

4663	ISSSTY_v1a_7367_02May011_6281	70951-83-6	c12c(c3c(c4c([C@@]5[C@]([C@](O)[C@@]4O)O5)cc3)cc1)cccc2	3
4664	ISSSTY_v1a_7367_02May011_6282	83830-70-0	c12c(c3c(c4c(C5C(C(O)C4O)O5)cc3)cc1)cccc2	3
4665	ISSSTY_v1a_7367_02May011_6283	90421-79-7	HC1C(C(H)OC2c3c(cccc3)SN=2)O1	3
4666	ISSSTY_v1a_7367_02May011_6284	60768-66-3	c12c(C=NS1)cc(N(=O)=O)cc2	3
4667	ISSSTY_v1a_7367_02May011_6285	89641-97-4	c1(N(=O)=O)c2c(C=NS2)ccc1	3
4668	ISSSTY_v1a_7367_02May011_6287	53473-85-1	c12c(C=NS1)cc(N)cc2	3
4669	ISSSTY_v1a_7367_02May011_6288	89795-79-9	c1(N)c2c(C=NS2)ccc1	3
4670	ISSSTY_v1a_7367_02May011_6289	76919-33-0	HC1C(C(H)Oc2cc3c(cc2)SN=C3)O1	3
4671	ISSSTY_v1a_7367_02May011_6290	148193-29-7	HC1C(C(H)Oc2c3c(C=NS3)ccc2)O1	3
4672	ISSSTY_v1a_7367_02May011_6291	30747-87-6	C1(Cl)c2c(ccc(N(=O)=O)c2)SN=1	3
4673	ISSSTY_v1a_7367_02May011_6292	19331-27-2	C1(Cl)c2c(cc(N(=O)=O)cc2)SN=1	3
4674	ISSSTY_v1a_7367_02May011_6293	720-69-4	c1(C2=CC=C(N(=O)=O)O2)nc(N)nc(N)n1	3
4675	ISSSTY_v1a_7367_02May011_6294	41533-75-9	C1(Cl)c2c(c(N(=O)=O)ccc2)SN=1	3
4676	ISSSTY_v1a_7367_02May011_6295	148193-30-0	C1(Cl)c2c(ccc(N)c2)SN=1	3
4677	ISSSTY_v1a_7367_02May011_6296	148193-31-1	C1(Cl)c2c(c(N)ccc2)SN=1	3
4678	ISSSTY_v1a_7367_02May011_6297	64099-26-9	HC(H)OC1c2c(ccc(N(=O)=O)c2)SN=1	3
4679	ISSSTY_v1a_7367_02May011_6298	148193-32-2	HC(H)OC1c2c(cc(N(=O)=O)cc2)SN=1	3
4680	ISSSTY_v1a_7367_02May011_6299	64099-25-8	HC(H)OC1c2c(c(N(=O)=O)ccc2)SN=1	3
4681	ISSSTY_v1a_7367_02May011_6300	64099-28-1	HC(H)OC1c2c(ccc(N)c2)SN=1	3
4682	ISSSTY_v1a_7367_02May011_6301	148193-33-3	HC(H)OC1c2c(cc(N)cc2)SN=1	3
4683	ISSSTY_v1a_7367_02May011_6302	64099-27-0	HC(H)OC1c2c(c(N)ccc2)SN=1	3
4684	ISSSTY_v1a_7367_02May011_6303	148193-34-4	HC(H)OC1c2c(ccc(OC(H)C3C(H)O3)c2)SN=1	3
4685	ISSSTY_v1a_7367_02May011_6304	148193-35-5	HC(H)OC1c2c(cc(OC(H)C3C(H)O3)cc2)SN=1	3
4686	ISSSTY_v1a_7367_02May011_6305	148193-36-6	HC(H)OC1c2c(c(OC(H)C3C(H)O3)ccc2)SN=1	3
4687	ISSSTY_v1a_7367_02May011_6306	4337-51-3	C1(=O)c2c(cc(N(=O)=O)cc2)SN1	3
4688	ISSSTY_v1a_7367_02May011_6307	817-99-2	HC(C(N)=O)NC(=O)C=[N+]=[N-]	3
4689	ISSSTY_v1a_7367_02May011_6308	148193-38-8	HC1C(C(H)N2C(=O)c3c(cc(OC(H)C4C(H)O4)cc3)S2)O1	3
4690	ISSSTY_v1a_7367_02May011_6309	110021-94-8	HC(H)S(=O)(=O)Nc1ccc(Nc2c3c(ccc(N=N_N)c3)nc3c2cccc3)cc1	3
4691	ISSSTY_v1a_7367_02May011_6310	64894-90-2	HC(H)S(=O)(=O)Nc1ccc(Nc2c3c(cc(N=N_N)cc3)nc3c2cccc3)cc1	3
4692	ISSSTY_v1a_7367_02May011_6312	110004-65-4	HC(H)S(=O)(=O)Nc1ccc(Nc2c3c(cc(N=N_N)cc3)nc3c2ccc(N=N_N)c3)cc1	3
4693	ISSSTY_v1a_7367_02May011_6314	145531-23-3	HC(C(H)C(H)N)S(=O)(=O)Nc1ccc(Nc2c3c(cc(N=N_N)cc3)nc3c2ccc(N=N_N)c3)cc1	3
4694	ISSSTY_v1a_7367_02May011_6315	145531-24-4	HC(H)Oc1c(Nc2c3c(ccc(N=N_N)c3)nc3c2cccc3)ccc(NS(=O)(=O)C(H)H)c1	3
4695	ISSSTY_v1a_7367_02May011_6316	999-29-1	HC(H)C(H)OC(=O)C(H)NC(=O)C=[N+]=[N-]	3
4696	ISSSTY_v1a_7367_02May011_6317	80266-02-0	HC(H)Oc1c(Nc2c3c(cc(N=N_N)cc3)nc3c2cccc3)ccc(NS(=O)(=O)C(H)H)c1	3
4697	ISSSTY_v1a_7367_02May011_6318	110004-69-8	HC(H)c1c2c(c(Nc3c(OC(H)H)cc(NS(=O)(=O)C(H)H)cc3)c3c(cc(N=N_N)cc3)n2)ccc1	3
4698	ISSSTY_v1a_7367_02May011_6319	64894-89-9	C(=O)(O)c1ccc(Nc2c3c(cc(N=N_N)cc3)nc3c2cccc3)cc1	3
4699	ISSSTY_v1a_7367_02May011_6320	89873-24-5	c12c(c(Nc3ccc(N=N_N)cc3)c3c(cccc3)n1)cccc2	3
4700	ISSSTY_v1a_7367_02May011_6321	14618-80-5	HC(c1cccc1)OC(H)[C@@]1C(H)O1	3
4701	ISSSTY_v1a_7367_02May011_6322	16495-13-9	HC(c1cccc1)OC(H)[C@]1C(H)O1	3
4702	ISSSTY_v1a_7367_02May011_6323	820-75-7	HC(C(=O)NN)NC(=O)C=[N+]=[N-]	3
4703	ISSSTY_v1a_7367_02May011_6324	56715-28-7	HC1[C@](C(H)Oc2c3c(cccc3)ccc2)O1	3
4704	ISSSTY_v1a_7367_02May011_6325	61249-00-1	HC1[C@@](C(H)Oc2c3c(cccc3)ccc2)O1	3

4705	ISSSTY_v1a_7367_02May011_6326	115314-17-5	HC1[C@](C(H)OS(=O)(=O)c2cc(N(=O)=O)ccc2)O1	3
4706	ISSSTY_v1a_7367_02May011_6327	115314-14-2	HC1[C@@](C(H)OS(=O)(=O)c2cc(N(=O)=O)ccc2)O1	3
4707	ISSSTY_v1a_7367_02May011_6328	106268-95-5	HC1[C@@](C(H)OC(=O)c2ccc(N(=O)=O)cc2)O1	3
4708	ISSSTY_v1a_7367_02May011_6329	115459-65-9	HC1[C@@](C(H)OC(=O)c2ccc(N(=O)=O)cc2)O1	3
4709	ISSSTY_v1a_7367_02May011_6330	125279-81-4	HC1[C@](C(H)Oc2ccc(N(=O)=O)cc2)O1	3
4710	ISSSTY_v1a_7367_02May011_6331	125279-82-5	HC1[C@@](C(H)Oc2ccc(N(=O)=O)cc2)O1	3
4711	ISSSTY_v1a_7367_02May011_6332	92180-79-5	HC(H)c1c(C(H)H)nc2c(c3c(cc2)N(C(H)H)C(N)=N3)n1	3
4712	ISSSTY_v1a_7367_02May011_6333	108354-48-9	HC(H)c1c2c(c3c(c1)nccn3)N=C(N)N2C(H)H	3
4713	ISSSTY_v1a_7367_02May011_6334	97389-17-8	HC(H)c1c2c(c3c(c1)nc(C(H)H)cn3)N=C(N)N2C(H)H	3
4714	ISSSTY_v1a_7367_02May011_6335	146177-57-3	HC(H)c1c2c(c3c(c1)N(C(H)H)C(N)=N3)nccn2	3
4715	ISSSTY_v1a_7367_02May011_6336	103139-94-2	HC(H)c1c2c(c3c(c1)N(C(H)H)C(N)=N3)nc(C(H)H)cn2	3
4716	ISSSTY_v1a_7367_02May011_6337	115609-71-7	HC(H)c1c2c(c3c(c1)N(C(H)H)C(N)=N3)ncc(C(H)H)n2	3
4717	ISSSTY_v1a_7367_02May011_6338	146177-59-5	HC(H)c1c2c(c3c(c1C(H)H)N(C(H)H)C(N)=N3)nccn2	3
4718	ISSSTY_v1a_7367_02May011_6339	95896-78-9	HC(H)c1c2c(c3c(c1)ncc(C(H)H)n3)N=C(N)N2C(H)H	3
4719	ISSSTY_v1a_7367_02May011_6340	132898-07-8	HC(H)c1c2c(c3c(c1)nc(C(H)H)c(C(H)H)n3)N=C(N)N2C(H)H	3
4720	ISSSTY_v1a_7367_02May011_6341	146177-58-4	HC(H)c1c2c(c3c(c1)N(C(H)H)C(N)=N3)nc(C(H)H)c(C(H)H)n2	3
4721	ISSSTY_v1a_7367_02May011_6342	146177-60-8	HC(H)c1c2c(c3c(c1C(H)H)N(C(H)H)C(N)=N3)nc(C(H)H)cn2	3
4722	ISSSTY_v1a_7367_02May011_6343	146177-61-9	HC(H)c1c2c(c3c(c1C(H)H)N(C(H)H)C(N)=N3)ncc(C(H)H)n2	3
4723	ISSSTY_v1a_7367_02May011_6344	88193-04-8	HC(H)c1c2c(c3-c4c5c(c(C(H)H)cc4Nc3c1)cccc5)cccc2	3
4724	ISSSTY_v1a_7367_02May011_6345	146177-64-2	HC(H)c1c2c(c3c(c1)N(C(H)H)C(N)=N3)nc(-c1cccc1)cn2	3
4725	ISSSTY_v1a_7367_02May011_6346	146177-62-0	HC(H)c1c2c(c3c(c1C(H)H)N(C(H)H)C(N)=N3)nc(C(H)H)c(C(H)H)n2	3
4726	ISSSTY_v1a_7367_02May011_6348	146177-65-3	HC(H)c1c2c(c3c(c1)N(C(H)H)C(N)=N3)ncc(-c1cccc1)n2	3
4727	ISSSTY_v1a_7367_02May011_6349	101021-43-6	HC(H)c1cc2c(c3-c4c5c(ccc4Nc3cc2)cccc5)cc1	3
4728	ISSSTY_v1a_7367_02May011_6350	145763-35-5	HC(H)C(C(=O)C12C(=O)N[C@](O)(C(H)C(H)O)[C@@]1O2)=CC=CC(C(H)H)=CC(C(H)H)=CC1C(=O)OC(H)C=1	3
4729	ISSSTY_v1a_7367_02May011_6352	111901-42-9	HC(H)c1c2c(c3c([C@](O)[C@@](O)[C@@]4[C@@]3O4)c1)ccc1c2cccc1	3
4730	ISSSTY_v1a_7367_02May011_6353	111901-40-7	HC(H)c1c2c(c3c(ccc3)c1)ccc1c2[C@@]2[C@]([C@](O)[C@@]1O)O2	3
4731	ISSSTY_v1a_7367_02May011_6358	6850-22-2	HC(H)N1C=C2C(C=C(N(=O)=O)C=C2)=N1	3
4732	ISSSTY_v1a_7367_02May011_6359	13436-58-3	HC(H)N1C=C2C(C(N(=O)=O)=CC=C2)=N1	3
4733	ISSSTY_v1a_7367_02May011_6360	6146-52-7	c12c(C=CN1)cc(N(=O)=O)cc2	3
4734	ISSSTY_v1a_7367_02May011_6361	114460-38-7	HC(H)N1c2c3c4c(ccc(O)c4)ccc3ccc2C=C1	3
4735	ISSSTY_v1a_7367_02May011_6362	5709-68-2	HC(H)N1c2c(cccc2)N=C1N(=O)=O	3
4736	ISSSTY_v1a_7367_02May011_6363	7597-18-4	c12c(C=NN1)ccc(N(=O)=O)c2	3
4737	ISSSTY_v1a_7367_02May011_6364	114460-39-8	HC(H)C1N(C(H)H)c2c3c4c(ccc(O)c4)ccc3ccc2N=1	3
4738	ISSSTY_v1a_7367_02May011_6365	114460-40-1	HC(H)c1c2c(c3c(ccc(O)c3)cc2)c2c(c1)NC(C(H)H)=N2	3
4739	ISSSTY_v1a_7367_02May011_6366	114460-41-2	HC(H)C(H)C1=Nc2c3c4c(ccc(O)c4)ccc3ccc2N1	3
4740	ISSSTY_v1a_7367_02May011_6367	149922-82-7	C12C(c3c4C(=Cc5c4c(ccc5)cc3)C=1)=CC(Cl)C=C2	3
4741	ISSSTY_v1a_7367_02May011_6368	10387-13-0	HC(Cl)c1c2c(c(C(H)Cl)c3c1cccc3)cccc2	3
4742	ISSSTY_v1a_7367_02May011_6369	19727-83-4	HC1c2c(cc(N(=O)=O)cc2)NC1H	3
4743	ISSSTY_v1a_7367_02May011_6370	32692-19-6	HC1c2c(ccc(N(=O)=O)c2)NC1H	3
4744	ISSSTY_v1a_7367_02May011_6371	5709-67-1	c12c(cccc1)N=C(N(=O)=O)N2	3
4745	ISSSTY_v1a_7367_02May011_6372	2942-42-9	c1(N(=O)=O)c2c(C=NN2)ccc1	3
4746	ISSSTY_v1a_7367_02May011_6377	5381-79-3	HC(H)N1c2c(ccc(N(=O)=O)c2)N=C1	3

4747	ISSSTY_v1a_7367_02May011_6378	136911-37-0	HC(H)N1C(H)C(H)N=N1	3
4748	ISSSTY_v1a_7367_02May011_6379	17886-23-6	HC(H)C(H)N1C(H)C(H)N=N1	3
4749	ISSSTY_v1a_7367_02May011_6380	17886-25-8	HC(c1ccccc1)N1C(H)C(H)N=N1	3
4750	ISSSTY_v1a_7367_02May011_6381	3585-32-8	HC(H)N=NNC(H)H	3
4751	ISSSTY_v1a_7367_02May011_6382	63980-20-1	HC(H)C(H)N=NNC(H)C(H)H	3
4752	ISSSTY_v1a_7367_02May011_6383	29814-12-8	HC(H)C(C(H)H)OC(=O)C(CI)=C(CI)C=O	3
4753	ISSSTY_v1a_7367_02May011_6384	115044-41-2	HC(H)C1=CNC2c(c3c(cc2)N(C(H)H)C(N=O)=N3)N1	3
4754	ISSSTY_v1a_7367_02May011_6385	108283-47-2	HC(H)C(C(H)H)(C(H)H)OC(=O)[C@@](N)C(H)N=N_N	3
4755	ISSSTY_v1a_7367_02May011_6386	91897-48-2	HC(H)N1C(H)C(C(H)O)=C[C@@]2c3c4C(C(H)[C@]12)=CN(C(H)C=CH)c4ccc3	3
4756	ISSSTY_v1a_7367_02May011_6387	87633-43-0	HC(H)N1c2c3C(C(H)[C@@]4C(c3ccc2)=C[C@@](C(H)OC(H)H)C(H)N4C(H)H)=C1	3
4757	ISSSTY_v1a_7367_02May011_6388	18523-47-2	HC(C(=O)O)C(H)N=N_N	3
4758	ISSSTY_v1a_7367_02May011_6389	569-26-6	HC(H)[C@]1C(H)[C@@]2c3c4C(C(H)[C@]2N(C(H)H)C1H)=CNC4ccc3	3
4759	ISSSTY_v1a_7367_02May011_6390	129134-96-9	HC(H)[C@]1C(H)C2c3c4C(C(H)[C@]2N(C(H)H)C1H)=CN(C1C(H)C(H)C(H)C1H)c4ccc3	3
4760	ISSSTY_v1a_7367_02May011_6392	98931-06-7	HC(H)C(H)C(H)N1c2c3C(C(H)[C@@]4C(c3ccc2)C(H)[C@@](C(H)H)C(H)N4C_N)=C1	3
4761	ISSSTY_v1a_7367_02May011_6393	108283-49-4	HC(H)C(C(H)H)(C(H)H)OC(=O)N([C@](C(=O)O)C(H)H)N=N_N	3
4762	ISSSTY_v1a_7367_02May011_6394	98931-07-8	HC(H)[C@]1C(H)C2c3c4C(C(H)[C@]2N(C_N)C1H)=CN(C(H)C=CH)c4ccc3	3
4763	ISSSTY_v1a_7367_02May011_6395	52517-34-7	HC(H)N1C(H)[C@](C(H)Br)C(H)C2c3c4C(C(H)[C@]12)=CNC4ccc3	3
4764	ISSSTY_v1a_7367_02May011_6396	108283-48-3	HC(H)C(C(H)H)(C(H)H)OC(=O)[C@](C(H)H)N(C(=O)OC(C(H)H)(C(H)H)C(H)H)N=N_N	3
4765	ISSSTY_v1a_7367_02May011_6398	149127-58-2	HC(H)C(C(H)H)(N=NC(H)C(H)C(H)H)OO	3
4766	ISSSTY_v1a_7367_02May011_6399	117135-59-8	HC(H)C(C(H)H)(N=NC(H)C(H)C(H)H)OO	3
4767	ISSSTY_v1a_7367_02May011_6400	142628-08-8	HC([C@](N)C(=O)O)SC(F)(F)C(CI)Br	3
4768	ISSSTY_v1a_7367_02May011_6401	126637-65-8	HC([C@](N)C(=O)O)SC(F)(F)C(Br)Br	3
4769	ISSSTY_v1a_7367_02May011_6402	153342-07-5	HC([C@](N)C(=O)O)SC(F)(F)C(F)Br	3
4770	ISSSTY_v1a_7367_02May011_6409	153260-28-7	HC(H)C1(C(H)H)C2=C(c3c(C1H)nccc3)N=C(N)S2	3
4771	ISSSTY_v1a_7367_02May011_6411	488-11-9	C(=O)O)C(Br)=C(Br)C=O	3
4772	ISSSTY_v1a_7367_02May011_6412	149418-41-7	HC1C(Br)=C(Br)C(=O)O1	3
4773	ISSSTY_v1a_7367_02May011_6413	26049-69-4	HC(H)N(C(H)H)NC1=NC(C2=CC=C(N(=O)=O)O2)=CS1	3
4774	ISSSTY_v1a_7367_02May011_6414	191-26-4	c12c3c4c5c6c(cc4ccc3ccc1)cccc6ccc5c2	3
4775	ISSSTY_v1a_7367_02May011_6415	155014-05-4	c1(N)c2c(ccc1)ncc(F)c2	3
4776	ISSSTY_v1a_7367_02May011_6416	155014-06-5	HC(H)C(=O)Nc1c2c(cc(F)cn2)ccc1	3
4777	ISSSTY_v1a_7367_02May011_6417	147293-13-8	HC(H)N1c2c(c3c(cccn3)cc2)N=C1N	3
4778	ISSSTY_v1a_7367_02May011_6418	147293-14-9	HC(H)N1c2c(c3c(ccnc3)cc2)N=C1N	3
4779	ISSSTY_v1a_7367_02May011_6419	147293-15-0	HC(H)N1c2c(c3c(cc2)cncc3)N=C1N	3
4780	ISSSTY_v1a_7367_02May011_6425	505-57-7	HC(H)C(H)C(H)C=CC=O	3
4781	ISSSTY_v1a_7367_02May011_6426	20930-10-3	HC(H)C_CC(c1ccccc1)(c1ccccc1)OC(=O)NC1C(H)C(H)C(H)C1H	3
4782	ISSSTY_v1a_7367_02May011_6427	10087-89-5	HC1C(H)C(H)C(H)C(H)C1NC(=O)OC(c1ccccc1)(c1ccccc1)C_C	3
4783	ISSSTY_v1a_7367_02May011_6428	330-54-1	HC(H)N(C(=O)Nc1cc(Cl)c(Cl)cc1)C(H)H	3
4784	ISSSTY_v1a_7367_02May011_6429	185-75-1	HC1C2(C(H)C(H)C(H)OC2H)O1	3
4785	ISSSTY_v1a_7367_02May011_6433	215-62-3	c12c(c3c(c4c1cc1c(cccc1)n4)cccc3)cccc2	3
4786	ISSSTY_v1a_7367_02May011_6434	1146-04-9	HC(H)C1C2(C(O)C(H)H)C(=O)C3C=1C(O)C(C(H)H)(C(H)H)C=3)C(H)C2H	3
4787	ISSSTY_v1a_7367_02May011_6435	1149-99-1	HC(H)C1C2(C(O)C(H)H)C(=O)C3C=1C(O)C(C(H)H)(C(H)O)C=3)C(H)C2H	3
4788	ISSSTY_v1a_7367_02May011_6436	224-53-3	c12c(c3c(cc4c(c5c(cccc5)cc4)n3)cc1)cccc2	3

4789	ISSSTY_v1a_7367_02May011_6437	54897-63-1	HC(H)C(H)N(C(H)C(H)C(H)C(=O)O)N=O	3
4790	ISSSTY_v1a_7367_02May011_6438	142762-84-3	HC(H)OC(=O)[C@]1C(H)S[C@@]2C(Cl)=C(Cl)C(=O)N12	3
4791	ISSSTY_v1a_7367_02May011_6439	152612-74-3	HC(H)OC(=O)[C@@]1C(H)S[C@]2C(Cl)=C(Cl)C(=O)N12	3
4792	ISSSTY_v1a_7367_02May011_6440	152612-73-2	HC(H)OC(=O)C1C(H)SC2C(Cl)=C(Cl)C(=O)N12	3
4793	ISSSTY_v1a_7367_02May011_6441	54897-62-0	HC(H)C(H)N(C(H)C(H)C(H)C(H)O)N=O	3
4794	ISSSTY_v1a_7367_02May011_6443	4559-64-2	c1(N)c(N)cc2c(c1)nc1c(cc(Cl)cc1)n2	3
4795	ISSSTY_v1a_7367_02May011_6444	13147-25-6	HC(H)C(H)N(C(H)C(H)O)N=O	3
4796	ISSSTY_v1a_7367_02May011_6445	5836-85-1	HC(H)Oc1c2c(c3c(C(=O)C(H)C3H)c1)ccc1c2cccc1	3
4797	ISSSTY_v1a_7367_02May011_6447	125239-64-7	HC(H)Oc1c(N)cc2c(c1)nc1c(cc(OC(H)H)c(N)c1)n2	3
4798	ISSSTY_v1a_7367_02May011_6450	125239-65-8	HC(H)Oc1c(N)cc2c(c1)nc1c(ccc(N)c1)n2	3
4799	ISSSTY_v1a_7367_02May011_6451	159714-85-9	HC(H)C(H)c1c2c3c(c4c(c2cc2c1cccc2)cccc4)O3	3
4800	ISSSTY_v1a_7367_02May011_6452	159714-86-0	HC(H)C(H)c1c2c3c(c4c(c2cc2c1cccc2)cccc4)N3	3
4801	ISSSTY_v1a_7367_02May011_6453	146683-80-9	HC(H)c1c2c(c3c(c4c2cc2c(cccc2)c4)O3)ccc1	3
4802	ISSSTY_v1a_7367_02May011_6454	159714-84-8	HC(H)c1c2c(c3c(c4c2cc2c(cccc2)c4)N3)ccc1	3
4803	ISSSTY_v1a_7367_02May011_6455	71382-46-2	HC(H)c1c2c(c(C(H)H)c3c4c(c5c(c13)cccc5)N4)cccc2	3
4804	ISSSTY_v1a_7367_02May011_6456	39834-38-3	HC(H)c1c2-c3c(C4C(c2c(C(H)H)c2c1cccc2)O4)cccc3	3
4805	ISSSTY_v1a_7367_02May011_6457	109527-10-8	HC(H)C(=O)O[C@]1C(H)OC(Nc2ccc(N(=O)=O)cc2)[C@](OC(=O)C(H)H)[C@]1OC(=O)C(H)H	3
4806	ISSSTY_v1a_7367_02May011_6459	111858-64-1	HC1[C@@](O)[C@@](O)[C@](O)C(N(c2ccc(C(=O)O)cc2)N=O)O1	3
4807	ISSSTY_v1a_7367_02May011_6460	111858-68-5	HC(H)c1ccc(N(C(H)C2(O)[C@@](O)[C@](O)C(H)O2)N=O)cc1	3
4808	ISSSTY_v1a_7367_02May011_6461	145667-72-7	HC(Br)[C@](Br)C(H)Cl	3
4809	ISSSTY_v1a_7367_02May011_6462	145667-73-8	HC(Br)[C@@](Br)C(H)Cl	3
4810	ISSSTY_v1a_7367_02May011_6463	111858-66-3	HC(C1c2c(cccc2)NC=1)C(H)N(C1[C@](O)[C@@](O)[C@](O)C(H)O1)N=O	3
4811	ISSSTY_v1a_7367_02May011_6466	163401-68-1	HC(H)C(H)C(H)C(Cl)C(=O)S	3
4812	ISSSTY_v1a_7367_02May011_6467	125157-97-3	HC(H)C1c2c(c(C(H)H)ccc2)N(C(H)H)C2C=1c1c(cccc1)N=2	3
4813	ISSSTY_v1a_7367_02May011_6468	55738-54-0	HC(H)N(C(H)H)C=NC1=NN=C(C=CC2=CC=C(N(=O)=O)O2)O1	3
4814	ISSSTY_v1a_7367_02May011_6469	1516-74-1	c12c(cccc1)N=C(N=N_N)N2	3
4815	ISSSTY_v1a_7367_02May011_6470	1516-73-0	HC(H)N1c2c(cccc2)N=C1N=N_N	3
4816	ISSSTY_v1a_7367_02May011_6473	126420-92-6	HC(c1ccc(F)cc1)N1C2c3c(-c4c(cccc4)C12)cccc3	3
4817	ISSSTY_v1a_7367_02May011_6474	126370-96-5	HC(c1ccc(Cl)cc1)N1C2c3c(-c4c(cccc4)C12)cccc3	3
4818	ISSSTY_v1a_7367_02May011_6475	126420-93-7	HC(c1ccc(Br)cc1)N1C2c3c(-c4c(cccc4)C12)cccc3	3
4819	ISSSTY_v1a_7367_02May011_6476	126370-97-6	HC(c1c(C(F)(F)F)ccc1)N1C2c3c(-c4c(cccc4)C12)cccc3	3
4820	ISSSTY_v1a_7367_02May011_6477	126420-94-8	HC(H)c1ccc(C(H)N2C3c4c(-c5c(cccc5)C23)cccc4)cc1	3
4821	ISSSTY_v1a_7367_02May011_6478	126370-98-7	HC(H)Oc1cc(C(H)N2C3c4c(-c5c(cccc5)C23)cccc4)ccc1	3
4822	ISSSTY_v1a_7367_02May011_6479	160543-14-6	HC(H)c1c2c(c3c([C@](O)[C@@](O)C=C3)cc2)nc2c1cc(C(H)O)cc2	3
4823	ISSSTY_v1a_7367_02May011_6480	126370-99-8	HC(H)Oc1ccc(C(H)N2C3c4c(-c5c(cccc5)C23)cccc4)cc1	3
4824	ISSSTY_v1a_7367_02May011_6481	160543-15-7	HC(H)c1cc2c(C(H)O)c3c(c4c([C@](O)[C@@](O)C=C4)cc3)nc2cc1	3
4825	ISSSTY_v1a_7367_02May011_6483	126420-95-9	HC(H)c1c(C(H)N2C3c4c(-c5c(cccc5)C23)cccc4)c(C(H)H)cc(C(H)H)c1	3
4826	ISSSTY_v1a_7367_02May011_6484	160637-28-5	HC(H)c1c2c(c3c([C@](O)[C@@](O)C=C3)cc2)nc2c1cc(C(H)H)cc2	3
4827	ISSSTY_v1a_7367_02May011_6486	126371-00-4	HC(c1ccc(N(=O)=O)cc1)N1C2c3c(-c4c(cccc4)C12)cccc3	3
4828	ISSSTY_v1a_7367_02May011_6487	160543-00-0	HC(H)c1cc2c(C(H)O)c3c(c4c(cccc4)cc3)nc2cc1	3
4829	ISSSTY_v1a_7367_02May011_6488	160543-02-2	HC(H)c1c2c(c3c(cccc3)cc2)nc2c1cc(C(H)O)cc2	3
4830	ISSSTY_v1a_7367_02May011_6489	160543-04-4	HC(O)c1c2c(c3c(cccc3)cc2)nc2c1cc(C(H)O)cc2	3

4831	ISSSTY_v1a_7367_02May011_6490	160637-30-9	HC(H)c1c2c(c3c([C@](O)[C@@](O)C=C3)cc2)nc2c1ccc(C(H)H)c2	3
4832	ISSSTY_v1a_7367_02May011_6491	160637-29-6	HC(H)c1c2c(c3c(cccc3)cc2)nc2c1[C@](O)[C@@](O)C(C(H)H)=C2	3
4833	ISSSTY_v1a_7367_02May011_6493	160543-08-8	HC(H)c1c2c(c3c(cccc3)cc2)nc2c1ccc(C(H)O)c2	3
4834	ISSSTY_v1a_7367_02May011_6496	394-70-7	c1(F)c2c(cccc2)nc1	3
4835	ISSSTY_v1a_7367_02May011_6498	57-74-9	HC1C2C3(CI)C(CI)(CI)C(CI)(C(CI)=C3CI)C2C(CI)C1CI	3
4836	ISSSTY_v1a_7367_02May011_6499	95741-57-4	HC(H)c1cc2c3c(c4c(c3ccc2)cc2c(cccc2)c4)c1	3
4837	ISSSTY_v1a_7367_02May011_6500	95741-56-3	HC(H)c1c2c(c(C(H)H)c3c4c5c(c13)cccc5ccc4)cccc2	3
4838	ISSSTY_v1a_7367_02May011_6501	32818-80-7	HC(H)N(C(H)O)N(=O)=O	3
4839	ISSSTY_v1a_7367_02May011_6502	36239-01-7	HC(H)C(=O)OC(H)N(C(H)H)N(=O)=O	3
4840	ISSSTY_v1a_7367_02May011_6503	157996-62-8	c12c(c(N)c3c(ccc([N+](=O)[O-])c3)n1)cc([N+](=O)[O-])cc2	3
4841	ISSSTY_v1a_7367_02May011_6504	790-60-3	c12c(c3c(c4c1cc1c(cccc1)c4)cccc3)O2	3
4842	ISSSTY_v1a_7367_02May011_6505	1193-54-0	C1(=O)C(CI)=C(CI)C(=O)N1	3
4843	ISSSTY_v1a_7367_02May011_6506	170660-62-5	HC1C(=C(CI)CI)C(=O)NC1=O	3
4844	ISSSTY_v1a_7367_02May011_6507	170660-63-6	C1(=O)C(=C(CI)CI)C(CI)C(=O)N1	3
4845	ISSSTY_v1a_7367_02May011_6509	28342-33-8	HC(H)N1C(=O)c2c(-c3c1c1c(cc4c(c1)OC(H)O4)cc3)ccc(OC(H)H)c2OC(H)H	3
4846	ISSSTY_v1a_7367_02May011_6510	816-57-9	HC(H)C(H)C(H)N(C(N)=O)N=O	3
4847	ISSSTY_v1a_7367_02May011_6512	7132-67-4	c12c(c(N)c3c(ccc(O)c3)n1)cccc2	3
4848	ISSSTY_v1a_7367_02May011_6513	15444-20-9	HC(H)Oc1c2-c3c(C(=O)c4c2c(cc1OC(H)H)ccn4)cccc3	3
4849	ISSSTY_v1a_7367_02May011_6514	70403-81-5	HC(H)Oc1c2-c3c(C(=O)c4c2c(cc1OC(H)H)ccn4)cc(OC(H)H)cc3	3
4850	ISSSTY_v1a_7367_02May011_6515	88741-67-7	HC(H)Oc1c(O)c2C(=O)c3c(-c4c2c(ccn4)c1)cc(OC(H)H)cc3	3
4851	ISSSTY_v1a_7367_02May011_6516	88741-68-8	HC(H)Oc1c2C(=O)c3c(-c4c2c(cc1OC(H)H)ccn4)cc(OC(H)H)cc3	3
4852	ISSSTY_v1a_7367_02May011_6522	72100-19-7	c12c(c3c(c4c1cc1c(c(O)c(O)cc1)c4)cccc3)cccc2	3
4853	ISSSTY_v1a_7367_02May011_6523	132172-57-7	c1(O)c(O)c2c(c3c(c4c2cc2c(cccc2)c4)cccc3)cc1	3
4854	ISSSTY_v1a_7367_02May011_6524	132172-58-8	c1(O)c(O)c2c(c3c(c4c2cccc4)cc2c(cccc2)c3)cc1	3
4855	ISSSTY_v1a_7367_02May011_6525	88488-97-5	c12c(c3c(c4c1cc1c(cccc1)c4)ccc(O)c3)cccc2	3
4856	ISSSTY_v1a_7367_02May011_6526	113058-38-1	c12c(c3c(c4c1cc1c(cccc1)c4)cc(O)cc3)cccc2	3
4857	ISSSTY_v1a_7367_02May011_6528	113058-39-2	c1(O)c2c(c3c(c4c2cccc4)cc2c(cccc2)c3)ccc1	3
4858	ISSSTY_v1a_7367_02May011_6529	39081-15-7	c12c(c3c(c4c1cc1c(c(O)ccc1)c4)cccc3)cccc2	3
4859	ISSSTY_v1a_7367_02May011_6530	39147-43-8	c12c(c3c(c4c1cc1c(cc(O)cc1)c4)cccc3)cccc2	3
4860	ISSSTY_v1a_7367_02May011_6531	132172-56-6	c12c(c3c(c4c1C=CC=CO4)cccc3)cc1c(cccc1)c2	3
4861	ISSSTY_v1a_7367_02May011_6532	117022-35-2	HC(H)c1c2c(c3c(c4c(C(O)C(O)C5C4O5)cc3)c(C(H)H)c2)ccc1	3
4862	ISSSTY_v1a_7367_02May011_6533	129176-04-1	HC(Br)[C@]1[C@](Cl)O1	3
4863	ISSSTY_v1a_7367_02May011_6534	129176-05-2	HC(Br)C1C(Cl)O1	3
4864	ISSSTY_v1a_7367_02May011_6535	90745-27-0	HC(H)c1c2c(N(=O)=O)cccc2ccc1	3
4865	ISSSTY_v1a_7367_02May011_6536	54755-21-4	HC(H)c1cc2c(N(=O)=O)cccc2cc1	3
4866	ISSSTY_v1a_7367_02May011_6537	13615-38-8	HC(H)c1cc2c(N(=O)=O)cccc2cc1	3
4867	ISSSTY_v1a_7367_02May011_6538	91137-27-8	HC(H)c1c2c(c(N(=O)=O)ccc2)ccc1	3
4868	ISSSTY_v1a_7367_02May011_6539	1951-56-0	HC(H)C(C(H)H)NC(=O)C=CC1=CC=C(N(=O)=O)O1	3
4869	ISSSTY_v1a_7367_02May011_6540	54755-20-3	HC(H)c1cc2c(c(N(=O)=O)ccc2)cc1	3
4870	ISSSTY_v1a_7367_02May011_6541	880-93-3	HC(H)c1c2c(c(N(=O)=O)cc1)cccc2	3
4871	ISSSTY_v1a_7367_02May011_6543	105752-67-8	HC(H)c1c2c(cc(N(=O)=O)cc2)ccc1	3
4872	ISSSTY_v1a_7367_02May011_6544	63017-87-8	HC(H)c1c2c(ccc1N(=O)=O)cccc2	3

4873	ISSSTY_v1a_7367_02May011_6545	41037-13-2	HC(H)c1c2c(cc(N(=O)=O)c1)cccc2	3
4874	ISSSTY_v1a_7367_02May011_6546	116530-07-5	HC(H)c1c2c(ccc(N(=O)=O)c2)ccc1	3
4875	ISSSTY_v1a_7367_02May011_6547	91137-28-9	HC(H)c1cc2c(ccc(N(=O)=O)c2)cc1	3
4876	ISSSTY_v1a_7367_02May011_6548	54357-08-3	HC(H)c1cc2c(cc(N(=O)=O)cc2)cc1	3
4877	ISSSTY_v1a_7367_02May011_6552	19655-56-2	HC(H)C(H)c1c2c(cccn2)ccc1	3
4878	ISSSTY_v1a_7367_02May011_6553	134109-03-8	c12c(c(Cl)c3c(c4c([C@](O)[C@@](O)C=C4)cc3)c1)cccc2	3
4879	ISSSTY_v1a_7367_02May011_6554	35509-27-4	C(N)c1c2c(cccn2)ccc1	3
4880	ISSSTY_v1a_7367_02May011_6558	60657-25-2	c12c3c4c(c5c(C=C[C@](O)[C@]5O)cc4ccc3ccc1)cc2	3
4881	ISSSTY_v1a_7367_02May011_6561	32795-84-9	c12c(c(Br)c3c(c4c(cccc4)cc3)c1)cccc2	3
4882	ISSSTY_v1a_7367_02May011_6563	94339-56-7	HC1c2c(c3c4c5c(ccc4c2)cccc5cc3)C=CC1O	3
4883	ISSSTY_v1a_7367_02May011_6564	94339-55-6	HC1C(O)c2c(c3c4c5c(ccc4c2)cccc5cc3)C=C1	3
4884	ISSSTY_v1a_7367_02May011_6565	199536-62-4	HC(Br)C1=C(Br)C(=O)OC1H	3
4885	ISSSTY_v1a_7367_02May011_6567	199536-64-6	HC(Br)C1=C(Br)C(=O)OC1O	3
4886	ISSSTY_v1a_7367_02May011_6568	199536-79-3	HC1C(C(Br)Br)=C(Br)C(=O)O1	3
4887	ISSSTY_v1a_7367_02May011_6569	199536-82-8	HC1C(C(Br)Br)=C(Cl)C(=O)O1	3
4888	ISSSTY_v1a_7367_02May011_6570	199536-84-0	HC(Cl)C1=C(Br)C(=O)OC1H	3
4889	ISSSTY_v1a_7367_02May011_6571	199536-65-7	HC(Br)C1=C(Cl)C(=O)OC1H	3
4890	ISSSTY_v1a_7367_02May011_6573	230-46-6	c12c(c3c(cccn3)cc1)cccn2	3
4891	ISSSTY_v1a_7367_02May011_6574	191861-16-2	c1(F)c2c(c3c(cccn3)c1)cccn2	3
4892	ISSSTY_v1a_7367_02May011_6575	191861-17-3	c12c(c3c(cccn3)cc1)cc(F)cn2	3
4893	ISSSTY_v1a_7367_02May011_6577	191861-19-5	c1(F)c2c(c3c(cccn3)c1)nccc2	3
4894	ISSSTY_v1a_7367_02May011_6579	163275-58-9	c1(F)c2c(c3c(cccc3)c1)nccc2	3
4895	ISSSTY_v1a_7367_02May011_6580	163275-59-0	c1(F)c2c(c3c(cccn3)c1)cccc2	3
4896	ISSSTY_v1a_7367_02May011_6581	163275-60-3	c1(F)c2c(c3c(cccn3)cc2)ccc1	3
4897	ISSSTY_v1a_7367_02May011_6582	163275-61-4	c12c(c3c(ccc(F)c3)cc1)nccc2	3
4898	ISSSTY_v1a_7367_02May011_6584	163275-64-7	c12c(c3c(c(F)ccc3F)cc1)nccc2	3
4899	ISSSTY_v1a_7367_02May011_6585	163275-65-8	c12c(c3c(cccc3)cc1)cc(F)cn2	3
4900	ISSSTY_v1a_7367_02May011_6586	163275-66-9	c12c(c3c(c(F)ccc3)cc1)cccn2	3
4901	ISSSTY_v1a_7367_02May011_6587	163275-67-0	c1(F)c2c3c(ccc2ccc1)nccc3	3
4902	ISSSTY_v1a_7367_02May011_6588	163275-68-1	c12c(c3c(c(F)ccc3F)cc1)cccn2	3
4903	ISSSTY_v1a_7367_02May011_6589	88492-34-6	HC(C(O)C(H)N1c2c(c(N)ncn2)N=C1)N=N_N	3
4904	ISSSTY_v1a_7367_02May011_6590	87009-12-9	C1(=O)C=CNC(=O)N1	3
4905	ISSSTY_v1a_7367_02May011_6591	133762-80-8	HC(H)C1C(=O)NC(=O)N(C(H)C(O)C(H)N=N_N)C=1	3
4906	ISSSTY_v1a_7367_02May011_6593	66927-03-5	HC([C@@](O)[C@](O)[C@](O)[C@@](O)C=O)N=N_N	3
4907	ISSSTY_v1a_7367_02May011_6594	20847-05-6	HC([C@@](O)[C@@](O)[C@](O)[C@@](O)C=O)N=N_N	3
4908	ISSSTY_v1a_7367_02May011_6595	2381-39-7	HC(H)c1c2c(c3c4c5c(ccc14)cccc5cc3)cccc2	3
4909	ISSSTY_v1a_7367_02May011_6596	117333-21-8	HC(C1c2c(cccc2)N(N=O)C=1)C(O)C(=O)O	3
4910	ISSSTY_v1a_7367_02May011_6598	7068-83-9	HC(H)C(H)C(H)C(H)N(C(H)H)N=O	3
4911	ISSSTY_v1a_7367_02May011_6599	13088-34-1	C(Cl)(Cl)=C1C=CC(=O)O1	3
4912	ISSSTY_v1a_7367_02May011_6600	112654-68-9	C1(=O)C(Cl)=CC(=C(Cl)Cl)O1	3
4913	ISSSTY_v1a_7367_02May011_6601	31555-54-1	C1(=O)C(Cl)=C(Cl)C(=C(Cl)Cl)O1	3
4914	ISSSTY_v1a_7367_02May011_6602	101328-96-5	C1(=O)C(Cl)(Cl)C(=O)C=C1	3

4915	ISSSTY_v1a_7367_02May011_6603	61445-55-4	HC(H)N(C(H)C(H)C(H)C(=O)O)N=O	3
4916	ISSSTY_v1a_7367_02May011_6604	88552-47-0	C1(=O)C(Cl)(Cl)C(=O)C(Cl)=C1	3
4917	ISSSTY_v1a_7367_02May011_6609	202345-21-9	HC(H)c1c(NO)nc2c(-c3c(cccc3)N2)c1	3
4918	ISSSTY_v1a_7367_02May011_6610	23045-12-7	HC(H)c1cc2c(N)c3c(cccc3)nc2cc1	3
4919	ISSSTY_v1a_7367_02May011_6611	194479-75-9	HC(H)c1cc2c(N)c3c(ccc(C(H)H)c3)nc2cc1	3
4920	ISSSTY_v1a_7367_02May011_6612	23250-39-7	c12c(c(N)c3c(ccc(Cl)c3)n1)cccc2	3
4921	ISSSTY_v1a_7367_02May011_6613	157996-59-3	c12c(c(N)c3c(ccc(Br)c3)n1)cccc2	3
4922	ISSSTY_v1a_7367_02May011_6614	194479-79-3	c12c(c(N)c3c(ccc(l)c3)n1)cccc2	3
4923	ISSSTY_v1a_7367_02May011_6616	55090-44-3	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)N=O	3
4924	ISSSTY_v1a_7367_02May011_6619	97170-07-5	HC(H)c1c2c(c3c(cccc3)c1)ccc1c2[C@]2[C@@]([C@@](O)[C@@]1O)O2	3
4925	ISSSTY_v1a_7367_02May011_6621	7258-52-8	HC1c2c(c3c4c(ccc3cc2)cccc4)C(H)C1H	3
4926	ISSSTY_v1a_7367_02May011_6622	183249-37-8	HC1c2c(c3c4c(ccc3cc2)cccc4)C=C1	3
4927	ISSSTY_v1a_7367_02May011_6624	212-54-4	HC1c2c(-c3c1c1c4c(ccc1cc3)cccc4)cccc2	3
4928	ISSSTY_v1a_7367_02May011_6628	611-35-8	c1(Cl)c2c(cccc2)ncc1	3
4929	ISSSTY_v1a_7367_02May011_6630	635-27-8	c1(Cl)c2c(ccc1)nccc2	3
4930	ISSSTY_v1a_7367_02May011_6631	612-57-7	c12c(cc(Cl)cc1)cccn2	3
4931	ISSSTY_v1a_7367_02May011_6633	622-79-7	HC(c1ccccc1)N=N_N	3
4932	ISSSTY_v1a_7367_02May011_6635	51938-16-0	HC(H)N(C(H)C(H)C(H)C(H)O)N=O	3
4933	ISSSTY_v1a_7367_02May011_6636	173216-43-8	HC(H)[C@@](c1ccccc1)C(H)C(H)N=N_N	3
4934	ISSSTY_v1a_7367_02May011_6637	173216-44-9	HC(C(H)C(c1ccccc1)c1ccccc1)N=N_N	3
4935	ISSSTY_v1a_7367_02May011_6638	134625-72-2	HC([C@](O)c1ccccc1)N=N_N	3
4936	ISSSTY_v1a_7367_02May011_6639	124817-06-7	HC([C@@](O)c1ccccc1)N=N_N	3
4937	ISSSTY_v1a_7367_02May011_6640	173216-45-0	HC(c1ccccc1)[C@](C(H)N=N_N)C(H)O	3
4938	ISSSTY_v1a_7367_02May011_6641	173216-46-1	HC(c1ccccc1)[C@@](C(H)N=N_N)C(H)O	3
4939	ISSSTY_v1a_7367_02May011_6642	84506-41-2	HC(H)[C@@](C(=O)OC(H)H)C(H)N=N_N	3
4940	ISSSTY_v1a_7367_02May011_6643	107747-84-2	HC(H)[C@](C(=O)OC(H)H)C(H)N=N_N	3
4941	ISSSTY_v1a_7367_02May011_6644	121745-57-1	HC(O)[C@](O)[C@@](c1ccccc1)N=N_N	3
4942	ISSSTY_v1a_7367_02May011_6645	116911-14-9	HC(O)[C@@](O)[C@](c1ccccc1)N=N_N	3
4943	ISSSTY_v1a_7367_02May011_6646	6367-36-8	HC(H)C(C(H)H)(C(H)H)OC(=O)C(H)N=N_N	3
4944	ISSSTY_v1a_7367_02May011_6647	134874-62-7	c1([N+](=O)[O-])c2c3c(c4c(c5c3c(ccc5)cc2)cccc4)c([N+](=O)[O-])c1	3
4945	ISSSTY_v1a_7367_02May011_6648	120014-85-9	HC1c2c3c4c5c(c(N(=O)=O)ccc5ccc4cc2C(O)C(H)C1H)cc3	3
4946	ISSSTY_v1a_7367_02May011_6649	134998-76-8	HC1c2c(c3c4c5c(c(N=O)ccc5cc3)ccc4c2)C(H)C(H)C1H	3
4947	ISSSTY_v1a_7367_02May011_6650	67616-44-8	HC(C(H)O)SN=O	3
4948	ISSSTY_v1a_7367_02May011_6652	115-02-6	HC(C(N)C(=O)O)OC(=O)C=[N+]=[N-]	3
4949	ISSSTY_v1a_7367_02May011_6653	21638-36-8	HC(H)C1C(H)N(N=CC2=CC=C(N(=O)=O)O2)C(=O)N1	3
4950	ISSSTY_v1a_7367_02May011_6654	89930-59-6	HC(H)C1C(H)N(C(H)H)[C@@]2C(H)C3c4c(cccc4[C@]2C=1)N(C(H)C(H)C(H)H)C=3	3
4951	ISSSTY_v1a_7367_02May011_6655	53757-29-2	HC(H)C1=NC(C2=CC=C(N(=O)=O)O2)=CS1	3
4952	ISSSTY_v1a_7367_02May011_6656	101328-75-0	HC(H)C1C(H)N(C(H)H)[C@@]2C(H)C3c4c(cccc4[C@]2C=1)N(C(H)C(H)C(H)C(H)H)C=3	3
4953	ISSSTY_v1a_7367_02May011_6657	82617-23-0	HC1C(OC(N)=O)O1	3
4954	ISSSTY_v1a_7367_02May011_6658	239-35-0	c12-c3c(c4c(cccc4)cc3)Sc1cccc2	3
4955	ISSSTY_v1a_7367_02May011_6662	92078-92-7	HC(H)NN=O	3
4956	ISSSTY_v1a_7367_02May011_6665	333-27-7	HC(H)OS(=O)(=O)C(F)(F)F	3

4957	ISSSTY_v1a_7367_02May011_6670	184582-64-7	HC(H)C(=O)NSc1c2c(cccc(O)c2)nc2c1cc(O)cc2	3
4958	ISSSTY_v1a_7367_02May011_6671	29700-20-7	HC(O)C1=CC=C(c2c3c(-c4c(ccccc4)N3)ccn2)O1	3
4959	ISSSTY_v1a_7367_02May011_6673	66267-19-4	c12c(c3c([C@@](O)[C@](O)C=C3)cc1)cc1c(c3c(cccc3)cc1)c2	3
4960	ISSSTY_v1a_7367_02May011_6676	28657-80-9	HC(H)C(H)N1c2c(C(=O)C(C(=O)O)=N1)cc1c(c2)OC(H)O1	3
4961	ISSSTY_v1a_7367_02May011_6677	70458-92-3	HC(H)C(H)N1c2c(C(=O)C(C(=O)O)=C1)cc(F)c(N1C(H)C(H)N(C(H)H)C(H)C1H)c2	3
4962	ISSSTY_v1a_7367_02May011_6678	125369-79-1	C(N)C(c1c(Cl)cccc1)=CC=Cc1cccc1	3
4963	ISSSTY_v1a_7367_02May011_6679	155144-64-2	HC(H)c1cc(-c2c(F)cc3c(c2)N(C2C(H)C2H)C2=CC(=O)N(O)C(=O)N32)cc(C(H)H)n1	3
4964	ISSSTY_v1a_7367_02May011_6680	115550-35-1	HC(H)N1C(H)C(H)N(c2c3c4c(C(=O)C(C(=O)O)=CN4N(C(H)H)C(H)O3)cc2F)C(H)C1H	3
4965	ISSSTY_v1a_7367_02May011_6681	103978-08-1	HC(H)C(H)N1c2c(C(=O)C(C(=O)O)=C1)cc(F)c(-c1ccc(O)cc1)c2F	3
4966	ISSSTY_v1a_7367_02May011_6682	93106-60-6	HC(H)C(H)N1C(H)C(H)N(c2c(F)cc3C(=O)C(C(=O)O)=CN(C4C(H)C4H)c3c2)C(H)C1H	3
4967	ISSSTY_v1a_7367_02May011_6685	42286-46-4	c12C(=O)C(=O)c3c4c(c5c(cccc5)c3)ccc(c14)ccc2	3
4968	ISSSTY_v1a_7367_02May011_6686	34522-72-0	c1(F)c2c(cc(F)c1)nccc2	3
4969	ISSSTY_v1a_7367_02May011_6694	139347-89-0	HC(H)c1c2c(c3c(c4c(C(O)C(O)C5C4O5)cc3)c1C(H)H)cccc2	3
4970	ISSSTY_v1a_7367_02May011_6695	139627-44-4	HC(H)c1c2c(c3c(c4c(C(O)C(O)C5C4O5)cc3)c(C(H)H)c2)ccc1	3
4971	ISSSTY_v1a_7367_02May011_6696	91540-29-3	HC(H)C(H)C(H)C(H)C(H)N1C2c3c(-c4c(cccc4)C12)cccc3	3
4972	ISSSTY_v1a_7367_02May011_6697	139493-54-2	HC(H)c1c2c(c3c(ccc(C(H)H)c3)c1)ccc1c2[C@@]2[C@]([C@](O)[C@@]1O)O2	3
4973	ISSSTY_v1a_7367_02May011_6698	81593-13-7	HC(H)C(H)OP(=O)(N1C2c3c(-c4c(cccc4)C12)cccc3)OC(H)C(H)H	3
4974	ISSSTY_v1a_7367_02May011_6699	106686-67-3	HC(c1cccc1)S(=O)(=O)N1C2c3c(-c4c(cccc4)C12)cccc3	3
4975	ISSSTY_v1a_7367_02May011_6702	8004-87-3	HC(H)N(c1ccc([C+](c2ccc(N(C(H)H)C(H)H)cc2)c2ccc(NC(H)H)cc2)cc1)C(H)H	3
4976	ISSSTY_v1a_7367_02May011_6703	128753-82-2	HC(H)C12C(OC(H)H)(c3c(cccc3)O1)OO2	3
4977	ISSSTY_v1a_7367_02May011_6704	128753-83-3	HC(H)C12c3c(cccc3)OC1OO2	3
4978	ISSSTY_v1a_7367_02May011_6705	772-43-0	C(N)(C1=CC=C(N(=O)=O)O1)=NO	3
4979	ISSSTY_v1a_7367_02May011_6706	128753-86-6	HC(H)C12C(C(H)H)(c3c(c(C(=O)C(H)H)ccc3)O1)OO2	3
4980	ISSSTY_v1a_7367_02May011_6707	128753-87-7	HC(H)C12C(C(H)H)(c3c(cccc3OC(H)H)O1)OO2	3
4981	ISSSTY_v1a_7367_02May011_6708	128753-88-8	HC(H)C12C(C(H)H)(c3c(c(OC(H)H)ccc3)O1)OO2	3
4982	ISSSTY_v1a_7367_02May011_6709	128753-90-2	HC(H)C12C(C(H)H)(c3c(cc(OC(=O)C(H)H)cc3)O1)OO2	3
4983	ISSSTY_v1a_7367_02May011_6711	128753-91-3	HC(H)C12C(C(H)H)(c3c(ccc(OC(=O)C(H)H)c3)O1)OO2	3
4984	ISSSTY_v1a_7367_02May011_6714	128753-95-7	HC(H)C12c3c(cccc3)OC1(C(H)OC(H)H)OO2	3
4985	ISSSTY_v1a_7367_02May011_6715	128753-96-8	HC(H)C12c3c(cccc3)OC1(C(H)OC(=O)C(H)H)OO2	3
4986	ISSSTY_v1a_7367_02May011_6716	128753-99-1	HC(H)C12c3c(cccc3)OC1(C(H)OC(=O)Nc1ccc(Cl)cc1)OO2	3
4987	ISSSTY_v1a_7367_02May011_6717	129812-24-4	HC(H)C12C(C(H)H)(c3c(cc4c(C(C(H)H)=CC(=O)O4)c3)O1)OO2	3
4988	ISSSTY_v1a_7367_02May011_6718	129833-00-7	HC(H)C12C(C(H)H)(c3c(c4c(C(C(H)H)=CC(=O)O4)cc3)O1)OO2	3
4989	ISSSTY_v1a_7367_02May011_6719	2578-75-8	HC(H)C(=O)NC1=NN=C(C2=CC=C(N(=O)=O)O2)S1	3
4990	ISSSTY_v1a_7367_02May011_6720	129812-26-6	HC(H)C12C(C(H)H)(c3c4C(C(H)H)=CC(=O)Oc4ccc3O1)OO2	3
4991	ISSSTY_v1a_7367_02May011_6725	710-25-8	C(N)(=O)C=CC1=CC=C(N(=O)=O)O1	3
4992	ISSSTY_v1a_7367_02May011_6726	3675-13-6	C(=O)C=CC=O	3
4993	ISSSTY_v1a_7367_02May011_6729	53757-28-1	C1(C2=CC=C(N(=O)=O)O2)=CSC=N1	3
4994	ISSSTY_v1a_7367_02May011_6732	220042-15-9	C1(C2C(=O)C=C(Nc3ccc(N(=O)=O)cc3)C(=O)C=2)=NN=C(NC(=O)c2cccc2)S1	3
4995	ISSSTY_v1a_7367_02May011_6734	128350-00-5	HC(H)C(C(c1cccc1)C(c1cc(Cl)c(Cl)cc1)C_N)C=C(c1cc(Cl)c(Cl)cc1)C_N	3
4996	ISSSTY_v1a_7367_02May011_6736	3741-15-9	c1(N(=O)=O)c2c(cccc2)ncc1	3
4997	ISSSTY_v1a_7367_02May011_6738	125847-46-3	c12-c3c(c4c([C@@](O)[C@](O)C=C4)cc3)Sc1cccc2	3
4998	ISSSTY_v1a_7367_02May011_6742	96563-10-9	HC(H)C1c2c(-c3c1cc(F)cc3)ccc(F)c2	3

4999	ISSSTY_v1a_7367_02May011_6743	2523-37-7	HC(H)C1c2c(-c3c1cccc3)cccc2	3
5000	ISSSTY_v1a_7367_02May011_6744	96563-11-0	HC(H)C1c2c(-c3c1cc(F)cc3)cccc2	3
5001	ISSSTY_v1a_7367_02May011_6745	504-78-9	HC1C(H)[N+](H)C(H)S1	3
5002	ISSSTY_v1a_7367_02May011_6746	102234-07-1	HC1C2(C(=O)N(C(H)C(H)N3C(H)C3H)C(=O)N2)C(H)C(H)C(H)C1H	3
5003	ISSSTY_v1a_7367_02May011_6749	923-32-0	HC(C(N)C(=O)O)SSC(H)C(N)C(=O)O	3
5004	ISSSTY_v1a_7367_02May011_6750	70-54-2	HC(N)C(H)C(H)C(H)C(N)C(=O)O	3
5005	ISSSTY_v1a_7367_02May011_6752	609-36-9	HC1C(H)C(H)C(C(=O)O)N1	3
5006	ISSSTY_v1a_7367_02May011_6753	80-68-2	HC(H)C(O)C(N)C(=O)O	3
5007	ISSSTY_v1a_7367_02May011_6758	141691-42-1	HC(H)N1c2c(ccc(C_N)c2)N=C1N	3
5008	ISSSTY_v1a_7367_02May011_6759	139953-95-0	HC(H)C(H)C(H)OC=CC=CC=CC=CC(H)C(H)H	3
5009	ISSSTY_v1a_7367_02May011_6760	225366-91-6	c1(F)c(F)c2c(cc1)ncccc2	3
5010	ISSSTY_v1a_7367_02May011_6761	1234799	HC(H)C1C(C(O)=C2C(=O)C(=O)N(C(H)c3ccnc3)C2c2ccc(Cl)cc2)=C(C(H)H)NC=1C(=O)OC(H)C(H)H	3
5011	ISSSTY_v1a_7367_02May011_6762	139953-97-2	HC(H)C(H)C=CC=CC=CC=CC=COC(H)C(O)C(H)H	3
5012	ISSSTY_v1a_7367_02May011_6763	145241-76-5	c1(F)c(F)c2c(cccn2)cc1	3
5013	ISSSTY_v1a_7367_02May011_6764	139953-98-3	HC(H)C(H)C=CC=CC=CC=CC=COC(H)C(O)c1cccc1	3
5014	ISSSTY_v1a_7367_02May011_6765	139259-93-1	HC(H)C(c1ccc(C(H)ON(C(=O)c2ccccc2)OC(=O)C(H)H)cc1)(C(H)H)C(H)H	3
5015	ISSSTY_v1a_7367_02May011_6766	220168-39-8	HC(c1cccc1)ON(C(=O)c1cccc1)OC(=O)c1cccc1	3
5016	ISSSTY_v1a_7367_02May011_6768	145241-75-4	c1(F)c2c(cc(F)c1)cccn2	3
5017	ISSSTY_v1a_7367_02May011_6769	1234712	c1(F)c(F)c(F)c(F)c2c1cccn2	3
5018	ISSSTY_v1a_7367_02May011_6770	220168-56-9	HC(H)C(c1ccc(C(=O)ON(C(=O)c2ccccc2)OC(H)c2ccccc2)cc1)(C(H)H)C(H)H	3
5019	ISSSTY_v1a_7367_02May011_6771	25413-64-3	HC(H)C(H)C(H)C(H)N(C(H)C(H)C(H)H)N=O	3
5020	ISSSTY_v1a_7367_02May011_6772	56316-37-1	HC(H)C(H)C(H)N(C(H)C(H)C(H)C(=O)O)N=O	3
5021	ISSSTY_v1a_7367_02May011_6773	66-75-1	HC(Cl)C(H)N(C1C(=O)NC(=O)NC=1)C(H)C(H)Cl	3
5022	ISSSTY_v1a_7367_02May011_6774	339152-94-2	C1(=O)C(Cl)=C(C(Cl)Cl)C(=O)N1	3
5023	ISSSTY_v1a_7367_02May011_6775	339152-95-3	HC(Cl)C1C(=O)NC(=O)C=1Cl	3
5024	ISSSTY_v1a_7367_02May011_6777	339152-96-4	HC(Br)C1C(=O)NC(=O)C=1Cl	3
5025	ISSSTY_v1a_7367_02May011_6778	60883-97-8	HC(H)c1ccc(S(=O)(=O)N2C3c4c(-c5c(cccc5)C23)cccc4)cc1	3
5026	ISSSTY_v1a_7367_02May011_6780	51938-12-6	HC(H)C(H)C(H)N(C(H)C(H)C(H)C(H)O)N=O	3
5027	ISSSTY_v1a_7367_02May011_6798	106626-55-5	HC(H)N(C(H)H)C(H)C(H)NC(=O)c1c2c(ccc1)nc1c(cccc1)c2	3
5028	ISSSTY_v1a_7367_02May011_6799	89459-25-6	HC(H)N(C(H)H)C(H)C(H)NC(=O)c1c2c(cc3c(cccc3)n2)ccc1	3
5029	ISSSTY_v1a_7367_02May011_6800	103942-97-8	HC(H)N(C(H)H)C(H)C(H)NC(=O)c1c2c(ccc1)nc1c(cccc1)n2	3
5030	ISSSTY_v1a_7367_02May011_6801	112022-05-6	HC(H)N(C(H)H)C(H)C(H)NC(=O)c1c2c(cc3c(cccc3)c2)ccc1	3
5031	ISSSTY_v1a_7367_02May011_6802	112022-09-0	HC(H)N(C(H)H)C(H)C(H)NC(=O)C1C2N(C(=O)c3c(cccc3)N=2)C=CC=1	3
5032	ISSSTY_v1a_7367_02May011_6804	103554-58-1	HC(H)N(C(H)H)C(H)C(H)NC(=O)c1c2c(C(=O)c3c(cccc3)N2)ccc1	3
5033	ISSSTY_v1a_7367_02May011_6805	112022-08-9	HC(H)N(C(H)H)C(H)C(H)NC(=O)c1c2c(C(=O)c3c(cccc3)O2)ccc1	3
5034	ISSSTY_v1a_7367_02May011_6807	112022-07-8	HC(H)N(C(H)H)C(H)C(H)NC(=O)c1c2c(C(=O)c3c(cccc3)S2)ccc1	3
5035	ISSSTY_v1a_7367_02May011_6808	112022-06-7	HC(H)N(C(H)H)C(H)C(H)NC(=O)c1c2C(=O)c3c(C(=O)c2ccc1)cccc3	3
5036	ISSSTY_v1a_7367_02May011_6810	112022-13-6	HC(H)N(C(H)H)C(H)C(H)NC(=O)c1c2c(ccc1)Oc1c(cccc1)N2	3
5037	ISSSTY_v1a_7367_02May011_6811	112022-10-3	HC(H)N(C(H)H)C(H)C(H)NC(=O)c1c2c(ccc1)Oc1c(cccc1)O2	3
5038	ISSSTY_v1a_7367_02May011_6812	131862-15-2	HC(H)N(C(H)H)C(H)C(H)NC(=O)c1c2c(c3c(cccc3)cn2)ccc1	3
5039	ISSSTY_v1a_7367_02May011_6813	131862-17-4	HC(H)N(C(H)H)C(H)C(H)NC(=O)c1c2c(c3c(cccc3)c1)cccn2	3
5040	ISSSTY_v1a_7367_02May011_6814	131862-18-5	HC(H)N(C(H)H)C(H)C(H)NC(=O)c1ccc2c(c3c(cccn3)cc2)n1	3

5041	ISSSTY_v1a_7367_02May011_6816	107027-12-3	HC(H)N(C(H)H)C(H)C(H)NC(=O)c1c2c(ccc(-c3ccccc3)n2)ccc1	3
5042	ISSSTY_v1a_7367_02May011_6817	124340-47-2	HC(H)N(C(H)H)C(H)C(H)NC(=O)c1c2c(ccc1)NC(c1ccccc1)=N2	3
5043	ISSSTY_v1a_7367_02May011_6820	131862-21-0	HC(H)N(C(H)H)C(H)C(H)NC(=O)C1C2N(C=C(c3ccccc3)N=2)C=CC=1	3
5044	ISSSTY_v1a_7367_02May011_6821	107027-31-6	HC(H)N(C(H)H)C(H)C(H)NC(=O)c1c2c(ccc1)ncc(-c1ccccc1)n2	3
5045	ISSSTY_v1a_7367_02May011_6822	131862-22-1	HC(H)N(C(H)H)C(H)C(H)NC(=O)c1c2c(C=C(c3ccccc3)O2)ccc1	3
5046	ISSSTY_v1a_7367_02May011_6823	130942-88-0	HC(H)c1c2c(c(C(H)OS(=O)(=O)O)c3c1cccc3)cccc2	3
5047	ISSSTY_v1a_7367_02May011_6824	105708-79-0	HC(H)C(=O)OC(H)c1c2c3c4c(ccc3cc1)cccc4cc2	3
5048	ISSSTY_v1a_7367_02May011_6826	85431-61-4	HC(H)[C@@]12C(C(H)C(H)[C@@](O)[C@]1C(H)H)=CC(=O)[C@]1([C@]3(C(H)O)C(H)O3)[C@@]2O1	3
5049	ISSSTY_v1a_7367_02May011_6829	42011-48-3	C1(C2=CC=C(N(=O)=O)O2)=CSC(NC(=O)C(F)(F)F)=N1	3
5050	ISSSTY_v1a_7367_02May011_6831	61421-83-8	c12c(c(Nc3ccc(O)cc3)c3c(cccc3)n1)cccc2	3
5051	ISSSTY_v1a_7367_02May011_6832	61421-82-7	HC(H)Oc1ccc(Nc2c3c(cccc3)nc3c2cccc3)cc1	3
5052	ISSSTY_v1a_7367_02May011_6833	58658-11-0	c12c(c(Nc3ccc(N)cc3)c3c(cccc3)n1)cccc2	3
5053	ISSSTY_v1a_7367_02May011_6834	75776-00-0	HC(H)Nc1ccc(Nc2c3c(cccc3)nc3c2cccc3)cc1	3
5054	ISSSTY_v1a_7367_02May011_6835	106063-42-7	HC(H)Oc1c(Nc2c3c(cccc3)nc3c2cccc3)ccc(O)c1	3
5055	ISSSTY_v1a_7367_02May011_6838	116169-87-0	HC(H)N1C(N=O)=NC=C1	3
5056	ISSSTY_v1a_7367_02May011_6839	1671-82-5	HC(H)N1C(N(=O)=O)=NC=C1	3
5057	ISSSTY_v1a_7367_02May011_6840	3328-25-4	HC(H)[C@@]12C(O)C(H)[C@@](O)C(H)C1H)C=C[C@]1[C@@]3[C@@](C(H)H)(C(H)C(H)[C@@]21)[C@@]([C@@](C(H)H)C(H)C(H)C(H)C(H)C(H)C(H)C3H	3
5058	ISSSTY_v1a_7367_02May011_6841	2846-29-9	HC(H)[C@@]12C(C(H)[C@@](O)C(H)C1H)=C[C@@](OO)[C@]1[C@@]3[C@@](C(H)H)(C(H)C(H)[C@@]21)[C@@]([C@@](C(H)H)C(H)C(H)C(H)C(H)C(H)C(H)C3H	3
5059	ISSSTY_v1a_7367_02May011_6853	31647-36-6	HC(H)c1c2c3c(c4c(cccc4)c2)ccc2c3c(ccc2)c1	3
5060	ISSSTY_v1a_7367_02May011_6856	589-41-3	HC(H)C(H)OC(=O)NO	3
5061	ISSSTY_v1a_7367_02May011_6857	112380-29-7	HC(H)C(H)N(C(C=O)=NO)N=O	3
5062	ISSSTY_v1a_7367_02May011_6859	99601-33-9	HC(H)C(H)N1c2c(c3c(cc2)nccc3)N=C1N	3
5063	ISSSTY_v1a_7367_02May011_6860	14129-84-1	C(Cl)(Cl)=C(C=O)C(Cl)Cl	3
5064	ISSSTY_v1a_7367_02May011_6861	99601-32-8	HC(H)c1c2c(c3c(c1)nccc3)N=C(N)N2C(H)C(H)H	3
5065	ISSSTY_v1a_7367_02May011_6862	100924-64-9	HC(c1c2c(c3c(cccc3)c1)ccc1c2cccc1)OS(=O)(=O)O	3
5066	ISSSTY_v1a_7367_02May011_6863	99520-58-8	c12c3c4c(c(O)c5c6c(c(c35)cc1)cccc6)cccc4cc2	3
5067	ISSSTY_v1a_7367_02May011_6864	99520-59-9	c1(O)c2c(c3c4c5c6c(cc24)cccc6ccc5cc3)ccc1	3

