Supporting Information

Explorations of Substituted Urea Functionality for Discovery of New Activators of the Heme Regulated Inhibitor Kinase

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I. **Table S1.** Effect of agents on F/R ratio in the ternary complex assay.

Mol_ ID	Formula	MolWeight	Origin	Normalized F/R Fold Ratio (normalized to DMSO)	
				33 µM	10 µM
2	C23H38N2O3	390.559	KIH-271-00-2	1.20715108	1.049791243
6	C22H38N2O3	378.549	KIH-271-41	1.271459453	1.125531824
7	C34H58N4O2	554.85	KIH-271-24 B	1.029022708	-1.120683604
10	C19H34N2O3	338.485	KIH-271-53	1.002897901	-1.038022774
11	C22H38N2O2	362.549	KIH-271-55 B	1.055001455	1.099896937
12	C23H42N2O2	378.592	KIH-271-61	1.33299008	1.060198905
13	C23H38N2O3	390.559	KIH-271-11	1.089668569	-1.032227733
15	C23H32N2O3	384.512	KIH-271-01	-1.256846431	-1.029811398
16	C20H36N2O2	336.512	KIH-258-96	1.975743565	-1.135501372
18	C22H36N2O5	408.532	KIH-258-92	-1.038246611	1.086463393
23	C29H50N2O5	506.718	KIH-271-13	-1.211665514	1.01128348
24	C20H36N2O2	336.512	KIH-258-98	2.523315074	-1.023009769
25	C20H36N2O2	336.512	KIH-271-02	1.115285408	1.086978378
26	C20H36N2O2	336.512	KIH-271-03	-1.17567983	-1.23493713
27	C20H36N2O2	336.512	KIH-258-99	-1.075537537	-1.021620663
29	C18H28N2O3	320.427	KIH-271-11-A	1.02011574	-1.023301487
30	C13H22N2O2	238.326	KIH-258-98-OH	-1.254473531	-1.173004229
31	C14H24N2O2	252.353	KIH-258-96-OH	-1.017620058	-1.054205139
32	C15H26N2O2	266.379	KIH-271-02-OH	1.130878288	-1.193033957
33	C16H28N2O2	280.406	KIH-271-03-OH	1.12973756	1.044301803
34	C17H30N2O2	294.432	KIH-258-75-OH	-1.031636046	1.006342763
35	C16H26N2O3	294.389	KIH-271-13	-1.028833853	-1.045843694
36	C12H22N2O3	242.315	KIH-258-83	1.226092797	1.134050032
720	C20H26N2O2	326.433	KIH-271-30B	-1.181140812	-1.237317991
729	C3H6N2O	86.0925	Aldrich	1.098347529	-1.014538954
730	C7H6N2O	134.135	Aldrich	-1.001880328	1.14306097
731	C4H8N2O	100.119	Aldrich	-1.092887235	-1.083114159
732	C16H10N2O2	262.263	Aldrich	1.269612712	1.091870643
735	C11H20ClF6N2P	360.707	Aldrich	-1.004338899	-1.071706635
736	C10H8N2	156.184	Aldrich	-1.041999366	-1.109831841
737	C11H8N2O	184.194	Aldrich	1.106404164	-1.17278931
738	C7H13NO	127.184	Aldrich	-1.03002608	1.10073912
739	C13H10O3	214.217	Aldrich	-1.095212622	-1.099434974
740	C14H10N2O2	238.241	Aldrich	-1.042992668	1.013471079
742	C14H12O2	212.244	Aldrich	-1.097167137	-1.001166252
743	C15H14O	210.271	Aldrich	-1.033114871	1.038469225
744	C15H17N3	239.316	Aldrich	-1.099632513	-1.052317273
747	C13H15NO6	281.261	MG-XXXI-37B	-1.158368808	1.058712367
748	C14H14OS	230.325	MG-XXXI-67A	-1.017519313	1.105990699

749	C2H8NO2PS	141.129	Chem Service (Monitor)	-1.017457607	1.0987501
750	C4H10NO3PS	183.166	Chem Service (acephate)	-1.02971787	1.007411614
752	C22H30Cl2N10	505.447	Aldrich (chlorohexidine)	1.781518283	1.101221782
753	C14H29NO	227.386	DLD-01-41-127A	-1.1601148	-1.025669015
762	C13H22N2O	222.327	MG-XXXII-44B	-1.276508735	-1.108041141
763	C9H14O2	154.206	BB-01	-1.126408909	1.057241821
765	C17H17NO	251.323	MG-XXXIII-60D	1.838115105	1.256461614
766	C13H29NO2S	263.44	MG-XXXIII-96B	1.149715379	-1.00843112
767	C19H33NO2S	339.536	MG-XXXIV-66B	-1.340086208	-1.160244979
769	C12H26	170.335	Aldrich	-1.112573175	-1.117756164
770	C12H25Br	249.231	Aldrich	1.11987533	1.29294881
774	C19H41NO2S	347.599	MG-XXXIV-80B	1.001938054	1.10319167
775	C16H35NO2S	305.52	MG-XXXIV-81B	-1.086025178	1.119301328
776	C12H17NO2S	239.334	MG-XXXIV-85A	-1.961615949	-1.217655745
777	C14H16N2O2	244.289	JRS	-1.05531291	1.145317639
778	C15H31N2OP	286.393	JRS-09-01A	-1.280142062	1.049169256
779	C7H8Cl2NO3P	256.023	TM-1 (Toru)	1.01730921	1.108990784
780	C8H10Cl2NO3P	270.05	TM-2	1.003382154	1.169502917
781	C9H12Cl2NO3P	284.076	TM-3	-1.01681899	1.14111761
782	C10H14Cl2NO3P	298.103	TM-4	-1.064667936	-1.070755352
783	C10H14Cl2NO3P	298.103	TM-5	1.125552127	-1.003608486
784	C11H16Cl2NO3P	312.129	TM-6	-1.423034861	-1.10678313
785	C11H16Cl2NO3P	312.129	TM-7	1.074400209	1.037771717
786	C11H15Cl2O4P	313.114	TM-8	-1.123965199	1.139662876
787	C11H25NO2S	235.387	Cri-48.8-A	1.029522982	-1.084363594
789	C12H26N2	198.348	Cri-54.8-A	1.0139561	-1.255868705
790	C12H24O2	200.318	CM-02-7	-1.04401583	1.070949922
791	C17H21IN2O	396.266	CW-87-KY	3.515050779	1.057976008
792	C13H16Cl2N2O2	303.184	CW-25-KY	-1.264591648	-1.297957457
793	C15H21BrN2O	325.244	CW-13-KY	1.354132709	1.007516758
794	C14H15Cl2F3N2O	355.183	CW-20-KY	1.042398381	1.152018628
795	C14H16ClF3N2O	320.738	CW-31-KY	1.045875684	-1.088791494
796	C14H15BrClF3N2O	399.634	CW-19-KY	1.058307061	-1.171965848
797	C13H15Cl3N2O	321.63	CW-67-KY	1.328754821	1.060712229
798	C15H20Br2N2O	404.14	CW-16-KY	1.152771188	1.275480398
799	C13H16ClFN2O	270.73	CW-40-KY	-1.203411045	-1.278915457
800	C13H16Cl2N2O	287.185	CW-68-KY	-1.017989831	1.063943
801	C13H16Cl2N2O	287.185	CW-74-KY	1.054717075	1.035224268
802	C14H18ClN3O3	311.764	CW-22-KY	1.033839802	-1.157278325
803	C19H30N2O	302.454	CW-99-KY	-1.123746254	1.003554585
804	C18H28N2O	288.428	CW-56-KY	-1.047361133	1.088831536
805	C14H14N2O	226.274	CW-7-KY	1.338734437	1.180251304
806	C14H14N2O2	242.273	CW-11-KY	1.065408226	1.109845661
807	C15H16N2O3	272.299	CW-10-KY	1.035723823	-1.06022033
808	C13H10Cl2N2O	281.137	CW-8-KY	6.016378159	1.109333863

809	C15H16N2O	240.3	CW-9-KY	1.273204041	1.062157907
810	C14H13ClN2O	260.719	CW-6-KY	1.117345958	-1.097037206
811	C14H13ClN2O2	276.718	CW-3-KY	-1.034908495	-1.091085605
812	C13H10Cl2N2O	281.137	CW-2-KY	1.221477048	-1.034598889
813	C15H16N2O3	272.299	CW-12-KY	1.237568174	-1.34203136
814	C15H31NO	241.413	BDH	1.077284046	1.080552617
815	C16H33NO	255.439	BDH	-1.184710104	1.039810469
816	C21H41NO	323.556	CM-18.7-A	1.04819186	1.097562459
817	C22H43NO	337.583	CM-18.7-B	-1.079641214	1.273018068
818	C22H43NO	337.583	CM-18.7-C	-1.075352313	-1.234255022
819	C23H45NO	351.61	CM-18.7-D	-1.071169396	-1.011640877
820	C23H45NO	351.61	CM-18.7-E	1.14967251	1.110306094
821	C24H45NO	363.62	CM-18.7-F	-1.185471906	-1.039253607
824	C17H34N2O2	298.464	CM-30.7-A	-1.338483827	1.068437377
825	C20H40N2O2	340.544	CM-27.7-A	1.087943454	1.004093858
826	C18H37NO2	299.492	CM-29.7-A	1.193042792	1.239919737
828	C10H22N2O2	202.294	MG-XXXII-12A	1.037036408	1.228582646
829	C16H33BrN2O	349.35	MG-XXXII-15A	3.36423696	1.023340045
832	C9H8N4OS	220.251	Chem service	1.047074837	1.217585227
843	C14H10F2N2O2	276.238	Y1-01	1.48366487	1.200939833
844	C15H12F2N2O2	290.265	Y1-02	1.096274567	1.017703559
845	C16H14F2N2O2	304.291	Y1-03	1.24002205	1.267407921
846	C17H16F2N2O2	318.318	Y1-05	1.106010949	-1.290771277
847	C18H18F2N2O2	332.345	Y1-07	1.063174869	-1.018150678
848	C20H22F2N2O2	360.398	Y1-08	-1.070243986	1.016589341
849	C26H34F2N2O2	444.557	Y1-11	1.00861173	-1.127664661
850	C20H13BrF2N2O2	431.23	Y1-43	-1.014175671	1.187168091
851	C16H14F2N2O3	320.291	Y1-12	1.08561339	1.023088615
852	C21H16F2N2O3	382.36	Y1-14	-1.02244703	-1.107843924
853	C21H15ClF2N2O3	416.805	Y1-15	1.264238874	-1.028067374
854	C22H18F2N2O3	396.387	Y1-16	1.084307164	-1.452338127
855	C22H17ClF2N2O3	430.832	Y1-17	-1.150741365	-1.103619438
856	C23H20F2N2O3	410.413	Y1-18	-1.096532155	-1.006162732
857	C24H22F2N2O3	424.44	Y1-19	-1.005914618	-1.011463322
858	C14H9F3N2O2	294.229	Y1-48	1.207777785	1.112844084
91	C15H21ClN2O4	328.791	KIH-237-09	-1.713145772	-1.091161787
92	C16H23ClN2O3	326.818	KIH-237-12	1.055658342	1.088340261
93	C15H22ClN3O3	327.806	KIH-237-49	-1.659548837	-1.222938189
94	C14H20ClN3O3	313.78	KIH-237-24	-1.072336194	-1.127900895
96	C16H24ClN3O2	325.834	KIH-237-48	-1.041961569	-1.021212857
97	C15H23ClN4O2	326.822	KIH-237-51	1.189140204	-1.451839282
98	C16H23ClN2O3	326.818	KIH-237-15	-1.499334109	-1.017650136
99	C16H24ClN3O2	325.834	KIH-237-52	-1.003585643	1.294369878
100	C14H20ClN3O3	313.78	KIH-237-46	-1.591798123	-1.031170828
101	C13H10Cl2N2O	281.137	KIH-237-14	1.267454349	1.389474749

103	C16H30N2O3	298.421	KIH-237-22	-1.201951058	1.101972547
104	C12H15ClN2O3	270.712	KIH-237-19	1.032874986	1.166581882
105	C12H22N2O3	242.315	KIH-237-23	-1.127910944	-1.070307099
108	C15H22ClN3O3	327.806	KIH-237-40'	-1.459980944	-1.141259658
109	C24H42N2O3	406.602	KIH-237-59	1.058405026	1.038792096
110	C26H44N2O3	432.639	KIH-237-60	1.056698872	1.122019637
111	C30H45ClN2O3	517.143	KIH-237-61	1.023403529	-1.110227505
112	C26H46N2O3	434.655	KIH-237-62	-1.057338068	1.24386277
113	C25H44N2O3	420.628	KIH-237-63	-1.2382528	1.039773814
115	C33H54N2O3	526.793	KIH-237-65	1.048784678	-1.047857325
116	C34H48N2O3	532.757	KIH-237-66	-1.022996339	-1.255092856
117	C26H42N2O3	430.623	KIH-237-68	-1.031132448	-1.032305174
118	C20H34N2O3	350.496	KIH-237-71	1.048426108	1.123591051
120	C17H34N2O	282.465	KIH-237-73	1.089837125	1.089984352
121	C26H47N3O2	433.67	KIH-237-77	1.202744143	-1.269661241
122	C25H45N3O2	419.644	KIH-237-76	1.045873506	1.30623158
124	C21H16F21NO2	713.324	KIH-237-79	-1.050496831	-1.140539318
125	C21H37NO2	335.524	KIH-237-80	1.061677611	-1.011419489
126	C16H22N2O3	290.357	JRS	-1.048416987	-1.008524189
127	C29H51N3O7	553.731	Blankfield	1.00953468	-1.190791142
128	C27H48N2O3	448.682	KIH-258-08	-1.188817417	-1.216939665
130	C27H48N2O3	448.682	KIH-258-10	-1.126834906	-1.085184466
131	C27H48N2O3	448.682	KIH-258-12	-1.262798091	-1.009580426
132	C30H46N2O3	482.698	KIH-237-98	-1.116726281	1.010393145
133	C23H38N2O5	422.558	KIH-237-95	1.357918409	1.190643908
134	C15H24N2O3	280.363	KIH-237-92	-1.016254291	-1.014857024
137	C16H22ClNO4	327.803	KIH-237-93	1.159911879	-1.374002505
138	C25H30N2O3	406.517	KIH-258-18	1.179983738	-1.053167488
139	C17H23ClO4	326.815	KIH-237-94	1.029880703	1.054574503
140	C16H21ClO5	328.788	KIH-237-96	1.024429074	1.208398892
142	C25H30N2O5	438.516	KIH-258-20	1.299193111	-1.182833359
143	C23H29N3O3	395.495	KIH-258-28	1.309681722	1.862690098
144	C13H16ClNO4	285.723	KIH-258-01	-1.166350323	1.023633974
147	C21H35NO3	349.507	KIH-258-35	1.049601359	1.063659876
148	C33H54N2O3	526.793	KIH-258-37	1.046031034	1.02082198
149	C24H41N3O4	435.6	KIH-258-34	-1.004862786	-1.01287397
150	C21H35NO3	349.507	KIH-258-32	1.043481387	1.070354234
151	C26H30N2O4	434.527	KIH-258-74	-1.0381418	1.06352488
157	C29H38N4O7	554.635	JP-435	1.194990301	-1.100557716
159	C24H33N3O4	427.537	KIH-258-47	1.11980127	1.119323668
160	C16H25ClN2O2	312.835	KIH-258-45	-1.338761784	-1.225508763
162	C25H34N2O5	442.548	KIH-258-55	1.350909374	1.21247148
164	C26H34N2O5	454.559	KIH-258-68	1.281993031	-1.026999664
167	C13H24N2O3	256.341	KIH-258-85	-1.03325785	-1.119291749
170	C19H30N2O5	366.452	KIH-258-89	1.135412775	1.083759383

171	C21H34N2O5	394.505	KIH-258-91	-1.019243875	-1.090319027
172	C7H8N2S	152.217	Aldrich	-1.136673988	1.128991966
177	C10H20N2S4	296.539	Disulfiram Sigma	1.214899105	1.225971636
178	C13H24N2S	240.408	MG-XXX-73B	-1.284830811	-1.184877929
180	C14H20N2S	248.387	MG-XXXV-17A	1.780562607	1.357594208
181	C16H24N2S	276.44	MG-XXXIV-54B	-1.374090275	-1.310942094
187	CH4N2O	60.0553	Aldrich	1.053831087	1.078137416
188	C2H2N3NaO	107.047	Aldrich	1.166542311	1.01329589
190	C7H8N2O	136.151	Aldrich	-1.027937994	-1.0044169
191	C3H8N2O	88.1084	Aldrich	-1.323798663	1.203488237
193	C5H12N2O	116.162	Aldrich	-1.153826097	-1.046523592
195	C7H16N2O	144.215	DLD-01-31-140A	-1.035105929	-1.111282183
196	C7H16N2O	144.215	Aldrich	1.297750075	1.13290404
197	C7H12N2O	140.183	Aldrich	-1.038520256	1.015766433
198	C9H20N2O	172.268	CM-42-6-A	-1.20095504	1.001884424
199	C8H18N2O3	190.24	DD-01-31-151A	-1.002156065	-1.011166429
200	C11H24N2O3	232.32	DD-01-31-104A	1.093069486	1.14007917
201	C15H30N2O	254.411	MG-XXXII-54A	1.178460293	-1.000717888
202	C16H32N2O	268.438	MG-XXXII-9A	1.488905656	1.020977328
203	C9H20N2O	172.268	MG-XXXIII-35A	1.123455634	1.034134752
204	C11H24N2O	200.321	MG-XXXII-42B	-1.076427886	1.044100242
205	C17H36N2O	284.481	MG-XXXII-34A	-1.154617871	1.007150571
206	C19H34N2O	306.486	MG-XXXII-78B	-1.124591045	1.192768686
207	C7H16N2O	144.215	MG-XXXII-10A	1.017995019	1.055483826
208	C8H18N2O	158.241	MG-XXX-13A	-1.117180533	1.10918952
209	C8H18N2O2	174.241	MG-XXXII-23A	-1.074414627	-1.181554962
210	C11H24N2O	200.321	MG-XXXI-6B	1.092067938	-1.090087134
211	C12H26N2O	214.348	MG-XXXI-39A	-1.236159995	-1.150094508
212	C13H20N2O	220.311	DD-01-31-17A	-1.122367557	1.034998434
213	C17H22N2O	270.369	DD-01-31-129A	1.117114725	1.162291117
214	C13H19ClN2O	254.756	DD-01-31-33A	3.000206858	1.149734854
215	C9H20N2O	172.268	MG-XXXI-11C	1.077568915	-1.00698457
216	C10H22N2O	186.294	MG-XXX-33A	-1.257623511	-1.056202459
217	C11H24N2O	200.321	DD-01-31-110A	-1.100294848	1.021302734
218	C12H26N2O	214.348	MG-XXXII-98A	-1.208781512	1.136885076
219	C12H24N2O	212.332	MG-XXXIII-12A	1.019725744	1.09289635
220	C14H30N2O	242.401	MG-XXXI-55A	-1.01352121	-1.065419865
222	C15H32N2O	256.427	DD-01-31-81A	-1.05541425	-1.009267137
223	C15H29N3O	267.41	MG-XXXV-32A	-1.002886174	-1.020089353
224	C15H31N3O2	285.426	MG-XXXV-33A	-1.256674052	-1.193576223
225	C13H26N2O	226.358		1.031207445	1.003348901
227	C15H30N2O	254.411	DD-01-31-174A	-1.075139747	-1.011443367
228	C15H24N2O	248.364	DD-01-31-30A	1.036514391	-1.196779001
229	C15H23ClN2O	282.809	DD-01-31-46A	3.266865254	-1.186383277
230	C13H28N2O	228.374	MG-XXXII-83A	1.113174557	1.140507617

232	C12H26N2O	214.348	MG-XXX-11B	-1.114341425	-1.05831702
233	C13H28N2O	228.374	MG-XXX-14A	1.334274802	-1.117576924
234	C14H30N2O	242.401	MG-XXX-38A	-1.036692325	-1.153857366
235	C17H34N2O	282.465	DD-01-31-175A	1.084627062	1.056084507
236	C17H28N2O	276.417	DD-01-31-31A	1.163099876	-1.169257267
237	C17H27ClN2O	310.862	DD-01-31-47A	4.134380891	-1.133085769
238	C15H32N2O	256.427	MG-XXXIII-82A	-1.140696924	1.045451059
239	C16H34N2O	270.454	MG-XXXIV-57A	-1.102371529	-1.063562512
241	C16H34N2O	270.454	MG-XXXIV-92A	1.092155177	-1.103385533
242	C17H36N2O	284.481	MG-XXXIV-83A	-1.019881143	1.303515268
243	C15H31BrN2O	335.323	MG-XXXV-20A	3.597921293	-1.057027719
244	C16H34N2O	270.454	MG-XXXIII-25A	1.131687987	-1.001518288
245	C16H32N2O	268.438	MG-XXXII-88B	1.047852784	1.15228709
246	C16H30N2O	266.422	MG-XXXIV-55A	1.069180789	1.096356799
247	C17H36N2O	284.481	MG-XXXV-27A	-1.080581963	1.089540684
248	C17H36N2O	284.481	MG-XXXIII-83A	-1.164866519	-1.042298163
249	C18H38N2O	298.507	MG-XXXIV-79A	1.188913696	-1.01876037
250	C18H38N2O	298.507	MG-XXXIV-73A	1.094054412	1.03362761
251	C15H29ClN2O2	304.856	MG-XXXIV-56A	1.058354794	1.111959023
252	C15H30N2O4	302.41	MG-XXXV-19A	1.0336549	1.112885479
253	C17H36N2O	284.481	MG-XXXII-56A	1.184572926	1.018696241
254	C18H38N2O	298.507	MG-XXXV-26A	1.185367798	1.124931898
255	C19H40N2O	312.534	MG-XXXIV-68A	-1.060462611	-1.137026772
256	C21H44N2O	340.587	MG-XXXIV-76A	-1.09978107	-1.071491567
258	C17H34N2O	282.465	MG-XXXIII-94B	-1.00252355	1.111711883
259	C18H36N2O	296.491	MG-XXXIV-90A	-1.073878456	-1.093305168
260	C16H34N2O	270.454	MG-XXXII-11A	-1.165930414	1.057631363
261	C16H33ClN2O	304.899	MG-XXXII-28A	4.274192497	1.037124169
262	C17H36N2O	284.481	MG-XXXIV-26A	1.263245523	-1.028137119
263	C18H38N2O	298.507	MG-XXXIV-58A	-1.069208086	1.088434649
264	C15H32N2O	256.427	CM-36-6	-1.002023953	1.269495033
265	C16H34N2O	270.454	DLD-01-41-9B	-1.11992503	-1.100910492
267	C17H36N2O	284.481	CM-36-6	1.101308081	1.077944654
268	C18H38N2O	298.507	DLD-01-41-10B	1.0373133	-1.08532503
271	C19H40N2O	312.534	CM-36-6	-1.196173864	-1.141998949
272	C19H38N2O	310.518	MG-XXXII-55A	1.093247568	1.09319927
273	C22H44N2O	352.598	MG-XXXIV-62B	-1.056745597	-1.008086959
275	C9H18N2O	170.252	DD-01-31-147A	1.029709543	1.002985742
276	C9H18N2O	170.252	DD-01-17G	1.118336731	-1.001515422
277	C8H16N2O2	172.225	MG-XXXIII-76A	1.110999827	1.105598459
378	C14H17N3O	243.304	MG-XXX-82A	1.196827848	-1.101011235
379	C15H20N2O2	260.332	MG-XXXI-52A	1.052328989	1.02094865
380	C15H20N2O2	260.332	BDH25	1.025077196	-1.501980803
381	C14H18N2O3	262.304	JRS-01-08	-2.499108368	-1.266256406
382	C16H24N2O	260.375	MG-XXX-69A	1.426529963	1.09105049

383	C17H26N2O	274.401	DD-01-31-179A	4.884153299	1.349087918
384	C17H26N2O	274.401	MG-XXX-81A	2.85719759	1.259143829
385	C19H30N2O	302.454	MG-XXXIII-91B	-1.078807234	-1.36868778
386	C13H17FN2O	236.285	MG-XXX-65A	-1.086242219	-1.137609917
387	C13H17ClN2O	252.74	MG-XXX-15A	-1.0701542	1.087469283
388	C14H19ClN2O	266.766	BH-147-10-02	1.015394319	1.006633872
389	C15H21ClN2O	280.793	MG-XXXII-75B	1.110435357	-1.061892239
390	C13H17ClN2O	252.74	DD-01-09E	1.146004651	-1.013302029
391	C14H19ClN2O	266.766	DD-01-31-35A	3.93785068	-1.041225532
393	C13H17IN2O	344.191	MG-XXX-48B	-1.121114638	1.099876126
394	C13H19N3O	233.309	MG-XXXIII-17A	1.084561599	-1.01887832
395	C14H21N3O	247.336	MG-XXXII-90A	-1.055489062	-1.045089432
396	C15H23N3O	261.363	MG-XXXII-77A	1.074577228	1.362267939
397	C13H17N3O3	263.292	MG-XXX-32B	1.271273939	-1.150522612
278	C10H20N2O	184.279	MG-XXX-29A	-1.092731402	-1.00906254
279	C9H16N2O3	200.235	MG-XXXIV-86A	-1.046575881	-1.091103713
280	C9H17N3O2	199.25	MG-XXXIV-97A	-1.045534521	-1.065936762
281	C9H15F3N2O	224.223	MG-XXXV-15A	1.102705137	-1.03729663
282	C10H20N2O	184.279	DD-01-08D	1.149008661	1.00804096
283	C11H22N2O	198.305	MG-XXXIII-87A	1.059581242	-1.007896478
284	C12H24N2O	212.332	MG-XXXV-25A	-1.306266763	-1.152037218
285	C11H22N2O	198.305	MG-XXXI-16A	1.042896156	-1.125867579
286	C11H22N2O	198.305	MG-XXX-40A	1.027901438	1.21098818
287	C10H18N2O	182.263	MG-XXX-92A	-1.120959318	1.043505728
288	C10H16N2O	180.247	MG-XXXIII-21A	-1.081396865	-1.044733458
289	C9H15N3O	181.235	MG-XXXIII-71A	1.045766248	1.176836604
290	C11H22N2O	198.305	MG-XXXI-88A	1.01047435	1.132655454
291	C11H23N3O	213.32	MG-XXXI-14A	-1.031890275	2.044770901
292	C15H30N2O	254.411	MG-XXXII-33A	-1.096180128	-1.049034204
293	C10H20N2O2	200.278	MG-XXX-46A	-1.016132816	-1.007459751
294	C12H26IN3O	355.259	MG-XXXII-27A	-1.084666774	-1.035623207
295	C16H29N3O3	311.42	BDH21	-1.102200121	1.127677308
296	C16H30N4O2	310.435	BDH20	-1.004947169	1.245754518
297	C13H26N2O3	258.357	DD-01-31-167A	-1.130368266	1.079104596
298	C10H18N2O3	214.262	MG-XXXIV-47A	-1.04564932	1.021939432
299	C13H24N2O3	256.341	MG-XXXIII-65A	1.006508362	-1.113218539
300	C10H18N2O3	214.262	MG-XXXI-29A	-1.070245078	1.073679718
301	C11H20N2O3	228.288	MG-XXXV-10B	-1.194937644	1.129769277
302	C14H27N3O3	285.382	MG-XXXI-59A	-1.078798342	-1.110931744
303	C11H20N2O3	228.288	MG-XXXIV-99A	1.147009853	1.159537296
304	C12H24N2O	212.332	MG-XXXIV-12A	-1.180345865	1.022832557
306	C13H26N2O2	242.358	MG-XXXII-26B	1.011159599	-1.088013315
307	C13H24N2O3	256.341	MG-XXX-52A	-1.212034231	-1.223075243
308	C13H23N3O	237.341	MG-XXXI-50A	-1.000445887	1.197516769
309	C14H28N2O	240.385	MG-XXXIV-10A	1.020103597	1.225213891

310	C14H26N2O3	270.368	MG-XXXV-9A	1.030462183	1.202604325
311	C15H28N2O3	284.394	MG-XXXV-11A	-1.066593628	1.048574487
312	C16H30N2O3	298.421	MG-XXXV-13A	1.090041927	1.026398223
313	C16H32N2O	268.438	MG-XXXIII-72A	1.220386856	-1.11352783
314	C18H34N2O3	326.474	MG-XXXIV-98A	1.111438542	-1.126319653
315	C19H36N2O3	340.501	MG-XXXV-5B	-1.040887922	1.253168572
316	C18H35N3O2	325.489	MG-XXXV-18B	-1.000244478	-1.004997607
317	C19H38N2O	310.518	CM-29-5	1.030376512	1.084251059
318	C19H36N2O3	340.501	MG-XXX-64B	-1.063515354	1.027949513
319	C23H42N2O	362.592		-1.012325028	1.025511402
320	C20H40N2O	324.544	MG-XXXII-47A	1.036044581	1.233402062
321	C21H42N2O	338.571	MG-XXXIII-80A	-1.018294838	1.015690713
322	C11H20N2OS	228.354	MG-XXX-50A	-1.089291805	1.013218293
323	C10H18N2O	182.263	MG-XXX-89A	-1.047736082	1.265751969
324	C11H20N2O	196.289	MG-XXXI-41A	-1.132428954	1.096038588
325	C12H22N2O	210.316	MG-XXX-24A	-1.336776099	1.032549543
326	C12H23N3O	225.331	MG-XXXII-35A	1.012459413	-1.141932302
327	C13H24N2O2	240.342	MG-XXXIII-13A	1.128758755	1.269252215
329	C14H26N2O	238.369	MG-XXXIV-24A	1.055115689	1.028570489
330	C14H26N2O	238.369	MG-XXXIV-49A	-1.294580216	1.145031604
331	C14H26N2O	238.369	MG-XXX-53A	-1.017707686	1.14734508
332	C15H28N2O	252.396	MG-XXXII-69B	1.329485197	1.339883525
333	C15H26N2O	250.38	MG-XXXII-68A	1.354743619	1.172057639
334	C12H20N4O	236.313	MG-XXXIII-23A	-1.030957476	1.465391427
335	C8H14N6O	210.236	MG-XXXIV-5B	-1.003737344	-1.171768675
336	C15H23N3O	261.363	MG-XXXIII-50A	1.01956067	-1.062271586
337	C14H27N3O2	269.383	MG-XXXII-84A	-1.118748527	1.024883487
338	C17H32N2O	280.449	MG-XXXII-79A	1.315170277	1.404069794
340	C15H28N2O	252.396	MG-XXX-54A	-1.110118288	1.132415298
341	C19H36N2O	308.502	MG-XXXI-40A	-1.111258516	1.047169051
342	C14H24N2O	236.353	MG-XXXIV-33B	1.114900637	1.125560046
343	C17H28N2O	276.417	BH-147-10-01	1.065637683	1.240852405
345	C19H32N2O	304.47	MG-XXXII-61B	-1.03320461	1.162459452
346			DD-01-06B	-1.042107613	1.075250393
347	C13H18N2O	218.295	MG-XXX-16A	-1.084500278	-1.125747518
348	C15H22N2O	246.348	MG-XXXIII-33A	-1.092362016	-1.010359265
349	C14H20N2O	232.321	CM-26.5-01	1.034321861	-1.025684324
350	C15H23N2OS-	279.421	MG-XXXIV-37A	-1.017515894	1.373664197
351	C15H22N2O	246.348	MG-XXXIV-38A	1.128099419	1.012875484
352	C16H23N3O	273.373	BDH24	-1.031856225	1.094328653
353	C13H19N3O	233.309	MG-XXXIV-39B	-1.094720537	1.10223119
354	C18H30N2O	290.444	MG-XXXIII-36A	-1.076060744	-1.058575049
355	C14H20N2O	232.321	DD-01-31-19A	1.16811498	1.109467071
356	C16H24N2O	260.375	MG-XXXV-28A	1.009780791	-1.026286443
357	C16H24N2O	260.375	MG-XXXIII-70B	-1.110219196	1.336192194

358	C15H22N2O	246.348	MG-XXX-35A	1.346964599	1.356053219
359	C16H24N2O	260.375	MG-XXXI-7A	1.005149278	1.061989561
360	C17H26N2O	274.401	MG-XXXI-5A	-1.000180022	-1.089249497
362	C13H19N3O	233.309	MG-XXXI-80A	1.21878741	-1.001054765
363	C17H24N2O	272.385	MG-XXXIII-29A	1.004511612	1.008074781
364	C17H20N2O	268.354	MG-XXX-63A	-1.202695275	-1.497104792
365	C17H20N2O2	284.353	MG-XXXIV-31B	1.163187951	-1.028790088
366	C17H20N2O2	284.353	MG-XXXIV-35A	-1.044904608	-1.152686729
367	C17H20N2O2	284.353	MG-XXXIV-78A	3.775231861	-1.107544461
368	C20H21N3O	319.4	MG-XXXIV-64A	-2.658393599	-1.445511338
369	C18H22N2O	282.38	DD-01-31-131A	-1.280418721	-1.224118581
371	C20H22N2O2	322.401	MG-XXXI-64A	2.67352039	-1.032075399
372	C14H20N2O	232.321	MG-XV-22A	-1.210515983	1.059724933
373	C14H17F3N2O	286.293	MG-XXXIV-72C	-1.138507002	-1.038563082
374	C14H17F3N2O	286.293	MG-XXXIV-94A	1.612445818	-1.226804971
375	C14H20N2O2	248.321	MG-XXX-70A	-1.335394078	1.22123265
376	C17H26N2O3	306.4	MG-XXXIII-14A	-1.030879142	1.141403473
377	C14H17F3N2O2	302.292	MG-XXXII-24A	1.14558593	-1.054923999
398	C14H19N3O3	277.319	MG-XXXII-22C	1.056332181	1.162253652
399	C13H18N2O2	234.294	MG-XXXI-60A	1.111980966	1.039948028
400	C14H20N2O2	248.321	JRS	-1.033109427	1.13109154
401	C13H18N2O4S	298.358	MG-XXXI-13A	-1.032718734	1.163489725
402	C13H19N3O3S	297.373	MG-XXXI-56B	1.01489324	1.101135723
403	C14H20N2O	232.321	Chem-Service (Siduron)	-1.226303289	-1.298606431
404	C21H32N2O	328.492	CM-11-6	1.048125789	1.069197776
405	C22H34N2O	342.518	CM-11-6	1.056449092	1.010079798
406	C23H40N2O	360.577	CM-11-6	1.142995409	-1.000629919
407	C20H28N2O	312.449	MG-XXXIII-37A	1.369786506	1.146977564
408	C11H22N2O	198.305	MG-XXXII-46A	1.018705621	-1.050464556
409	C9H12N2O	164.204	Lancaster	1.045912244	1.031908467
411	C13H18N2O3	250.294	MG-XXXIII-44A	-1.503730975	1.030106521
412	C14H20N2O3	264.32	MG-XXXI-71B	-1.106796021	1.145913578
413	C13H20N2O3	252.31	DD-01-31-23A	1.022010077	1.015589613
414	C15H24N2O3	280.363	DD-01-31-24A	1.032675489	1.107867189
416	C14H14N2O	226.274	CM-10.6-01	-1.145278716	-1.143964413
417	C15H16N2O	240.3	Aldrich	1.079103965	1.089035539
418	C17H20N2O	268.354	Aldrich	-1.016215894	1.062706874
419	C15H16N2O	240.3	DD-01-31-20A	1.100638454	1.100450242
420	C16H18N2O	254.327	MG-XXXII-92B	-1.232530233	1.298635798
422	C10H14N2O2	194.23	DD-01-31-21A	-1.112119951	1.255469736
423	C15H14N2O3	270.283	DD-01-31-28A	-1.103745119	-1.120411889
424	C16H18N2O	254.327	MG-XXXIII-68A	-1.006222883	1.020965765
425	C16H22N2O	258.359	MG-XXXIII-69A	1.079343981	-1.056296682
426	C12H18N2O	206.284	BH-147-10-08	-1.096057665	-1.022534434
427	C16H18N2O	254.327	OH-1	1.191368192	1.028138366

428	C18H22N2O	282.38	OH-3	1.059405203	1.116271305
429	C19H24N2O	296.407	OH-5	-1.053829857	1.018954671
430	C15H15FN2O	258.291	OH-7	-1.261520319	1.043528354
431	C15H14Cl2N2O	309.19	OH-9	2.394487737	1.213464178
432	C16H17FN2O	272.317	OH-11	1.069471937	1.368935349
433	C16H20N2OS	288.408	OH2	1.135674923	1.138565185
434	C18H24N2OS	316.461	OH-4	-1.081567114	-1.138774781
435	C19H26N2OS	330.488	OH-6	1.164512643	1.127821332
436	C15H17FN2OS	292.372	OH-8	-1.15166738	-1.32546923
437	C15H16Cl2N2OS	343.271	OH-10	1.83745733	1.053083159
438	C16H19FN2OS	306.398	OH-12	1.102079564	-1.007973373
439	C11H16N2O	192.258	MG-XXXV-12C	-1.018097755	1.071751203
440	C13H20N2O2	236.31	DD-01-31-181A	1.133551625	-1.10786706
441	C16H26N2O3	294.389	DD-01-31-183A	1.221936461	1.003378659
442	C18H22N2O	282.38	DD-01-31-180A	2.628109914	1.115321892
447	C8H8ClN3O	197.622	MG-XXXIII-60A	-1.046796832	-1.021237635
448	C10H13ClN2O2	228.675	DD-01-31-37A	1.210570865	-1.019704703
449	C9H11ClN2O	198.649	BH-147-10-04	-1.16775165	1.078070381
452	C13H19ClN2O3	286.755	DD-01-31-39A	-1.362762343	-1.006990989
454	C15H23ClN2O3	314.808	DD-01-31-40A	-1.238428163	1.033431263
459	C26H36Cl2N4O2	507.496	BDH-reaction 2	1.092420621	-1.092240398
460	C13H17ClN2O3	284.739	BDH-reaction 17	1.390153976	-1.183835025
461	C16H16Cl2N4O2	367.23	BDH-reaction 16	-1.0316018	1.136085727
463	C15H15ClN2O	274.745	DD-01-31-36A	-1.324058245	-1.27334708
464	C13H10Cl2N2O	281.137	CM-10.6-02	1.363015538	1.186726693
466	C13H8Cl4N2O	350.027	CM-10.6-03	10.49066094	1.876917079
467	C8H8Cl2N2O	219.068	MG-XXX-43B	1.102590647	1.085069719
472	C14H12Cl2N2O2	311.163	BH-147-10-09	1.027307383	1.054117407
473	C19H14Cl2N2O2	373.233	BH-147-10-10	-1.071150342	1.182100322
474	C15H16N4O3	300.313	MG-XXXIII-46A	-1.021041401	-1.093838922
475	C14H13N3O4	287.271	MG-XXXIII-47B	1.139713266	-1.049295728
476	C13H10N4O5	302.242	Aldrich	1.148905564	-1.093982274
477	C12H12N2O	200.236	DLD-01-41-16B	-1.10124666	1.02177492
478	C13H14N2O	214.263	BH-147-10-07	-1.11637146	1.003055481
479	C14H16N2O	228.29	DLD-01-41-18B	1.298307605	1.084274414
481	C15H18N2O3	274.315	DLD-01-31-135A	-1.265865397	-1.024843764
486	C19H24N2O	296.407	DLD-01-31-132A	-1.395362527	-1.030983088
491	C10H14N2O	178.231	DD-01-31-148A	-1.058503346	-1.206798661
492	C12H18N2O	206.284	DD-01-31-116A	1.040309106	-1.10172225
493	C14H17ClN2O2	280.75	DLD-01-41-29B	1.094150998	1.227979808
495	C8H8N2O2	164.161	Lancaster	-1.021922922	1.100057635
497	C14H9ClF2N2O2	310.683		1.193253786	-1.002395743
498	C20H9Cl3F5N3O3	540.655	Chlorfluazuron (Shuo Wang)	2.458359772	1.055432081
499	C21H10Cl2F6N2O3	523.212	Fluofenoxuron (Shuo Wang)	4.047409251	-1.088028364

500	C17H7Cl2F9N2O3	529.141	Lufenuron (Shuo Wang)	2.277756398	-1.172101204
501	C14H6Cl2F4N2O2	381.109	Teflubenzuron (Shuo Wang)	-1.01733144	1.134705467
506	C5H11NO2	117.146	MG-XXXII-41C	-1.244809791	1.073655411
508	C10H21NO2	187.279	DD-01-240	-1.01696379	1.094212471
509	C12H25NO2	215.332	DLD-01-41-22B	-1.071107999	1.09693969
510	C12H25NO2	215.332	CM-08-6	-1.168649057	-1.052254395
511	C15H31NO2	257.412	MG-XXXIV-29A	-1.023525718	-1.104513993
512	C16H33NO2	271.439	MG-XXXIV-30A	-1.018010437	1.177363533
513	C16H33NO2	271.439	MG-XXXV-53A	1.08957139	1.120595913
514	C16H23N3O2	289.373	Eserine Aldrich	-1.035057114	-1.001274858
515	C14H29NO2	243.386	DLD-01-41-21B	1.016422748	-1.034972749
517	C13H23NO2	225.327	DD-01-14J	1.274002039	1.049166091
518	C15H20N2O3	276.331	MG-XXXIII-53A	1.043240273	1.104164597
522	C13H16ClNO2	253.725	DLD-01-41-37B	-1.094077496	1.086535988
523	C16H23NO2	261.359	MG-XXXIII-27A	1.326693925	-1.002171137
524	C17H31NO2	281.434	DLD-01-41-42B	1.496084561	-1.008786673
525	C12H21NO2	211.301	DLD-01-41-46B	1.170530255	1.196691033
526	C17H25NO2	275.386	MG-XXXI-84A	1.165644642	1.370715305
527	C17H24N2O4	320.383	MG-XXXI-87A	1.148933756	1.123965517
529	C17H19NO2	269.338	MG-XXXV-22A	3.056337362	1.144339866
532	C17H31NO2	281.434	DLD-01-41-39B	1.116138207	1.138969717
533	C18H21NO2	283.365	DLD-01-41-40B	1.035943026	1.239157468
535	C21H23NO2	321.413	BDH Carbamate	1.118954825	1.041152818
536	C22H23NO2	333.424	DLD-01-41-41B	1.242415646	-1.014558729
537	C9H17NO2	171.237	DLD-01-41-26B	-1.029062664	-1.141672135
538	C8H9NO2	151.163	DD-01-22M	-1.047646516	1.037004533
540	C16H17NO2	255.312	MG-XXXIII-45A	-1.1206731	1.006993435
541	C14H12ClNO2	261.704	CM-26.5-02	1.460104454	1.42331471
543	C14H12ClNO2	261.704	CM-26.5-04	-1.086259687	1.057807218
544	C12H11NO2	201.221	DLD-01-41-19B	-1.165998758	1.056891544
545	C2H2N2O2	86.0495	MG-XXXII-41D	1.072253533	-1.042450187
546	C8H15NO3	173.21	MG-XXXIII-60B	-1.051021896	1.042483503
547	C14H29NO	227.386	MG-XXXIII-65A	3.019428832	1.276808776
548	C20H39NO	309.53	MG-XXXII-98A	1.759578446	1.39700963
549	C14H26F3NO	281.358	MG-XXXIV-11B	1.209658462	1.14496708
550	C16H33NO	255.439	MG-XXXV-23A	1.003542269	-1.049554919
551	C8H18N2O	158.241	MG-XXXV-12A	1.00801866	1.095463536
553	C13H27NO	213.36	Cri-51.8-A	1.151210979	1.234373804
554	C11H23NOS	217.371	CEW	-1.095957778	1.007032547
555	C12H25NOS	231.398	Cri-55.8-A	-1.041114821	1.160149345
556	C11H23NOS	217.371	CEW	1.107736518	-1.05872469
557	C15H31NO	241.413	MG-XXXIV-40B	-1.006691256	-1.017813693
558	C17H35NO	269.466	TFS-011701-1	1.090982943	-1.031313304
559	C17H35NO	269.466	MG-XXXV-55A	-1.078405488	1.048480071

560	C12H25NO2	215.332	MG-XXXIV-42B	-1.020594022	1.070767329
561	C13H27NO2	229.359	MG-XXXIV-53B	1.165857656	1.021120727
562	C12H26N2O	214.348	Cri-24.8-A	-1.055969245	1.020743226
563	C14H28N2O2	256.384	Cri-25.8-A	1.157756218	1.303818656
564	C16H34N2O	270.454	MG-XXXV-12B	-1.015210895	1.021287258
566	C14H28ClNO	261.831	MG-XXXIV-63B	-1.039700452	-1.04719939
567	C19H39NO	297.519	MG-XXXIV-67B	-1.095905299	1.075403779
568	C18H37NO	283.492	CM-08-6	1.026651103	1.014635187
570	C18H35NO	281.477	CM-08-6	-1.24428945	1.124776202
571	C18H35NO2	297.476	CM52.7A	1.054919361	-1.011509125
572	C21H41NO2	339.556	CM 53.7A	1.270719042	1.02216466
573	C21H43NO2	341.572	Aldrich	1.457170779	-1.153121148
574	C18H33NO	279.461	CM-08-6	-1.414353444	1.007415332
575	C19H37NO	295.503	CM-08-6	1.076842389	-1.009150027
577	C18H31NO	277.445	CM-08-6	1.141385259	1.006051997
578	C18H31NO	277.445	CM-08-6	1.136102895	1.375334872
579	C18H33NO	279.461	CM-08-6	1.022798501	1.015153006
580	C22H37NO	331.535	CM-08-6	3.42624563	1.01760648
581	C22H33NO	327.504	CM-08-6	1.10635568	1.257358861
583	C18H35NO2	297.476	CM-26-6	1.0583479	1.239411969
584	C18H37NO3	315.491	CM-18-6	-1.007684776	1.085293165
588	C7H13NO	127.184	MG-XXXIV-16A	1.036430672	1.250443412
589	C8H15NO	141.211	MG-XXXV-31A	-1.027850728	-1.006890525
592	C13H23NO	209.328	MG-XXXII-74A	-1.073912534	1.055065331
593	C14H25NO	223.354	MG-XXXI-77B	-1.026922612	1.027329108
594	C14H25NO	223.354	MG-XXXII-76B	-1.08395795	1.037220654
595	C13H17NO	203.28	MG-XXXIV-18B	-1.229574488	1.111734368
596	C20H41NO2	327.545	CM-61-6	1.52774807	1.17627358
597	C19H39NO2	313.518	CM-62-6	4.76670948	1.002294046
598	C15H21NO2	247.333	JRS	1.014048	1.119488859
599	C14H19NO2	233.306	JRS	1.048686851	1.125228836
600	C15H21NO	231.333	MG-XXXIV-06A	-1.142114377	-1.15630842
602	C15H21NO	231.333	MG-XXXIV-13B	1.007539855	1.119418898
603	C15H19NO	229.317	MG-XXXIV-82B	1.399186841	1.236814764
604	C14H19NO	217.307	MG-XXXIV-19A	1.012227074	1.007812734
605	C17H25NO	259.387	MG-XXXII-95A	1.043659135	-1.005219823
606	C17H25NO	259.387	MG-XXXIII-6A	1.059127599	-1.084462372
607	C17H25NO	259.387	MG-XXXIII-90A	-1.288711352	1.032018873
608	C9H9NO	147.174	MG-XXXIV-48B	1.031646967	1.011621962
609	C13H11NO	197.233	Aldrich	-1.013724126	1.094998137
610	C14H13NO	211.259	MG-XXXIV-21A	-1.000910186	-1.008318225
611	C17H19NO	253.339	MG-XXXIII-92B	1.052411212	-1.273784973
614	C6H13NO2S	163.238	MG-XV-22A	-1.143397469	1.010186127
621	C13H16ClNOS	269.79	MG-XXX-5B	7.02367346	1.819317112
622	C13H23NOS	241.393	MG-XXX-21A	1.982950915	1.768511825

623	C13H16ClNOS	269.79	MG-XXX-49B	1.430400302	1.053909392
633	C17H16F2N2O2	318.318	Y1-04	1.223164678	1.104152001
634	C18H18F2N2O2	332.345	Y1-06	-1.09109492	-1.05961143
635	C22H26F2N2O2	388.451	Y1-10	1.009566218	-1.050419581
636	C20H14F2N2O3	368.334	Y1-13	-1.102997171	1.045731398
637	C21H23F2N3O2S	419.488	Y1-28	-1.406995388	-1.276924083
638	C15H9F2N3O2	301.248	Y1-36	1.093859879	1.015952827
639	C20H14F2N2O2	352.334	Y1-42	1.281761346	-1.022703788
640	C14H8ClF3N2O2	328.674	Y2-01	1.161029623	-1.019878056
641	C17H16Cl2N2O2	351.227	Y3-04	1.010246488	1.080907126
642	C18H18Cl2N2O2	365.254	Y3-06	2.182820096	1.139120867
2015	C17H28N2O2	292.416	Atrazine - Chemservice	-1.117377852	-1.084178301
2016	C26H36N2O4	440.575	Simazine - Chemservice	1.064835056	1.065559497
2017	C24H32N2O4	412.522	Simetryn	1.179895974	-1.218309208
2018	C24H31N3O2	393.522	Cyanuric acid	-1.242783437	1.00530512
2019	C21H21F3N2O5	438.397	Propazine	-1.402476279	-1.25087205
2020	C21H21F3N2O5	438.397	Ametryn	1.008795195	-1.297642349
2021	C21H22N2O6	398.409	Prometryn	-1.408905092	-1.326407437
2022	C23H32FN3O	385.518	2-chloro-4-isopropyl-6-amino-s-triazine	-1.000433931	-1.359755549
2023	C17H16N2O3S	328.386	2-chloro-4-ethylamino-6-amino-s-triazine	-1.15427319	-1.063872164
2024	C16H14N2O	250.295	Ammelide	-1.151743133	-1.024946019
2025	C21H40N2O3	368.554	Ammeline	1.136466922	-1.009332013
2026	C19H36N2O2S	356.566	Cyanazine	-1.307853043	-1.021383495
2027	C19H35NO4	341.486	Terbutryn	-1.095480376	-1.05647066
2028	C22H36O3	348.519	Prometon	-1.055118718	-1.345580605
2029	C20H38N2O3	354.527	2-chloro-4,6-diamino-s-triazine	1.025865042	-1.002796607
2030	C19H35NO4	341.486	Dazomet - Chemservice	-1.022992844	1.008466594
2031	C20H37NO3	339.513	Carbaryl - Chemservice	1.625679683	1.20236306
2032	C19H28N2O2	316.438	Propoxur - Chemservice	1.077785103	-1.054115487
2033	C14H9Cl2F3N2O	349.135	Aldicarb - Chemservice	-1.019859947	-1.103961576
2034	C21H39O6P	418.505	Aldoxycarb	-1.122739985	1.03919888
2035	C20H26F3N3O4	429.433	Isopropyl-N-[m-chlorophenyl]carbamate - Chemservice	1.31987479	-1.039081622
643	C20H22Cl2N2O2	393.307	Y3-08	-1.104345529	-1.017833661
644	C16H14Cl2N2O3	353.2	Y3-13	1.080795457	-1.115636975
645	C18H19Cl2N3O4S	444.332	Y3-14	1.113889128	-1.149637921
646	C18H17Cl2N3O4S	442.316	Y3-16	1.221306841	1.062493064
647	C14H9Cl3N2O2	343.592	Y3-24	1.194528237	-1.064642713
648	C14H9Cl2N3O4	354.145	Y3-25	1.024197911	1.16199331
649	C14H9Cl3N2O2	343.592	Y3-27	1.186494764	1.2785782
650	C14H9Cl2N3O4	354.145	Y3-28	1.221364275	-1.093528921
651	C18H12Cl2N2O2	359.206	Y3-29	1.001990606	-1.032258674
652	C14H11ClN2O2	274.702	Y4-01	1.127216266	1.165298415

653	C16H16ClN3O2	317.77	Y4-17	-1.041874021	1.001577896
654	C14H10ClFN2OS	308.758	Y4-37	1.123321531	-1.04298333
655	C14H11ClN2OS	290.768	Y4-38	1.037644366	1.13616332
656	C16H14F2N2O3	320.291	Y5-04	-1.069523211	1.29441128
657	C17H16IN3O4S	485.296	Y6-11	-1.135196768	1.1298875
658	C17H16N4O6S	404.397	Y6-12	1.149338414	1.17191666
659	C14H18N2O2	246.305	Y7-02	1.06046109	1.392898399
660	C20H30N2O2	330.464	Y7-03	-1.093060871	-1.150580012
661	C20H29ClN2O2	364.909	Y7-06	-1.071210541	1.006219326
662	C15H16N2O	240.3	Y7-04	-1.026081081	-1.167251846
663	C14H17ClN2O2	280.75	Y7-05	1.127766821	1.020620508
664	C14H14N2O	226.274	Y7-07	-1.068036056	-1.016690621
665	C14H13ClN2O	260.719	Y7-08	1.075071166	1.22469099
666	C15H13ClN2O2	288.729	Y7-09	-1.345216352	-1.003913002
667	C20H15ClN2O3	366.798	Y7-10	-1.436203928	-1.518924112
668	C20H16N2O3	332.353	Y7-11	1.099673893	1.061604077
669	C15H14N2O2	254.284	Y7-12	-1.115333119	-1.0705348
670	C18H20N2O2	296.364	Y7-13	1.492150037	1.374011705
671	C9H13N	135.206	Aldrich	-1.154133848	1.092268864
2036	C17H22F3N3O4	389.369	Isopropyl-N-phenylcarbamate - Chemservice	-1.05570906	-1.334971094
2037	C19H30N2O2	318.454	Oryzalin	-1.014454704	1.073983922
2038	C21H39O6P	418.505	2-methylheptyl-4,6-dinitrophenyl Crotonate-chemser	1.490642964	-1.117986831
2039	C19H37O6P	392.467	DNBP - Chemservice	1.947956549	-1.070616938
2040	C21H39O5P	402.505	4.6-Dinitro-o-cresol - Chemservice	1.17025813	-1.080541474
2041	C20H39O5P	390.494	Triclopyr - Chemservice	-1.012170288	-1.2284196
2042	C22H41O5P	416.532	Fluroxypyr	-1.001908164	-1.060432162
2043	C22H42NaO6P	456.529	Clopyralid	1.037368275	-1.096022908
2044	C20H39ClNaO6P	464.937	Picloram	-1.082370048	1.004189354
2045	C22H41FNaO6P	474.519	Mecoprop	-1.118237653	1.007649411
2046	C20H40NaO7P	446.491	Glyphosate	-1.037734124	-1.034864867
2047	C12H26O3S	250.398	Paraquat dichloride	-1.018179718	-1.100255405
2048	C20H39BrNaO6P	509.388	Diethyl phthalate	1.013915931	-1.011071605
2049	C20H40NaO7P	446.491	Bromacil	1.091818823	1.098301284
2050	C12H7Cl3O2	289.542	Rotenone	3.691221816	-1.276305392
2051	C24H35N3O3	413.553	Captan - Chemservice	1.110013353	-1.005220909
2052	C30H31N3O3	481.585	Folpet - Chemservice	16.20047243	1.717682584
2053	C26H31N3O2	417.543	Cacodylic acid, Na salt - Chemservice	-1.011385981	1.169664186
2055	C16H14N4O3S	342.372	Chloranocryl - Chemservice	1.189989889	-1.069239042
2056	C17H15N3O3S	341.384	Diphenylacetonitrile - Chemservice	1.067895002	1.015771029
2057	C16H24N2O	260.375	Maleic acid hydrazide - Chemservice	1.080543585	1.07862235

2059	C19H19N5O	333.387	Nicotine - Chemservice	1.036584187	-1.147901352
2060	C20H30N2O3	346.464	Ziram - Chemservice	24.38574274	-1.052273802
2061	C18H28N2O3	320.427	Nabam - Chemservice	-1.133650414	1.164299113
2062	C17H14N2O4S	342.369	Metam sodium - Chemservice	-1.152547261	-1.254425043
2063	C21H20N2O4S	396.459	Molinate - Chemservice	-1.293474458	-1.128142101
2064	C19H18N2O4S	370.422	Thiobencarb - Chemservice	-1.02945433	1.080870161
2065	C6H7NO2S	157.19	Eptam - Chemservice	-1.072992245	1.310693022
2066	C17H16N2O3S	328.386	CDEC - Chemservice	-1.106587144	1.094361067
2067	C24H27N3O3S	437.554	Ferbam - Chemservice	1.227851702	-1.131492982
2068	C28H32N4O3S	504.644	Maneb - Chemservice	1.367449922	1.325674084
2069	C25H21F3N4O3S	514.519	Zineb - Chemservice	1.134778078	-1.000116175
2070	C27H25F3N4O3S	542.573	Tetramethylthiuram disulfide - Chemservice	1.194106777	-1.124086776
2071	C27H23N3O4S	485.554	s-propyl butylethylthiocarbamate - Chemservice	-1.074177761	-1.109930432
2072	C17H14F3N3O2S	381.372	Pirimiphos - methyl - Chemservice	-1.104946566	-1.055799312
2073	C18H29N3O2	319.442	Pirimiphos - ethyl - Chemservice	1.269532507	1.03457947
2074	C15H18F3N3O3	345.317	Diazinon - Chemservice	1.077257955	1.019610223
2075	C17H20F3N3O5	403.353	Malathion	1.051036657	-1.011662733
2076	C23H37N3O3	403.558	Chlorpyrifos - Chemservice	1.006156019	-1.19681576
2077	C17H28N2O2	292.416	Chlorpyrifos oxon - Chemservice	1.059682849	-1.245006349
2078	C17H28N2O2	292.416	2-diethylamino-6-methylpyrimidin-4-ol	-1.143812873	-1.222749253
2079	C26H36N2O4	440.575	Methamidophos - Chemservice	-1.126998184	1.122333938
688	C10H9N	143.185	Aldrich	1.228461253	-1.027782677
689	C10H24N2	172.311	Aldrich	-1.078194852	-1.043571526
690	C12H27N	185.349	Aldrich	-1.008520441	-1.054787792
692	C10H9N	143.185	Aldrich	4.777865603	1.113708415
697	C8H19N	129.243	Aldrich	-1.035436782	1.062324759
2080	C24H32N2O4	412.522	Diethyl phosphate - Chemservice	-1.181656418	1.066895054
2081	C24H31N3O2	393.522	3,5,6-trichloro-2-pyridinol	1.00821137	-1.111116002
2082	C21H21F3N2O5	438.397	Methidathion	1.029083898	1.184144954
2083	C21H21F3N2O5	438.397	6-chloromethyl-4-hydroxy-2-isopropyl pyrimidine	-1.045429841	-1.015552637
2084	C21H22N2O6	398.409	2-methoxy-3,5,6-trichloropyridine	1.005749973	-1.108759891
2085	C23H32FN3O	385.518	Parathion	-1.100872316	-1.008549187
2086	C17H16N2O3S	328.386	Des-N-isopropyl isophenphos oxygen analog	-1.240403697	-1.134217676
2087	C16H14N2O	250.295	Des-N-isopropyl isophenphos	-1.214731678	1.095256854
2088	C21H40N2O3	368.554	o,o-diethylthiophosphate	1.056648134	1.089148134
2089	C19H36N2O2S	356.566	Tributyl (2,4-	1.768824223	1.102758254

			dichlorobenzyl)phosphonium chloride		
2090	C19H35NO4	341.486	Tributyl phosphorotrithioite	-1.002599335	-1.039203432
2091	C22H36O3	348.519	Phosdrin - Chemservice	1.122018735	-1.116839669
2092	C20H38N2O3	354.527	Carbophenothion - Chemservice	1.51211785	1.101302886
2093	C19H35NO4	341.486	DDVP - Chemservice	-1.142796682	-1.104179163
2094	C20H37NO3	339.513	o,o-dimethyl phosphochloridothioate	-1.053563141	1.063052599
2095	C19H28N2O2	316.438	Dichlorprop - Chemservice	-1.119228913	1.035434302
2096	C14H9Cl2F3N2O	349.135	2,4-D - Chemservice	-1.415725063	1.002515426
2097	C21H39O6P	418.505	2,4,5-T	1.280146022	-1.002821315
2098	C20H26F3N3O4	429.433	p,p-DDT	-1.029424654	-1.172431339
2099	C17H22F3N3O4	389.369	o,p'-DDD	1.578001016	-1.046182168
2100	C19H30N2O2	318.454	p,p-DDD	3.70330036	-1.007918778
2101	C21H39O6P	418.505	p,p-DDE	-1.305487447	-1.015308605
2102	C19H37O6P	392.467	o,p'-DDE	-1.112383085	-1.115335358
2103	C21H39O5P	402.505	2,4-DB	1.000969298	1.127962327
2104	C20H39O5P	390.494	Dalapon	-1.247594829	1.044112855
2105	C22H41O5P	416.532	Heptachlor	1.337017621	1.198771722
2106	C22H42NaO6P	456.529	Heptachlor epoxide	3.392046302	1.133823517
2107	C20H39ClNaO6P	464.937	Aldrin	1.255754244	1.079930856
2108	C22H41FNaO6P	474.519	Dieldrin	2.591730576	1.031659568
2109	C20H40NaO7P	446.491	2,2'-methylenebis(4-chlorophenol) - Chemservice	1.11778608	1.126579725
2110	C12H26O3S	250.398	Pentachlorophenol - Chemservice	6.638174987	1.019887347
2111	C20H39BrNaO6P	509.388	2,3,4,6-Tetrachlorophenol - Chemservice	3.006485512	-1.080107134
2112	C20H40NaO7P	446.491	2,4,5-trichlorophenol - Chemservice	1.286144148	-1.261988422
859	C14H9BrF2N2O2	355.134	Y1-47	1.416563023	1.33538423
860	C15H9F5N2O2	344.236	Y1-45	1.475318972	1.007200879
861	C15H9F5N2O2	344.236	Y1-46	1.038477172	-1.338751152
862	C20H14F2N2O4S	416.398	Y1-24	-1.538463042	-1.604397156
863	C20H13F2N3O6S	461.396	Y1-23	-1.054483514	-1.230125762
864	C18H17F2N3O4S	409.407	Y1-29	-1.218349656	1.064079964
865	C16H15F2N3O4S	383.37	Y1-26	-1.980727636	-1.069483474
866	C18H19F2N3O4S	411.423	Y1-21	-1.58162161	-1.247153093
867	C22H19F2N3O4S	459.466	Y1-22	2.853807227	-1.807287757
868	C20H13ClF2N2O5S	466.842	Y1-27	-1.016281988	-1.147981126
869	C19H13F2N3O3	369.322	Y1-20	1.284211317	1.114602804
2113	C12H7Cl3O2	289.542	2,4,6-trichlorophenol - Chemservice	1.270019729	1.336420673
2114	C24H35N3O3	413.553	Chloranil - Chemservice	2.418171979	-1.133689892
2115	C30H31N3O3	481.585	Dichlone - Chemservice	7.541895191	-1.006484304
2116	C26H31N3O2	417.543	o-Chlorophenoxyaceric acid - Chemservice	1.321767285	1.014271156

2117	C16H13N3O4S	343.357	p-Chlorophenoxyaceric acid - Chemservice	1.503758969	-1.063610398
2118	C16H14N4O3S	342.372	MCPA - Chemservice	1.252122033	-1.006968424
2119	C17H15N3O3S	341.384	2,4-Dichlorophenoxyacetic acid, butyl ester	-1.122039105	-1.065026348
2120	C16H24N2O	260.375	2,4-Dichlorophenoxyacetic acid, isopropyl ester	-1.037066182	-1.031360103
2121	C22H38N2O	346.55	2,4,5-Trichlorophenoxyacetic acid, isopropyl ester	1.068226539	1.20392904
2122	C19H19N5O	333.387	Silvex - Chemservice	1.349046552	1.011305327
2129	C17H16N2O3S	328.386	Tedion - Chemservice	1.474184521	1.084716431
870	C18H16F2N2O3	346.328	Y1-39	1.082697462	1.075397231
871	C14H9F3N2O2	294.229	Y1-30	-1.064202611	-1.061117819
872	C14H9BrF2N2O2	355.134	Y1-32	-1.044948045	-1.375020203
873	C15H9F5N2O2	344.236	Y1-35	-1.09861516	-1.246782852
874	C20H14F2N4O2	380.348	Y1-41	-1.01099243	-1.187550947
875	C16H12F2N2O3	318.275	Y1-37	1.070578956	1.035780359
876	C16H12F2N2O4	334.274	Y1-44	1.044596123	1.277858191
877	C14H9F2IN2O2	402.135	Y1-33	-1.030580763	1.015735932
878	C14H9F2N3O4	321.236	Y1-34	-1.1858192	1.217099137
879	C16H11F2N3O2	315.274	Y1-38	1.384940992	1.20754542
880	C15H11ClF2N2O2	324.71	Y2-04	1.149220163	-1.024588327
881	C16H14F2N2O2	304.291	Y2-18	1.17509945	-1.169498396
882	C14H8Cl2F2N2O2	345.128	Y2-17	1.015371408	1.139721593
883	C15H11ClF2N2O2	324.71	Y2-19	1.023938773	-1.01758664
884	C14H8Cl2F2N2O2	345.128	Y2-02	1.015652579	-1.13278668
885	C16H14F2N2O2	304.291	Y2-03	1.153032722	-1.213159594
886	C15H8F6N2O2	362.227	Y2-16	1.000811176	1.073058141
887	C14H8Cl2F2N2O2	345.128	Y2-20	1.049151539	1.053048483
888	C16H14F2N2O2	304.291	Y2-27	-1.022194084	1.086958828
889	C16H14F2N2O2	304.291	Y2-13	-1.042414568	1.46330405
890	C18H17BrF2N2O2	411.241	Y2-07	3.35657024	1.297763165
891	C15H11BrF2N2O3	385.16	Y2-10	2.408969496	1.229355927
892	C15H8ClF5N2O2	378.681	Y2-09	2.443486507	-1.034910379
893	C15H11BrF2N2O2	369.161	Y2-12	1.45012672	-1.329237391
894	C14H8Cl2F2N2O2	345.128	Y2-06	1.898475612	-1.0749967
895	C19H20F2N2O2	346.371	Y2-14	4.409694216	1.404846062
896	C18H17F2N3O4	377.342	Y2-08	1.145165668	-1.074382619
897	C15H11BrF2N2O2S	401.226	Y2-11	1.026571221	-1.051473817
898	C16H13BrF2N2O2	383.187	Y2-15	1.487446214	1.413280956
899	C14H8ClF3N2O2	328.674	Y2-05	-1.003820021	1.916306276
900	C15H11BrF2N2O2	369.161	Y2-25	-1.07714809	1.05729885
901	C15H8ClF5N2O2	378.681	Y2-22	-1.029806302	-1.097115013
902	C15H8BrF5N2O3	439.132	Y2-24	-1.081144907	1.025744292
903	C16H13BrF2N2O2	383.187	Y2-28	-1.036203323	-1.001970874

904	C16H14F2N2O2	304.291	Y2-29	1.177480017	1.481150575
905	C15H11ClF2N2O2	324.71	Y2-26	-1.056253579	-1.036011347
906	C15H8F6N2O2	362.227	Y2-23	1.061839186	1.14182561
907	C18H17BrF2N2O2	411.241	Y2-21	1.012291325	1.489189008
908	C14H8Cl2F2N2O2	345.128	Y2-30	1.094162783	1.105300698
909	C16H8F8N2O2	412.234	Y2-31	1.545475624	-1.228715784
910	C15H10BrClF2N2O2	403.606	Y2-34	-1.067762372	1.122970179
911	C14H7BrClF3N2O2	407.57	Y2-33	1.014956119	1.007821913
912	C15H7F7N2O2	380.217	Y2-46	1.033027789	-1.089964138
913	C15H7BrF6N2O2	441.123	Y2-45	-1.011298505	1.273419739
914	C15H7BrF6N2O3	457.122	Y2-51	1.127242278	1.016701969
915	C15H10BrClF2N2O2	403.606	Y2-35	1.160897574	-1.047771306
916	C14H7Cl3F2N2O2	379.573	Y2-32	1.036469489	-1.192553626
917	C15H7F7N2O3	396.217	Y2-49	-1.043973968	-1.195033724
918	C14H7BrF3N3O4	418.122	Y2-50	1.115828628	-1.054414838
919	C17H14ClF3N2O3	386.753	Y2-44	1.298188806	-1.053058974
920	C21H24F2N2O2	374.424	Y1-09	-1.030469545	1.22854621
921	C21H14F2N2O3	380.344	Y1-40	1.091477245	-1.115806766
922	C16H7BrF8N2O2	491.13	Y2-40	1.441707923	-1.089982722
923	C15H7BrClF5N2O2	457.577	Y2-41	1.046453561	-1.147543273
924	C15H7Cl2F5N2O2	413.126	Y2-39	-1.06395347	-1.170877831
925	C15H7Cl2F5N2O2	413.126	Y2-38	-1.055513622	1.048842256
926	C15H7ClF6N2O2	396.672	Y2-48	1.03138272	-1.032467126
927	C14H7BrCl2F2N2O2	424.024	Y2-43	-1.109492335	1.018606997
928	C15H7ClF6N2O2	396.672	Y2-42	1.046810598	-1.135046389
929	C15H7ClF6N2O2	396.672	Y2-36	-1.10095147	1.033398207
930	C15H7BrClF5N2O2	457.577	Y2-37	-1.145589936	1.144023379
931	C15H7Cl2F5N2O2	413.126	Y2-47	-1.022739871	1.086339379
932	C15H7BrF6N2O2	441.123	Y2-56	1.180576215	1.143571601
933	C14H7BrF4N2O2	391.115	Y2-55	1.184442455	-1.043929905
934	C14H7Cl3F2N2O2	379.573	Y2-53	-1.056147099	1.68929499
1174	C16H24OS	264.426	CRI-19-12	-1.102007839	-1.082320055
935	C16H13BrF2N2O2	383.187	Y2-54	1.032331971	1.056282779
936	C14H6Cl2F4N2O2	381.109	Y2-60	-1.094977824	-1.170552567
937	C16H13BrF2N2O2	383.187	Y2-57	-1.019464604	1.024934868
938	C17H16F2N2O2	318.318	Y2-52	-1.018335559	-1.048726577
939	C16H7BrF8N2O2	491.13	Y2-58	6.301048533	1.012120539
940	C15H6Br2F6N2O2	520.019	Y2-59	1.499666499	-1.108744862
941	C15H12Cl2N2O2	323.174	Y3-02	1.537188007	-1.068201537
942	C22H26Cl2N2O2	421.36	Y3-10	-1.765080113	1.003203775
943	C15H12Cl2N2O3	339.173	Y3-12	1.170665959	1.233090377
944	C14H9Cl2FN2O2	327.138	Y3-18	-1.133200869	-1.170567622
945	C14H9Cl2IN2O2	435.044	Y3-20	5.625309192	1.061612723
946	C16H14Cl2N2O2	337.201	Y3-03	-1.022884917	1.038986278
947	C21H24Cl2N2O2	407.333	Y3-09	2.6279653	-1.081193384

948	C26H34Cl2N2O2	477.466	Y3-11	-1.055206176	1.017135164
949	C14H9Cl3N2O2	343.592	Y3-19	-1.043006828	1.209666583
950	C14H10Cl2N2O2	309.147	Y3-01	1.007455717	1.12940811
951	C14H9Cl2N3O4	354.145	Y3-22	-1.03030354	-1.017782822
952	C20H14Cl2N4O2	413.257	Y3-17	1.321211435	1.009253761
953	C16H15Cl2N3O4S	416.279	Y3-15	-1.722361829	-1.249389951
954	C15H9Cl2F3N2O2	377.145	Y3-21	1.092606383	-1.045694866
955	C15H9Cl2N3O2	334.157	Y3-23	-1.09845261	1.040773115
956	C20H14Cl2N2O2	385.243	Y3-26	-1.146853681	1.021248834
957	C14H8Cl4N2O2	378.038	Y3-34	-1.04509394	-1.023976932
958	C14H8Cl2F2N2O2	345.128	Y3-31	-1.07117422	-1.045419998
959	C20H9Cl3F5N3O3	540.655	Y1-52	1.669382804	-1.033549113
960	C14H9ClF2N2O2	310.683	Y1-51	1.475538488	1.98492887
961	C16H13ClF2N2O2	338.736	Y1-49	1.415052418	1.09947088
962	C14H8Cl4N2O2	378.038	Y3-33	1.202697194	1.040807532
963	C14H8Cl4N2O2	378.038	Y3-32	-1.030169868	1.082724729
964	C13H9Cl2N3O2	310.135	Y3-30	1.174569433	1.364346425
965	C22H14F2N2O2	376.356	Y1-53	1.083442783	-1.143712555
966	C15H11ClF2N2O2	324.71	Y1-50	1.006577167	-1.109025576
967	C13H8BrF2N3O2	356.122	Y1-54	-1.093507198	1.145369707
968	C14H11ClN2OS	290.768	Y4-34	-1.10169876	1.1568736
969	C15H13ClN2OS	304.795	Y4-36	-1.050924853	-1.214813839
970	C14H10Cl2N2OS	325.213	Y4-35	1.014961927	-1.198666604
972	C14H10Cl2N2O2	309.147	Y4-08	1.153741495	-1.08128023
973	C14H10ClIN2O2	400.599	Y4-02	1.247327586	1.209191157
974	C14H10ClN3O4	319.7	Y4-19	-1.085781417	-1.131173839
975	C15H13ClN2O2S	320.794	Y4-07	1.003678324	1.029678641
976	C15H13ClN2O2	288.729	Y4-06	-1.00211925	-1.002612655
977	C14H10ClFN2O2	292.693	Y4-15	1.016914908	1.260889288
979	C15H10ClF3N2O2	342.7	Y4-13	-1.00087969	-1.190689838
980	C15H10ClN3O2	299.712	Y4-14	1.152050324	-1.321183913
981	C16H13ClN2O3	316.739	Y4-03	-1.075442099	-1.092828404
982	C16H15ClN2O2	302.755	Y4-18	1.099034625	1.355339057
983	C17H17ClN2O2	316.782	Y4-11	-1.020923634	1.091415654
1175	C24H33BrN2O2	461.435	SHH-01-003	-1.003372663	1.104186126
984	C15H13ClN2O3	304.728	Y4-04	-1.038566591	-1.055690614
985	C14H10ClFN2O2	292.693	Y4-10	1.088466761	1.105966907
986	C14H10ClFN2O2	292.693	Y4-28	1.131227177	-1.065748198
987	C14H10BrClN2O2	353.598	Y4-24	-1.109403462	-1.062454555
988	C15H13ClN2O2	288.729	Y4-25	-1.053935278	-1.069756553
989	C14H9BrClFN2O2	371.589	Y4-21	1.486327518	-1.002461651
990	C20H15ClN2O2	350.798	Y4-12	1.320133949	1.083242062
991	C16H15ClN2O3	318.755	Y4-05	-1.048083866	-1.103245482
992	C15H10ClN3O2	299.712	Y4-09	-1.0850148	-1.015635292
993	C14H10Cl2N2O2	309.147	Y4-27	1.06341134	-1.121074232

994	C14H10ClN3O4	319.7	Y4-26	1.063168647	1.128356892
995	C15H12Cl2N2O2	323.174	Y4-22	1.595584244	1.03621021
996	C18H19ClN2O2	330.809	Y4-23	-1.016986294	1.008425123
997	C28H23ClN2O4	486.946	Y4-20	3.320145562	-1.192795924
998	C13H9Cl2N3O2	310.135	Y4-32	-1.007359111	-1.014557771
999	C12H9ClN2O3	264.664	Y4-33	1.221634943	-1.060268749
1000	C12H13ClN2O2	252.697	Y4-30	1.200705903	-1.139332563
1001	C11H11ClN2O2	238.67	Y4-29	-1.070669303	1.056652241
1002	C12H15ClN2O2	254.713	Y4-31	-1.080254887	-1.062116179
1003	C14H9ClF2N2O2	310.683	Y5-06	1.359752646	1.383129448
1004	C15H12F2N2O3	306.264	Y5-03	-1.034523265	1.00518594
1005	C21H16F2N2O3	382.36	Y5-05	-1.005685127	-1.057427514
1006	C18H19ClN2O2	330.809	Y5-10	1.071618464	-1.163933136
1007	C14H10ClFN2O2	292.693	Y5-11	1.247656481	-1.194140197
1008	C16H15ClN2O2	302.755	Y5-12	-1.094373754	1.471725252
1009	C15H12F2N2O2	290.265	Y5-01	1.559203871	-1.064745991
1010	C20H22F2N2O2	360.398	Y5-02	1.180701833	-1.158569607
1011	C14H9Cl3N2O2	343.592	Y5-09	1.112288181	1.054209669
1012	C14H10BrClN2O2	353.598	Y5-07	1.160838023	1.017413892
1013	C16H15ClN2O3	318.755	Y5-08	-1.003293293	-1.015271379
1014	C21H10Cl3F5N2O3	539.667	Y5-14	1.046407485	1.356013651
1015	C21H10Cl5F3N2O3	572.576	Y5-17	1.011470366	1.003038614
1016	C25H20Cl3F3N2O3	559.792	Y5-16	1.016619063	-1.109774614
1017	C21H11BrCl3F3N2O3	582.582	Y5-15	1.310637838	1.219931798
1018	C23H16Cl3F3N2O4	547.738	Y5-13	-1.045353934	1.261311321
1019	C15H10F3N3O2S	353.319	Y6-01	1.073441745	1.216702734
1020	C15H10BrF2N3O2S	414.225	Y6-03	1.133691724	1.484633341
1021	C15H10ClF2N3O2S	369.774	Y6-02	1.063556634	1.113865777
1022	C15H10F2IN3O2S	461.225	Y6-04	1.387032492	-1.010091729
1023	C15H10Cl3N3O2S	402.683	Y6-06	-1.091322788	-1.091657602
1024	C17H15N3O3S	341.384	Y6-13	1.058538597	1.072874031
1025	C17H14ClN3O3S	375.829	Y6-19	-1.044172237	1.083619828
1026	C17H14N4O5S	386.382	Y6-21	1.003054569	1.144647798
1027	C18H17N3O3S	355.411	Y6-14	1.235096384	1.031285915
1028	C18H17N3O4S	371.41	Y6-16	-1.182374962	-1.344119983
1029	C17H14FN3O3S	359.375	Y6-18	1.183654233	-1.07788492
1030	C17H14BrN3O3S	420.28	Y6-20	-1.069323618	1.115563952
1031	C18H14N4O3S	366.394	Y6-22	-1.036584928	-1.275272958
1032	C20H21N3O3S	383.464	Y6-15	1.314642783	-1.037661943
1033	C19H19N3O4S	385.437	Y6-17	-1.358523954	-1.045744236
1034	C15H9ClFN3OS	333.768	Y6-25	-1.081893023	-1.203346744
1035	C16H12ClN3OS	329.804	Y6-28	-1.097219089	1.036886897
1036	C15H8ClF2N3OS	351.758	Y6-23	1.009086532	-1.115577488
1037	C15H9ClIN3OS	441.674	Y6-26	-1.075799668	1.264993057
1038	C15H9ClN4O3S	360.775	Y6-27	-1.065629939	1.031310991

1039	C15H8Cl3N3OS	384.668	Y6-24	-1.108035094	1.068006465
1040	C18H20N2O2	296.364	Y6-31	-1.09268559	1.019005156
1041	C22H28N2O3	368.469	Y6-32	1.004777002	1.037012437
1042	C22H28N2O2	352.47	Y6-30	-1.028678083	-1.093411493
1043	C8H9N3S	179.242	Y6-29	-1.008368293	1.221721122
1044	C17H17N3O4S	359.4	Y6-07	1.167162623	1.104894272
1045	C17H16ClN3O4S	393.845	Y6-09	1.098555683	-1.010533899
1046	C17H16FN3O4S	377.39	Y6-08	-1.050771472	1.039056387
1047	C17H16BrN3O4S	438.296	Y6-10	1.108968934	1.03765752
1048	C8H9NO2	151.163	Y6-33	-1.132469884	1.10298709
1049	C11H15NO3	209.242	Y6-37	1.070695518	-1.010777036
1050	C13H19NO2	221.295	Y6-34	-1.204238611	1.137327918
1051	C13H19NO2	221.295	Y6-39	-1.188135103	-1.098324375
1052	C9H10N2O4	210.187	Y6-38	-1.012444142	-1.067014834
1053	C9H10N2O4	210.187	Y6-36	-1.028803111	1.21169284
1054	C9H10N2O4	210.187	Y6-35	-1.200018077	-1.199384792
1191	C24H36N4O	396.569	LH-19	1.027278748	1.234531793
1060	C13H18O2	206.281		1.186164267	-1.47602476
1063	C14H24N2O2	252.353	LH-1	-1.153781702	-1.022883152
1064	C16H28N2O2	280.406	LH-2	1.02805602	1.027054376
1065	C12H20N2O4	256.298	LH-3	1.074249078	1.051757926
1066	C10H20N2O2	200.278	LH-5	-1.023981574	-1.119702234
1067	C14H17N3O4	291.302	LH-6	-1.053982178	-1.079156944
1068	C15H20N2O2	260.332	LH-8	-1.169713554	-1.177622642
1069	C12H22N2O2	226.315	LH-7	-1.004334854	1.004004874
1070	C18H24N2O4	332.394	LH-9	1.093243507	1.141573301
1071	C15H22N4O4	322.36	LH-10	-1.28459419	1.097946484
1072	C14H24N2O4	284.351	LH-11	-1.064263077	-1.187240146
1073	C14H22N2O6	314.334	LH-12	1.007389198	1.00145382
1074	C15H12N4O6	344.279	LH-13	-1.315428734	-1.125680127
1075	C17H18N2O4	314.336	LH-14	-1.469053678	-1.031211863
1076	C15H12Cl2N2O2	323.174	LH-15	-1.329781393	-1.047877896
1077	C11H22N2O2	214.305	LH-16	-1.449262538	1.169835414
1078	C17H22N2O2	286.369	LH-17	-1.008467172	1.259895093
1079	C13H22N2O2	238.326	LH-18	1.244079714	-1.106001487
1081	C22H41N3O4S	443.644	KIH-271-70	-1.128466514	1.041428483
1082	C28H38N2O5	482.612	KIH-271-69B	1.415324272	1.083093715
1084	C21H33N3O3	375.505	KIH-271-67C	-1.155137673	-1.042779624
1085	C22H30N2O3	370.485	KIH-271-81	-1.307451766	-1.0696429
1087	C26H33N3O5	467.557	KIH-271-79C	1.108320221	-1.159534619
1088	C26H36N2O5	456.574	KIH-271-77	-1.085480496	1.418129163
1089	C31H38N2O5	518.644	KIH-271-78	-1.115701834	-1.053964916
1090	C22H40N2O4	396.564	KIH-271-86	1.072120934	-1.107343994
1093	C8H16O2	144.211	ALDRICH	1.003309723	1.129772543
1096	C30H46N2O6	530.696	KIH-284-13	-1.002316385	-1.200077307

1099	C27H42N2O4	458.633	KIH-284-12	-1.160135032	-1.134766601
1100	C23H39N3O2	389.575	KIH-284-03	-1.030753073	1.172951439
1102	C10H17NO3	199.247	FH-010B-1	-1.138025201	-1.028841485
1103	C11H19NO3	213.273	FH-014A-1	-1.163466439	1.272619617
1104	C14H19NO	217.307	FH-015A-1	-1.071727655	-1.068978678
1105	C15H21NO2	247.333	FH-016A-1	-1.075628067	-1.035122826
1106	C14H18ClNO	251.752	FH-015B-1	1.154476996	1.109807775
1107	C21H29NO	311.461	FH-017A-1	1.088821825	1.11474978
1108	C14H19NO	217.307	FH-019-1	1.092387252	-1.374010129
1109	C14H18ClNO	251.752	FH-022A-1	1.05888721	-1.101529288
1110	C15H21NO2	247.333	FH-022B-1	-1.19526289	-1.130821079
1111	C16H23NO	245.36	FH-023A-1	1.373463158	1.184535789
1113	C28H44N2O4	472.66	KIH-284-19	1.508862484	1.087074384
1114	C23H42N2O4	410.591	KIH-284-22	1.152844604	-1.041058461
1116	C32H48N4O5S	600.812	KIH-284-29	1.390413536	-1.055626266
1117	C13H26N2O2	242.358	PDJ-II-38	-1.00157648	-1.03772047
1118	C13H19ClN2O2	270.755	PDJ-II-44	1.048769952	-1.046500453
1119	C21H36N2O2	348.523	PDJ-I-2	-1.163447527	-1.072094525
1120	C13H17ClN2O	252.74	PDJ-II-47	1.348194186	-1.079213811
1122	C20H32N2O2	332.48	KIH-284-32	-1.050390831	1.215580197
1123	C22H36N2O2	360.533	KIH-284-33	1.178947007	1.128186055
1126	C31H46N4O4S	570.786	KIH-284-43	1.054067695	1.042838327
1127	C17H24ClNO3	325.83	KIH-284-36	1.005193797	-1.188061538
1128	C17H24ClNO3	325.83	KIH-284-37	-1.062420215	-1.170251798
1129	C22H39NO	333.551	KIH-284-44	-1.066047121	1.007792785
1130	C17H25NO	259.387	FH-025B-1	-1.043104892	-1.01217914
1131	C21H29NO	311.461	FH-026A-1	1.490170394	1.101918092
1132	C17H25NO	259.387	FH-020B-1	-1.014414937	1.238261791
1133	C16H23NO	245.36	FH-025A-1	1.138126051	-1.022094641
1135	C14H22N2O2	250.337	PDJ-II-81	1.195841738	-1.201073214
1136	C25H42N6O4S	522.704	PDJ-II-62	-1.018200716	-1.169256959
1139	C20H15ClF3N3O5	469.798	Dupont JT333	-1.096601601	-1.016984175
1140	C22H17ClF3N3O7	527.834	Dupont MP062	1.303834743	1.046779672
1141	C33H59N3O4	561.839	AUDA-Laa	3.222831334	-1.189305566
1142	C39H69N3O9	723.98	AUDA-Laa-GLC	1.078163582	-1.057971144
1143	C26H48N2O4	452.67	KIH-284-45	1.010146131	-1.079021827
1144	C23H39F3N2O3	448.563	KIH-284-51	1.598924417	1.116230896
1148	C22H38N2O4	394.548	KIH-284-56	1.085661094	-1.205207588
1149	C29H37N3O5	507.621	KIH-284-60-trans	1.501359509	1.291657204
1151	C26H38N6O5	514.617	CRI-01-12	1.208823982	1.016832373
1152	C26H40N6O5S	548.698	CRI-03-12	1.104204763	-1.023015137
1155	C18H31N3O2	321.458	KIH-284-76	-1.113375072	-1.133606319
1156	C21H35NO3	349.507	KIH-284-77	-1.112914578	1.209162615
1157	C22H39NO	333.551	KIH-284-78	1.052664408	1.277132783
1159	C15H23NO2	249.349	CRI-13-12-A	-1.027892212	-1.039154207

1160	C15H22N2O	246.348	JRS-Amide-1	1.381046256	-1.080692548
1162	C24H35NO2	369.54	KIH-284-71	1.736117816	1.453103729
1163	C15H25N3O2	279.378	KIH-284-74	1.071756209	-1.017694498
1164	C23H34N2O4	402.527	KIH-284-79	-1.012322002	-1.022580074
1165	C23H34N2O4	402.527	KIH-284-80	1.069108892	-1.001043181
1166	C26H39NO2	397.593	KIH-284-82	1.680751953	-1.091122142
1167	C27H41NO2	411.62	KIH-284-83	1.109697094	1.018159629
1169	C21H32N2O2	344.491	KIH-284-86A	1.014501213	1.139641436
1170	C25H45N3O4S	483.707	KIH-284-87	1.083938221	1.077609685
1171	C24H34N2O2	382.539	SHH-01-001	1.179006688	1.125735491
1173	C23H40N2O3	392.575	Cri-76-7	1.064271376	-1.109041318
1176	C17H26N2O	274.401	SHH-01-004	-1.070748126	-1.030530872
1177	C14H19N3O	245.32	SHH-01-009	-1.109606043	-1.077434046
1178	C24H32F2N2O2	418.52	SHH-01-013	-1.054541891	2.204369124
1179	C24H32Cl2N2O2	451.429	SHH-01-014	1.023961093	-1.076319629
1180	C17H28N2O2	292.416	SHH-01-017	1.104496646	-1.032280101
1181	C24H33ClN2O2	416.984	SHH-01-018	1.11616965	-1.134405363
1182	C19H26N2O	298.423	SHH-01-022	-1.281659356	-1.215409017
1183	C19H26N2O	298.423	SHH-01-023	-1.071850594	1.13193946
1185	C15H22N2O	246.348	SHH-01-024	-1.021922891	-1.06262349
1186	C15H22N2O	246.348	SHH-01-025	1.020573178	-1.047383389
1188	C25H36N2O2	396.566	SHH-01-027	-1.120954514	-1.231913944
1189	C24H40N2O2	388.587	SHH-01-028	1.318993278	1.030053237
1190	C18H30N2O2	306.443	SHH-01-030	1.240213444	1.024388048
1192	C20H36N4O	348.526	LH-20	-1.053717279	1.017937498
1193	C20H34N4O	346.51	LH-21	1.008547893	-1.117553958
1194	C20H36N4O2	364.525	LH-22	-1.204485692	-1.145369407
1195	C41H60N8O13	872.961	PW-01--Tb	1.123133845	-1.127646153
1196	C41H60N8O13Tb	1,031.89	PW-01-+Tb	-1.082270864	-1.068020943
1197	C17H20N2O	268.354	SHH-01-032	1.057721642	1.003341715
1198	C17H20N2O	268.354	SHH-01-033	-1.035641315	-1.275850715
1199	C17H20N2O	268.354	SHH-01-036	1.093177387	-1.068230875
1200	C17H20N2O	268.354	SHH-01-033+036	-1.012438483	1.025208889
1201	C28H43NO4	457.645	KIH-284-92	-1.107288814	-1.049009104
1202	C24H41N3O3	419.601	KIH 284-94	-1.135546217	1.196925535
1203	C28H43NO2	425.647	KIH-284-95	1.221069386	1.037937725
1204	C18H29NO2	291.428	KIH-284-97	1.001618325	-1.059643595
1205	C22H33NO2	343.503	KIH-284-98	-1.018798822	-1.100971207
1206	C20H27NO	297.434	KIH-320-02	1.066688098	-1.184583235
1207	C34H42N2O5	558.708	KIH-320-04	1.071700506	-1.172027252
1208	C31H56N2O6	552.786	KIH-320-05	1.093979896	-1.0292499
1209	C20H33NO3	335.481	KIH-320-06	-1.175836486	1.074724653
1210	C17H28N2O2	292.416	KIH-271-55A	-1.020287389	1.168563955
1211	C25H37NO2	383.567	KIH-320-03	1.971205761	-1.103630783
2014	C17H28N2O2	292.416			

1225	C37H47N5O5	641.8	CRI-37-12B	-1.174558007	-1.252229237
1337	C23H38N2O3	390.559	KIH-271-00	-1.215570436	1.203885904
1212	C20H18BrNO3	400.266	SHH-01-035	1.295306737	-1.13694453
1213	C21H19NO4	349.38	SHH-01-039	1.128770163	-1.233864128
1214	C23H31BrN2O2	447.408	SHH-01-43	-1.058154138	-1.097805272
1215	C24H32N2O3	396.522	SHH-01-046	-1.096526869	-1.148182688
1216	C21H18N2O6	394.377	SHH-01-057	1.110185901	-1.054648742
1217	C24H31N3O5	441.52	SHH-01-060	1.067913156	-1.096725013
1218	C17H28N2O2	292.416	SHH-01-061	1.073838669	-1.308899452
1219	C24H34N2O2	382.539	SHH-01-062	1.125215395	-1.059563433
1220	C19H27ClN2O2	350.883	PDJ-IV-52B	1.247878542	1.108714092
1221	C19H25ClN2O3	364.866	PDJ-IV-53	5.926997215	1.167062618
1222	C19H27ClN2O2	350.883	PDJ-IV-56B	-1.19839121	-1.176536413
1223	C19H27ClN2O	334.883	PDJ-IV-55	1.18473511	-1.01345222
1224	C19H29ClN2O	336.899	PDJ-IV-62	-1.393455103	-1.210556433
1226	C11H18N2O3	226.272	BB-1	-1.104755125	-1.244700416
1227	C11H18N2O2S	242.338	BB-2	1.106595203	-1.196716279
1228	C10H16N2O3	212.246	BB-3	1.018358378	-1.038565087
1229	C10H16N2O2S	228.311	BB-4	-1.077122955	-1.117624185
1230	C9H14N2O2S	214.285	BB-5	-1.038343641	1.065747287
1231	C9H14N2O3	198.219	BB-6	-1.196447103	1.00462226
1232	C8H12N2OS	184.259	BB-7	1.042940103	-1.07184001
1233	C13H14N2OS	246.328	BB-8	-1.068579866	1.36362508
1234	C13H14N2OS	246.328	BB-9	1.060918966	-1.003118713
1235	C14H16N2O3	260.288	BB-10	-1.001594032	-1.275860264
1236	C14H16N2O2S	276.354	BB-11	1.119234064	1.065247366
1237	C24H32F2N2O2	418.52	SHH-01-079	1.770728899	1.206829588
1238	C23H38N2O2	374.56	SHH-01-080	-1.02093381	-1.165399309
1239	C18H30N2O2	306.443	SHH-01-082	-1.022341591	1.198200037
1240	C24H32Cl2N2O2	451.429	SHH-01-090	-1.040082492	1.254290636
1241	C25H36N2O2	396.566	SHH-01-091	-1.016065751	-1.220486378
1242	C27H38F2N2O3	476.599	SHH-01-095	-1.012001169	-1.018893528
1243	C27H38F2N2O3	476.599	SHH-01-096	1.196288201	1.25505974
1244	C24H33BrN2O2	461.435	SHH-01-098	1.187341408	1.155880953
1245	C24H33ClN2O2	416.984	SHH-01-099	1.311265793	1.132357509
1246	C26H36F2N2O4	478.572	SHH-02-006	1.259546479	-1.052551745
1247	C26H36F2N2O4	478.572	SHH-02-007	1.481395702	1.159547379
1248	C24H33BrN2O2	461.435	SHH-02-009	1.03910905	1.19951826
1249	C24H37N3O2	399.569	JRS-06	-1.08805528	-1.154784681
1250	C16H24N2O	260.375	JRS-07	1.047222282	-1.015178219
1251	C16H24N2O	260.375	JRS-08	-1.13019516	-1.097062331
1252	C14H14ClN3O2S	323.798	WY14643	1.086140546	-1.066038971
1253	C29H46N2O3S	502.752	GW 7647	1.495684427	1.003802651
1254	C15H22N4O	274.361	PDJ-4-95	-1.048247694	1.01655681
1255	C18H28N4O	316.441	PDJ-4-96	-1.154282466	-1.046711024

1256	C22H28N4O	364.484	PDJ-4-87	1.028930526	-1.02395155
1257	C19H26N2O2	314.422	PDJ-4-79	1.116602617	-1.014788322
1258	C27H28N2O3	428.523	PDJ-4-77	-1.256670908	-1.083299454
1259	C17H30N3O+	292.439	pdj-iv-97	1.035622863	-1.031923884
1260	C24H35N3O	381.554	pdj-v-2	1.079523674	-1.146746047
1261	C21H35N3O2	361.522	pdj-v-5	1.139884503	-1.09199497
1262	C24H33N3O2	395.538	pdj-v-3	1.094425982	-1.012362498
1263	C20H35N3O	333.511	pdj-v-11	-1.073813317	-1.06755894
1264	C24H35N3O	381.554	pdj-v-7	-1.04053958	-1.133714031
1265	C17H29N3O	291.432	pdj-v-4	1.023670355	1.03252462
1266	C29H45NO2	439.673	KIH 320-11	1.095649746	-1.137723944
1267	C17H26N2O2	290.401	KIH 320-12	1.124102471	-1.122571446
1268	C18H27NO2	289.412	KIH 320-13	1.153727381	-1.01957537
1269	C22H40N2O4	396.564	KIH 320-29	-1.012645653	1.121720949
1270	C24H35N3O3	413.553	KIH 320-32	1.023479488	-1.113499078
1271	C23H42N2O4	410.591	KIH 320-31	-1.137546854	1.054113722
1272	C23H41N3O4S	455.654	KIH 320-20	1.136764828	-1.092874193
1273	C23H39N3O3	405.574	KIH 320-36	-1.16549873	1.004607046
1274	C23H40N4O3	420.589	KIH 320-35	1.007683848	-1.199125743
1275	C20H24N4O	336.431	KIH 320-37	1.095614304	-1.174572438
1276	C23H31FN2O2	386.503	SHH02-033	1.076143047	-1.27166656
1277	C23H31FN2O2	386.503	SHH02-034	1.15208832	-1.04423839
1278	C23H32N3O4	414.518	SHH02-035	-1.028791188	-1.142940461
1279	C24H34N2O3	398.538	SHH02-036	1.193977907	1.101653815
1280	C13H24N2O3	256.341	SHH02-037	1.059211882	1.114616952
1281	C23H32N3O4	414.518	SHH02-043	1.2486294	-1.01332511
1282	C23H30F2N2O2	404.493	SHH02-044	1.040557639	-1.220369997
1283	C17H27NO2	277.402	SHH02-048	1.029443695	-1.009553064
1284	C25H33F3N2O2	450.537	SHH02-054	-1.058596063	-1.04444089
1285	C25H33F3N2O3	466.536	SHH02-055	-1.148250116	-1.189318712
1286	C24H34N2O3	398.538	SHH02-063	-1.002189327	-1.02522268
1287	C23H30F2N2O2	404.493	SHH02-064	-1.312613009	-1.050271055
1288	C20H22F2N2O2	360.398	SHH02-065	-1.031543602	-1.009615071
1289	C20H22F2N2O2	360.398	SHH02-065_2	1.056978548	-1.163323475
1290	C25H33F2NO2	417.532	SHH02-066	2.292773956	1.042163427
1291	C24H33FN2O2	400.529	SHH02-067	1.05074395	1.076710236
1292	C16H27N3O	277.405	pdj-v-24	-1.092663052	-1.149629
1293	C18H31N3O	305.458	pdj-v-43	-1.064117952	1.069944379
1294	C18H29N3O2	319.442	pdj-v-44	-1.136170474	-1.141168205
1295	C19H33N3O	319.485	pdj-v-42	-1.102202173	1.014890849
1296	C19H33N3O	319.485	pdj-v-46	-1.005855478	-1.05675454
1297	C19H31N3O2	333.468	pdj-v-40	1.075085425	1.093586737
1298	C20H33N3O2	347.495	pdj-v-45	1.011772825	1.474821004
1299	C23H33N3O	367.528	pdj-v-27	1.150844286	-1.026087007
1300	C23H31N3O2	381.511	pdj-v-26	-1.057618042	-1.233576394

1301	C20H35N3O	333.511	pdj-v-52	-1.003844242	1.208531274
1302	C21H37N3O	347.538	pdj-v-53	-1.021916245	-1.170912989
1303	C20H33N3O2	347.495	pdj-v-54	1.031037234	1.074798821
1304	C19H31N3O2	333.468	pdj-v-52	-1.029013062	1.088876869
1305	C28H34N2O3	446.581	KIH-320-44	-1.068512547	1.257630011
1306	C24H34N4O3	426.552	KIH-320-57	1.265437734	1.160210389
1307	C25H36N4O3	440.578	KIH-320-58	1.126212718	1.12625124
1308	C21H29N3O2	355.474	KIH-320-40	1.006490802	-1.026043405
1309	C27H44N4O3	472.663	KIH-320-42	1.123320762	-1.082676613
1310	C20H33N3O2	347.495	KIH-320-46	-1.068278105	-1.080382974
1311	C15H24N2O2	264.363	KIH-320-55	-1.205531543	1.157867148
1312	C23H41NO4	395.576	KIH-320-26	-1.126614967	-1.122864531
1313	C22H40N2O4	396.564	KIH-320-50	1.210319146	1.019799042
1314	C18H28N2O3	320.427	PAW-01-76	1.013398977	1.040318426
1315	C20H33N3O3	363.494	PAW-01-78	1.119034612	1.076340406
1316	C16H28ClN3O	313.866	pdj-v-68b	-1.018551992	1.003900161
1317	C18H22N2O3	314.379	PAW-02-11-1M	1.261096547	1.179308815
1318	C18H22N2O3	314.379	PAW-02-11-1P	1.379763059	-1.221518771
1319	C19H24N2O3	328.405	PAW-02-11-2P	-1.160304098	1.048730245
1320	C22H29N3O3	383.484	KIH 320-45	1.125792547	-1.018146544
1321	C27H38N4O3	466.616	KIH 320-49	1.018266248	-1.212623672
1322	C18H22N2O3	314.379	KIH 320-43	-1.03800874	1.396901248
1323	C31H32N2O3	480.597	KIH 320-48	1.041855366	1.014949464
1324	C17H22N2O2	286.369	KIH 284-80A	1.039547737	1.132659411
1325	C21H28N2O4	372.458	KIH 320-51	1.313183392	-1.156006723
1326	C19H24N2O4	344.405	KIH 320-51B	1.014745786	1.185121269
1327	C22H30N2O4	386.485	KIH 320-52	1.248558065	1.296423229
1328	C20H26N2O4	358.431	KIH 320-52B	1.013095635	-1.091245471
1329	C7H10N2	122.168	KIH 320-59B	-1.151994127	1.214966029
1330	C17H21ClN2O2	320.814	TK 1	1.891424053	-1.233863769
1331	C18H24N2O2	300.395	TK 2	1.208721275	1.212178969
1332	C18H24N2O3	316.395	TK 3	1.126929485	1.043574727
1333	C19H24N2O2	312.406	TK 4	-1.312311112	1.132145966
1334	C19H24N2O3	328.405	TK 5	1.269838331	1.176545729
1335	C20H26N2O3	342.432	TK 6	-1.067330039	1.152164574
1336	C23H26N2O2	362.465	TK 7	1.79686602	1.017665323
1338	C22H39N3O3	393.563	KIH 320-66	-1.025066437	1.066482274
1339	C23H33N3O3	399.526	KIH 320-63	-1.070635939	-1.123381318
1340	C24H34N4O2	410.552	KIH 320-67	1.154454357	-1.004603372
1341	C25H36N4O3	440.578	KIH 320-68	1.294835849	1.146664561
1342	C23H32N4O2	396.526	KIH 320-59	-1.00574287	-1.184276886
1343	C22H30N4O2	382.499	pdj-v-73b	-1.193348711	1.186261895
1344	C25H33N3O4	439.547	pdj-v-77b	1.099977817	1.018479507
1345	C25H33N3O4	439.547	pdj-v-82b	-1.096148969	-1.091168273
1346	C25H33N3O4	439.547	pdj-v-76	-1.076499364	-1.177105119

1347	C21H33N3O4	391.504	pdj-v-80b	-1.18828334	-1.159794648
1348	C22H35N3O4	405.531	pdj-v-79b	1.061530496	1.059495117
1349	C23H32N4O2	396.526	pdj-v-73	1.006305829	-1.087734274
1350	C22H35N3O4	405.531	pdj-v-80a	1.054849044	1.049017287
1351	C26H35N3O4	453.574	pdj-v-82a	1.070132371	1.009387876
1352	C26H35N3O4	453.574	pdj-v-77a	1.043141918	2.22070442
1353	C26H35N3O4	453.574	pdj-v-74	-1.081070663	1.015864346
1354	C23H37N3O4	419.558	pdj-v-79a	1.083719248	1.081134891
1355	C17H28N2O3	308.416	CRI-07-12C	1.484766946	-1.025019278
1356	C19H32N2O3	336.469	CRI-70-12A	-2.696325713	-1.655563147
1357	C23H43N3O	377.607	CRI-70-12C	-1.069756394	1.138644415
1359	C19H24N2O2	312.406	TK8	2.314929472	1.334720755
1360	C24H26N2O2	374.475	TK9	4.223293392	1.034990031
1376	C21H36N2O3	364.522	KIH-271-74	1.633148242	1.011382792
1361	C24H26N2O2	374.475	TK10	4.982256987	1.004325315
1362	C19H24N2O3	328.405	TK11	1.028302442	1.053736011
1363	C20H26N2O3	342.432	TK12	-1.004283495	1.067430642
1364	C24H26N2O3	390.475	TK13	1.495689133	1.012998487
1365	C20H26N2O3	342.432	PAW-02-11-3P	-1.445190497	-1.358095246
1366	C21H28N2O3	356.459	PAW-02-11-4P	-2.809935167	-3.255034425
1367	C19H24N2O3	328.405	PAW-02-11-2M	-1.020274347	-1.007223805
1368	C20H26N2O3	342.432	PAW-02-11-3M	1.029697642	-1.100904262
1369	C22H27NO2	337.455	HHZ-001	2.137610951	-1.017569394
1370	C20H23NO2	309.402	HHZ-002	3.525679557	1.2019929
1371	C19H21NO2	295.376	HHZ-003	1.557784919	-1.172462829
1372	C21H25NO2	323.429	HHZ-004	5.67212374	1.125217497
1373	C23H29NO2	351.482	HHZ-005	3.360353135	1.216404436
1374	C21H25NO2	323.429	HHZ-006	2.805681986	1.175910833
1377	C17H25FN2O2	308.391	SHH-CC-1-1	-1.25411461	1.100660058
1378	C19H20F2N2O2	346.371	SHH-CC-1-2	1.199436308	-1.266490166
1379	C19H20F2N2O2	346.371	SHH-CC-1-3	5.779660333	-1.079110574
1380	C20H20F4N2O2	396.379	SHH-CC-4-1	1.431933504	-1.038881016
1381	C20H20F4N2O2	396.379	SHH-CC-1-5	7.234719909	1.139558246
1382	C23H23FN2O2	378.439	SHH-CC-1-6	1.680082299	1.021464834
1383	C19H21FN2O2	328.381	SHH-CC-1-7	-1.217191952	1.013978174
1384	C20H23FN2O2	342.407	SHH-CC-1-8	-1.225569473	-1.126167479
1385	C20H20F4N2O2	396.379	SHH-CC-1-9	6.210013864	1.026164292
1386	C20H23FN2O2	342.407	SHH-CC-1-10	1.25268724	1.107463983
1387	C20H23FN2O2	342.407	SHH-CC-1-11	1.074820848	-1.023937121
1388	C19H20ClFN2O2	362.826	SHH-CC-1-12	-1.035049546	-1.16560352
1389	C21H25FN2O2	356.434	SHH-CC-1-13	1.039929322	-1.066446975
1390	C20H23FN2O3	358.407	SHH-CC-1-14	1.083607463	-1.215127299
1391	C19H20FN3O4	373.378	SHH-CC-1-15	1.545217553	-1.183535648
1392	C19H20FN3O4	373.378	SHH-CC-1-16	5.341912627	1.051383621
1393	C19H20FN3O4	373.378	SHH-CC-1-17	3.832064612	-1.025723275

1394	C19H19F3N2O2	364.362	SHH-CC-1-18	1.046554919	-1.066334604
1395	C19H20BrFN2O2	407.277	SHH-CC-1-19	1.083249304	-1.171633082
1396	C20H23FN2O3	358.407	SHH-CC-1-20	1.141083097	-1.211902332
1397	C20H23FN2O3	358.407	SHH-CC-1-21	1.366069344	1.124961788
1398	C19H20ClFN2O2	362.826	SHH-CC-1-22	6.115272273	1.194086304
1399	C20H20F4N2O3	412.378	SHH-CC-1-23	1.305437945	1.099814766
1400	C20H20F4N2O3	412.378	SHH-CC-1-24	8.397600204	1.400264553
1401	C19H20BrFN2O2	407.277	SHH-CC-1-25	1.740197603	1.149722687
1402	C19H19Cl2FN2O2	397.271	SHH-CC-1-26	1.083876398	1.041811889
1403	C19H20ClFN2O2	362.826	SHH-CC-1-27	2.622255033	1.002901999
1404	C19H20BrFN2O2	407.277	SHH-CC-1-28	5.289507476	-1.060664981
1405	C23H31FN2O2	386.503	SHH-CC-1-29	1.576983489	1.142565609
1406	C25H33FN2O2	412.54	SHH-CC-1-30	1.01973248	1.027631732
1407	C21H25FN2O2	356.434	SHH-CC-1-31	1.186953891	-1.047167429
1408	C23H23FN2O2	378.439	SHH-CC-1-32	1.014241018	1.04001178
1409	C19H20FIN2O2	454.277	SHH-CC-1-33	2.224984696	1.121280884
1410	C20H23FN2O2S	374.472	SHH-CC-1-34	1.557342137	-1.019163869
1411	C26H25FN2O2	416.487	SHH-CC-1-35	-1.070927538	1.148181665
1412	C26H27FN2O2	418.503	SHH-CC-1-36	1.284275233	1.267578623
1413	C18H25FN2O2	320.402	SHH-CC-1-37	1.05622662	1.04343067
1414	C22H27FN2O2	370.46	SHH-CC-1-38	2.170420917	1.062028796
1415	C20H29FN2O2	348.455	SHH-CC-1-39	2.366900928	-1.051350547
1416	C21H31FN2O2	362.481	SHH-CC-1-40	1.946950382	1.116452615
1417	C25H39FN2O2	418.588	SHH-CC-1-41	-1.065175223	-1.10343787
1418	C19H20FIN2O2	454.277	SHH-CC-1-42	7.35858886	1.119135423
1419	C19H20FIN2O2	454.277	SHH-CC-1-43	1.566774423	1.053428857
1420	C20H23FN2O2S	374.472	SHH-CC-1-44	1.241750911	1.177930986
1421	C19H27FN2O2	334.428	SHH-CC-1-45	1.326452043	1.257002091
1422	C19H20F2N2O2	346.371	SHH-CC-1-46	1.071975987	-1.085319678
1423	C20H23FN2O2S	374.472	SHH-CC-1-47	3.730999461	-1.031523519
1424	C20H23FN2O2	342.407	SHH-CC-1-48	1.103212786	1.058170639
1426	C20H21F3N2O2	378.388	SHH-CC-2-2	-1.112399166	1.242667576
1427	C20H21F3N2O2	378.388	SHH-CC-2-3	1.066667186	1.008014965
1428	C21H21F5N2O2	428.396	SHH-CC-2-4	-1.133497722	-1.143685602
1429	C21H21F5N2O2	428.396	SHH-CC-2-5	2.596539678	-1.053861812
1430	C24H24F2N2O2	410.456	SHH-CC-2-6	1.276554688	1.08701645
1431	C20H22F2N2O2	360.398	SHH-CC-2-7	1.060379842	-1.127165297
1432	C21H24F2N2O2	374.424	SHH-CC-2-8	1.059960178	1.152889488
1433	C21H21F5N2O2	428.396	SHH-CC-2-9	1.067986559	-1.06825476
1434	C21H24F2N2O2	374.424	SHH-CC-2-10	1.191652714	1.411324802
1435	C21H24F2N2O2	374.424	SHH-CC-2-11	1.114150701	1.196266333
1436	C20H21ClF2N2O2	394.843	SHH-CC-2-12	-1.016480141	-1.226011006
1437	C22H26F2N2O2	388.451	SHH-CC-2-13	-1.020161515	-1.074582968
1438	C21H24F2N2O3	390.424	SHH-CC-2-14	1.124007759	1.012018252
1439	C20H21F2N3O4	405.395	SHH-CC-2-15	-1.060673269	1.109837796

1440	C20H21F2N3O4	405.395	SHH-CC-2-16	1.121695294	1.356324634
1441	C20H21F2N3O4	405.395	SHH-CC-2-17	1.010556767	-1.122200661
1442	C20H20F4N2O2	396.379	SHH-CC-2-18	1.067048878	-1.109691238
1443	C20H21BrF2N2O2	439.294	SHH-CC-2-19	1.156637712	-1.0059609
1444	C21H24F2N2O3	390.424	SHH-CC-2-20	1.088163324	-1.043585889
1445	C21H24F2N2O3	390.424	SHH-CC-2-21	5.307618248	-1.054244921
1446	C20H21ClF2N2O2	394.843	SHH-CC-2-22	1.563230782	-1.074299051
1447	C21H21F5N2O3	444.395	SHH-CC-2-23	1.029481651	1.148380076
1448	C21H21F5N2O3	444.395	SHH-CC-2-24	1.227781741	-1.013717259
1449	C20H21BrF2N2O2	439.294	SHH-CC-2-25	1.042892791	1.101400657
1450	C20H20Cl2F2N2O2	429.288	SHH-CC-2-26	-1.0809353	1.250488668
1451	C20H21ClF2N2O2	394.843	SHH-CC-2-27	1.021163861	-1.207467371
1452	C20H21BrF2N2O2	439.294	SHH-CC-2-28	1.610574847	-1.212634414
1454	C26H34F2N2O2	444.557	SHH-CC-2-30	-1.141661754	-1.108653273
1455	C22H26F2N2O2	388.451	SHH-CC-2-31	1.067411206	1.005041573
1456	C24H24F2N2O2	410.456	SHH-CC-2-32	2.665671281	-1.01646597
1457	C20H21F2IN2O2	486.294	SHH-CC-2-33	1.000747668	1.024328145
1458	C21H24F2N2O2S	406.489	SHH-CC-2-34	1.091548287	1.207571238
1459	C27H26F2N2O2	448.504	SHH-CC-2-35	1.088107133	1.716534127
1460	C27H28F2N2O2	450.52	SHH-CC-2-36	-1.267678346	-1.022093791
1462	C23H28F2N2O2	402.477	SHH-CC-2-38	-1.051145522	-1.060688447
1466	C20H21F2IN2O2	486.294	SHH-CC-2-42	1.332030255	1.034791751
1467	C20H21F2IN2O2	486.294	SHH-CC-2-43	-1.053675396	-1.146874027
1468	C21H24F2N2O2S	406.489	SHH-CC-2-44	-1.025402724	-1.068688513
1469	C20H28F2N2O2	366.445	SHH-CC-2-45	1.139512884	-1.086852918
1471	C21H24F2N2O2S	406.489	SHH-CC-2-47	-1.086789265	-1.139279263
1472	C21H24F2N2O2	374.424	SHH-CC-2-48	1.067505027	1.43458649
1474	C21H23FN4O3S	430.496	SHH-CC-3-2	-1.445710033	-1.194691455
1475	C21H23FN4O3S	430.496	SHH-CC-3-3	-1.250373784	-1.243797009
1476	C22H23F3N4O3S	480.503	SHH-CC-3-4	-1.107381334	-1.032169574
1477	C22H23F3N4O3S	480.503	SHH-CC-3-5	-1.506994728	1.008903903
1478	C25H26N4O3S	462.564	SHH-CC-3-6	-1.174004616	1.023983353
1479	C21H24N4O3S	412.505	SHH-CC-3-7	-1.993178427	-1.015448565
1480	C22H26N4O3S	426.532	SHH-CC-3-8	-1.292392704	-1.114879853
1481	C22H23F3N4O3S	480.503	SHH-CC-3-9	-1.034726997	1.045671346
1482	C22H26N4O3S	426.532	SHH-CC-3-10	-1.320798115	1.029130354
1483	C22H26N4O3S	426.532	SHH-CC-3-11	1.009598125	-1.132022376
1484	C21H23ClN4O3S	446.95	SHH-CC-3-12	1.184417306	-1.072723238
1485	C23H28N4O3S	440.558	SHH-CC-3-13	1.022364557	1.040198162
1486	C22H26N4O4S	442.531	SHH-CC-3-14	-1.463367294	-1.097238005
1487	C21H23N5O5S	457.503	SHH-CC-3-15	-1.700395852	-1.06090815
1489	C21H23N5O5S	457.503	SHH-CC-3-17	-1.594969996	1.079458676
1490	C21H22F2N4O3S	448.486	SHH-CC-3-18	-1.128323947	1.056593164
1491	C21H23BrN4O3S	491.401	SHH-CC-3-19	-1.419083522	-1.163117126
1492	C22H26N4O4S	442.531	SHH-CC-3-20	-1.415039914	1.076568728

1494	C21H23ClN4O3S	446.95	SHH-CC-3-22	-1.751340613	1.190846315
1495	C22H23F3N4O4S	496.503	SHH-CC-3-23	-1.369783583	1.090918094
1496	C22H23F3N4O4S	496.503	SHH-CC-3-24	1.038378023	-1.014862779
1497	C21H23BrN4O3S	491.401	SHH-CC-	-1.344382599	-1.017779881
1498	C21H22Cl2N4O3S	481.395	SHH-CC-3-26	-1.336004355	-1.024508789
1499	C21H23ClN4O3S	446.95	SHH-CC-3-27	-1.543007804	1.346911365
1500	C21H23BrN4O3S	491.401	SHH-CC-3-28	-1.748260677	1.009126042
1501	C25H34N4O3S	470.627	SHH-CC-3-29	-1.462062205	1.034599279
1502	C27H36N4O3S	496.665	SHH-CC-3-30	2.329171392	1.148117721
1503	C23H28N4O3S	440.558	SHH-CC-3-31	-1.093157485	1.157586371
1504	C25H26N4O3S	462.564	SHH-CC-3-32	-1.461903545	-1.124485293
1505	C21H23IN4O3S	538.402	SHH-CC-3-33	-1.572134293	-1.139463664
1506	C22H26N4O3S2	458.597	SHH-CC-3-34	-1.457058104	-1.165361148
1507	C28H28N4O3S	500.612	SHH-CC-3-35	-1.028590584	2.452243517
1508	C28H30N4O3S	502.628	SHH-CC-3-36	1.778934563	1.103507025
1509	C20H28N4O3S	404.526	SHH-CC-3-37	-1.330195279	1.055871618
1510	C24H30N4O3S	454.585	SHH-CC-3-38	-1.251025026	-1.028075592
1511	C22H32N4O3S	432.579	SHH-CC-3-39	-1.115733149	1.283140256
1512	C23H34N4O3S	446.606	SHH-CC-3-40	-1.147423596	1.196061358
1513	C27H42N4O3S	502.712	SHH-CC-3-41	1.44387328	-1.005777889
1514	C21H23IN4O3S	538.402	SHH-CC-3-42	-1.972507808	1.015754067
1515	C21H23IN4O3S	538.402	SHH-CC-3-43	-1.759836427	-1.026938726
1516	C22H26N4O3S2	458.597	SHH-CC-3-44	-1.508211851	1.083978847
1517	C21H30N4O3S	418.553	SHH-CC-3-45	-1.147475939	-1.078477876
1518	C21H23FN4O3S	430.496	SHH-CC-3-46	-1.00360043	-1.205814997
1519	C22H26N4O3S2	458.597	SHH-CC-3-47	-1.28041064	1.026360951
1520	C22H26N4O3S	426.532	SHH-CC-3-48	-1.343123692	-1.017727412
1521	C13H20N2O	220.311	SHH-CC-4-1	1.071526518	1.043599074
1522	C15H15FN2O	258.291	SHH-CC-4-2	1.079437377	-1.160302976
1523	C15H15FN2O	258.291	SHH-CC-4-3	-1.13237529	1.195860235
1524	C16H15F3N2O	308.298	SHH-CC-4-4	-1.070384773	-1.086917174
1525	C16H15F3N2O	308.298	SHH-CC-4-5	2.352970026	-1.278907078
1526	C19H18N2O	290.359	SHH-CC-4-6	1.403117516	1.179205893
1527	C15H16N2O	240.3	SHH-CC-4-7	-1.013864376	1.09919449
1528	C16H18N2O	254.327	SHH-CC-4-8	-1.140181635	-1.011471447
1529	C16H15F3N2O	308.298	SHH-CC-4-9	3.096545492	1.319662786
1530	C16H18N2O	254.327	SHH-CC-4-10	1.111832232	1.135755389
1531	C16H18N2O	254.327	SHH-CC-4-11	1.014560936	1.125520753
1532	C15H15ClN2O	274.745	SHH-CC-4-12	-1.196777907	-1.008404672
2124	C18H28N2O3	320.427	Benzene hexachloride - Chemservice	1.263341146	-1.116924746
2125	C17H14N2O4S	342.369	Lindane - Chemservice	5.263558618	1.069379671
2126	C21H20N2O4S	396.459	Chlorodane - Chemservice	1.386075685	1.14935124
2127	C19H18N2O4S	370.422	Endrin - Chemservice	8.324802718	1.292042836
2128	C6H7NO2S	157.19	Toxaphene - Chemservice	1.116296056	1.030572647

2130	C24H27N3O3S	437.554	Thiodan - Chemservice	1.726321311	1.15178904
2131	C28H32N4O3S	504.644	4,4'-Dichloro-a-(trichloromethyl)benzhydrol	12.3446442	-1.018845312
2132	C25H21F3N4O3S	514.519	Methoxychlor - Chemservice	4.509423196	-1.147784607
2133	C27H25F3N4O3S	542.573	Baythroid - Chemservice	-1.016007399	-1.024107116
2134	C27H23N3O4S	485.554	a-Cypermethrin	1.070259756	-1.203505542
2135	C17H14F3N3O2S	381.372	d-(cis/trans)phenothrin	3.715540558	1.059913216
1533	C17H20N2O	268.354	SHH-CC-4-13	-1.110153519	-1.074148905
1534	C16H18N2O2	270.326	SHH-CC-4-14	-1.118093402	-1.135507431
1535	C15H15N3O3	285.298	SHH-CC-4-15	-1.016552016	1.179019105
1536	C15H15N3O3	285.298	SHH-CC-4-16	1.065212482	1.044339402
1537	C15H15N3O3	285.298	SHH-CC-4-17	1.21186093	1.063110747
1538	C15H14F2N2O	276.281	SHH-CC-4-18	1.150942126	-1.01225423
1539	C15H15BrN2O	319.196	SHH-CC-4-19	-1.407120176	-1.044879117
1540	C16H18N2O2	270.326	SHH-CC-4-20	-1.028391363	-1.188836523
1541	C16H18N2O2	270.326	SHH-CC-4-21	-1.046225447	-1.020360544
1542	C15H15ClN2O	274.745	SHH-CC-4-22	1.135094971	1.073319893
1543	C16H15F3N2O2	324.298	SHH-CC-4-23	1.07804263	1.030458565
1544	C16H15F3N2O2	324.298	SHH-CC-4-24	1.928819384	-1.038309977
1545	C15H15BrN2O	319.196	SHH-CC-4-25	-1.031956574	1.015548374
1546	C15H14Cl2N2O	309.19	SHH-CC-4-26	-1.001936636	1.012084699
1547	C15H15ClN2O	274.745	SHH-CC-4-27	-1.012440689	-1.011050653
1548	C15H15BrN2O	319.196	SHH-CC-4-28	-1.019573703	-1.119340442
1549	C19H26N2O	298.423	SHH-CC-4-29	-1.015393603	-1.02270883
1550	C21H28N2O	324.46	SHH-CC-4-30	-1.160721662	-1.18665337
1551	C17H20N2O	268.354	SHH-CC-4-31	1.072143139	1.021870501
1552	C19H18N2O	290.359	SHH-CC-4-32	1.484037613	1.045301677
1553	C15H15IN2O	366.197	SHH-CC-4-33	1.35982327	1.109359477
1554	C16H18N2OS	286.392	SHH-CC-4-34	1.007821622	1.091216404
1555	C22H20N2O	328.407	SHH-CC-4-35	-1.212656384	1.124377321
1556	C22H22N2O	330.423	SHH-CC-4-36	-1.232989135	-1.029712165
1557	C14H20N2O	232.321	SHH-CC-4-37	-1.035452693	1.15726655
1558	C18H22N2O	282.38	SHH-CC-4-38	-1.165559904	-1.007038917
1559	C16H24N2O	260.375	SHH-CC-4-39	1.105960001	1.187139273
1560	C17H26N2O	274.401	SHH-CC-4-40	-1.07422359	-1.045628954
1562	C15H15IN2O	366.197	SHH-CC-4-42	-1.065495276	1.105861521
1563	C15H15IN2O	366.197	SHH-CC-4-43	-1.132514542	1.049053333
1564	C16H18N2OS	286.392	SHH-CC-4-44	-1.094910631	1.337878973
1566	C15H15FN2O	258.291	SHH-CC-4-46	1.041069445	1.073218306
1567	C16H18N2OS	286.392	SHH-CC-4-47	1.041128123	-1.087909355
1568	C16H18N2O	254.327	SHH-CC-4-48	1.115486281	1.147202255
1569	C39H43N5O5	661.789	Cri-02-13	1.055465427	-1.203907547
1578	C22H30N4O2	382.499	pdj-vi-12b	1.368067946	1.100588254
1579	C22H30N4O2	382.499	pdj-vi-12a	1.05303599	1.01299917

1580	C23H32N4O2	396.526	pdj-vi-13b	-1.010166614	-1.09843639
1581	C23H32N4O2	396.526	pdj-vi-13a	-1.083464279	-1.090862531
1582	C31H38N2O3	486.645	KIH-320-73	-1.113181717	1.144554822
1583	C34H46N2O6	578.739	KIH-320-80B	1.235896164	-1.047163771
1584	C27H40N2O5	472.617	KIH-320-85B	-1.523149491	1.130366032
1585	C28H34N4O3	474.595	KIH-320-54	1.153011805	1.100508595
1586	C28H34N2O4	462.581	KIH-320-69	1.298094884	-1.115550617
1587	C21H28N2O4	372.458	KIH-320-69B	1.074752279	1.088011628
1588	C21H26F2N2O4	408.439	KIH-320-74	3.697899532	1.100796036
1589	C19H22F2N2O4	380.386	KIH-320-74B	1.102512087	1.060171905
1590	C21H26N2O4	370.442	KIH-320-83	5.054372041	1.132781729
1591	C17H21ClN2O2	320.814	KIH-320-64	1.743822095	1.072815293
1592	C23H32ClN3O3	433.971	KIH-320-64B	-1.007287448	-1.061311207
1593	C23H32ClN3O3	433.971	KIH-320-65B	-1.429765929	-1.161629615
1594	C19H34N2O2	322.485	KIH-320-84A	-1.329331027	-1.075579359
1595	C20H36N2O2	336.512	KIH-320-84-2	-1.126077421	1.236813806
1596	C21H38N2O2	350.539	KIH-320-84-1	-1.000082734	1.053005904
1597	C21H27NO3	341.444	KIH-320-86A	1.485055988	1.334108348
1598	C19H23NO3	313.391	KIH-320-86B	1.67691994	1.004398103
1599	C18H23NO2	285.381	KIH-320-87	1.010253569	-1.150734123
1600	C18H22N2O3	314.379	KIH-320-43-Re	-1.034767808	1.182277871
1601	C24H31NO2	365.508	HHZ-007	1.574241179	1.027257744
1602	C22H27NO2	337.455	HHZ-008	1.210582732	1.251419596
1603	C15H15NO2	241.285	HHZ-009	1.081219561	1.291817587
1604	C17H19NO2	269.338	HHZ-010	-1.319098701	-1.083927415
1605	C19H23NO2	297.391	HHZ-011	1.810433476	1.061694253
1606	C25H19NO2	365.424	HHZ-012	1.694269629	-1.011131454
1607	C20H17NO2	303.354	HHZ-013	1.589138732	-1.01597803
1608	C17H19NO2	269.338	HHZ-014	1.257452983	1.003337284
1609	C19H23NO2	297.391	HHZ-015	3.296109735	1.303495699
1610	C21H27NO2	325.445	HHZ-016	2.798035115	1.100697705
1611	C27H23NO2	393.477	HHZ-017	-1.155683387	-1.053577797
1612	C22H21NO2	331.408	HHZ-018	4.638603542	-1.0157475
1613	C28H31NO3	429.551	HHZ-019	1.707947326	1.044648298
1614	C26H36N2O4	440.575	SHH02-084	1.270021243	1.36174017
1615	C26H36N2O4	440.575	SHH02-085	1.245621058	-1.000297259
1616	C24H32N2O4	412.522	SHH02-090	1.080008554	1.046711521
1643	C21H17F2NO2	353.362	HHZ-020	-1.160437512	1.06709958
1648	C22H35N3O4	405.531	PDJ-vi-29a	1.081750446	1.04468234
1649	C21H33N3O4	391.504	PDJ-vi-29b	-1.08271924	1.28629387
1650	C21H33N3O4	391.504	PDJ-vi-27	-1.013569154	-1.145381391
1651	C20H31N3O4	377.478	PDJ-vi-28	1.027637208	1.118489607
1652	C25H33N3O4	439.547	PDJ-vi-31b	-1.019700258	1.024217099
1653	C24H31N3O4	425.521	PDJ-vi-31a	-1.068222167	1.307637986
1654	C25H33N3O4	439.547	PDJ-vi-30b	-1.023846859	-1.049013834

1655	C24H31N3O4	425.521	PDJ-vi-30a	-1.017890583	1.177251533
1656	C6H7NO	109.126	SHH-pyr-001	1.000730571	1.061960816
1657	C6H4F3NO	163.097	SHH-pyr-002	1.010737576	-1.053696835
1658	C6H7NO2	125.125	SHH-pyr-003	-1.061390328	-1.002315383
1659	C10H6F3NO	213.156	SHH-Ind-002	1.140037514	-1.257007543
1660	C10H9NO2	175.184	SHH-Ind-003	1.237355885	-1.11673153
1661	C23H30F3N3O2	437.498	SHH-02-095	1.83936621	1.100690515
1662	C19H20ClFN2O2	362.826	SHH-02-093_Cl	1.105161198	1.036772366
1663	C20H29FN2O2	348.455	SHH-02-093_cHep	2.495529055	1.014583914
1664	C19H20BrFN2O2	407.277	SHH-02-093_Br	-1.097512456	-1.036424559
1665	C20H20F4N2O2	396.379	SHH-02-093_CF3	7.230142519	1.381797427
1666	C19H20FIN2O2	454.277	SHH-02-093_I	1.09895193	-1.162244937
1667	C20H20F4N2O3	412.378	SHH-02-093_OCF3	10.79360855	1.148394299
1668	C19H28N2O	300.438	JRS-prop-1	1.109361125	-1.024514272
1669	C20H39N5O	365.557	CRI-05-13A	1.621186128	1.124428067
1670	C25H33N3O4	439.547	pdj-vi-32b	1.049997107	1.057790966
1671	C24H31N3O4	425.521	pdj-vi-32a	1.04061365	1.060625141
1686	C19H23NO3	313.391	KIH-320-86B	1.510322111	1.352322544
1697	C14H25N5O	279.381	CRI-05-13B	-1.089309701	1.09220729
1698	C18H37N3O	311.506	CRI-08-13-A1	-1.144983633	-1.006864246
1699	C17H31N3O3	325.446	CRI-08-13-B1	1.120761856	-1.049572649
1701	C21H33N3O	343.506	CRI-08-13-C	1.367823033	-1.135137669
1702	C15H19N3O	257.331	CRI-08-13-D	1.282102923	-1.029771972
1703	C15H18F3N3O3	345.317	PDJ-6-41	-1.020304476	-1.013336051
1704	C19H28F3N3O2	387.44	PDJ-vi-42-2	-1.059861927	1.02192971
1705	C19H16N2O2	304.343	HHZ-021	1.164151392	1.097808353
1706	C21H20N2O2	332.396	HHZ-022	1.020443028	1.215393721
1707	C19H16N2O2	304.343	HHZ-023	1.001774408	1.012676737
1766	C30H38N4O3	502.648	KIH-320-91	2.732659333	-1.107012535
1708	C21H20N2O2	332.396	HHZ-024	1.826093807	1.036232345
1709	C17H17NO3	283.322	HHZ-025	-1.022234621	-1.038417967
1710	C18H19NO3	297.348	HHZ-026	2.62370499	1.475301208
1711	C20H15F2NO2	339.335	HHZ-027	-1.00258872	-1.045986988
1712	C17H26N2O2	290.401	SHH-03-001	1.01722299	-1.091590311
1713	C24H36N2O5	432.553	SHH-03-001	-1.052964057	-1.019318694
1714	C23H30F3N3O2	437.498	SHH-03-000	1.040366272	-1.001754403
1716	C20H32N4O	344.494	CRI-12-13-A	1.168043695	-1.04826692
1717	C14H18N4O	258.319	CRI-12-13-B	1.480691181	1.063183961
1718	C13H16F3N3O2	303.28	PDJ-vi-40B	1.10501681	1.061941435
1719	C16H27N3O	277.405	PDJ-iv-1A	-1.104823497	1.156030309
1881	C19H21NO2	295.376	HHZ-031	1.148343521	1.003804018
1720	C22H19F2NO2	367.389	HHZ-028	4.563870896	1.084617745
1738	C18H26F3N3O2	373.413	pdj-vi-51	-1.021277569	1.185092771
1739	C15H15F6N3O3	399.288	pdj-vi-53	1.048139699	1.197109194
1747	C19H24N2O3	328.405	CRI-13-13-A1	1.496605191	1.129917099

1748	C18H22N2O3	314.379	CRI-13-13-A2	-1.061199991	1.039319453
1749	C17H29N3O	291.432	CRI-13-13-B	1.045962785	-1.287455431
1750	C12H23N3O	225.331	CRI-08-13-B3	1.086899477	1.128080545
1751	C18H29N3O2	319.442	pdj-vi-62	-1.0577884	1.786315417
1752	C11H24Cl2N4O	299.24	pdj-vi-56-1	1.01364379	-1.041178041
1753	C25H30N4O3	434.531	pdji-vi-57	1.121815462	-1.079644276
1754	C18H26F3N3O2	373.413	pdj-vi-54	1.035398715	1.167141401
1755	C17H29N3O	291.432	pdj-vi-1b-fb	1.056261812	-1.143914055
1756	C19H20FN3O4	373.378	SHH-030311	4.835570919	1.106471271
1757	C21H23FN2O4	386.417	SHH-03014	-1.003513955	-1.016732619
1758	C20H21FN2O4	372.39	SHH-03016	4.539937841	-1.071983942
1759	C26H36N2O4	440.575	SHH-03023	1.021581204	-1.086898638
1760	C23H25F3N2O5	466.45	SHH-03024	5.873042887	-1.109697889
1761	C24H28N2O6	440.489	SHH-03025	1.07710062	1.104462269
1762	C27H36N2O6	484.585	SHH-03026	-1.120612767	-1.254753958
1763	C24H25F3N2O7	510.46	SHH-03027	5.761529818	-1.018977216
1764	C25H28N2O8	484.498	SHH-03028	1.256709983	1.004008052
1765	C16H29N3O	279.421	CRI-13-13E	-1.035359965	-1.255318223
1767	C23H40N2O4	408.575	KIH-320-88	-1.698228221	1.154529671
1768	C24H42N2O4	422.601	KIH-320-99	-1.352154505	-1.09920318
1769	C23H38F2N2O4	444.556	KIH-320-96	-1.536117534	-1.013101101
1770	C23H31F3N2O4	456.498	KIH-320-93	1.433461242	-1.311755753
1771	C18H21FN2O3	332.369	KIH-320-89	1.102943136	1.690078181
1772	C19H22FNO3	331.381	KIH-320-90	1.228044127	1.481875096
1773	C18H22N2O3	314.379	KIH-320.95	-1.125720371	1.494089883
1789	C18H28N2O2	304.427	PDJ-VI-74B	-1.039975225	1.120929927
1790	C19H30N2O2	318.454	PDJ-VI-74A	-1.164792983	1.189404532
1791	C18H25F3N2O2	358.399	PDJ-VI-73B	1.0671605	1.067992735
1792	C19H27F3N2O2	372.425	PDJ-VI-73A	-1.068171711	-1.020816901
1793	C15H27N3O2	281.394	PDJ-VI-77	1.176338925	1.095212955
1794	C24H26N2O3	390.475	TK-14	1.067900013	-1.05087727
1795	C18H24N2O2	300.395	TK-15	-1.113918442	1.243064874
1796	C18H21F3N2O2	354.367	TK-16	4.585799921	1.180134051
1797	C18H22F2N2O2	336.376	TK-17	2.221156755	1.197730781
1798	C19H22F4N2O2	386.384	TK-18	2.479665621	1.689557588
1799	C18H21F3N2O	338.367	TK-19	2.958799057	1.006669868
1800	C19H23F3N2O2	368.393	TK-20	2.432149769	1.038356387
1801	C18H22N2O3	314.379	TK-22	1.011748652	1.157211022
1802	C15H20N2O3	276.331	TK-23	-1.049285468	1.16614582
1803	C15H11F3N2O3	324.255	TK-24	1.293402778	1.19265854
1804	C19H24N2O3	328.405	TK-25	1.834700451	1.053283884
1805	C16H22N2O3	290.357	TK-26	1.258667096	1.168693472
1806	C16H13F3N2O3	338.281	TK-27	-1.042378376	1.175552224
1807	C21H40N2O3	368.554	TK-28	-1.205873036	1.051676436
1808	C25H48N2O3	424.66	TK-29	1.026992521	1.004789215

1809	C20H29F3N2O3	402.451	TK-30	1.055312167	-1.049436288
1810	C24H37F3N2O3	458.557	TK-31	1.193678613	1.237141178
1811	C20H29F3N2O4	418.45	TK-32	1.067257987	-1.045237908
1812	C24H37F3N2O4	474.557	TK-33	1.116913053	1.03547384
1813	C19H24N2O3	328.405	TK-34	1.281977841	1.060449442
1814	C20H26N2O3	342.432	TK-35	1.11958793	1.219961857
1815	C20H26N2O3	342.432	TK-36	-1.931677019	-1.334067452
1816	C21H28N2O3	356.459	TK-37	-1.215107595	-1.455046347
1817	C16H13F3N2O4	354.281	TK-38	5.644724765	1.213498421
1818	C15H11F3N2O4	340.254	TK-39	1.202533709	-1.169633757
1819	C19H24N2O4	344.405	TK-40	4.895920989	1.053415796
1820	C18H22N2O4	330.378	TK-41	-1.014948942	1.013886966
1821	C25H28N2O2	388.502	TK-42	2.919617775	1.246218734
1822	C21H25FN2O2	356.434	SHH-03-047	1.002348723	-1.013617117
1823	C24H32N2O4	412.522	SHH-03-042	-1.051190102	-1.047038165
1824	C21H22N2O6	398.409	SHH-03-044	-1.037321657	-1.047415915
1825	C24H31FN2O	382.514	SHH-03-032	1.062535577	-1.097004537
1826	C24H33FN2O	384.53	SHH-03-040	1.255760921	1.050221571
1827	C21H23FN2O4	386.417	SHH-03-014	3.482612015	1.033993636
1828	C24H32FNO2	385.515	SHH-03-035	3.082995843	1.1549126
1829	C20H21FN2O4	372.39	SHH-03-016	1.093966071	-1.026394355
1830	C16H22N2O3	290.357	SHH-03-033	1.105872355	1.234065063
1831	C9H8F2O4	218.154	SHH-03-057_MOM	-1.240493882	1.16480757
1832	C21H23FN2O4	386.417	SHH-03-039	2.271740741	-1.148309662
1833	C14H20N2O	232.321	SHH-03-029	1.075555175	-1.068645401
1834	C21H21F3N2O5	438.397	SHH-03-043	1.573809732	-1.02844308
1835	C20H21FN2O4	372.39	SHH-03-046	1.090162152	1.147703846
1836	C15H28N2O	252.396	SHH-03-056_cHep	1.133146327	1.170222307
1837	C15H26N2O2	266.379	SHH-03-049	-1.038160989	1.097156572
1838	C13H10Br2N2O	370.039	SHH-03-056_Br	-1.241900509	1.199599546
1839	C21H20N2O9	444.392	SHH-03-056_mpCO2Me	-1.111383749	-1.184118066
1840	C13H10I2N2O	464.04	SHH-03-056_I	-1.170364638	-1.106211642
1841	C17H16N2O5	328.319	SHH-03-056_pCO2Me	1.046166091	-1.117407048
1842	C13H10Cl2N2O	281.137	SHH-03-056_Cl	1.083541573	-1.020894749
1843	C17H16N2O5	328.319	SHH-03-056_MCO2Me	1.242029773	1.086406288
1844	C15H10F6N2O	348.243	SHH-03-056_CF3	9.443480774	2.479402028
1845	C23H25FN2O6	444.453	SHH-03-038	1.448766944	-1.166936359
1846	C15H10F6N2O3	380.242	SHH-03-056_OCF3	6.269757144	-1.204749464
1847	C21H21FN2O6	416.4	SHH-03-045	1.061523448	-1.020075785
1848			Cri-26-13A	-1.075568591	-1.116127603
1849	C17H29N3O3S	355.495	PDJ-VI-87	-1.035990988	1.04437022
1850	C18H29N3O3	335.441	PDJ-VI-89	1.092455292	-1.049064062
1851	C21H22N2O6	398.409	SHH-03-044	-1.007068397	-1.01218315
1852	C17H12N2O9	388.285	SHH-03-060	1.093397001	-1.015280555
1853	C23H32FN3O	385.518	SHH-03-022	1.026011271	-1.280514771

1854	C15H12N2O5	300.266	SHH-03-058	-1.145666835	-1.041686679
1855	C21H29FN2O2	360.466	SHH-03-062	1.297735426	1.021773875
1856	C15H12N2O5	300.266	SHH-03-058	-1.193928331	-1.026608182
1857	C14H18F3N3O4S	381.371	PDJ-VII-3b	1.02788663	-1.010925584
1858	C25H27F3N4O4S	536.566	PDJ-VII-5	10.53892076	1.133760354
1859	C20H22F3N3O4S	457.467	PDJ-VII-3a	5.370647683	1.038000283
1860	C15H18F3N3O3	345.317	PDJ-VII-4	1.122095152	1.140540549
1861	C19H30N2O	302.454	JRS-Pr-2	1.054475475	-1.062380532
1862	C25H42N2O	386.614	JRS-Pr-4	-1.169487886	1.01242085
1863	C25H44N2O	388.63	JRS-Pr-7	-1.157625413	1.000676843
1864	C22H26N2O3	366.453	JRS-Pr-3	1.049677649	-1.186478176
1865	C22H28N2O3	368.469	JRS-Pr-6	1.072753027	1.240800507
1866	C20H22N2O3	338.4	JRS-Pr-5	1.32250906	1.14266384
1867	C20H24N2O3	340.416	JRS-Pr-8	1.068717666	1.173738303
1868	C23H25FN2O2	380.455	SHH-03_070	3.878358764	-1.003699008
1869	C10H9NO2	175.184	SHH-In-3-OAc	1.325079109	1.165543445
1870	C9H7NO	145.158	SHH-In-3-CHO	-1.007277482	1.063752433
1871	C17H25NO3	291.385	Capsaicin	1.163490501	1.086474272
1872	C19H21ClN2O2S	376.9	capsazepine	1.137033356	1.064803125
1873	C9H7NO2	161.157	5-methylisatin	1.066683832	-1.038276207
1874	CH3N5	85.068	5-aminotetrazole	1.039380372	1.075898842
1875	C8H9N5	175.191	SHH-03-084	-1.044420939	-1.052595083
1876	C21H21F3N2O5	438.397	SHH-03-078	1.128544633	1.125369111
1877	C20H20F4N2O3	412.378	SHH-03-079	1.649356838	1.326184427
1878	C19H19Cl2FN2O2	397.271	SHH-03-080	1.306339773	1.092044373
1879	C24H30FN2O2	397.506	SHH-03-081	1.00601907	-1.048080047
1880	C21H25FN2O2	356.434	SHH-03-082	1.049944908	-1.064635989
1882	C19H29N3O	315.453	HHZ-032	1.014121362	1.025200345
1884	C16H19N3O2	285.341	HHZ-034	-1.009469087	1.071031352
1885	C17H21N3O2	299.368	HHZ-035	1.034636519	-1.126572055
1886	C18H23N3O2	313.394	HHZ-036	1.004450475	-1.106690194
1887	C19H25N3O2	327.421	HHZ-037	1.026257125	1.03740778
1888	C18H23N3O	297.395	HHZ-038	-1.025848122	-1.137964262
1889	C18H23N3O	297.395	HHZ-039	-1.171575071	-1.241852071
1890	C16H18N2O2	270.326	HHZ-040	1.067056081	-1.089207945
1891	C14H27N3O3S	317.447	PDJ-vii-45	1.060032349	-1.001813407
1892	C22H22F3N3O5	465.422	PDJ-vii-42e	1.011624883	-1.229932606
1893	C18H22F3N3O5	417.38	PDJ-vii-50	1.028838928	1.034020095
1894	C22H22F3N3O5	465.422	PDJ-vii-42c	-1.070440081	-1.131000082
1895	C22H22F3N3O5	465.422	PDJ-vii-42d	-1.142801417	1.101927241
1896	C18H22F3N3O5	417.38	PDJ-vii_42a	-1.118577775	1.094262097
1897	C21H20F3N3O5	451.396	PDJ-vii-46d	1.060784665	-1.129121825
1898	C17H20F3N3O5	403.353	PDJ-vii-49a	-1.156760423	1.082789574
1899	C19H24F3N3O5	431.406	PDJ-vii-42b	-1.035072498	-1.085114858
1900	C21H20F3N3O5	451.396	PDJ-vii-46e	-1.038033292	1.104452579

1901	C21H20F3N3O5	451.396	PDJ-vii-49b	-1.140933323	1.018952232
1902	C23H31FN2O2	386.503	SHH-03-091	-1.091009329	-1.152665195
1903	C25H34N2O4	426.548	SHH-03-093	1.080910863	-1.185526051
1904	C24H32N2O4	412.522	SHH-04-002	1.113375236	-1.118538755
1905	C21H21F3N2O5	438.397	SHH-03-097	1.517212134	-1.076333662
1906	C24H32F2N2O2	418.52	SHH-03-086	1.007666139	-1.049672603
1907	C25H32N2O	376.534	PR-9	-1.030597714	1.181715184
1908	C25H36N2O	380.566	PR-10	-2.489051245	-2.340273995
1909	C19H20F3N3O4S	443.44	PDJ-vii-61	1.894760818	-1.050831956
1910	C14H21N3O3S	311.4	PDJ-vii-71-1	1.340151096	-1.331756823
1911	C15H23N3O3S	325.426	PDJ-vii-74	1.063003404	-1.017008131
1912	C12H17N3O3S	283.347	PDJ-vii-76	-1.018091964	-1.087882881
1913	C16H20F3N3O3	359.344	PDJ-vII-58a	-1.099682501	1.010006881
1914	C17H22F3N3O3	373.37	PDJ-vii-58B	-1.066456491	1.080791728
1915	C19H16ClNO4	357.788	Indometacin	-1.021726514	1.015758794
1916	C14H14O3	230.259	Naproxen	-1.718727754	-1.165457327
1917	C16H13F3N2O5	370.28	TK-43	4.639903786	-1.179978498
1918	C15H11F3N2O5	356.253	TK-44	-1.119002843	-1.115806135
1919	C17H22N2O	270.369	TK-45	1.133990699	1.073651783
1920	C17H22N2O2	286.369	TK-46	-1.157734605	-1.131176723
1921	C17H22N2O2	286.369	TK-47	1.17047399	1.006716398
1922	C18H24N2O	284.396	TK-48	-1.151809467	1.060611855
1923	C23H26N2O2	362.465	TK-49	3.605833779	1.012104182
1924	C18H24N2O2	300.395	TK-50	1.116578876	-1.16926604
1925	C22H30N2O3	370.485	TK-51	-1.741887092	-3.926142526
1926	C21H28N2O3	356.459	TK-52	-2.395639491	-2.69492617
1927	C29H52N2O3	476.735	KIH-354-04-1	-1.081227807	1.231158235
1928	C28H50N2O3	462.708	KIH-354-04-3	1.172162049	1.173190625
1929	C23H32N2O3	384.512	KIH-354-11	-1.550636933	-1.469163598
1930	C30H44N2O5	512.681	KIH-354-08	-1.030732571	1.029532151
1931	C25H28N2O3	404.501	KIH-354-06	5.224484965	1.241008156
1932	C29H40N2O5	496.638	KIH-354-10	-1.008176553	-1.030587481
1933	C37H50N2O6	618.803	KIH-354-09	-1.006932692	1.058020752
1934	C25H34N2O3	410.549	KIH-354-07	-4.189449044	-2.345746448
1935	C26H30N2O3	418.528	KIH-354-13	1.561998058	1.016003733
1936	C18H24N2O2	300.395	KIH-354-18	1.256772614	-1.308724714
1937	C20H29F3N2O4	418.45	KIH-354-15	-1.064305255	1.065246751
1938	C18H24N2OS	316.461	KIH-354-20	1.579441209	1.336372104
1939	C19H24N2O4	344.405	KIH-354-25	-2.686020035	-1.727273713
1940	C19H24N2O3	328.405	KIH-354-17	2.535349333	1.141469015
1941	C18H22N2O4	330.378	KIH-354-26	-1.033227903	-1.027121351
1942	C22H32N2O2	356.502	KIH-354-14	-2.529979032	-1.976612409
1943	C19H25N3O2	327.421	KIH-354-22	1.243996396	1.171775966
1944	C29H56N2O2	464.767	KR-I-88-22	1.003581934	-1.039295248
1945	C29H50N2O2	458.719	KR-I-77-22	-1.249951104	1.005735285

1946	C29H56N2O3	480.767	KR-I-104-28	-1.237230971	-1.664456447
1947	C19H36N2O3	340.501	KR-I-58-23	-1.111194593	-1.122828453
1948	C23H32N2O	352.513	JRS-PR-11	2.622357715	1.048920791
1949	C24H39N3O3	417.585	JRS-PR-12	1.227108929	-1.073765392
1950	C22H28N2O3	368.469	JRS-PR-13	-1.834105805	-1.116842215
1951	C25H42N2O3	418.613	JRS-PR-14	-1.145264085	1.230109025
1952	C25H38N4O2	426.595	LH-23	-1.052642791	-1.094329172
1953	C24H36N4O2	412.568	LH-24	1.034395301	1.077575177
1954	C29H44N4O4	512.684	LH-25	-1.02257619	-1.17149013
1955	C26H38N4O3	454.605	LH-26	-1.742293881	-1.11438311
1956	C25H38N4O2	426.595	LH-27	-2.610828287	-1.368987286
1957	C24H36N4O2	412.568	LH-28	-1.839935999	-1.552096151
1958	C29H44N4O4	512.684	LH-29	-2.182062496	-1.537683367
1959	C26H38N4O3	454.605	LH-30	-1.190376729	-1.131525145
1960	C25H38N4OR	410.595	LH-31	1.050049308	-1.268715377
1961	C24H36N4OR	396.569	LH-32	-1.152740508	-1.023552585
1962	C29H44N4O3R	496.685	LH-33	-1.753114699	-1.067085692
1963	C26H38N4O2R	438.606	LH-34	-1.127978302	-1.24350258
1964	C26H40N4O2	440.621	LH-35	1.031307525	1.086140588
1965	C25H38N4O2	426.595	LH-36	-1.020938412	1.061252711
1966	C30H46N4O4	526.711	LH-37	-1.7990689	-2.062792758
1967	C27H40N4O3	468.632	LH-38	1.05529138	1.645097
1968	C26H40N4O2	440.621	LH-39	1.110364573	1.156900963
1969	C25H38N4O2	426.595	LH-40	1.139866767	1.061677334
1970	C30H46N4O4	526.711	LH-41	-1.154007153	-1.033304321
1971	C27H40N4O3	468.632	LH-42	1.085715408	1.178584477
1972	C26H40N4O2	440.621	LH-43	-1.088357152	1.181735746
1973	C25H38N4O2	426.595	LH-44	-1.182762695	1.14723139
1974	C30H46N4O4	526.711	LH-45	-2.239725359	-1.677848348
1975	C27H40N4O3	468.632	LH-46	-2.283335954	-1.078892562
1976	C16H27N3O	277.405	LH-47	1.066413656	-1.072709364
1977	C15H25N3O	263.378	LH-48	-1.005834742	-1.025626577
1978	C21H35N3O3	377.521	LH-49	1.129931542	1.072427208
1979	C16H27N3O	277.405	LH-50	-1.008418903	-1.049345926
1980	C18H23F3N2O3	372.382	LH-51	-1.335783728	-1.064113212
1981	C13H15F3N2O	272.266	LH-52	-1.333961928	-1.016006828
1982	C25H41N5O3	459.625	LH-53	-1.774933542	-1.595728423
1983	C30H49N5O5	559.741	LH-54	-2.002876132	1.012540611
1984	C27H43N5O4	501.661	LH-55	-2.77738284	-1.273368991
1985	C19H30ClN3O2	367.913	LH-56	1.361909874	1.001693802
1986	C23H41N3O2	391.591	TK-358-27-54	-1.247545006	-1.230437785
1987	C23H41N3O3	407.59	TK-358-32-55	-1.058951031	1.001301269
1988	C24H40N4O2	416.6	TK-358-49-59	-1.103966355	-1.026818975
1989	C19H24N2O3	328.405	TK-358-39-56	1.079287069	1.075194509
1990	C18H22N2O3	314.379	TK-358-48-58	-1.102307321	1.147958313

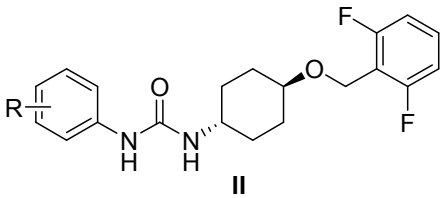
1991	C19H24N2O2	312.406	TK-358-42-57	-1.103859822	-1.012462648
1992	C26H28N2O5	448.511	TK-358-23-53	3.122670195	-1.129103957
1993	C9H8O4	180.157	Aspirin	1.030765137	1.012158492
1994	C14H26N2O	238.369	MG-XXX-19A	1.731957226	-1.066111869
1995	C13H17BrN2O	297.191	MG-XXX-66A	1.2038546	1.107376682
2136	C18H29N3O2	319.442	Resmethrin	1.530277027	-1.066053814
2137	C15H18F3N3O3	345.317	Bifenthrin	1.192495912	-1.027762911
2138	C17H20F3N3O5	403.353	Asana - Chemservice	1.105372493	1.322594995
2139	C23H37N3O3	403.558	zeta-cypermethrin	1.342053734	-1.049490247
2140	C17H28N2O2	292.416	Deltamethrin	1.130496821	1.06983749
2141	C17H28N2O2	292.416	Pyrethrum	1.15544164	-1.002966089
2142	C26H36N2O4	440.575	Pyrethrum	2.412639306	-1.08359278
2143	C24H32N2O4	412.522	Cypermethin (mix of isomers)	-1.100819573	1.152749098
2144	C24H31N3O2	393.522	trans-Cypermethrin	1.001953955	-1.345085717
2145	C21H21F3N2O5	438.397	Sanmarton	1.085579186	-1.036045254
2146	C21H21F3N2O5	438.397	cis-cypermethrin	1.132464107	1.166185452
2147	C21H22N2O6	398.409	Oxyfluorfen	1.731710879	1.058056861
2148	C23H32FN3O	385.518	Diuron	1.085429054	-1.108483072
2149	C17H16N2O3S	328.386	Diflubenzuron	-1.104256671	1.060960262
2150	C16H14N2O	250.295	Monuron - Chemservice	1.086930963	1.096937949
2151	C21H40N2O3	368.554	Fenuron - Chemservice	1.136908742	-1.107353866
2152	C19H36N2O2S	356.566	1-Naphthaleneacetamide	-1.059654859	1.006813616
2153	C19H35NO4	341.486	1-Naphthaleneacetic acid	1.093155361	-1.011896875
2154	C22H36O3	348.519	1-Naphthaleneacetic acid, methyl ester	1.053962576	1.015418372
2155	C20H38N2O3	354.527	Chloracetic acid	1.192895232	-1.115444796
2156	C19H35NO4	341.486	2,2-dichloropropionic acid	1.199096394	-1.081786309
2158	C19H28N2O2	316.438	Trichloroacetic acid	1.075011799	-1.026530051
2159	C14H9Cl2F3N2O	349.135	2-Naphthoxyacetic acid	-1.054343146	-1.126729638
2160	C21H39O6P	418.505	Phenoxyacetic acid	-1.012647339	-1.136080688
2161	C20H26F3N3O4	429.433	2-Phenoxypropionic acid	1.042690285	-1.032278402
2162	C17H22F3N3O4	389.369	3-Indolebutyric acid	1.158738443	1.121639898
2163	C19H30N2O2	318.454	Gibberellic acid	-1.085533275	1.036890387
2164	C21H39O6P	418.505	N-m-Tolylphthalamic acid	1.310745126	-1.027140067
2166	C21H39O5P	402.505	o-Dichlorobenzene	-1.022088173	-1.141659986
2167	C20H39O5P	390.494	p-Dichlorobenzene	1.097673863	-1.057296673
2171	C22H41FNaO6P	474.519	Naphthalene	-1.023888916	-1.04883344
2170	C20H39ClNaO6P	464.937	3,4,4'-trichlorocarbanilide	9.783635058	2.019966309
2172	C20H40NaO7P	446.491	1-Nitronaphthalene	1.075415001	-1.169901509
2173	C12H26O3S	250.398	Siduron	-1.23382839	1.098371305
1994	C14H26N2O	238.369	CH223191	1.015982956	1.181260321
1995	C13H17BrN2O	297.191	JRS-Pr-15	-1.115596653	1.02602009
1996	C19H19N5O	333.387	JRS	-1.013667524	-1.121843142
1997	C20H30N2O3	346.464	SHH-04-022	-1.058130688	1.008343899
1998	C18H28N2O3	320.427	SHH-04-029	-1.193670236	-1.050766412

1999	C17H14N2O4S	342.369	SHH-04-021	-1.277480146	-1.087673046
2000	C21H20N2O4S	396.459	MTPC	-1.12973183	1.055296429
2001	C19H18N2O4S	370.422	SHH-04-024	-1.21032182	-1.096686901
2002	C6H7NO2S	157.19	SHH-04-037	-1.045983589	-1.103734586
2003	C17H16N2O3S	328.386	SHH-04-032I	1.313029291	-1.09667029
2004	C24H27N3O3S	437.554	SHH-04-032II	3.651481682	-1.171379636
2005	C28H32N4O3S	504.644	SHH-04-042	1.980061038	-1.122542459
2006	C25H21F3N4O3S	514.519	SHH-04-036	-1.119113427	-1.140688622
2007	C27H25F3N4O3S	542.573	Celecoxib	-1.078878817	-1.015926758
2008	C27H23N3O4S	485.554	SHN-01-023	1.268092859	1.177622367
2009	C17H14F3N3O2S	381.372	SHN-01-025	1.004422893	-1.074029897
2010	C18H29N3O2	319.442	PDJ-vii-49a	-1.028371319	1.087501782
2011	C15H18F3N3O3	345.317	JRS-Pr-16	1.031963668	1.125673509
2012	C17H20F3N3O5	403.353	HSH-2	-1.158236965	-1.239090194
2013	C23H37N3O3	403.558	HSH-8	-1.100847294	-1.125311742
2014	C17H28N2O2	292.416	SHH-04-051	2.899704106	1.037299585
2015	C17H28N2O2	292.416	SHH-04-055	1.004871286	-1.031547761
2016	C26H36N2O4	440.575	HSH-03-074	-1.21770624	-1.011053912
2017	C24H32N2O4	412.522	HSH-37A	1.000863146	-1.23818224
2018	C24H31N3O2	393.522	HSH-37B	1.451792233	1.0570052
2019	C21H21F3N2O5	438.397	HSH-37D	-1.20810393	-1.064506173
2020	C21H21F3N2O5	438.397	HSH-34	1.104575005	-1.041417671
2021	C21H22N2O6	398.409	SHH-04-053-top	-1.153414668	1.049343959
2022	C23H32FN3O	385.518	SHH-04-053mid	-1.181523549	1.041145629
2023	C17H16N2O3S	328.386	KR-II-3-21	1.713694095	1.067101434
2024	C16H14N2O	250.295	KR-II-4-21	1.128672224	1.048901435
2025	C21H40N2O3	368.554	KR-I-188-23	4.180372213	-1.075548908
2026	C19H36N2O2S	356.566	KR-II-5-21	1.300770425	1.034347965
2027	C19H35NO4	341.486	KR-II-2-20	1.042007666	-1.036670023
2028	C22H36O3	348.519	KR-I-197-22	-1.004102798	1.152124529
2029	C20H38N2O3	354.527	KR-I-185-20	1.007665922	1.055728619
2030	C19H35NO4	341.486	JRS-Pr-17	-1.13648935	1.18357448
2031	C20H37NO3	339.513	TCC-8	-1.10854513	-1.398352556
2032	C19H28N2O2	316.438	Gabor tygrii	1.199556512	-1.2878351
2033	C14H9Cl2F3N2O	349.135	HHz-D001	1.076189114	-1.017758514
2034	C21H39O6P	418.505	HHZ-D004	2.908377245	1.100473933
2035	C20H26F3N3O4	429.433	JRS-PR-18	-1.162970482	1.099261143
2036	C17H22F3N3O4	389.369	gabor Tygrii	-1.096671731	1.085372271
2037	C19H30N2O2	318.454	Gabor Tygrii	-1.218449618	1.099970744
2038	C21H39O6P	418.505	gabor Tygrii	-1.114223645	1.11862817
2039	C19H37O6P	392.467	gabor Tygrii	-1.08556835	1.045144247
2040	C21H39O5P	402.505	Gabor Tygrii	4.2870171	-1.182408265
2041	C20H39O5P	390.494	JGW-9	2.659687275	1.147596357
2042	C22H41O5P	416.532	JGW-18	-1.199872499	-1.004021526
2043	C22H42NaO6P	456.529	xy-17	-1.242756381	-1.597154014

2044	C20H39ClNaO6P	464.937	JG-34 (SS)	-1.040655432	1.040018789
2045	C22H41FNaO6P	474.519	aLDRICH	-1.009272334	1.006672238
2046	C20H40NaO7P	446.491	JGW-8	-1.285479543	1.008635182
2047	C12H26O3S	250.398	JG-35(SR)	1.003215159	1.054918443
2048	C20H39BrNaO6P	509.388	Triclosan	-1.181156988	-1.249839723
2049	C20H40NaO7P	446.491	HHZ-D005	-1.004452601	-1.376868055
2050	C12H7Cl3O2	289.542	HHZ-D006	1.122913693	1.148292053
2051	C24H35N3O3	413.553	SHH-04-058	1.274644136	1.06150066
2052	C30H31N3O3	481.585	SHH-04-062	-1.052406072	-1.069566216
2053	C26H31N3O2	417.543	SHH-04-066NH2	-1.043516837	1.078361075
2054	C16H13N3O4S	343.357	SHH-04-066-Me	-1.173494789	1.159106326
2055	C16H14N4O3S	342.372	JRS-PR-19	-1.209827168	-1.113724255
2056	C17H15N3O3S	341.384	JRS-PR-20	-1.152252868	1.018300746
1996	C19H19N5O	333.387		-1.066424571	1.157903265
1997	C20H30N2O3	346.464		1.335059779	-1.033978117
1998	C18H28N2O3	320.427		-1.03918649	1.073575546
1999	C17H14N2O4S	342.369		2.517203622	-1.104024813
2000	C21H20N2O4S	396.459		1.394597002	-1.065122573
2174	C20H39BrNaO6P	509.388	Irgasan	6.997283045	1.121476064
2175	C20H40NaO7P	446.491	Finasteride	1.031228024	-1.063369661
2176	C12H7Cl3O2	289.542	Clomipramine	1.285395133	1.059819445
2177	C24H35N3O3	413.553	Anthracene	1.296574673	-1.040116963
2178	C30H31N3O3	481.585	BEHP	1.506368365	-1.12328208
2179	C26H31N3O2	417.543	BHA	1.254214231	1.050276896
2180	C16H13N3O4S	343.357	BHT	1.190503864	1.040258175
2181	C16H14N4O3S	342.372	Bisphenol A	1.1387244	-1.137260702
2183	C16H24N2O	260.375	Triton X-100	1.766025899	1.646465561
2184	C22H38N2O	346.55	SDS	1.120598942	-1.162476375
2185	C14H10	178.229	Phenanthrene	1.147406495	1.378554969
2186	C24H46O10	494.616	Tween - 20	1.484575733	1.229511321
2187	C12H27O4P	266.314	n-dodecyl phosphoric acid	1.800700515	1.046496
2188	C10H11ClO3	214.646	Clofibric acid	1.016236925	-1.114658102
2190	C12H6Br4O	485.791	PBDE-47	1.137221398	1.085270468
2191	C6H14NO5P	211.153	Pyrovatex CP	-1.161095757	1.057920737
2192	C9H15Cl6O4P	430.905	Amgard CJ	1.103082907	1.338121331
2193	C18H15O4P	326.283	Phosphoric acid triphenyl ester	-1.059900136	1.162532904
2194	C15H12N2O	236.269	Carbamazepine	-1.011240437	-1.070590735
2195	C17H19ClF3NO	345.787	Fluoxetine HCl	1.145310693	1.051091129
2196	C8H12Br4	427.797	1,2-dibromo-4-(1,2-dibromoethyl)cyclohexane	1.161598472	1.125830085
2197	C13H16N2S2	264.41	N-cyclohexyl-2-benzothiazyl sulfenamide	-1.08013246	1.116835414
2198	C13H8ClNS	245.727	2-(4-chlorophenyl)-benzothiazole	1.603840235	1.141127279
2199	C7H5NOS	151.186	2-hydroxy-benzothiazole	1.061315234	-1.029525469

2200	C26H28N2O2	400.513	JRS-Pr-21	-1.01849127	-1.018235078
2201	C26H30N2O2	402.529	JRS-Pr-22	1.011364667	1.694111436
2202	C26H34N2O4	438.559	SHH04080	1.127512232	1.160500233
2203	C5H7NS	113.181	4,5-dimethylthiazole	-1.090010467	1.079244157
2204	C12H14ClNS	239.764	SHH04067	-1.002493184	-1.076292293
2205	C27H46O2	402.653	CHOLESTAN-5?, 6?-EPOXY-3?-OL	1.30244855	1.061625074
2206	C21H32O3	332.477	PREGNAN-5a, 6a-EPOXY-3?-OL-20-ONE	1.448784669	-1.076740558
2207	C21H30O4	346.461	5a-PREGNAN-16, 17-EPOXY-3?-OL-11, 20-DIONE	1.410620203	-1.101987114
2208	C21H32O3	332.477	5a-PREGNAN-16, 17-EPOXY-3?-OL-20-ONE	-1.084544433	-1.022935595
2209	C27H46O2	402.653	CHOLESTAN-5a, 6a-EPOXY-3?-OL	-1.094111145	1.05830178
2210	C21H32O4	348.476	5?-PREGNAN-16, 17-EPOXY-3a, 12a-DIOL-20-ONE	-1.179446606	1.093257945
2211	C21H32O3	332.477	5?-PREGNAN-16, 17-EPOXY-3?-OL-20-ONE	1.205463463	1.033963771
2212	C22H32O3	344.488	5-PREGNEN-16, 17-EPOXY-16?-METHYL-3?-OL-20-ONE	-1.091998617	1.171694864
2213	C11H9NOS	203.26	Cri-14-16	-1.067058393	1.052591212
2214	C12H7F3OS	256.244	HHZ	-1.20265312	-1.116584229
2215	C18H34N2O4	342.474	AKR-I-46-24	1.062111396	1.04694024
2216	C19H34N2O4	354.484	AKR-I-27-28	-1.205447202	-1.039128204
2217	C19H36N2O3	340.501	KR-II-149-23	-1.137163333	1.06949656
2218	C19H36N2O3	340.501	MRK-I-147-31	-1.02054007	1.009909348
2219	C19H36N2O3	340.501	MRK-I-145-10	-1.086672416	-1.066015152
2220	C20H35N3O2	349.511	PN-II-91-35	1.042687389	1.161761131
2221	C9H12N4O3	224.217	SHH-04-089	1.154169891	1.026823307
2222	C15H11NO5	285.252	SHH-04-098	-1.546764215	-1.185983024
2223	C28H40N2O4	468.628	SHH-04-091	-1.083516512	1.129857502
2224	C30H44N2O6	528.68	SHH-04-092	1.278675945	-1.101964235
2225	C16H13N3O4S	343.357	AG-1-0	1.244711313	1.163155816
2226	C21H23N3O3S	397.491	AG-1-10	-1.211722565	-1.01895849
2227	C19H19N3O4S	385.437	AG-1-13	-1.010529088	-1.099480545
2228	C23H27N3O3S	425.544	AG-1-14	1.335040343	1.007752229
2229	C9H10Cl2N2O	233.095	DIURON	1.0256666	-1.166240861
2230	C14H20N2O	232.321	SIDURON	1.114762296	-1.023795779
2231	C9H11ClN2O	198.649	MONURON	-1.014254112	-1.459057022
2232	C14H9ClF2N2O2	310.683	DIMILIN	1.022916351	-1.028577398

II. **Table S2:** Activity of *N*-phenyl-*N′*-(4-((2,6-difluorobenzyl)oxy)cyclohexyl) ureas **II**, in the ternary complex and cell proliferation assay.



II

Compound	R	*Emax* (F/R) (μM)			IC_{50} (μM)
		30	15	7.5	
II-1o	*o*-F	0.89	0.98	0.96	>20
II-1m	*m*-F	0.67	0.77	0.72	>20
II-2o	*o*-Cl	0.81	0.69	0.81	>20
II-2m	m-Cl	0.75	0.78	0.79	>20
II-2p	*p*-Cl	0.74	0.96	0.95	>20
II-3o	*o*-Br	0.96	0.99	0.96	>20
II-3m	*m*-Br	0.98	1.04	1.07	>20
II-3p	*p*-Br	0.73	0.85	0.76	>20
II-4o	*o*-I	0.81	0.74	0.81	>20
II-4m	*m*-I	0.72	0.75	0.69	>20
II-4p	*p*-I	0.67	0.82	0.76	>20
II-5o	*o*-CF_3	0.64	0.80	0.95	>20

II-5m	*m*-CF_3	1.11	1.15	1.13	>20
II-5p	*p*-CF_3	0.85	0.79	0.91	>20
II-6o	*o*-CF_3O	0.76	0.93	0.93	>20
II-6p	*p*-CF_3O	0.98	0.80	0.81	>20
II-7o	*o*-Me	0.83	0.79	0.78	>20
II-7m	*m*-Me	0.81	0.89	0.82	>20
II-7p	*p*-Me	0.77	0.81	0.81	>20
II-8o	*o*-MeO	0.84	0.88	0.94	>20
II-8m	*m*-MeO	0.74	0.97	0.84	>20
II-8p	*p*-MeO	0.68	0.71	0.74	>20
II-9o	*o*-NO_2	0.74	0.90	0.96	>20
II-9m	*m*-NO_2	0.94	0.76	0.96	>20
II-9p	*p*-NO_2	0.83	0.83	0.87	>20
II-10o	*o*-MeS	0.83	0.90	0.82	>20
II-10m	*m*-MeS	1.06	0.73	1.01	>20
II-10p	*p*-MeS	1.07	0.98	0.94	>20
II-11	H	0.81	0.88	0.89	>20

III. **Figure S1:** Time response studies of the selected *N*-aryl,*N'*-cyclohexylarylureas in the surrogate eIF2α phosphorylation assays.

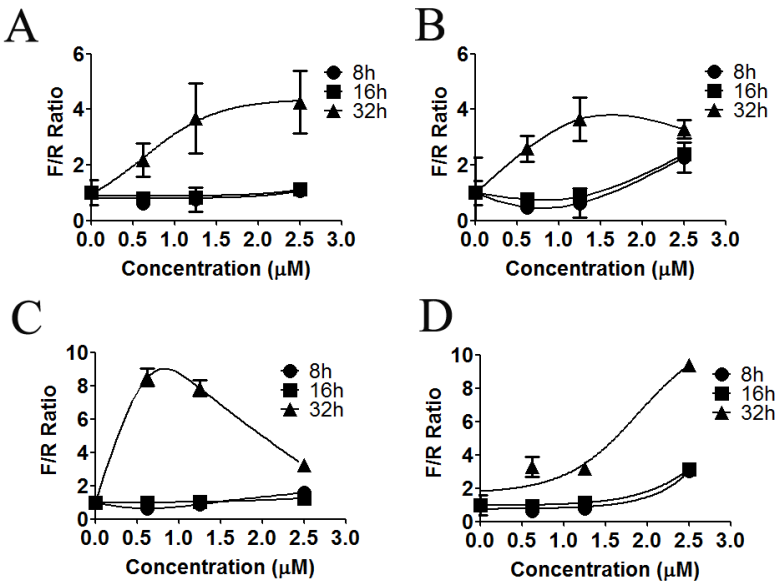
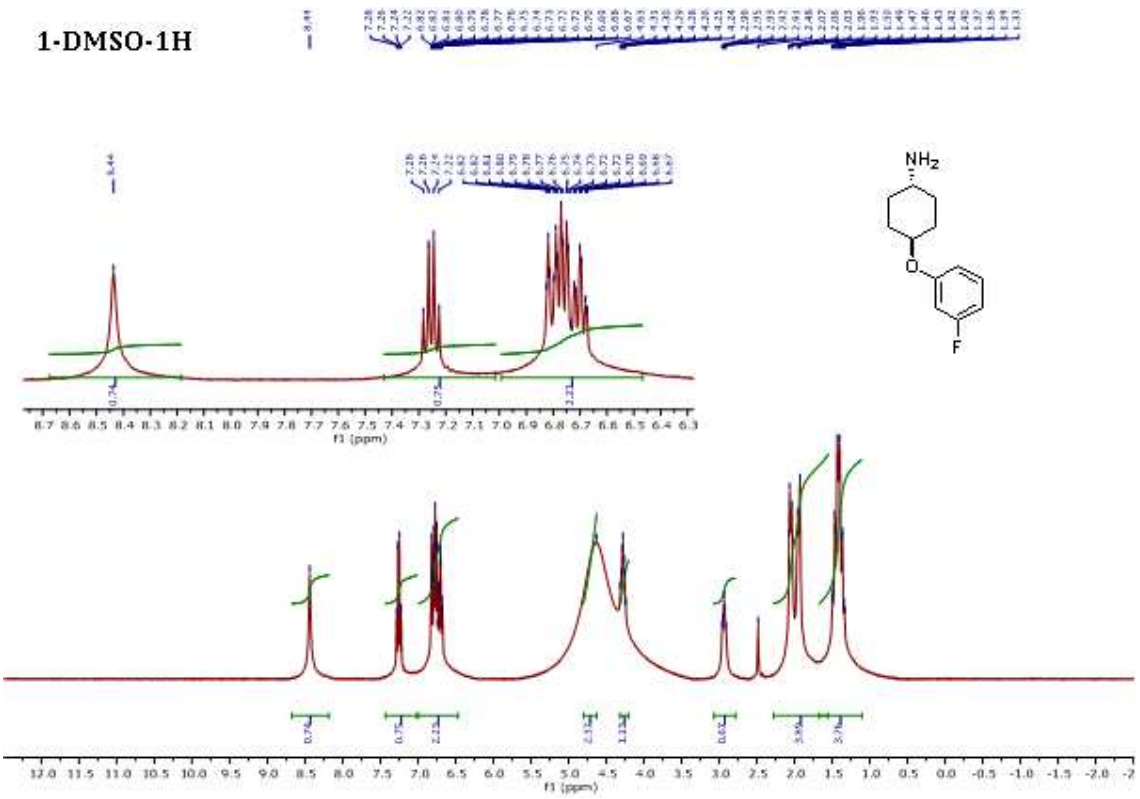
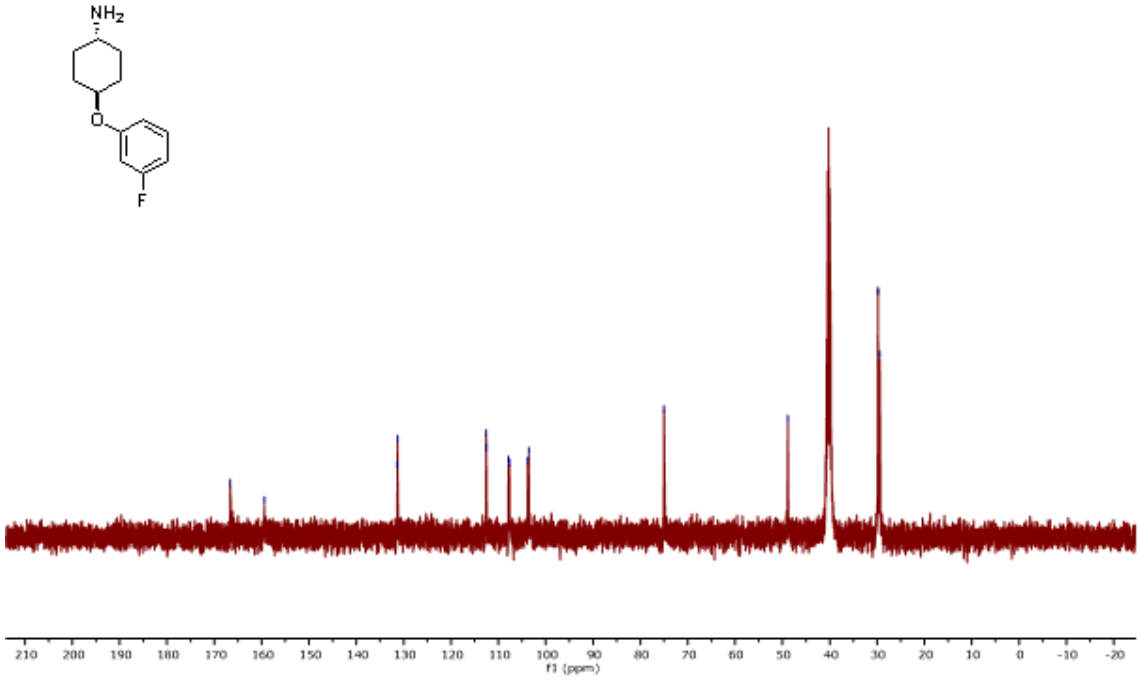


Figure S1. Time response studies of the selected *N*-aryl,*N'*-cyclohexylarylureas **in the surrogate eIF2α phosphorylation assays.** Reporter cells were incubated with (A) **I-14**, (B) **I-15**, (C) **III-3** and (D) **III-4** for 8, 16, or 32 hours and the F/R was determined by DLR assay. The experiment was conducted in triplicate and each experiment was independently performed three times; Data are shown as Mean±S.E.M.

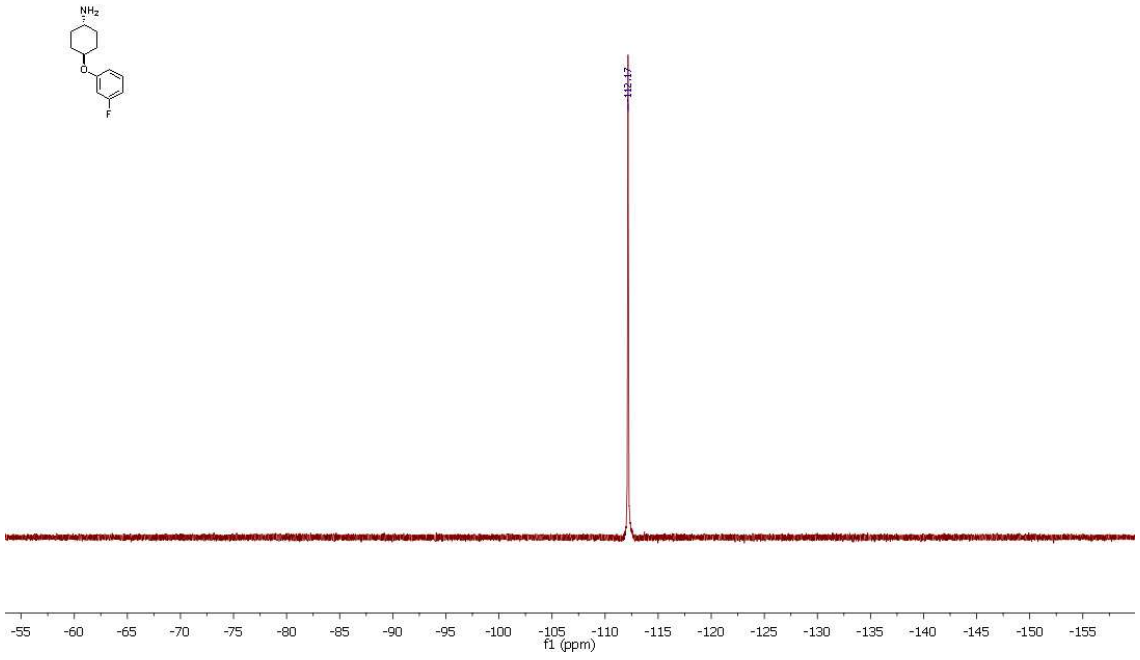
IV. ^{1}H-NMR, ^{13}C-NMR and ^{19}F –NMR (if any) spectra for compounds **1-10**.



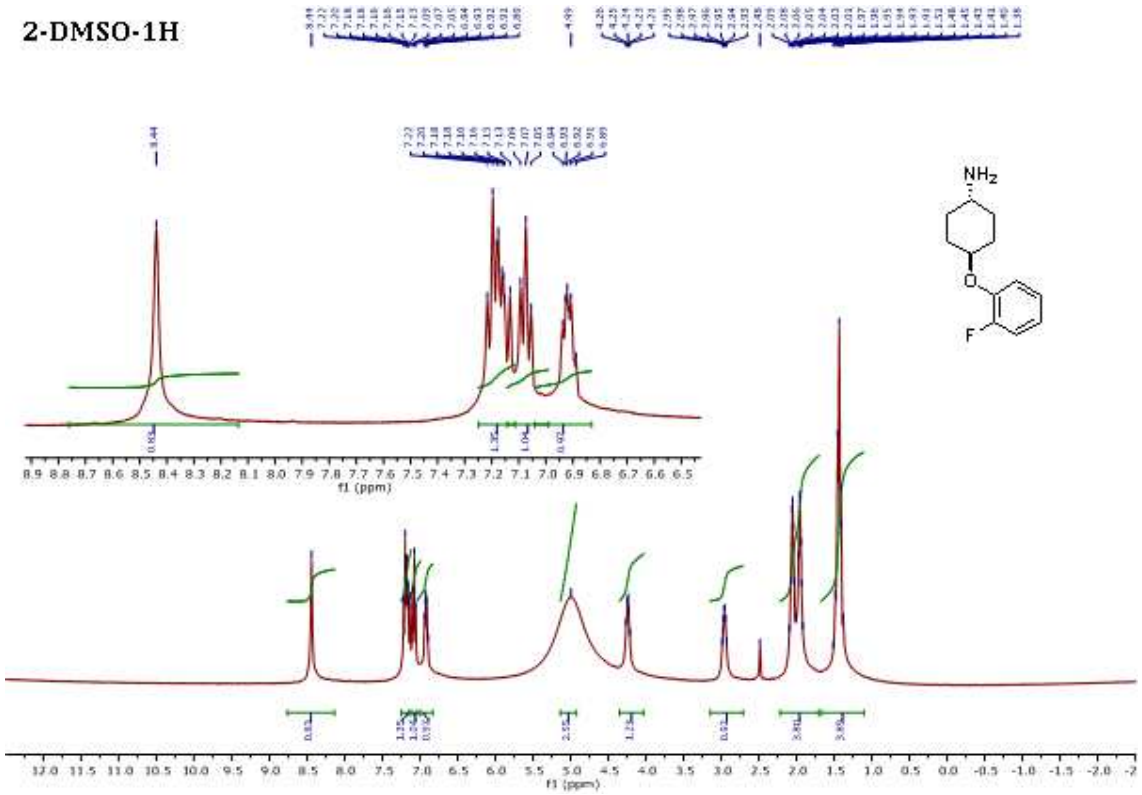
1-DMSO-13C



1-DMSO-19F



2-DMSO-1H



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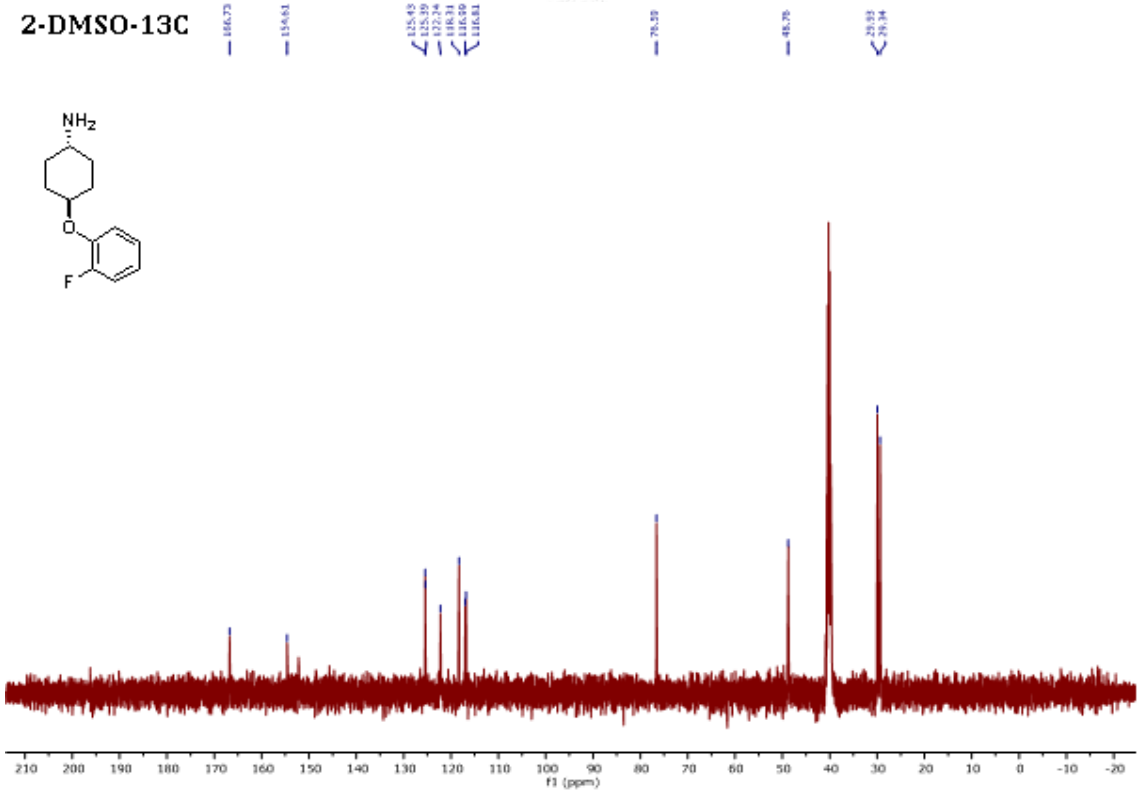

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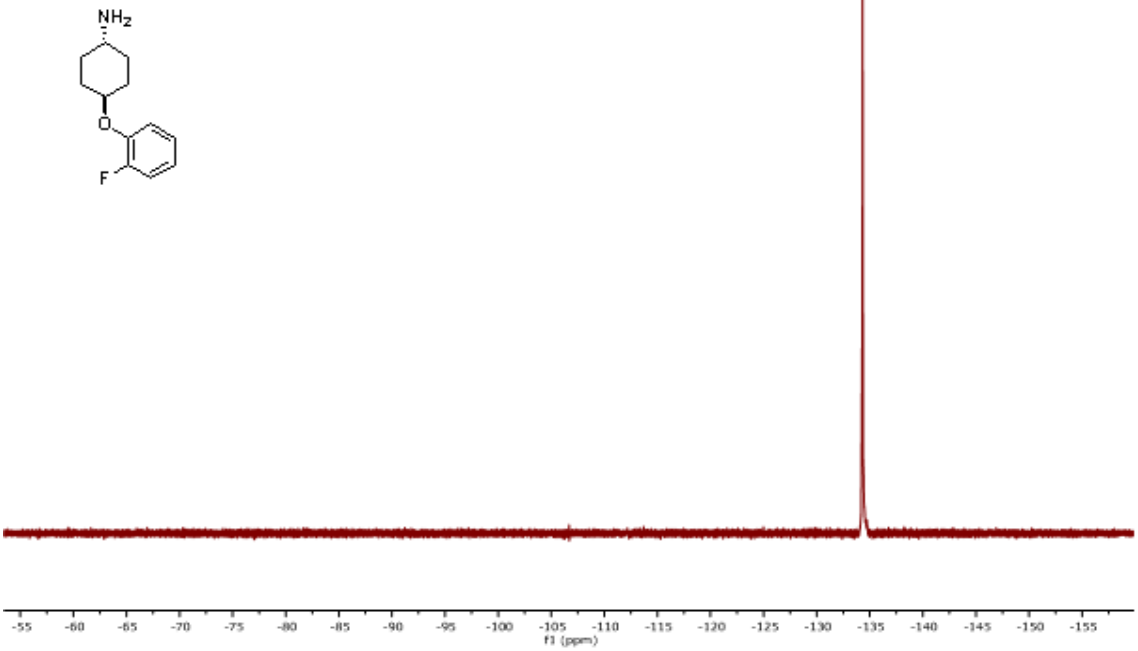
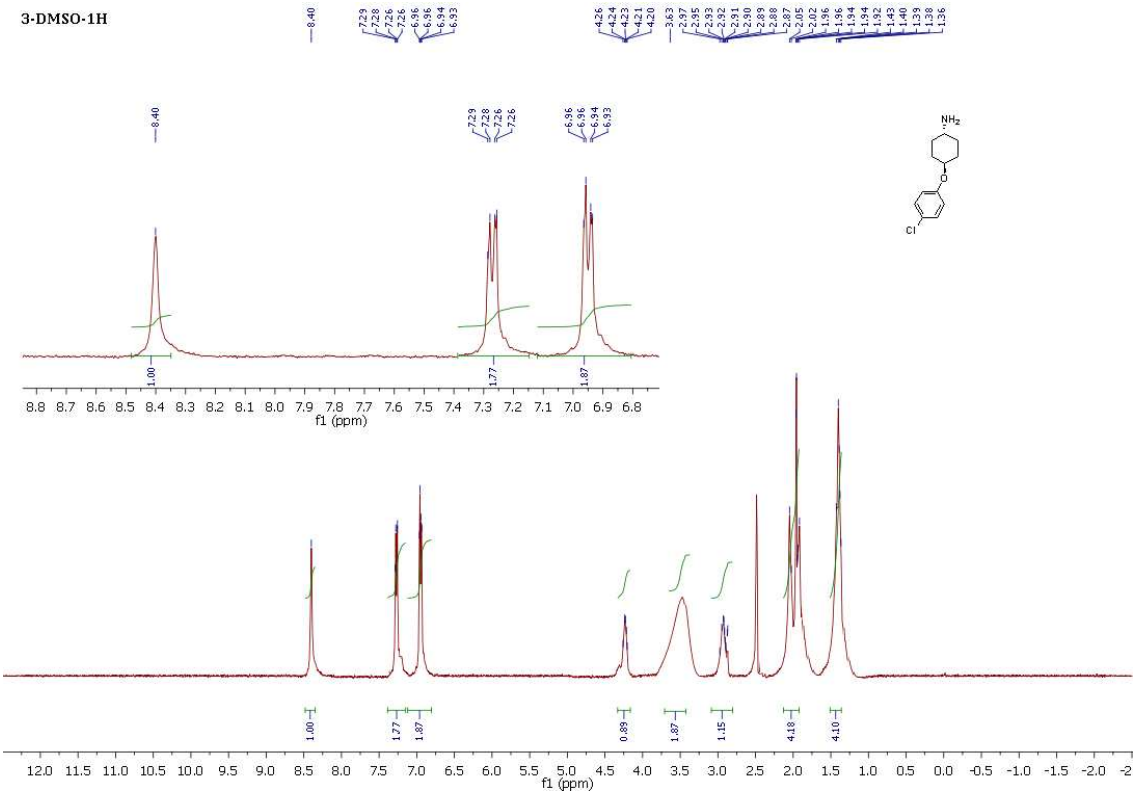
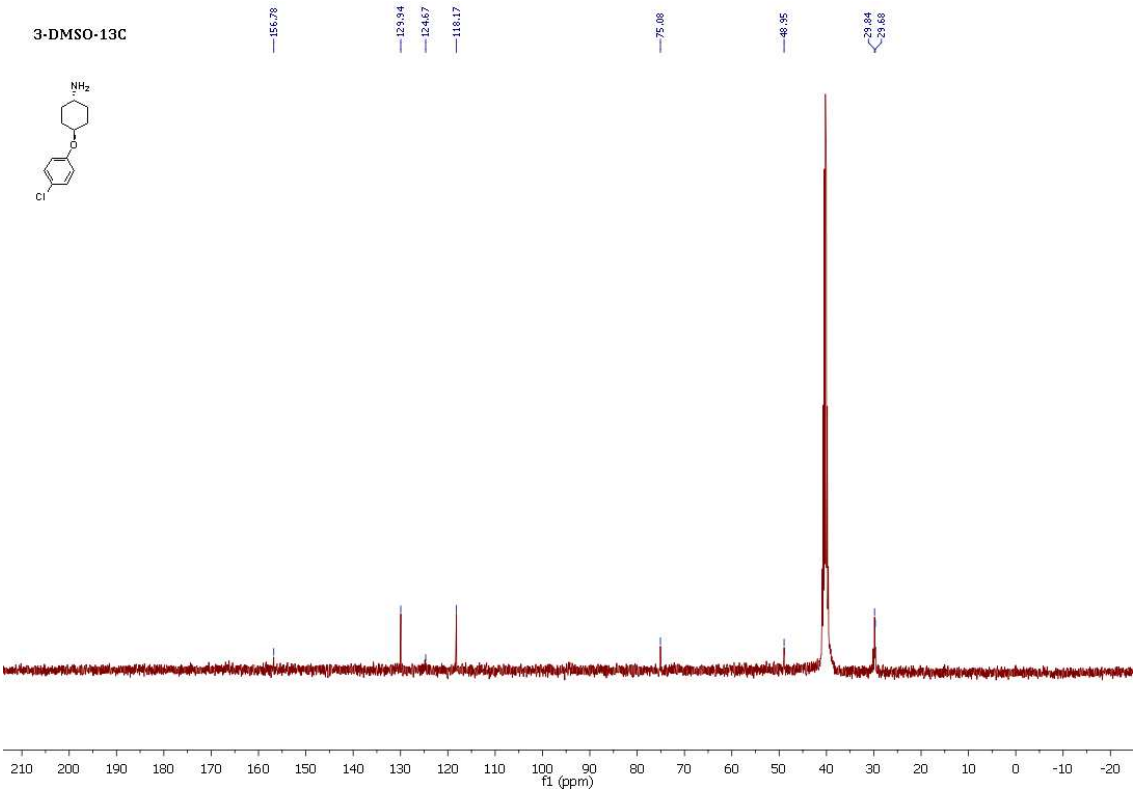
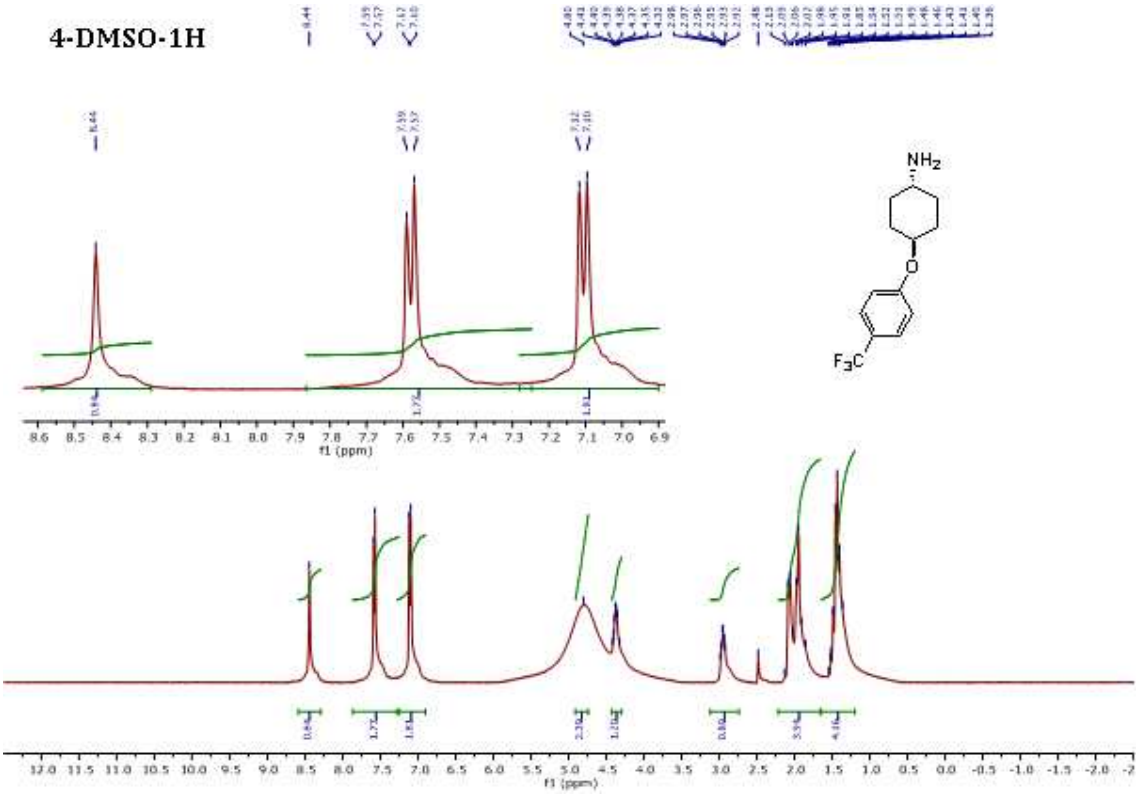


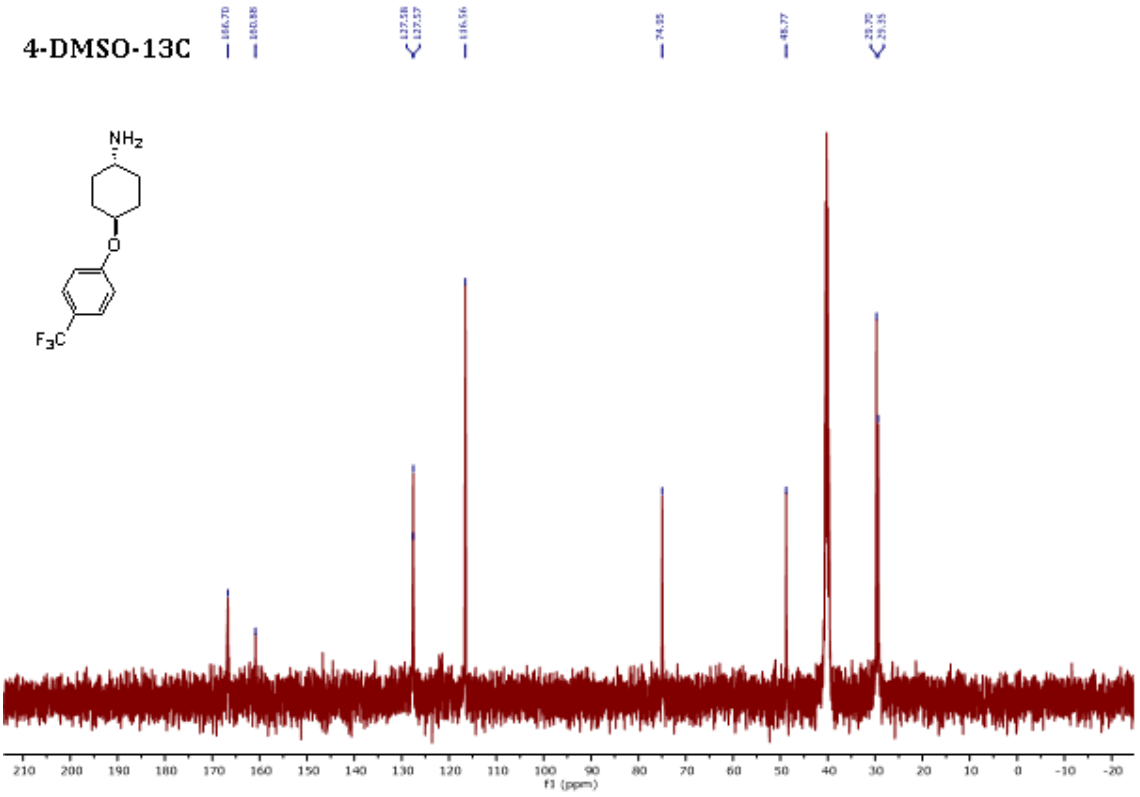
3-DMSO-1H



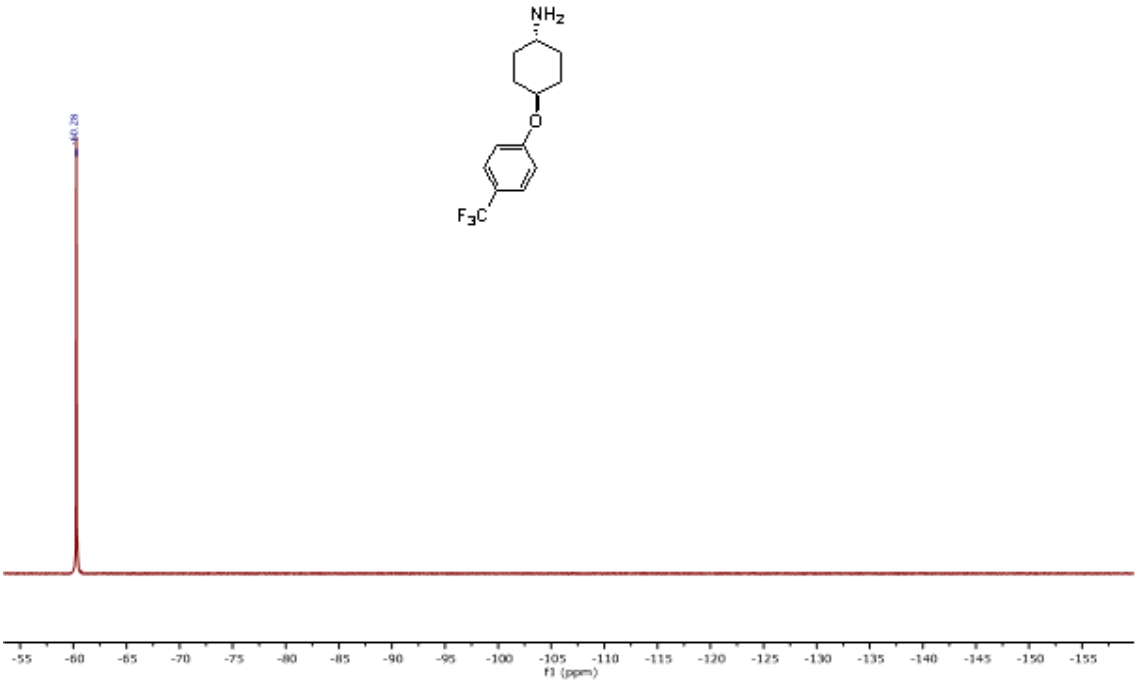

3-DMSO-13C
156.78
129.94
124.67
118.17
75.08
48.95
29.84
29.68
NH2
O
Cl
f1 (ppm)


4-DMSO-1H
8.44
7.59
7.57
7.42
7.40
NH2
O
F3C
f1 (ppm)

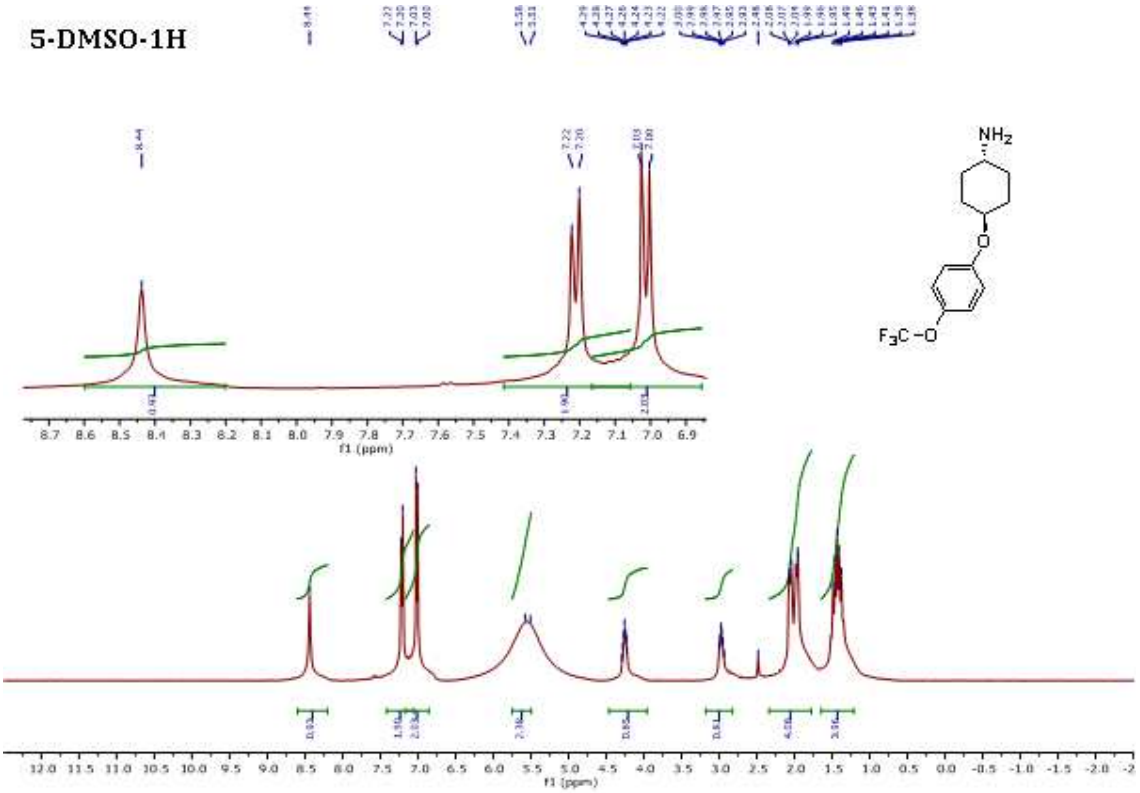
4-DMSO-13C



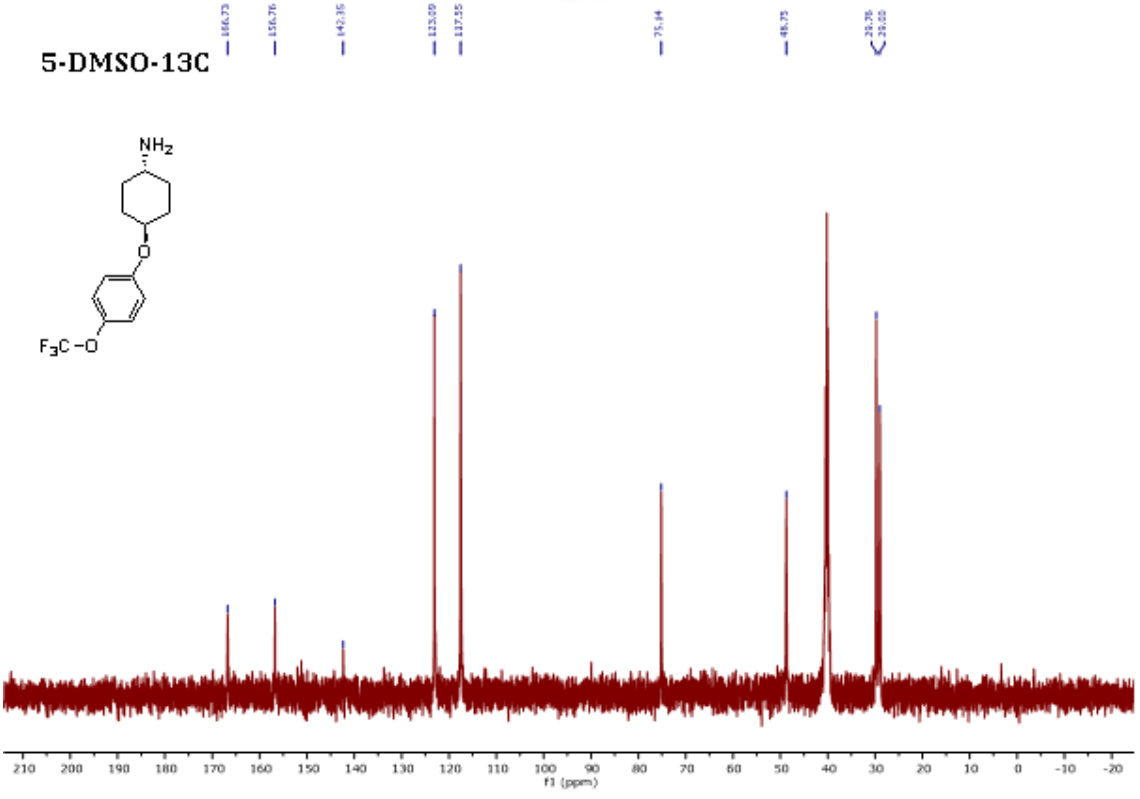
4-DMSO-19F



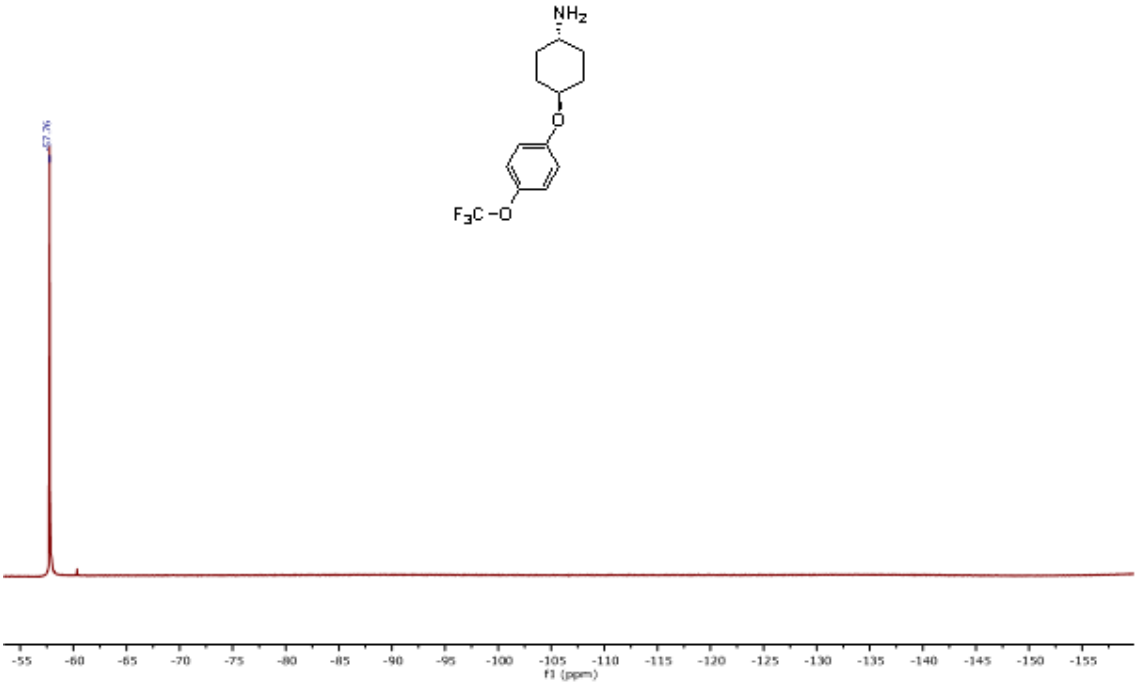
5-DMSO-1H



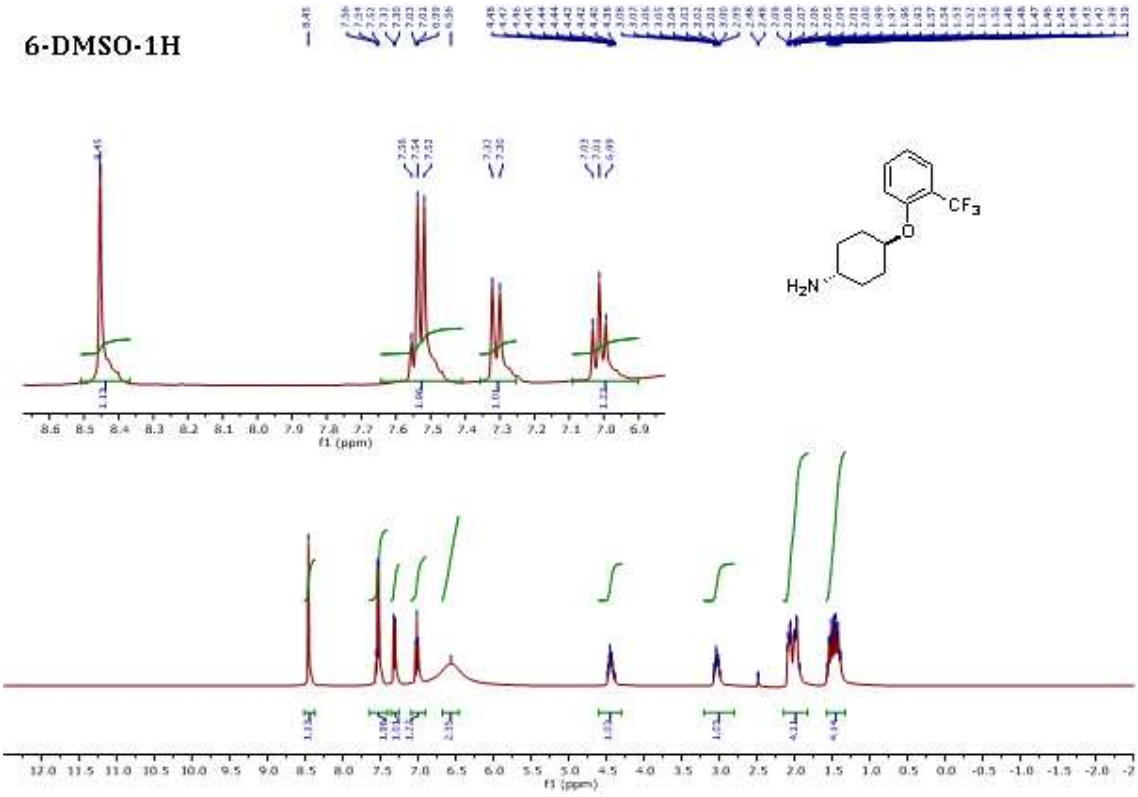
5-DMSO-13C



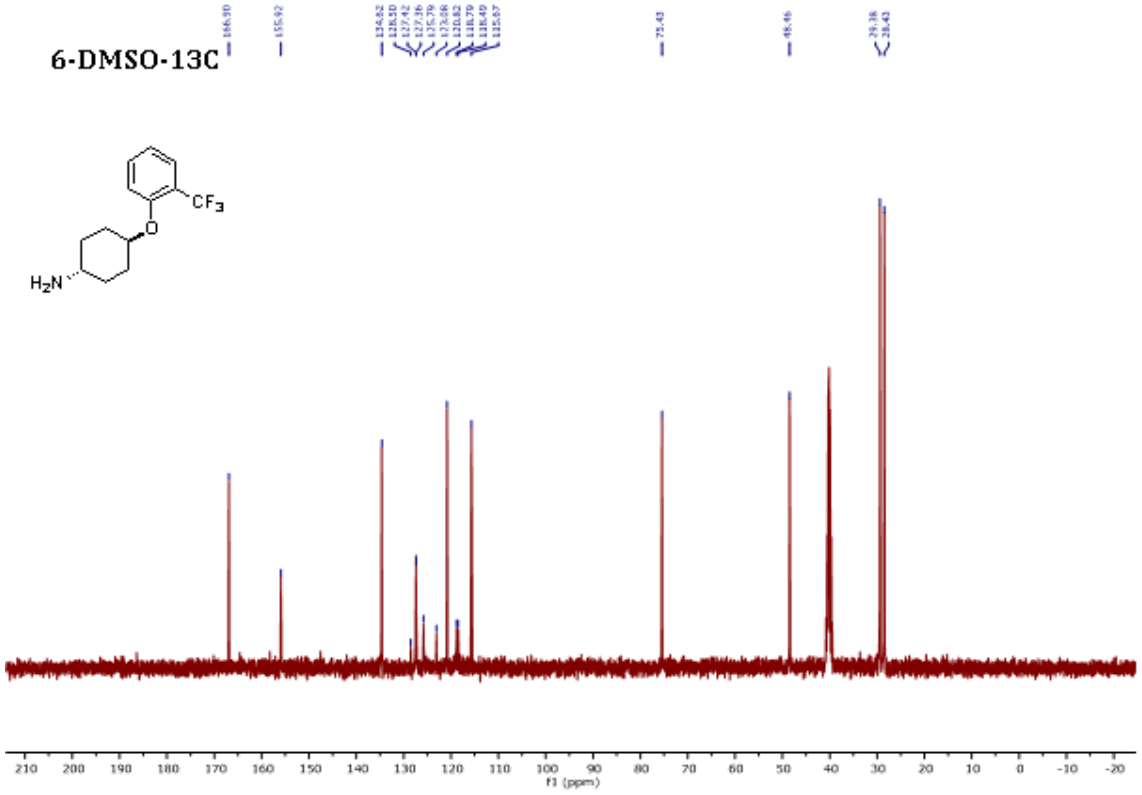
5-DMSO-19F



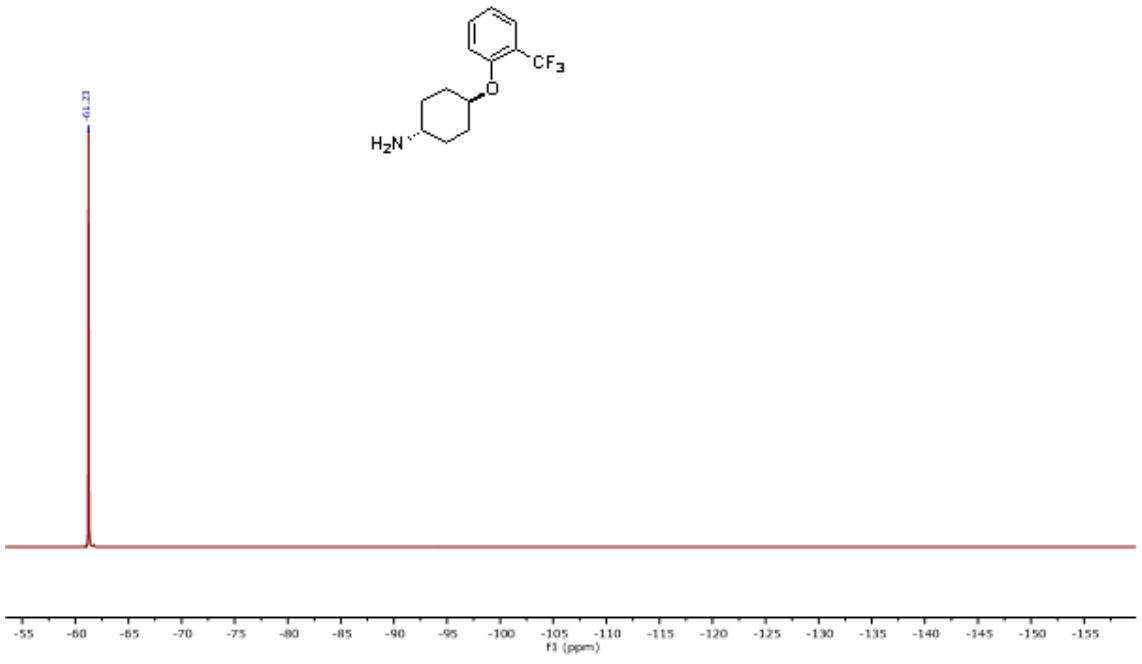
6-DMSO-1H



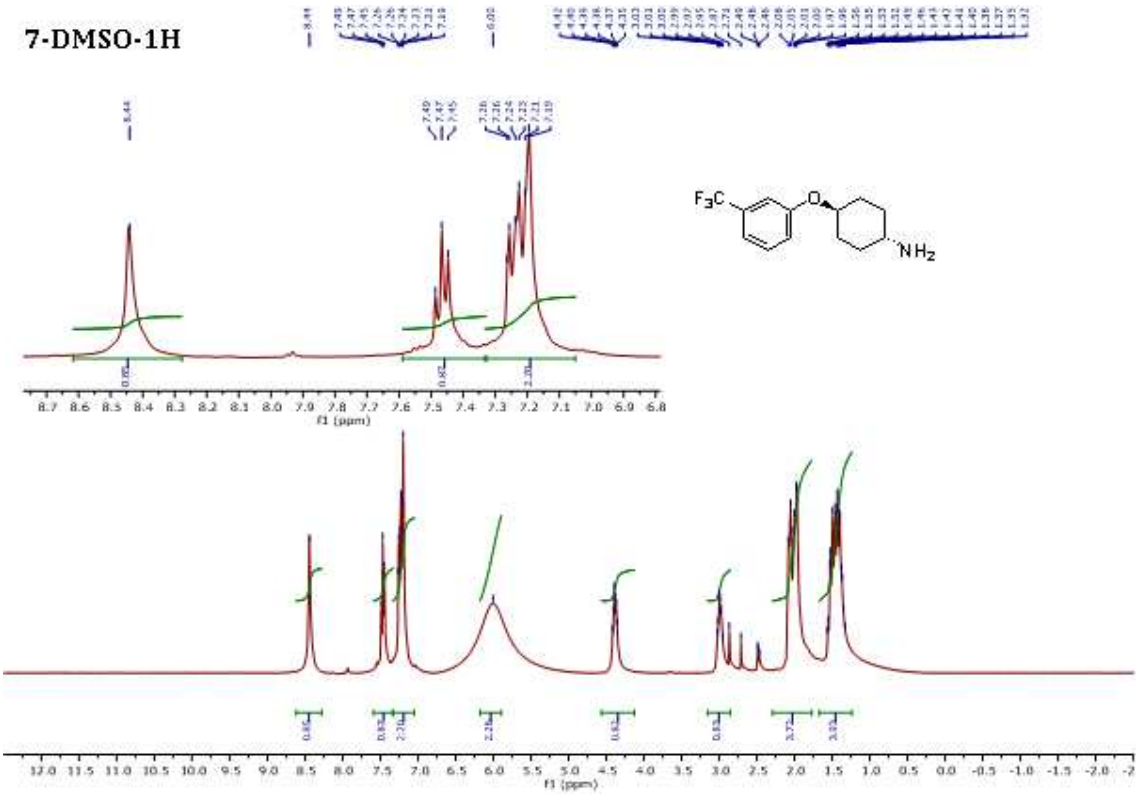
6-DMSO-13C



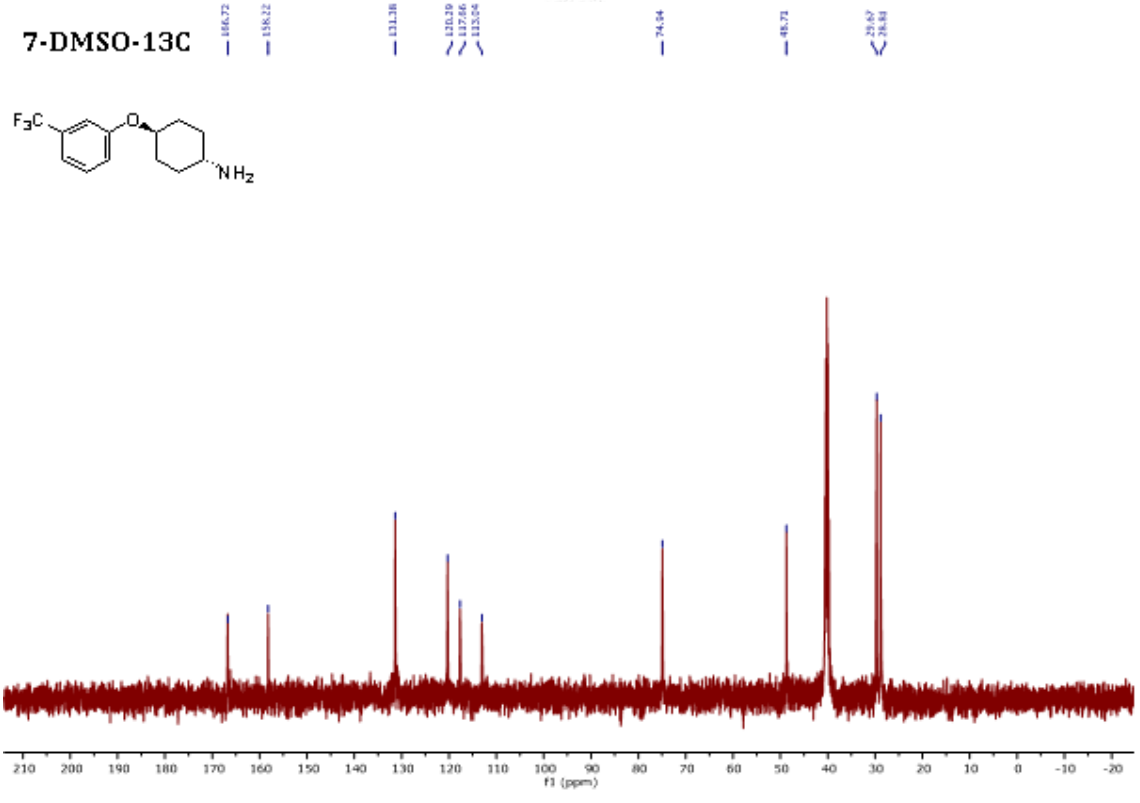
6-DMSO-19F



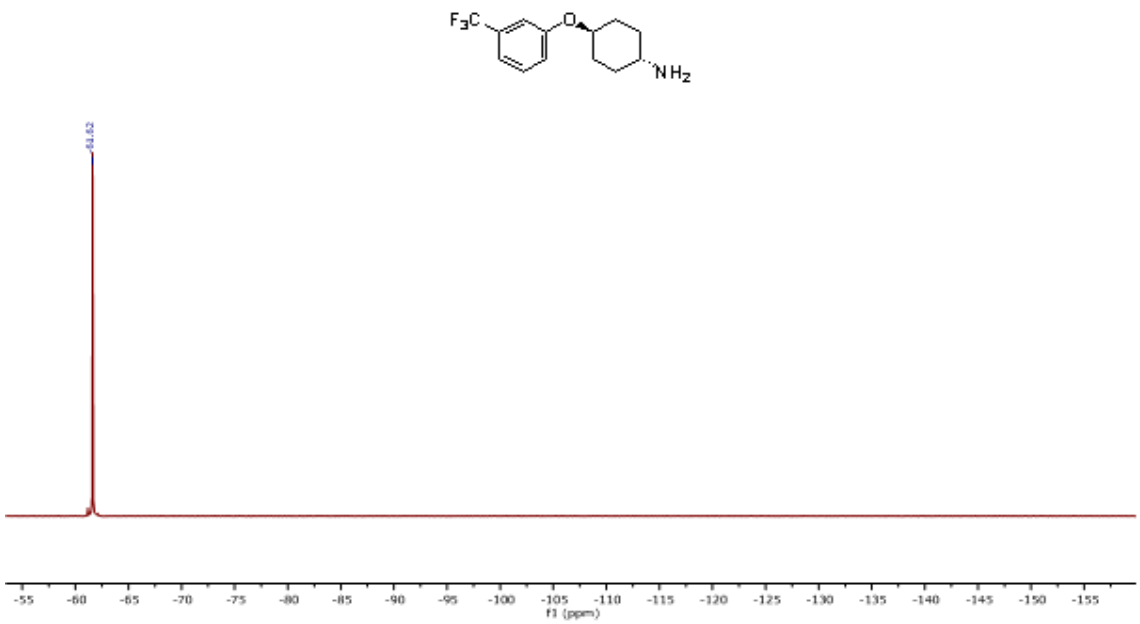
7-DMSO-1H



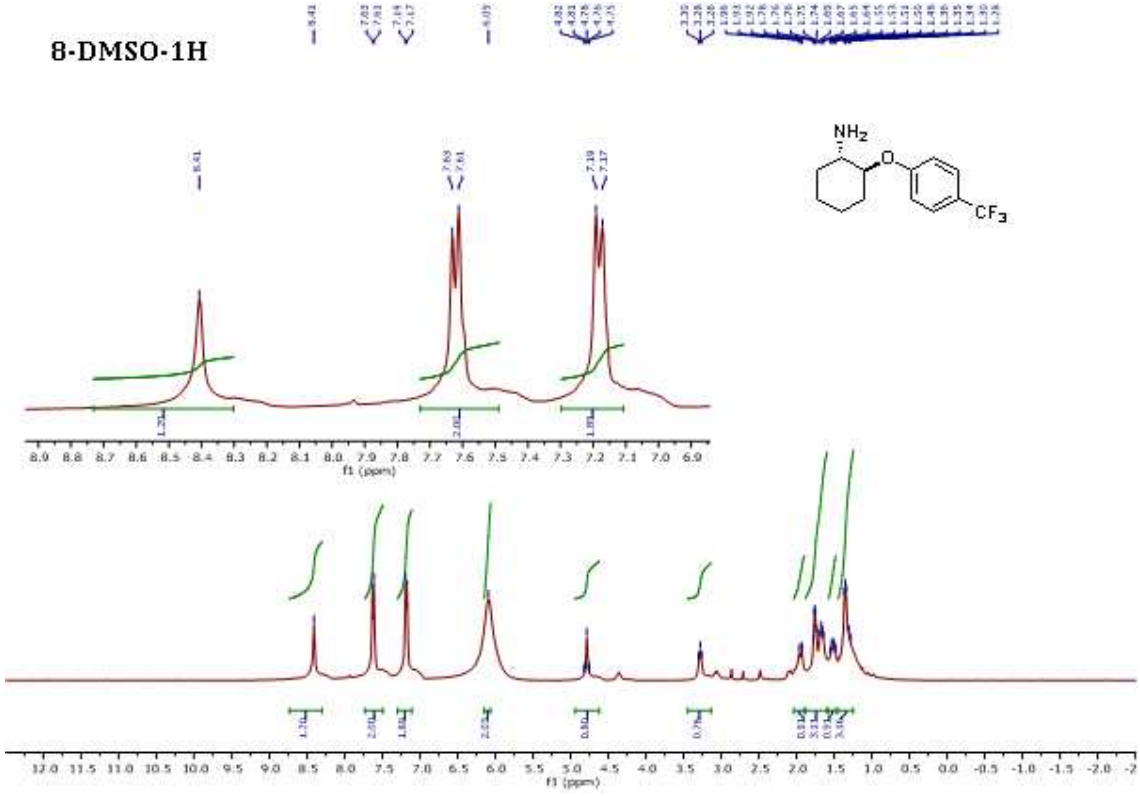
7-DMSO-13C



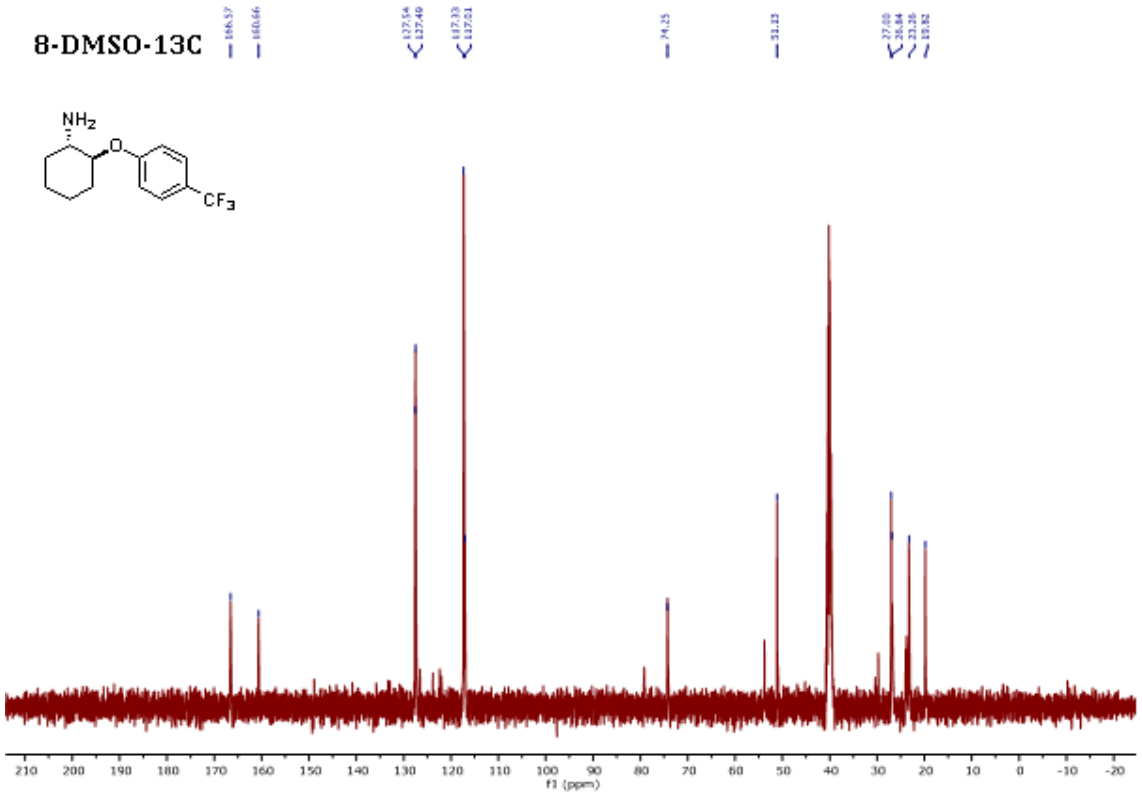
7-DMSO-19F



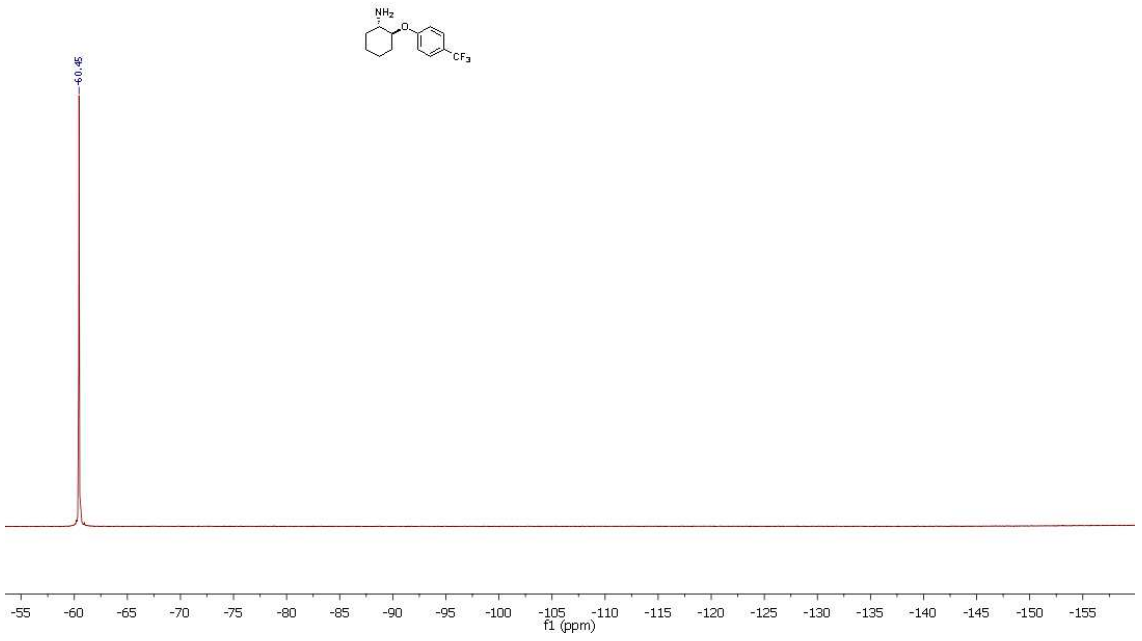
8-DMSO-1H



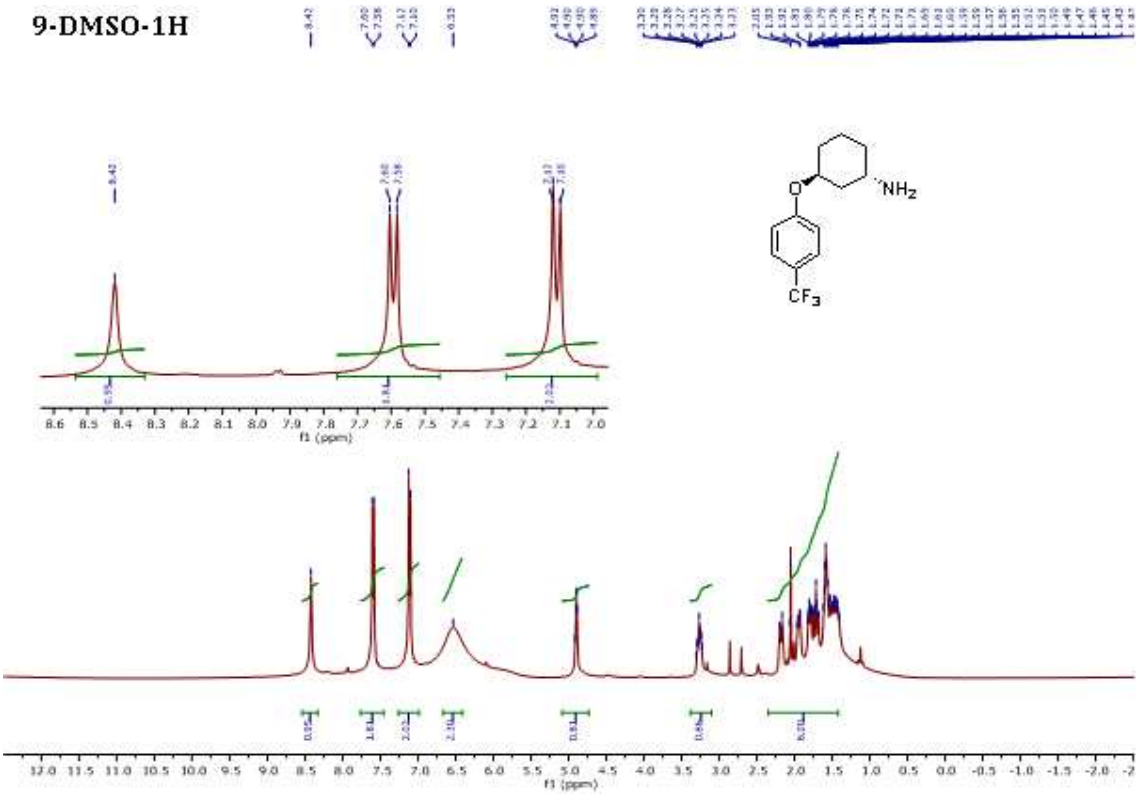
8-DMSO-13C



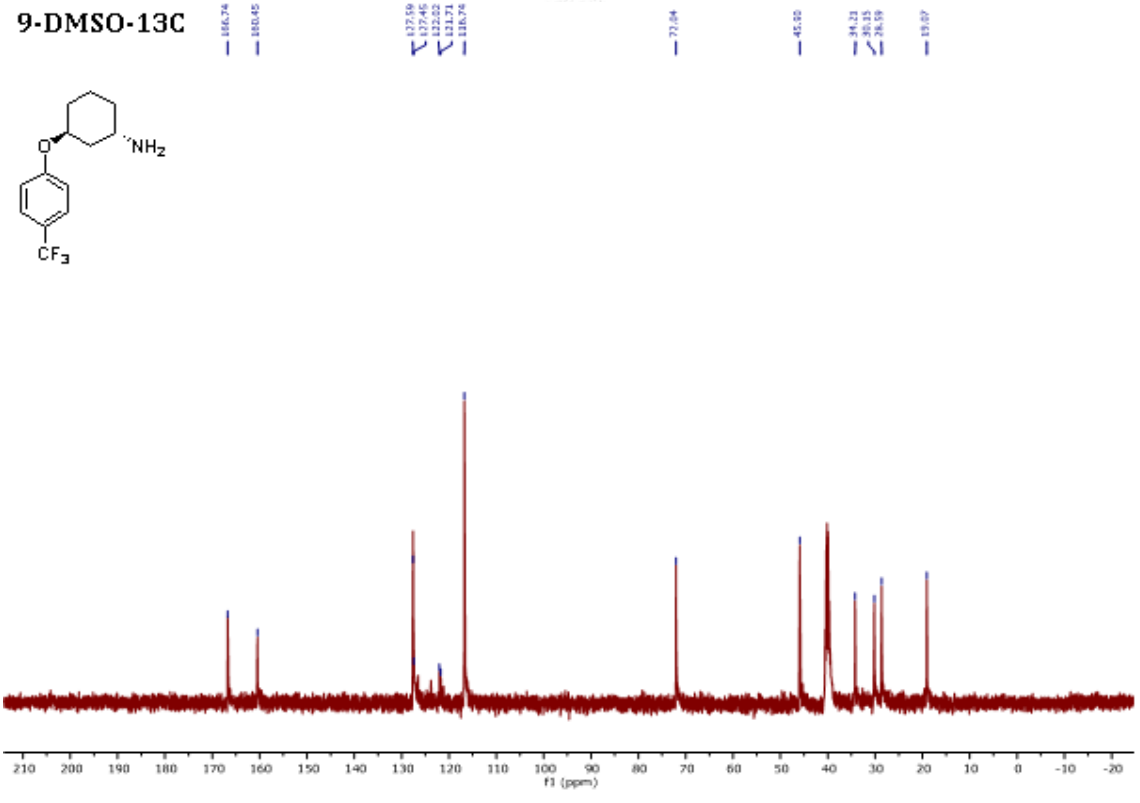
8-DMSO-19F



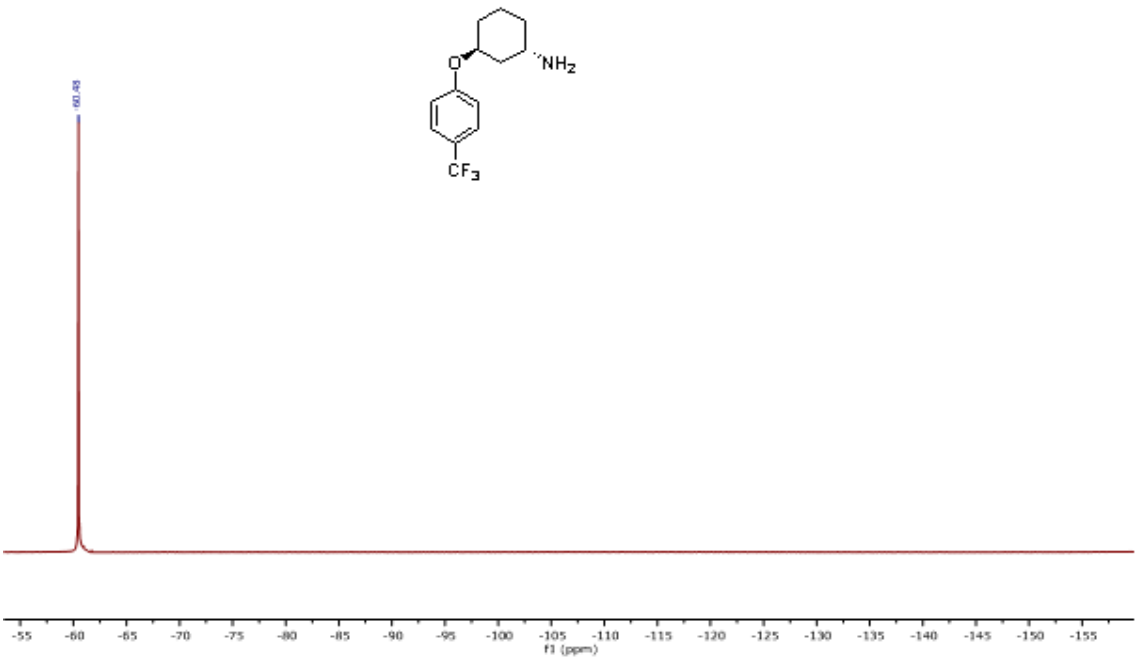
9-DMSO-1H



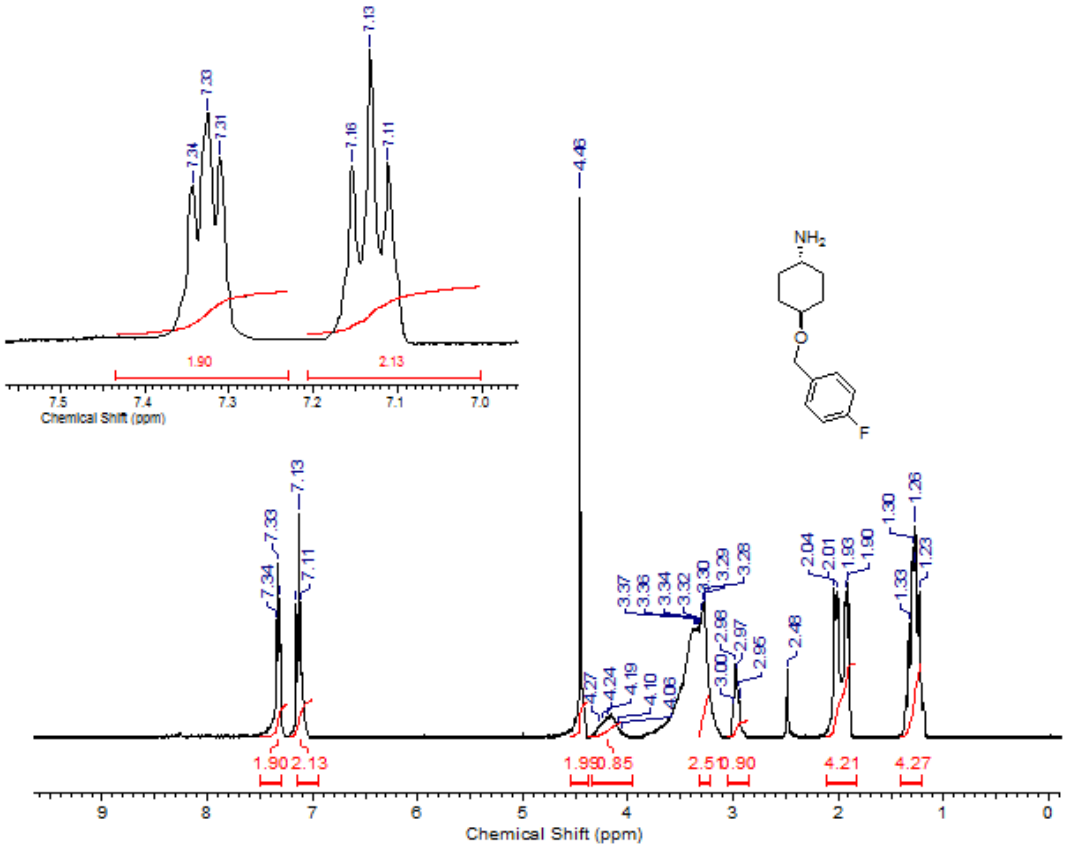
9-DMSO-13C



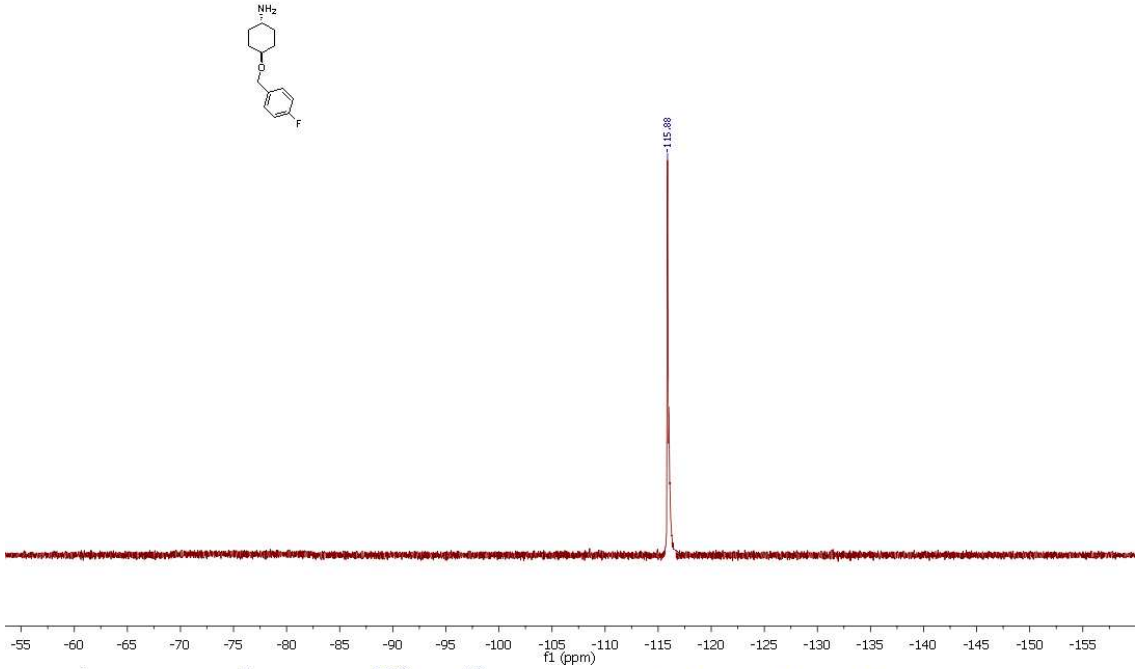
9-DMSO-19F


O
NH2
CF3
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
f1 (ppm)

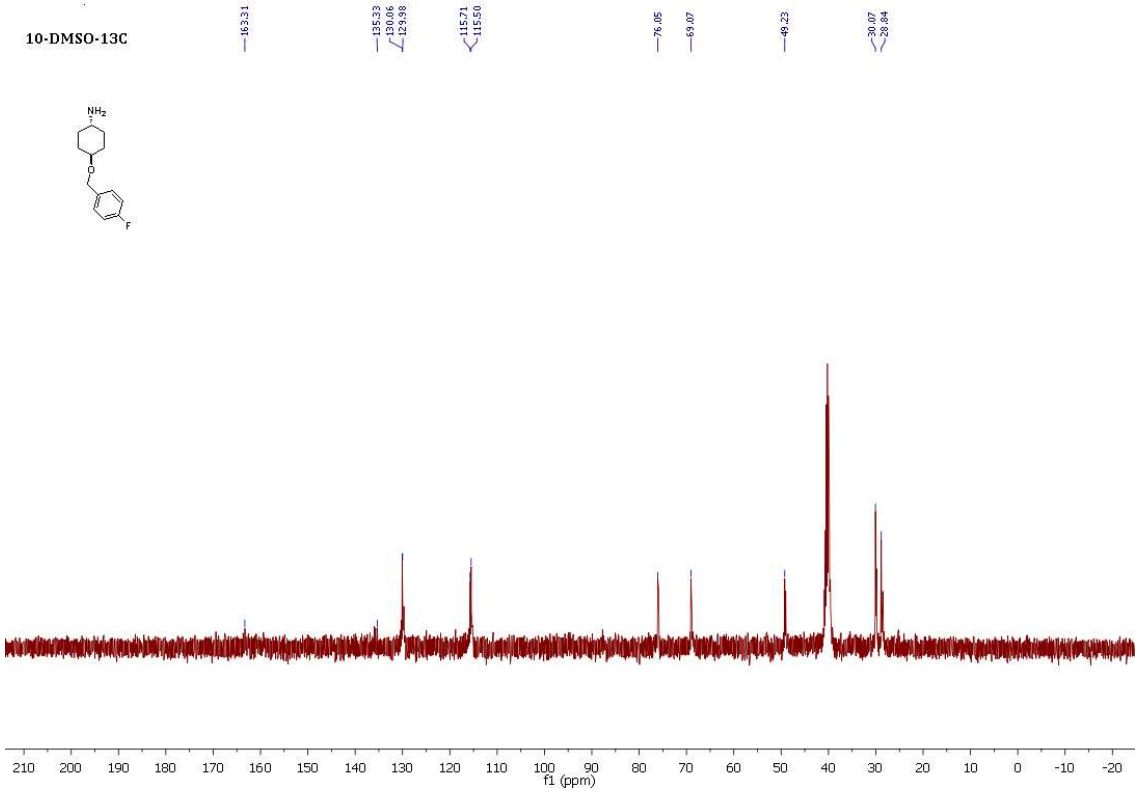
10-DMSO-1H


7.34
7.33
7.31
7.16
7.13
7.11
1.90
2.13
7.5
7.4
7.3
7.2
7.1
7.0
Chemical Shift (ppm)
4.46
NH2
O
F
3.37
3.36
3.34
3.32
3.30
3.29
3.28
2.98
2.97
2.95
4.27
4.24
4.19
4.10
4.06
3.00
2.48
2.04
2.01
1.93
1.90
1.33
1.30
1.26
1.23
1.90
2.13
1.99
0.85
2.51
0.90
4.21
4.27
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

10-DMSO-19F

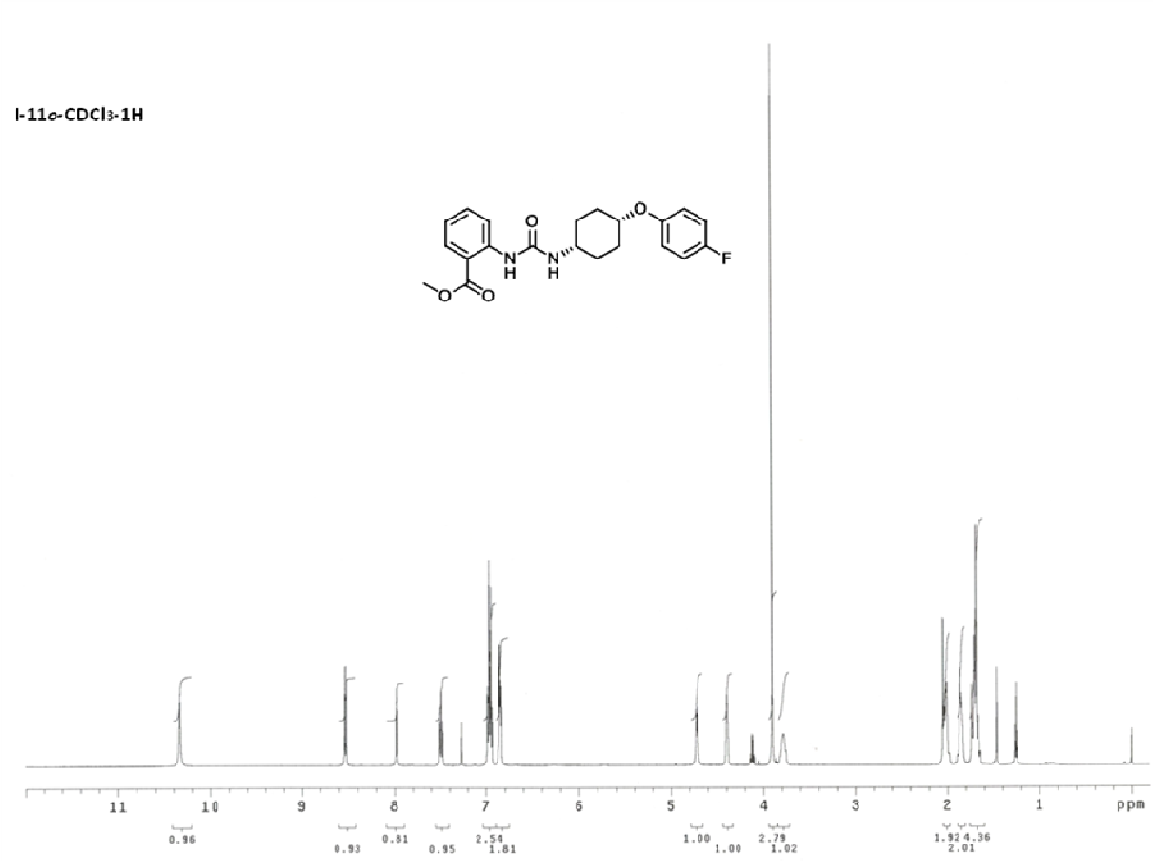


10-DMSO-13C

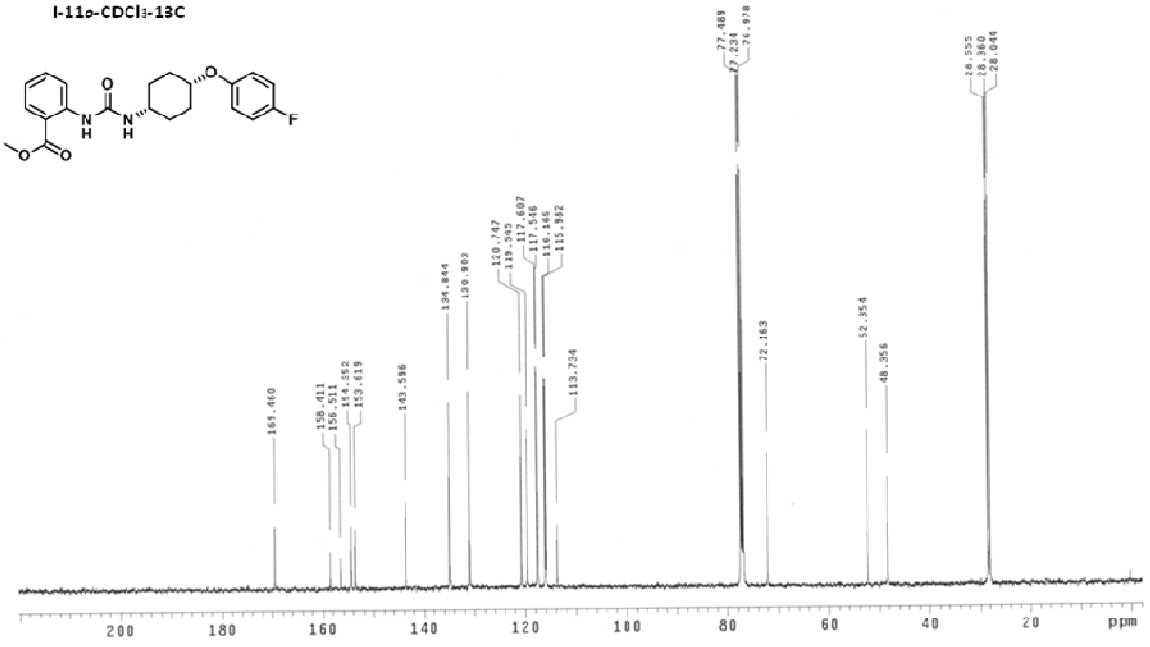


V. Structural confirmation data for the synthesized ureas**: I-11*o*, I-12*o*, I-14-20** and **III-1-5**.

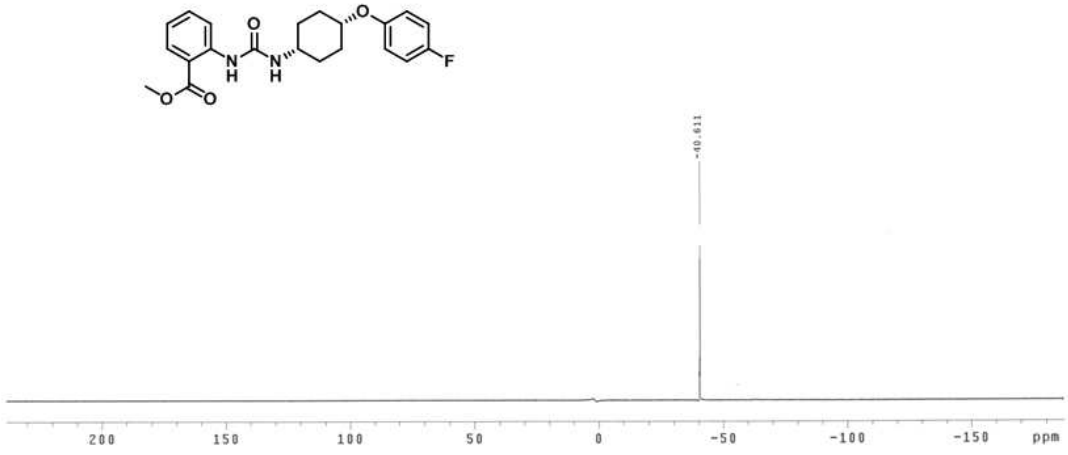
***V*.1**. ^{1}H-NMR, ^{13}C-NMR and ^{19}F –NMR Spectra *for compounds* **I-11o, I-12o, I-14-20** and **III-1-5**.



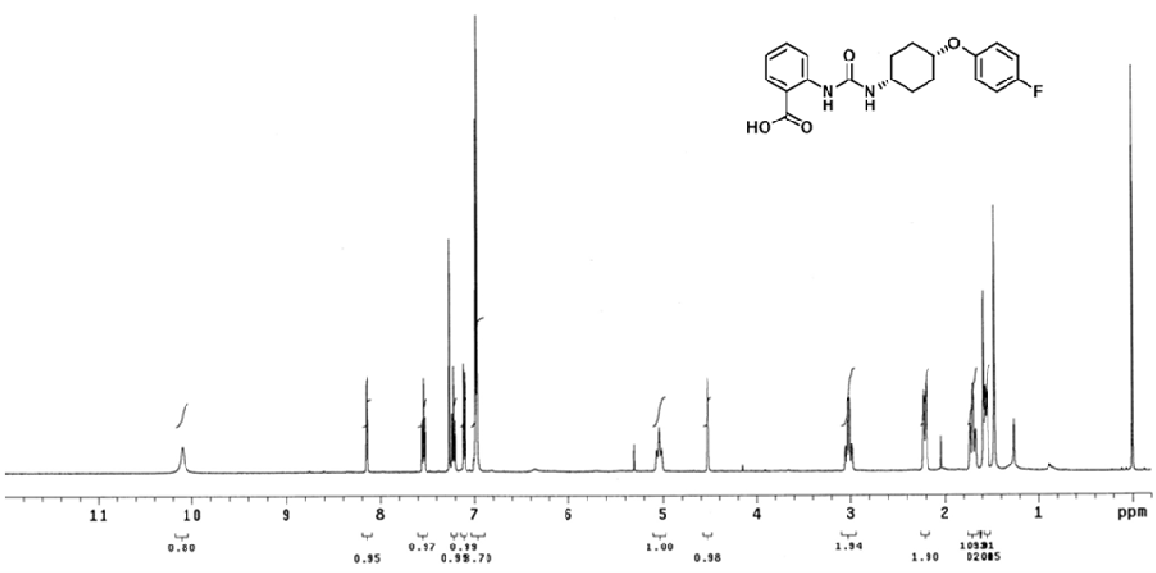
I-11*o*-CDCl3-13C



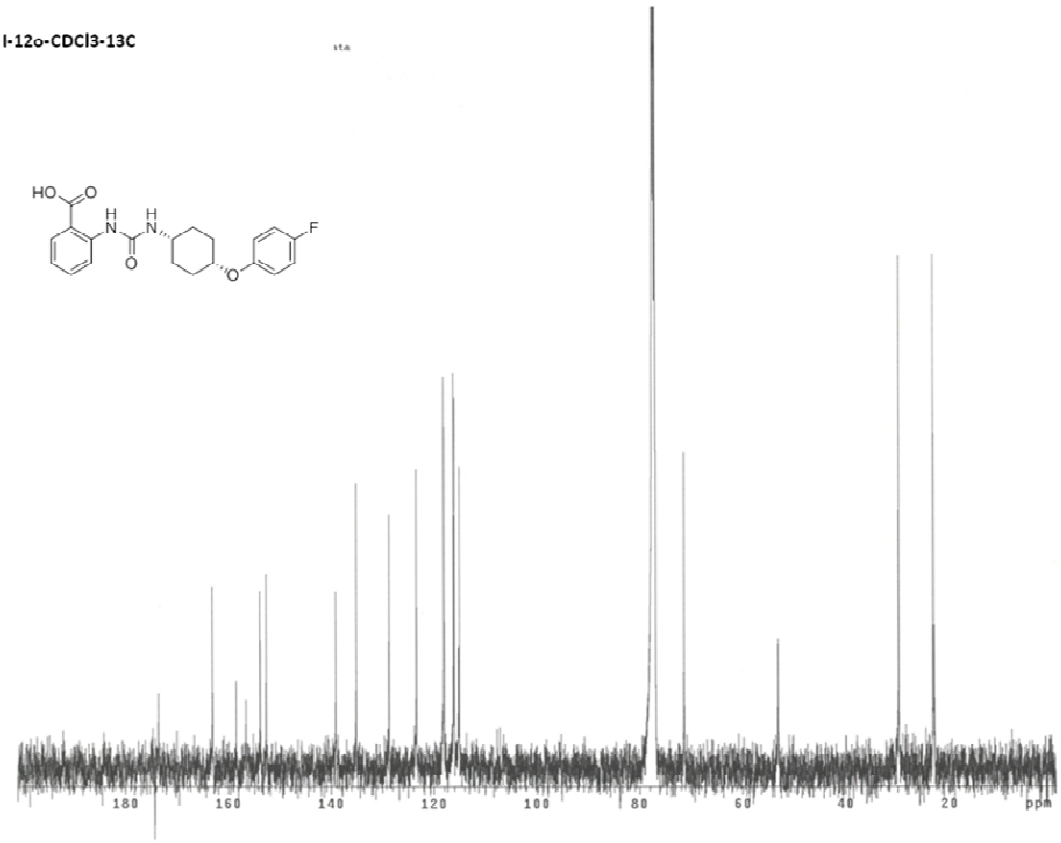
I-11-*o*-CDCl3-19F



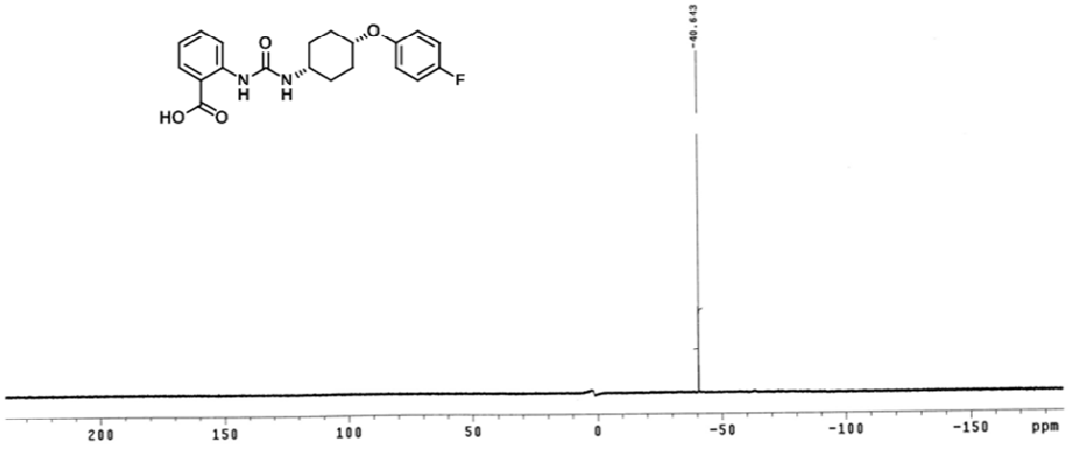
I-12e-CDCl3-1H



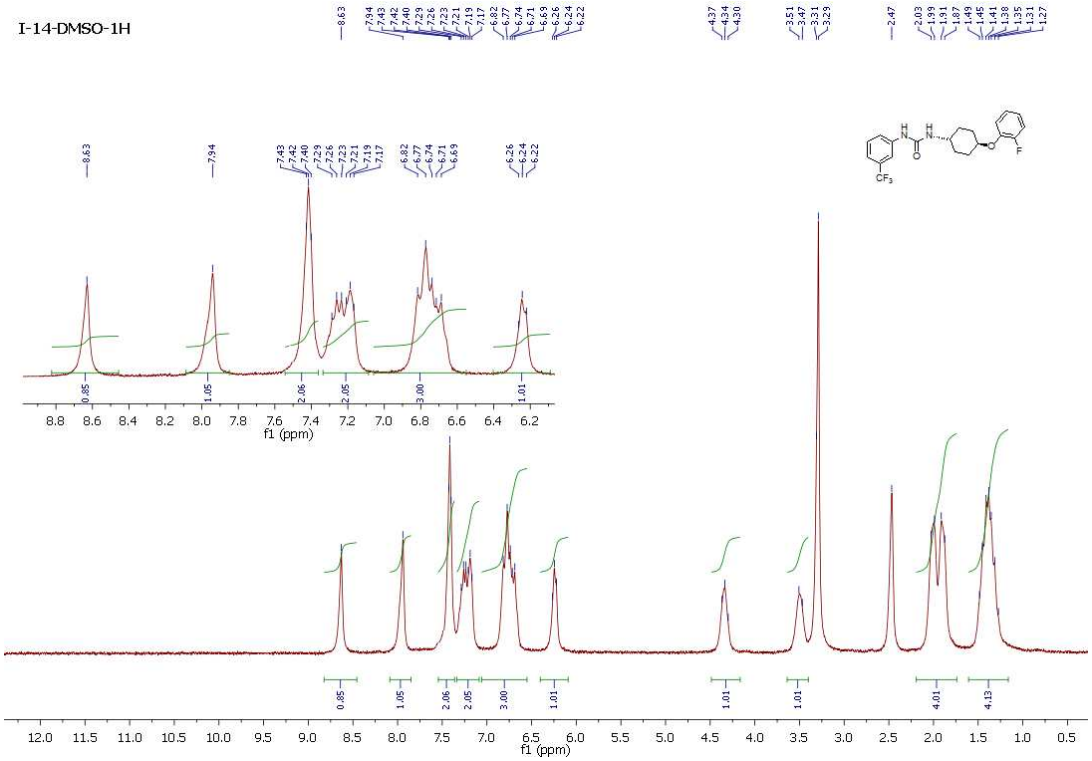
I-12o-CDCl3-13C



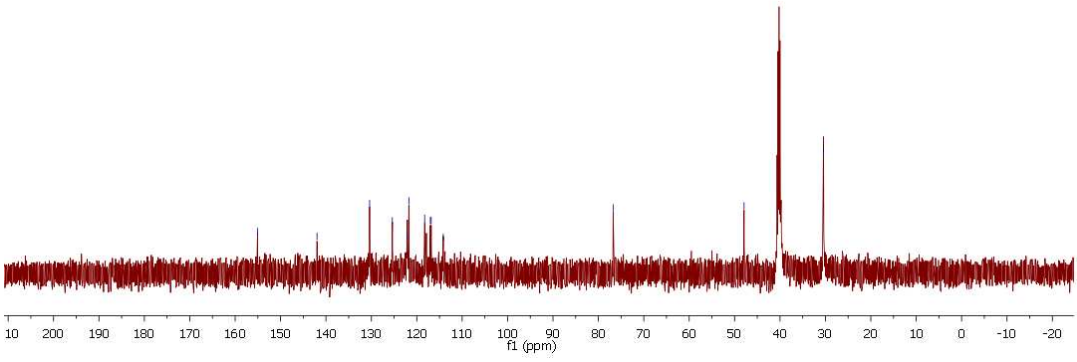
I-12o-CDCl3-19F



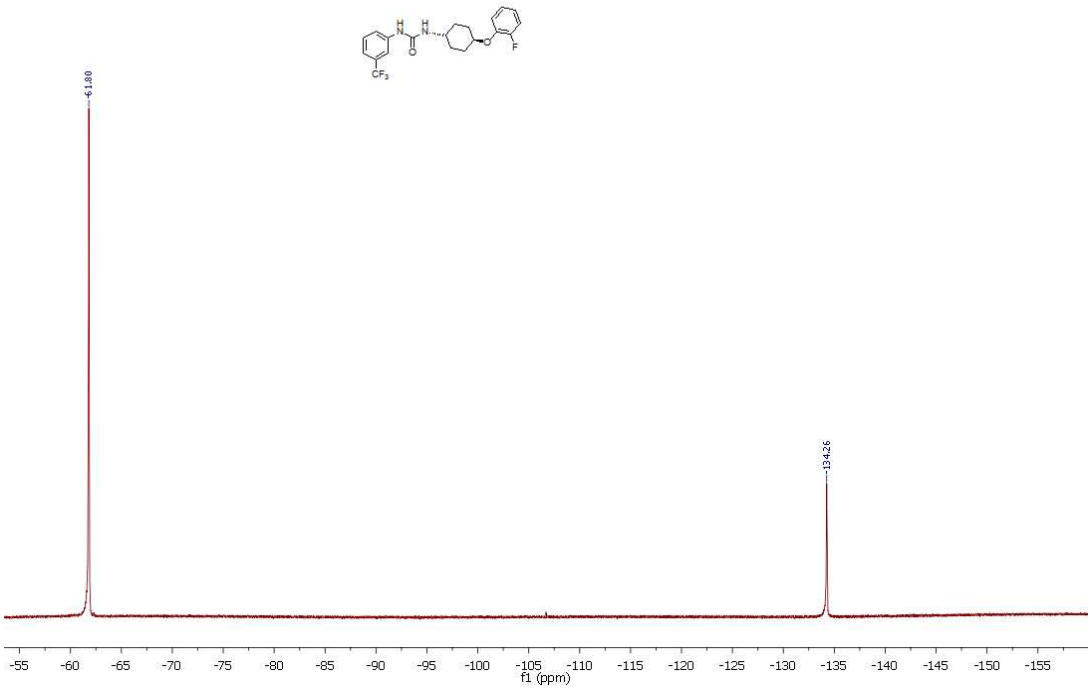
I-14-DMSO-1H



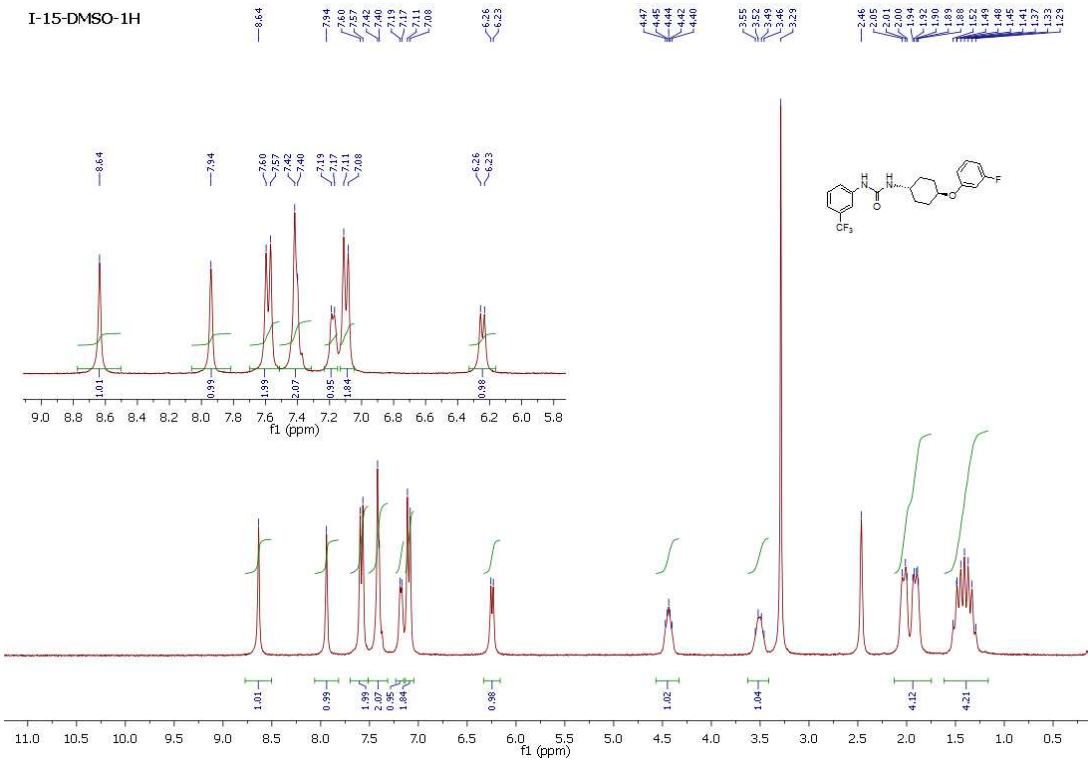
I-14-DMSO-13C



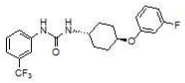
I-14-DMSO-19F



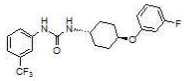
I-15-DMSO-1H

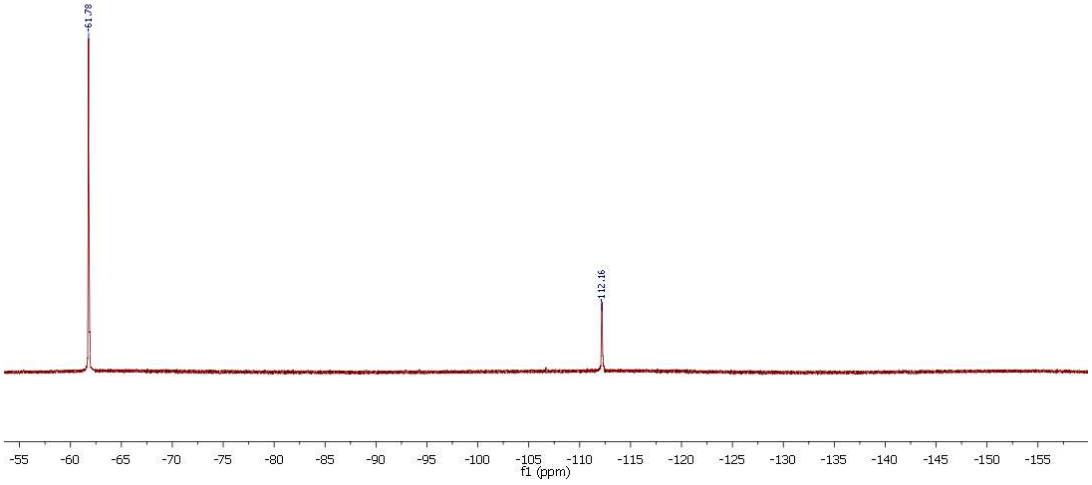


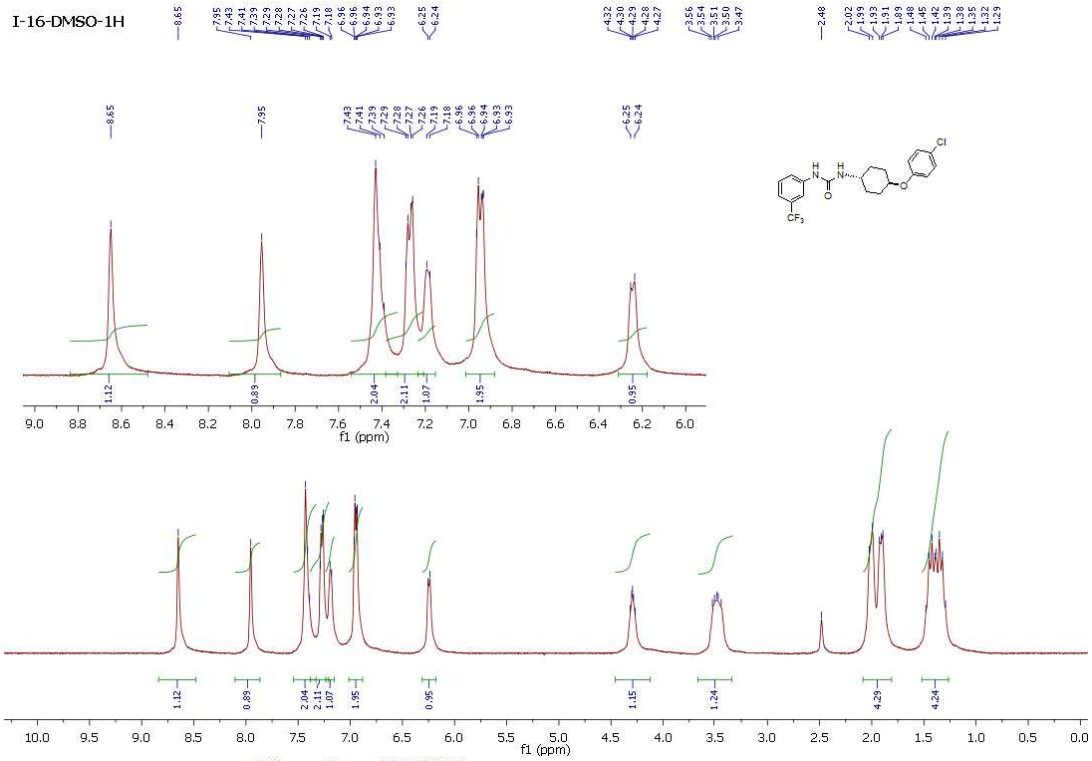
I-15-DMSO-13C

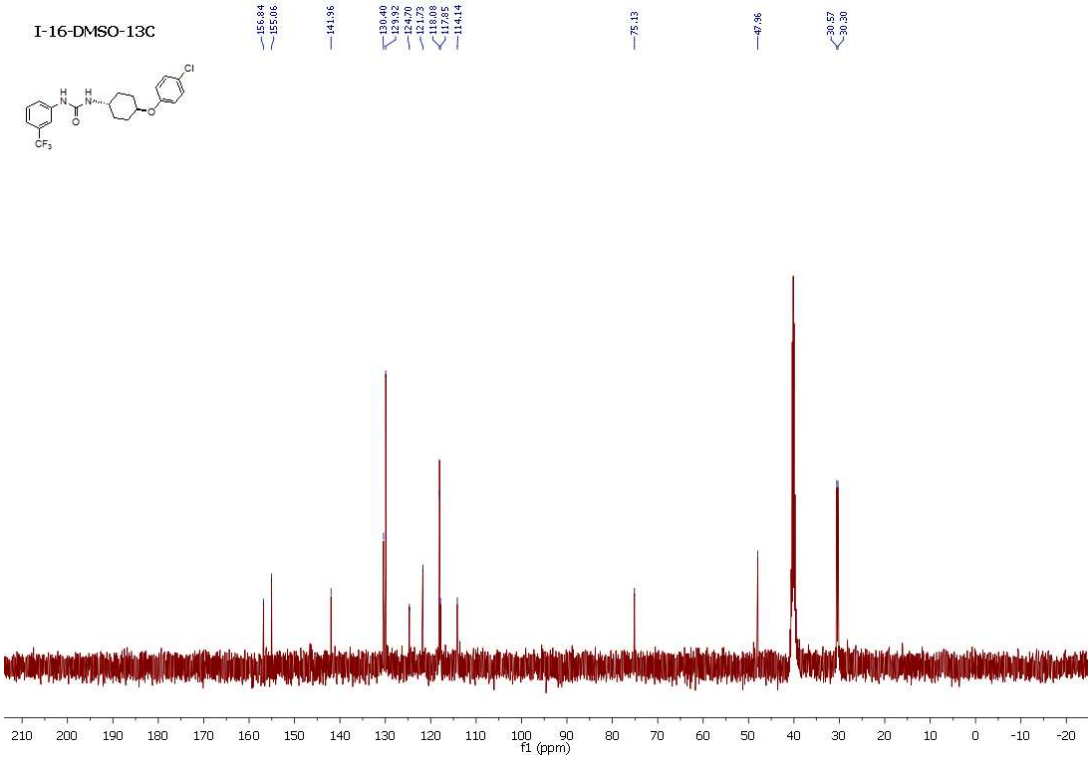


I-15-DMSO-19F

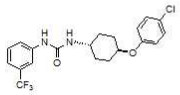


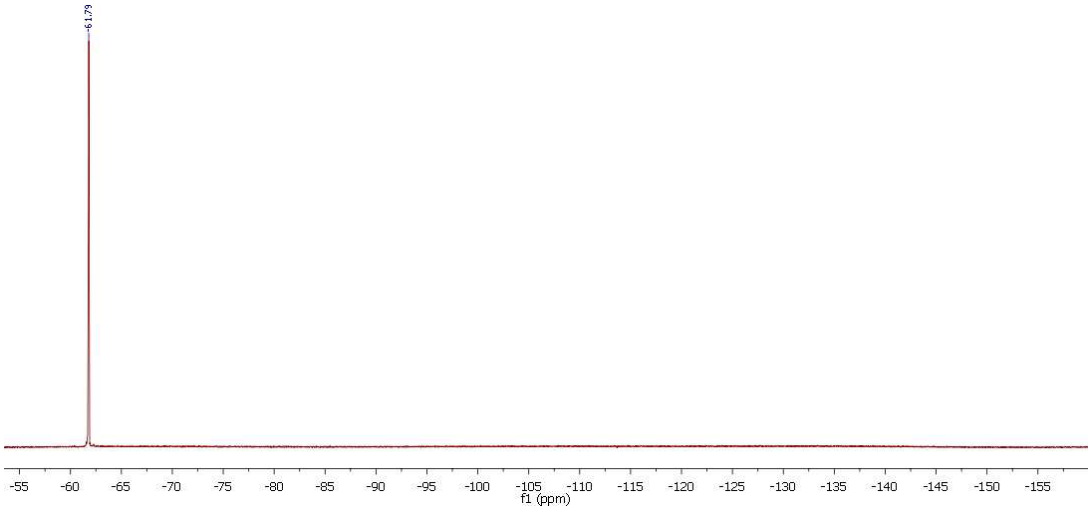



I-16-DMSO-1H
f1 (ppm)

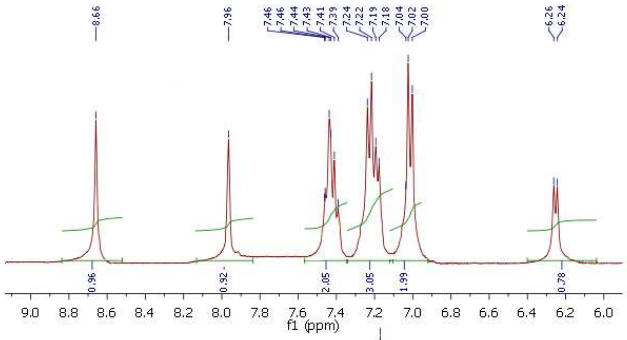

I-16-DMSO-13C
f1 (ppm)

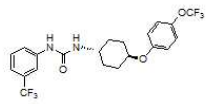
I-16-DMSO-19F

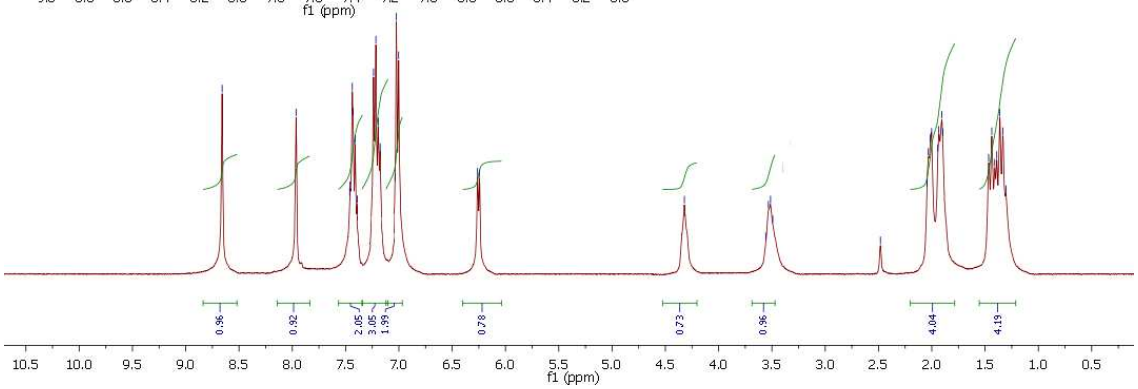




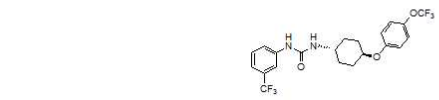
I-17-DMSO-1H

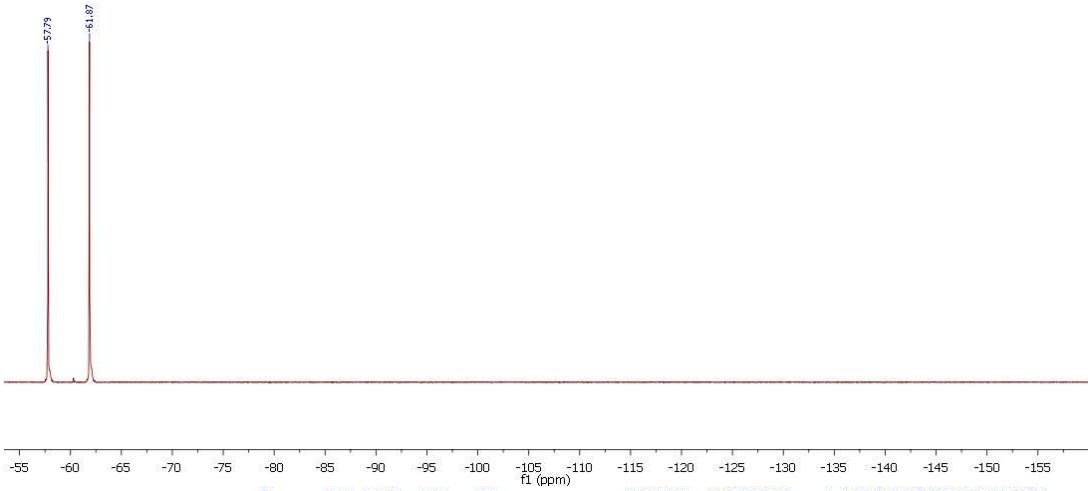




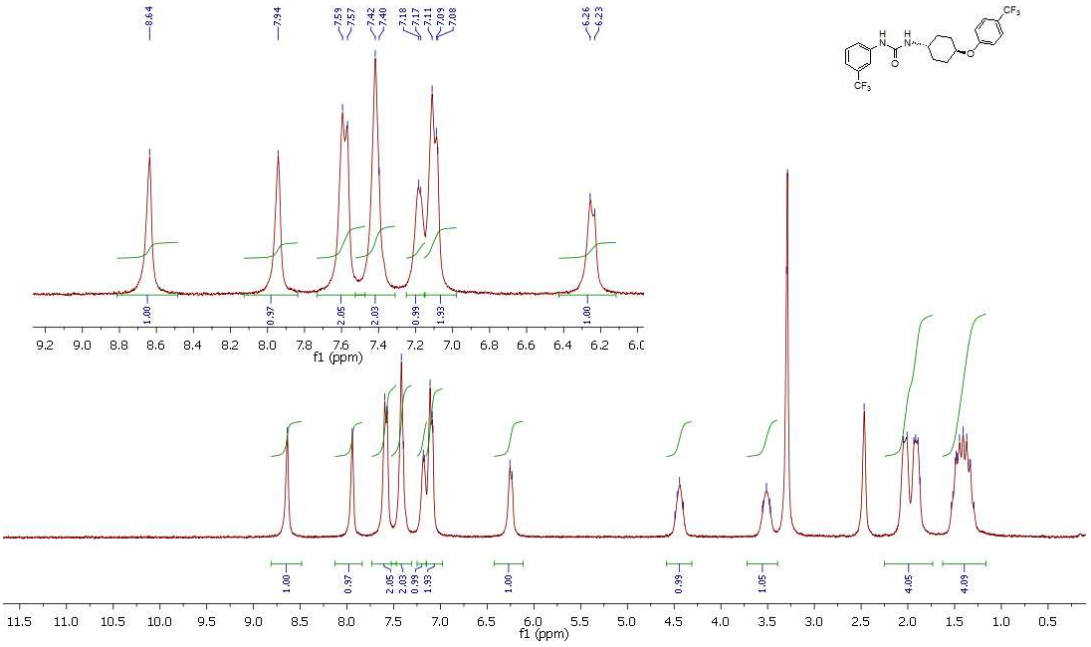


I-17-DMSO-19F

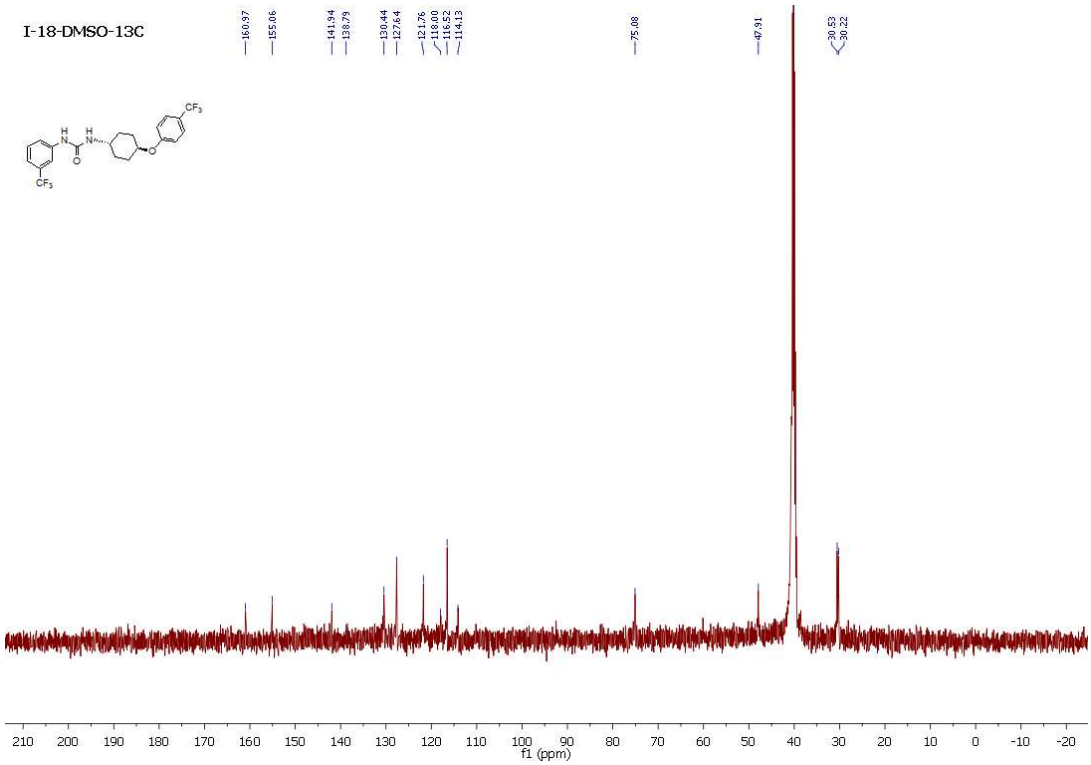




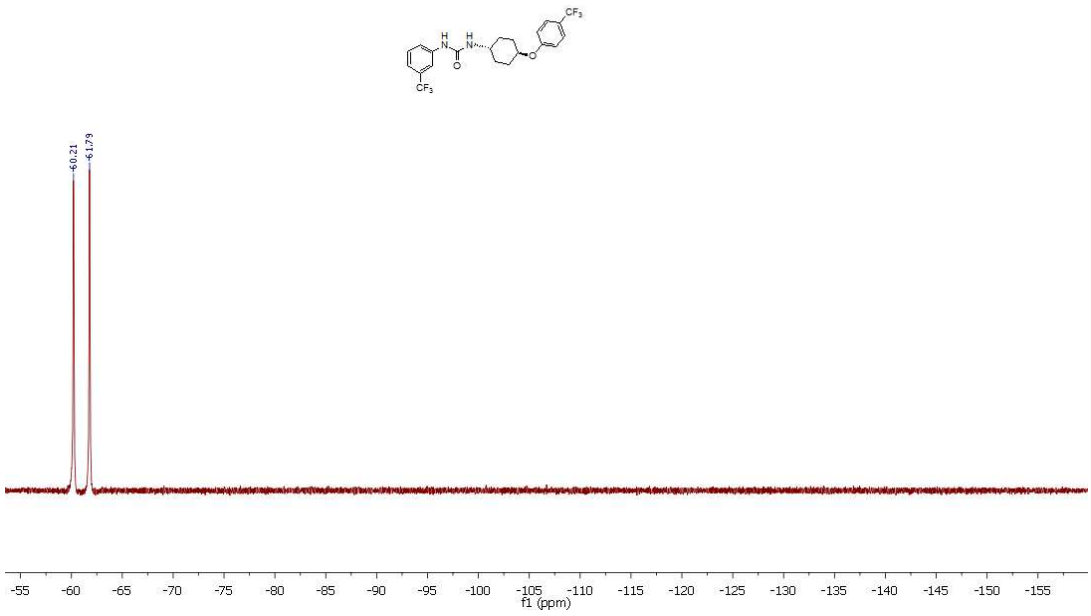
I-18-DMSO-1H



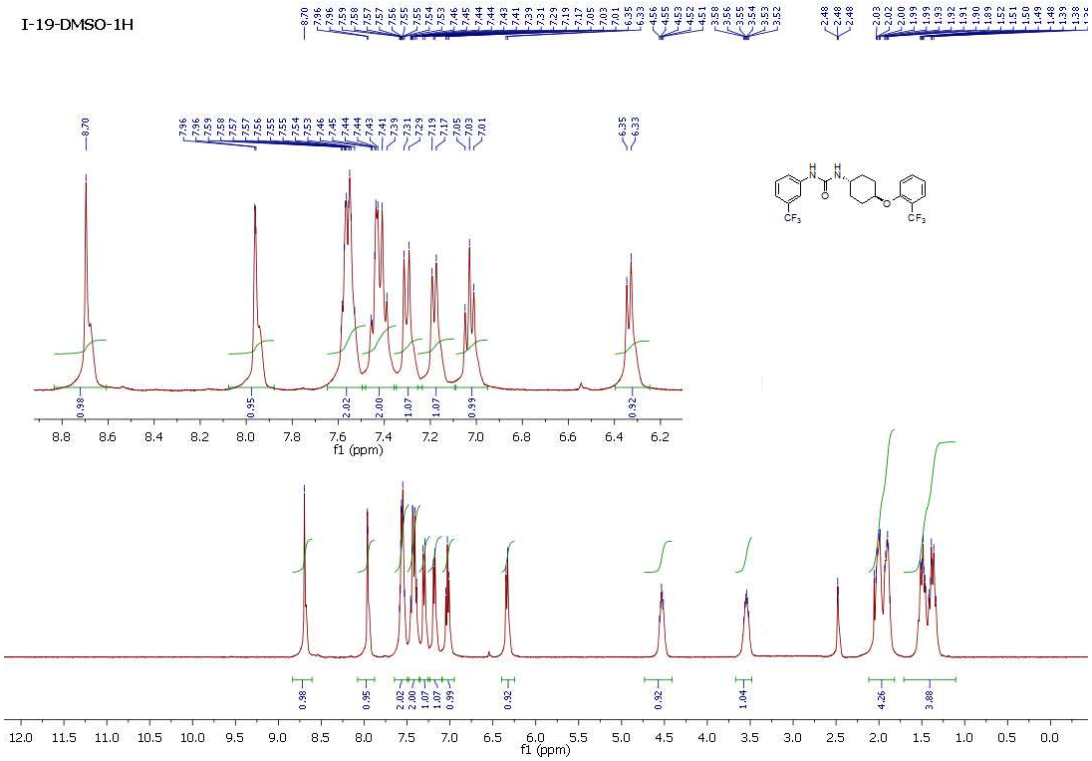
I-18-DMSO-13C



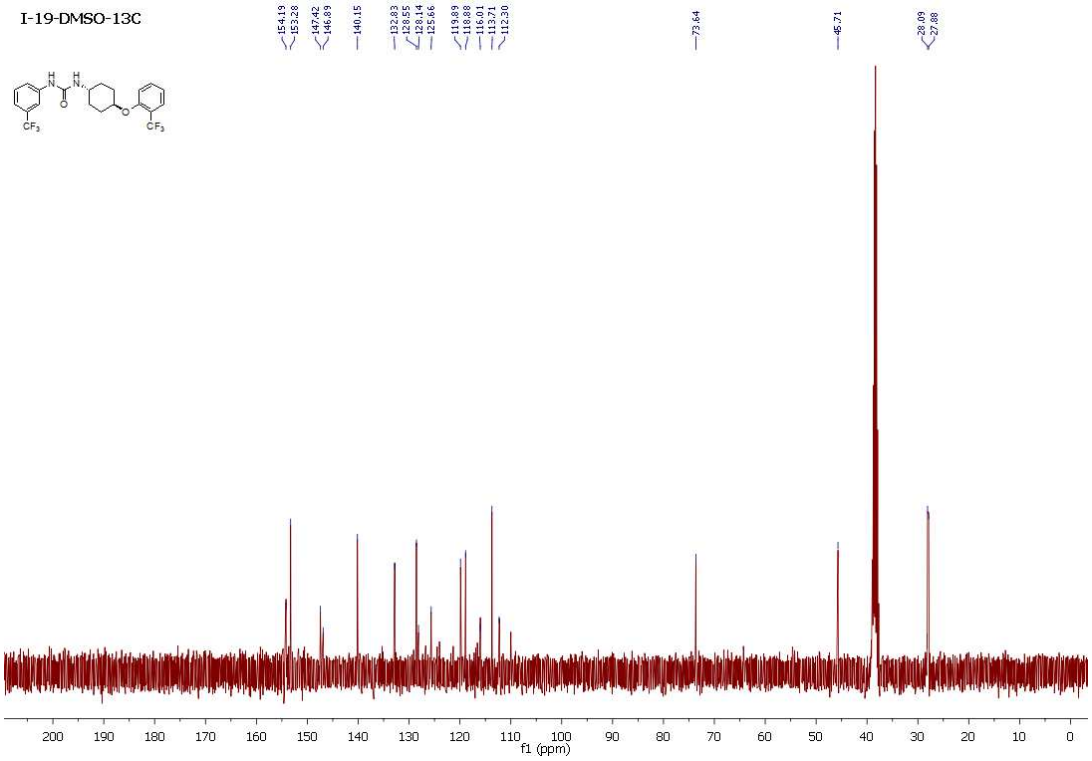
I-18-DMSO-19F



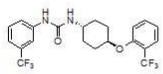
I-19-DMSO-1H

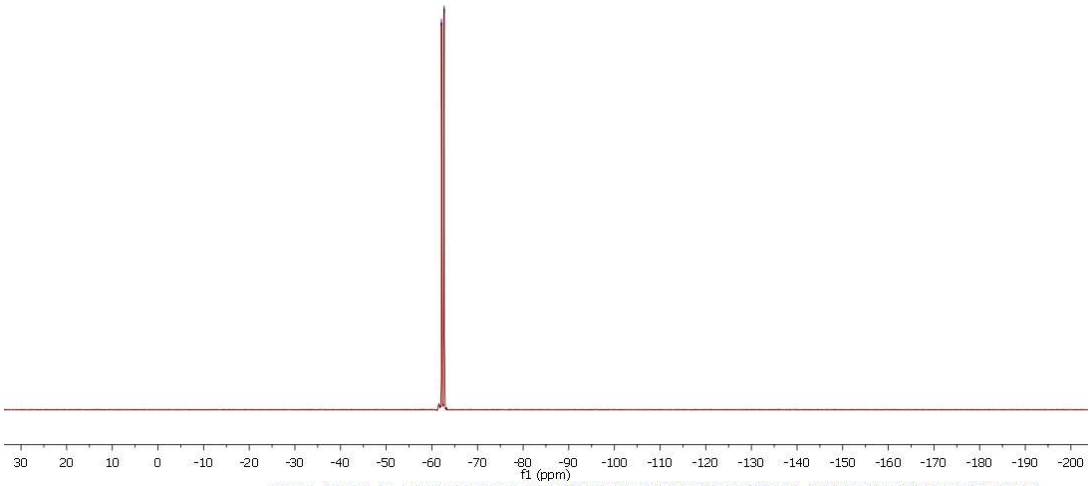


I-19-DMSO-13C

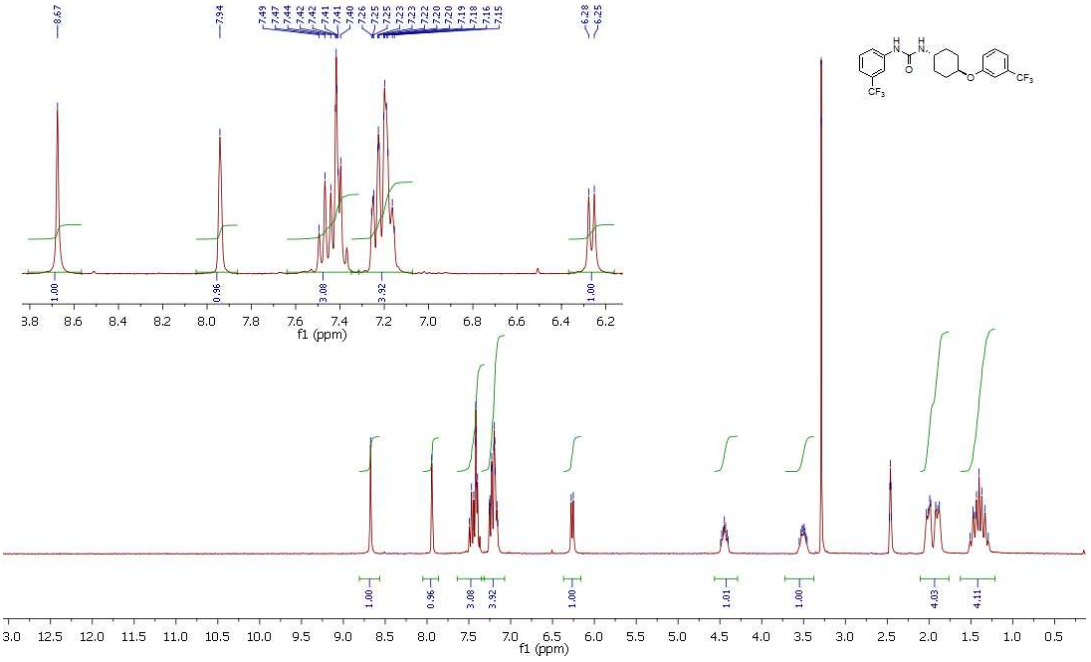


I-19-DMSO-19F

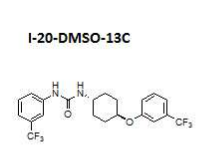




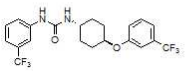
I-20-DMSO-1H

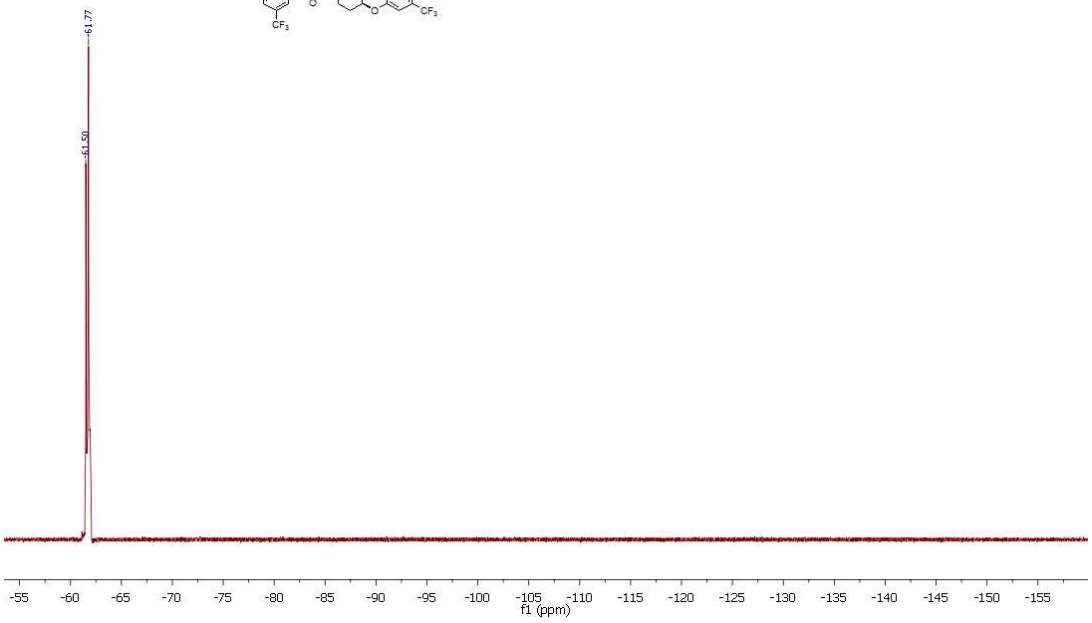


I-20-DMSO-13C

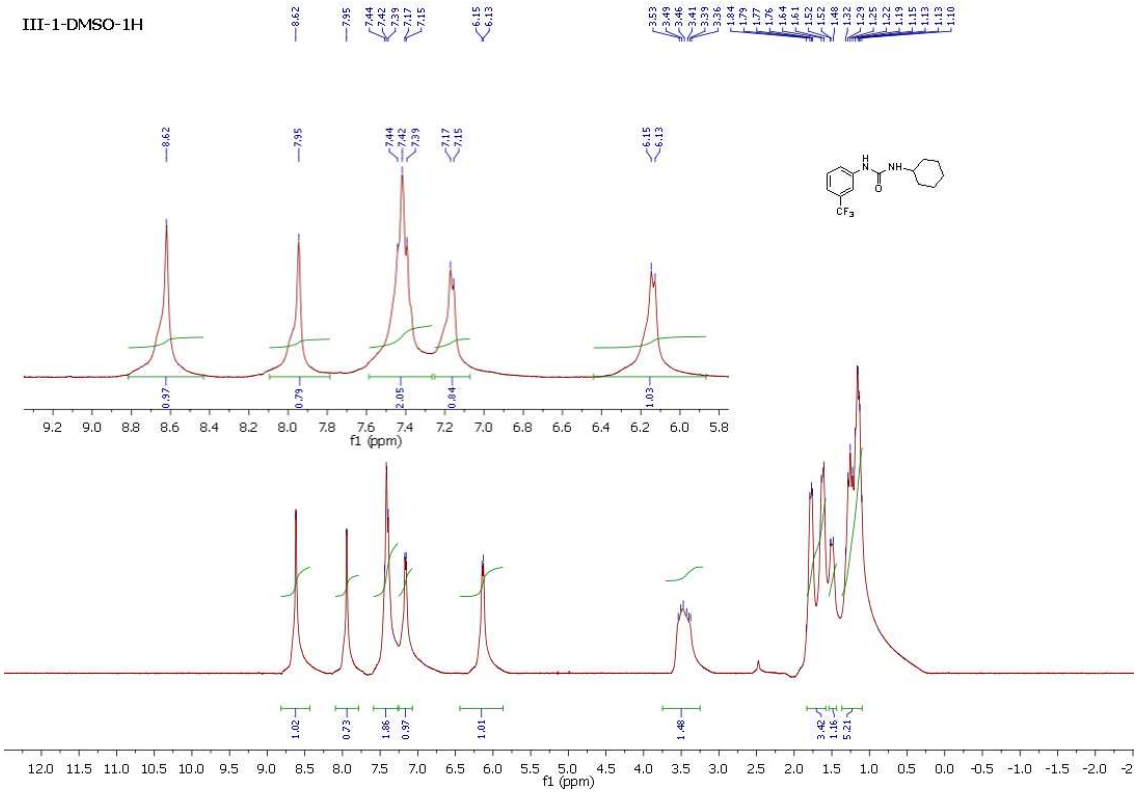


I-20-DMSO-19F

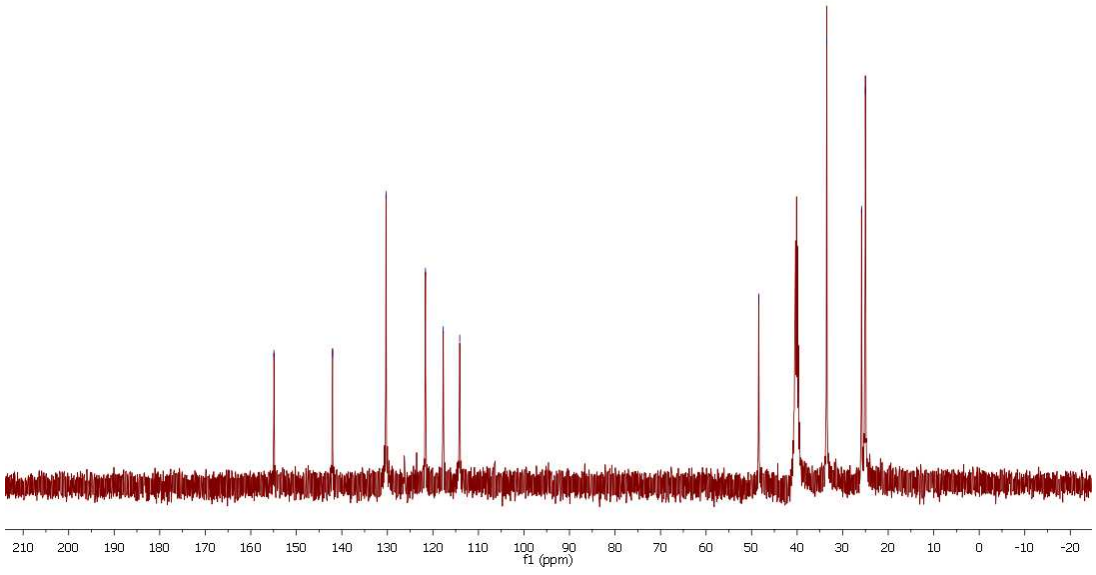




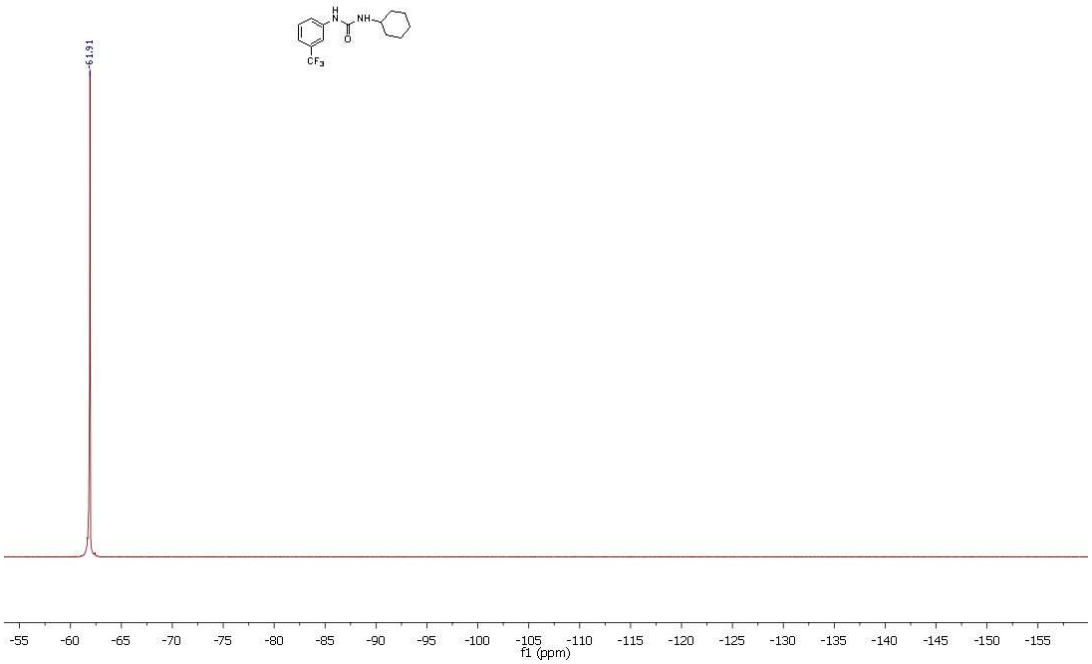
III-1-DMSO-1H



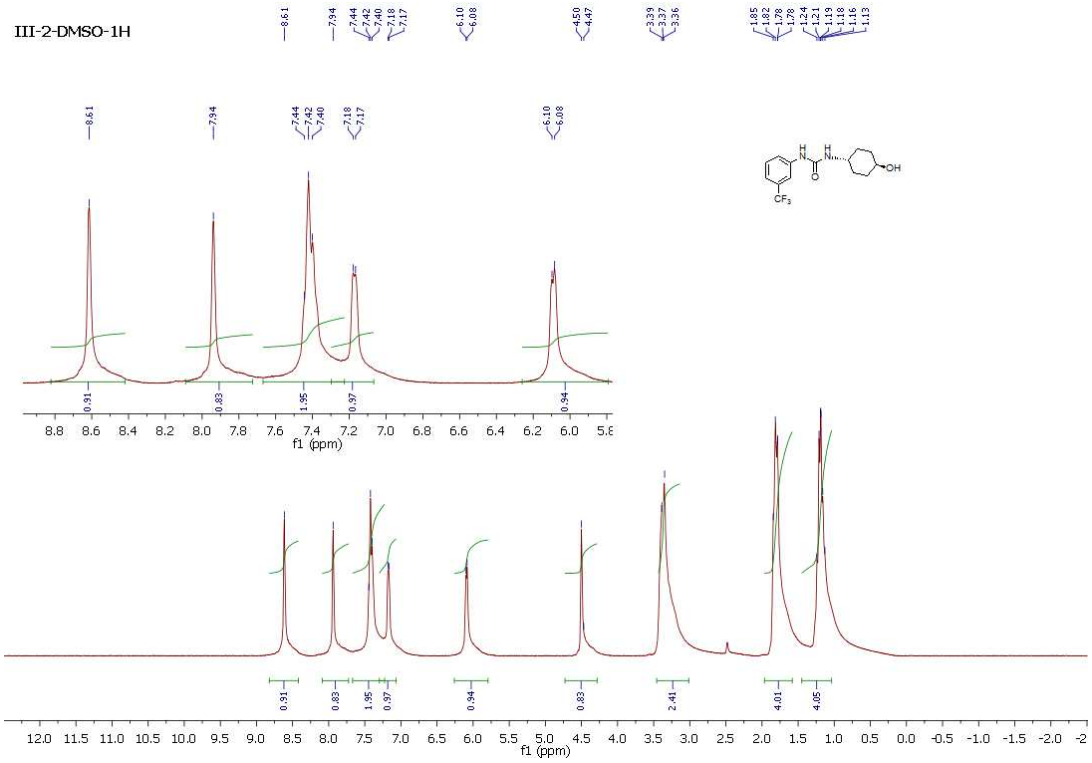
III-1-DMSO-13C



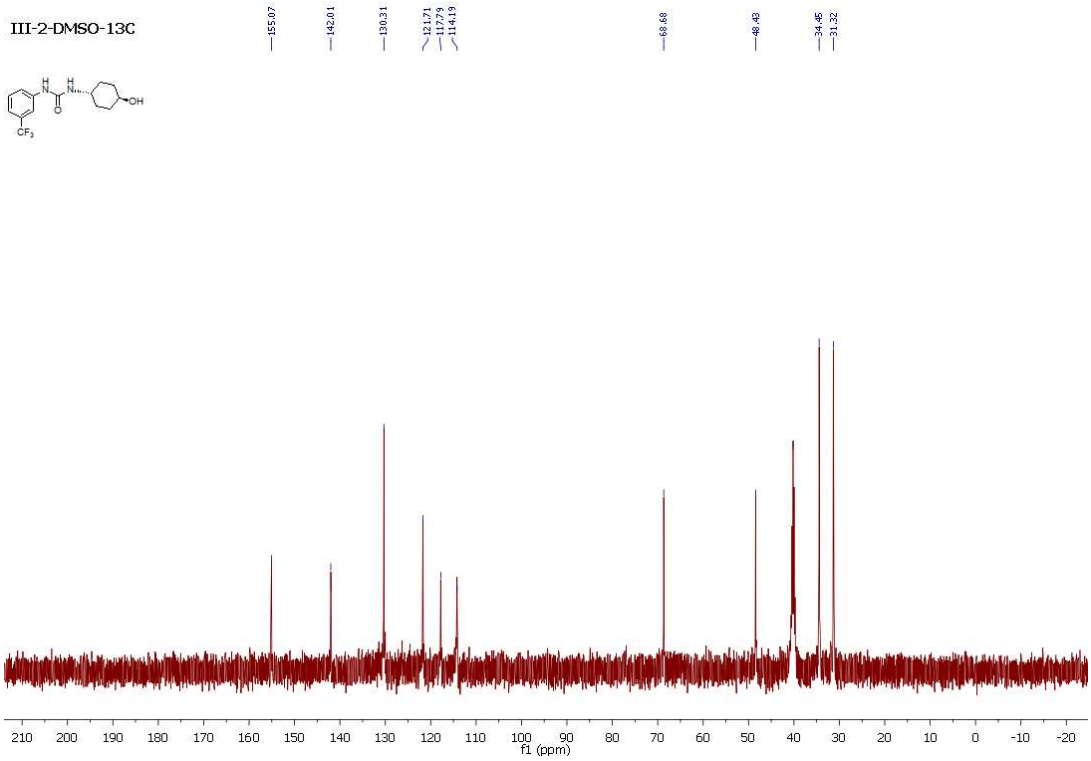
III-1-DMSO-19F



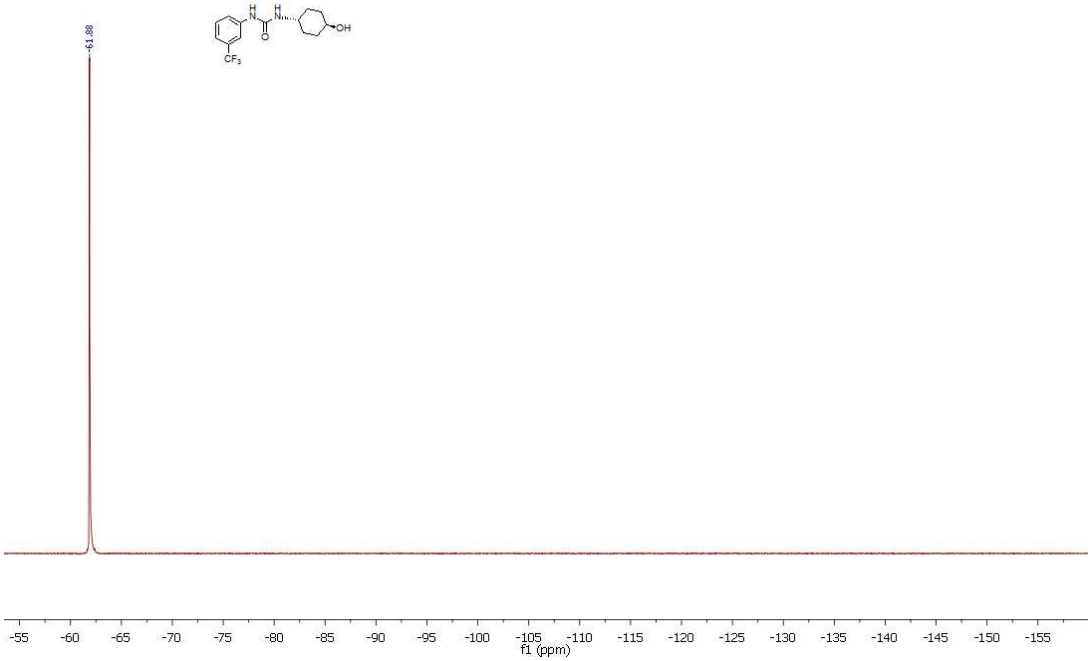
III-2-DMSO-1H

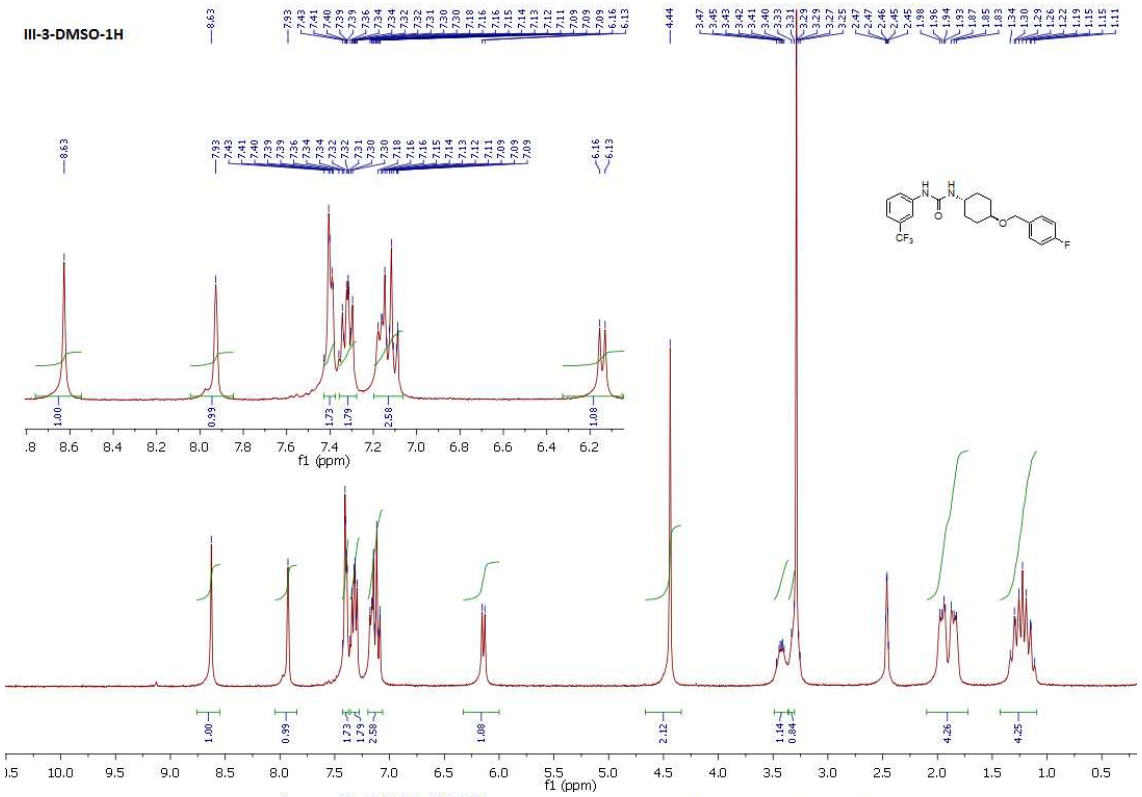


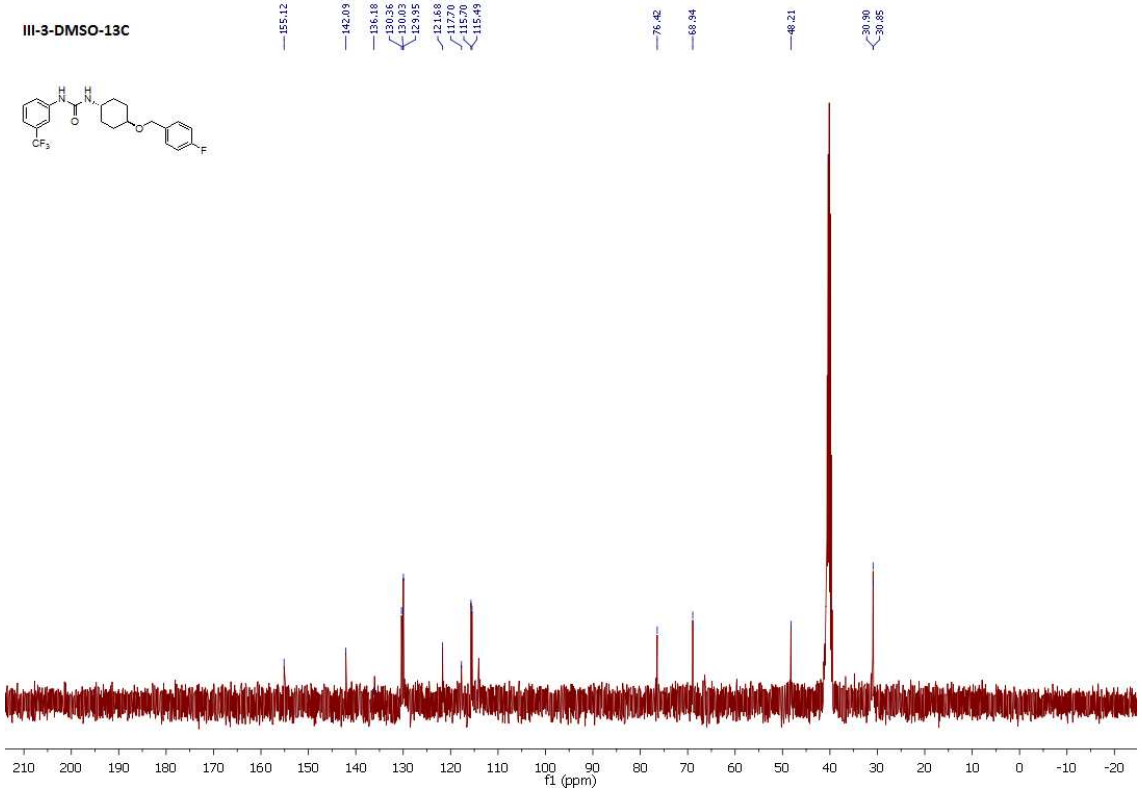
III-2-DMSO-13C



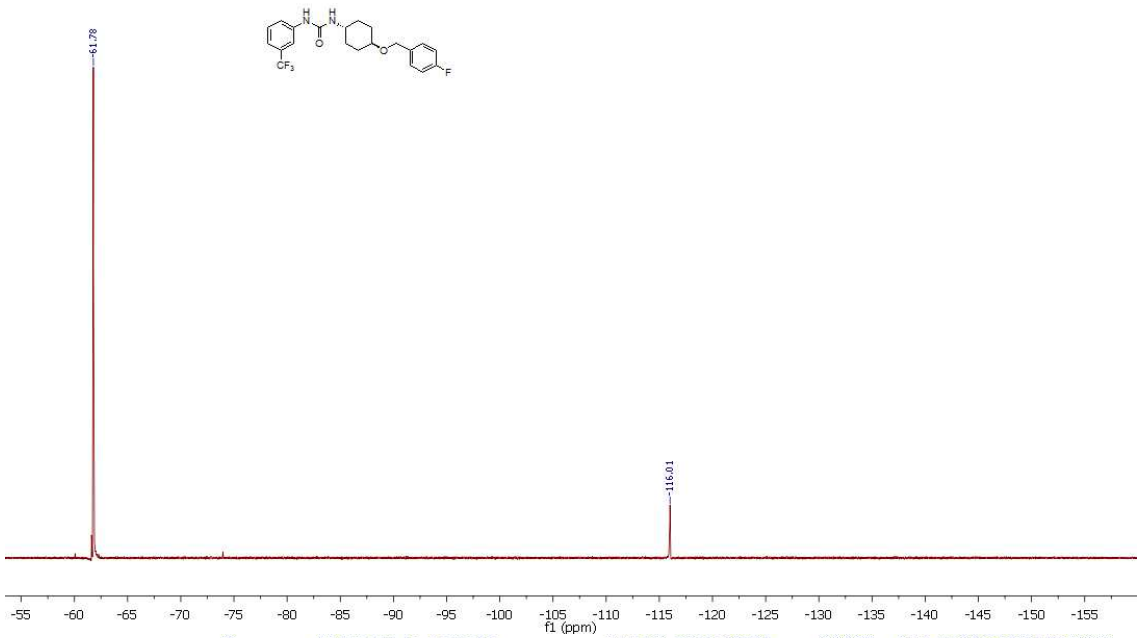
III-2-DMSO-19F



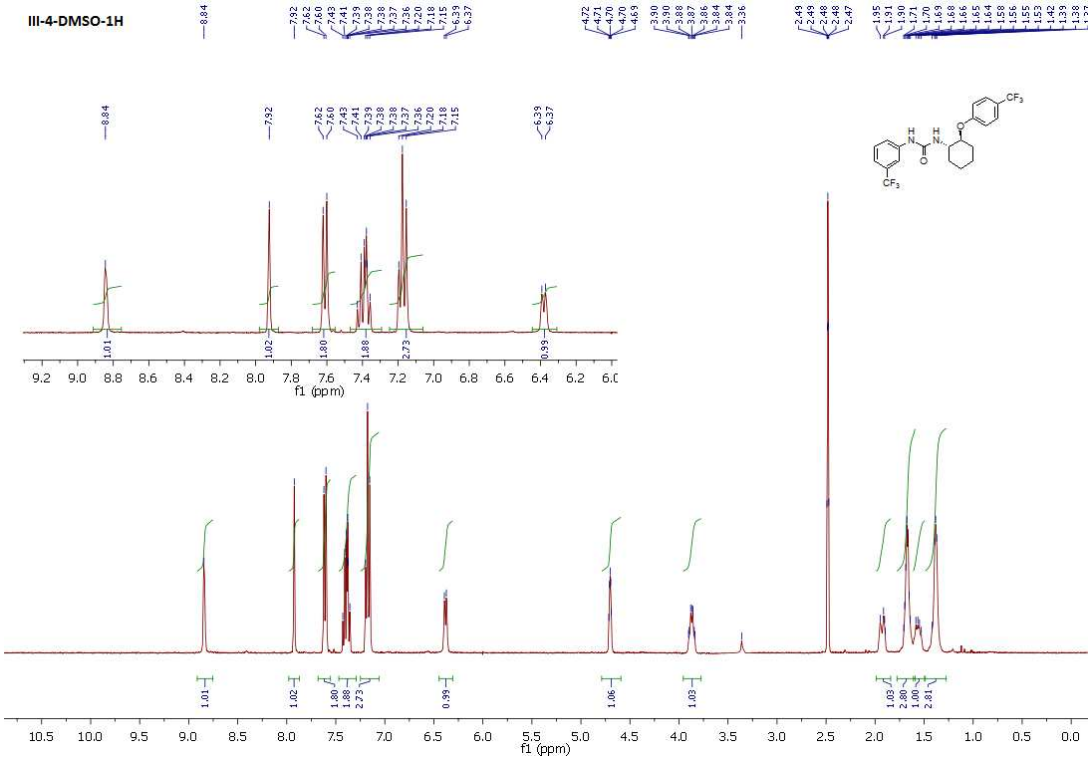

III-3-DMSO-1H
f1 (ppm)


III-3-DMSO-13C
f1 (ppm)

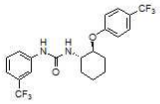
III-3-DMSO-19F



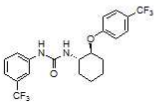
III-4-DMSO-1H



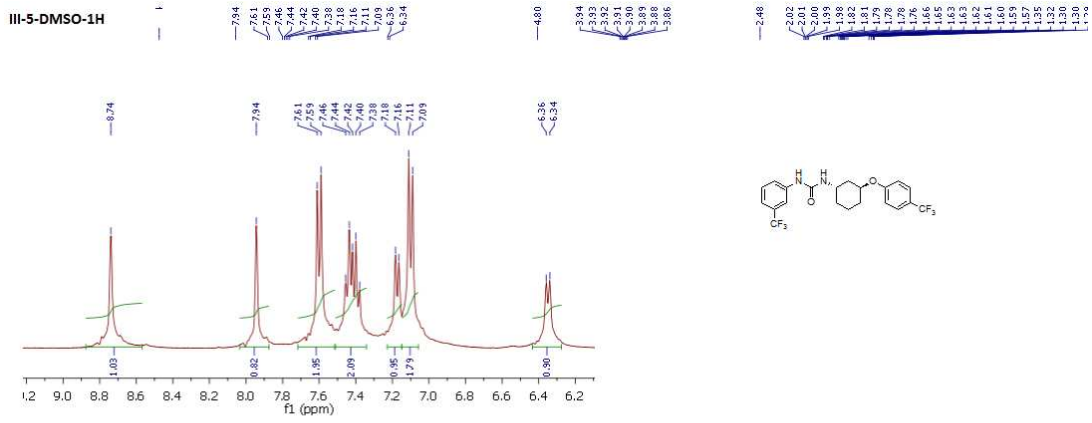
III-4-DMSO-13C

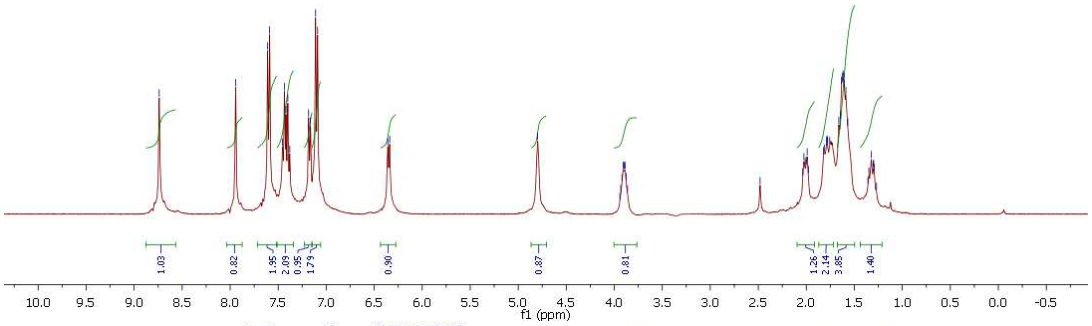


III-4-DMSO-19F

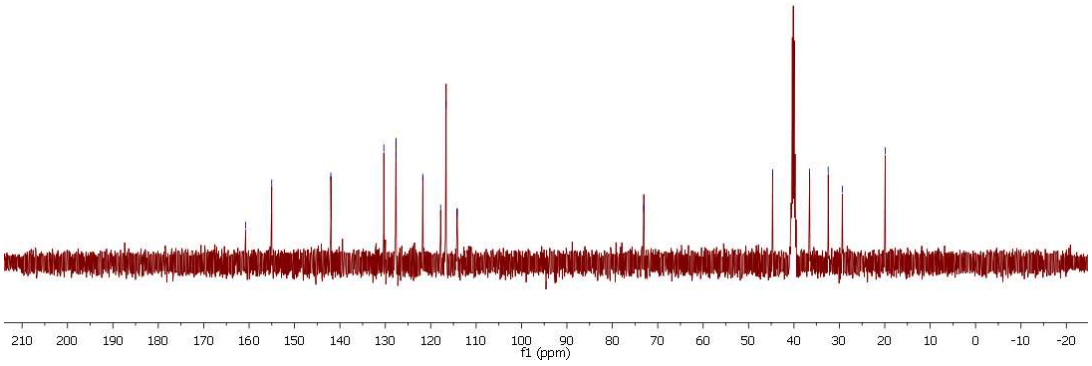


III-5-DMSO-1H

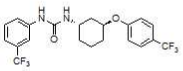


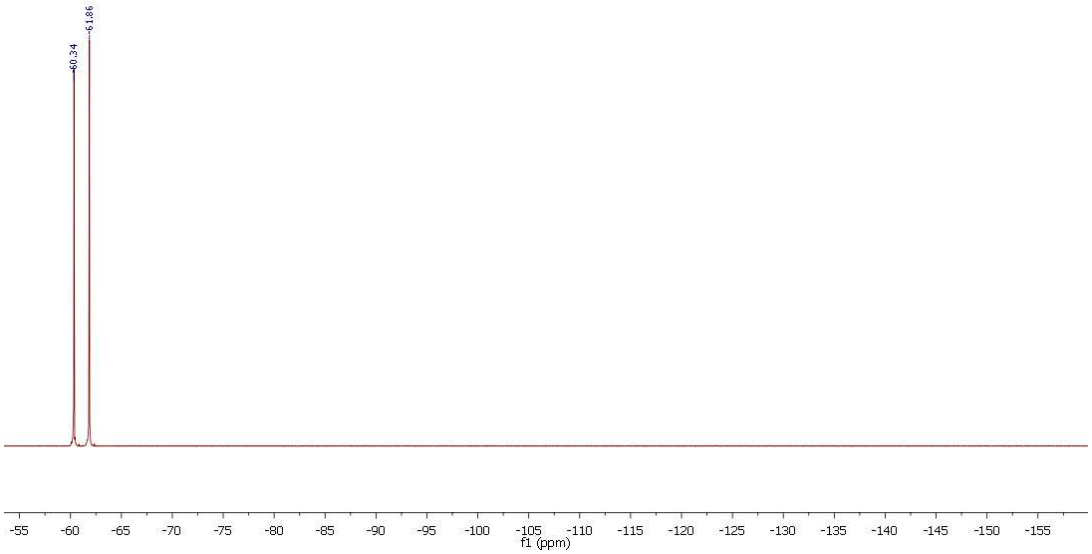


III-5-DMSO-13C



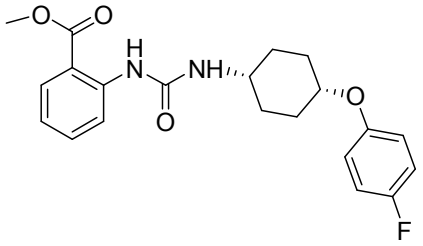
III-5-DMSO-19F





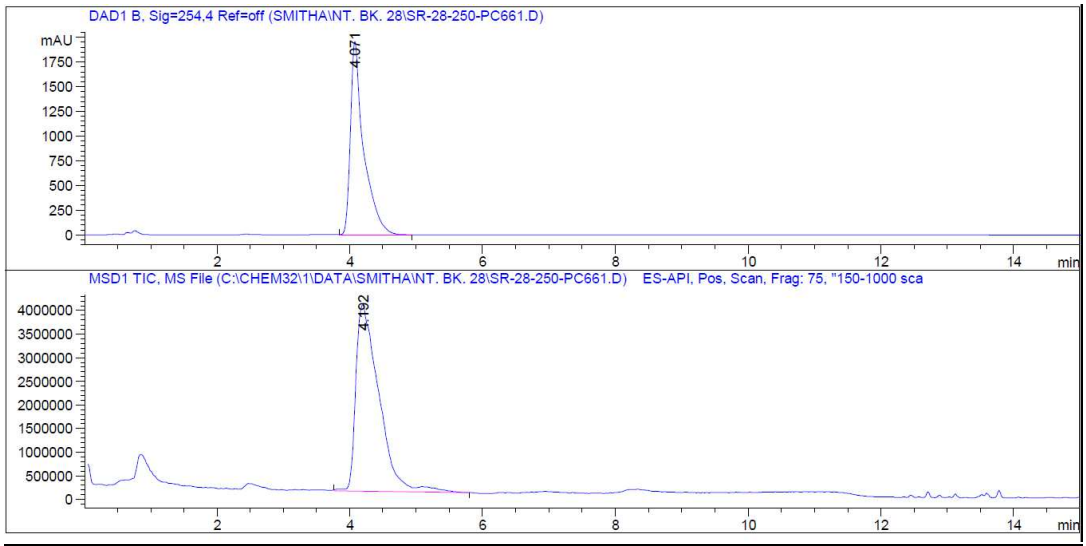
V.2. Mass confirmation data for compounds **I-11o, I-12o, I-14-20** and **III-1-5**.

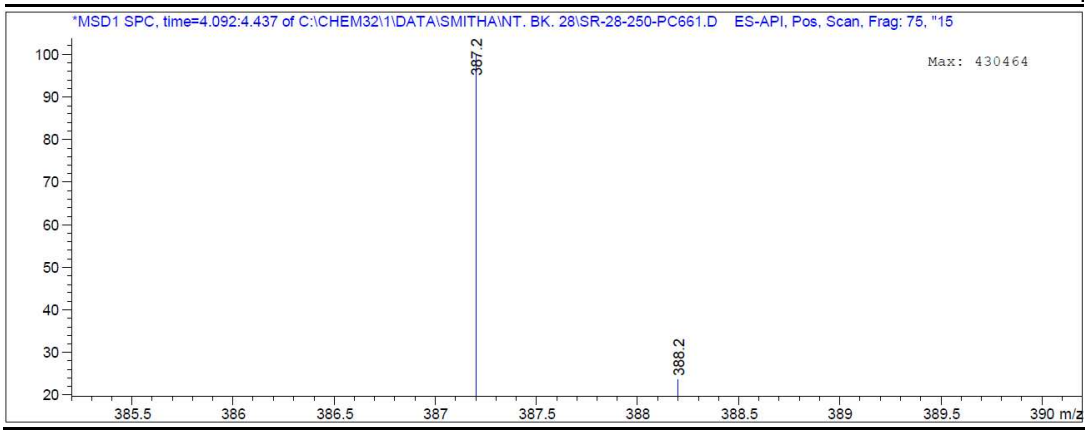
I-11o



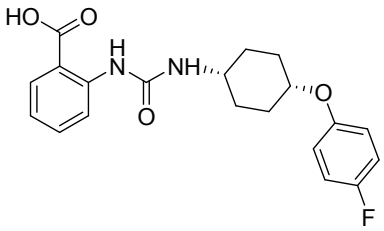
Chemical Formula: $C_{21}H_{23}FN_2O_4$

m/z: 386.16419 (100.0%), 387.16754 (22.7%), 388.17090 (2.5%)





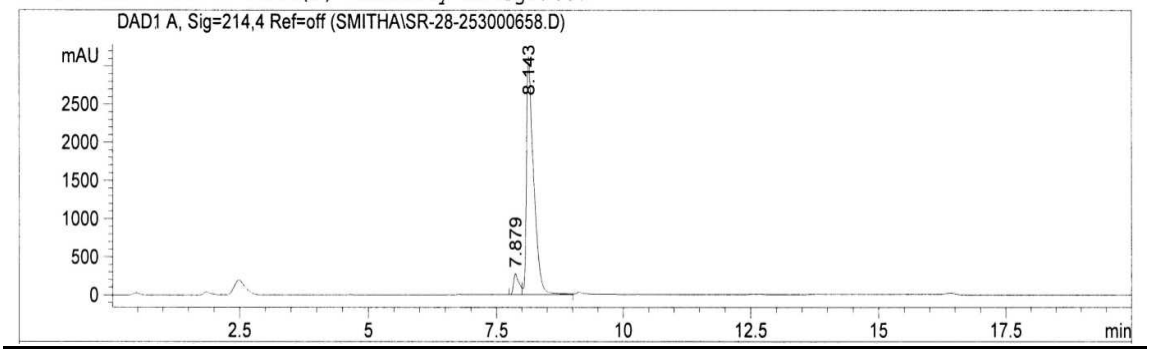
I-12o

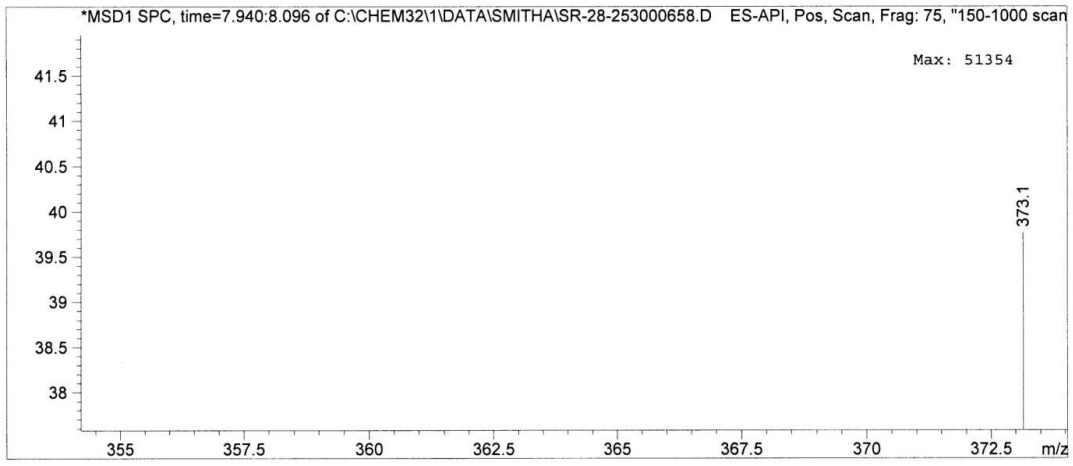


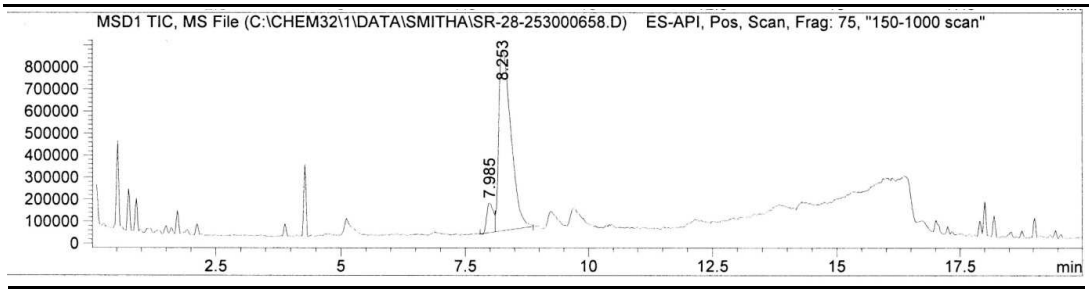
Chemical Formula: $C_{20}H_{21}FN_2O_4$

m/z: 372.14854 (100.0%), 373.15189 (21.6%), 374.15525 (2.2%)

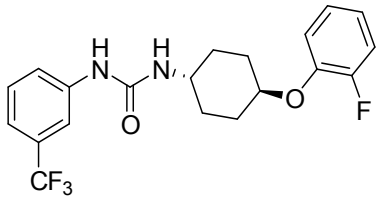
Additional Info : Peak(s) manually integrated





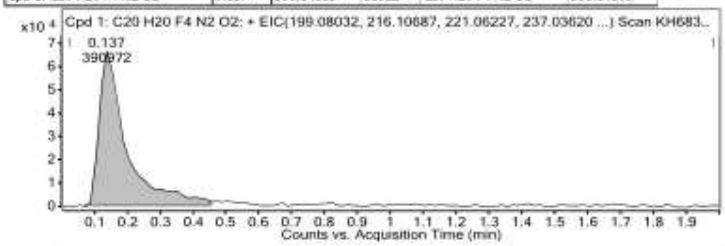


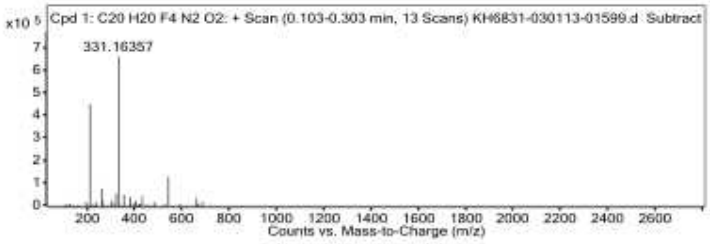
I-14

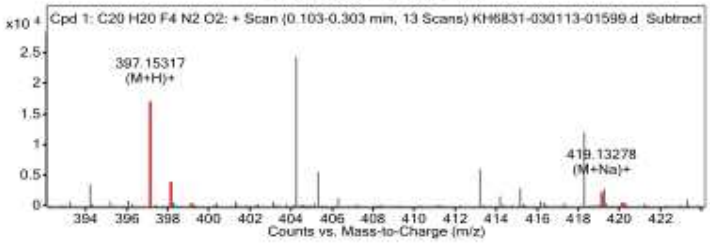


Chemical Formula: $C_{20}H_{20}F_4N_2O_2$
m/z: 396.15 (100.0%), 397.15 (21.9%), 398.15 (2.8%)

Compound Label	RT	Mass	Abund	Formula	Tgt Mass
Cpd 1: C20 H20 F4 N2 O2	0.137	396.14619	16922	C20 H20 F4 N2 O2	396.14609

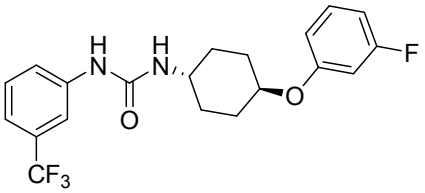






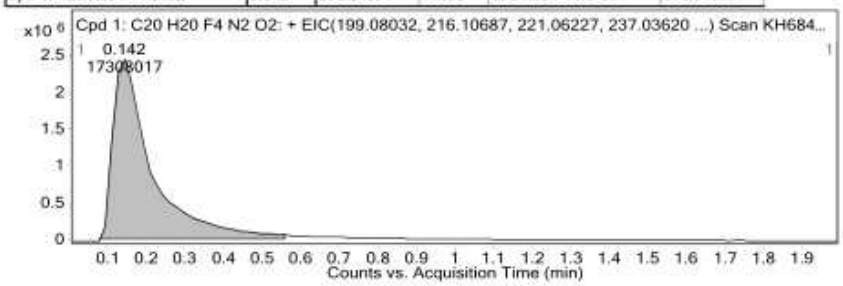
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
331.16357				664049.69		
397.15317	397.15337	-0.49	1	16922.39	C20H21F4N2O2	(M+H)+
398.15783	398.15655	3.2	1	3960.71	C20H21F4N2O2	(M+H)+
399.17392	399.15942	36.32	1	425.66	C20H21F4N2O2	(M+H)+
419.13278	419.13531	-6.04	1	2012.98	C20H20F4N2NaO2	(M+Na)+
420.13794	420.1385	-1.33	1	608.65	C20H20F4N2NaO2	(M+Na)+

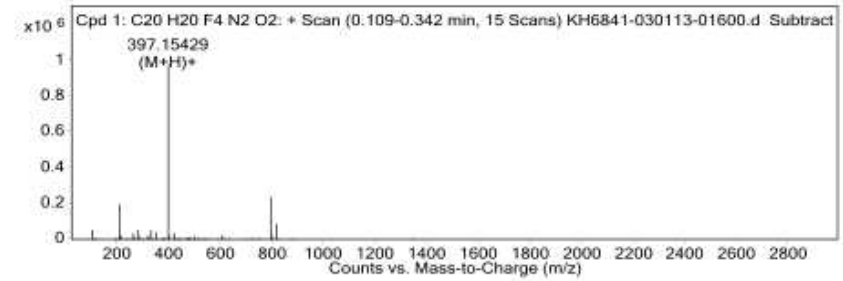
I-15

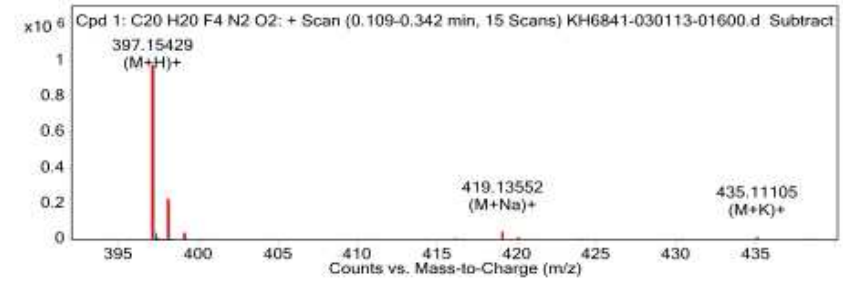


Chemical Formula: $C_{20}H_{20}F_4N_2O_2$
m/z: 396.15 (100.0%), 397.15 (21.9%), 398.15 (2.8%)

Compound Label	RT	Mass	Abund	Formula	Tgt Mass
Cpd 1: C20 H20 F4 N2 O2	0.142	396.14694	32693	C20 H20 F4 N2 O2	396.14609

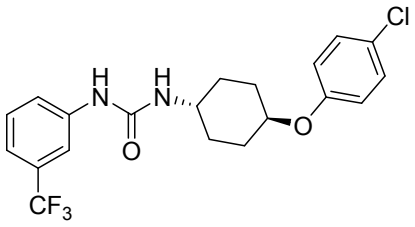






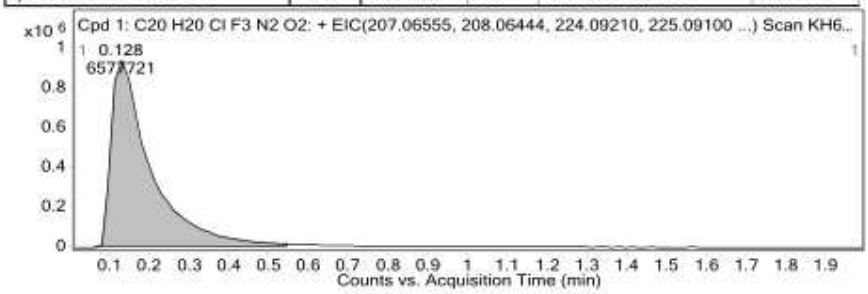
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
397.15429	397.15337	2.33	1	977477.69	C20H21F4N2O2	(M+H)+
398.15719	398.15655	1.59	1	214577.05	C20H21F4N2O2	(M+H)+
399.15987	399.15942	1.12	1	25948.84	C20H21F4N2O2	(M+H)+
400.16305	400.16215	2.27	1	3228.28	C20H21F4N2O2	(M+H)+
419.13552	419.13531	0.5	1	32693.39	C20H20F4N2NaO2	(M+Na)+
420.13895	420.1385	1.08	1	7319.85	C20H20F4N2NaO2	(M+Na)+
421.14318	421.14137	4.3	1	1153.46	C20H20F4N2NaO2	(M+Na)+
435.11105	435.10925	4.15	1	4112.49	C20H20F4KN2O2	(M+K)+
436.1099	436.11243	-5.81	1	1231.01	C20H20F4KN2O2	(M+K)+

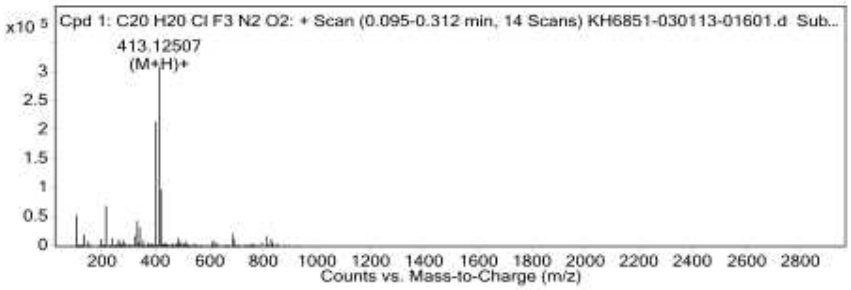
I-16

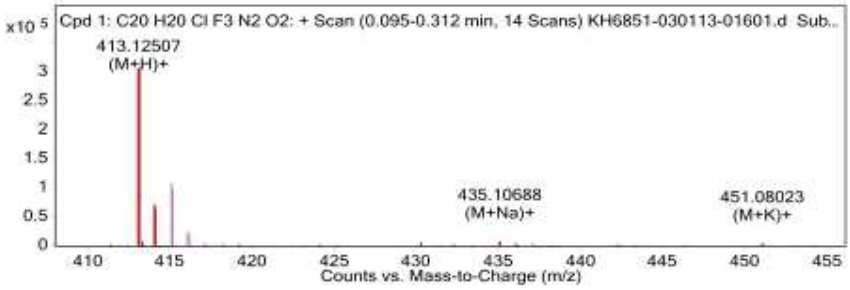


Chemical Formula: $C_{20}H_{20}ClF_3N_2O_2$
m/z: 412.11654 (100.0%), 414.11359 (32.0%)

Compound Label	RT	Mass	Abund	Formula	Tgt Mass
Cpd 1: C20 H20 Cl F3 N2 O2	0.128	412.11772	2333	C20 H20 Cl F3 N2 O2	412.11654

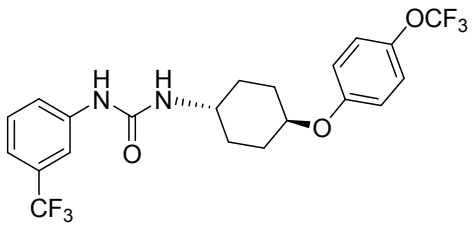




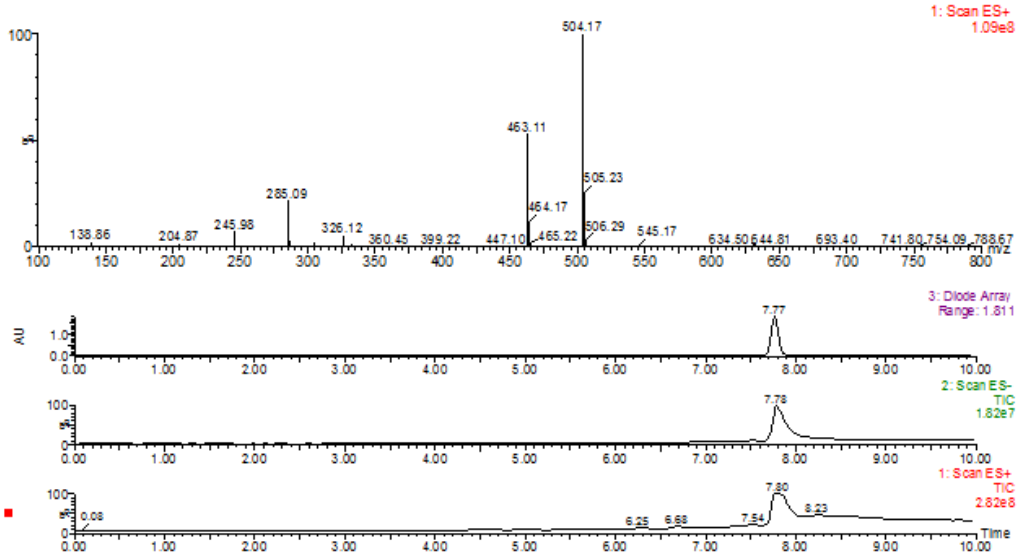


m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
413.12507	413.12382	3.04	1	310100.78	C20H21ClF3N2O2	(M+H)+
414.12788	414.127	2.13	1	64170.29	C20H21ClF3N2O2	(M+H)+
435.10688	435.10576	2.58	1	6200.94	C20H20ClF3N2NaO2	(M+Na)+
436.10867	436.10894	-0.62	1	1674.95	C20H20ClF3N2NaO2	(M+Na)+
451.08023	451.0797	1.17	1	2333.49	C20H20ClF3KN2O2	(M+K)+
452.08295	452.08288	0.16	1	630.5	C20H20ClF3KN2O2	(M+K)+

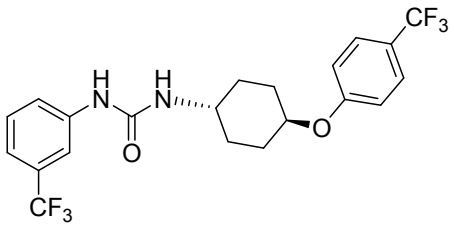
I-17:



Chemical Formula: $C_{21}H_{20}F_6N_2O_3$
Exact Mass: 462.14

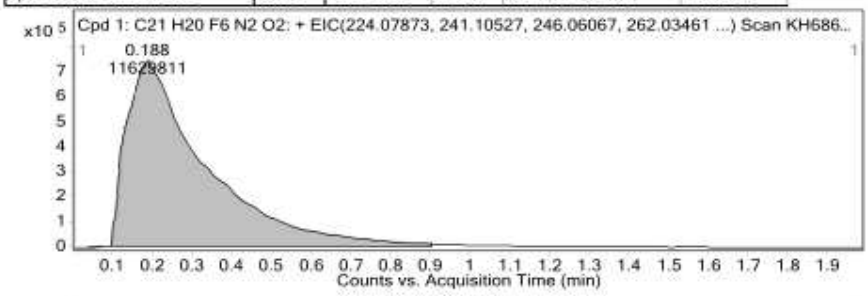


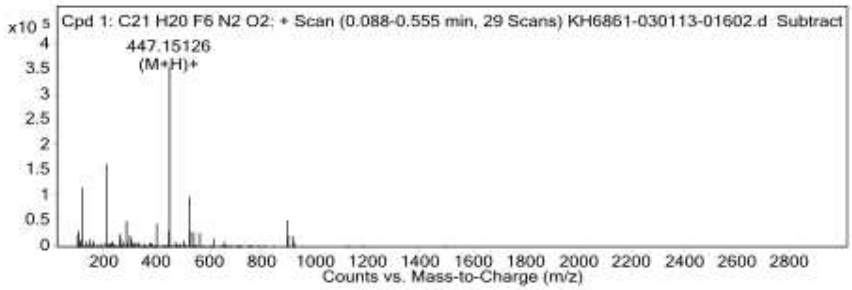
I-18:

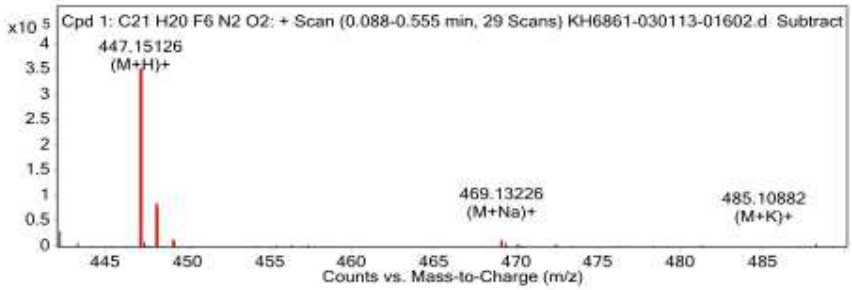


Chemical Formula: $C_{21}H_{20}F_6N_2O_2$
m/z: 446.14290

Compound Label	RT	Mass	Abund	Formula	Tgt Mass
Cpd 1: C21 H20 F6 N2 O2	0.188	446.14388	355351	C21 H20 F6 N2 O2	446.1429

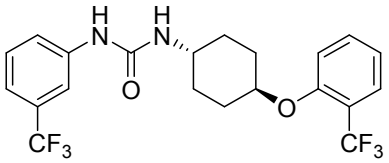






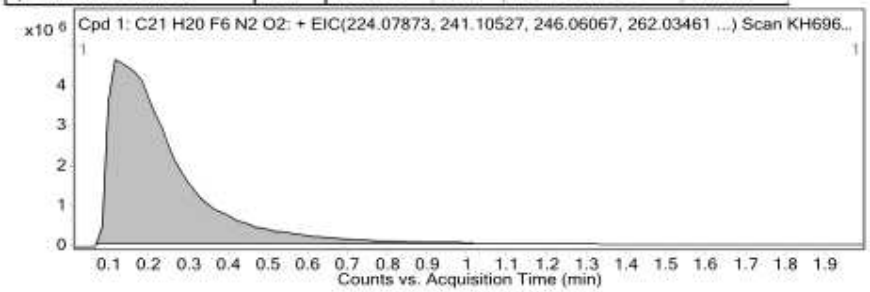
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
447.15126	447.15017	2.44	1	355351.28	C21H21F6N2O2	(M+H)+
448.15389	448.15337	1.17	1	77688.22	C21H21F6N2O2	(M+H)+
449.15752	449.15627	2.78	1	10099.43	C21H21F6N2O2	(M+H)+
450.15844	450.15902	-1.3	1	1145.79	C21H21F6N2O2	(M+H)+
464.17712	464.17672	0.85	1	116.16	C21H24F6N3O2	(M+NH4)+
469.13226	469.13212	0.31	1	10118.34	C21H20F6N2NaO2	(M+Na)+
470.13829	470.13531	6.35	1	2563.38	C21H20F6N2NaO2	(M+Na)+
471.139	471.13821	1.67	1	475.37	C21H20F6N2NaO2	(M+Na)+
485.10882	485.10606	5.69	1	1012.07	C21H20F6KN2O2	(M+K)+

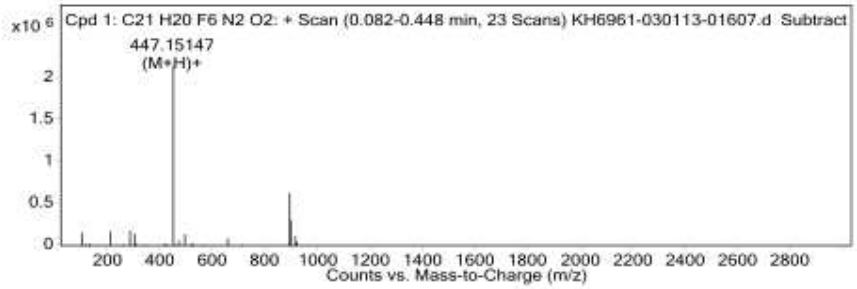
I-19:

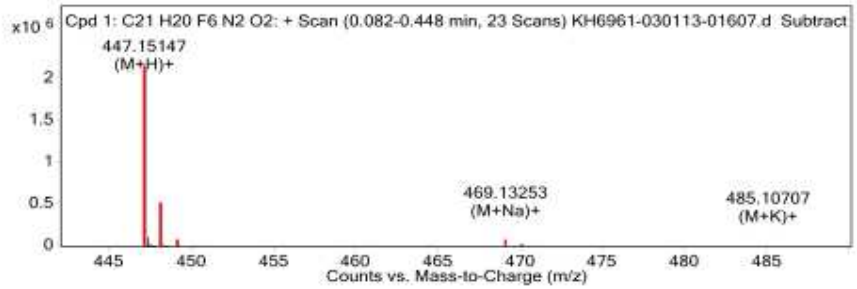


Chemical Formula: $C_{21}H_{20}F_6N_2O_2$
Exact Mass: 446.14290

Compound Label	RT	Mass	Abund	Formula	Tgt Mass
Cpd 1: C21 H20 F6 N2 O2	0.115	446.14414	69682	C21 H20 F6 N2 O2	446.1429

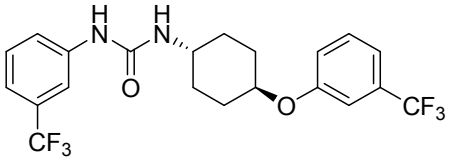






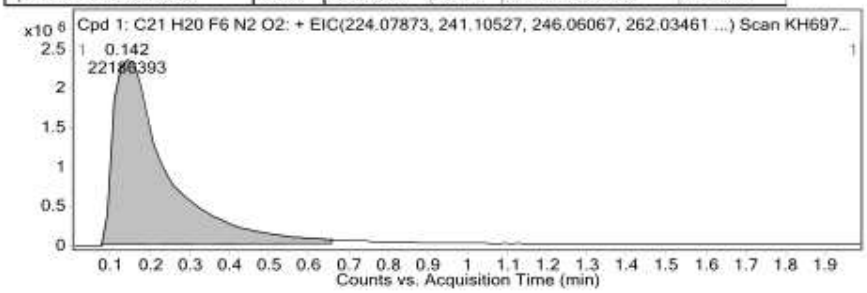
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
447.15147	447.15017	2.9	1	2142253	C21H21F6N2O2	(M+H)+
448.15462	448.15337	2.79	1	507455	C21H21F6N2O2	(M+H)+
449.15696	449.15627	1.53	1	64374.13	C21H21F6N2O2	(M+H)+
450.15957	450.15902	1.22	1	7699.52	C21H21F6N2O2	(M+H)+
469.13253	469.13212	0.89	1	69682.2	C21H20F6N2NaO2	(M+Na)+
470.13573	470.13531	0.9	1	16057.05	C21H20F6N2NaO2	(M+Na)+
471.13433	471.13821	-8.24	1	2203.28	C21H20F6N2NaO2	(M+Na)+
472.12687	472.14096	-29.83	1	89.38	C21H20F6N2NaO2	(M+Na)+
485.10707	485.10606	2.08	1	3086.53	C21H20F6KN2O2	(M+K)+
486.11164	486.10925	4.92	1	858.75	C21H20F6KN2O2	(M+K)+

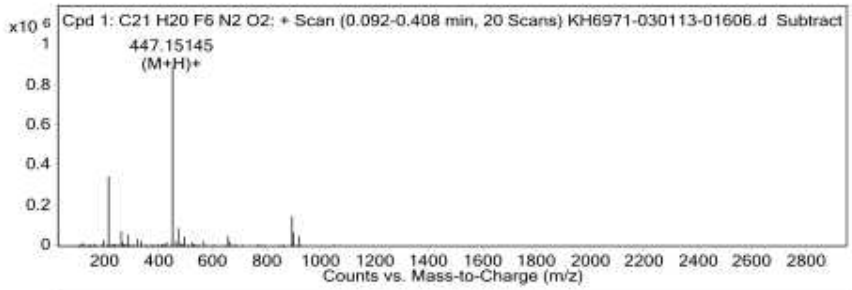
I-20

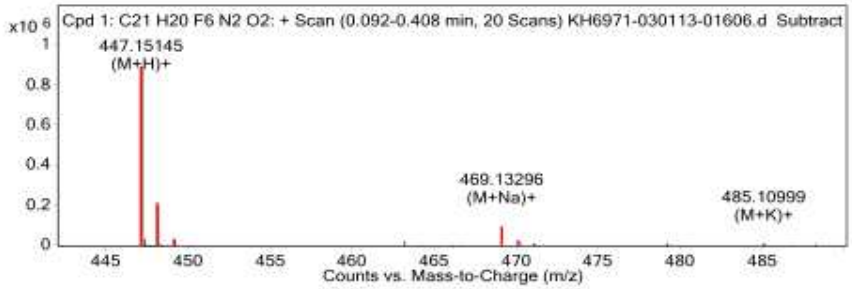


Chemical Formula: $C_{21}H_{20}F_6N_2O_2$
m/z: 446.1429 (100.0%), 447.1463 (22.7%), 448.1496 (2.5%)

Compound Label	RT	Mass	Abund	Formula	Tgt Mass
Cpd 1: C21 H20 F6 N2 O2	0.142	446.14407	93400	C21 H20 F6 N2 O2	446.1429

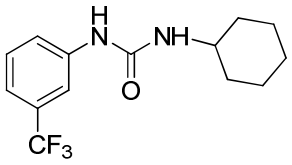






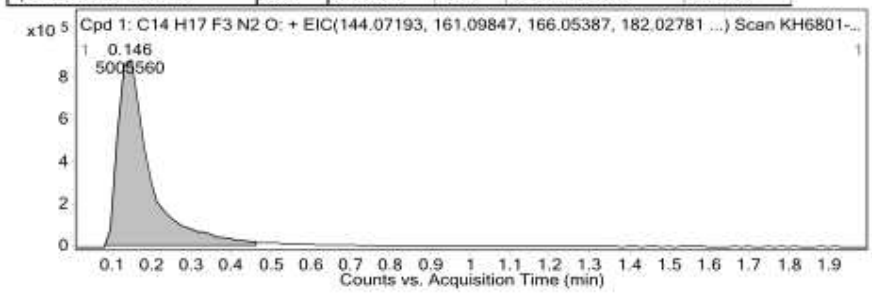
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
447.15145	447.15017	2.86	1	895293.13	C21H21F6N2O2	(M+H)+
448.15428	448.15337	2.05	1	204839.61	C21H21F6N2O2	(M+H)+
449.15674	449.15627	1.06	1	26027.81	C21H21F6N2O2	(M+H)+
450.15899	450.15902	-0.06	1	3311.36	C21H21F6N2O2	(M+H)+
469.13296	469.13212	1.8	1	93400.25	C21H20F6N2NaO2	(M+Na)+
470.13576	470.13531	0.95	1	20852.15	C21H20F6N2NaO2	(M+Na)+
471.13512	471.13821	-6.55	1	2840.53	C21H20F6N2NaO2	(M+Na)+
472.14521	472.14096	8.99	1	687.08	C21H20F6N2NaO2	(M+Na)+
485.10999	485.10606	8.12	1	6114.42	C21H20F6KN2O2	(M+K)+
486.11795	486.10925	17.92	1	1749.07	C21H20F6KN2O2	(M+K)+

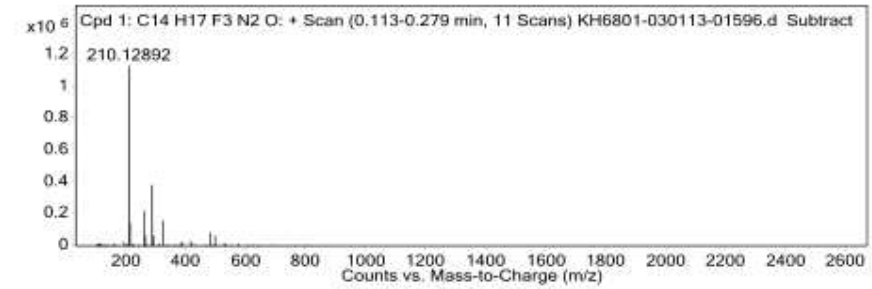
III-1

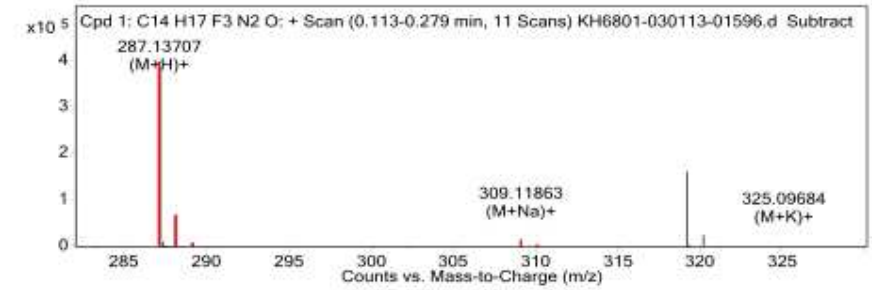


Chemical Formula: $C_{14}H_{17}F_3N_2O$
m/z: 286.13 (100.0%), 287.13 (15.9%), 288.14 (1.1%)

Compound Label	RT	Mass	Abund	Formula	Tgt Mass
Cpd 1: C14 H17 F3 N2 O	0.146	286.12951	12043	C14 H17 F3 N2 O	286.1293

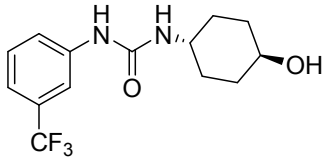






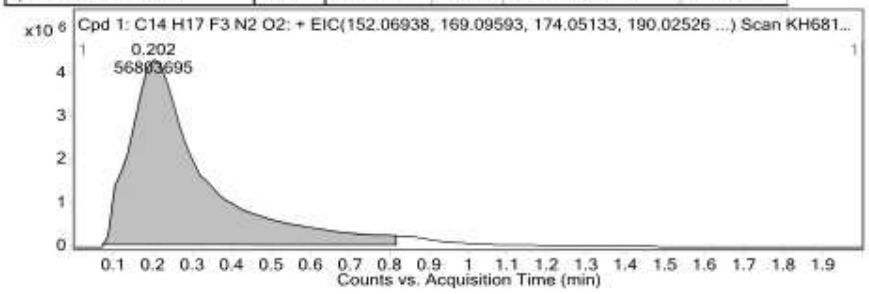
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
210.12892				1128544.75		
287.13707	287.13657	1.72	1	385535.19	C14H18F3N2O	(M+H)+
288.13862	288.13968	-3.68	1	69285.71	C14H18F3N2O	(M+H)+
289.1398	289.14249	-9.31	1	6882.78	C14H18F3N2O	(M+H)+
290.14293	290.14513	-7.6	1	1163.47	C14H18F3N2O	(M+H)+
309.11863	309.11852	0.35	1	12042.55	C14H17F3N2NaO	(M+Na)+
310.12218	310.12162	1.78	1	2226.52	C14H17F3N2NaO	(M+Na)+
311.12779	311.12443	10.8	1	248.71	C14H17F3N2NaO	(M+Na)+
325.09684	325.09246	13.49	1	145.31	C14H17F3KN2O	(M+K)+

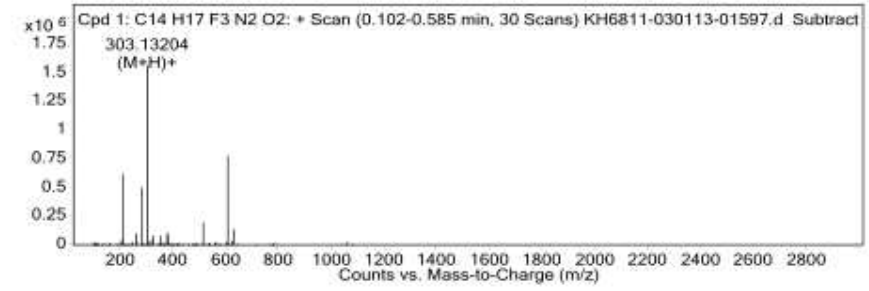
III-2

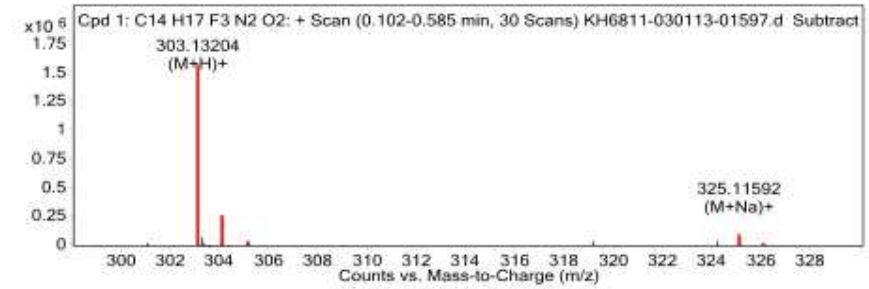


Chemical Formula: $C_{14}H_{17}F_3N_2O_2$
m/z: 302.12 (100.0%), 303.13 (15.4%), 304.13 (1.5%)

Compound Label	RT	Mass	Abund	Formula	Tgt Mass
Cpd 1: C14 H17 F3 N2 O2	0.202	302.12499	1562579	C14 H17 F3 N2 O2	302.12421

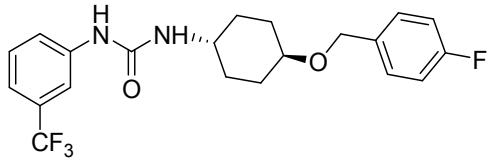




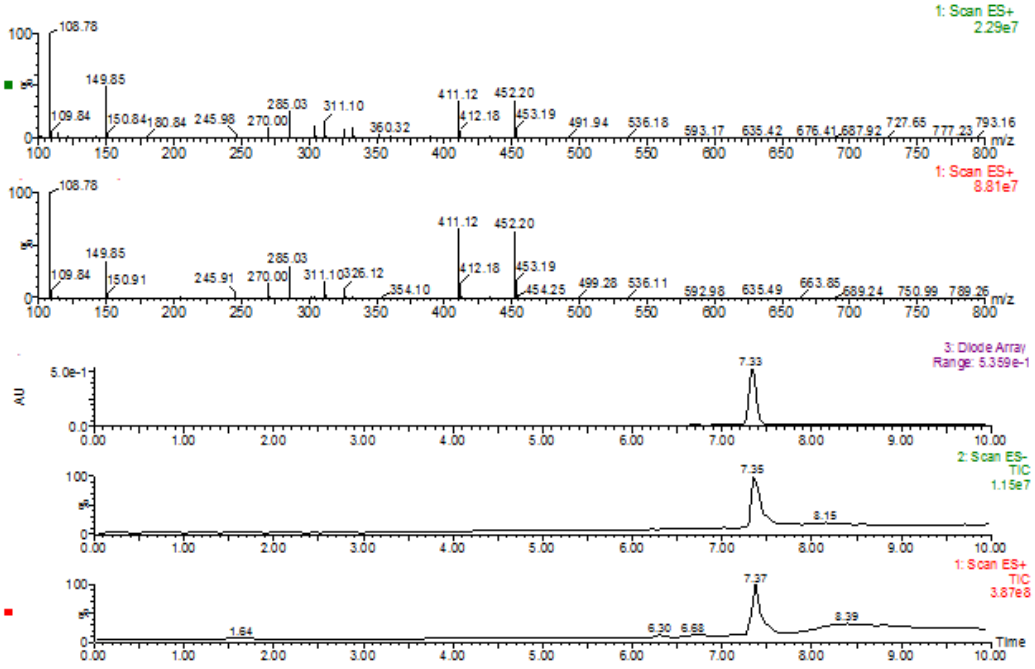


m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
303.13204	303.13149	1.82	1	1562579.13	C14H18F3N2O2	(M+H)+
304.13505	304.1346	1.49	1	252341.16	C14H18F3N2O2	(M+H)+
305.14506	305.1372	25.78	1	33592.56	C14H18F3N2O2	(M+H)+
306.15229	306.13973	41.03	1	3734.81	C14H18F3N2O2	(M+H)+
325.11592	325.11343	7.64	1	80122.33	C14H17F3N2NaO2	(M+Na)+
326.11845	326.11654	5.86	1	12455.17	C14H17F3N2NaO2	(M+Na)+
327.1209	327.11914	5.39	1	1455.75	C14H17F3N2NaO2	(M+Na)+

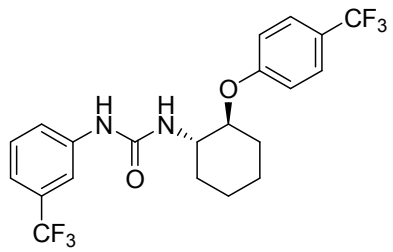
III-3:



Chemical Formula: $C_{21}H_{22}F_4N_2O_2$
Exact Mass: 410.16174

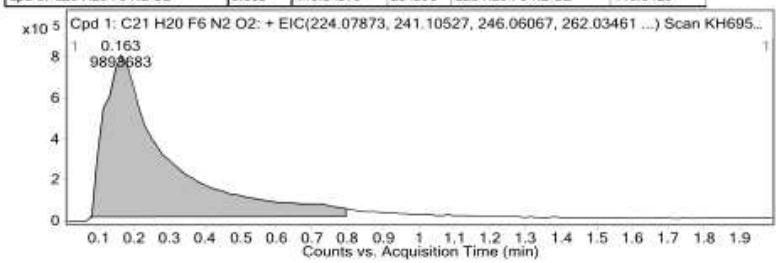


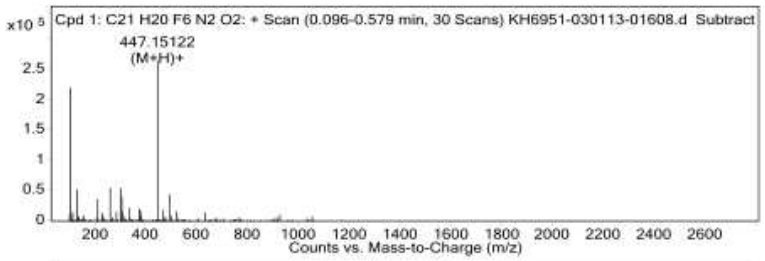
III-4:

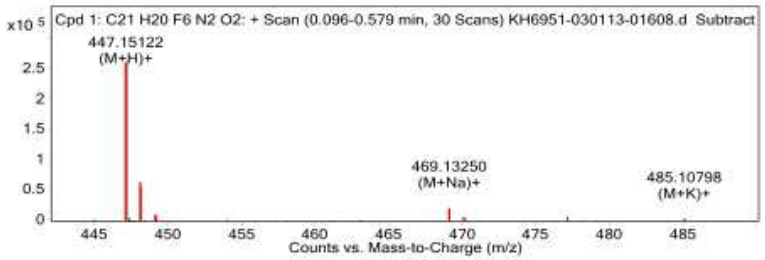


Chemical Formula: $C_{21}H_{20}F_6N_2O_2$
m/z: 446.1429 (100.0%), 447.1463 (22.7%), 448.1496 (2.5%)

Compound Label	RT	Mass	Abund	Formula	Tgt Mass
Cpd 1: C21 H20 F6 N2 O2	0.163	446.14379	264596	C21 H20 F6 N2 O2	446.1429

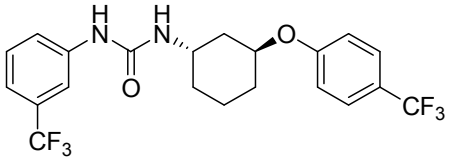






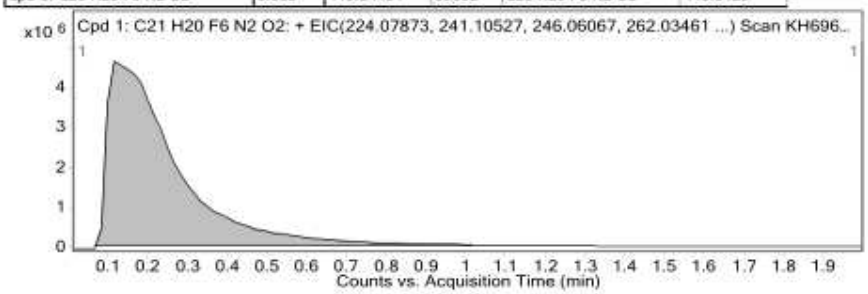
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
447.15122	447.15017	2.35	1	264596.22	C21H21F6N2O2	(M+H)+
448.15389	448.15337	1.17	1	57477.33	C21H21F6N2O2	(M+H)+
449.15673	449.15627	1.04	1	7478.51	C21H21F6N2O2	(M+H)+
450.15916	450.15902	0.32	1	1230.6	C21H21F6N2O2	(M+H)+
469.1325	469.13212	0.81	1	19527.89	C21H20F6N2NaO2	(M+Na)+
470.13622	470.13531	1.94	1	4643.88	C21H20F6N2NaO2	(M+Na)+
471.12403	471.13821	-30.09	1	632.95	C21H20F6N2NaO2	(M+Na)+
472.13839	472.14096	-5.44	1	88.47	C21H20F6N2NaO2	(M+Na)+
485.10798	485.10606	3.96	1	1427.72	C21H20F6KN2O2	(M+K)+
486.11266	486.10925	7.03	1	458.79	C21H20F6KN2O2	(M+K)+

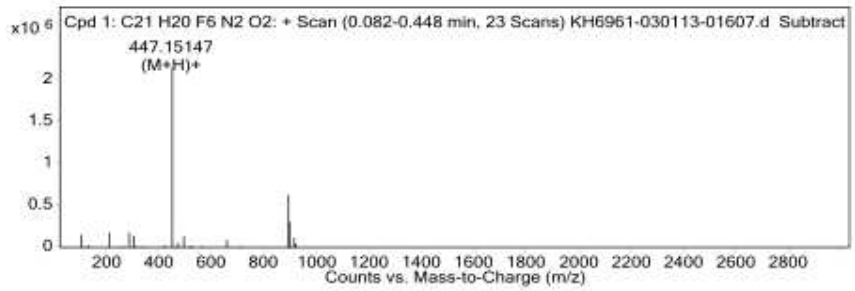
III-5

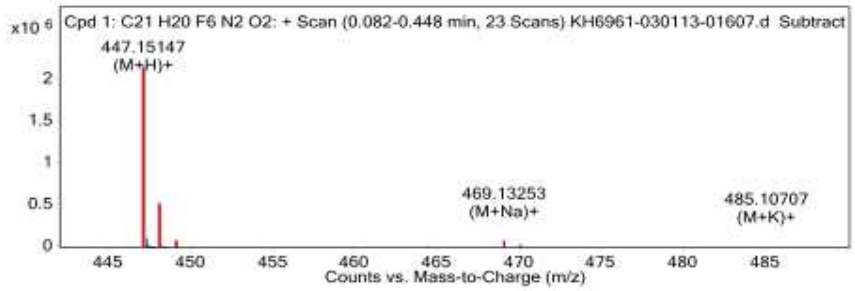


Chemical Formula: $C_{21}H_{20}F_6N_2O_2$
m/z: 446.1429 (100.0%), 447.1463 (22.7%), 448.1496 (2.5%)

Compound Label	RT	Mass	Abund	Formula	Tgt Mass
Cpd 1: C21 H20 F6 N2 O2	0.115	446.14414	69682	C21 H20 F6 N2 O2	446.1429





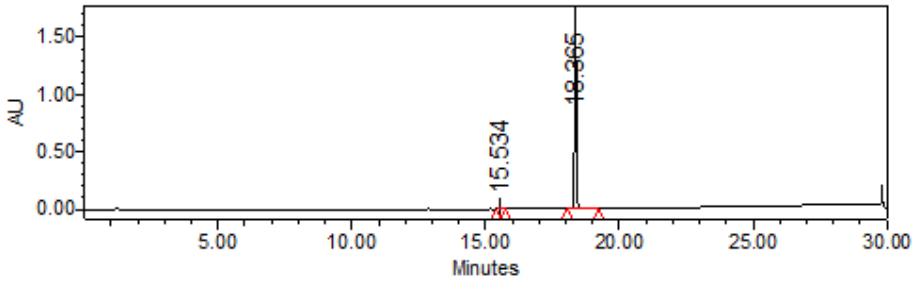


m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
447.15147	447.15017	2.9	1	2142253	C21H21F6N2O2	(M+H)+
448.15462	448.15337	2.79	1	507455	C21H21F6N2O2	(M+H)+
449.15696	449.15627	1.53	1	64374.13	C21H21F6N2O2	(M+H)+
450.15957	450.15902	1.22	1	7699.52	C21H21F6N2O2	(M+H)+
469.13253	469.13212	0.89	1	69682.2	C21H20F6N2NaO2	(M+Na)+
470.13573	470.13531	0.9	1	16057.05	C21H20F6N2NaO2	(M+Na)+
471.13433	471.13821	-8.24	1	2203.28	C21H20F6N2NaO2	(M+Na)+
472.12687	472.14096	-29.83	1	89.38	C21H20F6N2NaO2	(M+Na)+
485.10707	485.10606	2.08	1	3086.53	C21H20F6KN2O2	(M+K)+
486.11164	486.10925	4.92	1	858.75	C21H20F6KN2O2	(M+K)+

VI. HPLC purity confirmation data for compounds **I-14-20** and **III-1-5.**

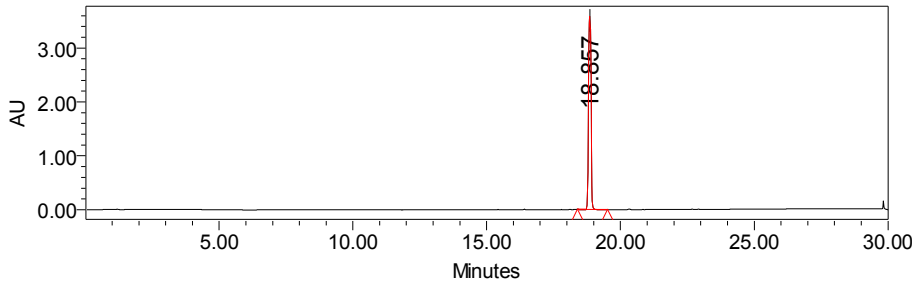
The compounds monitored at 254 nanometers with a reversed phase column (column XBridge BEH130 C18, 4.6 x 100 mm, 5 µm particle size) using a Waters Alliance 2695 with the binary system water/acetonitrile containing 0.1 % of trifluoracetic acid (TFA) as eluent running with a gradient increase of acetonitrile from 0 to 100% in 25 min at a flow rate of 1 mL/min. Then 5 min wash at 100% acetonitrile.

I-14:



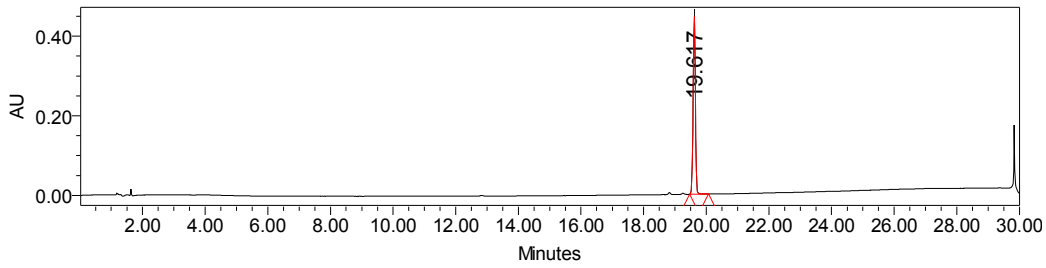
	Retention Time	Area	% Area	Height
1	15.534	47849	0.54	10146
2	18.365	8878632	99.46	1656798

I-15:



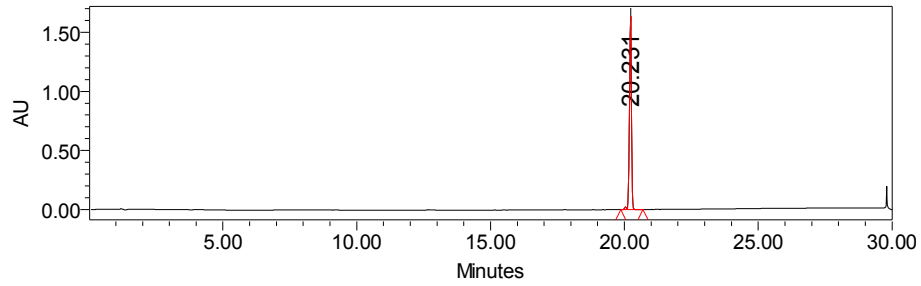
	Retention Time	Area	% Area	Height
1	18.857	23623602	100.00	3590094

I-16:



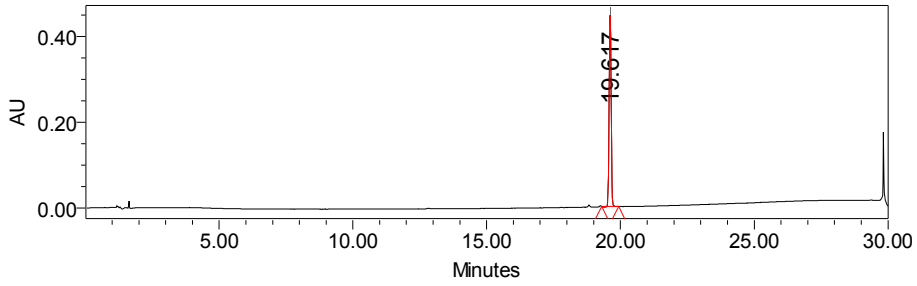
	Retention Time	Area	% Area	Height
1	19.617	2291443	100.00	440112

I-17:



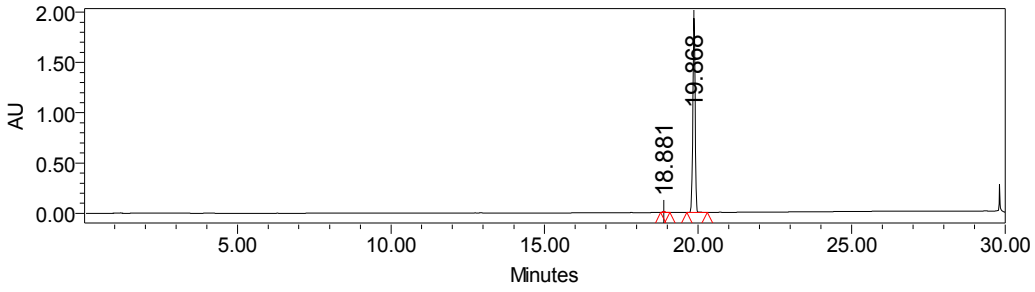
	Retention Time	Area	% Area	Height
1	20.231	8438792	100.00	1615064

I-18:



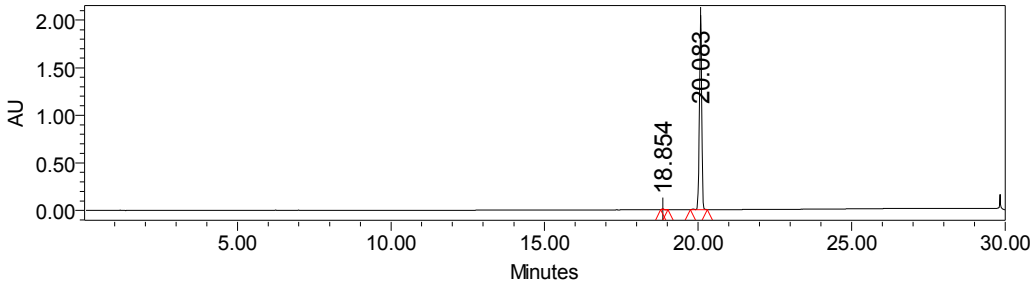
	Retention Time	Area	% Area	Height
1	19.617	2280164	100.00	439224

I-19:



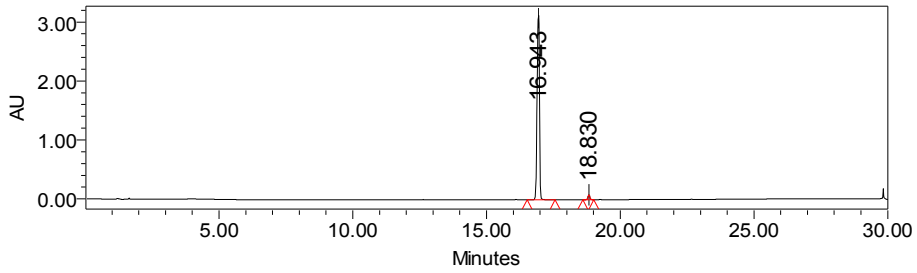
	Retention Time	Area	% Area	Height
1	18.881	56315	0.57	11249
2	19.868	9888316	99.43	1905711

I-20:



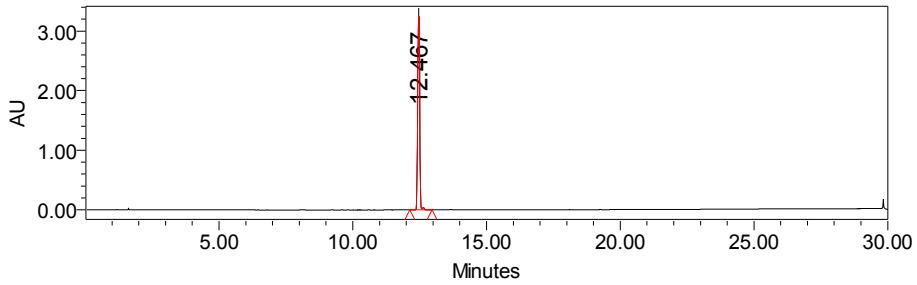
	Retention Time	Area	% Area	Height
1	18.854	31165	0.29	6716
2	20.083	10594192	99.71	2018778

III-1:



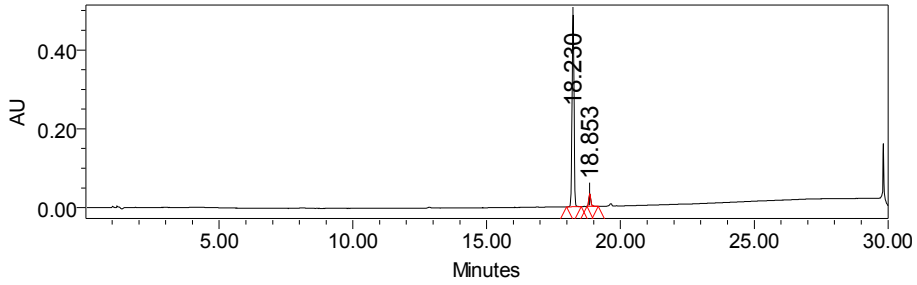
	Retention Time	Area	% Area	Height
1	16.943	20328440	98.08	3201563
2	18.830	398995	1.92	79956

III-2:



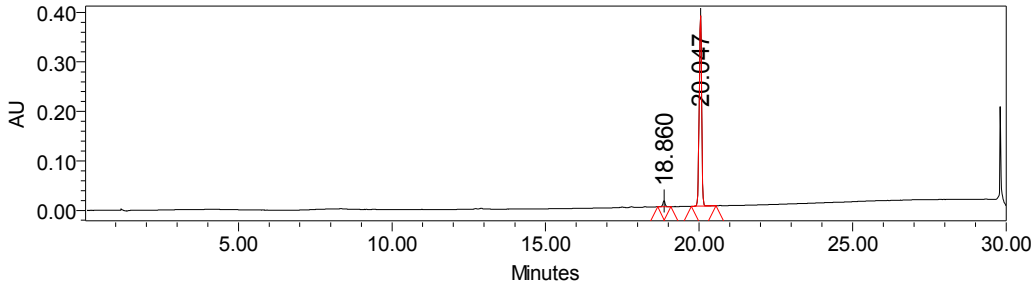
	Retention Time	Area	% Area	Height
1	12.467	17231425	100.00	3329693

III-3:



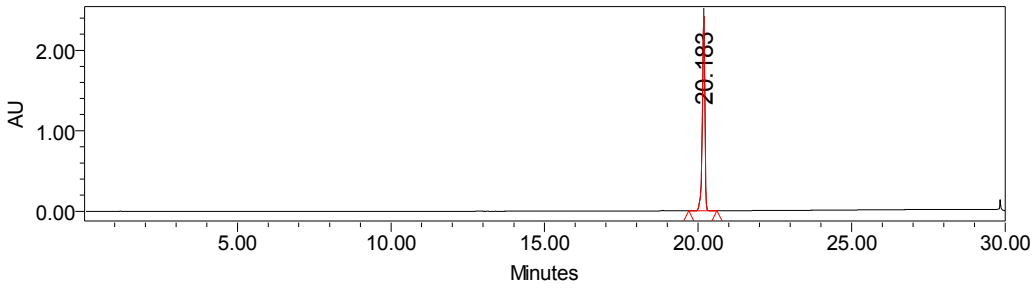
	Retention Time	Area	% Area	Height
1	18.230	2409731	95.57	480771
2	18.853	165630	4.43	31614

III-4:



	Retention Time	Area	% Area	Height
1	18.860	62768	2.88	11825
2	20.047	2114743	97.12	380954

III-5:



	Retention Time	Area	% Area	Height
1	20.183	13748186	100.00	2403688