

3,841	ISSSTY_v1a_7367_02May011_4934	2381-16-0	HC(H)c1cc2c(cc3c4c(ccc3c2)cccc4)cc1	3
3,842	ISSSTY_v1a_7367_02May011_4935	50618-02-5	HC(H)[C@]1[C@@](c2ccc(OC(H)H)cc2)O1	3
3,843	ISSSTY_v1a_7367_02May011_4936	6111-78-0	HC(H)c1c2c(cc3c(c4c(cccc4)cc3)c2)ccc1	3
3,844	ISSSTY_v1a_7367_02May011_4940	151378-32-4	c12C34c5c(c6c(cccc6)cc5)-c1cccc2C(O)C(O)C3O4	3
3,845	ISSSTY_v1a_7367_02May011_4941	151378-33-5	c12c3c(c4c(c5c(C(O)C(O)C6C5O6)cc4)c3ccc1)ccc2	3
3,846	ISSSTY_v1a_7367_02May011_4943	151378-34-6	c12c3c(c4c(c5c(C(O)C(O)C6C5O6)cc4)c3ccc1)ccc2	3
3,847	ISSSTY_v1a_7367_02May011_4945	80-40-0	HC(H)c1ccc(S(=O)(=O)OC(H)C(H)H)cc1	3
3,848	ISSSTY_v1a_7367_02May011_4948	159091-35-7	HC(C1=CC=C(C=O)O1)OS(=O)(=O)O	3
3,849	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
3,850	ISSSTY_v1a_7367_02May011_4951	39501-62-7	c1(Oc2cccc2)ccc(NO)cc1	3
3,851	ISSSTY_v1a_7367_02May011_4952	1147-55-3	HC(H)C(=O)Nc1cc2c(-c3c(O)cccc3C2H)cc1	3
3,852	ISSSTY_v1a_7367_02May011_4954	97606-15-0	C12C(C3C(C4C1N4)=CSC=3)=CSC=2	3
3,853	ISSSTY_v1a_7367_02May011_4955	23102-68-3	C12C(C3C(C4C1O4)=CSC=3)=CSC=2	3
3,854	ISSSTY_v1a_7367_02May011_4956	13345-23-8	c1(O)c2c3c4c(c5c(cc4ccc3cc1)cccc5)cc2	3
3,855	ISSSTY_v1a_7367_02May011_4957	57-57-8	HC1C(=O)OC1H	3
3,856	ISSSTY_v1a_7367_02May011_4958	78400-41-6	HC(H)c1c2c3c(c4c(-c5c(C6C4N6)cccc5)cc3cc1)C(H)C2H	3
3,857	ISSSTY_v1a_7367_02May011_4959	928-51-8	HC(Cl)C(H)C(H)C(H)O	3
3,858	ISSSTY_v1a_7367_02May011_4960	71382-49-5	c12-c3c(C4C(c1cc1c5c(ccc1c2)cccc5)N4)cccc3	3
3,859	ISSSTY_v1a_7367_02May011_4961	75-55-8	HC(H)C1C(H)N1	3
3,860	ISSSTY_v1a_7367_02May011_4963	103088-83-1	C1(=O)C(=O)c2c3c(c4c(cccc4)cc3)ccc2C=C1	3
3,861	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
3,862	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
3,863	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
3,864	ISSSTY_v1a_7367_02May011_4968	30269-02-4	c1(N)c2c3c4c(c(N(=O)=O)ccc4ccc3cc1)cc2	3
3,865	ISSSTY_v1a_7367_02May011_4969	20268-52-4	c12c(c(Cl)c3c(c4c(cccc4)cc3)c1)cccc2	3
3,866	ISSSTY_v1a_7367_02May011_4970	83504-80-7	c1(Sc2cccc2)ccc(N=O)cc1	3
3,867	ISSSTY_v1a_7367_02May011_4972	21229-99-2	c1(Sc2cccc2)ccc(NO)cc1	3
3,868	ISSSTY_v1a_7367_02May011_4973	590-96-5	HC(H)[N+](=O)[N-]C(H)O	3
3,869	ISSSTY_v1a_7367_02May011_4974	57011-48-0	HC(C(O)C(H)N=N_N)N=N_N	3
3,870	ISSSTY_v1a_7367_02May011_4975	709-49-9	c1(I)c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3

3,871	ISSSTY_v1a_7367_02May011_4985	25125-72-8	c1([C@]2[C@](c3ccccc3)N2)ccccc1	3
3,872	ISSSTY_v1a_7367_02May011_4986	3416-21-5	HC(H)c1c2c3c(c4c(-c5c(C6C4O6)ccccc5)cc3cc1)C(H)C2H	3
3,873	ISSSTY_v1a_7367_02May011_4988	1605-06-7	c1([C@]2[C@@](c3ccccc3)N2)ccccc1	3
3,874	ISSSTY_v1a_7367_02May011_4989	1919899	c12c3c(C4C(c3ccc1)N4)ccc2	3
3,875	ISSSTY_v1a_7367_02May011_4991	81851-68-5	HC(H)c1c2c(c3c(cccc3)c1)ccc1c2C2[C@]([C@](O)[C@@]1O)O2	3
3,876	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
3,877	ISSSTY_v1a_7367_02May011_4995	108670-78-6	HC(H)C(H)C=CC=CC=CC=COC(H)C(O)C(H)O	3
3,878	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
3,879	ISSSTY_v1a_7367_02May011_4998	1488-21-7	HC1C23C(C(H)C1H)(C=CC=C2)O3	3
3,880	ISSSTY_v1a_7367_02May011_5000	114451-08-0	HC(H)N1c2c(c3c(cc2)nccc3)N=C1N(=O)=O	3
3,881	ISSSTY_v1a_7367_02May011_5001	540-80-7	HC(H)C(C(H)H)(C(H)H)ON=O	3
3,882	ISSSTY_v1a_7367_02May011_5002	33611-88-0	c1([N+](=O)[O-])c([N+](=O)[O-])c2c3c(c4c2c(ccc4)c1)cccc3	3
3,883	ISSSTY_v1a_7367_02May011_5003	110419-21-1	c1([N+](=O)[O-])c2c3c(c4c(c3c([N+](=O)[O-])c1)cccc4)ccc2	3
3,884	ISSSTY_v1a_7367_02May011_5004	64810-99-7	c1(OS(=O)(=O)O)c2c3c4c(c5c(cc4ccc3cc1)cccc5)cc2	3
3,885	ISSSTY_v1a_7367_02May011_5006	151751-83-6	HC(H)C(H)OC(=O)N(C(H)C(H)C=O)N=O	3
3,886	ISSSTY_v1a_7367_02May011_5007	90-15-3	c1(O)c2c(cccc2)ccc1	3
3,887	ISSSTY_v1a_7367_02May011_5008	71432-00-3	C1(=O)c2c3c(c4c(cccc4)c2)ccc2c3c(ccc2)O1	3
3,888	ISSSTY_v1a_7367_02May011_5010	112309-62-3	C(=O)(O)C=C(C(Cl)Cl)C(Cl)Cl	3
3,889	ISSSTY_v1a_7367_02May011_5011	203-33-8	c12c(c3c4c(c5c3c(ccc5)c1)cccc4)cccc2	3
3,890	ISSSTY_v1a_7367_02May011_5013	215226-70-3	HC(Cl)C(=C(Cl)C(=O)O)C=O	3
3,891	ISSSTY_v1a_7367_02May011_5014	64188-64-3	HC(c1ccccc1)N1C2c3c(-c4c(cccc4)C12)cccc3	3
3,892	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)Cl)C(H)C(H)Cl)cc2)N4)N3)C(H)C1H	3
3,893	ISSSTY_v1a_7367_02May011_5021	166546-22-1	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)Cl)C(H)C(H)Cl)cc2)N4)N3)C(H)C1H	3
3,894	ISSSTY_v1a_7367_02May011_5023	1672-88-4	HC1C(=O)NC(=O)N1N=CC=CC1=CC=C(N(=O)=O)O1	3
3,895	ISSSTY_v1a_7367_02May011_5028	8001-35-2	HC(Cl)C1(C(H)Cl)C(=CH)C2(Cl)C(Cl)(Cl)C1(Cl)C(Cl)C2Cl	3
3,896	ISSSTY_v1a_7367_02May011_5030	771-29-9	HC1c2c(C(OO)C(H)C1H)cccc2	3
3,897	ISSSTY_v1a_7367_02May011_5031	75-21-8	HC1C(H)O1	3
3,898	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
3,899	ISSSTY_v1a_7367_02May011_5035	5496-41-3	HC(H)Oc1c(OC(H)H)cc(C2=NC(c3ccccc3)=C(c3ccccc3)N2)cc1	3
3,900	ISSSTY_v1a_7367_02May011_5037	2687-25-4	HC(H)c1c(N)c(N)ccc1	3

3,901	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
3,902	ISSSTY_v1a_7367_02May011_5041	2125597	O=S(Cl)Cl	3
3,903	ISSSTY_v1a_7367_02May011_5043	101688-02-2	HC(Cl)C(H)N(c1cc2c(c3c(cc2)OC(N(=O)=O)=C3)cc1)C(H)C(H)Cl	3
3,904	ISSSTY_v1a_7367_02May011_5044	116505-02-3	HC(H)C(=O)N(c1ccc(Sc2ccccc2)cc1)OC(=O)C(H)H	3
3,905	ISSSTY_v1a_7367_02May011_5045	843-23-2	HC(H)C(=O)N(O)c1ccc(C=Cc2ccccc2)cc1	3
3,906	ISSSTY_v1a_7367_02May011_5046	16110-13-7	HC(O)c1c2c(c3c(cccc3)cc2)cc2c1cccc2	3
3,907	ISSSTY_v1a_7367_02May011_5049	78246-54-5	HC(O)c1ccc([N+]_N)cc1	3
3,908	ISSSTY_v1a_7367_02May011_5051	68006-83-7	HC(H)c1c(N)nc2c(-c3c(cccc3)N2)c1	3
3,909	ISSSTY_v1a_7367_02May011_5053	138331-98-3	HC([C@]1[C@@](O)[C@](O)[C@@](O)[C@@](O)O1)N=N_N	3
3,910	ISSSTY_v1a_7367_02May011_5054	120202-54-2	HC([C@]1[C@@](O)[C@](O)[C@@](O)[C@@](O)O1)N=N_N	3
3,911	ISSSTY_v1a_7367_02May011_5055	138331-99-4	HC([C@]1[C@@](O)[C@@](O)[C@](O)[C@@](O)O1)N=N_N	3
3,912	ISSSTY_v1a_7367_02May011_5056	138332-01-1	HC([C@]1[C@@](O)[C@@](O)[C@@](O)[C@@](O)O1)N=N_N	3
3,913	ISSSTY_v1a_7367_02May011_5057	138332-00-0	HC([C@@]1[C@@](O)[C@](O)[C@@](O)[C@@](O)O1)N=N_N	3
3,914	ISSSTY_v1a_7367_02May011_5058	73174-38-6	HC([C@]1[C@](O)[C@](O)[C@@](O)[C@@](O)O1)N=N_N	3
3,915	ISSSTY_v1a_7367_02May011_5059	138245-73-5	HC([C@@](O)[C@](O)[C@](O)[C@@](O)C(=O)O)N=N_N	3
3,916	ISSSTY_v1a_7367_02May011_5060	98736-45-9	HC(H)N(C(H)c1cc(OC(H)H)ccc1)N=O	3
3,917	ISSSTY_v1a_7367_02May011_5061	62783-49-7	HC(H)c1cc(C(H)N(C(H)H)N=O)ccc1	3
3,918	ISSSTY_v1a_7367_02May011_5062	98736-46-0	HC(H)N(C(H)c1cc(Cl)ccc1)N=O	3
3,919	ISSSTY_v1a_7367_02May011_5063	98736-47-1	HC(H)N(C(H)c1cc(Br)ccc1)N=O	3
3,920	ISSSTY_v1a_7367_02May011_5064	98736-48-2	HC(H)N(C(H)c1cc(C(F)(F)F)ccc1)N=O	3
3,921	ISSSTY_v1a_7367_02May011_5065	98736-49-3	HC(H)N(C(H)c1cc(C_N)ccc1)N=O	3
3,922	ISSSTY_v1a_7367_02May011_5068	84174-21-0	HC(H)N(C(H)c1ccc(F)cc1)N=O	3
3,923	ISSSTY_v1a_7367_02May011_5069	84174-22-1	HC(H)N(C(H)c1ccc(Cl)cc1)N=O	3
3,924	ISSSTY_v1a_7367_02May011_5070	98736-50-6	HC(H)N(C(H)c1ccc(Br)cc1)N=O	3
3,925	ISSSTY_v1a_7367_02May011_5071	84174-23-2	HC(H)N(C(H)c1ccc(C_N)cc1)N=O	3
3,926	ISSSTY_v1a_7367_02May011_5072	84174-24-3	HC(H)N(C(H)c1ccc(N(=O)=O)cc1)N=O	3
3,927	ISSSTY_v1a_7367_02May011_5077	10517-47-2	HC(H)C(=O)c1ccc(NO)cc1	3
3,928	ISSSTY_v1a_7367_02May011_5079	69245-38-1	HC(H)C([C@](O)(O)C(H)2c(O)c3C(=O)c4c(C(=O)c3c(O)c2C(OC2C(H)C(N3C(H)C(H)OC(H)C3C_N)C(O)C(C(H)H)O2)C1H)c(OC(H)H)ccc4	3
3,929	ISSSTY_v1a_7367_02May011_5080	94730-47-9	HC(H)C(=O)C1(O)C(H)c2c(O)c3C(=O)c4c(C(=O)c3c(O)c2C(OC2C(H)C(N3C(H)C(H)OC(H)C3C_N)C(O)C(C(H)H)O2)C1H)c(OC(H)H)ccc4	3
3,930	ISSSTY_v1a_7367_02May011_5083	28860-95-9	HC(H)[C@@](C(=O)O)(C(H)c1cc(O)c(O)cc1)NN	3

3,931	ISSSTY_v1a_7367_02May011_5086	92887-88-2	HC(H)N(c1ccc(N=Nc2cc3c(cc2)N=CS3)cc1)C(H)C(H)C_N	3
3,932	ISSSTY_v1a_7367_02May011_5088	20983-67-9	c1(Nc2ccc(Cl)cc2)ccc(N(=O)=O)cc1	3
3,933	ISSSTY_v1a_7367_02May011_5093	2950-43-8	NOS(=O)(=O)O	3
3,934	ISSSTY_v1a_7367_02May011_5095	103395-25-1	HC(Cl)c1c2c3c(c4c2c(ccc4)cc1)cccc3	3
3,935	ISSSTY_v1a_7367_02May011_5097	103393-70-0	HC(Cl)c1cc2c3c(c4c(c3ccc2)cccc4)c1	3
3,936	ISSSTY_v1a_7367_02May011_5099	957-52-8	HC(Cl)c1c2c3c(c4c(c3ccc2)cccc4)cc1	3
3,937	ISSSTY_v1a_7367_02May011_5101	103393-71-1	HC(Cl)c1c2c(c3c4c(cccc24)ccc3)ccc1	3
3,938	ISSSTY_v1a_7367_02May011_5103	103393-72-2	HC(Cl)c1cc2c(c3c4c(cccc24)ccc3)cc1	3
3,939	ISSSTY_v1a_7367_02May011_5104	135295-00-0	HC(O)c1cc2c(c3c4c(cccc24)ccc3)cc1	3
3,940	ISSSTY_v1a_7367_02May011_5106	142741-10-4	HC(H)c1c2c(-c3c(c([N+](=O)[O-])cc([N+](=O)[O-])c3)N2)cc(N(=O)=O)n1	3
3,941	ISSSTY_v1a_7367_02May011_5109	6375-16-2	HC(H)c1c(N)cc(NC(=O)C(H)H)cc1	3
3,942	ISSSTY_v1a_7367_02May011_5111	592-62-1	HC(H)C(=O)OC(H)[N-][N+](=O)C(H)H	3
3,943	ISSSTY_v1a_7367_02May011_5112	1622-62-4	HC(H)N1c2c(C(c3c(F)cccc3)=NC(H)C1=O)cc(N(=O)=O)cc2	3
3,944	ISSSTY_v1a_7367_02May011_5113	2278-22-0	HC(H)C(=O)OON(=O)=O	3
3,945	ISSSTY_v1a_7367_02May011_5115	20324-66-7	HC(H)c1cc2C(=O)c3c(C(=O)c2c(O)c1)c(O)cc(O)c3O	3
3,946	ISSSTY_v1a_7367_02May011_5117	133831-60-4	c1(SSC(Cl)=C(Cl)Cl)c(N(=O)=O)cccc1	3
3,947	ISSSTY_v1a_7367_02May011_5119	133831-62-6	C(F)(F)(F)C(Cl)=C(Cl)SSc1c(N(=O)=O)cccc1	3
3,948	ISSSTY_v1a_7367_02May011_5120	133831-61-5	c1(SSC(F)=C(Cl)Cl)c(N(=O)=O)cccc1	3
3,949	ISSSTY_v1a_7367_02May011_5121	6098-45-9	HC(H)C(=O)N(c1cc2c(-c3c(cccc3)C2H)cc1)OC(=O)c1cccc1	3
3,950	ISSSTY_v1a_7367_02May011_5122	136861-00-2	c1(-c2c([N+](=O)[O-])cc(N)cc2[N+](=O)[O-])cccc1	3
3,951	ISSSTY_v1a_7367_02May011_5123	136861-01-3	c1(-c2c(N)cc(N)cc2N(=O)=O)cccc1	3
3,952	ISSSTY_v1a_7367_02May011_5124	5855-71-0	c1(-c2c([N+](=O)[O-])cc(N)cc2)c([N+](=O)[O-])cc(N)cc1	3
3,953	ISSSTY_v1a_7367_02May011_5125	133561-39-4	c1(-c2c(N)cc([N+](=O)[O-])cc2)c([N+](=O)[O-])cc(N)cc1	3
3,954	ISSSTY_v1a_7367_02May011_5127	98151-91-8	c1(N(=O)=O)c2c3c4c(c5c(C=C[C@](O)[C@@]5O)cc4cc2)ccc3cc1	3
3,955	ISSSTY_v1a_7367_02May011_5128	6098-46-0	HC(H)N(c1ccc(N=Nc2cccc2)cc1)OC(=O)c1cccc1	3
3,956	ISSSTY_v1a_7367_02May011_5129	97576-08-4	c1(N(=O)=O)c2c3c4c(c5c([C@](O)[C@@](O)C=C5)cc4cc2)ccc3cc1	3
3,957	ISSSTY_v1a_7367_02May011_5135	154-93-8	HC(Cl)C(H)N(C(=O)NC(H)C(H)Cl)N=O	3
3,958	ISSSTY_v1a_7367_02May011_5137	3096-63-7	HC(H)c1c(NO)c(C(H)H)ccc1	3
3,959	ISSSTY_v1a_7367_02May011_5138	3096-64-8	HC(H)c1c(NO)cc(C(H)H)cc1	3
3,960	ISSSTY_v1a_7367_02May011_5139	43192-07-0	HC(H)c1c(C(H)H)cc(NO)cc1	3

3,961	ISSSTY_v1a_7367_02May011_5140	42471-28-3	HC(H)c1nc(N)c(C(H)NC(=O)N(C(H)C(H)Cl)N=O)cn1	3
3,962	ISSSTY_v1a_7367_02May011_5141	3096-62-6	HC(H)c1c(C(H)H)c(NO)ccc1	3
3,963	ISSSTY_v1a_7367_02May011_5142	70853-94-0	HC(H)c1c(NO)ccc(C(H)H)c1	3
3,964	ISSSTY_v1a_7367_02May011_5146	115664-51-2	c1(O)c2c3c(c4c5c(ccc(c25)cc1)ccc4N(=O)=O)cccc3	3
3,965	ISSSTY_v1a_7367_02May011_5151	5221-17-0	HC(Br)C(Br)C=O	3
3,966	ISSSTY_v1a_7367_02May011_5154	33372-39-3	HC(O)C(H)N(c1c2c(cccc2)nc(C2=CC=C(N(=O)=O)S2)n1)C(H)C(H)O	3
3,967	ISSSTY_v1a_7367_02May011_5155	107-04-0	HC(Br)C(H)Cl	3
3,968	ISSSTY_v1a_7367_02May011_5157	298-18-0	HC1C(C2C(H)O2)O1	3
3,969	ISSSTY_v1a_7367_02May011_5158	96563-06-3	HC(H)c1c(C(H)H)cc2-c3c(C(C(H)H)c2c1)cccc3	3
3,970	ISSSTY_v1a_7367_02May011_5160	95791-46-1	c1(Cl)c2c(c3c(c4c(cccc4)cc3)c1)cccc2	3
3,971	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
3,972	ISSSTY_v1a_7367_02May011_5162	34244-14-9	c12c3c4c(c(Cl)ccc4ccc3ccc1)cc2	3
3,973	ISSSTY_v1a_7367_02May011_5163	716-53-0	c12c(c(Cl)c3c(cccc3)c1)cccc2	3
3,974	ISSSTY_v1a_7367_02May011_5164	42978-43-8	HC(H)C(=O)OC(H)c1c2c(c3c4c5c(ccc14)cccc5cc3)cccc2	3
3,975	ISSSTY_v1a_7367_02May011_5165	105708-73-4	HC(H)C(=O)OC(H)c1c2c3c4c5c6c(cc4ccc3ccc2)cccc6ccc15	3
3,976	ISSSTY_v1a_7367_02May011_5166	49852-85-9	HC(Br)c1c2c(c3c4c5c(ccc14)cccc5cc3)cccc2	3
3,977	ISSSTY_v1a_7367_02May011_5167	105708-74-5	HC(Br)c1c2c3c4c5c6c(cc4ccc3ccc2)cccc6ccc15	3
3,978	ISSSTY_v1a_7367_02May011_5168	2564-64-9	HC(H)c1c2c(c(C(H)OC(=O)C(H)H)c3c4c(ccc13)cccc4)cccc2	3
3,979	ISSSTY_v1a_7367_02May011_5170	17526-33-9	HC(H)C(=O)OC(H)c1c2c3c(ccc2cc2c1cccc2)cccc3	3
3,980	ISSSTY_v1a_7367_02May011_5171	16430-32-3	HC(H)C(=O)OC(H)c1c2c(cc3c1cccc3)cccc2	3
3,981	ISSSTY_v1a_7367_02May011_5173	31688-71-8	HC(H)c1c2c(c(C(H)OC(=O)C(H)H)c3c1cccc3)cccc2	3
3,982	ISSSTY_v1a_7367_02May011_5174	24961-39-5	HC(Br)c1c2c(c3c(cccc3)cc2)cc2c1cccc2	3
3,983	ISSSTY_v1a_7367_02May011_5175	2517-98-8	HC(H)c1c2c(c(C(H)OC(=O)C(H)H)c3c1c1c(cccc1)cc3)cccc2	3
3,984	ISSSTY_v1a_7367_02May011_5176	17526-24-8	HC(H)C(=O)OC(H)c1c2c(c3c(cccc3)cc2)cc2c1cccc2	3
3,985	ISSSTY_v1a_7367_02May011_5177	78533-30-9	HC(Br)c1c2c3c(ccc2cc2c1cccc2)cccc3	3
3,986	ISSSTY_v1a_7367_02May011_5178	34331-95-8	HC(H)c1c2c(c(C(H)Br)c3c1cccc3)cccc2	3
3,987	ISSSTY_v1a_7367_02May011_5179	59230-81-8	HC(H)c1c2c(c(C(H)Br)c3c4c(ccc13)cccc4)cccc2	3
3,988	ISSSTY_v1a_7367_02May011_5180	105708-67-6	HC(H)C(=O)OC1c2c3c4c5c(cc3C1H)cccc5ccc4cc2	3
3,989	ISSSTY_v1a_7367_02May011_5181	7319-59-7	HC(H)c1c2c3c(c4c(c5c(cccc5)cc4)cc3cc1)C(OC(=O)C(H)H)C2H	3
3,990	ISSSTY_v1a_7367_02May011_5182	105708-68-7	HC(H)C(=O)OC1c2c3c4c5c(ccc4ccc3C1H)cccc5c2	3

3,991	ISSSTY_v1a_7367_02May011_5183	7390-93-4	HC(H)c1c2c3c(c4c(c5c(cccc5)cc4)cc3cc1)C(H)C2OC(=O)C(H)H	3
3,992	ISSSTY_v1a_7367_02May011_5184	16169-17-8	c1(-c2c(NO)cccc2)cccc1	3
3,993	ISSSTY_v1a_7367_02May011_5185	115453-72-0	HC([C@](N)C(=O)O)SC(Cl)=C(Cl)C(Cl)(Cl)Cl	3
3,994	ISSSTY_v1a_7367_02May011_5187	21711-71-7	c1(-c2c(N=O)cccc2)cccc1	3
3,995	ISSSTY_v1a_7367_02May011_5188	105361-86-2	c1(-c2cc(N=O)ccc2)cccc1	3
3,996	ISSSTY_v1a_7367_02May011_5192	6341-85-1	HC(H)C1(C2C(H)O2)C(H)O1	3
3,997	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
3,998	ISSSTY_v1a_7367_02May011_5195	3198-41-2	HC1c2c(C(H)C(H)C1H)cc1c(c(N)ccc1)n2	3
3,999	ISSSTY_v1a_7367_02May011_5196	13109-99-4	HC1C(=O)N(C2=NC=C(N(=O)=O)S2)C(H)C1H	3
4,000	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
4,001	ISSSTY_v1a_7367_02May011_5199	120812-48-8	c1([N+](=O)[O-])c2c3c(c4c(c5c([N+](=O)[O-])ccc(c35)cc2)cccc4)cc1	3
4,002	ISSSTY_v1a_7367_02May011_5200	3311-98-6	HC(Cl)C(H)NC(=O)NC1=NC=C(N(=O)=O)S1	3
4,003	ISSSTY_v1a_7367_02May011_5201	10560-74-4	HC(H)C1C(H)NC(=O)N1C1=NC=C(N(=O)=O)S1	3
4,004	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
4,005	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
4,006	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
4,007	ISSSTY_v1a_7367_02May011_5207	120812-46-6	HC1c2c(c3c4c5c(ccc(N(=O)=O)c25)ccc4ccc3)C(H)C(H)C1H	3
4,008	ISSSTY_v1a_7367_02May011_5208	57-92-1	HC(H)[C@@]1[C@@](O)(C=O)[C@@]2[C@@](NC(H)H)[C@@](O)[C@@]3[C@@](O)C2[C@@]2[C@@](O)[C@@]4[C@@](N=C(N)N)[C@@](O)[C@@]2N=C(N)N)O1	3
4,009	ISSSTY_v1a_7367_02May011_5210	6558-78-7	HC(H)C(H)C(H)C(H)N(C(=O)OC(H)C(H)H)N=O	3
4,010	ISSSTY_v1a_7367_02May011_5212	111712-45-9	HC(H)C(C(Br)C(H)Br)OP(=O)(OC(C(H)H)C(Br)C(H)Br)OC(C(H)H)C(Br)C(H)Br	3
4,011	ISSSTY_v1a_7367_02May011_5213	60102-37-6	HC(H)C1(O)C(=O)OC(H)C2C(=O)C(C(H)C(H)N(C(H)H)C(H)C=2)OC(=O)C2(C(H)C1C(H)H)C(C(H)H)O2	3
4,012	ISSSTY_v1a_7367_02May011_5214	33979-15-6	HC(H)[C@@]1(OC(=O)C(H)H)C(=O)OC(H)C2C3([O-])[C@](C(H)C(H)[N+](3(C(H)H)C(H)C=2)OC(=O)C(C=CH)=C[C@]1C(H)H	3
4,013	ISSSTY_v1a_7367_02May011_5216	60872-63-1	HC(H)[C@@]1(OC(=O)C(H)H)C(=O)OC(H)C2C(=O)[C@](C(H)C(H)N(C(H)H)C(H)C=2)OC(=O)C(=CC(H)H)C(H)[C@@]1C(H)H	3
4,014	ISSSTY_v1a_7367_02May011_5219	91575-28-9	HC(H)C(=O)Nc1c(Cl)cc(C(H)c2cc(Cl)c(N)cc2)cc1	3
4,015	ISSSTY_v1a_7367_02May011_5220	111712-47-1	HC(H)C(Br)C(Br)C(H)OP(=O)(OC(H)C(Br)C(Br)C(H)H)OC(H)C(Br)C(Br)C(H)H	3
4,016	ISSSTY_v1a_7367_02May011_5223	166664-83-1	HC(H)N1c2c(N=C1N)nc1c(cccn1)c2	3
4,017	ISSSTY_v1a_7367_02May011_5224	111712-50-6	HC(H)C(Br)C(Br)C(H)Cl	3
4,018	ISSSTY_v1a_7367_02May011_5227	87261-28-7	c12c(c(N(=O)=O)c3c(c4c([C@@](O)[C@](O)C=C4)cc3)c1)cccc2	3
4,019	ISSSTY_v1a_7367_02May011_5229	97166-13-7	HC(H)C(Cl)C(Br)C(H)Br	3
4,020	ISSSTY_v1a_7367_02May011_5230	87259-00-5	c12c(c3c(c(N(=O)=O)c4c(C=C[C@@](O)[C@]4O)c3)cc1)cccc2	3

4,021	ISSSTY_v1a_7367_02May011_5233	64625-66-7	HC(H)c1c2c(c3c(C(O)C(O)[C@]4[C@@]3O4)cc2)cc2c1cccc2	3
4,022	ISSSTY_v1a_7367_02May011_5234	120693-41-6	HC(H)C(H)c1c2c(c3c([C@](O)[C@@](O)[C@@]4[C@@]3O4)cc2)cc2c1cccc2	3
4,023	ISSSTY_v1a_7367_02May011_5235	21919-05-1	HC1C(H)N1c1c([N+](=O)[O-])cc([N+](=O)[O-])c(C(N)=O)c1	3
4,024	ISSSTY_v1a_7367_02May011_5236	13417-43-1	HC(H)C(C(H)Cl)=CC(H)H	3
4,025	ISSSTY_v1a_7367_02May011_5237	119943-51-0	HC(H)C(H)C(C(H)H)OS(=O)(=O)C(H)H	3
4,026	ISSSTY_v1a_7367_02May011_5238	66194-68-1	HC(H)C(H)[C@](C(H)H)OS(=O)(=O)C(H)H	3
4,027	ISSSTY_v1a_7367_02May011_5239	50599-13-8	HC(H)C(H)[C@@](C(H)H)OS(=O)(=O)C(H)H	3
4,028	ISSSTY_v1a_7367_02May011_5240	13345-62-5	HC(H)c1c2c(c(C(H)Cl)c3c1c1c(cccc1)cc3)cccc2	3
4,029	ISSSTY_v1a_7367_02May011_5242	191-30-0	c12c3c(c4c(c5c6c(cc(c35)cc1)cccc6)cccc4)ccc2	3
4,030	ISSSTY_v1a_7367_02May011_5243	75-29-6	HC(H)C(Cl)C(H)H	3
4,031	ISSSTY_v1a_7367_02May011_5244	91379-15-6	HC(H)C(H)C(H)C(H)C=CC=CC=CC=CC=CCOC(H)[C@@](O)C(H)O	3
4,032	ISSSTY_v1a_7367_02May011_5245	78-89-7	HC(H)C(Cl)C(H)O	3
4,033	ISSSTY_v1a_7367_02May011_5246	19770-52-6	c12c(c3c4c(c5c(cc4c1)cccc5)C=C3)cccc2	3
4,034	ISSSTY_v1a_7367_02May011_5247	1791337	HC(H)OC(=O)N=NC=C1C=[N+](O-)]c2c(cccc2)N1O	3
4,035	ISSSTY_v1a_7367_02May011_5248	119631-01-5	HC(H)c1c(N)c2c(cc1)nc1c(cc(N)c(C(H)H)c1)n2	3
4,036	ISSSTY_v1a_7367_02May011_5249	6270-13-9	HC(O)C(H)N(c1cc2c(cccc2)cc1)C(H)C(H)O	3
4,037	ISSSTY_v1a_7367_02May011_5250	192-65-4	c12c(c3c4c(c5c(c6c4c(ccc6)cc3)cccc5)c1)cccc2	3
4,038	ISSSTY_v1a_7367_02May011_5251	2876-24-6	c12c(c(N(=O)=O)ccc1)nc1c(cccc1)n2	3
4,039	ISSSTY_v1a_7367_02May011_5252	3442-62-4	c12c(cc(N(=O)=O)cc1)nc1c(cccc1)n2	3
4,040	ISSSTY_v1a_7367_02May011_5254	105836-99-5	c1([N+](=O)[O-])c2c(ccc1)nc1c(ccc([N+](=O)[O-])c1)n2	3
4,041	ISSSTY_v1a_7367_02May011_5255	58718-48-2	c1([N+](=O)[O-])c2c(ccc1)nc1c(c([N+](=O)[O-])ccc1)n2	3
4,042	ISSSTY_v1a_7367_02May011_5256	72848-48-7	c12c(cc([N+](=O)[O-])cc1)nc1c(cc([N+](=O)[O-])cc1)n2	3
4,043	ISSSTY_v1a_7367_02May011_5257	105837-00-1	c12c(cc([N+](=O)[O-])cc1)nc1c(ccc([N+](=O)[O-])c1)n2	3
4,044	ISSSTY_v1a_7367_02May011_5258	2876-22-4	c1(N)c2c(ccc1)nc1c(cccc1)n2	3
4,045	ISSSTY_v1a_7367_02May011_5259	2876-23-5	c12c(cc(N)cc1)nc1c(cccc1)n2	3
4,046	ISSSTY_v1a_7367_02May011_5260	16582-03-9	c1(N)c2c(ccc1)nc1c(N)cccc1n2	3
4,047	ISSSTY_v1a_7367_02May011_5261	28124-29-0	c1(N)c2c(ccc1)nc1c(ccc(N)c1)n2	3
4,048	ISSSTY_v1a_7367_02May011_5263	7704-40-7	c12c(cc(N)cc1)nc1c(ccc(N)c1)n2	3
4,049	ISSSTY_v1a_7367_02May011_5264	619-17-0	C(=O)(O)c1c(N)cc(N(=O)=O)cc1	3
4,050	ISSSTY_v1a_7367_02May011_5265	60784-46-5	HC(Cl)C(H)N(C(=O)NC(H)C(H)O)N=O	3

4,051	ISSSTY_v1a_7367_02May011_5266	65267-04-1	HC(C(N)=O)NC(=O)N(C(H)C(H)Cl)N=O	3
4,052	ISSSTY_v1a_7367_02May011_5267	76014-81-8	HC(H)N(C(H)C(H)C(H)C(O)c1cccnc1)N=O	3
4,053	ISSSTY_v1a_7367_02May011_5268	5385-75-1	c12c(c3c4c(c5c(c4c4c(cccc4)c3)cccc5)c1)cccc2	3
4,054	ISSSTY_v1a_7367_02May011_5269	74340-04-8	c12c(c3c4c(c5c(c4c4c(cccc4)c3)cccc5)c1)C=C[C@](O)[C@@]2O	3
4,055	ISSSTY_v1a_7367_02May011_5270	74339-98-3	c12c(c3c4c(c5c(c4c4c([C@](O)[C@@](O)C=C4)c3)cccc5)c1)cccc2	3
4,056	ISSSTY_v1a_7367_02May011_5273	5422-34-4	HC(H)C(O)C(=O)NC(H)C(H)O	3
4,057	ISSSTY_v1a_7367_02May011_5274	17309-86-3	HC(H)N(c1ccc(N=Nc2cc3c(cc2)NN=C3)cc1)C(H)H	3
4,058	ISSSTY_v1a_7367_02May011_5278	93673-32-6	HC1c2c(C3=C4C(=C5C=C6C(=C1C35)C=CC=C6)O4)cccc2	3
4,059	ISSSTY_v1a_7367_02May011_5279	93673-31-5	HC1c2c(C3=C4C(=C5C=CC=C1C35)O4)ccc1c2cccc1	3
4,060	ISSSTY_v1a_7367_02May011_5280	93673-34-8	HC1c2c(C3C4C(=C5C(C1=4)O5)C=CC=3)cc1c(cccc1)c2	3
4,061	ISSSTY_v1a_7367_02May011_5281	51-75-2	HC(H)N(C(H)C(H)Cl)C(H)C(H)Cl	3
4,062	ISSSTY_v1a_7367_02May011_5283	126-85-2	HC(H)[N+](=[O-])(C(H)C(H)Cl)C(H)C(H)Cl	3
4,063	ISSSTY_v1a_7367_02May011_5285	1197-55-3	HC(c1ccc(N)cc1)C(=O)O	3
4,064	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
4,065	ISSSTY_v1a_7367_02May011_5287	149573-80-8	HC(C1=CN(N=O)C=N1)C(=O)NO	3
4,066	ISSSTY_v1a_7367_02May011_5290	3029-19-4	c12c3c4c(c(C=O)ccc4ccc3ccc1)cc2	3
4,067	ISSSTY_v1a_7367_02May011_5299	428856	c12C(=O)c3c(-c1cc1c(cccc1)c2)cccc3	3
4,068	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
4,069	ISSSTY_v1a_7367_02May011_5306	93673-39-3	c1(O)c2c(c3c(c4c5c(C=C4)cccc5c3)cc2)ccc1	3
4,070	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
4,071	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
4,072	ISSSTY_v1a_7367_02May011_5313	26651-23-0	c12c3c4c(c(S(=O)(=O)O)ccc4ccc3ccc1)cc2	3
4,073	ISSSTY_v1a_7367_02May011_5314	81424-67-1	HC(H)C(=O)N(C(=O)NC(H)H)OC(=O)NC(H)H	3
4,074	ISSSTY_v1a_7367_02May011_5316	4543-63-9	HC(H)N(C(=O)NC(H)H)C(=O)ON	3
4,075	ISSSTY_v1a_7367_02May011_5320	104145-44-0	HC(H)OC(=O)c1cc2-c3c(cccc3)Nc2c(-c2ccc3C(=O)C=CC(=O)c3n2)n1	3
4,076	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
4,077	ISSSTY_v1a_7367_02May011_5325	4081-23-6	HC1c2c(cccc2)OP(=O)(Oc2cccc2)O1	3
4,078	ISSSTY_v1a_7367_02May011_5326	3571-31-1	HC(H)c1cc(O)c2C(=O)c3c(C(H)c2c1)cc(OC(H)H)cc3O	3
4,079	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
4,080	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

4,081	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
4,082	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
4,083	ISSSTY_v1a_7367_02May011_5334	30461-65-5	c12C(=O)c3c(c4c(cc3O)O[C@@]3[C@]4C=CO3)Oc1cccc2O	3
4,084	ISSSTY_v1a_7367_02May011_5335	111901-39-4	HC(H)c1c2c(c3c(cccc3)c1)ccc1c2[C@]2[C@@]([C@@](O)[C@]1O)O2	3
4,085	ISSSTY_v1a_7367_02May011_5338	58086-32-1	HC(H)C(=O)Oc1c2C(=O)c3c(c4c(cc3OC(H)H)OC3C4C=CO3)Oc2ccc1	3
4,086	ISSSTY_v1a_7367_02May011_5339	36050-09-6	C(N)(=O)C1C=C(N(=O)=O)SC=1	3
4,087	ISSSTY_v1a_7367_02May011_5340	146795-48-4	HC(H)N(C(=O)C1C=C(N(=O)=O)SC=1)c1cccc1	3
4,088	ISSSTY_v1a_7367_02May011_5341	146795-44-0	C(=O)(C1C=C([N+](=O)[O-])SC=1)Nc1ccc([N+](=O)[O-])cc1	3
4,089	ISSSTY_v1a_7367_02May011_5342	146795-38-2	C(=O)(C1C=C(N(=O)=O)SC=1)Nc1ccc(Cl)cc1	3
4,090	ISSSTY_v1a_7367_02May011_5343	146795-41-7	C(=O)(C1C=C(N(=O)=O)SC=1)Nc1ccc(Br)cc1	3
4,091	ISSSTY_v1a_7367_02May011_5344	146795-35-9	C(=O)(C1C=C(N(=O)=O)SC=1)Nc1ccc(F)cc1	3
4,092	ISSSTY_v1a_7367_02May011_5345	146818-20-4	HC(H)C(H)c1ccc(NC(=O)C2C=C(N(=O)=O)SC=2)cc1	3
4,093	ISSSTY_v1a_7367_02May011_5346	146795-29-1	HC(H)c1ccc(NC(=O)C2C=C(N(=O)=O)SC=2)cc1	3
4,094	ISSSTY_v1a_7367_02May011_5347	146795-26-8	HC(H)Oc1ccc(NC(=O)C2C=C(N(=O)=O)SC=2)cc1	3
4,095	ISSSTY_v1a_7367_02May011_5348	122089-49-0	HC(H)c1c2c(c3c(C(O)C(O)C4C3O4)cc2)c(C(H)H)cc1	3
4,096	ISSSTY_v1a_7367_02May011_5349	146795-45-1	C(=O)(C1C=C([N+](=O)[O-])SC=1)Nc1cc([N+](=O)[O-])ccc1	3
4,097	ISSSTY_v1a_7367_02May011_5350	146795-39-3	C(=O)(C1C=C(N(=O)=O)SC=1)Nc1cc(Cl)ccc1	3
4,098	ISSSTY_v1a_7367_02May011_5351	122033-85-6	HC(H)c1c2c(c3c(C(O)C(O)C4C3O4)cc2)c(C(H)H)cc1	3
4,099	ISSSTY_v1a_7367_02May011_5352	146795-42-8	C(=O)(C1C=C(N(=O)=O)SC=1)Nc1cc(Br)ccc1	3
4,100	ISSSTY_v1a_7367_02May011_5353	146795-36-0	C(=O)(C1C=C(N(=O)=O)SC=1)Nc1cc(F)ccc1	3
4,101	ISSSTY_v1a_7367_02May011_5354	146795-32-6	HC(H)C(H)c1cc(NC(=O)C2C=C(N(=O)=O)SC=2)ccc1	3
4,102	ISSSTY_v1a_7367_02May011_5355	146795-30-4	HC(H)c1cc(NC(=O)C2C=C(N(=O)=O)SC=2)ccc1	3
4,103	ISSSTY_v1a_7367_02May011_5356	146795-27-9	HC(H)Oc1cc(NC(=O)C2C=C(N(=O)=O)SC=2)ccc1	3
4,104	ISSSTY_v1a_7367_02May011_5357	146795-46-2	C(=O)(C1C=C([N+](=O)[O-])SC=1)Nc1c([N+](=O)[O-])cccc1	3
4,105	ISSSTY_v1a_7367_02May011_5359	146795-40-6	C(=O)(C1C=C(N(=O)=O)SC=1)Nc1c(Cl)cccc1	3
4,106	ISSSTY_v1a_7367_02May011_5360	146795-43-9	C(=O)(C1C=C(N(=O)=O)SC=1)Nc1c(Br)cccc1	3
4,107	ISSSTY_v1a_7367_02May011_5361	146795-37-1	C(=O)(C1C=C(N(=O)=O)SC=1)Nc1c(F)cccc1	3
4,108	ISSSTY_v1a_7367_02May011_5362	146795-33-7	HC(H)C(H)c1c(NC(=O)C2C=C(N(=O)=O)SC=2)cccc1	3
4,109	ISSSTY_v1a_7367_02May011_5363	146795-31-5	HC(H)c1c(NC(=O)C2C=C(N(=O)=O)SC=2)cccc1	3
4,110	ISSSTY_v1a_7367_02May011_5364	146795-28-0	HC(H)Oc1c(NC(=O)C2C=C(N(=O)=O)SC=2)cccc1	3

4,111	ISSSTY_v1a_7367_02May011_5365	98033-22-8	HC(H)C1c2c3c(c(O)cc2NC1H)ccc1c3cccc1	3
4,112	ISSSTY_v1a_7367_02May011_5366	98033-24-0	HC(H)C1=Nc2c(c3c4c(ccc(O)c4)ccc3cc2)O1	3
4,113	ISSSTY_v1a_7367_02May011_5367	84-68-4	c1(-c2c(Cl)cc(N)cc2)c(Cl)cc(N)cc1	3
4,114	ISSSTY_v1a_7367_02May011_5368	98033-23-9	HC(H)Nc1cc2c3c(ccc(O)c3)ccc2cc1	3
4,115	ISSSTY_v1a_7367_02May011_5369	98033-26-2	HC(H)C1=Nc2c3c4c(ccc(O)c4)ccc3ccc2N1	3
4,116	ISSSTY_v1a_7367_02May011_5371	507-19-7	HC(H)C(Br)(C(H)H)C(H)H	3
4,117	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
4,118	ISSSTY_v1a_7367_02May011_5386	81677-51-2	HC(H)OC(=O)c1cc2-c3c(ccc(N(=O)=O)c3)Nc2c(-c2ccccc2)n1	3
4,119	ISSSTY_v1a_7367_02May011_5389	4332-51-8	HC(c1ccccc1)SC(H)C(H)Cl	3
4,120	ISSSTY_v1a_7367_02May011_5390	111959-96-7	HC(c1ccccc1)SC(Cl)=C(Cl)C(Cl)=C(Cl)Cl	3
4,121	ISSSTY_v1a_7367_02May011_5391	91085-62-0	HC(c1ccccc1)SC(Cl)=CCl	3
4,122	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
4,123	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
4,124	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
4,125	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
4,126	ISSSTY_v1a_7367_02May011_5396	33389-33-2	C1(=O)c2c(cccc2)NC(C2=CC=C(N(=O)=O)S2)N1	3
4,127	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
4,128	ISSSTY_v1a_7367_02May011_5398	107210-40-2	HC(H)N(C(H)H)C(H)C(H)C(H)Nc1c2c(c(N(C(H)C(H)O)C(H)C(H)O)ccc2N(=O)=O)nc2c1cccc2	3
4,129	ISSSTY_v1a_7367_02May011_5399	107210-39-9	HC(H)C(=O)OC(H)C(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)C(H)OC(=O)C(H)H	3
4,130	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
4,131	ISSSTY_v1a_7367_02May011_5405	513-31-5	HC(Br)C(Br)=CH	3
4,132	ISSSTY_v1a_7367_02May011_5406	766-40-5	C1(=O)C(Cl)=C(Cl)C(O)O1	3
4,133	ISSSTY_v1a_7367_02May011_5409	381740	HC(c1ccccc1)NC(=O)C(H)Br	3
4,134	ISSSTY_v1a_7367_02May011_5413	5875-25-2	HC(H)C(Br)C(N)=O	3
4,135	ISSSTY_v1a_7367_02May011_5414	42308-20-3	HC(H)C(Br)C(=O)Nc1ccccc1	3
4,136	ISSSTY_v1a_7367_02May011_5415	6653-71-0	HC(H)C(Br)C(=O)NC(H)c1ccccc1	3
4,137	ISSSTY_v1a_7367_02May011_5417	91687-67-1	HC(H)C(Br)C(=O)NC(H)c1ccc(Cl)cc1	3
4,138	ISSSTY_v1a_7367_02May011_5418	27798	C(Cl)(Cl)(Cl)C(=O)Cl	3
4,139	ISSSTY_v1a_7367_02May011_5419	25413-02-9	HC(H)C(H)OC(=O)C(H)NC(=O)C(Br)C(H)H	3
4,140	ISSSTY_v1a_7367_02May011_5427	242683	HC(c1ccccc1)NC(=O)C(H)Cl	3

4,141	ISSSTY_v1a_7367_02May011_5429	27946-19-6	HC(c1cccc1)NC(=O)C(Cl)c1cccc1	3
4,142	ISSSTY_v1a_7367_02May011_5430	105427-03-0	HC1C(C(=O)Nc2cccc2)O1	3
4,143	ISSSTY_v1a_7367_02May011_5431	105427-02-9	HC(c1cccc1)NC(=O)C1C(H)O1	3
4,144	ISSSTY_v1a_7367_02May011_5432	105427-01-8	HC(H)C1(C(=O)Nc2cccc2)C(H)O1	3
4,145	ISSSTY_v1a_7367_02May011_5433	105427-00-7	HC(H)C1(C(=O)NC(H)c2cccc2)C(H)O1	3
4,146	ISSSTY_v1a_7367_02May011_5435	92-69-3	c1(-c2ccc(O)cc2)cccc1	3
4,147	ISSSTY_v1a_7367_02May011_5436	1343853	HC(H)NC(=O)Oc1ccc(-c2cccc2)cc1	3
4,148	ISSSTY_v1a_7367_02May011_5439	53175-28-3	HC(H)C=C(Cl)C=O	3
4,149	ISSSTY_v1a_7367_02May011_5440	484-17-3	c1(O)c2c(c3c(cccc3)c1)cccc2	3
4,150	ISSSTY_v1a_7367_02May011_5442	109032-48-6	HC(H)NC(=O)Oc1c2c(c3c(cccc3)c1)cccc2	3
4,151	ISSSTY_v1a_7367_02May011_5443	620-25-7	HC(H)c1cc(NO)ccc1	3
4,152	ISSSTY_v1a_7367_02May011_5445	108278-71-3	HC(C(=O)O)C(H)N(C(N)=O)N=O	3
4,153	ISSSTY_v1a_7367_02May011_5446	4164-28-7	HC(H)N(C(H)H)N(=O)=O	3
4,154	ISSSTY_v1a_7367_02May011_5447	108278-72-4	HC(C(=O)O)C(H)C(H)N(C(N)=O)N=O	3
4,155	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)C(H)H)N=O	3
4,156	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
4,157	ISSSTY_v1a_7367_02May011_5452	7227-91-0	HC(H)N(C(H)H)N=Nc1cccc1	3
4,158	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
4,159	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
4,160	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)C(H)C3(O[C@@]3[C@](O)(C(=O)C(H)H)[C@@](O)[C@](OC(=O)C=C4ccc(O)cc4)[C@@](C(H)O)O3)C=1)C(H)C2H	3
4,161	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
4,162	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
4,163	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)C(H)C3(O[C@@]3[C@](O)(C(=O)C(H)H)[C@@](O)[C@](OC(=O)C=C4ccc(O)cc4)[C@@](C(H)O)O3)C=1)C(H)C2H	3
4,164	ISSSTY_v1a_7367_02May011_5459	1001985	HC(O)C=CCl	3
4,165	ISSSTY_v1a_7367_02May011_5460	1002017	HC(O)C=CCl	3
4,166	ISSSTY_v1a_7367_02May011_5461	2345-61-1	C(=O)(O)C=CCl	3
4,167	ISSSTY_v1a_7367_02May011_5462	1609-93-4	C(=O)(O)C=CCl	3
4,168	ISSSTY_v1a_7367_02May011_5463	85340-40-5	HC(C(H)Sc1c(N)cccc1)Sc1c(N)cccc1	3
4,169	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
4,170	ISSSTY_v1a_7367_02May011_5467	97135-11-0	C1(O)C(=O)C2=C(C3=C4C(C=CC=13)=Cc1c3c(ccc1N4)cccc3)O2	3

4,171	ISSSTY_v1a_7367_02May011_5469	524-89-0	HC(H)Oc1c2c(cc3c(c2)OC(H)O3)nc2c1C=CO2	3
4,172	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
4,173	ISSSTY_v1a_7367_02May011_5471	523-66-0	HC(H)Oc1c2c(cc(OC(H)H)cc2)nc2c1C=CO2	3
4,174	ISSSTY_v1a_7367_02May011_5472	2221-41-2	HC(H)Oc1c2c(ccc(OC(H)H)c2)nc2c1C=CO2	3
4,175	ISSSTY_v1a_7367_02May011_5473	522-06-5	HC(H)Oc1c2c(c(OC(H)H)c3c(c2)OC(H)O3)nc2c1C=CO2	3
4,176	ISSSTY_v1a_7367_02May011_5474	484-08-2	HC(H)Oc1c2c(cc(OC(H)H)c(OC(H)H)c2)nc2c1C=CO2	3
4,177	ISSSTY_v1a_7367_02May011_5477	157730-35-3	HC(H)N1c2c(N=C1N)nc1c(ccnc1)c2	3
4,178	ISSSTY_v1a_7367_02May011_5478	157730-36-4	HC(H)N1c2c(N=C1N)nc1c(cnc1)c2	3
4,179	ISSSTY_v1a_7367_02May011_5479	157730-37-5	HC(H)N1c2c(N=C1N)nc1c(c2)nccc1	3
4,180	ISSSTY_v1a_7367_02May011_5480	156215-58-6	HC(H)N1c2c(N=C1N)nc1c(cccc1)c2	3
4,181	ISSSTY_v1a_7367_02May011_5481	30489-67-9	HC(H)N1c2c(cc3c(cccc3)c2)N=C1N	3
4,182	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
4,183	ISSSTY_v1a_7367_02May011_5483	921-03-9	HC(Cl)C(=O)C(Cl)Cl	3
4,184	ISSSTY_v1a_7367_02May011_5485	165606-93-9	C1(=O)C(Cl)(Cl)C(=C(Cl)Cl)C(=O)N1	3
4,185	ISSSTY_v1a_7367_02May011_5486	64201-68-9	C1(c2ccc(N(=O)=O)cc2)=CSC(NC=O)=N1	3
4,186	ISSSTY_v1a_7367_02May011_5487	115453-71-9	HC([C@](N)C(=O)O)SC=CCl	3
4,187	ISSSTY_v1a_7367_02May011_5488	114414-79-8	HC(H)C1c2c(cccc2)N(C(H)H)C2C=1c1c(cccc1)N=2	3
4,188	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
4,189	ISSSTY_v1a_7367_02May011_5490	125372-28-3	HC(H)N1c2c3c(ccc2N=C1N=N_N)nccc3	3
4,190	ISSSTY_v1a_7367_02May011_5491	1516-71-8	HC(H)N1c2c(c3c(cccc3)cc2)N=C1N=N_N	3
4,191	ISSSTY_v1a_7367_02May011_5492	95389-75-6	HC(H)N1c2c3c(ccc2N=C1N=N_N)cccc3	3
4,192	ISSSTY_v1a_7367_02May011_5493	125372-29-4	HC(H)c1c2c(c3c(c1)nccc3)N=C(N=N_N)N2C(H)H	3
4,193	ISSSTY_v1a_7367_02May011_5495	160543-12-4	HC(H)c1c2c3c(c4c(c2nc2c1cc(C(H)H)cc2)cccc4)O3	3
4,194	ISSSTY_v1a_7367_02May011_5496	77287-29-7	HC(H)[C@](Cl)C(=O)OC(H)H	3
4,195	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
4,196	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
4,197	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
4,198	ISSSTY_v1a_7367_02May011_5501	6312-87-4	HC(H)C(=O)Nc1ccc(Oc2cccc2)cc1	3
4,199	ISSSTY_v1a_7367_02May011_5502	76543-08-3	HC(H)C(=O)Nc1ccc(Oc2ccc(Cl)cc2)cc1	3
4,200	ISSSTY_v1a_7367_02May011_5503	56120-26-4	HC(H)C(=O)Nc1ccc(Oc2c(Cl)cc(Cl)cc2)cc1	3

4,201	ISSSTY_v1a_7367_02May011_5504	26049-71-8	C1(c2ccc(N)cc2)=CSC(NN)=N1	3
4,202	ISSSTY_v1a_7367_02May011_5505	51489-62-4	c1(Oc2ccc(Cl)cc2)ccc(NC=O)cc1	3
4,203	ISSSTY_v1a_7367_02May011_5506	68906-23-0	c1(Cl)c(Oc2ccc(NC=O)cc2)c(Cl)cc(Cl)c1	3
4,204	ISSSTY_v1a_7367_02May011_5508	98911-09-2	HC(H)C(=O)N(O)c1ccc(Oc2c(Cl)cc(Cl)cc2Cl)cc1	3
4,205	ISSSTY_v1a_7367_02May011_5509	165550-82-3	c1(Oc2ccccc2)ccc(N(O)C=O)cc1	3
4,206	ISSSTY_v1a_7367_02May011_5510	105801-28-3	c1(Oc2ccc(Cl)cc2)ccc(N(O)C=O)cc1	3
4,207	ISSSTY_v1a_7367_02May011_5511	26049-70-7	C1(c2ccc(N(=O)=O)cc2)=CSC(NN)=N1	3
4,208	ISSSTY_v1a_7367_02May011_5512	165550-83-4	c1(Oc2ccc(N(O)C=O)cc2)c(Cl)cc(Cl)cc1	3
4,209	ISSSTY_v1a_7367_02May011_5513	165550-84-5	c1(Cl)c(Oc2ccc(N(O)C=O)cc2)c(Cl)cc(Cl)c1	3
4,210	ISSSTY_v1a_7367_02May011_5514	396-32-7	c12c(cc(F)cc1)nccc2	3
4,211	ISSSTY_v1a_7367_02May011_5515	79-44-7	HC(H)N(C(=O)Cl)C(H)H	3
4,212	ISSSTY_v1a_7367_02May011_5516	164200-11-7	HC(H)[C@]12[C@@](C=O)(C(C=O)=CC(H)C1H)C2H	3
4,213	ISSSTY_v1a_7367_02May011_5517	164200-12-8	HC(H)[C@@]12[C@](C=O)(C(C=O)=CC(H)C1H)C2H	3
4,214	ISSSTY_v1a_7367_02May011_5518	143347-57-3	HC(H)C12C(C=O)(C(C=O)=CC(H)C1H)C2H	3
4,215	ISSSTY_v1a_7367_02May011_5526	62690-96-4	HC1c2c(C3C(C(H)C(H)C(H)C=3)C1H)cccc2	3
4,216	ISSSTY_v1a_7367_02May011_5527	10353-53-4	HC(C(H)C1C(H)O1)C=CH	3
4,217	ISSSTY_v1a_7367_02May011_5528	97-52-9	HC(H)Oc1c(N)ccc(N(=O)=O)c1	3
4,218	ISSSTY_v1a_7367_02May011_5529	19600-63-6	HC(C(H)C(H)C(H)C1C(H)O1)C=CH	3
4,219	ISSSTY_v1a_7367_02May011_5531	93-27-6	HC(H)C(=O)Nc1c(OC(H)H)cc(N(=O)=O)cc1	3
4,220	ISSSTY_v1a_7367_02May011_5532	1888-89-7	HC(C(H)C1C(H)O1)C1C(H)O1	3
4,221	ISSSTY_v1a_7367_02May011_5533	2224-15-9	HC(C(H)OC(H)C1C(H)O1)OC(H)C1C(H)O1	3
4,222	ISSSTY_v1a_7367_02May011_5534	1244421	HC(H)Oc1c(N)ccc(N)c1	3
4,223	ISSSTY_v1a_7367_02May011_5535	5329-15-7	HC(H)C(=O)Nc1c(OC(H)H)cc(N)cc1	3
4,224	ISSSTY_v1a_7367_02May011_5539	63390-11-4	c1(-c2cc(Cl)c(N)c(Cl)c2)ccc(N)cc1	3
4,225	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
4,226	ISSSTY_v1a_7367_02May011_5543	26196-04-3	HC(H)C1(C(H)H)C(OC(H)H)O1	3
4,227	ISSSTY_v1a_7367_02May011_5544	98151-92-9	c1(N)c2c3c4c(c5c(cc4cc2)cccc5)ccc3cc1	3
4,228	ISSSTY_v1a_7367_02May011_5545	1120-71-4	HC1C(H)C(H)OS1(=O)=O	3
4,229	ISSSTY_v1a_7367_02May011_5546	1768-31-6	C(Cl)(Cl)(Cl)C(=O)C(Cl)Cl	3
4,230	ISSSTY_v1a_7367_02May011_5547	3787-28-8	C(Cl)(Cl)=C(Cl)C=O	3

4,231	ISSSTY_v1a_7367_02May011_5550	23045-35-4	c12c(c(N)c3c(ccc(N(=O)=O)c3)n1)cccc2	3
4,232	ISSSTY_v1a_7367_02May011_5553	1466-88-2	c1(N(=O)=O)c(C=CC=O)cccc1	3
4,233	ISSSTY_v1a_7367_02May011_5555	52411-33-3	HC(C(H)Sc1c(N)cccc1)Sc1c(N)cccc1	3
4,234	ISSSTY_v1a_7367_02May011_5557	33389-36-5	HC(O)C(H)Nc1c2c(cccc2)nc(C2=CC=C(N(=O)=O)S2)n1	3
4,235	ISSSTY_v1a_7367_02May011_5558	1214-32-0	HC1c2c(-c3c1cc(N(=O)=O)cc3)ccc(N)c2	3
4,236	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
4,237	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
4,238	ISSSTY_v1a_7367_02May011_5562	19322-27-1	HC(H)C1=C(O)C(=O)C(H)O1	3
4,239	ISSSTY_v1a_7367_02May011_5563	95050-14-9	c1(N(=O)=O)c2c(c3c4c5c6c(ccc5ccc24)cccc6c3)ccc1	3
4,240	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
4,241	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
4,242	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
4,243	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
4,244	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
4,245	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
4,246	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
4,247	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
4,248	ISSSTY_v1a_7367_02May011_5573	23740-25-2	HC(H)Oc1cc2C(=O)c3c4c(c5c(cc4ccn3)OC(H)O5)-c2cc1	3
4,249	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
4,250	ISSSTY_v1a_7367_02May011_5575	83287-02-9	HC(H)Oc1c2C(=O)c3c(-c4c2c(cc1OC(H)H)ccn4)ccc(OC(H)H)c3	3
4,251	ISSSTY_v1a_7367_02May011_5576	961-29-5	C(=O)(c1c(O)cc(O)cc1)C=Cc1ccc(O)cc1	3
4,252	ISSSTY_v1a_7367_02May011_5577	179073-71-3	HC(H)c1c2c3c(c4c(c5c(cccc5)cc4)cc3cc1)C(OS(=O)(=O)O)C2H	3
4,253	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
4,254	ISSSTY_v1a_7367_02May011_5579	3475-63-6	HC(H)N(C(=O)N(C(H)H)C(H)H)N=O	3
4,255	ISSSTY_v1a_7367_02May011_5581	105-11-3	c1(NO)ccc(N=O)cc1	3
4,256	ISSSTY_v1a_7367_02May011_5585	97672-08-7	HC(C1c2c(cccc2)N(N=O)C=1)C_N	3
4,257	ISSSTY_v1a_7367_02May011_5586	127128-50-1	HC(H)C(H)C=CC=CC=CC=COC(H)C(O)C(H)O	3
4,258	ISSSTY_v1a_7367_02May011_5587	127072-58-6	HC(H)C(H)C=CC=CC=CC=CC=CC=COC(H)C(O)C(H)O	3
4,259	ISSSTY_v1a_7367_02May011_5589	116-54-1	HC(H)OC(=O)C(Cl)Cl	3
4,260	ISSSTY_v1a_7367_02May011_5590	75-17-2	HC=NO	3

4,261	ISSSTY_v1a_7367_02May011_5600	89415-69-0	HC(Br)C(H)OC(=O)C(=O)OC(H)C(H)Br	3
4,262	ISSSTY_v1a_7367_02May011_5601	127923-98-2	HC(Br)C(H)OC(=O)C(O)C(O)C(=O)OC(H)C(H)Br	3
4,263	ISSSTY_v1a_7367_02May011_5602	127924-00-9	HC(C(O)(C(=O)OC(H)C(H)Br)C(H)C(=O)OC(H)C(H)Br)C(=O)OC(H)C(H)Br	3
4,264	ISSSTY_v1a_7367_02May011_5603	3022-61-5	HC(H)C(=O)C1c2c(C(=O)c3c(O)cccc13)c(O)ccc2	3
4,265	ISSSTY_v1a_7367_02May011_5604	131229-61-3	HC(H)c1ccc(C(=O)N(OC(=O)C(H)H)OC(H)C(H)C(H)C(H)H)cc1	3
4,266	ISSSTY_v1a_7367_02May011_5605	75464-10-7	HC(H)C(H)C(=O)C1c2c(C(=O)c3c(O)cccc13)c(O)ccc2	3
4,267	ISSSTY_v1a_7367_02May011_5606	2318-18-5	HC(H)[C@@]1(O)C(=O)OC(H)C2C(=O)[C@](C(H)C(H)N(C(H)H)C(H)C=2)OC(=O)C(=CC(H)H)C(H)[C@@]1C(H)H	3
4,268	ISSSTY_v1a_7367_02May011_5607	75464-11-8	HC(H)C(H)C(H)C(=O)C1c2c(C(=O)c3c(O)cccc13)c(O)ccc2	3
4,269	ISSSTY_v1a_7367_02May011_5608	14628-90-1	HC(H)OC1C(=O)C=CC(N(=O)=O)=CC=1	3
4,270	ISSSTY_v1a_7367_02May011_5609	16650-32-1	c1(F)c2c(c(F)cc1)cccn2	3
4,271	ISSSTY_v1a_7367_02May011_5610	54818-87-0	HC(H)C(=O)Nc1ccc(Sc2ccccc2)cc1	3
4,272	ISSSTY_v1a_7367_02May011_5611	220168-55-8	HC(c1ccccc1)ON(C(=O)c1ccccc1)OC(=O)c1ccc(N(=O)=O)cc1	3
4,273	ISSSTY_v1a_7367_02May011_5612	130040-14-1	HC(H)C(=O)N(O)c1ccc(Sc2ccccc2)cc1	3
4,274	ISSSTY_v1a_7367_02May011_5613	1135-14-4	c1(Sc2ccccc2)ccc(N)cc1	3
4,275	ISSSTY_v1a_7367_02May011_5614	101-59-7	c1(Sc2ccc(N)cc2)ccc(N(=O)=O)cc1	3
4,276	ISSSTY_v1a_7367_02May011_5622	575-44-0	c1(O)c2c(cc(O)cc2)ccc1	3
4,277	ISSSTY_v1a_7367_02May011_5623	571-60-8	c1(O)c2c(c(O)cc1)cccc2	3
4,278	ISSSTY_v1a_7367_02May011_5624	10159-46-3	HC(H)N(C(H)H)P(=O)(N(C(H)H)C(H)H)NC(H)H	3
4,279	ISSSTY_v1a_7367_02May011_5625	153117-08-9	HC(H)C(H)C(H)C(H)N(C(H)[C@@](C(H)c1ccccc1)C(H)O)N=O	3
4,280	ISSSTY_v1a_7367_02May011_5627	17177-50-3	HC(O)C(O)C1C(H)O1	3
4,281	ISSSTY_v1a_7367_02May011_5628	7144-65-2	HC1C(C(H)Oc2c(-c3ccccc3)cccc2)O1	3
4,282	ISSSTY_v1a_7367_02May011_5629	312304-87-3	HC(H)C(=O)OC(H)N(C(H)C(H)C(H)Cl)N=O	3
4,283	ISSSTY_v1a_7367_02May011_5630	4698-96-8	HC1C(C(H)Oc2ccc(-c3ccccc3)cc2)O1	3
4,284	ISSSTY_v1a_7367_02May011_5631	2461-43-0	HC(c1c(OC(H)C2C(H)O2)cccc1)c1ccccc1	3
4,285	ISSSTY_v1a_7367_02May011_5632	5296-38-8	HC(c1ccc(OC(H)C2C(H)O2)cc1)c1ccccc1	3
4,286	ISSSTY_v1a_7367_02May011_5633	165550-81-2	c1(Oc2ccccc2)ccc(NC=O)cc1	3
4,287	ISSSTY_v1a_7367_02May011_5634	5234-06-0	HC1C(C(H)Oc2cc3c(cccc3)cc2)O1	3
4,288	ISSSTY_v1a_7367_02May011_5635	53552-01-5	c1(Oc2ccc(NC=O)cc2)c(Cl)cc(Cl)cc1	3
4,289	ISSSTY_v1a_7367_02May011_5636	66931-57-5	HC(c1c2c(cccc2)ccc1)OC(H)C1C(H)O1	3
4,290	ISSSTY_v1a_7367_02May011_5637	98911-08-1	HC(H)C(=O)N(O)c1ccc(Oc2c(Cl)cc(Cl)cc2)cc1	3

4,291	ISSSTY_v1a_7367_02May011_5639	91254-97-6	c1(N(=O)=O)c2c3c4c(c(O)cc3cc1)cccc4cc2	3
4,292	ISSSTY_v1a_7367_02May011_5640	91254-93-2	c1(O)c2c3c4c(c(N(=O)=O)ccc4ccc3ccc2)c1	3
4,293	ISSSTY_v1a_7367_02May011_5641	91254-92-1	c12c3c4c(c(O)cc3ccc1)c(N(=O)=O)ccc4cc2	3
4,294	ISSSTY_v1a_7367_02May011_5642	54235-20-0	c1(O)c(N(=O)=O)c2c3c(c4c(c3ccc2)cccc4)c1	3
4,295	ISSSTY_v1a_7367_02May011_5643	192705-52-5	HC(H)C(=O)Nc1c2c3c(c4c(c3cc1O)cccc4)ccc2	3
4,296	ISSSTY_v1a_7367_02May011_5644	192705-53-6	HC(H)C(=O)Nc1c2c3c(c4c(c3ccc2)cc(O)cc4)cc1	3
4,297	ISSSTY_v1a_7367_02May011_5645	192705-54-7	HC(H)C(=O)Nc1c2c3c(c4c(c3ccc2)ccc(O)c4)cc1	3
4,298	ISSSTY_v1a_7367_02May011_5647	51118-04-8	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
4,299	ISSSTY_v1a_7367_02May011_5648	99585-29-2	HC1c2c(-c3c(O)cccc13)ccc(N(=O)=O)c2	3
4,300	ISSSTY_v1a_7367_02May011_5649	6633-40-5	HC1c2c(-c3c1cc(N(=O)=O)cc3)ccc(O)c2	3
4,301	ISSSTY_v1a_7367_02May011_5650	28149-15-7	c12-c3c(C(O)c1cc(N(=O)=O)cc2)cccc3	3
4,302	ISSSTY_v1a_7367_02May011_5652	164733-82-8	HC1C2(C=O)C(C=O)=CC(H)C(H)C12	3
4,303	ISSSTY_v1a_7367_02May011_5653	91605-35-5	HC(H)C(H)C=CC=CC=CC=CC=CCOC(H)[C@@](O)C(H)O	3
4,304	ISSSTY_v1a_7367_02May011_5654	87576-94-1	HC(H)[Si](C(H)H)(C(H)H)C(H)N=N_N	3
4,305	ISSSTY_v1a_7367_02May011_5655	6926-44-9	HC(c1cccc1)C(H)N=N_N	3
4,306	ISSSTY_v1a_7367_02May011_5657	173216-42-7	HC(H)[C@](c1cccc1)C(H)N=N_N	3
4,307	ISSSTY_v1a_7367_02May011_5658	74669-74-2	HC(H)[C@@](c1cccc1)C(H)N=N_N	3
4,308	ISSSTY_v1a_7367_02May011_5661	131321-84-1	HC(O)[C@](O)C(H)N=N_N	3
4,309	ISSSTY_v1a_7367_02May011_5662	85820-84-4	HC(O)[C@@](O)C(H)N=N_N	3
4,310	ISSSTY_v1a_7367_02May011_5663	4648-54-8	HC(H)[Si](C(H)H)(C(H)H)N=N_N	3
4,311	ISSSTY_v1a_7367_02May011_5664	16804-85-6	HC1C(H)C(H)C(H)C2c3c(C=CC12)cccc3	3
4,312	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
4,313	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
4,314	ISSSTY_v1a_7367_02May011_5669	134998-79-1	HC1c2c(c3c4c5c(c(N(=O)=O)cc4ccc3)cccc25)C(H)C(H)C1H	3
4,315	ISSSTY_v1a_7367_02May011_5670	134998-77-9	c1(N(=O)=O)c2c3c(c4c(c5c3c(ccc5)c1)cccc4)ccc2	3
4,316	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
4,317	ISSSTY_v1a_7367_02May011_5672	115084-47-4	HC(c1cc(Cl)c(NO)cc1)c1cc(Cl)c(N)cc1	3
4,318	ISSSTY_v1a_7367_02May011_5675	59485-08-4	HC1C(Oc2ccc(N(=O)=O)cc2)O1	3
4,319	ISSSTY_v1a_7367_02May011_5676	155379-82-1	HC(H)c1c(N)c(N(=O)=O)cc(N)c1	3
4,320	ISSSTY_v1a_7367_02May011_5677	1070-66-2	HC(H)C(H)C(H)C(H)C(C=O)=CH	3

4,321	ISSSTY_v1a_7367_02May011_5681	28564-83-2	HC(H)C1=C(O)C(=O)C(O)C(H)O1	3
4,322	ISSSTY_v1a_7367_02May011_5682	214130	c1(-c2c([N+](=O)[O-])cc([N+](=O)[O-])cc2)ccccc1	3
4,323	ISSSTY_v1a_7367_02May011_5685	109897-79-2	c12c([C@@](O)[C@](O)C=C1)cc1c(cc(N(=O)=O)cc1)c2	3
4,324	ISSSTY_v1a_7367_02May011_5687	109897-78-1	C12C([C@](O)[C@@](O)C=C1)=CC1C=C(N(=O)=O)C=CC1C=2	3
4,325	ISSSTY_v1a_7367_02May011_5688	632-21-3	C(=O)(C(Cl)Cl)C(Cl)Cl	3
4,326	ISSSTY_v1a_7367_02May011_5698	125369-82-6	C(_N)C(c1ccc(F)cc1)=CC=Cc1ccccc1	3
4,327	ISSSTY_v1a_7367_02May011_5699	125369-84-8	C(_N)C(c1ccc(Br)cc1)=CC=Cc1c(N(=O)=O)ccccc1	3
4,328	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
4,329	ISSSTY_v1a_7367_02May011_5701	20780-53-4	HC1[C@@](c2ccccc2)O1	3
4,330	ISSSTY_v1a_7367_02May011_5702	20780-54-5	HC1[C@](c2ccccc2)O1	3
4,331	ISSSTY_v1a_7367_02May011_5703	81593-15-9	c12-c3c(G4C(c1ccccc2)N4Cl)ccccc3	3
4,332	ISSSTY_v1a_7367_02May011_5704	64188-66-5	HC(H)C(H)C(H)C(H)N1C2c3c(-c4c(ccccc4)C12)ccccc3	3
4,333	ISSSTY_v1a_7367_02May011_5705	91540-30-6	HC(C=CH)N1C2c3c(-c4c(ccccc4)C12)ccccc3	3
4,334	ISSSTY_v1a_7367_02May011_5706	64188-65-4	HC1C(H)C(H)C(H)C(H)C1N1C2c3c(-c4c(ccccc4)C12)ccccc3	3
4,335	ISSSTY_v1a_7367_02May011_5707	187585-11-1	HC(H)Oc1c(N)cc(C2=C(N)C(=O)c3c(ccccc3)O2)cc1	3
4,336	ISSSTY_v1a_7367_02May011_5708	187585-43-9	HC(H)Oc1c([N+](=O)[O-])cc(C2=C([N+](=O)[O-])C(=O)c3c(ccccc3)O2)cc1	3
4,337	ISSSTY_v1a_7367_02May011_5709	607-30-7	c1(NO)c2c(ccccc2)ccc1	3
4,338	ISSSTY_v1a_7367_02May011_5711	81593-11-5	HC(H)S(=O)(=O)N1C2c3c(-c4c(ccccc4)C12)ccccc3	3
4,339	ISSSTY_v1a_7367_02May011_5712	36712-35-3	c1(-c2c([N+](=O)[O-])cc([N+](=O)[O-])cc2)c([N+](=O)[O-])ccccc1	3
4,340	ISSSTY_v1a_7367_02May011_5713	102873-32-5	c1(-c2c([N+](=O)[O-])cc([N+](=O)[O-])cc2)cc([N+](=O)[O-])ccccc1	3
4,341	ISSSTY_v1a_7367_02May011_5714	36712-34-2	c1(-c2c([N+](=O)[O-])cc([N+](=O)[O-])cc2)ccc([N+](=O)[O-])cc1	3
4,342	ISSSTY_v1a_7367_02May011_5715	145627-68-5	HC1c2c(c3c(c4c([C@](O)[C@@](O)C=C4)cc3)cc2)C(H)C1H	3
4,343	ISSSTY_v1a_7367_02May011_5718	1010-93-1	HC(H)C1N(C(H)C(=O)O)C(N(=O)=O)=CN=1	3
4,344	ISSSTY_v1a_7367_02May011_5719	4812-40-2	HC(O)C1N(C(H)C(H)O)C(N(=O)=O)=CN=1	3
4,345	ISSSTY_v1a_7367_02May011_5720	1874-23-3	HC(H)OC(=O)C1=CC=C(N(=O)=O)O1	3
4,346	ISSSTY_v1a_7367_02May011_5722	52101-40-3	c1(C2C(c3ccccc3)=C(C(=O)O)OC=2N(=O)=O)ccccc1	3
4,347	ISSSTY_v1a_7367_02May011_5730	1794-84-9	HC(Cl)N(=O)=O	3
4,348	ISSSTY_v1a_7367_02May011_5731	7119-89-3	C(Cl)(Cl)N(=O)=O	3
4,349	ISSSTY_v1a_7367_02May011_5733	771-97-1	c1(N)c(N)cc2c(ccccc2)c1	3
4,350	ISSSTY_v1a_7367_02May011_5738	2255-50-7	HC(H)Oc1c2c(c(O)ccc2)nc2c1C=CO2	3

4,351	ISSSTY_v1a_7367_02May011_5741	82911-12-4	c12C3c4c(-c1cccc2[C@@](O)[C@](O)C=3)cccc4	3
4,352	ISSSTY_v1a_7367_02May011_5742	105777-13-7	C12c3c4c(C=1[C@](O)[C@@](O)C=C2)cccc4ccc3	3
4,353	ISSSTY_v1a_7367_02May011_5745	79526-11-7	HC1C(Oc2cccc2)O1	3
4,354	ISSSTY_v1a_7367_02May011_5746	5386-28-7	C1(=O)C(=O)c2c3C(c4c(-c3ccc2)cccc4)=C1	3
4,355	ISSSTY_v1a_7367_02May011_5748	83349-67-1	c12[C@@]34c5c(-c1cccc2C(O)C(O)[C@@]3O4)cccc5	3
4,356	ISSSTY_v1a_7367_02May011_5749	83349-66-0	c12[C@@]34c5c(-c1cccc2C(O)C(O)[C@@]3O4)cccc5	3
4,357	ISSSTY_v1a_7367_02May011_5756	1629-58-9	HC(H)C(H)C(=O)C=CH	3
4,358	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
4,359	ISSSTY_v1a_7367_02May011_5759	590-21-6	HC(H)C=CCl	3
4,360	ISSSTY_v1a_7367_02May011_5763	96918-15-9	c12c3c4c(c5c(C=CO5)cc4ccc3ccc1)cc2	3
4,361	ISSSTY_v1a_7367_02May011_5765	96918-24-0	c12c3c4c(c5c(cc4ccc3ccc1)OC=C5)cc2	3
4,362	ISSSTY_v1a_7367_02May011_5769	96563-08-5	HC(H)c1c2-c3c(C(C(H)H)c2ccc1)cccc3	3
4,363	ISSSTY_v1a_7367_02May011_5770	21846-26-4	HC(H)c1cc2c(-c3c(cccc3)C2C(H)H)cc1	3
4,364	ISSSTY_v1a_7367_02May011_5771	96563-07-4	HC(H)c1cc2-c3c(C(C(H)H)c2cc1)cccc3	3
4,365	ISSSTY_v1a_7367_02May011_5772	22994-85-0	HC(c1cccc1)NC(=O)C(H)N1C(N(=O)=O)=NC=C1	3
4,366	ISSSTY_v1a_7367_02May011_5773	17057-98-6	HC(H)c1c2c(-c3c(cccc3)C2C(H)H)ccc1	3
4,367	ISSSTY_v1a_7367_02May011_5781	229-87-8	c12c(c3c(cccc3)cn1)cccc2	3
4,368	ISSSTY_v1a_7367_02May011_5785	51-18-3	HC1C(H)N1c1nc(N2C(H)C2H)nc(N2C(H)C2H)n1	3
4,369	ISSSTY_v1a_7367_02May011_5789	59283-76-0	HC(H)c1c(NO)cc([N+](=O)[O-])cc1[N+](=O)[O-]	3
4,370	ISSSTY_v1a_7367_02May011_5790	185376-54-9	HC(H)c1c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
4,371	ISSSTY_v1a_7367_02May011_5791	1622-57-7	HC(H)N1c2c(cccc2)N=C1N	3
4,372	ISSSTY_v1a_7367_02May011_5792	6285-68-3	HC(H)c1cc2c(cc1)N=C(N)N2	3
4,373	ISSSTY_v1a_7367_02May011_5794	20921-50-0	HC(H)c1c(C(H)H)cc(C(c2cccc2)(C_C)OC(=O)NC2C(H)C(H)C(H)C(H)C2H)cc1	3
4,374	ISSSTY_v1a_7367_02May011_5795	63655-40-3	C(_N)c1cc2c(cc1)N=C(N)N2	3
4,375	ISSSTY_v1a_7367_02May011_5797	51276-85-8	c12c(cc(O)cc1)NC(N)=N2	3
4,376	ISSSTY_v1a_7367_02May011_5798	76215-00-4	HC(H)C(=O)OC(H)N(C(H)C(H)Cl)N=O	3
4,377	ISSSTY_v1a_7367_02May011_5799	39860-12-3	HC(H)c1cc2c(cc1)N(C(H)H)C(N)=N2	3
4,378	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
4,379	ISSSTY_v1a_7367_02May011_5801	103748-25-0	HC(H)N1c2c(cc(Cl)cc2)N=C1N	3
4,380	ISSSTY_v1a_7367_02May011_5802	141691-41-0	HC(H)N1c2c(cc(C_N)cc2)N=C1N	3

4,381	ISSSTY_v1a_7367_02May011_5805	1805-02-3	HC(H)N1c2c(cc(OC(H)H)cc2)N=C1N	3
4,382	ISSSTY_v1a_7367_02May011_5806	102408-26-4	HC(H)N1c2c(c3c(cc2)nccc3)N=C1NC(H)H	3
4,383	ISSSTY_v1a_7367_02May011_5807	102408-27-5	HC(H)N1c2c(c3c(cc2)nccc3)N=C1N(C(H)H)C(H)H	3
4,384	ISSSTY_v1a_7367_02May011_5808	102408-25-3	HC(H)N1c2c3c(ccc2N=C1N)nccc3	3
4,385	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
4,386	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
4,387	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
4,388	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
4,389	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
4,390	ISSSTY_v1a_7367_02May011_5815	139259-92-0	HC(H)C(=O)ON(C(=O)c1ccccc1)OC(H)c1ccc(Oc2ccccc2)cc1	3
4,391	ISSSTY_v1a_7367_02May011_5817	139259-94-2	HC(H)c1ccc(C(H)ON(C(=O)c2ccccc2)OC(=O)C(H)H)cc1	3
4,392	ISSSTY_v1a_7367_02May011_5819	139259-96-4	HC(H)C(=O)ON(C(=O)c1ccccc1)OC(H)c1ccc(Cl)cc1	3
4,393	ISSSTY_v1a_7367_02May011_5820	139259-98-6	HC(H)C(=O)ON(C(=O)c1ccccc1)OC(H)c1ccc(N(=O)=O)cc1	3
4,394	ISSSTY_v1a_7367_02May011_5821	139259-91-9	HC(H)C(=O)ON(C(=O)c1ccccc1)OC(H)c1ccc(OC(H)H)cc1	3
4,395	ISSSTY_v1a_7367_02May011_5822	139259-97-5	HC(H)C(=O)ON(C(=O)c1ccccc1)OC(H)c1ccc(Br)cc1	3
4,396	ISSSTY_v1a_7367_02May011_5823	220168-52-5	HC(c1ccccc1)ON(C(=O)c1ccccc1)OC(=O)c1ccc(C_N)cc1	3
4,397	ISSSTY_v1a_7367_02May011_5824	220168-41-2	HC(H)Oc1ccc(C(=O)ON(C(=O)c2ccccc2)OC(H)c2ccccc2)cc1	3
4,398	ISSSTY_v1a_7367_02May011_5825	220168-43-4	HC(H)c1ccc(C(=O)ON(C(=O)c2ccccc2)OC(H)c2ccccc2)cc1	3
4,399	ISSSTY_v1a_7367_02May011_5826	220168-45-6	HC(c1ccccc1)ON(C(=O)c1ccccc1)OC(=O)c1ccc(Cl)cc1	3
4,400	ISSSTY_v1a_7367_02May011_5827	220168-47-8	HC(c1ccccc1)ON(C(=O)c1ccccc1)OC(=O)c1ccc(C=O)cc1	3
4,401	ISSSTY_v1a_7367_02May011_5828	115689-52-6	HC1c2c(C3=C(C1H)SC(N)=N3)cccn2	3
4,402	ISSSTY_v1a_7367_02May011_5829	357204-48-9	HC(c1ccccc1)ON(C(=O)c1ccccc1)OC(=O)c1cc(N(=O)=O)ccc1	3
4,403	ISSSTY_v1a_7367_02May011_5830	141890-75-7	c12c(c3c(cc1)nccc3)N=C(N)S2	3
4,404	ISSSTY_v1a_7367_02May011_5831	357204-49-0	HC(H)c1cc(C(=O)ON(C(=O)c2ccccc2)OC(H)c2ccccc2)ccc1	3
4,405	ISSSTY_v1a_7367_02May011_5832	244775-76-6	HC(H)C(=O)ON(C(=O)c1ccccc1)OC(H)C(H)C(H)H	3
4,406	ISSSTY_v1a_7367_02May011_5833	139259-64-6	HC(H)C(=O)ON(C(=O)c1ccccc1)OC(C(H)H)C(H)H	3
4,407	ISSSTY_v1a_7367_02May011_5834	357204-50-3	HC(H)C(=O)ON(C(=O)c1cc2c(cccc2)cc1)OC(H)C(H)C(H)C(H)H	3
4,408	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
4,409	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
4,410	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

