Supporting Information

Incorporation of a QM/MM Buffer Zone in the Variational Double Self-Consistent Field Method

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Cartesian coordinates obtained from the X-Pol optiminizations (Table S1) and from full AM1 optimizations (Table S2) are given in CHARMM format for all compounds described in this paper.

Table S1. Cartesian coordinates optimized using the X-Pol potential with AM1 model for all compounds described in the main paper. Coordinates are given in angstroms in CHARMM format.

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water dimer
    1    1 WATE OH2   -6.33964   2.04925   0.85798 WATE 40     0.00000
    2    1 WATE H1    -7.06441   2.30632   1.43486 WATE 40     0.00000
    3    1 WATE H2    -5.88641   1.36153   1.35375 WATE 40     0.00000
    4    2 WATE OH2   -5.63910   3.16024  -1.90934 WATE 48     0.00000
    5    2 WATE H1    -6.21540   2.42275  -1.68803 WATE 48     0.00000
    6    2 WATE H2    -5.33688   3.46307  -1.04798 WATE 48     0.00000

propane
    1    1 PROP H11    5.84587 -13.20124  -5.74231 PROP 1      0.00000
    2    1 PROP H12    4.39756 -12.30026  -5.13086 PROP 1      0.00000
    3    1 PROP H13    5.38375 -13.31011  -3.99402 PROP 1      0.00000
    4    1 PROP C1     4.98653 -13.24079  -5.03210 PROP 1      0.00000
    5    1 PROP HB1    3.22882 -14.46626  -4.63314 PROP 1      0.00000
    6    1 PROP CB     4.09499 -14.43506  -5.32714 PROP 1      0.00000
    7    1 PROP HB2    3.69578 -14.31610  -6.35552 PROP 1      0.00000
    8    1 PROP C3     4.87207 -15.73161  -5.18497 PROP 1      0.00000
    9    1 PROP H31    5.26215 -15.84964  -4.14652 PROP 1      0.00000
   10    1 PROP H32    4.20520 -16.59362  -5.41642 PROP 1      0.00000
   11    1 PROP H33    5.73168 -15.74051  -5.89294 PROP 1      0.00000

2-methylpropane
    1    1 IBUT C1    -6.19373  -6.33881   6.78862 IBUT 1      0.00000
    2    1 IBUT H11   -6.87613  -6.66887   7.60696 IBUT 1      0.00000
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     3    1 IBUT H12    -6.78961   -5.78982    6.02396 IBUT 1       0.00000
     4    1 IBUT H13    -5.73889   -7.23811    6.31489 IBUT 1       0.00000
     5    1 IBUT C2     -4.18694   -4.94027    6.21847 IBUT 1       0.00000
     6    1 IBUT H21    -4.78788   -4.39480    5.45525 IBUT 1       0.00000
     7    1 IBUT H22    -3.40749   -4.25156    6.62149 IBUT 1       0.00000
     8    1 IBUT H23    -3.68448   -5.80638    5.73121 IBUT 1       0.00000
     9    1 IBUT CB     -5.10072   -5.43005    7.33286 IBUT 1       0.00000
    10    1 IBUT HB     -5.59827   -4.53631    7.77387 IBUT 1       0.00000
    11    1 IBUT C3     -4.28983   -6.16252    8.39026 IBUT 1       0.00000
    12    1 IBUT H31    -4.96014   -6.49112    9.21703 IBUT 1       0.00000
    13    1 IBUT H32    -3.78747   -7.05961    7.95795 IBUT 1       0.00000
    14    1 IBUT H33    -3.51197   -5.48189    8.80559 IBUT 1       0.00000

2,2-dimethylpropane
     1    1 NPNT C1     -6.95571   -6.49691    6.95802 NPNT 1       0.00000
     2    1 NPNT H11    -7.49476   -7.05959    7.75584 NPNT 1       0.00000
     3    1 NPNT H12    -7.68711   -5.86038    6.40990 NPNT 1       0.00000
     4    1 NPNT H13    -6.50529   -7.22533    6.24595 NPNT 1       0.00000
     5    1 NPNT C2     -5.13556   -4.85860    6.45104 NPNT 1       0.00000
     6    1 NPNT H21    -5.86082   -4.21655    5.90121 NPNT 1       0.00000
     7    1 NPNT H22    -4.33149   -4.21235    6.87475 NPNT 1       0.00000
     8    1 NPNT H23    -4.67783   -5.58045    5.73694 NPNT 1       0.00000
     9    1 NPNT CB     -5.86041   -5.61960    7.55746 NPNT 1       0.00000
    10    1 NPNT C3     -4.85946   -6.50250    8.29798 NPNT 1       0.00000
    11    1 NPNT H31    -5.37910   -7.05682    9.11235 NPNT 1       0.00000
    12    1 NPNT H32    -4.39041   -7.23845    7.60372 NPNT 1       0.00000
    13    1 NPNT H33    -4.05963   -5.86917    8.74483 NPNT 1       0.00000
    14    1 NPNT C4     -6.49086   -4.62045    8.52276 NPNT 1       0.00000
    15    1 NPNT H41    -7.22538   -3.96755    7.99555 NPNT 1       0.00000
    16    1 NPNT H42    -5.69704   -3.98015    8.97047 NPNT 1       0.00000
    17    1 NPNT H43    -7.01655   -5.16784    9.33800 NPNT 1       0.00000

1,3,5-trifluolohexane
     1    1 HEXF C1    -14.75975    2.45496   -5.35362 HEXF 1       0.00000
     2    1 HEXF F1    -14.14446    2.25906   -4.13255 HEXF 1       0.00000
     3    1 HEXF H12   -15.18177    3.49803   -5.38137 HEXF 1       0.00000
     4    1 HEXF H13   -15.60754    1.72049   -5.44834 HEXF 1       0.00000
     5    1 HEXF C2    -13.77653    2.26548   -6.50373 HEXF 1       0.00000
     6    1 HEXF H21   -12.92971    2.98998   -6.39640 HEXF 1       0.00000
     7    1 HEXF H22   -13.35318    1.23155   -6.46789 HEXF 1       0.00000
     8    1 HEXF H31   -15.43442    1.89166   -7.84748 HEXF 1       0.00000
     9    1 HEXF C3    -14.48331    2.48135   -7.85031 HEXF 1       0.00000
    10    1 HEXF F2    -14.82291    3.83283   -7.98621 HEXF 1       0.00000
    11    1 HEXF H41   -13.23724    0.97249   -8.79783 HEXF 1       0.00000
    12    1 HEXF C4    -13.60188    2.00954   -9.00686 HEXF 1       0.00000
    13    1 HEXF H42   -12.72068    2.69230   -9.08831 HEXF 1       0.00000
    14    1 HEXF C5    -14.36685    2.02342  -10.33332 HEXF 1       0.00000
    15    1 HEXF F3    -15.33029    1.02266  -10.36278 HEXF 1       0.00000
    16    1 HEXF H52   -14.90257    3.01462  -10.43042 HEXF 1       0.00000
    17    1 HEXF C6    -13.38883    1.86386  -11.49373 HEXF 1       0.00000
    18    1 HEXF H61   -12.80099    0.92251  -11.38108 HEXF 1       0.00000
    19    1 HEXF H62   -13.94886    1.81983  -12.45786 HEXF 1       0.00000
    20    1 HEXF H63   -12.68960    2.73188  -11.51609 HEXF 1       0.00000
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Ala-Gly-Leu-Phe-Ser extended linear conformation. The C-terminal is caped by the peptide unit -CONH(CH3); and the N-terminal is caped by -NHCOCH3.

1	1	ALA	CAY	-2.14580	0.53881	0.65149	PEP5	1	0.00000
2	1	ALA	HY1	-2.63346	0.72964	1.63825	PEP5	1	0.00000
3	1	ALA	HY2	-2.31377	1.41878	-0.01455	PEP5	1	0.00000
4	1	ALA	HY3	-2.60784	-0.36453	0.18562	PEP5	1	0.00000
5	1	ALA	CY	-0.66812	0.32266	0.88140	PEP5	1	0.00000
6	1	ALA	OY	-0.17376	0.38296	2.02500	PEP5	1	0.00000
7	1	ALA	N	0.09100	0.01759	-0.22858	PEP5	1	0.00000
8	1	ALA	HN	-0.29661	0.10935	-1.13566	PEP5	1	0.00000
9	1	ALA	CA	1.54648	-0.09046	-0.15925	PEP5	1	0.00000
10	1	ALA	HA	1.73848	-0.81589	0.68002	PEP5	1	0.00000
11	1	ALA	CB	2.26439	1.22433	0.17515	PEP5	1	0.00000
12	1	ALA	HB1	3.35631	1.04329	0.31305	PEP5	1	0.00000
13	1	ALA	HB2	2.11298	1.96757	-0.64008	PEP5	1	0.00000
14	1	ALA	HB3	1.84836	1.63237	1.12767	PEP5	1	0.00000
15	1	ALA	C	2.13595	-0.65437	-1.48541	PEP5	1	0.00000
16	1	ALA	O	1.54513	-0.54037	-2.57430	PEP5	1	0.00000
17	2	GLY	N	3.30887	-1.35320	-1.34123	PEP5	2	0.00000
18	2	GLY	HN	3.84229	-1.26502	-0.50868	PEP5	2	0.00000
19	2	GLY	CA	4.00533	-1.85009	-2.52050	PEP5	2	0.00000
20	2	GLY	HA1	3.85019	-2.95993	-2.49123	PEP5	2	0.00000
21	2	GLY	HA2	3.55062	-1.43543	-3.45188	PEP5	2	0.00000
22	2	GLY	C	5.51930	-1.53844	-2.51969	PEP5	2	0.00000
23	2	GLY	O	6.10725	-1.14258	-1.49821	PEP5	2	0.00000
24	3	LEU	N	6.17040	-1.86824	-3.68569	PEP5	3	0.00000
25	3	LEU	HN	5.64440	-1.98010	-4.52049	PEP5	3	0.00000
26	3	LEU	CA	7.58710	-1.55354	-3.88216	PEP5	3	0.00000
27	3	LEU	HA	8.10509	-2.00010	-2.99286	PEP5	3	0.00000
28	3	LEU	CB	7.88671	-0.03729	-3.92407	PEP5	3	0.00000
29	3	LEU	HB1	7.62780	0.35047	-4.94285	PEP5	3	0.00000
30	3	LEU	HB2	7.20416	0.46765	-3.18890	PEP5	3	0.00000
31	3	LEU	CG	9.31791	0.35050	-3.57643	PEP5	3	0.00000
32	3	LEU	HG	10.03649	-0.32178	-4.12198	PEP5	3	0.00000
33	3	LEU	CD1	9.56815	1.77282	-4.04443	PEP5	3	0.00000
34	3	LEU	HD11	10.61797	2.07446	-3.81289	PEP5	3	0.00000
35	3	LEU	HD12	9.41082	1.85777	-5.14628	PEP5	3	0.00000
36	3	LEU	HD13	8.87434	2.47990	-3.52961	PEP5	3	0.00000
37	3	LEU	CD2	9.59584	0.24508	-2.09082	PEP5	3	0.00000
38	3	LEU	HD21	10.57997	0.71682	-1.85193	PEP5	3	0.00000
39	3	LEU	HD22	8.80108	0.76307	-1.50161	PEP5	3	0.00000
40	3	LEU	HD23	9.63550	-0.82054	-1.76376	PEP5	3	0.00000
41	3	LEU	C	8.08386	-2.22329	-5.20988	PEP5	3	0.00000
42	3	LEU	O	7.39765	-2.14258	-6.24448	PEP5	3	0.00000
43	4	PHE	N	9.29637	-2.85767	-5.11343	PEP5	4	0.00000
44	4	PHE	HN	9.72777	-2.93901	-4.22148	PEP5	4	0.00000
45	4	PHE	CA	9.78970	-3.81353	-6.10371	PEP5	4	0.00000
46	4	PHE	HA	9.52350	-3.36923	-7.10290	PEP5	4	0.00000
47	4	PHE	CB	9.09353	-5.19966	-5.99819	PEP5	4	0.00000
48	4	PHE	HB1	9.47103	-5.71774	-5.07850	PEP5	4	0.00000
49	4	PHE	HB2	7.99480	-5.01128	-5.85749	PEP5	4	0.00000
50	4	PHE	CG	9.27046	-6.07102	-7.19276	PEP5	4	0.00000
51	4	PHE	CD1	10.16020	-7.15198	-7.14924	PEP5	4	0.00000
52	4	PHE	HD1	10.74296	-7.34401	-6.23572	PEP5	4	0.00000
53	4	PHE	CD2	8.51801	-5.85202	-8.35418	PEP5	4	0.00000
54	4	PHE	HD2	7.80328	-5.01535	-8.39050	PEP5	4	0.00000

55	4	PHE	CE1	10.31247	-7.98438	-8.25633	PEP5	4	0.00000
56	4	PHE	HE1	11.01407	-8.83027	-8.21227	PEP5	4	0.00000
57	4	PHE	CE2	8.67265	-6.68553	-9.45990	PEP5	4	0.00000
58	4	PHE	HE2	8.08015	-6.50434	-10.36896	PEP5	4	0.00000
59	4	PHE	CZ	9.57436	-7.74890	-9.41573	PEP5	4	0.00000
60	4	PHE	HZ	9.70178	-8.40104	-10.29192	PEP5	4	0.00000
61	4	PHE	C	11.33802	-3.98839	-5.98027	PEP5	4	0.00000
62	4	PHE	O	11.91362	-4.12210	-4.88222	PEP5	4	0.00000
63	5	SER	N	12.02934	-3.96493	-7.16269	PEP5	5	0.00000
64	5	SER	HN	11.55441	-3.88862	-8.03629	PEP5	5	0.00000
65	5	SER	CA	13.45868	-4.14215	-7.20233	PEP5	5	0.00000
66	5	SER	HA	13.92079	-3.37378	-6.50689	PEP5	5	0.00000
67	5	SER	CB	13.92852	-5.54092	-6.72122	PEP5	5	0.00000
68	5	SER	HB1	13.24576	-5.93015	-5.91985	PEP5	5	0.00000
69	5	SER	HB2	13.96980	-6.26964	-7.57326	PEP5	5	0.00000
70	5	SER	OG	15.25528	-5.45192	-6.24268	PEP5	5	0.00000
71	5	SER	HG1	15.21989	-5.02438	-5.37730	PEP5	5	0.00000
72	5	SER	C	14.01016	-3.90110	-8.62783	PEP5	5	0.00000
73	5	SER	O	13.25645	-3.67350	-9.59657	PEP5	5	0.00000
74	5	SER	NT	15.37957	-3.92374	-8.75028	PEP5	5	0.00000
75	5	SER	HNT	15.91780	-4.25615	-7.97987	PEP5	5	0.00000
76	5	SER	CAT	16.02532	-3.85142	-10.02388	PEP5	5	0.00000
77	5	SER	HT1	16.93100	-3.19389	-9.93656	PEP5	5	0.00000
78	5	SER	HT2	16.34870	-4.87193	-10.36724	PEP5	5	0.00000
79	5	SER	HT3	15.32567	-3.41925	-10.78857	PEP5	5	0.00000

Ala-Gly-Leu-Phe-Ser beta turn conformation. The C-terminal is caped by the peptide unit -CONH(CH3); and the N-terminal is caped by -NHCOCH3.

1	1	ALA	CAY	0.78029	3.54076	-8.73330	PEP5	1	0.00000
2	1	ALA	HY1	-0.19064	3.81578	-8.25411	PEP5	1	0.00000
3	1	ALA	HY2	1.06486	4.33624	-9.46288	PEP5	1	0.00000
4	1	ALA	HY3	0.65658	2.57411	-9.27833	PEP5	1	0.00000
5	1	ALA	CY	1.82809	3.40511	-7.65346	PEP5	1	0.00000
6	1	ALA	OY	1.53126	3.53150	-6.44661	PEP5	1	0.00000
7	1	ALA	N	3.10477	3.08451	-8.06257	PEP5	1	0.00000
8	1	ALA	HN	3.33990	3.13986	-9.02443	PEP5	1	0.00000
9	1	ALA	CA	4.23328	3.11077	-7.13498	PEP5	1	0.00000
10	1	ALA	HA	3.90165	2.49122	-6.25722	PEP5	1	0.00000
11	1	ALA	CB	4.59759	4.50724	-6.61397	PEP5	1	0.00000
12	1	ALA	HB1	5.40380	4.42588	-5.84725	PEP5	1	0.00000
13	1	ALA	HB2	4.94534	5.15671	-7.44872	PEP5	1	0.00000
14	1	ALA	HB3	3.69733	4.96402	-6.13880	PEP5	1	0.00000
15	1	ALA	C	5.50585	2.47869	-7.77215	PEP5	1	0.00000
16	1	ALA	O	5.72634	2.55223	-8.99531	PEP5	1	0.00000
17	2	GLY	N	6.31211	1.79233	-6.89876	PEP5	2	0.00000
18	2	GLY	HN	6.17160	1.89417	-5.91006	PEP5	2	0.00000
19	2	GLY	CA	7.63076	1.38830	-7.36019	PEP5	2	0.00000
20	2	GLY	HA1	7.48536	0.40111	-7.86647	PEP5	2	0.00000
21	2	GLY	HA2	8.04712	2.11374	-8.10354	PEP5	2	0.00000
22	2	GLY	C	8.68591	1.28804	-6.23699	PEP5	2	0.00000
23	2	GLY	O	9.63355	2.09557	-6.20578	PEP5	2	0.00000
24	3	LEU	N	8.52103	0.26478	-5.34493	PEP5	3	0.00000
25	3	LEU	HN	7.71232	-0.30815	-5.39035	PEP5	3	0.00000
26	3	LEU	CA	9.58488	-0.19905	-4.45575	PEP5	3	0.00000
27	3	LEU	HA	9.35966	-1.29316	-4.31402	PEP5	3	0.00000
28	3	LEU	CB	11.01020	-0.07449	-5.03579	PEP5	3	0.00000
29	3	LEU	HB1	10.95615	-0.20994	-6.14836	PEP5	3	0.00000

30	3	LEU	HB2	11.38978	0.96559	-4.86726	PEP5	3	0.00000
31	3	LEU	CG	11.99017	-1.09258	-4.46417	PEP5	3	0.00000
32	3	LEU	HG	11.71571	-1.32296	-3.39554	PEP5	3	0.00000
33	3	LEU	CD1	11.96834	-2.38609	-5.25293	PEP5	3	0.00000
34	3	LEU	HD11	12.68618	-3.11660	-4.80705	PEP5	3	0.00000
35	3	LEU	HD12	10.95042	-2.84255	-5.24170	PEP5	3	0.00000
36	3	LEU	HD13	12.26359	-2.20478	-6.31496	PEP5	3	0.00000
37	3	LEU	CD2	13.38907	-0.50656	-4.47349	PEP5	3	0.00000
38	3	LEU	HD21	14.12283	-1.25661	-4.09227	PEP5	3	0.00000
39	3	LEU	HD22	13.68511	-0.21445	-5.50988	PEP5	3	0.00000
40	3	LEU	HD23	13.43702	0.39906	-3.82224	PEP5	3	0.00000
41	3	LEU	C	9.48814	0.44435	-3.03794	PEP5	3	0.00000
42	3	LEU	O	9.38397	-0.31725	-2.06323	PEP5	3	0.00000
43	4	PHE	N	9.51082	1.81278	-2.98709	PEP5	4	0.00000
44	4	PHE	HN	9.66722	2.32608	-3.82181	PEP5	4	0.00000
45	4	PHE	CA	9.32089	2.62588	-1.78644	PEP5	4	0.00000
46	4	PHE	HA	9.74438	3.62558	-2.08506	PEP5	4	0.00000
47	4	PHE	CB	10.15229	2.12312	-0.57222	PEP5	4	0.00000
48	4	PHE	HB1	9.61982	1.24372	-0.12132	PEP5	4	0.00000
49	4	PHE	HB2	11.13630	1.74888	-0.96225	PEP5	4	0.00000
50	4	PHE	CG	10.41203	3.17116	0.45355	PEP5	4	0.00000
51	4	PHE	CD1	9.65160	3.20778	1.62955	PEP5	4	0.00000
52	4	PHE	HD1	8.83556	2.48138	1.77079	PEP5	4	0.00000
53	4	PHE	CD2	11.45219	4.09457	0.28500	PEP5	4	0.00000
54	4	PHE	HD2	12.06498	4.06364	-0.62820	PEP5	4	0.00000
55	4	PHE	CE1	9.91839	4.16007	2.61148	PEP5	4	0.00000
56	4	PHE	HE1	9.31578	4.18226	3.53128	PEP5	4	0.00000
57	4	PHE	CE2	11.71566	5.04702	1.26729	PEP5	4	0.00000
58	4	PHE	HE2	12.53185	5.77035	1.12548	PEP5	4	0.00000
59	4	PHE	CZ	10.94815	5.08271	2.43132	PEP5	4	0.00000
60	4	PHE	HZ	11.15646	5.83438	3.20614	PEP5	4	0.00000
61	4	PHE	C	7.80451	2.78257	-1.44584	PEP5	4	0.00000
62	4	PHE	O	7.24285	2.23514	-0.48721	PEP5	4	0.00000
63	5	SER	N	7.12874	3.69170	-2.26754	PEP5	5	0.00000
64	5	SER	HN	7.51917	3.81738	-3.17885	PEP5	5	0.00000
65	5	SER	CA	5.68485	3.76905	-2.27194	PEP5	5	0.00000
66	5	SER	HA	5.41833	4.76669	-2.74595	PEP5	5	0.00000
67	5	SER	CB	5.08089	3.75622	-0.85164	PEP5	5	0.00000
68	5	SER	HB1	4.91863	2.70548	-0.49230	PEP5	5	0.00000
69	5	SER	HB2	5.76236	4.28686	-0.13391	PEP5	5	0.00000
70	5	SER	OG	3.83936	4.44337	-0.94170	PEP5	5	0.00000
71	5	SER	HG1	3.53584	4.58008	-0.03678	PEP5	5	0.00000
72	5	SER	C	5.03674	2.70086	-3.19360	PEP5	5	0.00000
73	5	SER	O	5.72287	2.14820	-4.08965	PEP5	5	0.00000
74	5	SER	NT	3.70833	2.43309	-3.03738	PEP5	5	0.00000
75	5	SER	HNT	3.18781	2.95005	-2.36260	PEP5	5	0.00000
76	5	SER	CAT	2.99519	1.46986	-3.81829	PEP5	5	0.00000
77	5	SER	HT1	2.46657	0.75295	-3.13344	PEP5	5	0.00000
78	5	SER	HT2	2.23607	1.98620	-4.46807	PEP5	5	0.00000
79	5	SER	HT3	3.70471	0.89133	-4.46694	PEP5	5	0.00000

Table S2. Cartesian coordinates from AM1 geometry optimizations for all compounds described in the main paper. Coordinates are given in angstroms in CHARMM format.

```
water dimer
    1    1 WATE OH2   -6.05189   1.92824   0.65797 WATE 40     0.00000
    2    1 WATE H1    -6.79495   2.54132   0.68802 WATE 40     0.00000
    3    1 WATE H2    -6.10268   1.45695   1.49335 WATE 40     0.00000
    4    2 WATE OH2   -6.09087   3.23186  -1.40355 WATE 48     0.00000
    5    2 WATE H1    -6.16349   2.28154  -1.53829 WATE 48     0.00000
    6    2 WATE H2    -5.27795   3.32324  -0.89627 WATE 48     0.00000

propane
    1    1 PROP H11    5.84338 -13.19156  -5.73133 PROP 1      0.00000
    2    1 PROP H12    4.39381 -12.29097  -5.13165 PROP 1      0.00000
    3    1 PROP H13    5.37850 -13.28696  -3.98697 PROP 1      0.00000
    4    1 PROP C1     4.98159 -13.23136  -5.02644 PROP 1      0.00000
    5    1 PROP HB1    3.23877 -14.44172  -4.62260 PROP 1      0.00000
    6    1 PROP CB     4.10815 -14.43409  -5.32499 PROP 1      0.00000
    7    1 PROP HB2    3.70253 -14.34655  -6.36280 PROP 1      0.00000
    8    1 PROP C3     4.86843 -15.73920  -5.19375 PROP 1      0.00000
    9    1 PROP H31    5.26251 -15.85771  -4.15848 PROP 1      0.00000
   10    1 PROP H32    4.19934 -16.60082  -5.41919 PROP 1      0.00000
   11    1 PROP H33    5.72738 -15.76231  -5.90284 PROP 1      0.00000

2-methylpropane
    1    1 IBUT C1    -6.19415  -6.33873   6.77907 IBUT 1      0.00000
    2    1 IBUT H11   -6.86969  -6.66901   7.60064 IBUT 1      0.00000
    3    1 IBUT H12   -6.79742  -5.79236   6.01884 IBUT 1      0.00000
    4    1 IBUT H13   -5.75054  -7.24080   6.29940 IBUT 1      0.00000
    5    1 IBUT C2    -4.19036  -4.94228   6.20978 IBUT 1      0.00000
    6    1 IBUT H21   -4.78531  -4.39011   5.44718 IBUT 1      0.00000
    7    1 IBUT H22   -3.41144  -4.25894   6.61812 IBUT 1      0.00000
    8    1 IBUT H23   -3.68448  -5.80094   5.71242 IBUT 1      0.00000
    9    1 IBUT CB    -5.09702  -5.43694   7.32898 IBUT 1      0.00000
   10    1 IBUT HB    -5.58479  -4.54447   7.80131 IBUT 1      0.00000
   11    1 IBUT C3    -4.29050  -6.15698   8.40154 IBUT 1      0.00000
   12    1 IBUT H31   -4.95813  -6.48650   9.22984 IBUT 1      0.00000
   13    1 IBUT H32   -3.78773  -7.05339   7.97230 IBUT 1      0.00000
   14    1 IBUT H33   -3.51199  -5.47868   8.81898 IBUT 1      0.00000

2,2-dimethylpropane
    1    1 NPNT C1    -6.95486  -6.49531   6.95038 NPNT 1      0.00000
    2    1 NPNT H11   -7.48928  -7.05456   7.75154 NPNT 1      0.00000
    3    1 NPNT H12   -7.69183  -5.86583   6.40188 NPNT 1      0.00000
    4    1 NPNT H13   -6.51130  -7.22794   6.23854 NPNT 1      0.00000
    5    1 NPNT C2    -5.13939  -4.86121   6.44471 NPNT 1      0.00000
    6    1 NPNT H21   -5.85771  -4.21495   5.89102 NPNT 1      0.00000
    7    1 NPNT H22   -4.33788  -4.21800   6.87377 NPNT 1      0.00000
    8    1 NPNT H23   -4.67718  -5.57706   5.72768 NPNT 1      0.00000
    9    1 NPNT CB    -5.86044  -5.61957   7.55746 NPNT 1      0.00000
   10    1 NPNT C3    -4.86024  -6.49951   8.30481 NPNT 1      0.00000
   11    1 NPNT H31   -5.37315  -7.05880   9.11988 NPNT 1      0.00000
   12    1 NPNT H32   -4.39517  -7.23219   7.60688 NPNT 1      0.00000
   13    1 NPNT H33   -4.05587  -5.87313   8.75297 NPNT 1      0.00000
   14    1 NPNT C4    -6.48725  -4.62225   8.52992 NPNT 1      0.00000
   15    1 NPNT H41   -7.21941  -3.97354   7.99764 NPNT 1      0.00000
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16	1	NPNT	H42	-5.69959	-3.97659	8.98039	NPNT	1	0.00000
17	1	NPNT	H43	-7.01687	-5.16226	9.34730	NPNT	1	0.00000

Ala-Gly-Leu-Phe-Ser extended linear conformation. The C-terminal is caped by the peptide unit -CONH(CH3); and the N-terminal is caped by -NHCOCH3.

1	1	ALA	CAY	-2.02562	-0.03633	0.26618	PEP5	1	0.00000
2	1	ALA	HY1	-2.65828	-0.67539	0.92925	PEP5	1	0.00000
3	1	ALA	HY2	-2.22503	1.03743	0.49811	PEP5	1	0.00000
4	1	ALA	HY3	-2.29540	-0.23784	-0.79867	PEP5	1	0.00000
5	1	ALA	CY	-0.57598	-0.37583	0.50818	PEP5	1	0.00000
6	1	ALA	OY	-0.23679	-1.28495	1.29104	PEP5	1	0.00000
7	1	ALA	N	0.36973	0.39770	-0.14754	PEP5	1	0.00000
8	1	ALA	HN	0.07670	1.00930	-0.87454	PEP5	1	0.00000
9	1	ALA	CA	1.77386	0.08172	-0.11285	PEP5	1	0.00000
10	1	ALA	HA	1.91963	-0.75767	0.63519	PEP5	1	0.00000
11	1	ALA	CB	2.64678	1.26717	0.30592	PEP5	1	0.00000
12	1	ALA	HB1	3.71194	0.93616	0.35091	PEP5	1	0.00000
13	1	ALA	HB2	2.55939	2.10563	-0.42615	PEP5	1	0.00000
14	1	ALA	HB3	2.34165	1.63532	1.31436	PEP5	1	0.00000
15	1	ALA	C	2.27842	-0.35341	-1.51376	PEP5	1	0.00000
16	1	ALA	O	1.88601	0.22134	-2.54865	PEP5	1	0.00000
17	2	GLY	N	3.15553	-1.41883	-1.56344	PEP5	2	0.00000
18	2	GLY	HN	3.55745	-1.75726	-0.71712	PEP5	2	0.00000
19	2	GLY	CA	3.82600	-1.79156	-2.77283	PEP5	2	0.00000
20	2	GLY	HA1	3.60638	-2.87824	-2.99125	PEP5	2	0.00000
21	2	GLY	HA2	3.43131	-1.16644	-3.62489	PEP5	2	0.00000
22	2	GLY	C	5.35806	-1.68545	-2.65888	PEP5	2	0.00000
23	2	GLY	O	5.94317	-1.92676	-1.58281	PEP5	2	0.00000
24	3	LEU	N	6.04601	-1.34003	-3.79893	PEP5	3	0.00000
25	3	LEU	HN	5.55940	-1.16493	-4.64755	PEP5	3	0.00000
26	3	LEU	CA	7.48717	-1.31636	-3.86204	PEP5	3	0.00000
27	3	LEU	HA	7.88039	-1.71181	-2.87596	PEP5	3	0.00000
28	3	LEU	CB	8.05344	0.09639	-4.08797	PEP5	3	0.00000
29	3	LEU	HB1	7.82884	0.41434	-5.14092	PEP5	3	0.00000
30	3	LEU	HB2	7.53743	0.81480	-3.39742	PEP5	3	0.00000
31	3	LEU	CG	9.55361	0.17256	-3.84539	PEP5	3	0.00000
32	3	LEU	HG	10.06314	-0.64993	-4.42436	PEP5	3	0.00000
33	3	LEU	CD1	10.07460	1.50260	-4.35578	PEP5	3	0.00000
34	3	LEU	HD11	11.18003	1.56327	-4.21140	PEP5	3	0.00000
35	3	LEU	HD12	9.85173	1.61956	-5.44347	PEP5	3	0.00000
36	3	LEU	HD13	9.59790	2.34743	-3.80275	PEP5	3	0.00000
37	3	LEU	CD2	9.89853	0.01008	-2.37946	PEP5	3	0.00000
38	3	LEU	HD21	10.99183	0.17830	-2.22344	PEP5	3	0.00000
39	3	LEU	HD22	9.33448	0.74517	-1.75646	PEP5	3	0.00000
40	3	LEU	HD23	9.65190	-1.01889	-2.02302	PEP5	3	0.00000
41	3	LEU	C	7.96091	-2.20523	-5.04219	PEP5	3	0.00000
42	3	LEU	O	7.44857	-2.09073	-6.17335	PEP5	3	0.00000
43	4	PHE	N	8.92234	-3.15815	-4.76812	PEP5	4	0.00000
44	4	PHE	HN	9.43612	-3.08780	-3.91660	PEP5	4	0.00000
45	4	PHE	CA	9.55013	-3.91940	-5.82315	PEP5	4	0.00000
46	4	PHE	HA	9.15255	-3.53716	-6.81624	PEP5	4	0.00000
47	4	PHE	CB	9.23831	-5.42841	-5.71835	PEP5	4	0.00000
48	4	PHE	HB1	9.96625	-5.91305	-5.01616	PEP5	4	0.00000
49	4	PHE	HB2	8.21185	-5.56879	-5.28045	PEP5	4	0.00000
50	4	PHE	CG	9.27019	-6.08980	-7.05101	PEP5	4	0.00000
51	4	PHE	CD1	10.19138	-7.10971	-7.31470	PEP5	4	0.00000

52	4	PHE	HD1	10.91249	-7.41149	-6.54063	PEP5	4	0.00000
53	4	PHE	CD2	8.34895	-5.72363	-8.04129	PEP5	4	0.00000
54	4	PHE	HD2	7.61484	-4.92826	-7.83722	PEP5	4	0.00000
55	4	PHE	CE1	10.19589	-7.75007	-8.55344	PEP5	4	0.00000
56	4	PHE	HE1	10.92594	-8.54787	-8.75439	PEP5	4	0.00000
57	4	PHE	CE2	8.35841	-6.36273	-9.27931	PEP5	4	0.00000
58	4	PHE	HE2	7.63660	-6.06467	-10.05418	PEP5	4	0.00000
59	4	PHE	CZ	9.28195	-7.37621	-9.53774	PEP5	4	0.00000
60	4	PHE	HZ	9.29077	-7.87698	-10.51678	PEP5	4	0.00000
61	4	PHE	C	11.08659	-3.72520	-5.81392	PEP5	4	0.00000
62	4	PHE	O	11.67277	-3.12144	-4.88902	PEP5	4	0.00000
63	5	SER	N	11.78844	-4.25889	-6.86747	PEP5	5	0.00000
64	5	SER	HN	11.32239	-4.74065	-7.60699	PEP5	5	0.00000
65	5	SER	CA	13.20738	-4.04400	-6.99458	PEP5	5	0.00000
66	5	SER	HA	13.42375	-2.96949	-6.69618	PEP5	5	0.00000
67	5	SER	CB	14.04694	-4.95861	-6.06427	PEP5	5	0.00000
68	5	SER	HB1	13.48855	-5.16878	-5.11398	PEP5	5	0.00000
69	5	SER	HB2	14.30710	-5.92381	-6.57328	PEP5	5	0.00000
70	5	SER	OG	15.28789	-4.34363	-5.78279	PEP5	5	0.00000
71	5	SER	HG1	15.11674	-3.61479	-5.17254	PEP5	5	0.00000
72	5	SER	C	13.68892	-4.23833	-8.45169	PEP5	5	0.00000
73	5	SER	O	12.91800	-4.60739	-9.36029	PEP5	5	0.00000
74	5	SER	NT	15.01160	-3.94126	-8.68759	PEP5	5	0.00000
75	5	SER	HNT	15.61298	-3.80027	-7.90580	PEP5	5	0.00000
76	5	SER	CAT	15.62338	-4.15511	-9.96156	PEP5	5	0.00000
77	5	SER	HT1	16.30145	-3.29023	-10.19225	PEP5	5	0.00000
78	5	SER	HT2	16.23177	-5.10042	-9.96106	PEP5	5	0.00000
79	5	SER	HT3	14.83822	-4.23280	-10.76058	PEP5	5	0.00000

Ala-Gly-Leu-Phe-Ser beta turn conformation. The C-terminal is caped by the peptide unit -CONH(CH3); and the N-terminal is caped by -NHCOCH3.

1	1	ALA	CAY	0.98957	3.28525	-8.92608	PEP5	1	0.00000
2	1	ALA	HY1	-0.01743	3.03194	-8.51395	PEP5	1	0.00000
3	1	ALA	HY2	0.95375	4.30910	-9.36980	PEP5	1	0.00000
4	1	ALA	HY3	1.25152	2.55045	-9.72559	PEP5	1	0.00000
5	1	ALA	CY	2.00253	3.21220	-7.80979	PEP5	1	0.00000
6	1	ALA	OY	1.69095	2.79946	-6.67291	PEP5	1	0.00000
7	1	ALA	N	3.28143	3.65915	-8.08745	PEP5	1	0.00000
8	1	ALA	HN	3.53441	3.84909	-9.03046	PEP5	1	0.00000
9	1	ALA	CA	4.37236	3.49777	-7.15959	PEP5	1	0.00000
10	1	ALA	HA	3.95432	3.07661	-6.18964	PEP5	1	0.00000
11	1	ALA	CB	5.09199	4.80924	-6.83713	PEP5	1	0.00000
12	1	ALA	HB1	5.84461	4.60726	-6.03594	PEP5	1	0.00000
13	1	ALA	HB2	5.61174	5.21513	-7.73744	PEP5	1	0.00000
14	1	ALA	HB3	4.36586	5.57055	-6.46493	PEP5	1	0.00000
15	1	ALA	C	5.44962	2.54269	-7.73606	PEP5	1	0.00000
16	1	ALA	O	5.74394	2.55189	-8.94887	PEP5	1	0.00000
17	2	GLY	N	6.05018	1.67193	-6.85088	PEP5	2	0.00000
18	2	GLY	HN	5.84864	1.75716	-5.87848	PEP5	2	0.00000
19	2	GLY	CA	7.17842	0.88038	-7.23716	PEP5	2	0.00000
20	2	GLY	HA1	6.83816	-0.18235	-7.40671	PEP5	2	0.00000
21	2	GLY	HA2	7.60634	1.26490	-8.21124	PEP5	2	0.00000
22	2	GLY	C	8.31728	0.92834	-6.20161	PEP5	2	0.00000
23	2	GLY	O	9.04074	1.93877	-6.09633	PEP5	2	0.00000
24	3	LEU	N	8.50132	-0.19298	-5.42332	PEP5	3	0.00000
25	3	LEU	HN	7.82688	-0.92026	-5.47419	PEP5	3	0.00000
26	3	LEU	CA	9.61964	-0.42947	-4.54841	PEP5	3	0.00000

27	3	LEU	HA	9.61782	-1.54186	-4.31711	PEP5	3	0.00000
28	3	LEU	CB	10.98791	-0.07448	-5.15129	PEP5	3	0.00000
29	3	LEU	HB1	11.04026	-0.45873	-6.20428	PEP5	3	0.00000
30	3	LEU	HB2	11.09781	1.04119	-5.20394	PEP5	3	0.00000
31	3	LEU	CG	12.12860	-0.67691	-4.34200	PEP5	3	0.00000
32	3	LEU	HG	11.88003	-0.58935	-3.24450	PEP5	3	0.00000
33	3	LEU	CD1	12.32482	-2.14267	-4.67090	PEP5	3	0.00000
34	3	LEU	HD11	13.15700	-2.56493	-4.05734	PEP5	3	0.00000
35	3	LEU	HD12	11.39829	-2.72577	-4.45245	PEP5	3	0.00000
36	3	LEU	HD13	12.58106	-2.27415	-5.74982	PEP5	3	0.00000
37	3	LEU	CD2	13.40840	0.09003	-4.60808	PEP5	3	0.00000
38	3	LEU	HD21	14.25247	-0.35954	-4.03160	PEP5	3	0.00000
39	3	LEU	HD22	13.66486	0.05920	-5.69442	PEP5	3	0.00000
40	3	LEU	HD23	13.29707	1.15744	-4.30049	PEP5	3	0.00000
41	3	LEU	C	9.47985	0.25489	-3.16112	PEP5	3	0.00000
42	3	LEU	O	9.54416	-0.45623	-2.14045	PEP5	3	0.00000
43	4	PHE	N	9.32072	1.62096	-3.12707	PEP5	4	0.00000
44	4	PHE	HN	9.29370	2.12134	-3.98989	PEP5	4	0.00000
45	4	PHE	CA	9.25441	2.41112	-1.92496	PEP5	4	0.00000
46	4	PHE	HA	9.64226	3.44546	-2.18776	PEP5	4	0.00000
47	4	PHE	CB	10.10638	1.88753	-0.75464	PEP5	4	0.00000
48	4	PHE	HB1	9.56636	1.03129	-0.26318	PEP5	4	0.00000
49	4	PHE	HB2	11.07481	1.48153	-1.15446	PEP5	4	0.00000
50	4	PHE	CG	10.39661	2.96701	0.22780	PEP5	4	0.00000
51	4	PHE	CD1	9.78366	2.95573	1.48632	PEP5	4	0.00000
52	4	PHE	HD1	9.05582	2.16434	1.72682	PEP5	4	0.00000
53	4	PHE	CD2	11.30750	3.98425	-0.08247	PEP5	4	0.00000
54	4	PHE	HD2	11.79441	3.99809	-1.06887	PEP5	4	0.00000
55	4	PHE	CE1	10.08438	3.94419	2.42251	PEP5	4	0.00000
56	4	PHE	HE1	9.60208	3.92620	3.41079	PEP5	4	0.00000
57	4	PHE	CE2	11.60344	4.97303	0.85384	PEP5	4	0.00000
58	4	PHE	HE2	12.31995	5.76856	0.60266	PEP5	4	0.00000
59	4	PHE	CZ	10.99458	4.95309	2.10887	PEP5	4	0.00000
60	4	PHE	HZ	11.23296	5.73083	2.84881	PEP5	4	0.00000
61	4	PHE	C	7.77999	2.55743	-1.44545	PEP5	4	0.00000
62	4	PHE	O	7.32498	1.87671	-0.51163	PEP5	4	0.00000
63	5	SER	N	7.04457	3.55839	-2.07468	PEP5	5	0.00000
64	5	SER	HN	7.35141	3.81121	-2.99178	PEP5	5	0.00000
65	5	SER	CA	5.62429	3.74908	-1.89344	PEP5	5	0.00000
66	5	SER	HA	5.42921	4.85993	-2.04065	PEP5	5	0.00000
67	5	SER	CB	5.13004	3.38266	-0.48023	PEP5	5	0.00000
68	5	SER	HB1	4.91866	2.28393	-0.39889	PEP5	5	0.00000
69	5	SER	HB2	5.89872	3.66510	0.28871	PEP5	5	0.00000
70	5	SER	OG	3.93869	4.13102	-0.26774	PEP5	5	0.00000
71	5	SER	HG1	3.70805	4.01888	0.66140	PEP5	5	0.00000
72	5	SER	C	4.79878	3.06047	-3.01293	PEP5	5	0.00000
73	5	SER	O	5.34332	2.79976	-4.11430	PEP5	5	0.00000
74	5	SER	NT	3.47813	2.79159	-2.79119	PEP5	5	0.00000
75	5	SER	HNT	3.05413	3.10731	-1.94758	PEP5	5	0.00000
76	5	SER	CAT	2.62111	2.24830	-3.80166	PEP5	5	0.00000
77	5	SER	HT1	1.87219	1.56574	-3.31993	PEP5	5	0.00000
78	5	SER	HT2	2.07458	3.06353	-4.35137	PEP5	5	0.00000
79	5	SER	HT3	3.22128	1.66701	-4.55191	PEP5	5	0.00000