The following tables show the coformers found in the red and yellow clusters described at the end of the results section. Where possible, the CSD refcode is provided. For coformers that do not have an identifiable refcode, the canonical SMILES code is provided instead.

This table holds the coformers for the red cluster:

| # | degree | CSD refcode/canonical SMILES code |
|---|---|---|
| 1 | 13 | DOCDAC |
| 2 | 10 | AMXBPM10 |
| 3 | 9 | Fc1c(F)c(C(=O)O)c(c(c1Br)F)F |
| 4 | 9 | TEKKUP |
| 5 | 8 | ETYNBZ |
| 6 | 8 | Oc1c(F)c(F)c(c(c1F)F)I |
| 7 | 7 | Fc1cc(F)c(c(c1F)I)F |
| 8 | 7 | DNEDAM |
| 9 | 7 | Oc1c(F)c(F)c(c(c1F)F)Br |
| 10 | 7 | OC(=O)[C@@H]1C[C@@H](C[C@@H](C1)C(=O)O)C(=O)O |
| 11 | 7 | Oc1cc(cc(c1)O)c1c2ccccc2c(c2c1cccc2)c1cc(O)cc(c1)O |
| 12 | 6 | KOFJUK |
| 13 | 6 | DOCCOP |
| 14 | 6 | VITKAL |
| 15 | 6 | NAPHOL |
| 16 | 6 | NOMBEA |
| 17 | 5 | AWEXOQ |
| 18 | 5 | WEBNUO |
| 19 | 5 | WEBMIB |
| 20 | 5 | IC#Cc1cccc2c1cc1c(cccc1c2)C#CI |
| 21 | 5 | EGEPEO |
| 22 | 5 | AJEYAQ |
| 23 | 5 | Oc1ccc(cc1)[C@@]12C[C@H]3C[C@@H](C1)C[C@@](C2)(C3)c1ccc(cc1)O |
| 24 | 5 | Nc1ccc(cc1)/N=N/c1ccccc1 |
| 25 | 4 | TELXAJ |
| 26 | 4 | SILGOK |
| 27 | 4 | IC#Cc1ccccc1C#CI |
| 28 | 4 | WEBNOI |
| 29 | 4 | WEBMUN |
| 30 | 4 | WEBNAU |

| | | |
|---|---|---|
| 31 | 4 | WEBMOH |
| 32 | 4 | PIDGOZ |
| 33 | 4 | TETBBZ22 |
| 34 | 4 | VITJUE |
| 35 | 4 | VAMBOA |
| 36 | 4 | C[Te]C#Cc1cccc2c1cc1c(cccc1c2)C#C[Te]C |
| 37 | 4 | RIJHIE |
| 38 | 4 | ZEHGEY |
| 39 | 4 | N#Cc1cc(O)cc(c1)O |
| 40 | 4 | TICHUI |
| 41 | 4 | IKACUT |
| 42 | 4 | GIMBOT |
| 43 | 4 | Oc1ccc(cc1Sc1cc(Cl)ccc1O)Cl |
| 44 | 4 | OHADAD |
| 45 | 4 | GUWCOQ |
| 46 | 4 | PEXBZA |
| 47 | 4 | MAMPOL |
| 48 | 4 | WINWUL |
| 49 | 4 | SAFNIW |
| 50 | 3 | CC(=O)c1c(O)cc(cc1O)O |
| 51 | 3 | JOQKEF |
| 52 | 3 | CROTAC |
| 53 | 3 | BIFFAZ |
| 54 | 3 | TERRUD01 |
| 55 | 3 | UNADUK |
| 56 | 3 | PEYRAP |
| 57 | 3 | WEBNEY |
| 58 | 3 | IKAYEZ |
| 59 | 3 | OC(=O)COc1cccc(c1)C(=O)O |
| 60 | 3 | CC([Si](c1cc(cc(c1)[Si](C(C)C)(C(C)C)O)[Si](C(C)C)(C(C)C)O)(C(C)C)O)C |
| 61 | 3 | DOCCUV |
| 62 | 3 | ATUVIU |
| 63 | 3 | XAPVOA |
| 64 | 3 | OC(=O)[C@@H]1[C@@H](C(=O)O)[C@@H]2c3c([C@H]1c1c2cccc1)cccc3 |

| | | |
|---|---|---|
| 65 | 3 | TUVXAM |
| 66 | 3 | DOYJEH |
| 67 | 3 | QQQBSS01 |
| 68 | 3 | OC(=O)c1c[nH]c(=O)[nH]c1=O |
| 69 | 3 | TAJPAW |
| 70 | 3 | MIQVUF |
| 71 | 3 | ABEGEU |
| 72 | 3 | IC#Cc1cccc(c1)N(=O)=O |
| 73 | 3 | IC#Cc1ccc(cc1)I |
| 74 | 3 | BUXBZA |
| 75 | 3 | ZZZLAO10 |
| 76 | 3 | IC#C[C@@]1(O)CC[C@](CC1)(O)C#CI |
| 77 | 3 | HIXVIW |
| 78 | 3 | O=C(c1c(F)c(F)c(c(c1F)F)I)Nc1c(F)c(F)c(c(c1F)F)Br |
| 79 | 3 | OC(=O)c1ccc(cc1)Oc1nc(nc(n1)Oc1ccc(cc1)C(=O)O)Oc1ccc(cc1)C(=O)O |
| 80 | 3 | Oc1ccc(cc1Cl)[C@]12C[C@@H]3C[C@H](C1)C[C@](C2)(C3)c1ccc(c(c1)Cl)O |
| 81 | 3 | DEBJUQ |
| 82 | 3 | IMOQIN |
| 83 | 3 | LURNOB |
| 84 | 3 | WUMHAQ01 |
| 85 | 3 | Fc1cc(F)c(c(c1F)Br)F |
| 86 | 3 | SULDAZ |
| 87 | 3 | ETEYUX02 |
| 88 | 3 | PAXNIL |
| 89 | 2 | O[C@H]([C@@H](C(O)O)O)C(O)O |
| 90 | 2 | VAPBIY |
| 91 | 2 | WIGPUZ |
| 92 | 2 | Clc1c(Cl)c(Cl)c(c(c1Cl)I)I |
| 93 | 2 | Brc1cc(Br)c(c(c1)Br)O |
| 94 | 2 | CCc1c(C(=O)O)c(CC)c(c(c1C(=O)O)CC)C(=O)O |
| 95 | 2 | N#C[Se]CC#CC#CC[Se]C#N |
| 96 | 2 | UYIREB |
| 97 | 2 | UYIRAX |
| 98 | 2 | BOLNEW |

| | | |
|---|---|---|
| 99 | 2 | FESNOG |
| 100 | 2 | OC(=O)c1ccc(c(c1)C(=O)O)O |
| 101 | 2 | F[C@@H]1[C@H](Br)[C@@H](F)[C@H]([C@H]([C@@H]1F)Br)F |
| 102 | 2 | F[C@H]1[C@@H](Br)[C@H](F)[C@@H]([C@@H]([C@H]1F)Br)F |
| 103 | 2 | WEBNIC |
| 104 | 2 | Cl[C@@H]1[C@H](I)[C@@H](Cl)[C@H]([C@H]([C@@H]1Cl)I)Cl |
| 105 | 2 | SUGYEZ |
| 106 | 2 | DOCCEF |
| 107 | 2 | PUYTEI |
| 108 | 2 | KEQTIL |
| 109 | 2 | OC(=O)CCC[Si](O[Si](CCCC(=O)O)(C)C)(C)C |
| 110 | 2 | C#CCCCC(=O)O |
| 111 | 2 | BOXMUZ |
| 112 | 2 | IHAHIL |
| 113 | 2 | HIHJIR |
| 114 | 2 | MAGHIO |
| 115 | 2 | C#C[C@@]1(O)CC[C@](CC1)(O)C#C |
| 116 | 2 | TOYPUS |
| 117 | 2 | WACJUF |
| 118 | 2 | OJURAO |
| 119 | 2 | OC(=O)c1cc(O)c(c(c1)O)Br |
| 120 | 2 | C[Te]C#Cc1c(F)c(F)c(c(c1F)F)C#C[Te]C |
| 121 | 2 | IMOQOT |
| 122 | 2 | ADOGUW |
| 123 | 2 | PINPIL01 |
| 124 | 2 | IGALUY |
| 125 | 2 | OJIHAQ |
| 126 | 2 | C[C@@]12CC[C@@](c3c1cc(O)c(c3)O)(c1c2cc(O)c(c1)O)C |
| 127 | 2 | C[C@H]1c2cc(c(cc2O)O)[C@@H](C)c2cc(c(cc2O)O)[C@@H](c2cc([C@@H](c3cc1c(O)cc3O)C)c(O)cc2O)C |
| 128 | 2 | FC(C(C(C(C(I)(F)F)(F)F)(F)F)(F)F)(C(C(C(C(C(I)(F)F)(F)F)(F)F)(F)F)(F)F)F |
| 129 | 2 | Fc1c(OCc2ccc(cc2)OP2(=NP(=NP(=N2)(Oc2ccc(cc2)COc2c(F)c(F)c(c(c2F)F)I)Oc2ccc(cc2)COc2c(F)c(F)c(c(c2F)F)I)(Oc2ccc(cc2)COc2c(F)c(F)c(c(c2F)F)I)Oc2ccc(cc2)COc2c(F)c(F)c(c(c2F)F)I)Oc2ccc(cc2)COc2c (F)c(F)c(c(c2F)F)I)c(F)c(c(c1F)I)F |
| 130 | 2 | POXYEH |
| 131 | 2 | FEDHUU |

| | | |
|---|---|---|
| 132 | 2 | GEMXEB |
| 133 | 2 | UHELOI |
| 134 | 2 | RASCEU |
| 135 | 2 | Oc1cc2O[C@H](c3cc(O)c(c(c3)O)O)[C@H](C(=O)c2c(c1)O)O |
| 136 | 2 | OTATAF |

This table holds the coformers for the yellow cluster:

| # | degree | CSD refcode/canonical SMILES code |
|---|---|---|
| 1 | 18 | PENDAM |
| 2 | 17 | AZSTBA |
| 3 | 16 | CICYOD |
| 4 | 15 | O=C1N(c2ccncc2)C(=O)c2c3c1ccc1c3c(cc2)C(=O)N(C1=O)c1ccncc1 |
| 5 | 12 | OWOHAL |
| 6 | 12 | GURCOL |
| 7 | 10 | LIZCUS |
| 8 | 9 | QARYEO |
| 9 | 9 | PHENAT |
| 10 | 8 | CC(=O)c1ccncc1 |
| 11 | 8 | PYRBTA |
| 12 | 8 | O=N(=O)c1ccc(cc1)C(c1ccc(cc1)N(=O)=O)(c1ccc(cc1)N(=O)=O)c1ccc(cc1)N(=O)=O |
| 13 | 8 | EDEQAG |
| 14 | 8 | c1ccc(cn1)c1ncc[nH]1 |
| 15 | 7 | TPPOSS |
| 16 | 7 | n1ccc(cc1)/C=C/c1ccccn1 |
| 17 | 7 | WEFBOZ |
| 18 | 7 | VIQBOM |
| 19 | 7 | GENYIH |
| 20 | 7 | Brc1cnc(c(n1)Br)N |
| 21 | 6 | TPPHSE |
| 22 | 6 | Cc1cc2ncn(c2cc1C)Cc1cccnc1 |
| 23 | 6 | JEHGUB |
| 24 | 6 | Cc1cc2ncn(c2cc1C)Cc1ccncc1 |
| 25 | 6 | RIBGIS |
| 26 | 6 | CN1CCC[C@H]1c1cccnc1 |
| 27 | 6 | n1ccc(cc1)c1ccc(s1)c1ccco1 |
| 28 | 5 | CNC(=S)NC |
| 29 | 5 | O/C(=C\C(=O)c1ccccc1)/c1ccncc1 |
| 30 | 5 | O=C(NCc1cccnc1)NCc1cccnc1 |
| 31 | 5 | YIJBEZ |
| 32 | 5 | VAPPIP |
| 33 | 5 | KAQCAJ |

| | | |
|---|---|---|
| 34 | 5 | DPHDSE |
| 35 | 5 | IVEJUO |
| 36 | 5 | COUMAR01 |
| 37 | 5 | n1ccc(cc1)c1ccc(s1)c1cccs1 |
| 38 | 4 | c1ccc(cn1)Cn1cnc2c1cccc2 |
| 39 | 4 | ON1C(=C(C)N(C(=C1C)C)O)C |
| 40 | 4 | Cc1cc(C)cc(c1N#C)C |
| 41 | 4 | POWGEQ |
| 42 | 4 | CC(=O)NCc1ccncc1 |
| 43 | 4 | HAKNAJ |
| 44 | 4 | HUVHAJ |
| 45 | 4 | SUSWUB |
| 46 | 4 | YADJIY |
| 47 | 4 | MANTHR01 |
| 48 | 4 | WIZFOA |
| 49 | 4 | OKILEB |
| 50 | 4 | HEQXOR |
| 51 | 4 | NEXBOI |
| 52 | 4 | FINNEW |
| 53 | 3 | PACLAK |
| 54 | 3 | QESZUK |
| 55 | 3 | c1ccc(cc1)c1nccn1Cc1ccncc1 |
| 56 | 3 | CIJXAX |
| 57 | 3 | c1ccc(cn1)c1cc(c2cccnc2)c(cc1c1cccnc1)c1cccnc1 |
| 58 | 3 | GUQYID |
| 59 | 3 | C1CCSCS1 |
| 60 | 3 | Cc1nc(nc(c1)C)c1nc(C)cc(n1)C |
| 61 | 3 | SLCPYA |
| 62 | 3 | ZEFHOK |
| 63 | 3 | RECFIS |
| 64 | 3 | CEQVAY |
| 65 | 3 | [H]1[S@]23N41[CH2]2[CH2]1[S@@]25[CH2]([CH2]34)N12[H]5 |
| 66 | 3 | DPHSOX03 |
| 67 | 3 | CNITBZ02 |

| | | |
|---|---|---|
| 68 | 3 | BERTIB |
| 69 | 3 | Nc1ncc(nc1)Br |
| 70 | 3 | SOBKOL |
| 71 | 3 | JULZAR |
| 72 | 3 | ZORSEG |
| 73 | 3 | c1ccc2c(c1)ccc1c2nccc1 |
| 74 | 3 | C=Cc1ccncc1 |
| 75 | 3 | BEYGUK |
| 76 | 3 | OFIZEK |
| 77 | 3 | n1ccc(cc1)Cn1cncc1 |
| 78 | 3 | ON1C(=N(C(C1(C)C)(C)C)O)c1ccccc1 |
| 79 | 3 | LIDCAN10 |
| 80 | 3 | Cc1ccc(cc1)C(=O)C |
| 81 | 3 | NERDUN |
| 82 | 3 | WIFKIF |
| 83 | 3 | O=C1N2Cc3cccc(n3)CN3CN(CN(Cc4nc(CN1CN(C2)C(C)(C)C)ccc4)C3=O)C(C)(C)C |
| 84 | 2 | RIVPOE |
| 85 | 2 | CC(=O)c1cccnc1 |
| 86 | 2 | YIZZIT |
| 87 | 2 | Clc1ccc2c(n1)c1ncccc1cc2 |
| 88 | 2 | C/C(=C/C(=O)C)/NCCN1CCNCC1 |
| 89 | 2 | C/C(=C/C(=O)C)/NCCN1CCOCC1 |
| 90 | 2 | C/C(=C/C(=O)c1ccccc1)/NCCN1CCNCC1 |
| 91 | 2 | BENJUD |
| 92 | 2 | PACNEQ |
| 93 | 2 | TASKIL |
| 94 | 2 | NN1CCOCC1 |
| 95 | 2 | DADMBP |
| 96 | 2 | O1CCN(CC1)CCN=C1CCSCC1 |
| 97 | 2 | OWEKEH |
| 98 | 2 | BENLUD |
| 99 | 2 | c1ccc2n(c1)nnc2 |
| 100 | 2 | NEDXAX |
| 101 | 2 | Cc1cc(c(cc1c1ccc(cc1)c1cc(C)c(cc1C)c1ccncc1)C)c1ccncc1 |

| | | |
|---|---|---|
| 102 | 2 | DMHTEZ10 |
| 103 | 2 | SUBTIS01 |
| 104 | 2 | FEXRIK |
| 105 | 2 | n1cc(cc(c1)c1ccncc1)c1ccncc1 |
| 106 | 2 | KENDOA |
| 107 | 2 | C1CNCCS1 |
| 108 | 2 | VAZMOB |
| 109 | 2 | COc1cccc(c1O)/C=N/c1ccc(cc1)C#N |
| 110 | 2 | EXUPOE |
| 111 | 2 | EHELOT |
| 112 | 2 | WIFXIU |
| 113 | 2 | DIXREH |
| 114 | 2 | CASHOT |
| 115 | 2 | ATAKOY |
| 116 | 2 | c1ccc(cn1)c1ccc(cc1)C(=C(c1ccc(cc1)c1cccnc1)c1ccc(cc1)c1cccnc1)c1ccc(cc1)c1cccnc1 |
| 117 | 2 | c1cnc2c(c1)nc[nH]2 |
| 118 | 2 | PAPSEG |
| 119 | 2 | TEHZIP |
| 120 | 2 | CCCCCc1ccc(cc1)C#Cc1ccncc1 |
| 121 | 2 | PUQYEH |
| 122 | 2 | c1ccc(cn1)Cn1cncc1 |
| 123 | 2 | COc1cncc(c1)C#Cc1cccnc1 |
| 124 | 2 | ZOHFEK |
| 125 | 2 | NIQDOG |
| 126 | 2 | AMIPYR |
| 127 | 2 | HIWLEH |
| 128 | 2 | VABDOR |
| 129 | 2 | n1ccc(cc1)/C=C/c1cccc2c1cccc2 |
| 130 | 2 | IQUGUY |
| 131 | 2 | Cc1ccnc2c1ccc1c2nccc1C |
| 132 | 2 | XECYEM |
| 133 | 2 | JITPIL |
| 134 | 2 | AMACPH |
| 135 | 2 | SEUREA |

| | | |
|---|---|---|
| 136 | 2 | OLUNOA |
| 137 | 2 | FOFDIN |
| 138 | 2 | DPHDTE |
| 139 | 2 | EHUKIC |
| 140 | 2 | n1ccc(cc1)Cn1cnc2c1cccc2 |
| 141 | 2 | NMKPIP |
| 142 | 2 | COc1cc(C=O)cc(c1Br)OC |
| 143 | 2 | CALXEW |
| 144 | 2 | [H]1[O@]23N41[CH2]2[CH2]1[O@@]25[CH2]([CH2]34)N12[H]5 |
| 145 | 2 | TUDHAE |
| 146 | 2 | MESITN |
| 147 | 2 | [S-]C1=CC[NH+](C=C1)c1ccncc1 |