

ID	SMILES	Split 1	Split 2	Split 3	Split 4	Exp.	Prd. 1	Prd. 2	Prd. 3	Prd. 4
1	[Cl-]^Cn1cc[nH+]c1	+	+	+	+	345.15	344.454	357.3358	338.7871	349.263
2	[Br-]^Cn1cc[nH+]c1	+	-	#	#	314.15	321.6739	339.5925	316.9577	337.6344
3	Cn1cc[nH+]c1^[O-]Cl(=O)(=O)=O	+	+	+	+	430.15	359.4713	377.0482	379.378	357.4868
4	Cn1cc[nH+]c1^F[B-](F)(F)F	#	+	-	-	310.15	299.9001	319.8652	328.2873	326.9787
5	Cn1cc[nH+]c1^FC(F)(F)S(=O)(=O)NS(=O)(=O)C(F)(F)F	#	+	#	-	282.15	281.9808	273.4981	286.5396	280.0366
6	Cn1cc[nH+]c1^FC(F)(F)C(F)(F)S(=O)(=O)NS(=O)(=O)C(F)(F)C(F)(F)F	-	#	-	+	284.15	293.1343	291.3098	281.5566	296.5291
7	Cn1cc[nH+]c1^[O-]N(=O)=O	-	#	-	+	343.15	337.0763	341.6925	336.1084	341.3067
8	Cn1cc[nH+]c1^[O-]S(=O)(=O)C(F)(F)F	+	+	+	+	357.15	316.8292	331.7675	321.1204	325.6585
9	Cn1cc[nH+]c1^F[P-](F)(F)(F)F	+	-	+	-	389.15	333.7375	329.8861	348.9548	349.7061
10	Cn1cc[nH+]c1^[O-]C(=O)C(F)(F)F	+	+	-	+	324.15	278.5965	292.5118	268.891	281.9284
11	CC(=O)[O-]^Cn1cc[nH+]c1	-	#	-	#	250.15	272.9482	283.3392	248.1404	281.7608
12	[Cl-]^CCn1cc[nH+]c1	+	#	+	#	331.15	341.6835	336.5565	327.3342	339.6687
13	[Br-]^CCn1cc[nH+]c1	-	-	*	#	333.15	314.0295	325.3046	333.15	320.9809
14	CCn1cc[nH+]c1^[O-]Cl(=O)(=O)=O	-	#	+	+	294.15	340.3314	324.2884	350.5743	334.8429
15	CCn1cc[nH+]c1^[O-]N(=O)=O	#	-	+	#	304.15	325.6153	318.7535	315.6405	327.3142
16	CCn1cc[nH+]c1^[O-]S(=O)(=O)C(F)(F)F	+	-	+	+	281.15	297.6893	279.0077	292.3168	303.0146
17	[Cl-]^C[n+]1ccn(C)c1	-	-	+	*	398.15	387.2984	387.74	396.5541	368.4128
18	[Br-]^C[n+]1ccn(C)c1	+	#	+	+	382.65	364.5183	369.9967	374.7246	380.0413
19	C[n+]1ccn(C)c1.F[B-](F)(F)F					376.55	Outlier			
20	C[n+]1ccn(C)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	+	-	#	+	295.15	271.3912	278.4686	287.8038	280.0661
21	C[n+]1ccn(C)c1^[O-]S(=O)(=O)C(F)(F)F	*	-	-	-	312.15	325.0721	313.1679	322.0747	314.5993
22	Cc1ccc(cc1)S(=O)(=O)[O-]^C[n+]2ccn(C)c2	*	+	*	-	372.6	345.9729	354.5074	342.3696	361.7015
23	C[n+]1ccn(C)c1^[O-]C(=O)C(F)(F)F	-	-	-	+	325.15	289.3483	284.3099	278.4154	267.1545
24	C[n+]1ccn(C)c1^F[B-](F)(F)C(F)(F)F	#	-	+	+	288.15	285.2457	278.7856	278.0686	278.4741
25	C[n+]1ccn(C)c1^F[B-](F)(F)C(F)(F)C(F)(F)F	#	*	-	*	300.15	277.6794	279.3619	272.8494	<b>286.5918</b>
26	C[n+]1ccn(C)c1^F[B-](F)(F)C(F)(F)C(F)(F)C(F)(F)F	#	-	-	*	284.15	283.8644	285.3977	291.5086	<b>283.0363</b>
27	C[n+]1ccn(C)c1^F[B-](F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	-	+	-	-	289.15	283.3626	284.3397	293.256	287.4611

28	[Cl-]^Cc1[nH+]ccn1C	*	*	+	-	454.15	458.2799	437.1076	452.2186	441.9198
29	[Br-]^Cc1[nH+]ccn1C	+	*	-	+	449.15	435.4998	419.3643	430.3892	430.2913
30	Cc1[nH+]ccn1C^Cl(=O)(=O)=O	-	-	*	+	337.15	372.6461	359.3162	387.4290	373.945
31	Cc1[nH+]ccn1C^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	-	*	+	+	295.15	328.8891	311.3991	332.8015	317.9951
32	Cc1[nH+]ccn1C^FC(F)(F)C(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)C(F)(F)F	-	-	+	+	288.15	325.087	306.7695	318.1134	318.7034
33	Cc1[nH+]ccn1C^O-N(=O)=O	-	-	+	-	357.15	369.0798	349.9904	384.4979	366.9082
34	Cc1[nH+]ccn1C^O-S(=O)(=O)C(F)(F)F	+	+	#	-	392.15	367.4497	351.6514	382.3542	373.8762
35	Cc1[nH+]ccn1C^F[P-](F)(F)(F)F	+	-	+	+	388.15	371.5571	342.0852	365.1983	359.4195
36	[Cl-]^CC[n+]1ccn(C)c1	+	+	-	+	357.15	356.5707	335.1658	334.9672	341.1301
37	[Br-]^CC[n+]1ccn(C)c1	#	+	-	#	338.05	328.9167	323.9139	315.2934	322.4424
38	[I-]^CC[n+]1ccn(C)c1	-	-	#	#	352.15	362.8283	303.1623	338.8677	349.6015
39	CC[n+]1ccn(C)c1^F[B-](F)(F)F	-	+	*	-	287.57	285.097	288.0383	318.0926	302.2261
40	CCn1cc[n+](C)c1^F[B-](F)(F)C(F)(F)F	#	-	-	+	253.15	260.295	247.0787	239.8757	259.5588
41	CCn1cc[n+](C)c1^F[B-](F)(F)C(F)(F)C(F)(F)F	-	-	-	+	274.15	252.7287	247.655	234.6565	267.6764
42	CCn1cc[n+](C)c1^F[B-](F)(F)C(F)(F)C(F)(F)C(F)(F)F	-	+	+	-	281.15	258.9137	253.6908	253.3157	264.121
43	CCn1cc[n+](C)c1^F[B-](F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	-	+	-	+	269.15	258.412	252.6328	255.0631	268.5457
44	CCC[B-](F)(F)F^CCn1cc[n+](C)c1	-	-	+	+	259.15	255.8166	247.5865	249.5014	268.8584
45	CCCC[B-](F)(F)F^CCn1cc[n+](C)c1	#	-	*	#	264.15	258.3392	258.2108	253.7070	270.8018
46	CCCCC[B-](F)(F)F^CCn1cc[n+](C)c1	-	+	-	-	289.15	256.3089	261.7407	250.446	272.0791
47	CCn1cc[n+](C)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	+	+	+	+	256.15	246.4405	246.7617	249.6109	261.1507
48	CCn1cc[n+](C)c1^FC(F)(F)C(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)C(F)(F)F	*	*	-	*	272.15	257.594	264.5733	244.6279	277.6432
49	CCn1cc[n+](C)c1^N#C[N-]C#N	*	#	-	#	261.15	253.7204	255.6346	251.4775	269.0647
50	CCn1cc[n+](C)c1^FC(F)(F)C(=O)[N-]S(=O)(=O)C(F)(F)F	+	#	+	+	275.75	278.1193	262.6311	249.8484	280.3598
51	CCn1cc[n+](C)c1^O-N=O	+	#	-	-	328.15	294.408	281.5915	272.5039	307.5228
52	CCn1cc[n+](C)c1^O-N(=O)=O	#	#	+	+	311.15	313.4315	311.0502	305.9516	317.8048
53	CCn1cc[n+](C)c1^FC(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)F	*	*	#	-	298.15	260.7189	261.5083	280.2248	281.252
54	CCn1cc[n+](C)c1^FS(=O)(=O)[N-]S(=O)(=O)F	*	+	-	*	260.1	226.3293	256.0471	235.9345	260.8511
55	CCn1cc[n+](C)c1^CCn2cc[n+](C)c2^O-S(=O)(=O)[O-]	+	+	+	-	343.15	336.9883	354.0159	359.5672	322.9162



83	CC[n+] <sub>1</sub> ccn(CC)c1^[O-]S(=O)(=O)C(F)(F)F	#	+	+	#	296.15	306.3158	278.5638	300.518	311.7178
84	[Cl-]^CCC[n+] <sub>1</sub> ccn(C)c1	-	#	+	-	333.15	349.8508	342.9637	339.5386	342.9389
85	CCC[n+] <sub>1</sub> ccn(C)c1^F[B-](F)(F)F	-	#	*	+	256.15	280.9529	284.9577	311.9987:	293.3968
86	CCC[n+] <sub>1</sub> ccn(C)c1^F[B-](F)(F)C(F)(F)F	+	-	*	#	252.15	267.0024	258.2847	255.7577:	264.4162
87	CCC[n+] <sub>1</sub> ccn(C)c1^F[B-](F)(F)C(F)(F)C(F)(F)F	-	+	#	#	231.15	259.436	258.861	250.5385	272.5338
88	CCC[n+] <sub>1</sub> ccn(C)c1^F[B-](F)(F)C(F)(F)C(F)(F)C(F)(F)F	-	-	-	*	268.15	265.6211	264.8968	269.1977	<b>268.9784</b>
89	CCC[n+] <sub>1</sub> ccn(C)c1^F[B-](F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	*	-	+	*	261.15	265.1193	263.8389	270.9451	<b>273.4031</b>
90	CCC[n+] <sub>1</sub> ccn(C)c1^FC(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	+	*	+	-	277.15	267.4263	272.7143	296.1068	286.1093
91	CCC[n+] <sub>1</sub> ccn(C)c1^[O-]S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	-	#	+	*	306.15	281.4971	294.2851	309.4805	304.3381
92	CCC[n+] <sub>1</sub> ccn(C)c1^F[P-](F)(F)(F)(F)F	#	#	#	#	294.15	324.9841	306.1411	312.9504	316.1616
93	[I-]^CC(C)[n+] <sub>1</sub> ccn(C)c1	#	-	+	-	387.15	397.2428	332.5751	380.5177	375.1068
94	CC(C)[n+] <sub>1</sub> ccn(C)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	-	-	*	*	289.15	284.1284	289.889	285.9447	<b>283.2413</b>
95	CC(C)[n+] <sub>1</sub> ccn(C)c1^FC(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	-	+	*	*	301.15	298.4068	304.6356	316.5586	<b>303.3426</b>
96	CC(C)[n+] <sub>1</sub> ccn(C)c1^[O-]S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	-	-	-	+	298.15	312.4776	326.2064	329.9323	321.5714
97	CC(C)[n+] <sub>1</sub> ccn(C)c1^F[P-](F)(F)(F)(F)F	*	+	+	+	375.15	353.5882	339.284	352.7584	326.241
98	[Cl-]^COCCn1cc[n+](C)c1	*	+	+	#	338.15	327.8881	339.6434	320.108	359.1577
99	COCCn1cc[n+](C)c1^F[B-](F)(F)C(F)(F)F	#	-	-	-	275.15	265.1931	255.9256	239.5313	274.1513
100	COCCn1cc[n+](C)c1^F[B-](F)(F)C(F)(F)C(F)(F)F	-	*	#	*	264.15	257.6267	256.5019	234.3121	<b>282.2689</b>
101	COCCn1cc[n+](C)c1^[O-]S(=O)(=O)C(F)(F)F	-	-	*	*	300.15	305.3997	287.374	286.2432	<b>290.0432</b>
102	COCCn1cc[n+](C)c1^F[P-](F)(F)(F)(F)F	+	#	-	-	299.15	306.369	319.9404	295.4176	319.5297
103	[Cl-]^CCCC[n+] <sub>1</sub> ccn(C)c1	+	+	+	-	314.15	337.5032	340.0408	327.2164	341.7281
104	[I-].CCCC[n+] <sub>1</sub> ccn(C)c1					<b>201.15</b>	Outlier			
105	CCCC[n+] <sub>1</sub> ccn(C)c1.F[B-](F)(F)F					<b>192.15</b>	Outlier			
106	CCCC[n+] <sub>1</sub> ccn(C)c1^FC(F)(F)c2cc(cc(c2)C(F)(F)F)[B-](c3cc(cc(c3)C(F)(F)C(F)(F)F)(c4cc(cc(c4)C(F)(F)F)C(F)(F)F)c5cc(cc(c5)C(F)(F)F)C(F)(F)F	*	-	-	#	382.15	352.9459	352.8987	357.4812	355.668
107	CCCC[n+] <sub>1</sub> ccn(C)c1^C[Si](C)(CCC(F)(F)F)c2ccc(cc2)[B-	+	+	-	+	377.15	387.1974	398.9636	368.6903	378.4972

	](c3ccc(cc3)[Si](C)(C)CCC(F)(F)F)(c4ccc(cc4)[Si](C)(C)CCC(F)(F)F)c5ccc(cc5)[Si](C)(C)CCC(F)(F)F									
108	CCCC[n+]1ccn(C)c1^FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)c2ccc(cc2)[B-](c3ccc(cc3)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)(c4ccc(cc4)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)c5ccc(cc5)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F~:	+	#	-	+	316.0673	47.0827	33.7638	336.6887	365.7086
109	CCCC[n+]1ccn(C)c1^F[B-](F)(F)C(F)(F)C(F)(F)F	-	-	*	-	231.15	256.3075	263.9761	240.4441	271.2383
110	CCCC[n+]1ccn(C)c1^CC(CC#N)[B-](F)(F)F	-	-	#	-	188.65	208.2285	210.9042	238.3208	214.9754
111	CCCC[n+]1ccn(C)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	-	*	#	-	271.15	250.0193	263.0828	255.3985	264.7126
112	CCCC[n+]1ccn(C)c1^N#C[N-]C#N	+	*	#	+	267.15	257.2992	271.9558	257.2651	272.6266
113	CCCC[n+]1ccn(C)c1^FC(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	+	+	-	#	298.15	264.2978	277.8295	286.0124	284.8138
114	CCCC[n+]1ccn(C)c1^[O-]S(=O)(=O)C(F)(F)F	#	+	*	-	289.55	303.7003	297.7822	289.6694	299.2458
115	CCCC[n+]1ccn(C)c1^[O-]S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	*	-	#	-	293.15	278.3686	299.4002	299.3861	303.0426
116	CCCCOS(=O)(=O)[O-]^CCCC[n+]1ccn(C)c1	+	-	#	+	256.15	246.4671	254.3391	251.1817	257.0572
117	CCCC[n+]1ccn(C)c1^[O-]S(=O)(=O)OCCCC(F)(F)C(F)(F)F	#	-	#	*	258.05	239.4596	260.7205	215.6371	243.5846
118	CCCC[n+]1ccn(C)c1^[O-]S(=O)(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)F	-	+	-	+	211.95	230.4464	240.0646	233.5362	245.9761
119	CCCC[n+]1ccn(C)c1^COS(=O)(=O)[O-]	+	+	+	#	253.15	252.2536	257.8468	243.9968	264.8137
120	CCCC[n+]1ccn(C)c1.F[P-](F)(F)(F)(F)F					212.15	Outlier			
121	CCCC[n+]1ccn(C)c1^[O-]C(=O)C(F)(F)F	+	#	-	-	233.15	263.6658	268.2763	264.3272	261.5277
122	CCCC[n+]1ccn(C)c1^CC(=O)[O-]	*	#	#	+	253.15	281.9549	284.7494	250.0908	274.2053
123	CCCC[n+]1ccn(C)c1^Cl[Al-](Cl)(Cl)Cl	+	-	+	#	263.15	318.2596	271.9829	259.9514	276.3123
124	CC(C)C[n+]1ccn(C)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	+	+	+	#	233.15	269.5029	255.6983	266.3927	268.7069
125	CC(C)C[n+]1ccn(C)c1^FC(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)-+F	-	+	*	-	277.15	283.7814	270.4449	297.0066	288.8082
126	CCCC[n+]1ccn(C)c1^FC(F)(F)c2cc(cc-c2)C(F)(F)F[B-](c3+cc(ccc3)C(F)(F)C(F)(F)F)(c4cc(ccc4)C#(F)(F)C(F)(F)F)c5cc(ccc5)C(F)(F)C(F)(F)F	#	+	+	+	355.15	340.5983	349.9757	346.5709	354.4571
127	CCCC[n+]1ccn(C)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	+	+	+	-	264.15	237.6718	260.1599	244.4882	263.5017

128	CCCCC[n+] <sub>1</sub> ccn(C)c1^FC(F)(F)C(F)(F)C(F)(F)C(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	-	-	+	-	298.15	251.9502	274.9065	275.1021	283.6030
129	CCCCC[n+] <sub>1</sub> ccn(C)c1^O=C2[N-]S(=O)(=O)c3ccccc23	-	+	#	*	337.15	326.7087	317.6166	317.2346	338.3526
130	CCCCC[n+] <sub>1</sub> ccn(C)c1^FC(F)(F)C(F)(F)[P-](F)(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	*	#	-	-	223.15	216.198	199.1484	208.0832	226.9447
131	CCCCC[n+] <sub>1</sub> ccn(CC)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	+	*	*	+	233.15	233.0147	242.976	239.1485	265.8488
132	CCCCC[n+] <sub>1</sub> ccn(CC)c1^[O-]S(=O)(=O)C(F)(F)F	-	+	-	-	275.15	286.6956	277.6753	273.4194	300.3821
133	CCCCC[n+] <sub>1</sub> ccn(CC)c1^[O-]S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	+	*	+	#	294.15	261.3639	279.2934	283.1361	304.1789
134	CCCCC[n+] <sub>1</sub> ccn(CC)c1^[O-]C(=O)C(F)(F)F	#	+	+	-	233.15	243.0772	245.4629	239.832	253.6557
135	[Br-]^CCCC[n+] <sub>1</sub> ccn(C=C)c1	#	+	+	-	356.15	301.0684	327.0023	335.3442	326.381
136	[Cl-].CCCCCn1cc[n+](C)c1					<b>198.15</b>	Outlier			
137	CCCCCn1cc[n+](C)c1.F[B-](F)(F)F					<b>191.15</b>	Outlier			
138	CCCCCn1cc[n+](C)c1^FC(F)(F)c2cc(cc(c2)C(F)(F)F)[B-](c3cc(cc(c3)C(F)(F)C(F)(F)F)(c4cc(cc(c4)C(F)(F)C(F)(F)F)c5cc(cc(c5)C(F)(F)F)C(F)(F)F	+	+	-	#	355.15	332.7621	338.3137	326.5788	342.3127
139	CCCCCn1cc[n+](C)c1^F[B-](F)(F)C(F)(F)C(F)(F)F	#	-	#	+	263.15	236.1237	249.3911	209.5417	257.883
140	CCCCCn1cc[n+](C)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F		-	-	#	266.00	229.8355	248.4978	224.4961	251.3573
141	CCCCCn1cc[n+](C)c1^[O-]S(=O)(=O)C(F)(F)F	-	-	-	*	302.15	283.5164	283.1972	258.767	285.89.05
142	CCCCCn1cc[n+](C)c1^F[P-](F)(F)(F)F	+	+	-	+	212.15	301.6717	296.6713	271.9535	301.5108
143	CCCCCn1cc[n+](C)c1^FC(F)(F)C(F)(F)[P-](F)(F)(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	+	+	#	#	223.15	208.3617	187.4864	188.0912	214.8003
144	[Br-]^Cn1cc[n+](CC(=O)c2ccccc2)c1	#	#	+	*	322.15	347.4291	332.4208	332.6466	349.3296
145	C^CCCCCn1cc[n+](C)c1^FC(F)(F)c2cc(cc(c2)C(F)(F)F)[B-](c3cc(cc(c3)C(F)(F)C(F)(F)F)(c4cc(cc(c4)C(F)(F)C(F)(F)F)c5cc(cc(c5)C(F)(F)F)C(F)(F)F	*	-	-	+	342.15	342.3.79	340.6063	347.4855	333.8753
146	CCCCCn1cc[n+](C)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	-	+	*	-	280.15	232.8507	251.1225	226.4800	252.8996
147	[Cl-]^CCCC[n+] <sub>1</sub> ccn(CCCC)c1	#	-	#	+	328.15	320.2623	301.0881	282.3356	314.1461
148	[Br-]^C[n+] <sub>1</sub> ccn(Cc2ccccc2)c1	#	#	#	+	399.15	404.0049	415.1495	389.748	416.0577
149	C[n+] <sub>1</sub> ccn(Cc2ccccc2)c1.[O-]S(=O)(=O)C(F)(F)F					<b>300.15</b>	Outlier			

150	C[n+] <sub>1</sub> ccn(Cc2cccc2)c1^F[P-](F)(F)(F)F	-	*	#	-	403.15	381.1002	390.4904	382.1009	378.3363
151	COc1ccc(Cn2cc[n+](C)c2)cc1^[O-]S(=O)(=O)C(F)(F)F	-	-	-	+	318.15	326.8112	297.2003	306.0243	324.3893
152	[Cl-].CCCCCCCCn1cc[n+](C)c1					<b>191.15</b>	Outlier			
153	CCCCCCCCn1cc[n+](C)c1.F[B-](F)(F)F					<b>193.15</b>	Outlier			
154	CCCCCCCCn1cc[n+](C)c1^FC(F)(F)c2cc(cc(c2)C(F)(F)F)[B-](c3cc(cc(c3)C(F)(F)F)C(F)(F)F)(c4cc(cc(c4)C(F)(F)F)C(F)(F)F)c5cc(cc(c5)C(F)(F)F)C(F)(F)F	+	-	*	+	348.15	338.7925	343.563	330.5467	345.3973
155	CCCCCCCCn1cc[n+](C)c1.F[P-](F)(F)(F)F					<b>198.15</b>	Outlier			
156	C[n+] <sub>1</sub> ccn(Cc2cccc2)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	+	#	*	*	310.15	304.0629	320.2758	327.7324	314.6667
157	C[n+] <sub>1</sub> ccn(Cc2cccc2)c1^F[P-](F)(F)(F)F	-	+	#	+	376.15	375.8991	368.4492	375.1898	364.8202
158	CCCCCCCCn1cc[n+](C)c1^F[P-](F)(F)(F)F	*	-	*	-	310.15	293.9561	316.6027	288.3345	315.4198
159	CCC[n+] <sub>1</sub> ccn(CC(=O)c2cccc2)c1.F[B-](F)(F)F					<b>422.15</b>	Outlier			
160	CCCCOCn1cc[n+](COCCC)c1^F[P-](F)(F)(F)F	+	-	#	-	320.15	282.4933	286.4184	278.4782	298.829
161	CCCCCCCC[n+] <sub>1</sub> ccn(C)c1^F[P-](F)(F)(F)F	#	-	-	-	287.15	321.5688	318.832	299.8813	319.8244
162	CCCCCCCC[n+] <sub>1</sub> ccn(CC)c1^C2ccc(cc2)S(=O)(=O)[O-]	+	+	#	+	343.15	336.5199	310.9473	335.5736	347.5279
163	CCCCCCCC[n+] <sub>1</sub> ccn(CC)c1.F[P-](F)(F)(F)F					<b>223.15</b>	Outlier			
164	Cn1cc[n+](CCc2cccc2)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	+	+	+	+	321.15	289.0612	303.1116	305.9023	302.6142
165	Cn1cc[n+](CCc2cccc2)c1^F[P-](F)(F)(F)F	-	+	+	+	325.15	360.8974	351.2851	353.3597	352.7676
166	CCCCOC[n+] <sub>1</sub> ccn(COCCC)c1^F[P-](F)(F)(F)F	-	+	#	-	330.15	324.5665	300.6241	321.4469	326.6597
167	CCCCCCCC[n+] <sub>1</sub> ccn(CCC)c1^F[P-](F)(F)(F)F	+	+	+	-	243.15	307.3759	297.1644	305.82	304.646
168	[Cl-]^CCCCCCCCC[n+] <sub>1</sub> ccn(C)c1	+	+	#	-	311.17	345.6734	328.4614	334.8949	341.9252
169	CCCCCCCCC[n+] <sub>1</sub> ccn(C)c1.F[B-](F)(F)F					<b>195.65</b>	Outlier			
170	C^CCCCCCCCC[n+] <sub>1</sub> ccn(C)c1^FC(F)(F)c2cc(cc(c2)C(F)(F)F)[B-](c3cc(cc(c3)C(F)(F)F)C(F)(F)F)(c4cc(cc(c4)C(F)(F)F)C(F)(F)F)c5cc(cc(c5)C(F)(F)F)C(F)(F)F	+	*	+	+	358.15	362.205	362.767	375.4133	352.1889
171	CCCCCCCCC[n+] <sub>1</sub> ccn(C)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	#	*	#	+	244.15	252.7478	273.2833	254.4078	271.2132
172	CCCCCCCCC[n+] <sub>1</sub> ccn(C)c1^C2ccc(cc2)S(=O)(=O)[O-]	#	-	+	-	352.14	350.7914	336.0872	353.1264	357.2736
173	CCCCCCCCC[n+] <sub>1</sub> ccn(C)c1^F[P-](F)(F)(F)F	+	+	-	*	305.15	324.5841	321.4567	301.8652	<b>321.3666</b>
174	CCCCCCCCC[n+] <sub>1</sub> ccn(C)c1^F[B-](F)(F)F	-	-	+	*	294.55	283.568	302.8979	302.8975	<b>300.1442</b>

175	[Cl-]^CCCCCCCCCCCC[n+]1ccn(C)c1	-	+	+	#	369.78	345.9395	328.1006	338.8627	342.1949
176	[Br-]^CCCCCCCCCCCC[n+]1ccn(C)c1	+	-	+	-	267.85	318.2856	316.8487	319.1889	323.5071
177	CCCCCCCCCCCC[n+]1ccn(C)c1^F[B-](F)(F)F	-	-	+	-	312.15	286.5833	305.5226	304.8814	301.6864
178	CCCCCCCCCCCC[n+]1ccn(C)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	-	-	#	+	289.85	258.7783	278.5326	258.3756	274.2977
179	CCCCCCCCCCCC[n+]1ccn(C)c1^F[O-]S(=O)(=O)C(F)(F)F	-	-	#	+	312.85	312.4592	313.232	292.6465	308.831
180	CCCCCCCCCCCC[n+]1ccn(C)c1^F[P-](F)(F)(F)F	+	+	-	*	323.15	330.6145	326.7061	305.8331	324.4512
181	CCCCCCCCCCCC[n+]1ccn(C)c1^FC(F)(F)c2cc(cc(c2)C(F)(F)F)[B-](c3cc(cc(c3)C(F)(F)F)C(F)(F)F)(c4cc(cc(c4)C(F)(F)F)C(F)(F)F)c5cc(cc(c5)C(F)(F)F)C(F)(F)F	+	+	+	-	345.15	361.7048	368.3485	360.4584	365.2531
182	CCCCCCCCCCCC[n+]1ccn(C)c1^F[B-](F)F	*	-	-	+	322.15	289.5985	308.1473	306.8653	303.2287
183	[Cl-]^CCCCCCCCCCCCCCCC[n+]1ccn(C)c1	+	+	+	#	292.55	346.2057	327.7399	342.8305	342.4646
184	[Br-]^CCCCCCCCCCCCCCCC[n+]1ccn(C)c1	-	*	+	*	293.95	318.5517	316.488	323.1567	323.7768
185	CCCCCCCCCCCCCCCC[n+]1ccn(C)c1^F[B-](F)(F)F	+	+	+	-	315.15	292.6137	310.772	308.8492	304.771
186	CCCCCCCCCCCCCCCC[n+]1ccn(C)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	+	-	+	+	307.45	264.8087	283.782	262.3435	277.3823
187	CCCCCCCCCCCCCCCC[n+]1ccn(C)c1^F[O-]S(=O)(=O)C(F)(F)F	+	+	-	-	323.15	318.4896	318.4813	296.6143	311.9156
188	CCCCCCCCCCCCCCCC[n+]1ccn(C)c1^F[P-](F)(F)F		*	-	+	347.15	336.6449	331.9554	309.8009	327.5358
189	CCCCCCCCCCCCCCCC[n+]1ccn(C)c1^F[B-](F)(F)F	+	+	*	-	328.35	295.6289	313.3967	310.8331	306.3133
190	[Cl-]^CCCCCCCCCCCCCCCC[n+]1ccn(C)c1	*	#	-	#	315.15	373.6858	327.3792	346.7984	342.7343
191	[Br-]^CCCCCCCCCCCCCCCC[n+]1ccn(C)c1	-	*	+	+	313.35	318.8178	360.285	327.1246	324.0465
192	CCCCCCCCCCCCCCCC[n+]1ccn(C)c1^F[B-](F)(F)F	*	#	-	-	322.15	298.6441	316.0213	312.8171	307.8556
193	CCCCCCCCCCCCCCCC[n+]1ccn(C)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	+	-	#	#	315.25	270.8391	289.0314	266.3113	280.4669
194	CCCCCCCCCCCCCCCC[n+]1ccn(C)c1^F[O-]S(=O)(=O)C(F)(F)F	-	*	+	#	331.25	324.52	323.7307	300.5822	315.0001
195	CCCCCCCCCCCCCCCC[n+]1ccn(C)c1^F[P-](F)(F)(F)F	#	*	-	#	348.15	342.6753	337.2048	313.7688	330.6204
196	[Cl-]^CCCCCCCCCCCCCCCC[n+]1ccn(C)c1	-	*	-	+	348.15	346.738	376.7863	350.7662	343.004
197	CCCCCCCCCCCCCCCC[n+]1ccn(C)c1^F[B-](F)(F)F	+	+	+	#	339.95	304.6745	321.2707	316.7849	310.9402
198	CCCCCCCCCCCCCCCC[n+]1ccn(C)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	*	*	-	-	317.95	276.8695	294.2807	270.2792	283.5515
199	CCCCCCCCCCCCCCCC[n+]1ccn(C)c1^F[O-]S(=O)(=O)C(F)(F)F	#	#	-	-	339.15	330.5504	328.98	304.55	318.0847



200	CCCCCCCCCCCCCCCC[n+] <sub>1</sub> ccn(C)c1^F[P-](F)(F)(F)F	*	#	*	+	353.15	348.7057	342.4541	317.7366	333.705
201	[Br-]^CCCCCCCCCCCCCCCC[n+] <sub>1</sub> ccn(C)c1	*	-	+	+	333.35	319.3501	315.4058	335.0603	324.5859
202	[Cl-]^COCn1cc[n+](C)c1	-	+	-	*	290.15	323.0908	330.5113	332.3464	<b>355.3531</b>
203	COCn1cc[n+](C)c1^F[B-](F)(F)C(F)(F)F	+	#	*	*	290.15	262.2469	264.5021	237.1719	<b>281.3568</b>
204	COCn1cc[n+](C)c1^F[B-](F)(F)C(F)(F)CC(F)(F)F	#	*	-	#	252.15	270.3509	280.4052	250.0608	278.2695
205	[I-]^C[N]1=C[NH+](C=C1)C(F)(F)C(F)F	-	-	-	-	413.15	400.8167	363.2319	384.7078	377.4028
206	C[N]1=C[NH+](C=C1)C(F)(F)C(F)F^F[B-](F)(F)F	#	-	*	-	337.15	316.5185	335.9633	345.3083	327.3271
207	C[N]1=C[NH+](C=C1)C(F)(F)C(F)F^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	-	+	+	+	314.15	291.5222	302.4346	290.9669	314.5053
208	[I-]^CC[N]1=C[NH+](C=C1)C(F)(F)C(F)F	*	-	-	#	363.15	377.4349	340.1042	350.2038	372.5286
209	#:CC[N]1=C[NH+](C=C1)C(F)(F)C(F)F^F[B-](F)(F)F	#	#	+	+	298.15	314.2347	329.9743	323.7266	304.79
210	CC[N]1=C[NH+](C=C1)C(F)(F)C(F)F^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	-	+	-	+	288.15	289.2383	296.4455	269.3852	291.9682
211	[I-]^CCCC[N]1=C[NH+](C=C1)C(F)(F)C(F)F	+	-	-	+	350.15	370.7151	347.9021	356.1871	374.3373
212	[I-]^CCCC[N]1=C[NH+](C=C1)C(F)(F)C(F)F	-	-	*	#	346.15	358.3675	344.9792	326.2523	373.1265
213	CCOC(=O)[C@@H](C)[NH+] <sub>1</sub> C=C[N](=C1)C^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	-	-	#	-	318.15	298.089	308.3921	280.8362	310.5945
214	CCOC(=O)[C@@H](C)[NH+] <sub>1</sub> C=C[N](=C1)C^[O-]S(=O)(=O)C(F)(F)F	*	-	-	#	346.15	341.5871	332.7003	355.5708	347.0086
215	CCCCCCCCCOC[n+] <sub>1</sub> ccn(COCCCCCCC)c1^F[B-](F)(F)F	-	*	-	+	326.15	323.8392	283.0581	318.3166	329.7541
216	CCCCCCCCCOC[n+] <sub>1</sub> ccn(COCCCCCCC)c1^F[B-](F)(F)F	-	#	+	-	328.15	329.8696	288.3075	322.2845	332.8387
217	CCCCCCCCCOC[n+] <sub>1</sub> ccn(COCCCCCCC)c1^F[B-](F)(F)F	-	*	*	-	340.15	335.9	293.5569	326.2523	335.9233
218	CCCCCCCCCOC[n+] <sub>1</sub> ccn(COCCCCCCC)c1^F[B-](F)(F)F	+	#	#	+	343.15	341.9305	298.8062	330.2202	339.0079
219	CCCCCCCCCOC[n+] <sub>1</sub> ccn(COCCCCCCC)c1^F[B-](F)(F)F	#	*	-	*	351.15	347.9609	304.0556	334.188	342.0924
220	[Cl-]^C[NH+] <sub>1</sub> C=C[N](=C1)CCO	-	+	#	-	333.95	359.762	329.5942	333.0218	342.2985
221	C[NH+] <sub>1</sub> C=C[N](=C1)CCO^F[P-](F)(F)(F)F	+	-	+	+	296.15	321.7014	314.0215	298.731	313.2133
222	COC(=O)C[n+] <sub>1</sub> ccn(C)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	+	+	-	+	230.65	297.1413	286.43	270.2397	291.1305
223	COC(=O)C[n+] <sub>1</sub> ccn(C)c1^F[P-](F)(F)(F)F	+	+	#	+	349.15	348.0448	333.7009	297.1233	330.61
224	CCC(C)Cn1cc[n+](C)c1^FC(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	-	-	-	-	227.15	278.6504	273.8998	294.0859	272.5024
225	CCC(C)Cn1cc[n+](C)c1^[O-]S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	*	#	+	*	315.15	292.7212	295.4706	307.4596	290.7312

226	CC(C)CCn1cc[n+](C)c1^FC(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	-	-	+	+	312.15	265.7357	263.8446	266.6579	286.8568
227	[I-]^C[n+]1ccn(CCO[Si](C)(C)C)c1	+	-	-	+	342.15	384.9122	375.9919	370.436	368.3959
228	[Br-]^C[n+]1ccn(CCO[Si](C)(C)C)c1	-	+	#	-	399.15	376.8406	388.3894	345.8682	383.8699
229	[I-]^C[Si](C)(C)OCCn1cc[n+](CCC(F)(F)F)c1	+	-	+	+	406.15	364.2915	361.6372	393.4866	401.2041
230	CCOCCn1cc[n+](CCC(F)(F)F)c1.FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F					<b>401.15</b>	Outlier			
231	C[n+]1ccn(Cc2ccccc2[Cr](C=O)(C=O)C=O)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	-	+	-	#	311.15	315.6296	297.1595	309.3436	322.1923
232	C[n+]1ccn(CC#N)c1^F[B-](F)(F)F	-	-	+	+	308.15	264.441	251.655	275.6674	264.532
233	C[n+]1ccn(CC#N)c1^F[P-](F)(F)(F)F	#	+	+	#	351.15	308.6751	342.4443	357.2196	311.3587
234	[Cl-]^C[n+]1ccn(CCC#N)c1	+	*	-	+	323.15	354.5944	329.1794	344.0269	330.4205
235	C[n+]1ccn(CCC#N)c1^F[B-](F)(F)F	+	-	+	+	293.15	261.3125	256.7702	265.5729	263.2365
236	C[n+]1ccn(CCC#N)c1^F[P-](F)(F)(F)F	-	#	*	+	308.15	305.5466	347.5595	347.1252	310.0631
237	[Cl-]^C[n+]1ccn(CCCC#N)c1	+	*	+	+	353.15	339.3647	326.2564	333.1166	327.8022
238	C[n+]1ccn(CCCC#N)c1^F[B-](F)(F)F	-	+	+	-	201.25	248.9649	253.8472	254.6626	262.0256
239	CC(CC#N)[B-](F)(F)F^C[n+]1ccn(CCCC#N)c1	*	-	+	#	196.55	204.1224	199.8155	191.8809	209.0723
240	C[n+]1ccn(CCCC#N)c1^F[P-](F)(F)(F)F	#	+	-	#	348.15	293.199	344.6365	336.2149	308.8523
241	[Cl-]^C[n+]1ccn(CCCCC#N)c1	-	#	*	#	305.15	339.4978	315.3289	335.1005	327.937
242	C[n+]1ccn(CCCCC#N)c1^F[B-](F)(F)F	+	+	+	-	201.25	251.9801	256.4719	256.6466	263.5679
243	C[n+]1ccn(CCCCC#N)c1.F[P-](F)(F)(F)F					<b>212.85</b>	Outlier			
244	CCCCn1cc[n+](CCP(=O)(OCC)OCC)c1^F[B-](F)(F)F	+	-	*	+	192.65	189.1204	187.7107	171.4218	202.0669
245	CCCCn1cc[n+](CCP(=O)(OCC)OCC)c1^F[P-](F)(F)(F)F 187.4124	*	*	-	#	222.95	218.6578	206.5105	199.2273	210.5509
246	CCn1cc[n+](CCCP(=O)(OC)OCC)c1^F[B-](F)(F)F	+	#	*	-	208.85	194.8551	191.334	236.2249	217.6214
247	CCn1cc[n+](CCCP(=O)(OC)OCC)c1^F[P-](F)(F)(F)F	-	-	*	+	220.65	224.3925	210.1338	264.0305	226.1055
248	CCCCCn1cc[n+](CCP(=O)(OCC)OCC)c1^F[B-](F)(F)F	#	*	-	*	190.55	179.788	187.4124	162.4954	202.3983
249	CCCCCn1cc[n+](CCP(=O)(OCC)OCC)c1^F[P-](F)(F)(F)F	*	+	-	#	210.85	209.3255	206.2122	190.3009	210.8824
250	CCCCCn1cc[n+](CCCP(=O)(OCC)OCC)c1^F[B-](F)(F)F	+	*	-	+	197.65	164.7298	176.1969	171.2192	196.8412
251	CCCCCn1cc[n+](CCCP(=O)(OCC)OCC)c1^F[P-](F)(F)(F)F	#	+	#	+	206.95	194.2673	194.9967	199.0247	205.3252

252	CCCCCCCn1cc[n+](CCP(=O)(OCC)OC)C)c1^F[B-](F)(F)F	-	#	-	#	193.35	185.8185	192.6617	166.4633	205.4829
253	CCCCCCCn1cc[n+](CCP(=O)(OCC)OC)C)c1^F[P-](F)(F)(F)F	+	-	*	*	208.95	215.3559	211.4616	194.2688	213.9670
254	CCCCCCCn1cc[n+](CCCP(=O)(OCC)OC)C)c1^F[B-](F)(F)F	-	-	*	#	208.65	170.7602	181.4463	175.1870	199.9258
255	CCCCCCCn1cc[n+](CCCP(=O)(OCC)OC)C)c1^F[P-](F)(F)(F)F	+	+	+	-	180.65	200.2977	200.2461	202.9926	208.4098
256	C[n+]1ccn(CCC(F)(F)C(F)(F)S(F)(F)(F)F)F)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	#	*	-	-	217.65	227.829	246.2365	202.5411	236.8359
257	C[n+]1ccn(CCC(F)(F)C(F)(F)S(F)(F)(F)F)F)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	+	+	-	-	216.45	210.6204	231.1087	197.846	231.2906
258	C[n+]1ccn(CCC(F)(F)C(F)(F)C(F)(F)C(F)(F)S(F)(F)(F)F)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	+	-	*	-	223.15	219.5577	236.0866	234.8897	229.4563
259	C[n+]1ccn(CCCSC(=S)N(c2cccc2)c3ccc3)c1^F[P-](F)(F)(F)F	-	#	-	-	326.15	350.4469	355.7799	327.7083	332.0974
260	C[n+]1ccn(CCCSC(=S)N2CCOCC2)c1^F[P-](F)(F)(F)F	+	+	+	#	323.15	338.027	342.0708	328.7385	354.8025
261	C[n+]1ccn(CCCSC(=S)[N]2=CC=CC=C2)c1^F[P-](F)(F)(F)F	+	+	-	+	409.15	368.3583	404.3382	400.4231	408.4817
262	C[n+]1ccn(CCCSC(=S)n2ccnc2)c1^F[P-](F)(F)(F)F	-	-	+	-	397.15	380.7159	351.4657	381.0373	384.5667
263	C[n+]1ccn(CCCBr)c1^F[P-](F)(F)(F)F	*	#	-	+	318.15	347.1549	339.1284	325.8133	326.4561
264	[Cl-]^CCCC[n+]1ccn(CC(C)O)c1	-	-	-	+	409.65	357.8307	354.1434	366.2424	380.5664
265	CCCCNC(=O)Cn1cc[n+](C)c1^F[P-](F)(F)(F)F	+	-	-	+	337.15	328.8838	316.3748	294.6634	330.1076
266	CCCCN(C)C(=O)Cn1cc[n+](C)c1^F[P-](F)(F)(F)F	+	+	*	*	335.15	322.8845	338.5646	330.6583	309.4347
267	[Br-]^CCN(CC)C(=O)Cn1cc[n+](C)c1	-	#	+	-	339.15	340.9681	309.4338	336.3574	306.7862
268	CCN(CC)C(=O)Cn1cc[n+](C)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	#	#	-	**	316.15	280.8924	284.3222	281.1725	277.044
269	CCN(CC)C(=O)Cn1cc[n+](C)c1^F[P-](F)(F)(F)F	-	-	+	*	337.15	322.8793	309.8241	318.6953	303.4517
270	CC(CC#N)[B-](F)(F)F^Cn1cc[n+](CC#C)c1	*	+	*	-	192.75	209.0572	175.2705	170.0991	194.3163
271	Cn1cc[n+](CC=C)c1^F[B-](F)(F)F	+	+	+	#	192.05	253.4413	234.0386	263.824	276.1735
272	CC(CC#N)[B-](F)(F)F^Cn1cc[n+](CC=C)c1	+	-	+	#	183.95	210.5775	184.2206	171.6457	205.6569
273	CC(CC#N)[B-](F)(F)F^Cn1cc[n+](CCCC(=O)O)c1	*	-	+	-	214.55	260.2984	237.8173	236.641	254.6508
274	F[B-](F)(F)F^C#CC[n+]1ccn(CC#C)c1	+	+	#	+	340.15	294.8343	280.9447	275.0572	285.7076
275	CC(CC#N)[B-](F)(F)F^C#CC[n+]1ccn(CC#C)c1	+	*	#	*	218.05	224.5401	197.1684	198.9374	201.0723
276	CC(CC#N)[B-](F)(F)F^C=CC[n+]1ccn(CC=C)c1	*	#	*	-	185.85	<b>229.58 24</b>	193.6651	224.6441	213.2767
277	CC(CC#N)[B-](F)(F)F^N#CCCC[n+]1ccn(CCCC#N)c1	#	#	*	+	203.35	193.8422	187.9574	166.2351	188.5725
278	CC(CC#N)[B-](F)(F)F^OC(=O)CCC[n+]1ccn(CCCC(=	-	+	#	+	311.15	284.5332	255.7986	267.5251	276.3407

	O)O)c1									
279	[Br-] ]C[C@@H](CC[n+]1ccn(C)c1)OCc2ccc ce2	+	-	#	*	330.15	362.7377	350.177	373.9961	348.2042
280	C[C@@H](CC[n+]1ccn(C)c1)OCc2ccccc 2^F[B-](F)(F)F	*	*	*	-	314.15	317.8555	298.5681	330.2970	318.9476
281	C[C@@H](CC[n+]1ccn(C)c1)OCc2ccccc 2^F[P-](F)(F)(F)F	-	+	*	+	365.15	348.2669	347.1103	345.4393	363.3004
282	C[n+]1ccn(CC(Br)CBr)c1^F[P-] (F)(F)(F)F	-	+	#	+	343.85	364.5814	360.3356	346.8735	362.3697
283	C[n+]1ccn(CC(Br)CBr)c1^F[Sb-] (F)(F)(F)F	-	-	#	-	337.55	358.5214	332.653	311.6875	336.2064
284	[Cl-]^C#CCCC[n+]1ccn(CCCC#C)c1	-	*	-	*	338.15	289.7382	307.1201	286.5218	321.3588
285	F[B-] (F)(F)F^C#CCCC[n+]1ccn(CCCC#C)c1	+	+	+	+	250.15	281.7973	291.069	274.098	289.39
286	[O-] S(=O)(=O)C(F)(F)F^C(c1ccccc1)[n+]2cc n(Cc3ccccc3)c2	#	-	+	-	346.5	367.6693	331.7637	349.94	324.9473
287	Cc1ccc(cc1)S(=O)(=O)[O-] ]^C(c2ccccc2)[n+]3ccn(Cc4ccccc4)c3	-	#	+	-	386.69	389.7471	363.3043	392.0767	380.6015
288	[Cl-]^CC1NC(C)C(C)[NH2+] <sup>1</sup>	-	*	#	+	467.15	464.9687	406.4246	408.9917	472.2543
289	[Cl-]^CC1N(C)CC[NH+] <sup>1</sup> C	#	+	#	+	462.15	440.4277	452.2352	488.9398	456.5055
290	[Cl-].CC[n+]1ccn(C)c1C					<b>461.15</b>	Outlier			
291	[Br-]^CC[n+]1ccn(C)c1C	+	-	-	-	414.15	329.0073	351.1018	346.8524	350.312
292	CC[n+]1ccn(C)c1C^FC(F)(F)S(=O)(=O)[ N-]S(=O)(=O)C(F)(F)F	#	*	+	#	300.15	284.4478	271.2005	286.745	274.6389
293	CC[n+]1ccn(C)c1C^FC(F)(F)C(F)(F)S(= O)(=O)[N-]S(=O)(=O)C(F)(F)C(F)(F)F	-	*	-	#	298.15	280.6457	266.5709	272.0569	275.3473
294	CC[n+]1ccn(C)c1C^[O-] ]S(=O)(=O)C(F)(F)F	#	-	+	-	382.15	323.0084	311.4528	336.2977	330.52
295	CC[n+]1ccn(C)c1C^[O-]C(=O)C(F)(F)F	#	-	*	+	332.15	295.3002	297.3135	278.3903	300.8331
296	CC[n+]1cn(C)cc1C^FC(F)(F)S(=O)(=O)[ N-]S(=O)(=O)C(F)(F)F	-	+	#	-	270	284.3017	278.0206	269.6281	290.4637
297	CC[n+]1cn(C)cc1C^[O-] ]S(=O)(=O)C(F)(F)F	+	-	+	+	279	322.8623	318.2729	319.1808	346.3448
298	CCN1CCN(C)C1C^FC(F)(F)S(=O)(=O)[ N-]S(=O)(=O)C(F)(F)F	+	+	#	+	298.15	291.4078	286.3352	262.4093	281.7323
299	CCN1CCN(C)C1C^[O-]C(=O)c2ccccc2	#	+	+	+	288.91	351.3291	323.3831	305.4529	325.8192
300	CCN1CCN(CC)C1C^FC(F)(F)S(=O)(=O)[ N-]S(=O)(=O)C(F)(F)F	#	-	-	+	251	278.8561	265.7969	267.1414	284.7978
301	CCN1CC(C)N(CC)C1^[O-] ]S(=O)(=O)C(F)(F)F	#	#	+	-	308.15	349.6842	294.9671	313.8055	312.7349
302	[Cl-]^CCCN1CCN(C)C1C	+	+	+	-	411.15	393.8899	396.0165	394.0002	385.1994
303	CCCN1CCN(C)C1C^FC(F)(F)S(=O)(=O)[ N-]S(=O)(=O)C(F)(F)F	-	*	*	*	284.44	287.2637	283.2546	256.3153	<b>272.903</b>
304	CCC[n+]1ccn(C)c1C^F[P-](F)(F)(F)F	-	+	-	*	351.15	331.0136	311.2128	304.7877	<b>309.4416</b>
305	CCC[n+]1ccn(C)c1C^FC(F)(F)C(F)(F)S(= O)(=O)[N-]S(=O)(=O)C(F)(F)C(F)(F)F	#	#	#	#	307.15	276.5016	263.4902	265.963	266.518

306	CCc1[n+](CC)ccn1C^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	*	-	-	*	301.15	333.1588	304.0477	291.7903	312.1592
307	CCc1[n+](CC)ccn1C^O-]S(=O)(=O)C(F)(F)F	-	-	*	+	386.15	371.7195	344.3	341.3430	368.0403
308	CCCC[n+]1ccn(C)c1C^F[B-](F)(F)F	-	#	#	+	312.8	314.4432	311.1299	337.0688	301.7797
309	CCCC[n+]1ccn(C)c1C^O=C2[N-S(=O)(=O)c3ccccc23	+	-	*	#	343.15	363.2834	344.1345	356.9429	351.2364
310	CCCC[n+]1ccn(C)c1C^O-]S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	*	+	+	#	332.15	293.4317	313.9874	322.7544	315.8555
311	CCCC[n+]1ccn(C)c1C^O-]S(=O)(=O)OCCCC(F)(F)C(F)(F)F	-	-	-	-	285.75	266.7332	261.7028	246.6091	275.778
312	CCCC[n+]1ccn(C)c1C^O-]S(=O)(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)F	+	-	+	*	258.95	257.72	241.0469	264.5082	278.1695
313	CCCCCOCCOCCOCC^CCCC[n+]1ccn(C)c1C^CCOC^COCCOCCOCCOCCOCCOCCOS(=O)(=O)[O-]	+	+	#	-	308.15	325.1638	313.6725	361.2187	310.9474
314	CCCC[n+]1ccn(C)c1C^F[P-](F)(F)(F)(F)F	#	#	#	+	313	327.8851	316.328	294.6932	308.1461
315	CCCC[n+]1ccn(C)c1C^F[Sb-](F)(F)(F)F	+	-	*	*	317.5	312.8178	286.1699	267.7832	281.1149
316	CCCCCCCC[n+]1ccn(C)c1C.[O-]S(=O)(=O)C(F)(F)F					235.15	Outlier			
317	[Cl-]^Cc1[n+](CCCC#N)ccn1C	*	*	+	-	378.15	399.4342	363.1265	369.7858	374.4393
318	Cc1[n+](CCCC#N)ccn1C^F[B-](F)(F)F	-	-	+	-	313.15	311.01	288.8904	279.4859	312.9334
319	Cc1[n+](CCCC#N)ccn1C^F[P-](F)(F)(F)F	-	+	#	#	358.15	316.6129	351.2874	325.9711	341.154
320	C[n+]1cn(C)cc1N(=O)=O^O-]Cl(=O)(=O)=O	+	#	-	+	445.15	414.3143	434.0649	430.2144	413.924
321	C[n+]1cn(C)cc1N(=O)=O^O-]N(=O)=O	#	+	+	*	436.15	403.0867	396.9622	404.04	371.9591
322	Cn1cc[n+]2CCCCc12^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	-	-	-	-	356.15	353.6158	335.829	326.9022	334.5376
323	CCCCCn1cc[n+](C)c1C^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	*	#	#	+	268.15	256.9913	258.65	239.6542	251.1588
324	Cc1[n+](C)ccn1Cc2cccc(c2)[Cr](C=O)(C=O)C=O^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	*	+	*	#	341.15	339.5418	380.265	339.3320	377.7622
325	[Br-]^CCn1cc[n+](c1)C(C)CO	+	+	*	+	278.15	340.1809	301.2273	272.4659	313.6321
326	[Br-]^CCn1cc[n+](c1)C(C)(CO)C(C)C	*	-	-	+	284.15	314.9462	275.5284	278.1521	299.8934
327	[Br-]^CCn1cc[n+](c1)C(C)(CO)CC(C)C	#	#	#	+	288.15	318.5358	249.414	276.3995	290.8069
328	Cc1[n+](C)ccn1CC(F)Cn2cc[n+](C)c2C^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	+	#	#	+	359.35	383.9441	395.8652	422.0263	376.2219
329	C[n+]1ccn(C)c1c2[n+](C)ccn2C^F[P-](F)(F)(F)F^F[P-](F)(F)(F)F	#	-	-	*	390.15	406.2294	388.4336	385.7337	368.0916
330	C[n+]1ccn(C)c1c2[n+](C)ccn2C^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	+	+	-	-	366.15	397.5173	401.2408	390.9668	389.5623

331	CCCCn1cc[n+](C)c1c2[n+](C)ccn2CCCC ^F[P-](F)(F)(F)(F)F^F[P-](F)(F)(F)(F)F	-	+	-	-	348.15	377.2369	368.9439	347.2146	348.5621
332	+:CCCC[n+]1ccn(CCCC)c1c2[n+](CCCC )ccn2CCCC^FC(F)(F)S(=O)(=O)[N- ]S(=O)(=O)C(F)(F)F^FC(F)(F)S(=O)(=O) [N-]S(=O)(=O)C(F)(F)F	-	-	+	*	368.15	350.7916	358.4652	342.3669	354.7059
333	CCCCn1cc[n+](CCCC(F)(F)F)c1c2[n+](C CCC(F)(F)F)ccn2CCCC^FC(F)(F)S(=O)( =O)[N- ]S(=O)(=O)C(F)(F)F^FC(F)(F)S(=O)(=O) [N-]S(=O)(=O)C(F)(F)F	+	+	-	+	392.15	340.7591	358.0286	368.8274	352.1366
334	C[n+] <sup>1</sup> ccn2CCCCc12^FC(F)(F)S(=O)(=O) )N-]S(=O)(=O)C(F)(F)F	*	-	*	+	319.15	318.2878	333.2805	291.4444	342.9971
335	CC[n+] <sup>1</sup> ccn(CC)c1C^FC(F)(F)S(=O)(=O) [N-]S(=O)(=O)C(F)(F)F	-	+	-	*	251.15	271.896	250.6622	291.4772	277.7044
336	Cc1[n+](C)cc(N(=O)=O)n1C^[O- ]Cl(=O)(=O)=O	*	+	+	*	459.15	401.9288	446.5323	460.7164	446.7793
337	Cc1[n+](C)cc(N(=O)=O)n1C^[O- ]N(=O)=O	*	*	#	+	434.15	400.0475	429.0342	431.4499	413.7543
338	CCn1c(C)[n+](C)cc1N(=O)=O^[O- ]Cl(=O)(=O)=O	+	+	*	#	419.15	396.8987	426.8623	411.3445	411.6182
339	CCn1c(C)[n+](C)cc1N(=O)=O^[O- ]N(=O)=O	-	+	+	-	338.15	385.6711	389.7596	385.1701	369.6533
340	[I-]^Cc1c(C)n(C)c(C)[n+] <sup>1</sup> C	+	-	#	+	486.15	479.7531	464.764	495.0438	507.076
341	Cc1c(C)n(C)c(C)[n+] <sup>1</sup> C^FC(F)(F)S(=O)( =O)[N-]S(=O)(=O)C(F)(F)F	*	#	-	*	391.15	338.5004	382.0706	385.3817	393.7692
342	Cc1c(C)n(C)c(C)[n+] <sup>1</sup> C^F[P- ](F)(F)(F)(F)F	*	*	*	+	439.15	389.2103	425.1636	409.5184	437.4013
343	+:C[n+] <sup>1</sup> c(Br)c(Br)n(C)c1Br^F[B- ](F)(F)F	+	-	-	#	541.15	529.9626	493.3267	475.0117	489.4413
344	[Br-]^Br- ]^CCCCCCCCCCCCCn1cc[n+](CCCC[ n+] <sup>2</sup> ccn(CCCCCCCCCCCC)c2)c1	-	+	#	-	331.15	355.329	333.3043	304.2208	356.4602
345	CCCCn1cc[n+](CC(F)(F)C(F)(F)C(F)(F)C [n+] <sup>2</sup> ccn(CCCC)c2)c1^FC(F)(F)S(=O)(=O) [N- ]S(=O)(=O)C(F)(F)F^FC(F)(F)S(=O)(=O) [N-]S(=O)(=O)C(F)(F)F	+	*	*	+	322.35	307.7707	362.4192	328.2382	318.4926
346	CCCCn1cc[n+](CC(F)(F)C(F)(F)C(F)(F)C (F)(F)C[n+] <sup>2</sup> ccn(CCCC)c2)c1^FC(F)(F)S (=O)(=O)[N- ]S(=O)(=O)C(F)(F)F^FC(F)(F)S(=O)(=O) [N-]S(=O)(=O)C(F)(F)F	*	+	+	#	347.55	305.714	355.4343	341.6811	316.8074
347	CCCCn1cc[n+](Cc2ccc(C[n+] <sup>3</sup> ccn(CCCC )c3)cc2)c1^FC(F)(F)S(=O)(=O)[N- ]S(=O)(=O)C(F)(F)F^FC(F)(F)S(=O)(=O) [N-]S(=O)(=O)C(F)(F)F	-	-	-	*	322.45	330.4326	304.7207	319.5595	328.6356
348	CCCCCCCCCCCCCn1cc[n+](Cc2ccc(C[n+] 3ccn(CCCCCCCCCC)c3)cc2)c1^FC(F)(F) )S(=O)(=O)[N- ]S(=O)(=O)C(F)(F)F^FC(F)(F)S(=O)(=O) [N-]S(=O)(=O)C(F)(F)F	#	*	-	-	341.55	338.9047	327.7462	319.5621	343.1791
349	CCCCCCCCCCCCCn1cc[n+](Cc2ccc(C [n+] <sup>3</sup> ccn(CCCCCCCCCCCC)c3)cc2)c 1^FC(F)(F)S(=O)(=O)[N- ]S(=O)(=O)C(F)(F)F^FC(F)(F)S(=O)(=O) [N-]S(=O)(=O)C(F)(F)F	+	+	-	*	356.15	360.0112	346.119	333.4495	353.9751

350	CCCCn1cc[n+](Cc2c(F)c(F)c(C[n+]3ccn(CCCC)c3)c(F)c2F)c1^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F^FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	-	*	#	-	345.15	368.379	293.1122	354.3587	345.3024
351	[Br-]^Br-]^Cn1cc[n+](C[C@@H](OC(=O)c2ccccc2)[C@@H](C[n+]3ccn(C)c3)OC(=O)c4ccccc4)c1	+	#	#	*	455.15	428.3282	429.8707	370.137	389.6705
352	Cn1cc[n+](C[C@@H](OC(=O)c2ccccc2)[C@@H](C[n+]3ccn(C)c3)OC(=O)c4ccccc4)c1^F[B-](F)(F)F^F[B-](F)(F)F	-	+	-	-	402.15	<b>378.1604</b>	395.9311	407.4105	390.4497
353	Cn1cc[n+](C[C@@H](OC(=O)c2ccccc2)[C@@H](C[n+]3ccn(C)c3)OC(=O)c4ccccc4)c1^F[P-](F)(F)(F)F^F[P-](F)(F)(F)F	+	+	-	-	361.15	390.1121	372.5588	374.0089	355.1117