Supplementary Material (ESI) for Organic & Biomolecular Chemistry


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TITLE     TWO DIFFERENT CONFORMATIONS OF COMPOUND 20
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: (1S,8S)-11-(2,4-Dimethoxy-benzyl)-3-oxa-9,11-diaza-
bicyclo[6.2.2]dodec-5-ene-10,12-dione (16)
COMPND    MOL_ID: 2;
COMPND   2 MOLECULE: (1S,8S)-11-(2,4-Dimethoxy-benzyl)-3-oxa-9,11-diaza-
bicyclo[6.2.2]dodec-5-ene-10,12-dione (16)
EXPDTA    THEORETICAL MODEL
AUTHOR    STEFANO COSTANZI
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JRNL        AUTH   P. BESADA, L.MAMEDOVA, C.J. THOMAS, S.COSTANZI,K.A.JACOBSON
JRNL        TITL   DESIGN AND SYNTHESIS OF NEW BICYCLIC DIKETOPIPERAZINES AS
SCAFFOLDS
JRNL        TITL 2 FOR RECEPTOR PROBES OF STRUCTURALLY DIVERSE FUNCTIONALITY
JRNL        REF    ORGANIC & BIOMOLECULAR CHEMISTRY
HETATM    1  N   MOL     1      -4.968  -0.419  -1.350  1.00  0.00
HETATM    2  C   MOL     1      -4.808   0.941  -1.509  1.00  0.00
HETATM    3  O   MOL     1      -4.157   1.400  -2.444  1.00  0.00
HETATM    4  C1  MOL     1      -5.490   1.882  -0.476  1.00  0.00
HETATM    5  C2  MOL     1      -4.418   2.436   0.492  1.00  0.00
HETATM    6  N1  MOL     1      -6.717   1.238   0.107  1.00  0.00
HETATM    7  C3  MOL     1      -7.841   2.119   0.495  1.00  0.00
HETATM    8  C4  MOL     1      -6.870  -0.142   0.153  1.00  0.00
HETATM    9  O1  MOL     1      -7.915  -0.693   0.500  1.00  0.00
HETATM   10  C5  MOL     1      -5.631  -1.035  -0.201  1.00  0.00
HETATM   11  C6  MOL     1      -4.831  -1.271   1.110  1.00  0.00
HETATM   12  C7  MOL     1      -3.342  -1.511   0.929  1.00  0.00
HETATM   13  C8  MOL     1      -2.372  -0.587   0.808  1.00  0.00
HETATM   14  C9  MOL     1      -2.482   0.925   0.756  1.00  0.00
HETATM   15  O2  MOL     1      -3.700   1.486   1.291  1.00  0.00
HETATM   16  C10 MOL     1      -8.651   2.666  -0.667  1.00  0.00
HETATM   17  C11 MOL     1      -8.485   3.974  -1.165  1.00  0.00
HETATM   18  O3  MOL     1      -7.537   4.806  -0.558  1.00  0.00
HETATM   19  C12 MOL     1      -7.272   6.094  -1.104  1.00  0.00
HETATM   20  C13 MOL     1      -9.261   4.410  -2.240  1.00  0.00
HETATM   21  C14 MOL     1     -10.206   3.574  -2.844  1.00  0.00
HETATM   22  O4  MOL     1     -11.002   3.952  -3.915  1.00  0.00
HETATM   23  C15 MOL     1     -10.848   5.260  -4.458  1.00  0.00
HETATM   24  C16 MOL     1     -10.361   2.280  -2.341  1.00  0.00
HETATM   25  C17 MOL     1      -9.593   1.852  -1.276  1.00  0.00
HETATM   26  N   MOL     2      -4.998  -0.428  -1.371  1.00  0.00
HETATM   27  C   MOL     2      -4.849   0.934  -1.537  1.00  0.00
HETATM   28  O   MOL     2      -4.249   1.397  -2.501  1.00  0.00
HETATM   29  C1  MOL     2      -5.491   1.877  -0.475  1.00  0.00
HETATM   30  C2  MOL     2      -4.375   2.401   0.463  1.00  0.00
HETATM   31  N1  MOL     2      -6.722   1.249   0.108  1.00  0.00
HETATM   32  C3  MOL     2      -7.848   2.134   0.477  1.00  0.00
HETATM   33  C4  MOL     2      -6.846  -0.131   0.212  1.00  0.00
HETATM   34  O1  MOL     2      -7.874  -0.687   0.600  1.00  0.00
HETATM   35  C5  MOL     2      -5.626  -1.041  -0.203  1.00  0.00
HETATM   36  C6  MOL     2      -4.716  -1.385   1.021  1.00  0.00
HETATM   37  C7  MOL     2      -5.237  -0.828   2.334  1.00  0.00
HETATM   38  C8  MOL     2      -4.829   0.283   2.967  1.00  0.00
HETATM   39  C9  MOL     2      -3.741   1.249   2.549  1.00  0.00
HETATM   40  O2  MOL     2      -3.585   1.407   1.127  1.00  0.00
HETATM   41  C10 MOL     2      -7.605   3.029   1.680  1.00  0.00
HETATM   42  C11 MOL     2      -7.750   2.570   3.005  1.00  0.00
HETATM   43  O3  MOL     2      -8.145   1.246   3.213  1.00  0.00
HETATM   44  C12 MOL     2      -8.475   0.799   4.525  1.00  0.00
HETATM   45  C13 MOL     2      -7.494   3.434   4.071  1.00  0.00
HETATM   46  C14 MOL     2      -7.106   4.759   3.857  1.00  0.00
HETATM   47  O4  MOL     2      -6.834   5.662   4.873  1.00  0.00
HETATM   48  C15 MOL     2      -6.945   5.225   6.225  1.00  0.00
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HETATM   49  C16 MOL     2      -6.986   5.209   2.539  1.00  0.00
HETATM   50  C17 MOL     2      -7.236   4.351   1.486  1.00  0.00
CONECT    1    2   10
CONECT    2    3    4
CONECT    4    5    6
CONECT    5   15
CONECT    6    7    8
CONECT    7   16
CONECT    8    9   10
CONECT   10   11
CONECT   11   12
CONECT   12   13
CONECT   13   14
CONECT   14   15
CONECT   16   17   25
CONECT   17   18   20
CONECT   18   19
CONECT   20   21
CONECT   21   22   24
CONECT   22   23
CONECT   24   25
CONECT   26   27   35
CONECT   27   28   29
CONECT   29   30   31
CONECT   30   40
CONECT   31   32   33
CONECT   32   41
CONECT   33   34   35
CONECT   35   36
CONECT   36   37
CONECT   37   38
CONECT   38   39
CONECT   39   40
CONECT   41   42   50
CONECT   42   43   45
CONECT   43   44
CONECT   45   46
CONECT   46   47   49
CONECT   47   48
CONECT   49   50
END
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