nc2cccc2)ccc1N	3
3471	ISSSTY_v1a_7367_02May011_4436	70634-28-5	HC(H)C(c1c(N(=O)=O)ccc(-c2cccc2)c1)(C(H)H)C(H)H	1
3472	ISSSTY_v1a_7367_02May011_4437	279242-17-0	HC(H)C(c1ccc(-c2ccc(N=O)cc2)cc1)(C(H)H)C(H)H	3
3473	ISSSTY_v1a_7367_02May011_4438	59282-34-7	HC(H)C(c1c(O)c(N(=O)=O)cc(OC(H)H)c1)(C(H)H)C(H)H	1
3474	ISSSTY_v1a_7367_02May011_4439	2940-63-8	HC(H)C(C1C(=O)C(=O)C=C(OC(H)H)C=1)(C(H)H)C(H)H	1
3475	ISSSTY_v1a_7367_02May011_4440	962-58-3	HC(H)c1cc(OP(=O)(OC(H)C(H)H)OC(H)C(H)H)nc(C(C(H)H)C(H)H)n1	3
3476	ISSSTY_v1a_7367_02May011_4441	2255-17-6	HC(H)c1c(N(=O)=O)ccc(OP(=O)(OC(H)H)OC(H)H)c1	3
3477	ISSSTY_v1a_7367_02May011_4442	105553-32-0	HC(H)C(=O)C(C(=O)N(c1cccc1)N(C(H)H)N=O)=NO	3
3478	ISSSTY_v1a_7367_02May011_4444	32306-29-9	HC(H)C(H)OP(=O)(OC1C=C(c2cccc2)ON=1)OC(H)C(H)H	1
3479	ISSSTY_v1a_7367_02May011_4445	311-45-5	HC(H)C(H)OP(=O)(Oc1ccc(N(=O)=O)cc1)OC(H)C(H)H	3
3480	ISSSTY_v1a_7367_02May011_4446	83-75-0	HC(H)C(H)OC(=O)O[C@](c1c2c(ccc(OC(H)H)c2)nc1)[C@@]1C(H)[C@]2C(H)C(H)N1C(H)[C@]2C=CH	1
3481	ISSSTY_v1a_7367_02May011_4448	41069-00-5	c1(C(=O)[C@@]2[C@](c3cccc3)O2)ccc(N(=O)=O)cc1	3
3482	ISSSTY_v1a_7367_02May011_4449	90811-87-3	c1(C(=O)C=Cc2ccc(Oc3cccc3)cc2)ccccc1	1
3483	ISSSTY_v1a_7367_02May011_4450	2453-44-3	c1(C(=O)C=Cc2cccc2)ccc(-c2cccc2)cc1	1
3484	ISSSTY_v1a_7367_02May011_4451	952-97-6	c1(Sc2cccc2)ccc(N(=O)=O)cc1	3
3485	ISSSTY_v1a_7367_02May011_4452	86-87-3	HC(c1c2c(cccc2)ccc1)C(=O)O	1
3486	ISSSTY_v1a_7367_02May011_4453	82414-03-7	HC(H)c1c(N(=O)=O)cc(N=O)cc1	1

3487	ISSSTY_v1a_7367_02May011_4454	128531-59-9	HC(H)C(H)N(C=S)SSC(H)[C@@](C(=O)NC(H)C(=O)O)NC(=O)C(H)C(H)[C@](N)(C(=O)O)C(H)C(H)H	1
3488	ISSSTY_v1a_7367_02May011_4455	188970-78-7	c12-c3c4c(c(N(=O)=O)cc3Nc1ccc1c2cccc1)cccc4	3
3489	ISSSTY_v1a_7367_02May011_4456	188970-86-7	c12-c3c4c(c(N(=O)=O)cc3Nc1ccc1c2cccc1)ccc(O)c4	3
3490	ISSSTY_v1a_7367_02May011_4457	188970-88-9	c12-c3c4c(c(N(=O)=O)cc3Nc1ccc1c2cc(O)cc1)cccc4	3
3491	ISSSTY_v1a_7367_02May011_4458	188970-81-2	c12-c3c4c(c(N(=O)=O)cc3Nc1ccc1c2cccc1)cc(O)cc4	3
3492	ISSSTY_v1a_7367_02May011_4459	188970-84-5	c12-c3c4c(c(N(=O)=O)cc3Nc1ccc1c(O)cccc21)cccc4	3
3493	ISSSTY_v1a_7367_02May011_4460	138805-29-5	HC(H)c1c(N=Nc2c(C(H)H)ccc(N)c2)cc(N)cc1	3
3494	ISSSTY_v1a_7367_02May011_4462	59863-59-1	HC1C(Cl)C(Cl)C(H)N1N=O	3
3495	ISSSTY_v1a_7367_02May011_4463	73018-98-1	HC(O)C(O)C(H)N=N_N	3
3496	ISSSTY_v1a_7367_02May011_4465	4273-73-8	HC(H)C1(C(H)H)C(C=CC(C(H)H)=CC=CC(C(H)H)=CC=CC=C(C(H)H)C=CC=C(C(=O)OC(H)H)C(H)H)=C(C(H)H)C(H)C(H)C1H	1
3497	ISSSTY_v1a_7367_02May011_4468	96614-59-4	HC(C(=O)N[C@](C(=O)NC(H)C(=O)O)C(H)SC(Cl)=CCl)C(H)[C@](N)(C(=O)O	3
3498	ISSSTY_v1a_7367_02May011_4469	619-90-9	HC(H)C(=O)OC(H)c1ccc(N(=O)=O)cc1	3
3499	ISSSTY_v1a_7367_02May011_4470	35300-54-0	HC(H)C(H)C(H)C(=O)OC(H)c1ccc(N(=O)=O)cc1	3
3500	ISSSTY_v1a_7367_02May011_4471	4457-41-4	HC(c1ccc(N(=O)=O)cc1)OC(=O)c1cccc1	3
3501	ISSSTY_v1a_7367_02May011_4472	55-80-1	HC(H)c1cc(N=Nc2ccc(N(C(H)H)C(H)H)cc2)ccc1	3
3502	ISSSTY_v1a_7367_02May011_4473	60259-80-5	c1(N(=O)=O)ccc(CNN=Nc2ccc(C)cc2)cc1	3
3503	ISSSTY_v1a_7367_02May011_4474	17564-64-6	HC(Cl)N1C(=O)c2c(C1=O)cccc2	3
3504	ISSSTY_v1a_7367_02May011_4475	54455-37-7	HC(Cl)N1C(=O)c2c(C1=O)cc(N(=O)=O)cc2	3
3505	ISSSTY_v1a_7367_02May011_4476	394039	HC(H)C(C(H)H)N=C(NC(C(H)H)C(H)H)OC(H)c1ccc(N(=O)=O)cc1	3
3506	ISSSTY_v1a_7367_02May011_4477	309459	HC(H)C(=O)Oc1cc2c(C(C(H)Br)=CC(=O)O2)cc1	1
3507	ISSSTY_v1a_7367_02May011_4478	35231-44-8	HC(H)Oc1cc2c(C(C(H)Br)=CC(=O)O2)cc1	1
3508	ISSSTY_v1a_7367_02May011_4479	491-64-5	HC(H)Oc1cc2C(=O)c3c(O)cc(O)cc3Oc2cc1	3
3509	ISSSTY_v1a_7367_02May011_4480	5000-65-7	HC(H)Oc1cc(C(=O)C(H)Br)ccc1	1
3510	ISSSTY_v1a_7367_02May011_4481	4436-24-2	HC(c1cccc1)C1C(H)O1	3
3511	ISSSTY_v1a_7367_02May011_4482	18458-01-0	HC(H)c1ccc(C(H)C2C(H)O2)cc1	3
3512	ISSSTY_v1a_7367_02May011_4483	4106-66-5	c12-c3c(cc(N)ccc3)Oc1cccc2	3
3513	ISSSTY_v1a_7367_02May011_4492	36519-91-2	HC(c1ccc(Cl)cc1)C1C(H)O1	3
3514	ISSSTY_v1a_7367_02May011_4494	389104-54-5	HC(H)C(c1c2c(ccc1N)cccc2)C(H)H	3
3515	ISSSTY_v1a_7367_02May011_4499	129018-59-3	HC(H)N1c2c(N=C1N(=O)=O)ncc(-c1cccc1)c2	3
3516	ISSSTY_v1a_7367_02May011_4500	135577-57-0	HC(H)N1c2c(N=C1N=N_N)ncc(-c1cccc1)c2	3
3517	ISSSTY_v1a_7367_02May011_4502	66452-61-7	HC(H)C(C(H)H)Sc1c(N)ccc(C(H)c2cc(SC(C(H)H)C(H)H)c(N)cc2)c1	3
3518	ISSSTY_v1a_7367_02May011_4503	548-42-5	HC(H)C1C(H)N(C(H)H)[C@@]2C(H)C3c4c(cccc4[C@]2C=1)NC=3	3
3519	ISSSTY_v1a_7367_02May011_4504	6756-41-8	HC(H)c1ccc(NN=C2c3c(C=CC2=O)cccc3)cc1	1
3520	ISSSTY_v1a_7367_02May011_4506	529-49-7	c12C(=O)c3c(O)cc(O)cc3Oc1ccc(O)c2	3
3521	ISSSTY_v1a_7367_02May011_4508	111017-06-2	HC(H)Oc1c(OC(H)H)c2c3c(C(H)C(H)N(C=O)c3cc3c2cccc3)c1	3
3522	ISSSTY_v1a_7367_02May011_4509	62826-28-2	HC(H)Oc1c(C(H)C2C(H)O2)cccc1	3
3523	ISSSTY_v1a_7367_02May011_4510	499-75-2	HC(H)c1c(O)cc(C(C(H)H)C(H)H)cc1	1
3524	ISSSTY_v1a_7367_02May011_4511	53940-49-1	HC(H)Oc1c(O)ccc(C(H)C2C(H)O2)c1	3
3525	ISSSTY_v1a_7367_02May011_4512	91-63-4	HC(H)c1ccc2c(cccc2)n1	3
3526	ISSSTY_v1a_7367_02May011_4514	10102-44-0	N(=O)=O	3
3527	ISSSTY_v1a_7367_02May011_4515	27602-80-8	HC(H)Oc1c(OC(H)H)cc(C(H)C2C(H)O2)cc1	3
3528	ISSSTY_v1a_7367_02May011_4517	548-04-9	HC(H)c1c2c3c(C(=O)c4c5c(c6c7c(C(=O)c8c(c7c35)c2c(C(H)H)cc8O)c(O)cc6O)c(O)cc4O)c(O)c1	1

3571	ISSSTY_v1a_7367_02May011_4568	91991-22-9	HC(H)C(H)C(H)C(H)C(=O)NC1=C2C(C=CC(Cl)=C2)=NS1	1
3572	ISSSTY_v1a_7367_02May011_4569	91991-23-0	HC(H)C(C(H)H)C(H)C(=O)NC1=C2C(C=CC(Cl)=C2)=NS1	1
3573	ISSSTY_v1a_7367_02May011_4570	98447-34-8	HC(H)C(H)C(H)C(=O)NC1=C2C(C=C(Cl)C=C2)=NS1	1
3574	ISSSTY_v1a_7367_02May011_4571	87619-82-7	HC([C@](N)C(=O)O)SC(Cl)=C(Cl)C(Cl)=C(Cl)Cl	3
3575	ISSSTY_v1a_7367_02May011_4572	98025-31-1	HC([C@](N)C(=O)O)SC(Cl)=C(Cl)Cl	3
3576	ISSSTY_v1a_7367_02May011_4573	20589-85-9	C(Cl)C(Cl)Cl)=CCl	3
3577	ISSSTY_v1a_7367_02May011_4575	132832-27-0	c12c(c3c(c4c(c5c3cccc5)cccc4)cc1)[C@@]1[C@](C@@)(O)[C@]2O)O1	3
3578	ISSSTY_v1a_7367_02May011_4576	76024-59-4	c12c(c3c(c4c1[C@](O)[C@@](O)[C@@]1[C@@]4O1)cccc3)cccc2	3
3579	ISSSTY_v1a_7367_02May011_4577	132769-75-6	c12c(c3c4c(c5c6c(c(O)c(O)c5cc4)O6)ccc3cc1)cccc2	3
3580	ISSSTY_v1a_7367_02May011_4578	127-90-2	HC(C(Cl)(Cl)Cl)C(Cl)OC(Cl)C(H)C(Cl)(Cl)Cl	3
3581	ISSSTY_v1a_7367_02May011_4579	1447-88-7	HC(H)Oc1c(O)c2C(=O)C=C(c3ccc(O)cc3)Oc2cc1O	1
3582	ISSSTY_v1a_7367_02May011_4580	123442-39-7	HC(H)Oc1c(OC(H)H)cc2C(=O)C(O)=C(c3ccc(O)cc3)Oc2c1	1
3583	ISSSTY_v1a_7367_02May011_4583	122341-55-3	HC(H)C(H)N(C(H)C(O)C1C=CC(=[N+]=[N-])C(=O)C=1)N=O	3
3584	ISSSTY_v1a_7367_02May011_4584	76144-81-5	HC(H)[N+](C(H)H)(C(H)H)NC(H)C(H)C(=O)[O-]	1
3585	ISSSTY_v1a_7367_02May011_4585	63-91-2	HC(c1cccc1)C(N)C(=O)O	1
3586	ISSSTY_v1a_7367_02May011_4586	24385-10-2	HC(H)Oc1c2C(=O)c3c(C(=O)c2ccc1)c(O)c1c(c3O)[C@@](O)C(H)[C@@](O)C(=O)C(H)O)C1H	3
3587	ISSSTY_v1a_7367_02May011_4587	18774-09-9	HC(H)C1(OO)c2c(-c3c1cccc3)cccc2	3
3588	ISSSTY_v1a_7367_02May011_4588	96918-27-3	c12c3c4c(c5c(cc4ccc3ccc1)OC(N(=O)=O)=C5)cc2	3
3589	ISSSTY_v1a_7367_02May011_4589	533-30-2	c12c(cc(N)cc1)SC=N2	3
3590	ISSSTY_v1a_7367_02May011_4591	86674-50-2	c1(N(=O)=O)c2c3c4c([C@@](O)[C@](O)c3cc1)cccc4cc2	3
3591	ISSSTY_v1a_7367_02May011_4592	56183-12-1	c12c3c4c([C@](O)[C@@](O)c3ccc1)cccc4cc2	1
3592	ISSSTY_v1a_7367_02May011_4593	16156-54-0	HC(H)C(H)C(C(H)H)OS(=O)(=O)C(H)H	3
3593	ISSSTY_v1a_7367_02May011_4594	102822-04-8	c12C(=O)C(=O)c3c4c(c(N(=O)=O)cc3)ccc(c14)ccc2	3
3594	ISSSTY_v1a_7367_02May011_4595	102791-32-2	c12C(=O)C(=O)c3c4c(ccc(c14)ccc2N(=O)=O)ccc3	3
3595	ISSSTY_v1a_7367_02May011_4596	6217-22-7	c12C(=O)C(=O)c3c4c(ccc(c14)ccc2)ccc3	1
3596	ISSSTY_v1a_7367_02May011_4598	94764-55-3	c12-c3c(cc(N(=O)=O)cc3)Sc1cccc2	3
3597	ISSSTY_v1a_7367_02May011_4599	23702-49-0	C1(=O)c2c3c4c(ccc3ccc2)cccc4O1	1
3598	ISSSTY_v1a_7367_02May011_4600	137-17-7	HC(H)c1c(C(H)H)cc(N)c(C(H)H)c1	3
3599	ISSSTY_v1a_7367_02May011_4603	18024-11-8	HC(H)c1c2-c3c(cccc3)N(C(H)H)c2c(C(H)H)cc1	3
3600	ISSSTY_v1a_7367_02May011_4604	188107-70-2	HC(H)N1c2c(-c3c1cc(N(=O)=O)cc3)cccc2	3
3601	ISSSTY_v1a_7367_02May011_4605	188107-71-3	HC(H)c1c2-c3c(cccc3)N(C(H)H)c2c(C(H)H)cc1N(=O)=O	3
3602	ISSSTY_v1a_7367_02May011_4606	94-41-7	c1(C(=O)C=Cc2cccc2)cccc1	1
3603	ISSSTY_v1a_7367_02May011_4607	7570-86-7	c1(C(=O)C2C(c3cccc3)O2)cccc1	3
3604	ISSSTY_v1a_7367_02May011_4608	111249-52-6	HC(H)c1c2-c3c(cccc3)Nc2c(C(H)H)cc1N	3
3605	ISSSTY_v1a_7367_02May011_4609	102059-18-7	HC(H)C(=O)Nc1ccc(C=CC(=O)c2cccc2)cc1	3
3606	ISSSTY_v1a_7367_02May011_4610	19337-19-0	HC(H)C(=O)Nc1ccc(C(=O)C=Cc2cccc2)cc1	1
3607	ISSSTY_v1a_7367_02May011_4611	82389-36-4	HC(H)C(=O)Nc1ccc([C@]2[C@@](C(=O)c3cccc3)O2)cc1	3
3608	ISSSTY_v1a_7367_02May011_4612	82389-38-6	HC(H)C(=O)Nc1ccc(C(=O)[C@]2[C@@](c3cccc3)O2)cc1	3
3609	ISSSTY_v1a_7367_02May011_4613	215245-16-2	HC(H)C(=O)Nc1c(N2N=C3C(C(Cl)=C(N)C=C3Br)=N2)cc(OC(H)H)c(N(C(H)C(H)H)C(H)C(H)C(H)C_N)c1	3
3610	ISSSTY_v1a_7367_02May011_4614	76002-91-0	HC(H)C(c1ccc(OC(H)C2C(H)O2)cc1)(c1ccc(OC(H)C(O)C(H)O)cc1)C(H)H	3
3611	ISSSTY_v1a_7367_02May011_4615	1774-66-9	c1(C(=O)C=Cc2ccc(Br)cc2)cccc1	1
3612	ISSSTY_v1a_7367_02May011_4616	484-47-9	c1(C2=C(c3cccc3)N=C(c3cccc3)N2)cccc1	3

3613	ISSSTY_v1a_7367_02May011_4617	120-66-1	HC(H)c1c(NC(=O)C(H)H)cccc1	1
3614	ISSSTY_v1a_7367_02May011_4618	1728-96-7	HC(H)Oc1ccc(C2=C(c3ccc(OC(H)H)cc3)N=C(c3ccc(OC(H)H)cc3)N2)cc1	3
3615	ISSSTY_v1a_7367_02May011_4619	27730-00-3	c1(C(=O)C=Cc2ccc(Br=O)cc2)ccccc1	1
3616	ISSSTY_v1a_7367_02May011_4620	32157-71-4	c1(C(=O)[C@@]2[C@](c3ccccc3)O2)ccc(Br)cc1	1
3617	ISSSTY_v1a_7367_02May011_4621	70786-65-1	HC(H)c1c(N(O)C(=O)C(H)H)cccc1	3
3618	ISSSTY_v1a_7367_02May011_4622	112077-92-6	HC(H)c1c(N(C(=O)C(H)H)OC(=O)C(H)H)cccc1	1
3619	ISSSTY_v1a_7367_02May011_4623	399-10-0	c1(C(=O)C=Cc2ccccc2)ccc(F)cc1	1
3620	ISSSTY_v1a_7367_02May011_4624	362-05-0	HC(H)[C@]12C(H)C(H)[C@@]3c4c(C(H)C(H)[C@]3[C@@]1C(H)C(H)[C@]2O)cc(O)c(O)c4	1
3621	ISSSTY_v1a_7367_02May011_4625	5976-61-4	HC(H)[C@]12C(H)C(H)[C@@]3c4c(c(O)c(O)cc4)C(H)C(H)[C@]3[C@@]1C(H)C(H)[C@]2O	1
3622	ISSSTY_v1a_7367_02May011_4626	73936-27-3	c1(C(=O)[C@@]2[C@](c3ccccc3)O2)ccc(F)cc1	3
3623	ISSSTY_v1a_7367_02May011_4627	101821-44-7	C12C(C=C(Br)C=C1)=NC(=C(N)N)C=2	1
3624	ISSSTY_v1a_7367_02May011_4628	63-75-2	HC(H)N1C(H)C(C(=O)OC(H)H)=CC(H)C1H	3
3625	ISSSTY_v1a_7367_02May011_4629	2657-25-2	c1(C(=O)C=Cc2ccccc2)ccc(O)cc1	1
3626	ISSSTY_v1a_7367_02May011_4630	959-33-1	HC(H)Oc1ccc(C=CC(=O)c2ccccc2)cc1	1
3627	ISSSTY_v1a_7367_02May011_4631	275795-16-9	HC(H)C(c1c(N=O)ccc(-c2ccccc2)c1)(C(H)H)C(H)H	3
3628	ISSSTY_v1a_7367_02May011_4632	279242-11-4	HC(H)C(c1ccc(-c2ccc(N(=O)=O)cc2)cc1)(C(H)H)C(H)H	1
3629	ISSSTY_v1a_7367_02May011_4633	959-23-9	HC(H)Oc1ccc(C(=O)C=Cc2ccccc2)cc1	1
3630	ISSSTY_v1a_7367_02May011_4634	18873-03-5	HC(H)Oc1ccc(C(=O)C2C(c3ccccc3)O2)cc1	1
3631	ISSSTY_v1a_7367_02May011_4635	27730-03-6	c1(C(=O)C2C(c3ccc(N(=O)=O)cc3)O2)ccccc1	1
3632	ISSSTY_v1a_7367_02May011_4636	109143-18-2	HC(H)Oc1c2c(c(N(C(H)C(H)Cl)C(H)C(H)Cl)cc1)OC(N(=O)=O)=C2	3
3633	ISSSTY_v1a_7367_02May011_4637	33942-93-7	HC(H)c1cc2c(cc1)nc1c3c(ccc1c2)cccc3	3
3634	ISSSTY_v1a_7367_02May011_4638	7230-71-9	Cc1ccc2cc3ccc4ccccc4c3nc2c1	3
3635	ISSSTY_v1a_7367_02May011_4639	13911-90-5	HC(H)c1c2c(ccc1)nc1c3c(ccc1c2)cccc3	3
3636	ISSSTY_v1a_7367_02May011_4640	10567-95-0	HC(H)c1c2c(c3c(c(C(H)H)c4c(cccc4)n3)c1)cccc2	3
3637	ISSSTY_v1a_7367_02May011_4641	86711-50-4	c1(C(=O)C2C(c3ccc(OC4ccccc4)cc3)O2)ccccc1	1
3638	ISSSTY_v1a_7367_02May011_4643	3340-94-1	HC(H)c1c2c(c3c(cccc3)cc2)nc2c1cccc2	3
3639	ISSSTY_v1a_7367_02May011_4644	2403-28-3	c1(C(=O)C=Cc2ccc(-c3ccccc3)cc2)ccccc1	1
3640	ISSSTY_v1a_7367_02May011_4645	51787-42-9	HC(H)c1c2c(c(C(H)H)c3c(c4c(cccc4)cc3)n2)cc(C(H)H)c1	3
3641	ISSSTY_v1a_7367_02May011_4646	58430-01-6	HC(H)c1c2c(c3c(cccc3)cc2)nc2c1cc(C(H)H)c(C(H)H)c2	3
3642	ISSSTY_v1a_7367_02May011_4647	32740-01-5	HC(H)c1c2c(c(C(H)H)c3c(c4c(cccc4)cc3)n2)ccc1	3
3643	ISSSTY_v1a_7367_02May011_4648	82389-34-2	c1(C(=O)C2C(c3ccc(-c4ccccc4)cc3)O2)ccccc1	1
3644	ISSSTY_v1a_7367_02May011_4649	82389-37-5	c1(C(=O)C2C(c3ccccc3)O2)ccc(-c2ccccc2)cc1	1
3645	ISSSTY_v1a_7367_02May011_4651	95860-07-4	HC(H)c1c(NO)cc(N(=O)=O)cc1	1
3646	ISSSTY_v1a_7367_02May011_4653	43192-03-6	HC(H)c1c(N(=O)=O)cc(NO)cc1	1
3647	ISSSTY_v1a_7367_02May011_4654	13379-35-6	HC(H)Oc1cc2C(=O)c3c(O)cc(OC(H)H)cc3Oc2cc1	3
3648	ISSSTY_v1a_7367_02May011_4655	67151-57-9	HC(H)c1c([N-][N+](=O)c2c(C(H)H)ccc([N+](=O)[O-])c2)cc(N(=O)=O)cc1	1
3649	ISSSTY_v1a_7367_02May011_4656	5679-89-0	HC(H)c1c(N(=O)=O)cc([N-][N+](=O)c2cc([N+](=O)[O-])c(C(H)H)cc2)cc1	1
3650	ISSSTY_v1a_7367_02May011_4658	5042-54-6	HC(H)c1c(N)cc(N)c(N=Nc2ccccc2)c1	3
3651	ISSSTY_v1a_7367_02May011_4659	389104-60-3	HC(H)C(H)c1c(N)ccc(-c2ccccc2)c1	3
3652	ISSSTY_v1a_7367_02May011_4660	127502-69-6	HC(H)C(c1c(N)ccc(-c2ccccc2)c1)C(H)H	3
3653	ISSSTY_v1a_7367_02May011_4661	54810-82-1	HC(H)c1c(N)c(C(H)H)cc(-c2ccccc2)c1	3
3654	ISSSTY_v1a_7367_02May011_4662	314084-63-4	HC(H)C(H)c1c(N)c(C(H)C(H)H)cc(-c2ccccc2)c1	1

3655	ISSSTY_v1a_7367_02May011_4664	389104-62-5	HC(H)C(c1c(N)c(C(C(H)H)C(H)H)cc(-c2ccccc2)c1)C(H)H	1
3656	ISSSTY_v1a_7367_02May011_4665	313-80-4	c12c3c4c(ccc3ccc1)ccnc4cc2	3
3657	ISSSTY_v1a_7367_02May011_4666	125701-97-5	HC(H)c1c(C2=NC(c3ccc(OC(H)H)cc3)=C(c3ccc(OC(H)H)cc3)N2)ccc(C(H)H)c1	3
3658	ISSSTY_v1a_7367_02May011_4668	105360-93-8	C12c3c4c(C=C1)cccc4ccc3NC(=O)C=2	3
3659	ISSSTY_v1a_7367_02May011_4669	668-17-7	HC(H)C(H)[C@]1(O)C(H)[C@](OC2C(H)C(N(C(H)H)C(H)H)C(O)C(C(H)H)O2)c2c(O)c3C(=O)c4c(C(=O)c3cc2[C@@]1C(=O)OC(H)H)c(O)ccc4O	3
3660	ISSSTY_v1a_7367_02May011_4670	5598-15-2	HC(H)C(H)OP(=O)(Oc1c(Cl)cc(Cl)c(Cl)n1)OC(H)C(H)H	1
3661	ISSSTY_v1a_7367_02May011_4672	2012-00-2	HC(H)C(H)OP(=O)(c1ccccc1)Oc1ccc(N(=O)=O)cc1	3
3662	ISSSTY_v1a_7367_02May011_4673	54738-93-1	c1(N(=O)=O)c2c(cc3c(cccc3)c2)ccc1	3
3663	ISSSTY_v1a_7367_02May011_4674	31120-85-1	HC(H)C(H)OP(=O)(NC(C(H)H)C(H)H)Oc1c(C(=O)OC(C(H)H)C(H)H)cccc1	3
3664	ISSSTY_v1a_7367_02May011_4675	27729-95-9	HC(H)Oc1ccc([C@@]2[C@](C(=O)c3ccccc3)O2)cc1	3
3665	ISSSTY_v1a_7367_02May011_4676	51868-46-3	HC(H)C(=O)Nc1c(N=Nc2c(Br)cc([N+](=O)[O-])cc2[N+](=O)[O-])cc(OC(H)H)c(N(C(H)C=CH)C(H)C=CH)c1	3
3666	ISSSTY_v1a_7367_02May011_4677	13301-61-6	HC(H)C(H)N(c1ccc(N=Nc2c(Cl)cc(N(=O)=O)cc2Cl)cc1)C(H)C(H)C_N	3
3667	ISSSTY_v1a_7367_02May011_4678	932-97-8	C1(=O)C=CC(=[N+]=[N-])C=C1	3
3668	ISSSTY_v1a_7367_02May011_4679	6375-47-9	HC(H)C(=O)Nc1cc(N)c(OC(H)H)cc1	3
3669	ISSSTY_v1a_7367_02May011_4680	17420-30-3	C(N)c1c(N)ccc(N(=O)=O)c1	3
3670	ISSSTY_v1a_7367_02May011_4683	6214-18-2	HC(H)C(C(H)H)C(H)OS(=O)(=O)c1ccccc1	3
3671	ISSSTY_v1a_7367_02May011_4685	109143-20-6	HC(H)Oc1c2c(c(N(C(H)C(H)Cl)C(H)C(H)Cl)cc1)C=C(N(=O)=O)O2	3
3672	ISSSTY_v1a_7367_02May011_4686	109143-16-0	HC(Cl)C(H)N(c1cc2c(cc1)OC(N(=O)=O)=C2)C(H)C(H)Cl	3
3673	ISSSTY_v1a_7367_02May011_4687	605-32-3	c12C(=O)c3c(C(=O)c1cc(O)cc2)cccc3	3
3674	ISSSTY_v1a_7367_02May011_4688	109143-19-3	HC(H)Oc1c(N(C(H)C(H)Cl)C(H)C(H)Cl)c2c(cc1)OC(N(=O)=O)=C2	3
3675	ISSSTY_v1a_7367_02May011_4689	109143-17-1	HC(Cl)C(H)N(c1cc2c(C=C(N(=O)=O)O2)cc1)C(H)C(H)Cl	3
3676	ISSSTY_v1a_7367_02May011_4690	152-84-1	HC([C@]1[C@@](O)[C@](O)[C@@](O)[C@](Oc2c(O)c3C(=O)c4c(C(=O)c3cc2)cccc4)O1)O[C@@]1[C@](O)[C@@](O)[C@](O)C(H)O1	1
3677	ISSSTY_v1a_7367_02May011_4691	29706-59-0	HC(O)c1c(O)c2C(=O)c3c(C(=O)c2cc1O[C@@]1[C@](O)[C@@](O)[C@@](O)[C@@](C(H)O[C@@]2[C@](O)[C@@](O)[C@](O)C(H)O2)O1)cccc3	3
3678	ISSSTY_v1a_7367_02May011_4692	3131-23-5	HC(H)C12C(=O)C(H)C(H)[C@]1C1C(H)C(H)c3c(O)c(O)ccc3[C@]1C(H)C2H	1
3679	ISSSTY_v1a_7367_02May011_4693	362-06-1	HC(H)[C@@]12C(=O)C(H)C(H)[C@]1[C@@]1C(H)C(H)c3c(cc(O)c(O)c3)[C@]1C(H)C2H	1
3680	ISSSTY_v1a_7367_02May011_4694	72076-98-3	c12c3c4c(c5c(cc4Sc3ccc1)cccc5)cc2	3
3681	ISSSTY_v1a_7367_02May011_4695	142022-84-2	c12c3c4c(c5c(cc4S(=O)(=O)c3ccc1)cccc5)cc2	3
3682	ISSSTY_v1a_7367_02May011_4696	63348-71-0	HC(H)c1c([N+](=O)[O-])c(S(=O)(=O)O)c([N+](=O)[O-])cc1	1
3683	ISSSTY_v1a_7367_02May011_4697	52146-86-8	HC(H)c1c([N+](=O)[O-])cc([N+](=O)[O-])c(S(=O)(=O)O)c1	1
3684	ISSSTY_v1a_7367_02May011_4698	99346-47-1	c1(O)c2c3c4c(c5c([C@@](O)[C@](O)C=C5)cc4cc2)ccc3cc1	3
3685	ISSSTY_v1a_7367_02May011_4702	138261-41-3	HC(c1ccc(Cl)nc1)N1C(NN(=O)=O)=NC(H)C1H	3
3686	ISSSTY_v1a_7367_02May011_4704	98046-73-2	HC1C(N=O)=CC2=C(N3C(C=CC=C3)=N2)N1	3
3687	ISSSTY_v1a_7367_02May011_4705	482-35-9	HC(O)[C@]1[C@@](O)[C@](O)[C@@](O)[C@](OC2C(=O)c3c(O)cc(O)cc3OC=2c2cc(O)c(O)cc2)O1	3
3688	ISSSTY_v1a_7367_02May011_4707	96287-03-5	HC(H)C1C2N(c3c(c(C(H)H)c(N)cn3)N=2)C=CC=1	3
3689	ISSSTY_v1a_7367_02May011_4708	10265-92-6	HC(H)OP(N)(=O)SC(H)H	3
3690	ISSSTY_v1a_7367_02May011_4710	27758-60-7	HC(H)c1ccc(N(N)c2ccc(C(H)H)cc2)cc1	3
3691	ISSSTY_v1a_7367_02May011_4711	16596-38-6	HC(H)C(C(H)H)C(H)N(N)C(H)C(C(H)H)C(H)H	3
3692	ISSSTY_v1a_7367_02May011_4713	644-21-3	HC(H)C(H)N(N)c1ccccc1	3
3693	ISSSTY_v1a_7367_02May011_4717	1576-87-0	HC(H)C(H)C=CC=O	3
3694	ISSSTY_v1a_7367_02May011_4719	188970-77-6	c12-c3c4c(c([N+](=O)[O-])cc3Nc1cc([N+](=O)[O-])c1c2cccc1)cccc4	3
3695	ISSSTY_v1a_7367_02May011_4720	89784-39-4	HC(H)C(=O)N[C@](C(=O)O)C(H)SC(Cl)=C(Cl)C(Cl)=C(Cl)Cl	3
3696	ISSSTY_v1a_7367_02May011_4721	481-73-2	HC(O)c1cc2C(=O)c3c(C(=O)c2c(O)c1)c(O)cc(O)c3	3

3697	ISSSTY_v1a_7367_02May011_4722	138805-30-8	HC(H)c1c([N-][N+](=O)c2c(C(H)H)ccc(N)c2)cc(N)cc1	3
3698	ISSSTY_v1a_7367_02May011_4723	188970-83-4	c12-c3c4c(c(N(=O)=O)cc3Nc1ccc1c2cccc1)c(O)ccc4	3
3699	ISSSTY_v1a_7367_02May011_4735	626-43-7	c1(Cl)cc(Cl)cc(N)c1	1
3700	ISSSTY_v1a_7367_02May011_4737	634-67-3	c1(Cl)c(Cl)c(Cl)c(N)cc1	1
3701	ISSSTY_v1a_7367_02May011_4738	3333-66-2	HC(H)c1c2c(c3c(c(Cl)c4c(cccc4)n3)c1C(H)H)cccc2	3
3702	ISSSTY_v1a_7367_02May011_4739	634-91-3	c1(Cl)c(Cl)c(Cl)cc(N)c1	1
3703	ISSSTY_v1a_7367_02May011_4741	17722-52-0	HC(C(=O)Nc1ccc(Cl)cc1)C(H)C(=O)O	1
3704	ISSSTY_v1a_7367_02May011_4742	17722-71-3	HC(C(=O)Nc1cc(Cl)c(Cl)cc1)C(H)C(N)=O	1
3705	ISSSTY_v1a_7367_02May011_4743	53219-95-7	HC(C(=O)Nc1cc(Cl)cc(Cl)c1)C(H)C(=O)O	1
3706	ISSSTY_v1a_7367_02May011_4744	112368-25-9	HC(C(=O)Nc1c(Cl)c(Cl)c(Cl)cc1)C(H)C(N)=O	1
3707	ISSSTY_v1a_7367_02May011_4746	112368-26-0	HC(C(=O)Nc1cc(Cl)c(Cl)c(Cl)c1)C(H)C(N)=O	1
3708	ISSSTY_v1a_7367_02May011_4747	6943-00-6	HC1C(=O)N(c2ccc(Cl)cc2)C(=O)C1H	1
3709	ISSSTY_v1a_7367_02May011_4749	15386-58-0	HC1C(=O)N(c2cc(Cl)c(Cl)cc2)C(=O)C1H	1
3710	ISSSTY_v1a_7367_02May011_4750	24096-53-5	HC1C(=O)N(c2cc(Cl)cc(Cl)c2)C(=O)C1H	1
3711	ISSSTY_v1a_7367_02May011_4751	112368-27-1	HC1C(=O)N(c2c(Cl)c(Cl)c(Cl)cc2)C(=O)C1H	1
3712	ISSSTY_v1a_7367_02May011_4752	27746-63-0	HC1C(=O)N(c2cc(Cl)c(Cl)c(Cl)c2)C(=O)C1H	1
3713	ISSSTY_v1a_7367_02May011_4754	1068-57-1	HC(H)C(=O)NN	3
3714	ISSSTY_v1a_7367_02May011_4755	19315-64-1	HC(H)C(=O)N(O)c1ccc(OC(H)C(H)H)cc1	3
3715	ISSSTY_v1a_7367_02May011_4758	14634-93-6	HC(H)C(H)N(c1cccc1)C([S-])=S[Zn++]=S=C([S-])N(c1cccc1)C(H)C(H)H	1
3716	ISSSTY_v1a_7367_02May011_4759	95-33-0	HC1C(H)C(H)C(H)C(H)C1NSC1=Nc2c(cccc2)S1	1
3717	ISSSTY_v1a_7367_02May011_4760	102-77-2	HC1C(H)N(SC2=Nc3c(cccc3)S2)C(H)C(H)O1	1
3718	ISSSTY_v1a_7367_02May011_4761	26780-96-1	HC(H)C1c2c(cccc2)NC(C(H)H)(C(H)H)C=1	1
3719	ISSSTY_v1a_7367_02May011_4762	61788-44-1	HC=Cc1c(O)ccc(C=CH)c1	1
3720	ISSSTY_v1a_7367_02May011_4764	85-60-9	HC(H)C(c1c(O)cc(C(H)H)c(C(c2c(C(H)H)cc(O)c(C(C(H)H)(C(H)H)C(H)H)c2)C(H)C(H)C(H)H)c1)(C(H)H)C(H)H	1
3721	ISSSTY_v1a_7367_02May011_4765	843-55-0	HC1C(c2ccc(O)cc2)(c2ccc(O)cc2)C(H)C(H)C(H)C1H	1
3722	ISSSTY_v1a_7367_02May011_4766	119-47-1	HC(H)C(c1c(O)c(C(H)c2c(O)c(C(C(H)H)(C(H)H)C(H)H)cc(C(H)H)c2)cc(C(H)H)c1)(C(H)H)C(H)H	1
3723	ISSSTY_v1a_7367_02May011_4767	91-53-2	HC(H)C1c2c(ccc(OC(H)C(H)H)c2)NC(C(H)H)(C(H)H)C=1	1
3724	ISSSTY_v1a_7367_02May011_4768	548-39-0	C1(=O)c2c3c(C=C1)cccc3ccc2	3
3725	ISSSTY_v1a_7367_02May011_4769	66291-31-4	HC(H)c1c(C(H)H)c2c3c(ccc2cc1)cccc3	1
3726	ISSSTY_v1a_7367_02May011_4770	15254-64-5	HC(H)c1c2c3c(ccc2cc(C(H)H)c1)cccc3	3
3727	ISSSTY_v1a_7367_02May011_4771	16664-45-2	HC(H)c1c2c(c3c(cccc3)cc2)cc(C(H)H)c1	3
3728	ISSSTY_v1a_7367_02May011_4772	22349-59-3	HC(H)c1c2c(c3c(cccc3)cc2)c(C(H)H)cc1	3
3729	ISSSTY_v1a_7367_02May011_4773	1070-13-9	HC(H)C(H)C(H)C(C=O)=CH	3
3730	ISSSTY_v1a_7367_02May011_4774	922-63-4	HC(H)C(H)C(C=O)=CH	3
3731	ISSSTY_v1a_7367_02May011_4775	94500-54-6	HC(Cl)c1c2c3c4c(ccc3cc3c2cccc3)cccc4c1	3
3732	ISSSTY_v1a_7367_02May011_4778	94500-44-4	HC(Cl)c1c2c3c4c(c5c(cc4ccc3ccc5)cccc5)c1	3
3733	ISSSTY_v1a_7367_02May011_4782	1107-26-2	HC(H)C1(C(H)H)C(C=CC(C(H)H)=CC=CC(C(H)H)=CC=CC(C(H)H)C=CC(C(H)H)C=O)=C(C(H)H)C(H)C(H)C1H	1
3734	ISSSTY_v1a_7367_02May011_4785	7269-58-1	HC(O)[C@]1[C@@](O)[C@@](O)[C@](N2c3c(c(NO)nc(N)n3)N=C2)O1	3
3735	ISSSTY_v1a_7367_02May011_4792	27762-78-3	HC(H)C(H)OC(C(=O)C(O)O)C(H)H	3
3736	ISSSTY_v1a_7367_02May011_4793	6149-34-4	c1(Nc2ccc(N)cc2)ccc(N(=O)=O)cc1	3
3737	ISSSTY_v1a_7367_02May011_4794	60516-11-2	HC(H)C(=O)Nc1ccc(Nc2ccc(N(=O)=O)cc2)cc1	3
3738	ISSSTY_v1a_7367_02May011_4795	620-89-3	HC(H)c1ccc(Nc2ccc(N(=O)=O)cc2)cc1	3

3739	ISSSTY_v1a_7367_02May011_4797	962-32-3	c12-c3c(C4C(c1cc1c(cccc1)c2)O4)cccc3	3
3740	ISSSTY_v1a_7367_02May011_4798	138835-35-5	c12c(c3c4c5c(c(N(=O)=O)ccc5ccc4n1)cc3)cccc2	3
3741	ISSSTY_v1a_7367_02May011_4799	138835-36-6	c12c(c3c4c5c(c(N(=O)=O)ccc5ccc3)ccc4n1)cccc2	3
3742	ISSSTY_v1a_7367_02May011_4800	138835-33-3	c12c(c3c4c5c(c([N+](=O)[O-])ccc5ccc4[n+])1[O-])cc3)cccc2	3
3743	ISSSTY_v1a_7367_02May011_4801	138835-34-4	c12c(c3c4c5c(c([N+](=O)[O-])ccc5ccc3)ccc4[n+])1[O-])cccc2	3
3744	ISSSTY_v1a_7367_02May011_4802	125974-01-8	HC(C)C1=C(C)C(=O)OC1H	3
3745	ISSSTY_v1a_7367_02May011_4804	93673-37-1	c12c3c(c4c(c5c([C@](O)[C@@](O)C=C5)cc4)cc3ccc1)C=C2	3
3746	ISSSTY_v1a_7367_02May011_4806	24279-91-2	HC(H)C1C(=O)C(N2C(H)C2H)=C(C(C(H)OC(N)=O)OC(H)H)C(=O)C=1N1C(H)C1H	3
3747	ISSSTY_v1a_7367_02May011_4807	488-41-5	HC(Br)C(O)C(O)C(O)C(O)C(H)Br	3
3748	ISSSTY_v1a_7367_02May011_4809	3697-30-1	HC(H)C(H)c1c2c(c3c(cccc3)cc2)cc2c1cccc2	3
3749	ISSSTY_v1a_7367_02May011_4814	71708-92-4	HC(H)C(=O)N(O)c1ccc(Oc2ccccc2)cc1	3
3750	ISSSTY_v1a_7367_02May011_4816	2417-77-8	HC(Br)c1c2c(cc3c1cccc3)cccc2	3
3751	ISSSTY_v1a_7367_02May011_4818	114924-37-7	HC(H)[C@@]12[C@](C=O)(C(C=O)=C3[C@](O)(C(H)C(C(H)H)(C(H)H)C3H)[C@]1O)C2H	3
3752	ISSSTY_v1a_7367_02May011_4819	114838-69-6	HC(H)[C@]12[C@@](C=O)(C(C=O)=C3[C@](O)(C(H)C(C(H)H)(C(H)H)C3H)[C@]1OC(=O)C(H)H)C2H	3
3753	ISSSTY_v1a_7367_02May011_4820	108893-58-9	HC(H)[C@@]12[C@](C=O)(C(C=O)=C3[C@](O)(C(H)C(C(H)H)(C(H)H)C3H)[C@]1O)C2H	3
3754	ISSSTY_v1a_7367_02May011_4823	114882-46-1	c1(N=O)c2c3c4c(c5c(cc4ccc3cc1)cccc5)cc2	3
3755	ISSSTY_v1a_7367_02May011_4824	120388-69-4	c1(N=O)c2c3c4c(c5c(cc4cc2)cccc5)ccc3cc1	3
3756	ISSSTY_v1a_7367_02May011_4825	120812-47-7	HC1c2c(c3c4c5c(c(N(=O)=O)ccc25)ccc4ccc3)C(H)C(H)C1H	3
3757	ISSSTY_v1a_7367_02May011_4826	215226-71-4	HC(H)C(=C(C)C(=O)O)C=O	3
3758	ISSSTY_v1a_7367_02May011_4827	215226-73-6	HC(C)C(=C(C)C(=O)O)C(C)C1	3
3759	ISSSTY_v1a_7367_02May011_4828	215226-72-5	HC(C)C(C(C)C)C1=CC(=O)O	3
3760	ISSSTY_v1a_7367_02May011_4829	491-35-0	HC(H)c1c2c(cccc2)ncc1	3
3761	ISSSTY_v1a_7367_02May011_4833	97931-39-0	HC1c2c3c4c(c(N(=O)=O)c5c(c4ccc3ccc2)cccc5)C1H	3
3762	ISSSTY_v1a_7367_02May011_4834	67587-52-4	HC1C(H)N(N=O)C(H)C(O)O1	3
3763	ISSSTY_v1a_7367_02May011_4835	88598-56-5	HC1c2c(c3c4c5c(c(N(=O)=O)ccc5ccc4c2)cc3)C(H)C(H)C1H	3
3764	ISSSTY_v1a_7367_02May011_4836	88598-57-6	HC1c2c(c3c4c5c(c(N(=O)=O)ccc5ccc3)ccc4c2)C(H)C(H)C1H	3
3765	ISSSTY_v1a_7367_02May011_4837	107-20-0	HC(C)C=O	3
3766	ISSSTY_v1a_7367_02May011_4839	95840-05-4	[C@]1(O)[C@@](O)[C@@]2[C@](C=C1)O2	3
3767	ISSSTY_v1a_7367_02May011_4840	121153-48-8	[C@]1(O)[C@@](O)[C@]2[C@@](C=C1)O2	3
3768	ISSSTY_v1a_7367_02May011_4841	121153-49-9	[C@@]1(O)[C@](O)[C@@]2[C@](C=C1)O2	3
3769	ISSSTY_v1a_7367_02May011_4843	120209-97-4	c12c(cc(N)cc1)nc1c(cc(N)cc1)n2	3
3770	ISSSTY_v1a_7367_02May011_4850	93673-33-7	HC1c2c(C3=C4C(=C5C=CC=C1C35)O4)c1c(cccc1)cc2	3
3771	ISSSTY_v1a_7367_02May011_4851	577-19-5	c1(Br)c(N(=O)=O)cccc1	3
3772	ISSSTY_v1a_7367_02May011_4852	585-79-5	c1(Br)cc(N(=O)=O)cccc1	3
3773	ISSSTY_v1a_7367_02May011_4853	96910-71-3	HC(H)[C@@]12[C@@](C=O)(C(C=O)=C[C@@]3(O)C(H)C(C(H)H)(C(H)H)C(H)[C@@]13)C2H	3
3774	ISSSTY_v1a_7367_02May011_4855	2213-00-5	HC(H)C1(C(H)H)C(H)[C@@]2C3(C(=O)OC(H)H)[C@](C=O)(C(C=O)=C[C@@]2C1H)C3H	3
3775	ISSSTY_v1a_7367_02May011_4857	109883-99-0	HC(H)C1(C(H)H)C(H)C2(O)C(C34C(C(C=O)=C2)(C(O)OC3=O)C4H)C1H	3
3776	ISSSTY_v1a_7367_02May011_4858	603-02-1	HC(H)c1c([N+](=O)[O-])c(C(H)H)c([N+](=O)[O-])cc1	3
3777	ISSSTY_v1a_7367_02May011_4860	610-28-6	C(=O)(O)c1c([N+](=O)[O-])ccc([N+](=O)[O-])c1	3
3778	ISSSTY_v1a_7367_02May011_4861	96910-73-5	HC(H)C1(C(H)H)C(H)[C@]2(O)C=C(C=O)C(C=O)=C[C@](C(H)H)[C@]2C1H	3
3779	ISSSTY_v1a_7367_02May011_4867	99-33-2	C(=O)(C)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1	3
3780	ISSSTY_v1a_7367_02May011_4872	96910-70-2	HC(H)[C@]12[C@@](C=O)(C(C(H)O)=C[C@@]3C(H)C(C(H)H)(C(H)H)C(H)[C@@]13)C2H	3

3781	ISSSTY_v1a_7367_02May011_4874	30074	c12C(=O)c3c(-c4c1c(ccc4)ccc2)cccc3	3
3782	ISSSTY_v1a_7367_02May011_4875	90-44-8	HC1c2c(C(=O)c3c1cccc3)cccc2	3
3783	ISSSTY_v1a_7367_02May011_4877	104671-59-2	HC(H)C(=O)NOC(=O)NC(H)H	3
3784	ISSSTY_v1a_7367_02May011_4878	106807-80-1	HC(H)C(=O)N(O)C(=O)NC(H)H	3
3785	ISSSTY_v1a_7367_02May011_4881	51594-55-9	HC(CI)[C@@]1C(H)O1	3
3786	ISSSTY_v1a_7367_02May011_4882	67843-74-7	HC(CI)[C@]1C(H)O1	3
3787	ISSSTY_v1a_7367_02May011_4883	57044-25-4	HC(O)[C@]1C(H)O1	3
3788	ISSSTY_v1a_7367_02May011_4884	60456-23-7	HC(O)[C@]1C(H)O1	3
3789	ISSSTY_v1a_7367_02May011_4886	113826-06-5	HC(H)c1ccc(S(=O)(=O)OC(H)[C@@]2C(H)O2)cc1	3
3790	ISSSTY_v1a_7367_02May011_4887	70987-78-9	HC(H)c1ccc(S(=O)(=O)OC(H)[C@]2C(H)O2)cc1	3
3791	ISSSTY_v1a_7367_02May011_4888	129286-36-8	c1(F)c2c3c(c4c(c5c(ccc5)cc4)c3ccc2)cc1	3
3792	ISSSTY_v1a_7367_02May011_4889	129286-37-9	c12c3c(c4c(c5c(cc(F)cc5)cc4)c3ccc1)ccc2	3
3793	ISSSTY_v1a_7367_02May011_4890	28361-96-8	HC(CI)C(H)SC(H)C(N)C(=O)O	3
3794	ISSSTY_v1a_7367_02May011_4892	101043-65-6	c1(N(=O)=O)c2c3c4c(c(N=O)ccc4cc2)ccc3cc1	3
3795	ISSSTY_v1a_7367_02May011_4893	105500-28-5	c12c(c3c([C@@](O)[C@](O)[C@@]4[C@@]3O4)cc1)cc1c3c(ccc1n2)cccc3	3
3796	ISSSTY_v1a_7367_02May011_4894	105467-73-0	c12c(c3c([C@@](O)[C@](O)[C@]4[C@]3O4)cc1)cc1c3c(ccc1n2)cccc3	3
3797	ISSSTY_v1a_7367_02May011_4895	118745-11-2	c1(C=Cc2ccc(N(O)C=O)cc2)ccccc1	3
3798	ISSSTY_v1a_7367_02May011_4896	78281-06-8	c1(-c2ccc(NC(=O)O)cc2)ccccc1	3
3799	ISSSTY_v1a_7367_02May011_4897	1707-31-9	c12c(cc(N(O)C=O)cc1)cccc2	3
3800	ISSSTY_v1a_7367_02May011_4899	118745-12-3	HC(H)C(H)C(=O)N(O)c1ccc(C=Cc2ccccc2)cc1	3
3801	ISSSTY_v1a_7367_02May011_4902	5329-87-3	HC1c2c(-c3c(cc(N(=O)=O)cc3)C1H)cccc2	3
3802	ISSSTY_v1a_7367_02May011_4903	10549-22-1	HC1c2c3-c4c(C(H)C(H)c3cc(N(=O)=O)c2)cccc4C1H	3
3803	ISSSTY_v1a_7367_02May011_4904	117929-14-3	HC1c2c3c4c(cc(N(=O)=O)cc4ccc3ccc2)C1H	3
3804	ISSSTY_v1a_7367_02May011_4905	149127-56-0	HC(H)C(C(H)H)(N=NC(H)H)OO	3
3805	ISSSTY_v1a_7367_02May011_4906	69533-68-2	HC1c2c(-c3c(cc([N+](=O)[O-])cc3)C1H)ccc([N+](=O)[O-])c2	3
3806	ISSSTY_v1a_7367_02May011_4907	17573-23-8	HC1c2c(c3c4c5c(ccc4c2)cccc5cc3)C=CC1H	3
3807	ISSSTY_v1a_7367_02May011_4908	117929-13-2	HC1c2c3-c4c(C(H)C(H)c3cc([N+](=O)[O-])c2)cc([N+](=O)[O-])cc4C1H	3
3808	ISSSTY_v1a_7367_02May011_4909	117929-12-1	HC1c2c3c4c(cc([N+](=O)[O-])cc4ccc3cc([N+](=O)[O-])c2)C1H	3
3809	ISSSTY_v1a_7367_02May011_4910	119-27-7	HC(H)Oc1c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
3810	ISSSTY_v1a_7367_02May011_4911	2363-23-7	HC(H)Sc1c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
3811	ISSSTY_v1a_7367_02May011_4912	581437	c1(Oc2ccc(Oc3ccc(N)cc3)cc2)ccc(N)cc1	3
3812	ISSSTY_v1a_7367_02May011_4913	23815-63-6	HC([C@](N)C(=O)O)Sc1c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
3813	ISSSTY_v1a_7367_02May011_4920	151378-31-3	c12C34c5c(c6c(cccc6)cc5)-c1cccc2C(O)C(O)C3O4	3
3814	ISSSTY_v1a_7367_02May011_4921	132335-15-0	c12-c3c(c4c(cccc4)cc3)C3C(c1cccc2)N3	3
3815	ISSSTY_v1a_7367_02May011_4922	84850-16-8	c12c(c3c(c4c5c(c6c(c14)cccc6)cccc5)cccc3)O2	3
3816	ISSSTY_v1a_7367_02May011_4923	132335-20-7	c12-c3c4c(c5c(c3C3C(c1cccc2)N3)cccc5)cccc4	3
3817	ISSSTY_v1a_7367_02May011_4927	623-10-9	HC(H)c1ccc(NO)cc1	3
3818	ISSSTY_v1a_7367_02May011_4929	2498-77-3	HC(H)c1c2c3c(cc4c(cccc4)c3)ccc2ccc1	3
3819	ISSSTY_v1a_7367_02May011_4930	2498-76-2	HC(H)c1cc2c3c(cc4c(cccc4)c3)ccc2cc1	3
3820	ISSSTY_v1a_7367_02May011_4931	2498-75-1	HC(H)c1cc2c(c3c(cc4c(cccc4)c3)cc2)cc1	3
3821	ISSSTY_v1a_7367_02May011_4932	316-49-4	HC(H)c1c2c(c3c(cccc3)c1)cc1c(cccc1)c2	3
3822	ISSSTY_v1a_7367_02May011_4933	2381-31-9	HC(H)c1c2c(cc3c4c(ccc3c2)cccc4)ccc1	3