

241	ISSSTY_v1a_7367_02May011_281	111-44-4	HC(Cl)C(H)OC(H)C(H)Cl	3
242	ISSSTY_v1a_7367_02May011_282	118-91-2	C(=O)(O)c1c(Cl)cccc1	1
243	ISSSTY_v1a_7367_02May011_284	75-00-3	HC(H)C(H)Cl	3
244	ISSSTY_v1a_7367_02May011_286	684-93-5	HC(H)N(C(N)=O)N=O	3
245	ISSSTY_v1a_7367_02May011_288	95-85-2	c1(O)c(N)cc(Cl)cc1	3
246	ISSSTY_v1a_7367_02May011_289	131-11-3	HC(H)OC(=O)c1c(C(=O)OC(H)H)cccc1	1
247	ISSSTY_v1a_7367_02May011_290	91-66-7	HC(H)C(H)N(c1cccc1)C(H)C(H)H	1
248	ISSSTY_v1a_7367_02May011_291	96-48-0	HC1C(=O)OC(H)C1H	1
249	ISSSTY_v1a_7367_02May011_292	92-93-3	c1(-c2ccc(N(=O)=O)cc2)cccc1	3
250	ISSSTY_v1a_7367_02May011_293	29007	HC=CC(N)=O	1
251	ISSSTY_v1a_7367_02May011_294	389-08-2	HC(H)c1ccc2C(=O)C(C(=O)O)=CN(C(H)C(H)H)c2n1	3
252	ISSSTY_v1a_7367_02May011_295	104-76-7	HC(H)C(H)C(H)C(H)C(C(H)C(H)H)C(H)O	1
253	ISSSTY_v1a_7367_02May011_296	121-14-2	HC(H)c1c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
254	ISSSTY_v1a_7367_02May011_297	134682-95-4	HC(H)C(H)C(H)C(H)C(C(H)C(H)H)C(H)OC(=O)c1cc(N(=O)=O)c(N(C(H)H)C(H)H)cc1	3
255	ISSSTY_v1a_7367_02May011_298	892-21-7	c1(N(=O)=O)c2c3c(c4c(c3ccc2)cccc4)cc1	3
256	ISSSTY_v1a_7367_02May011_299	106-42-3	HC(H)c1ccc(C(H)H)cc1	1
257	ISSSTY_v1a_7367_02May011_300	100-61-8	HC(H)Nc1cccc1	1
258	ISSSTY_v1a_7367_02May011_301	344-07-0	c1(Cl)c(F)c(F)c(F)c(F)c1F	1
259	ISSSTY_v1a_7367_02May011_302	604-75-1	c1(C2c3c(ccc(Cl)c3)NC(=O)C(O)N=2)cccc1	1
260	ISSSTY_v1a_7367_02May011_303	532-27-4	HC(Cl)C(=O)c1cccc1	1
261	ISSSTY_v1a_7367_02May011_305	110-80-5	HC(H)C(H)OC(H)C(H)O	1
262	ISSSTY_v1a_7367_02May011_306	16543-55-8	HC1C(H)C(H)C(c2cccnc2)N1N=O	3
263	ISSSTY_v1a_7367_02May011_307	119-36-8	HC(H)OC(=O)c1c(O)cccc1	1
264	ISSSTY_v1a_7367_02May011_308	79-43-6	C(=O)(O)C(Cl)Cl	3
265	ISSSTY_v1a_7367_02May011_309	30516-87-1	HC(H)C1C(=O)NC(=O)N([C@@]2C(H)[C@](N=N_N)[C@@](C(H)O)O2)C=1	3
266	ISSSTY_v1a_7367_02May011_310	4180-23-8	HC(H)C=Cc1ccc(OC(H)H)cc1	1
267	ISSSTY_v1a_7367_02May011_311	8003-22-3	C1(=O)c2c(C(=O)C1c1ccc3c(cccc3)n1)cccc2	3
268	ISSSTY_v1a_7367_02May011_312	99-61-6	c1(C=O)cc(N(=O)=O)ccc1	3
269	ISSSTY_v1a_7367_02May011_313	89-98-5	c1(Cl)c(C=O)cccc1	1
270	ISSSTY_v1a_7367_02May011_314	141-32-2	HC(H)C(H)C(H)C(H)OC(=O)C=CH	1

271	ISSSTY_v1a_7367_02May011_315	535-80-8	C(=O)(O)c1cc(Cl)ccc1	1
272	ISSSTY_v1a_7367_02May011_316	101-72-4	HC(H)C(C(H)H)Nc1ccc(Nc2ccccc2)cc1	1
273	ISSSTY_v1a_7367_02May011_317	17924-92-4	HC(H)[C@@]1C(H)C(H)C(H)C(=O)C(H)C(H)C(H)C=Cc2c(C(=O)O1)c(O)cc(O)c2	1
274	ISSSTY_v1a_7367_02May011_318	18420	HC(H)C(H)C1(c2ccccc2)C(=O)NC(=O)NC1=O	3
275	ISSSTY_v1a_7367_02May011_319	97-56-3	HC(H)c1c(N)ccc(N=Nc2c(C(H)H)cccc2)c1	3
276	ISSSTY_v1a_7367_02May011_320	625-48-9	HC(O)C(H)N(=O)=O	3
277	ISSSTY_v1a_7367_02May011_321	52645-53-1	HC(H)C1(C(H)H)[C@](C(=O)OC(H)c2cc(Oc3ccccc3)ccc2)[C@]1C=C(Cl)Cl	1
278	ISSSTY_v1a_7367_02May011_322	110-02-1	C1C=CSC=1	1
279	ISSSTY_v1a_7367_02May011_323	96-18-4	HC(Cl)C(Cl)C(H)Cl	3
280	ISSSTY_v1a_7367_02May011_324	552-89-6	c1(N(=O)=O)c(C=O)cccc1	1
281	ISSSTY_v1a_7367_02May011_325	36015	C(F)(F)(F)c1cccc1	1
282	ISSSTY_v1a_7367_02May011_326	51264-14-3	HC(H)Oc1c(Nc2c3c(cccc3)nc3c2cccc3)ccc(NS(=O)(=O)C(H)H)c1	3
283	ISSSTY_v1a_7367_02May011_327	75411-83-5	HC(H)C(O)C(H)N(C(H)H)N=O	3
284	ISSSTY_v1a_7367_02May011_328	609-31-4	HC(H)C(H)C(C(H)O)N(=O)=O	1
285	ISSSTY_v1a_7367_02May011_329	584-79-2	HC(H)C1=C(C(H)C=CH)C(=O)C(H)C1OC(=O)C1C(C(H)H)(C(H)H)C1C=C(C(H)H)C(H)H	3
286	ISSSTY_v1a_7367_02May011_330	19287-45-7	HB(H)B(H)H	3
287	ISSSTY_v1a_7367_02May011_331	134308-13-7	HC(H)c1ccc(C(=O)c2cc(O)c(O)c(N(=O)=O)c2)cc1	1
288	ISSSTY_v1a_7367_02May011_332	61499-28-3	HC(H)C(=O)C(H)N(C(H)C(O)C(H)H)N=O	3
289	ISSSTY_v1a_7367_02May011_333	68-22-4	HC(H)[C@@]12[C@](O)(C)C(H)C(H)[C@]1[C@@]1C(H)C(H)C3[C@@](C(H)C(H)C(=O)C=3)[C@]1C(H)C2H	1
290	ISSSTY_v1a_7367_02May011_334	117-80-6	C1(Cl)C(=O)c2c(C(=O)C=1Cl)cccc2	3
291	ISSSTY_v1a_7367_02May011_335	149-57-5	HC(H)C(H)C(H)C(H)C(C(=O)O)C(H)C(H)H	1
292	ISSSTY_v1a_7367_02May011_336	298-81-7	HC(H)Oc1c2c(C=CC(=O)O2)cc2c1OC=C2	3
293	ISSSTY_v1a_7367_02May011_337	122-14-5	HC(H)c1c(N(=O)=O)ccc(OP(=S)(OC(H)H)OC(H)H)c1	3
294	ISSSTY_v1a_7367_02May011_338	107-31-3	HC(H)OC=O	1
295	ISSSTY_v1a_7367_02May011_340	95-76-1	c1(Cl)c(Cl)cc(N)cc1	1
296	ISSSTY_v1a_7367_02May011_341	57-14-7	HC(H)N(N)C(H)H	3
297	ISSSTY_v1a_7367_02May011_342	1071-83-6	HC(C(=O)O)NC(H)P(=O)(O)O	1
298	ISSSTY_v1a_7367_02May011_343	60-80-0	HC(H)C1=CC(=O)N(c2ccccc2)N1C(H)H	1
299	ISSSTY_v1a_7367_02May011_344	60414-81-5	HC(H)C(=O)OC(C(H)H)C(H)N(C(H)C(C(H)H)OC(=O)C(H)H)N=O	3
300	ISSSTY_v1a_7367_02May011_346	96-69-5	HC(H)C(c1c(O)cc(C(H)H)c(Sc2c(C(H)H)cc(O)c(C(C(H)H)(C(H)H)C(H)H)c2)c1)(C(H)H)C(H)H	1

331	ISSSTY_v1a_7367_02May011_382	35311	HC1C(c2ccccc2)O1	3
332	ISSSTY_v1a_7367_02May011_384	2784-27-2	C1(=O)C(c2ccc(O)cc2)(c2ccccc2)NC(=O)N1	1
333	ISSSTY_v1a_7367_02May011_385	693-13-0	HC(H)C(C(H)H)N=C=NC(C(H)H)C(H)H	1
334	ISSSTY_v1a_7367_02May011_386	141-78-6	HC(H)C(=O)OC(H)C(H)H	1
335	ISSSTY_v1a_7367_02May011_387	112-55-0	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)S	1
336	ISSSTY_v1a_7367_02May011_388	97-63-2	HC(H)C(C(=O)OC(H)C(H)H)=CH	1
337	ISSSTY_v1a_7367_02May011_389	67730-11-4	HC(H)C1C2N(c3c(ccc(N)n3)N=2)C=CC=1	3
338	ISSSTY_v1a_7367_02May011_390	95-84-1	HC(H)c1cc(N)c(O)cc1	3
339	ISSSTY_v1a_7367_02May011_391	118-79-6	c1(Br)c(O)c(Br)cc(Br)c1	1
340	ISSSTY_v1a_7367_02May011_392	1122-58-3	HC(H)N(c1cc[n+](cc1)C(H)H	1
341	ISSSTY_v1a_7367_02May011_393	91-64-5	c12c(C=CC(=O)O1)cccc2	3
342	ISSSTY_v1a_7367_02May011_395	111-76-2	HC(H)C(H)C(H)C(H)OC(H)C(H)O	1
343	ISSSTY_v1a_7367_02May011_396	142-09-6	HC(H)C(C(=O)OC(H)C(H)C(H)C(H)C(H)H)=CH	1
344	ISSSTY_v1a_7367_02May011_398	491-70-3	C1(=O)c2c(O)cc(O)cc2OC(c2cc(O)c(O)cc2)=C1	1
345	ISSSTY_v1a_7367_02May011_399	603-34-9	c1(N(c2ccccc2)c2ccccc2)cccc1	1
346	ISSSTY_v1a_7367_02May011_400	693-98-1	HC(H)C1=NC=CN1	1
347	ISSSTY_v1a_7367_02May011_401	54827-17-7	HC(H)c1c(N)c(C(H)H)cc(-c2cc(C(H)H)c(N)c(C(H)H)c2)c1	1
348	ISSSTY_v1a_7367_02May011_402	134-32-7	c1(N)c2c(cccc2)ccc1	3
349	ISSSTY_v1a_7367_02May011_403	5989-27-5	HC(H)C1C(H)C(H)[C@@](C(C(H)H)=CH)C(H)C=1	1
350	ISSSTY_v1a_7367_02May011_404	37151-16-9	HC(O)[C@]1[C@@](O)[C@@](O)[C@](N2c3c(c(N)nc(-c4ccc(N(=O)=O)cc4)n3)N=C2)O1	3
351	ISSSTY_v1a_7367_02May011_406	90-34-6	HC(H)C(C(H)C(H)C(H)N)Nc1c2c(cc(OC(H)H)c1)cccn2	3
352	ISSSTY_v1a_7367_02May011_407	91-94-1	c1(-c2cc(Cl)c(N)cc2)cc(Cl)c(N)cc1	3
353	ISSSTY_v1a_7367_02May011_408	109-06-8	HC(H)c1ccccn1	1
354	ISSSTY_v1a_7367_02May011_410	100-19-6	HC(H)C(=O)c1ccc(N(=O)=O)cc1	3
355	ISSSTY_v1a_7367_02May011_411	108-03-2	HC(H)C(H)C(H)N(=O)=O	1
356	ISSSTY_v1a_7367_02May011_412	554-84-7	c1(O)cc(N(=O)=O)ccc1	3
357	ISSSTY_v1a_7367_02May011_413	552-16-9	C(=O)(O)c1c(N(=O)=O)cccc1	3
358	ISSSTY_v1a_7367_02May011_414	86-30-6	c1(N(c2ccccc2)N=O)cccc1	3
359	ISSSTY_v1a_7367_02May011_415	69304-47-8	HC(O)[C@]1[C@@](O)C(H)[C@@](N2C(=O)NC(=O)C(C=CBr)=C2)O1	1
360	ISSSTY_v1a_7367_02May011_416	305-03-3	HC(c1ccc(N(C(H)C(H)Cl)C(H)C(H)Cl)cc1)C(H)C(H)C(=O)O	3

361	ISSSTY_v1a_7367_02May011_417	83-66-9	HC(H)C(c1c(OC(H)H)c([N+](=O)[O-])c(C(H)H)c([N+](=O)[O-])c1)(C(H)H)C(H)H	3
362	ISSSTY_v1a_7367_02May011_418	62-56-6	C(N)(N)=S	1
363	ISSSTY_v1a_7367_02May011_419	1319-77-3	HC(H)c1ccc(O)cc1	1
364	ISSSTY_v1a_7367_02May011_420	101-68-8	HC(c1ccc(N=C=O)cc1)c1ccc(N=C=O)cc1	1
365	ISSSTY_v1a_7367_02May011_421	36373	HC(H)c1cc(N(=O)=O)ccc1	1
366	ISSSTY_v1a_7367_02May011_422	111-41-1	HC(O)C(H)NC(H)C(H)N	3
367	ISSSTY_v1a_7367_02May011_423	110-86-1	c1cccn1	1
368	ISSSTY_v1a_7367_02May011_424	105650-23-5	HC(H)N1c2c(N=C1N)ncc(-c1ccccc1)c2	3
369	ISSSTY_v1a_7367_02May011_425	96-23-1	HC(Cl)C(O)C(H)Cl	3
370	ISSSTY_v1a_7367_02May011_426	112-57-2	HC(N)C(H)NC(H)C(H)NC(H)C(H)NC(H)C(H)N	3
371	ISSSTY_v1a_7367_02May011_427	38083-17-9	HC(H)C(C(=O)C(N1C=CN=C1)Oc1ccc(Cl)cc1)(C(H)H)C(H)H	1
372	ISSSTY_v1a_7367_02May011_428	128-37-0	HC(H)C(c1c(O)c(C(C(H)H)(C(H)H)C(H)H)cc(C(H)H)c1)(C(H)H)C(H)H	1
373	ISSSTY_v1a_7367_02May011_429	15687-27-1	HC(H)C(c1ccc(C(H)C(C(H)H)C(H)H)cc1)C(=O)O	1
374	ISSSTY_v1a_7367_02May011_430	2122-77-2	HC(O)C(H)Oc1c(Cl)cc(Cl)c(Cl)c1	1
375	ISSSTY_v1a_7367_02May011_431	75-77-4	HC(H)[Si](Cl)(C(H)H)C(H)H	1
376	ISSSTY_v1a_7367_02May011_433	75-78-5	HC(H)[Si](Cl)(Cl)C(H)H	1
377	ISSSTY_v1a_7367_02May011_434	78-67-1	HC(H)C(C_N)(C(H)H)N=NC(C_N)(C(H)H)C(H)H	1
378	ISSSTY_v1a_7367_02May011_435	67-21-0	HC(H)C(H)SC(H)C(H)C(N)C(=O)O	1
379	ISSSTY_v1a_7367_02May011_436	2524-03-0	HC(H)OP(=S)(Cl)OC(H)H	1
380	ISSSTY_v1a_7367_02May011_437	98-56-6	C(F)(F)(F)c1ccc(Cl)cc1	1
381	ISSSTY_v1a_7367_02May011_439	92-52-4	c1(-c2ccccc2)ccccc1	1
382	ISSSTY_v1a_7367_02May011_440	3096-52-4	c12C(=O)c3c(-c1ccc(N(=O)=O)c2)ccccc3	3
383	ISSSTY_v1a_7367_02May011_441	3290-92-4	HC(H)C(C(=O)OC(H)C(C(H)C(H)H)(C(H)OC(=O)C(C(H)H)=CH)C(H)OC(=O)C(C(H)H)=CH)=CH	1
384	ISSSTY_v1a_7367_02May011_442	25103-58-6	HC(H)C(S)(C(C(C(H)H)(C(H)H)C(C(H)H)C(H)H)(C(H)H)C(H)H)C(H)H	1
385	ISSSTY_v1a_7367_02May011_443	52-90-4	HC(S)C(N)C(=O)O	3
386	ISSSTY_v1a_7367_02May011_444	124-07-2	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(=O)O	1
387	ISSSTY_v1a_7367_02May011_445	140-29-4	HC(c1ccccc1)C_N	1
388	ISSSTY_v1a_7367_02May011_446	1116-54-7	HC(O)C(H)N(C(H)C(H)O)N=O	3
389	ISSSTY_v1a_7367_02May011_447	79-46-9	HC(H)C(C(H)H)N(=O)=O	3
390	ISSSTY_v1a_7367_02May011_448	75-35-4	HC=C(Cl)Cl	3

421	ISSSTY_v1a_7367_02May011_487	108-90-7	c1(Cl)cccc1	1
422	ISSSTY_v1a_7367_02May011_488	552-30-7	C1(=O)c2c(C(=O)O1)cc(C(=O)O)cc2	1
423	ISSSTY_v1a_7367_02May011_489	51-21-8	C1(=O)C(F)=CNC(=O)N1	1
424	ISSSTY_v1a_7367_02May011_490	625-86-5	HC(H)C1=CC=C(C(H)H)O1	1
425	ISSSTY_v1a_7367_02May011_492	5410-97-9	c12-c3c(cc(N(=O)=O)cc3)Oc1cccc2	3
426	ISSSTY_v1a_7367_02May011_494	396-01-0	c1(-c2c(N)nc3c(c(N)nc(N)n3)n2)cccc1	1
427	ISSSTY_v1a_7367_02May011_498	67-72-1	C(Cl)(Cl)(Cl)C(Cl)(Cl)Cl	1
428	ISSSTY_v1a_7367_02May011_499	628-34-2	HC(H)C(H)OC(H)C(H)Cl	3
429	ISSSTY_v1a_7367_02May011_500	421-70-5	C(F)(F)(I)C(F)(F)Br	3
430	ISSSTY_v1a_7367_02May011_502	822-06-0	HC(C(H)C(H)C(H)C(H)C(H)N=C=O)N=C=O	1
431	ISSSTY_v1a_7367_02May011_503	4337-65-9	HC(H)C(H)C(H)C(H)C(C(H)C(H)H)C(H)OC(=O)C(H)C(H)C(H)C(H)C(=O)O	1
432	ISSSTY_v1a_7367_02May011_504	63-25-2	HC(H)NC(=O)Oc1c2c(cccc2)ccc1	3
433	ISSSTY_v1a_7367_02May011_505	109-69-3	HC(H)C(H)C(H)C(H)Cl	1
434	ISSSTY_v1a_7367_02May011_506	15625-89-5	HC(H)C(H)C(C(H)OC(=O)C=CH)(C(H)OC(=O)C=CH)C(H)OC(=O)C=CH	3
435	ISSSTY_v1a_7367_02May011_508	77-47-4	C1(Cl)C(Cl)(Cl)C(Cl)=C(Cl)C=1Cl	1
436	ISSSTY_v1a_7367_02May011_509	524-42-5	C1(=O)C(=O)c2c(C=C1)cccc2	3
437	ISSSTY_v1a_7367_02May011_510	28376	c1(C2(c3ccc(O)cc3)c3c(C(=O)O2)cccc3)ccc(O)cc1	1
438	ISSSTY_v1a_7367_02May011_511	136112-71-5	C1(c2ccc([N+](=O)[O-])cc2)N(c2ccc([N+](=O)[O-])cc2)c2c(c(N)ncn2)N=1	3
439	ISSSTY_v1a_7367_02May011_512	108-88-3	HC(H)c1cccc1	1
440	ISSSTY_v1a_7367_02May011_513	108171-26-2	HC(H)C(H)C(Cl)C(Cl)C(Cl)C(H)C(Cl)C(Cl)C(Cl)C(H)H	1
441	ISSSTY_v1a_7367_02May011_514	21314-05-6	c1(N)c2c(N(c3ccc(N(=O)=O)cc3)C=N2)ncn1	3
442	ISSSTY_v1a_7367_02May011_516	934-32-7	c12c(cccc1)N=C(N)N2	1
443	ISSSTY_v1a_7367_02May011_517	103-23-1	HC(H)C(H)C(H)C(H)C(C(H)C(H)H)C(H)OC(=O)C(H)C(H)C(H)C(H)C(=O)OC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)H	1
444	ISSSTY_v1a_7367_02May011_518	120-32-1	HC(c1c(O)ccc(Cl)c1)c1cccc1	1
445	ISSSTY_v1a_7367_02May011_520	102-71-6	HC(O)C(H)N(C(H)C(H)O)C(H)C(H)O	1
446	ISSSTY_v1a_7367_02May011_521	109875-50-5	c1(-c2ccc(N(=O)=O)cc2)nc(N)c2c(N=CN2)n1	3
447	ISSSTY_v1a_7367_02May011_522	125-33-7	HC(H)C(H)C1(c2ccccc2)C(=O)NC(H)NC1=O	3
448	ISSSTY_v1a_7367_02May011_523	58-15-1	HC(H)C1=C(N(C(H)H)C(H)H)C(=O)N(c2ccccc2)N1C(H)H	1
449	ISSSTY_v1a_7367_02May011_524	50-81-7	HC(O)C(O)C1C(=O)C(O)=C(O)O1	1
450	ISSSTY_v1a_7367_02May011_525	14191-22-1	c12-c3c(cc(N(=O)=O)cc3)Nc1cccc2	3

451	ISSSTY_v1a_7367_02May011_526	33457	HC(H)c1c(N=C=O)cccc1N=C=O	3
452	ISSSTY_v1a_7367_02May011_527	136-77-6	HC(H)C(H)C(H)C(H)C(H)C(H)c1c(O)cc(O)cc1	1
453	ISSSTY_v1a_7367_02May011_528	100-69-6	HC=Cc1ccccn1	1
454	ISSSTY_v1a_7367_02May011_529	140-67-0	HC(H)Oc1ccc(C(H)C=CH)cc1	1
455	ISSSTY_v1a_7367_02May011_530	136112-69-1	c1(Nc2ccc(N(=O)=O)cc2)c2c(N=CN2)ncn1	1
456	ISSSTY_v1a_7367_02May011_531	764-42-1	C(N)C=CC_N	1
457	ISSSTY_v1a_7367_02May011_532	1143-38-0	HC1c2c(C(=O)c3c(O)cccc13)c(O)ccc2	3
458	ISSSTY_v1a_7367_02May011_533	112-24-3	HC(N)C(H)NC(H)C(H)NC(H)C(H)N	3
459	ISSSTY_v1a_7367_02May011_534	83-79-4	HC(H)C([C@]1C(H)c2c3c(C(=O)[C@]4c5c(cc(OC(H)H)c(OC(H)H)c5)OC(H)[C@]4O3)ccc2O1)=CH	1
460	ISSSTY_v1a_7367_02May011_535	64-19-7	HC(H)C(=O)O	1
461	ISSSTY_v1a_7367_02May011_538	100-40-3	HC1C(H)C(C=CH)C(H)C=C1	1
462	ISSSTY_v1a_7367_02May011_539	27735	C(N)=O	1
463	ISSSTY_v1a_7367_02May011_540	54-31-9	HC(C1=CC=CO1)Nc1c(C(=O)O)cc(S(N)(=O)=O)c(Cl)c1	1
464	ISSSTY_v1a_7367_02May011_541	599-79-1	C(=O)(O)C1C(=O)C=CC(=NNc2ccc(S(=O)(=O)Nc3ccccn3)cc2)O=1	1
465	ISSSTY_v1a_7367_02May011_542	98-55-5	HC(H)C(O)(C(H)H)[C@]1C(H)C(H)C(C(H)H)=CC1H	1
466	ISSSTY_v1a_7367_02May011_544	98-85-1	HC(H)C(O)c1cccc1	1
467	ISSSTY_v1a_7367_02May011_545	5134-49-6	HC(c1ccc(N(=O)=O)cc1)Nc1c2c(N=CN2)ncn1	3
468	ISSSTY_v1a_7367_02May011_546	124-09-4	HC(N)C(H)C(H)C(H)C(H)C(H)N	1
469	ISSSTY_v1a_7367_02May011_548	100-41-4	HC(H)C(H)c1cccc1	1
470	ISSSTY_v1a_7367_02May011_550	354656	HC(O)C(H)Nc1c(N(=O)=O)cc(N)cc1	3
471	ISSSTY_v1a_7367_02May011_551	93-45-8	c12c(cc(Nc3ccc(O)cc3)cc1)cccc2	1
472	ISSSTY_v1a_7367_02May011_553	99-75-2	HC(H)c1ccc(C(=O)OC(H)H)cc1	1
473	ISSSTY_v1a_7367_02May011_554	109875-45-8	HC(O)[C@]1C(O)C(c2ccc(N(=O)=O)cc2)[C@](N2c3c(c(N)ncn3)N=C2)O1	3
474	ISSSTY_v1a_7367_02May011_555	2832-40-8	HC(H)C1C=CC(=O)C(=NNc2ccc(NC(=O)C(H)H)cc2)C=1	3
475	ISSSTY_v1a_7367_02May011_556	73215-03-9	HC(c1ccc(N(=O)=O)cc1)N1c2c(c(N)ncn2)N=C1	3
476	ISSSTY_v1a_7367_02May011_558	130-26-7	c1(I)c(O)c2c(c(Cl)c1)ccc2	1
477	ISSSTY_v1a_7367_02May011_559	75-34-3	HC(H)C(Cl)Cl	1
478	ISSSTY_v1a_7367_02May011_561	309-00-2	HC1C2C3C4(Cl)C(Cl)(Cl)C(Cl)(C(Cl)=C4Cl)C3C1C=C2	1
479	ISSSTY_v1a_7367_02May011_562	191906	HC1C2C(=O)N(SC(Cl)(Cl)C(Cl)Cl)C(=O)C2C(H)C=C1	3
480	ISSSTY_v1a_7367_02May011_563	21313-86-0	C1(c2ccc(N(=O)=O)cc2)=Nc2c(c(N)ncn2)N1	3

481	ISSSTY_v1a_7367_02May011_565	81-64-1	c12C(=O)c3c(C(=O)c1c(O)ccc2O)cccc3	3
482	ISSSTY_v1a_7367_02May011_566	77500-04-0	HC(H)c1cnc2c(c3c(cc2)N(C(H)H)C(N)=N3)n1	3
483	ISSSTY_v1a_7367_02May011_567	75-36-5	HC(H)C(=O)Cl	1
484	ISSSTY_v1a_7367_02May011_568	10373-78-1	HC(H)C1(C(H)H)C2(C(H)H)C(=O)C(=O)C1C(H)C2H	1
485	ISSSTY_v1a_7367_02May011_569	16529-56-9	HC(H)C(C_N)C=CH	1
486	ISSSTY_v1a_7367_02May011_570	82-62-2	c1(Cl)c(Cl)c(N(=O)=O)c(O)c(Cl)c1	1
487	ISSSTY_v1a_7367_02May011_571	124-19-6	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C=O	1
488	ISSSTY_v1a_7367_02May011_572	131-57-7	HC(H)Oc1cc(O)c(C(=O)c2ccccc2)cc1	1
489	ISSSTY_v1a_7367_02May011_573	29465	c1(S(=O)(=O)c2ccc(O)cc2)ccc(O)cc1	1
490	ISSSTY_v1a_7367_02May011_574	104-94-9	HC(H)Oc1ccc(N)cc1	3
491	ISSSTY_v1a_7367_02May011_575	22227	HC(H)N(c1ccc(N=Nc2ccccc2)cc1)C(H)H	3
492	ISSSTY_v1a_7367_02May011_576	3420-97-1	HC(H)C(H)Oc1ccc(N=O)cc1	3
493	ISSSTY_v1a_7367_02May011_577	598-21-0	HC(Br)C(=O)Br	3
494	ISSSTY_v1a_7367_02May011_578	29102	HC(H)C(H)C(=O)O	1
495	ISSSTY_v1a_7367_02May011_580	9002-98-6	HC1C(H)N1	1
496	ISSSTY_v1a_7367_02May011_581	25013-15-4	HC(H)c1cc(C=CH)ccc1	1
497	ISSSTY_v1a_7367_02May011_582	118-75-2	C1(Cl)C(=O)C(Cl)=C(Cl)C(=O)C=1Cl	3
498	ISSSTY_v1a_7367_02May011_583	95-64-7	HC(H)c1c(C(H)H)cc(N)cc1	1
499	ISSSTY_v1a_7367_02May011_584	839-90-7	HC(O)C(H)N1C(=O)N(C(H)C(H)O)C(=O)N(C(H)C(H)O)C1=O	1
500	ISSSTY_v1a_7367_02May011_586	31055	c12c(c3c(cccc3)cc1)cccc2	1
501	ISSSTY_v1a_7367_02May011_587	591-17-3	HC(H)c1cc(Br)ccc1	1
502	ISSSTY_v1a_7367_02May011_588	99-54-7	c1(Cl)c(Cl)cc(N(=O)=O)cc1	3
503	ISSSTY_v1a_7367_02May011_589	83-32-9	HC1c2c3c(cccc3ccc2)C1H	1
504	ISSSTY_v1a_7367_02May011_590	106-38-7	HC(H)c1ccc(Br)cc1	1
505	ISSSTY_v1a_7367_02May011_592	86674-49-9	c12c3c4c(c(O)cc(N(=O)=O)c4ccc3ccc1)cc2	3
506	ISSSTY_v1a_7367_02May011_594	584-84-9	HC(H)c1c(N=C=O)cc(N=C=O)cc1	3
507	ISSSTY_v1a_7367_02May011_595	53-95-2	HC(H)C(=O)N(O)c1cc2c(-c3c(cccc3)C2H)cc1	3
508	ISSSTY_v1a_7367_02May011_596	13674-84-5	HC(H)C(C(H)Cl)OP(=O)(OC(C(H)H)C(H)Cl)OC(C(H)H)C(H)Cl	1
509	ISSSTY_v1a_7367_02May011_597	81-55-0	c12C(=O)c3c(C(=O)c1c(O)ccc2[N+](=O)[O-])c(O)ccc3[N+](=O)[O-]	3
510	ISSSTY_v1a_7367_02May011_598	112-56-1	HC(H)C(H)C(H)C(H)OC(H)C(H)OC(H)C(H)SC_N	1

511	ISSSTY_v1a_7367_02May011_599	439-14-5	HC(H)N1c2c(C(c3ccccc3)=NC(H)C1=O)cc(Cl)cc2	1
512	ISSSTY_v1a_7367_02May011_600	111-71-7	HC(H)C(H)C(H)C(H)C(H)C(H)C=O	1
513	ISSSTY_v1a_7367_02May011_601	111-14-8	HC(H)C(H)C(H)C(H)C(H)C(H)C(=O)O	1
514	ISSSTY_v1a_7367_02May011_602	38178-41-5	c12c(cc(N(=O)=O)cc1)Oc1c(cccc1)O2	3
515	ISSSTY_v1a_7367_02May011_603	609-19-8	c1(Cl)c(Cl)c(Cl)cc(O)c1	1
516	ISSSTY_v1a_7367_02May011_604	78-97-7	HC(H)C(O)C_N	1
517	ISSSTY_v1a_7367_02May011_605	626-17-5	C(_N)c1cc(C_N)ccc1	1
518	ISSSTY_v1a_7367_02May011_607	4569-77-1	C1(N)C(=O)C=C2C(G=1)=Nc1c(cccc1)N2	3
519	ISSSTY_v1a_7367_02May011_608	2043937	c1(N(=O)=O)c2c(c3c(c4c(cccc4)cc3)c1)cccc2	3
520	ISSSTY_v1a_7367_02May011_609	498-21-5	HC(H)C(C(=O)O)C(H)C(=O)O	1
521	ISSSTY_v1a_7367_02May011_610	759-73-9	HC(H)C(H)N(C(N)=O)N=O	3
522	ISSSTY_v1a_7367_02May011_611	577-59-3	HC(H)C(=O)c1c(N(=O)=O)cccc1	1
523	ISSSTY_v1a_7367_02May011_612	891986	HC(H)N(C(H)H)NN=C1C(C(N)=O)=NC=N1	3
524	ISSSTY_v1a_7367_02May011_614	631-64-1	C(=O)(O)C(Br)Br	3
525	ISSSTY_v1a_7367_02May011_615	434-13-9	HC(H)[C@@]12c(H)C(H)[C@@]3[C@@]4(C(H)H)C(H)C(H)[C@@](O)C(H)[C@@]4(C(H)C(H)C(H)C(H)C(=O)O	1
526	ISSSTY_v1a_7367_02May011_616	143-07-7	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(=O)O	1
527	ISSSTY_v1a_7367_02May011_617	136112-72-6	c1(Nc2ccc([N+](=O)[O-])cc2)c2c(N(c3ccc([N+](=O)[O-])cc3)C=N2)ncn1	3
528	ISSSTY_v1a_7367_02May011_618	129-00-0	c12c3c4c(ccc3ccc1)cccc4cc2	3
529	ISSSTY_v1a_7367_02May011_619	1504-74-1	HC(H)Oc1c(C=CC=O)cccc1	1
530	ISSSTY_v1a_7367_02May011_620	7203-90-9	HC(H)N(C(H)H)N=Nc1ccc(Cl)cc1	3
531	ISSSTY_v1a_7367_02May011_621	15176-29-1	HC(H)C(H)C1C(=O)NC(=O)N([C@@]2C(H)[C@](O)[C@@](C(H)O)O2)C=1	1
532	ISSSTY_v1a_7367_02May011_624	119-93-7	HC(H)c1c(N)ccc(-c2cc(C(H)H)c(N)cc2)c1	3
533	ISSSTY_v1a_7367_02May011_625	126-73-8	HC(H)C(H)C(H)C(H)OP(=O)(OC(H)C(H)C(H)C(H)H)OC(H)C(H)C(H)C(H)H	1
534	ISSSTY_v1a_7367_02May011_626	478-08-0	HC(O)c1c(O)c2C(=O)c3c(C(=O)c2cc1O)cccc3	3
535	ISSSTY_v1a_7367_02May011_627	1606-67-3	c12c3c4c(c(N)ccc4ccc3ccc1)cc2	3
536	ISSSTY_v1a_7367_02May011_628	75-83-2	HC(H)C(C(H)H)(C(H)H)C(H)C(H)H	1
537	ISSSTY_v1a_7367_02May011_629	120-71-8	HC(H)c1cc(N)c(OC(H)H)cc1	3
538	ISSSTY_v1a_7367_02May011_630	2461-15-6	HC(H)C(H)C(H)C(H)C(C(H)C(H)H)C(H)OC(H)C1C(H)O1	1
539	ISSSTY_v1a_7367_02May011_631	103-84-4	HC(H)C(=O)Nc1cccc1	1
540	ISSSTY_v1a_7367_02May011_632	121-39-1	HC(H)C(H)OC(=O)C1C(c2ccccc2)O1	1

541	ISSSTY_v1a_7367_02May011_633	70021-99-7	c1(N(=O)=O)c2c3c4c(c5c(cc4ccc3cc1)cccc5)cc2	3
542	ISSSTY_v1a_7367_02May011_634	91423-46-0	HC(H)C(H)C=CC=CC=CC=CC=CCOC(H)[C@@](O)C(H)O	3
543	ISSSTY_v1a_7367_02May011_635	634-93-5	c1(Cl)c(N)c(Cl)cc(Cl)c1	1
544	ISSSTY_v1a_7367_02May011_636	140-10-3	C(=O)(O)C=Cc1cccc1	1
545	ISSSTY_v1a_7367_02May011_637	105-59-9	HC(H)N(C(H)C(H)O)C(H)C(H)O	1
546	ISSSTY_v1a_7367_02May011_638	98-95-3	c1(N(=O)=O)cccc1	1
547	ISSSTY_v1a_7367_02May011_639	71-58-9	HC(H)C(=O)[C@]1(Oc(=O)C(H)H)[C@]2(C(H)H)C(H)C(H)[C@@]3[C@@]4(C(H)H)C([C@@](C(H)H)C(H)[C@]3[C@@]2(C(H)C1H)=CC(=O)C(H)O)4H	1
548	ISSSTY_v1a_7367_02May011_640	101-96-2	HC(H)C(H)C(C(H)H)Nc1ccc(NC(C(H)H)C(H)C(H)H)cc1	1
549	ISSSTY_v1a_7367_02May011_641	90-04-0	HC(H)Oc1c(N)cccc1	3
550	ISSSTY_v1a_7367_02May011_642	35572-78-2	HC(H)c1c(N)cc([N+](=O)[O-])cc1[N+](=O)[O-]	3
551	ISSSTY_v1a_7367_02May011_643	732-11-6	HC(H)OP(=S)(OC(H)H)SC(H)N1C(=O)c2c(C1=O)cccc2	3
552	ISSSTY_v1a_7367_02May011_644	112-34-5	HC(H)C(H)C(H)C(H)OC(H)C(H)OC(H)C(H)O	1
553	ISSSTY_v1a_7367_02May011_645	79-29-8	HC(H)C(C(H)H)C(C(H)H)C(H)H	1
554	ISSSTY_v1a_7367_02May011_646	25174	HC(H)N(C(H)H)C=O	1
555	ISSSTY_v1a_7367_02May011_647	101-77-9	HC(c1ccc(N)cc1)c1ccc(N)cc1	3
556	ISSSTY_v1a_7367_02May011_648	89-75-8	C(=O)(Cl)c1c(Cl)cc(Cl)cc1	3
557	ISSSTY_v1a_7367_02May011_649	98-00-0	HC(O)C1=CC=CO1	1
558	ISSSTY_v1a_7367_02May011_650	1455-77-2	C1(N)N=C(N)NN=1	3
559	ISSSTY_v1a_7367_02May011_651	110-88-3	HC1OC(H)OC(H)O1	1
560	ISSSTY_v1a_7367_02May011_653	117-10-2	c12C(=O)c3c(C(=O)c1c(O)ccc2)c(O)ccc3	3
561	ISSSTY_v1a_7367_02May011_654	19406-51-0	HC(H)c1c([N+](=O)[O-])cc(N)cc1[N+](=O)[O-]	3
562	ISSSTY_v1a_7367_02May011_655	194-59-2	c12-c3c4c(ccc3Nc1ccc1c2cccc1)cccc4	1
563	ISSSTY_v1a_7367_02May011_656	123-92-2	HC(H)C(=O)OC(H)C(H)C(C(H)H)C(H)H	1
564	ISSSTY_v1a_7367_02May011_657	141-43-5	HC(O)C(H)N	1
565	ISSSTY_v1a_7367_02May011_658	92-59-1	HC(H)C(H)N(c1cccc1)C(H)c1cccc1	1
566	ISSSTY_v1a_7367_02May011_660	19881-18-6	c1(Oc2ccc(N(=O)=O)cc2)ccc(N=C=S)cc1	3
567	ISSSTY_v1a_7367_02May011_661	13463-41-7	c1([S-][Zn++][S-]c2cccc[n+]2[O-])cccc[n+]1[O-]	1
568	ISSSTY_v1a_7367_02May011_662	115-77-5	HC(O)C(C(H)O)(C(H)O)C(H)O	1
569	ISSSTY_v1a_7367_02May011_663	65-45-2	C(N)(=O)c1c(O)cccc1	1
570	ISSSTY_v1a_7367_02May011_665	7227-92-1	HC(H)N(C(H)H)N=Nc1ccc(N(=O)=O)cc1	3

691	ISSSTY_v1a_7367_02May011_809	104-85-8	HC(H)c1ccc(C_N)cc1	1
692	ISSSTY_v1a_7367_02May011_810	98-82-8	HC(H)C(c1ccccc1)C(H)H	1
693	ISSSTY_v1a_7367_02May011_811	101-39-3	HC(H)C(C=O)=Cc1ccccc1	1
694	ISSSTY_v1a_7367_02May011_812	77-73-6	HC1C2C3C(H)C(C=C3)C2C=C1	1
695	ISSSTY_v1a_7367_02May011_814	94-82-6	HC(C(=O)O)C(H)C(H)Oc1c(Cl)cc(Cl)cc1	1
696	ISSSTY_v1a_7367_02May011_815	22204-53-1	HC(H)C(c1cc2c(cc(OC(H)H)cc2)cc1)C(=O)O	1
697	ISSSTY_v1a_7367_02May011_816	135768-83-1	HC(H)[C@@]12[C@@]3(O)C(H)C(H)C1(C(H)[C@]3O)[C@@]1C(H)C(H)c3c(ccc(O)c3)[C@]1C(H)C2H	1
698	ISSSTY_v1a_7367_02May011_817	121-79-9	HC(H)C(H)C(H)OC(=O)c1cc(O)c(O)c(O)c1	1
699	ISSSTY_v1a_7367_02May011_819	1187-42-4	C(_N)C(N)=C(N)C_N	1
700	ISSSTY_v1a_7367_02May011_820	15356-70-4	HC(H)C(C(H)H)C1C(H)C(H)C(C(H)H)C(H)C1O	1
701	ISSSTY_v1a_7367_02May011_822	123-05-7	HC(H)C(H)C(H)C(H)C(C(H)C(H)H)C=O	1
702	ISSSTY_v1a_7367_02May011_826	97-54-1	HC(H)C=Cc1cc(OC(H)H)c(O)cc1	1
703	ISSSTY_v1a_7367_02May011_827	253-52-1	c12c(ccc1)cnnc2	1
704	ISSSTY_v1a_7367_02May011_830	616-23-9	HC(Cl)C(Cl)C(H)O	3
705	ISSSTY_v1a_7367_02May011_831	20927-95-1	c12-c3c(ccc(N(=O)=O)c3)Oc1cccc2	3
706	ISSSTY_v1a_7367_02May011_832	555-16-8	c1(C=O)ccc(N(=O)=O)cc1	3
707	ISSSTY_v1a_7367_02May011_833	3694-52-8	c1(N)c(N)c(N(=O)=O)ccc1	3
708	ISSSTY_v1a_7367_02May011_834	3018-12-0	C(_N)C(Cl)Cl	3
709	ISSSTY_v1a_7367_02May011_835	3380-34-5	c1(Oc2c(Cl)cc(Cl)cc2)c(O)cc(Cl)cc1	1
710	ISSSTY_v1a_7367_02May011_836	107-15-3	HC(N)C(H)N	3
711	ISSSTY_v1a_7367_02May011_837	38848-76-9	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(=O)N[N+](C(H)H)(C(H)H)C(H)C([O-])C(H)H	1
712	ISSSTY_v1a_7367_02May011_838	954-46-1	c1(N(=O)=O)c2c(c3c(cccc3)c1)cccc2	3
713	ISSSTY_v1a_7367_02May011_839	13171-21-6	HC(H)C(=C(Cl)C(=O)N(C(H)C(H)H)C(H)C(H)H)OP(=O)(OC(H)H)OC(H)H	3
714	ISSSTY_v1a_7367_02May011_840	54-85-3	C(=O)(c1ccncc1)NN	3
715	ISSSTY_v1a_7367_02May011_841	367-25-9	c1(N)c(F)cc(F)cc1	1
716	ISSSTY_v1a_7367_02May011_842	66-81-9	HC(H)[C@]1C(=O)[C@@]([C@](O)C(H)C2C(H)C(=O)NC(=O)C2H)C(H)[C@@](C(H)H)C1H	1
717	ISSSTY_v1a_7367_02May011_843	75321-20-9	c12c3c4c(c([N+](=O)[O-])cc([N+](=O)[O-])c4ccc3ccc1)cc2	3
718	ISSSTY_v1a_7367_02May011_845	87-66-1	c1(O)c(O)c(O)ccc1	3
719	ISSSTY_v1a_7367_02May011_847	110-00-9	C1C=COC=1	1
720	ISSSTY_v1a_7367_02May011_848	119-75-5	c1(Nc2cccc2)c(N(=O)=O)cccc1	1

781	ISSSTY_v1a_7367_02May011_917	15972-60-8	HC(H)C(H)c1c(N(C(=O)C(H)Cl)C(H)OC(H)H)c(C(H)C(H)H)ccc1	3
782	ISSSTY_v1a_7367_02May011_918	555-30-6	HC(H)[C@](N)(C(=O)O)C(H)c1cc(O)c(O)cc1	1
783	ISSSTY_v1a_7367_02May011_919	42135-22-8	c12C(=O)c3c(-c1cc(N(=O)=O)cc2)cccc3	3
784	ISSSTY_v1a_7367_02May011_920	76-38-0	HC(H)OC(F)(F)C(Cl)Cl	1
785	ISSSTY_v1a_7367_02May011_921	818-61-1	HC(O)C(H)OC(=O)C=CH	1
786	ISSSTY_v1a_7367_02May011_922	1119-48-8	HC(H)NC(H)C(H)C(H)C(=O)O	1
787	ISSSTY_v1a_7367_02May011_924	3296-90-0	HC(Br)C(C(H)O)(C(H)O)C(H)Br	1
788	ISSSTY_v1a_7367_02May011_925	27522	HC(H)C_N	1
789	ISSSTY_v1a_7367_02May011_927	8021-39-4	HC(H)Oc1c(O)cccc1	1
790	ISSSTY_v1a_7367_02May011_928	105-45-3	HC(H)C(=O)C(H)C(=O)OC(H)H	1
791	ISSSTY_v1a_7367_02May011_929	56-55-3	c12c(c3c(cc4c(cccc4)c3)cc1)cccc2	3
792	ISSSTY_v1a_7367_02May011_930	109-77-3	HC(C_N)C_N	1
793	ISSSTY_v1a_7367_02May011_931	130-80-3	HC(H)C(H)C(c1ccc(OC(=O)C(H)C(H)H)cc1)=C(c1ccc(OC(=O)C(H)C(H)H)cc1)C(H)C(H)H	1
794	ISSSTY_v1a_7367_02May011_932	88-19-7	HC(H)c1c(S(N)(=O)=O)cccc1	1
795	ISSSTY_v1a_7367_02May011_934	29743-15-5	HC(H)C(H)c1ccc(N=Cc2ccc(OC(H)C(H)C(H)C(H)H)cc2)cc1	1
796	ISSSTY_v1a_7367_02May011_936	70021-98-6	c1(N(=O)=O)c2c3c4c(c5c(cc4cc2)cccc5)ccc3cc1	3
797	ISSSTY_v1a_7367_02May011_938	101-90-6	HC1C(C(H)Oc2cc(OC(H)C3C(H)O3)ccc2)O1	3
798	ISSSTY_v1a_7367_02May011_939	479-13-0	C1(=O)C2c3c(cc(O)cc3)OC=2c2c(cc(O)cc2)O1	1
799	ISSSTY_v1a_7367_02May011_940	320-67-2	HC(O)[C@]1[C@@](O)[C@@](O)[C@](N2C(=O)N=C(N)N=C2)O1	3
800	ISSSTY_v1a_7367_02May011_941	15121-84-3	HC(c1c(N(=O)=O)cccc1)C(H)O	1
801	ISSSTY_v1a_7367_02May011_942	87-51-4	HC(C1c2c(cccc2)NC=1)C(=O)O	1
802	ISSSTY_v1a_7367_02May011_943	78-08-0	HC(H)C(H)O[Si](C=CH)(OC(H)C(H)H)OC(H)C(H)H	1
803	ISSSTY_v1a_7367_02May011_945	71-55-6	HC(H)C(Cl)(Cl)Cl	3
804	ISSSTY_v1a_7367_02May011_946	75-26-3	HC(H)C(Br)C(H)H	3
805	ISSSTY_v1a_7367_02May011_948	107-29-9	HC(H)C=NO	1
806	ISSSTY_v1a_7367_02May011_949	121-75-5	HC(H)C(H)OC(=O)C(H)C(C(=O)OC(H)C(H)H)SP(=S)(OC(H)H)OC(H)H	1
807	ISSSTY_v1a_7367_02May011_950	5336-53-8	HC(c1cccc1)N(C(H)c1cccc1)N=O	3
808	ISSSTY_v1a_7367_02May011_951	81840-15-5	HC(H)Oc1c(OC(H)H)cc(O)N2C(H)C(H)N(c3cc4c(cc3)NC(=O)C(H)C4H)C(H)C2H)cc1	1
809	ISSSTY_v1a_7367_02May011_952	102-96-5	c1(C=CN(=O)=O)cccc1	1
810	ISSSTY_v1a_7367_02May011_955	124-18-5	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)H	1

811	ISSSTY_v1a_7367_02May011_956	924-16-3	HC(H)C(H)C(H)C(H)N(C(H)C(H)C(H)C(H)H)N=O	3
812	ISSSTY_v1a_7367_02May011_957	120-83-2	c1(O)c(Cl)cc(Cl)cc1	1
813	ISSSTY_v1a_7367_02May011_958	93878	HC(H)C(C(=O)OC(H)C(H)C(H)C(H)C(H)C(H)C(H)H)=CH	1
814	ISSSTY_v1a_7367_02May011_960	128-95-0	c12C(=O)c3c(C(=O)c1c(N)ccc2N)cccc3	3
815	ISSSTY_v1a_7367_02May011_962	67730-10-3	c12c(ccc(N)n1)N=C1C=CC=CN21	3
816	ISSSTY_v1a_7367_02May011_964	122-80-5	HC(H)C(=O)Nc1ccc(N)cc1	3
817	ISSSTY_v1a_7367_02May011_965	2608-48-2	c1(C=CC=CC=O)ccc(N(=O)=O)cc1	3
818	ISSSTY_v1a_7367_02May011_968	1732-29-2	c1(O)c2c3c4c(c(N(=O)=O)ccc4ccc3cc1)cc2	3
819	ISSSTY_v1a_7367_02May011_969	2499-95-8	HC(H)C(H)C(H)C(H)C(H)C(H)OC(=O)C=CH	1
820	ISSSTY_v1a_7367_02May011_970	4463-22-3	HC(H)C(=O)N(O)c1ccc(-c2ccccc2)cc1	3
821	ISSSTY_v1a_7367_02May011_971	64-17-5	HC(H)C(H)O	1
822	ISSSTY_v1a_7367_02May011_973	92-24-0	c12c(cc3c(cc4c(ccccc4)c3)c1)cccc2	3
823	ISSSTY_v1a_7367_02May011_974	75-45-6	C(F)(F)Cl	3
824	ISSSTY_v1a_7367_02May011_976	85721-33-1	HC1C(H)C1N1c2c(C(=O)C(C(=O)O)=C1)cc(F)c(N1C(H)C(H)NC(H)C1H)c2	3
825	ISSSTY_v1a_7367_02May011_977	126-07-8	HC(H)[C@@]1[C@]2(C(=O)c3c(Cl)c(OC(H)H)cc3OC(H)H)O2)C(OC(H)H)C(H)C(=O)C1H	1
826	ISSSTY_v1a_7367_02May011_978	121-90-4	C(=O)(Cl)c1cc(N(=O)=O)ccc1	3
827	ISSSTY_v1a_7367_02May011_979	107-94-8	HC(C(=O)O)C(H)Cl	3
828	ISSSTY_v1a_7367_02May011_980	60719-84-8	c1(C2C=C(N)C(=O)NC=2)ccncc1	1
829	ISSSTY_v1a_7367_02May011_981	100-22-1	HC(H)N(c1ccc(N(C(H)H)C(H)H)cc1)C(H)H	3
830	ISSSTY_v1a_7367_02May011_983	13395-02-3	HC(H)Oc1c2c(c3c4c(C(=O)Nc4c2)cc2c3OC(H)O2)ccc1	3
831	ISSSTY_v1a_7367_02May011_984	73-31-4	HC(H)C(=O)NC(H)C(H)C1c2c(ccc(OC(H)H)c2)NC=1	1
832	ISSSTY_v1a_7367_02May011_986	105-53-3	HC(H)C(H)OC(=O)C(H)C(=O)OC(H)C(H)H	1
833	ISSSTY_v1a_7367_02May011_992	93-76-5	HC(C(=O)O)Oc1c(Cl)cc(Cl)c(Cl)c1	1
834	ISSSTY_v1a_7367_02May011_994	82-68-8	c1(Cl)c(Cl)c(Cl)c(Cl)c(Cl)c1N(=O)=O	1
835	ISSSTY_v1a_7367_02May011_995	28281	HC(H)C12C(=O)O[C@]3([C@@]4[C@]5(C(H)C(=CH)[C@](O)(C(H)C4H)C5H)[C@@](C(=O)O)[C@]13)C=C[C@]2O	1
836	ISSSTY_v1a_7367_02May011_996	2832-19-1	HC(Cl)C(=O)NC(H)O	1
837	ISSSTY_v1a_7367_02May011_997	10043-35-3	B(O)(O)O	1
838	ISSSTY_v1a_7367_02May011_998	75-91-2	HC(H)C(C(H)H)(C(H)H)OO	3
839	ISSSTY_v1a_7367_02May011_999	110-85-0	HC1C(H)NC(H)C(H)N1	1
840	ISSSTY_v1a_7367_02May011_1000	2373-98-0	c1(-c2cc(O)c(N)cc2)cc(O)c(N)cc1	3