Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

Partition analysis of dipole moments in solution applied to functional groups in polypeptide motifs

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Table S1. Coordinates for α-(Ala)$_{10}$.

atom	*x*	*y*	*z*
H	0.089480	0.269339	-0.153996
C	-0.076694	1.341304	-0.096417
H	0.839990	1.862725	-0.355924
H	-0.827347	1.604084	-0.840450
C	-0.550254	1.760937	1.266233
O	-0.346667	2.925556	1.705171
N	-1.201491	0.853696	2.042608
H	-1.447803	-0.057880	1.654894
C	-1.903564	1.277190	3.269700
H	-2.807157	1.848234	2.981490
C	-0.990114	2.204989	4.121585
O	-1.358717	3.348366	4.475239
C	-2.338492	0.035495	4.048259
H	-2.894715	0.319969	4.935883
H	-2.974145	-0.596273	3.433667
H	-1.478422	-0.553022	4.359901
N	0.197334	1.673438	4.523492
H	0.437366	0.734610	4.201181
C	1.221248	2.404833	5.281706
H	0.925946	2.449934	6.344958
C	1.393304	3.847673	4.757697
O	1.479907	4.824834	5.537462
C	2.543579	1.636549	5.158504
H	3.323156	2.125104	5.734674
H	2.429866	0.620971	5.528693
H	2.865982	1.587189	4.120936
N	1.588827	3.967865	3.418679
H	1.327871	3.178493	2.818453
C	1.688162	5.273033	2.750692
H	2.558092	5.803122	3.171765
C	0.439673	6.139660	2.990264
O	0.540566	7.309985	3.435084
C	1.901504	5.055304	1.248510
H	1.967694	6.008395	0.732781
H	2.822137	4.505865	1.070378
H	1.076972	4.483997	0.825812
N	-0.758473	5.611905	2.646209
H	-0.812460	4.622183	2.362980
C	-2.000609	6.365109	2.854310
H	-2.048284	7.178509	2.109492
C	-2.014596	7.000520	4.259351
O	-2.270335	8.213865	4.448388
C	-3.198687	5.432241	2.653528
H	-4.131411	5.962743	2.817732
H	-3.203465	5.035391	1.641642

H	-3.148504	4.591679	3.343661
N	-1.780251	6.119473	5.262717
H	-1.549828	5.152063	5.011747
C	-1.727120	6.465671	6.683697
H	-2.724317	6.809684	7.006633
C	-0.722212	7.607161	6.947914
O	-1.082925	8.713491	7.419374
C	-1.343961	5.197091	7.453572
H	-1.275385	5.393874	8.519287
H	-2.089831	4.422375	7.295043
H	-0.384596	4.813903	7.108481
N	0.581676	7.331569	6.701713
H	0.837344	6.444714	6.250176
C	1.647692	8.315970	6.917398
H	1.819808	8.438846	7.999869
C	1.246267	9.681315	6.324242
O	1.320697	10.749220	6.980787
C	2.916267	7.785904	6.240991
H	3.742406	8.479987	6.362653
H	3.202455	6.830203	6.672510
H	2.745143	7.634235	5.176828
N	0.887205	9.662795	5.014961
H	0.773037	8.765254	4.530093
C	0.452138	10.875188	4.318468
H	1.308602	11.565521	4.235536
C	-0.638283	11.585957	5.131809
O	-0.533770	12.801760	5.438991
C	-0.045078	10.506233	2.917426
H	-0.388117	11.388441	2.385684
H	0.753324	10.045115	2.342275
H	-0.866428	9.794285	2.982194
N	-1.717210	10.855493	5.494710
H	-1.768389	9.851799	5.274156
C	-2.805706	11.449189	6.272729
H	-3.315564	12.207618	5.655875
C	-2.264611	12.156525	7.533494
O	-2.669560	13.295078	7.869173
C	-3.797779	10.351691	6.661099
H	-4.614232	10.759655	7.249552
H	-4.212841	9.884349	5.771179
H	-3.296765	9.579972	7.242036
N	-1.379842	11.466321	8.297906
H	-1.003673	10.576158	7.950168
C	-0.718405	12.092938	9.444767
H	-1.481213	12.312659	10.209962
C	-0.048918	13.432594	9.089582
O	-0.050885	14.381485	9.909250

C	0.290297	11.101307	10.032436
H	0.804473	11.535583	10.884899
H	-0.218864	10.198597	10.359975
H	1.027498	10.822582	9.281836
N	0.566970	13.532492	7.885911
H	0.562314	12.739712	7.232317
C	1.168925	14.793223	7.443430
H	1.681643	15.244119	8.308898
C	0.120465	15.826445	6.958769
O	0.411699	17.050423	6.951766
C	2.182991	14.513793	6.337576
H	2.614976	15.441832	5.976331
H	2.984181	13.876768	6.703072
H	1.701017	14.005444	5.504848
N	-1.081176	15.371890	6.536151
H	-1.284280	14.372558	6.581186
C	-2.162902	16.255932	6.163732
H	-1.810856	17.284739	6.218489
H	-2.507346	16.051335	5.144067
H	-3.018639	16.131392	6.836570

Table S2. Coordinates for extended-$(Ala)_{10}$.

atom	*x*	*y*	*z*
H	-0.422035	-0.171698	-0.279294
C	0.050425	0.782513	-0.063577
H	1.085316	0.585665	0.211746
H	0.058837	1.386550	-0.964874
C	-0.650222	1.511432	1.063609
O	-0.690210	2.762513	1.120772
N	-1.197019	0.732978	2.038475
H	-1.159348	-0.289477	1.990146
C	-1.878728	1.260293	3.221940
H	-1.169153	1.899270	3.784799
C	-2.283299	0.039121	4.095353
O	-2.040945	-1.125306	3.704089
C	-3.085745	2.136579	2.846712
H	-3.547876	2.548815	3.740138
H	-2.760571	2.956683	2.212974
H	-3.832927	1.559603	2.308695
N	-2.901108	0.289522	5.275718
H	-3.068303	1.256125	5.585749
C	-3.377580	-0.723663	6.214556
H	-4.082908	-1.389219	5.681994
C	-4.121774	-0.014151	7.377850
O	-4.152049	1.233690	7.443606
C	-2.221279	-1.602745	6.733223
H	-2.598591	-2.381774	7.391400

H	-1.710564	-2.072717	5.897183
H	-1.499533	-1.007127	7.286137
N	-4.760171	-0.839551	8.242070
H	-4.705283	-1.861203	8.111947
C	-5.546402	-0.461463	9.412216
H	-4.913561	0.155492	10.078917
C	-5.939470	-1.771223	10.153732
O	-5.658414	-2.880458	9.649589
C	-6.769040	0.389465	9.034224
H	-7.309360	0.698262	9.925524
H	-6.447952	1.279267	8.499429
H	-7.450519	-0.166627	8.395774
N	-6.549394	-1.630287	11.352765
H	-6.751800	-0.691852	11.732202
C	-7.047219	-2.707299	12.207655
H	-7.781098	-3.304788	11.633664
C	-7.768039	-2.026501	13.407063
O	-7.811270	-0.777936	13.464998
C	-5.914648	-3.656058	12.635769
H	-6.305494	-4.475331	13.234461
H	-5.431561	-4.070997	11.755280
H	-5.166587	-3.129571	13.222871
N	-8.306876	-2.835127	14.351946
H	-8.279268	-3.859151	14.237313
C	-9.131517	-2.407628	15.482025
H	-8.509804	-1.781210	16.151249
C	-9.558390	-3.685586	16.260178
O	-9.297213	-4.816016	15.793854
C	-10.324465	-1.543028	15.043813
H	-10.892253	-1.216193	15.911212
H	-9.969234	-0.665768	14.510276
H	-10.990375	-2.097823	14.387874
N	-10.174090	-3.496426	17.450850
H	-10.341325	-2.542026	17.803489
C	-10.600113	-4.535705	18.384952
H	-11.313861	-5.204898	17.868022
C	-11.318912	-3.832925	19.570979
O	-11.356091	-2.583967	19.624497
C	-9.410116	-5.398710	18.842338
H	-9.745474	-6.198729	19.497951
H	-8.923598	-5.841669	17.977487
H	-8.679023	-4.799672	19.378971
N	-11.852900	-4.645299	20.513620
H	-11.805434	-5.670437	20.402192
C	-12.584774	-4.244259	21.711066
H	-11.917014	-3.640019	22.354646
C	-12.979800	-5.549521	22.460557

O	-12.703713	-6.659496	21.954984
C	-13.806831	-3.374180	21.368458
H	-14.316578	-3.057758	22.275157
H	-13.489345	-2.489412	20.823189
H	-14.513757	-3.922525	20.751363
N	-13.578356	-5.407522	23.664828
H	-13.777795	-4.468558	24.044742
C	-14.073111	-6.482914	24.523678
H	-14.807538	-7.082847	23.953192
C	-14.792009	-5.798496	25.721530
O	-14.832905	-4.549757	25.777108
C	-12.939552	-7.429355	24.954358
H	-13.329002	-8.244811	25.558631
H	-12.458979	-7.849494	24.074966
H	-12.189894	-6.899493	25.536215
N	-15.333509	-6.602125	26.670130
H	-15.309373	-7.624775	26.559010
C	-16.150574	-6.154577	27.797855
H	-15.523401	-5.517288	28.450599
C	-16.591459	-7.390878	28.604978
O	-16.356650	-8.544008	28.183259
C	-17.344839	-5.294761	27.349531
H	-17.903381	-4.944007	28.213419
H	-16.989389	-4.433055	26.791733
H	-18.018252	-5.863247	26.713422
N	-17.215018	-7.151507	29.783446
H	-17.354276	-6.195038	30.123662
C	-17.631517	-8.199468	30.714813
H	-18.357446	-8.863684	30.209516
C	-18.336241	-7.498698	31.887598
O	-18.378814	-6.247916	31.947401
C	-16.442799	-9.055974	31.180444
H	-16.780317	-9.845399	31.845996
H	-15.959433	-9.509858	30.320040
H	-15.711948	-8.449411	31.707606
N	-18.876754	-8.291704	32.847248
H	-18.833339	-9.304648	32.746222
C	-19.559786	-7.756243	34.007072
H	-19.527281	-6.669687	33.954830
H	-20.604257	-8.083145	34.033956
H	-19.078036	-8.086716	34.932806

Table S3. Coordinates for β-(Ala)$_{10}$.

atom	*x*	*y*	*z*
C	-0.812969	2.510062	0.511889
H	0.197950	2.838490	0.743432
H	-1.115812	3.020046	-0.398797

H	-0.793055	1.441032	0.323761
C	-1.739460	2.864479	1.647763
O	-1.979403	4.064741	1.955217
N	-2.266813	1.851454	2.375000
H	-2.091347	0.869046	2.149684
C	-3.143603	2.090558	3.522933
H	-2.671349	2.852024	4.172973
C	-3.279983	0.749229	4.282572
O	-2.965565	-0.327339	3.720926
C	-4.504501	2.651066	3.083314
H	-5.092741	2.925779	3.954730
H	-4.355742	3.534970	2.469866
H	-5.060992	1.918599	2.504279
N	-3.741294	0.791092	5.554266
H	-3.982089	1.687544	6.003614
C	-3.863076	-0.397943	6.398044
H	-4.356504	-1.187203	5.803667
C	-4.708875	-0.049184	7.644974
O	-4.929808	1.147318	7.948239
C	-2.474230	-0.929357	6.802539
H	-2.569063	-1.831143	7.402431
H	-1.895600	-1.164266	5.913395
H	-1.929317	-0.188532	7.381695
N	-5.188572	-1.092127	8.358947
H	-4.959532	-2.056769	8.088501
C	-5.938699	-0.964827	9.609534
H	-5.482073	-0.153918	10.205202
C	-5.868820	-2.303322	10.382251
O	-5.554349	-3.360568	9.788577
C	-7.407198	-0.582395	9.336241
H	-7.932133	-0.410448	10.272317
H	-7.450258	0.325384	8.740623
H	-7.917792	-1.373418	8.793250
N	-6.157833	-2.250941	11.700386
H	-6.439368	-1.359437	12.139096
C	-6.217961	-3.412239	12.582208
H	-6.684803	-4.237725	12.014350
C	-7.096765	-3.055943	13.796223
O	-7.567955	-1.903363	13.924376
C	-4.811586	-3.890429	12.989505
H	-4.871519	-4.785781	13.602427
H	-4.232069	-4.120881	12.100207
H	-4.285286	-3.123354	13.552284
N	-7.316561	-4.032213	14.716543
H	-6.985457	-4.980209	14.527182
C	-8.255754	-3.855053	15.830415
H	-9.281975	-4.033795	15.461096

C	-8.217877	-2.416453	16.400772
O	-9.273552	-1.807899	16.672706
C	-7.957940	-4.886082	16.925955
H	-8.678193	-4.799792	17.733281
H	-8.012701	-5.893953	16.523189
H	-6.962855	-4.739524	17.339516
N	-6.990103	-1.879023	16.644579
H	-6.160575	-2.442356	16.449931
C	-6.805172	-0.607122	17.335826
H	-7.839674	-0.239695	17.478011
C	-6.037657	0.538945	16.602773
O	-5.499117	1.431565	17.292283
C	-6.238550	-0.837793	18.747074
H	-6.093468	0.115172	19.246627
H	-6.919487	-1.446647	19.334146
H	-5.278461	-1.346732	18.703882
N	-6.035726	0.577575	15.240884
H	-6.482480	-0.166078	14.684787
C	-5.311216	1.608520	14.480544
H	-5.624419	2.596405	14.864886
C	-5.610582	1.516007	12.959127
O	-6.220952	0.533254	12.477693
C	-3.789917	1.484362	14.720762
H	-3.252858	2.271790	14.197273
H	-3.573771	1.564674	15.782718
H	-3.422097	0.524710	14.365657
N	-5.136978	2.518590	12.181674
H	-4.652301	3.325723	12.599020
C	-5.228563	2.564273	10.721629
H	-4.812492	1.624569	10.309210
C	-4.414632	3.782640	10.213351
O	-4.026282	4.653960	11.025728
C	-6.694971	2.660739	10.251002
H	-6.746260	2.569246	9.169594
H	-7.279169	1.861447	10.698368
H	-7.134558	3.612087	10.540984
N	-4.195284	3.864718	8.879017
H	-4.490638	3.097234	8.256498
C	-3.437159	4.938701	8.233711
H	-3.909120	5.903159	8.499485
C	-3.462037	4.770412	6.702285
O	-3.960574	3.750988	6.168543
C	-1.991082	4.981568	8.767041
H	-1.437835	5.801192	8.314434
H	-2.001569	5.122747	9.844083
H	-1.470488	4.053526	8.545576
N	-2.924113	5.782416	5.982095

H	-2.481397	6.582908	6.443237
C	-2.760798	5.728244	4.528865
H	-2.433860	4.711013	4.248873
C	-1.655222	6.724735	4.141994
O	-1.269595	7.598796	4.956763
C	-4.074199	6.019649	3.787437
H	-3.937402	5.880798	2.718686
H	-4.848415	5.338887	4.130407
H	-4.408081	7.038257	3.967023
N	-1.163450	6.627878	2.883780
H	-1.444261	5.824126	2.308218
C	-0.078757	7.461326	2.407955
H	0.866498	6.906771	2.368348
H	-0.293191	7.833255	1.402598
H	0.038667	8.305949	3.085414