

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
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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

