Supplementary Material (ESI) for PCCP

A Matrix Isolation Study on Ac-Gly-NHMe and Ac-L-Ala-NHMe, the Simplest Chiral and Achiral Building Blocks of Petides and Proteins

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Supporting information

Table set S1. Optimized geometries of Ac-Gly-NHMe conformers at the B3LYP/6-31G* level of theory (Descartes coordinates in Angstroms):

β_{DL}

Atom	X	Y	Z
N	-1.193841	0.224334	-0.000491
H	-0.939983	1.204386	-0.000674
C	-0.086347	-0.696033	-0.000563
C	1.215746	0.108938	-0.000381
H	-0.121874	-1.355156	0.877891
H	-0.121790	-1.355014	-0.879132
O	1.213222	1.337062	-0.000229
C	-2.481154	-0.216930	0.000149
O	-2.758025	-1.412716	0.000562
N	2.347942	-0.643248	-0.000114
H	2.257016	-1.648509	-0.000216
C	3.679787	-0.062041	0.000392
H	4.241983	-0.361522	0.891339
H	4.242546	-0.361211	-0.890304
H	3.562948	1.021590	0.000547
C	-3.548451	0.866084	0.000259
H	-4.182418	0.734525	0.881252
H	-3.143928	1.881618	-0.000349
H	-4.183380	0.733844	-0.879939

$\delta_{D=L}$

Atom	X	Y	Z
N	0.893573	-0.557540	-0.449054
H	0.943931	-0.341071	-1.433902
C	-0.169950	-1.441171	-0.000878
C	-1.573601	-0.823773	0.043508
H	-0.239382	-2.335728	-0.627126
H	0.095884	-1.759708	1.011644

O	-2.563429	-1.545068	0.034271
C	1.995396	-0.284714	0.333527
O	2.079390	-0.642913	1.498738
N	-1.613552	0.534522	0.117728
H	-0.731843	1.022650	0.170601
C	-2.855787	1.268897	0.266618
H	-2.935784	1.729114	1.258349
H	-2.942093	2.053381	-0.492703
H	-3.672089	0.556476	0.142489
C	3.100501	0.500259	-0.354716
H	3.955154	-0.163580	-0.517532
H	2.803164	0.931330	-1.314756
H	3.430518	1.298636	0.313191

$\gamma_{D=L}$

Atom	**X**	**Y**	**Z**
N	-0.993551	-1.092113	-0.028680
H	-1.268766	-1.763515	0.671469
C	0.209253	-1.363457	-0.810556
C	1.492584	-0.739955	-0.225366
H	0.367226	-2.441271	-0.849328
H	0.041515	-0.984597	-1.823499
O	2.391343	-1.440645	0.228171
C	-1.691554	0.069449	-0.149556
O	-1.331044	0.974180	-0.905594
N	1.516368	0.617774	-0.278864
H	0.688608	1.082685	-0.641816
C	2.616556	1.395917	0.258138
H	3.384145	0.698089	0.594349
H	3.041194	2.055237	-0.506654
H	2.296346	2.010726	1.107685
C	-2.949080	0.187986	0.691316
H	-3.797428	0.362893	0.024343
H	-3.154581	-0.692973	1.304761
H	-2.859133	1.063590	1.339681

Table S2. Scaled vibrational frequencies of Ac-Gly-NHMe conformers at the B3LYP/6-31G* level of theory

β_{DL}		$\delta_{D=L}$		$\gamma_{D=L}$	
Wavenumber (cm^{-1})	IR intensity (km/mol)	Wavenumber (cm^{-1})	IR intensity (km/mol)	Wavenumber (cm^{-1})	IR intensity (km/mol)
20	0.1	36.4	3.6	51	2.9
41	7.8	49.0	4.7	59	5.5
53	2.7	56.8	7.7	71	0.5
74	0.0	84.6	0.5	77	6.3

112	14.6	86.5	1.1	122	16.9
139	4.0	152.6	8.7	152	4.1
169	16.8	223.1	2.3	232	3.4
248	5.3	273.2	10.2	272	4.5
285	2.9	314.0	4.9	311	11.2
376	24.4	366.4	14.7	388	8.2
438	65.9	435.0	96.7	425	91.8
488	11.0	519.3	22.3	462	25.8
498	102.6	524.6	57.6	567	11.1
590	0.0	578.1	10.9	615	5.1
615	7.0	615.0	16.6	624	5.5
630	4.2	650.8	1.9	692	91.4
689	0.4	678.6	12.0	778	4.1
868	3.9	843.8	10.2	821	2.9
963	8.6	860.6	7.1	869	5.5
974	19.6	964.1	6.9	957	4.7
984	0.8	1020.3	11.9	991	2.3
1025	4.0	1029.0	6.3	1031	8.8
1032	9.1	1066.9	1.8	1061	3.7
1124	0.7	1082.0	13.8	1085	2.1
1138	9.9	1123.9	3.2	1122	1.5
1152	35.0	1146.9	28.0	1155	35.5
1201	0.0	1210.1	45.8	1215	29.0
1205	108.3	1224.9	91.4	1260	75.6
1233	26.1	1249.5	133.3	1277	36.1
1334	33.1	1324.6	1.1	1334	3.4
1357	33.5	1354.5	28.8	1357	22.3
1395	17.4	1392.8	12.4	1392	15.2
1427	5.1	1421.1	27.1	1421	18.2
1437	44.8	1424.0	9.6	1424	6.0
1451	86.1	1441.1	10.7	1439	18.5
1454	7.0	1448.3	59.3	1453	25.7
1461	8.2	1456.2	13.2	1455	9.6
1492	439.4	1489.5	197.3	1506	173.7
1535	130.4	1526.8	160.7	1555	176.6
1702	368.2	1725.6	270.2	1685	148.1
1721	81.2	1728.8	216.3	1724	332.0
2895	32.9	2907.7	60.8	2906	61.0
2914	55.7	2927.6	6.8	2931	6.3
2917	16.4	2941.9	22.0	2947	11.9
2929	7.4	2961.2	33.8	2957	35.8
2968	30.3	2992.9	8.0	3007	4.3
3004	7.2	2997.7	12.1	3010	15.6
3008	18.5	3016.7	8.5	3023	6.4
3037	0.8	3028.9	1.5	3028	2.9
3463	99.7	3494.7	19.6	3389	165.9
3498	27.3	3500.6	35.1	3514	30.4

Table set S3. Optimized geometries of Ac-L-Ala-NHMe conformers at the B3LYP/6-31G* level of theory (Descartes coordinates in Angstroms):

α_D

Atom	X	Y	Z
N	-1.024337	0.624809	-0.692456
H	-1.436028	0.946321	-1.554931
C	0.243755	1.267504	-0.299493
C	1.495715	0.370934	-0.473862
H	0.402914	2.061762	-1.031132
O	2.436278	0.770448	-1.155248
C	-1.689662	-0.343632	-0.009300
O	-1.254184	-0.872509	1.017625
N	1.476448	-0.805804	0.199813
H	0.631904	-1.039002	0.718312
C	2.585015	-1.740597	0.149313
H	2.984567	-1.932184	1.151530
H	2.278865	-2.697076	-0.290054
H	3.367447	-1.298488	-0.468135
C	-3.035439	-0.753491	-0.584189
H	-3.809524	-0.538096	0.157629
H	-3.292381	-0.250508	-1.519974
H	-3.032212	-1.834280	-0.746191
C	0.177558	1.893828	1.101750
H	1.124268	2.397286	1.317356
H	-0.626239	2.635021	1.145642
H	-0.004728	1.137753	1.865996

$\beta_{L(D)}$

Atom	X	Y	Z
N	-1.180963	-0.407485	0.151458
H	-0.925728	-1.325374	0.494820
C	-0.069798	0.495981	-0.067527
C	1.210018	-0.355038	-0.043735
H	-0.192412	0.957906	-1.055480
O	1.218541	-1.488280	0.432380
C	-2.448557	-0.093369	-0.234153
O	-2.732977	0.992339	-0.733704
N	2.313275	0.250589	-0.557462
H	2.212326	1.171204	-0.957784
C	3.621981	-0.380491	-0.576581
H	3.981824	-0.514342	-1.602384
H	4.355178	0.212148	-0.019067
H	3.519453	-1.358047	-0.105521

C	-3.493288	-1.173422	-0.000097
H	-3.089522	-2.086129	0.445694
H	-4.273437	-0.772344	0.652585
H	-3.963921	-1.419090	-0.955899
C	-0.019202	1.616575	0.989699
H	-0.958474	2.171912	0.956180
H	0.111807	1.192210	1.989388
H	0.803876	2.312546	0.797191

δ_D

Atom	**X**	**Y**	**Z**
N	-0.923163	-0.192089	-0.198594
H	-0.561954	-1.090543	-0.489472
C	-0.035104	0.958883	-0.420623
C	1.410658	0.483321	-0.619287
H	-0.311765	1.472469	-1.347504
O	2.154437	1.021518	-1.426905
C	-2.293557	-0.059951	-0.194931
O	-2.857582	1.024837	-0.171627
N	1.797941	-0.558559	0.183815
H	1.183482	-0.817442	0.942917
C	3.175379	-1.023563	0.217412
H	3.738201	-0.580291	1.047948
H	3.206802	-2.112830	0.310282
H	3.648064	-0.723570	-0.717891
C	-3.068023	-1.370463	-0.217038
H	-3.532298	-1.492227	-1.200790
H	-2.451557	-2.248769	-0.006723
H	-3.872589	-1.310747	0.518742
C	-0.092790	1.969347	0.738413
H	-1.103698	2.366384	0.827454
H	0.186515	1.494674	1.684800
H	0.602600	2.789612	0.539600

δ_L

Atom	**X**	**Y**	**Z**
N	0.887496	0.170572	-0.248898
H	0.933570	0.180988	-1.258963
C	-0.167185	0.969213	0.373561
C	-1.561962	0.314987	0.267536
H	0.086310	0.984169	1.439730
O	-2.580581	0.984861	0.399277
C	2.022591	-0.204708	0.438732
O	2.133593	-0.075519	1.649117
N	-1.562292	-1.029683	0.058587
H	-0.665859	-1.489567	0.004943

C	-2.781598	-1.815441	0.045453
H	-3.619602	-1.118935	0.087848
H	-2.854946	-2.412765	-0.869744
H	-2.835689	-2.488446	0.909078
C	3.129013	-0.803356	-0.415539
H	2.806093	-1.078246	-1.423568
H	3.945199	-0.078286	-0.494464
H	3.524204	-1.685882	0.091477
C	-0.198923	2.402980	-0.162549
H	0.740432	2.913965	0.064003
H	-0.350935	2.414382	-1.248104
H	-1.028930	2.944716	0.292488

γ_L

Atom	**X**	**Y**	**Z**
N	1.012280	0.653798	-0.179304
H	1.273793	1.230234	-0.965718
C	-0.212047	1.008976	0.548244
C	-1.429958	0.226352	-0.010253
H	-0.047824	0.691230	1.583154
O	-2.299564	0.773606	-0.681110
C	1.753559	-0.446885	0.117247
O	1.424864	-1.245484	0.998248
N	-1.425214	-1.091263	0.322136
H	-0.594592	-1.445742	0.789684
C	-2.429324	-2.016500	-0.169379
H	-2.018739	-2.697397	-0.925154
H	-2.838088	-2.614852	0.651253
H	-3.230360	-1.431453	-0.622237
C	3.023437	-0.637990	-0.692000
H	2.972041	-1.600663	-1.207661
H	3.202326	0.152334	-1.425572
H	3.870985	-0.683010	-0.002972
C	-0.448736	2.512784	0.480024
H	-1.322054	2.782389	1.077478
H	0.420890	3.055586	0.861153
H	-0.657675	2.823951	-0.547259

γ_D

Atom	**X**	**Y**	**Z**
N	-1.024063	0.624608	-0.693013
H	-1.435322	0.945365	-1.555975
C	0.244052	1.267333	-0.300181
C	1.495771	0.370313	-0.474009
H	0.403472	2.061154	-1.032239
O	2.436145	0.768772	-1.156261

C	-1.689644	-0.343335	-0.009398
O	-1.254535	-0.871469	1.018066
N	1.476491	-0.805613	0.201107
H	0.631810	-1.038308	0.719611
C	2.584584	-1.740981	0.150807
H	2.982508	-1.934144	1.153350
H	2.278633	-2.696718	-0.290350
H	3.368117	-1.298451	-0.464946
C	-3.035387	-0.753311	-0.584275
H	-3.290557	-0.253307	-1.522139
H	-3.033530	-1.834668	-0.742333
H	-3.810032	-0.534073	0.155857
C	0.177735	1.894417	1.100708
H	1.124499	2.397822	1.316206
H	-0.625930	2.635786	1.144060
H	-0.004818	1.138806	1.865346

Table set S4. Scaled vibrational frequencies of Ac-L-Ala-NHMe conformers at the B3LYP/6-31G* level of theory

α_D

Wavenumber (cm^{-1})	IR intensity (km/mol)	VCR rotatory strength (
45	1.3	25.2
53	4.5	-28.5
65	0.6	-7.0
77	6.7	0.5
128	8.4	3.1
143	3.7	-2.6
195	7.5	-4.3
219	1.0	1.4
243	1.2	10.8
259	9.4	-21.5
333	12.6	-9.5
369	5.2	0.6
390	9.5	30.4
439	72.7	-7.9
517	18.1	-32.2
602	5.6	72.2
635	1.2	-11.0
675	7.0	16.6
708	69.3	23.0
769	17.9	22.6
821	0.4	1.4
882	4.8	13.9
914	7.2	19.0

970	7.3	-18.0
1006	7.5	-4.1
1031	10.3	-2.8
1068	5.8	-4.2
1107	7.9	33.0
1120	17.4	-58.3
1123	7.6	-22.3
1158	19.4	24.6
1248	60.5	-89.3
1271	59.5	158.9
1288	7.3	42.1
1351	31.1	-7.8
1354	17.2	1.8
1364	37.0	-20.5
1391	13.1	8.1
1423	6.0	-1.7
1438	24.0	-2.1
1445	5.7	1.1
1454	27.6	-7.4
1455	6.8	-1.0
1465	1.8	-1.6
1510	160.0	19.3
1563	182.9	-50.5
1680	126.9	0.4
1714	332.3	1.3
2906	66.6	-8.2
2929	19.6	-2.0
2931	6.5	-2.0
2956	34.9	2.0
2980	8.3	5.2
2995	19.7	-2.1
3005	7.8	6.4
3011	12.0	-5.6
3029	3.1	0.4
3032	8.0	-0.8
3350	253.9	-13.6
3510	27.4	1.5

$\beta_{L(D)}$

36	1.3	-2.4
49	0.4	-10.1
64	9.8	17.0
77	0.1	-3.3
97	8.2	-1.7
131	3.3	7.6
135	11.6	-13.3
230	3.1	19.9
242	2.3	-22.7

284	9.0	23.9
303	4.6	-23.8
378	23.1	7.9
395	17.8	-56.3
478	61.0	29.8
508	10.7	-2.7
520	87.0	34.5
611	7.2	-43.1
639	6.5	16.7
673	0.5	7.7
733	3.2	-6.5
841	1.6	-6.0
888	2.0	-7.0
957	29.9	25.7
980	3.2	-6.6
1019	4.5	8.1
1031	8.5	-3.1
1051	3.2	8.8
1076	2.3	-5.1
1124	1.1	2.0
1146	26.0	-8.5
1163	39.8	0.1
1198	65.0	65.3
1229	19.7	-107.9
1303	66.5	-70.8
1340	0.5	6.0
1353	11.3	-18.9
1361	23.5	23.7
1396	16.4	3.9
1426	5.2	-0.3
1434	73.3	-16.4
1443	2.5	-2.7
1450	90.0	-23.1
1455	8.3	3.1
1462	10.7	1.3
1491	401.5	41.4
1533	124.1	27.0
1696	348.3	-11.0
1713	70.3	5.4
2913	66.8	-2.8
2917	8.3	6.4
2921	22.6	-3.3
2929	7.0	0.7
2967	29.5	0.2
2991	29.1	-9.9
3004	7.1	-1.9
3008	17.6	2.3
3019	7.4	0.3

3036	0.8	0.1
3458	92.1	-7.2
3504	24.9	0.3

δ_D

44	3.3	0.8
47	8.5	32.1
63	1.6	-19.2
73	0.6	0.4
104	1.5	3.6
127	1.8	-1.6
172	7.0	14.9
223	14.7	-4.3
241	0.9	-9.6
266	4.7	10.5
310	3.4	-0.4
373	15.4	-23.3
377	14.7	-20.9
456	128.0	-42.6
527	8.1	32.3
573	29.2	-21.4
620	8.3	-4.9
628	34.4	-74.6
672	5.9	29.1
740	6.4	23.9
834	1.2	4.9
883	2.1	-6.7
946	8.3	19.2
961	18.5	-59.4
999	3.0	-8.5
1028	9.3	-1.9
1076	15.1	4.6
1087	9.7	-19.1
1118	15.0	-31.7
1122	10.5	28.9
1149	23.4	-3.2
1227	103.2	33.0
1242	75.8	33.6
1285	22.3	-55.6
1334	26.3	-64.2
1352	16.9	-3.4
1355	22.5	11.1
1395	10.6	30.5
1424	20.6	-7.0
1438	30.6	11.6
1442	10.9	-7.9
1444	67.9	15.9
1457	29.0	22.8

1468	16.5	10.6
1481	235.2	73.7
1517	143.0	-67.6
1724	211.8	182.4
1729	209.0	-214.5
2909	57.1	13.8
2924	18.2	7.2
2927	6.3	-1.1
2944	10.8	-8.9
2972	29.8	-0.5
2995	22.3	-5.8
2996	14.2	11.3
3017	9.0	-3.7
3035	1.7	-1.5
3038	2.4	0.6
3471	22.0	-7.6
3484	19.9	0.6

δ_L

34	6.2	-20.6
47	5.3	15.3
54	3.7	-3.5
82	0.1	7.3
86	1.0	-7.4
129	3.1	-3.9
188	5.6	19.7
210	7.8	19.3
224	0.8	-4.2
307	3.3	15.1
335	6.6	5.2
374	14.1	-32.5
420	9.5	7.9
458	70.5	47.7
520	19.3	-102.9
566	36.4	101.6
573	54.5	-71.5
614	15.2	55.4
655	9.3	13.7
744	2.0	-6.8
840	0.9	4.6
884	2.9	-16.5
933	4.2	1.5
976	11.6	25.8
1016	8.2	-21.3
1027	7.1	-1.6
1073	3.5	18.0
1101	6.3	-18.7
1124	8.5	-11.3

1133	73.7	-28.2
1153	17.9	2.0
1214	89.0	24.9
1219	83.7	19.6
1305	1.6	23.2
1310	33.2	9.4
1354	37.4	2.1
1359	7.2	9.7
1392	12.4	-9.6
1424	12.5	5.1
1441	10.2	-11.2
1446	44.3	-29.5
1449	39.1	-23.7
1452	29.0	-30.0
1456	10.7	-5.4
1483	194.9	-95.2
1523	177.8	38.7
1714	244.0	40.9
1726	215.9	-11.5
2907	65.9	-4.9
2918	20.6	-2.5
2927	6.8	1.8
2948	14.9	31.9
2960	33.5	1.4
2989	19.4	-8.7
2996	13.0	-5.4
3018	8.6	1.9
3029	1.3	0.9
3030	6.3	-0.3
3474	15.8	-4.7
3503	38.4	7.3

γ_D

45	1.3	25.6
53	4.5	-29.0
65	0.6	-6.9
77	6.7	0.6
128	8.4	3.1
143	3.7	-2.6
195	7.5	-4.3
219	1.0	1.4
243	1.2	10.8
259	9.4	-21.5
333	12.6	-9.5
369	5.2	0.6
390	9.5	30.4
439	72.7	-8.1
517	18.1	-32.1

602	5.6	72.1
635	1.2	-11.0
675	7.0	16.6
708	69.4	23.0
770	17.9	22.5
821	0.4	1.3
882	4.8	13.9
914	7.2	19.0
969	7.3	-18.0
1006	7.5	-4.0
1031	10.3	-2.9
1068	5.8	-4.2
1107	7.8	33.0
1120	17.4	-58.4
1123	7.6	-22.2
1158	19.4	24.7
1248	60.5	-89.1
1271	59.4	158.9
1288	7.3	42.1
1351	31.0	-7.9
1354	17.2	1.8
1364	37.0	-20.5
1391	13.1	7.8
1423	6.1	-1.9
1438	23.9	-1.9
1445	5.7	1.1
1454	28.2	-6.8
1455	6.2	-1.6
1465	1.8	-1.6
1510	160.0	19.3
1563	182.8	-50.5
1680	126.9	0.2
1714	332.3	1.5
2906	66.6	-8.3
2929	19.6	-2.0
2931	6.5	-2.0
2956	34.9	1.9
2980	8.3	5.2
2995	19.7	-2.1
3005	7.9	6.5
3011	11.8	-5.7
3029	3.1	0.4
3032	8.0	-0.8
3350	253.8	-13.7
3510	27.4	1.5

γ_L

51	2.5	-31.7

59	5.1	38.1
72	0.3	9.7
78	5.3	-7.8
111	11.4	-21.5
149	2.0	18.1
183	7.6	-2.7
202	2.3	8.1
231	4.8	15.8
290	3.9	11.1
321	1.7	4.3
350	16.5	-12.5
427	43.9	77.3
434	55.7	-66.7
491	7.3	-23.9
575	7.8	6.8
616	4.5	-54.6
648	20.5	-17.7
703	89.9	-64.0
773	1.5	-9.8
846	1.1	4.8
888	1.3	-1.9
936	4.9	-6.1
986	3.6	10.2
1018	4.8	-25.9
1029	10.9	4.4
1034	1.1	11.9
1110	14.0	57.2
1121	5.1	18.7
1147	22.2	-43.1
1160	28.2	-3.2
1219	52.5	10.7
1239	54.0	-60.5
1323	13.7	-15.1
1340	3.7	-21.7
1357	28.1	-5.6
1368	5.1	12.1
1393	13.3	3.0
1424	6.1	-1.3
1439	23.7	5.8
1440	10.1	7.8
1449	9.1	-1.9
1451	22.2	-3.6
1457	12.8	0.9
1497	230.8	32.5
1556	178.2	38.1
1680	153.9	-59.0
1719	293.8	22.0
2904	63.1	17.7

2930	15.2	-6.4
2930	7.3	4.2
2946	4.6	8.0
2960	35.3	-1.0
3003	17.3	-4.1
3006	4.9	2.9
3009	15.2	-4.2
3013	14.1	2.7
3029	3.1	-1.5
3382	157.9	25.4
3499	26.3	1.9

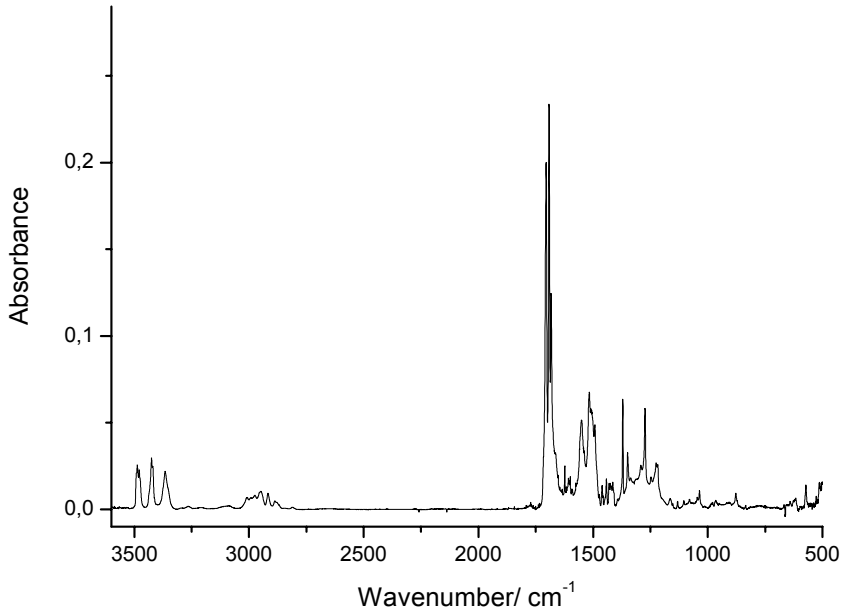

Figure S1. Spectrum of Ac-Gly-NHMe recorded in Ar.

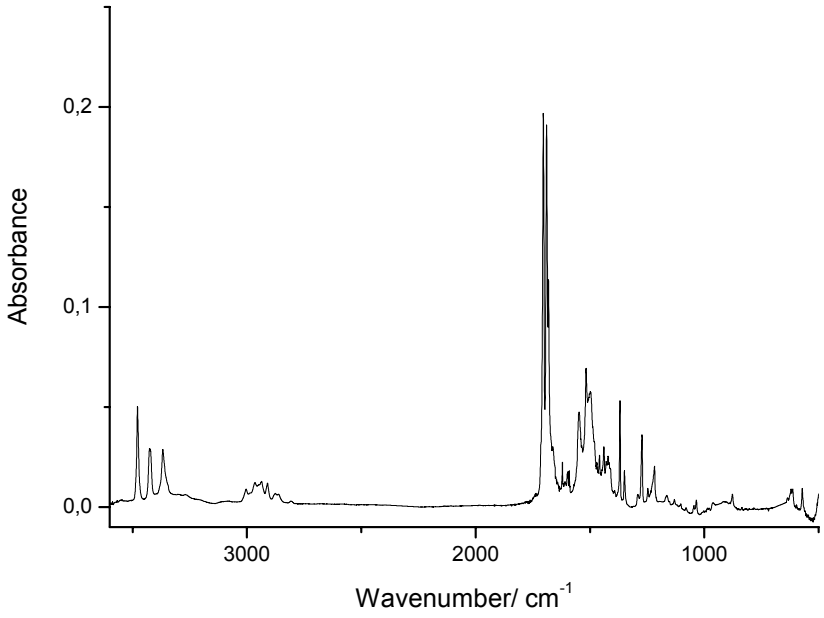

Figure S2. Spectrum of Ac-Gly-NHMe recorded in Kr.

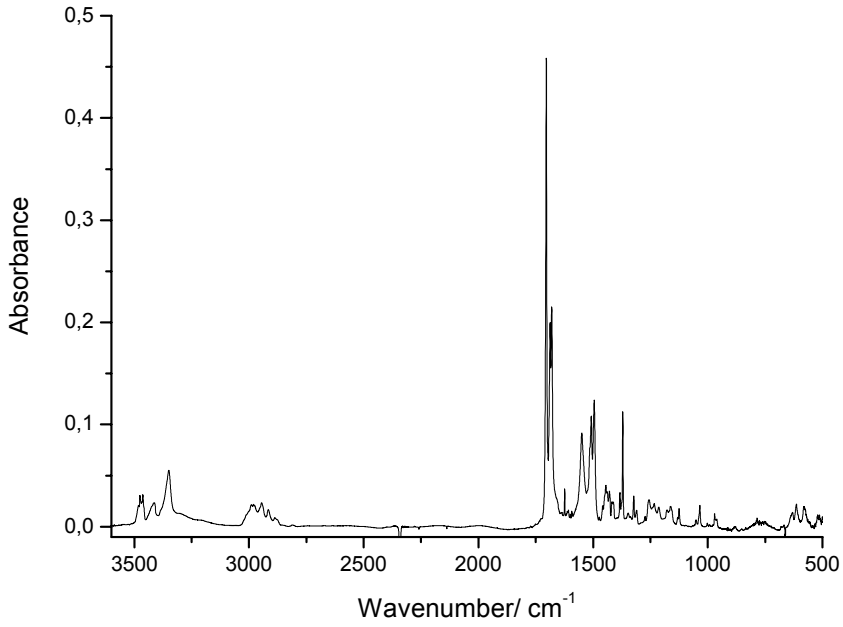

Figure S3. Spectrum of Ac-L-Ala-NHMe recorded in Ar.

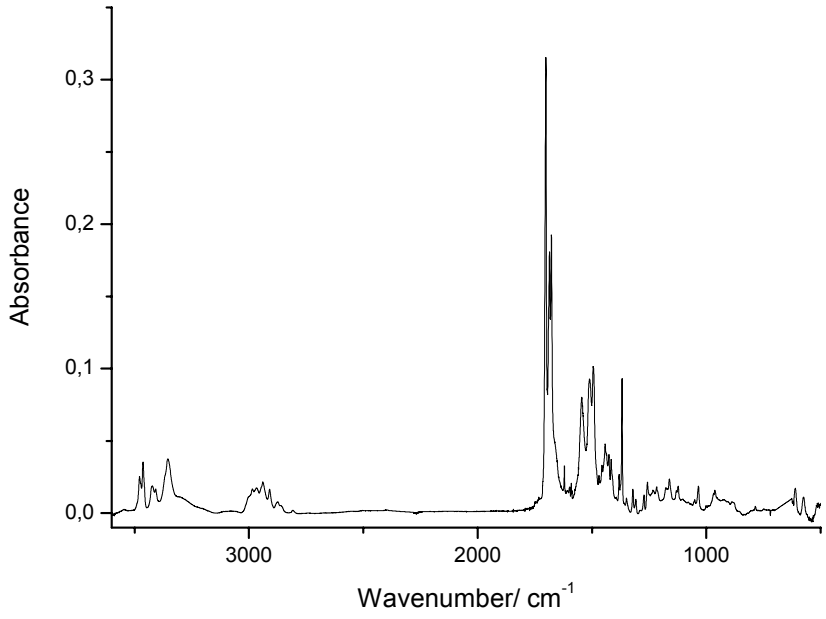

Figure S4. Spectrum of Ac-L-Ala-NHMe recorded in Kr.

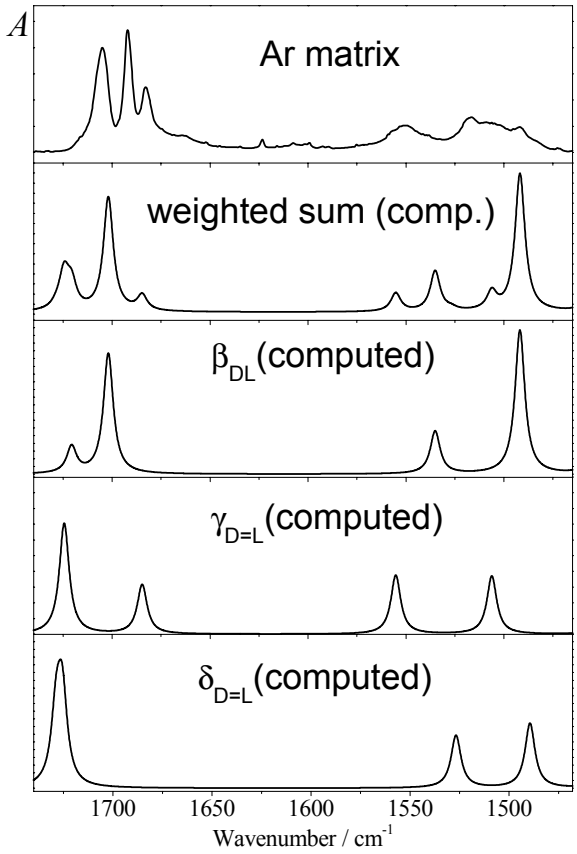

Figure S5. Experimental and computed IR spectra Ac-Gly-NHMe in the amide I and amide II regions.

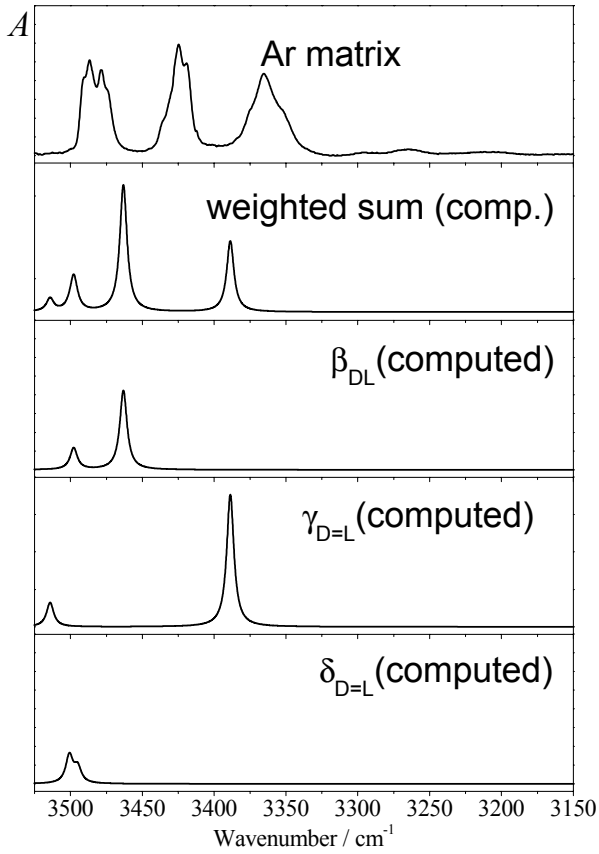

Figure S6. Experimental and computed IR spectra Ac-Gly-NHMe in the amide A region.

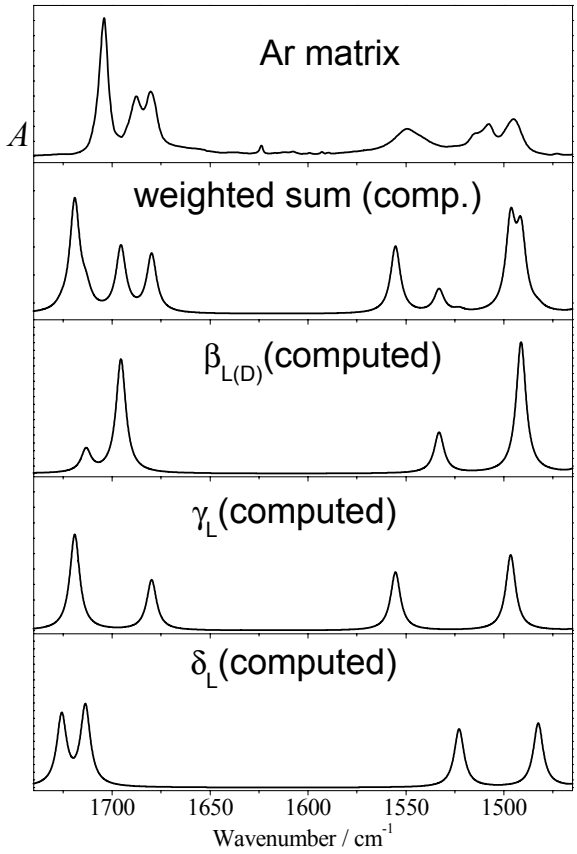

Figure S7. Experimental and computed IR spectra Ac-L-Ala-NHMe in the amide I and amide II regions.

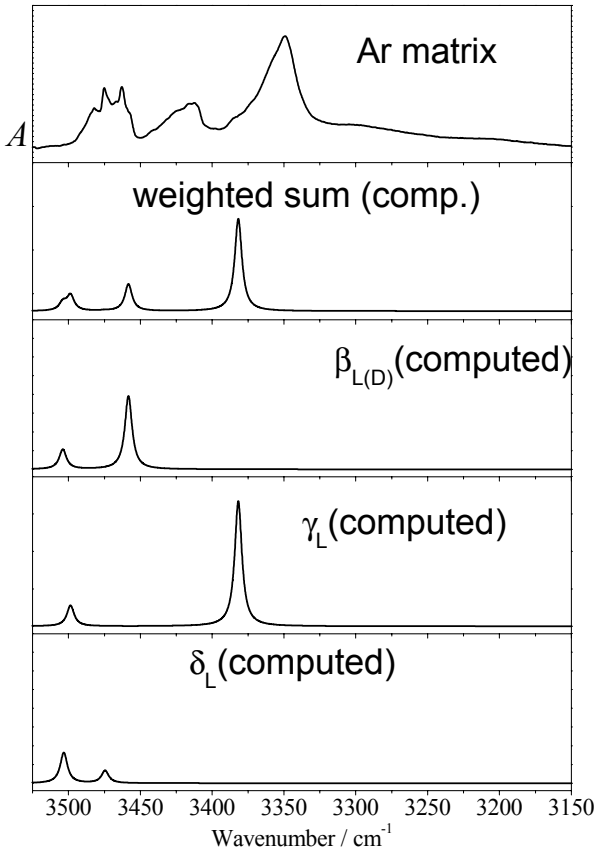

Figure S8. Experimental and computed IR spectra Ac-L-Ala-NHMe in the amide A region.

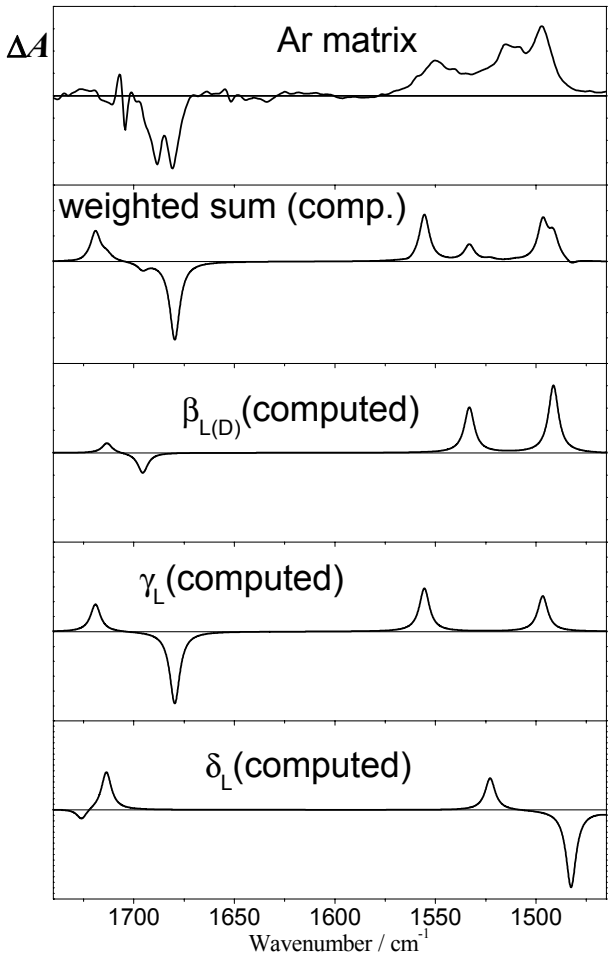

Figure S9. Experimental and computed IR spectra Ac-L-Ala-NHMe in the amide I and amide II regions.

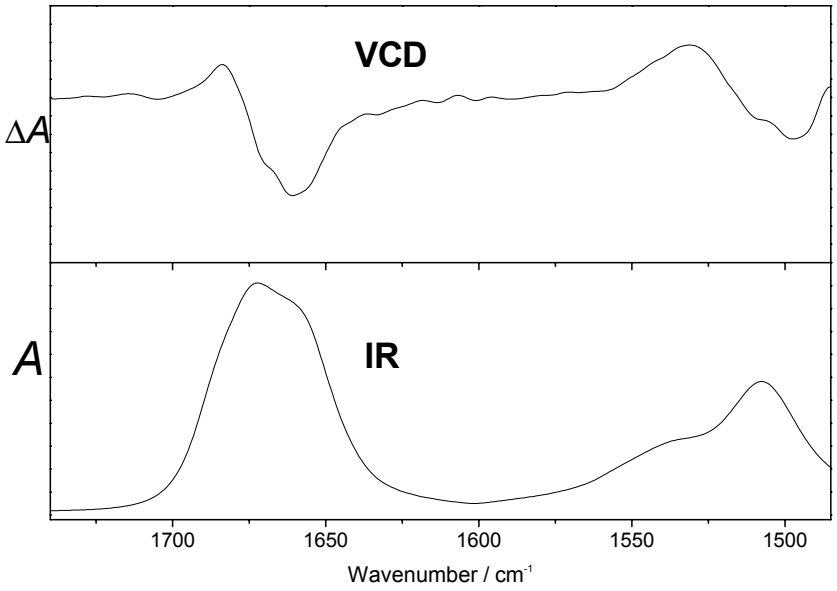

Figure S10. IR and VCD spectra Ac-L-Ala-NHMe as recorded in 2 mg ml^{-1} $CDCl_3$ solution.