**TODO: UPDATE**

Table 2. Examples of InChI for polymers.

Numbering follows numbers of records in the file PZ.SDF included in this distribution.

InChI and InChIKey strings are generated using inchi-1 v. 1.06 with options ‘Polymers’, ‘NPZZ’, and ‘OutErrINCHI’. For comparison, InChI v. 1.05 strings generated with inchi-1 v. 1.05 option ‘Polymers’ is shown in red (the same results are obtained by using inchi-1 v. 1.06 with option ‘Polymer105’).

To obtain round-trip result structures in the last column of table, the structures were back-converted from InChI using inchi-1 with options ‘InChI2Struct’ and ‘OutputSDF’, then imported (as *xyz*-less and stereo-less Molfiles) to Biovia / Draw 18.1 & where ‘Chemistry->Clean’ was applied.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Name | pzx | Structure | InChI/Key | Comment and/or structure as back-converted from InChI\* |
| zz.sdf/ zz01 |  |  |  |  |
| zz02 |  |  |  |  |
| zz03 |  |  |  |  |
| zz04 |  |  |  |  |
| zz05 |  |  |  |  |
| zz06 |  |  |  |  |
| zz07 |  |  |  |  |
| zz08 |  |  |  |  |
| zz09 |  |  |  |  |
| zz010 |  |  |  |  |
| zz011 |  |  |  |  |
| zz012 |  |  |  |  |
| zz013 |  |  |  |  |
| zz014 |  |  |  |  |
| zz015 |  |  | InChI=1B/C2H4/c1-2/h1-2H2/z200-1-2  InChIKey=VGGSQFUCUMXWEO-JEIJVWOYBA-N |  |
| zz016 |  |  | InChI=1B/C8H8/c1-2-8-6-4-3-5-7-8/h2-7H,1H2/z200-1-8  InChIKey=PPBRXRYQALVLMV-ZMQGHSLKBA-N |  |
| zz017 |  |  | InChI=1B/C8H8.C3H6.C2H4O/c1-2-8-6-4-3-5-7-8;1-3-2;1-2-3-1/h2-7H,1H2;3H,1H2,2H3;1-2H2/z200-9-11;200-12-14;200-1-8;320-1-14  InChIKey=MYPPWGFYCAYBAJ-CALUOSFZBA-N |  |
| zz018 |  |  | InChI=1B/C8H8.C3H6.C2H4O/c1-2-8-6-4-3-5-7-8;1-3-2;1-2-3-1/h2-7H,1H2;3H,1H2,2H3;1-2H2/z200-9-11;200-12-14;200-1-8;310-1-14  InChIKey=MYPPWGFYCAYBAJ-WRCKSDIVBA-N |  |
| zz019 |  |  | InChI=1B/C8H8.C3H6.C2H4O/c1-2-8-6-4-3-5-7-8;1-3-2;1-2-3-1/h2-7H,1H2;3H,1H2,2H3;1-2H2/z200-9-11;200-12-14;200-1-8;330-1-14  InChIKey=MYPPWGFYCAYBAJ-CQPMJGTBBA-N |  |
| zz020 |  |  | InChI=1B/C8H8.C3H6.C2H4O/c1-2-8-6-4-3-5-7-8;1-3-2;1-2-3-1/h2-7H,1H2;3H,1H2,2H3;1-2H2/z200-9-11;200-12-14;200-1-8;320-1-11;330-1-14  InChIKey=MYPPWGFYCAYBAJ-MCGIIRCZBA-N |  |
| zz021 |  |  | InChI=1B/C8H6O4.C6H6O2/c9-7(10)5-1-2-6(4-3-5)8(11)12;7-5-1-2-6(8)4-3-5/h1-4H,(H,9,10)(H,11,12);1-4,7-8H/z200-1-20  InChIKey=RYGHNMANMHVMMN-NRYBNUJIBA-N |  |
| zz022 |  |  | InChI=1B/C8H6O4.C6H6O2/c9-7(10)5-1-2-6(4-3-5)8(11)12;7-5-1-2-6(8)4-3-5/h1-4H,(H,9,10)(H,11,12);1-4,7-8H/z600-13-20;600-1-12;200-1-20  InChIKey=RYGHNMANMHVMMN-AMBOAQDBBA-N |  |
| zz023 |  |  | InChI=1B/C2H3Cl.C2H4/c1-2-3;1-2/h2H,1H2;1-2H2/z200-4-5;400-1-3;320-1-5  InChIKey=KRGNPJFAKZHQPS-PIORLKTDBA-N |  |
|  |  |  |  |  |
| zz024 |  |  | InChI=1B/C10H10.C8H8/c1-3-9-5-7-10(4-2)8-6-9;1-2-8-6-4-3-5-7-8/h3-8H,1-2H2;2-7H,1H2/z200-11-18;500-1-10;320-1-18  InChIKey=KOLSKAPZYPZSGC-AVCIZLQUBA-N |  |
| zz025 |  |  | InChI=1B/C8H8.C4H6/c1-2-8-6-4-3-5-7-8;1-3-4-2/h2-7H,1H2;3-4H,1-2H2/z200-9-12;200-1-8;330-1-12  InChIKey=MTAZNLWOLGHBHU-ZNVYRHKRBA-N |  |
| zz026 |  |  | InChI=1B/C8H8.C4H6/c1-2-8-6-4-3-5-7-8;1-3-4-2/h2-7H,1H2;3-4H,1-2H2/z200-9-12;200-1-8;330-1-12  InChIKey=MTAZNLWOLGHBHU-ZNVYRHKRBA-N | ‘hh’ is ignored |
| zz027 |  |  | InChI=1S/C8H8.C4H6/c1-2-8-6-4-3-5-7-8;1-3-4-2/h2-7H,1H2;3-4H,1-2H2  InChIKey=MTAZNLWOLGHBHU-UHFFFAOYSA-N | Not a polymer. Note the same 1st block as the previous entry |
| zz028 |  |  | InChI=1B/C8H8.C3H3N/c1-2-8-6-4-3-5-7-8;1-2-3-4/h2-7H,1H2;2H,1H2/z200-9-12;200-1-8  InChIKey=SCUZVMOVTVSBLE-BEPCRINZBA-N | Considered as mixture of polymers |
| zz029 |  |  | InChI=1B/C8H8.C3H3N/c1-2-8-6-4-3-5-7-8;1-2-3-4/h2-7H,1H2;2H,1H2/z200-9-12;200-1-8;330-1-12  InChIKey=SCUZVMOVTVSBLE-ZNVYRHKRBA-N | Block copolymer |
| zz030 |  |  | InChI=1B/C8H8.C3H3N/c1-2-8-6-4-3-5-7-8;1-2-3-4/h2-7H,1H2;2H,1H2/z200-9-12;200-1-8;310-1-12  InChIKey=SCUZVMOVTVSBLE-YMBOZTOTBA-N | Alternating copolymer |
| zz031 |  |  | InChI=1B/C10H14O2/c1-9(8-11-2)12-10-6-4-3-5-7-10/h3-7,9H,8H2,1-2H3/z101-1,8-9,12(10-12,11-8)  InChIKey=WGAOQOCTPHKPGH-VUBNIWPLBA-N |  |
| zz032 |  |  | InChI=1B/C16H22O2/c1-12(2)5-4-6-13(3)7-8-14-9-10-15(17)11-16(14)18/h5,7,9-11,17-18H,4,6,8H2,1-3H3/z101-3,6-8,13(4-6,14-8)/b13-7+  InChIKey=RGUSQESFCCLNEG-HDMSAIMJBA-N |  |
| zz033 |  |  | InChI=1B/C12H26O16P2/c13-1-6(15)3-25-30(22,23)26-5-7(4-24-29(19,20)21)27-12-11(18)10(17)9(16)8(2-14)28-12/h6-18H,1-5H2,(H,22,23)(H2,19,20,21)/z101-2,4-5,7-12,14,16-19,21,24,26-29(20-29,30-26)/t6?,7?,8-,9-,10+,11-,12+/m1/s1  InChIKey=CVGGAOGCVJSXBB-OHILBRHSBA-N |  |
| zz034 |  |  | InChI=1S/C12H26O16P2/c13-1-6(15)3-25-30(22,23)26-5-7(4-24-29(19,20)21)27-12-11(18)10(17)9(16)8(2-14)28-12/h6-18H,1-5H2,(H,22,23)(H2,19,20,21)/t6?,7?,8-,9-,10+,11-,12+/m1/s1  InChIKey=CVGGAOGCVJSXBB-XMDCDNQBSA-N | Not a polymer. Note the same 1st block tas the previous entry |
| zz035 |  |  | InChI=1B/S3/c1-3-2/z101-3(1-3,2-3)  InChIKey=NVSDADJBGGUCLP-IVYKBIFBBA-N |  |
| zz036 |  |  | InChI=1B/C24H30N8O9/c25-24-31-19-18(21(37)32-24)28-13(10-27-19)9-26-12-3-1-11(2-4-12)20(36)30-15(23(40)41)5-7-16(33)29-14(22(38)39)6-8-17(34)35/h1-4,13-15,26,28H,5-10H2,(H,29,33)(H,30,36)(H,34,35)(H,38,39)(H,40,41)(H4,25,27,31,32,37)/z103-5,7,15-16,23,30,33,40-41(20-30,29-16)  InChIKey=ZAOGJXDWOQXFBW-LLEXUJLJBA-N |  |
| zz037 |  |  | InChI=1B/C6H14O3/c1-5(8)4-9-6(2)3-7/h5-8H,3-4H2,1-2H3/z101-2-3,6,9(4-9,7-3)  InChIKey=DUFKCOQISQKSAV-QZIZWDOBBA-N |  |
| zz038 |  |  | InChI=1B/C4H10O2/c1-5-3-4-6-2/h3-4H2,1-2H3/z101-3-5(1-5,6-4)  InChIKey=XTHFKEDIFFGKHM-MYPDUYLMBA-N |  |
| zz039 |  |  | InChI=1B/C4H10O3/c5-1-3-7-4-2-6/h5-6H,1-4H2/z101-3-4,7(1-3,2-4)  InChIKey=MTHSVFCYNBDYFN-ZQIFOVHGBA-N |  |
| zz040 |  |  | InChI=1B/C4H6O2/c1-3-6-4(2)5/h3H,1H2,2H3/z101-1-6(1.3)  InChIKey=XTXRWKRVRITETP-IKXXVMLBBA-N |  |
| zz041 |  |  | InChI=1B/C3H5NO/c1-2-3(4)5/h2H,1H2,(H2,4,5)/z101-1-5(1.2)  InChIKey=HRPVXLWXLXDGHG-YZJLBCBGBA-N |  |
| zz042 |  |  | InChI=1B/C2H3BrO/c3-2-1-4-2/h2H,1H2/z101-1-4(1,2,1,4,2,4)  InChIKey=XOOVDXMNWOFROX-UAKBPNCWBA-N |  |
| zz043 |  |  | InChI=1B/C2H3BrO/c3-2-1-4-2/h2H,1H2/z101-1-4(1,2,1,4,2,4)  InChIKey=XOOVDXMNWOFROX-UAKBPNCWBA-N |  |
| zz044 |  |  | InChI=1B/C2H3BrO/c3-2-1-4-2/h2H,1H2/z101-1-4(1,2,1,4,2,4)  InChIKey=XOOVDXMNWOFROX-UAKBPNCWBA-N |  |
| zz045 |  |  | InChI=1B/C10H10O2/c11-10-9-5-3-8(4-6-9)2-1-7-12-10/h3-6H,1-2,7H2/z101-1-12(1,2,1,7,2,8,7,12,9,10,10,12)  InChIKey=MZCUXAXPLLHRKB-WSHGCIBBBA-N |  |
| zz046 |  |  | InChI=1B/C10H10O2/c11-10-9-5-3-8(4-6-9)2-1-7-12-10/h3-6H,1-2,7H2/z101-1-12(1,2,1,7,2,8,7,12,9,10,10,12)  InChIKey=MZCUXAXPLLHRKB-WSHGCIBBBA-N |  |
| zz047 |  |  | InChI=1B/C10H10O2/c11-10-9-5-3-8(4-6-9)2-1-7-12-10/h3-6H,1-2,7H2/z101-1-12(1,2,1,7,2,8,7,12,9,10,10,12)  InChIKey=MZCUXAXPLLHRKB-WSHGCIBBBA-N |  |
| zz048 |  |  | InChI=1B/C6H5N/c1-2-6-4-3-5(1)7-6/h1-4,7H/z101-1-7(5,7,6,7)  InChIKey=MRPDSIUDKSQKSH-DNFXZTSDBA-N |  |
| zz049 |  |  | InChI=1B/C6H5N/c1-2-6-4-3-5(1)7-6/h1-4,7H/z101-1-7(5,7,6,7)/i1D  InChIKey=MRPDSIUDKSQKSH-JTPWJMIPBA-N |  |
| zz050 |  |  | InChI=1B/C6H5N/c1-2-6-4-3-5(1)7-6/h1-4,7H/z101-1-7(5,7,6,7)/i1D  InChIKey=MRPDSIUDKSQKSH-JTPWJMIPBA-N |  |
| zz051 |  |  | InChI=1B/C6H10O2/c7-6-4-2-1-3-5-8-6/h1-5H2/z101-1-8(1,2,1,3,2,4,3,5,4,6,5,8,6,8)  InChIKey=PAPBSGBWRJIAAV-CMRMDLKMBA-N |  |
| zz052 |  |  | InChI=1B/C5H8O2/c1-4(2)5(6)7-3/h1H2,2-3H3/z101-1-7(1.4)  InChIKey=VVQNEPGJFQJSBK-KCAOANCDBA-N |  |
| zz053 |  |  | InChI=1B/C2H3Cl/c1-2-3/h2H,1H2/z101-1-3(1.2)  InChIKey=BZHJMEDXRYGGRV-QLSTWJNGBA-N |  |
| zz054 |  |  | InChI=1B/C2H3Cl/c1-2-3/h2H,1H2/z101-1-3(1.2)  InChIKey=BZHJMEDXRYGGRV-QLSTWJNGBA-N |  |
| zz055 |  |  | InChI=1B/C13H8/c1-3-12-10-5-8(1)9-2-4-13(12)11(6-9)7-10/h1-6H,7H2/z101-1-13(8,9)  InChIKey=JFICTVGWKKNZIQ-XVERVCKYBA-N |  |
| zz056 |  |  | InChI=1B/C16H18N2O6/c19-13-9-7-10(12(16(23)24)8-11(9)15(21)22)14(20)18-6-4-2-1-3-5-17-13/h7-8H,1-6H2,(H,17,19)(H,18,20)(H,21,22)(H,23,24)/z101-1-24(1,2,1,3,2,4,3,5,4,6,5,17,6,18,9,13,10,14)  InChIKey=NRXUBKMTMFYTLT-HYQSQRQEBA-N |  |
| zz057 |  |  | InChI=1B/C62H98O2/c1-39(2)13-11-15-41(5)51-23-25-53-49-21-19-45-37-47(27-31-59(45,7)55(49)29-33-61(51,53)9)63-57-35-44-18-17-43(57)36-58(44)64-48-28-32-60(8)46(38-48)20-22-50-54-26-24-52(42(6)16-12-14-40(3)4)62(54,10)34-30-56(50)60/h17-18,35-36,39-42,45-56H,11-16,19-34,37-38H2,1-10H3/z101-1-64(17,18,17,43,18,44)/t41-,42-,45+,46+,47+,48+,49+,50+,51-,52-,53+,54+,55+,56+,59+,60+,61-,62-/m1/s1  InChIKey=PYGFEFGUKGGHSU-DBPKQELEBA-N |  |
| zz058 |  |  | InChI=1B/C53H64N2O6/c1-4-7-9-16-20-24-36(25-21-17-10-8-5-2)55-52(59)43-32-28-39-37-26-30-41-48-42(31-27-38(46(37)48)40-29-33-44(53(55)60)49(43)47(39)40)51(58)54(50(41)57)34-22-18-14-12-11-13-15-19-23-35-61-45(56)6-3/h6,26-33,36H,3-5,7-25,34-35H2,1-2H3/z101-1-61(3.6)  InChIKey=CXJULOVRHUZQEG-PHGMDXHZBA-N |  |
| zz059 |  |  | InChI=1B/C26H40N2O36S5/c1-4(30)27-7-9(31)12-6(3-53-66(41,42)43)55-23(7)58-15-10(32)18(64-69(50,51)52)26(61-19(15)21(34)35)57-13-5(2-29)54-24(8(28-65(38,39)40)14(13)62-67(44,45)46)59-16-11(33)17(63-68(47,48)49)25(56-12)60-20(16)22(36)37/h5-20,23-26,28-29,31-33H,2-3H2,1H3,(H,27,30)(H,34,35)(H,36,37)(H,38,39,40)(H,41,42,43)(H,44,45,46)(H,47,48,49)(H,50,51,52)/z101-1-69(12,56,13,57,15,58,16,59,23,58,24,59,25,56,26,57)/t5-,6-,7-,8-,9-,10+,11+,12-,13-,14-,15+,16+,17-,18-,19-,20+,23?,24-,25-,26-/m1/s1  InChIKey=RTKRRPJNBRRQDW-XTCKGPBSBA-N |  |
| zz060 |  |  | InChI=1B/C3H5Cl.C2H4O/c4-3-1-2-3;1-2-3-1/h3H,1-2H2;1-2H2/z101-5-7(5,6,5,7,6,7);101-1-4(1,2,1,3,2,3)  InChIKey=KVIOBMVNVRVGPK-JKXHHPFUBA-N | NB: mixture of polymers, not copolymer |
| zz061 |  |  | InChI=1B/C3H5Cl.C2H4O/c4-3-1-2-3;1-2-3-1/h3H,1-2H2;1-2H2/z101-5-7(5,6,5,7,6,7);101-1-4(1,2,1,3,2,3)  InChIKey=KVIOBMVNVRVGPK-JKXHHPFUBA-N | NB: mixture of polymers, not copolymer |
| zz062 |  |  | InChI=1B/C3H5Cl.C2H4O/c4-3-1-2-3;1-2-3-1/h3H,1-2H2;1-2H2/z101-5-7(5,6,5,7,6,7);101-1-4(1,2,1,3,2,3)  InChIKey=KVIOBMVNVRVGPK-JKXHHPFUBA-N | NB: mixture of polymers, not copolymer |
| zz063 |  |  | InChI=1B/C8H8.C3H6/c1-2-8-6-4-3-5-7-8;1-3-2/h2-7H,1H2;3H,1H2,2H3/z101-9-11(9.11);101-1-8(1.2);311-1-15  InChIKey=YARNEMCKJLFQHG-NTLSNBPHBA-N |  |
| zz064 |  |  | InChI=1B/C8H8.C3H6/c1-2-8-6-4-3-5-7-8;1-3-2/h2-7H,1H2;3H,1H2,2H3/z101-9-11(9.11);101-1-8(1.2);321-1-15  InChIKey=YARNEMCKJLFQHG-AESXVLFWBA-N |  |
| zz065 |  |  | InChI=1B/C19H12O3.C16H14O3/c20-19-13-1-5-15(6-2-13)21-17-9-11-18(12-10-17)22-16-7-3-14(19)4-8-16;1-16(2)11-3-7-13(8-4-11)18-15(17)19-14-9-5-12(16)6-10-14/h1-12H;3-10H,1-2H3/z101-23-41(33,38,34,38,35,40,36,41,37,40,37,41);101-1-22(13,19,14,19,15,21,16,22,17,21,18,22)  InChIKey=HHFXSTKAFNJYEC-JELLZUPSBA-N | NB: mixture of polymers, not copolymer |
| zz066 |  |  | InChI=1B/C19H12O3.C16H14O3/c20-19-13-1-5-15(6-2-13)21-17-9-11-18(12-10-17)22-16-7-3-14(19)4-8-16;1-16(2)11-3-7-13(8-4-11)18-15(17)19-14-9-5-12(16)6-10-14/h1-12H;3-10H,1-2H3/z401-23-41(33,38,34,38,35,40,36,41,37,40,37,41);101-1-22(13,19,14,19,15,21,16,22,17,21,18,22);331-1-45  InChIKey=HHFXSTKAFNJYEC-FBXUJDOCBA-N | Block-copolymer |
| zz067 |  |  | InChI=1B/C8H4/c1-2-8-5-3-7(1)4-6-8/h1-3,5H/z101-1-8(4,6,4,7,6,8)  InChIKey=GQEZFUOMAFZPSC-BVCYNDGCBA-N |  |
| zz068 |  |  | InChI=1B/C3H5NO/c5-3-1-2-4-3/h1-2H2,(H,4,5)/z101-1-5(1,2,1,3,2,4) InChIKey=MNFORVFSTILPAW-GKSSZUKRBA-N |  |
| zz069 |  |  | InChI=1B/C3H5NO/c5-3-1-2-4-3/h1-2H2,(H,4,5)/z101-1-5(1,2,1,3,2,4  InChIKey=MNFORVFSTILPAW-GKSSZUKRBA-N |  |
| zz070 |  |  | InChI=1B/C3H5NO/c5-3-1-2-4-3/h1-2H2,(H,4,5)/z101-1-5(1,2,1,3,2,4)  InChIKey=MNFORVFSTILPAW-GKSSZUKRBA-N |  |
| zz071 |  |  | InChI=1B/C5H7NO3/c7-4-2-1-3(6-4)5(8)9/h3H,1-2H2,(H,6,7)(H,8,9)/z101-1-9(1,2,1,3,2,4,3,6)/t3-/m1/s1  InChIKey=ODHCTXKNWHHXJC-AQUWEPPIBA-N |  |
| zz072 |  |  | InChI=1B/C16H18N2O6/c19-13-9-7-10(12(16(23)24)8-11(9)15(21)22)14(20)18-6-4-2-1-3-5-17-13/h7-8H,1-6H2,(H,17,19)(H,18,20)(H,21,22)(H,23,24)/z101-1-24(1,2,1,3,2,4,3,5,4,6,5,17,6,18,9,13,10,14)  InChIKey=NRXUBKMTMFYTLT-HYQSQRQEBA-N |  |
| zz073 |  |  | InChI=1B/Cl2NP/c1-4(2)3/z101-1-4(3.4)  InChIKey=UXJHQBVRZUANLK-KBEGDARSBA-N |  |
| zz074 |  |  | InChI=1B/C3H4O2.Na/c1-2-3(4)5;/h2H,1H2,(H,4,5);/q;+1/p-1/z101-1-6(1.2)  InChIKey=NNMHYFLPFNGQFZ-GJEZIXODBA-M |  |
| zz075 |  |  | InChI=1B/C18H13N/c1-2-4-16(5-3-1)19-17-10-6-14(7-11-17)15-8-12-18(19)13-9-15/h1-13H/z101-1-19(14,15,17,19,18,19)  InChIKey=WUTRCYSYTJLPJT-DUOYJIBFBA-N |  |
| zz076 |  |  | InChI=1B/C8H10N.HI/c1-3-8-6-4-5-7-9(8)2;/h3-7H,1H2,2H3;1H/q+1;/p-1/z101-1-10(1.3)  InChIKey=DWMSYQDOPYSCJR-DDSQTIRRBA-M |  |
| zz077 |  |  | InChI=1B/C8H6O5/c9-7-5-1-2-6(13-5)8(10)12-4-3-11-7/h1-2H,3-4H2/z101-1-13(3,4,3,11,4,12,5,7,6,8,7,11,8,12)  InChIKey=DVVGBNZLQNDSPA-XVRIZPPSBA-N |  |
| zz078 |  |  | InChI=1B/C4H8N2S4.Zn/c7-3(8)5-1-2-6-4(9)10;/h1-2H2,(H2,5,7,8)(H2,6,9,10);/q;+2/p-2/z101-1-11(1,5)  InChIKey=AMHNZOICSMBGDH-SJNBWECRBA-L |  |
|  |  | Same with /RecMet | InChI=1B/C4H8N2S4.Zn/c7-3(8)5-1-2-6-4(9)10;/h1-2H2,(H2,5,7,8)(H2,6,9,10);/q;+2/p-2/z101-1-11(1,5)/rC4H6N2S4Zn/c1-2-6-4-9-11(10-4)7-3(5-1)8-11/h5-6H,1-2H2/z101-1-11(1,5)  InChIKey=AMHNZOICSMBGDH-ZPQHTIIXBA-L |  |
| zz079 |  |  | InChI=1B/O2.2O.V/c1-2;;;/q-2;;-1;+2/z101-1-5(1,2)  InChIKey=PIZXTTZLZREQOK-OXOBPHIVBA-N |  |
|  |  | Same with /RecMet | InChI=1B/O2.2O.V/c1-2;;;/q-2;;-1;+2/z101-1-5(1,2)/rO4V/c1-5(2)3-4-5/q-1/z101-1-5(3,4)  InChIKey=PIZXTTZLZREQOK-LFGDFKGNBA-N |  |
| zz080 |  |  | InChI=1B/C12H10N2O.2ClH.Cu/c1-3-9-7-15-8-10-4-2-6-12(14-10)11(5-1)13-9;;;/h1-6H,7-8H2;2\*1H;/q;;;+2/p-2/z101-1-18(7,9,7,15,8,10,8,15,11,12)  InChIKey=SJLWIGOSCVCHFV-VDYOQJQMBA-L |  |
|  |  | Same with /RecMet | InChI=1B/C12H10N2O.2ClH.Cu/c1-3-9-7-15-8-10-4-2-6-12(14-10)11(5-1)13-9;;;/h1-6H,7-8H2;2\*1H;/q;;;+2/p-2/z101-1-18(7,9,7,15,8,10,8,15,11,12)/rC12H10Cl2CuN2O/c13-15(14)16-9-3-1-5-11(16)12-6-2-4-10(17(12)15)8-18-7-9/h1-6H,7-8H2/z101-1-18(7,9,7,18,8,10,8,18,11,12)  InChIKey=SJLWIGOSCVCHFV-VIBYZETQBA-L |  |
| zz081 |  |  | InChI=1B/C9H10/c1-4-9-5-2-7(1)8(9)3-6-9/h1,3-4,6-8H,2,5H2/z101-1-9(7,8)  InChIKey=RQMLRGLXQHWVQB-WCYUVGCXBA-N |  |
| zz082 |  |  | InChI=1B/C2H6N/c1-3-2/h1-2H3/q+1/z101-1-3(3)  InChIKey=JLBDYIULKDRRIS-DJAGSJGEBA-N |  |
| zz083 |  |  | InChI=1B/C2H2/c1-2/h1-2H/z101-1-2(1.2)  InChIKey=HSFWRNGVRCDJHI-SIBUVIRQBA-N |  |
| zz084 |  |  | InChI=1B/C2H2/c1-2/h1-2H/z101-1-2(1.2)  InChIKey=HSFWRNGVRCDJHI-SIBUVIRQBA-N |  |
| zz085 |  |  | InChI=1B/C8H10N.C3H4O2.ClH.Na/c1-9-5-7-2-3-8(4-7)6-9;1-2-3(4)5;;/h4-6H,2-3H2,1H3;2H,1H2,(H,4,5);1H;/q+1;;;+1/p-2/z101-10-14,16(10.11);101-1-9,15(2,3,2,7,3,8);321-1-20  InChIKey=RHMLQKOGNDZGNR-QNNKLHLLBA-L |  |
| zz086 |  |  | InChI=1B/C3H6/c1-3-2/h3H,1H2,2H3/z200-1-3  InChIKey=QQONPFPTGQHPMA-DJNVOPQRBA-N |  |
| zz087 |  |  | InChI=1B/C3H6/c1-3-2/h3H,1H2,2H3/z101-1-3(1.3)  InChIKey=QQONPFPTGQHPMA-KDIWSDSHBA-N |  |
| zz088 |  |  | InChI=1S/C3H6/c1-3-2/h3H,1H2,2H3  InChIKey=QQONPFPTGQHPMA-UHFFFAOYSA-N | Not a polymer |
| zz089 |  |  | InChI=1B/C6H11NO/c8-6-4-2-1-3-5-7-6/h1-5H2,(H,7,8)/z200-1-8  InChIKey=JBKVHLHDHHXQEQ-ZMQGHSLKBA-N |  |
|  |  | Same with /FixedH | InChI=1B/C6H11NO/c8-6-4-2-1-3-5-7-6/h1-5H2,(H,7,8)/z200-1-8/f/h7H  InChIKey=JBKVHLHDHHXQEQ-ZWBUTNKYBA-N |  |
| zz090 |  |  | InChI=1B/C6H11NO/c8-6-4-2-1-3-5-7-6/h1-5H2,(H,7,8)/z101-1-8(1,2,1,3,2,4,3,5,4,6,5,7)  InChIKey=JBKVHLHDHHXQEQ-DZWZRWJOBA-N |  |
|  |  | Same with /FixedH | Structure: 76  InChI=1B/C6H11NO/c8-6-4-2-1-3-5-7-6/h1-5H2,(H,7,8)/z101-1-8(1,2,1,3,2,4,3,5,4,6,5,7)/f/h7H  InChIKey=JBKVHLHDHHXQEQ-VWJAHPQWBA-N |  |
| zz091 |  |  | InChI=1S/C6H11NO/c8-6-4-2-1-3-5-7-6/h1-5H2,(H,7,8)  InChIKey=JBKVHLHDHHXQEQ-UHFFFAOYSA-N | Not a polymer |
| zz092 |  |  | InChI=1B/C17H15NOS/c1-3-14-16-7-10(1)5-11-6-13(18-9-11)12-2-4-15(19-14)17(8-12)20-16/h1-4,7-8,11,13,18H,5-6,9H2/z101-1-20(5,10,5,11,12,13)  InChIKey=NVAVLZKTSMLUDJ-ALPRJYBXBA-N |  |
| zz093 |  |  | InChI=1B/C5H13NOSSi/c1-2-7-4-9-5-8-3-6-1/h6H,1-5,9H2/z101-1-9(1,2,1,6,2,7,3,6,3,8,4,7,4,9,5,8,5,9)  InChIKey=ZCYFYWGBNPBAHW-RUMMOZOHBA-N |  |
| zz094 |  |  | InChI=1B/C23H14O/c1-2-20-21-12-17-6-7-18(21)13-22(20)23(3-1)24-19-9-8-15-10-14(17)4-5-16(15)11-19/h1-12H,13H2/z101-1-24(14,17,19,24,23,24)  InChIKey=IKWWVSMTFFXWKZ-GSYXJMKABA-N |  |
| zz095 |  |  | **105=** |  |
| zz096 |  |  | **105=** |  |
| zz097 |  |  | **105=** |  |
| zz098 |  |  | **105=** |  |
| zz099 |  |  | **105=** |  |
| zz100 |  |  | **105=** |  |
| zz101 |  |  | **105=** |  |
| zz102 |  |  | **105=** |  |
| zz103 |  |  | **105=** |  |
| zz104 |  |  | **105=** |  |
| zz105 |  |  | **105=** |  |
| zz106 |  |  | **105=** |  |
| zz107 |  |  | **105=** |  |
| zz108 |  |  | **105=** |  |
| zz109 |  |  | **105=** |  |
| zz110 |  |  | **105=** |  |
| zz111 |  |  | **105=** |  |
| zz112 |  |  | **105=** |  |
| zz113 |  |  | **105=** |  |
| zz114 |  |  | **105=** |  |
| zz115 |  |  | **105=** |  |
| zz116 |  |  | **105=** |  |
| zz117 |  |  | **105=** |  |
| zz118 |  |  | **105=** |  |
| zz119 |  |  | **105=** |  |
| zz120 |  |  | **105=** |  |
| zz121 |  |  | **105=** |  |
| zz122 |  |  | **105=InChI=1B/C3H6O/c1-3-2-4-3/h3H,2H2,1H3/z101-1-4(2,3,2,4,3,4)/t3-/m0/s1**  **InChIKey=GOOHAUXETOMSMM-IFHZNEBOBA-N** |  |
| zz123 |  |  | **105=1B/C3H6O/c1-3-2-4-3/h3H,2H2,1H3/z101-1-4(2,3,2,4,3,4)/t3-/m1/s1**  **InChIKey=GOOHAUXETOMSMM-NALVCCAMBA-N** |  |
| zz124 |  |  | **105=1B/C3H6O/c1-3-2-4-3/h3H,2H2,1H3/z101-1-4(2,3,2,4,3,4)**  **InChIKey=GOOHAUXETOMSMM-KUWDYTNTBA-N** |  |
| zz125 |  |  | **105=1B/C3H6O/c1-3-2-4-3/h3H,2H2,1H3/z101-1-4(2,3,2,4,3,4)/t3-/m1/s1**  **InChIKey=GOOHAUXETOMSMM-NALVCCAMBA-N** |  |
| zz126 |  |  | **105=1B/C3H6O/c1-3-2-4-3/h3H,2H2,1H3/z101-1-4(2,3,2,4,3,4)/t3-/m0/s1**  **InChIKey=GOOHAUXETOMSMM-IFHZNEBOBA-N** |  |
| zz127 |  |  | **105=** |  |
| zz128 |  |  | **105=** |  |
| zz129 |  |  | **105=** |  |
| zz130 |  |  | **105=** |  |
| zz131 |  |  | **105=** |  |
| zz132 |  |  | **105=** |  |
| zz133 |  |  | **105=** |  |
| zz134 |  |  | **105=** |  |
| zz135 |  |  | **105=** |  |
| zz136 |  |  | **105=1B/C3H3BrFIO/c4-3(5,6)2-1-7-2/h2H,1H2/z101-1-7(1,2,1,7,2,7)/t2?,3-/m0/s1**  **InChIKey=KSEKWBIZSFPODQ-MPCUZTEDBA-N** |  |
| zz137 |  |  | **105=1B/C3H3BrFIO/c4-3(5,6)2-1-7-2/h2H,1H2/z101-1-7(1,2,1,7,2,7)/t2?,3-/m0/s1**  **InChIKey=KSEKWBIZSFPODQ-MPCUZTEDBA-N** |  |
| zz138 |  |  | **105=1B/C3H3BrFIO/c4-3(5,6)2-1-7-2/h2H,1H2/z101-1-7(1,2,1,7,2,7)/t2?,3-/m0/s1**  **InChIKey=KSEKWBIZSFPODQ-MPCUZTEDBA-N** |  |
| zz139 |  |  | **105=InChI=1B/C3H3BrFIO/c4-3(5,6)2-1-7-2/h2H,1H2/z101-1-7(1,2,1,7,2,7)/t2?,3-/m1/s1**  **InChIKey=KSEKWBIZSFPODQ-MGWLQIOJBA-N** |  |
| zz140 |  |  | **105=InChI=1B/C6H12N2O/c7-4-2-1-3-5-6(9)8-5/h5H,1-4,7H2,(H,8,9)/z101-1-9(5,6,5,8)/t5-/m0/s1**  **InChIKey=XWKCFGKXBDJAPI-FHPVQWQBBA-N** |  |
| zz141 |  |  | **105=InChI=1B/C6H12N2O/c7-4-2-1-3-5-6(9)8-5/h5H,1-4,7H2,(H,8,9)/z101-1-9(5,6,5,8)/t5-/m1/s1**  **InChIKey=XWKCFGKXBDJAPI-TVOWTXMKBA-N** |  |
| zz142 |  |  | **105=** |  |
| zz143 |  |  | **105=** |  |
| zz144 |  |  | **105=** |  |
| zz145 |  |  | **105=** |  |
| zz146 |  |  | **105=** |  |
| zz147 |  |  | **105=** |  |
| zz148 |  |  | **105=** |  |
| zz149 |  |  | **105=** |  |
| zz150 |  |  | **105=** |  |
| zz151 |  |  | **105=** |  |
| zz152 |  |  | **105=** |  |
| zz153 |  |  | **105=InChI=1B/C2H2N2/c1-3-2-4-1/h1-2H/z101-1-4(1,3,1,4,2,3,2,4)** |  |
| zz154 |  |  | **105=** |  |
| zz155 |  |  | **105=** |  |
| zz156 |  |  | **105=** |  |
| zz157 |  |  | **105=** |  |
| zz158 |  |  |  |  |
| zz159 |  |  | **105=** |  |
| zz160 |  |  | **105=InChI=1B/C10H16/c1-2-8-5-7(1)9-3-4-10(8)6-9/h7-10H,1-6H2/z101-1-10(7,9,8,10)**  **InChIKey=RKBXEEWDGKTVPH-YYOHJBEHBA-N** |  |
| zz161 |  |  | **105=InChI=1B/C25H40/c1-2-17-11-16(1)18-3-4-20(12-18)22-7-8-24(14-22)25-10-9-23(15-25)21-6-5-19(17)13-21/h16-25H,1-15H2/z101-1-25(16,18,17,19,20,22,21,23,24,25)**  **InChIKey=AEINYIBNCTXDFV-FUCNMZATBA-N** |  |
| zz162 |  |  | **105=InChI=1B/C30H48/c1-2-20-13-19(1)21-3-4-23(14-21)25-7-8-27(16-25)29-11-12-30(18-29)28-10-9-26(17-28)24-6-5-22(20)15-24/h19-30H,1-18H2/z101-1-30(19,21,20,22,23,25,24,26,27,29,28,30)**  **InChIKey=MLSNKSBTJIMAQG-OJEFRDRRBA-N** |  |
| zz163 |  |  | **105=InChI=1B/C30H45Br3/c31-28-22-7-8-24(28)18-3-4-20(14-18)26-11-12-27(30(26)33)21-6-5-19(15-21)25-10-9-23(29(25)32)17-2-1-16(22)13-17/h16-30H,1-15H2/z101-1-33(16,22,17,23,18,24,19,25,20,26,21,27)**  **InChIKey=SMOQSZJYSNOPBP-ALIFQNQQBA-N** |  |
| zz164 |  |  | **105=InChI=1B/C30H46Br2/c31-29-25-9-10-27(29)23-7-3-19(15-23)20-4-8-24(16-20)28-12-11-26(30(28)32)22-6-2-18(14-22)17-1-5-21(25)13-17/h17-30H,1-16H2/z101-1-32(17,18,19,20,21,25,22,26,23,27,24,28)**  **InChIKey=NLYAOKQDJQEFEL-CUBMEBPLBA-N** |  |
| zz165 |  |  | **105=InChI=1B/C30H45Br3/c31-28-22-7-8-24(28)18-3-4-20(14-18)26-11-12-27(30(26)33)21-6-5-19(15-21)25-10-9-23(29(25)32)17-2-1-16(22)13-17/h16-30H,1-15H2/z101-1-33(16,22,17,23,18,24,19,25,20,26,21,27)/t16?,17?,18?,19?,20?,21?,22?,23?,24?,25?,26?,27?,28-,29-,30-**  **InChIKey=SMOQSZJYSNOPBP-CHMWFNIOBA-N** |  |
| zz166 |  |  | **105=InChI=1B/C30H45Br3/c31-28-22-7-8-24(28)18-3-4-20(14-18)26-11-12-27(30(26)33)21-6-5-19(15-21)25-10-9-23(29(25)32)17-2-1-16(22)13-17/h16-30H,1-15H2/z101-1-33(16,22,17,23,18,24,19,25,20,26,21,27)/t16?,17?,18?,19?,20?,21?,22?,23?,24?,25?,26?,27?,28-,29-,30-**  **InChIKey=SMOQSZJYSNOPBP-CHMWFNIOBA-N** |  |
| zz167 |  |  | **105=InChI=1B/C30H45Br3/c31-28-22-7-8-24(28)18-3-4-20(14-18)26-11-12-27(30(26)33)21-6-5-19(15-21)25-10-9-23(29(25)32)17-2-1-16(22)13-17/h16-30H,1-15H2/z101-1-33(16,22,17,23,18,24,19,25,20,26,21,27)/t16?,17?,18?,19?,20?,21?,22?,23?,24?,25?,26?,27?,28-,29-,30-**  **InChIKey=SMOQSZJYSNOPBP-CHMWFNIOBA-N** |  |