



1345	ISSSTY_v1a_7367_02May011_1655	67-99-2	HC(H)N1C(=O)[C@@]23C(H)C4[C@]([C@@](O)C=CC=4)N2C(=O)[C@]1(C(H)O)SS3	1
1346	ISSSTY_v1a_7367_02May011_1656	88-96-0	C(N)(=O)c1c(C(N)=O)cccc1	1
1347	ISSSTY_v1a_7367_02May011_1657	32534-81-9	c1(Br)c(Br)cc(Br)c(Oc2c(Br)cc(Br)cc2)c1	1
1348	ISSSTY_v1a_7367_02May011_1658	75-31-0	HC(H)C(N)C(H)H	1
1349	ISSSTY_v1a_7367_02May011_1659	144-80-9	HC(H)C(=O)NS(=O)(=O)c1ccc(N)cc1	1
1350	ISSSTY_v1a_7367_02May011_1661	71-36-3	HC(H)C(H)C(H)C(H)O	1
1351	ISSSTY_v1a_7367_02May011_1662	78-63-7	HC(H)C(C(H)H)C(C(H)H)OOC(C(H)H)C(C(H)H)C(H)C(C(H)H)C(C(H)H)OOC(C(H)H)C(C(H)H)C(H)H	1
1352	ISSSTY_v1a_7367_02May011_1663	6358-23-2	c1(Nc2c(O)cccc2)c([N+](=O)[O-])cc([N+](=O)[O-])cc1	3
1353	ISSSTY_v1a_7367_02May011_1665	99-07-0	HC(H)N(c1cc(O)ccc1)C(H)H	3
1354	ISSSTY_v1a_7367_02May011_1666	134998-71-3	HC(H)C(H)C(C(H)C(H)C(O)C(H)H)C(H)OC(=O)C(H)C(H)C(H)C(=O)O	1
1355	ISSSTY_v1a_7367_02May011_1667	32861-85-1	HC(H)Oc1c(N(=O)=O)ccc(Oc2c(Cl)cc(Cl)cc2)c1	3
1356	ISSSTY_v1a_7367_02May011_1668	40809-41-4	HC(H)C(H)C(C(H)C(H)C(H)C(=O)O)C(H)OC(=O)c1c(C(=O)O)cccc1	1
1357	ISSSTY_v1a_7367_02May011_1669	120-37-6	HC(H)c1c(NC(H)C(H)H)cc(O)cc1	3
1358	ISSSTY_v1a_7367_02May011_1670	9002-92-0	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)OC(H)C(H)O	1
1359	ISSSTY_v1a_7367_02May011_1671	1694-20-8	c1(C=Cc2ccc(N(=O)=O)cc2)cccc1	3
1360	ISSSTY_v1a_7367_02May011_1672	9003-39-8	HC1C(=O)N(C=CH)C(H)C1H	1
1361	ISSSTY_v1a_7367_02May011_1673	109-76-2	HC(N)C(H)C(H)N	1
1362	ISSSTY_v1a_7367_02May011_1674	94-20-2	HC(H)C(H)C(H)NC(=O)NS(=O)(=O)c1ccc(Cl)cc1	1
1363	ISSSTY_v1a_7367_02May011_1676	131-14-6	c12C(=O)c3c(C(=O)c1cc(N)cc2)ccc(N)c3	3
1364	ISSSTY_v1a_7367_02May011_1677	620-88-2	c1(Oc2cccc2)ccc(N(=O)=O)cc1	3
1365	ISSSTY_v1a_7367_02May011_1678	140-66-9	HC(H)C(c1ccc(O)cc1)(C(H)H)C(H)C(C(H)H)C(H)H)C(H)H	1
1366	ISSSTY_v1a_7367_02May011_1681	121-60-8	HC(H)C(=O)Nc1ccc(S(=O)(=O)Cl)cc1	1
1367	ISSSTY_v1a_7367_02May011_1682	828-00-2	HC(H)C(=O)OC1C(H)C(C(H)H)OC(C(H)H)O1	3
1368	ISSSTY_v1a_7367_02May011_1683	134998-72-4	HC(H)C(=O)C(H)C(H)C(C(H)C(H)H)C(H)OC(=O)C(H)C(H)C(H)C(=O)O	1
1369	ISSSTY_v1a_7367_02May011_1684	88321-09-9	HC(H)C(H)OC(=O)[C@]1[C@@](C(=O)N[C@](C(=O)NC(H)C(C(H)H)C(H)H)C(H)C(C(H)H)C(H)H)O1	1
1370	ISSSTY_v1a_7367_02May011_1685	645-62-5	HC(H)C(H)C(C=O)=CC(H)C(H)C(H)H	1
1371	ISSSTY_v1a_7367_02May011_1687	110-18-9	HC(H)N(C(H)H)C(H)C(H)N(C(H)H)C(H)H	1
1372	ISSSTY_v1a_7367_02May011_1688	583-78-8	c1(Cl)c(O)cc(Cl)cc1	1
1373	ISSSTY_v1a_7367_02May011_1689	1769-41-1	C(=O)(C=NO)Nc1cccc1	1
1374	ISSSTY_v1a_7367_02May011_1690	87-82-1	c1(Br)c(Br)c(Br)c(Br)c(Br)c1Br	1
1375	ISSSTY_v1a_7367_02May011_1691	393-52-2	C(=O)(Cl)c1c(F)cccc1	3
1376	ISSSTY_v1a_7367_02May011_1692	150-69-6	HC(H)C(H)Oc1ccc(NC(N)=O)cc1	1
1377	ISSSTY_v1a_7367_02May011_1693	5273-86-9	HC(H)C=Cc1c(OC(H)H)cc(OC(H)H)c(OC(H)H)c1	3
1378	ISSSTY_v1a_7367_02May011_1694	301-12-2	HC(H)C(H)S(=O)C(H)C(H)SP(=O)(OC(H)H)OC(H)H	3
1379	ISSSTY_v1a_7367_02May011_1695	25990-37-8	HC(H)C12C3=C(C(H)H)C(C4C=COC=4)C(H)C3OC1C1C3C(C(H)H)C(=O)C=CC3(C(H)H)C(=O)O1)C2C(H)C(=O)OC(H)H	1
1380	ISSSTY_v1a_7367_02May011_1696	4802-20-4	HC(H)C1C(H)C(H)C(C(C(H)H)C(H)S)C(H)C1S	1
1381	ISSSTY_v1a_7367_02May011_1697	5589-96-8	C(=O)(O)C(Cl)Br	3
1382	ISSSTY_v1a_7367_02May011_1698	75-50-3	HC(H)N(C(H)H)C(H)H	1
1383	ISSSTY_v1a_7367_02May011_1699	26091-73-6	HC(H)C1(C(H)H)[C@](C(H)O)c2c3c(cc4c2C=CC(=O)O4)OC=C3)O1	1
1384	ISSSTY_v1a_7367_02May011_1700	106-02-5	HC1C(=O)OC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C1H	1
1385	ISSSTY_v1a_7367_02May011_1702	531-75-9	HC(O)[C@]1[C@@](O)[C@](O)[C@@](O)[C@](O)c2c(O)cc3c(C=CC(=O)O3)c2)O1	1
1386	ISSSTY_v1a_7367_02May011_1703	25143	HC(S)C(=O)O	1

1387	ISSSTY_v1a_7367_02May011_1704	2385-85-5	C12(CI)C3(CI)C4(CI)C(CI)(CI)C5(CI)C(CI)(C(CI)(C35CI)C1(CI)CI)C24CI	1
1388	ISSSTY_v1a_7367_02May011_1705	634-66-2	c1(CI)c(CI)c(CI)c(CI)cc1	1
1389	ISSSTY_v1a_7367_02May011_1706	117-18-0	c1(CI)c(CI)c(N(=O)=O)c(CI)c(CI)c1	1
1390	ISSSTY_v1a_7367_02May011_1707	129-43-1	c12C(=O)c3c(C(=O)c1c(O)ccc2)cccc3	3
1391	ISSSTY_v1a_7367_02May011_1708	106-92-3	HC1C(C(H)OC(H)C=CH)O1	3
1392	ISSSTY_v1a_7367_02May011_1712	26446-35-5	HC(H)C(=O)OC(H)C(O)C(H)O	3
1393	ISSSTY_v1a_7367_02May011_1713	108-86-1	c1(Br)cccc1	1
1394	ISSSTY_v1a_7367_02May011_1714	92-66-0	c1(-c2ccc(Br)cc2)cccc1	1
1395	ISSSTY_v1a_7367_02May011_1715	55705	c1(-c2c(Br)cccc2)cccc1	1
1396	ISSSTY_v1a_7367_02May011_1716	94-25-7	HC(H)C(H)C(H)C(H)OC(=O)c1ccc(N)cc1	1
1397	ISSSTY_v1a_7367_02May011_1717	111-83-1	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)Br	1
1398	ISSSTY_v1a_7367_02May011_1718	523-47-7	HC(H)C1C(H)[C@@]2[C@@](C(C(H)H)=CC(H)[C@@]2C(C(H)H)C(H)H)C(H)C=1	1
1399	ISSSTY_v1a_7367_02May011_1719	628-94-4	HC(C(N)=O)C(H)C(H)C(H)C(N)=O	1
1400	ISSSTY_v1a_7367_02May011_1720	108-93-0	HC1C(H)C(H)C(H)C(H)C1O	1
1401	ISSSTY_v1a_7367_02May011_1721	1116-40-1	HC(H)C(C(H)H)C(H)N(C(H)C(C(H)H)C(H)H)C(H)C(C(H)H)C(H)H	1
1402	ISSSTY_v1a_7367_02May011_1722	108-80-5	C1(=O)NC(=O)NC(=O)N1	1
1403	ISSSTY_v1a_7367_02May011_1723	17433-31-7	HC(H)C(=O)NNC(=O)c1ccccn1	1
1404	ISSSTY_v1a_7367_02May011_1724	95-77-2	c1(CI)c(CI)cc(O)cc1	1
1405	ISSSTY_v1a_7367_02May011_1725	57-83-0	HC(H)[C@]12C(C(H)C(H)[C@]3[C@]4[C@](C(H)H)(C(H)C(H)[C@@]13)[C@@](C(=O)C(H)H)C(H)C4H)=CC(=O)C(H)C2H	1
1406	ISSSTY_v1a_7367_02May011_1726	576-24-9	c1(CI)c(CI)c(O)ccc1	1
1407	ISSSTY_v1a_7367_02May011_1727	111-42-2	HC(O)C(H)NC(H)C(H)O	1
1408	ISSSTY_v1a_7367_02May011_1728	118-52-5	HC(H)C1(C(H)H)C(=O)N(CI)C(=O)N1CI	1
1409	ISSSTY_v1a_7367_02May011_1729	1488-25-1	C1C2C(C=CC=1)O2	3
1410	ISSSTY_v1a_7367_02May011_1731	517-28-2	HC1c2c([C@]3c4c(c(O)c(O)cc4)OC(H)[C@]13O)cc(O)c(O)c2	1
1411	ISSSTY_v1a_7367_02May011_1732	756-79-6	HC(H)OP(=O)(C(H)H)OC(H)H	1
1412	ISSSTY_v1a_7367_02May011_1733	118-56-9	HC(H)C1(C(H)H)C(H)C(C(H)H)C(H)C(OC(=O)c2c(O)cccc2)C1H	1
1413	ISSSTY_v1a_7367_02May011_1734	3268-87-9	c1(CI)c(CI)c(CI)c(CI)c2c1Oc1c(CI)c(CI)c(CI)c(CI)c1O2	1
1414	ISSSTY_v1a_7367_02May011_1736	90-33-5	HC(H)C1c2c(cc(O)cc2)OC(=O)C=1	1
1415	ISSSTY_v1a_7367_02May011_1737	57-55-6	HC(H)C(O)C(H)O	1
1416	ISSSTY_v1a_7367_02May011_1738	150-78-7	HC(H)Oc1ccc(OC(H)H)cc1	1
1417	ISSSTY_v1a_7367_02May011_1739	621-77-2	HC(H)C(H)C(H)C(H)C(H)N(C(H)C(H)C(H)C(H)C(H)H)C(H)C(H)C(H)C(H)H	1
1418	ISSSTY_v1a_7367_02May011_1741	879-39-0	c1(CI)c(CI)c(CI)c(CI)c(N(=O)=O)c1	1
1419	ISSSTY_v1a_7367_02May011_1742	36355-01-8	c1(-c2c(Br)c(Br)c(Br)cc2)c(Br)c(Br)c(Br)cc1	1
1420	ISSSTY_v1a_7367_02May011_1743	53-94-1	HC1c2c(-c3c1cc(NO)cc3)cccc2	3
1421	ISSSTY_v1a_7367_02May011_1744	3322-93-8	HC1C(H)C(C(Br)C(H)Br)C(H)C(Br)C1Br	1
1422	ISSSTY_v1a_7367_02May011_1745	133-18-6	HC(c1cccc1)C(H)OC(=O)c1c(N)cccc1	1
1423	ISSSTY_v1a_7367_02May011_1746	603-35-0	c1(P(c2cccc2)c2cccc2)cccc1	1
1424	ISSSTY_v1a_7367_02May011_1747	1122-54-9	HC(H)C(=O)c1ccncc1	1
1425	ISSSTY_v1a_7367_02May011_1748	126-30-7	HC(H)C(C(H)H)(C(H)O)C(H)O	1
1426	ISSSTY_v1a_7367_02May011_1749	78-51-3	HC(H)C(H)C(H)C(H)OC(H)C(H)OP(=O)(OC(H)C(H)OC(H)C(H)C(H)H)OC(H)C(H)OC(H)C(H)C(H)H	1
1427	ISSSTY_v1a_7367_02May011_1750	60-00-4	HC(C(=O)O)N(C(H)C(=O)O)C(H)C(H)N(C(H)C(=O)O)C(H)C(=O)O	1
1428	ISSSTY_v1a_7367_02May011_1751	101-84-8	c1(Oc2cccc2)cccc1	1





















1807	ISSSTY_v1a_7367_02May011_2244	98-57-7	HC(H)S(=O)(=O)c1ccc(Cl)cc1	1
1808	ISSSTY_v1a_7367_02May011_2245	57-13-6	C(N)(N)=O	1
1809	ISSSTY_v1a_7367_02May011_2246	1942394	HC(H)c1c(N)c(C(H)H)cc(N)c1	1
1810	ISSSTY_v1a_7367_02May011_2247	57835-92-4	c12c3c4c(c(N(=O)=O)cc3ccc1)cccc4cc2	3
1811	ISSSTY_v1a_7367_02May011_2248	1198-61-4	c1(Cl)c(F)c(Cl)c(F)c(F)c1F	1
1812	ISSSTY_v1a_7367_02May011_2249	17479-19-5	HC(H)C([C@@H]1NC(=O)[C@H]2C(H)[C@@H]3c4c5C(C(H)[C@H]3NC(H)H)C2H)=CNc5ccc4C(=O)N2[C@@H]1O)([C@@H]3C(H)C(H)C(H)N3C(=O)[C@H]2C(H)c2cccc2O)1C(H)H	1
1813	ISSSTY_v1a_7367_02May011_2250	97629-64-6	HC(H)c1c(N)c(C(H)H)c(N(=O)=O)c(N)c1	1
1814	ISSSTY_v1a_7367_02May011_2251	84-54-8	HC(H)c1cc2C(=O)c3c(C(=O)c2cc1)cccc3	1
1815	ISSSTY_v1a_7367_02May011_2252	115-39-9	c1(C2(c3cc(Br)c(O)c(Br)c3)c3c(cccc3)S(=O)(=O)O2)cc(Br)c(O)c(Br)c1	1
1816	ISSSTY_v1a_7367_02May011_2253	610-88-8	HC(H)C(=O)C1C(=O)C(C(C(H)H)C(H)C(H)H)NC=1O	1
1817	ISSSTY_v1a_7367_02May011_2254	59702-31-7	HC(H)C(H)N1C(=O)C(=O)NC(H)C1H	1
1818	ISSSTY_v1a_7367_02May011_2255	50264-69-2	HC(c1c(Cl)cc(Cl)cc1)N1c2c(C(C(=O)O)=N1)cccc2	1
1819	ISSSTY_v1a_7367_02May011_2257	6422-86-2	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)OC(=O)c1ccc(C(=O)OC(H)C(C(H)H)C(H)C(H)C(H)C(H)C(H)H)cc1	1
1820	ISSSTY_v1a_7367_02May011_2258	25057-89-0	HC(H)C(C(H)H)N1C(=O)c2c(cccc2)NS1(=O)=O	1
1821	ISSSTY_v1a_7367_02May011_2259	695-99-8	C1(C)C(=O)C=CC(=O)C=1	1
1822	ISSSTY_v1a_7367_02May011_2261	67-45-8	HC1C(H)N(N=CC2=CC=C(N(=O)=O)O2)C(=O)O1	3
1823	ISSSTY_v1a_7367_02May011_2263	79-34-5	C(Cl)(Cl)C(Cl)Cl	3
1824	ISSSTY_v1a_7367_02May011_2264	74-88-4	HC(H)I	3
1825	ISSSTY_v1a_7367_02May011_2268	155603-50-2	HC(H)C(H)C(H)C(H)C(C(H)C(H)H)C(H)OC(=O)c1ccc(C(=O)O)cc1	1
1826	ISSSTY_v1a_7367_02May011_2269	85-86-9	C1(=O)C(=NNc2ccc(N=Nc3ccccc3)cc2)c2c(C=C1)cccc2	1
1827	ISSSTY_v1a_7367_02May011_2270	2921-88-2	HC(H)C(H)OP(=S)(Oc1c(Cl)cc(Cl)c(Cl)n1)OC(H)C(H)H	1
1828	ISSSTY_v1a_7367_02May011_2271	137-18-8	HC(H)C1C(=O)C=C(C(H)H)C(=O)C=1	1
1829	ISSSTY_v1a_7367_02May011_2272	605-94-7	HC(H)C1C(=O)C(OC(H)H)=C(OC(H)H)C(=O)C=1	1
1830	ISSSTY_v1a_7367_02May011_2273	90098-04-7	HC(C1c2c(cccc2)NC(=O)C=1)C(C(=O)O)NC(=O)c1ccc(Cl)cc1	1
1831	ISSSTY_v1a_7367_02May011_2274	86451-37-8	HC(H)N(C(H)C(O)C(H)O)N=O	3
1832	ISSSTY_v1a_7367_02May011_2275	527-61-7	HC(H)C1C(=O)C(C(H)H)=CC(=O)C=1	1
1833	ISSSTY_v1a_7367_02May011_2278	64224-21-1	HC(H)C1C(=S)SSC=1c1cncn1	1
1834	ISSSTY_v1a_7367_02May011_2279	64896-26-0	C(=O)(O)C1C(=O)C=CC(=NNc2ccc(C(=O)O)cc2)C=1	1
1835	ISSSTY_v1a_7367_02May011_2282	602-64-2	c12C(=O)c3c(C(=O)c1c(O)c(O)c2)cccc3	3
1836	ISSSTY_v1a_7367_02May011_2283	28911-01-5	HC(H)C1N2c3c(C(c4c(Cl)cccc4)=NC(H)C2=NN=1)cc(Cl)cc3	1
1837	ISSSTY_v1a_7367_02May011_2284	106871-13-0	HC(H)c1c(N(C(H)C(H)Cl)C(H)Cl)cc(C(O)P(=O)(O)O)P(=O)(O)O)cc1	3
1838	ISSSTY_v1a_7367_02May011_2286	82-39-3	HC(H)Oc1c2C(=O)c3c(C(=O)c2ccc1)cccc3	3
1839	ISSSTY_v1a_7367_02May011_2287	384-22-5	C(F)(F)(F)c1c(N(=O)=O)cccc1	1
1840	ISSSTY_v1a_7367_02May011_2288	57749	c12C(=O)c3c(C(=O)c1c(N)c(C(=O)O)cc2N(=O)=O)cccc3	3
1841	ISSSTY_v1a_7367_02May011_2289	320-51-4	C(F)(F)(F)c1c(Cl)ccc(N)c1	1
1842	ISSSTY_v1a_7367_02May011_2290	393-75-9	C(F)(F)(F)c1cc([N+](=O)[O-])c(Cl)c([N+](=O)[O-])c1	1
1843	ISSSTY_v1a_7367_02May011_2291	98-46-4	C(F)(F)(F)c1cc(N(=O)=O)ccc1	1
1844	ISSSTY_v1a_7367_02May011_2292	109-64-8	HC(Br)C(H)C(H)Br	3
1845	ISSSTY_v1a_7367_02May011_2293	202-33-5	c12c(c3c(c4c5c(C=C4)cccc5c3)cc1)cccc2	3
1846	ISSSTY_v1a_7367_02May011_2295	55028-70-1	HC(H)[C@@H](O)C(C(H)C(H)C(H)C(H)H)C=CC1[C@@H](C(H)C=CC(H)C(H)C(H)C(=O)O)C(=O)C(H)[C@@H]1O	1
1847	ISSSTY_v1a_7367_02May011_2296	918-00-3	HC(H)C(=O)C(Cl)(Cl)Cl	3
1848	ISSSTY_v1a_7367_02May011_2297	811-97-2	HC(F)C(F)(F)F	1

1849	ISSSTY_v1a_7367_02May011_2298	5633-20-5	HC(H)C(H)N(C(H)C_CC(H)OC(=O)C(O)(c1ccccc1)C1C(H)C(H)C(H)C(H)C1H)C(H)C(H)H	1
1850	ISSSTY_v1a_7367_02May011_2299	994-05-8	HC(H)C(C(H)H)(C(H)C(H)H)OC(H)H	1
1851	ISSSTY_v1a_7367_02May011_2300	60129-67-1	HC(O)C(H)N(c1ccc(N=Nc2c([N+](=O)[O-])cc([N+](=O)[O-])cc2)cc1)C(H)C(H)O	3
1852	ISSSTY_v1a_7367_02May011_2301	121808-62-6	HC1C(=O)N[C@](C(=O)N2C(H)SC(H)[C@@]2C(=O)O)C1H	1
1853	ISSSTY_v1a_7367_02May011_2302	79748-81-5	HC(H)C(C(=O)[C@@]12C(=O)N[C@@](O)(C(H)C(H)O)[C@@]1O2)=CC=CC(C(H)H)=CC(C(H)H)=CC(C(=O)OC(H)H)=CC(H)H	3
1854	ISSSTY_v1a_7367_02May011_2303	59283-75-9	HC(H)c1c([N+](=O)[O-])cc(NO)cc1[N+](=O)[O-]	3
1855	ISSSTY_v1a_7367_02May011_2304	111753-73-2	HC(H)Oc1ccc(C(c2ccc(OC(H)H)cc2)=C(C_N)C(H)C(H)C(=O)O)cc1	1
1856	ISSSTY_v1a_7367_02May011_2307	50330-59-1	HC(H)N(C(=O)C1N=C2C(H)N=C(c3c(Cl)cccc3)c3c(ccc(Cl)c3)N2N=1)C(H)H	1
1857	ISSSTY_v1a_7367_02May011_2308	146-22-5	HC1C(=O)Nc2c(C(c3ccccc3)=N1)cc(N(=O)=O)cc2	1
1858	ISSSTY_v1a_7367_02May011_2309	35212-22-7	HC(H)C(C(H)H)Oc1cc2c(C(=O)C(c3ccccc3)=CO2)cc1	1
1859	ISSSTY_v1a_7367_02May011_2310	19392	HC(H)C(S)C(=O)NC(H)C(=O)O	1
1860	ISSSTY_v1a_7367_02May011_2311	95-69-2	HC(H)c1c(N)ccc(Cl)c1	3
1861	ISSSTY_v1a_7367_02May011_2314	86439-49-8	c12-c3c(cc(N)c(N(=O)=O)c3)Nc1cccc2	3
1862	ISSSTY_v1a_7367_02May011_2315	158321-20-1	c12-c3c(c(N(=O)=O)c(N)cc3)Nc1cccc2	3
1863	ISSSTY_v1a_7367_02May011_2319	29590-42-9	HC(H)C(C(H)H)C(H)C(H)C(H)C(H)C(H)OC(=O)C=CH	1
1864	ISSSTY_v1a_7367_02May011_2320	34834-67-8	HC(H)N1C(=O)C(O)C(H)C1c1cccnc1	1
1865	ISSSTY_v1a_7367_02May011_2322	4245-76-5	HC(H)N=C(N)NN(=O)=O	1
1866	ISSSTY_v1a_7367_02May011_2323	123-09-1	HC(H)Sc1ccc(Cl)cc1	1
1867	ISSSTY_v1a_7367_02May011_2325	32055	C(=O)(c1c(O)c(Br)cc(Br)c1)Nc1ccc(Br)cc1	1
1868	ISSSTY_v1a_7367_02May011_2326	2277-92-1	C(=O)(c1c(Cl)c(Cl)cc(Cl)c1O)Nc1c(O)c(Cl)cc(Cl)c1	1
1869	ISSSTY_v1a_7367_02May011_2328	852-20-0	c1(Sc2c(O)c([N+](=O)[O-])cc(Cl)c2)c(O)c([N+](=O)[O-])cc(Cl)c1	1
1870	ISSSTY_v1a_7367_02May011_2330	29975-16-4	HC1C2N(c3c(C(c4ccccc4)=N1)cc(Cl)cc3)C=NN=2	1
1871	ISSSTY_v1a_7367_02May011_2331	479-50-5	HC(H)c1c2c(C(=O)c3c(cccc3)S2)c(NC(H)C(H)N(C(H)C(H)H)C(H)C(H)H)cc1	3
1872	ISSSTY_v1a_7367_02May011_2332	594-20-7	HC(H)C(Cl)(Cl)C(H)H	1
1873	ISSSTY_v1a_7367_02May011_2333	21672	HC(H)N(c1ccc(C(=O)N[C@](C(=O)O)C(H)C(H)C(=O)O)cc1)C(H)c1cnc2c(c(N)nc(N)n2)n1	1
1874	ISSSTY_v1a_7367_02May011_2335	142-28-9	HC(Cl)C(H)C(H)Cl	1
1875	ISSSTY_v1a_7367_02May011_2336	21466-07-9	c1(-c2c(OP(=O)(O)O)c(Br)cc(Br)c2)c(O)c(Br)cc(Br)c1	1
1876	ISSSTY_v1a_7367_02May011_2337	540-88-5	HC(H)C(C(H)H)(C(H)H)OC(=O)C(H)H	1
1877	ISSSTY_v1a_7367_02May011_2338	12771-68-5	HC(H)Oc1ccc(C(O)(c2cncnc2)C2C(H)C2H)cc1	1
1878	ISSSTY_v1a_7367_02May011_2339	2475-46-9	HC(H)Nc1c2C(=O)c3c(C(=O)c2c(NC(H)C(H)O)cc1)cccc3	3
1879	ISSSTY_v1a_7367_02May011_2340	2106-54-9	C(F)(F)(Cl)C(F)(Cl)C(F)(F)C(F)(Cl)C(F)(F)C(=O)O	1
1880	ISSSTY_v1a_7367_02May011_2342	2923-68-4	C(F)(F)(Cl)C(F)(Cl)C(F)(F)C(F)(Cl)C(F)(F)C(F)(Cl)C(F)(F)C(=O)O	1
1881	ISSSTY_v1a_7367_02May011_2343	335-76-2	C(F)(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(=O)O	1
1882	ISSSTY_v1a_7367_02May011_2345	74-31-7	c1(Nc2ccccc2)ccc(Nc2ccccc2)cc1	3
1883	ISSSTY_v1a_7367_02May011_2347	54567-09-8	HC(O)C(H)N(c1ccc(N=Nc2c(C_N)cc(N(=O)=O)cc2)cc1)C(H)C(H)O	3
1884	ISSSTY_v1a_7367_02May011_2348	112-59-4	HC(H)C(H)C(H)C(H)C(H)C(H)OC(H)C(H)OC(H)C(H)O	1
1885	ISSSTY_v1a_7367_02May011_2350	159860-07-8	HC(H)C(H)N(c1ccc(N=Nc2c(Cl)cc([N+](=O)[O-])cc2[N+](=O)[O-])cc1)C(H)C(H)H	3
1886	ISSSTY_v1a_7367_02May011_2352	5216-25-1	C(Cl)(Cl)(Cl)c1ccc(Cl)cc1	3
1887	ISSSTY_v1a_7367_02May011_2354	386523	HC(H)[C@@]12C(H)C(H)[C@@]3[C@@]4(C(H)C(H)C(H)C(H)[C@@](O)C(H)[C@@]4[C@@](O)C(H)[C@@]3[C@@]1)C(H)C(H)[C@@]2[C@@](C(H)H)C(H)C(H)C(=O)NC(H)C(H)S(=O)(=O)O	1
1888	ISSSTY_v1a_7367_02May011_2355	110-72-5	HC(H)C(H)[N+](H)C(H)C(H)[N+](H)H	1
1889	ISSSTY_v1a_7367_02May011_2357	26196-45-2	c1(N)c(Cl)cc(N)c(N(=O)=O)c1	3
1890	ISSSTY_v1a_7367_02May011_2358	17626-02-7	HC(H)Oc1c(N)cc(OC(H)H)c(N)c1	3





1933	ISSSTY_v1a_7367_02May011_2414	120-52-5	C(=O)(c1ccccc1)ON=C1C=CC(=NOC(=O)c2ccccc2)C=C1	3
1934	ISSSTY_v1a_7367_02May011_2415	103-34-4	HC1C(H)N(SSN2C(H)C(H)OC(H)C2H)C(H)C(H)O1	1
1935	ISSSTY_v1a_7367_02May011_2417	13060-14-5	HC(H)Oc1c(OC(H)H)c(OC(H)H)cc([C@]2[C@]3C(H)O[C@@]1(c4cc(OC(H)H)c(OC(H)H)c(OC(H)H)c4)[C@]3C(H)O2)c1	1
1936	ISSSTY_v1a_7367_02May011_2418	2314-97-8	C(F)(F)(F)I	3
1937	ISSSTY_v1a_7367_02May011_2419	3268-49-3	HC(H)SC(H)C(H)C=O	1
1938	ISSSTY_v1a_7367_02May011_2420	106-97-8	HC(H)C(H)C(H)C(H)H	1
1939	ISSSTY_v1a_7367_02May011_2421	76-43-7	HC(H)[C@]12[C@@](O)(C(H)H)C(H)C(H)[C@]1[C@]1[C@@](F)([C@]3C(H)H)C(C(H)C1H)=CC(=O)C(H)C3H)[C@@](O)C2H	1
1940	ISSSTY_v1a_7367_02May011_2422	3032-55-1	HC(H)C(C(H)ON(=O)=O)(C(H)ON(=O)=O)C(H)ON(=O)=O	1
1941	ISSSTY_v1a_7367_02May011_2423	95186-19-9	HC(C1C2N(C(N)=NC=1c1ccccc1)N=CN=2)C(H)O	1
1942	ISSSTY_v1a_7367_02May011_2424	82486-82-6	HC(H)C(H)C(H)C(H)N(C(H)C(H)ON(=O)=O)[N+](=O)[O-]	3
1943	ISSSTY_v1a_7367_02May011_2425	650166	HC(H)S(=O)(=O)C=CH	1
1944	ISSSTY_v1a_7367_02May011_2426	104485-01-0	HC(H)C(H)C(H)C(H)C(H)Oc1cc(NC(=O)OC2C(H)C(H)C(H)C(H)[C@@]2N2C(H)C(H)C(H)C2H)ccc1	1
1945	ISSSTY_v1a_7367_02May011_2428	195-52-8	c12c(c3c4c(ccc3cc1)cccc4)C=CS2	3
1946	ISSSTY_v1a_7367_02May011_2430	627-05-4	HC(H)C(H)C(H)C(H)N(=O)=O	1
1947	ISSSTY_v1a_7367_02May011_2431	612-24-8	C(N)c1c(N(=O)=O)cccc1	1
1948	ISSSTY_v1a_7367_02May011_2433	619-72-7	C(N)c1ccc(N(=O)=O)cc1	1
1949	ISSSTY_v1a_7367_02May011_2434	621-52-3	HC(H)C(H)Oc1cc(N(=O)=O)ccc1	1
1950	ISSSTY_v1a_7367_02May011_2435	100-29-8	HC(H)C(H)Oc1ccc(N(=O)=O)cc1	3
1951	ISSSTY_v1a_7367_02May011_2436	1877-73-2	HC(c1cc(N(=O)=O)ccc1)C(=O)O	1
1952	ISSSTY_v1a_7367_02May011_2437	21399	HC(H)N1C(=O)C2=C(N(C(H)H)C1=O)N=CN2C(H)H	1
1953	ISSSTY_v1a_7367_02May011_2438	1013-96-3	c1(N(=O)=O)c(C=CC(=O)O)cccc1	1
1954	ISSSTY_v1a_7367_02May011_2439	1849-36-1	c1(S)ccc(N(=O)=O)cc1	3
1955	ISSSTY_v1a_7367_02May011_2440	80830-42-8	HC(C(=O)N1[C@](c2c(O)cccc2)SC(H)[C@@]1C(=O)O)C(H)S	1
1956	ISSSTY_v1a_7367_02May011_2442	78-62-6	HC(H)C(H)O[Si](C(H)H)(C(H)H)OC(H)C(H)H	1
1957	ISSSTY_v1a_7367_02May011_2443	75-79-6	HC(H)[Si](Cl)(Cl)Cl	1
1958	ISSSTY_v1a_7367_02May011_2444	2031-67-6	HC(H)C(H)O[Si](C(H)H)(OC(H)C(H)H)OC(H)C(H)H	1
1959	ISSSTY_v1a_7367_02May011_2445	18883-66-4	HC(H)N(C(=O)N[C@]1[C@@](O)[C@](O)[C@@](C(H)O)O[C@]1O)N=O	3
1960	ISSSTY_v1a_7367_02May011_2446	112-53-8	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)C(H)O	1
1961	ISSSTY_v1a_7367_02May011_2447	10026-04-7	[Si](Cl)(Cl)(Cl)Cl	1
1962	ISSSTY_v1a_7367_02May011_2448	107-46-0	HC(H)[Si](C(H)H)(C(H)H)O[Si](C(H)H)(C(H)H)C(H)H	1
1963	ISSSTY_v1a_7367_02May011_2449	26538-44-3	HC(H)[C@@]1C(H)C(H)C(H)C(O)C(H)C(H)C(H)C(H)C(H)c2c(C(=O)O1)c(O)cc(O)c2	1
1964	ISSSTY_v1a_7367_02May011_2450	541-05-9	HC(H)[Si]1(C(H)H)O[Si](C(H)H)(C(H)H)O[Si](C(H)H)(C(H)H)O1	1
1965	ISSSTY_v1a_7367_02May011_2451	60564-31-0	c12-c3c(cc(N(=O)=O)c(N)c3)Nc1cccc2	3
1966	ISSSTY_v1a_7367_02May011_2452	541-02-6	HC(H)[Si]1(C(H)H)O[Si](C(H)H)(C(H)H)O[Si](C(H)H)(C(H)H)O[Si](C(H)H)(C(H)H)O1	1
1967	ISSSTY_v1a_7367_02May011_2454	81-15-2	HC(H)C(c1c([N+](=O)[O-])c(C(H)H)c([N+](=O)[O-])c(C(H)H)c1[N+](=O)[O-])(C(H)H)C(H)H	1
1968	ISSSTY_v1a_7367_02May011_2455	112-80-1	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C=CC(H)C(H)C(H)C(H)C(H)C(=O)O	1
1969	ISSSTY_v1a_7367_02May011_2456	96014-34-5	HC(H)C(=O)Nc1c(N(=O)=O)c2-c3c(cccc3)Nc2cc1	3
1970	ISSSTY_v1a_7367_02May011_2457	738-70-5	HC(H)Oc1c(OC(H)H)c(OC(H)H)cc(C(H)c2c(N)nc(N)nc2)c1	3
1971	ISSSTY_v1a_7367_02May011_2458	96014-35-6	HC(H)C(=O)Nc1c(N(=O)=O)cc2c(-c3c(cccc3)N2)c1	3
1972	ISSSTY_v1a_7367_02May011_2459	205-82-3	c12c(c3c(c4c5c(cccc35)ccc4)cc1)cccc2	3
1973	ISSSTY_v1a_7367_02May011_2461	21416-67-1	HC(H)C(C(H)N1C(H)C(=O)NC(=O)C1H)N1C(H)C(=O)NC(=O)C1H	1
1974	ISSSTY_v1a_7367_02May011_2462	646-06-0	HC1C(H)OC(H)O1	1



1975	ISSSTY_v1a_7367_02May011_2463	63358-49-6	HC(H)C1(C(H)H)[C@@](C(=O)O)N2C(=O)[C@@](NC(=O)[C@@](c3ccc(O)cc3)NC(=O)[C@](N)C(H)C(=O)NC(H)H)[C@]2S1	1
1976	ISSSTY_v1a_7367_02May011_2464	81486-22-8	HC(H)C(C(H)H)NC(H)C(O)C(H)Oc1c2c(C(H)C(ON(=O)=O)C(H)O2)ccc1	1
1977	ISSSTY_v1a_7367_02May011_2465	86247-86-1	HC(H)C(C(H)H)NC(H)C(O)C(H)Oc1c2c(C(H)C(O)C(H)O2)ccc1	1
1978	ISSSTY_v1a_7367_02May011_2468	115688-97-6	HC(H)N1C(H)C(H)C=C2C3=C(C(H)C(H)C12)SC(N)=N3	3
1979	ISSSTY_v1a_7367_02May011_2470	14703-71-0	c1(O)c(N(=O)=O)c(N)ccc1	1
1980	ISSSTY_v1a_7367_02May011_2471	58-85-5	HC(C(=O)O)C(H)C(H)C1C2C(C(H)S1)NC(=O)N2	1
1981	ISSSTY_v1a_7367_02May011_2472	603-85-0	c1(O)c(N)c(N(=O)=O)ccc1	1
1982	ISSSTY_v1a_7367_02May011_2473	603-87-2	c1(N)c(O)c(N(=O)=O)ccc1	1
1983	ISSSTY_v1a_7367_02May011_2474	143343-83-3	HC(H)Oc1c(OC(H)H)cc(C(H)NC(H)C(O)C(H)Oc2cc3c(cc2)NC(=O)C=C3)cc1	1
1984	ISSSTY_v1a_7367_02May011_2475	117-02-2	HC(H)c1c(O)c2C(=O)c3c(C(=O)c2cc1O)cccc3	3
1985	ISSSTY_v1a_7367_02May011_2476	581-89-5	c12c(cc(N(=O)=O)cc1)cccc2	3
1986	ISSSTY_v1a_7367_02May011_2477	77121-90-5	HC(H)C1C(OC(H)H)C(N)C(H)C(OC2c3c(O)c4C(=O)c5c(C(=O)c4c(O)c3C(H)C(O)C(=O)C(H)O2)H)cccc5OC(H)H)O1	3
1987	ISSSTY_v1a_7367_02May011_2478	79660-72-3	HC(H)N1C(H)C(H)N(c2c(F)c3c(C(=O)C(C(=O)O)=CN3C(H)C(H)F)cc2F)C(H)C1H	3
1988	ISSSTY_v1a_7367_02May011_2479	74011-58-8	HC(H)C(H)N1c2c(C(=O)C(C(=O)O)=C1)cc(F)c(N1C(H)C(H)NC(H)C1H)n2	3
1989	ISSSTY_v1a_7367_02May011_2480	110-52-1	HC(Br)C(H)C(H)C(H)Br	3
1990	ISSSTY_v1a_7367_02May011_2482	86674-51-3	c12c3c4c(c(N=O)ccc4ccc3ccc1)cc2	3
1991	ISSSTY_v1a_7367_02May011_2483	785-30-8	C(=O)(c1ccc(N)cc1)Nc1ccc(N)cc1	3
1992	ISSSTY_v1a_7367_02May011_2484	75453-80-4	C1C(O)C(O)C=CC=1	3
1993	ISSSTY_v1a_7367_02May011_2485	125974-08-5	HC(Cl)C1=C(Cl)C(=O)OC1O	3
1994	ISSSTY_v1a_7367_02May011_2487	118517-20-7	HC(H)[C@@]12[C@@]3(C(H)[C@@](OC(=O)C(H)H)C(H)[C@@]4(C)C(C)C(H)C(H)[C@]21)[C@](C(H)H)C(H)C(H)C(H)C(H)C(H)C4)HN3N1C(=O)c2c(C1=O)cccc2	3
1995	ISSSTY_v1a_7367_02May011_2488	152-18-1	HC(H)OP(=S)(OC(H)H)OC(H)H	1
1996	ISSSTY_v1a_7367_02May011_2489	22608-53-3	HC(H)OP(=O)(SC(H)H)SC(H)H	1
1997	ISSSTY_v1a_7367_02May011_2490	491-59-8	HC(H)c1cc(O)c2c(O)c3c(cc2c1)cccc3O	3
1998	ISSSTY_v1a_7367_02May011_2491	81-63-0	HC1C(N)=C2C(C(=O)c3c(C2=O)cccc3)=C(N)C1H	3
1999	ISSSTY_v1a_7367_02May011_2492	4947-27-7	HC(H)c1c(Nc2cccc2)c2C(=O)c3c(C(=O)c2cc1)cccc3	3
2000	ISSSTY_v1a_7367_02May011_2493	129-44-2	c12C(=O)c3c(C(=O)c1c(N)ccc2)cccc3N	3
2001	ISSSTY_v1a_7367_02May011_2494	82-50-8	c12C(=O)c3c(C(=O)c1c(N(=O)=O)ccc2)cccc3S(=O)(=O)O	3
2002	ISSSTY_v1a_7367_02May011_2495	6483-86-9	c12C(=O)c3c(C(=O)c1c(N(=O)=O)ccc2)ccc(S(=O)(=O)O)c3	3
2003	ISSSTY_v1a_7367_02May011_2496	527751	HC(H)C(H)OC(=O)C(H)C(C(=O)OC(H)C(H)H)SP(=O)(OC(H)H)SC(H)H	1
2004	ISSSTY_v1a_7367_02May011_2497	152-20-5	HC(H)OP(=O)(OC(H)H)SC(H)H	1
2005	ISSSTY_v1a_7367_02May011_2498	118745-15-6	c12c3c4c(c(N=O)c5c(c4ccc3ccc1)cccc5)cc2	3
2006	ISSSTY_v1a_7367_02May011_2499	89-80-5	HC(H)C(C(H)H)C1C(=O)C(H)C(C(H)H)C(H)C1H	3
2007	ISSSTY_v1a_7367_02May011_2500	52-67-5	HC(H)C(S)(C(H)H)[C@@](N)C(=O)O	3
2008	ISSSTY_v1a_7367_02May011_2501	5405-53-8	HC1c2c(-c3c1cc([N+](=O)[O-])cc3)ccc([N+](=O)[O-])c2	3
2009	ISSSTY_v1a_7367_02May011_2502	932-53-6	HC(H)C1C(=O)NC(=O)NN=1	1
2010	ISSSTY_v1a_7367_02May011_2503	27032-78-6	HC1NC(=O)NC(=O)N1	3
2011	ISSSTY_v1a_7367_02May011_2504	216-48-8	c12c(c3c(c4c5c(C=Cc5ccc4)c3)cc1)cccc2	3
2012	ISSSTY_v1a_7367_02May011_2505	551-92-8	HC(H)C1N(C(H)H)C(N(=O)=O)=CN=1	3
2013	ISSSTY_v1a_7367_02May011_2506	1836-75-5	c1(OC2ccc(N(=O)=O)cc2)c(Cl)cc(Cl)cc1	3
2014	ISSSTY_v1a_7367_02May011_2507	82-71-3	c1([N+](=O)[O-])c(O)c([N+](=O)[O-])c(O)c([N+](=O)[O-])c1	1
2015	ISSSTY_v1a_7367_02May011_2508	99-30-9	c1(Cl)c(N)c(Cl)cc(N(=O)=O)c1	3
2016	ISSSTY_v1a_7367_02May011_2509	123016-76-2	C(=O)(O)c1ccc(N(c2cccc2)C(N)=O)cc1	1

2017	ISSSTY_v1a_7367_02May011_2512	192-97-2	c12c3c(c4c(c5c3c(ccc5)cc1)cccc4)ccc2	3
2018	ISSSTY_v1a_7367_02May011_2513	76150-91-9	c1(Oc2ccc(Oc3c(Cl)cc(Cl)cn3)cc2)c(Cl)cc(Cl)cn1	1
2019	ISSSTY_v1a_7367_02May011_2514	63020-20-2	HC(H)C(=O)Nc1cc2c(-c3c(cccc3)N2)cc1	3
2020	ISSSTY_v1a_7367_02May011_2515	85068-73-1	HC(H)C(H)N(C(H)C(H)ON(=O)=O)[N+](=O)[O-]	3
2021	ISSSTY_v1a_7367_02May011_2516	1464-53-5	HC1C(C2C(H)O2)O1	3
2022	ISSSTY_v1a_7367_02May011_2517	145439-03-8	HC(H)N(C(=O)C1=C(NC(H)H)N=CN1C(H)H)N=O	3
2023	ISSSTY_v1a_7367_02May011_2518	645-12-5	C(=O)(O)C1=CC=C(N(=O)=O)O1	3
2024	ISSSTY_v1a_7367_02May011_2519	51940-44-4	HC(H)C(H)N1c2c(C(=O)C(C(=O)O)=C1)cnc(N1C(H)C(H)NC(H)C1H)n2	3
2025	ISSSTY_v1a_7367_02May011_2520	71-33-0	C1(=O)N=CNC(=O)N1	1
2026	ISSSTY_v1a_7367_02May011_2523	490-91-5	HC(H)C1C(=O)C=C(C(C(H)H)C(H)H)C(=O)C=1	1
2027	ISSSTY_v1a_7367_02May011_2524	84-58-2	C(N)C1C(=O)C(CI)=C(CI)C(=O)C=1C_N	3
2028	ISSSTY_v1a_7367_02May011_2526	476-60-8	c1(O)c2c(O)c3c(c(O)c2c(O)cc1)cccc3	3
2029	ISSSTY_v1a_7367_02May011_2528	96563-01-8	HC([C@](N)C(=O)O)SC(F)(F)C(F)CI	1
2030	ISSSTY_v1a_7367_02May011_2529	91-62-3	HC(H)c1cc2c(cc1)nccc2	3
2031	ISSSTY_v1a_7367_02May011_2530	13010-08-7	HC(H)C(H)C(H)C(H)N(C(N)=NN(=O)=O)N=O	3
2032	ISSSTY_v1a_7367_02May011_2531	51640-90-5	C1(=O)c2c(-c3c(c(N(=O)=O)ccc3)O1)cccc2	3
2033	ISSSTY_v1a_7367_02May011_2532	74-95-3	HC(Br)Br	3
2034	ISSSTY_v1a_7367_02May011_2533	129401-88-3	HC1C(H)N(C(=O)C=CH)C(H)C(H)N1c1cccc1	1
2035	ISSSTY_v1a_7367_02May011_2535	612-60-2	HC(H)c1cc2c(cccn2)cc1	3
2036	ISSSTY_v1a_7367_02May011_2536	3544-23-8	HC(H)Oc1c(N)ccc(N=Nc2cccc2)c1	3
2037	ISSSTY_v1a_7367_02May011_2537	133331-34-7	HC(H)[C@@]12C(H)C(H)[C@@]3[C@@]4(C(H)H)C(H)C(=O)[C@]5(C)C(=O)1C(H)C(H)[C@@]2[C@@](C(H)H)C(H)C(H)C(H)H)S(=O)(=O)C(H)C(H)S4(=O)=O	3
2038	ISSSTY_v1a_7367_02May011_2538	55691-69-5	c1([N+](=O)[O-])c2c3c(c4c(c3ccc2[N+](=O)[O-])cccc4)cc1	3
2039	ISSSTY_v1a_7367_02May011_2539	105735-71-5	c1([N+](=O)[O-])c2c3c(c4c(c([N+](=O)[O-])ccc4)c3ccc2)cc1	3
2040	ISSSTY_v1a_7367_02May011_2540	22506-53-2	c1([N+](=O)[O-])c2c3c(c4c(c3ccc2)ccc([N+](=O)[O-])c4)cc1	3
2041	ISSSTY_v1a_7367_02May011_2541	50-53-3	HC(H)N(C(H)H)C(H)C(H)C(H)N1c2c(ccc(Cl)c2)Sc2c1cccc2	1
2042	ISSSTY_v1a_7367_02May011_2542	13010-07-6	HC(H)C(H)C(H)N(C(N)=NN(=O)=O)N=O	3
2043	ISSSTY_v1a_7367_02May011_2543	13177-29-2	c12c3c(c4c(c3cc(N(=O)=O)c1)cccc4)ccc2	3
2044	ISSSTY_v1a_7367_02May011_2544	578-06-3	c1(N)c2c(ccc1)nc1c(cccc1)c2	3
2045	ISSSTY_v1a_7367_02May011_2545	23043-62-1	c12c(c(N)c3c(ccc(N)c3)n1)cccc2	3
2046	ISSSTY_v1a_7367_02May011_2546	117823-31-1	C(=O)(O)C(CI)=C(C(=O)C(CI)CI	3
2047	ISSSTY_v1a_7367_02May011_2547	4539-51-9	c12-c3c(cc(N)cc3)Nc1cccc2	3
2048	ISSSTY_v1a_7367_02May011_2548	2310-17-0	HC(H)C(H)OP(=S)(OC(H)C(H)H)SC(H)N1c2c(cc(Cl)cc2)OC1=O	1
2049	ISSSTY_v1a_7367_02May011_2549	71382-45-1	HC(H)c1c2c(-c3c(C4C2N4)cccc3)cc2c1cccc2	3
2050	ISSSTY_v1a_7367_02May011_2551	91598-91-3	HC(H)C(=O)Nc1c2c3c4c(c(O)ccc4cc2)ccc3cc1	3
2051	ISSSTY_v1a_7367_02May011_2553	106-60-5	HC(N)C(=O)C(H)C(H)C(=O)O	3
2052	ISSSTY_v1a_7367_02May011_2554	79-27-6	C(Br)(Br)C(Br)Br	3
2053	ISSSTY_v1a_7367_02May011_2555	521-61-9	HC(H)c1cc2C(=O)c3c(C(=O)c2c(O)c1)c(O)cc(OC(H)H)c3	3
2054	ISSSTY_v1a_7367_02May011_2556	35983	C(Cl)(Cl)(Cl)c1cccc1	3
2055	ISSSTY_v1a_7367_02May011_2557	205-99-2	c12c(c3c4c(c5c(c4ccc3)cccc5)c1)cccc2	3
2056	ISSSTY_v1a_7367_02May011_2559	85-83-6	HC(H)c1c(NN=C2c3c(C=CC2=O)cccc3)ccc(N=Nc2c(C(H)H)cccc2)c1	3
2057	ISSSTY_v1a_7367_02May011_2560	207-08-9	c12c3c(c4c(c3ccc1)cc1c(cccc1)c4)ccc2	3
2058	ISSSTY_v1a_7367_02May011_2561	630-17-1	HC(H)C(C(H)H)(C(H)H)C(H)Br	1

2059	ISSSTY_v1a_7367_02May011_2562	3228-99-7	HC(Cl)C(C(H)Cl)(C(H)Cl)C(H)Cl	1
2060	ISSSTY_v1a_7367_02May011_2564	155506-70-0	HC(H)C1=C(C(=O)OC(H)C(H)C(c2cc(Cl)ccc2)C(C(=O)OC(H)C2C(H)OC3(C(H)C(H)C(H)C3H)O2)=C(C(H)H)N1	1
2061	ISSSTY_v1a_7367_02May011_2565	55706-61-1	C(N)(=O)c1c2c(cccn2)ccc1	3
2062	ISSSTY_v1a_7367_02May011_2567	17948-33-3	HC(H)C(C1C(H)c2c3c(C(=O)c4c(cccc4)N3C(H)H)c(O)cc2O1)=CH	3
2063	ISSSTY_v1a_7367_02May011_2570	155-09-9	HC1C(c2ccccc2)[C@]1N	1
2064	ISSSTY_v1a_7367_02May011_2571	38579-27-0	HC(C1c2c(cccc2)NC=1)[C@@](C(=O)N[C@](C(=O)O)C(H)C(H)C(H)N)NC(=O)[C@@](N)C(H)C(H)C(H)N	1
2065	ISSSTY_v1a_7367_02May011_2572	5845-67-0	HC(H)C(C(H)H)C(H)C1C(=O)NC(H)C(=O)N1	1
2066	ISSSTY_v1a_7367_02May011_2573	22008-60-2	HC(H)SC(H)C(H)[C@@](C(=O)N[C@](C(=O)O)C(H)c1ccccc1)NC=O	1
2067	ISSSTY_v1a_7367_02May011_2574	60254-83-3	HC(H)C(C(H)H)C(H)C(C(=O)O)NC(=O)C(C(H)c1ccccc1)NC(=O)C(H)NC(=O)C(H)N	1
2068	ISSSTY_v1a_7367_02May011_2575	298-12-4	C(=O)(O)C=O	3
2069	ISSSTY_v1a_7367_02May011_2576	501-53-1	HC(c1ccccc1)OC(=O)Cl	1
2070	ISSSTY_v1a_7367_02May011_2577	41840-28-2	HC(H)C(C(H)H)(C(H)H)OC(=O)Sc1nc(C(H)H)cc(C(H)H)n1	1
2071	ISSSTY_v1a_7367_02May011_2578	58632-95-4	HC(H)C(C(H)H)(C(H)H)OC(=O)ON=C(c1ccccc1)C_N	1
2072	ISSSTY_v1a_7367_02May011_2580	3343-64-4	HC(H)C(H)C(H)C(H)SC(H)C(H)[C@@](C(=O)[O-])[N+](H)H	1
2073	ISSSTY_v1a_7367_02May011_2581	6066-82-6	HC1C(=O)N(O)C(=O)C1H	1
2074	ISSSTY_v1a_7367_02May011_2582	87679-37-6	HC(H)C(H)OC(=O)[C@@](C(H)C(H)c1ccccc1)N[C@](C(=O)N1[C@](C(=O)O)C(H)[C@]2C(H)C(H)C(H)[C@@]12)C(H)H	1
2075	ISSSTY_v1a_7367_02May011_2584	103-17-3	HC(c1ccc(Cl)cc1)Sc1ccc(Cl)cc1	1
2076	ISSSTY_v1a_7367_02May011_2585	530-62-1	C(=O)(N1C=CN=C1)N1C=CN=C1	1
2077	ISSSTY_v1a_7367_02May011_2586	102694-32-6	[C@]12(O)c3c(-c4c5c(C(=O)C6C([C@]15)O6)c(O)cc4)ccc(O)c3C(=O)C=C2	3
2078	ISSSTY_v1a_7367_02May011_2587	28920-43-6	HC(C1c2c(-c3c1cccc3)cccc2)OC(=O)Cl	3
2079	ISSSTY_v1a_7367_02May011_2589	33213-65-9	HC1[C@]2C3(Cl)C(Cl)(Cl)[C@@](Cl)(C(Cl)=C3Cl)[C@]2C(H)OS(=O)O1	1
2080	ISSSTY_v1a_7367_02May011_2590	2550-75-6	HC(Cl)C1C2(Cl)C(Cl)(Cl)C(Cl)(C(Cl)=C2Cl)C1C(H)Cl	1
2081	ISSSTY_v1a_7367_02May011_2591	94-81-5	HC(H)c1c(OC(H)C(H)C(H)C(=O)O)ccc(Cl)c1	1
2082	ISSSTY_v1a_7367_02May011_2592	7085-19-0	HC(H)c1c(OC(C(=O)O)C(H)H)ccc(Cl)c1	1
2083	ISSSTY_v1a_7367_02May011_2593	93-72-1	HC(H)C(C(=O)O)Oc1c(Cl)cc(Cl)c(Cl)c1	1
2084	ISSSTY_v1a_7367_02May011_2594	2386-87-0	HC1C(H)C(C(=O)OC(H)C2C(H)C(H)C3C(C2H)O3)C(H)C2C1O2	3
2085	ISSSTY_v1a_7367_02May011_2595	1194-65-6	C(N)c1c(Cl)cccc1Cl	1
2086	ISSSTY_v1a_7367_02May011_2600	1733-13-7	HC(H)N(c1ccc(C(c2ccc(N(C(H)H)C(H)H)cc2)=C2C=CC(=NC(H)H)C=C2)cc1)C(H)H	1
2087	ISSSTY_v1a_7367_02May011_2601	77996-03-3	HC(H)C1(C2C(H)c3c4c(C(=O)c5c(cccc5)N4C(H)H)c(O)cc3O2)C(H)O1	3
2088	ISSSTY_v1a_7367_02May011_2602	18234-46-3	HC(H)C(=O)OC(H)C1C2C(C(=O)=CC=2)=COC=1	3
2089	ISSSTY_v1a_7367_02May011_2603	5002-47-1	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(=O)OC(H)C(H)N1C(H)C(H)N(C(H)C(H)C(H)N2c3c(ccc(C(F)F)F)c3)Sc3c2ccccc3)C(H)C1H	1
2090	ISSSTY_v1a_7367_02May011_2604	938-55-6	HC(H)N(c1c2c(N=CN2)ncn1)C(H)H	3
2091	ISSSTY_v1a_7367_02May011_2605	67910-07-0	HC(H)C(C(H)H)C(H)C(=O)OC(H)C1C2C(C(C=O)=CC=2)=COC=1	3
2092	ISSSTY_v1a_7367_02May011_2608	1121-55-7	HC=Cc1ccnc1	1
2093	ISSSTY_v1a_7367_02May011_2609	83463-62-1	C(N)C(Cl)Br	3
2094	ISSSTY_v1a_7367_02May011_2610	138580-44-6	HC(H)c1c2-c3c(cccc3)Nc2c2C(=O)C=CC(=O)c2n1	3
2095	ISSSTY_v1a_7367_02May011_2611	138580-46-8	HC(H)C1C(=O)c2c(C(=O)C=1)nc(C(H)H)c1-c3c(cccc3)Nc21	3
2096	ISSSTY_v1a_7367_02May011_2612	5694-00-8	HC1C(C(N)=O)O1	3
2097	ISSSTY_v1a_7367_02May011_2614	138580-48-0	HC(H)c1c2-c3c(cccc3)Nc2c2C(=O)C(N3C(H)C(H)N(C(H)H)C(H)C3H)=CC(=O)c2n1	3
2098	ISSSTY_v1a_7367_02May011_2615	87406-72-2	HC1C(C(H)N(C(=O)C=CH)C(H)C2C(H)O2)O1	3
2099	ISSSTY_v1a_7367_02May011_2616	73-24-5	c1(N)c2c(N=CN2)ncn1	3
2100	ISSSTY_v1a_7367_02May011_2617	1845-30-3	HC(H)C1(C(H)H)[C@]2C(C(H)H)=C[C@@](O)[C@@]1C2H	1

2101	ISSSTY_v1a_7367_02May011_2618	65071-98-9	HC(H)C(=O)OC(H)C(H)O	1
2102	ISSSTY_v1a_7367_02May011_2619	57471-01-9	HC(H)C(=O)c1c(OC(H)C(O)C(H)NC(C(H)H)(C(H)H)C(H)H)ccc(N(C(C(H)H)(C(H)H)C(H)H)C(N)=O)c1	1
2103	ISSSTY_v1a_7367_02May011_2620	2541-69-7	HC(H)c1c2c(c3c(cccc3)cc2)cc2c1cccc2	3
2104	ISSSTY_v1a_7367_02May011_2621	24305-27-9	HC(C1=CN=CN1)[C@](C(=O)N1C(H)C(H)C(H)[C@@]1C(N)=O)NC(=O)[C@]1C(H)C(H)C(=O)N1	1
2105	ISSSTY_v1a_7367_02May011_2622	1456-55-9	HC(H)[C@@]12C(=O)N3[C@@](C(=O)N1C(H)H)([C@](O)[C@@]1(O)c4c(c(OC(H)H)c(OC(H)H)c(Cl)c4)N(C(H)H)[C@@]31)SS2	1
2106	ISSSTY_v1a_7367_02May011_2624	24424-99-5	HC(H)C(C(H)H)(C(H)H)OC(=O)OC(=O)OC(C(H)H)(C(H)H)C(H)H	1
2107	ISSSTY_v1a_7367_02May011_2626	1928-38-7	HC(H)OC(=O)C(H)Oc1c(Cl)cc(Cl)cc1	1
2108	ISSSTY_v1a_7367_02May011_2627	101901-07-9	HC(H)C(H)c1c2c(C3=C(C(C(H)C(=O)OC(H)C(H)H)OC(H)C3H)N2)ccc1O	3
2109	ISSSTY_v1a_7367_02May011_2628	101901-08-0	HC(H)C(H)OC(=O)C(H)C1C2=C(c3c(c(C(O)C(H)H)ccc3)N2)C(H)C(H)O1	1
2110	ISSSTY_v1a_7367_02May011_2629	41340-36-7	HC(H)C(H)c1c2c(C(C(H)C(H)O)=CN2)ccc1	1
2111	ISSSTY_v1a_7367_02May011_2630	115066-03-0	HC(H)C1(C(H)C(H)H)C2=C(c3c(c(C(H)C(H)H)ccc3)N2)C(H)C(H)O1	1
2112	ISSSTY_v1a_7367_02May011_2631	41340-19-6	HC(H)c1c2c(C3=C(C(C(H)C(=O)OC(H)C(H)H)OC(H)C3H)N2)ccc1	1
2113	ISSSTY_v1a_7367_02May011_2632	135086-99-6	C1(N)c2c(cccc2)NC=1C(=O)NN=Cc1cccc1	1
2114	ISSSTY_v1a_7367_02May011_2633	21096	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)O	1
2115	ISSSTY_v1a_7367_02May011_2634	959-98-8	HC1[C@@]2C3(CI)C(CI)(CI)[C@](CI)(C(CI)=C3CI)[C@@]2C(H)OS(=O)O1	1
2116	ISSSTY_v1a_7367_02May011_2635	2517-43-3	HC(H)C(C(H)C(H)O)OC(H)H	1
2117	ISSSTY_v1a_7367_02May011_2637	92134-93-5	HC1C(H)N(N=O)C(C(H)O)S1	3
2118	ISSSTY_v1a_7367_02May011_2638	92134-95-7	HC(H)C(O)C(O)C(O)C1N(N=O)C(H)C(H)S1	1
2119	ISSSTY_v1a_7367_02May011_2639	75-37-6	HC(H)C(F)F	1
2120	ISSSTY_v1a_7367_02May011_2640	92134-97-9	HC1C(C(=O)O)N(N=O)C(C(O)C(O)C(O)C(O)C(H)O)S1	1
2121	ISSSTY_v1a_7367_02May011_2641	526-73-8	HC(H)c1c(C(H)H)c(C(H)H)ccc1	3
2122	ISSSTY_v1a_7367_02May011_2642	108-67-8	HC(H)c1cc(C(H)H)cc(C(H)H)c1	1
2123	ISSSTY_v1a_7367_02May011_2643	76-14-2	C(F)(F)(Cl)C(F)(F)Cl	1
2124	ISSSTY_v1a_7367_02May011_2644	84736-60-7	c1(N(=O)=O)ccc(N(O)C=O)cc1	3
2125	ISSSTY_v1a_7367_02May011_2645	125-46-2	HC(H)C(=O)c1c2c(C3(C(H)H)C(=O)C(C(=O)C(H)H)C(=O)C=C3O2)c(O)c(C(H)H)c1O	1
2126	ISSSTY_v1a_7367_02May011_2646	90689-60-4	HC(H)c1c2C(=O)Oc3c(c(C(H)H)c(C(=O)O)c(O)c3C(H)OC(=O)C(H)H)Oc2c(C=O)c(O)c1	3
2127	ISSSTY_v1a_7367_02May011_2647	122-88-3	HC(C(=O)O)Oc1ccc(Cl)cc1	1
2128	ISSSTY_v1a_7367_02May011_2648	27113-22-0	HC(H)C(H)C(H)C(H)C(H)C(H)C(H)C(=O)C(H)C(H)c1cc(OC(H)H)c(O)cc1	1
2129	ISSSTY_v1a_7367_02May011_2650	33089-61-1	HC(H)c1c(N=CN(C(H)H)C=Nc2c(C(H)H)cc(C(H)H)cc2)ccc(C(H)H)c1	1
2130	ISSSTY_v1a_7367_02May011_2652	4435-53-4	HC(H)C(=O)OC(H)C(H)C(C(H)H)OC(H)H	1
2131	ISSSTY_v1a_7367_02May011_2653	4189-44-0	C(=N)(N)S(=O)[O-]	3
2132	ISSSTY_v1a_7367_02May011_2654	84-60-6	c12C(=O)c3c(C(=O)c1cc(O)cc2)ccc(O)c3	1
2133	ISSSTY_v1a_7367_02May011_2655	577-33-3	c1(O)c(O)c2c(c(O)c3c(cccc3)c2)cc1	3
2134	ISSSTY_v1a_7367_02May011_2656	13593-03-8	HC(H)C(H)OP(=S)(Oc1cnc2c(cccc2)n1)OC(H)C(H)H	1
2135	ISSSTY_v1a_7367_02May011_2657	81-61-8	c12C(=O)c3c(C(=O)c1c(O)c(O)cc2)c(O)ccc3O	3
2136	ISSSTY_v1a_7367_02May011_2658	28932-22-1	C1(=O)c2c(C(=O)C3C(O)=CC=C(O)C13)c(O)ccc2O	3
2137	ISSSTY_v1a_7367_02May011_2659	68641-49-6	HC1C(H)N(P(=O)(Cl)N2C(=O)OC(H)C2H)C(=O)O1	3
2138	ISSSTY_v1a_7367_02May011_2660	116-85-8	c12C(=O)c3c(C(=O)c1c(O)ccc2N)cccc3	3
2139	ISSSTY_v1a_7367_02May011_2662	68884-32-2	HC(c1c2c(cccc2)ccc1)C1C(H)O1	3
2140	ISSSTY_v1a_7367_02May011_2663	7774-68-7	HC(Cl)C(Cl)C(H)OC(H)C(Cl)C(H)Cl	3
2141	ISSSTY_v1a_7367_02May011_2666	155164-54-8	HC(H)C(H)S(=O)(=O)N1C(=O)C(Cl)=C(Cl)C=N1	3
2142	ISSSTY_v1a_7367_02May011_2669	155164-57-1	C1(=O)C(Cl)=C(Cl)C=NN1S(=O)(=O)c1cccc1	1