Supplementary information

SI 1. The dataset

In the following table we present the name, the chemical formula, SMILES, reported Tg and reference of the molecules in the dataset.

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| --- | --- | --- | --- | --- |
| Name | Chemical  Formula | SMILES | Tg [K] | Reference |
| Training | | | | |
| (S) Glycerol acetonide | C6H12O3 | CC1(C)OC[C@H](CO)O1 | 282 | (1) |
| (S)(-)Methyl lactate | C4H8O3 | COC(=O)[C@H](C)O | 286 | (1) |
| 1,1,1,2,3,3-Hexafluoropropane | C3H2F6 | FC(F)C(F)C(F)(F)F | 95 | (2) (SI 2) |
| 1,1,1,2-Tetrafluoroethane | C2H2F4 | FCC(F)(F)F | 71 | (2) (SI 2) |
| 1,1-dichloro-1-fluoroethane | C2H3Cl2F | CC(F)(Cl)Cl | 41 | (2) (SI 2) |
| 1,2-diphenylcyclobutene | C16H14 | c1ccc(C2=C(c3ccccc3)CC2)cc1 | 216 | (3) |
| 1,2-diphenylcycloheptene | C19H20 | c1ccc(C2=C(c3ccccc3)CCCCC2)cc1 | 233 | (3) |
| 1,2-Pentanediol | C5H12O2 | CCCC(O)CO | 181 | (4)(SI 5) |
| 1,2-propanediamine | C3H10N2 | CC(N)CN | 144.1 | (5) |
| 1,3,5-Tri(1-naphthyl)benzene | C36H24 | c1ccc2c(-c3cc(-c4cccc5ccccc45)cc(-c4cccc5ccccc45)c3)cccc2c1 | 342 | (4)(SI 19) |
| 1,3,5-Tri-2-naphthylbenzene | C36H24 | c1ccc2cc(-c3cc(-c4ccc5ccccc5c4)cc(-c4ccc5ccccc5c4)c3)ccc2c1 | 337 | (6)(13) |
| 1,3,5-Tris[(3-methylphenyl)phenylamino]benzene | C45H39N3 | Cc1cccc(N(c2ccccc2)c2cc(N(c3ccccc3)c3cccc(C)c3)cc(N(c3ccccc3)c3cccc(C)c3)c2)c1 | 334 | (7) |
| 1,3-Di(1-naphthyl)-5-(2-naphthyl)benzene | C36H24 | c1ccc2cc(-c3cc(-c4cccc5ccccc45)cc(-c4cccc5ccccc45)c3)ccc2c1 | 350.15 | (8) |
| 1,3-Dinitro-4,6-bis-(R-1’-phenylethylamino)benzene | C22H22N4O4 | C[C@H](Nc1cc(N[C@@H](C)c2ccccc2)c([N+](=O)[O-])cc1[N+](=O)[O-])c1ccccc1 | 316 | (1) |
| 1,3-propanediol | C3H8O2 | OCCCO | 154 | (9)(10) |
| 1,4-Pentanediol | C5H12O2 | CC(O)CCCO | 175.8 | (4)(SI 5) |
| 1,5-Hexanediol | C6H14O2 | CC(O)CCCCO | 179.4 | (4)(SI 5) |
| 1,5-pentanediol | C5H12O2 | OCCCCCO | 163.65 | (10) |
| 1ª | C20H12N6 | CNc1nc(Nc2cc(C)cc(C)c2)nc(Nc2cc(C)cc(C)c2)n1 | 367.15 | (11) |
| 1b | C21H13N5 | CCc1nc(Nc2cc(C)cc(C)c2)nc(Nc2cc(C)cc(C)c2)n1 | 314.15 | (11) |
| 1-Butene | C4H8 | C=CCC | 61 | (4)(SI 4) |
| 1-butoxy-2-propanol | C7H16O2 | CCCCOCC(C)O | 155.1 | (10)(34) |
| 1-chloro-1,1-difluoroethane | C2H3ClF2 | CC(F)(F)Cl | 27 | (2)(SI 2) |
| 1-Ethyl-2-phenyl-1H-indole | C16H15N | CCn1c(-c2ccccc2)cc2ccccc21 | 280.75 | (12) |
| 1-ethylcarbazole | C14H13N | CCc1cccc2c1[nH]c1ccccc12 | 271.95 | (12) |
| 1-methoxy-2-propanol | C4H10O2 | COCC(C)O | 145.2 | (13) |
| 1-Methylbenzimidazole | C8H8N2 | Cn1cnc2ccccc21 | 164.45 | (12) |
| 1-methylindole | C9H9N | Cn1ccc2ccccc21 | 184.7 | (10) |
| 1-methylpyrazole | C4H6N2 | Cn1cccn1 | 148.45 | (12) |
| 1-Naphthylamine | C10H9N | Nc1cccc2ccccc12 | 306 | (1) |
| 1-phenyl-1-propanol | C9H12O | CCC(O)c1ccccc1 | 193.65 | (14) |
| 1-propoxy-2-propanol | C6H14O2 | CCCOCC(C)O | 153.7 | (10)(34) |
| 1-tert-butoxy-2-propanol | C7H16O2 | CC(O)COC(C)(C)C | 174.15 | (10) |
| 2-(2-ethylhexyloxy) ethanol | C10H22O2 | CCCCC(CC)COCCO | 158.6 | (13) |
| 2,2,2-Tris(chloromethyl)ethyl-p-nitrophenylurethane | C14H11N2O4Cl3 | CCOC(=O)N(CC(CCl)(CCl)CCl)c1ccc([N+](=O)[O-])cc1 | 293 | (1) |
| 2,3,4,5,6-Pentabromotoluene | C7H3Br5 | Cc1c(Br)c(Br)c(Br)c(Br)c1Br | 202 | (15) |
| 2,3-Dimethylbutane | C6H14 | CC(C)C(C)C | 76 | (4)(SI 4) |
| 2,3-dimethylindole | C10H11N | Cc1[nH]c2ccccc2c1C | 151.25 | (12) |
| 2,4-lutidine | C7H9N | Cc1ccnc(C)c1 | 150.05 | (12) |
| 2,4-Pentanediol | C5H12O2 | CC(O)CC(C)O | 205 | (4)(SI 5) |
| 2,5-Hexanediol | C6H14O2 | CC(O)CCC(C)O | 203.5 | (4)(SI 5) |
| 2a | C16H16N6 | CNc1nc(Nc2ccccc2)nc(Nc2ccccc2)n1 | 329.15 | (11) |
| 2b | C18H20N6 | CNc1nc(Nc2ccccc2C)nc(Nc2ccccc2C)n1 | 328.15 | (11) |
| 2-Benzylphenol (alpha-phenyl-o-cresol) | C13H12O | Oc1ccccc1Cc1ccccc1 | 220 | (4)(SI 6) |
| 2-Bromobutane | C4H9Br | CCC(C)Br | 97 | (4)(SI 3) |
| 2c | C18H20N6 | CNc1nc(Nc2cccc(C)c2)nc(Nc2cccc(C)c2)n1 | 333.15 | (11) |
| 2-Chloro-4-nitroaniline | C6H5ClN2O2 | Nc1ccc([N+](=O)[O-])cc1Cl | 324 | (1) |
| 2-Chloroaniline | C6H6ClN | Nc1ccccc1Cl | 292 | (1) |
| 2-ethyl-1,3-hexanediol | C8H18O2 | CCCC(O)C(CC)CO | 213.3 | (10)(24) |
| 2-ethyl-1-hexanol | C8H18O | CCCCC(CC)CO | 146 | (4)(SI 5) |
| 2-ethylhexylamine | C8H19N | CCCCC(CC)CN | 141 | (4)(SI 14) |
| 2f | C20H24N6 | CNc1nc(Nc2ccc(C)cc2C)nc(Nc2ccc(C)cc2C)n1 | 327.15 | (11) |
| 2g | C20H24N6 | CNc1nc(Nc2cc(C)ccc2C)nc(Nc2cc(C)ccc2C)n1 | 339.15 | (11) |
| 2h | C20H24N6 | CNc1nc(Nc2c(C)cccc2C)nc(Nc2c(C)cccc2C)n1 | 362.15 | (11) |
| 2i | C20H24N6 | CNc1nc(Nc2ccc(C)c(C)c2)nc(Nc2ccc(C)c(C)c2)n1 | 344.15 | (11) |
| 2-iso-propoxyethanol | C5H12O2 | CC(C)OCCO | 141 | (4)(SI 5) |
| 2l | C16H12N6Cl2 | CNc1nc(Nc2cc(Cl)cc(Cl)c2)nc(Nc2cc(Cl)cc(Cl)c2)n1 | 356.15 | (11) |
| 2m | C16H12N6Br2 | CNc1nc(Nc2cc(Br)cc(Br)c2)nc(Nc2cc(Br)cc(Br)c2)n1 | 367.15 | (11) |
| 2-Methyl-1-heptanol | C8H18O | CCCCCC(C)CO | 144.15 | (14) |
| 2-Methyl-1-pyrroline | C5H9N | CC1=NCCC1 | 139.55 | (12) |
| 2-methyl-2,4-pentanediol | C6H14O2 | CC(O)CC(C)(C)O | 191.55 | (10) |
| 2-Methyl-2-butene | C5H10 | CC=C(C)C | 73 | (4)(SI 3) |
| 2-Methyl-3-heptanol | C8H18O | CCCCC(O)C(C)C | 158.15 | (14) |
| 2-methyl-4-heptanol | C8H18O | CCCC(O)CC(C)C | 167 | (16) |
| 2-methylheptane | C8H18 | CCCCCC(C)C | 80 | (17) |
| 2-methylindole | C9H9N | Cc1cc2ccccc2[nH]1 | 148.25 | (12) |
| 2-methylpentane | C6H14 | CCCC(C)C | 78 | (4)(SI 5) |
| 2-Methyltetrahydrofuran | C5H10O | CC1CCCO1 | 91 | (4)(SI 6) |
| 2n | C16H12N6I2 | CNc1nc(Nc2cc(I)cc(I)c2)nc(Nc2cc(I)cc(I)c2)n1 | 401.15 | (11) |
| 2-Naphthylamine | C10H9N | Nc1ccc2ccccc2c1 | 304 | (1) |
| 2-Nitroaniline | C6H6N2O2 | Nc1ccccc1[N+](=O)[O-] | 299 | (1) |
| 2o | C20H24N6O2 | CNc1nc(Nc2cc(OC)cc(OC)c2)nc(Nc2cc(OC)cc(OC)c2)n1 | 338.15 | (11) |
| 2-phenylethyl N-phenylcarbamate | C15H15NO2 | O=C(Nc1ccccc1)OCCc1ccccc1 | 235 | (17) |
| 2-picoline | C6H7N | Cc1ccccn1 | 136.3 | (10) |
| 2q | C32H48N6 | CNc1nc(Nc2cc(C(C)(C)C)cc(C(C)(C)C)c2)nc(Nc2cc(C(C)(C)C)cc(C(C)(C)C)c2)n1 | 402.15 | (11) |
| 3,3',5,5'-Tetrachlorobiphenyl (Aroclor 1248) | C12H6Cl4 | Clc1cc(Cl)cc(-c2cc(Cl)cc(Cl)c2)c1 | 229 | (6)(29) |
| 3,3-Bis(4-methoxyphenyl)phthalide (phenylphthalein dimethylether) | C22H18O4 | COc1ccc(C2(c3ccc(OC)cc3)OC(=O)c3ccccc32)cc1 | 294 | (4) (SI 6) |
| 3,3-Dimethyl-1-butanol | C6H14O | CC(C)(C)CCO | 146 | (18) |
| 3-amino-1-propanol | C3H9NO | NCCCO | 168.15 | (19) |
| 3c | C16H28N6 | CNc1nc(NC2CCCCC2)nc(NC2CCCCC2)n1 | 331.15 | (11) |
| 3-Chloroaniline | C6H6ClN | Nc1cccc(Cl)c1 | 286 | (1) |
| 3-ethoxy-1,2-propanediol | C5H12O3 | CCOCC(O)CO | 187.05 | (10) |
| 3-Methyl-3-heptanol | C8H18O | CCCCC(C)(O)CC | 151.15 | (14) |
| 3-methylbenzophenone | C14H12O | Cc1cccc(C(=O)c2ccccc2)c1 | 215.45 | (10) |
| 3-methylheptane | C8H18 | CCCCC(C)CC | 98 | (17) |
| 3-methylpentane | C6H14 | CCC(C)CC | 77 | (4)(SI 5) |
| 3-Nitroaniline | C6H6N2O2 | Nc1cccc([N+](=O)[O-])c1 | 301 | (1) |
| 3-Trifluoromethylaniline | C7H6F3N | Nc1cccc(C(F)(F)F)c1 | 280 | (1) |
| 4-(4-Chlorophenyl)-4-hydroxypiperidine (T263) | C11H14ClNO | OC1(c2ccc(Cl)cc2)CCNCC1 | 292.2 | (20) |
| 4-(Diglycidylamino)phenyl glycidyl ether (DGGOA) | C15H19NO4 | c1cc(N(CC2CO2)CC2CO2)ccc1OCC1CO1 | 244 | (4)(SI 17) |
| 4,4'-dimethoxytetraphenylmethane | C27H24O2 | COc1ccc(C(c2ccccc2)(c2ccccc2)c2ccc(OC)cc2)cc1 | 297 | (1) |
| 4-[bis(4-methylphenyl)amino]acetophenone | C22H21NO | CC(=O)c1ccc(N(c2ccc(C)cc2)c2ccc(C)cc2)cc1 | 282.15 | (21) |
| 4a | C17H17N5 | CCc1nc(Nc2ccccc2)nc(Nc2ccccc2)n1 | 300.15 | (11) |
| 4-amino-1-butanol | C4H11NO | NCCCCO | 158.15 | (19) |
| 4-Biphenylcarboxaldehyde | C13H10O | O=Cc1ccc(-c2ccccc2)cc1 | 223.15 | (22) |
| 4-Biphenylcarboxylic acid | C13H10O2 | O=C(O)c1ccc(-c2ccccc2)cc1 | 342.15 | (22) |
| 4-biphenylmethanol | C13H12O | OCc1ccc(-c2ccccc2)cc1 | 251.15 | (22) |
| 4-Chloroaniline | C6H6ClN | Nc1ccc(Cl)cc1 | 297 | (1) |
| 4-Cyanoaniline | C7H6N2 | N#Cc1ccc(N)cc1 | 314 | (1) |
| 4e | C21H25N5 | CCc1nc(Nc2cccc(C)c2C)nc(Nc2cccc(C)c2C)n1 | 319.15 | (11) |
| 4f | C21H25N5 | CCc1nc(Nc2ccc(C)cc2C)nc(Nc2ccc(C)cc2C)n1 | 312.15 | (11) |
| 4g | C21H25N5 | CCc1nc(Nc2cc(C)ccc2C)nc(Nc2cc(C)ccc2C)n1 | 305.15 | (11) |
| 4i | C21H25N5 | CCc1nc(Nc2ccc(C)c(C)c2)nc(Nc2ccc(C)c(C)c2)n1 | 307.15 | (11) |
| 4j | C23H29N5 | CCc1nc(Nc2c(C)cc(C)cc2C)nc(Nc2c(C)cc(C)cc2C)n1 | 333.15 | (11) |
| 4k | C17H12N5F2 | CCc1nc(Nc2cc(F)cc(F)c2)nc(Nc2cc(F)cc(F)c2)n1 | 298.15 | (11) |
| 4l | C17H12N5Cl2 | CCc1nc(Nc2cc(Cl)cc(Cl)c2)nc(Nc2cc(Cl)cc(Cl)c2)n1 | 325.15 | (11) |
| 4m | C17H12N5Br2 | CCc1nc(Nc2cc(Br)cc(Br)c2)nc(Nc2cc(Br)cc(Br)c2)n1 | 339.15 | (11) |
| 4-Methoxyaniline | C7H9NO | COc1ccc(N)cc1 | 287 | (1) |
| 4-methyl-1-pentanol | C6H14O | CC(C)CCCO | 131.85 | (10) |
| 4-methyl-3-heptanol | C8H18O | CCCC(C)C(O)CC | 162.2 | (4)(SI 5) |
| 4-Methylcyclohexene | C7H12 | CC1CC=CCC1 | 94 | (4)(SI 3) |
| 4-methylnonane | C10H22 | CCCCCC(C)CCC | 118 | (16) |
| 4n | C17H12N5I2 | CCc1nc(Nc2cc(I)cc(I)c2)nc(Nc2cc(I)cc(I)c2)n1 | 369.15 | (11) |
| 4-Nitro-1-naphthylamine | C10H8N2O2 | Nc1ccc([N+](=O)[O-])c2ccccc12 | 305 | (1) |
| 4o | C21H25N5O2 | CCc1nc(Nc2cc(OC)cc(OC)c2)nc(Nc2cc(OC)cc(OC)c2)n1 | 308.15 | (11) |
| 4p | C23H29N5O3 | CCc1nc(Nc2cc(OC)c(OC)c(OC)c2)nc(Nc2cc(OC)c(OC)c(OC)c2)n1 | 336.15 | (11) |
| 4-phenylphenol | C12H10O | Oc1ccc(-c2ccccc2)cc1 | 294.15 | (22) |
| 4-Tert-Butylpyridine | C9H13N | CC(C)(C)c1ccncc1 | 166 | (4)(SI 16) |
| 5H-5-Methyl-6,7-dihydrocyclopentapyrazine | C8H10N2 | CC1CCc2nccnc21 | 170.4 | (23) |
| 5H-cyclopentapyrazine | C7H6N2 | C1=Cc2nccnc2C1 | 173.85 | (10) |
| 5-Methyl-3-heptanol | C8H18O | CCC(C)CC(O)CC | 159.15 | (14) |
| 6-Methyl-1-heptanol | C8H18O | CC(C)CCCCCO | 140.15 | (14) |
| 6-methyl-2-heptanol | C8H18O | CC(C)CCCC(C)O | 160 | (16) |
| 6-Methyl-3-heptanol | C8H18O | CCC(O)CCC(C)C | 159.15 | (14) |
| 9,9'-bis-(9,9-dimethyl-9H-fluoren-2-yl)-9H,9'H-[3,3']bicarbazolyl | C54H40N2 | CC1(C)c2ccccc2-c2ccc(-n3c4ccccc4c4cc(-c5ccc6c(c5)c5ccccc5n6-c5ccc6c(c5)C(C)(C)c5ccccc5-6)ccc43)cc21 | 450.95 | (24) |
| 9,9-Bis(p-aminophenyl)fluorene | C25H20N2 | Nc1ccc(C2(c3ccc(N)cc3)c3ccccc3-c3ccccc32)cc1 | 360 | (1) |
| 9-bromophenanthrene | C14H9Br | Brc1cc2ccccc2c2ccccc12 | 225 | (4)(SI 10) |
| Aceclofenac | C16H13Cl2NO4 | O=C(O)COC(=O)Cc1ccccc1Nc1c(Cl)cccc1Cl | 283 | (22) |
| Acemetacin | C21H18ClNO6 | COc1ccc2c(c1)c(CC(=O)OCC(=O)O)c(C)n2C(=O)c1ccc(Cl)cc1 | 310 | (25) |
| acetaldehyde | C2H4O | CC=O | 82 | (4)(SI 3) |
| Acetaminophen (Paracetamol) | C8H9NO2 | CC(=O)Nc1ccc(O)cc1 | 299.35 | (10)(49) |
| acetic acid | C2H4O2 | CC(=O)O | 150 | (2)(SI 1) |
| Acetohexamide | C15H20N2O4S | CC(=O)c1ccc(S(=O)(=O)NC(=O)NC2CCCCC2)cc1 | 299 | (26) |
| acetone | C3H6O | CC(C)=O | 93 | (4)(SI 3) |
| Acetyl tributyl citrate | C20H34O8 | CCCCOC(=O)CC(CC(=O)OCCCC)(OC(C)=O)C(=O)OCCCC | 187 | (27) |
| Acetyl triethyl citrate | C14H22O8 | CCOC(=O)CC(CC(=O)OCC)(OC(C)=O)C(=O)OCC | 202 | (27) |
| Albendazole | C12H15N3O2S | CCCSc1ccc2nc(NC(=O)OC)[nH]c2c1 | 333 | (26) |
| Ammonia | NH3 | N | 30 | (2)(SI) |
| Amobarbital | C11H18N2O3 | CCC1(CCC(C)C)C(=O)NC(=O)NC1=O | 286 | (28) |
| aniline | C6H7N | Nc1ccccc1 | 192 | (4)(SI 3) |
| Anilinephthalein | C20H16N2O2 | Nc1ccc(C2(c3ccc(N)cc3)OC(=O)c3ccccc32)cc1 | 353 | (1) |
| Anisole | C7H8O | COc1ccccc1 | 122 | (4)(SI 3) |
| Anthranilic acid | C7H7NO2 | Nc1ccccc1C(=O)O | 278.15 | (22) |
| Antipyrine | C11H12N2O | Cc1cc(=O)n(-c2ccccc2)n1C | 256 | (29) |
| Aprepitant | C23H21F7N4O3 | C[C@@H](O[C@H]1OCCN(Cc2n[nH]c(=O)[nH]2)[C@H]1c1ccc(F)cc1)c1cc(C(F)(F)F)cc(C(F)(F)F)c1 | 309 | (30) |
| Arabinose | C5H10O5 | OC1OC[C@H](O)[C@H](O)[C@H]1O | 276.15 | (31) |
| Aripiprazole | C23H27Cl2N3O2 | O=C1CCc2ccc(OCCCCN3CCN(c4cccc(Cl)c4Cl)CC3)cc2N1 | 363 | (25) |
| Aspirin | C9H8O4 | CC(=O)Oc1ccccc1C(=O)O | 243 | (29) |
| Atropine | C17H23NO3 | CN1[C@H]2CC[C@@H]1CC(OC(=O)C(CO)c1ccccc1)C2 | 281 | (29) |
| Beclomethasone dipropionate | C28H37ClO7 | CCC(=O)OCC(=O)[C@@]1(OC(=O)CC)[C@@H](C)C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(Cl)[C@@H](O)C[C@@]21C | 339.15 | (32)(60) |
| benzaldehyde | C7H6O | O=Cc1ccccc1 | 149 | (4)(SI 3) |
| Benzamide | C7H7NO | NC(=O)c1ccccc1 | 263.15 | (22) |
| benzene | C6H6 | c1ccccc1 | 131 | (4)(SI 3) |
| Benzocaine | C9H11NO2 | CCOC(=O)c1ccc(N)cc1 | 242.15 | (22) |
| benzoin isobutylether | C18H20O2 | CC(C)COC(C(=O)c1ccccc1)c1ccccc1 | 220.15 | (33) |
| benzophenone | C13H10O | O=C(c1ccccc1)c1ccccc1 | 212 | (4)(SI 9) |
| Benzyl alcohol | C7H8O | OCc1ccccc1 | 171 | (4)(SI 3) |
| Benzyl phenylcarbamate | C14H13NO2 | O=C(Nc1ccccc1)OCc1ccccc1 | 233 | (17) |
| Bezafibrate | C19H20ClNO4 | CC(C)(Oc1ccc(CCNC(=O)c2ccc(Cl)cc2)cc1)C(=O)O | 346 | (26) |
| Bicalutamide | C18H14F4N2O4S | CC(O)(CS(=O)(=O)c1ccc(F)cc1)C(=O)Nc1ccc(C#N)c(C(F)(F)F)c1 | 323 | (25) |
| Bis(hydroxymethyl)p-cresol (BMPC) | C9H12O3 | Cc1ccc(O)c(CO)c1CO | 241 | (4)(SI 6) |
| Bisphenol A diglycidyl ether | C21H24O4 | CC(C)(c1ccc(OCC2CO2)cc1)c1ccc(OCC2CO2)cc1 | 257 | (4)(SI 17) |
| Bisphenol C dimethyl ether | C19H24O2 | COc1ccc(C(C)(C)c2ccc(OC)c(C)c2)cc1C | 240 | (4)(SI 6) |
| BNIBPC | C37H22O4N2 | O=C1c2cccc3cccc(c23)C(=O)N1c1ccc(Cc2ccc(N3C(=O)c4cccc5cccc(c45)C3=O)cc2)cc1 | 443 | (17) |
| Bromobenzene | C6H5Br | Brc1ccccc1 | 138 | (4)(SI 3) |
| Brucine | C23H26N2O4 | COc1cc2c(cc1OC)[C@@]13CCN4CC5=CCO[C@H]6CC(=O)N2[C@H]1[C@H]6[C@H]5C[C@H]43 | 365 | (28) |
| Bucindolol | C22H25N3O2 | CC(C)(Cc1c[nH]c2ccccc12)NCC(O)COc1ccccc1C#N | 356 | (25) |
| Budesonide | C25H34O6 | CCCC1O[C@@H]2C[C@H]3[C@@H]4CCC5=CC(=O)C=C[C@]5(C)[C@H]4[C@@H](O)C[C@]3(C)[C@]2(C(=O)CO)O1 | 368 | (25) |
| Butethal | C10H16N2O3 | CCCCC1(CC)C(=O)NC(=O)NC1=O | 278.15 | (34) |
| Butyronitrile | C4H7N | CCCC#N | 100 | (4)(SI 6) |
| C1 | C44H34N2 | C(=C(c1ccc(N(c2ccccc2)c2ccccc2)cc1)c1ccc(N(c2ccccc2)c2ccccc2)cc1)c1ccccc1 | 345 | (17) |
| C2 | C50H46N2 | CC(C)c1ccc(C=C(c2ccc(N(c3ccccc3)c3ccccc3)cc2)c2ccc(N(c3ccccc3)c3ccccc3)cc2)c(C(C)C)c1 | 344 | (17) |
| C3 | C48H42N2 | CC(C)(C)c1ccc(C=C(c2ccc(N(c3ccccc3)c3ccccc3)cc2)c2ccc(N(c3ccccc3)c3ccccc3)cc2)cc1 | 355 | (17) |
| Caffeine | C8H10N4O2 | Cn1c(=O)c2c(ncn2C)n(C)c1=O | 260 | (35) |
| Captopril | C9H15NO3S | C[C@H](CS)C(=O)N1CCC[C@H]1C(=O)O | 277 | (25) |
| Carbamazepine | C15H12N2O | NC(=O)N1c2ccccc2C=Cc2ccccc21 | 334.15 | (22) |
| carbazole | C12H9N | c1ccc2c(c1)[nH]c1ccccc12 | 268.85 | (12) |
| carvedilol | C24H26N2O4 | COc1ccccc1OCCNCC(O)COc1cccc2[nH]c3ccccc3c12 | 310.15 | (36) |
| Celecoxib | C17H14F3N3O2S | Cc1ccc(-c2cc(C(F)(F)F)nn2-c2ccc(S(N)(=O)=O)cc2)cc1 | 331.25 | (32)(71) |
| Chenodeoxycholic acid | C24H40O4 | C[C@H](CCC(=O)O)[C@H]1CC[C@H]2[C@H]3[C@H](CC[C@@]21C)[C@@]1(C)CC[C@@H](O)C[C@H]1C[C@H]3O | 371 | (28) |
| Chloramphenicol | C11H12Cl2N2O5 | O=C(N[C@H](CO)[C@H](O)c1ccc([N+](=O)[O-])cc1)C(Cl)Cl | 304 | (25) |
| Chlorhexidine | C22H30Cl2N10 | NC(=NCCCCCCN=C(N)/N=C(\N)Nc1ccc(Cl)cc1)/N=C(\N)Nc1ccc(Cl)cc1 | 336 | (25) |
| Chlormadinone acetate | C23H29ClO4 | CC(=O)O[C@]1(C(C)=O)CC[C@H]2[C@@H]3C=C(Cl)C4=CC(=O)CC[C@]4(C)[C@H]3CC[C@@]21C | 334 | (28) |
| chlorobenzene | C6H5Cl | Clc1ccccc1 | 128 | (4)(SI 3) |
| Chlorotrianisene | C23H21ClO3 | COc1ccc(C(Cl)=C(c2ccc(OC)cc2)c2ccc(OC)cc2)cc1 | 298 | (28) |
| chlorotrifluoromethane | CF3Cl | FC(F)(F)Cl | 18 | (2)(SI 2) |
| Chlorpropamide | C10H13ClN2O3S | CCCNC(=O)NS(=O)(=O)c1ccc(Cl)cc1 | 289.15 | (22) |
| Chlorzoxazone | C7H4ClNO2 | O=c1[nH]c2cc(Cl)ccc2o1 | 311.15 | (22) |
| Cholecalciferol | C27H44O | C=C1CC[C@H](O)C/C1=C/C=C1\CCC[C@@]2(C)[C@H]1CC[C@@H]2[C@H](C)CCCC(C)C | 296 | (29) |
| Cholesterol | C27H46O | CC(C)CCC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3CC=C4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@@]21C | 332 | (1) |
| Cholic acid | C24H40O5 | C[C@H](CCC(=O)O)[C@H]1CC[C@H]2[C@H]3[C@H](C[C@H](O)[C@@]21C)[C@@]1(C)CC[C@@H](O)C[C@H]1C[C@H]3O | 393 | (28) |
| Cinchonidine | C19H22N2O | C=CC1CN2CCC1CC2C(O)c1ccnc2ccccc12 | 377 | (1) |
| Cinchonine | C19H22N2O | C=C[C@H]1CN2CC[C@H]1C[C@@H]2[C@@H](O)c1ccnc2ccccc12 | 395 | (1) |
| Cinnarizine | C26H28N2 | C(=C/c1ccccc1)\CN1CCN(C(c2ccccc2)c2ccccc2)CC1 | 280 | (25) |
| Citric acid | C6H8O7 | O=C(O)CC(O)(CC(=O)O)C(=O)O | 283 | (28) |
| Clofoctol | C21H26Cl2O | CC(C)(C)CC(C)(C)c1ccc(O)c(Cc2ccc(Cl)cc2Cl)c1 | 269 | (22) |
| Clotrimazole | C22H17ClN2 | Clc1ccccc1C(c1ccccc1)(c1ccccc1)n1ccnc1 | 303 | (25) |
| Colchicine | C22H25NO6 | COc1cc2c(c(OC)c1OC)-c1ccc(OC)c(=O)cc1[C@@H](NC(C)=O)CC2 | 374.5 | (37) |
| cresolphthalein dimethylether | C24H22O4 | COc1ccc(C2(c3ccc(OC)c(C)c3)OC(=O)c3ccccc32)cc1C | 314 | (4)(SI 6) |
| Cresyl glycidyl ether | C10H12O2 | Cc1ccc(OCC2CO2)cc1 | 204 | (4)(SI 17) |
| Cyclobarbital | C12H16N2O3 | CCC1(C2=CCCCC2)C(=O)NC(=O)NC1=O | 314.65 | (34) |
| cycloheptane | C7H14 | C1CCCCCC1 | 83 | (17) |
| cycloheptanol | C7H14O | OC1CCCCCC1 | 140 | (17) |
| d,l-Lactic acid | C3H6O3 | CC(O)C(=O)O | 204 | (16) |
| D1 | C36H28N2 | c1ccc(N(c2ccccc2)c2ccc(-c3ccc(N(c4ccccc4)c4ccccc4)cc3)cc2)cc1 | 346 | (17) |
| D3 | C38H30N2 | C(=C/c1ccc(N(c2ccccc2)c2ccccc2)cc1)\c1ccc(N(c2ccccc2)c2ccccc2)cc1 | 344 | (17) |
| D4 | C38H32N2 | c1ccc(N(c2ccccc2)c2ccc(CCc3ccc(N(c4ccccc4)c4ccccc4)cc3)cc2)cc1 | 317 | (17) |
| D5 | C39H34N2 | c1ccc(N(c2ccccc2)c2ccc(CCCc3ccc(N(c4ccccc4)c4ccccc4)cc3)cc2)cc1 | 308 | (17) |
| Danazol | C22H27NO2 | C#C[C@]1(O)CC[C@H]2[C@@H]3CCC4=Cc5oncc5C[C@]4(C)[C@H]3CC[C@@]21C | 352 | (25) |
| Decahydroisoquinoline | C9H17N | C1CCC2CNCCC2C1 | 180 | (4)(SI 14) |
| Decahydronaphthalene | C10H18 | C1CCC2CCCCC2C1 | 150 | (4)(SI 2) |
| Decane | C10H22 | CCCCCCCCCC | 54 | (2)(SI 2) |
| Dehydrocholic acid | C24H34O5 | C[C@H](CCC(=O)O)[C@H]1CC[C@H]2[C@@H]3C(=O)C[C@@H]4CC(=O)CC[C@]4(C)[C@H]3CC(=O)[C@@]21C | 348 | (29) |
| Deoxycholic acid | C24H40O4 | C[C@H](CCC(=O)O)[C@H]1CC[C@H]2[C@@H]3CC[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3C[C@H](O)[C@@]21C | 377 | (28) |
| deuterium Oxide | H2O | [2H]O[2H] | 160 | (2) (SI 2) |
| Dexketoprofen ((S)-(+)-ketoprofen) | C16H14O3 | C[C@H](C(=O)O)c1cccc(C(=O)c2ccccc2)c1 | 272.75 | (10)(49) |
| di-2-ethylhexylphthalate | C24H38O4 | CCCCC(CC)COC(=O)c1ccccc1C(=O)OCC(CC)CCCC | 187 | (4)(SI 6) |
| DIAMINE | C46H46N2 | Cc1ccc(N(c2ccc(C)cc2)c2ccc(C3(c4ccc(N(c5ccc(C)cc5)c5ccc(C)cc5)cc4)CCCCC3)cc2)cc1 | 351 | (17) |
| Diazepam | C16H13ClN2O | CN1C(=O)CN=C(c2ccccc2)c2cc(Cl)ccc21 | 319.15 | (32)(75) |
| Dibucaine | C20H29N3O2 | CCCCOc1cc(C(=O)NCCN(CC)CC)c2ccccc2n1 | 238.15 | (22) |
| dibutyl phthalate | C16H22O4 | CCCCOC(=O)c1ccccc1C(=O)OCCCC | 179 | (4)(SI 6) |
| diclrodifluoromethane | CF2Cl2 | FC(F)(Cl)Cl | 18 | (2)(SI 2) |
| Diethyl phthalate | C12H14O4 | CCOC(=O)c1ccccc1C(=O)OCC | 178 | (4)(SI 8) |
| Diisobutyl phthalate | C16H22O4 | CC(C)COC(=O)c1ccccc1C(=O)OCC(C)C | 191.1 | (4)(SI 5) |
| dimethyl acetamide | C4H9NO | CC(=O)N(C)C | 146.1 | (4)(SI 3) |
| dimethyl formamide | C3H7NO | CN(C)C=O | 129 | (4)(SI 3) |
| dimethyl phthalate | C10H10O4 | COC(=O)c1ccccc1C(=O)OC | 194.18 | (4)(SI 15) |
| dimethyl sulfone | C2H6O2S | CS(C)(=O)=O | 190 | (4)(SI 3) |
| Dimethyl sulfoxide | (CH3)2SO | CS(C)=O | 150 | (4)(SI 3) |
| Diphylline | C10H14N4O4 | Cn1c(=O)c2c(ncn2CC(O)CO)n(C)c1=O | 315 | (28) |
| Dodecane | C12H26 | CCCCCCCCCCCC | 76 | (2)(SI 2) |
| DPH | C31H24N3 | C(=N/N(c1ccccc1)c1ccccc1)\c1ccc(N(c2ccccc2)c2ccccc2)cc1 | 323 | (17) |
| Droperidol | C22H22FN3O2 | O=C(CCCN1CC=C(n2c(=O)[nH]c3ccccc32)CC1)c1ccc(F)cc1 | 302.15 | (22) |
| Emtricitabine | C8H10FN3O3S | Nc1nc(=O)n([C@@H]2CS[C@H](CO)O2)cc1F | 344 | (25) |
| Ergocalciferol | C28H44O | C=C1CC[C@H](O)C/C1=C/C=C1\CCC[C@@]2(C)[C@H]1CC[C@@H]2[C@H](C)/C=C/[C@H](C)C(C)C | 290 | (29) |
| Estradiol | C18H24O2 | CC12CCC3c4ccc(O)cc4CCC3C1CCC2O | 358 | (25) |
| Estradiol benzoate | C25H28O3 | C[C@]12CC[C@@H]3c4ccc(OC(=O)c5ccccc5)cc4CC[C@H]3[C@@H]1CC[C@@H]2O | 336 | (28) |
| Ethacrynic acid | C13H12Cl2O4 | C=C(CC)C(=O)c1ccc(OCC(=O)O)c(Cl)c1Cl | 282 | (28) |
| Ethane, 2,2-dichloro-1,1,1-trifluoro- | C2HCl2F3 | FC(F)(F)C(Cl)Cl | 59 | (2)(SI 2) |
| Ethanol | C2H6O | CCO | 97 | (38) |
| ethylbenzene | C8H10 | CCc1ccccc1 | 115 | (4)(SI 3) |
| ethylcyclohexane | C8H16 | CCC1CCCCC1 | 98 | (4)(SI 3) |
| Ethylene glycol | C2H6O2 | OCCO | 155 | (4)(SI 3) |
| ethylether | C4H10O | CCOCC | 92 | (4)(SI 3) |
| Etoricoxib | C18H15ClN2O2S | Cc1ccc(-c2ncc(Cl)cc2-c2ccc(S(C)(=O)=O)cc2)cn1 | 313.95 | (32)(73) |
| Eugenol | C10H12O2 | C=CCc1ccc(O)c(OC)c1 | 192.7 | (4) (SI 5) |
| Ezetimibe | C24H21F2NO3 | O=C1[C@H](CC[C@H](O)c2ccc(F)cc2)[C@@H](c2ccc(O)cc2)N1c1ccc(F)cc1 | 338 | (25) |
| Famotidine | C8H15N7O2S3 | NC(N)=Nc1nc(CSCCC(N)=NS(N)(=O)=O)cs1 | 323 | (26) |
| Felbinac | C14H12O2 | O=C(O)Cc1ccc(-c2ccccc2)cc1 | 297.15 | (22) |
| Felodipine | C18H19Cl2NO4 | CCOC(=O)C1=C(C)NC(C)=C(C(=O)OC)C1c1cccc(Cl)c1Cl | 315.85 | (32)(65) |
| fenofibrate | C20H21ClO4 | CC(C)OC(=O)C(C)(C)Oc1ccc(C(=O)c2ccc(Cl)cc2)cc1 | 255.3 | (10)(49) |
| flufenamic acid | C14H10F3NO2 | O=C(O)c1ccccc1Nc1cccc(C(F)(F)F)c1 | 285 | (10)(49) |
| Fluorescamine | C17H10O4 | O=C1OC2(OC=C(c3ccccc3)C2=O)c2ccccc21 | 299 | (25) |
| Flurbiprofen | C15H13FO2 | CC(C(=O)O)c1ccc(-c2ccccc2)c(F)c1 | 268.5 | (32)(74) |
| flutamide | C11H11F3N2O3 | CC(C)C(=O)Nc1ccc([N+](=O)[O-])c(C(F)(F)F)c1 | 274 | (39) |
| Fructose | C6H12O6 | OCC1(O)OC[C@@H](O)[C@@H](O)[C@@H]1O | 283.15 | (31) |
| Fucose | C6H12O5 | C[C@@H]1OC(O)[C@@H](O)[C@H](O)[C@@H]1O | 304.15 | (31) |
| Galactose | C6H12O6 | OC[C@H]1OC(O)[C@H](O)[C@@H](O)[C@H]1O | 311.15 | (31) |
| Glafenine | C19H17ClN2O4 | O=C(OCC(O)CO)c1ccccc1Nc1ccnc2cc(Cl)ccc12 | 337 | (25) |
| Glibenclamide | C23H28ClN3O5S | COc1ccc(Cl)cc1C(=O)NCCc1ccc(S(=O)(=O)NC(=O)NC2CCCCC2)cc1 | 333 | (25) |
| Glycerol | C3H8O3 | OCC(O)CO | 189.15 | (40) |
| Griseofulvin | C17H17ClO6 | COC1=CC(=O)CC(C)C12Oc1c(Cl)c(OC)cc(OC)c1C2=O | 359 | (39) |
| H3 | C26H20N3 | Cn1c2ccccc2c2cc(/C=N/N(c3ccccc3)c3ccccc3)ccc21 | 333 | (17) |
| H4 | C28H24N3 | CC(C)n1c2ccccc2c2cc(/C=N/N(c3ccccc3)c3ccccc3)ccc21 | 337 | (17) |
| H5 | C28H23N3 | Cn1c2ccccc2c2cc(/C=C/C=N/N(c3ccccc3)c3ccccc3)ccc21 | 334 | (17) |
| Heptabarbital | C13H18N2O3 | CCC1(C2=CCCCCC2)C(=O)NC(=O)NC1=O | 305.15 | (34) |
| heptane | C7H16 | CCCCCCC | 44 | (2)(SI 2) |
| hexane | C6H14 | CCCCCC | 23 | (2)(SI 2) |
| Hexobarbital | C12H16N2O3 | CN1C(=O)NC(=O)C(C)(C2=CCCCC2)C1=O | 286 | (28) |
| HMHPPD (1,3,4,6,7,8-Hexahydro-2H-pyrimido[1,2-a]pyrimidine) | C7H13N3 | C1CN=C2NCCCN2C1 | 184.05 | (10) |
| Hydrochlorothiazide | C7H8ClN3O4S2 | NS(=O)(=O)c1cc2c(cc1Cl)NCNS2(=O)=O | 391 | (25) |
| Hydrocortisone | C21H30O5 | C[C@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)CC[C@@]43C)[C@@H]1CC[C@]2(O)C(=O)CO | 359 | (25) |
| Hydroflumethiazide | C8H8F3N3O4S2 | NS(=O)(=O)c1cc2c(cc1C(F)(F)F)NCNS2(=O)=O | 373 | (25) |
| Indapamide | C16H16ClN3O3S | CC1Cc2ccccc2N1NC(=O)c1ccc(Cl)c(S(N)(=O)=O)c1 | 371.15 | (41) |
| Indoprofen | C17H15NO3 | CC(C(=O)O)c1ccc(N2Cc3ccccc3C2=O)cc1 | 323.15 | (22) |
| Ioperamide (T1001) | C29H33ClN2O2 | CN(C)C(=O)C(CCN1CCC(O)(c2ccc(Cl)cc2)CC1)(c1ccccc1)c1ccccc1 | 336.9 | (20) |
| iso-amyl bromide | C5H12Br | CC(C)CCBr | 109 | (4)(SI 5) |
| isobutane | C6H10 | CC(C)C | 20 | (2)(SI 2) |
| Isopentane | C5H12 | CCC(C)C | 69 | (4)(SI 3) |
| Isopropanol | C3H8O | CC(C)O | 115 | (42) |
| isopropylbenzene | C9H12 | CC(C)c1ccccc1 | 125 | (4)(SI 5) |
| isopropylcyclohexane | C9H18 | CC(C)C1CCCCC1 | 108 | (4)(SI 3) |
| Isradipine | C19H21N3O5 | COC(=O)C1=C(C)NC(C)=C(C(=O)OC(C)C)C1c1cccc2nonc12 | 316 | (25) |
| Itraconazole | C35H38Cl2N8O4 | CCC(C)n1ncn(-c2ccc(N3CCN(c4ccc(OC[C@H]5CO[C@](Cn6cncn6)(c6ccc(Cl)cc6Cl)O5)cc4)CC3)cc2)c1=O | 332.4 | (43) |
| Ketoconazole | C26H28Cl2N4O4 | CC(=O)N1CCN(c2ccc(OC[C@H]3CO[C@](Cn4ccnc4)(c4ccc(Cl)cc4Cl)O3)cc2)CC1 | 318.6 | (44) |
| Ketoprofen | C16H14O3 | CC(C(=O)O)c1cccc(C(=O)c2ccccc2)c1 | 259.15 | (32)(60) |
| Lamotrigine | C9H7Cl2N5 | Nc1nnc(-c2cccc(Cl)c2Cl)c(N)n1 | 367.15 | (45) |
| Lidocaine | C14H22N2O | CCN(CC)CC(=O)Nc1c(C)cccc1C | 234.15 | (22) |
| Linaprazan | C21H26N4O2 | Cc1cccc(C)c1CNc1cc(C(=O)NCCO)cn2c(C)c(C)nc12 | 373 | (25) |
| l-menthyl-3-nitrophenyluretane | C15H18O4N2 | C[C@@H]1CC[C@@H](C)[C@H](OC(=O)Nc2cccc([N+](=O)[O-])c2)C1 | 288 | (1) |
| Loratadine | C22H23ClN2O2 | CCOC(=O)N1CCC(=C2c3ccc(Cl)cc3CCc3cccnc32)CC1 | 305.15 | (36) |
| Lyxose | C5H10O5 | OC1OC[C@@H](O)[C@H](O)[C@@H]1O | 277.1 | (46) |
| Maltitol | C12H24O11 | OC[C@H](O)[C@@H](O)[C@H](O[C@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O)[C@H](O)CO | 317.15 | (31) |
| Maltose | C12H22O11 | OC[C@H]1O[C@H](O[C@@H]2[C@@H](CO)O[C@@H](O)[C@H](O)[C@H]2O)[C@H](O)[C@@H](O)[C@@H]1O | 365.15 | (31) |
| Mannose | C6H12O6 | OC[C@H]1OC(O)[C@@H](O)[C@@H](O)[C@@H]1O | 304.15 | (31) |
| m-cresol | C7H8O | Cc1cccc(O)c1 | 198.5 | (4)(SI 6) |
| Meglumine | C7H17NO5 | CNC[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO | 292.05 | (32)(71) |
| Melibiose | C12H22O11 | OC[C@H]1O[C@H](OC[C@H]2OC(O)[C@H](O)[C@@H](O)[C@@H]2O)[C@H](O)[C@@H](O)[C@H]1O | 364.15 | (31) |
| Mephenesin | C10H14O3 | Cc1ccccc1OCC(O)CO | 247 | (28) |
| Mephobarbital | C13H14N2O3 | CCC1(c2ccccc2)C(=O)NC(=O)N(C)C1=O | 270.15 | (34) |
| Methanol | COH4 | CO | 103 | (47) |
| methyl n-phenylcarbamate | C8H9NO2 | COC(=O)Nc1ccccc1 | 218 | (4)(SI 4) |
| methyl o-toluate | C9H10O2 | COC(=O)c1ccccc1C | 167.25 | (10)(43) |
| Methylcyclohexane | C7H14 | CC1CCCCC1 | 87 | (4)(SI 3) |
| methyl-m-toluate | C9H10O2 | COC(=O)c1cccc(C)c1 | 165 | (4)(SI 14) |
| Methyltestosterone | C20H30O2 | C[C@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@@]21C | 270 | (29) |
| Metolazone | C16H16ClN3O3S | Cc1ccccc1N1C(=O)c2cc(S(N)(=O)=O)c(Cl)cc2NC1C | 382 | (25) |
| m-fluoroaniline | C6H6FN | Nc1cccc(F)c1 | 173 | (48) |
| m-fluorophenol | C6H5FO | Oc1cccc(F)c1 | 191 | (48) |
| m-fluorotoluene | C7H7F | Cc1cccc(F)c1 | 117 | (4)(SI 6) |
| Miconazole | C18H14Cl4N2O | Clc1ccc(COC(Cn2ccnc2)c2ccc(Cl)cc2Cl)c(Cl)c1 | 274.8 | (43) |
| m-MTDAB | C45H39N3 | Cc1cccc(N(c2ccccc2)c2cc(N(c3ccccc3)c3ccccc3)cc(N(c3cccc(C)c3)c3cccc(C)c3)c2)c1 | 322 | (17) |
| Monoethanolamine | C2H7NO | NCCO | 146.15 | (19) |
| MTDATA | C57H48N4 | Cc1cccc(N(c2ccccc2)c2ccc(N(c3ccc(N(c4ccccc4)c4cccc(C)c4)cc3)c3ccc(N(c4ccccc4)c4cccc(C)c4)cc3)cc2)c1 | 348 | (17) |
| m-toluidine | C7H9N | Cc1cccc(N)c1 | 187 | (4)(SI 6) |
| m-xylene | C8H10 | Cc1cccc(C)c1 | 120 | (4)(SI 6) |
| N-(R-1-Naphthylethyl)-2,2'-diphenic imide | C26H19O2N | C[C@@H](c1ccc2ccccc2c1)n1c(=O)c2ccccc2c2ccccc2c1=O | 333 | (1) |
| N-(R-1-Phenylethyl)-1,8-naphthalimide | C20H15NO2 | C[C@@H](c1ccccc1)N1C(=O)c2cccc3cccc(c23)C1=O | 319 | (1) |
| N-(R-1-Phenylethyl)-3-nitrophthalimide | C16H12N2O4 | C[C@@H](c1ccccc1)N1C(=O)c2cccc([N+](=O)[O-])c2C1=O | 289 | (1) |
| N-(R-1-Phenylethyl)-4-nitro-1,8-naphthalimide | C20H14N2O4 | C[C@@H](c1ccccc1)N1C(=O)c2cccc3c([N+](=O)[O-])ccc(c23)C1=O | 320 | (1) |
| N-(R-1-Phenylethyl)-N’- (p-nitrophenyl)thiourea | C15H15N3O2 | C[C@H](NC(=S)Nc1ccc([N+](=O)[O-])cc1)c1ccccc1 | 313 | (1) |
| N-(R-1-Phenylethyl)-tetrabromophthalimide | C16H9NO2Br4 | C[C@@H](c1ccccc1)N1C(=O)c2c(Br)c(Br)c(Br)c(Br)c2C1=O | 330 | (1) |
| N-(R-1-Phenylethyl)-tetrachlorophthalimide | C16H9NO2Cl4 | C[C@@H](c1ccccc1)N1C(=O)c2c(Cl)c(Cl)c(Cl)c(Cl)c2C1=O | 313 | (1) |
| N-(R-1-Phenylethyl)-tetraiodophthalimide | C16H9NO2I4 | C[C@@H](c1ccccc1)N1C(=O)c2c(I)c(I)c(I)c(I)c2C1=O | 370 | (1) |
| N-(S-1-Naphthylethyl)-2,2'-diphenic imide | C26H19O2N | C[C@H](c1ccc2ccccc2c1)n1c(=O)c2ccccc2c2ccccc2c1=O | 356 | (1) |
| N-(S-1-Naphthylethyl)-tetrachlorophthalimide | C20H11NO2Cl4 | C[C@H](c1cccc2ccccc12)N1C(=O)c2c(Cl)c(Cl)c(Cl)c(Cl)c2C1=O | 362 | (1) |
| N,N′-bis(3-methylphenyl)-N,N′-diphenylbenzidine | C38H32N2 | Cc1cccc(N(c2ccccc2)c2ccc(-c3ccc(N(c4ccccc4)c4cccc(C)c4)cc3)cc2)c1 | 342 | (7) |
| N,N′-diphenyl-N,N′-di-p-tolylbenzene-1,4-diamine | C32H28N2 | Cc1ccc(N(c2ccccc2)c2ccc(N(c3ccccc3)c3ccc(C)cc3)cc2)cc1 | 325 | (7) |
| Nandrolone | C18H26O2 | C[C@]12CC[C@@H]3[C@H]4CCC(=O)C=C4CC[C@H]3[C@@H]1CC[C@@H]2O | 310 | (25) |
| Naproxen | C14H14O3 | COc1ccc2cc([C@H](C)C(=O)O)ccc2c1 | 302.15 | (32)(60) |
| n-butyl bromide | C4H9Br | CCCCBr | 96.5 | (4)(SI 6) |
| n-butylbenzene | C10H14 | CCCCc1ccccc1 | 129 | (4)(SI 3) |
| n-butylcyclohexane | C10H20 | CCCCC1CCCCC1 | 119 | (4)(SI 3) |
| n-ethylacetamide | C4H9NO | CCNC(C)=O | 158 | (4)(SI 6) |
| n-hexanol | C6H14O | CCCCCCO | 125 | (17) |
| n-hexylbenzene | C12H18 | CCCCCCc1ccccc1 | 140 | (4)(SI 3) |
| Nialamide | C16H18N4O2 | O=C(CCNNC(=O)c1ccncc1)NCc1ccccc1 | 297 | (28) |
| Nifedipine | C17H18N2O6 | COC(=O)C1=C(C)NC(C)=C(C(=O)OC)C1c1ccccc1[N+](=O)[O-] | 321.15 | (32)(67) |
| Nilutamide | C12H10F3N3O4 | CC1(C)NC(=O)N(c2ccc([N+](=O)[O-])c(C(F)(F)F)c2)C1=O | 306 | (22) |
| Nimesulide | C13H12N2O5S | CS(=O)(=O)Nc1ccc([N+](=O)[O-])cc1Oc1ccccc1 | 296 | (25) |
| Nimodipine | C21H26N2O7 | COCCOC(=O)C1=C(C)NC(C)=C(C(=O)OC(C)C)C1c1cccc([N+](=O)[O-])c1 | 293.15 | (32)(66) |
| Nisoldipine | C20H24N2O6 | COC(=O)C1=C(C)NC(C)=C(C(=O)OCC(C)C)C1c1ccccc1[N+](=O)[O-] | 307 | (39) |
| nitrobenzene | C6H5NO2 | O=[N+]([O-])c1ccccc1 | 161 | (4)(SI 3) |
| Nizatidine | C12H21N5O2S2 | CN/C(=C\[N+](=O)[O-])NCCSCc1csc(CN(C)C)n1 | 286 | (25) |
| Nordazepam | C15H11ClN2O | O=C1CN=C(c2ccccc2)c2cc(Cl)ccc2N1 | 346.8 | (49) |
| n-Pentyl-p-nitrophenylurethane | C14H20N2O4 | CCCCCN(C(=O)OCC)c1ccc([N+](=O)[O-])cc1 | 243 | (1) |
| n-propylbenzene | C9H12 | CCCc1ccccc1 | 125 | (4)(SI 3) |
| o-fluoroaniline | C6H6FN | Nc1ccccc1F | 174 | (48) |
| Omeprazole | C17H19N3O3S | COc1ccc2nc(S(=O)Cc3ncc(C)c(OC)c3C)[nH]c2c1 | 324 | (26) |
| Orlistat | C29H53NO5 | CCCCCCCCCCC[C@@H](C[C@@H]1OC(=O)[C@H]1CCCCCC)OC(=O)[C@H](CC(C)C)NC=O | 228 | (25) |
| ortho-terphenyl | C18H14 | c1ccc(-c2ccccc2-c2ccccc2)cc1 | 243 | (4)(SI 7) |
| o-Toluidine | C7H9N | Cc1ccccc1N | 189 | (50)(21) |
| OXD-6 | C32H28O2N6 | CN(C)c1ccc(-c2nnc(-c3ccc(-c4ccc(-c5nnc(-c6ccc(N(C)C)cc6)o5)cc4)cc3)o2)cc1 | 402 | (17) |
| OXD-7 | C30H30O2N4 | CC(C)(C)c1ccc(-c2nnc(-c3ccc(-c4nnc(-c5ccc(C(C)(C)C)cc5)o4)cc3)o2)cc1 | 350 | (17) |
| OXD-8 | C26H24O2N6 | CN(C)c1ccc(-c2nnc(-c3ccc(-c4nnc(-c5ccc(N(C)C)cc5)o4)cc3)o2)cc1 | 369 | (17) |
| OXD-S0 | C30H18O3N6 | c1ccc(-c2nnc(-c3cc(-c4nnc(-c5ccccc5)o4)cc(-c4nnc(-c5ccccc5)o4)c3)o2)cc1 | 372 | (17) |
| OXD-S1 | C42H41O3N6 | CC(C)(C)c1ccc(-c2nnc(-c3cc(-c4nnc(-c5ccc(C(C)(C)C)cc5)o4)cc(-c4nnc(-c5ccc(C(C)(C)C)cc5)o4)c3)o2)cc1 | 412 | (17) |
| OXD-S7 | C33H15O3N6F9 | FC(F)(F)c1ccc(-c2nnc(-c3cc(-c4nnc(-c5ccc(C(F)(F)F)cc5)o4)cc(-c4nnc(-c5ccc(C(F)(F)F)cc5)o4)c3)o2)cc1 | 411 | (17) |
| OXD-S8 | C42H24O3N6 | c1ccc2c(-c3nnc(-c4cc(-c5nnc(-c6cccc7ccccc67)o5)cc(-c5nnc(-c6cccc7ccccc67)o5)c4)o3)cccc2c1 | 418 | (17) |
| OXD-S9 | C36H30O9N6 | COc1ccc(-c2nnc(-c3cc(-c4nnc(-c5ccc(OC)cc5OC)o4)cc(-c4nnc(-c5ccc(OC)cc5OC)o4)c3)o2)c(OC)c1 | 405 | (17) |
| o-xylene | C8H10 | Cc1ccccc1C | 123 | (4)(SI 6) |
| Pentachloronitrobenzene | C6Cl5NO2 | O=[N+]([O-])c1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl | 201 | (15) |
| Pentobarbital | C11H18N2O3 | CCCC(C)C1(CC)C(=O)NC(=O)NC1=O | 279 | (28) |
| Phenacetin | C10H13NO2 | CCOc1ccc(NC(C)=O)cc1 | 275.15 | (22) |
| Phenobarbital | C12H12N2O3 | CCC1(c2ccccc2)C(=O)NC(=O)NC1=O | 321 | (29) |
| phenol | C6H6O | Oc1ccccc1 | 198 | (4)(SI 3) |
| phenolphthalein | C20H14O4 | O=C1OC(c2ccc(O)cc2)(c2ccc(O)cc2)c2ccccc21 | 363 | (9) |
| Phenylbutazone | C19H20N2O2 | CCCCC1C(=O)N(c2ccccc2)N(c2ccccc2)C1=O | 277 | (29) |
| Physostigmine; Eserine | C15H21N3O2 | CNC(=O)Oc1ccc2c(c1)[C@]1(C)CCN(C)[C@@H]1N2C | 293 | (25) |
| Pimozide | C28H29F2N3O | O=c1[nH]c2ccccc2n1C1CCN(CCCC(c2ccc(F)cc2)c2ccc(F)cc2)CC1 | 335 | (25) |
| Piperine | C17H19NO3 | O=C(/C=C/C=C/c1ccc2c(c1)OCO2)N1CCCCC1 | 284 | (1) |
| p-MTDAB | C45H39N3 | Cc1ccc(N(c2ccccc2)c2cc(N(c3ccccc3)c3ccccc3)cc(N(c3ccc(C)cc3)c3ccc(C)cc3)c2)cc1 | 331 | (17) |
| PPCP | C35H26 | c1ccc(C2=C(c3ccccc3)C(c3ccccc3)C(c3ccccc3)=C2c2ccccc2)cc1 | 330 | (17) |
| Prednisone | C21H26O5 | C[C@]12CC(=O)[C@H]3[C@@H](CCC4=CC(=O)C=C[C@@]43C)[C@@H]1CC[C@]2(O)C(=O)CO | 366 | (30) |
| Probucol | C31H48O2S2 | CC(C)(Sc1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1)Sc1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1 | 295 | (51) |
| Procaine | C13H20N2O2 | CCN(CC)CCOC(=O)c1ccc(N)cc1 | 234 | (22) |
| Propanol | C3H8O | CCCO | 98 | (42) |
| Propenylguaiacol (isoeugenol) | C10H12O2 | CC=Cc1ccc(O)c(OC)c1 | 220.1 | (4)(SI 5) |
| propyl N-phenylcarbamate | C10H13NO2 | CCCOC(=O)Nc1ccccc1 | 203 | (17) |
| propylene carbonate | C4H6O3 | CC1COC(=O)O1 | 159 | (4)(SI 8) |
| Proxyphylline | C10H14N4O3 | CC(O)Cn1cnc2c1c(=O)n(C)c(=O)n2C | 295 | (28) |
| pyridine | C5H5N | c1ccncc1 | 128 | (4)(SI 3) |
| Quinaldine | C10H9N | Cc1ccc2ccccc2n1 | 180 | (23) |
| Quinidine | C20H24N2O2 | C=C[C@H]1CN2CC[C@H]1C[C@@H]2[C@@H](O)c1ccnc2ccc(OC)cc12 | 326 | (29) |
| Quinine Ethylcarbonate | C23H28N2O4 | C=C[C@H]1CN2CC[C@H]1C[C@H]2[C@H](OC(=O)OCC)c1ccnc2ccc(OC)cc12 | 278 | (29) |
| Rhamnose | C6H12O5 | C[C@@H]1OC(O)[C@H](O)[C@H](O)[C@H]1O | 273.15 | (31) |
| Ribose | C5H10O5 | OC1OC[C@@H](O)[C@@H](O)[C@H]1O | 260.15 | (31) |
| Ritonavir | C37H48N6O5S2 | CC(C)c1nc(CN(C)C(=O)N[C@H](C(=O)N[C@@H](Cc2ccccc2)C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OCc2cncs2)C(C)C)cs1 | 322 | (22) |
| Salicin | C13H18O7 | OCc1ccccc1O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O | 333 | (29) |
| Salol | C13H10O3 | O=C(Oc1ccccc1)c1ccccc1O | 219.15 | (40) |
| Santonin | C15H18O3 | CC1=C2C3OC(=O)C(C)C3CCC2(C)C=CC1=O | 290 | (29) |
| S-Benzoyl-3-mercapto-2-methylpropanoyl chloride (BMMPC) | C11H11ClO2S | C[C@H](CSC(=O)c1ccccc1)C(=O)Cl | 261 | (4)(SI 6) |
| sec-butyl alcohol | C4H10O | CCC(C)O | 100 | (17) |
| sec-butylbenzene | C10H14 | CCC(C)c1ccccc1 | 128 | (17) |
| Simvastatin | C25H38O5 | CCC(C)(C)C(=O)O[C@H]1C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H]3C[C@@H](O)CC(=O)O3)[C@H]21 | 309 | (25) |
| Sorbitol | C6H14O6 | OC[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO | 266 | (9) |
| Sorbose | C6H12O6 | OCC1(O)OC[C@H](O)[C@@H](O)[C@@H]1O | 300.15 | (31) |
| Spironolactone | C24H32O4S | CC(=O)S[C@@H]1CC2=CC(=O)CC[C@]2(C)[C@H]2CC[C@@]3(C)[C@@H](CC[C@@]34CCC(=O)O4)[C@@H]21 | 364 | (25) |
| Squalane | C30H62 | CC(C)CCCC(C)CCCC(C)CCCCC(C)CCCC(C)CCCC(C)C | 167.4 | (6)(26) |
| Stilbestrol | C18H20O2 | CCC(=C(CC)c1ccc(O)cc1)c1ccc(O)cc1 | 308 | (29) |
| Sucrose 1'-benzoate(sucrose benzoate) | C19H26O12 | O=C(OC[C@@]1(O[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)O[C@H](CO)[C@@H](O)[C@@H]1O)c1ccccc1 | 337 | (4)(SI 6) |
| Sulfathiazole | C9H9N3O2S2 | Nc1ccc(S(=O)(=O)Nc2nccs2)cc1 | 334 | (29) |
| Sulfisoxazole | C11H13N3O3S | Cc1noc(NS(=O)(=O)c2ccc(N)cc2)c1C | 306 | (29) |
| Sulindac | C20H17FO3S | CC1=C(CC(=O)O)c2cc(F)ccc2/C1=C\c1ccc(S(C)=O)cc1 | 348 | (25) |
| Tamoxifen | C26H29NO | CC/C(=C(\c1ccccc1)c1ccc(OCCN(C)C)cc1)c1ccccc1 | 263 | (25) |
| Tartaric acid | C4H6O6 | O=C(O)C(O)C(O)C(=O)O | 289 | (29) |
| TCTA | C42H27N3 | c1ccc2c(c1)c1ccccc1n2-c1cc(-n2c3ccccc3c3ccccc32)cc(-n2c3ccccc3c3ccccc32)c1 | 424 | (17) |
| TDP | C38H32N2 | Cc1cccc(N(c2ccccc2)c2ccc(-c3ccc(N(c4ccccc4)c4cccc(C)c4)cc3)cc2)c1 | 333 | (17) |
| Telmisartan | C33H30N4O2 | CCCc1nc2c(C)cc(-c3nc4ccccc4n3C)cc2n1Cc1ccc(-c2ccccc2C(=O)O)cc1 | 400.3 | (52) |
| Tenofovir | C9H14N5O4P | C[C@H](Cn1cnc2c(N)ncnc21)OCP(=O)(O)O | 416 | (25) |
| tert-Butyl alcohol | C4H10O | CC(C)(C)O | 180 | (17) |
| tert-Butyl chloride | C4H9Cl | CC(C)(C)Cl | 130 | (17) |
| Tert-Butylbenzene | C10H14 | CC(C)(C)c1ccccc1 | 140 | (4)(SI 3) |
| Testosterone | C19H28O2 | C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@@]43C)[C@@H]1CC[C@@H]2O | 315 | (25) |
| Tetrahydroisoquinoline | C9H11N | c1ccc2c(c1)CCNC2 | 191.15 | (10) |
| Tetrahydroquinoline | C9H11N | c1ccc2c(c1)CCCN2 | 195.1 | (10) |
| Tetraphenylbenzidine | C36H28N2 | c1ccc(N(c2ccccc2)c2ccc(-c3ccc(N(c4ccccc4)c4ccccc4)cc3)cc2)cc1 | 350 | (7) |
| Tetrazepam | C16H17ClN2O | CN1C(=O)CN=C(C2=CCCCC2)c2cc(Cl)ccc21 | 313 | (49) |
| Theophylline | C7H8N4O2 | Cn1c(=O)c2[nH]cnc2n(C)c1=O | 367.15 | (22) |
| Tinidazole | C8H13N3O4S | CCS(=O)(=O)CCn1c([N+](=O)[O-])cnc1C | 266 | (25) |
| Tolazamide | C14H21N3O3S | Cc1ccc(S(=O)(=O)NC(=O)NN2CCCCCC2)cc1 | 297 | (25) |
| Tolbudamide | C12H18N2O3S | CCCCNC(=O)NS(=O)(=O)c1ccc(C)cc1 | 277.15 | (22) |
| Tolfenamic acid | C14H12ClNO2 | Cc1c(Cl)cccc1Nc1ccccc1C(=O)O | 336.15 | (22) |
| Tolnaftate | C19H17NOS | Cc1cccc(N(C)C(=S)Oc2ccc3ccccc3c2)c1 | 287 | (28) |
| Toluene | C7H8 | Cc1ccccc1 | 117 | (53) |
| TPTTA | C54H36N4S3 | c1cc(N2C3CCCCC3SC3CCCCC32)ccc1N(c1ccc(N2C3CCCCC3SC3CCCCC32)cc1)c1ccc(N2C3CCCCC3SC3CCCCC32)cc1 | 414 | (17) |
| Trehalose | C12H22O11 | OC[C@H]1O[C@H](O[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@H](O)[C@@H](O)[C@@H]1O | 380.15 | (31) |
| Triacetate | C6H8O4 | CC(=O)CC(=O)CC(=O)O | 205.55 | (10)(48) |
| Tributyl citrate | C18H32O7 | CCCCOC(=O)CC(O)(CC(=O)OCCCC)C(=O)OCCCC | 184 | (27) |
| trifluoroethanol | C2H3F3O | OCC(F)(F)F | 144 | (4)(SI 3) |
| triphenylchloromethane | C19H15Cl | ClC(c1ccccc1)(c1ccccc1)c1ccccc1 | 243 | (4)(SI 6) |
| triphenylethene | C20H16 | C(=C(c1ccccc1)c1ccccc1)c1ccccc1 | 248 | (4)(SI 13) |
| triphenylphosphate | C18H15O4P | O=P(Oc1ccccc1)(Oc1ccccc1)Oc1ccccc1 | 205 | (4)(SI 6) |
| Tris-naphthylbenzene | C36H24 | c1cc(-c2cccc3ccccc23)c(-c2cccc3ccccc23)c(-c2cccc3ccccc23)c1 | 344.8 | (6)(26) |
| Ursodeoxycholic acid | C24H40O4 | C[C@H](CCC(=O)O)[C@H]1CC[C@H]2[C@@H]3[C@@H](O)C[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@@]21C | 379 | (51) |
| vinyl acetate | C4H6O2 | C=COC(C)=O | 125 | (17) |
| Vitamin A | C22H32O2 | CC(=O)OC/C=C(C)/C=C/C=C(C)/C=C/C1=C(C)CCCC1(C)C | 244.33 | (54) |
| Vitamin E | C31H52O3 | CC(=O)Oc1c(C)c(C)c2c(c1C)CC[C@@](C)(CCC[C@H](C)CCC[C@H](C)CCCC(C)C)O2 | 223 | (55) |
| xylose | C5H10O5 | OC1OC[C@@H](O)[C@H](O)[C@H]1O | 283 | (28) |
| Zolmitriptan | C16H21N3O2 | CN(C)CCc1c[nH]c2ccc(C[C@H]3COC(=O)N3)cc12 | 322 | (25) |
| Zoxazolamine | C7H5ClN2O | Nc1nc2cc(Cl)ccc2o1 | 284.15 | (26) |
| Validation | | | | |
| 1'-(Ethoxycarbonyl)ethyl-2-methyl-4-nitrophenyluretane | C13H16O6N2 | CCOC(=O)C(C)OC(=O)Nc1ccc([N+](=O)[O-])cc1C | 273 | (1) |
| 1,2,6-Hexanetriol | C6H14O3 | OCCCCC(O)CO | 202 | (4)(SI 6) |
| 1,3-Butanediol | C4H10O2 | CC(O)CCO | 173 | (4)(SI 6) |
| 2,2,3,3-Tetrafluoropropyl-p-nitrophenylurethane | C12H11N2O4F4 | CCOC(=O)N(CC(F)(F)C(F)F)c1ccc([N+](=O)[O-])cc1 | 261 | (1) |
| 2-ethyl-1-butanol | C6H14O | CCC(CC)CO | 132.5 | (10)(24) |
| 2-ethylhexyl acetate | C10H20O2 | CCCCC(CC)COC(C)=O | 146.45 | (10) |
| 2-methyl-1-pentanol | C6H14O | CCCC(C)CO | 139.75 | (10) |
| 3,4-Dichloroaniline | C6H5Cl2N | Nc1ccc(Cl)c(Cl)c1 | 296 | (1) |
| 3a | C10H18N6 | CNc1nc(NC(C)C)nc(NC(C)C)n1 | 295.15 | (11) |
| 3b | C12H24N6 | CNc1nc(NC(C)(C)C)nc(NC(C)(C)C)n1 | 312.15 | (11) |
| 4-(Dimethylamino)-N,N-dimethyl-2,2-diphenylbutanamide (R731) | C20H26N2O | CN(C)CCC(C(=O)N(C)C)(c1ccccc1)c1ccccc1 | 257 | (20) |
| 4-Nitroaniline | C6H6N2O2 | Nc1ccc([N+](=O)[O-])cc1 | 318 | (1) |
| 9,9-Bis(p-hydroxyphenyl)fluorene | C25H18O0 | Oc1ccc(C2(c3ccc(O)cc3)c3ccccc3-c3ccccc32)cc1 | 372 | (1) |
| Atenolol | C14H22N2O3 | CC(C)NCC(O)COc1ccc(CC(N)=O)cc1 | 295.15 | (22) |
| Bifonazole | C22H18N2 | c1ccc(-c2ccc(C(c3ccccc3)n3ccnc3)cc2)cc1 | 290 | (22) |
| Clemastine | C21H26ClNO | CN1CCC[C@@H]1CCO[C@](C)(c1ccccc1)c1ccc(Cl)cc1 | 308 | (25) |
| Ethyl N-phenylcarbamate | C9H11NO2 | CCOC(=O)Nc1ccccc1 | 213 | (17) |
| Haloperidol | C21H23ClFNO2 | O=C(CCCN1CCC(O)(c2ccc(Cl)cc2)CC1)c1ccc(F)cc1 | 306.15 | (22) |
| Ibuprofen | C13H18O2 | CC(C)Cc1ccc(C(C)C(=O)O)cc1 | 228 | (22) |
| Indomethacin | C19H16ClNO4 | COc1ccc2c(c1)c(CC(=O)O)c(C)n2C(=O)c1ccc(Cl)cc1 | 314 | (4)(SI 12) |
| Nitrendipine | C18H20N2O6 | CCOC(=O)C1=C(C)NC(C)=C(C(=O)OC)C1c1cccc([N+](=O)[O-])c1 | 303 | (28) |
| Norethynodrel | C20H26O2 | C#C[C@]1(O)CC[C@H]2[C@@H]3CCC4=C(CCC(=O)C4)[C@H]3CC[C@@]21C | 324 | (28) |
| Progesterone | C21H30O2 | CC(=O)[C@H]1CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C | 279 | (29) |
| Sulfadimethoxine | C12H14N4O4S | COc1cc(NS(=O)(=O)c2ccc(N)cc2)nc(OC)n1 | 339 | (29) |
| TDATA | C54H42N4 | c1ccc(N(c2ccccc2)c2ccc(N(c3ccc(N(c4ccccc4)c4ccccc4)cc3)c3ccc(N(c4ccccc4)c4ccccc4)cc3)cc2)cc1 | 362 | (17) |
| Tri(biphenyl-4-yl)amine | C36H27N | c1ccc(-c2ccc(N(c3ccc(-c4ccccc4)cc3)c3ccc(-c4ccccc4)cc3)cc2)cc1 | 349.15 | (56) |
| Tributyl phosphate | C12H27O4P | CCCCOP(=O)(OCCCC)OCCCC | 142.85 | (10) |
| Tripropylene glycol | C9H20O4 | CC(O)COC(C)COC(C)CO | 193 | (4)(SI 14) |
| Warfarin | C19H16O4 | CC(=O)CC(c1ccccc1)c1c(O)c2ccccc2oc1=O | 345 | (25) |
| Xylitol | C5H12O5 | OC[C@H](O)C(O)[C@H](O)CO | 250.15 | (31) |
| Test | | | | |
| 1,1,1,2,3,3,3-heptafluoropropane | C3HF7 | FC(C(F)(F)F)C(F)(F)F | 47 | (2)(SI 2) |
| 1,2-diphenylcyclohexene | C18H18 | c1ccc(C2=C(c3ccccc3)CCCC2)cc1 | 230 | (3) |
| 1,2-diphenylcyclopentene | C17H16 | c1ccc(C2=C(c3ccccc3)CCC2)cc1 | 222 | (3) |
| 2-butyl-1-octanol | C12H26O | CCCCCCC(CO)CCCC | 164.1 | (10) |
| 2d | C18H20N6 | CNc1nc(Nc2ccc(C)cc2)nc(Nc2ccc(C)cc2)n1 | 340.15 | (11) |
| 2e | C20H24N6 | CNc1nc(Nc2cccc(C)c2C)nc(Nc2cccc(C)c2C)n1 | 343.15 | (11) |
| 2-hexanol | C6H14O | CCCCC(C)O | 145.85 | (10) |
| 2j | C22H28N6 | CNc1nc(Nc2c(C)cc(C)cc2C)nc(Nc2c(C)cc(C)cc2C)n1 | 356.15 | (11) |
| 2k | C16H12N6F2 | CNc1nc(Nc2cc(F)cc(F)c2)nc(Nc2cc(F)cc(F)c2)n1 | 327.15 | (11) |
| 2-Methoxy-4-nitroaniline | C7H8N2O3 | COc1cc([N+](=O)[O-])ccc1N | 331 | (1) |
| 2p | C22H28N6O3 | CNc1nc(Nc2cc(OC)c(OC)c(OC)c2)nc(Nc2cc(OC)c(OC)c(OC)c2)n1 | 367.15 | (11) |
| 3-Bromopentane | C5H11Br | CCC(Br)CC | 108 | (4)(SI 6) |
| 3-dimethylamino-1-propanol | C5H13NO | CN(C)CCCO | 146 | (4)(SI 14) |
| 3-Methoxy-1-butanol | C5H12O2 | COC(C)CCO | 145.3 | (4)(SI 5) |
| 3-methyl-2-pentanol | C6H14O | CCC(C)C(C)O | 148.85 | (10)(24) |
| 3-methylhexane | C7H16 | CCCC(C)CC | 88 | (4)(SI 3) |
| 4c | C19H21N5 | CCc1nc(Nc2cccc(C)c2)nc(Nc2cccc(C)c2)n1 | 292.15 | (11) |
| 4d | C19H21N5 | CCc1nc(Nc2ccc(C)cc2)nc(Nc2ccc(C)cc2)n1 | 308.15 | (11) |
| 4-methyl-2-heptanol | C8H18O | CCCC(C)CC(C)O | 148 | (16) |
| 4-methyl-2-pentanol | C6H14O | CC(C)CC(C)O | 157.5 | (10) |
| 4-methyl-4-heptanol | C8H18O | CCCC(C)(O)CCC | 167 | (16) |
| 5-methyl-1-heptanol | C8H18O | CCC(C)CCCCO | 138 | (16) |
| 5-methyl-2-heptanol | C8H18O | CCC(C)CCC(C)O | 155.85 | (10)(24) |
| Lactose | C12H22O11 | OC[C@H]1O[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1O[C@@H]1O[C@H](CO)[C@H](O)[C@H](O)[C@H]1º | 374.15 | (31) |
| Mannitol | C6H14O6 | OC[C@@H](O)[C@@H](O)[C@H](O)[C@H](O)CO | 282 | (9) |
| OXD-S2 | C36H33O3N9 | CN(C)c1ccc(-c2nnc(-c3cc(-c4nnc(-c5ccc(N(C)C)cc5)o4)cc(-c4nnc(-c5ccc(N(C)C)cc5)o4)c3)o2)cc1 | 442 | (17) |
| OXD-S3 | C48H30O3N6 | c1ccc(-c2ccc(-c3nnc(-c4cc(-c5nnc(-c6ccc(-c7ccccc7)cc6)o5)cc(-c5nnc(-c6ccc(-c7ccccc7)cc6)o5)c4)o3)cc2)cc1 | 420 | (17) |
| OXD-S4 | C30H12O3N6Cl3Br3 | Clc1ccc(Br)cc1-c1nnc(-c2cc(-c3nnc(-c4cc(Br)ccc4Cl)o3)cc(-c3nnc(-c4cc(Br)ccc4Cl)o3)c2)o1 | 413 | (17) |
| OXD-S6 | C33H24O6N6 | COc1ccc(-c2nnc(-c3cc(-c4nnc(-c5ccc(OC)cc5)o4)cc(-c4nnc(-c5ccc(OC)cc5)o4)c3)o2)cc1 | 381 | (17) |
| Sucrose | C12H22O11 | OC[C@H]1O[C@H](O[C@]2(CO)O[C@H](CO)[C@@H](O)[C@@H]2O)[C@H](O)[C@@H](O)[C@@H]1O | 340.15 | (31) |

Figure SI 1 shows the Tg distribution for the molecular glass formers in the dataset.

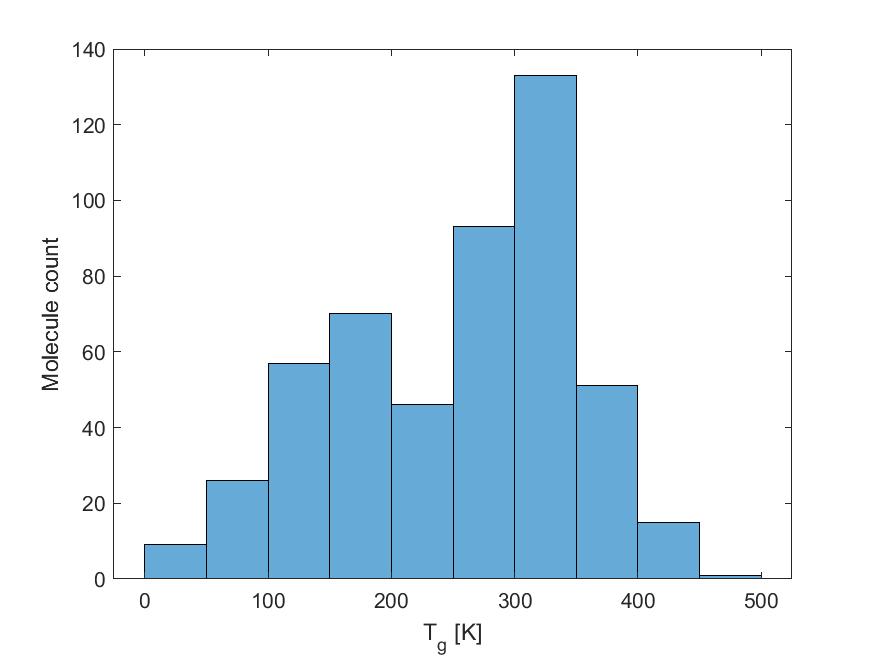
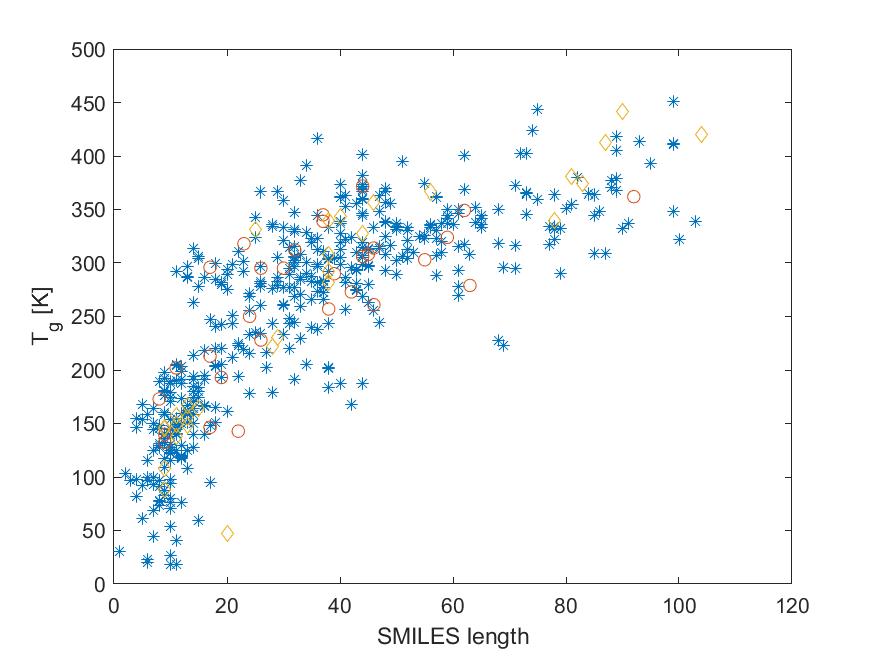


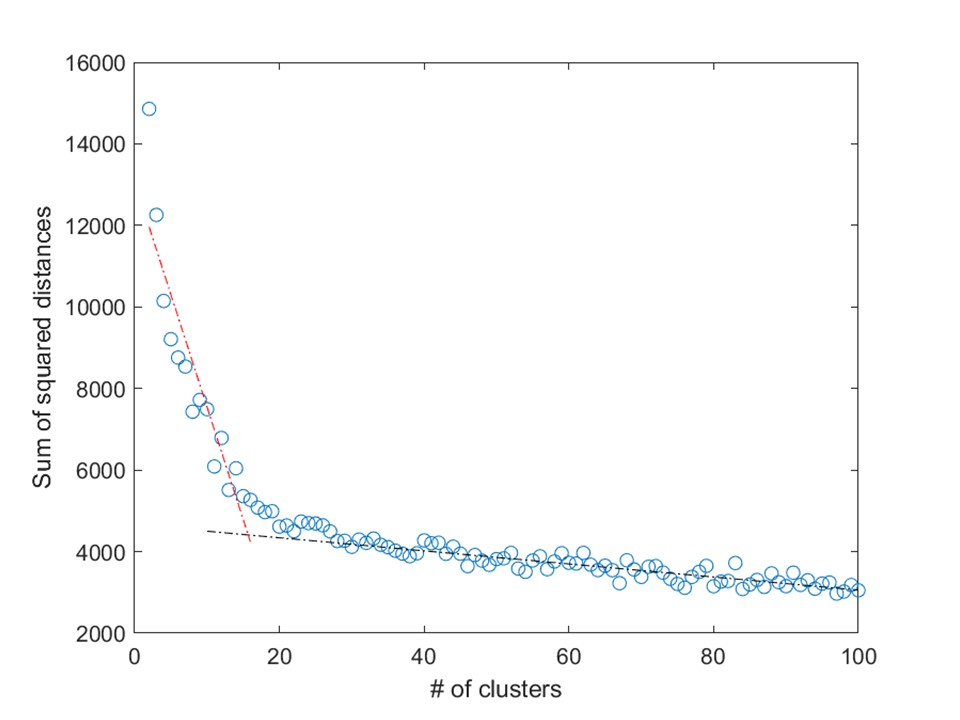
Figure SI 1

Figure SI 2 shows the SMILES length dependence of the Tg. Blue, orange and yellow symbols represent training, validation and test sets, respectively.

  
Figure SI 2

SI 2. The Elbow method

The Elbow method is a heuristic way to establish the number of clusters necessary for the clusterization to be informative without overfitting. In our case, we calculated the sum of the squared distances of each vector from the respective centroid and chose the number of clusters at which the graph changes its slope. To do so, we solved the system for 2 trend lines and took the intersection point (16 ; 4427). We show the results in Figure SI 3.

  
Figure SI 3

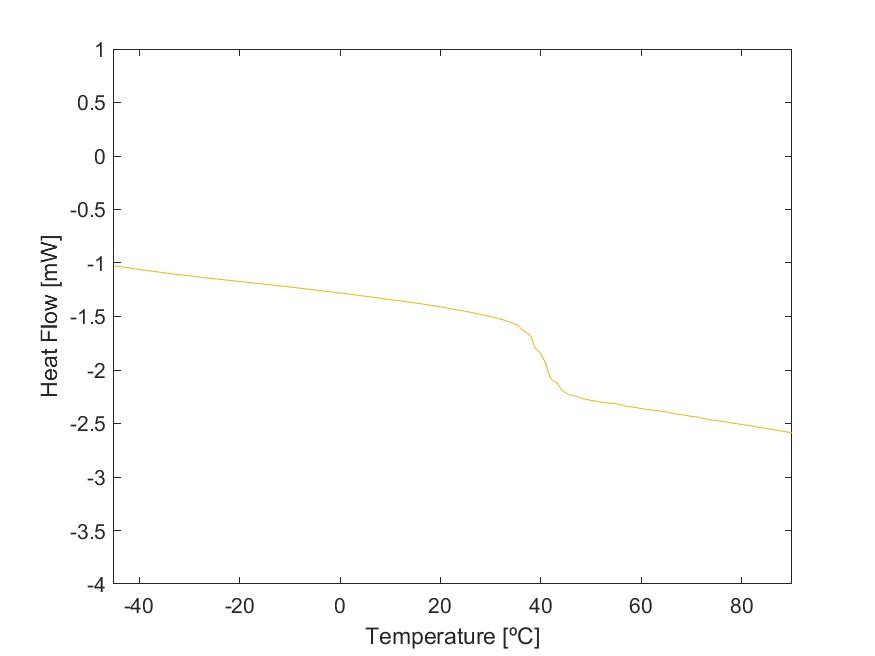
**SI3: 3-Lys glass transition**

**3-Lys sample preparation**

3-Lys is a 3 peptide of the amino acid lysine (i.e.: an oligomer with a chain length equivalent to 3 lysine monomers. For this work, 3-Lys was obtained from Merck.

**Differential scanning calorimetry (DSC)**

A Q2000 TMDSC from TA Instruments was used for measuring the of pure 3-Lys. Samples of about 6 to 10 mg were prepared in sealed pans and melted in situ by heating up to 150 ºC. The glass transition temperature of the melted samples was then determined by employing heating rates of 10 K/min. Figure SI4 shows the heat flow as a function of the temperature. The experimental glass transition (41.2ºC) was determined as the inflection point during the heating cycle.

  
Figure SI 4

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