Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Influence of a Fluorine Substituent on the Physicochemical Properties and Chemical Reactivity of Fluorinated Amino Acids. 1. The Conformers of 3-Fluoroalanine. A Theoretical Study

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Table of Contents

Table S-1. Dipole moments and NBO charges of alanine conformers **1**-**4** in the gas phase [B3LYP 6-311++G(d,p)].

Conformer	Dipole [D]	C1	C2	C3	H4	N	O6	O7	H8	H9	H10	H11	H12	H13
1	1.305	0.793	-0.119	-0.573	0.199	-0.831	-0.607	-0.693	0.478	0.357	0.358	0.210	0.216	0.212
2	5.582	0.789	-0.128	-0.580	0.204	-0.880	-0.591	-0.686	0.499	0.372	0.370	0.205	0.200	0.231
3	1.632	0.791	-0.116	-0.574	0.201	-0.831	-0.602	-0.704	0.484	0.356	0.358	0.210	0.216	0.210
4	3.319	0.782	-0.128	-0.576	0.208	-0.830	-0.574	-0.679	0.469	0.359	0.361	0.191	0.219	0.198

Table S-2. Structural parameters for alanine conformers **1**-**4** in the gas phase [6-311++G(d,p)].

Conformer	Rel. Energies [kcal/mol]	Level	Bond lengths [Å]								Angle [°]	Dihedral angles [°]	
			5,8	6,9	7,9	6,10	7,10	7,8	5,9	5,10	9,5,10	9,5,2,1	5,2,1,6*
1	0.00	RHF	-	2.857	-	2.692	-	0.946	0.999	1.000	106.77	-60.12	-14.47
		B3LYP	-	2.934	-	2.687	-	0.969	1.015	1.016	106.42	-61.13	-18.62
2	1.28	RHF	2.053	-	-	-	-	0.949	1.000	0.998	107.85	-86.72	161.35
		B3LYP	1.918	-	-	-	-	0.983	1.014	1.013	107.89	-96.02	167.88
3	1.00	RHF	-	-	3.097	-	2.566	0.946	0.999	0.999	108.07	-61.95	135.88
		B3LYP	-	-	3.106	-	2.576	0.969	1.014	1.015	107.55	-60.36	135.68
4	5.47	RHF	-	2.859	-	2.648	-	0.942	1.000	1.001	106.57	-60.41	-17.38
		B3LYP	-	2.920	-	2.653	-	0.965	1.015	1.016	106.19	-60.76	-20.17

* atom numbers according to Fig. 3

Table S-3a. Selected bond lengths, intramolecular atom distances (Å) and dipole moments (D) of twenty 3-fluoroalanine conformers **1Fa**-**4Fc** [B3LYP 6-311++G(d,p)].

Conformer / Parameter	**1Fa**	**1Fb-1**	**1Fb-2**	**1Fb-3**	**1Fc**	**2Fa-1**	**2Fa-2**	**2Fa-3**	**2Fb**	**2Fc**
Dipole [D]	2.424	2.015	2.000	2.537	1.932	5.602	3.215	4.189	3.752	6.047
C-F	1.405	1.405	1.402	1.393	1.399	1.406	1.423	1.408	1.403	1.394
O-H	0.969	0.970	0.970	0.969	0.970	0.982	0.970	0.970	0.982	0.978
N-H9	1.014	1.013	1.014	1.013	1.013	1.012	1.014	1.008	1.013	1.013
N-H10	1.015	1.014	1.015	1.015	1.016	1.016	1.015	1.009	1.016	1.016
N···H-O	-	-	-	-	-	1.921	-	2.228	1.930	1.994
C=O···H-O	2.306	2.300	2.307	2.307	2.308	-	-	-	-	2.308
N-H9···O-H	-	-	-	-	-	-	-	-	-	-
N-H10···O-H	-	-	-	-	-	-	-	-	-	-
N-H9···O=C	2.701	-	-	3.138	3.342	-	3.134	-	-	-
N-H10···O=C	2.876	2.381	2.423	2.514	2.570	-	-	-	-	-
C-F···H9-N	3.775	2.619	2.485	3.703	-	3.493	-	-	2.888	-
C-F···H10-N	2.539	-	-	3.583	-	2.345	2.591	2.461	2.983	-
C-F···H-O	-	-	-	-	3.870	-	1.918	-	-	-
C-F···H11	-	-	-	-	2.665	-	-	-	-	2.439

Table S-3a:

Conformer / Parameter	**3Fa**	**3Fb-1**	**3Fb-2**	**3Fb-3**	**3Fb-4**	**3Fb-5**	**3Fc**	**4Fa**	**4Fb**	**4Fc**
Dipole [D]	1.874	2.354	2.225	2.871	2.962	3.288	2.882	4.248	2.022	3.641
C-F	1.406	1.406	1.401	1.395	1.393	1.393	1.399	1.399	1.393	1.422
O-H	0.969	0.969	0.969	0.970	0.969	0.969	0.969	0.965	0.965	0.971
N-H9	1.013	1.015	1.014	1.014	1.013	1.013	1.013	1.014	1.014	1.011
N-H10	1.014	1.014	1.015	1.015	1.015	1.014	1.014	1.016	1.016	1.016
N···H-O	-	-	-	-	-	-	-	-	-	-
C=O···H-O	2.294	2.302	2.304	2.303	2.306	2.288	2.306	-	-	-
N-H9···O-H	2.629	-	-	2.898	-	2.691	-	-	-	-
N-H10···O-H	2.763	2.429	2.417	-	2.603	2.694	2.657	-	-	-
N-H9···O=C	-	-	-	-	3.532	-	3.409	2.704	3.170	3.469
N-H10···O=C	-	-	-	3.142	-	-	-	2.788	2.494	2.179
C-F···H9-N	3.760	2.489	2.550	-	-	3.781	-	3.792	3.746	-
C-F···H10-N	2.510	-	-	-	-	3.427	-	2.568	3.592	-
C-F···H-O	-	-	-	-	-	-	-	-	-	1.896
C-F···H11	-	-	-	-	-	-	2.677	-	-	2.586

Table S-3b. Dipole moments and NBO charges of 3-fluoroalanine conformers **1Fa**-**4Fc** in the gas phase [B3LYP 6-311++G(d,p)].

Conf.	Dipole [D]	C1	C2	C3	Fa (H4)*	N5	O6	O7	H8	H9	H10	H11	Fb (H12)*	Fc (H13)*
1Fa	2,424	0,795	-0,159	0,091	-0,401	-0,833	-0,593	-0,697	0,486	0,364	0,366	0,224	0,176	0,179
1Fb-1	2,015	0,807	-0.154	0.093	0.173	-0.847	-0.591	-0.690	0.488	0.367	0.376	0.203	-0.402	0.178
1Fb-2	2,000	0,803	-0,154	0,086	0,164	-0,837	-0,591	-0,685	0,486	0,366	0,369	0,218	-0,399	0,174
1Fb-3	2,537	0,789	-0,158	0,100	0,165	-0,828	-0,596	-0,689	0,482	0,360	0,365	0,227	-0,388	0,171
1Fc	1,932	0,794	-0,152	0,099	0,167	-0,833	-0,608	-0,673	0,480	0,362	0,367	0,216	0,175	-0,395
2Fa-1	5,602	0,793	-0,171	0,081	-0,401	-0,880	-0,588	-0,676	0,501	0,374	0,381	0,228	0,161	0,197
2Fa-2	3,215	0,777	-0,169	0,078	-0,414	-0,830	-0,570	-0,686	0,487	0,369	0,360	0,230	0,189	0,178
2Fa-3	4,189	0,785	-0,173	0,093	-0,404	-0,879	-0,579	-0,668	0,474	0,367	0,380	0,232	0,173	0,189
2Fb	3,752	0,788	-0,169	0,084	0,161	-0,872	-0,584	-0,677	0,501	0,382	0,366	0,227	-0,402	0,194
2Fc	6,047	0,787	-0,172	0,086	0,177	-0,870	-0,566	-0,681	0,497	0,374	0,365	0,231	0,157	-0,386
3Fa	1,874	0,794	-0,159	0,093	-0,402	-0,835	-0,604	-0,687	0,487	0,363	0,366	0,227	0,175	0,183
3Fb-1	2,354	0,811	-0,151	0,093	0,176	-0,844	-0,594	-0,690	0,488	0,367	0,368	0,199	-0,404	0,181
3Fb-2	2,225	0,804	-0,152	0,086	0,163	-0,835	-0,587	-0,693	0,489	0,366	0,362	0,223	-0,399	0,175
3Fb-3	2,871	0,786	-0,153	0,097	0,170	-0,815	-0,603	-0,688	0,484	0,364	0,355	0,221	-0,390	0,171
3Fb-4	2,962	0,786	-0,152	0,098	0,168	-0,822	-0,586	-0,704	0,487	0,362	0,360	0,225	-0,387	0,166
3Fb-5	3,288	0,787	-0,159	0,098	0,157	-0,824	-0,602	-0,689	0,487	0,363	0,354	0,231	-0,388	0,185
3Fc	2,882	0,792	-0,150	0,095	0,168	-0,829	-0,586	-0,704	0,487	0,366	0,361	0,219	0,174	-0,394
4Fa	4,248	0,784	-0,169	0,090	-0,395	-0,832	-0,558	-0,674	0,467	0,366	0,369	0,213	0,185	0,153
4Fb	2,022	0,778	-0,164	0,097	0,174	-0,827	-0,565	-0,673	0,472	0,360	0,368	0,206	-0,388	0,160
4Fc	3,641	0,795	-0,169	0,086	0,179	-0,855	-0,578	-0,675	0,493	0,363	0,390	0,206	0,179	-0,414

* according to Figure 3C

Table S-4. Structural parameters[a,b,c] for 3-fluoroalanine conformers in the gas phase [6-311++G(d,p)].

Conformer	Level	Bond lengths [Å]								Angle [°]	Dihedral angles [°]		
		3,F	5,8	6,9	6,10	F,(9)10	7,8	5,9	5,10	9,5,10	F,3,2,5	9,5,2,1	5,2,1,6
1Fa	RHF	1.373	-	2.684	2.832	2.544	0.946	0.999	1.000	106.91	64.78	-53.70	1.94
	B3LYP	1.405	-	2.701	2.876	2.539	0.969	1.014	1.015	106.60	64.22	-51.74	1.07
1Fb-1	RHF	1.372	-	-	2.403	(2.550)	0.946	0.998	0.999	109.61	-61.57	-166.81	22.14
	B3LYP	1.405	-	-	2.381	(2.619)	0.970	1.013	1.014	109.69	-63.22	-163.56	20.33
1Fb-2	RHF	1.369	-	-	2.459	(2.517)	0.946	0.998	0.999	109.49	-59.60	170.68	-27.61
	B3LYP	1.402	-	-	2.423	(2.485)	0.970	1.014	1.015	109.48	-57.76	165.73	-24.71
1Fb-3	RHF	1.361	-	3.018	2.567	-	0.946	0.999	1.000	107.41	-69.14	-73.13	-14.01
	B3LYP	1.393	-	3.138	2.515	-	0.969	1.013	1.015	107.24	-70.26	-78.96	-16.37
1Fc	RHF	1.368	-	3.287	2.559	-	0.947	0.999	1.001	107.98	177.82	-76.73	-43.60
	B3LYP	1.399	-	3.342	2.570	-	0.970	1.013	1.016	107.71	178.94	-77.33	-45.04
2Fa-1	RHF	1.373	2.034	-	-	2.381	0.949	0.998	1.001	108.46	52.61	-145.94	-168.64
	B3LYP	1.406	1.921	-	-	2.345	0.982	1.012	1.016	108.60	49.68	-141.10	-171.19
2Fa-2	RHF	1.385	-	-	-	2.542	0.944	0.999	0.999	108.74	61.54	-56.65	104.446
	B3LYP	1.423	-	-	-	2.591	0.970	1.014	1.015	108.18	64.03	55.55	95.92
2Fa-3	RHF	1.376	2.321	-	-	2.465	0.942	0.996	0.997	112.57	60.35	-59.83	167.44
	B3LYP	1.408	2.228	-	-	2.461	0.970	1.008	1.009	114.75	58.14	-65.29	171.84
2Fb	RHF	1.371	2.071	-	-	-	0.949	0.998	1.002	107.34	-57.81	-156.83	-157.61
	B3LYP	1.403	1.930	-	-	-	0.983	1.013	1.016	107.16	-60.36	-149.55	-164.89
2Fc	RHF	1.362	2.147	-	-	-	0.947	0.999	1.001	108.28	-157.55	-161.41	-143.61
	B3LYP	1.394	1.994	-	-	-	0.978	1.013	1.016	108.07	-152.47	-156.26	-153.91
			6,8	7,9	7,10								
3Fa	RHF	1.374	2.269	2.616	2.747	2.512	0.946	0.998	0.999	107.69	62.11	-57.78	-179.46
	B3LYP	1.406	2.294	2.629	2.763	2.511	0.969	1.013	1.014	107.37	61.72	-53.85	178.38
3Fb-1	RHF	1.375	2.280	-	2.470	(2.452)	0.946	0.999	0.999	108.48	-62.83	177.29	-130.66
	B3LYP	1.406	2.302	-	2.429	(2.498)	0.969	1.015	1.014	108.38	-63.59	-179.03	-136.06
3Fb-2	RHF	1.369	2.283	-	2.491	(2.602)	0.946	0.999	1.000	108.61	-60.17	-175.01	134.78
	B3LYP	1.401	2.304	-	2.417	2.550	0.969	1.014	1.015	108.43	-58.69	178.19	146.49
3Fb-3	RHF	1.364	2.278	2.673	-	-	0.946	0.998	1.000	108.82	-67.04	-63.94	-116.81
	B3LYP	1.395	2.303	2.897	-	-	0.970	1.014	1.015	108.69	-68.77	-67.18	-96.51
3Fb-4	RHF	1.361	2.282	-	2.568	-	0.946	0.998	0.999	108.94	-69.77	-69.82	125.61
	B3LYP	1.393	2.306	-	2.603	-	0.969	1.013	1.015	108.59	-70.14	-68.80	120.43
3Fb-5	RHF	1.364	2.278	2.672	3.225	-	0.946	0.998	1.000	108.82	-67.04	-63.93	-116.81
	B3LYP	1.393	2.288	2.692	2.694	-	0.969	1.013	1.014	107.42	-67.99	-64.48	-172.41
3Fc	RHF	1.368	2.283	-	2.636	-	0.946	0.998	0.999	108.63	177.79	-70.57	112.61
	B3LYP	1.399	2.306	-	2.657	-	0.969	1.013	1.015	108.25	179.43	-69.97	109.98
			F,8	6,9	6,10								
4Fa	RHF	1.366	-	2.708	2.735	2.555	0.941	0.999	1.001	106.63	65.64	-55.49	-4.93
	B3LYP	1.399	-	2.704	2.788	2.568	0.965	1.014	1.016	106.24	66.25	-53.43	-3.04
4Fb	RHF	1.361	-	3.086	2.518	-	0.942	0.999	1.001	107.43	-72.89	-73.95	-24.32
	B3LYP	1.393	-	3.170	2.494	-	0.956	1.014	1.016	107.17	-73.49	-77.44	-25.23
4Fc	RHF	1.381	2.021	2.950	2.471	-	0.944	0.998	1.001	106.38	-172.81	-78.18	-1.07
	B3LYP	1.422	1.896	3.469	2.179	-	0.971	1.011	1.016	108.81	-173.71	-130.45	12.28

[a)] atom numbers according to Fig. 3, [b)] distance F,8 is 1.896 Å in **4Fc**, 1.918 Å in **2Fa-2** and > 3.9 Å in all other conformers

Table S-5. Dipole moments and NBO charges of alanine conformers $\mathbf{1}_{aq}$-$\mathbf{4}_{aq}$ in water, [B3LYP, 6-311++G(d,p)] CPCM model

Conf.	Dipole [D]	C1	C2	C3	H4	N5	O6	O7	H8	H9	H10	H11	H12	H13
$\mathbf{1}_{aq}$	2.110	0,814	-0,125	-0,575	0,201	-0,870	-0,670	-0,711	0,535	0,379	0,373	0,224	0,213	0,213
$\mathbf{2}_{aq}$	7.545	0,812	-0,137	-0,585	0,204	-0,898	-0,671	-0,709	0,520	0,403	0,390	0,242	0,210	0,220
$\mathbf{3}_{aq}$	2.686	0,814	-0,121	-0,576	0,203	-0,870	-0,674	-0,710	0,537	0,380	0,374	0,219	0,214	0,211
$\mathbf{4}_{aq}$	4.823	0,809	-0,130	-0,577	0,205	-0,867	-0,662	-0,711	0,537	0,380	0,375	0,217	0,215	0,210

Table S-6. Optimized bond lengths, bond angles and dihedral angles for selected alanine conformers **1**-**4** in water [B3LYP level with 6-311++G(d,p)]. CPCM model

Conformer	Rel. Energy	Bond lengths [Å]								Angle [°]	Dihedral angles [°]	
		5,8	6,9	7,9	6,10	7,10	7,8	5,9	5,10	9,5,10	9,5,2,1	5,2,1,6*
$\mathbf{1}_{aq}$	0.00	-	2.914	-	2.716	-	0.993	1.021	1.021	106.53	-58.78	-19.84
$\mathbf{2}_{aq}$	1.69	1.862	-	-	-	-	0.996	1.020	1.019	107.53	-99.23	169.72
$\mathbf{3}_{aq}$	0.73	-	-	3.018	-	2.598	0.993	1.021	1.020	106.98	-57.07	140.27
$\mathbf{4}_{aq}$	2.56	-	3.042	-	2.685	-	0.989	1.021	1.021	106.75	-59.76	-35.18

* atom numbers according to Fig. 3

Table S-7. Dipole moments and NBO charges of 3-fluoroalanine conformers $\mathbf{1Fa}_{aq}$-$\mathbf{4Fc}_{aq}$ in water obtained with CPCM model [B3LYP 6-311++G(d,p)].

Conform.	Dipole [D]	C1	C2	C3	Fa (H4)*	N5	O6	O7	H8	H9	H10	H11	Fb (H12)*	Fc (H13)*
$\mathbf{1Fa}_{aq}$	3,886	0,815	-0,171	0,087	-0,426	-0,870	-0,655	-0,709	0,539	0,385	0,379	0,254	0,185	0,188
$\mathbf{1Fb\text{-}1}_{aq}$	3,302	0,824	-0,163	0,087	0,179	-0,879	-0,648	-0,705	0,542	0,383	0,386	0,227	-0,423	0,189
$\mathbf{1Fb\text{-}2}_{aq}$	2,907	0,820	-0,165	0,079	0,176	-0,869	-0,646	-0,704	0,541	0,384	0,379	0,241	-0,422	0,186
$\mathbf{1Fb\text{-}3}_{aq}$	3,749	0,811	-0,165	0,089	0,177	-0,867	-0,652	-0,707	0,540	0,384	0,378	0,244	-0,419	0,187
$\mathbf{1Fc}_{aq}$	2,814	0,811	-0,158	0,091	0,177	-0,864	-0,665	-0,697	0,537	0,389	0,381	0,231	0,185	-0,419
$\mathbf{2Fa\text{-}1}_{aq}$	7,904	0,813	-0,183	0,079	-0,423	-0,896	-0,660	-0,699	0,523	0,406	0,396	0,267	0,185	0,193
$\mathbf{2Fa\text{-}2}_{aq}$ [a)]	5,521	0,812	-0,179	0,088	-0,425	-0,885	-0,657	-0,694	0,526	0,394	0,386	0,259	0,186	0,190
$\mathbf{2Fa\text{-}3}_{aq}$ [a)]	5,550	0,812	-0,180	0,088	-0,425	-0,885	-0,657	-0,694	0,526	0,394	0,386	0,260	0,186	0,190
$\mathbf{2Fb}_{aq}$	5,306	0,816	-0,178	0,081	0,178	-0,894	-0,659	-0,699	0,523	0,406	0,395	0,257	-0,420	0,193
$\mathbf{2Fc}_{aq}$	8,634	0,813	-0,177	0,080	0,181	-0,889	-0,652	-0,701	0,524	0,404	0,393	0,257	0,182	-0,416
$\mathbf{3Fa}_{aq}$	3,007	0,815	-0,170	0,088	-0,426	-0,871	-0,669	-0,698	0,540	0,385	0,380	0,254	0,185	0,188
$\mathbf{3Fb\text{-}1}_{aq}$	3,567	0,828	-0,161	0,088	0,179	-0,879	-0,657	-0,701	0,543	0,382	0,386	0,227	-0,424	0,190
$\mathbf{3Fb\text{-}2}_{aq}$	2,932	0,820	-0,161	0,081	0,176	-0,871	-0,660	-0,694	0,542	0,384	0,378	0,240	-0,421	0,185
$\mathbf{3Fb\text{-}3}_{aq}$	4,366	0,810	-0,160	0,088	0,180	-0,858	-0,661	-0,702	0,538	0,386	0,379	0,236	-0,421	0,183
$\mathbf{3Fb\text{-}4}_{aq}$	4,468	0,809	-0,157	0,087	0,181	-0,862	-0,653	-0,710	0,541	0,386	0,379	0,233	-0,418	0,183
$\mathbf{3Fb\text{-}5}_{aq}$	4,885	0,812	-0,165	0,091	0,176	-0,868	-0,667	-0,697	0,541	0,385	0,378	0,246	-0,420	0,188
$\mathbf{3Fc}_{aq}$	4,144	0,811	-0,157	0,088	0,180	-0,861	-0,657	-0,711	0,541	0,391	0,381	0,231	0,184	-0,420
$\mathbf{4Fa}_{aq}$	6,837	0,809	-0,176	0,086	-0,423	-0,868	-0,645	-0,709	0,538	0,386	0,382	0,248	0,189	0,184
$\mathbf{4Fb}_{aq}$	3,461	0,804	-0,168	0,088	0,181	-0,865	-0,646	-0,704	0,541	0,385	0,380	0,235	-0,416	0,183
$\mathbf{4Fc}_{aq}$	5,132	0,807	-0,166	0,091	0,179	-0,864	-0,655	-0,700	0,540	0,390	0,382	0,229	0,187	-0,419

* according to Figure 3C; [a)] upon optimization conformer $\mathbf{2Fa\text{-}2}_{aq}$ gives conformer $\mathbf{2Fa\text{-}3}_{aq}$

Table S-8. Bond lengths, bond angles and dihedral angles of 3-fluoroalanine conformers **1Fa$_{aq}$**-**4Fc$_{aq}$** in water obtained with the CPCM model [B3LYP 6-311++G(d,p)].

Conformer	E_{rel}	Bond lengths [Å]								Angle [°]	Dihedral angles [°]		
	[kcal/mol]	3,F	5,8	6,9	6,10	F,(9)10	7,8	5,9	5,10	9,5,10	F,3,2,5	9,5,2,1	5,2,1,6*
1Fa$_{aq}$	0.00	1.420	-	2.856	2.736	2.664	0.994	1.020	1.020	106.65	64.95	-61.33	-6.18
1Fb-1$_{aq}$	1.44	1.418	-	-	2.492	-	0.995	1.020	1.020	106.94	-62.12	-167.21	12.40
1Fb-2$_{aq}$	1.32	1.415	-	-	2.683	(2.593)	0.994	1.020	1.022	107.54	-59.42	-177.37	-15.79
1Fb-3$_{aq}$	1.13	1.412	-	2.921	2.679	-	0.994	1.020	1.021	106.90	-66.62	-65.59	-8.19
1Fc$_{aq}$	1.17	1.415	-	3.328	2.652	-	0.995	1.021	1.021	107.40	178.62	-71.70	-49.30
2Fa-1$_{aq}$	0.50	1.418	1.888	-	-	2.516	0.994	1.019	1.021	108.28	58.02	-140.87	-170.87
2Fa-2$_{aq}$[a)]	3.97	1.420	2.392	-	-	2.621	0.982	1.020	1.021	109.75	63.81	-61.68	172.66
2Fa-3$_{aq}$[a)]	3.97	1.420	2.389	-	-	2.620	0.982	1.020	1.021	109.78	63.60	-62.20	173.68
2Fb$_{aq}$	1.05	1.413	1.883	-	-	-	0.995	1.019	1.022	108.04	-64.39	-142.34	-168.92
2Fc$_{aq}$	2.67	1.412	1.954	-	-	-	0.989	1.020	1.023	108.09	-161.94	-151.76	-160.73
			6,8	7,9	7,10								
3Fa$_{aq}$	0.82	1.420	2.327	2.724	2.656	2.636	0.994	1.019	1.020	106.92	63.63	-59.95	175.30
3Fb-1$_{aq}$	2.19	1.417	2.334	-	2.417	(2.522)	0.995	1.021	1.020	106.30	-63.29	-175.32	-144.91
3Fb-2$_{aq}$	2.23	1.413	2.331	-	2.570	(2.625)	0.995	1.020	1.022	107.29	-61.09	-174.75	161.89
3Fb-3$_{aq}$	2.00	1.413	2.337	2.892	-	-	0.995	1.021	1.023	107.63	-67.10	-67.63	-97.09
3Fb-4$_{aq}$	2.14	1.412	2.343	-	2.658	-	0.995	1.021	1.021	107.65	-68.49	-63.32	116.81
3Fb-5$_{aq}$	2.03	1.411	2.333	2.859	2.665	-	0.994	1.020	1.021	107.18	-67.10	-63.16	164.28
3Fc$_{aq}$	1.47	1.415	2.340	-	2.676	-	0.994	1.020	1.021	107.70	178.91	-67.89	111.37
			4,8	6,9	6,10								
4Fa$_{aq}$	3.07	1.415	-	2.934	2.660	2.647	0.990	1.020	1.020	106.77	64.02	-62.60	-22.60
4Fb$_{aq}$	3.83	1.409	-	3.117	2.616	-	0.991	1.021	1.021	107.21	-68.14	-67.05	-33.29
4Fc$_{aq}$	3.21	1.412	2.583	3.761	2.585	-	0.989	1.021	1.020	107.29	-173.18	-161.33	-17.40

* atom numbers according to Fig. 3; [a)] upon optimization conformer **2Fa-2$_{aq}$** gives conformer **2Fa-3$_{aq}$**

Table S-9. Structural parameters for alanine zwitterionic forms in water [CPCM, B3LYP 6-311++G(d,p)].

Bond lengths [Å]			Bond angles [°]			Dihedral angles [°]		
Atom*)	**zwAl$_{aq}$**	**zwAr$_{aq}$**	Atom*)	**zwAl$_{aq}$**	**zwAr$_{aq}$**	Atom*)	**zwAl$_{aq}$**	**zwAr$_{aq}$**
1,2	1.559	1.555	2,1,6	115.963	115.487	8,5,2,1	-25.859	41.318
2,5	1.511	1.511	2,1,7	115.735	116.055	10,5,2,1	90.585	163.673
1,6	1.247	1.249	5,2,1	107.524	107.843	5,2,1,6	-171.134	163.043
1,7	1.259	1.257	6,1,7	128.266	128.437	5,2,1,7	10.840	-18.513
5,8	1.035	1.033	8,5,2	106.559	108.486	8,5,1,6	170.603	-170.678
5,9	1.029	1.030	8,5,9	110.319	106.426	8,5,1,7	-16.016	22.725
5,10	1.030	1.030	8,5,10	106.668	109.938	11,2,1,7	-102,079	-134.331
2,11	1.096	1.093	9,5,2	112.924	110.956	10,5,1,7	86.499	134.529
7,8	2.013	2.187	10,5,2	112.294	113.270	9,5,2,1	-147.130	-75.254
7,10(9)	3.012	(2.880)	11,2,1	106.887	109.800	Ha,3,2,5	61.641	60.673
Ha,3	1.094	1.094	3,2,1	114.986	111.643	Ha,3,2,11	178.309	178.293
Hb,3	1.093	1.094	Ha,3,2	111.122	111.179	Ha,3,5,10	22.124	92.318
Hc,3	1.089	1.090	Hb,3,2	111.282	111.269	Ha,3,2,1	-60.647	-58.896
Ha,10(8)	2.467	(2.717)	Hc,3,2	108.926	108.933	Hb,3,2,5	-59.748	-60.763
Hb,9(10)	2.856	(2.470)				Hb,3,2,11	56.921	56.858
Hc,11	2.499	2.507				Hb,3,5,10	-86.787	-16.579
Hc,6	2.674	2.858				Hb,3,5,9	19.990	97.756
						Hb,3,2,1	177.965	179.668
						Hc,3,2,11	-62.684	-62.380
						Hc,3,2,1	58.360	60.430
						Hc,3,1,6	12.464	-9.149

*) The atomic numbering scheme is given in Fig. 3, with H8 at the amino group also in Fig. 11.

Table S-10. Dipole moments, NBO charges of alanine zwitterionic forms **zwAr$_{aq}$** and **zwAl$_{aq}$** in water, [B3LYP, 6-311++G(d,p)] CPCM model

Conform.	Dipole [D]	C1	C2	C3	H4	N5	O6	O7	H8 (N)_zw	H9	H10	H11	H12	H13
zwAr$_{aq}$	14,237	0,765	-0,115	-0,596	0,212	-0,700	-0,798	-0,817	0,460	0,457	0,448	0,238	0,213	0,232
zwAl$_{aq}$	14,064	0,769	-0,119	-0,597	0,209	-0,703	-0,793	-0,818	0,465	0,453	0,446	0,242	0,212	0,235

Table S-11. Structural parameters for the 3-fluoroalanine zwitterionic form **zwAFa$_{aq}$** position in aqueous media [CPCM, B3LYP 6-311++G(d,p)].

Bond lengths [Å]		Bond angles [°]		Dihedral angles [°]	
Atom*)		Atom*)		Atom*)	
1,2	1.566	2,1,6	115.658	8,5,2,1	-19.852
2,3	1.51	2,1,7	115.009	9,5,2,1	-140.208
2,5	1.505	5,2,1	107.978	10,5,2,1	96.411
1,6	1.244	6,1,7	129.212	5,2,1,6	-171.725
1,7	1.253	8,5,2	105.427	5,2,1,7	10.379
5,8	1.039	9,5,2	113.125	8,5,1,7	-10.772
5,9	1.030	10,5,2	112.519	11,2,1,6	72.911
5,10	1.031	8,5,9	110.094	10,5,1,7	90.422
7,8	1.959	8,5,10	106.987	F,3,2,5	60.394
2,11	1.098	3,2,1	114.357	F,3,2,11	178.042
F,3	1.416	11,2,1	107.383	F,3,5,10	27.586
F,10	2.457	F,3,2	109.109	F,3,2,1	-62.263
12,3	1.093	12,3,2	112.440	12,3,2,5	-57.854
13,3	1.089	F,3,12	106.761	12,3,2,11	59.795
13,6	2.636	13,3,2	109.679	12,3,5,9	27.634
				12,3,2,1	179.489
				13,3,2,11	-63.869
				13,3,2,1	55.825
				13,3,1,6	9.638

*) The atomic numbering scheme is given in Fig. 3, with H8 at amino group, and Fig 9.

Table S-12. Structural parameters for the 3-fluoroalanine zwitterionic forms **zwAFbl$_{aq}$** and **zwAFbr$_{aq}$** position in water [CPCM, B3LYP 6-311++G(d,p)].

Bond lengths [Å]			Bond angles [°]			Dihedral angles [°]		
Atom*)	**zwAFbl$_{aq}$**	**zwAFbr$_{aq}$**	Atom*)	**zwAFbl$_{aq}$**	**zwAFbr$_{aq}$**	Atom*)	**zwAFbl$_{aq}$**	**zwAFbr$_{aq}$**
1,2	1.566	1.565	2,1,6	115.655	114.964	8,5,2,1	-149.610	158.731
2,5	1.504	1.504	2,1,7	115.040	115.559	9,5,2,1	-28.597	-80.649
1,6	1.246	1.247	5,2,1	108.328	108.848	10,5,2,1	87.900	36.042
1,7	1.254	1.253	6,1,7	129.278	129.464	5,2,1,6	-167.877	168.248
5,8	1.030	1.031	8,5,2	112.887	113.131	5,2,1,7	13.838	-12.950
5,9	1.036	1.031	9,5,2	106.461	110.716	9,5,1,7	-15.848	-81.998
5,10	1.032	1.034	10,5,2	112.518	108.617	11,2,1,6	77.511	50.724
7,9	2.044	2.92	8,5,9	110.183	107.406	10,5,1,7	87.182	22.873
7,10		1.166	8,5,10	107.951	110.199	4,3,2,5	56.763	56.539
2,11	1.097	1.094	3,2,1	113.161	110.253	4,3,2,11	174.271	174.810
4,3	1.094	1.094	11,2,1	107.589	110.071	4,3,5,10	16.651	-24.512
4,10	2.436	2.753	4,3,2	112.308	112.375	4,3,2,1	-65.499	-63.541
F,3	1.417	1.415	F,3,2	109.411	109.486	F,3,2,5	-61.607	-61.920
F,10	2.984	-	F,3,4	106.766	106.764	F,3,2,11	55.901	56.351
F,8	2.860	2.476	13,3,2	109.917	109.721	F,3,5,10	-90.162	-131.309
13,3	1.088	1.089				F,3,5,8	16.888	-21.803
13,6	2.605	2.759				F,3,2,1	176.131	178.000
						13,3,2,11	-62.502	-61.844
						13,3,2,1	57.728	59.804
						13,3,1,6	13.897	-6.193

*) The atomic numbering scheme is given in Fig. 3, with H8 at amino group, and Fig 9 (for left and right structures).

Table S-13. Structural parameters for the 3-fluoroalanine zwitterionic forms **zwAFcl$_{aq}$** and **zwAFcr$_{aq}$** in water [CPCM, B3LYP 6-311++G(d,p)].

Bond lengths [Å]			Bond angles [°]			Dihedral angles [°]		
Atom*)	**zwAFcl$_{aq}$**	**zwAFcr$_{aq}$**	Atom*)	**zwAFcl$_{aq}$**	**zwAFcr$_{aq}$**	Atom*)	**zwAFcl$_{aq}$**	**zwAFcr$_{aq}$**
1,2	1.561	1.561	2,1,6	116.040	116.330	8,5,2,1	-149.946	161.184
2,5	1.504	1.503	2,1,7	114.972	114.641	9,5,2,1	-29.047	-77.966
1,6	1.245	1.246	5,2,1	107.684	107.410	10,5,2,1	87.079	38.531
1,7	1.257	1.257	6,1,7	128.963	129.016	5,2,1,6	-162.692	152.327
5,8	1.031	1.032	8,5,2	113.108	114.096	5,2,1,7	18.924	-28.881
5,9	1.037	1.032	9,5,2	105.809	110.480	9,5,1,7	-11.889	-94.437
5,10	1.032	1.036	10,5,2	112.823	107.863	10,5,1,7	90.923	11.023
7,9	2.014	2.992	8,5,9	110.337	107.198	11,2,1,6	83.232	34.276
7,10	3.032	2.128	8,5,10	108.009	110.093	4,3,2,5	93.160	66.123
2,11	1.097	1.093	3,2,1	115.787	112.079	4,3,2,11	-150.764	-176.348
4,3	1.091	1.094	11,2,1	107.626	111.353	4,3,5,10	42.691	-14.679
4,10	2.877	2.726	4,3,2	112.169	111.556	4,3,2,1	-29.747	-51.778
12,3	1.094	1.095	12,3,2	111.173	110.926	12,3,2,5	-30.759	-56.897
12,10	2.515	-	F,3,2	108.938	109.035	12,3,2,11	85.317	60.632
12,8	2.691	2.368	F,3,4	107.333	107.773	12,3,5,8	41.673	-15.143
F,3	1.405	1.400	F,3,12	106.780	107.397	12,3,5,10	-65.704	-124.711
F,11	2.436	2.632	12,3,4	111.173	110.009	12,3,2,1	-153.666	-174.808
F,6	3.153	3.131				F,3,2,5	-148.160	-174.964
						F,3,2,11	-32.084	-57.435
						F,3,2,1	88.933	67.125
						F,3,1,6	44.923	-13.618

*) The atomic numbering scheme is given in Fig. 3 with H8 at amino group and Fig 9 (for left right structures).

Table S-14. Dipole moments and NBO charges of 3-fluoroalanine zwitterionic forms **zwAFa$_{aq}$** to **zwAFcr$_{aq}$** in water, [B3LYP, 6-311++G(d,p)] CPCM model

Conformer	Dipole [D]	C1	C2	C3	Fa (H4)*	N5	O6	O7	H8 (-N)_zw	H9	H10	H11	Fb (H12)*	Fc (H13)*
zwAFa$_{aq}$	14,203	0,774	-0,169	0,067	-0,418	-0,708	-0,805	-0,783	0,467	0,458	0,452	0,267	0,189	0,208
zwAFbl$_{aq}$	11,672	0,773	-0,163	0,067	0,186	-0,704	-0,800	-0,783	0,468	0,459	0,452	0,257	-0,418	0,208
zwAFbr$_{aq}$	11,872	0,767	-0,160	0,066	0,188	-0,702	-0,799	-0,785	0,464	0,462	0,454	0,253	-0,416	0,206
zwAFcl$_{aq}$	14,766	0,770	-0,162	0,076	0,192	-0,703	-0,809	-0,780	0,470	0,459	0,452	0,261	0,183	-0,407
zwAFcr$_{aq}$	15,559	0,761	-0,150	0,077	0,186	-0,703	-0,811	-0,779	0,466	0,465	0,455	0,248	0,185	-0,399

* according to Figure 3C

Table S-15. Structural parameters for protonated alanine conformers in the gas phase.

Confor	E_{rel}	Bond lengths [Å]								Angle [°]	Dihedral angles [°]		
	[kcal/mol]	6(7),9[10]*	6,8	1,6	1,7	7,8	5,9	5,10	5,14	6,1,7	14,5,2,1	9,5,1,6(7)*	10,5,1,6(7)*
p1	0.00	1.911	2.381	1.208	1.319	0.973	1.041	1.024	1.022	126.803	-128.113	-6.068	93.221
p3	2.58	2.222	2.386	1.190	1.352	0.973	1.026	1.025	1.024	126.139	-168.470	-29.089	77.442
p4	8.94	1.854	-	1.204	1.321	0.967	1.046	1.022	1.023	122.498	-102.726	-94.064	5.671

* The notation (7) is used for conformer **p3** and [10] for conformer **p4** (Figure 11).

Table S-16. Dipole moments and NBO charges of protonated alanine conformers **p1**, **p3** and **p4** in the gas phase [6-311++G(d,p)].

Conform.	Dipole [D]	C1	C2	C3	H4	N5	O6	O7	H8	H9	H10	H11	H12	H13	H14 (-N+)
p1	4,950	0,798	-0,104	-0,604	0,225	-0,696	-0,584	-0,639	0,516	0,466	0,438	0,250	0,231	0,262	0,441
p3	7,136	0,781	-0,102	-0,607	0,224	-0,681	-0,506	-0,716	0,523	0,458	0,440	0,250	0,227	0,271	0,440
p4	7,277	0,794	-0,119	-0,606	0,235	-0,699	-0,555	-0,610	0,494	0,442	0,468	0,239	0,235	0,244	0,439

Table S-17. Relative Energies and structural parameters for protonated alanine conformers in water (CPCM-Model)

Conformer	rel. Energy [kcal/mol]	Bond lengths [Å]								
		6(7),9*	6(7),10*	6,8	1,6	1,7	7,8	5,9	5,10	5,14
$p1_{aq}$	0.00	2.578	2.647	2.369	1.211	1.324	0.998	1.034	1.034	1.033
$p3_{aq}$	1.47	2.478	2.578	2.377	1.207	1.330	0.999	1.033	1.034	1.034
$p4_{aq}$	4.03	2.831	2.444	-	1.209	1.327	0.995	1.034	1.034	1.034

	Angle [°]			Dihedral angles [°]		
	9,6(7),10*	6,1,7	9,5,10	14,5,2,1	9,5,1,6(7)*	10,5,1,6(7)*
$p1_{aq}$	37.029	125.722	106.844	-175.476	-53.684	53.125
$p3_{aq}$	38.348	125.547	107.147	-176.081	-50.953	56.322
$p4_{aq}$	35.808	121.243	107.012	176.076	-77.804	29.155

* The notation (7) is used for conformer **p3** (Figure 11).

Table S-18. Dipole moments and NBO charges of protonated alanine conformers **$p1_{aq}$**, **$p3_{aq}$** and **$p4_{aq}$** in water

Conf.	Dipole [D]	C1	C2	C3	H4	N5	O6	O7	H8	H9	H10	H11	H12	H13	H14 (-N+)
$p1_{aq}$	6,512	0,813	-0,114	-0,596	0,220	-0,695	-0,635	-0,686	0,553	0,470	0,463	0,272	0,226	0,242	0,466
$p3_{aq}$	9,250	0,816	-0,113	-0,595	0,220	-0,698	-0,625	-0,703	0,559	0,471	0,463	0,273	0,225	0,242	0,466
$p4_{aq}$	10,017	0,809	-0,122	-0,597	0,224	-0,696	-0,626	-0,682	0,551	0,470	0,466	0,268	0,230	0,238	0,466

Table S-19. Structural parameters and relative energy (kcal/mol) for protonated 3-fluoroalanine conformers in the gas phase

Conformer	Relative energy	Bond lengths [Å]							Angle [°]	Dihedral angles [°]			
		1,6	1,7	6(7),9	6(7),10	5,9	5,10	5,14	6,1,7	9,5,2,1	10,5,2,1	9,5,1,6(7)	10,5,1,6(7)
p1Fa	0.00	1.204	1.319	1.979	-	1.038	1.029	1.022	127.469	-19.738	95.938	-11.108	91.146
p1Fb	0.37	1.204	1.321	3.035	2.102	1.024	1.034	1.028	127.618	-90.478	27.219	-85.864	17.580
p1Fc	7.02	1.209	1.313	3.110	1.915	1.024	1.044	1.024	127.490	-99.369	17.626	-95.301	5.816
p3Fa	2.59	1.190	1.347	(2.136)	(2.908)	1.027	1.029	1.024	126.852	-36.803	81.320	-19.390	87.345
p3Fb	2.94	1.191	1.346	(2.571)	(2.487)	1.024	1.025	1.028	127.014	-66.236	53.242	-52.758	54.138
p3Fc	9.97	1.188	1.355	(2.957)	(2.202)	1.025	1.029	1.026	126.773	-70.188	48.068	-95.754	10.872
p4Fa	10.71	1.202	1.320	1.866	-	1.044	1.028	1.022	122.717	-15.440	99.521	-9.202	91.089
p4Fb	10.09	1.201	1.323	3.033	2.013	1.024	1.037	1.027	123.080	-90.068	27.190	-91.305	11.949
p4Fc	12.20	1.207	1.311	-	1.795	1.024	1.054	1.023	123.629	-10.188	106.279	-4.324	93.456

* The notation (7) is used for fluorine conformers correspond to **p3** (Figure 11).

Table S-20. Dipole moments and NBO charges of protonated 3-fluoroalanine conformers in the gas phase

Conf.	Dipole, D	C1	C2	C3	Fa (H4)*	N5	O6	O7	H8	H9	H10	H11	Fb (H12)*	Fc (H13)*	H14 (N+)
p1Fa	5,155	0,797	-0,146	0,069	-0,377	-0,696	-0,570	-0,643	0,520	0,468	0,453	0,264	0,194	0,225	0,442
p1Fb	3,047	0,787	-0,142	0,073	0,192	-0,690	-0,567	-0,641	0,518	0,446	0,462	0,258	-0,373	0,221	0,454
p1Fc	6,814	0,792	-0,140	0,085	0,189	-0,696	-0,584	-0,619	0,516	0,447	0,469	0,259	0,184	-0,341	0,439
p3Fa	7,093	0,785	-0,145	0,068	-0,379	-0,689	-0,504	-0,710	0,527	0,463	0,456	0,264	0,192	0,232	0,442
p3Fb	5,858	0,777	-0,141	0,073	0,190	-0,682	-0,504	-0,703	0,524	0,452	0,447	0,260	-0,377	0,228	0,456
p3Fc	9,476	0,770	-0,134	0,082	0,188	-0,683	-0,478	-0,722	0,525	0,450	0,461	0,258	0,183	-0,340	0,441
p4Fa	7,216	0,796	-0,160	0,067	-0,368	-0,700	-0,545	-0,606	0,492	0,472	0,451	0,259	0,201	0,199	0,443
p4Fb	4,528	0,783	-0,155	0,070	0,200	-0,693	-0,541	-0,610	0,495	0,446	0,467	0,245	-0,369	0,210	0,454
p4Fc	8,018	0,796	-0,158	0,070	0,195	-0,702	-0,558	-0,606	0,512	0,473	0,438	0,257	0,201	-0,364	0,446

* according to Figure 3C

Table S-21. Relative energy (kcal/mol) and structural parameters for protonated 3-fluoroalanine conformers in water (CPCM-model)

Conf.	Relative energy	Bond lengths [Å]							Angle [°]		Dihedral angles [°]		
		1,6	1,7	6(7),9	6(7),10	5,9	5,10	5,14	6,1,7	9,5,2,1	10,5,2,1	9,5,1,6(7)	10,5,1,6(7)
p1Fa$_{aq}$	0.00	1.208	1.322	2.514	2.716	1.034	1.035	1.035	126.406	-53.403	66.020	-46.776	59.983
p1Fb$_{aq}$	0.70	1.208	1.322	2.578	2.672	1.034	1.035	1.034	126.476	-57.922	61.781	-50.153	56.876
p1Fc$_{aq}$	3.37	1.210	1.321	2.613	2.595	1.035	1.036	1.035	126.165	-57.323	61.798	-58.953	47.652
p3Fa$_{aq}$	1.29	1.205	1.326	(2.464)	(2.619)	1.034	1.034	1.035	126.259	-55.991	64.291	-48.147	59.174
p3Fb$_{aq}$	2.02	1.206	1.326	(2.475)	(2.625)	1.034	1.035	1.035	126.295	-59.381	61.114	-45.515	61.964
p3Fc$_{aq}$	4.47	1.205	1.329	(2.722)	(2.451)	1.035	1.035	1.036	126.095	-57.941	62.160	-76.367	30.776
p4Fa$_{aq}$	4.52	1.207	1.326	2.704	2.513	1.035	1.035	1.035	121.660	-59.860	59.545	-68.050	38.942
p4Fb$_{aq}$	5.20	1.207	1.324	2.883	2.435	1.035	1.035	1.035	121.912	-66.652	52.968	-80.800	26.326
p4Fc$_{aq}$	6.53	1.208	1.323	2.863	2.428	1.036	1.036	1.036	121.753	-65.663	53.442	-80.916	25.949

* The notation (7) is used for 3-fluoroalanine cation corresponding to conformer **p3** (Figure 12).

Table S-22. Dipole moments and NBO charges of protonated 3-fluoroalanine conformers in water

Conf.	Dipole [D]	C1	C2	C3	Fa (H4)*	N5	O6	O7	H8	H9	H10	H11	Fb (H12)*	Fc (H13)*	H14-(N+)
p1Fa$_{aq}$	7,692	0,815	-0,159	0,068	-0,404	-0,698	-0,624	-0,684	0,557	0,475	0,468	0,297	0,202	0,215	0,471
p1Fb$_{aq}$	4,074	0,813	-0,154	0,070	0,197	-0,697	-0,620	-0,683	0,558	0,475	0,468	0,286	-0,400	0,215	0,471
p1Fc$_{aq}$	8,620	0,810	-0,151	0,077	0,197	-0,696	-0,628	-0,677	0,554	0,477	0,472	0,285	0,197	-0,386	0,470
p3Fa$_{aq}$	9,921	0,817	-0,159	0,070	-0,404	-0,700	-0,616	-0,698	0,562	0,475	0,469	0,297	0,202	0,215	0,471
p3Fb$_{aq}$	8,348	0,816	-0,154	0,071	0,197	-0,699	-0,614	-0,696	0,562	0,475	0,468	0,287	-0,400	0,215	0,471
p3Fc$_{aq}$	12,306	0,808	-0,146	0,078	0,196	-0,699	-0,606	-0,703	0,561	0,477	0,471	0,280	0,199	-0,388	0,473
p4Fa$_{aq}$	11,377	0,809	-0,167	0,067	-0,399	-0,698	-0,614	-0,679	0,552	0,475	0,471	0,294	0,206	0,211	0,472
p4Fb$_{aq}$	6,659	0,805	-0,161	0,069	0,201	-0,699	-0,611	-0,673	0,554	0,475	0,471	0,281	-0,395	0,211	0,472
p4Fc$_{aq}$	11,462	0,805	-0,157	0,076	0,198	-0,698	-0,620	-0,672	0,554	0,478	0,472	0,278	0,202	-0,389	0,473

* according to Figure 3C

Table S-23. Structural parameters for the alanine anion conformers in the gas phase

Conformer	rel. energy [kcal/mol]	Bond lengths [Å]								Angle [°]		Dihedral angles [°]	
		1,6	1,7	5,9	5,10	6,11	6,13	7,9	7,10	9,5,10	6,1,7	10,5,1,7	9,5,1,7
a1r	0.00	1.253	1.258	1.017	1.023	2,550	2.833	3.048	2.206	103.451	129.050	11.781	-90.133
a1l	0.26	1.253	1.257	1.023	1.019	2.703	2.567	2.140	3.080	103.711	128.919	82.024	-14.116

Table S-24. Dipole moments and NBO charges of alanine anion conformers in the gas phase

Conf.	Dipole [D]	C1	C2	C3	H4	N5	O6	O7	H9	H10	H11	H12	H13
a1r	4,576	0,743	-0,122	-0,572	0,186	-0,881	-0,789	-0,804	0,331	0,367	0,165	0,176	0,200
a1l	4,944	0,747	-0,124	-0,581	0,175	-0,879	-0,792	-0,801	0,374	0,321	0,167	0,172	0,220

Table S-25. Structural parameters for the alanine anion conformer **a1l** in water (CPCM-model)

Conf.	Bond lengths [Å]								Angle [°]		Dihedral angles [°]	
	1,6	1,7	5,9	5,10	6,11	6,13	7,10	7,9	9,5,10	6,1,7	10,5,1,7	9,5,1,7
a1l$_{aq}$	1.264	1.261	1.021	1.021	2.508	2.943	2.564	2.998	105.277	125.612	22.447	-82.789

Table S-26. Dipole moments and NBO charges of alanine anion conformer **a1l** in water

Conf.	Dipole [D]	C1	C2	C3	H4	N5	O6	O7	H9	H10	H11	H12	H13
a1l$_{aq}$	6,861	0,759	-0,121	-0,575	0,194	-0,885	-0,852	-0,846	0,367	0,365	0,192	0,199	0,203

Table S-27. Relative energy [kcal/mol], optimized bond lengths, bond angles and dihedral angles for 3-fluoroalanine anion conformers [B3LYP 6-311++G(d,p)] in the gas phase

Conformer	Relative	Bond lengths [Å]							Angle [Å]		Dihedral angles [Å]		
	energy	F,9	F,10	5,9	5,10	6,13	7,9	7,10	9,5,10	5,2,1,7	9,5,2,1	10,5,2,1	10,5,1,7
a1Fa	1.96	-	2.361	1.022	1.018	2.468	2.182	3.090	103.708	10.599	-22.921	86.487	87.019
a1Fbl	0.15	-	2.514	1.021	1.015	2.647	2.085	3.488	109.909	-13.756	18.412	137.828	106.395
a1Fcl	5.58	-	-	1.021	1.018	-	2.154	-	108.655	-42.899	33.353	151.423	94.935
a1Fbr	0.00	3.047	-	1.013	1.021	2.460	3.469	2.065	109.347	18.228	-139.487	-20.961	-4.749
a1Fcr	3.84	-	-	1.016	1.022	-	-	2.282	105.072	-47.951	-76.078	35.342	-7.542

Table S-28. Dipole moments and NBO charges of 3-fluoroalanine anion conformers in the gas phase

Conf.	Dipole [D]	C1	C2	C3	Fa (H4)*	N5	O6	O7	H9	H10	H11	Fb (H12)*	Fc (H13)*
a1Fa	5,530	0,753	-0,167	0,083	-0,433	-0,879	-0,787	-0,788	0,375	0,339	0,182	0,135	0,188
a1Fbl	5.429	0.758	-0.165	0.080	0.147	-0.879	-0.778	-0.780	0.379	0.332	0.178	-0.446	0.175
a1Fcl	7.048	0.756	-0.157	0.087	0.163	-0.862	0.754	0.806	0.378	0.316	0.176	0.121	-0.418
a1Fbr	4,981	0,761	-0,167	0,086	0,152	-0,883	-0,781	-0,781	0,331	0,383	0,167	-0,448	0,178
a1Fcr	5,613	0,741	-0,155	0,096	0,161	-0,875	-0,764	-0,809	0,340	0,367	0,177	0,140	-0,420

* according to Figure 3C

Table S-29. Relative energy [kcal/mol], optimized bond lengths, bond angles and dihedral angles for 3-fluoroalanine anion conformers in water [B3LYP 6-311++G(d,p), CPCM model]

Conformer	E_{rel}	Bond lengths [Å]						Angle [°]	Dihedral angles [°]			
	[kcal/ mol]	7,9	7,10	F,10(9)	6,13	5,9	5,10	9,5,10	5,2,1,7	9,5,2,1	10,5,2,1	10,5,1,7
a1Fa$_{aq}$	0.00	2.819	2.640	2.679	2.646	1.020	1.021	105.126	-6.847	-61.151	53.118	43.116
a1Fbl$_{aq}$	0.28	2.380	-	2.524	2.792	1020	1.020	107.992	-24.462	46.800	165.605	134.916
a1Fcl$_{aq}$	0.79	2.574	-	-	-	1.021	1.022	107.550	-57.278	59.552	178.082	127.382
a1Fbr$_{aq}$	0.56	-	2.250	(2.781)	2.534	1.019	1.018	107.946	16.804	-152.657	-34.438	-18.161
a1Fcr$_{aq}$	0.75	3.346	2.549	-	-	1.020	1.021	106.466	-53.653	-72.290	43.829	-5.229

Table S-30. Dipole moments and NBO charges of 3-fluoroalanine anion conformers in water

Conf.	Dipole [D]	C1	C2	C3	Fa (H4)*	N5	O6	O7	H9	H10	H11	Fb (H12)*	Fc (H13)*
a1Fal$_{aq}$	7,744	0,761	-0,177	0,088	-0,441	-0,882	-0,844	-0,828	0,374	0,370	0,225	0,171	0,182
a1Fbl$_{aq}$	8,407	0,767	-0,163	0,078	0,169	-0,886	-0,833	-0,823	0,376	0,369	0,205	-0,438	0,179
a1Fcl$_{aq}$	10.879	0.768	-0.155	0.076	0.172	-0.875	-0.830	-0.837	0.374	0.372	0.200	0.168	-0.433
a1Fbr$_{aq}$	7,393	0,771	-0,167	0,088	0,167	-0,895	-0,832	-0,823	0,371	0,382	0,199	-0,443	0,182
a1Fcr$_{aq}$	8,288	0,757	-0,157	0,090	0,170	-0,880	-0,834	-0,841	0,379	0,373	0,203	0,171	-0,431

* according to Figure 3C

Table S-31. Total energies [au], relative energies [kcal/mol], dipole moments [D] at the B3LYP/6-311++G(d,P)//B3LYP/6-311++G(d,p) MP2/6-311++G(d,P)//B3LYP/6-311++G(d,p) level of theory including zero point energies (ZPE) of alanine and 3-fluoroalanine in the gas phase

Alanine

Compound	B3LYP/6-311++G(d,p)	E_{rel}	Dipole Moment	B3LYP/6-311++G(d,p) + ZPE	E_{rel} (ZPE)	SCS-MP2/6-311++G(d,p)	E_{rel}	E_{rel} (ZPE)
Neutrals								
1	-323,85608	0,00	1,3053	-323,74849	0,00	-322,96501	0,00	0,00
2	-323,85606	0,01	5,5837	-323,74795	0,34	-322,96349	0,96	1,28
3	-323,85438	1,07	1,6309	-323,74669	1,13	-322,96353	0,93	1,00
4	-323,84696	5,72	3,3195	-323,73981	5,44	-322,95585	5,75	5,47
Protonated								
p1	-324,21157	0,00	4,9503	-324,08962	0,00	-323,32196	0,00	0,00
p3	-324,20554	3,78	7,1362	-324,08364	3,75	-323,31780	2,61	2,58
p4	-324,19722	9,00	1,3053	-324,07588	8,62	-323,30710	9,32	8,94
Anionic								
AIr	-323,30308	0,00	4,5762	-323,20883	0,00	-322,40548	0,00	0,00
AII	-323,30291	0,10	4,9439	-323,20877	0,04	-322,40496	0,32	0,26

3-Fluoroalanine

Compound	B3LYP/6-311++G(d,p)	E_{rel}	Dipole Moment	B3LYP/6-311++G(d,p) + ZPE	E_{rel} (ZPE)	SCS-MP2/6-311++G(d,p)	E_{rel}	E_{rel} (ZPE)
Neutrals								
1Fa	-42312022	0,34	2,4242	-423,01954	-0,08	-422,02942	0,00	0,00
Fb-1	-423,11832	1,53	2,0152	-423,01783	1,00	-422,02695	1,55	1,43
1Fb-2	-423,11832	1,53	2,0002	-423,01771	1,07	-422,02695	1,55	1,50
1Fb-3	-423,11651	2,67	2,5371	-423,01622	2,00	-422,02497	2,80	2,55
1Fc	-423,11826	1,57	1,9318	-423,01753	1,19	-422,02738	1,28	1,31
2Fa-1	-423,12076	0,00	5,6016	-423,01942	0,00	-422,02809	0,83	1,25
2Fa-2	-423,11244	5,22	3,2156	-423,01147	4,98	-422,02041	5,65	5,83
2Fa-3	-423,11179	5,62	4,1893	-423,01181	4,77	-422,01897	6,56	6,12
2Fb	-423,12065	0,07	3,7516	-423,01944	-0,01	-422,02808	0,84	1,18
2Fc	-423,11343	4,60	6,0474	-423,01243	4,38	-422,02124	5,13	5,33
3Fa	-423,11880	1,23	1,8736	-423,01800	0,89	-422,02766	1,10	1,18
3Fb-1	-423,11789	1,80	2,3546	-423,01734	1,30	-422,02709	1,47	1,38
3Fb-2	-423,11663	2,59	2,2253	-423,01606	2,11	-422,02564	2,37	2,30
3Fb-3	-423,11499	3,62	2,8714	-423,01454	3,06	-422,02369	3,59	3,45
3Fb-4	-423,11456	3,89	2,9621	-423,01420	3,27	-422,02357	3,67	3,47
3Fb-5	-423,11445	3,96	3,2881	-423,01404	3,37	-422,02272	4,21	4,04
3Fc	-423,11705	2,33	2,8819	-423,01633	1,94	-422,02646	1,86	1,89
4Fa	-423,10874	7,54	4,2475	-423,00854	6,83	-422,01772	7,34	7,04
4Fb	-423,10703	8,61	2,0220	-423,00703	7,77	-422,01548	8,75	8,32
4Fc	-423,11513	3,53	3,6414	-423,01441	3,14	-422,02235	4,44	4,47
Protonated								
p1Fa	-423,46903	0,00	5,1552	-423,35389	0,00	-422,38023	0,00	0,00
p1Fb	-423,46816	0,55	3,0475	-423,35310	0,50	-422,37956	0,42	0,37
p1Fc	-423,45758	7,19	6,8146	-423,34284	6,93	-422,36863	7,28	7,02
p3Fa	-423,46349	3,48	7,0928	-423,34853	3,37	-422,37592	2,71	2,59
p3Fb	-423,46267	3,99	5,8578	-423,34773	3,87	-422,37534	3,07	2,94
p3Fc	-423,45024	11,80	9,4762	-423,33550	11,54	-422,36393	10,23	9,97
p4Fa	-423,45212	10,62	7,2159	-423,33777	10,12	-422,36237	11,21	10,71
p4Fb	-423,45273	10,23	4,5279	-423,33823	9,82	-422,36351	10,49	10,09
p4Fc	-423,45082	11,43	8,0177	-423,33622	11,09	-422,36025	12,54	12,20

Anionic								
a1Fa	-422,57564	2,18	5,5304	-422,48814	2,40	-421,47701	1,75	1,96
a1Fbl	-422,57872	0,25	5,4288	-422,49151	0,28	-421,47960	0,12	0,15
a1Fbr	-422,57912	0,00	4,9813	-422,49196	0,00	-421,47979	0,00	0,00
a1Fcr	-422,57148	4,79	5,6128	-422,48404	4,97	-421,47395	3,66	3,84
a1Fcl	-422,56905	6,32	7,0480	-422,48192	6,30	-421,47086	5,60	5,58

Table S-32. Total energies [au], relative energies [kcal/mol], Dipole moments [D] at the B3LYP/6-311++G(d,P)//B3LYP/6-311++G(d,p) MP2/6-311++G(d,P)//B3LYP/6-311++G(d,p) level of theory including zero point energies (ZPE) of alanine and 3-fluoroalanine in water

Alanine

Conformer	B3LYP/6-311++G(d,p)	E_{rel}	Dipole Moment	B3LYP-Solvatation	SCS-MP2/6-311++G(d,p)-CPCM	E_{rel}	Solvatation CPCM-MP2
Neutrals							
1_{aq}	-323,87753	0,00	2,1083	-15,89	-322,98559	0,00	-17,34
2_{aq}	-323,87691	0,38	7,5667	-16,54	-322,98289	1,69	-18,54
3_{aq}	-323,87627	0,79	2,6991	-16,58	-322,98443	0,73	-18,04
4_{aq}	-323,87375	2,37	4,8241	-21,63	-322,98152	2,56	-24,06
Zwitterions							
$zwAr_{aq}$	-323,87803	0,00	14,3185	-51,71	-322,98339	0,00	-52,00
$zwAl_{aq}$	-323,87787	0,10	14,0642	-45,35	-322,98249	0,57	-50,15
Protonated							
$p1_{aq}$	-324,32911	0,00	6,5125	-78,34	-323,44073	0,00	-80,35
$p3_{aq}$	-324,32716	1,23	9,2505	-82,06	-323,43839	1,47	-84,43
$p4_{aq}$	-324,32313	3,76	10,0172	-87,34	-323,43431	4,03	-90,72
Anionic							
all_{aq}	-323,41060	0,00	6,8609	-72,45	-322,51311	0,00	-75,96

3-Fluoroalanines

Conformer	B3LYP/6-311++G(d,p)	E_{rel}	Dipole Moment	B3LYP-Solvatation	SCS-MP2/6-311++G(d,p)-CPCM	E_{rel}l	CPCM-MP2-Solvatation
Neutrals							
$1Fa_{aq}$	-423.14523	0,00	3.8860	-18,99	-422,05312	0,00	-21,04
$1Fb\text{-}1_{aq}$	-423.14293	1,44	3.3023	-19,11	-422,05064	1,55	-21,08
$1Fb\text{-}2_{aq}$	-423.14313	1,32	2.9074	-19,38	-422,05078	1,46	-21,40
$1Fb\text{-}3_{aq}$	-423.14344	1,13	3.7518	-20,39	-422,05095	1,36	-22,45
$1Fc_{aq}$	-423.14337	1,17	2.8087	-18,72	-422,05140	1,07	-20,64
$2Fa\text{-}1_{aq}$	-423.14444	0,50	7.9027	-19,18	-422,05018	1,84	-21,60
$2Fa\text{-}2_{aq}$	-423.13891	3.97	5.5499	-22,35	-422,04540	4,84	-25,24
$2Fa\text{-}3_{aq}$	-423.13890	3.97	5.3058	-22,41	-422,04536	4,86	-25,31
$2Fb_{aq}$	-423.14356	1,05	5.2982	-17,45	-422,04937	2,35	-19,81
$2Fc_{aq}$	-423.14099	2,67	8.6342	-22,37	-422,04709	3,78	-25,52
$3Fa_{aq}$	-423.14392	0,82	3.0076	-19,01	-422,05150	1,01	-20,91
$3Fb\text{-}1_{aq}$	-423.14174	2.19	3.5673	-18,14	-422,04964	2,18	-19,88
$3Fb\text{-}2_{aq}$	-423.14169	2.23	2.9321	-19,05	-422,04930	2,40	-20,96
$3Fb\text{-}3_{aq}$	-423.14205	2.00	4.3665	-20,46	-422,04984	2,06	-22,51
$3Fb\text{-}4_{aq}$	-423.14183	2.14	4.4683	-20,89	-422,04972	2,13	-22,94
$3Fb\text{-}5_{aq}$	-423.14201	2,02	4.8946	-21,04	-422,04925	2,43	-23,11
$3Fc_{aq}$	-423.14289	1,47	4.1446	-19,68	-422,05097	1,34	-21,61
$4Fa_{aq}$	-423.14034	3,07	6.8371	-26,47	-422,04798	3,22	-29,85
$4Fb_{aq}$	-423.13911	3,84	3.4606	-25,54	-422,04644	4,19	-28,52
$4Fc_{aq}$	-423.14013	3,21	5.1355	-23,58	-422,04781	3,33	-26,47

Zwitterions							
zwAFa$_{aq}$	-423,14434	0,00	14,2031	-46,95	-422,04876	0,08	-52,50
zwAFbl$_{aq}$	-423,14416	0,12	11,6721	-43,19	-422,04860	0,18	-48,09
zwAFcl$_{aq}$	-423,13844	3,70	14,7659	-51,65	-422,04296	3,72	-57,70
zwAFcr$_{aq}$	-423,13811	3,91	15,5597	-54,40	-422,04366	3,28	-60,68
zwAFbr$_{aq}$	-423,14392	0,27	11,8722	-43,95	-422,04889	0,00	-48,77
Protonated							
p1Fa$_{aq}$	-423,59169	0,00	7,6919	-83,63	-422,50360	0,00	-86,48
p1Fb$_{aq}$	-423,59085	0,53	4,0745	-81,99	-422,50248	0,70	-84,58
p1Fc$_{aq}$	-423,58637	3,34	8,6202	-87,56	-422,49823	3,37	-90,88
p3Fa$_{aq}$	-423,58994	1,10	9,9214	-86,76	-422,50154	1,29	-89,85
p3Fb$_{aq}$	-423,58898	1,70	8,3484	-85,37	-422,50039	2,02	-88,24
p3Fc$_{aq}$	-423,58437	4,60	12,3062	-92,52	-422,49647	4,47	-96,35
p4Fa$_{aq}$	-423,58483	4,30	11,3776	-94,49	-422,49640	4,52	-99,06
p4Fb$_{aq}$	-423,58409	4,77	6,6589	-90,76	-422,49532	5,20	-94,70
p4Fc$_{aq}$	-423,58161	6,33	11,4618	-94,27	-422,49319	6,53	-98,72
Anionic							
a1Fa$_{aq}$	-422,68163	0,00	7,7444	-72,72	-421,58356	0,00	-76,63
a1Fbl$_{aq}$	-422,68143	0,12	8,4074	-70,38	-421,58311	0,28	-73,97
a1Fbr$_{aq}$	-422,68145	0,11	7,3933	-69,06	-421,58267	0,56	-72,51
a1Fcr$_{aq}$	-422,68005	0,99	8,2887	-74,15	-421,58236	0,75	-78,17
a1Fcl$_{aq}$	-422,67994	1,06	10,8685	-78,55	-421,58230	0,79	-83,05

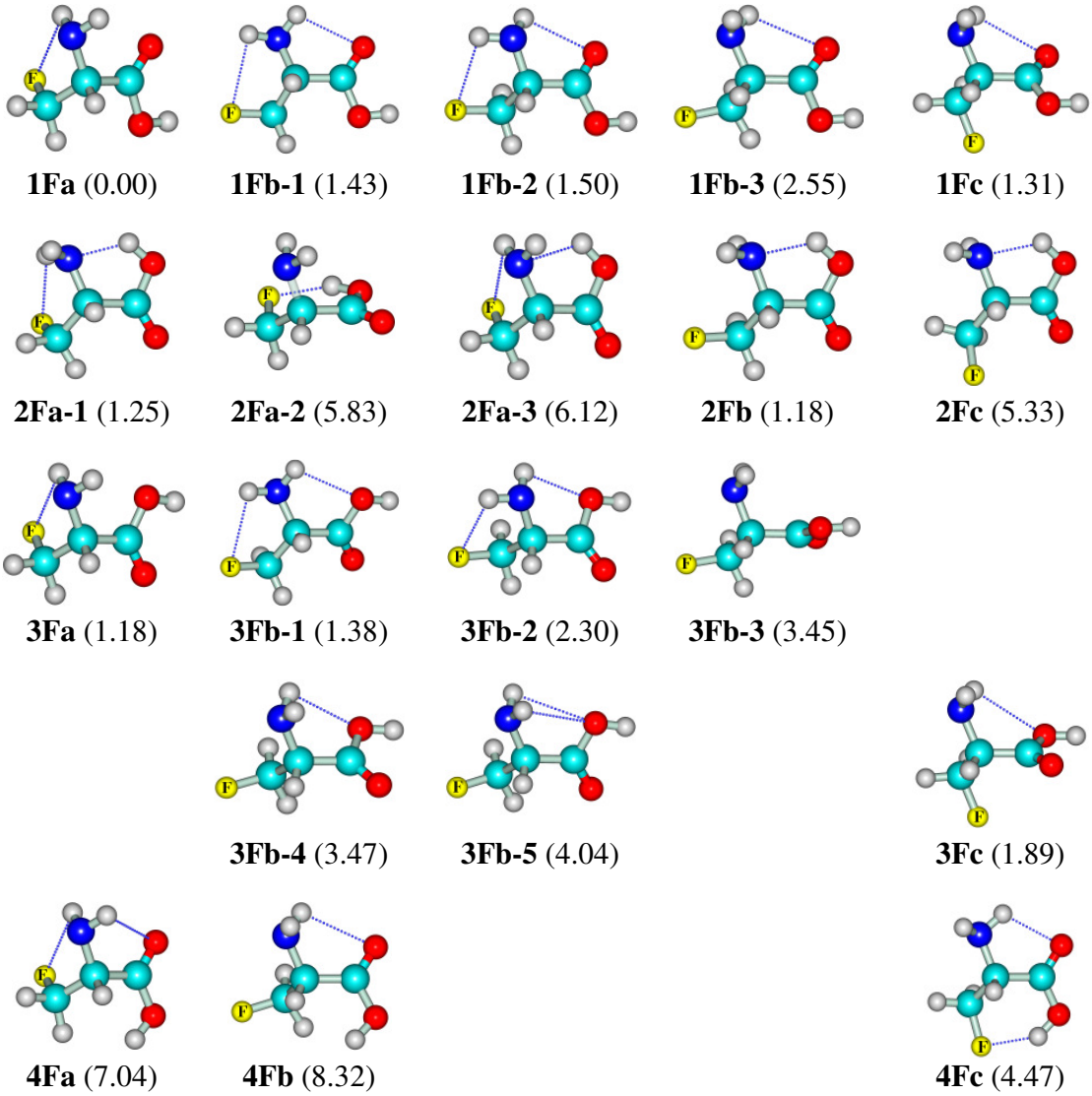
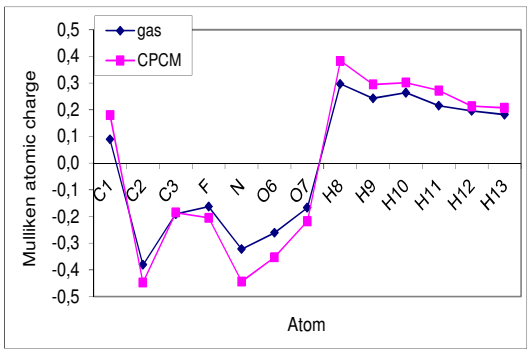
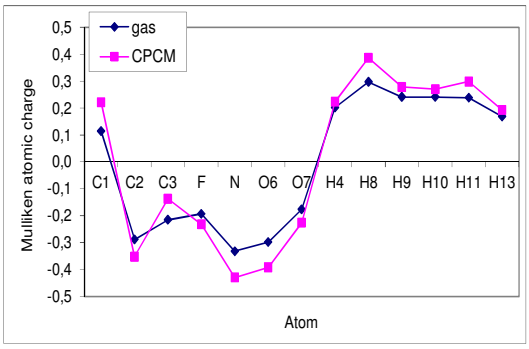


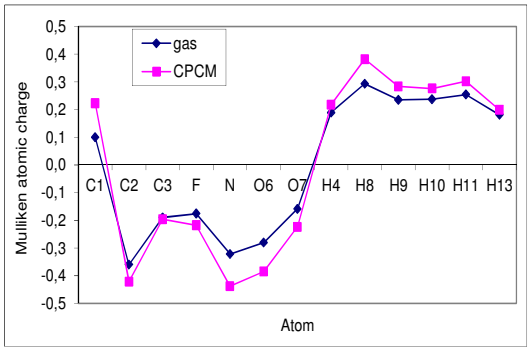
Figure S-1. Twenty 3-fluoroalanine conformers **1Fa**-**4Fc** (basic types **1**-**4** of alanine) and relative energies [kcal/mol] of (SCS-MP2/B3LYP 6-311++G(d,p). The (*S*)-enantiomer is drawn.



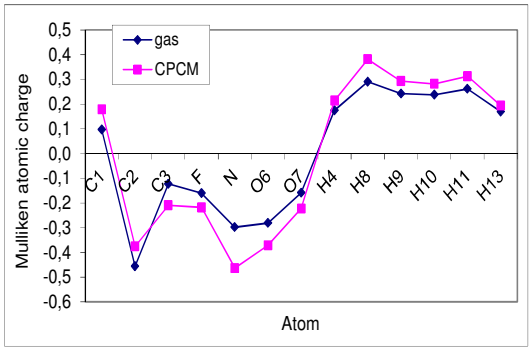
1Fa



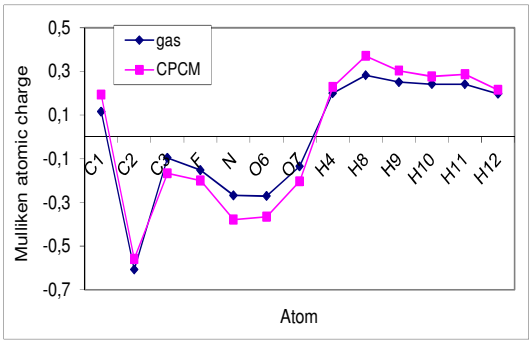
1Fb-1



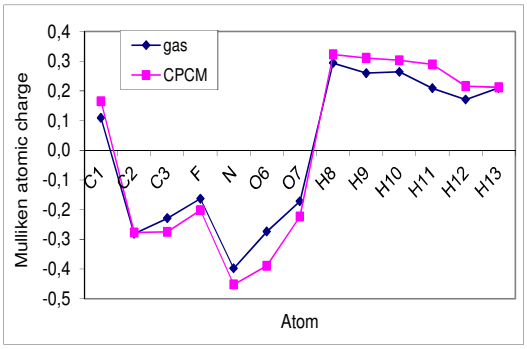
1Fb-2



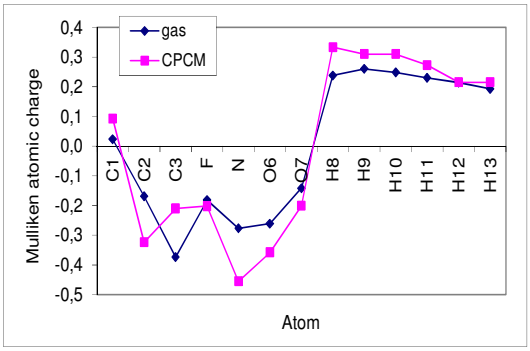
1Fb-3



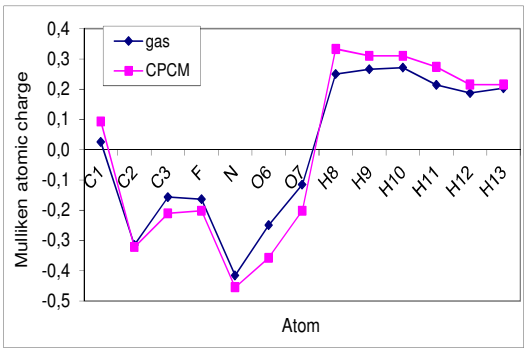
1Fc



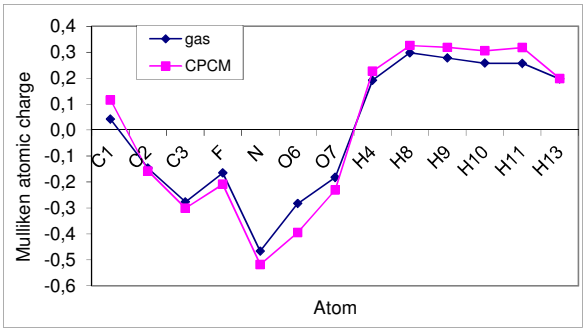
2Fa-1



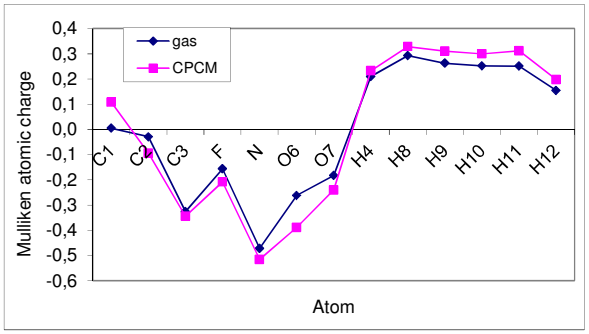
2Fa-2



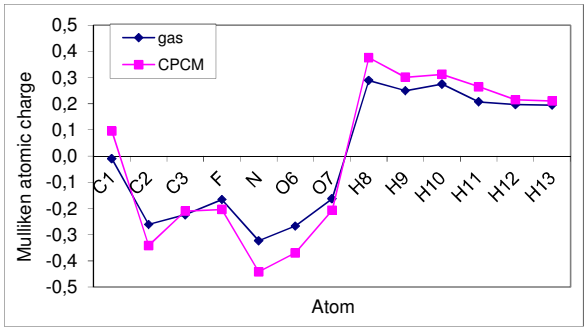
2Fa-3



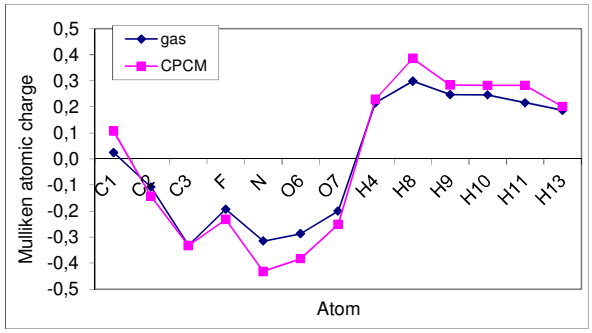
2Fb



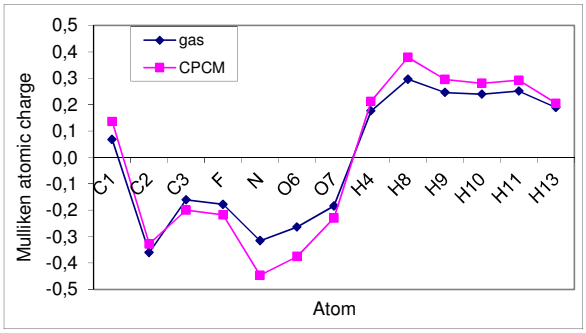
2Fbc



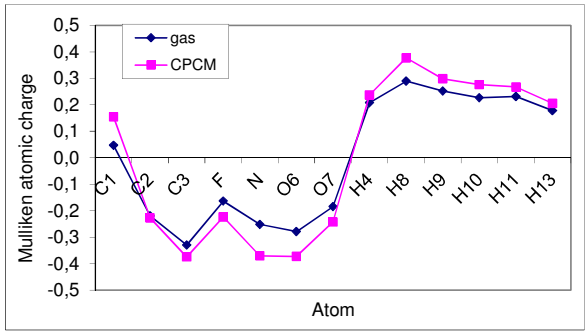
3Fa



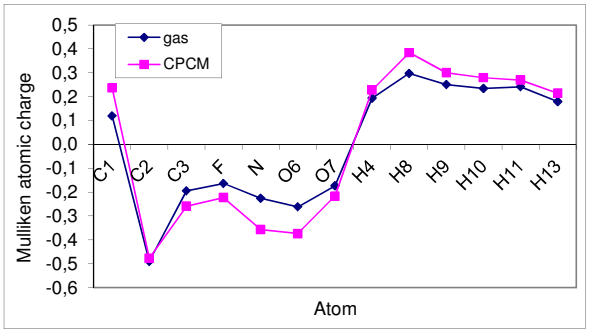
3Fb-1



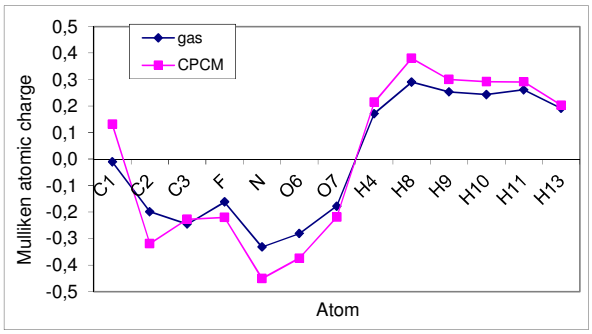
3Fb-2



3Fb-3



3Fb-4



3Fb-5

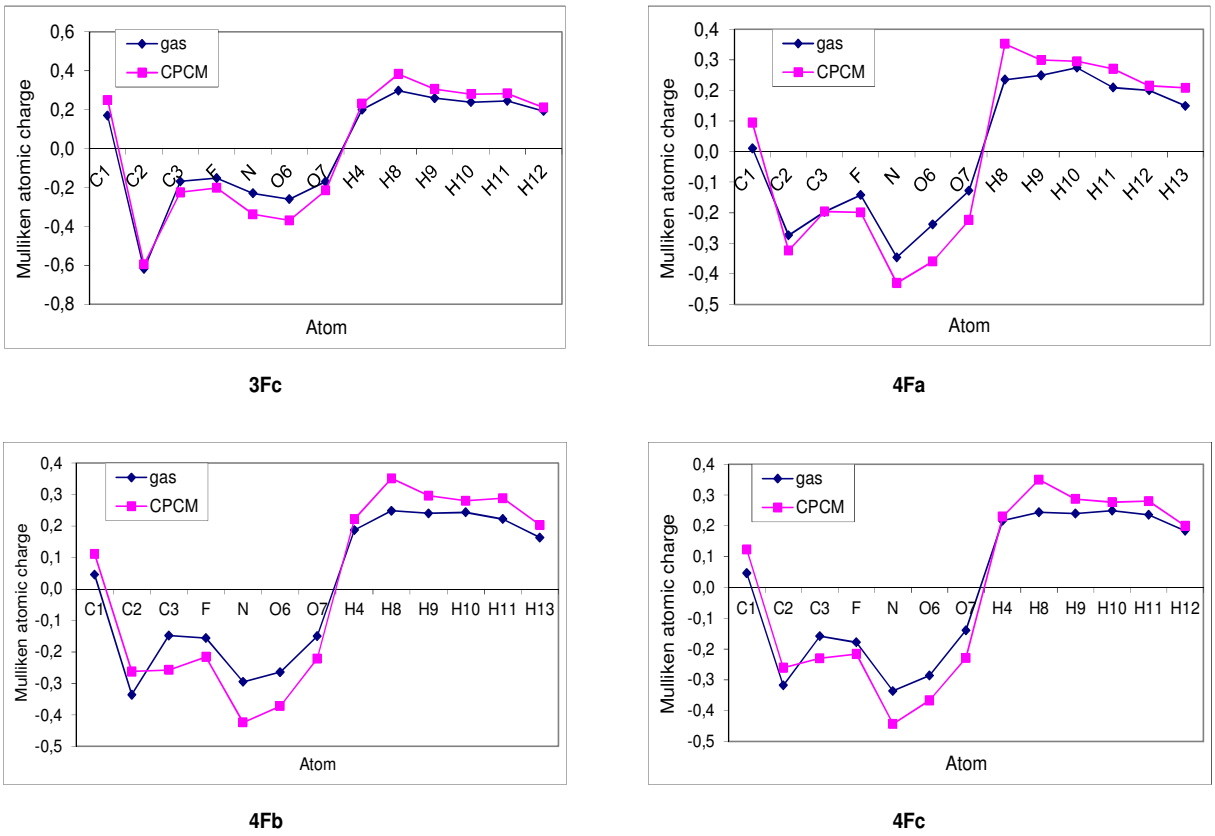


Figure S-2. Variation of Mulliken atomic charges for 3-fluoroalanine conformers **1Fa**-**4Fc** in the gas phase and in aqueous solution.

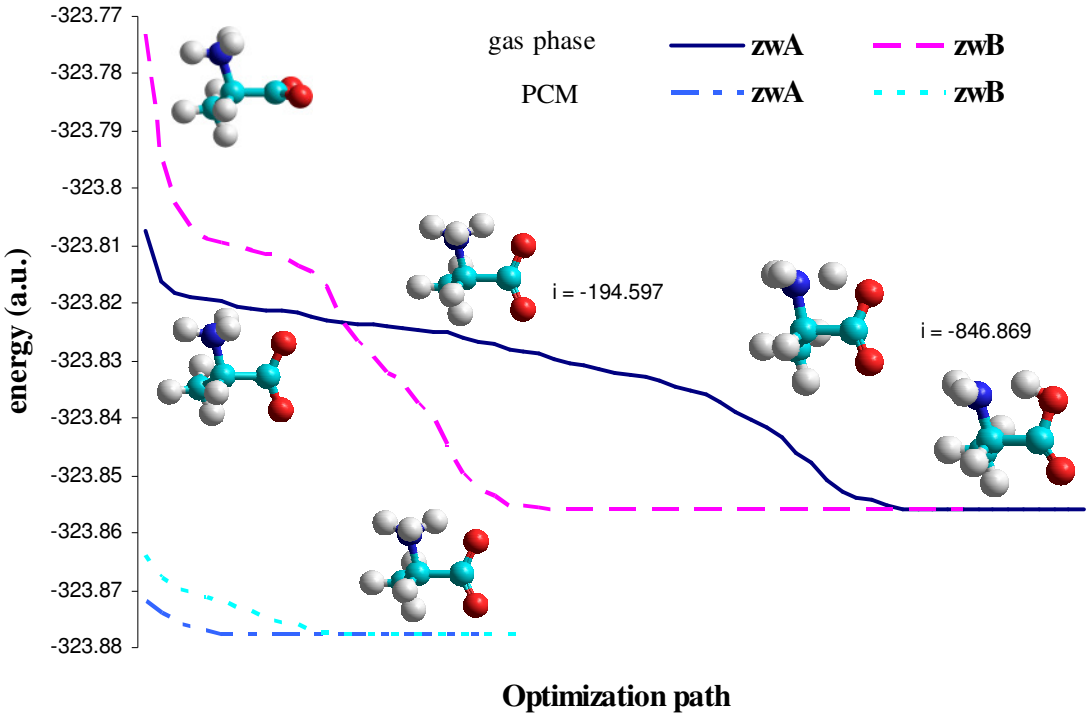


Figure S-3. B3LYP 6-311++G(d,p) optimized of two forms of alanine zwitterions in gas phase (upper part) and aqueous solution (CPCM) (lower part). Intramolecular proton transfer from NH_3^+ to COO^- group in the gas phase and imaginary frequencies for this.

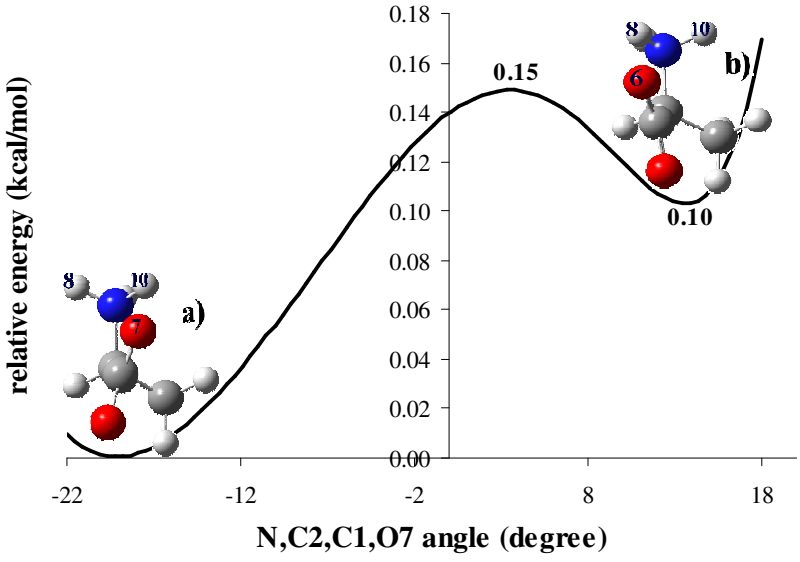
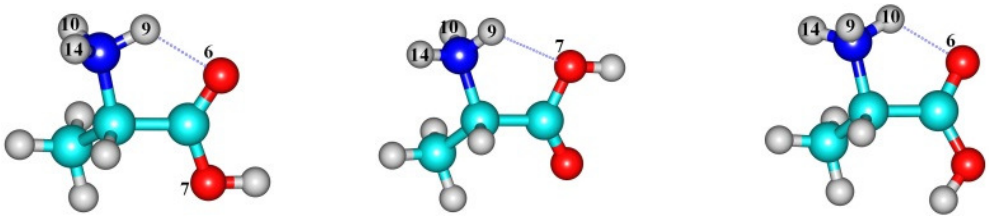
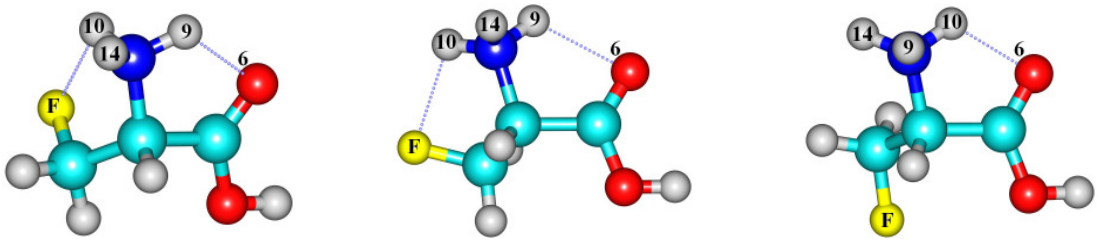


Figure S-4. Stable structures for the alanine zwitterion in aqueous solution, relative energy and rotation barrier (kcal/mol): a) **zwAr**$_{aq}$; b) **zwAl**$_{aq}$.

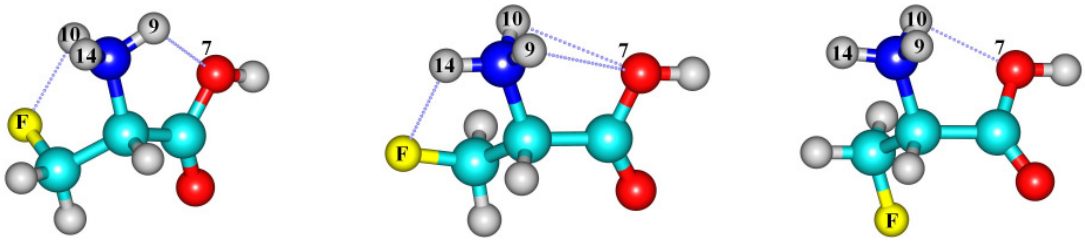


p1 (0.00) **p3** (2.58) **p4** (8.94)

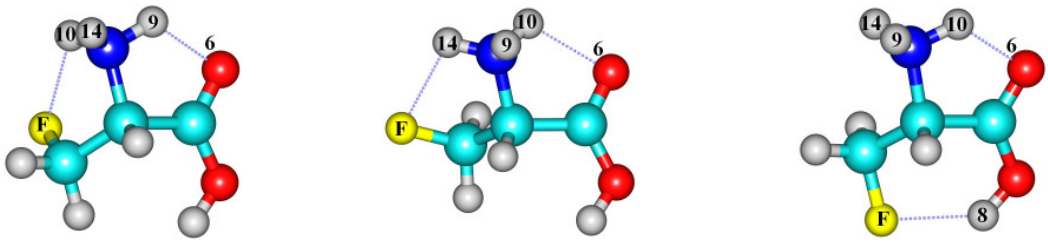
Figure S-5. Conformers of protonated alanine with relative energies [kcal/mol].



p1Fa (0.00) **p1Fb** (0.37) **p1Fc** (7.02)



p3Fa (2.59) **p3Fb** (2.94) **p3Fc** (9.97)



p4Fa (10.71) **p4Fb** (10.09) **p4Fc** (12.20)

Figure S-6. Nine conformers of protonated 3-fluoroalanine with relative energies [kcal/mol].

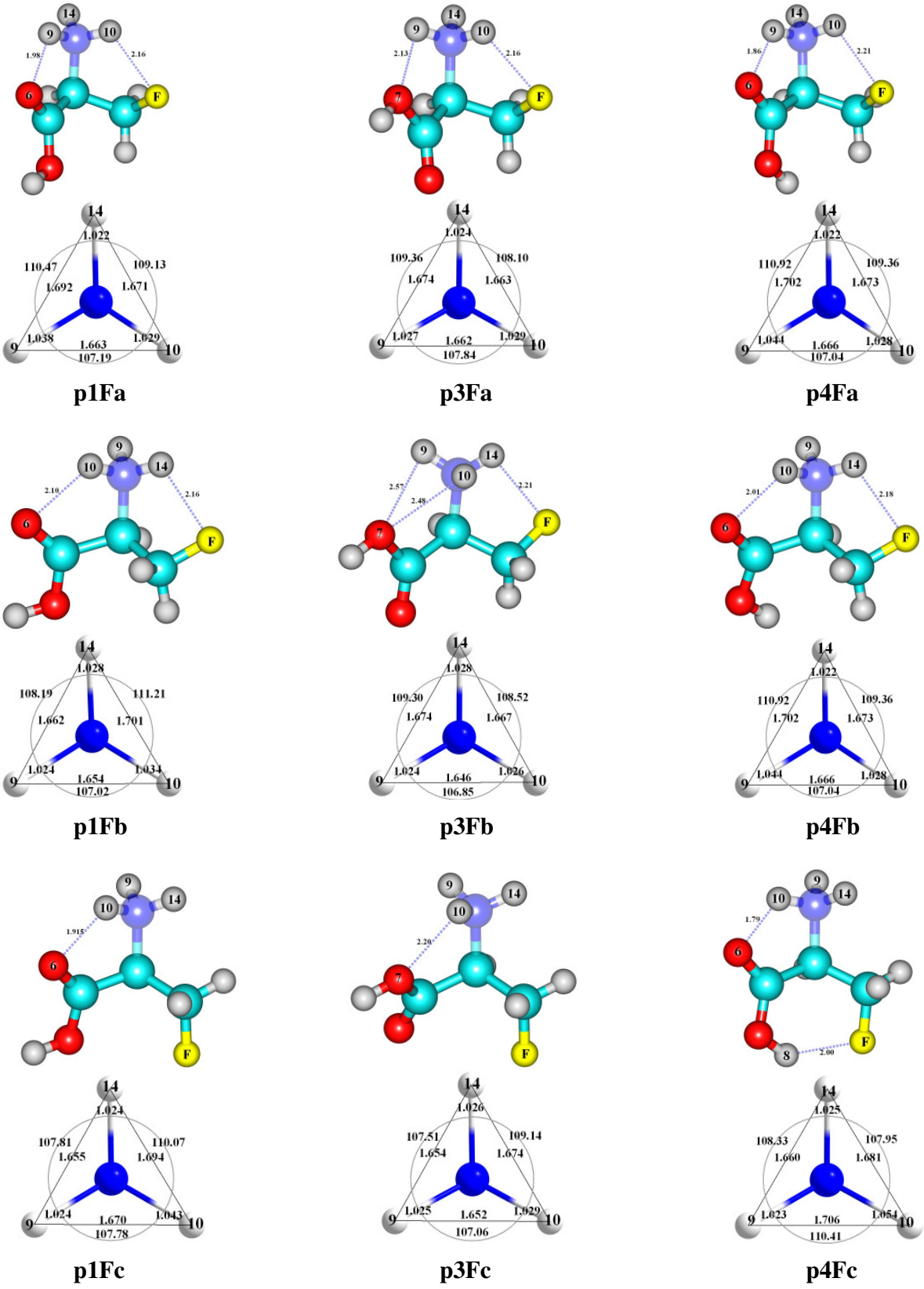


Figure S-7. Hydrogen bridges and structural parameters of NH_3^+ group for optimized protonate alanine conformers in gaseous phase [B3LYP/6-311++G(d,p) levels].

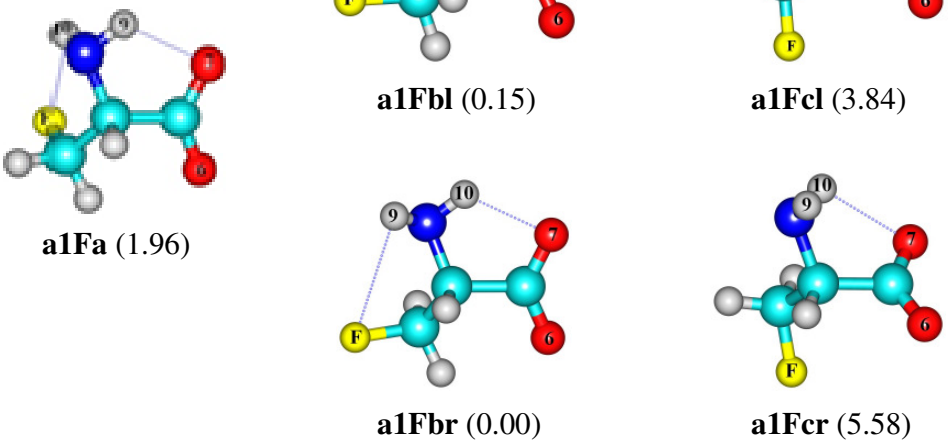


Figure S-8 3-Fluoroalanine anion conformers and relative energies [kcal/mol] in the gas phase.

Calculated Structures (energy [a.u.], xyz coordinates and NBO charges)

Alanines, Gas Phase

1 -323.8560796				
	x	y	z	NBO
1	-1.5255	1.4205	0.6032	0.3577
7	-1.5479	1.0175	-0.3294	-0.8305
6	-0.6655	0.1370	0.3984	-0.1195
6	0.7812	-0.1725	-0.0020	0.7932
8	1.1453	-1.1317	0.6311	-0.6068
6	-1.2032	1.2703	0.4906	-0.5725
1	-1.2407	-1.7471	-0.9646	0.3567
8	1.6392	0.7837	-0.4369	-0.6932
1	2.5254	0.5407	-0.1281	0.4779
1	-0.6427	0.4922	-1.4331	0.2100
1	-0.5773	2.1612	0.4196	0.2117
1	-1.2366	0.9526	1.5372	0.1989
1	-2.2180	1.5179	0.1765	0.2164

2 -323.856035				
	X	y	z	NBO
8	1.4613	-1.1887	0.0847	-0.5913
6	0.8645	-0.1446	0.0572	0.7894
6	-0.6447	-0.0285	0.3771	-0.1306
7	-1.1220	1.3201	0.0139	-0.8796
6	-1.4328	-1.1812	-0.2481	-0.5862
8	1.4557	1.0265	-0.2175	-0.6853
1	-1.5717	1.3220	-0.8966	0.3650
1	-1.7870	1.6842	0.6856	0.3734
1	-0.6988	-0.1110	1.4681	0.2139
1	-1.4256	-1.1054	-1.3402	0.1988
1	-2.4706	-1.1643	0.0935	0.1996
1	-0.9851	-2.1378	0.0220	0.2334
1	0.7353	1.6947	-0.1848	0.4996

3 -323.8543779				
	x	y	z	NBO
8	-1.7002	-0.6606	-0.7015	-0.6015
6	-0.8260	-0.0667	-0.1210	0.7911
6	0.6693	-0.1656	-0.4306	-0.1160
7	1.3822	1.1092	-0.4654	-0.8311
6	1.3353	-1.1125	0.5771	-0.5742
8	-1.0828	0.7695	0.9191	-0.7039
1	1.3089	1.5895	0.4260	0.3577
1	1.0057	1.7262	-1.1775	0.3560
1	0.7244	-0.6125	-1.4257	0.2104
1	0.8379	-2.0850	0.5928	0.2095

1	1.3004	-0.6908	1.5853	0.2016
1	2.3805	-1.2528	0.2968	0.2163
1	-2.040438	0.758792	1.066532	0.48427

4 -323.8469574				
	x	y	z	NBO
1	-1.5316	-1.4203	0.5451	0.3611
7	-1.5413	-0.9918	-0.3766	-0.8297
6	-0.6434	0.1510	-0.3963	-0.1279
6	0.8029	-0.1944	0.0137	0.7819
8	1.1088	-1.1695	0.6406	-0.5739
6	-1.1851	1.2557	0.5273	-0.5759
1	-1.2273	-1.7073	-1.0247	0.3585
8	1.7579	0.7033	-0.3574	-0.6791
1	1.3706	1.4187	-0.8769	0.4688
1	-0.6195	0.5348	-1.4245	0.1913
1	-0.5630	2.1541	0.5085	0.1979
1	-1.2248	0.8977	1.5598	0.2076
1	-2.1959	1.5211	0.2154	0.2194

Alanines, CPCM

$\mathbf{1}_{aq}$ -323.8775264				
	x	y	z	NBO
1	-1.5573	-1.4115	0.6049	0.3727
7	-1.5466	-1.0207	-0.3388	-0.8705
6	-0.6643	0.1376	-0.3980	-0.1251
6	0.7849	-0.1653	-0.0030	0.8138
8	1.1445	-1.1297	0.6412	-0.6698
6	-1.2035	1.2685	0.4937	-0.5753
1	-1.2063	-1.7597	-0.9555	0.3788
8	1.6314	0.7779	-0.4419	-0.7107
1	2.5512	0.5582	-0.1376	0.5349
1	-0.6349	0.4951	-1.4346	0.2244
1	-0.5704	2.1557	0.4372	0.2126
1	-1.2539	0.9438	1.5377	0.2013
1	-2.2114	1.5328	0.1684	0.2130

$\mathbf{2}_{aq}$ -323.8769267				
	x	y	z	NBO
8	1.4995	-1.1664	0.1023	-0.6706
6	0.8570	-0.1368	0.0590	0.8117
6	-0.6453	-0.0424	0.3783	-0.1374
7	-1.1147	1.3076	0.0321	-0.8982
6	-1.4321	-1.1882	-0.2647	-0.5852

8	1.4243	1.0311	-0.2415	-0.7088
1	-1.6029	1.3240	-0.8650	0.3901
1	-1.7506	1.6770	0.7380	0.4029
1	-0.6963	-0.1441	1.4717	0.2422
1	-1.4225	-1.0995	-1.3556	0.2035
1	-2.4696	-1.1608	0.0749	0.2103
1	-1.0015	-2.1539	0.0044	0.2198
1	0.6781	1.6913	-0.2154	0.5198

3_{aq} -323.8762695				
	x	y	z	NBO
8	-1.6760	-0.7517	-0.6352	-0.6738
6	-0.8241	-0.0585	-0.1122	0.8136
6	0.6720	-0.1667	-0.4221	-0.1207
7	1.3994	1.1000	-0.4645	-0.8695
6	1.3199	-1.1181	0.5954	-0.5763
8	-1.1053	0.8606	0.8196	-0.7105
1	1.3644	1.5686	0.4417	0.3735
1	0.9792	1.7351	-1.1447	0.3796
1	0.7253	-0.6240	-1.4161	0.2194
1	0.8056	-2.0817	0.6207	0.2109
1	1.2949	-0.6855	1.5999	0.2031
1	2.3624	-1.2850	0.3172	0.2136
1	-2.0838	0.8611	0.9904	0.5371

4_{aq} -323.8737476				
	x	y	z	NBO
1	-1.5497	-1.4675	0.4067	0.3747
7	-1.5061	-0.9890	-0.4948	-0.8673
6	-0.6362	0.1773	-0.4057	-0.1303
6	0.7958	-0.1577	0.0403	0.8087
8	1.0624	-1.0298	0.8391	-0.6621
6	-1.2216	1.2009	0.5816	-0.5767
1	-1.1351	-1.6619	-1.1676	0.3800
8	1.7906	0.5949	-0.4623	-0.7114
1	1.4782	1.2222	-1.1610	0.5367
1	-0.5803	0.6354	-1.4021	0.2172
1	-0.6007	2.0979	0.6479	0.2100
1	-1.3025	0.7620	1.5802	0.2050
1	-2.2195	1.4910	0.2478	0.2155

3-**Fluoroalanines Gasphase**

1Fa -423.1202222				
	x	y	z	NBO
1	1.0605	1.6583	0.7257	0.3660
7	0.8165	1.6731	-0.2601	-0.8327
6	0.2836	0.3842	-0.6561	-0.1592
6	-1.0585	0.0267	0.0035	0.7949
8	-1.6634	0.7290	0.7695	-0.5931
6	1.3213	-0.7085	-0.4285	0.0912
1	0.1192	2.4007	-0.3750	0.3645
8	-1.5160	-1.1783	-0.4146	-0.6966
1	-2.3642	-1.3387	0.0265	0.4862
1	0.0914	0.3938	-1.7372	0.2241
1	0.9657	-1.6805	-0.7696	0.1791
9	1.5906	-0.8143	0.9468	-0.4008
1	2.2550	-0.4366	-0.9225	0.1765

1Fb-1 -423.1183171				
	x	y	z	NBO
9	-2.4962	-0.3884	0.0951	-0.4022
8	2.0914	0.7475	-0.1435	-0.5907
6	-0.2319	0.2694	0.3242	-0.1539
7	-0.5085	1.6183	-0.1408	-0.8466
6	1.2268	-0.0668	0.0462	0.8066
6	-1.1968	-0.7182	-0.3259	0.0927
8	1.4651	-1.3981	0.0904	-0.6904
1	-0.3401	0.1432	1.4172	0.2031
1	-1.3694	1.9696	0.2600	0.3667
1	0.2547	2.2460	0.0855	0.3759
1	-1.1736	-0.6242	-1.4132	0.1731
1	-1.0018	-1.7445	-0.0167	0.1779
1	2.4164	-1.5267	-0.0454	0.4878

1Fb-2 -423.1183178				
	x	y	z	NBO
7	0.5614	1.5933	-0.4256	-0.8372
6	0.2373	0.1786	-0.4348	-0.1538
6	-1.2099	-0.0128	-0.0083	0.8029
8	-1.7090	-1.1905	-0.4473	-0.6850
8	-1.8356	0.7568	0.6734	-0.5911
6	1.1220	-0.6925	0.4748	0.0861
1	0.1991	2.0450	0.4081	0.3691

1	1.5644	1.7306	-0.4758	0.3660
1	0.3418	-0.2097	-1.4530	0.2184
1	0.8836	-1.7538	0.3791	0.1738
9	2.4563	-0.5213	0.0792	-0.3995
1	1.0503	-0.3753	1.5188	0.1641
1	-2.6148	-1.2680	-0.1100	0.4860

1Fb-3 -423.1165083				
	x	y	z	NBO
8	-1.5495	-1.3189	-0.4268	-0.6887
6	-1.2007	-0.0788	-0.0116	0.7894
6	0.2523	0.2605	-0.3714	-0.1581
7	0.5601	1.6742	-0.2752	-0.8277
6	1.1879	-0.5680	0.5202	0.1002
1	0.1149	2.0818	0.5418	0.3648
1	0.2228	2.1808	-1.0853	0.3599
1	0.4217	-0.0781	-1.3976	0.2272
8	-1.9531	0.6511	0.5816	-0.5960
1	0.8628	-1.6089	0.5744	0.1708
1	1.2427	-0.1368	1.5237	0.1646
9	2.4737	-0.5581	-0.0156	-0.3879
1	-2.4663	-1.4756	-0.1519	0.4816

1Fc -423.1182566				
	x	y	z	NBO
1	0.0000	2.2066	0.6554	0.3673
7	0.3408	1.9736	-0.2731	-0.8332
6	0.3129	0.5276	-0.4735	-0.1516
6	-0.9608	-0.1227	0.0730	0.7943
8	-1.4346	0.1329	1.1530	-0.6084
6	1.5344	-0.0551	0.2427	0.0991
1	-0.2488	2.4492	-0.9465	0.3624
8	-1.5072	-1.0051	-0.7863	-0.6733
1	-2.2846	-1.3940	-0.3551	0.4797
1	0.3929	0.3082	-1.5394	0.2158
9	1.5582	-1.4481	0.1114	-0.3945
1	1.5017	0.1777	1.3101	0.1675
1	2.4442	0.3492	-0.2019	0.1749

2Fa-1 -423.120757				
	x	y	z	NBO
6	-1.3993	-0.6142	0.4364	0.0811
6	-0.2056	0.3061	0.6582	-0.1714
6	1.0859	-0.3088	0.0605	0.7929
8	1.8646	0.5733	-0.5714	-0.6759

7	-0.3962	1.6728	0.1581	-0.8796
1	-1.0342	1.6842	-0.6325	0.3805
1	-0.7497	2.3031	0.8673	0.3745
1	-0.0201	0.3451	1.7372	0.2278
8	1.3702	-1.4685	0.1992	-0.5876
1	-1.1335	-1.6524	0.6343	0.1973
9	-1.7979	-0.5163	-0.9085	-0.4012
1	-2.2537	-0.3081	1.0445	0.1612
1	1.3808	1.4278	-0.5332	0.5006

2Fa-2 -423.1124388				
	x	y	z	NBO
1	-0.0547	-1.4415	-0.7711	0.4875
6	-1.3534	-0.0129	0.8306	0.0782
6	-0.1079	0.7267	0.3760	-0.1685
6	1.1111	-0.1857	0.1065	0.7768
8	0.8935	-1.3094	-0.6161	-0.6856
8	2.2203	0.1113	0.4588	-0.5699
7	-0.4350	1.5919	-0.7587	-0.8299
9	-1.7994	-0.8787	-0.2077	-0.4141
1	-1.1686	-0.6411	1.7036	0.1777
1	0.1960	1.3665	1.2090	0.2305
1	0.3662	2.1490	-1.0353	0.3690
1	-0.7434	1.0586	-1.5651	0.3596
1	-2.1647	0.6897	1.0189	0.1887

2Fa-3 -423.1117944				
	x	y	z	NBO
1	-1.0481	1.3928	0.9397	0.4745
6	1.3267	-0.7535	-0.3705	0.0926
6	0.2398	0.2571	-0.7153	-0.1727
6	-1.0995	-0.1988	-0.0762	0.7855
8	-1.6432	0.6351	0.8296	-0.6677
8	-1.6271	-1.2323	-0.3833	-0.5790
7	0.7067	1.5937	-0.4189	-0.8789
9	1.6543	-0.6169	0.9919	-0.4039
1	0.9795	-1.7736	-0.5309	0.1891
1	0.0720	0.1696	-1.7943	0.2319
1	0.1561	2.3698	-0.7512	0.3759
1	1.1332	1.7346	0.4851	0.3799
1	2.2332	-0.5481	-0.9412	0.1728

2Fb -423.1206509				
	x	y	z	NBO
8	-1.4704	-1.5113	-0.0433	-0.5845
6	-1.2130	-0.3366	-0.0640	0.7883
6	0.2063	0.2074	-0.3400	-0.1686
7	0.2883	1.6208	0.0481	-0.8723
6	1.2512	-0.7033	0.2931	0.0838
8	-2.1283	0.6207	0.1199	-0.6766
1	0.5879	1.7270	1.0135	0.3665
1	0.9510	2.1260	-0.5281	0.3816
1	0.3313	0.1561	-1.4271	0.2269
1	1.2037	-0.6691	1.3859	0.1609
9	2.5261	-0.2561	-0.0845	-0.4015
1	1.1331	-1.7315	-0.0457	0.1945
1	-1.6371	1.4709	0.0781	0.5009

2Fc -423.113427				
	x	y	z	NBO
1	1.3505	-0.1742	1.4024	0.1774
6	1.4662	0.2974	0.4238	0.0858
6	0.1152	0.5355	-0.2610	-0.1717
6	-0.8782	-0.6202	-0.0122	0.7871
7	-0.5373	1.8101	0.0681	-0.8701
8	-2.1669	-0.2590	-0.1394	-0.6809
1	1.9988	1.2474	0.5247	0.1570
9	2.2604	-0.5405	-0.3581	-0.3861
1	0.3035	0.5341	-1.3403	0.2312
8	-0.5396	-1.7414	0.2465	-0.5660
1	-2.1726	0.7127	-0.2510	0.4973
1	-0.5181	2.0065	1.0649	0.3651
1	-0.1122	2.5931	-0.4149	0.3738

3Fa -423.1187987				
	x	y	z	NBO
8	-1.4763	-1.3121	-0.4016	-0.6040
6	-1.0410	-0.2243	-0.1199	0.7943
6	0.2737	0.3429	-0.6859	-0.1594
7	0.6632	1.6835	-0.2885	-0.8353
6	1.4035	-0.6376	-0.3949	0.0933
8	-1.6790	0.6326	0.7064	-0.6873
1	0.8637	1.7149	0.7057	0.3664
1	-0.0758	2.3527	-0.4694	0.3625
1	0.1346	0.3234	-1.7743	0.2269
1	1.1360	-1.6514	-0.6920	0.1832
9	1.6550	-0.6508	0.9887	-0.4023
1	2.3182	-0.3070	-0.8880	0.1751
1	-2.4892	0.1912	1.0048	0.4866

3Fb-1 -423.117889				
	x	y	z	NBO
9	-2.5374	-0.2163	0.1952	-0.4044
8	1.4180	-1.4529	-0.2021	-0.5937
6	-0.2216	0.2688	0.2940	-0.1513
7	-0.3902	1.5385	-0.4110	-0.8442
6	1.1680	-0.3017	0.0490	0.8112
6	-1.2774	-0.7250	-0.1674	0.0933
8	2.1229	0.6448	0.1915	-0.6903
1	-0.3127	0.3618	1.3912	0.1991
1	-1.3149	1.9116	-0.2236	0.3667
1	0.2967	2.2191	-0.1068	0.3683
1	-1.2668	-0.8327	-1.2530	0.1763
1	-1.1560	-1.6942	0.3144	0.1809
1	2.9802	0.2225	0.0292	0.4881

3Fb-2 -423.1166286				
	x	y	z	NBO
7	0.4820	1.5515	-0.5094	-0.8353
6	0.2430	0.1156	-0.4663	-0.1518
6	-1.2043	-0.2110	-0.1241	0.8040
8	-1.8128	-1.1581	-0.5501	-0.5872
8	-1.7236	0.6554	0.7767	-0.6928
6	1.1475	-0.6652	0.5032	0.0860
1	0.2484	1.9940	0.3735	0.3620
1	1.4597	1.7330	-0.7102	0.3660
1	0.4106	-0.2936	-1.4656	0.2226
1	0.9594	-1.7401	0.4530	0.1746
9	2.4800	-0.4491	0.1265	-0.3994
1	1.0373	-0.3060	1.5301	0.1628
1	-2.6353	0.3793	0.9565	0.4886

3Fb-3 -423.1149888				
	x	y	z	NBO
1	-2.9575	0.0048	-0.5130	0.4841
6	1.3055	-0.7034	0.0390	0.0974
6	0.2327	0.3482	-0.2236	-0.1525
6	-1.1508	-0.2738	-0.0367	0.7862
8	-1.4066	-1.2139	0.6756	-0.6029

8	-2.0998	0.4052	-0.7245	-0.6882
7	0.4204	1.5133	0.6417	-0.8149
9	2.5415	-0.2280	-0.3985	-0.3899
1	1.3888	-0.9315	1.1040	0.1696
1	0.3254	0.6843	-1.2592	0.2214
1	-0.1835	2.2819	0.3735	0.3643
1	0.2463	1.2877	1.6161	0.3550
1	1.0905	-1.6237	-0.5083	0.1705

3Fb-4 -423.1145609				
	x	y	z	NBO
1	-2.4799	-0.1810	1.2443	0.4869
6	1.2014	-0.6301	0.4291	0.0982
6	0.2547	0.2195	-0.4215	-0.1524
6	-1.1919	-0.2001	-0.1440	0.7859
8	-1.9424	-0.7109	-0.9344	-0.5864
8	-1.5557	0.0899	1.1333	-0.7041
7	0.5107	1.6408	-0.2202	-0.8222
9	2.4976	-0.5379	-0.0724	-0.3868
1	1.2164	-0.2847	1.4658	0.1680
1	0.4406	-0.0222	-1.4693	0.2251
1	0.0453	2.2093	-0.9182	0.3616
1	0.2129	1.9493	0.6993	0.3598
1	0.9117	-1.6844	0.3982	0.1663

3Fb-5 -423.1144466				
	x	y	z	NBO
8	-2.0881	0.5983	0.1968	-0.6895
6	-1.1513	-0.3363	-0.0842	0.7875
6	0.2427	0.2702	-0.3313	-0.1588
7	0.4184	1.6810	-0.0426	-0.8238
6	1.2784	-0.5795	0.4103	0.0983
8	-1.4060	-1.5129	-0.1503	-0.6022
1	0.4276	0.1152	-1.4011	0.2309
1	0.1647	1.9002	0.9149	0.3541
1	-0.1523	2.2593	-0.6476	0.3630
1	1.0615	-1.6403	0.2877	0.1849
1	1.3028	-0.3235	1.4744	0.1573
9	2.5479	-0.3354	-0.1088	-0.3884
1	-2.9304	0.1309	0.3091	0.4867

3Fc -423.1170466				
	x	y	z	NBO
8	-1.7208	-0.7226	-0.9382	-0.5859
6	-0.9592	-0.2716	-0.1228	0.7919
6	0.2670	0.5879	-0.4348	-0.1503
7	0.1102	1.9820	-0.0152	-0.8290
6	1.5370	0.0413	0.2117	0.0945
8	-1.1360	-0.4223	1.2152	-0.7038
1	-0.1907	2.0472	0.9518	0.3614
1	-0.5667	2.4680	-0.5920	0.3664
1	0.3823	0.5628	-1.5194	0.2192
9	1.7168	-1.2979	-0.1539	-0.3940
1	1.4771	0.0815	1.3016	0.1680
1	2.3989	0.6115	-0.1373	0.1745
1	-1.9383	-0.9495	1.3469	0.4873

4Fa -423.1087448				
	x	y	z	NBO
8	-1.6622	-1.1621	-0.3216	-0.6743
6	-1.0768	0.0128	0.0359	0.7842
6	0.2609	0.3553	-0.6689	-0.1687
6	1.3324	-0.6985	-0.4026	0.0901
7	0.7793	1.6673	-0.3368	-0.8316
1	1.0378	-1.7005	-0.7283	0.1531
9	1.5915	-0.7704	0.9702	-0.3946
1	2.2589	-0.4079	-0.8998	0.1845
1	0.0645	0.3232	-1.7504	0.2134
8	-1.6109	0.7350	0.8257	-0.5582
1	-1.1277	-1.6410	-0.9664	0.4668
1	0.9967	1.7083	0.6548	0.3689
1	0.0757	2.3791	-0.5027	0.3664

4Fb -423.1070317				
	x	y	z	NBO
8	-1.8879	0.6295	0.7021	-0.5648
6	-1.2161	-0.0904	0.0190	0.7777
6	0.2372	0.2421	-0.3864	-0.1640
7	0.5296	1.6623	-0.3911	-0.8268
6	1.1828	-0.4990	0.5703	0.0974
8	-1.7055	-1.2834	-0.4097	-0.6732
1	0.1016	2.1076	0.4162	0.3685
1	0.1517	2.1131	-1.2168	0.3601
1	0.4273	-0.1546	-1.3903	0.2062
1	0.8503	-1.5234	0.7616	0.1599
1	1.2624	0.0412	1.5167	0.1744
9	2.4554	-0.5753	0.0095	-0.3876
1	-1.0764	-1.7275	-0.9921	0.4721

4Fc -423.1151317				
	x	y	z	NBO
1	1.6708	1.6483	-0.2482	0.3896
7	0.7099	1.8662	-0.0003	-0.8549
6	0.0092	0.6439	0.3622	-0.1686
6	0.8755	-0.5875	0.0320	0.7953
8	2.0397	-0.5000	-0.2516	-0.5777
6	-1.3339	0.6401	-0.3772	0.0862
1	0.7127	2.5422	0.7523	0.3628
8	0.2654	-1.7835	0.1046	-0.6755
1	-0.6859	-1.6773	0.2686	0.4930
1	-0.2056	0.5804	1.4391	0.2059
9	-2.1232	-0.4622	0.0517	-0.4138
1	-1.2017	0.5481	-1.4560	0.1785
1	-1.8955	1.5439	-0.1449	0.1794

3-Fluoroalanines, CPCM

1Fa$_{aq}$ -423.1452346				
	x	y	z	NBO
1	0.9511	1.7276	0.7314	0.3793
7	0.8400	1.6680	-0.2817	-0.8699
6	0.2880	0.3791	-0.6597	-0.1712
6	-1.0513	0.0345	0.0131	0.8147
8	-1.5773	0.6978	0.8796	-0.6553
6	1.3016	-0.7342	-0.4344	0.0873
1	0.2024	2.4177	-0.5505	0.3845
8	-1.5814	-1.0890	-0.4856	-0.7093
1	-2.4415	-1.2803	-0.0254	0.5392
1	0.0913	0.3812	-1.7429	0.2537
1	0.9296	-1.7024	-0.7699	0.1876
9	1.5757	-0.8534	0.9540	-0.4257
1	2.2449	-0.4864	-0.9230	0.1850

1Fb-1$_{aq}$ -423.1429371				
	x	y	z	NBO
9	2.4948	-0.4237	-0.0494	-0.4235
8	-2.0625	0.7580	0.2681	-0.6482
6	0.2291	0.2619	-0.3413	-0.1631
7	0.5323	1.6307	0.0615	-0.8786
6	-1.2283	-0.0663	-0.0340	0.8239
6	1.1686	-0.7151	0.3576	0.0875
8	-1.4918	-1.3692	-0.1813	-0.7051
1	0.3317	0.0909	-1.4300	0.2273
1	1.4301	1.9088	-0.3353	0.3832
1	-0.1691	2.2694	-0.3139	0.3862
1	1.1378	-0.5896	1.4425	0.1788
1	0.9685	-1.7482	0.0764	0.1892
1	-2.4597	-1.5273	-0.0142	0.5423

1Fb-2$_{aq}$ -423.1431169				
	x	y	z	NBO
7	0.5479	1.6364	-0.3277	-0.8691
6	0.2328	0.2183	-0.4045	-0.1648
6	-1.2252	-0.0260	-0.0246	0.8201
8	-1.6259	-1.2522	-0.3812	-0.7045
8	-1.9315	0.7726	0.5493	-0.6459
6	1.1185	-0.6918	0.4601	0.0789

1	0.4642	1.9783	0.6314	0.3786
1	1.5114	1.7898	-0.6258	0.3841
1	0.3506	-0.1092	-1.4466	0.2407
1	0.8732	-1.7474	0.3320	0.1865
9	2.4624	-0.5262	0.0494	-0.4218
1	1.0736	-0.4099	1.5160	0.1764
1	-2.5668	-1.3876	-0.0896	0.5407

1Fb-3$_{aq}$ -423.1434418				
	x	y	z	NBO
8	-1.5075	-1.3513	-0.3472	-0.7072
6	-1.2129	-0.0882	-0.0180	0.8108
6	0.2450	0.2665	-0.3626	-0.1649
7	0.5687	1.6748	-0.2306	-0.8674
6	1.1826	-0.5928	0.4862	0.0895
1	0.3030	2.0204	0.6934	0.3781
1	0.0480	2.2251	-0.9143	0.3845
1	0.3882	-0.0348	-1.4098	0.2442
8	-2.0060	0.6801	0.4797	-0.6520
1	0.8934	-1.6438	0.4676	0.1869
1	1.2292	-0.2291	1.5167	0.1769
9	2.4925	-0.5180	-0.0355	-0.4193
1	-2.4550	-1.5427	-0.1135	0.5400

1Fc$_{aq}$ -423.1433629				
	x	y	z	NBO
1	0.1114	2.2050	0.7187	0.3810
7	0.3535	1.9780	-0.2477	-0.8636
6	0.3132	0.5341	-0.4654	-0.1576
6	-0.9580	-0.1243	0.0844	0.8107
8	-1.3663	0.0454	1.2153	-0.6654
6	1.5415	-0.0661	0.2156	0.0909
1	-0.3229	2.4481	-0.8505	0.3894
8	-1.5727	-0.8960	-0.8158	-0.6968
1	-2.3837	-1.2998	-0.4040	0.5375
1	0.3705	0.3369	-1.5403	0.2311
9	1.5433	-1.4725	0.0627	-0.4195
1	1.5413	0.1403	1.2891	0.1774
1	2.4510	0.3187	-0.2471	0.1849

2Fa-1$_{aq}$ -423.1444436				
	x	y	z	NBO
6	-1.4517	-0.4858	0.4681	0.0791
6	-0.2087	0.3707	0.6395	-0.1826
6	1.0432	-0.3379	0.0848	0.8127
8	1.8799	0.4675	-0.5631	-0.6991
7	-0.2915	1.7208	0.0823	-0.8961
1	-0.9185	1.7661	-0.7231	0.3957
1	-0.6117	2.3971	0.7749	0.4061
1	-0.0295	0.4464	1.7235	0.2668
8	1.2780	-1.5162	0.2472	-0.6603
1	-1.2997	-1.4960	0.8499	0.1934
9	-1.7550	-0.5997	-0.9128	-0.4231
1	-2.3146	-0.0173	0.9449	0.1849
1	1.4492	1.3634	-0.5583	0.5225

2Fa-2$_{aq}$ -423.1389029				
	x	y	z	NBO
1	-1.2636	1.3596	1.0318	0.5261
6	1.3772	-0.6614	-0.3949	0.0882
6	0.2585	0.3264	-0.6928	-0.1795
6	-1.0623	-0.2160	-0.0987	0.8115
8	-1.7134	0.5152	0.8101	-0.6941
8	-1.5205	-1.2828	-0.4475	-0.6572
7	0.6619	1.6757	-0.3515	-0.8846

9	1.6327	-0.6755	1.0015	-0.4249
1	1.1078	-1.6777	-0.6823	0.1898
1	0.1019	0.2753	-1.7808	0.2592
1	-0.0056	2.3811	-0.6617	0.3935
1	0.8632	1.8041	0.6408	0.3858
1	2.2996	-0.3451	-0.8835	0.1862

2Fa-3$_{aq}$ -423.1389025				
	x	y	z	NBO
1	-1.2863	1.3656	1.0116	0.5260
6	1.3802	-0.6554	-0.3960	0.0883
6	0.2572	0.3284	-0.6908	-0.1797
6	-1.0613	-0.2213	-0.0986	0.8116
8	-1.7264	0.5143	0.7965	-0.6941
8	-1.5066	-1.2966	-0.4378	-0.6573
7	0.6560	1.6777	-0.3445	-0.8848
9	1.6383	-0.6692	1.0000	-0.4250
1	1.1142	-1.6725	-0.6834	0.1898
1	0.1008	0.2806	-1.7791	0.2595
1	-0.0096	2.3831	-0.6589	0.3935
1	0.8505	1.8050	0.6492	0.3860
1	2.3005	-0.3350	-0.8858	0.1861

2Fb$_{aq}$ -423.1435629				
	x	y	z	NBO
8	-1.4845	-1.5174	-0.0716	-0.6593
6	-1.2030	-0.3376	-0.0659	0.8159
6	0.2110	0.2096	-0.3331	-0.1776
7	0.2631	1.6253	0.0278	-0.8937
6	1.2543	-0.6787	0.3331	0.0809
8	-2.1161	0.6062	0.1410	-0.6987
1	0.6021	1.7686	0.9820	0.3945
1	0.8648	2.1532	-0.6031	0.4062
1	0.3420	0.1281	-1.4228	0.2570
1	1.2380	-0.5736	1.4219	0.1785
9	2.5376	-0.2745	-0.1001	-0.4198
1	1.1291	-1.7240	0.0510	0.1932
1	-1.6253	1.4703	0.1173	0.5229

$2Fc_{aq}$ -423.1409855				
	x	y	z	NBO
1	1.3549	0.1240	1.4398	0.1813
6	1.4525	0.4129	0.3901	0.0801
6	0.0954	0.5497	-0.3031	-0.1768
6	-0.8428	-0.6345	-0.0252	0.8128
7	-0.6007	1.7976	0.0119	-0.8894
8	-2.1381	-0.3136	-0.0048	-0.7006
1	1.9953	1.3570	0.3090	0.1822
9	2.2435	-0.5703	-0.2435	-0.4163
1	0.2732	0.5274	-1.3890	0.2569
8	-0.4732	-1.7770	0.1337	-0.6516
1	-2.1923	0.6702	-0.0980	0.5240
1	-0.5055	2.0548	0.9978	0.3932
1	-0.2525	2.5726	-0.5529	0.4042

$3Fa_{aq}$ -423.1439201				
	x	y	z	NBO
8	-1.4796	-1.2977	-0.4515	-0.6687
6	-1.0399	-0.2151	-0.1194	0.8150
6	0.2755	0.3575	-0.6796	-0.1704
7	0.6487	1.7035	-0.2756	-0.8712
6	1.4074	-0.6210	-0.4055	0.0884
8	-1.6491	0.5947	0.7466	-0.6981
1	0.7313	1.7690	0.7393	0.3795
1	-0.0669	2.3730	-0.5580	0.3850
1	0.1382	0.3454	-1.7720	0.2543
1	1.1617	-1.6307	-0.7351	0.1876
9	1.6477	-0.6869	0.9930	-0.4263
1	2.3301	-0.2694	-0.8688	0.1847
1	-2.4930	0.1657	1.0515	0.5401

3Fb-1$_{aq}$	-423.1417317			
	x	y	z	NBO
9	-2.5440	-0.2424	0.1607	-0.4241
8	1.4158	-1.4767	-0.1056	-0.6566
6	-0.2204	0.2650	0.3000	-0.1613
7	-0.3958	1.5765	-0.3287	-0.8786
6	1.1750	-0.2976	0.0537	0.8276
6	-1.2622	-0.7138	-0.2192	0.0878
8	2.1142	0.6496	0.0831	-0.7009
1	-0.3170	0.2982	1.4031	0.2265
1	-1.3125	1.9464	-0.0727	0.3821
1	0.2912	2.2365	0.0356	0.3859
1	-1.2549	-0.7663	-1.3101	0.1792
1	-1.1407	-1.7040	0.2177	0.1896
1	3.0067	0.2300	-0.0466	0.5425

3Fb-2$_{aq}$	-423.1417008			
	x	y	z	NBO
7	0.4500	1.6149	-0.3697	-0.8710
6	0.2394	0.1744	-0.4281	-0.1612
6	-1.1979	-0.2357	-0.1146	0.8204
8	-1.6501	-1.3218	-0.4159	-0.6603
8	-1.8842	0.6910	0.5532	-0.6942
6	1.1607	-0.6549	0.4809	0.0809
1	0.3479	1.9649	0.5846	0.3784
1	1.4003	1.8312	-0.6720	0.3839
1	0.4211	-0.1579	-1.4583	0.2405
1	0.9717	-1.7257	0.3841	0.1853
9	2.4981	-0.4306	0.0832	-0.4207
1	1.0832	-0.3412	1.5258	0.1764
1	-2.7958	0.3427	0.7469	0.5415

3Fb-3$_{aq}$	-423.1420554			
	x	y	z	NBO
1	-2.9920	0.0244	-0.4997	0.5385
6	1.2910	-0.7128	0.0271	0.0880
6	0.2302	0.3481	-0.2300	-0.1599
6	-1.1586	-0.2663	-0.0415	0.8102

8	-1.3979	-1.2233	0.6682	-0.6608
8	-2.0997	0.4116	-0.7077	-0.7017
7	0.4319	1.5103	0.6413	-0.8576
9	2.5502	-0.2209	-0.3830	-0.4208
1	1.3714	-0.9592	1.0880	0.1798
1	0.3151	0.6839	-1.2702	0.2361
1	-0.1720	2.2838	0.3607	0.3865
1	0.2098	1.2806	1.6128	0.3786
1	1.0983	-1.6177	-0.5524	0.1831

3Fb-4$_{aq}$	-423.1418378			
	x	y	z	NBO
1	-2.4831	-0.3230	1.2736	0.5414
6	1.1935	-0.6735	0.3649	0.0870
6	0.2505	0.2466	-0.4050	-0.1570
6	-1.1997	-0.1802	-0.1417	0.8093
8	-1.9689	-0.5600	-1.0000	-0.6532
8	-1.5303	-0.0660	1.1501	-0.7096
7	0.5183	1.6486	-0.0909	-0.8617
9	2.5083	-0.5145	-0.1239	-0.4183
1	1.2147	-0.4300	1.4298	0.1809
1	0.4196	0.0912	-1.4756	0.2332
1	-0.0330	2.2644	-0.6903	0.3861
1	0.2776	1.8630	0.8782	0.3789
1	0.9281	-1.7246	0.2255	0.1830

3Fb-5$_{aq}$	-423.1420085			
	x	y	z	NBO
8	-2.0497	0.6057	0.2863	-0.6971
6	-1.1632	-0.3176	-0.0860	0.8122
6	0.2433	0.2538	-0.3505	-0.1649
7	0.4435	1.6734	-0.1148	-0.8685
6	1.2521	-0.5796	0.4384	0.0907
8	-1.4372	-1.4933	-0.2248	-0.6666
1	0.4225	0.0495	-1.4168	0.2464
1	0.1703	1.9274	0.8358	0.3777
1	-0.1297	2.2284	-0.7501	0.3850
1	1.0496	-1.6456	0.3390	0.1882
1	1.2685	-0.2909	1.4934	0.1758
9	2.5500	-0.3544	-0.0688	-0.4198
1	-2.9338	0.1690	0.4179	0.5409

3Fc$_{aq}$ -423.1428936				
	x	y	z	NBO
8	-1.6967	-0.7450	-0.9447	-0.6571
6	-0.9582	-0.2642	-0.1096	0.8106
6	0.2703	0.5899	-0.4388	-0.1568
7	0.1275	1.9903	-0.0371	-0.8609
6	1.5343	0.0420	0.2139	0.0876
8	-1.1527	-0.3903	1.2082	-0.7107
1	-0.1464	2.0715	0.9434	0.3814
1	-0.5878	2.4541	-0.5983	0.3909
1	0.3859	0.5522	-1.5266	0.2305
9	1.6956	-1.3216	-0.1314	-0.4202
1	1.4844	0.0938	1.3037	0.1795
1	2.4087	0.5807	-0.1539	0.1844
1	-1.9812	-0.9143	1.3726	0.5408

4Fa$_{aq}$ -423.1403441				
	x	y	z	NBO
8	-1.8763	-0.8794	-0.4200	-0.7086
6	-1.0509	0.0508	0.0887	0.8085
6	0.2497	0.3346	-0.6891	-0.1763
6	1.2524	-0.7908	-0.4485	0.0865
7	0.8516	1.6235	-0.3982	-0.8675
1	0.8479	-1.7718	-0.7078	0.1835
9	1.6033	-0.8375	0.9219	-0.4232
1	2.1684	-0.5933	-1.0074	0.1888
1	0.0090	0.2912	-1.7629	0.2479
8	-1.3406	0.5988	1.1271	-0.6449
1	-1.6198	-1.1776	-1.3286	0.5379
1	1.0127	1.7235	0.6050	0.3816
1	0.2203	2.3776	-0.6719	0.3857

4Fb$_{aq}$ -423.1391095				
	x	y	z	NBO
8	-1.8075	0.6352	0.8187	-0.6461
6	-1.2140	-0.0745	0.0382	0.8038
6	0.2377	0.2010	-0.4072	-0.1680
7	0.5813	1.6109	-0.4663	-0.8647
6	1.1625	-0.5405	0.5610	0.0883
8	-1.8139	-1.1691	-0.4511	-0.7037

1	0.3325	2.0767	0.4085	0.3803
1	0.0617	2.0737	-1.2133	0.3854
1	0.3775	-0.2382	-1.4047	0.2355
1	0.8509	-1.5775	0.7086	0.1829
1	1.2185	-0.0242	1.5231	0.1812
9	2.4682	-0.5775	0.0317	-0.4156
1	-1.2698	-1.6357	-1.1358	0.5406

$4Fc_{aq}$ -423.1401263				
	x	y	z	NBO
1	-0.0667	2.2422	0.6212	0.3824
7	0.2218	1.9917	-0.3263	-0.8642
6	0.2734	0.5439	-0.4794	-0.1663
6	-0.9698	-0.1797	0.0711	0.8065
8	-1.5017	0.1391	1.1123	-0.6548
6	1.5172	0.0488	0.2609	0.0908
1	-0.4619	2.3936	-0.9688	0.3899
8	-1.4594	-1.2056	-0.6359	-0.7001
1	-0.9593	-1.3615	-1.4766	0.5405
1	0.3838	0.3078	-1.5454	0.2290
9	1.6029	-1.3602	0.1782	-0.4189
1	1.4745	0.3081	1.3221	0.1786
1	2.4151	0.4638	-0.1982	0.1865

Alanine Zwitterion, CPCM

zwAr$_{aq}$ -323.8780279				
	x	y	z	NBO
8	1.1154	-1.1193	0.6358	-0.8169
6	0.9254	-0.0728	-0.0346	0.7654
6	-0.5505	0.2353	-0.4155	-0.1146
7	-1.3416	-1.0436	-0.2722	-0.6999
6	-1.1483	1.3171	0.4801	-0.5959
1	-1.1506	-1.6850	-1.0560	0.4571
1	-2.3600	-0.8910	-0.2370	0.4485
1	-1.0279	-1.5278	0.5848	0.4600
1	-0.6091	0.5237	-1.4685	0.2377
8	1.7657	0.7721	-0.4108	-0.7984
1	-1.1187	1.0199	1.5326	0.2118
1	-2.1844	1.5329	0.2040	0.2128
1	-0.5670	2.2325	0.3654	0.2324

zwAl$_{aq}$ -323.8778686				
	X	y	z	NBO
1	0.5100	-1.9116	0.0923	0.4647
7	1.2409	-1.1808	0.0311	-0.7035
6	0.5774	0.1287	0.3899	-0.1188
6	-0.9351	0.0032	0.0333	0.7692
6	1.2970	1.2993	-0.2639	-0.5973
8	-1.3356	-1.1561	-0.2524	-0.8183
8	-1.6017	1.0553	0.1045	-0.7928
1	0.6424	0.2008	1.4823	0.2417
1	2.0304	-1.4128	0.6499	0.4530
1	1.5862	-1.1900	-0.9400	0.4458
1	1.2637	1.2229	-1.3552	0.2090
1	2.3420	1.3501	0.0536	0.2119
1	0.8017	2.2251	0.0263	0.2353

3-Fluoroalanines, Zwitterions CPCM

zwAFa$_{aq}$ -423.1443442				
	X	y	z	NBO
8	1.8155	0.5654	-0.6125	-0.8045
6	1.1286	-0.2664	0.0307	0.7741
6	-0.1859	0.3045	0.6620	-0.1689
7	-0.4081	1.6844	0.1038	-0.7081
6	-1.4020	-0.5683	0.4640	0.0675
1	-0.7535	2.3541	0.8061	0.4581
8	1.3651	-1.4645	0.2700	-0.7827
1	-0.0113	0.4137	1.7404	0.2673
1	0.5181	1.9896	-0.2556	0.4671
1	-1.0575	1.6865	-0.6971	0.4515
1	-1.2041	-1.5667	0.8523	0.2078
9	-1.6695	-0.6833	-0.9218	-0.4180
1	-2.2986	-0.1451	0.9240	0.1889

zwAFbr$_{aq}$ -423.1441575				
	X	y	z	NBO
1	1.0567	-1.7637	0.0385	0.2082
6	1.2000	-0.7240	0.3268	0.0668
6	0.1752	0.1463	-0.3604	-0.1633
6	-1.3009	-0.2746	-0.0462	0.7729
7	0.3453	1.5926	0.0173	-0.7042
8	-2.0883	0.6761	0.1748	-0.8000
8	-1.5326	-1.4982	-0.0838	-0.7831
1	0.3109	0.0927	-1.4479	0.2565
1	0.6179	1.7137	1.0055	0.4521
1	1.0409	2.0798	-0.5659	0.4586
1	-0.5852	2.0357	-0.0907	0.4678
1	1.1669	-0.6236	1.4161	0.1857
9	2.4996	-0.3324	-0.0806	-0.4180

zwAFb1$_{aq}$ -423.1439166				
	X	y	z	NBO
9	2.4612	-0.4511	0.0377	-0.4156
6	1.1279	-0.7110	0.4358	0.0662
6	0.1776	0.0930	-0.4259	-0.1599
6	-1.3051	-0.2196	-0.0344	0.7666
7	0.4301	1.5639	-0.2379	-0.7016
8	-1.9059	0.6926	0.5794	-0.7994

8	-1.7075	-1.3536	-0.3606	-0.7846
1	0.3431	-0.1358	-1.4831	0.2534
1	0.0723	2.1011	-1.0422	0.4619
1	1.4303	1.7933	-0.1340	0.4540
1	-0.0982	1.8863	0.5907	0.4643
1	0.9391	-1.7752	0.2972	0.2064
1	1.0570	-0.4443	1.4944	0.1884

zwAFcl$_{aq}$ -423.1384438				
	X	y	z	NBO
1	1.2793	-0.2081	1.4295	0.1921
6	1.4183	0.2898	0.4682	0.0758
6	0.1043	0.4504	-0.2930	-0.1623
6	-0.9745	-0.6458	-0.0244	0.7695
7	-0.5201	1.7876	-0.0001	-0.7031
8	-2.1610	-0.2295	-0.0051	-0.8094
8	-0.5506	-1.8088	0.1091	-0.7804
1	0.3236	0.4445	-1.3682	0.2606
1	-0.4391	2.0586	0.9928	0.4524
1	-0.1285	2.5509	-0.5717	0.4585
1	-1.5330	1.6751	-0.1940	0.4697
1	1.9132	1.2554	0.6106	0.1831
9	2.2921	-0.5056	-0.2929	-0.4066

zwAFcr$_{aq}$ -423.1381092				
	X	y	z	NBO
8	-1.7149	-0.2101	0.8661	-0.8112
6	-0.9199	-0.6052	-0.0237	0.7612
6	0.1294	0.4580	-0.4777	-0.1498
7	-0.4923	1.8137	-0.2871	-0.7026
6	1.4033	0.4077	0.3699	0.0769
1	-1.1551	2.0177	-1.0514	0.4646
1	0.1887	2.5896	-0.2583	0.4546
1	-1.0427	1.7904	0.5902	0.4656
1	0.3772	0.3458	-1.5367	0.2478
8	-0.8437	-1.7238	-0.5669	-0.7792
1	1.1767	0.4534	1.4393	0.1864
1	2.0869	1.2180	0.0969	0.1848
9	2.0673	-0.8003	0.1250	-0.3992

Alanines, protonated Gasphase

p1	-324.2115677			
	x	y	z	NBO
1	0.6805	-1.8029	-0.1268	0.4656
7	1.3933	-1.0782	0.1007	-0.6964
6	0.6134	0.1977	0.4028	-0.1040
6	-0.8358	-0.1526	0.0291	0.7981
8	-1.1364	-1.2569	-0.3572	-0.5838
6	1.1894	1.4012	-0.3368	-0.6040
1	1.9666	-1.3909	0.8870	0.4414
8	-1.6478	0.8722	0.2020	-0.6387
1	-2.5610	0.6218	-0.0224	0.5162
1	0.6562	0.3497	1.4835	0.2499
1	0.5997	2.2845	-0.0914	0.2623
1	1.1519	1.2610	-1.4207	0.2247
1	2.2205	1.5894	-0.0305	0.2308
1	2.0036	-0.9651	-0.7134	0.4378

p3	-324.2055391			
	x	y	z	NBO
8	1.3816	1.0417	-0.1753	-0.7164
6	0.8630	-0.1833	0.0676	0.7806
6	-0.6341	-0.0932	0.3963	-0.1015
7	-1.1687	1.2846	-0.0028	-0.6812
6	-1.4559	-1.1978	-0.2523	-0.6071
1	-1.2238	1.3749	-1.0226	0.4399
1	-0.5444	2.0280	0.3297	0.4579
1	-2.1078	1.4390	0.3757	0.4401
1	-0.7217	-0.1306	1.4859	0.2496
8	1.4623	-1.2119	0.0678	-0.5064
1	-1.0390	-2.1586	0.0502	0.2706
1	-1.4121	-1.1460	-1.3435	0.2244
1	-2.4976	-1.1609	0.0733	0.2266
1	2.3376	0.9701	-0.3397	0.5229

p4	-324,1972222			
	x	y	z	NBO
1	0.7971	-1.6452	-0.3316	0.4676
7	1.4111	-1.0138	0.2335	-0.6994
6	0.5883	0.2526	0.4208	-0.1189
6	-0.8415	-0.1812	0.0096	0.7942
8	-1.0042	-1.2474	-0.5262	-0.5552

6	1.1358	1.3888	-0.4452	-0.6055
1	1.6189	-1.4849	1.1175	0.4423
8	-1.8369	0.6565	0.2403	-0.6099
1	-1.5795	1.4661	0.7034	0.4939
1	0.6227	0.5121	1.4808	0.2386
1	0.5349	2.2898	-0.3105	0.2440
1	1.1091	1.1285	-1.5063	0.2352
1	2.1585	1.6403	-0.1558	0.2345
1	2.2929	-0.8447	-0.2563	0.4386

Alanine Protonated-CPCM

$p1_{aq}$ -324.329114				
	x	y	z	NBO
1	-1.1063	-1.8319	-0.6841	0.4704
7	-1.4570	-1.0146	-0.1573	-0.6949
6	-0.6003	0.1975	-0.3918	-0.1136
6	0.8323	-0.1769	-0.0239	0.8131
8	1.1382	-1.2510	0.4433	-0.6352
6	-1.1315	1.3936	0.3968	-0.5963
1	-2.4299	-0.8442	-0.4616	0.4660
8	1.6659	0.8190	-0.2842	-0.6857
1	2.5955	0.5552	-0.0347	0.5527
1	-0.6373	0.3969	-1.4709	0.2724
1	-0.5208	2.2686	0.1753	0.2415
1	-1.0971	1.2061	1.4735	0.2205
1	-2.1617	1.6105	0.1052	0.2261
1	-1.4787	-1.2877	0.8399	0.4629

$p3_{aq}$ -324.3271564				
	x	y	z	NBO
8	1.2760	-1.0803	0.3450	-0.7028
6	0.8694	0.1108	-0.0847	0.8156
6	-0.6263	0.1492	-0.3929	-0.1134
7	-1.2673	-1.1889	-0.1248	-0.6977
6	-1.3438	1.2505	0.3836	-0.5953
1	-1.2194	-1.4564	0.8729	0.4632
1	-0.8151	-1.9448	-0.6648	0.4706
1	-2.2646	-1.1756	-0.3969	0.4657
1	-0.7224	0.3157	-1.4743	0.2730
8	1.5727	1.0802	-0.2353	-0.6249

1	-0.8742	2.2073	0.1566	0.2420
1	-1.2846	1.0789	1.4620	0.2200
1	-2.3936	1.3014	0.0864	0.2254
1	2.2596	-1.0667	0.5183	0.5587

$p4_{aq}$ -324.3231288				
	x	y	z	NBO
1	-1.4151	-1.4127	0.5802	0.4661
7	-1.4515	-0.9581	-0.3482	-0.6957
6	-0.5701	0.2575	-0.3994	-0.1220
6	0.8351	-0.1874	0.0119	0.8085
8	1.0136	-1.1652	0.7003	-0.6265
6	-1.1057	1.3377	0.5440	-0.5968
1	-1.1599	-1.6663	-1.0436	0.4704
8	1.8479	0.5826	-0.3661	-0.6816
1	1.6056	1.2794	-1.0333	0.5507
1	-0.5738	0.6042	-1.4408	0.2683
1	-0.4712	2.2238	0.4882	0.2380
1	-1.1204	0.9827	1.5778	0.2239
1	-2.1170	1.6266	0.2488	0.2302
1	-2.4359	-0.7173	-0.5527	0.4664

3-Fluoroalanines, protonated, Gasphase

p1Fa -423.4690334				
	x	y	z	NBO
1	-1.3209	1.4463	-0.6101	0.4525
7	-0.6831	1.5756	0.1867	-0.6958
6	-0.2402	0.2226	0.7006	-0.1456
6	1.1151	-0.0311	0.0115	0.7973
8	1.6742	0.8437	-0.5991	-0.5704
6	-1.3206	-0.8180	0.4137	0.0689
1	0.1659	2.0513	-0.1741	0.4680
8	1.5411	-1.2617	0.2211	-0.6431
1	2.4099	-1.3984	-0.1959	0.5197
1	-0.0655	0.2969	1.7770	0.2639
1	-0.9311	-1.8233	0.5698	0.2248
9	-1.6856	-0.6658	-0.9249	-0.3769
1	-2.2109	-0.6591	1.0258	0.1943
1	-1.1431	2.1529	0.8938	0.4423

p1Fb -423.4681597				
	x	y	z	NBO
9	-2.4348	-0.4622	-0.0972	-0.3728
6	-1.1268	-0.8573	-0.3719	0.0729
6	-0.2091	0.0520	0.4562	-0.1417
7	-0.6301	1.4904	0.2468	-0.6901
6	1.2553	-0.0345	0.0087	0.7871
8	1.7825	-1.2023	0.3306	-0.6410
1	-0.0563	1.8884	-0.5153	0.4622
1	-0.4615	2.0626	1.0790	0.4462
1	-1.6318	1.5386	0.0220	0.4542
1	-0.3136	-0.1792	1.5168	0.2581
8	1.7827	0.8720	-0.5823	-0.5670
1	-0.9618	-0.7460	-1.4467	0.1925
1	-0.9927	-1.8969	-0.0747	0.2214
1	2.7038	-1.2588	0.0206	0.5182

p1Fc -423.4575808				
	x	y	z	NBO
7	0.5170	1.8503	0.2320	-0.6963
6	-0.1560	0.5087	0.4458	-0.1396
6	0.9058	-0.5174	0.0113	0.7920
8	1.8729	-0.1612	-0.6209	-0.5844

8	0.6067	-1.7368	0.3948	-0.6188
6	-1.4504	0.4363	-0.3959	0.0848
1	-0.0995	2.5554	-0.1819	0.4386
1	0.8925	2.2351	1.1033	0.4473
1	1.3213	1.6596	-0.4049	0.4688
1	-0.4047	0.3936	1.5010	0.2591
1	1.2734	-2.3703	0.0747	0.5164
1	-1.2312	0.4380	-1.4686	0.1893
9	-2.1004	-0.7252	-0.0733	-0.3411
1	-2.1008	1.2816	-0.1467	0.1837

p3Fa -423.4634874				
	x	y	z	NBO
8	1.4181	-1.4396	0.1707	-0.5041
6	1.0860	-0.3000	0.0894	0.7849
6	-0.2302	0.2146	0.7008	-0.1453
7	-0.5606	1.5996	0.1651	-0.6886
6	-1.4040	-0.7152	0.4047	0.0677
8	1.7807	0.7055	-0.4768	-0.7102
1	-1.0030	1.4995	-0.7590	0.4555
1	0.2970	2.1514	0.0452	0.4629
1	-1.2085	2.1072	0.7748	0.4418
1	-0.0753	0.3029	1.7793	0.2639
1	-1.1045	-1.7512	0.5606	0.2324
9	-1.7362	-0.5256	-0.9396	-0.3794
1	-2.2835	-0.4756	1.0060	0.1921
1	2.6265	0.3761	-0.8272	0.5266

p3Fb -423.4626721				
	x	y	z	NBO
9	-2.4777	-0.3055	-0.0390	-0.3768
6	-1.2129	-0.8214	-0.3212	0.0731
6	-0.2101	0.0689	0.4163	-0.1415
6	1.2375	-0.2986	0.0838	0.7773
7	-0.5238	1.5208	0.0906	-0.6823
8	1.9375	0.7872	-0.2944	-0.7033
8	1.6382	-1.4175	0.1653	-0.5039
1	-0.3576	-0.0353	1.4940	0.2600
1	-0.2802	1.7516	-0.8785	0.4471
1	0.0020	2.1637	0.6901	0.4516
1	-1.5312	1.6812	0.2213	0.4563
1	-1.0735	-0.8031	-1.4053	0.1904

1	-1.1433	-1.8443	0.0462	0.2282
1	2.8581	0.5400	-0.4912	0.5238

p3Fc -423.450235				
	x	y	z	NBO
7	-0.2571	1.8846	-0.3008	-0.6833
6	0.2388	0.4573	-0.4950	-0.1340
6	-0.8863	-0.5228	-0.1354	0.7700
8	-1.0574	-1.5621	-0.6847	-0.4785
8	-1.6042	-0.0248	0.8997	-0.7223
6	1.4911	0.2475	0.3831	0.0822
1	0.5055	2.5683	-0.3603	0.4413
1	-0.9530	2.1359	-1.0107	0.4497
1	-0.7163	1.9704	0.6156	0.4606
1	0.4930	0.3303	-1.5471	0.2583
1	-2.2901	-0.6592	1.1703	0.5248
1	1.2573	0.3631	1.4462	0.1881
9	1.9397	-1.0278	0.1624	-0.3398
1	2.2779	0.9530	0.0943	0.1830

p4Fa -423.4521168				
	x	y	z	NBO
1	-1.3260	1.5013	-0.5342	0.4510
7	-0.6391	1.5794	0.2265	-0.7003
6	-0.2331	0.2034	0.7057	-0.1605
6	1.1291	-0.0516	-0.0075	0.7965
8	1.6392	0.8486	-0.6187	-0.5446
6	-1.3535	-0.7900	0.4013	0.0669
1	0.2284	1.9900	-0.1854	0.4716
8	1.6946	-1.2373	0.1209	-0.6061
1	1.1944	-1.8748	0.6484	0.4925
1	-0.0563	0.2514	1.7840	0.2588
1	-1.0424	-1.8219	0.5767	0.1991
9	-1.6878	-0.6399	-0.9391	-0.3684
1	-2.2443	-0.5863	1.0005	0.2009
1	-1.0147	2.1822	0.9616	0.4426

p4Fb -423.45273				
	x	y	z	NBO
9	-2.4320	-0.4690	-0.1002	-0.3692
6	-1.1263	-0.8289	-0.4187	0.0695

6	-0.2028	0.0198	0.4675	-0.1549
7	-0.6162	1.4676	0.3294	-0.6932
6	1.2677	-0.0345	-0.0146	0.7831
8	1.9780	-1.1131	0.2732	-0.6099
1	-0.0365	1.8740	-0.4287	0.4667
1	-0.4265	2.0063	1.1794	0.4462
1	-1.6187	1.5419	0.1176	0.4537
1	-0.3203	-0.2612	1.5156	0.2447
8	1.6957	0.8766	-0.6690	-0.5412
1	-0.9678	-0.6302	-1.4818	0.1999
1	-0.9935	-1.8923	-0.2158	0.2096
1	1.5437	-1.7373	0.8718	0.4951

p4Fc -423.4508212				
	x	y	z	NBO
7	0.9531	1.6956	0.0757	-0.7019
6	-0.0162	0.5792	0.3859	-0.1583
6	0.7750	-0.7133	0.0234	0.7963
8	1.9418	-0.6011	-0.2636	-0.5577
8	0.1469	-1.8632	0.0736	-0.6060
6	-1.3517	0.7520	-0.3520	0.0698
1	1.0615	2.3640	0.8420	0.4463
1	1.8585	1.1841	-0.0969	0.4731
1	0.7175	2.2161	-0.7749	0.4380
1	-0.1994	0.5836	1.4632	0.2565
1	-0.8035	-1.7781	0.2620	0.5120
1	-1.2364	0.6994	-1.4385	0.1952
9	-2.1521	-0.3124	0.0507	-0.3642
1	-1.8535	1.6793	-0.0677	0.2008

3-Fluoroalanine, protonated CPCM

p1Fa$_{aq}$ -423.591693				
	x	y	z	NBO
1	0.9467	1.6096	0.8662	0.4680
7	0.7399	1.6391	-0.1473	-0.6976
6	0.2729	0.3128	-0.6643	-0.1591
6	-1.0796	0.0034	-0.0181	0.8146
8	-1.6328	0.7680	0.7365	-0.6242
6	1.3213	-0.7602	-0.4280	0.0683
1	0.0178	2.3665	-0.2854	0.4753
8	-1.5320	-1.1743	-0.4127	-0.6837
1	-2.4190	-1.3581	0.0088	0.5569
1	0.1240	0.4178	-1.7502	0.2971
1	0.9872	-1.7083	-0.8504	0.2149
9	1.5015	-0.9295	0.9566	-0.4041
1	2.2857	-0.4719	-0.8549	0.2022
1	1.5954	1.9498	-0.6398	0.4715

p1Fb$_{aq}$ -423.5908547				
	x	y	z	NBO
9	2.4737	-0.4828	-0.0205	-0.3999
6	1.1597	-0.7712	0.3834	0.0697
6	0.2170	0.1502	-0.3800	-0.1542
7	0.5443	1.5836	-0.0983	-0.6973
6	-1.2532	-0.0855	-0.0331	0.8134
8	-1.5851	-1.3513	-0.2236	-0.6827
1	0.4228	1.8240	0.9015	0.4679
1	-0.0695	2.2169	-0.6388	0.4752
1	1.5213	1.7965	-0.3625	0.4715
1	0.3489	-0.0011	-1.4613	0.2865
8	-1.9820	0.7979	0.3508	-0.6197
1	1.1057	-0.6114	1.4647	0.1973
1	0.9451	-1.8113	0.1385	0.2145
1	-2.5518	-1.4874	-0.0081	0.5579

p1Fc$_{aq}$ -423.5863661				
	x	y	z	NBO
7	-0.3996	1.8865	-0.2047	-0.6963
6	0.1480	0.5054	-0.3869	-0.1506
6	-0.9565	-0.4839	-0.0176	0.8097
8	-1.9997	-0.1355	0.4864	-0.6284

8	-0.6094	-1.7240	-0.3134	-0.6769
6	1.4251	0.3506	0.4563	0.0772
1	0.2869	2.6055	-0.4934	0.4720
1	-1.2489	2.0232	-0.7799	0.4769
1	-0.6724	2.0754	0.7763	0.4699
1	0.4053	0.3935	-1.4488	0.2847
1	-1.3376	-2.3515	-0.0409	0.5540
1	1.2028	0.1854	1.5144	0.1969
9	2.1420	-0.7478	-0.0143	-0.3861
1	2.0557	1.2373	0.3390	0.1971

p3Fa$_{aq}$ -423.58994				
	x	y	z	NBO
8	-1.4533	-1.3597	-0.3991	-0.6164
6	-1.0609	-0.2536	-0.1236	0.8165
6	0.2593	0.2851	-0.6831	-0.1588
7	0.5626	1.6634	-0.1669	-0.7002
6	1.4161	-0.6565	-0.4000	0.0698
8	-1.6786	0.6272	0.6517	-0.6975
1	0.7130	1.6737	0.8567	0.4685
1	-0.2086	2.3213	-0.3695	0.4752
1	1.4150	2.0445	-0.6148	0.4714
1	0.1416	0.3694	-1.7744	0.2971
1	1.1873	-1.6500	-0.7871	0.2150
9	1.5977	-0.7516	0.9918	-0.4045
1	2.3480	-0.2817	-0.8313	0.2019
1	-2.5450	0.2532	0.9818	0.5619

p3Fb$_{aq}$ -423.5889773				
	x	y	z	NBO
9	2.5173	-0.3444	-0.0378	-0.3999
6	1.2304	-0.7358	0.3639	0.0714
6	0.2199	0.1307	-0.3753	-0.1541
6	-1.2112	-0.3202	-0.0805	0.8159
7	0.4331	1.5795	-0.0452	-0.6993
8	-2.0013	0.6967	0.2353	-0.6957
8	-1.5355	-1.4794	-0.1566	-0.6140
1	0.3780	0.0329	-1.4597	0.2872
1	0.2760	1.7839	0.9575	0.4678
1	-0.2045	2.1871	-0.5865	0.4754
1	1.3998	1.8667	-0.2778	0.4711
1	1.1698	-0.6063	1.4488	0.1971

1	1.0857	-1.7816	0.0940	0.2149
1	-2.9332	0.3747	0.4027	0.5624

p3Fc$_{aq}$ -423.5843673				
	x	y	z	NBO
7	-0.3242	1.8721	-0.2828	-0.6991
6	0.2027	0.4765	-0.4521	-0.1460
6	-0.8695	-0.5614	-0.1210	0.8083
8	-0.8406	-1.6805	-0.5672	-0.6064
8	-1.7752	-0.0782	0.7237	-0.7031
6	1.4486	0.3154	0.4346	0.0781
1	0.3849	2.5746	-0.5612	0.4727
1	-1.1540	2.0308	-0.8813	0.4771
1	-0.6089	2.0770	0.6911	0.4706
1	0.4845	0.3610	-1.5052	0.2795
1	-2.4536	-0.7780	0.9452	0.5611
1	1.1945	0.3108	1.4988	0.1960
9	2.0549	-0.9010	0.1279	-0.3877
1	2.1636	1.1155	0.2201	0.1987

p4Fa$_{aq}$ -423.5848344				
	x	y	z	NBO
1	0.9905	1.6113	0.7197	0.4708
7	0.8172	1.5690	-0.2995	-0.6984
6	0.2450	0.2452	-0.7069	-0.1669
6	-1.0752	0.0569	0.0518	0.8091
8	-1.3413	0.7239	1.0217	-0.6141
6	1.2454	-0.8664	-0.4159	0.0673
1	0.1707	2.3439	-0.5284	0.4753
8	-1.8866	-0.8990	-0.3793	-0.6789
1	-1.6484	-1.2820	-1.2661	0.5524
1	0.0642	0.2803	-1.7922	0.2942
1	0.8508	-1.8295	-0.7481	0.2110
9	1.4746	-0.9345	0.9659	-0.3992
1	2.2023	-0.6670	-0.9064	0.2058
1	1.7100	1.7576	-0.7888	0.4717

p4Fbaq -423.5840921				
	x	y	z	NBO
9	2.4459	-0.5583	0.0549	-0.3952
6	1.1298	-0.7155	0.5108	0.0690

6	0.2091	0.0737	-0.4171	-0.1608
7	0.5712	1.5266	-0.3719	-0.6985
6	-1.2544	-0.0630	0.0268	0.8054
8	-1.9088	-1.1416	-0.3743	-0.6731
1	0.3561	1.9432	0.5514	0.4705
1	0.0444	2.0655	-1.0817	0.4751
1	1.5778	1.6663	-0.5669	0.4715
1	0.3412	-0.2624	-1.4548	0.2812
8	-1.7638	0.7616	0.7463	-0.6114
1	1.0874	-0.3441	1.5391	0.2009
1	0.8804	-1.7783	0.4781	0.2113
1	-1.4250	-1.6834	-1.0556	0.5542

p4Fc$_{aq}$ -423.581608				
	x	y	z	NBO
7	-0.4140	1.8904	-0.2967	-0.6975
6	0.1491	0.5142	-0.4608	-0.1567
6	-0.9140	-0.4823	0.0204	0.8046
8	-1.7410	-0.1580	0.8399	-0.6199
8	-0.8592	-1.7120	-0.4644	-0.6722
6	1.4364	0.4043	0.3717	0.0756
1	0.2831	2.6213	-0.5270	0.4730
1	-1.2230	2.0350	-0.9269	0.4779
1	-0.7512	2.0524	0.6694	0.4723
1	0.3768	0.3743	-1.5260	0.2781
1	-0.1884	-1.8367	-1.1893	0.5541
1	1.2350	0.5213	1.4408	0.1977
9	1.9744	-0.8668	0.1675	-0.3887
1	2.1688	1.1441	0.0365	0.2019

Alanine Anions Gasphase

a1r -323.3030773				
	X	y	z	NBO
1	-0.9743	-1.6201	0.4370	0.3668
7	-1.4181	-1.0948	-0.3209	-0.8814
6	-0.6185	0.1492	-0.4087	-0.1215
6	0.8963	-0.0540	-0.0325	0.7428
8	1.1444	-1.0541	0.6899	-0.8038
6	-1.2289	1.2165	0.5078	-0.5722
1	-1.2122	-1.6519	-1.1470	0.3307
8	1.6820	0.8192	-0.4689	-0.7889
1	-0.6567	0.5156	-1.4401	0.1649
1	-0.6505	2.1422	0.4476	0.2003
1	-1.2139	0.8699	1.5473	0.1865
1	-2.2709	1.4173	0.2338	0.1758

a1l -323.3029148				
	x	y	z	NBO
1	-0.5124	1.9515	0.1210	0.3744
7	-1.2839	1.2805	0.1424	-0.8793
6	-0.6235	-0.0186	0.3989	-0.1236
6	0.9112	-0.0284	0.0265	0.7467
8	1.4041	1.0872	-0.2807	-0.8006
6	-1.3846	-1.1577	-0.2767	-0.5807
8	1.4789	-1.1416	0.1171	-0.7916
1	-0.6528	-0.1947	1.4836	0.1667
1	-0.8918	-2.1068	-0.0634	0.2199
1	-1.3885	-1.0222	-1.3666	0.1752
1	-2.4268	-1.1995	0.0640	0.1721
1	-1.6232	1.2719	-0.8182	0.3207

Alanine Anions CPCM

all_{aq} -323.410603				
	X	y	z	NBO
1	-1.3352	-1.5196	0.5058	0.3649
7	-1.4351	-1.0653	-0.4037	-0.8852
6	-0.6098	0.1516	-0.4125	-0.1215
6	0.8820	-0.0586	-0.0244	0.7592
8	1.1541	-0.9779	0.7945	-0.8463
6	-1.2296	1.1960	0.5258	-0.5751
1	-1.0599	-1.7322	-1.0802	0.3674
8	1.7170	0.7357	-0.5435	-0.8521
1	-0.6207	0.5504	-1.4328	0.1924
1	-0.6519	2.1235	0.5180	0.2034
1	-1.2559	0.8185	1.5536	0.1935
1	-2.2552	1.4196	0.2202	0.1994

Fluoroalanines, Anions, Gasphase

a1Fal -422.5756392				
	X	y	z	NBO
6	-1.3550	-0.5710	0.4572	0.0831
6	-0.1616	0.3375	0.6416	-0.1673
6	1.1617	-0.2403	-0.0125	0.7530
8	1.8797	0.6034	-0.5981	-0.7877
7	-0.4830	1.7235	0.2623	-0.8794
1	0.4161	2.1155	-0.0234	0.3746
1	-1.0147	1.6819	-0.6046	0.3392
1	0.0415	0.3105	1.7235	0.1825
8	1.3604	-1.4587	0.1917	-0.7872
1	-1.0620	-1.6027	0.6472	0.1878
9	-1.8434	-0.5129	-0.8810	-0.4334
1	-2.2012	-0.2678	1.0835	0.1348

alFar -422.5787216				
	X	y	z	NBO
9	2.4839	-0.4070	0.0880	-0.4462
6	1.1016	-0.6483	0.4015	0.0800
6	0.1860	0.1826	-0.4693	-0.1648
6	-1.2955	-0.1964	-0.0369	0.7576
7	0.4210	1.6252	-0.3673	-0.8791
1	0.9931	-0.3865	1.4583	0.1471

1	0.9264	-1.7124	0.2469	0.1750
1	0.3101	-0.1504	-1.5062	0.1778
8	-1.9256	0.7006	0.5683	-0.7804
8	-1.6376	-1.3631	-0.3268	-0.7783
1	-0.3119	1.9825	0.2473	0.3792
1	1.3332	1.8260	0.0293	0.3323

a1Fbr -422.5791161				
	X	y	z	NBO
9	2.5353	-0.2924	-0.1021	-0.4476
6	1.2103	-0.6219	0.3461	0.0864
6	0.1859	0.2660	-0.3158	-0.1666
6	-1.2830	-0.2824	-0.0488	0.7612
7	0.3086	1.6579	0.1313	-0.8831
1	1.2147	-0.4727	1.4280	0.1518
1	1.0435	-1.6667	0.0922	0.1778
1	0.3261	0.1663	-1.4043	0.1675
8	-2.1504	0.6010	0.1374	-0.7805
8	-1.4054	-1.5258	-0.0936	-0.7807
1	0.8514	2.2114	-0.5215	0.3311
1	-0.6468	2.0161	0.1656	0.3827

alFcl -422.56904850				
	X	y	z	NBO
7	-0.2009	1.8765	-0.4481	-0.8624
6	0.1725	0.4533	-0.5249	-0.1571
6	-1.0451	-0.4079	-0.0052	0.7557
8	-1.3150	-1.4361	-0.6531	-0.7538
8	-1.5886	0.0604	1.0297	-0.8062
6	1.4074	0.2144	0.3412	0.0872
1	-0.8089	1.9558	0.3681	0.3779
1	0.6093	2.4769	-0.3099	0.3161
1	0.3957	0.1700	-1.5574	0.1759
1	2.1954	0.9427	0.1023	0.1208
1	1.1415	0.2894	1.3996	0.1633
9	1.9882	-1.0581	0.1394	-0.4176

a1Fcr -422.57147903				
	X	y	z	NBO
7	-0.1249	1.9227	-0.3029	-0.8747
6	0.1691	0.4784	-0.4903	-0.1549
6	-1.0162	-0.4181	0.0230	0.7415
8	-1.4308	-1.3040	-0.7525	-0.7641
8	-1.4254	-0.0984	1.1712	-0.8091
6	1.4562	0.2279	0.2814	0.0964
1	-0.7864	2.2023	-1.0221	0.3396
1	-0.6507	1.9641	0.5724	0.3671
1	0.3460	0.2823	-1.5517	0.1770
1	2.2349	0.9275	-0.0374	0.1397
1	1.2736	0.3267	1.3549	0.1612
9	1.9614	-1.0746	0.0634	-0.4197

3-Fluoroalanine Anion-CPCM

a1Fal$_{aq}$ -422.6816284				
	X	y	z	NBO
6	1.3248	-0.6387	-0.4439	0.0883
6	0.2099	0.3646	-0.6624	-0.1767
6	-1.1213	-0.1423	-0.0114	0.7614
8	-1.6553	0.5726	0.8729	-0.8284
7	0.6576	1.7056	-0.2821	-0.8819
1	-0.0625	2.3811	-0.5379	0.3740
1	0.7226	1.7589	0.7352	0.3704
1	0.0324	0.3606	-1.7475	0.2250
8	-1.5564	-1.2414	-0.4508	-0.8435
1	1.0357	-1.6371	-0.7705	0.1818
9	1.6260	-0.7375	0.9504	-0.4414
1	2.2483	-0.3168	-0.9287	0.1713

a1Fbl$_{aq}$ -422.6814324				
	X	y	z	NBO
9	2.4540	-0.4680	0.0757	-0.4384
6	1.0945	-0.6462	0.4745	0.0783
6	0.1841	0.1640	-0.4427	-0.1635
6	-1.2846	-0.1613	-0.0392	0.7671
7	0.4458	1.6035	-0.4237	-0.8856
1	1.0356	-0.3043	1.5114	0.1689
1	0.8914	-1.7164	0.4082	0.1787
1	0.3312	-0.2093	-1.4631	0.2054
8	-1.8870	0.6807	0.6725	-0.8225
8	-1.7326	-1.2695	-0.4367	-0.8327
1	0.0790	2.0022	0.4402	0.3755
1	1.4489	1.7865	-0.4543	0.3689

a1Fbr$_{aq}$ -422.6814488				
	X	y	z	NBO
9	-2.5036	-0.3105	0.0673	-0.4429
6	-1.1795	-0.6796	-0.3315	0.0875
6	-0.1796	0.2459	0.3317	-0.1672
6	1.2766	-0.2364	0.0465	0.7708
7	-0.3913	1.6269	-0.1087	-0.8954
1	-1.1541	-0.5844	-1.4195	0.1675
1	-1.0405	-1.7149	-0.0262	0.1823

1	-0.3052	0.1331	1.4234	0.1985
8	2.1358	0.6486	-0.1923	-0.8231
8	1.4784	-1.4770	0.1195	-0.8317
1	-1.1206	2.0720	0.4466	0.3714
1	0.4724	2.1475	0.0327	0.3822

a1Fcl$_{aq}$ -422.67994399				
	X	y	z	NBO
7	-0.0432	1.9430	-0.2859	-0.8841
6	0.2055	0.5063	-0.4796	-0.1583
6	-1.0320	-0.2930	0.0086	0.7717
8	-1.5946	-1.0553	-0.8208	-0.8112
8	-1.3753	-0.1086	1.2065	-0.8372
6	1.4658	0.0731	0.2633	0.0761
1	-0.2118	2.1317	0.7031	0.3796
1	0.7696	2.4928	-0.5702	0.3656
1	0.3424	0.3193	-1.5491	0.1916
1	2.3414	0.6229	-0.0920	0.1648
1	1.3482	0.1989	1.3421	0.1708
9	1.7374	-1.3082	0.0365	-0.4294

a1Fcr$_{aq}$ -422.68004928				
	X	y	z	NBO
7	0.0041	1.9758	-0.2092	-0.8799
6	0.1897	0.5387	-0.4696	-0.1573
6	-0.9957	-0.3432	0.0175	0.7569
8	-1.5318	-1.1113	-0.8258	-0.8341
8	-1.3345	-0.2076	1.2240	-0.8414
6	1.4874	0.1433	0.2213	0.0903
1	-0.7046	2.3490	-0.8416	0.3788
1	-0.3597	2.0974	0.7375	0.3730
1	0.3080	0.3991	-1.5488	0.2033
1	2.3335	0.6945	-0.1928	0.1715
1	1.4223	0.2988	1.3009	0.1703
9	1.7570	-1.2391	0.0232	-0.4312