

3823	ISSSTY_v1a_7367_02May011_4934	2381-16-0	HC(H)c1cc2c(cc3c4c(ccc3c2)cccc4)cc1	3
3824	ISSSTY_v1a_7367_02May011_4935	50618-02-5	HC(H)[C@]1[C@@](c2ccc(OC(H)H)cc2)O1	3
3825	ISSSTY_v1a_7367_02May011_4936	6111-78-0	HC(H)c1c2c(cc3c(c4c(cccc4)cc3)c2)ccc1	3
3826	ISSSTY_v1a_7367_02May011_4940	151378-32-4	c12C34c5c(c6c(cccc6)cc5)-c1cccc2C(O)C(O)C3O4	3
3827	ISSSTY_v1a_7367_02May011_4941	151378-33-5	c12c3c(c4c(c5c(C(O)C(O)C6C5O6)cc4)c3ccc1)ccc2	3
3828	ISSSTY_v1a_7367_02May011_4943	151378-34-6	c12c3c(c4c(c5c(C(O)C(O)C6C5O6)cc4)c3ccc1)ccc2	3
3829	ISSSTY_v1a_7367_02May011_4945	80-40-0	HC(H)c1ccc(S(=O)(=O)OC(H)C(H)H)cc1	3
3830	ISSSTY_v1a_7367_02May011_4948	159091-35-7	HC(C1=CC=C(C=O)O1)OS(=O)(=O)O	3
3831	ISSSTY_v1a_7367_02May011_4950	125157-96-2	HC(H)C1c2c(ccc(C(H)H)c2)N(C(H)H)C2C=1c1c(cccc1)N=2	3
3832	ISSSTY_v1a_7367_02May011_4951	39501-62-7	c1(Oc2ccccc2)ccc(NO)cc1	3
3833	ISSSTY_v1a_7367_02May011_4952	1147-55-3	HC(H)C(=O)Nc1cc2c(-c3c(O)cccc3C2H)cc1	3
3834	ISSSTY_v1a_7367_02May011_4954	97606-15-0	C12C(C3C(C4C1N4)=CSC=3)=CSC=2	3
3835	ISSSTY_v1a_7367_02May011_4955	23102-68-3	C12C(C3C(C4C1O4)=CSC=3)=CSC=2	3
3836	ISSSTY_v1a_7367_02May011_4956	13345-23-8	c1(O)c2c3c4c(c5c(cc4ccc3cc1)cccc5)cc2	3
3837	ISSSTY_v1a_7367_02May011_4957	57-57-8	HC1C(=O)OC1H	3
3838	ISSSTY_v1a_7367_02May011_4958	78400-41-6	HC(H)c1c2c3c(c4c(-c5c(C6C4N6)cccc5)cc3cc1)C(H)C2H	3
3839	ISSSTY_v1a_7367_02May011_4959	928-51-8	HC(Cl)C(H)C(H)C(H)O	3
3840	ISSSTY_v1a_7367_02May011_4960	71382-49-5	c12-c3c(C4C(c1cc1c5c(ccc1c2)cccc5)N4)cccc3	3
3841	ISSSTY_v1a_7367_02May011_4961	75-55-8	HC(H)C1C(H)N1	3
3842	ISSSTY_v1a_7367_02May011_4963	103088-83-1	C1(=O)C(=O)c2c3c(c4c(cccc4)cc3)ccc2C=C1	3
3843	ISSSTY_v1a_7367_02May011_4965	5461-85-8	HC(H)C(C(H)H)C(H)N(C(N)=NN(=O)=O)N=O	3
3844	ISSSTY_v1a_7367_02May011_4966	88847-41-0	c12c(c3c(c4c([C@](O)[C@@](O)[C@@]5[C@@]4O5)cc3)cc1)cc(O)cc2	3
3845	ISSSTY_v1a_7367_02May011_4967	127923-99-3	HC(C(=O)OC(H)C(H)Br)C(O)C(=O)OC(H)C(H)Br	3
3846	ISSSTY_v1a_7367_02May011_4968	30269-02-4	c1(N)c2c3c4c(c(N(=O)=O)ccc4ccc3cc1)cc2	3
3847	ISSSTY_v1a_7367_02May011_4969	20268-52-4	c12c(c(Cl)c3c(c4c(cccc4)cc3)c1)cccc2	3
3848	ISSSTY_v1a_7367_02May011_4970	83504-80-7	c1(Sc2ccccc2)ccc(N=O)cc1	3
3849	ISSSTY_v1a_7367_02May011_4972	21229-99-2	c1(Sc2ccccc2)ccc(NO)cc1	3
3850	ISSSTY_v1a_7367_02May011_4973	590-96-5	HC(H)[N+](=O)[N-]C(H)O	3
3851	ISSSTY_v1a_7367_02May011_4974	57011-48-0	HC(C(O)C(H)N=N_N)N=N_N	3
3852	ISSSTY_v1a_7367_02May011_4975	709-49-9	c1(l)c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
3853	ISSSTY_v1a_7367_02May011_4985	25125-72-8	c1([C@]2[C@](c3ccccc3)N2)ccccc1	3
3854	ISSSTY_v1a_7367_02May011_4986	3416-21-5	HC(H)c1c2c3c(c4c(-c5c(C6C4O6)cccc5)cc3cc1)C(H)C2H	3
3855	ISSSTY_v1a_7367_02May011_4988	1605-06-7	c1([C@]2[C@](c3ccccc3)N2)ccccc1	3
3856	ISSSTY_v1a_7367_02May011_4989	1919899	c12c3c(C4C(c3ccc1)N4)ccc2	3
3857	ISSSTY_v1a_7367_02May011_4991	81851-68-5	HC(H)c1c2c(c3c(cccc3)c1)ccc1c2C2[C@]([C@](O)[C@@]1O)O2	3
3858	ISSSTY_v1a_7367_02May011_4994	57564-91-7	HC(C(=O)N[C@](C(=O)NC(H)C(=O)O)C(H)SN=O)C(H)[C@](N)C(=O)O	3
3859	ISSSTY_v1a_7367_02May011_4995	108670-78-6	HC(H)C(H)C=CC=CC=CC=COC(H)C(O)C(H)O	3
3860	ISSSTY_v1a_7367_02May011_4996	89300-15-2	HC(H)C(H)C=CC=CC=CC=CC=COC(H)C(O)C(H)O	3
3861	ISSSTY_v1a_7367_02May011_4998	1488-21-7	HC1C23C(C(H)C1H)(C=CC=C2)O3	3
3862	ISSSTY_v1a_7367_02May011_5000	114451-08-0	HC(H)N1c2c(c3c(cc2)nccc3)N=C1N(=O)=O	3
3863	ISSSTY_v1a_7367_02May011_5001	540-80-7	HC(H)C(C(H)H)(C(H)H)ON=O	3
3864	ISSSTY_v1a_7367_02May011_5002	33611-88-0	c1([N+](=O)[O-])c([N+](=O)[O-])c2c3c(c4c2c(ccc4)c1)cccc3	3

3865	ISSSTY_v1a_7367_02May011_5003	110419-21-1	c1([N+](=O)[O-])c2c3c(c4c(c3c([N+](=O)[O-])c1)cccc4)ccc2	3
3866	ISSSTY_v1a_7367_02May011_5004	64810-99-7	c1(OS(=O)(=O)O)c2c3c4c(c5c(cc4ccc3cc1)cccc5)cc2	3
3867	ISSSTY_v1a_7367_02May011_5006	151751-83-6	HC(H)C(H)OC(=O)N(C(H)C(H)C=O)N=O	3
3868	ISSSTY_v1a_7367_02May011_5007	90-15-3	c1(O)c2c(cccc2)ccc1	3
3869	ISSSTY_v1a_7367_02May011_5008	71432-00-3	C1(=O)c2c3c(c4c(cccc4)c2)ccc2c3c(ccc2)O1	3
3870	ISSSTY_v1a_7367_02May011_5010	112309-62-3	C(=O)(O)C=C(C(CI)CI)C(CI)CI	3
3871	ISSSTY_v1a_7367_02May011_5011	203-33-8	c12c(c3c4c(c5c3c(ccc5)c1)cccc4)cccc2	3
3872	ISSSTY_v1a_7367_02May011_5013	215226-70-3	HC(CI)C(=C(CI)C(=O)O)C=O	3
3873	ISSSTY_v1a_7367_02May011_5014	64188-64-3	HC(c1cccc1)N1C2c3c(-c4c(cccc4)C12)cccc3	3
3874	ISSSTY_v1a_7367_02May011_5020	166546-21-0	HC(H)N1C(H)C(H)N(c2cc3c(cc2)N=C(C(H)C(H)c2cc4c(cc2)N=C(c2ccc(N(C(H)C(H)CI)C(H)C(H)CI)cc2)N4)N3)C(H)C1H	3
3875	ISSSTY_v1a_7367_02May011_5021	166546-22-1	HC(H)N1C(H)C(H)N(c2cc3c(cc2)N=C(C(H)C(H)C(H)c2cc4c(cc2)N=C(c2ccc(N(C(H)C(H)CI)C(H)C(H)CI)cc2)N4)N3)C(H)C1H	3
3876	ISSSTY_v1a_7367_02May011_5023	1672-88-4	HC1C(=O)NC(=O)N1N=CC=CC1=CC=C(N(=O)=O)O1	3
3877	ISSSTY_v1a_7367_02May011_5028	8001-35-2	HC(CI)C1(C(H)CI)C(=CH)C2(CI)C(CI)(CI)C1(CI)C(CI)C2CI	3
3878	ISSSTY_v1a_7367_02May011_5030	771-29-9	HC1c2c(C(OO)C(H)C1H)cccc2	3
3879	ISSSTY_v1a_7367_02May011_5031	75-21-8	HC1C(H)O1	3
3880	ISSSTY_v1a_7367_02May011_5033	13010-10-1	HC(H)C(H)C(H)C(H)C(H)N(C(N)=NN(=O)=O)N=O	3
3881	ISSSTY_v1a_7367_02May011_5035	5496-41-3	HC(H)Oc1c(OC(H)H)ccc(C2=NC(c3ccccc3)=C(c3ccccc3)N2)cc1	3
3882	ISSSTY_v1a_7367_02May011_5037	2687-25-4	HC(H)c1c(N)c(N)ccc1	3
3883	ISSSTY_v1a_7367_02May011_5040	104975-31-7	c12c(c3c(c4c([C@@](O)[C@](O)[C@@]5[C@@]4O5)cc3)cc1)cc(O)cc2	3
3884	ISSSTY_v1a_7367_02May011_5041	2125597	O=S(Cl)Cl	3
3885	ISSSTY_v1a_7367_02May011_5043	101688-02-2	HC(CI)C(H)N(c1cc2c(c3c(cc2)OC(N(=O)=O)=C3)cc1)C(H)C(H)Cl	3
3886	ISSSTY_v1a_7367_02May011_5044	116505-02-3	HC(H)C(=O)N(c1ccc(Sc2ccccc2)cc1)OC(=O)C(H)H	3
3887	ISSSTY_v1a_7367_02May011_5045	843-23-2	HC(H)C(=O)N(O)c1ccc(C=Cc2ccccc2)cc1	3
3888	ISSSTY_v1a_7367_02May011_5046	16110-13-7	HC(O)c1c2c(c3c(cccc3)cc2)cc2c1cccc2	3
3889	ISSSTY_v1a_7367_02May011_5049	78246-54-5	HC(O)c1ccc([N+]_N)cc1	3
3890	ISSSTY_v1a_7367_02May011_5051	68006-83-7	HC(H)c1c(N)nc2c(-c3c(cccc3)N2)c1	3
3891	ISSSTY_v1a_7367_02May011_5053	138331-98-3	HC([C@]1[C@@](O)[C@](O)[C@@](O)[C@@](O)O1)N=N_N	3
3892	ISSSTY_v1a_7367_02May011_5054	120202-54-2	HC([C@]1[C@@](O)[C@](O)[C@](O)[C@@](O)O1)N=N_N	3
3893	ISSSTY_v1a_7367_02May011_5055	138331-99-4	HC([C@]1[C@@](O)[C@@](O)[C@](O)[C@@](O)O1)N=N_N	3
3894	ISSSTY_v1a_7367_02May011_5056	138332-01-1	HC([C@]1[C@@](O)[C@@](O)[C@](O)[C@@](O)O1)N=N_N	3
3895	ISSSTY_v1a_7367_02May011_5057	138332-00-0	HC([C@@]1[C@@](O)[C@](O)[C@@](O)[C@@](O)O1)N=N_N	3
3896	ISSSTY_v1a_7367_02May011_5058	73174-38-6	HC([C@]1[C@](O)[C@](O)[C@@](O)[C@@](O)O1)N=N_N	3
3897	ISSSTY_v1a_7367_02May011_5059	138245-73-5	HC([C@@](O)[C@](O)[C@](O)[C@@](O)O)C(=O)O)N=N_N	3
3898	ISSSTY_v1a_7367_02May011_5060	98736-45-9	HC(H)N(C(H)c1cc(OC(H)H)ccc1)N=O	3
3899	ISSSTY_v1a_7367_02May011_5061	62783-49-7	HC(H)c1cc(C(H)N(C(H)H)N=O)ccc1	3
3900	ISSSTY_v1a_7367_02May011_5062	98736-46-0	HC(H)N(C(H)c1cc(Cl)ccc1)N=O	3
3901	ISSSTY_v1a_7367_02May011_5063	98736-47-1	HC(H)N(C(H)c1cc(Br)ccc1)N=O	3
3902	ISSSTY_v1a_7367_02May011_5064	98736-48-2	HC(H)N(C(H)c1cc(C(F)(F)F)ccc1)N=O	3
3903	ISSSTY_v1a_7367_02May011_5065	98736-49-3	HC(H)N(C(H)c1cc(C_N)ccc1)N=O	3
3904	ISSSTY_v1a_7367_02May011_5068	84174-21-0	HC(H)N(C(H)c1ccc(F)cc1)N=O	3
3905	ISSSTY_v1a_7367_02May011_5069	84174-22-1	HC(H)N(C(H)c1ccc(Cl)cc1)N=O	3
3906	ISSSTY_v1a_7367_02May011_5070	98736-50-6	HC(H)N(C(H)c1ccc(Br)cc1)N=O	3

3949	ISSSTY_v1a_7367_02May011_5155	107-04-0	HC(Br)C(H)Cl	3
3950	ISSSTY_v1a_7367_02May011_5157	298-18-0	HC1C(C2C(H)O2)O1	3
3951	ISSSTY_v1a_7367_02May011_5158	96563-06-3	HC(H)c1c(C(H)H)cc2-c3c(C(C(H)H)c2c1)cccc3	3
3952	ISSSTY_v1a_7367_02May011_5160	95791-46-1	c1(Cl)c2c(c3c(c4c(cccc4)cc3)c1)cccc2	3
3953	ISSSTY_v1a_7367_02May011_5161	61740-00-9	HC(H)Oc1c2C3=C(C(=O)Oc2c2c(c1)O[C@@]1[C@]2C=CO1)[C@](O)C(H)C3H	3
3954	ISSSTY_v1a_7367_02May011_5162	34244-14-9	c12c3c4c(c(Cl)ccc4ccc3ccc1)cc2	3
3955	ISSSTY_v1a_7367_02May011_5163	716-53-0	c12c(c(Cl)c3c(cccc3)c1)cccc2	3
3956	ISSSTY_v1a_7367_02May011_5164	42978-43-8	HC(H)C(=O)OC(H)c1c2c(c3c4c5c(ccc14)cccc5cc3)cccc2	3
3957	ISSSTY_v1a_7367_02May011_5165	105708-73-4	HC(H)C(=O)OC(H)c1c2c3c4c5c6c(cc4ccc3ccc2)cccc6ccc15	3
3958	ISSSTY_v1a_7367_02May011_5166	49852-85-9	HC(Br)c1c2c(c3c4c5c(ccc14)cccc5cc3)cccc2	3
3959	ISSSTY_v1a_7367_02May011_5167	105708-74-5	HC(Br)c1c2c3c4c5c6c(cc4ccc3ccc2)cccc6ccc15	3
3960	ISSSTY_v1a_7367_02May011_5168	2564-64-9	HC(H)c1c2c(c(C(H)OC(=O)C(H)H)c3c4c(ccc13)cccc4)cccc2	3
3961	ISSSTY_v1a_7367_02May011_5170	17526-33-9	HC(H)C(=O)OC(H)c1c2c3c(ccc2cc2c1cccc2)cccc3	3
3962	ISSSTY_v1a_7367_02May011_5171	16430-32-3	HC(H)C(=O)OC(H)c1c2c(cc3c1cccc3)cccc2	3
3963	ISSSTY_v1a_7367_02May011_5173	31688-71-8	HC(H)c1c2c(c(C(H)OC(=O)C(H)H)c3c1cccc3)cccc2	3
3964	ISSSTY_v1a_7367_02May011_5174	24961-39-5	HC(Br)c1c2c(c3c(cccc3)cc2)cc2c1cccc2	3
3965	ISSSTY_v1a_7367_02May011_5175	2517-98-8	HC(H)c1c2c(c(C(H)OC(=O)C(H)H)c3c1c1c(cccc1)cc3)cccc2	3
3966	ISSSTY_v1a_7367_02May011_5176	17526-24-8	HC(H)C(=O)OC(H)c1c2c(c3c(cccc3)cc2)cc2c1cccc2	3
3967	ISSSTY_v1a_7367_02May011_5177	78533-30-9	HC(Br)c1c2c3c(ccc2cc2c1cccc2)cccc3	3
3968	ISSSTY_v1a_7367_02May011_5178	34331-95-8	HC(H)c1c2c(c(C(H)Br)c3c1cccc3)cccc2	3
3969	ISSSTY_v1a_7367_02May011_5179	59230-81-8	HC(H)c1c2c(c(C(H)Br)c3c4c(ccc13)cccc4)cccc2	3
3970	ISSSTY_v1a_7367_02May011_5180	105708-67-6	HC(H)C(=O)OC1c2c3c4c5c(cc3C1H)cccc5ccc4cc2	3
3971	ISSSTY_v1a_7367_02May011_5181	7319-59-7	HC(H)c1c2c3c(c4c(c5c(cccc5)cc4)cc3cc1)C(OC(=O)C(H)H)C2H	3
3972	ISSSTY_v1a_7367_02May011_5182	105708-68-7	HC(H)C(=O)OC1c2c3c4c5c(ccc4ccc3C1H)cccc5c2	3
3973	ISSSTY_v1a_7367_02May011_5183	7390-93-4	HC(H)c1c2c3c(c4c(c5c(cccc5)cc4)cc3cc1)C(H)C2OC(=O)C(H)H	3
3974	ISSSTY_v1a_7367_02May011_5184	16169-17-8	c1(-c2c(NO)cccc2)cccc1	3
3975	ISSSTY_v1a_7367_02May011_5185	115453-72-0	HC([C@](N)C(=O)O)SC(Cl)=C(Cl)C(Cl)(Cl)Cl	3
3976	ISSSTY_v1a_7367_02May011_5187	21711-71-7	c1(-c2c(N=O)cccc2)cccc1	3
3977	ISSSTY_v1a_7367_02May011_5188	105361-86-2	c1(-c2cc(N=O)ccc2)cccc1	3
3978	ISSSTY_v1a_7367_02May011_5192	6341-85-1	HC(H)C1(C2C(H)O2)C(H)O1	3
3979	ISSSTY_v1a_7367_02May011_5193	38363-41-6	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
3980	ISSSTY_v1a_7367_02May011_5195	3198-41-2	HC1c2c(C(H)C(H)C1H)cc1c(c(N)ccc1)n2	3
3981	ISSSTY_v1a_7367_02May011_5196	13109-99-4	HC1C(=O)N(C2=NC=C(N(=O)=O)S2)C(H)C1H	3
3982	ISSSTY_v1a_7367_02May011_5198	92569-05-6	HC1C(H)N(C(=O)C(Cl)Cl)C(=O)N1C1=NC=C(N(=O)=O)S1	3
3983	ISSSTY_v1a_7367_02May011_5199	120812-48-8	c1([N+](=O)[O-])c2c3c(c4c(c5c([N+](=O)[O-])ccc(c35)cc2)cccc4)cc1	3
3984	ISSSTY_v1a_7367_02May011_5200	3311-98-6	HC(Cl)C(H)NC(=O)NC1=NC=C(N(=O)=O)S1	3
3985	ISSSTY_v1a_7367_02May011_5201	10560-74-4	HC(H)C1C(H)NC(=O)N1C1=NC=C(N(=O)=O)S1	3
3986	ISSSTY_v1a_7367_02May011_5203	120812-50-2	HC1c2c(c3c4c5c(c([N+](=O)[O-])cc([N+](=O)[O-])c25)ccc4ccc3)C(H)C(H)C1H	3
3987	ISSSTY_v1a_7367_02May011_5204	120812-51-3	HC1c2c(c3c4c5c(c([N+](=O)[O-])ccc25)ccc4ccc3[N+](=O)[O-])C(H)C(H)C1H	3
3988	ISSSTY_v1a_7367_02May011_5206	120812-52-4	HC1c2c(c3c4c5c(ccc([N+](=O)[O-])c25)ccc4ccc3[N+](=O)[O-])C(H)C(H)C1H	3
3989	ISSSTY_v1a_7367_02May011_5207	120812-46-6	HC1c2c(c3c4c5c(ccc(N(=O)=O)c25)ccc4ccc3)C(H)C(H)C1H	3
3990	ISSSTY_v1a_7367_02May011_5208	57-92-1	HC(H)[C@@]1[C@](O)C(=O)[C@@](O)C2[C@@](NC(H)H)[C@](O)[C@@](O)[C@](C(H)O)2[C@@](O)C2[C@@]1O[C@@](O)[C@](N=C(N)N)[C@@](O)[C@]2N=C(N)NO1	3

4033	ISSSTY_v1a_7367_02May011_5266	65267-04-1	HC(C(N)=O)NC(=O)N(C(H)C(H)Cl)N=O	3
4034	ISSSTY_v1a_7367_02May011_5267	76014-81-8	HC(H)N(C(H)C(H)C(H)C(O)c1cccnc1)N=O	3
4035	ISSSTY_v1a_7367_02May011_5268	5385-75-1	c12c(c3c4c(c5c(c4c4c(cccc4)c3)cccc5)c1)cccc2	3
4036	ISSSTY_v1a_7367_02May011_5269	74340-04-8	c12c(c3c4c(c5c(c4c4c(cccc4)c3)cccc5)c1)C=C[C@](O)[C@@]2O	3
4037	ISSSTY_v1a_7367_02May011_5270	74339-98-3	c12c(c3c4c(c5c(c4c4c([C@](O)[C@@](O)C=C4)c3)cccc5)c1)cccc2	3
4038	ISSSTY_v1a_7367_02May011_5273	5422-34-4	HC(H)C(O)C(=O)NC(H)C(H)O	3
4039	ISSSTY_v1a_7367_02May011_5274	17309-86-3	HC(H)N(c1ccc(N=Nc2cc3c(cc2)NN=C3)cc1)C(H)H	3
4040	ISSSTY_v1a_7367_02May011_5278	93673-32-6	HC1c2c(C3=C4C(=C5C=C6C(=C1C35)C=CC=C6)O4)cccc2	3
4041	ISSSTY_v1a_7367_02May011_5279	93673-31-5	HC1c2c(C3=C4C(=C5C=CC=C1C35)O4)ccc1c2cccc1	3
4042	ISSSTY_v1a_7367_02May011_5280	93673-34-8	HC1c2c(C3C4C(=C5C(C1=4)O5)C=CC=3)cc1c(cccc1)c2	3
4043	ISSSTY_v1a_7367_02May011_5281	51-75-2	HC(H)N(C(H)C(H)Cl)C(H)C(H)Cl	3
4044	ISSSTY_v1a_7367_02May011_5283	126-85-2	HC(H)[N+](=[O-])(C(H)C(H)Cl)C(H)C(H)Cl	3
4045	ISSSTY_v1a_7367_02May011_5285	1197-55-3	HC(c1ccc(N)cc1)C(=O)O	3
4046	ISSSTY_v1a_7367_02May011_5286	98079-51-7	HC(H)C(H)N1c2c(C(=O)C(C(=O)O)=C1)cc(F)c(N1C(H)C(H)NC(C(H)H)C1H)c2F	3
4047	ISSSTY_v1a_7367_02May011_5287	149573-80-8	HC(C1=CN(N=O)C=N1)C(=O)NO	3
4048	ISSSTY_v1a_7367_02May011_5290	3029-19-4	c12c3c4c(c(C=O)ccc4ccc3ccc1)cc2	3
4049	ISSSTY_v1a_7367_02May011_5299	428856	c12C(=O)c3c(-c1cc1c(cccc1)c2)cccc3	3
4050	ISSSTY_v1a_7367_02May011_5305	92118-27-9	HC(H)C(H)OP(=O)(C(C(H)H)NC(=O)N(C(H)C(H)Cl)N=O)OC(H)C(H)H	3
4051	ISSSTY_v1a_7367_02May011_5306	93673-39-3	c1(O)c2c(c3c(c4c5c(C=C4)cccc5c3)cc2)ccc1	3
4052	ISSSTY_v1a_7367_02May011_5308	38716-10-8	HC(C1C(=O)NC(=O)N([C@]2C(H)[C@](O)[C@@](C(H)O)O2)C=1)OO	3
4053	ISSSTY_v1a_7367_02May011_5312	85977-49-7	HC(H)N(C(H)H)S(=O)(=O)C(H)C(H)NC(=O)N(C(H)C(H)Cl)N=O	3
4054	ISSSTY_v1a_7367_02May011_5313	26651-23-0	c12c3c4c(c(S(=O)(=O)O)ccc4ccc3ccc1)cc2	3
4055	ISSSTY_v1a_7367_02May011_5314	81424-67-1	HC(H)C(=O)N(C(=O)NC(H)H)OC(=O)NC(H)H	3
4056	ISSSTY_v1a_7367_02May011_5316	4543-63-9	HC(H)N(C(=O)NC(H)H)C(=O)ON	3
4057	ISSSTY_v1a_7367_02May011_5320	104145-44-0	HC(H)OC(=O)c1cc2-c3c(cccc3)Nc2c(-c2ccc3C(=O)C=CC(=O)c3n2)n1	3
4058	ISSSTY_v1a_7367_02May011_5324	78-30-8	HC(H)c1c(OP(=O)(Oc2c(C(H)H)cccc2)Oc2c(C(H)H)cccc2)cccc1	3
4059	ISSSTY_v1a_7367_02May011_5325	4081-23-6	HC1c2c(cccc2)OP(=O)(Oc2cccc2)O1	3
4060	ISSSTY_v1a_7367_02May011_5326	3571-31-1	HC(H)c1cc(O)c2C(=O)c3c(C(H)c2c1)cc(OC(H)H)cc3O	3
4061	ISSSTY_v1a_7367_02May011_5327	476-57-3	HC(H)c1c(O)c2C(=O)c3c(C(=O)c2c(O)c1)c(O)cc(OC(H)H)c3	3
4062	ISSSTY_v1a_7367_02May011_5329	22897-08-1	HC(H)Oc1c2C(=O)c3c(c(OC(H)H)ccc3O)Oc2c2c(c1)O[C@]1[C@@]2C=CO1	3
4063	ISSSTY_v1a_7367_02May011_5331	55481-88-4	HC(H)C1(C(H)H)C=Cc2c(C(=O)OC(H)H)c(O)c3c(c2O1)cccc3	3
4064	ISSSTY_v1a_7367_02May011_5332	65176-75-2	HC(H)Oc1c2C(=O)c3c(c(OC(H)H)c(OC(H)H)cc3O)Oc2c2c(c1)OC1C2C=CO1	3
4065	ISSSTY_v1a_7367_02May011_5334	30461-65-5	c12C(=O)c3c(c4c(cc3O)O[C@@]3[C@]4C=CO3)Oc1cccc2O	3
4066	ISSSTY_v1a_7367_02May011_5335	111901-39-4	HC(H)c1c2c(c3c(cccc3)c1)ccc1c2[C@]2[C@@]([C@@](O)[C@]1O)O2	3
4067	ISSSTY_v1a_7367_02May011_5338	58086-32-1	HC(H)C(=O)Oc1c2C(=O)c3c(c4c(cc3OC(H)H)OC3C4C=CO3)Oc2ccc1	3
4068	ISSSTY_v1a_7367_02May011_5339	36050-09-6	C(N)(=O)C1C=C(N(=O)=O)SC=1	3
4069	ISSSTY_v1a_7367_02May011_5340	146795-48-4	HC(H)N(C(=O)C1C=C(N(=O)=O)SC=1)c1cccc1	3
4070	ISSSTY_v1a_7367_02May011_5341	146795-44-0	C(=O)(C1C=C([N+](=O)[O-])SC=1)Nc1ccc([N+](=O)[O-])cc1	3
4071	ISSSTY_v1a_7367_02May011_5342	146795-38-2	C(=O)(C1C=C(N(=O)=O)SC=1)Nc1ccc(Cl)cc1	3
4072	ISSSTY_v1a_7367_02May011_5343	146795-41-7	C(=O)(C1C=C(N(=O)=O)SC=1)Nc1ccc(Br)cc1	3
4073	ISSSTY_v1a_7367_02May011_5344	146795-35-9	C(=O)(C1C=C(N(=O)=O)SC=1)Nc1ccc(F)cc1	3
4074	ISSSTY_v1a_7367_02May011_5345	146818-20-4	HC(H)C(H)c1ccc(NC(=O)C2C=C(N(=O)=O)SC=2)cc1	3

4075	ISSSTY_v1a_7367_02May011_5346	146795-29-1	HC(H)c1ccc(NC(=O)C2C=C(N(=O)=O)SC=2)cc1	3
4076	ISSSTY_v1a_7367_02May011_5347	146795-26-8	HC(H)Oc1ccc(NC(=O)C2C=C(N(=O)=O)SC=2)cc1	3
4077	ISSSTY_v1a_7367_02May011_5348	122089-49-0	HC(H)c1c2c(c3c(C(O)C(O)C4C3O4)cc2)c(C(H)H)cc1	3
4078	ISSSTY_v1a_7367_02May011_5349	146795-45-1	C(=O)(C1C=C([N+](=O)[O-])SC=1)Nc1cc([N+](=O)[O-])ccc1	3
4079	ISSSTY_v1a_7367_02May011_5350	146795-39-3	C(=O)(C1C=C(N(=O)=O)SC=1)Nc1cc(Cl)ccc1	3
4080	ISSSTY_v1a_7367_02May011_5351	122033-85-6	HC(H)c1c2c(c3c(C(O)C(O)C4C3O4)cc2)c(C(H)H)cc1	3
4081	ISSSTY_v1a_7367_02May011_5352	146795-42-8	C(=O)(C1C=C(N(=O)=O)SC=1)Nc1cc(Br)ccc1	3
4082	ISSSTY_v1a_7367_02May011_5353	146795-36-0	C(=O)(C1C=C(N(=O)=O)SC=1)Nc1cc(F)ccc1	3
4083	ISSSTY_v1a_7367_02May011_5354	146795-32-6	HC(H)C(H)c1cc(NC(=O)C2C=C(N(=O)=O)SC=2)ccc1	3
4084	ISSSTY_v1a_7367_02May011_5355	146795-30-4	HC(H)c1cc(NC(=O)C2C=C(N(=O)=O)SC=2)ccc1	3
4085	ISSSTY_v1a_7367_02May011_5356	146795-27-9	HC(H)Oc1cc(NC(=O)C2C=C(N(=O)=O)SC=2)ccc1	3
4086	ISSSTY_v1a_7367_02May011_5357	146795-46-2	C(=O)(C1C=C([N+](=O)[O-])SC=1)Nc1c([N+](=O)[O-])cccc1	3
4087	ISSSTY_v1a_7367_02May011_5359	146795-40-6	C(=O)(C1C=C(N(=O)=O)SC=1)Nc1c(Cl)cccc1	3
4088	ISSSTY_v1a_7367_02May011_5360	146795-43-9	C(=O)(C1C=C(N(=O)=O)SC=1)Nc1c(Br)cccc1	3
4089	ISSSTY_v1a_7367_02May011_5361	146795-37-1	C(=O)(C1C=C(N(=O)=O)SC=1)Nc1c(F)cccc1	3
4090	ISSSTY_v1a_7367_02May011_5362	146795-33-7	HC(H)C(H)c1c(NC(=O)C2C=C(N(=O)=O)SC=2)cccc1	3
4091	ISSSTY_v1a_7367_02May011_5363	146795-31-5	HC(H)c1c(NC(=O)C2C=C(N(=O)=O)SC=2)cccc1	3
4092	ISSSTY_v1a_7367_02May011_5364	146795-28-0	HC(H)Oc1c(NC(=O)C2C=C(N(=O)=O)SC=2)cccc1	3
4093	ISSSTY_v1a_7367_02May011_5365	98033-22-8	HC(H)C1c2c3c(c(O)cc2NC1H)ccc1c3cccc1	3
4094	ISSSTY_v1a_7367_02May011_5366	98033-24-0	HC(H)C1=Nc2c(c3c4c(ccc(O)c4)ccc3cc2)O1	3
4095	ISSSTY_v1a_7367_02May011_5367	84-68-4	c1(-c2c(Cl)cc(N)cc2)c(Cl)cc(N)cc1	3
4096	ISSSTY_v1a_7367_02May011_5368	98033-23-9	HC(H)Nc1cc2c3c(ccc(O)c3)ccc2cc1	3
4097	ISSSTY_v1a_7367_02May011_5369	98033-26-2	HC(H)C1=Nc2c3c4c(ccc(O)c4)ccc3ccc2N1	3
4098	ISSSTY_v1a_7367_02May011_5371	507-19-7	HC(H)C(Br)(C(H)H)C(H)H	3
4099	ISSSTY_v1a_7367_02May011_5385	144605-96-9	HC(H)C1C2=C(c3c(ccc(N(=O)=O)c3)N2)C(H)C(C(=O)OC(H)H)N1N=O	3
4100	ISSSTY_v1a_7367_02May011_5386	81677-51-2	HC(H)OC(=O)c1cc2-c3c(ccc(N(=O)=O)c3)Nc2c(-c2cccc2)n1	3
4101	ISSSTY_v1a_7367_02May011_5389	4332-51-8	HC(c1cccc1)SC(H)C(H)Cl	3
4102	ISSSTY_v1a_7367_02May011_5390	111959-96-7	HC(c1cccc1)SC(Cl)=C(Cl)C(Cl)=C(Cl)Cl	3
4103	ISSSTY_v1a_7367_02May011_5391	91085-62-0	HC(c1cccc1)SC(Cl)=CCl	3
4104	ISSSTY_v1a_7367_02May011_5392	116374-65-3	HC(H)N(C(H)H)C(H)C(H)C(H)Nc1c2c(c(Cl)ccc2N(=O)=O)nc2c1cccc2	3
4105	ISSSTY_v1a_7367_02May011_5393	116374-66-4	HC(H)N(C(H)H)C(H)C(H)C(H)Nc1c2c(c(F)ccc2N(=O)=O)nc2c1cccc2	3
4106	ISSSTY_v1a_7367_02May011_5394	24400-01-9	HC(H)c1c2c(c(NC(H)C(H)C(H)N(C(H)H)C(H)H)c3c(cccc3)n2)c(N(=O)=O)cc1	3
4107	ISSSTY_v1a_7367_02May011_5395	25799-70-6	HC(H)N(C(H)H)C(H)C(H)C(H)Nc1c2c(c(OC(H)H)ccc2N(=O)=O)nc2c1cccc2	3
4108	ISSSTY_v1a_7367_02May011_5396	33389-33-2	C1(=O)c2c(cccc2)NC(C2=CC=C(N(=O)=O)S2)N1	3
4109	ISSSTY_v1a_7367_02May011_5397	116374-67-5	HC(H)N(c1c2c(c(NC(H)C(H)C(H)N(C(H)H)C(H)H)c3c(cccc3)n2)c(N(=O)=O)cc1)C(H)H	3
4110	ISSSTY_v1a_7367_02May011_5398	107210-40-2	HC(H)N(C(H)H)C(H)C(H)C(H)Nc1c2c(c(NC(H)C(H)O)C(H)C(H)O)ccc2N(=O)=O)nc2c1cccc2	3
4111	ISSSTY_v1a_7367_02May011_5399	107210-39-9	HC(H)C(=O)OC(H)C(H)Nc1c2c(c(NC(H)C(H)C(H)N(C(H)H)C(H)H)c3c(cccc3)n2)c(N(=O)=O)cc1)C(H)C(H)OC(=O)C(H)H	3
4112	ISSSTY_v1a_7367_02May011_5400	116374-64-2	HC(H)N(C(H)H)C(H)C(H)C(H)Nc1c2c(c(C(=O)OC(H)H)ccc2N(=O)=O)nc2c1cccc2	3
4113	ISSSTY_v1a_7367_02May011_5405	513-31-5	HC(Br)C(Br)=CH	3
4114	ISSSTY_v1a_7367_02May011_5406	766-40-5	C1(=O)C(Cl)=C(Cl)C(O)O1	3
4115	ISSSTY_v1a_7367_02May011_5409	381740	HC(c1cccc1)NC(=O)C(H)Br	3
4116	ISSSTY_v1a_7367_02May011_5413	5875-25-2	HC(H)C(Br)C(N)=O	3

4117	ISSSTY_v1a_7367_02May011_5414	42308-20-3	HC(H)C(Br)C(=O)Nc1ccccc1	3
4118	ISSSTY_v1a_7367_02May011_5415	6653-71-0	HC(H)C(Br)C(=O)NC(H)c1ccccc1	3
4119	ISSSTY_v1a_7367_02May011_5417	91687-67-1	HC(H)C(Br)C(=O)NC(H)c1ccc(Cl)cc1	3
4120	ISSSTY_v1a_7367_02May011_5418	27798	C(Cl)(Cl)(Cl)C(=O)Cl	3
4121	ISSSTY_v1a_7367_02May011_5419	25413-02-9	HC(H)C(H)OC(=O)C(H)NC(=O)C(Br)C(H)H	3
4122	ISSSTY_v1a_7367_02May011_5427	242683	HC(c1ccccc1)NC(=O)C(H)Cl	3
4123	ISSSTY_v1a_7367_02May011_5429	27946-19-6	HC(c1ccccc1)NC(=O)C(Cl)c1ccccc1	3
4124	ISSSTY_v1a_7367_02May011_5430	105427-03-0	HC1C(C(=O)Nc2ccccc2)O1	3
4125	ISSSTY_v1a_7367_02May011_5431	105427-02-9	HC(c1ccccc1)NC(=O)C1C(H)O1	3
4126	ISSSTY_v1a_7367_02May011_5432	105427-01-8	HC(H)C1(C(=O)Nc2ccccc2)C(H)O1	3
4127	ISSSTY_v1a_7367_02May011_5433	105427-00-7	HC(H)C1(C(=O)NC(H)c2ccccc2)C(H)O1	3
4128	ISSSTY_v1a_7367_02May011_5435	92-69-3	c1(-c2ccc(O)cc2)ccccc1	3
4129	ISSSTY_v1a_7367_02May011_5436	1343853	HC(H)NC(=O)Oc1ccc(-c2ccccc2)cc1	3
4130	ISSSTY_v1a_7367_02May011_5439	53175-28-3	HC(H)C=C(Cl)C=O	3
4131	ISSSTY_v1a_7367_02May011_5440	484-17-3	c1(O)c2c(c3c(cccc3)c1)cccc2	3
4132	ISSSTY_v1a_7367_02May011_5442	109032-48-6	HC(H)NC(=O)Oc1c2c(c3c(cccc3)c1)cccc2	3
4133	ISSSTY_v1a_7367_02May011_5443	620-25-7	HC(H)c1cc(NO)ccc1	3
4134	ISSSTY_v1a_7367_02May011_5445	108278-71-3	HC(C(=O)O)C(H)N(C(N)=O)N=O	3
4135	ISSSTY_v1a_7367_02May011_5446	4164-28-7	HC(H)N(C(H)H)N(=O)=O	3
4136	ISSSTY_v1a_7367_02May011_5447	108278-72-4	HC(C(=O)O)C(H)C(H)N(C(N)=O)N=O	3
4137	ISSSTY_v1a_7367_02May011_5448	13256-06-9	HC(H)C(H)C(H)C(H)C(H)N(C(H)C(H)C(H)C(H)H)N=O	3
4138	ISSSTY_v1a_7367_02May011_5451	298-04-4	HC(H)C(H)OP(=S)(OC(H)C(H)H)SC(H)C(H)SC(H)C(H)H	3
4139	ISSSTY_v1a_7367_02May011_5452	7227-91-0	HC(H)N(C(H)H)N=Nc1ccccc1	3
4140	ISSSTY_v1a_7367_02May011_5453	140460-98-6	c12c(c3c([C@@](O)[C@@](O)[C@@]4[C@@]3O4)cc1)nc1c(c3c(cccc3)cc1)c2	3
4141	ISSSTY_v1a_7367_02May011_5454	140460-96-4	c12c(c3c([C@@](O)[C@@](O)[C@@]4[C@@]3O4)cc1)nc1c(c3c(cccc3)cc1)c2	3
4142	ISSSTY_v1a_7367_02May011_5455	125676-80-4	HC(H)C1C2(C(O)(C(H)H)C3C(=O)C(C(H)H)(C(H)H)C3(O[C@@]3[C@@](OC(=O)C(H)H)[C@@](O)[C@@](OC(=O)C=Cc4ccc(O)cc4)[C@@](C(H)O)O3)C=1)C(H)C2H	3
4143	ISSSTY_v1a_7367_02May011_5456	140461-57-0	c12c(c3c([C@@](O)[C@@](O)[C@@]4[C@@]3O4)cc1)nc1c(c3c(cccc3)cc1)c2	3
4144	ISSSTY_v1a_7367_02May011_5457	140460-97-5	c12c(c3c([C@@](O)[C@@](O)[C@@]4[C@@]3O4)cc1)nc1c(c3c(cccc3)cc1)c2	3
4145	ISSSTY_v1a_7367_02May011_5458	125761-28-6	HC(H)C1C2(C(O)(C(H)H)C3C(=O)C(C(H)H)(C(H)H)C3(O[C@@]3[C@@](OC(=O)C(H)H)[C@@](O)[C@@](OC(=O)C=Cc4ccc(O)cc4)[C@@](C(H)O)O3)C=1)C(H)C2H	3
4146	ISSSTY_v1a_7367_02May011_5459	1001985	HC(O)C=CCI	3
4147	ISSSTY_v1a_7367_02May011_5460	1002017	HC(O)C=CCI	3
4148	ISSSTY_v1a_7367_02May011_5461	2345-61-1	C(=O)(O)C=CCI	3
4149	ISSSTY_v1a_7367_02May011_5462	1609-93-4	C(=O)(O)C=CCI	3
4150	ISSSTY_v1a_7367_02May011_5463	85340-40-5	HC(C(H)Sc1c(N)cccc1)Sc1c(N)cccc1	3
4151	ISSSTY_v1a_7367_02May011_5466	97169-68-1	c12c(c3c([C@@](O)[C@@](O)[C@@]4[C@@]3O4)cc1)nc1c(c3c(cccc3)cc1)c2	3
4152	ISSSTY_v1a_7367_02May011_5467	97135-11-0	C1(O)C(=O)C2=C(C3=C4C(C=CC=13)=Cc1c3c(ccc1N4)cccc3)O2	3
4153	ISSSTY_v1a_7367_02May011_5469	524-89-0	HC(H)Oc1c2c(cc3c(c2)OC(H)O3)nc2c1C=CO2	3
4154	ISSSTY_v1a_7367_02May011_5470	522-19-0	HC(H)Oc1c2c(c(OC(H)H)c3c(n2)OC=C3)cc(OC(H)H)c1	3
4155	ISSSTY_v1a_7367_02May011_5471	523-66-0	HC(H)Oc1c2c(cc(OC(H)H)cc2)nc2c1C=CO2	3
4156	ISSSTY_v1a_7367_02May011_5472	2221-41-2	HC(H)Oc1c2c(ccc(OC(H)H)c2)nc2c1C=CO2	3
4157	ISSSTY_v1a_7367_02May011_5473	522-06-5	HC(H)Oc1c2c(c(OC(H)H)c3c(c2)OC(H)O3)nc2c1C=CO2	3
4158	ISSSTY_v1a_7367_02May011_5474	484-08-2	HC(H)Oc1c2c(cc(OC(H)H)c(OC(H)H)c2)nc2c1C=CO2	3

4159	ISSSTY_v1a_7367_02May011_5477	157730-35-3	HC(H)N1c2c(N=C1N)nc1c(ccnc1)c2	3
4160	ISSSTY_v1a_7367_02May011_5478	157730-36-4	HC(H)N1c2c(N=C1N)nc1c(cnc1)c2	3
4161	ISSSTY_v1a_7367_02May011_5479	157730-37-5	HC(H)N1c2c(N=C1N)nc1c(c2)nccc1	3
4162	ISSSTY_v1a_7367_02May011_5480	156215-58-6	HC(H)N1c2c(N=C1N)nc1c(cccc1)c2	3
4163	ISSSTY_v1a_7367_02May011_5481	30489-67-9	HC(H)N1c2c(cc3c(cccc3)c2)N=C1N	3
4164	ISSSTY_v1a_7367_02May011_5482	115655-93-1	HC(H)C(C(H)H)=CC(H)C(H)[C@@](O)(C(H)H)[C@@]1C(=O)C=CC(H)C1H	3
4165	ISSSTY_v1a_7367_02May011_5483	921-03-9	HC(Cl)C(=O)C(Cl)Cl	3
4166	ISSSTY_v1a_7367_02May011_5485	165606-93-9	C1(=O)C(Cl)(Cl)C(=C(Cl)Cl)C(=O)N1	3
4167	ISSSTY_v1a_7367_02May011_5486	64201-68-9	C1(c2ccc(N(=O)=O)cc2)=CSC(NC=O)=N1	3
4168	ISSSTY_v1a_7367_02May011_5487	115453-71-9	HC([C@](N)C(=O)O)SC=CCl	3
4169	ISSSTY_v1a_7367_02May011_5488	114414-79-8	HC(H)C1c2c(cccc2)N(C(H)H)C2C=1c1c(cccc1)N=2	3
4170	ISSSTY_v1a_7367_02May011_5489	125157-98-4	HC(H)C1c2c(cccc2)N(C(H)H)C2C=1c1c(ccc(C(H)H)c1)N=2	3
4171	ISSSTY_v1a_7367_02May011_5490	125372-28-3	HC(H)N1c2c3c(ccc2N=C1N=N_N)nccc3	3
4172	ISSSTY_v1a_7367_02May011_5491	1516-71-8	HC(H)N1c2c(c3c(cccc3)cc2)N=C1N=N_N	3
4173	ISSSTY_v1a_7367_02May011_5492	95389-75-6	HC(H)N1c2c3c(ccc2N=C1N=N_N)cccc3	3
4174	ISSSTY_v1a_7367_02May011_5493	125372-29-4	HC(H)c1c2c(c3c(c1)nccc3)N=C(N=N_N)N2C(H)H	3
4175	ISSSTY_v1a_7367_02May011_5495	160543-12-4	HC(H)c1c2c3c(c4c(c2nc2c1cc(C(H)H)cc2)cccc4)O3	3
4176	ISSSTY_v1a_7367_02May011_5496	77287-29-7	HC(H)[C@](Cl)C(=O)OC(H)H	3
4177	ISSSTY_v1a_7367_02May011_5498	153117-09-0	HC(H)C(H)C(H)C(H)N(C(H)[C@](C(H)c1cccc1)C(H)O)N=O	3
4178	ISSSTY_v1a_7367_02May011_5499	153117-10-3	HC(H)C(H)C(H)C(H)N(C(H)[C@](C(H)O)OC(H)c1cccc1)N=O	3
4179	ISSSTY_v1a_7367_02May011_5500	153859-79-1	HC(H)C(H)C(H)C(H)N(C(H)[C@@](C(H)O)OC(H)c1cccc1)N=O	3
4180	ISSSTY_v1a_7367_02May011_5501	6312-87-4	HC(H)C(=O)Nc1ccc(Oc2cccc2)cc1	3
4181	ISSSTY_v1a_7367_02May011_5502	76543-08-3	HC(H)C(=O)Nc1ccc(Oc2ccc(Cl)cc2)cc1	3
4182	ISSSTY_v1a_7367_02May011_5503	56120-26-4	HC(H)C(=O)Nc1ccc(Oc2c(Cl)cc(Cl)cc2)cc1	3
4183	ISSSTY_v1a_7367_02May011_5504	26049-71-8	C1(c2ccc(N)cc2)=CSC(NN)=N1	3
4184	ISSSTY_v1a_7367_02May011_5505	51489-62-4	c1(Oc2ccc(Cl)cc2)ccc(NC=O)cc1	3
4185	ISSSTY_v1a_7367_02May011_5506	68906-23-0	c1(Cl)c(Oc2ccc(NC=O)cc2)c(Cl)cc(Cl)c1	3
4186	ISSSTY_v1a_7367_02May011_5508	98911-09-2	HC(H)C(=O)N(O)c1ccc(Oc2c(Cl)cc(Cl)cc2Cl)cc1	3
4187	ISSSTY_v1a_7367_02May011_5509	165550-82-3	c1(Oc2cccc2)ccc(N(O)C=O)cc1	3
4188	ISSSTY_v1a_7367_02May011_5510	105801-28-3	c1(Oc2ccc(Cl)cc2)ccc(N(O)C=O)cc1	3
4189	ISSSTY_v1a_7367_02May011_5511	26049-70-7	C1(c2ccc(N(=O)=O)cc2)=CSC(NN)=N1	3
4190	ISSSTY_v1a_7367_02May011_5512	165550-83-4	c1(Oc2ccc(N(O)C=O)cc2)c(Cl)cc(Cl)cc1	3
4191	ISSSTY_v1a_7367_02May011_5513	165550-84-5	c1(Cl)c(Oc2ccc(N(O)C=O)cc2)c(Cl)cc(Cl)c1	3
4192	ISSSTY_v1a_7367_02May011_5514	396-32-7	c12c(cc(F)cc1)nccc2	3
4193	ISSSTY_v1a_7367_02May011_5515	79-44-7	HC(H)N(C(=O)Cl)C(H)H	3
4194	ISSSTY_v1a_7367_02May011_5516	164200-11-7	HC(H)[C@]12[C@@](C(=O)(C(=O)=CC(H)C1H)C2H	3
4195	ISSSTY_v1a_7367_02May011_5517	164200-12-8	HC(H)[C@@]12[C@](C(=O)(C(=O)=CC(H)C1H)C2H	3
4196	ISSSTY_v1a_7367_02May011_5518	143347-57-3	HC(H)C12C(C=O)(C(=O)=CC(H)C1H)C2H	3
4197	ISSSTY_v1a_7367_02May011_5526	62690-96-4	HC1c2c(C3C(C(H)C(H)C(H)C=3)C1H)cccc2	3
4198	ISSSTY_v1a_7367_02May011_5527	10353-53-4	HC(C(H)C1C(H)O1)C=CH	3
4199	ISSSTY_v1a_7367_02May011_5528	97-52-9	HC(H)Oc1c(N)ccc(N(=O)=O)c1	3
4200	ISSSTY_v1a_7367_02May011_5529	19600-63-6	HC(C(H)C(H)C(H)C1C(H)O1)C=CH	3

4201	ISSSTY_v1a_7367_02May011_5531	93-27-6	HC(H)C(=O)Nc1c(OC(H)H)cc(N(=O)=O)cc1	3
4202	ISSSTY_v1a_7367_02May011_5532	1888-89-7	HC(C(H)C1C(H)O1)C1C(H)O1	3
4203	ISSSTY_v1a_7367_02May011_5533	2224-15-9	HC(C(H)OC(H)C1C(H)O1)OC(H)C1C(H)O1	3
4204	ISSSTY_v1a_7367_02May011_5534	1244421	HC(H)Oc1c(N)ccc(N)c1	3
4205	ISSSTY_v1a_7367_02May011_5535	5329-15-7	HC(H)C(=O)Nc1c(OC(H)H)cc(N)cc1	3
4206	ISSSTY_v1a_7367_02May011_5539	63390-11-4	c1(-c2cc(CI)c(N)c(CI)c2)ccc(N)cc1	3
4207	ISSSTY_v1a_7367_02May011_5542	98349-84-9	HC(H)C(H)Oc1ccc(N(O)C(=O)C(H)C(O)C(H)H)cc1	3
4208	ISSSTY_v1a_7367_02May011_5543	26196-04-3	HC(H)C1(C(H)H)C(OC(H)H)O1	3
4209	ISSSTY_v1a_7367_02May011_5544	98151-92-9	c1(N)c2c3c4c(c5c(cc4cc2)cccc5)ccc3cc1	3
4210	ISSSTY_v1a_7367_02May011_5545	1120-71-4	HC1C(H)C(H)OS1(=O)=O	3
4211	ISSSTY_v1a_7367_02May011_5546	1768-31-6	C(CI)(CI)(CI)C(=O)C(CI)CI	3
4212	ISSSTY_v1a_7367_02May011_5547	3787-28-8	C(CI)(CI)=C(CI)C=O	3
4213	ISSSTY_v1a_7367_02May011_5550	23045-35-4	c12c(c(N)c3c(ccc(N(=O)=O)c3)n1)cccc2	3
4214	ISSSTY_v1a_7367_02May011_5553	1466-88-2	c1(N(=O)=O)c(C=CC=O)cccc1	3
4215	ISSSTY_v1a_7367_02May011_5555	52411-33-3	HC(C(H)Sc1c(N)cccc1)Sc1c(N)cccc1	3
4216	ISSSTY_v1a_7367_02May011_5557	33389-36-5	HC(O)C(H)Nc1c2c(cccc2)nc(C2=CC=C(N(=O)=O)S2)n1	3
4217	ISSSTY_v1a_7367_02May011_5558	1214-32-0	HC1c2c(-c3c1cc(N(=O)=O)cc3)ccc(N)c2	3
4218	ISSSTY_v1a_7367_02May011_5559	138154-40-2	HC(H)C1N2c3c(C(=O)c4c(NC(H)C(H)N(C(H)C(H)H)C(H)C(H)H)ccc(c24)N=1)cc(O)cc3	3
4219	ISSSTY_v1a_7367_02May011_5560	138154-39-9	HC(H)C(H)N(C(H)C(H)H)C(H)C(H)Nc1c2C(=O)c3c(ccc(O)c3)N3c2c(cc1)N=C3	3
4220	ISSSTY_v1a_7367_02May011_5562	19322-27-1	HC(H)C1=C(O)C(=O)C(H)O1	3
4221	ISSSTY_v1a_7367_02May011_5563	95050-14-9	c1(N(=O)=O)c2c(c3c4c5c6c(ccc5ccc24)cccc6c3)ccc1	3
4222	ISSSTY_v1a_7367_02May011_5565	517-66-8	HC(H)N1C(H)C(H)c2c3c(-c4c(C(H)[C@@]13)cc(OC(H)H)c(OC(H)H)c4)c1c(c2)OC(H)O1	3
4223	ISSSTY_v1a_7367_02May011_5566	242895	HC(H)N1C(H)C(H)c2c3c(-c4c(C(H)[C@@]13)cc1c(c4)OC(H)O1)c(OC(H)H)c(OC(H)H)c2	3
4224	ISSSTY_v1a_7367_02May011_5567	3153-55-7	HC(H)N1C(H)C(H)c2c3c(-c4c(C(H)[C@@]13)cccc4)c(OC(H)H)c(O)c2	3
4225	ISSSTY_v1a_7367_02May011_5568	548-08-3	HC(H)N1C(H)C(H)c2c3c(-c4c(C(H)[C@@]13)cccc4)c1c(c2)OC(H)O1	3
4226	ISSSTY_v1a_7367_02May011_5569	24191-98-8	HC(H)N1C(H)[C@@](O)c2c3c(-c4c(C(H)[C@@]13)cccc4)c1c(c2)OC(H)O1	3
4227	ISSSTY_v1a_7367_02May011_5570	3175-89-1	HC(H)N1C(H)C(H)c2c3c(-c4c([C@@](O)[C@@]13)cccc4)c1c(c2)OC(H)O1	3
4228	ISSSTY_v1a_7367_02May011_5571	24260-08-0	HC(H)C(=O)NC1C(=O)C=C(OC(H)C(H)H)C(=O)C=1	3
4229	ISSSTY_v1a_7367_02May011_5572	77784-22-6	HC(H)N1c2c3c(c4c(c(OC(H)H)c(OC(H)H)cc4)c2)c2c(cc3C(H)C1H)OC(H)O2	3
4230	ISSSTY_v1a_7367_02May011_5573	23740-25-2	HC(H)Oc1cc2C(=O)c3c4c(c5c(cc4ccn3)OC(H)O5)-c2cc1	3
4231	ISSSTY_v1a_7367_02May011_5574	77784-21-5	HC(H)N1C(=O)C(=O)c2c3c(c4c(c(OC(H)H)c(OC(H)H)cc4)cc13)c1c(c2)OC(H)O1	3
4232	ISSSTY_v1a_7367_02May011_5575	83287-02-9	HC(H)Oc1c2C(=O)c3c(-c4c2c(cc1OC(H)H)ccn4)ccc(OC(H)H)c3	3
4233	ISSSTY_v1a_7367_02May011_5576	961-29-5	C(=O)(c1c(O)cc(O)cc1)C=Cc1ccc(O)cc1	3
4234	ISSSTY_v1a_7367_02May011_5577	179073-71-3	HC(H)c1c2c3c(c4c(c5c(cccc5)cc4)cc3cc1)C(OS(=O)(=O)O)C2H	3
4235	ISSSTY_v1a_7367_02May011_5578	50285-71-7	HC(H)C(H)N(C(=O)N(C(H)H)C(H)H)N=O	3
4236	ISSSTY_v1a_7367_02May011_5579	3475-63-6	HC(H)N(C(=O)N(C(H)H)C(H)H)N=O	3
4237	ISSSTY_v1a_7367_02May011_5581	105-11-3	c1(NO)ccc(N=O)cc1	3
4238	ISSSTY_v1a_7367_02May011_5585	97672-08-7	HC(C1c2c(cccc2)N(N=O)C=1)C_N	3
4239	ISSSTY_v1a_7367_02May011_5586	127128-50-1	HC(H)C(H)C=CC=CC=CC=COC(H)C(O)C(H)O	3
4240	ISSSTY_v1a_7367_02May011_5587	127072-58-6	HC(H)C(H)C=CC=CC=CC=CC=COC(H)C(O)C(H)O	3
4241	ISSSTY_v1a_7367_02May011_5589	116-54-1	HC(H)OC(=O)C(CI)CI	3
4242	ISSSTY_v1a_7367_02May011_5590	75-17-2	HC=NO	3

4285	ISSSTY_v1a_7367_02May011_5653	91605-35-5	HC(H)C(H)C=CC=CC=CC=CC=COC(H)[C@@](O)C(H)O	3
4286	ISSSTY_v1a_7367_02May011_5654	87576-94-1	HC(H)[Si](C(H)H)(C(H)H)C(H)N=N_N	3
4287	ISSSTY_v1a_7367_02May011_5655	6926-44-9	HC(c1ccccc1)C(H)N=N_N	3
4288	ISSSTY_v1a_7367_02May011_5657	173216-42-7	HC(H)[C@](c1ccccc1)C(H)N=N_N	3
4289	ISSSTY_v1a_7367_02May011_5658	74669-74-2	HC(H)[C@@](c1ccccc1)C(H)N=N_N	3
4290	ISSSTY_v1a_7367_02May011_5661	131321-84-1	HC(O)[C@](O)C(H)N=N_N	3
4291	ISSSTY_v1a_7367_02May011_5662	85820-84-4	HC(O)[C@@](O)C(H)N=N_N	3
4292	ISSSTY_v1a_7367_02May011_5663	4648-54-8	HC(H)[Si](C(H)H)(C(H)H)N=N_N	3
4293	ISSSTY_v1a_7367_02May011_5664	16804-85-6	HC1C(H)C(H)C(H)C2c3c(C=CC12)cccc3	3
4294	ISSSTY_v1a_7367_02May011_5665	121625-58-9	HC(H)C1c2c([C@@]3C(H)C(H)C(H)C(H)[C@]3C=1)cccc2	3
4295	ISSSTY_v1a_7367_02May011_5666	118326-95-7	HC(H)Oc1cc2c(C=C[C@@]3C(H)C(H)C(H)C(H)[C@]23)cc1	3
4296	ISSSTY_v1a_7367_02May011_5669	134998-79-1	HC1c2c(c3c4c5c(c(N(=O)=O)cc4ccc3)cccc25)C(H)C(H)C1H	3
4297	ISSSTY_v1a_7367_02May011_5670	134998-77-9	c1(N(=O)=O)c2c3c(c4c(c5c3c(ccc5)c1)cccc4)ccc2	3
4298	ISSSTY_v1a_7367_02May011_5671	134998-78-0	HC(H)C(=O)Oc1c(OC(=O)C(H)H)c2c3c(c4c(c5c3c1c(N(=O)=O)cc5)cccc4)ccc2	3
4299	ISSSTY_v1a_7367_02May011_5672	115084-47-4	HC(c1cc(Cl)c(NO)cc1)c1cc(Cl)c(N)cc1	3
4300	ISSSTY_v1a_7367_02May011_5675	59485-08-4	HC1C(Oc2ccc(N(=O)=O)cc2)O1	3
4301	ISSSTY_v1a_7367_02May011_5676	155379-82-1	HC(H)c1c(N)c(N(=O)=O)cc(N)c1	3
4302	ISSSTY_v1a_7367_02May011_5677	1070-66-2	HC(H)C(H)C(H)C(H)C(C=O)=CH	3
4303	ISSSTY_v1a_7367_02May011_5681	28564-83-2	HC(H)C1=C(O)C(=O)C(O)C(H)O1	3
4304	ISSSTY_v1a_7367_02May011_5682	214130	c1(-c2c([N+](=O)[O-])cc([N+](=O)[O-])cc2)cccc1	3
4305	ISSSTY_v1a_7367_02May011_5685	109897-79-2	c12c([C@@](O)[C@](O)C=C1)cc1c(cc(N(=O)=O)cc1)c2	3
4306	ISSSTY_v1a_7367_02May011_5687	109897-78-1	C12C([C@](O)[C@@](O)C=C1)=CC1C=C(N(=O)=O)C=CC1C=2	3
4307	ISSSTY_v1a_7367_02May011_5688	632-21-3	C(=O)(C(Cl)Cl)C(Cl)Cl	3
4308	ISSSTY_v1a_7367_02May011_5698	125369-82-6	C(N)C(c1ccc(F)cc1)=CC=Cc1ccccc1	3
4309	ISSSTY_v1a_7367_02May011_5699	125369-84-8	C(N)C(c1ccc(Br)cc1)=CC=Cc1c(N(=O)=O)cccc1	3
4310	ISSSTY_v1a_7367_02May011_5700	42509-80-8	HC(H)C(H)OP(=S)(OC1N=C(Cl)N(C(C(H)H)C(H)H)N=1)OC(H)C(H)H	3
4311	ISSSTY_v1a_7367_02May011_5701	20780-53-4	HC1[C@@](c2ccccc2)O1	3
4312	ISSSTY_v1a_7367_02May011_5702	20780-54-5	HC1[C@](c2ccccc2)O1	3
4313	ISSSTY_v1a_7367_02May011_5703	81593-15-9	c12-c3c(C4C(c1cccc2)N4Cl)cccc3	3
4314	ISSSTY_v1a_7367_02May011_5704	64188-66-5	HC(H)C(H)C(H)C(H)N1C2c3c(-c4c(cccc4)C12)cccc3	3
4315	ISSSTY_v1a_7367_02May011_5705	91540-30-6	HC(C=CH)N1C2c3c(-c4c(cccc4)C12)cccc3	3
4316	ISSSTY_v1a_7367_02May011_5706	64188-65-4	HC1C(H)C(H)C(H)C(H)C1N1C2c3c(-c4c(cccc4)C12)cccc3	3
4317	ISSSTY_v1a_7367_02May011_5707	187585-11-1	HC(H)Oc1c(N)cc(C2=C(N)C(=O)c3c(cccc3)O2)cc1	3
4318	ISSSTY_v1a_7367_02May011_5708	187585-43-9	HC(H)Oc1c([N+](=O)[O-])cc(C2=C([N+](=O)[O-])C(=O)c3c(cccc3)O2)cc1	3
4319	ISSSTY_v1a_7367_02May011_5709	607-30-7	c1(NO)c2c(cccc2)ccc1	3
4320	ISSSTY_v1a_7367_02May011_5711	81593-11-5	HC(H)S(=O)(=O)N1C2c3c(-c4c(cccc4)C12)cccc3	3
4321	ISSSTY_v1a_7367_02May011_5712	36712-35-3	c1(-c2c([N+](=O)[O-])cc([N+](=O)[O-])cc2)c([N+](=O)[O-])cccc1	3
4322	ISSSTY_v1a_7367_02May011_5713	102873-32-5	c1(-c2c([N+](=O)[O-])cc([N+](=O)[O-])cc2)cc([N+](=O)[O-])ccc1	3
4323	ISSSTY_v1a_7367_02May011_5714	36712-34-2	c1(-c2c([N+](=O)[O-])cc([N+](=O)[O-])cc2)ccc([N+](=O)[O-])cc1	3
4324	ISSSTY_v1a_7367_02May011_5715	145627-68-5	HC1c2c(c3c(c4c([C@](O)[C@@](O)C=C4)cc3)cc2)C(H)C1H	3
4325	ISSSTY_v1a_7367_02May011_5718	1010-93-1	HC(H)C1N(C(H)C(=O)O)C(N(=O)=O)=CN=1	3
4326	ISSSTY_v1a_7367_02May011_5719	4812-40-2	HC(O)C1N(C(H)C(H)O)C(N(=O)=O)=CN=1	3

4327	ISSSTY_v1a_7367_02May011_5720	1874-23-3	HC(H)OC(=O)C1=CC=C(N(=O)=O)O1	3
4328	ISSSTY_v1a_7367_02May011_5722	52101-40-3	c1(C2C(c3ccccc3)=C(C(=O)O)OC=2N(=O)=O)ccccc1	3
4329	ISSSTY_v1a_7367_02May011_5730	1794-84-9	HC(Cl)N(=O)=O	3
4330	ISSSTY_v1a_7367_02May011_5731	7119-89-3	C(Cl)(Cl)N(=O)=O	3
4331	ISSSTY_v1a_7367_02May011_5733	771-97-1	c1(N)c(N)cc2c(cccc2)c1	3
4332	ISSSTY_v1a_7367_02May011_5738	2255-50-7	HC(H)Oc1c2c(c(O)ccc2)nc2c1C=CO2	3
4333	ISSSTY_v1a_7367_02May011_5741	82911-12-4	c12C3c4c(-c1cccc2[C@@](O)[C@](O)C=3)cccc4	3
4334	ISSSTY_v1a_7367_02May011_5742	105777-13-7	C12c3c4c(C=1[C@](O)[C@@](O)C=C2)cccc4ccc3	3
4335	ISSSTY_v1a_7367_02May011_5745	79526-11-7	HC1C(Oc2ccccc2)O1	3
4336	ISSSTY_v1a_7367_02May011_5746	5386-28-7	C1(=O)C(=O)c2c3C(c4c(-c3ccc2)cccc4)=C1	3
4337	ISSSTY_v1a_7367_02May011_5748	83349-67-1	c12[C@@]34c5c(-c1cccc2C(O)C(O)[C@@]3O4)cccc5	3
4338	ISSSTY_v1a_7367_02May011_5749	83349-66-0	c12[C@@]34c5c(-c1cccc2C(O)C(O)[C@@]3O4)cccc5	3
4339	ISSSTY_v1a_7367_02May011_5756	1629-58-9	HC(H)C(H)C(=O)C=CH	3
4340	ISSSTY_v1a_7367_02May011_5757	106323-85-7	c1(-c2c([N+](=O)[O-])cc([N+](=O)[O-])cc2)cc([N+](=O)[O-])c([N+](=O)[O-])cc1	3
4341	ISSSTY_v1a_7367_02May011_5759	590-21-6	HC(H)C=CCl	3
4342	ISSSTY_v1a_7367_02May011_5763	96918-15-9	c12c3c4c(c5c(C=CO5)cc4ccc3ccc1)cc2	3
4343	ISSSTY_v1a_7367_02May011_5765	96918-24-0	c12c3c4c(c5c(cc4ccc3ccc1)OC=C5)cc2	3
4344	ISSSTY_v1a_7367_02May011_5769	96563-08-5	HC(H)c1c2-c3c(C(C(H)H)c2ccc1)cccc3	3
4345	ISSSTY_v1a_7367_02May011_5770	21846-26-4	HC(H)c1cc2c(-c3c(cccc3)C2C(H)H)cc1	3
4346	ISSSTY_v1a_7367_02May011_5771	96563-07-4	HC(H)c1cc2-c3c(C(C(H)H)c2cc1)cccc3	3
4347	ISSSTY_v1a_7367_02May011_5772	22994-85-0	HC(c1cccc1)NC(=O)C(H)N1C(N(=O)=O)=NC=C1	3
4348	ISSSTY_v1a_7367_02May011_5773	17057-98-6	HC(H)c1c2c(-c3c(cccc3)C2C(H)H)ccc1	3
4349	ISSSTY_v1a_7367_02May011_5781	229-87-8	c12c(c3c(cccc3)cn1)cccc2	3
4350	ISSSTY_v1a_7367_02May011_5785	51-18-3	HC1C(H)N1c1nc(N2C(H)C2H)nc(N2C(H)C2H)n1	3
4351	ISSSTY_v1a_7367_02May011_5789	59283-76-0	HC(H)c1c(NO)cc([N+](=O)[O-])cc1[N+](=O)[O-]	3
4352	ISSSTY_v1a_7367_02May011_5790	185376-54-9	HC(H)c1c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
4353	ISSSTY_v1a_7367_02May011_5791	1622-57-7	HC(H)N1c2c(cccc2)N=C1N	3
4354	ISSSTY_v1a_7367_02May011_5792	6285-68-3	HC(H)c1cc2c(cc1)N=C(N)N2	3
4355	ISSSTY_v1a_7367_02May011_5794	20921-50-0	HC(H)c1c(C(H)H)cc(C(c2ccccc2)(C_C)OC(=O)NC2C(H)C(H)C(H)C(H)C2H)cc1	3
4356	ISSSTY_v1a_7367_02May011_5795	63655-40-3	C(N)c1cc2c(cc1)N=C(N)N2	3
4357	ISSSTY_v1a_7367_02May011_5797	51276-85-8	c12c(cc(O)cc1)NC(N)=N2	3
4358	ISSSTY_v1a_7367_02May011_5798	76215-00-4	HC(H)C(=O)OC(H)N(C(H)C(H)Cl)N=O	3
4359	ISSSTY_v1a_7367_02May011_5799	39860-12-3	HC(H)c1cc2c(cc1)N(C(H)H)C(N)=N2	3
4360	ISSSTY_v1a_7367_02May011_5800	312304-89-5	HC(H)C(=O)OC(H)N(C(H)C(H)C(H)C(H)Cl)N=O	3
4361	ISSSTY_v1a_7367_02May011_5801	103748-25-0	HC(H)N1c2c(cc(Cl)cc2)N=C1N	3
4362	ISSSTY_v1a_7367_02May011_5802	141691-41-0	HC(H)N1c2c(cc(C_N)cc2)N=C1N	3
4363	ISSSTY_v1a_7367_02May011_5805	1805-02-3	HC(H)N1c2c(cc(OC(H)H)cc2)N=C1N	3
4364	ISSSTY_v1a_7367_02May011_5806	102408-26-4	HC(H)N1c2c(c3c(cc2)nccc3)N=C1NC(H)H	3
4365	ISSSTY_v1a_7367_02May011_5807	102408-27-5	HC(H)N1c2c(c3c(cc2)nccc3)N=C1N(C(H)H)C(H)H	3
4366	ISSSTY_v1a_7367_02May011_5808	102408-25-3	HC(H)N1c2c3c(ccc2N=C1N)nccc3	3
4367	ISSSTY_v1a_7367_02May011_5809	145142-71-8	HC(H)C(c1ccc(C(=O)N(OC(=O)C(H)H)OC(H)C(H)C(H)C(H)H)cc1)(C(H)H)C(H)H	3
4368	ISSSTY_v1a_7367_02May011_5810	131229-62-4	HC(H)C(=O)ON(C(=O)c1ccc(Cl)cc1)OC(H)C(H)C(H)C(H)H	3

4369	ISSSTY_v1a_7367_02May011_5811	131229-63-5	HC(H)C(=O)ON(C(=O)c1ccc(Br)cc1)OC(H)C(H)C(H)C(H)H	3
4370	ISSSTY_v1a_7367_02May011_5813	131229-64-6	HC(H)C(=O)ON(C(=O)c1ccc(N(=O)=O)cc1)OC(H)C(H)C(H)C(H)H	3
4371	ISSSTY_v1a_7367_02May011_5814	357204-47-8	HC(H)C(=O)ON(C(=O)c1cc(N(=O)=O)ccc1)OC(H)C(H)C(H)C(H)H	3
4372	ISSSTY_v1a_7367_02May011_5815	139259-92-0	HC(H)C(=O)ON(C(=O)c1ccccc1)OC(H)c1ccc(Oc2ccccc2)cc1	3
4373	ISSSTY_v1a_7367_02May011_5817	139259-94-2	HC(H)c1ccc(C(H)ON(C(=O)c2ccccc2)OC(=O)C(H)H)cc1	3
4374	ISSSTY_v1a_7367_02May011_5819	139259-96-4	HC(H)C(=O)ON(C(=O)c1ccccc1)OC(H)c1ccc(Cl)cc1	3
4375	ISSSTY_v1a_7367_02May011_5820	139259-98-6	HC(H)C(=O)ON(C(=O)c1ccccc1)OC(H)c1ccc(N(=O)=O)cc1	3
4376	ISSSTY_v1a_7367_02May011_5821	139259-91-9	HC(H)C(=O)ON(C(=O)c1ccccc1)OC(H)c1ccc(OC(H)H)cc1	3
4377	ISSSTY_v1a_7367_02May011_5822	139259-97-5	HC(H)C(=O)ON(C(=O)c1ccccc1)OC(H)c1ccc(Br)cc1	3
4378	ISSSTY_v1a_7367_02May011_5823	220168-52-5	HC(c1ccccc1)ON(C(=O)c1ccccc1)OC(=O)c1ccc(C_N)cc1	3
4379	ISSSTY_v1a_7367_02May011_5824	220168-41-2	HC(H)Oc1ccc(C(=O)ON(C(=O)c2ccccc2)OC(H)c2ccccc2)cc1	3
4380	ISSSTY_v1a_7367_02May011_5825	220168-43-4	HC(H)c1ccc(C(=O)ON(C(=O)c2ccccc2)OC(H)c2ccccc2)cc1	3
4381	ISSSTY_v1a_7367_02May011_5826	220168-45-6	HC(c1ccccc1)ON(C(=O)c1ccccc1)OC(=O)c1ccc(Cl)cc1	3
4382	ISSSTY_v1a_7367_02May011_5827	220168-47-8	HC(c1ccccc1)ON(C(=O)c1ccccc1)OC(=O)c1ccc(C=O)cc1	3
4383	ISSSTY_v1a_7367_02May011_5828	115689-52-6	HC1c2c(C3=C(C1H)SC(N)=N3)ccccn2	3
4384	ISSSTY_v1a_7367_02May011_5829	357204-48-9	HC(c1ccccc1)ON(C(=O)c1ccccc1)OC(=O)c1cc(N(=O)=O)ccc1	3
4385	ISSSTY_v1a_7367_02May011_5830	141890-75-7	c12c(c3c(cc1)nccc3)N=C(N)S2	3
4386	ISSSTY_v1a_7367_02May011_5831	357204-49-0	HC(H)c1cc(C(=O)ON(C(=O)c2ccccc2)OC(H)c2ccccc2)ccc1	3
4387	ISSSTY_v1a_7367_02May011_5832	244775-76-6	HC(H)C(=O)ON(C(=O)c1ccccc1)OC(H)C(H)C(H)H	3
4388	ISSSTY_v1a_7367_02May011_5833	139259-64-6	HC(H)C(=O)ON(C(=O)c1ccccc1)OC(C(H)H)C(H)H	3
4389	ISSSTY_v1a_7367_02May011_5834	357204-50-3	HC(H)C(=O)ON(C(=O)c1cc2c(ccc2)cc1)OC(H)C(H)C(H)C(H)H	3
4390	ISSSTY_v1a_7367_02May011_5836	37797-31-2	HC(H)C(=O)OC(H)c1c(N=Nc2ccc(C(H)OC(=O)C(H)H)cc2)cccc1	3
4391	ISSSTY_v1a_7367_02May011_5837	78914-74-6	HC(H)C(=O)OC(H)c1c(N=Nc2ccc(N(C(H)H)C(H)H)cc2)cccc1	3
4392	ISSSTY_v1a_7367_02May011_5838	78914-75-7	HC(H)C(=O)OC(H)c1ccc(N=Nc2ccc(N(C(H)H)C(H)H)cc2)cc1	3
4393	ISSSTY_v1a_7367_02May011_5839	35282-72-5	HC(H)N(c1ccc(N=Nc2cc(C(H)Cl)ccc2)cc1)C(H)H	3
4394	ISSSTY_v1a_7367_02May011_5840	493-52-7	HC(H)N(c1ccc(N=Nc2c(C(=O)O)cccc2)cc1)C(H)H	3
4395	ISSSTY_v1a_7367_02May011_5841	24554-26-5	C1(C2=CC=C(N(=O)=O)O2)=CSC(NC=O)=N1	3
4396	ISSSTY_v1a_7367_02May011_5843	39208-00-9	HC(H)N(c1ccc(N=Nc2ccc(C=O)cc2)cc1)C(H)H	3
4397	ISSSTY_v1a_7367_02May011_5846	33804-48-7	HC(H)C(=O)N(c1ccc(N=Nc2ccc(N(C(H)H)C(H)H)cc2)cc1)C(H)H	3
4398	ISSSTY_v1a_7367_02May011_5847	1591-56-6	HC(H)C(=O)Nc1ccc(N=Nc2ccc(N(C(H)H)C(H)H)cc2)cc1	3
4399	ISSSTY_v1a_7367_02May011_5849	53499-68-6	HC(H)C(=O)N(c1ccc(N=Nc2ccc(NC(H)H)cc2)cc1)C(H)H	3
4400	ISSSTY_v1a_7367_02May011_5850	775-11-1	HC(c1ccccc1)N(C(N)=O)N=O	3
4401	ISSSTY_v1a_7367_02May011_5854	130536-39-9	c12c(C3C(C=C1)O3)nccc2	3
4402	ISSSTY_v1a_7367_02May011_5855	142044-37-9	HC(H)[n+]1c2c([C@]3[C@@](C=C2)O3)ccc1	3
4403	ISSSTY_v1a_7367_02May011_5857	131229-60-2	HC(H)C(=O)ON(C(=O)c1ccc(OC(H)H)cc1)OC(H)C(H)C(H)C(H)H	3
4404	ISSSTY_v1a_7367_02May011_5865	63710-09-8	HC(H)C(H)C1(O)C(H)[C@](OC2C(H)C(N(C(H)H)C(H)H)C(OC3C(H)C(O)C(C(H)H)O3)C(C(H)H)O2)c2e(O)c3C(=O)c4c(C(=O)c3cc2[C@]1C(=O)OC(H)H)c(O)ccc4O	3
4405	ISSSTY_v1a_7367_02May011_5868	60504-57-6	HC(H)C(H)[C@]1(O)C(H)[C@](O[C@@]2C(H)C@](N(C(H)H)C(H)H)[C@](O)[C@](C(H)H)O2)c2e(O)c3C(=O)c4c(C(=O)c3cc2[C@]1C(=O)OC(H)H)ccc4O	3
4406	ISSSTY_v1a_7367_02May011_5871	14160-38-4	HC(H)C(C1C(=O)C(C2C(=O)C(C(C(H)H)(C(H)H)C(H)H)=CC(=O)C=2)=CC(=O)C=1)C(C(H)H)C(H)H	3
4407	ISSSTY_v1a_7367_02May011_5878	3031-73-0	HC(H)OO	3
4408	ISSSTY_v1a_7367_02May011_5879	3031-74-1	HC(H)C(H)OO	3
4409	ISSSTY_v1a_7367_02May011_5880	39300-45-3	C(C)C(c1c(OC(=O)C=CC)c([N+](=O)[O-])cc([N+](=O)[O-])c1)CC(C)C(C)	3
4410	ISSSTY_v1a_7367_02May011_5881	34041-03-7	HC(H)N(C(=S)SNC(H)C(H)NSC(=S)N(C(H)H)C(H)H)C(H)H	3

4411	ISSSTY_v1a_7367_02May011_5882	6068-96-8	HC(H)C(H)C(H)OO	3
4412	ISSSTY_v1a_7367_02May011_5883	4813-50-7	HC(H)C(H)C(H)C(H)OO	3
4413	ISSSTY_v1a_7367_02May011_5885	23245-64-9	C(N)c1c2c(c(N(=O)=O)ccc2)ccc1	3
4414	ISSSTY_v1a_7367_02May011_5886	3811-49-2	HC(H)OP1(=S)Oc2c(C(H)O1)cccc2	3
4415	ISSSTY_v1a_7367_02May011_5887	2227-17-0	C1(Cl)C(Cl)(C2(Cl)C(Cl)=C(Cl)C(Cl)=C2Cl)C(Cl)=C(Cl)C=1Cl	3
4416	ISSSTY_v1a_7367_02May011_5888	304-81-4	c12c(cccc1)nc1c(cccc1)n2=O	3
4417	ISSSTY_v1a_7367_02May011_5889	96-50-4	C1(N)=NC=CS1	3
4418	ISSSTY_v1a_7367_02May011_5890	6165-76-0	HC(H)c1ccc(S(=O)(=O)OC(H)C_C)cc1	3
4419	ISSSTY_v1a_7367_02May011_5891	778-28-9	HC(H)c1ccc(S(=O)(=O)OC(H)C(H)C(H)C(H)H)cc1	3
4420	ISSSTY_v1a_7367_02May011_5892	2307-69-9	HC(H)c1ccc(OS(=O)(=O)C(C(H)H)C(H)H)cc1	3
4421	ISSSTY_v1a_7367_02May011_5893	599-91-7	HC(H)c1ccc(S(=O)(=O)OC(H)C(H)C(H)H)cc1	3
4422	ISSSTY_v1a_7367_02May011_5894	80-48-8	HC(H)c1ccc(S(=O)(=O)OC(H)H)cc1	3
4423	ISSSTY_v1a_7367_02May011_5895	80-44-4	HC(H)C(H)C(H)C(H)OS(=O)(=O)c1ccccc1	3
4424	ISSSTY_v1a_7367_02May011_5896	515-46-8	HC(H)C(H)OS(=O)(=O)c1ccccc1	3
4425	ISSSTY_v1a_7367_02May011_5897	80-18-2	HC(H)OS(=O)(=O)c1ccccc1	3
4426	ISSSTY_v1a_7367_02May011_5898	16156-53-9	HC(H)C(C(H)H)C(H)OS(=O)(=O)C(H)H	3
4427	ISSSTY_v1a_7367_02May011_5899	1912-32-9	HC(H)C(H)C(H)C(H)OS(=O)(=O)C(H)H	3
4428	ISSSTY_v1a_7367_02May011_5900	1912-31-8	HC(H)C(H)C(H)OS(=O)(=O)C(H)H	3
4429	ISSSTY_v1a_7367_02May011_5901	80-42-2	HC(H)C(H)C(H)OS(=O)(=O)c1ccccc1	3
4430	ISSSTY_v1a_7367_02May011_5902	303-33-3	HC(H)[C@@]([C@@](O)(C(=O)OC(H)C1[C@@]2[C@@](O)C(H)C(H)N2C(H)C=1)C(C(H)H)C(H)H)OC(H)H	3
4431	ISSSTY_v1a_7367_02May011_5906	75965-74-1	HC(H)Oc1cc2c(c3c(cc2)OC(N(=O)=O)=C3)cc1	3
4432	ISSSTY_v1a_7367_02May011_5912	765-34-4	HC1C(C=O)O1	3
4433	ISSSTY_v1a_7367_02May011_5914	53478-38-9	HC(H)S(=O)(=O)Nc1ccc(Nc2c3c(cccc3)nc3c2cccc3)cc1	3
4434	ISSSTY_v1a_7367_02May011_5917	217-59-4	c12c(c3c(c4c1cccc4)cccc3)cccc2	3
4435	ISSSTY_v1a_7367_02May011_5918	7332-00-5	HC(H)C(H)C(H)C(H)N=N_N	3
4436	ISSSTY_v1a_7367_02May011_5919	6926-45-0	HC(H)C(H)C(H)C(H)C(H)C(H)N=N_N	3
4437	ISSSTY_v1a_7367_02May011_5920	2148-31-4	HC(H)C(=O)N[C@](C(=O)O)C(H)SC(Cl)=CCl	3
4438	ISSSTY_v1a_7367_02May011_5921	111348-61-9	HC(H)C(=O)N[C@](C(=O)O)C(H)SC(Cl)=C(Cl)Cl	3
4439	ISSSTY_v1a_7367_02May011_5922	93780-95-1	c12c(c3c([C@@](O)[C@](O)[C@@]4[C@@]3O4)cc1)nc1c3c(ccc1c2)cccc3	3
4440	ISSSTY_v1a_7367_02May011_5923	93781-00-1	c12c(c3c([C@](O)[C@@](O)[C@@]4[C@@]3O4)cc1)nc1c3c(ccc1c2)cccc3	3
4441	ISSSTY_v1a_7367_02May011_5924	93780-98-4	c12c(c3c([C@@](O)[C@](O)[C@]4[C@]3O4)cc1)nc1c3c(ccc1c2)cccc3	3
4442	ISSSTY_v1a_7367_02May011_5925	93780-96-2	c12c(c3c([C@](O)[C@@](O)[C@]4[C@]3O4)cc1)nc1c3c(ccc1c2)cccc3	3
4443	ISSSTY_v1a_7367_02May011_5926	99152-10-0	HC(H)C(=O)N[C@@](C(=O)N(C(H)C(=O)O)N=O)C(C(H)H)C(H)H	3
4444	ISSSTY_v1a_7367_02May011_5928	40568-90-9	HC(H)c1c2c3c4c(c5c(cc4ccc3cc1)cccc5)cc2	3
4445	ISSSTY_v1a_7367_02May011_5930	16757-82-7	HC(H)c1cc2c3c4c(c5c(cc4ccc3c1)cccc5)cc2	3
4446	ISSSTY_v1a_7367_02May011_5932	16757-81-6	HC(H)c1c2c3c4c(c5c(cc4cc2)cccc5)ccc3cc1	3
4447	ISSSTY_v1a_7367_02May011_5933	16757-83-8	HC(H)c1c2c3c4c(c5c(cc4c1)cccc5)ccc3ccc2	3
4448	ISSSTY_v1a_7367_02May011_5934	63041-77-0	HC(H)c1c2c(c3c4c5c(ccc4c2)cccc5cc3)ccc1	3
4449	ISSSTY_v1a_7367_02May011_5935	63041-76-9	HC(H)c1cc2c(c3c4c5c(ccc4c2)cccc5cc3)cc1	3
4450	ISSSTY_v1a_7367_02May011_5936	70644-19-8	HC(H)c1cc2c3c4c5c(ccc4cc2cc1)cccc5cc3	3
4451	ISSSTY_v1a_7367_02May011_5937	63104-32-5	HC(H)c1c2c3c4c5c(ccc4cc2ccc1)cccc5cc3	3
4452	ISSSTY_v1a_7367_02May011_5938	16757-80-5	HC(H)c1c2c3c4c(ccc3cc3c2cccc3)cccc4c1	3

4453	ISSSTY_v1a_7367_02May011_5939	4514-19-6	HC(H)c1c2c3c4c(c5c(cc4ccc3ccc2)cccc5)c1	3
4454	ISSSTY_v1a_7367_02May011_5940	24143-08-6	HC(H)C(=O)NC1C=NC(C2=CC=C(N(=O)=O)O2)=NO1	3
4455	ISSSTY_v1a_7367_02May011_5945	94500-46-6	HC(Cl)c1c2c3c4c(c5c(cc4c1)cccc5)ccc3ccc2	3
4456	ISSSTY_v1a_7367_02May011_5947	29852-26-4	HC(Cl)c1c2c3c(c4c(cccc4)c2)ccc2c3c(ccc2)c1	3
4457	ISSSTY_v1a_7367_02May011_5951	86803-19-2	HC(Cl)c1c2c3c4c5c(ccc4cc2ccc1)cccc5cc3	3
4458	ISSSTY_v1a_7367_02May011_5952	78411-56-0	HC(H)c1cnc2c3c(ccc2n1)N(C(H)H)C(N)=N3	3
4459	ISSSTY_v1a_7367_02May011_5957	303-34-4	HC(H)C(O)(C@)(O)(C(=O)O)C(H)C1[C@@]2[C@@](OC(=O)C(C(H)H)=CC(H)H)C(H)C(H)N2C(H)C=1)[C@](C(H)H)OC(H)H)C(H)H	3
4460	ISSSTY_v1a_7367_02May011_5961	41267-76-9	HC(H)C1c2c(c3c4c(C(H)C(H)C(H)N4C(H)C(H)C3H)c2)OC(=O)C=1	3
4461	ISSSTY_v1a_7367_02May011_5965	58336-35-9	HC1c2c3c(c4c(C=CC(=O)O4)c2)C(H)C(H)C(H)N3C(H)C1H	3
4462	ISSSTY_v1a_7367_02May011_5966	3365-85-3	c1(-c2ccc(-c3ccc(N)cc3)cc2)ccc(N)cc1	3
4463	ISSSTY_v1a_7367_02May011_5967	53693-66-6	HC(H)C(H)N(c1c(-c2cccc2)c(-c2cccc2)ccc1N(C(H)C(H)H)C(H)C(H)H)C(H)C(H)H	3
4464	ISSSTY_v1a_7367_02May011_5976	99520-64-6	c12C3C4c5c6c(ccc5C5C(C=4c1cccc2)O5)cccc6C=3	3
4465	ISSSTY_v1a_7367_02May011_5977	7696-62-0	HC(H)C(H)C(H)C(H)Oc1ccc(N=O)cc1	3
4466	ISSSTY_v1a_7367_02May011_5978	100690-33-3	HC(H)C(H)C(H)C(H)C(H)Oc1ccc(N=O)cc1	3
4467	ISSSTY_v1a_7367_02May011_5979	1517-05-1	HC(O)C(H)N=N_N	3
4468	ISSSTY_v1a_7367_02May011_5980	138245-74-6	HC(O)[C@](O)[C@@](O)[C@@](O)[C@](O)C(H)N=N_N	3
4469	ISSSTY_v1a_7367_02May011_5983	67019-41-4	C1(=NC(=O)c2ccc([N+](=O)[O-])cc2)c2c(cccc2)N(C(=O)c2ccc([N+](=O)[O-])cc2)S1	3
4470	ISSSTY_v1a_7367_02May011_5987	99523-84-9	HC(H)c1cc2C(=NC(=O)c3ccc([N+](=O)[O-])ccc3)SN(C(=O)c3cc([N+](=O)[O-])ccc3)c2cc1	3
4471	ISSSTY_v1a_7367_02May011_5988	99523-85-0	HC(H)c1cc2C(=NC(=O)c3ccc([N+](=O)[O-])cc3)SN(C(=O)c3ccc([N+](=O)[O-])ccc3)c2cc1	3
4472	ISSSTY_v1a_7367_02May011_5990	91991-31-0	HC(C(=O)N1c2c(C(=NC(=O)C(H)C(H)C(H)Cl)S1)cc(Cl)cc2)C(H)C(H)Cl	3
4473	ISSSTY_v1a_7367_02May011_5991	91991-42-3	C1(=NC(=O)c2ccc([N+](=O)[O-])cc2)c2c(cccc(Cl)c2)N(C(=O)c2ccc([N+](=O)[O-])cc2)S1	3
4474	ISSSTY_v1a_7367_02May011_5992	106532-60-9	HC(H)C(=O)N1c2c(C(=NC(=O)C(H)H)S1)cc(N(=O)=O)cc2	3
4475	ISSSTY_v1a_7367_02May011_5993	106532-61-0	HC(H)C(H)C(=O)N1c2c(C(=NC(=O)C(H)C(H)H)S1)cc(N(=O)=O)cc2	3
4476	ISSSTY_v1a_7367_02May011_5994	106532-63-2	HC(H)C(H)C(H)C(=O)N1c2c(C(=NC(=O)C(H)C(H)C(H)H)S1)cc(N(=O)=O)cc2	3
4477	ISSSTY_v1a_7367_02May011_5995	106532-64-3	HC(H)C(C(=O)N1c2c(C(=NC(=O)C(C(H)H)C(H)H)S1)cc(N(=O)=O)cc2)C(H)H	3
4478	ISSSTY_v1a_7367_02May011_5996	106532-66-5	HC(H)C(H)C(H)C(H)C(=O)N1c2c(C(=NC(=O)C(H)C(H)C(H)C(H)H)S1)cc(N(=O)=O)cc2	3
4479	ISSSTY_v1a_7367_02May011_5997	106532-67-6	HC(H)C(C(H)H)C(H)C(=O)N1c2c(C(=NC(=O)C(H)C(H)C(H)C(H)H)S1)cc(N(=O)=O)cc2	3
4480	ISSSTY_v1a_7367_02May011_5998	106532-68-7	HC(H)C(H)C(H)C(H)C(H)C(=O)N1c2c(C(=NC(=O)C(H)C(H)C(H)C(H)C(H)H)S1)cc(N(=O)=O)cc2	3
4481	ISSSTY_v1a_7367_02May011_5999	106532-69-8	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(=O)N1c2c(C(=NC(=O)C(H)C(H)C(H)C(H)C(H)C(H)H)S1)cc(N(=O)=O)cc2	3
4482	ISSSTY_v1a_7367_02May011_6000	106532-70-1	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(=O)N1c2c(C(=NC(=O)C(H)C(H)C(H)C(H)C(H)C(H)H)S1)cc(N(=O)=O)cc2	3
4483	ISSSTY_v1a_7367_02May011_6001	106532-62-1	HC(C(=O)N1c2c(C(=NC(=O)C(H)C(H)Cl)S1)cc(N(=O)=O)cc2)C(H)Cl	3
4484	ISSSTY_v1a_7367_02May011_6002	106532-65-4	HC(C(=O)N1c2c(C(=NC(=O)C(H)C(H)C(H)Cl)S1)cc(N(=O)=O)cc2)C(H)C(H)Cl	3
4485	ISSSTY_v1a_7367_02May011_6003	106532-71-2	C1(=NC(=O)c2cccc2)c2c(ccc(N(=O)=O)c2)N(C(=O)c2cccc2)S1	3
4486	ISSSTY_v1a_7367_02May011_6004	106532-72-3	C1(=NC(=O)c2c(Cl)cccc2)c2c(ccc(N(=O)=O)c2)N(C(=O)c2c(Cl)cccc2)S1	3
4487	ISSSTY_v1a_7367_02May011_6005	106532-73-4	C1(=NC(=O)c2cc(Cl)ccc2)c2c(ccc(N(=O)=O)c2)N(C(=O)c2cc(Cl)ccc2)S1	3
4488	ISSSTY_v1a_7367_02May011_6006	106532-74-5	C1(=NC(=O)c2ccc(Cl)cc2)c2c(ccc(N(=O)=O)c2)N(C(=O)c2ccc(Cl)cc2)S1	3
4489	ISSSTY_v1a_7367_02May011_6007	106532-75-6	C1(=NC(=O)c2cc(Cl)c(Cl)cc2)c2c(ccc(N(=O)=O)c2)N(C(=O)c2cc(Cl)c(Cl)cc2)S1	3
4490	ISSSTY_v1a_7367_02May011_6008	106532-76-7	C1(=NC(=O)c2c([N+](=O)[O-])cccc2)c2c(ccc([N+](=O)[O-])c2)N(C(=O)c2c(N(=O)=O)cccc2)S1	3
4491	ISSSTY_v1a_7367_02May011_6009	106532-77-8	C1(=NC(=O)c2cc([N+](=O)[O-])ccc2)c2c(ccc([N+](=O)[O-])c2)N(C(=O)c2cc([N+](=O)[O-])ccc2)S1	3
4492	ISSSTY_v1a_7367_02May011_6010	106532-78-9	C1(=NC(=O)c2ccc([N+](=O)[O-])cc2)c2c(ccc([N+](=O)[O-])c2)N(C(=O)c2ccc([N+](=O)[O-])cc2)S1	3
4493	ISSSTY_v1a_7367_02May011_6011	99601-31-7	HC(H)c1cnc2c(c3c(cc2)N(C(H)C(H)H)C(N)=N3)n1	3
4494	ISSSTY_v1a_7367_02May011_6012	99601-30-6	HC(H)c1cnc2c3c(ccc2n1)N(C(H)C(H)H)C(N)=N3	3

4495	ISSSTY_v1a_7367_02May011_6013	100-65-2	c1(NO)cccc1	3
4496	ISSSTY_v1a_7367_02May011_6015	89837-94-5	HC(H)C(=O)C(H)N(C(H)OC(=O)C(H)H)N=O	3
4497	ISSSTY_v1a_7367_02May011_6016	112725-15-2	HC(H)C(=O)C(N(C(H)H)N=O)OC(=O)C(H)H	3
4498	ISSSTY_v1a_7367_02May011_6017	31464-26-3	HC(H)N(c1ccc(N=Nc2ccccc2)cc1)C(H)C(H)C_N	3
4499	ISSSTY_v1a_7367_02May011_6018	92911-19-8	HC(H)Nc1ccc(N=Nc2cc3c(cc2)N=CS3)cc1	3
4500	ISSSTY_v1a_7367_02May011_6020	39720-27-9	HC(H)C(=O)Oc1ccc(C(H)Cl)cc1	3
4501	ISSSTY_v1a_7367_02May011_6027	80556-89-4	HC(C(=O)O)N(C(H)C(H)O)N=O	3
4502	ISSSTY_v1a_7367_02May011_6036	4450-68-4	HC(H)c1ccc(S(=O)(=O)OC(H)c2ccc(N(=O)=O)cc2)cc1	3
4503	ISSSTY_v1a_7367_02May011_6039	61734-86-9	HC(H)C(H)C(H)C(H)C(H)N(C(H)C(H)C(H)C(H)O)N=O	3
4504	ISSSTY_v1a_7367_02May011_6040	34424-65-2	HC(H)C(O)C=CC=O	3
4505	ISSSTY_v1a_7367_02May011_6041	105453-63-2	c12c(c3c(C=C[C@](O)[C@@]3O)cc1)cc1c(c3c(cccc3)cc1)c2	3
4506	ISSSTY_v1a_7367_02May011_6043	105453-65-4	c12c(c3c([C@](O)[C@@](O)C=C3)cc1)cc1c(c3c(cccc3)cc1)c2	3
4507	ISSSTY_v1a_7367_02May011_6044	105453-64-3	c12c(c3c([C@](O)[C@@](O)C=C3)cc1)cc1c(c3c(cccc3)cc1)c2	3
4508	ISSSTY_v1a_7367_02May011_6045	105453-66-5	c12-c3c([C@](O)[C@@](O)c1cc1c4c(ccc1c2)cccc4)cccc3	3
4509	ISSSTY_v1a_7367_02May011_6046	105453-67-6	c12-c3c([C@](O)[C@@](O)c1cc1c4c(ccc1c2)cccc4)cccc3	3
4510	ISSSTY_v1a_7367_02May011_6048	14953-62-9	c1(C2=C(N(=O)=O)N=CN2)cccc1	3
4511	ISSSTY_v1a_7367_02May011_6049	14953-63-0	HC(H)N1C(N(=O)=O)=C(c2ccccc2)N=C1	3
4512	ISSSTY_v1a_7367_02May011_6050	111380-09-7	HC(H)N1C(c2ccccc2)=C(N=O)N=C1	3
4513	ISSSTY_v1a_7367_02May011_6051	106232-36-4	c1(C2=C(N=O)N=CN2)cccc1	3
4514	ISSSTY_v1a_7367_02May011_6052	111380-08-6	HC(H)N1C(N=O)=C(c2ccccc2)N=C1	3
4515	ISSSTY_v1a_7367_02May011_6053	97055-38-4	HC(H)OC1C(C(Cl)Cl)=C(Cl)C(=O)O1	3
4516	ISSSTY_v1a_7367_02May011_6057	111955-16-9	HC(H)c1ccc(NC2[C@@](O)[C@](O)[C@](O)C(H)O2)cc1	3
4517	ISSSTY_v1a_7367_02May011_6058	3054-60-2	HC(H)c1ccc(NC2[C@@](O)[C@@](O)[C@](O)C(H)O2)cc1	3
4518	ISSSTY_v1a_7367_02May011_6059	111955-22-7	HC(C1c2c(ccc2)NC=1)C(H)NC1[C@](O)[C@@](O)[C@](O)C(H)O1	3
4519	ISSSTY_v1a_7367_02May011_6060	111955-14-7	HC1[C@@](O)[C@@](O)[C@@](O)C(N(c2ccc(N(=O)=O)cc2)N=O)O1	3
4520	ISSSTY_v1a_7367_02May011_6061	111955-18-1	HC1[C@@](O)[C@](O)[C@@](O)C(N(c2ccc(N(=O)=O)cc2)N=O)O1	3
4521	ISSSTY_v1a_7367_02May011_6062	111955-21-6	HC1[C@@](O)[C@](O)[C@](O)C(N(c2ccc(N(=O)=O)cc2)N=O)O1	3
4522	ISSSTY_v1a_7367_02May011_6063	111955-15-8	HC1[C@](O)[C@](O)[C@@](O)C(N(c2ccc(N(=O)=O)cc2)N=O)O1	3
4523	ISSSTY_v1a_7367_02May011_6064	125369-76-8	HC(H)c1ccc(C(C_N)=CC=Cc2c(N(=O)=O)cccc2)cc1	3
4524	ISSSTY_v1a_7367_02May011_6065	125369-77-9	HC(H)Oc1c(C=CC=C(c2ccc(Br)cc2)C_N)cccc1	3
4525	ISSSTY_v1a_7367_02May011_6068	116208-67-4	c1(F)c2c3c(c4c(c3ccc2)cc2c(cccc2)c4)cc1	3
4526	ISSSTY_v1a_7367_02May011_6069	113600-17-2	c12c3c(c4c(c3ccc1)cc1c(c(F)ccc1)c4)ccc2	3
4527	ISSSTY_v1a_7367_02May011_6070	113600-15-0	c12c3c(c4c(c3ccc1)cc1c(cc(F)cc1)c4)ccc2	3
4528	ISSSTY_v1a_7367_02May011_6071	112575-92-5	c12C3c4c(-c1cc1c(cccc1)c2)cccc4C(O)C(O)C=3	3
4529	ISSSTY_v1a_7367_02May011_6072	112309-61-2	HC(H)C1=C(Cl)C(=O)OC1O	3
4530	ISSSTY_v1a_7367_02May011_6073	88169-60-2	HC(H)OC(=O)[C@@](N)C(H)SC(H)C(H)Cl	3
4531	ISSSTY_v1a_7367_02May011_6074	58337-49-8	HC(H)C(=O)N[C@](C(=O)O)C(H)SC(H)C(H)Cl	3
4532	ISSSTY_v1a_7367_02May011_6075	75607-61-3	HC(C(=O)N(C(=O)[C@@](N)C(H)SC(H)C(H)Cl)C(H)C(=O)O)C(H)[C@](N)C(=O)O	3
4533	ISSSTY_v1a_7367_02May011_6076	112575-91-4	C1(=O)C(=O)c2c3C(c4c(-c3ccc2)cc2c(cccc2)c4)=C1	3
4534	ISSSTY_v1a_7367_02May011_6077	100310-95-0	c12c3c(c4c(c3ccc1)cc1c(C(O)C(O)C=C1)c4)ccc2	3
4535	ISSSTY_v1a_7367_02May011_6078	106428-28-8	HC(H)[C@]1(C(=O)O)C(H)C(H)C(H)[C@@]2(C(H)H)C3[C@@]4(C(=O)C(=CH)[C@](O)C(H)C3)C4)C(H)C(H)C12	3
4536	ISSSTY_v1a_7367_02May011_6079	6957-71-7	HC1c2c(-c3c1cc(NC=O)cc3)cccc2	3

4537	ISSSTY_v1a_7367_02May011_6080	3671-71-4	HC1c2c(-c3c1cc(N(O)C(=O)c1cccc1)cc3)cccc2	3
4538	ISSSTY_v1a_7367_02May011_6082	61064-66-2	HC1c2c(-c3c1cc(NCl)cc3)cccc2	3
4539	ISSSTY_v1a_7367_02May011_6084	7151-65-7	HC(H)C(=O)N(Cl)c1cc2c(-c3c(cccc3)C2H)cc1	3
4540	ISSSTY_v1a_7367_02May011_6087	125974-06-3	HC(Cl)C1C(O)OC(=O)C=1	3
4541	ISSSTY_v1a_7367_02May011_6088	125973-99-1	HC(Cl)C1C(H)OC(=O)C=1	3
4542	ISSSTY_v1a_7367_02May011_6089	92433-40-4	HC(H)C(=O)Nc1c(Cl)cc2-c3c(C(H)c2c1)cccc3	3
4543	ISSSTY_v1a_7367_02May011_6091	60129-60-4	HC(H)C1(C(=O)O)C(H)C(H)C(H)C2(C(H)H)C3C4(C(H)C(=CH)C(OC5C(O)C(O)C(O)C(C(H)O)O5)(C(H)C3H)C4H)C(H)C(H)C12	3
4544	ISSSTY_v1a_7367_02May011_6092	107759-11-5	HC(H)C(H)OC(=O)N(C(c1ccnc1)C(H)C(H)C=O)N=O	3
4545	ISSSTY_v1a_7367_02May011_6093	2085-88-3	HC(H)C1(c2cccc2)C(H)O1	3
4546	ISSSTY_v1a_7367_02May011_6095	1669-70-1	HC(H)C1(c2ccc(Cl)cc2)C(H)O1	3
4547	ISSSTY_v1a_7367_02May011_6096	104953-00-6	HC(H)C1C(c2ccc(C_N)cc2)O1	3
4548	ISSSTY_v1a_7367_02May011_6097	75590-19-1	HC(H)C1(c2ccc(N(=O)=O)cc2)C(H)O1	3
4549	ISSSTY_v1a_7367_02May011_6099	98600-98-7	HC(H)c1c2c(c3c([C@](O)[C@@](O)C=C3)c1)cc1c(ccc1)c2	3
4550	ISSSTY_v1a_7367_02May011_6100	64371-62-6	HC(H)C1(c2ccc(-c3cccc3)cc2)C(H)O1	3
4551	ISSSTY_v1a_7367_02May011_6101	98601-00-4	HC(H)c1c2c(c3c(ccc3)c1)cc1c([C@](O)[C@@](O)C=C1)c2	3
4552	ISSSTY_v1a_7367_02May011_6102	98601-01-5	HC(H)c1c2c(c3c(ccc3)c1)cc1c(C=C[C@](O)[C@@](O)C=C1)c2	3
4553	ISSSTY_v1a_7367_02May011_6103	78996-87-9	HC(H)c1c2c(c3c(c(O)ccc3)c1)cc1c(ccc1)c2	3
4554	ISSSTY_v1a_7367_02May011_6104	98601-02-6	HC(H)c1c2c(c3c(c(O)ccc3)c1)cc1c(C=C(O)C(H)C1O)c2	3
4555	ISSSTY_v1a_7367_02May011_6105	304-28-9	HC(H)C(=O)Nc1cc2c(-c3c(cc(NC(=O)C(H)H)cc3)C2H)cc1	3
4556	ISSSTY_v1a_7367_02May011_6109	68395-77-7	HC(H)c1cc(C(H)H)cc(NO)c1	3
4557	ISSSTY_v1a_7367_02May011_6110	39638-32-9	HC(H)C(Cl)(C(H)H)OC(Cl)(C(H)H)C(H)H	3
4558	ISSSTY_v1a_7367_02May011_6112	81943-37-5	HC(H)C(=O)OC(H)N(c1cccc1)N=O	3
4559	ISSSTY_v1a_7367_02May011_6114	430227	HC(H)c1ccc(N(C(H)C(H)O)C(H)C(H)O)cc1	3
4560	ISSSTY_v1a_7367_02May011_6115	3671-78-1	HC1c2c(-c3c1cc(NC(=O)c1cccc1)cc3)cccc2	3
4561	ISSSTY_v1a_7367_02May011_6120	99240-66-1	HC(H)C(=O)N(c1cc2c(-c3c(ccc3)C2H)cc1)C(H)C(H)H	3
4562	ISSSTY_v1a_7367_02May011_6121	24225-71-6	HC(H)C(=O)N(c1cc2c(-c3c(ccc3)C2H)cc1)Nc1cc2c(-c3c(ccc3)C2H)cc1	3
4563	ISSSTY_v1a_7367_02May011_6122	13177-32-7	c12c3c(c4c(c3ccc1)cc(N(=O)=O)cc4)ccc2	3
4564	ISSSTY_v1a_7367_02May011_6123	81316-80-5	c1(N(=O)=O)c2c3c(c4c(c3ccc2)cc2c(ccc2)c4)cc1	3
4565	ISSSTY_v1a_7367_02May011_6124	13177-28-1	c1(N(=O)=O)c2c3c(c4c2c(ccc4)cc1)cccc3	3
4566	ISSSTY_v1a_7367_02May011_6125	10353-98-7	c1(N(=O)=O)c2c3c(C=C2)cccc3cc1	3
4567	ISSSTY_v1a_7367_02May011_6126	10353-99-8	c1(N(=O)=O)c2c3c(C=Cc3ccc2)cc1	3
4568	ISSSTY_v1a_7367_02May011_6127	13177-31-6	c1(N(=O)=O)c2c(c3c4c(ccc24)ccc3)ccc1	3
4569	ISSSTY_v1a_7367_02May011_6128	3807-77-0	HC1c2c3c(c(N(=O)=O)ccc3ccc2)C1H	3
4570	ISSSTY_v1a_7367_02May011_6129	75476-80-1	HC1c2c(C=C1)ccc(N(=O)=O)c2	3
4571	ISSSTY_v1a_7367_02May011_6130	13132-28-0	C1(N(=O)=O)c2c3c(cccc3ccc2)C=1	3
4572	ISSSTY_v1a_7367_02May011_6142	550-60-7	c1(O)c(N(=O)=O)c2c(cccc2)cc1	3
4573	ISSSTY_v1a_7367_02May011_6144	496-14-0	HC1c2c(C(H)O1)cccc2	3
4574	ISSSTY_v1a_7367_02May011_6145	542-88-1	HC(Cl)OC(H)Cl	3
4575	ISSSTY_v1a_7367_02May011_6146	6281-23-8	C(=O)(O)C=CC1=CC=C(N(=O)=O)O1	3
4576	ISSSTY_v1a_7367_02May011_6147	1874-24-4	HC(H)OC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4577	ISSSTY_v1a_7367_02May011_6148	16339-05-2	HC(H)C(H)C(H)C(H)C(H)N(C(H)C(H)C(H)C(H)H)N=O	3
4578	ISSSTY_v1a_7367_02May011_6149	1874-12-0	HC(H)C(H)OC(=O)C=CC1=CC=C(N(=O)=O)O1	3

4579	ISSSTY_v1a_7367_02May011_6150	90147-18-5	HC(H)C(H)C(H)OC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4580	ISSSTY_v1a_7367_02May011_6151	90147-21-0	HC(H)C(C(H)H)OC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4581	ISSSTY_v1a_7367_02May011_6152	90147-19-6	HC(H)C(H)C(H)C(H)OC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4582	ISSSTY_v1a_7367_02May011_6153	91134-58-6	HC(H)C(C(H)H)C(H)OC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4583	ISSSTY_v1a_7367_02May011_6154	97461-38-6	HC(H)C(H)C(C(H)H)OC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4584	ISSSTY_v1a_7367_02May011_6155	97461-39-7	HC(H)C(C(H)H)(C(H)H)OC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4585	ISSSTY_v1a_7367_02May011_6156	91642-47-6	HC(H)C(H)C(H)C(H)C(H)OC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4586	ISSSTY_v1a_7367_02May011_6157	14308-65-7	HC(H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4587	ISSSTY_v1a_7367_02May011_6158	6755-13-1	HC(H)N(C(=O)C=CC1=CC=C(N(=O)=O)O1)C(H)H	3
4588	ISSSTY_v1a_7367_02May011_6159	6755-16-4	HC(H)C(H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4589	ISSSTY_v1a_7367_02May011_6160	90147-31-2	HC(H)C(H)C(H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4590	ISSSTY_v1a_7367_02May011_6161	91182-09-1	HC(H)C(H)C(H)C(H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4591	ISSSTY_v1a_7367_02May011_6162	39965-42-9	HC(H)C(C(H)H)(C(H)H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4592	ISSSTY_v1a_7367_02May011_6163	89811-25-6	HC(H)C(C(H)H)C(H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4593	ISSSTY_v1a_7367_02May011_6164	97461-40-0	HC(H)C(H)C(C(H)H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4594	ISSSTY_v1a_7367_02May011_6165	97461-41-1	HC(H)C(C(H)H)(C(H)H)C(H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4595	ISSSTY_v1a_7367_02May011_6166	97461-42-2	HC(H)C(H)C(H)C(H)C(H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4596	ISSSTY_v1a_7367_02May011_6167	68162-37-8	HC(H)OC(=O)C(=CC1=CC=C([N+](=O)[O-])O1)[N+](=O)[O-]	3
4597	ISSSTY_v1a_7367_02May011_6170	836-37-3	HC(H)OC(=O)C(C_N)=CC1=CC=C(N(=O)=O)O1	3
4598	ISSSTY_v1a_7367_02May011_6173	97461-43-3	HC(H)C(C(=O)OC(H)H)=CC1=CC=C(N(=O)=O)O1	3
4599	ISSSTY_v1a_7367_02May011_6174	69527-46-4	C(N)C(C_N)=CC1=CC=C(N(=O)=O)O1	3
4600	ISSSTY_v1a_7367_02May011_6175	122349-91-1	HC(H)c1c2c(cc(N)c(C(H)H)c2)nc(C(H)H)c1	3
4601	ISSSTY_v1a_7367_02May011_6176	830-07-9	C1(C=C[N+](=O)[O-])=CC=C([N+](=O)[O-])O1	3
4602	ISSSTY_v1a_7367_02May011_6178	75995-58-3	HC(H)C(Br)C(=O)NC(H)c1ccccc1	3
4603	ISSSTY_v1a_7367_02May011_6179	131432-91-2	HC(H)[C@@](Br)C(=O)NC(H)c1ccccc1	3
4604	ISSSTY_v1a_7367_02May011_6180	131432-92-3	HC(H)[C@](Br)C(=O)NC(H)c1ccccc1	3
4605	ISSSTY_v1a_7367_02May011_6181	51938-21-7	HC(H)C(H)C(H)C(H)N(C(H)C(H)C(=O)OC(H)H)N=O	3
4606	ISSSTY_v1a_7367_02May011_6182	142713-63-1	HC(H)C(Br)C(=O)NC(H)c1ccc(OC(H)H)cc1	3
4607	ISSSTY_v1a_7367_02May011_6183	142713-64-2	HC(H)C(Br)C(=O)NC(H)c1cc(OC(H)H)c(O)cc1	3
4608	ISSSTY_v1a_7367_02May011_6184	142713-65-3	HC(H)C(Br)C(=O)NC(H)c1cc(OC(H)H)c(OC(H)H)cc1	3
4609	ISSSTY_v1a_7367_02May011_6189	535-11-5	HC(H)C(H)OC(=O)C(Br)C(H)H	3
4610	ISSSTY_v1a_7367_02May011_6190	119613-62-6	HC(H)C(H)c1c2c(c3c(ccc3)c1)ccc1c2[C@@]2[C@]([C@](O)[C@@]1O)O2	3
4611	ISSSTY_v1a_7367_02May011_6192	51938-14-8	HC(H)C(H)C(H)C(H)N(C(H)C(H)O)N=O	3
4612	ISSSTY_v1a_7367_02May011_6193	80984-66-3	c12-c3c4C5C(c1cccc2C1C(c3ccc4)N1)N5	3
4613	ISSSTY_v1a_7367_02May011_6194	55400-88-9	c12c(c3c4c5c(c6c(cc5cc3)O6)ccc4c1)O2	3
4614	ISSSTY_v1a_7367_02May011_6195	80984-67-4	c12-c3c(C4C(c1cc1-c5c(C6C(c1c2)N6)cccc5)N4)cccc3	3
4615	ISSSTY_v1a_7367_02May011_6196	55400-87-8	c12c(c3c(c4c1cc1c(C5C(=C6C=CC=CC16)O5)c4)cccc3)O2	3
4616	ISSSTY_v1a_7367_02May011_6197	10227-50-6	HC1C(H)N(C2=NC=CS2)C(=O)N1	3
4617	ISSSTY_v1a_7367_02May011_6198	95741-47-2	HC(H)c1c2c3c4c(c5c(c4cc2ccc1)cccc5)ccc3	3
4618	ISSSTY_v1a_7367_02May011_6199	61734-89-2	HC(H)C(=O)C(H)C(H)N(C(H)C(H)C(H)C(H)H)N=O	3
4619	ISSSTY_v1a_7367_02May011_6201	51938-15-9	HC(H)C(=O)C(H)N(C(H)C(H)C(H)C(H)H)N=O	3
4620	ISSSTY_v1a_7367_02May011_6202	98033-25-1	HC(H)C1N(C(H)H)c2c(c3c4c(ccc(O)c4)ccc3cc2)N=1	3

4621	ISSSTY_v1a_7367_02May011_6205	97851-14-4	c1(-c2cc([N+](=O)[O-])c(O)cc2)cc([N+](=O)[O-])ccc1	3
4622	ISSSTY_v1a_7367_02May011_6209	4097-53-4	c1(-c2cc([N+](=O)[O-])c(O)c([N+](=O)[O-])c2)cccc1	3
4623	ISSSTY_v1a_7367_02May011_6210	39482-21-8	HC(H)[Si](C(H)H)(C(H)H)C(H)N(C(N)=O)N=O	3
4624	ISSSTY_v1a_7367_02May011_6211	5737-13-3	c12C(=O)c3c4c(ccc(c14)ccc2)ccc3	3
4625	ISSSTY_v1a_7367_02May011_6212	98090-89-2	HC(H)c1c2c3c4c(C(H)c3cc1)cccc4cc2	3
4626	ISSSTY_v1a_7367_02May011_6213	98096-09-4	HC(H)c1c2c3c(C(=O)c4c3c(ccc4)cc2)cc1	3
4627	ISSSTY_v1a_7367_02May011_6215	19246-18-5	HC(C(=O)O)NC(=O)[C@@](N)C(H)S	3
4628	ISSSTY_v1a_7367_02May011_6216	226-36-8	c12c(c3c(cc4c5c(ccc4n3)cccc5)cc1)cccc2	3
4629	ISSSTY_v1a_7367_02May011_6217	61203-01-8	HC(H)C(=O)C(Br)=CH	3
4630	ISSSTY_v1a_7367_02May011_6219	6325-54-8	HC(Cl)c1c2c(c3c(cccc3)cc2)cc2c1cccc2	3
4631	ISSSTY_v1a_7367_02May011_6220	5166-35-8	HC(H)C(C(Cl)C(H)H)=CH	3
4632	ISSSTY_v1a_7367_02May011_6222	19996-03-3	HC(Cl)c1c2c(c(Cl)c3c1cccc3)cccc2	3
4633	ISSSTY_v1a_7367_02May011_6223	25148-26-9	HC(H)c1c2c(c(C(H)Cl)c3c1cccc3)cccc2	3
4634	ISSSTY_v1a_7367_02May011_6225	113163-21-6	c12c(c3c([C@](O)[C@@](O)C=C3)cc1)nccc2	3
4635	ISSSTY_v1a_7367_02May011_6226	28622-66-4	c12c(c3c(C(O)C(O)C=C3)cc1)cccc2	3
4636	ISSSTY_v1a_7367_02May011_6230	113216-90-3	C1(O)C(=O)C2=C(C3=C4C(C=CC=13)=CC=CN4)O2	3
4637	ISSSTY_v1a_7367_02May011_6231	113163-22-7	c12c(c3c(C(O)C(O)C4C3O4)cc1)nccc2	3
4638	ISSSTY_v1a_7367_02May011_6234	119143-43-0	HC1c2c(c3c(cc2)nccc3)C2C(C1H)O2	3
4639	ISSSTY_v1a_7367_02May011_6237	113163-24-9	HC1c2c(c3c(ccn3)cc2)C2C(C1H)O2	3
4640	ISSSTY_v1a_7367_02May011_6242	112380-30-0	HC(H)C(H)C(H)C(H)N(C(C=O)=NO)N=O	3
4641	ISSSTY_v1a_7367_02May011_6243	38134-58-6	HC(C(=O)N[C@](C(=O)NC(H)C(=O)O)C(H)SC(=O)NC(H)C(H)Cl)C(H)[C@](N)C(=O)O	3
4642	ISSSTY_v1a_7367_02May011_6245	53330-03-3	HC(Cl)C(H)NC(=O)OC(=O)[C@@](N)C(H)S	3
4643	ISSSTY_v1a_7367_02May011_6248	689-98-5	HC(Cl)C(H)N	3
4644	ISSSTY_v1a_7367_02May011_6249	74339-99-4	c12c(c3c4c(c5c(c4c4c(cccc4)c3)ccc(O)c5)c1)cccc2	3
4645	ISSSTY_v1a_7367_02May011_6250	93285-74-6	HC1C2c3c4c(c5c(cc4c4c(cccc4)c3)cccc5)C=2C(H)C(H)C1H	3
4646	ISSSTY_v1a_7367_02May011_6251	15299-08-8	HC(H)c1cc2c(c3c4c(c5c(cc24)cccc5)cc2c3cccc2)cc1	3
4647	ISSSTY_v1a_7367_02May011_6252	60032-80-6	HC1c2c(c3c4c(c5c(cc4c4c3cccc4)cccc5)c2)C(H)C(H)C1H	3
4648	ISSSTY_v1a_7367_02May011_6253	138-89-6	HC(H)N(c1ccc(N=O)cc1)C(H)H	3
4649	ISSSTY_v1a_7367_02May011_6256	144730-01-8	HC1C(=O)c2c(c3c(c(C(F)(F)F)c2)c2c(cccc2)cc3)C1H	3
4650	ISSSTY_v1a_7367_02May011_6257	151109-62-5	HC1C(=O)c2c(c3c(c(C(F)(F)F)c2)c2c([C@](O)[C@@](O)C=C2)cc3)C1H	3
4651	ISSSTY_v1a_7367_02May011_6258	120-22-9	HC(H)C(H)N(c1ccc(N=O)cc1)C(H)C(H)H	3
4652	ISSSTY_v1a_7367_02May011_6262	531-82-8	HC(H)C(=O)NC1=NC(C2=CC=C(N(=O)=O)O2)=CS1	3
4653	ISSSTY_v1a_7367_02May011_6263	122-69-0	HC(C=Cc1cccc1)OC(=O)C=Cc1cccc1	3
4654	ISSSTY_v1a_7367_02May011_6264	86-57-7	c1(N(=O)=O)c2c(cccc2)ccc1	3
4655	ISSSTY_v1a_7367_02May011_6265	4437-51-8	HC(H)C(H)C(=O)C(=O)C(H)C(H)H	3
4656	ISSSTY_v1a_7367_02May011_6266	765-87-7	HC1C(=O)C(=O)C(H)C(H)C1H	3
4657	ISSSTY_v1a_7367_02May011_6271	100490-36-6	HC1C(H)C(N)C(H)N1c1c(F)cc2C(=O)C(C(=O)O)=CN(c3c(F)cc(F)cc3)c2n1	3
4658	ISSSTY_v1a_7367_02May011_6272	35282-68-9	HC(H)N(c1ccc(N=Nc2c(C(H)O)cccc2)cc1)C(H)H	3
4659	ISSSTY_v1a_7367_02May011_6277	6051-98-5	c12C(=O)c3c(c4c(cccc4)cc3)-c1cccc2	3
4660	ISSSTY_v1a_7367_02May011_6278	149996-82-7	HC(H)C(H)N(C=O)N=O	3
4661	ISSSTY_v1a_7367_02May011_6279	7417-67-6	HC(H)C(=O)N(C(H)H)N=O	3
4662	ISSSTY_v1a_7367_02May011_6280	67809-14-7	HC(H)N(C=O)N=O	3