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**Supporting Information**

# $CO_2$ Uptake Prediction in Metal–Organic Frameworks Using Quasi-SMILES Based on Monte Carlo Method

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## Supporting Information

**Table S1**. The $CO_2$ uptake capacity data in different physical conditions of temperature and pressure using MOFs with different BET and pore volume characteristics

| No. | MOF | Organic linker | Surface area, BET ($m^2/g$) | Pore volume ($cm^3/g$) | P(bar) | T(K) | $CO_2$ uptake (mol/kg) | Ref. |
|---|---|---|---|---|---|---|---|---|
| 1 | HKUST-1 (CuBTC) | BTC: Benzene-1,3,5-tricarboxylic acid, H3BTC, TMA,Trimesic acid | 1270 | 0.71 | 0.15 | 298 | 0.86 | [S1] |
| 2 | | | 1270 | 0.71 | 1 | 298 | 5.27 | [S2] |
| 3 | | | 1270 | 0.71 | 1 | 313 | 2.91 | [S3] |
| 4 | IRMOF-1 (MOF-5) | 1,4-benzendicarboxylic acid(Terephthalic acid ) | 2833 | 1.04 | 35 | 298 | 21.7 | [S4] |
| 5 | IRMOF-3 | 2-Aminoterephthalic acid | 1568 | 1.07 | 35 | 298 | 18.7 | [S4] |
| 6 | | | 1568 | 1.07 | 1 | 298 | 1.11 | [S5] |
| 7 | MIL-47 (V) (MIL= Materials of Institute Lavoisier) | 1,4-benzendicarboxylic acid(Terephthalic acid ) | 1049 | 0.36 | 20 | 304 | 11.5 | [S6] |
| 8 | MIL-53 (Cr) | TPA, H2BDC, Terephthalic acid | 1419 | 0.5 | 25 | 304 | 10 | [S6] |
| 9 | MIL-100 (Cr) | (Trimesic acid)(TMA)(1,3,5-BTC) | 1900 | 1.1 | 50 | 304 | 18 | [S7] |
| 10 | MIL-100 (Fe) | (Trimesic acid)(TMA)(1,3,5-BTC) | 1900 | 1.1 | 1 | 313 | 1.5 | [S3] |
| 11 | MIL-101 (Cr) | TPA, H2BDC, Terephthalic acid | 2988 | 1.853 | 50 | 304 | 40 | [S7] |
| 12 | | | 2988 | 1.853 | 1 | 298 | 2.16 | [S2] |
| 13 | MOF-74-Mg | H4DOBDC (2,5-dihydroxyterephthalic acid) | 1495 | 0.61 | 1 | 298 | 6.2 | [S2] |
| 14 | | | 1174 | 0.648 | 35 | 298 | 10.4 | [S4] |
| 15 | | | 1174 | 0.648 | 1 | 298 | 8.6 | |
| 16 | | | 1174 | 0.648 | 0.15 | 298 | 6.14 | |
| 17 | MOF-177 | 4-[3,5-bis(4-carboxyphenyl)phenyl]benzoic acid (BTB) | 4750 | 1.89 | 20 | 298 | 28 | [S5, S8] |
| 18 | | | 4750 | 1.89 | 20 | 273 | 33.5 | |
| 19 | MOF-200 | 4,4′,4″-[benzene-1,3,5-triyl-tris(benzene-4,1-diyl)]tribenzoate (BBC) | 4530 | 3.59 | 50 | 298 | 54.5 | [S9] |
| 20 | | | 4530 | 3.59 | 20 | 273 | 54.4 | |
| 21 | | | 4530 | 3.59 | 20 | 298 | 14.8 | |
| 22 | MOF-210 | BTE/biphenyl-4,4′-dicarboxylate (BPDC) | 6240 | 3.6 | 50 | 298 | 54.5 | [S9] |
| 23 | MOF-505 | H4BPTC(Biphenyl-3,3',5,5'-tetracarboxylic acid ) | 1547 | 0.63 | 35 | 298 | 10.2 | [S4] |
| 24 | NU-100 | large hexatopic carboxylate ligand (LH6): 5,5',5''-(((benzene-1,3,5-triyltris(ethyne-2,1-diyl))tris(benzene-4,1-diyl))tris(ethyne-2,1- | 6143 | 2.82 | 40 | 298 | 46.4 | [S10] |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | diyl))triisophthalic acid | | | | | | |
| 25 | UMCM-1 | H3BTB(1,3,5-Tris(4-carboxyphenyl)benzene ) | 4100 | 2.14 | 24 | 298 | 23.5 | [S11] |
| 26 | USO-2-Ni | 1,4-dicarboxylic-2-amino-benzene (2-aminoterephthalic acid) | 1925 | 0.74 | 25 | 298 | 13.6 | [S12] |
| 27 | Zn4O(FMA)3 | FMA: fumarate | 1120 | 0.586 | 28 | 300 | 15.7 | [S13] |
| 28 | | | 1120 | 0.586 | 1 | 298 | 0.89 | |
| 29 | Zn9O3(2,7-ndc)6(dmf)3 | 2,7-ndc: 2,7-naphthalene dicarboxylic acid ;dmf: dimethylformamide | 834 | 0.41 | 40 | 298 | 7.1 | [S14] |
| 30 | SIFSIX-2-Cu-i | Dipyridylacetylene(bis(4-pyridyl)acetylene)or(4,4'-(1,2-Ethynediyl)dipyridine) | 735 | 0.26 | 0.01 | 298 | 0.19 | [S15] |
| 31 | | | 735 | 0.26 | 1 | 298 | 5.41 | [S16] |
| 32 | PEI-MIL-101(Cr) | polyethylenimine-H2NDC (2,6-Naphthalenedicarboxylic acid) | 182.9 | 0.095 | 0.15 | 298 | 3.85 | [S17] |
| 33 | | | 182.9 | 0.095 | 1 | 298 | 4.38 | |
| 34 | UPC-12 | cyclohexane-1,2,3,4,5,6-hexacarboxylic acid and 4,4′-bipyridine | 271.8 | 0.126 | 1 | 273 | 1.5 | [S18] |
| 35 | NENU-520(NENU = Northeast Normal University) | 4'-(1H-tetrazol-5-yl)-[1,1'-biphenyl]-4-carboxylic acid | 387 | 0.27 | 1 | 298 | 2.71 | [S19] |
| 36 | SMT-1(‘single molecule trap’) | 3,3'-(naphthalene-2, 7-diyl)dibenzoic acid (H2L) | 153.7 | 0.097 | 1 | 196 | 2.32 | [S20] |
| 37 | | | 153.7 | 0.097 | 1 | 273 | 0.85 | |
| 38 | | | 153.7 | 0.097 | 1 | 296 | 0.63 | |
| 39 | MIL-120(Al4(OH)8(BTEC)) | (BTEC)=1,2,4,5-benzenetetracarboxylic acid | 308 | 0.11 | 1 | 303 | 3.152 | [S21] |
| 40 | Zn4(OH)2(1,2,4-BTC)2=MOF-1 | 1,2,4-BTC=benzene-1,2,4-tricarboxylate=Trimellitic acid | 408 | 0.205 | 1 | 295 | 1.879 | [S22] |
| 41 | Cu2(BTTCD)= PCN-80 | H8BTTCD= 9,9',9'',9'''-([1,1'-biphenyl]-3,3',5,5'-tetrayl)tetrakis(9H-carbazole-3,6-dicarboxylic acid) | 3850 | 1.47 | 1 | 296 | 3.036 | [S23] |
| 42 | MAF-X27ox | (OH)Cl2(bbta)[(OH)Cl2(benzo(1,2-d:4,5-d')bistriazole)] | 1167 | 0.56 | 1 | 298 | 6.7 | [S24] |
| 43 | MAF-X25ox | (OH)Cl2(bbta)[(OH)Cl2(benzo(1,2-d:4,5-d')bistriazole)] | 1286 | 0.46 | 1 | 298 | 7.1 | [S24] |
| 44 | MAF-66 | 3-amino-1,2,4-triazole (Hatz) | 1014 | 0.43 | 1 | 298 | 4.41 | [S25] |
| 45 | ZJNU-41 | (H4L1)= 5,5′-(Benzo[c][1,2,5]furanzan-4,7-diyl) diisophthalate (H4L1)(Oxadiazole functional group) | 2530 | 0.997 | 1 | 298 | 4.34821 | [S26] |
| 46 | | | 2530 | 0.997 | 1 | 288 | 5.54464 | |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 47 | ZJNU-40 | (H4L2)(Thiadiazole functional group)=5,5'-(benzo[c][1,2,5]thiadiazole-4,7-diyl)diisophthalic acid | 2072 | 0.837 | 1 | 298 | 3.82589 | [S26] |
| 48 | | | 2072 | 0.837 | 1 | 288 | 4.87054 | [S26] |
| 49 | | | 2072 | 0.837 | 1 | 296 | 3.92857 | [S27] |
| 50 | ZJNU-42 | 5,5′-(Benzo[c][1,2,5]selenadiazole-4,7-diyl) diisophthalate(H4L3)(Selenadiazole functional group) | 572 | 0.229 | 1 | 298 | 1.67857 | [S26] |
| 51 | | | 572 | 0.229 | 1 | 288 | 2.00446 | |
| 52 | QI-Cu | 2,5-Bis(hydroxymethyl)-3,6-dimethyl-1,4-diisophthalic acid (H4L2) | 1631 | 0.662 | 1 | 293 | 4.56 | [S28] |
| 53 | NOTT-101 | 1,1':4',1"-Terphenyl-3,3",5,5"-tetracarboxylic acid | 2522 | 1.014 | 1 | 293 | 3.93 | [S28] |
| 54 | NJU-Bai14(Cu2NTPTB) | H4NTPTB = 2′-nitro-1,1':4',1"-Terphenyl-3,3",5,5"-tetracarboxylic acid | 2384 | 0.924 | 1 | 298 | 4.46429 | [S29] |
| 55 | | | 2384 | 0.924 | 1 | 273 | 8.34821 | |
| 56 | MOF-505 | H4BPTC (Biphenyl-3,3',5,5'-tetracarboxylic acid) | 967 | 0.63 | 1 | 298 | 3.25893 | [S4] |
| 57 | HNUST-1(HNUST = Hunan University of Science and Technology) | H4BDPT(bis(3,5-dicarboxyphenyl) terephthalamide = H4BDPT) | 1400 | 0.571 | 1 | 298 | 4.15179 | [S30] |
| 58 | HNUST-3(=HNUST = Hunan University of Science and Technology) | N,N′-bis(3,5-dicarboxyphenyl)-oxalamide = H4BDPO | 2412 | 0.99 | 1 | 298 | 3.79464 | [S31] |
| 59 | NOTT-125 | H4L=oxalylbis(azanediyl)diisophthalic acid | 2471 | 1.1 | 1 | 298 | 4.13348 | [S32] |
| 60 | | | 2471 | 1.1 | 1 | 273 | 9.091 | |
| 61 | NOTT-122 | 5,5′,5″-(4,4′,4″-(benzene-1,3,5-triyl)tris(1H-1,2,3-triazole-4,1-diyl))triisophthalic acid (H6BTTI) | 3286 | 1.41 | 1 | 273 | 9.02273 | [S33] |
| 62 | | | 3286 | 1.41 | 1 | 298 | 4.63636 | |
| 63 | PCN-61 | BTEI=5,5',5"-(benzene-1,3,5-triyltris(ethyne-2,1-diyl))triisophthalic acid | 3350 | 1.37 | 1 | 273 | 4.86364 | [S34] |
| 64 | | | 3350 | 1.37 | 20 | 298 | 21.4 | [S35] |
| 65 | PCN-66 | NTEI=5,5',5"-((nitrilotris(benzene-4,1-diyl))tris(ethyne-2,1-diyl))triisophthalic acid | 4000 | 1.63 | 1 | 273 | 5.02273 | [S34] |
| 66 | | | 4000 | 1.63 | 20 | 298 | 22.1 | [S35] |
| 67 | PCN-68 | PTEI=5,5'-((5'-(4-((3,5-dicarboxyphenyl)ethynyl)phenyl)-[1,1':3',1"-terphenyl]-4,4"-diyl)bis(ethyne-2,1-diyl))diisophthalic acid | 5109 | 2.13 | 1 | 273 | 5.02273 | [S34] |
| 68 | | | 5109 | 2.13 | 20 | 298 | 22.1 | [S35] |
| 69 | Cu-TPBTM | TPBTM(N,N',N"-tris(isophthalyl)-1,3,5-benzenetricarboxamide)or(5,5',5"-[Benzene-1,3,5-triyltris(carbonylimino)]triisophthalic acid) | 3160 | 1.27 | 20 | 298 | 23.5 | [S35] |
| 70 | Cu-BTB(Cu3($BTB^{6-}$)) | H6BTB | 3288 | 1.77 | 20 | 273 | 35.6818 | [S36] |
| 71 | | | 3288 | 1.77 | 20 | 298 | 25.2 | |

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|---|---|---|---|---|---|---|---|---|
| 72 | Cu-TBT($Cu_3(TATB^{6-})$) | H6TBTB(5,5',5"-((4,4',4"-(1,3,5-triazine-2,4,6-triyl)tris(benzoyl))tris(azanediyl))triisophthalic acid) | 3360 | 1.91 | 20 | 273 | 35.6 | [S36] |
| 73 | | | 3360 | 1.91 | 20 | 298 | 25.2 | |
| 74 | MOF-205 | 4,4′,4″-benzene-1,3,5-triyl-tribenzoic acid (H3BTB)/2,6-naphthalenedicarboxylic acid (NDC) | 4460 | 2.16 | 50 | 298 | 38.1 | [S9] |
| 75 | | | 4460 | 2.16 | 20 | 273 | 33.9 | |
| 76 | | | 4460 | 2.16 | 20 | 298 | 26 | |
| 77 | MOF -210 | BTE/biphenyl-4,4′-dicarboxylate (BPDC) | 6240 | 3.6 | 20 | 273 | 54.5 | [S9] |
| 78 | | | 6240 | 3.6 | 20 | 298 | 16 | |
| 79 | NJU-Bai3(NJU-Bai3= Nanjing University Bai group) | 5-(4-carboxybenzoylamino)-isophthalic acid (H3L) | 2690 | 1.08 | 1 | 273 | 6.21 | [S37] |
| 80 | | | 2690 | 1.08 | 20 | 273 | 22.12 | |
| 81 | | | 2690 | 1.08 | 20 | 298 | 18.1 | |
| 82 | PCN-124 | 5,5'-((pyridine-3,5-dicarbonyl)bis(azanediyl))diisophthalic acid (H4PDAI) | 1372 | 0.579 | 1 | 273 | 6.5 | [S38] |
| 83 | | | 1372 | 0.579 | 1 | 283 | 5.40909 | |
| 84 | | | 1372 | 0.579 | 1 | 295 | 4.15909 | |
| 85 | Cu-TCMBT | N,N′,N″-tris(carboxymethyl)-1,3,5-benzenetricarboxamide (TCMBT)&bpp = 1,3-bis(4-pyridyl)propane | 808.5 | 0.32 | 1 | 298 | 2 | [S39] |
| 86 | | | 808.5 | 0.32 | 20 | 298 | 5.5 | |
| 87 | TMU-6 (TMU = Tarbiat Modares University) | 4,4"-oxybisbenzoic acid (H2oba)&N,N′-bis-(4-pyridylmethylene)-1,4-benzenediamine (bpmb) | 150 | 0.32 | 1 | 203 | 9 | [S40] |
| 88 | TMU-21 | 4,4"-oxybisbenzoic acid (H2oba)&N,N'-bis-(4-pyridylmethylene)-1,5-naphthalenediamine (bpm) | 0 | 0.16 | 1 | 203 | 4.5 | [S40] |
| 89 | TMU-22 | 4,4"-oxybisbenzoic acid (H2oba)&N,N'-bis(4-pyridinyl)-terephthalamide (bpta) | 680 | 0.25 | 1 | 203 | 7.2 | [S40] |
| 90 | TMU-23 | 4,4"-oxybisbenzoic acid (H2oba)& N,N'-(1,4-phenylene)diisonicotinamide (bpf) | 0 | 0.27 | 1 | 203 | 7.2 | [S40] |
| 91 | TMU-24 | 4,4"-oxybisbenzoic acid (H2oba)& N,N'-bis-(4-pyridylformamide)-1,5-naphthalenediamine (bpfn) | 0 | 0.22 | 1 | 203 | 6.3 | [S40] |
| 92 | WUF-1 | 2-((dimethylcarbamothioyl)oxy)-[1,1'-biphenyl]-4,4'-dicarboxylic acid, H2L1 | 1724 | 7.3 | 1 | 273 | 2.18182 | [S41] |
| 93 | WUF-2 | 2-((dimethylcarbamoyl)thio)-[1,1'-biphenyl]-4,4'-dicarboxylic acid | 1760 | 7.5 | 1 | 273 | 2.5 | [S41] |
| 94 | Ni(BPB) | H2BPB=1,4-Bis(4-pyrazolyl)benzene | 1600 | 0.38 | 30 | 273 | 10 | [S42] |
| 95 | Zn(BPB) | H2BPB=1,4-Bis(4-pyrazolyl)benzene | 2200 | 0.71 | 30 | 273 | 9.1 | [S42] |
| 96 | [Fe2(BPEB)3] | 1,4-bis(1H-pyrazol-4-ylethynyl)benzene (H2BPEB) | 1273 | 0.79 | 10 | 298 | 9.2 | [S42] |
| 97 | | | 1273 | 0.79 | 10 | 273 | 12 | |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 98 | | | 1273 | 0.79 | 1 | 195 | 13.6 | |
| 99 | [Ni(BPEB)] | 1,4-bis(1H-pyrazol-4-ylethynyl)benzene (H2BPEB) | 1900 | 1.05 | 10 | 298 | 5.9 | [S42] |
| 100 | | | 1900 | 1.05 | 10 | 273 | 8.5 | |
| 101 | | | 1900 | 1.05 | 1 | 195 | 11.6 | |
| 102 | α-[Zn(BPEB)] | 1,4-bis(1H-pyrazol-4-ylethynyl)benzene (H2BPEB) | 985 | 0.6 | 10 | 298 | 5.2 | [S42] |
| 103 | | | 985 | 0.6 | 10 | 273 | 8.2 | |
| 104 | | | 985 | 0.6 | 1 | 195 | 11.3 | |
| 105 | DMOF(Zn2(BDC)2 (DABCO)) | BDC = 1,4-benzenedicarboxylate, DABCO = diazabicyclo-octane | 1980 | 0.76 | 20 | 298 | 8.65909 | [S43] |
| 106 | DMOF-Br | (BDC-Br)(DABCO) | 1320 | 0.53 | 20 | 298 | 5.52273 | [S43] |
| 107 | DMOF-NO2 | (BDC-NO2)(DABCO) | 1310 | 0.53 | 20 | 298 | 7.27273 | [S43] |
| 108 | DMOF-TF | (BDC-TF)( DABCO) | 1210 | 0.49 | 20 | 298 | 3.68182 | [S43] |
| 109 | DMOF-Cl2 | (BDC-Cl2)DABCO) | 1180 | 0.45 | 20 | 298 | 6 | [S43] |
| 110 | DMOF-OH | (BDC-OH)(DABCO) | 1130 | 0.54 | 20 | 298 | 5.63636 | [S43] |
| 111 | DMOF-DM | (BDC-DM)(DABCO) | 1120 | 0.48 | 20 | 298 | 5.77273 | [S43] |
| 112 | DMOF-TM | (BDC-TM)(DABCO). | 1050 | 0.57 | 20 | 298 | 5.36364 | [S43] |
| 113 | DMOF-A | (BDC-A)(DABCO) | 760 | 0.33 | 20 | 298 | 3.88636 | [S43] |
| 114 | UiO-66(Zr100) | TPA= BDC= Terephthalic acid | 1390 | 0.7 | 1 | 298 | 1.40909 | [S44] |
| 115 | UiO-66(Ti56) | TPA= BDC= Terephthalic acid | 1844 | 1.18 | 1 | 298 | 2 | [S44] |
| 116 | (MgMOF-74) | dobdc4− = 2,5-dioxido-1,4-benzenedicarboxylate=2,5-Dioxidoterephthalate | 1495 | 0.572 | 0.1 | 296 | 5.36364 | [S3] |
| 117 | | | 1495 | 0.572 | 1 | 296 | 8 | |
| 118 | Ni-MOF-74 | dobdc4− = 2,5-dioxido-1,4-benzenedicarboxylate=2,5-Dioxidoterephthalate | 1070 | 0.54 | 0.1 | 296 | 2.63636 | [S3] |
| 119 | | | 1070 | 0.54 | 1 | 296 | 5.81818 | |
| 120 | Co-MOF-74 | dobdc4− = 2,5-dioxido-1,4-benzenedicarboxylate=2,5-Dioxidoterephthalate | 1080 | 0.5 | 0.1 | 296 | 2.63636 | [S3] |
| 121 | | | 1080 | 0.5 | 1 | 296 | 6.95455 | |
| 122 | Zn-MOF-74 | dobdc4− = 2,5-dioxido-1,4-benzenedicarboxylate=2,5-Dioxidoterephthalate | 816 | 0.58 | 0.1 | 296 | 1.31818 | [S3] |
| 123 | | | 816 | 0.58 | 1 | 296 | 5.54545 | |
| 124 | CPM-33a [Ni3OH(bdc)3tpt] | (bdc=Terephthalic acid )&(tpt=2,4,6-tri(4-pyridinyl)-1,3,5-triazine) | 966 | 0.463 | 0.1 | 273 | 0.73 | [S45] |
| 125 | | | 966 | 0.463 | 0.1 | 298 | 0.35 | |
| 126 | | | 966 | 0.463 | 1 | 273 | 6.09 | |
| 127 | | | 966 | 0.463 | 1 | 298 | 3.29 | |
| 128 | CPM-33b[Ni3OH(dhbdc)3tpt] | (dhbdc=2,5-dihydroxybenzene-1,4-dicarboxylate)&(tpt=2,4,6-tri(4-pyridinyl)-1,3,5-triazine) | 808 | 0.399 | 0.1 | 273 | 2.42 | [S45] |
| 129 | | | 808 | 0.399 | 0.1 | 298 | 1.03 | |
| 130 | | | 808 | 0.399 | 1 | 273 | 7.76 | |
| 131 | | | 808 | 0.399 | 1 | 298 | 5.63 | |
| 132 | CPM-33c[Ni3OH(NH2bdc)3tpt] | (NH2bdc=2-aminobenzene-1,4-dicarboxylate)&(tpt=2,4,6-tri(4-pyridinyl)-1,3,5-triazine) | 805 | 0.409 | 0.1 | 273 | 1.15 | [S45] |
| 133 | | | 805 | 0.409 | 0.1 | 298 | 0.59 | |
| 134 | | | 805 | 0.409 | 1 | 273 | 5.99 | |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 135 | | | 805 | 0.409 | 1 | 298 | 3.95 | |
| 136 | CPM-33d[Ni3OH(1,4-ndc)3tpt] | (1,4-ndc=naphthalene-1,4-dicarboxylate)&(tpt=2,4,6-tri(4-pyridinyl)-1,3,5-triazine) | 222 | 0.106 | 0.1 | 273 | 0.45 | [S45] |
| 137 | | | 222 | 0.106 | 0.1 | 298 | 0.22 | |
| 138 | | | 222 | 0.106 | 1 | 273 | 1.62 | |
| 139 | | | 222 | 0.106 | 1 | 298 | 1.1 | |
| 140 | CPM-34[Ni3OH(2,6-ndc)3tpt] | (2,6-ndc=naphthalene-2,6-dicarboxylate)&(tpt=2,4,6-tri(4-pyridinyl)-1,3,5-triazine) | 1002 | 0.487 | 0.1 | 273 | 0.45 | [S45] |
| 141 | | | 1002 | 0.487 | 0.1 | 298 | 0.23 | |
| 142 | | | 1002 | 0.487 | 1 | 273 | 3.13 | |
| 143 | | | 1002 | 0.487 | 1 | 298 | 1.96 | |
| 144 | CPM-35[Ni3OH(bpdc)3tpt] | (bpdc=biphenyl-4,4′-dicarboxylate)&(tpt=2,4,6-tri(4-pyridinyl)-1,3,5-triazine) | 724 | 0.311 | 0.1 | 273 | 0.35 | [S45] |
| 145 | | | 724 | 0.311 | 0.1 | 298 | 0.21 | |
| 146 | | | 724 | 0.311 | 1 | 273 | 1.93 | |
| 147 | | | 724 | 0.311 | 1 | 298 | 1.32 | |
| 148 | Fe2Ni-MIL-88B•Bp | BDC(1,4-benzenedicarboxylate)&4,4′-bipyridine (Bp) | 1120 | 0.448 | 1 | 273 | 4.50893 | [S46] |
| 149 | Fe2Ni-MIL-88B•Pz | BDC(1,4-benzenedicarboxylate)&pyrazine (Pz) | 465 | 0.186 | 1 | 273 | 2.41071 | [S46] |
| 150 | mmen-CuBTTri | (H3BTTri =1,3,5-tri(1H-1,2,3-triazol-4-yl)-benzene)&(mmen = N,N′-dimethylethylenediamine) | 870 | 0.363 | 1 | 298 | 4.13636 | [S47] |
| 151 | | | 870 | 0.363 | 0.15 | 298 | 2.39 | |
| 152 | CuBTTri | H3BTTri =1,3,5-tri(1H-1,2,3-triazol-4-yl)-benzene) | 1770 | 0.712 | 1 | 298 | 3.79545 | [S48] |
| 153 | | | 1770 | 0.712 | 0.15 | 298 | 0.68 | |
| 154 | UTSA-16 (K(H2O)2Co3(cit)(Hcit)) (UTSA=University of Texas at San Antonio) | H4cit=citric acid | 628 | 0.31 | 1 | 298 | 4.29545 | [S2] |
| 155 | UTSA-20[Cu3(BHB)] | H6BHB=3,3’,3’’,5,5’,5’’-benzene-1,3,5-triylhexabenzoic acid | 1156 | 0.635 | 1 | 298 | 3.33 | [S49] |
| 156 | | | 1156 | 0.635 | 0.15 | 300 | 0.575 | |
| 157 | UTSA-25a [Zn(BDC-OH)(DABCO)0.5·(DMF)2(H2O)] | [H2BDC-OH = 2-hydroxybenzenedicarboxylic acid]&[DABCO = 1,4-diazabicyclo[2.2.2]octane] | 994 | 0.607 | 1 | 298 | 3.11 | [S50] |
| 158 | UTSA-34b | H8L=1,2,4,5-tetra(5-isophthalate)benzene | 991 | 0.542 | 1 | 298 | 2.88 | [S51] |
| 159 | UTSA-33a | H8L=1,2,4,5-tetra(5-isophthalate)benzene | 660 | 0.367 | 1 | 298 | 2.37 | [S51] |
| 160 | UTSA-15a [Cu(BDC−OH)(4,4′-bipy) ] | ( H2BDC−OH = 2-hydroxy-benzenedicarboxylic acid)&(4,4′-bipy =4,4′-bipyridine) | 553 | 0.282 | 1 | 298 | 1.36 | [S52] |
| 161 | Zn4(OH)2(1,2,4- | 1,2,4-BTC = Benzene-1,2,4-tricarboxylate = | 408 | 0.216 | 1 | 298 | 1.75 | [S22] |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 162 | BTC)2 | Trimellitic acid | 408 | 0.216 | 0.15 | 295 | 0.31 | [S22] |
| 163 | Zn5(BTA)6(TDA)2 | HBTA = 1,2,3-benzenetriazole&H2TDA = thiophene-2,5-dicarboxylic acid | 414 | 0.225 | 1 | 298 | 1.55 | [S53] |
| 164 | Cu(BDC-OH) | H2BDC−OH = 2-hydroxy-benzenedicarboxylic acid | 397 | 0.214 | 1 | 298 | 2.21 | [S54] |
| 165 | Yb(BPT)=MOF 1 | BPT = biphenyl-3,4',5-tricarboxylate | 516 | 0.291 | 1 | 298 | 0.7 | [S55] |
| 166 | Bio-MOF-11 [Co2(ad)2(CO2CH3)2·2DMF·0.5H2O] | adenine&CH3CO2H | 1040 | 0.45 | 1 | 298 | 1.28 | [S56] |
| 167 | Zn(bdc)(dabco)0.5 | BDC = 1,4-benzyl dicarboxylate&DABCO = diazabicyclo-octane | 2022 | 0.8 | 1 | 298 | 2.04 | [S2] |
| 168 | Cu-TDPAT | 2,4,6-tris(3,5-dicarboxyphenylamino)-1,3,5-triazine=H6TDPAT | 1038 | 0.93 | 1 | 298 | 5.09 | [S2] |
| 169 | CPM-5(CPM =crystalline porous materials)([(CH3)2NH2][In3O(BTC)2(H2O)3]2) | BTC = 1,3,5-benzenetricarboxylate | 580 | 0.258 | 1 | 273 | 3.62946 | [S35] |
| 170 | | | 580 | 0.258 | 1 | 298 | 2.43304 | |
| 171 | PCN-6 | H3TATB=4,4',4"-s-triazine-2,4,6-triyl-tribenzoic acid | 3811 | 1.55 | 1 | 298 | 4.29545 | [S57] |
| 172 | IRMOF-9 | BPDC= 4,4'-biphenyldicarboxylic acid | 1918 | 1.18 | 1 | 298 | 1.79 | [S58] |
| 173 | Zn-DABCO | terephthalic acid=BDC=1,4-benzene dicarboxylate & DABCO = 1,4-diazabicyclo[2.2.2] | 1870 | 1.67 | 1 | 298 | 1.87 | [S59] |
| 174 | Ni-DABCO | terephthalic acid=BDC=1,4-benzene dicarboxylate & DABCO = 1,4-diazabicyclo[2.2.2] | 2120 | 1.78 | 1 | 298 | 2.17 | [S59] |
| 175 | Cu-DABCO | terephthalic acid=BDC=1,4-benzene dicarboxylate & DABCO = 1,4-diazabicyclo[2.2.2] | 1616 | 1.67 | 1 | 298 | 1.45 | [S59] |
| 176 | Co-DABCO | terephthalic acid=BDC=1,4-benzene dicarboxylate & DABCO = 1,4-diazabicyclo[2.2.2] | 2022 | 1.64 | 1 | 298 | 1.02 | [S59] |
| 177 | UTSA-62a [Yb3O(H2O)3(L)(NO3)] | H6L | 2190 | 0.9077 | 1 | 298 | 1.84091 | [S60] |
| 178 | UTSA-40a | H4L=5,5'-(6,6'-dichloro-2,2'-diethoxy-[1,1'- | 1630 | 0.65 | 30 | 300 | 12.7 | [S61] |

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|---|---|---|---|---|---|---|---|---|
| | | binaphthalene]-4,4'-diyl)diisophthalic acid | | | | | | |
| 179 | PCN-46 | H4L=5,5'-(buta-1,3-diyne-1,4-diyl)diisophthalic acid | 2500 | 1.02 | 30 | 298 | 22.5 | [S62] |
| 180 | SNU-50 | H4L=5,5'-(1,3,5,7-tetraoxopyrrolo[3,4-f]isoindole-2,6(1H,3H,5H,7H)-diyl)diisophthalic acid | 2300 | 1.08 | 55 | 298 | 17.5 | [S63] |
| 181 | | | 2300 | 1.08 | 1 | 298 | 3.6 | |
| 182 | | | 2300 | 1.08 | 0.15 | 298 | 0.65 | |
| 183 | NU-111 | H6L=5,5',5"-(benzene-1,3,5-triyltris(buta-1,3-diyne-4,1-diyl))triisophthalic acid | 4932 | 2.09 | 1 | 298 | 1.09091 | [S64] |
| 184 | UTSA-49=[Zn(mtz)2] | Hmtz = 5-methyl-1H-tetrazole | 710.5 | 0.407 | 1 | 298 | 3.09091 | [S65] |
| 185 | IRMOF-8 | 2,6-napthalenedicarboxylic acid = 2,6-H2NDC | 1599 | 0.66 | 1 | 298 | 1.77273 | [S66] |
| 186 | | | 1599 | 0.66 | 30 | 273 | 14.4 | |
| 187 | | | 1599 | 0.66 | 30 | 298 | 11.7 | |
| 188 | IRMOF-8-NO2 | 4,8-dinitro-2,6-napthalenedicarboxylic acid | 832 | 0.341 | 1 | 298 | 0.86364 | [S66] |
| 189 | | | 832 | 0.341 | 1 | 273 | 11 | |
| 190 | | | 832 | 0.341 | 1 | 298 | 7.2 | |
| 191 | ZJU-32 | H4L = 5′-((3,5-dicarboxyphenyl)ethynyl)-[1,1′:3′,1″-terphenyl]-4,4″-dicarboxylic acid | 3831 | 1.482 | 1 | 300 | 1.91 | [S67] |
| 192 | | | 3831 | 1.482 | 40 | 300 | 11.1364 | |
| 193 | rht-MOF-1 | 5-(2H-tetrazol-5-yl)isophthalic acid | 2847 | 1.01 | 1 | 298 | 2.5 | [S68] |
| 194 | Cu2dbip | 5-(3,5-dicarboxybenzyloxy)isophthalic acid (H4DBIP) | 1773 | 0.81 | 1 | 298 | 5.44643 | [S69] |
| 195 | ZJU-25[Cu2(FDDI)] ZJU = Zhejiang University) | H4FDDI = tetramethyl 5,5′-(9H-fluorene-2,7-diyl)diisophthalate acid | 2124 | 1.183 | 1 | 298 | 3.70536 | [S70] |
| 196 | ZJU-5 | H4PDDI = 5,5′-(pyridine-2,5-diyl)diisophthalic acid) | 2823 | 1.074 | 1 | 298 | 3.79464 | [S71] |
| 197 | CPM(200)-In | Trimesic acid(TMA, H3BTC, BTC) | 888 | 0.44 | 1 | 298 | 2.75446 | [S72] |
| 198 | | | 888 | 0.44 | 1 | 273 | 4.89286 | |
| 199 | CPM(200)-In/Ni | Trimesic acid(TMA, H3BTC, BTC) | 877 | 0.43 | 1 | 298 | 2.74554 | [S72] |
| 200 | | | 877 | 0.43 | 1 | 273 | 4.48214 | |
| 201 | CPM(200)-In/Co | Trimesic acid(TMA, H3BTC, BTC) | 1040 | 0.51 | 1 | 298 | 3.46429 | [S72] |
| 202 | | | 1040 | 0.51 | 1 | 273 | 6.11161 | |
| 203 | CPM(200)-In/Mn | Trimesic acid(TMA, H3BTC, BTC) | 941 | 0.45 | 1 | 298 | 3.24554 | [S72] |
| 204 | | | 941 | 0.45 | 1 | 273 | 5.64732 | |
| 205 | CPM(200)-In/Mg | Trimesic acid(TMA, H3BTC, BTC) | 1347 | 0.65 | 1 | 298 | 5.07589 | [S72] |
| 206 | | | 1347 | 0.65 | 1 | 273 | 8.51786 | |
| 207 | CPM(200)-Ga/Mg | Trimesic acid(TMA, H3BTC, BTC) | 1056 | 0.54 | 1 | 298 | 3.53571 | [S72] |
| 208 | | | 1056 | 0.54 | 1 | 273 | 6.08036 | |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 209 | CPM(200)-Fe/Mg | Trimesic acid(TMA, H3BTC, BTC) | 1459 | 0.72 | 1 | 273 | 9.26786 | [S72] |
| 210 | | | 1459 | 0.72 | 1 | 298 | 5.68304 | |
| 211 | CPM(200)-V/Mg | Trimesic acid(TMA, H3BTC, BTC) | 1011 | 0.5 | 1 | 273 | 6.9375 | [S72] |
| 212 | | | 1011 | 0.5 | 1 | 298 | 3.58929 | |
| 213 | CPM(200)-Sc/Mg | Trimesic acid(TMA, H3BTC, BTC) | 1041 | 0.51 | 1 | 298 | 2.74107 | [S72] |
| 214 | | | 1041 | 0.51 | 1 | 273 | 5.46429 | |
| 215 | CPM-20 | Trimesic acid(TMA, H3BTC, BTC)&1,4-Benzenedicarboxylic acid | 1009 | 0.404 | 1 | 298 | 2.13 | [S73] |
| 216 | | | 1009 | 0.404 | 1 | 273 | 4.07 | |
| 217 | CPM-21 | BTB=1,3,5-tri(4-carboxyphenyl)benzene | 272 | 0.133 | 1 | 273 | 1.71 | [S73] |
| 218 | CPM-13 | 4,4'-biphenyl-dicarboxylic acid | 904 | 0.487 | 1 | 273 | 2.03 | [S74] |
| 219 | IRMOF-74-III-CH3 | H4DH3PhDC-CH3 H4DH3PhDC = 2′,5′-dimethyl-3,3″-dihydroxy-[1,1′:4′,1″-terphenyl]-4,4″-dicarboxylic acid | 2640 | 1.37 | 1 | 298 | 2.95089 | [S75] |
| 220 | IRMOF-74-III-NH2 | H4DH3PhDC-NH2 H4DH3PhDC = 2′,5′-dimethyl-3,3″-dihydroxy-[1,1′:4′,1″-terphenyl]-4,4″-dicarboxylic acid | 2720 | 1.44 | 1 | 298 | 3.16964 | [S75] |
| 221 | IRMOF-74-III-CH2NHBoc | H4DH3PhDC-CH2NHBoc H4DH3PhDC = 2′,5′-dimethyl-3,3″-dihydroxy-[1,1′:4′,1″-terphenyl]-4,4″-dicarboxylic acid | 2170 | 0.95 | 1 | 298 | 2.08482 | [S75] |
| 222 | IRMOF-74-III-CH2NH2 | H4DH3PhDC-CH2NH2 H4DH3PhDC = 2′,5′-dimethyl-3,3″-dihydroxy-[1,1′:4′,1″-terphenyl]-4,4″-dicarboxylic acid | 2310 | 1.14 | 1 | 298 | 3.26786 | [S75] |
| 223 | IRMOF-74-III-CH2NMeBoc | H4DH3PhDC-CH2NMeBoc H4DH3PhDC = 2′,5′-dimethyl-3,3″-dihydroxy-[1,1′:4′,1″-terphenyl]-4,4″-dicarboxylic acid | 2220 | 0.89 | 1 | 298 | 1.90625 | [S75] |
| 224 | IRMOF-74-III-CH2NHMe | H4DH3PhDC-CH2NHMe H4DH3PhDC = 2′,5′-dimethyl-3,3″-dihydroxy-[1,1′:4′,1″-terphenyl]-4,4″-dicarboxylic acid | 2250 | 1.13 | 1 | 298 | 2.85268 | [S75] |
| 225 | MIL-53 (Al)(Basolite A100) | TPA, H2BDC, Terephthalic acid | 1500 | 0.581 | 25 | 298 | 6.8 | [S12] |
| 226 | | | 1500 | 0.581 | 30 | 304 | 10.4 | [S6] |
| 227 | | | 1500 | 0.581 | 1 | 318 | 1 | [S76] |
| 228 | UPG-1 | H6ttbmp=2,4,6-tris(4-phosphonomethyl)phenyl)-1,3,5-triazine | 410 | 0.2 | 10 | 273 | 3.39286 | [S77] |
| 229 | | | 410 | 0.2 | 10 | 298 | 3.08036 | |
| 230 | Bio-MOF-11 | adenine&CH3CO2H | 1040 | 0.45 | 1 | 273 | 6.56 | [S78] |
| 231 | | | 1040 | 0.45 | 1 | 298 | 4.06 | [S56] |
| 232 | Bio-MOF-12 | adenine&C2H5CO2H | 1008 | 0.42 | 1 | 273 | 4.46 | [S78] |
| 233 | | | 1008 | 0.42 | 1 | 298 | 3.17 | |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 234 | Bio-MOF-13 | adenine&C3H7CO2H | 412 | 0.2 | 1 | 273 | 2.68 | [S78] |
| 235 | | | 412 | 0.2 | 1 | 298 | 2.01 | |
| 236 | Bio-MOF-14 | adenine&C4H9CO2H | 17 | 0.035 | 1 | 273 | 2.01 | [S78] |
| 237 | | | 17 | 0.035 | 1 | 298 | 1.38 | |
| 238 | ZnAcBPDC | 2,2'-diacetamido-[1,1'-biphenyl]-4,4'-dicarboxylic acid | 920 | 0.5 | 0.9 | 273 | 4.65 | [S79] |
| 239 | | | 920 | 0.5 | 0.9 | 293 | 2.91 | |
| 240 | | | 920 | 0.5 | 0.9 | 313 | 2.06 | |
| 241 | ZnBuBPDC | 2,2'-dibutyramido-[1,1'-biphenyl]-4,4'-dicarboxylic acid | 850 | 0.43 | 0.9 | 293 | 1.73 | |
| 242 | PCN-26 | tetrakis[(3,5-dicarboxyphenyl)oxamethyl]methane=H8TDM | 1854 | 0.84 | 1 | 298 | 4.6875 | [S80] |
| 243 | MSO2Me-100 | H2L2 = 2-((methylsulfonyl)methyl)-[1,1'-biphenyl]-4,4'-dicarboxylic acid | 1776 | 0.78 | 1 | 196 | 18.5 | [S81] |
| 244 | | | 1776 | 0.78 | 1 | 298 | 1.4 | |
| 245 | | | 1776 | 0.78 | 10 | 298 | 6.5 | |
| 246 | MSO2Pr-100(WUF-10) WUF= Wollongong University Framework | H2L4=2-((propylsulfonyl)methyl)-[1,1'-biphenyl]-4,4'-dicarboxylic acid | 1514 | 0.65 | 1 | 196 | 15.5 | [S81] |
| 247 | | | 1514 | 0.65 | 1 | 298 | 0.98 | |
| 248 | | | 1514 | 0.65 | 10 | 298 | 6 | |
| 249 | MIL-140A | H2bdc= terephthalic acid=benzene-1,4-dicarboxylicacid | 396.4 | 0.16 | 0.15 | 293 | 0.16 | [S82] |
| 250 | MIL-140A-NH2 | H2bdc-NH2= 2-aminobenzene-1,4-dicarboxylicacid | 269.3 | 0.14 | 0.15 | 293 | 0.28 | [S82] |
| 251 | MIL-140A-F | H2bdc-F= 2-fluoroterephthalic acid | 350.3 | 0.16 | 0.15 | 293 | 0.1 | [S82] |
| 252 | MIL-140B | H2ndc= 2,6- Naphthalenedicarboxylic acid | 429.1 | 0.19 | 0.15 | 293 | 0.17 | [S82] |
| 253 | MIL-140C | H2bpdc=biphenyl-4,4'-dicarboxylic acid | 660.8 | 0.27 | 0.15 | 293 | 0.18 | [S82] |
| 254 | MIL-140C-Me | 2,2'-dimethyl-[1,1'-biphenyl]-4,4'-dicarboxylic acid | 574.4 | 0.26 | 0.15 | 293 | 0.21 | [S82] |
| 255 | MIL-140D | H2azobdc-Cl =4,4'-(diazene-1,2-diyl)bis(2-chlorobenzoic acid) | 830.6 | 0.37 | 0.15 | 293 | 0.1 | [S82] |
| 256 | [Cd2L7(H2O)]2 | 4,4'-(hexafluoroisopropylidene)diphthalate | 147 | 0.1 | 1 | 298 | 2.11 | [S83] |
| 257 | SNU-5 | abtc = 1,1'-azobenzene-3,3',5,5'-tetracarboxylic acid | 2850 | 1 | 1 | 273 | 8.75 | [S84] |
| 258 | | | 2850 | 1 | 0.15 | 273 | 1.83 | |
| 259 | SNU-30' | TCPBDA = N,N,N',N'-tetrakis(4-carboxyphenyl)-biphenyl-4,4'-diamine | 704 | 0.28 | 1 | 298 | 1.16 | [S85] |
| 260 | | | 704 | 0.28 | 0.15 | 298 | 0.21 | |

**Table S2.** Quasi-SMILES of MOFs, the set of each data, DCW, their experimental and predicted log ($CO_2$ uptake) for three splits

| **No.** | **Quasi-SMILES** | **Log ($CO_2$** | **Set** | **DCW (T*, N*)** | **Predicted log ($CO_2$ uptake)** |
|---|---|---|---|---|---|

| | | uptake) | 1 | 2 | 3 | Split 1 | Split 2 | Split 3 | Split 1 | Split 2 | Split 3 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | [Cu]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%12%20%30%49 | -0.07 | Outlier | | | | | | | | |
| 2 | [Cu]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%12%20%30%49 | 0.72 | * | # | - | 4.856 | 14.695 | -0.776 | 0.46 | 0.50 | 0.40 |
| 3 | [Cu]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%12%20%30%49 | 0.46 | + | # | + | 4.856 | 14.695 | -0.776 | 0.46 | 0.50 | 0.40 |
| 4 | [Zn]c1cc(ccc1C(=O)O)C(=O)O%14%21%36%49 | 1.34 | - | - | * | 23.368 | 34.602 | 14.909 | 1.19 | 1.24 | 1.12 |
| 5 | [Zn]c1cc(c(cc1C(=O)O)N)C(=O)O%12%21%36%49 | 1.27 | + | + | * | 23.857 | 37.073 | 14.428 | 1.21 | 1.33 | 1.10 |
| 6 | [Zn]c1cc(c(cc1C(=O)O)N)C(=O)O%12%21%30%49 | 0.05 | + | + | + | 5.072 | 14.964 | -0.728 | 0.47 | 0.51 | 0.40 |
| 7 | [V]c1cc(ccc1C(=O)O)C(=O)O%11%20%33%49 | 1.06 | + | + | + | 16.729 | 27.006 | 9.187 | 0.93 | 0.95 | 0.86 |
| 8 | [Cr]c1cc(ccc1C(=O)O)C(=O)O%12%20%34%49 | 1.00 | - | # | * | 16.577 | 28.225 | 20.146 | 0.92 | 1.00 | 1.36 |
| 9 | [Cr]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%13%21%39%49 | 1.26 | * | - | - | 28.072 | 40.914 | 16.611 | 1.38 | 1.47 | 1.20 |
| 10 | [Fe]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%13%21%30%49 | 0.18 | - | * | + | 3.911 | 12.670 | 0.158 | 0.42 | 0.42 | 0.44 |
| 11 | [Cr]c1cc(ccc1C(=O)O)C(=O)O%14%22%39%49 | 1.60 | + | - | - | 32.065 | 36.919 | 17.098 | 1.53 | 1.32 | 1.22 |
| 12 | [Cr]c1cc(ccc1C(=O)O)C(=O)O%14%22%30%49 | 0.33 | + | + | - | 5.575 | 14.756 | 6.385 | 0.49 | 0.50 | 0.73 |
| 13 | [Mg]c1c(c(cc(c1O)C(=O)O)O)C(=O)O%11%20%36%49 | 1.02 | # | * | + | 21.908 | 34.250 | 18.446 | 1.13 | 1.22 | 1.29 |
| 14 | [Mg]c1c(c(cc(c1O)C(=O)O)O)C(=O)O%11%20%30%49 | 0.93 | - | + | + | 5.632 | 17.864 | 0.988 | 0.49 | 0.61 | 0.48 |
| 15 | [Mg]c1c(c(cc(c1O)C(=O)O)O)C(=O)O%11%20%30%49 | 0.79 | * | - | * | 5.632 | 17.864 | 0.988 | 0.49 | 0.61 | 0.48 |
| 16 | [Zn]C1=CC(=CC=C1C2=CC(=CC(=C2)C3=CC=C(C=C3)C(=O)O)C4=CC=C(C=C4)C(=O)O)C(=O)O%17%22%33%49 | 1.45 | - | - | # | 15.483 | 31.867 | 18.557 | 0.88 | 1.13 | 1.29 |
| 17 | [Zn]C1=CC(=CC=C1C2=CC(=CC(=C2)C3=CC=C(C=C3)C(=O)O)C4=CC=C(C=C4)C(=O)O)C(=O)O%17%22%33%49 | 1.53 | * | * | - | 15.483 | 31.867 | 18.557 | 0.88 | 1.13 | 1.29 |
| 18 | [Zn]c1cc(ccc1c2ccc(cc2)C(=O)O)c3cc(cc(c3)c4ccc(cc4)c5ccc(cc5)C(=O)O)c6ccc(cc6)c7ccc(cc7)C(=O)O%17%24%39%49 | 1.74 | * | * | - | 36.922 | 57.071 | 23.868 | 1.72 | 2.07 | 1.54 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 19 | [Zn]c1cc(ccc1c2ccc(cc2)C(=O)O)c3cc(cc(c3)c4ccc(cc4)c5ccc(cc5)C(=O)O)c6ccc(cc6)c7ccc(cc7)C(=O)O%17%24%33%49 | 1.74 | - | # | - | 28.148 | 38.647 | 23.024 | 1.38 | 1.39 | 1.50 |
| 20 | [Zn]c1cc(ccc1c2ccc(cc2)C(=O)O)c3cc(cc(c3)c4ccc(cc4)c5ccc(cc5)C(=O)O)c6ccc(cc6)c7ccc(cc7)C(=O)O%17%24%33%49 | 1.17 | - | + | + | 28.148 | 38.647 | 23.024 | 1.38 | 1.39 | 1.50 |
| 21 | [Zn]c1cc(ccc1c2ccc(cc2)C(=O)O)C(=O)O%19%24%39%49 | 1.74 | + | + | - | 32.401 | 39.709 | 8.725 | 1.55 | 1.43 | 0.84 |
| 22 | [Cu]c1c(cc(cc1C(=O)O)C(=O)O)c2cc(cc(c2)C(=O)O)C(=O)O%12%20%36%49 | 1.01 | - | # | * | 20.239 | 38.172 | 20.907 | 1.07 | 1.37 | 1.40 |
| 23 | [Cu]OC(C1=CC(C(O)=O)=CC(C#CC(C=C2)=CC=C2C#CC3=CC(C#CC4=CC=C(C#CC5=CC(C(O)=O)=CC(C(O)=O)=C5)C=C4)=CC(C#CC6=CC=C(C#CC7=CC(C(O)=O)=CC(C(O)=O)=C7)C=C6)=C3)=C1)=O%19%23%37%49 | 1.67 | + | - | * | 40.148 | 42.949 | 27.095 | 1.85 | 1.55 | 1.68 |
| 24 | [Zn]C1=CC(=CC=C1C2=CC(=CC(=C2)C3=CC=C(C=C3)C(=O)O)C4=CC=C(C=C4)C(=O)O)C(=O)O%16%22%34%49 | 1.37 | # | + | - | 14.346 | 35.378 | 19.627 | 0.83 | 1.26 | 1.34 |
| 25 | [Ni]c1cc(c(cc1C(=O)O)N)C(=O)O%13%21%34%49 | 1.13 | - | - | + | 7.641 | 25.279 | 15.365 | 0.57 | 0.89 | 1.14 |
| 26 | [Zn]C(=C/C(=O)O)\C(=O)O%11%20%49 | 1.20 | + | * | - | 24.845 | 18.273 | 10.147 | 1.25 | 0.63 | 0.90 |
| 27 | [Zn]C(=C/C(=O)O)\C(=O)O%11%20%30%49 | -0.05 | + | - | + | 2.849 | 5.830 | -0.941 | 0.38 | 0.17 | 0.39 |
| 28 | [Zn]c1cc(cc2c1ccc(c2)C(=O)O)C(=O)O^CN(C)C=O%11%20%37%49 | 0.85 | Outlier | | | | | | | | |
| 29 | [Cu][Si]c1cnccc1C#Cc2ccncc2%11%20%30%49 | -0.72 | + | # | - | 14.089 | 11.018 | 7.970 | 0.82 | 0.36 | 0.80 |
| 30 | [Cu][Si]c1cnccc1C#Cc2ccncc3%11%20%30%49 | 0.73 | | | | | | | | | |
| 31 | [Cr]CCNCCNC^c1cc(cc2c1cc(cc2)C(=O)O)C(=O)O%10%20%30%49 | 0.59 | - | + | + | -2.264 | 13.243 | 2.462 | 0.18 | 0.44 | 0.55 |
| 32 | [Cr]CCNCCNC^c1cc(cc2c1cc(cc2)C(=O)O)C(=O)O%10%20%30%49 | 0.64 | - | # | - | 8.676 | 18.018 | 2.072 | 0.61 | 0.62 | 0.53 |
| 33 | [Zn]c1cnccc1c2ccncc2^OC(C1C(C(O)=O)C(C(O)=O)C(C(O)=O)C(C(O)=O)C1C(O)=O)=O%10%20%30%49 | 0.18 | # | - | + | 8.676 | 18.018 | 2.072 | 0.61 | 0.62 | 0.53 |
| 34 | [Mg]c1c(c(cc(c1O)C(=O)O)O)C(=O)O%12%20%30%49 | 0.79 | - | # | * | -5.152 | 11.028 | -12.907 | 0.07 | 0.36 | -0.16 |
| 35 | [Zn]OC(C1=CC=C(C2=CC=C(C3=NN=NN3)C=C2)C=C1)=O%10%20%30%49 | 0.43 | + | + | + | 8.912 | 20.263 | 2.088 | 0.62 | 0.70 | 0.53 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| 36 | [Cu]O=C(O)C1=CC=CC(C2=CC=C3C=CC(C4=CC(C(O)=O)=CC=C4)=CC3=C2)=C1%10%20%30%47 | 0.37 | - | - | # | -7.810 | -3.051 | -8.540 | -0.04 | -0.16 | 0.04 |
| 37 | [Cu]O=C(O)C1=CC=CC(C2=CC=C3C=CC(C4=CC(C(O)=O)=CC=C4)=CC3=C2)=C1%10%20%30%49 | -0.07 | * | # | + | 7.305 | 10.752 | 1.781 | 0.56 | 0.35 | 0.52 |
| 38 | [Cu]O=C(O)C1=CC=CC(C2=CC=C3C=CC(C4=CC(C(O)=O)=CC=C4)=CC3=C2)=C1%10%20%30%49 | -0.20 | * | - | - | -5.051 | -1.100 | -9.306 | 0.07 | -0.09 | 0.00 |
| 39 | [Al]O=C(C1=CC(C(O)=O)=C(C(O)=O)C=C1C(O)=O)O%10%20%30%49 | 0.50 | # | * | + | -5.051 | -1.100 | -9.306 | 0.07 | -0.09 | 0.00 |
| 40 | [Zn]c1cc(c(cc1C(=O)O)C(=O)O)C(=O)O%10%20%30%49 | 0.27 | * | + | - | -8.101 | 5.164 | -8.971 | -0.05 | 0.14 | 0.02 |
| 41 | [Cu]O=C(C1=CC2=C(C=C1)N(C3=CC(C4=CC(N5C6=C(C7=C5C=CC(C(O)=O)=C7)C=C(C(O)=O)C=C6)=CC(N8C9=C(C%10=C8C=CC(C(O)=O)=C%10)C=C(C(O)=O)C=C9)=C4)=CC(N%11C%12=C(C%13=C%11C=CC(C(O)=O)=C%13)C=C(C(O)=O)C=C%12)=C3)C%14=C2C=C(C(O)=O)C=C%14)O%16%21%30%49 | 0.48 | + | * | # | -2.536 | 9.420 | -4.313 | 0.17 | 0.30 | 0.23 |
| 42 | [Co(II)][Co(III)]C12=NN=NC1=CC3=NN=NC3=C2%11%20%30%49 | 0.83 | + | + | - | 0.963 | 15.446 | 0.347 | 0.31 | 0.52 | 0.45 |
| 43 | Mn(II)&Mn(III)C12=NN=NC1=CC3=NN=NC3=C2%12%20%30%49 | 0.85 | * | + | # | 18.733 | 26.273 | 14.930 | 1.01 | 0.93 | 1.12 |
| 44 | [Zn]NC1=NNC=N1%11%20%30%49 | 0.64 | + | - | + | 13.140 | 29.077 | 8.266 | 0.79 | 1.03 | 0.81 |
| 45 | [Cu]OC(C1=CC(C(O)=O)=CC(C2=CC=C(C3=CC(C(O)=O)=CC(C(O)=O)=C3)C4=NON=C42)=C1)=O%14%21%30%49 | 0.64 | + | - | * | -1.106 | 8.088 | -1.743 | 0.23 | 0.25 | 0.35 |
| 46 | [Cu]OC(C1=CC(C(O)=O)=CC(C2=CC=C(C3=CC(C(O)=O)=CC(C(O)=O)=C3)C4=NON=C42)=C1)=O%14%21%30%49 | 0.74 | - | - | + | 7.451 | 13.271 | 3.541 | 0.56 | 0.44 | 0.60 |
| 47 | [Cu]OC(C1=CC(C(O)=O)=CC(C2=CC=C(C3=CC(C(O)=O)=CC(C(O)=O)=C3)C4=NSN=C42)=C1)=O%13%21%30%49 | 0.58 | * | * | * | 7.451 | 13.271 | 3.541 | 0.56 | 0.44 | 0.60 |
| 48 | [Cu]OC(C1=CC(C(O)=O)=CC(C2=CC=C(C3=CC(C(O)=O)=CC(C(O)=O)=C3)C4=NSN=C42)=C1)=O%13%21%30%49 | 0.69 | + | + | - | 7.972 | 17.391 | 2.388 | 0.58 | 0.60 | 0.54 |
| 49 | [Cu]OC(C1=CC(C(O)=O)=CC(C2=CC=C(C3=CC(C(O)=O)=CC(C(O)=O)=C3)C4=NSN=C42)=C1)=O%13%21%30%49 | 0.59 | * | # | + | 7.972 | 17.391 | 2.388 | 0.58 | 0.60 | 0.54 |
| 50 | [Cu]OC(C1=CC(C(O)=O)=CC(C2=CC=C(C3=CC(C(O)=O)=CC(C(O)=O)=C3)C4=N[Se]N=C42)=C1)=O%10%20%30%49 | 0.22 | + | * | + | 7.972 | 17.391 | 2.388 | 0.58 | 0.60 | 0.54 |
| 51 | [Cu]OC(C1=CC(C(O)=O)=CC(C2=CC=C(C3=CC(C(O)=O)=CC(C(O)=O)=C3)C4=N[Se]N=C42)=C1)=O%10%20%30 | 0.30 | # | * | + | -1.929 | 5.177 | -3.083 | 0.19 | 0.14 | 0.29 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| | %49 | | | | | | | | | | |
| 52 | [Cu]O=C(C1=CC(C2=C(CO)C(C)=C(C3=CC(C(O)=O)=CC(C(O)=O)=C3)C(CO)=C2C)=CC(C(O)=O)=C1)O%12%20%30%49 | 0.66 | - | + | - | -1.929 | 5.177 | -3.083 | 0.19 | 0.14 | 0.29 |
| 53 | [Cu]c1cc(ccc1c2cc(cc(c2)C(=O)O)C(=O)O)c3cc(cc(c3)C(=O)O)C(=O)O%14%21%30%49 | 0.59 | + | * | + | 3.780 | 20.920 | 1.219 | 0.42 | 0.73 | 0.49 |
| 54 | [Cu]O=C(C1=CC(C2=CC=C(C3=CC(C(O)=O)=CC(C(O)=O)=C3)C=C2[N](O)=O)=CC(C(O)=O)=C1)O%13%21%30%49 | 0.65 | # | * | * | 5.148 | 24.130 | 7.601 | 0.47 | 0.85 | 0.78 |
| 55 | [Cu]O=C(C1=CC(C2=CC=C(C3=CC(C(O)=O)=CC(C(O)=O)=C3)C=C2[N](O)=O)=CC(C(O)=O)=C1)O%13%21%30%49 | 0.92 | - | * | - | 11.755 | 23.170 | 6.099 | 0.73 | 0.81 | 0.71 |
| 56 | [Cu]c1c(cc(cc1C(=O)O)C(=O)O)c2cc(cc(c2)C(=O)O)C(=O)O%11%20%30%49 | 0.51 | + | + | + | 11.755 | 23.170 | 6.099 | 0.73 | 0.81 | 0.71 |
| 57 | [Cu]O=C(NC1=CC(C(O)=O)=CC(C(O)=O)=C1)C2=CC=C(C(NC3=CC(C(O)=O)=CC(C(O)=O)=C3)=O)C=C2%12%20%30%49 | 0.62 | - | # | * | 0.683 | 19.387 | 2.349 | 0.30 | 0.67 | 0.54 |
| 58 | [Cu]O=C(NC1=CC(C(O)=O)=CC(C(O)=O)=C1)C(NC2=CC(C(O)=O)=CC(C(O)=O)=C2)=O%13%21%30%49 | 0.58 | - | - | - | 7.883 | 19.181 | 1.522 | 0.58 | 0.66 | 0.50 |
| 59 | [Cu]O=C(NC1=CC(C(O)=O)=CC(C(O)=O)=C1)C(NC2=CC(C(O)=O)=CC(C(O)=O)=C2)=O%13%21%30%49 | 0.62 | # | # | * | 8.765 | 17.894 | 4.574 | 0.62 | 0.61 | 0.64 |
| 60 | [Cu]O=C(NC1=CC(C(O)=O)=CC(C(O)=O)=C1)C(NC2=CC(C(O)=O)=CC(C(O)=O)=C2)=O%13%21%30%49 | 0.96 | + | + | + | 8.765 | 17.894 | 4.574 | 0.62 | 0.61 | 0.64 |
| 61 | [Cu]OC(C1=CC(C(O)=O)=CC([N](C2)=NN=C2C3=CC(C4=NN=[N](C5=CC(C(O)=O)=CC(C(O)=O)=C5)C4)=CC(C6=NN=[N](C7=CC(C(O)=O)=CC(C(O)=O)=C7)C6)=C3)=C1)=O%15%21%30%49 | 0.96 | - | + | # | 8.765 | 17.894 | 4.574 | 0.62 | 0.61 | 0.64 |
| 62 | [Cu]OC(C1=CC(C(O)=O)=CC([N](C2)=NN=C2C3=CC(C4=NN=[N](C5=CC(C(O)=O)=CC(C(O)=O)=C5)C4)=CC(C6=NN=[N](C7=CC(C(O)=O)=CC(C(O)=O)=C7)C6)=C3)=C1)=O%15%21%30%49 | 0.67 | + | # | # | 14.169 | 23.899 | 4.618 | 0.83 | 0.84 | 0.65 |
| 63 | [Cu]OC(C1=CC(C(O)=O)=CC(C#CC2=CC(C#CC3=CC(C(O)=O)=CC(C(O)=O)=C3)=CC(C#CC4=CC(C(O)=O)=CC(C(O)=O)=C4)=C2)=C1)=O%15%21%30%49 | 0.69 | + | - | - | 14.169 | 23.899 | 4.618 | 0.83 | 0.84 | 0.65 |
| 64 | [Cu]OC(C1=CC(C(O)=O)=CC(C#CC2=CC(C#CC3=CC(C(O)=O)=CC(C(O)=O)=C3)=CC(C#CC4=CC(C(O)=O)=CC(C(O)=O)=C4)=C2)=C1)=O%15%21%33%49 | 1.33 | # | * | - | 12.213 | 32.067 | 5.778 | 0.75 | 1.14 | 0.70 |
| 65 | [Cu]O=C(C1=CC(C(O)=O)=CC(C#CC2=CC=C(N(C3=CC=C(C#CC4=CC(C(O)=O)=CC(C(O)=O)=C4)C=C3)C5=CC=C | 0.70 | - | * | * | 25.138 | 43.775 | 18.736 | 1.26 | 1.58 | 1.30 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| | (C#CC6=CC(C(O)=O)=CC(C(O)=O)=C6)C=C5)C=C2)=C1)O%16%22%30%49 | | | | | | | | | | |
| 66 | [Cu]O=C(C1=CC(C(O)=O)=CC(C#CC2=CC=C(N(C3=CC=C(C#CC4=CC(C(O)=O)=CC(C(O)=O)=C4)C=C3)C5=CC=C(C#CC6=CC(C(O)=O)=CC(C(O)=O)=C6)C=C5)C=C2)=C1)O%16%22%33%49 | 1.34 | - | - | * | 10.248 | 19.377 | 1.191 | 0.67 | 0.67 | 0.49 |
| 67 | [Cu]O=C(C1=CC(C(O)=O)=CC(C#CC2=CC=C(C3=CC(C4=CC=C(C#CC5=CC(C(O)=O)=CC(C(O)=O)=C5)C=C4)=CC(C6=CC=C(C#CC7=CC(C(O)=O)=CC(C(O)=O)=C7)C=C6)=C3)C=C2)=C1)O%18%22%30%49 | 0.70 | - | # | - | 28.479 | 37.103 | 15.054 | 1.39 | 1.33 | 1.13 |
| 68 | [Cu]O=C(C1=CC(C(O)=O)=CC(C#CC2=CC=C(C3=CC(C4=CC=C(C#CC5=CC(C(O)=O)=CC(C(O)=O)=C5)C=C4)=CC(C6=CC=C(C#CC7=CC(C(O)=O)=CC(C(O)=O)=C7)C=C6)=C3)C=C2)=C1)O%18%22%33%49 | 1.34 | # | * | # | 9.616 | 18.640 | 7.416 | 0.65 | 0.64 | 0.78 |
| 69 | [Cu]OC(C1=CC(C(O)=O)=CC(NC(C2=CC(C(NC3=CC(C(O)=O)=CC(C(O)=O)=C3)=O)=CC(C(NC4=CC(C(O)=O)=CC(C(O)=O)=C4)=O)=C2)=O)=C1)=O%15%21%33%49 | 1.37 | # | * | - | 27.847 | 36.366 | 21.279 | 1.37 | 1.30 | 1.42 |
| 70 | [Cu]O=C(C1=CC=C(C2=CC(C3=CC=C(C(NC4=CC(C(O)=O)=CC(C(O)=O)=C4)=O)C=C3)=CC(C5=CC=C(C(NC6=CC(C(O)=O)=CC(C(O)=O)=C6)=O)C=C5)=C2)C=C1)NC7=CC(C(O)=O)=CC(C(O)=O)=C7%15%22%33%49 | 1.55 | * | # | - | 22.001 | 37.159 | 17.752 | 1.14 | 1.33 | 1.25 |
| 71 | [Cu]O=C(C1=CC=C(C2=CC(C3=CC=C(C(NC4=CC(C(O)=O)=CC(C(O)=O)=C4)=O)C=C3)=CC(C5=CC=C(C(NC6=CC(C(O)=O)=CC(C(O)=O)=C6)=O)C=C5)=C2)C=C1)NC7=CC(C(O)=O)=CC(C(O)=O)=C7%15%22%33%49 | 1.40 | # | * | # | 22.906 | 38.356 | 21.520 | 1.17 | 1.38 | 1.43 |
| 72 | [Cu]O=C(C1=CC=C(C2=NC(C3=CC=C(C(NC4=CC(C(O)=O)=CC(C(O)=O)=C4)=O)C=C3)=NC(C5=CC=C(C(NC6=CC(C(O)=O)=CC(C(O)=O)=C6)=O)C=C5)=N2)C=C1)NC7=CC(C(O)=O)=CC(C(O)=O)=C7%15%22%33%49 | 1.55 | # | + | + | 22.906 | 38.356 | 21.520 | 1.17 | 1.38 | 1.43 |
| 73 | [Cu]O=C(C1=CC=C(C2=NC(C3=CC=C(C(NC4=CC(C(O)=O)=CC(C(O)=O)=C4)=O)C=C3)=NC(C5=CC=C(C(NC6=CC(C(O)=O)=CC(C(O)=O)=C6)=O)C=C5)=N2)C=C1)NC7=CC(C(O)=O)=CC(C(O)=O)=C7%15%22%33%49 | 1.40 | # | # | * | 26.104 | 41.055 | 21.680 | 1.30 | 1.48 | 1.43 |
| 74 | [Zn]C1=CC(=CC=C1C2=CC(=CC(=C2)C3=CC=C(C=C3)C(=O)O)C4=CC=C(C=C4)C(=O)O)C(=O)O^c1cc(cc2c1cc(cc2)C(=O)O)C(=O)O%17%22%39%49 | 1.58 | # | # | + | 26.104 | 41.055 | 21.680 | 1.30 | 1.48 | 1.43 |
| 75 | [Zn]C1=CC(=CC=C1C2=CC(=CC(=C2)C3=CC=C(C=C3)C(=O)O)C4=CC=C(C=C4)C(=O)O)C(=O)O^c1cc(cc2c1cc(cc2)C(=O)O)C(=O)O%17%22%33%49 | 1.53 | - | - | # | 31.795 | 48.289 | 21.240 | 1.52 | 1.74 | 1.41 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| 76 | [Zn]C1=CC(=CC=C1C2=CC(=CC(=C2)C3=CC=C(C=C3)C(=O)O)C4=CC=C(C=C4)C(=O)O)C(=O)O^c1cc(cc2c1cc(cc2)C(=O)O)C(=O)O%17%22%33%49 | 1.41 | - | - | + | 23.536 | 43.852 | 24.390 | 1.20 | 1.58 | 1.56 |
| 77 | [Zn]<br>O=C(O)C(C=C1)=CC=C1C#CC2=CC(C#CC3=CC=C(C(O)=O)C=C3)=CC(C#CC4=CC=C(C(O)=O)C=C4)=C2^c1cc(ccc1c2ccc(cc2)C(=O)O)C(=O)O%19%24%33%49 | 1.74 | - | + | * | 23.536 | 43.852 | 24.390 | 1.20 | 1.58 | 1.56 |
| 78 | [Zn]<br>O=C(O)C(C=C1)=CC=C1C#CC2=CC(C#CC3=CC=C(C(O)=O)C=C3)=CC(C#CC4=CC=C(C(O)=O)C=C4)=C2^c1cc(ccc1c2ccc(cc2)C(=O)O)C(=O)O%19%24%33%49 | 1.20 | * | + | # | 34.958 | 40.512 | 17.635 | 1.65 | 1.46 | 1.25 |
| 79 | [Cu]O=C(O)C1=CC(C(O)=O)=CC(NC(C2=CC=C(C(O)=O)C=C2)=O)=C1%14%21%30%49 | 0.79 | # | - | # | 34.958 | 40.512 | 17.635 | 1.65 | 1.46 | 1.25 |
| 80 | [Cu]O=C(O)C1=CC(C(O)=O)=CC(NC(C2=CC=C(C(O)=O)C=C2)=O)=C1%14%21%33%49 | 1.34 | + | * | + | 10.315 | 20.988 | 3.388 | 0.68 | 0.73 | 0.59 |
| 81 | [Cu]O=C(O)C1=CC(C(O)=O)=CC(NC(C2=CC=C(C(O)=O)C=C2)=O)=C1%14%21%33%49 | 1.26 | * | - | * | 23.240 | 32.696 | 16.346 | 1.18 | 1.16 | 1.19 |
| 82 | [Cu]O=C(NC1=CC(C(O)=O)=CC(C(O)=O)=C1)C2=CN=CC(C(NC3=CC(C(O)=O)=CC(C(O)=O)=C3)=O)=C2%12%20%30%49 | 0.81 | - | - | + | 23.240 | 32.696 | 16.346 | 1.18 | 1.16 | 1.19 |
| 83 | [Cu]O=C(NC1=CC(C(O)=O)=CC(C(O)=O)=C1)C2=CN=CC(C(NC3=CC(C(O)=O)=CC(C(O)=O)=C3)=O)=C2%12%20%30%49 | 0.73 | - | + | + | 10.478 | 21.736 | 4.233 | 0.68 | 0.76 | 0.63 |
| 84 | [Cu]O=C(NC1=CC(C(O)=O)=CC(C(O)=O)=C1)C2=CN=CC(C(NC3=CC(C(O)=O)=CC(C(O)=O)=C3)=O)=C2%12%20%30%49 | 0.62 | + | * | # | 10.478 | 21.736 | 4.233 | 0.68 | 0.76 | 0.63 |
| 85 | [Cu]O=C(NCC(O)=O)C1=CC(C(NCC(O)=O)=O)=CC(C(NCC(O)=O)=O)=C1^C1(CCCC2=CC=NC=C2)=CC=NC=C1%11%20%30%49 | 0.30 | + | * | + | 10.478 | 21.736 | 4.233 | 0.68 | 0.76 | 0.63 |
| 86 | [Cu]O=C(NCC(O)=O)C1=CC(C(NCC(O)=O)=O)=CC(C(NCC(O)=O)=O)=C1^C1(CCCC2=CC=NC=C2)=CC=NC=C2%11%20%33%49 | 0.74 | + | + | # | 7.089 | 19.785 | 8.126 | 0.55 | 0.68 | 0.81 |
| 87 | [Zn]O=C(O)C1=CC=C(OC2=CC=C(C=C2)C(O)=O)C=C1^C1(/N=C/C2=CC=NC=C2)=CC=C(/N=C/C3=CC=NC=C3)C=C1%10%20%30%47 | 0.95 | - | + | # | 28.716 | 30.232 | 20.058 | 1.40 | 1.07 | 1.36 |
| 88 | [Zn]O=C(O)C1=CC=C(OC2=CC=C(C=C2)C(O)=O)C=C1^C1(/N=C/C2=CC=NC=C2)=C3C=CC=C(/N=C/C4=CC=NC=C4)C3=CC=C1%10%20%30%47 | 0.65 | + | # | + | 11.510 | 16.404 | 6.684 | 0.72 | 0.56 | 0.74 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 89 | [Zn]O=C(O)C1=CC=C(OC2=CC=C(C=C2)C(O)=O)C=C1^O=C(NC1=CC=NC=C1)C2=CC=C(C(NC3=CC=NC=C3)=O)C=C2%11%20%30%47 | 0.86 | # | # | + | 11.156 | 14.320 | 4.474 | 0.71 | 0.48 | 0.64 |
| 90 | [Zn]O=C(O)C1=CC=C(OC2=CC=C(C=C2)C(O)=O)C=C1^O=C(NC1=CC=C(NC(C2=CC=NC=C2)=O)C=C1)C3=CC=NC=C3%10%20%30%47 | 0.86 | # | * | - | 24.058 | 25.183 | 14.719 | 1.22 | 0.89 | 1.11 |
| 91 | [Zn]O=C(O)C1=CC=C(OC2=CC=C(C=C2)C(O)=O)C=C1^O=C(NC1=CC=CC2=C(NC(C3=CC=NC=C3)=O)C=CC=C12)C4=CC=NC=C4%10%20%30%47 | 0.80 | - | - | * | 17.507 | 21.813 | 8.810 | 0.96 | 0.76 | 0.84 |
| 92 | [Zn]O=C(C1=CC=C(C2=CC=C(C(O)=O)C=C2OC(N(C)C)=S)C=C1)O%12%24%30%49 | 0.34 | + | # | # | 19.041 | 14.191 | 9.121 | 1.02 | 0.48 | 0.85 |
| 93 | [Zn]O=C(C1=CC=C(C2=CC=C(C(O)=O)C=C2SC(N(C)C)=O)C=C1)O%12%29%30%49 | 0.40 | + | + | # | 0.615 | 9.034 | 1.307 | 0.29 | 0.29 | 0.49 |
| 94 | [Ni]C1(C2=CNN=C2)=CC=C(C3=CNN=C3)C=C1%12%20%35%49 | 1.00 | * | # | # | 3.488 | 8.896 | -1.580 | 0.41 | 0.28 | 0.36 |
| 95 | [Zn]C1(C2=CNN=C2)=CC=C(C3=CNN=C3)C=C1%13%20%35%49 | 0.96 | - | * | - | 16.381 | 24.387 | 12.762 | 0.92 | 0.86 | 1.02 |
| 96 | [Fe]C1(C#CC2=CNN=C2)=CC=C(C#CC3=CNN=C3)C=C1%12%21%31%49 | 0.96 | * | - | * | 18.385 | 27.641 | 15.814 | 0.99 | 0.98 | 1.16 |
| 97 | [Fe]C1(C#CC2=CNN=C2)=CC=C(C#CC3=CNN=C3)C=C1%12%21%31%49 | 1.08 | # | - | * | 19.099 | 26.533 | 15.611 | 1.02 | 0.94 | 1.15 |
| 98 | [Fe]C1(C#CC2=CNN=C2)=CC=C(C#CC3=CNN=C3)C=C1%12%21%30%47 | 1.13 | * | - | # | 19.099 | 26.533 | 15.611 | 1.02 | 0.94 | 1.15 |
| 99 | [Ni]C1(C#CC2=CNN=C2)=CC=C(C#CC3=CNN=C3)C=C1%13%21%31%49 | 0.77 | + | * | * | 21.874 | 28.484 | 13.367 | 1.13 | 1.01 | 1.05 |
| 100 | [Ni]C1(C#CC2=CNN=C2)=CC=C(C#CC3=CNN=C3)C=C1%13%21%31%49 | 0.93 | * | - | * | 19.730 | 25.020 | 15.105 | 1.05 | 0.88 | 1.13 |
| 101 | [Ni]C1(C#CC2=CNN=C2)=CC=C(C#CC3=CNN=C3)C=C1%13%21%30%47 | 1.06 | + | - | * | 19.730 | 25.020 | 15.105 | 1.05 | 0.88 | 1.13 |
| 102 | [Zn]C1(C#CC2=CNN=C2)=CC=C(C#CC3=CNN=C3)C=C1%11%20%31%49 | 0.72 | - | + | + | 22.505 | 26.971 | 12.861 | 1.16 | 0.95 | 1.03 |
| 103 | [Zn]C1(C#CC2=CNN=C2)=CC=C(C#CC3=CNN=C3)C=C1%11%20%31%49 | 0.91 | - | * | - | 16.302 | 28.829 | 7.816 | 0.91 | 1.02 | 0.79 |
| 104 | [Zn]C1(C#CC2=CNN=C2)=CC=C(C#CC3=CNN=C3)C=C1%11%20%30%47 | 1.05 | * | + | * | 16.302 | 28.829 | 7.816 | 0.91 | 1.02 | 0.79 |
| 105 | [Zn]c1cc(ccc1C(=O)O)C(=O)O^C1CN2CCN1CC2%13%21%33%49 | 0.94 | # | - | * | 19.057 | 30.927 | 13.609 | 1.02 | 1.10 | 1.06 |
| 106 | [Zn]O=C(C1=CC(Br)=C(C(O)=O)C=C1)O^C1CN2CCN1CC2%12%20%33%49 | 0.74 | # | # | # | 15.745 | 25.704 | 11.850 | 0.89 | 0.90 | 0.98 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| 107 | [Zn]O=C(C1=CC(N(=O)=O)=C(C(O)=O)C=C1)O^C1CN2CCN1CC2%12%20%33%49 | 0.86 | + | * | + | 14.611 | 24.299 | 8.744 | 0.85 | 0.85 | 0.84 |
| 108 | [Zn]O=C(C1=C(F)C(F)=C(C(O)=O)C(F)=C1F)O^C1CN2CCN1CC2%11%20%33%49 | 0.57 | - | + | + | 12.652 | 25.585 | 10.386 | 0.77 | 0.90 | 0.91 |
| 109 | [Zn]O=C(C1=CC(Cl)=C(C(O)=O)C=C1Cl)O^C1CN2CCN1CC2%11%20%33%49 | 0.78 | * | # | - | 9.555 | 14.416 | -1.489 | 0.65 | 0.49 | 0.36 |
| 110 | [Zn]O=C(C1=CC(O)=C(C(O)=O)C=C1)O^C1CN2CCN1CC2%11%20%33%49 | 0.75 | - | - | # | 23.607 | 30.836 | 9.196 | 1.20 | 1.10 | 0.86 |
| 111 | [Zn]O=C(C1=CC(C)=C(C(O)=O)C=C1C)O^C1CN2CCN1CC2%11%20%33%49 | 0.76 | + | # | + | 12.484 | 25.580 | 8.363 | 0.76 | 0.90 | 0.82 |
| 112 | [Zn]O=C(C1=C(C)C(C)=C(C(O)=O)C(C)=C1C)O^C1CN2CCN1CC2%11%20%33%49 | 0.73 | # | # | * | 13.476 | 25.962 | 10.168 | 0.80 | 0.91 | 0.90 |
| 113 | [Zn]O=C(C1=C(C=CC=C2)C2=C(C(O)=O)C3=C1C=CC=C3)O^C1CN2CCN1CC2%11%20%33%49 | 0.59 | + | # | - | 14.026 | 28.812 | 9.766 | 0.82 | 1.02 | 0.88 |
| 114 | [Zr]c1cc(ccc1C(=O)O)C(=O)O%12%20%30%49 | 0.15 | + | # | + | 12.444 | 27.205 | 7.484 | 0.76 | 0.96 | 0.78 |
| 115 | [Ti][Zr]c1cc(ccc1C(=O)O)C(=O)O%12%21%30%49 | 0.30 | # | + | # | -9.092 | 1.358 | -13.667 | -0.09 | 0.00 | -0.20 |
| 116 | [Mg]c1c(c(cc(c1[O])C(=O)[O])[O])C(=O)[O]%12%20%30%49 | 0.73 | # | * | + | -3.285 | 6.023 | -7.850 | 0.14 | 0.17 | 0.07 |
| 117 | [Mg]c1c(c(cc(c1[O])C(=O)[O])[O])C(=O)[O]%12%20%30%49 | 0.90 | * | # | # | 10.049 | 15.552 | 9.245 | 0.67 | 0.53 | 0.86 |
| 118 | [Ni]c1c(c(cc(c1[O])C(=O)[O])[O])C(=O)[O]%11%20%30%49 | 0.42 | + | # | + | 10.049 | 15.552 | 9.245 | 0.67 | 0.53 | 0.86 |
| 119 | [Ni]c1c(c(cc(c1[O])C(=O)[O])[O])C(=O)[O]%11%20%30%49 | 0.76 | - | - | - | 6.636 | 9.666 | -0.341 | 0.53 | 0.31 | 0.42 |
| 120 | [Co]c1c(c(cc(c1[O])C(=O)[O])[O])C(=O)[O]%11%20%30%49 | 0.42 | - | + | # | 6.636 | 9.666 | -0.341 | 0.53 | 0.31 | 0.42 |
| 121 | [Co]c1c(c(cc(c1[O])C(=O)[O])[O])C(=O)[O]%11%20%30%49 | 0.84 | # | # | * | 7.328 | 10.658 | 3.607 | 0.56 | 0.35 | 0.60 |
| 122 | [Zn]c1c(c(cc(c1[O])C(=O)[O])[O])C(=O)[O]%11%20%30%49 | 0.12 | + | * | - | 7.328 | 10.658 | 3.607 | 0.56 | 0.35 | 0.60 |
| 123 | [Zn]c1c(c(cc(c1[O])C(=O)[O])[O])C(=O)[O]%11%20%30%49 | 0.74 | + | + | + | 9.495 | 14.341 | 4.129 | 0.64 | 0.48 | 0.62 |
| 124 | [Ni]c1cc(ccc1C(=O)O)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc4%11%20%30%49 | -0.14 | # | - | # | 9.495 | 14.341 | 4.129 | 0.64 | 0.48 | 0.62 |
| 125 | [Ni]c1cc(ccc1C(=O)O)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc5%11%20%30%49 | -0.46 | * | + | * | -0.351 | 0.526 | -7.831 | 0.26 | -0.03 | 0.07 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| 126 | [Ni]c1cc(ccc1C(=O)O)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc6%11%20%30%49 | 0.78 | # | # | + | -16.185 | -2.850 | -19.986 | -0.37 | -0.16 | -0.49 |
| 127 | [Ni]c1cc(ccc1C(=O)O)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc7%11%20%30%49 | 0.52 | - | - | - | 9.138 | 11.622 | -0.941 | 0.63 | 0.38 | 0.39 |
| 128 | [Ni]O=C(C1=CC(O)=C(C(O)=O)C=C1O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc4%11%20%30%49 | 0.38 | - | + | + | -2.170 | 7.323 | 0.602 | 0.18 | 0.22 | 0.46 |
| 129 | [Ni]O=C(C1=CC(O)=C(C(O)=O)C=C1O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc4%11%20%30%49 | 0.01 | + | - | - | 0.530 | 4.146 | -7.085 | 0.29 | 0.10 | 0.11 |
| 130 | [Ni]O=C(C1=CC(O)=C(C(O)=O)C=C1O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc5%11%20%30%49 | 0.89 | Outlier | | | | | | | | |
| 131 | [Ni]O=C(C1=CC(O)=C(C(O)=O)C=C1O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc4%11%20%30%49 | 0.75 | + | - | + | 0.530 | 4.146 | -7.085 | 0.29 | 0.10 | 0.11 |
| 132 | [Ni]c1cc(c(cc1C(=O)O)N)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc4%11%20%30%49 | 0.06 | # | + | - | -0.236 | 4.200 | -4.951 | 0.26 | 0.11 | 0.20 |
| 133 | [Ni]c1cc(c(cc1C(=O)O)N)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc5%11%20%30%49 | -0.23 | * | # | + | -16.071 | 0.824 | -17.106 | -0.36 | -0.02 | -0.36 |
| 134 | [Ni]c1cc(c(cc1C(=O)O)N)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc6%11%20%30%49 | 0.78 | + | * | + | 9.253 | 15.296 | 1.939 | 0.63 | 0.52 | 0.52 |
| 135 | [Ni]c1cc(c(cc1C(=O)O)N)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc7%11%20%30%49 | 0.60 | - | + | - | -2.055 | 10.997 | 3.482 | 0.19 | 0.36 | 0.59 |
| 136 | [Ni]c1ccc2c(c1)c(ccc2C(=O)O)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc4%10%20%30%49 | -0.35 | + | - | # | -11.943 | -6.782 | -10.565 | -0.20 | -0.30 | -0.06 |
| 137 | [Ni]c1ccc2c(c1)c(ccc2C(=O)O)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc4%10%20%30%49 | -0.66 | + | - | - | -11.943 | -6.782 | -10.565 | -0.20 | -0.30 | -0.06 |
| 138 | [Ni]c1ccc2c(c1)c(ccc2C(=O)O)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc4%10%20%30%49 | 0.21 | - | + | # | -11.943 | -6.782 | -10.565 | -0.20 | -0.30 | -0.06 |
| 139 | [Ni]c1ccc2c(c1)c(ccc2C(=O)O)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc4%10%20%30%49 | 0.04 | + | + | - | -11.943 | -6.782 | -10.565 | -0.20 | -0.30 | -0.06 |
| 140 | [Ni]c1cc(cc2c1cc(cc2)C(=O)O)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc4%11%20%30%49 | -0.35 | - | # | + | -3.927 | -1.046 | -8.736 | 0.12 | -0.09 | 0.03 |
| 141 | [Ni]c1cc(cc2c1cc(cc2)C(=O)O)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc5%11%20%30%49 | -0.64 | + | + | - | -19.761 | -4.422 | -20.891 | -0.51 | -0.22 | -0.53 |
| 142 | [Ni]c1cc(cc2c1cc(cc2)C(=O)O)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc6%11%20%30%49 | 0.50 | * | + | + | 5.563 | 10.050 | -1.846 | 0.49 | 0.32 | 0.35 |
| 143 | [Ni]c1cc(cc2c1cc(cc2)C(=O)O)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc4%11%20%30%49 | 0.29 | + | - | # | -3.927 | -1.046 | -8.736 | 0.12 | -0.09 | 0.03 |
| 144 | [Ni]c1cc(ccc1c2ccc(cc2)C(=O)O)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc4%11%20%30%49 | -0.46 | - | + | - | -3.315 | -2.250 | -9.762 | 0.14 | -0.13 | -0.02 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| 145 | [Ni]c1cc(ccc1c2ccc(cc2)C(=O)O)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc5%11%20%30%49 | -0.68 | + | # | # | -19.150 | -5.626 | -21.917 | -0.48 | -0.26 | -0.58 |
| 146 | [Ni]c1cc(ccc1c2ccc(cc2)C(=O)O)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc6%11%20%30%49 | 0.29 | * | - | + | 6.174 | 8.846 | -2.872 | 0.51 | 0.28 | 0.30 |
| 147 | [Ni]c1cc(ccc1c2ccc(cc2)C(=O)O)C(=O)O^c1cnccc1c2nc(nc(n2)c3ccncc3)c4ccncc7%11%20%30%49 | 0.12 | - | # | # | -5.134 | 4.547 | -1.329 | 0.07 | 0.12 | 0.37 |
| 148 | [Ni]&[Fe]c1cc(ccc1C(=O)O)C(=O)O^c1cnccc1c2ccncc2%11%20%30%49 | 0.65 | # | # | - | 9.539 | -1.254 | -2.293 | 0.65 | -0.10 | 0.33 |
| 149 | [Ni][Fe]c1cc(ccc1C(=O)O)C(=O)O^c1cnccn1%10%20%30%49 | 0.38 | * | # | + | 9.763 | 2.210 | -2.930 | 0.65 | 0.03 | 0.30 |
| 150 | [Cu]C1(C2=CNN=N2)=CC(C3=CNN=N3)=CC(C4=CNN=N4)=C1^CNCCNC%11%20%30%49 | 0.62 | + | * | + | 13.433 | 8.299 | -0.453 | 0.80 | 0.26 | 0.41 |
| 151 | [Cu]C1(C2=CNN=N2)=CC(C3=CNN=N3)=CC(C4=CNN=N4)=C1^CNCCNC%11%20%30%49 | 0.38 | * | - | # | 13.433 | 8.299 | -0.453 | 0.80 | 0.26 | 0.41 |
| 152 | [Cu]C1(C2=CNN=N2)=CC(C3=CNN=N3)=CC(C4=CNN=N4)=C1%12%20%30%49 | 0.58 | - | + | * | 3.277 | 4.995 | -8.545 | 0.40 | 0.13 | 0.04 |
| 153 | [Cu]C1(C2=CNN=N2)=CC(C3=CNN=N3)=CC(C4=CNN=N4)=C1%12%20%30%49 | -0.17 | + | + | - | 3.277 | 4.995 | -8.545 | 0.40 | 0.13 | 0.04 |
| 154 | [K][Co]C(C(=O)O)C(CC(=O)O)(C(=O)O)O%11%20%30%49 | 0.63 | + | + | + | 9.951 | 15.471 | 1.988 | 0.66 | 0.52 | 0.52 |
| 155 | [Cu]OC(C1=CC(C(O)=O)=CC(C2=CC(C3=CC(C(O)=O)=CC(C(O)=O)=C3)=CC(C4=CC(C(O)=O)=CC(C(O)=O)=C4)=C2)=C1)=O%11%20%30%49 | 0.52 | - | * | * | 1.714 | 13.987 | 1.594 | 0.34 | 0.47 | 0.51 |
| 156 | [Cu]OC(C1=CC(C(O)=O)=CC(C2=CC(C3=CC(C(O)=O)=CC(C(O)=O)=C3)=CC(C4=CC(C(O)=O)=CC(C(O)=O)=C4)=C2)=C1)=O%11%20%30%49 | -0.24 | Outlier | | | | | | | | |
| 157 | [Zn]OC1=C(C(O)=O)C=CC=C1C(O)=O^C1CN2CCN1CC2%11%20%30%49 | 0.49 | # | + | * | -2.892 | 10.863 | -0.272 | 0.16 | 0.35 | 0.42 |
| 158 | [Cu]O=C(O)C1=CC(C2=C(C3=CC(C(O)=O)=CC(C(O)=O)=C3)C=C(C4=CC(C(O)=O)=CC(C(O)=O)=C4)C(C5=CC(C(O)=O)=CC(C(O)=O)=C5)=C2)=CC(C(O)=O)=C1%11%20%30%49 | 0.46 | * | # | - | 0.133 | 19.750 | -2.522 | 0.28 | 0.68 | 0.32 |
| 159 | [Zn]O=C(O)C1=CC(C2=C(C3=CC(C(O)=O)=CC(C(O)=O)=C3)C=C(C4=CC(C(O)=O)=CC(C(O)=O)=C4)C(C5=CC(C(O)=O)=CC(C(O)=O)=C5)=C2)=CC(C(O)=O)=C1%11%20%30%49 | 0.37 | - | + | # | 1.229 | 21.527 | -0.923 | 0.32 | 0.75 | 0.39 |
| 160 | [Cu]OC1=C(C(O)=O)C=CC=C1C(O)=O^C1(C2=CC=NC=C2)=CC=NC=C1%10%20%30%49 | 0.13 | + | # | * | -7.546 | -1.247 | -3.130 | -0.03 | -0.10 | 0.29 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| 161 | [Zn]c1cc(c(cc1C(=O)O)C(=O)O)C(=O)O%10%20%30%49 | 0.24 | - | # | * | -2.536 | 9.420 | -4.313 | 0.17 | 0.30 | 0.23 |
| 162 | [Zn]c1cc(c(cc1C(=O)O)C(=O)O)C(=O)O%10%20%30%49 | -0.51 | + | - | + | -2.536 | 9.420 | -4.313 | 0.17 | 0.30 | 0.23 |
| 163 | [Zn]C12=CC=CC=C1NN=N2^O=C(C1=CC=C(C(O)=O)S1)O%10%20%30%49 | 0.19 | - | # | - | -4.084 | 2.667 | -11.101 | 0.11 | 0.05 | -0.08 |
| 164 | [Cu]OC1=C(C(O)=O)C=CC=C1C(O)=O%10%20%30%49 | 0.34 | * | + | # | -11.131 | -2.012 | -6.995 | -0.17 | -0.13 | 0.11 |
| 165 | [Yb]O=C(C1=CC(C2=CC=C(C(O)=O)C=C2)=CC(C(O)=O)=C1)O%10%20%30%49 | -0.15 | * | # | - | -6.095 | -2.731 | -12.132 | 0.03 | -0.15 | -0.13 |
| 166 | [Co]c1[nH]c(c-2ncnc2n1)N^CC(=O)O%11%20%30%49 | 0.11 | # | # | * | -4.851 | -0.531 | -5.094 | 0.08 | -0.07 | 0.20 |
| 167 | [Zn]c1cc(ccc1C(=O)O)C(=O)O^C1CN2CCN1CC2%13%21%30%49 | 0.31 | - | * | - | 2.820 | 13.996 | -1.107 | 0.38 | 0.47 | 0.38 |
| 168 | [Cu]O=C(C1=CC(C(O)=O)=CC(NC2=NC(NC3=CC(C(O)=O)=CC(C(O)=O)=C3)=NC(NC4=CC(C(O)=O)=CC(C(O)=O)=C4)=N2)=C1)O%11%21%30%49 | 0.71 | + | * | # | 16.033 | 23.471 | 4.076 | 0.90 | 0.82 | 0.62 |
| 169 | [In]O=C(C1=CC(C(O)=O)=CC(C(O)=O)=C1)O%10%20%30%49 | 0.56 | + | # | + | -6.382 | 1.854 | -6.140 | 0.02 | 0.02 | 0.15 |
| 170 | [In]O=C(C1=CC(C(O)=O)=CC(C(O)=O)=C1)O%10%20%30%49 | 0.39 | - | - | + | -6.382 | 1.854 | -6.140 | 0.02 | 0.02 | 0.15 |
| 171 | [Cu]O=C(O)C1=CC=C(C2=NC(C3=CC=C(C=C3)C(O)=O)=NC(C4=CC=C(C=C4)C(O)=O)=N2)C=C1%16%22%30%49 | 0.63 | + | * | * | 2.387 | 9.402 | -2.224 | 0.36 | 0.30 | 0.33 |
| 172 | [Zn]O=C(C1=CC=C(C2=CC=C(C(O)=O)C=C2)C=C1)O%13%21%30%49 | 0.25 | * | + | + | -2.454 | 4.683 | -2.323 | 0.17 | 0.12 | 0.33 |
| 173 | [Zn]c1cc(ccc1C(=O)O)C(=O)O^C1CN2CCN1CC2%12%22%30%49 | 0.27 | - | + | # | -1.345 | 11.199 | 0.472 | 0.22 | 0.37 | 0.45 |
| 174 | [Ni]c1cc(ccc1C(=O)O)C(=O)O^C1CN2CCN1CC2%13%22%30%49 | 0.34 | * | # | * | -5.518 | 6.411 | -4.439 | 0.05 | 0.19 | 0.23 |
| 175 | [Cu]c1cc(ccc1C(=O)O)C(=O)O^C1CN2CCN1CC2%12%22%30%49 | 0.16 | - | + | - | -2.441 | 9.421 | -1.127 | 0.17 | 0.30 | 0.38 |
| 176 | [Co]c1cc(ccc1C(=O)O)C(=O)O^C1CN2CCN1CC2%13%22%30%49 | 0.01 | - | - | # | -4.825 | 7.402 | -0.491 | 0.08 | 0.22 | 0.41 |
| 177 | [Yb]OC(C(C=C1)=CC=C1C2=CC(C3=CC(C4=CC(C5=CC=C(C(O)=O)C=C5)=CC(C6=CC=C(C(O)=O)C=C6)=C4)=CC(C7=CC(C8=CC(C(O)=O)=CC=C8)=CC(C9=CC=C(C(O)=O)C=C9)=C7)=C3)=CC(C%10=CC=C(C(O)=O)C=C%10)=C2)=O%13%21%30%49 | 0.27 | + | # | # | -5.743 | 3.224 | -4.865 | 0.04 | 0.07 | 0.21 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| 178 | [Cu]OC(C1=CC(C2=C(C=C(Cl)C=C3)C3=C(C4=C(C=CC(Cl)=C5)C5=C(C6=CC(C(O)=O)=CC(C(O)=O)=C6)C=C4OCC)C(OCC)=C2)=CC(C(O)=O)=C1)=O%12%20%35%49 | 1.10 | + | + | # | 24.943 | 29.765 | 9.547 | 1.25 | 1.06 | 0.87 |
| 179 | [Cu]OC(C1=CC(C#CC#CC2=CC(C(O)=O)=CC(C(O)=O)=C2)=CC(C(O)=O)=C1)=O%14%21%35%49 | 1.35 | - | + | * | 26.410 | 36.961 | 23.245 | 1.31 | 1.32 | 1.51 |
| 180 | [Cu]OC(C1=CC(C(O)=O)=CC(N2C(C(C=C(C(N(C3=CC(C(O)=O)=CC(C(O)=O)=C3)C4=O)=O)C4=C5)=C5C2=O)=O)=C1)=O%13%21%39%49 | 1.24 | - | - | - | 17.990 | 30.425 | 8.143 | 0.98 | 1.08 | 0.81 |
| 181 | [Cu]OC(C1=CC(C(O)=O)=CC(N2C(C(C=C(C(N(C3=CC(C(O)=O)=CC(C(O)=O)=C3)C4=O)=O)C4=C5)=C5C2=O)=O)=C1)=O%13%21%30%49 | 0.56 | # | + | - | 1.752 | 9.965 | -3.453 | 0.34 | 0.32 | 0.27 |
| 182 | [Cu]OC(C1=CC(C(O)=O)=CC(N2C(C(C=C(C(N(C3=CC(C(O)=O)=CC(C(O)=O)=C3)C4=O)=O)C4=C5)=C5C2=O)=O)=C1)=O%13%21%30%49 | -0.19 | - | + | + | 1.752 | 9.965 | -3.453 | 0.34 | 0.32 | 0.27 |
| 183 | [Cu]OC(C1=CC(C#CC#CC2=CC(C#CC#CC3=CC(C(O)=O)=CC(C(O)=O)=C3)=CC(C#CC#CC4=CC(C(O)=O)=CC(C(O)=O)=C4)=C2)=CC(C(O)=O)=C1)=O%17%22%30%49 | 0.04 | Outlier | | | | | | | | |
| 184 | [Zn]Cc1[nH]nnn1%11%20%30%49 | 0.49 | * | - | - | -6.087 | 9.723 | -4.383 | 0.03 | 0.31 | 0.23 |
| 185 | [Zn]O=C(C1=CC=C2C=C(C(O)=O)C=CC2=C1)O%12%20%30%49 | 0.25 | - | # | # | -1.033 | 7.162 | -1.177 | 0.23 | 0.22 | 0.38 |
| 186 | [Zn]O=C(C1=CC=C2C=C(C(O)=O)C=CC2=C1)O%12%20%49 | 1.16 | # | + | - | 20.963 | 19.605 | 9.912 | 1.10 | 0.68 | 0.89 |
| 187 | [Zn]O=C(C1=CC=C2C=C(C(O)=O)C=CC2=C1)O%12%20%35%49 | 1.07 | + | # | - | 17.213 | 27.320 | 15.807 | 0.95 | 0.97 | 1.16 |
| 188 | [Zn]O=C(C1=CC([N](O)=O)=C2C=C(C(O)=O)C=C([N](O)=O)C2=C1)O%11%20%30%49 | -0.06 | - | + | - | 10.990 | 16.414 | 0.806 | 0.70 | 0.56 | 0.47 |
| 189 | [Zn]O=C(C1=CC([N](O)=O)=C2C=C(C(O)=O)C=C([N](O)=O)C2=C1)O%11%20%30%49 | 1.04 | + | # | - | 10.990 | 16.414 | 0.806 | 0.70 | 0.56 | 0.47 |
| 190 | [Zn]O=C(C1=CC([N](O)=O)=C2C=C(C(O)=O)C=C([N](O)=O)C2=C1)O%11%20%30%49 | 0.86 | + | + | - | 10.990 | 16.414 | 0.806 | 0.70 | 0.56 | 0.47 |
| 191 | [Cu]O=C(C1=CC=C(C2=CC(C3=CC=C(C(O)=O)C=C3)=CC(C#CC4=CC(C(O)=O)=CC(C(O)=O)=C4)=C2)C=C1)O%16%22%30%49 | 0.28 | * | * | - | 4.541 | 14.615 | 2.285 | 0.45 | 0.49 | 0.54 |
| 192 | [Cu]O=C(C1=CC=C(C2=CC(C3=CC=C(C(O)=O)C=C3)=CC(C#CC4=CC(C(O)=O)=CC(C(O)=O)=C4)=C2)C=C1)O%16%22%37%49 | 1.05 | + | * | * | 24.680 | 22.274 | 12.998 | 1.24 | 0.78 | 1.03 |
| 193 | [Cu]O=C(C1=CC(C(O)=O)=CC(C2=NNN=N2)=C1)O%14%21%30%49 | 0.40 | * | - | * | 3.470 | 8.644 | -1.835 | 0.41 | 0.27 | 0.35 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 194 | [Cu]O=C(O)C1=CC(OCC2=CC(C(O)=O)=CC(C(O)=O)=C2)=CC(C(O)=O)=C1%12%21%30%49 | 0.74 | # | * | + | 1.956 | 17.096 | 0.241 | 0.35 | 0.58 | 0.44 |
| 195 | [Cu]O=C(O)C1=CC(C2=CC(CC3=C4C=CC(C5=CC(C(O)=O)=CC(C(O)=O)=C5)=C3)=C4C=C2)=CC(C(O)=O)=C1%13%21%30%49 | 0.57 | + | - | - | 0.210 | 6.010 | -0.112 | 0.28 | 0.17 | 0.43 |
| 196 | [Cu]O=C(O)C1=CC(C2=NC=C(C3=CC(C(O)=O)=CC(C(O)=O)=C3)C=C2)=CC(C(O)=O)=C1%14%21%30%49 | 0.58 | * | + | * | 11.492 | 26.904 | 3.879 | 0.72 | 0.95 | 0.61 |
| 197 | [In]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%11%20%30%49 | 0.44 | - | - | * | 4.577 | 13.782 | -0.536 | 0.45 | 0.46 | 0.41 |
| 198 | [In][Ni]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%11%20%30%49 | 0.44 | + | # | # | 10.540 | 15.755 | 3.799 | 0.69 | 0.54 | 0.61 |
| 199 | [In][Co]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%11%20%30%49 | 0.54 | # | # | - | 11.233 | 16.746 | 7.747 | 0.71 | 0.57 | 0.79 |
| 200 | [In][Mn]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%11%20%30%49 | 0.51 | - | * | - | 10.485 | 15.926 | 0.642 | 0.68 | 0.54 | 0.46 |
| 201 | [In][Mg]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%12%20%30%49 | 0.71 | # | + | + | 15.265 | 20.880 | 8.335 | 0.87 | 0.73 | 0.82 |
| 202 | [Ga][Mg]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%11%20%30%49 | 0.55 | # | # | # | 5.344 | 14.267 | 2.376 | 0.48 | 0.48 | 0.54 |
| 203 | [Fe][Mg]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%12%21%30%49 | 0.75 | # | # | * | 12.805 | 19.188 | 5.800 | 0.77 | 0.66 | 0.70 |
| 204 | [V][Mg]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%11%20%30%49 | 0.56 | - | # | * | 11.310 | 25.597 | 9.544 | 0.72 | 0.90 | 0.87 |
| 205 | [Sc][Mg]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%11%20%30%49 | 0.44 | # | + | # | 9.266 | 17.821 | 0.330 | 0.64 | 0.61 | 0.45 |
| 206 | [In]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%11%20%30%49 | 0.69 | # | - | - | 4.577 | 13.782 | -0.536 | 0.45 | 0.46 | 0.41 |
| 207 | [In][Ni]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%11%20%30%49 | 0.65 | # | # | * | 10.540 | 15.755 | 3.799 | 0.69 | 0.54 | 0.61 |
| 208 | [In][Co]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%11%20%30%49 | 0.79 | # | + | - | 11.233 | 16.746 | 7.747 | 0.71 | 0.57 | 0.79 |
| 209 | [In][Mn]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%11%20%30%49 | 0.75 | # | * | # | 10.485 | 15.926 | 0.642 | 0.68 | 0.54 | 0.46 |
| 210 | [In][Mg]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%12%20%30%49 | 0.93 | # | - | + | 15.265 | 20.880 | 8.335 | 0.87 | 0.73 | 0.82 |
| 211 | [Ga][Mg]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%11%20%30%49 | 0.78 | * | * | - | 5.344 | 14.267 | 2.376 | 0.48 | 0.48 | 0.54 |
| 212 | [Fe][Mg]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%12%21%30%49 | 0.97 | - | - | * | 12.805 | 19.188 | 5.800 | 0.77 | 0.66 | 0.70 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 213 | [V][Mg]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%11%20%30%49 | 0.84 | + | + | - | 11.310 | 25.597 | 9.544 | 0.72 | 0.90 | 0.87 |
| 214 | [Sc][Mg]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%11%20%30%49 | 0.74 | + | + | * | 9.266 | 17.821 | 0.330 | 0.64 | 0.61 | 0.45 |
| 215 | [In][Co]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O^O=C(C1=CC=C(C(O)=O)C=C1)O%11%20%30%49 | 0.33 | * | - | + | 12.502 | 20.402 | 5.085 | 0.76 | 0.71 | 0.67 |
| 216 | [In][Co]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O^O=C(C1=CC=C(C(O)=O)C=C1)O%11%20%30%49 | 0.61 | - | * | * | 12.502 | 20.402 | 5.085 | 0.76 | 0.71 | 0.67 |
| 217 | [In][Nd]O=C(C1=CC=C(C2=CC(C3=CC=C(C(O)=O)C=C3)=CC(C4=CC=C(C(O)=O)C=C4)=C2)C=C1)O%10%20%30%49 | 0.23 | * | + | - | -3.913 | 1.952 | -6.050 | 0.12 | 0.02 | 0.15 |
| 218 | [In]O=C(C1=CC=C(C2=CC=C(C(O)=O)C=C2)C=C1)O%11%20%30%49 | 0.31 | * | * | # | -4.066 | 1.291 | -5.400 | 0.11 | 0.00 | 0.18 |
| 219 | [Mg]O=C(C1=CC=C(C2=C(C)C=C(C3=CC=C(C(O)=O)C(O)=C3)C=C2)C=C1O)O%14%21%30%49 | 0.47 | # | - | + | 3.771 | 16.482 | -3.467 | 0.42 | 0.56 | 0.27 |
| 220 | [Mg]O=C(C1=CC=C(C2=C(N)C=C(C3=CC=C(C(O)=O)C(O)=C3)C=C2)C=C1O)O%14%21%30%49 | 0.50 | # | # | * | 2.759 | 15.575 | -4.345 | 0.38 | 0.53 | 0.23 |
| 221 | [Mg]O=C(C1=CC=C(C2=C(CNC(OC(C)(C)C)=O)C=C(C3=CC=C(C(O)=O)C(O)=C3)C=C2)C=C1O)O%13%21%30%49 | 0.32 | - | * | + | 9.183 | 19.681 | -0.499 | 0.63 | 0.68 | 0.41 |
| 222 | [Mg]O=C(C1=CC=C(C2=C(CN)C=C(C3=CC=C(C(O)=O)C(O)=C3)C=C2)C=C1O)O%13%21%30%49 | 0.51 | - | - | + | 4.768 | 14.834 | -3.527 | 0.46 | 0.50 | 0.27 |
| 223 | [Mg]O=C(C1=CC=C(C2=C(CN(C)C(OC(C)(C)C)=O)C=C(C3=CC=C(C(O)=O)C(O)=C3)C=C2)C=C1O)O%13%21%30%49 | 0.28 | + | + | - | 6.608 | 18.854 | -3.122 | 0.53 | 0.65 | 0.29 |
| 224 | [Mg]O=C(C1=CC=C(C2=C(CNC)C=C(C3=CC=C(C(O)=O)C(O)=C3)C=C2)C=C1O)O%13%21%30%49 | 0.46 | # | - | * | 7.888 | 17.115 | -1.476 | 0.58 | 0.59 | 0.36 |
| 225 | [Al]c1cc(ccc1C(=O)O)C(=O)O%12%20%34%49 | 0.83 | - | * | + | 8.860 | 22.809 | 14.568 | 0.62 | 0.80 | 1.11 |
| 226 | [Al]c1cc(ccc1C(=O)O)C(=O)O%12%20%35%49 | 1.02 | - | * | + | 19.410 | 26.790 | 10.684 | 1.03 | 0.95 | 0.93 |
| 227 | [Al]c1cc(ccc1C(=O)O)C(=O)O%12%20%30%49 | 0.00 | + | * | + | 1.163 | 6.633 | -6.300 | 0.32 | 0.20 | 0.14 |
| 228 | [Zr]O=P(CC1=CC=C(C2=NC(C3=CC=C(CP(O)(O)=O)C=C3)=NC(C4=CC=C(CP(O)(O)=O)C=C4)=N2)C=C1)(O)O%10%20%31%49 | 0.53 | - | # | + | 3.828 | 14.201 | 1.362 | 0.42 | 0.48 | 0.50 |
| 229 | [Zr]O=P(CC1=CC=C(C2=NC(C3=CC=C(CP(O)(O)=O)C=C3)=NC(C4=CC=C(CP(O)(O)=O)C=C4)=N2)C=C1)(O)O%10%20%31%49 | 0.49 | + | + | # | 3.828 | 14.201 | 1.362 | 0.42 | 0.48 | 0.50 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 230 | [Co]NC1=NC=NC2=C1NC=N2^CC(O)=O%11%20%30%49 | 0.82 | + | + | - | 3.678 | 8.155 | 1.225 | 0.42 | 0.25 | 0.49 |
| 231 | [Co]NC1=NC=NC2=C1NC=N2^CC(O)=O%11%20%30%49 | 0.61 | + | - | - | 3.678 | 8.155 | 1.225 | 0.42 | 0.25 | 0.49 |
| 232 | [Co]NC1=NC=NC2=C1NC=N2^O=C(O)CC%11%20%30%49 | 0.65 | * | * | - | 3.493 | 6.738 | 2.126 | 0.41 | 0.20 | 0.53 |
| 233 | [Co]NC1=NC=NC2=C1NC=N2^O=C(O)CC%11%20%30%49 | 0.50 | + | - | - | 3.493 | 6.738 | 2.126 | 0.41 | 0.20 | 0.53 |
| 234 | [Co]NC1=NC=NC2=C1NC=N2^O=C(O)CCC%10%20%30%49 | 0.43 | # | - | # | 0.087 | 6.580 | -3.860 | 0.27 | 0.19 | 0.25 |
| 235 | [Co]NC1=NC=NC2=C1NC=N2^O=C(O)CCC%10%20%30%49 | 0.30 | * | * | * | 0.087 | 6.580 | -3.860 | 0.27 | 0.19 | 0.25 |
| 236 | [Co]NC1=NC=NC2=C1NC=N2^O=C(O)CCCC%10%20%30%49 | 0.30 | + | + | - | 0.622 | 6.707 | -3.531 | 0.29 | 0.20 | 0.27 |
| 237 | [Co]NC1=NC=NC2=C1NC=N2^O=C(O)CCCC%10%20%30%49 | 0.14 | + | - | * | 0.622 | 6.707 | -3.531 | 0.29 | 0.20 | 0.27 |
| 238 | [Zn]O=C(C1=CC(NC(C)=O)=C(C2=C(NC(C)=O)C=C(C(O)=O)C=C2)C=C1)O%11%20%30%49 | 0.67 | + | - | * | 1.568 | 9.732 | -1.374 | 0.33 | 0.31 | 0.37 |
| 239 | [Zn]O=C(C1=CC(NC(C)=O)=C(C2=C(NC(C)=O)C=C(C(O)=O)C=C2)C=C1)O%11%20%30%49 | 0.46 | - | # | # | 1.568 | 9.732 | -1.374 | 0.33 | 0.31 | 0.37 |
| 240 | [Zn]O=C(C1=CC(NC(C)=O)=C(C2=C(NC(C)=O)C=C(C(O)=O)C=C2)C=C1)O%11%20%30%49 | 0.31 | + | * | * | 1.568 | 9.732 | -1.374 | 0.33 | 0.31 | 0.37 |
| 241 | [Zn]O=C(C1=CC(NC(CCC)=O)=C(C2=C(NC(CCC)=O)C=C(C(O)=O)C=C2)C=C1)O%11%20%30%49 | 0.24 | # | # | * | 3.708 | 10.243 | -0.058 | 0.42 | 0.33 | 0.43 |
| 242 | [Cu]O=C(C1=CC(C(O)=O)=CC(OCC(COC2=CC(C(O)=O)=CC(C(O)=O)=C2)(COC3=CC(C(O)=O)=CC(C(O)=O)=C3)COC4=CC(C(O)=O)=CC(C(O)=O)=C4)=C1)O%12%21%30%49 | 0.67 | * | * | # | 8.541 | 23.640 | 5.531 | 0.61 | 0.83 | 0.69 |
| 243 | [Zn]O=C(C1=CC=C(C2=CC=C(C(O)=O)C=C2CS(C)(=O)=O)C=C1)O%12%21%30%47 | 1.27 | - | - | + | 18.734 | 26.788 | 12.736 | 1.01 | 0.95 | 1.02 |
| 244 | [Zn]O=C(C1=CC=C(C2=CC=C(C(O)=O)C=C2CS(C)(=O)=O)C=C1)O%12%21%30%49 | 0.15 | + | # | - | 6.378 | 14.936 | 1.648 | 0.52 | 0.50 | 0.51 |
| 245 | [Zn]O=C(C1=CC=C(C2=CC=C(C(O)=O)C=C2CS(C)(=O)=O)C=C1)O%12%21%31%49 | 0.81 | - | + | # | 15.959 | 24.837 | 14.980 | 0.90 | 0.87 | 1.12 |
| 246 | [Zn]O=C(C1=CC=C(C2=CC=C(C(O)=O)C=C2CS(CCC)(=O)=O)C=C1)O%12%20%30%47 | 1.19 | + | - | # | 18.083 | 24.522 | 13.805 | 0.98 | 0.86 | 1.07 |
| 247 | [Zn]O=C(C1=CC=C(C2=CC=C(C(O)=O)C=C2CS(CCC)(=O)=O)C=C1)O%12%20%30%49 | -0.01 | - | - | # | 5.727 | 12.670 | 2.717 | 0.50 | 0.42 | 0.56 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 248 | [Zn]O=C(C1=CC=C(C2=CC=C(C(O)=O)C=C2CS(CCC)(=O)=O)C=C1)O%12%20%31%49 | 0.78 | + | - | - | 15.327 | 22.425 | 8.013 | 0.87 | 0.78 | 0.80 |
| 249 | [Zr]c1cc(ccc1C(=O)O)C(=O)O%10%20%30%49 | -0.80 | - | + | # | -17.581 | -5.695 | -18.803 | -0.42 | -0.26 | -0.44 |
| 250 | [Zr]O=C(C1=CC=C(C(O)=O)C=C1N)O%10%20%30%49 | -0.55 | - | * | - | -22.712 | -8.884 | -20.250 | -0.62 | -0.38 | -0.50 |
| 251 | [Zr]O=C(C1=CC=C(C(O)=O)C=C1F)O%10%20%30%49 | -1.00 | - | + | + | -22.131 | -16.443 | -24.144 | -0.60 | -0.66 | -0.68 |
| 252 | [Zr]O=C(C1=CC=C2C=C(C(O)=O)C=CC2=C1)O%10%20%30%49 | -0.77 | - | + | # | -21.850 | -5.829 | -16.784 | -0.59 | -0.27 | -0.34 |
| 253 | [Zr]O=C(C1=CC=C(C2=CC=C(C(O)=O)C=C2)C=C1)O%11%20%30%49 | -0.74 | - | + | + | -18.298 | -6.000 | -15.612 | -0.45 | -0.27 | -0.29 |
| 254 | [Zr]O=C(C1=CC(C)=C(C2=CC=C(C(O)=O)C=C2C)C=C1)O%10%20%30%49 | -0.68 | - | - | # | -21.202 | 1.174 | -16.658 | -0.56 | -0.01 | -0.34 |
| 255 | [Zr]O=C(C1=CC=C(N=NC2=CC=C(C(O)=O)C(Cl)=C2)C=C1Cl)O%11%20%30%49 | -1.00 | Outlier | | | | | | | | |
| 256 | [Cu]FC(F)(F)C(C1=CC=C(C(C(O)=O)=C1)C(O)=O)(C2=CC=C(C(C(O)=O)=C2)C(O)=O)C(F)(F)F%10%20%30%49 | 0.32 | + | - | + | -2.587 | 18.580 | -3.990 | 0.17 | 0.64 | 0.25 |
| 257 | [Cu]O=C(C1=CC(/N=N/C2=CC(C(O)=O)=CC(C(O)=O)=C2)=CC(C(O)=O)=C1)O%14%21%30%49 | 0.94 | Outlier | | | | | | | | |
| 258 | [Cu]O=C(C1=CC(/N=N/C2=CC(C(O)=O)=CC(C(O)=O)=C2)=CC(C(O)=O)=C1)O%14%21%30%49 | 0.26 | # | + | - | 8.494 | 18.580 | 2.309 | 0.60 | 0.64 | 0.54 |
| 259 | [Zn]O=C(C1=CC=C(N(C2=CC=C(C(O)=O)C=C2)C3=CC=C(C4=CC=C(N(C5=CC=C(C(O)=O)C=C5)C6=CC=C(C(O)=O)C=C6)C=C4)C=C3)C=C1)O%11%20%30%49 | 0.06 | - | + | + | -12.270 | -8.122 | -16.877 | -0.21 | -0.35 | -0.35 |
| 260 | [Zn]O=C(C1=CC=C(N(C2=CC=C(C(O)=O)C=C2)C3=CC=C(C4=CC=C(N(C5=CC=C(C(O)=O)C=C5)C6=CC=C(C(O)=O)C=C6)C=C4)C=C3)C=C1)O%11%20%30%49 | -0.68 | + | + | + | -12.270 | -8.122 | -16.877 | -0.21 | -0.35 | -0.35 |

**Table S3.** Percentage of identity for three random splits

| | Set | Split 1 | Split 2 | Split 3 |
|---|---|---|---|---|
| Split 1 | Total | 100 | 28.7 | 26.4 |
| | Training | 100 | 33.3 | 33.8 |
| | Invisible training | 100 | 30.1 | 26.3 |
| | Calibration | 100 | 29.4 | 19.4 |
| | Validation | 100 | 18.6 | 22.2 |
| Split 2 | Total | | 100 | 23.6 |
| | Training | | 100 | 29.7 |
| | Invisible training | | 100 | 22.9 |
| | Calibration | | 100 | 21.1 |
| | Validation | | 100 | 18.9 |
| Split 3 | Total | | | 100 |
| | Training | | | 100 |
| | Invisible training | | | 100 |
| | Calibration | | | 100 |
| | Validation | | | 100 |

**Table S4.** Examples of quasi-SMILES and the relevant $CO_2$ uptake capacity

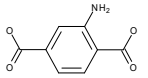
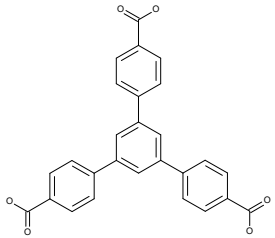
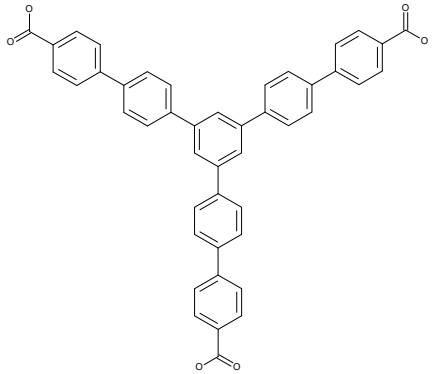
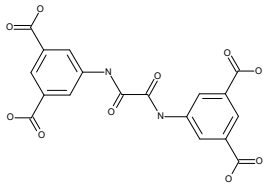
| No. | MOF | BET | Pore-volume | P (bar) | T(K) | Metal | Organic linker | Quasi-SMILES | $CO_2$ uptake capacity |
|---|---|---|---|---|---|---|---|---|---|
| 5 | IRMOF-3 | 1568 | 1.07 | 35 | 298 | Zn |  | [Zn]c1cc(c(cc1C(=O)O)N)C(=O)O%12%21%36%49 | 18.70 |
| 16 | MOF-177 | 4750 | 1.89 | 20 | 298 | Zn |  | [Zn]C1=CC(=CC=C1C2=CC(=CC(=C2)C3=CC=C(C=C3)C(=O)O)C4=CC=C(C=C4)C(=O)O)C(=O)O%17%22%33%49 | 28.00 |
| 18 | MOF-200 | 4530 | 3.59 | 50 | 298 | Zn |  | [Zn]c1cc(ccc1c2ccc(cc2)C(=O)O)c3cc(cc(c3)c4ccc(cc4)c5ccc(cc5)C(=O)O)c6ccc(cc6)c7ccc(cc7)C(=O)O%17%24%39%49 | 54.5 |
| 29 | SIFSIX-2-Cu-i | 735 | 0.26 | 0.01 | 298 | Cu and Si |  | [Cu][Si]c1cnccc1C#Cc2ccncc2%11%20%30%49 | 0.19 |
| 59 | NOTT-125 | 2471 | 1.1 | 1 | 298 | Cu |  | [Cu]O=C(NC1=CC(C(O)=O)=CC(C(O)=O)=C1)C(NC2=CC(C(O)=O)=CC(C(O)=O)=C2)=O%13%21%30%49 | 4.13 |

**Table S5**. The mathematical equations of various statistical criteria for predictive potential of the QSPR models

| Criterion of the predictive potential | Reference |
|---|---|
| $R^2 = 1 - \frac{\sum (Y_{obs} - Y_{prd})^2}{\sum (Y_{obs} - \bar{Y})^2}$ | [S86] |
| $Q^2 = 1 - \frac{\sum (Y_{prd} - Y_{obs})^2}{\sum (Y_{obs} - \overline{Y}_{train})^2}$ | [S87] |
| $Q^2_{F1} = 1 - \frac{\sum (Y_{per(test)} - Y_{obs(test)})^2}{\sum (Y_{obs(test)} - \overline{Y}_{train})^2}$ | [S88] |
| $Q^2_{F2} = 1 - \frac{\sum (Y_{prd(test)} - Y_{obs(test)})^2}{\sum (Y_{obs(test)} - \overline{Y}_{ext})^2}$ | [S88] |
| $Q^2_{F3} = 1 - \frac{\sum (Y_{prd(test)} - Y_{obs(test)})^2/n_{ext}}{\sum (Y_{obs(test)} - \overline{Y}_{train})^2/n_{train}}$ | [S88] |
| $r^2_m = r^2 \times \left(1 - \sqrt{r^2 - r_0^2}\right)$ | [S86] |
| $CCC = \frac{2\sum (X - \bar{X})(Y - \bar{Y})}{\sum (X - \bar{X})^2 + \sum (Y - \bar{Y})^2 + n((\bar{X} - \bar{Y})^2}$ | [S89] |
| $C_{R^2_p} = R\sqrt{\left(R^2 - R^2_r\right)}$ | [S86] |
| $MAE = \frac{1}{n} \times \sum \lvert Y_{obs} - Y_{prd} \rvert$ | [S86] |

**Table S6.** The calculation results of DCW(3, 14) of attributes for [Cu]c1c(cc(cc1C(=O)O)C(=O)O)C(=O)O%12%20%30%49, DCW= 4.856, split 1 and TF2

| AK | DCW(AK) | $N_{TRN}$ | $N_{iTRN}$ | $N_{CAL}$ |
|---|---|---|---|---|
| [..... | 0.9441 | 81 | 79 | 49 |
| Cu..... | 0.4246 | 23 | 20 | 14 |
| [..... | 0.9441 | 81 | 79 | 49 |
| c..... | 0.006 | 27 | 37 | 23 |
| 1..... | 0.139 | 78 | 79 | 49 |
| c..... | 0.006 | 27 | 37 | 23 |
| (..... | -0.6727 | 80 | 78 | 49 |
| c..... | 0.006 | 27 | 37 | 23 |
| c..... | 0.006 | 27 | 37 | 23 |
| (..... | -0.6727 | 80 | 78 | 49 |
| c..... | 0.006 | 27 | 37 | 23 |
| c..... | 0.006 | 27 | 37 | 23 |
| 1..... | 0.139 | 78 | 79 | 49 |
| C..... | 0.3737 | 81 | 79 | 49 |
| (..... | -0.6727 | 80 | 78 | 49 |
| =..... | 0.2556 | 81 | 78 | 49 |
| O..... | 0.3118 | 75 | 74 | 47 |
| (..... | -0.6727 | 80 | 78 | 49 |
| O..... | 0.3118 | 75 | 74 | 47 |
| (..... | -0.6727 | 80 | 78 | 49 |
| C..... | 0.3737 | 81 | 79 | 49 |
| (..... | -0.6727 | 80 | 78 | 49 |
| =..... | 0.2556 | 81 | 78 | 49 |
| O..... | 0.3118 | 75 | 74 | 47 |
| (..... | -0.6727 | 80 | 78 | 49 |
| O..... | 0.3118 | 75 | 74 | 47 |
| (..... | -0.6727 | 80 | 78 | 49 |
| C..... | 0.3737 | 81 | 79 | 49 |
| (..... | -0.6727 | 80 | 78 | 49 |
| =..... | 0.2556 | 81 | 78 | 49 |
| O..... | 0.3118 | 75 | 74 | 47 |
| (..... | -0.6727 | 80 | 78 | 49 |
| O..... | 0.3118 | 75 | 74 | 47 |
| %12..... | 0.4258 | 20 | 16 | 8 |
| %20..... | -0.986 | 57 | 50 | 28 |
| %30..... | -2.4445 | 64 | 55 | 37 |
| %49..... | -3.2085 | 77 | 76 | 46 |
| [...Cu..... | 1.6081 | 23 | 20 | 14 |

| | | | | |
|---|---|---|---|---|
| [...Cu..... | 1.6081 | 23 | 20 | 14 |
| c...[..... | 0.0675 | 25 | 33 | 21 |
| c...1..... | 0.0768 | 27 | 37 | 23 |
| c...1..... | 0.0768 | 27 | 37 | 23 |
| c...(..... | 0.9131 | 27 | 35 | 23 |
| c...(..... | 0.9131 | 27 | 35 | 23 |
| c...c..... | 0.2995 | 27 | 37 | 22 |
| c...(..... | 0.9131 | 27 | 35 | 23 |
| c...(..... | 0.9131 | 27 | 35 | 23 |
| c...c..... | 0.2995 | 27 | 37 | 22 |
| c...1..... | 0.0768 | 27 | 37 | 23 |
| C...1..... | -1.1973 | 66 | 69 | 43 |
| C...(..... | 0.2856 | 79 | 78 | 49 |
| =...(..... | 0.1224 | 76 | 78 | 48 |
| O...=..... | 0.6776 | 75 | 74 | 47 |
| O...(..... | 0.4192 | 75 | 73 | 47 |
| O...(..... | 0.4192 | 75 | 73 | 47 |
| O...(..... | 0.4192 | 75 | 73 | 47 |
| C...(..... | 0.2856 | 79 | 78 | 49 |
| C...(..... | 0.2856 | 79 | 78 | 49 |
| =...(..... | 0.1224 | 76 | 78 | 48 |
| O...=..... | 0.6776 | 75 | 74 | 47 |
| O...(..... | 0.4192 | 75 | 73 | 47 |
| O...(..... | 0.4192 | 75 | 73 | 47 |
| O...(..... | 0.4192 | 75 | 73 | 47 |
| C...(..... | 0.2856 | 79 | 78 | 49 |
| C...(..... | 0.2856 | 79 | 78 | 49 |
| =...(..... | 0.1224 | 76 | 78 | 48 |
| O...=..... | 0.6776 | 75 | 74 | 47 |
| O...(..... | 0.4192 | 75 | 73 | 47 |
| O...(..... | 0.4192 | 75 | 73 | 47 |
| O...%12..... | 2.2101 | 12 | 9 | 6 |
| %20.%12..... | 0.7037 | 14 | 11 | 4 |
| %30.%20..... | -1.3489 | 46 | 40 | 25 |
| %49.%30..... | -3.9033 | 60 | 52 | 34 |

**Table S7.** Correlation coefficient for training set ($R^2_{TRN}$), invisible training set ($R^2_{iTRN}$) and calibration set ($R^2_{CAL}$) after several Y-randomization test for models based on $TF_2$

| | Split 1 | | | Split 2 | | | Split 3 | | |
|---|---|---|---|---|---|---|---|---|---|
| | $R^2_{TRN}$ | $R^2_{iTRN}$ | $R^2_{CAL}$ | $R^2_{TRN}$ | $R^2_{iTRN}$ | $R^2_{CAL}$ | $R^2_{TRN}$ | $R^2_{iTRN}$ | $R^2_{CAL}$ |
| 1 | 0.0039 | 0.0029 | 0.0806 | 0.0119 | 0.0723 | 0.0146 | 0.0009 | 0.0066 | 0.0000 |
| 2 | 0.0073 | 0.0024 | 0.0171 | 0.0052 | 0.0020 | 0.0044 | 0.0350 | 0.0074 | 0.0123 |
| 3 | 0.0014 | 0.0003 | 0.0204 | 0.0153 | 0.0291 | 0.0114 | 0.0170 | 0.0002 | 0.0045 |
| 4 | 0.0121 | 0.0050 | 0.0019 | 0.0133 | 0.0001 | 0.0013 | 0.0062 | 0.0315 | 0.0000 |
| 5 | 0.0015 | 0.0388 | 0.0124 | 0.0009 | 0.0000 | 0.1216 | 0.0046 | 0.0025 | 0.0050 |
| 6 | 0.0001 | 0.0008 | 0.0182 | 0.0320 | 0.0001 | 0.0004 | 0.0250 | 0.0000 | 0.0181 |
| 7 | 0.0541 | 0.0050 | 0.0006 | 0.0005 | 0.0102 | 0.0216 | 0.0229 | 0.0196 | 0.0035 |
| 8 | 0.0076 | 0.0051 | 0.0070 | 0.0219 | 0.0039 | 0.0000 | 0.0001 | 0.0006 | 0.0000 |
| 9 | 0.0079 | 0.0381 | 0.0718 | 0.0076 | 0.0048 | 0.0124 | 0.0006 | 0.0087 | 0.0090 |
| 10 | 0.0001 | 0.0061 | 0.0229 | 0.0086 | 0.0034 | 0.0173 | 0.0002 | 0.0159 | 0.0006 |
| Average | 0.0096 | 0.0104 | 0.0253 | 0.0117 | 0.0126 | 0.0205 | 0.0112 | 0.0093 | 0.0053 |

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