SUPPORTING INFORMATION

Synthesis, In Silico and In Vitro Evaluation for Acetylcholinesterase and BACE-1 Inhibitory Activity of Some *N*-Substituted-4-Phenothiazine-Chalcones

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Figure S9. Alignment of re-dock ligands with the native one in the binding pocket of of 5HU1-chain B

Figure S10. The linear regression between docking score and pIC_{50} on AChE of synthesized chalcone derivatives (A. observed values from **AC1-3** and **AC5-10**, B. predicted values from **AC1, AC4, AC6, AC8, AC10, AC13**)

Table S1. Results of re-docking (RMSD in Å)

Ligand	AChE	BACE-1	
	1DX6	5HU1 (chain A)	5HU1 (chain B)
1	0.49	0.71	0.53
2	0.50	0.52	0.87
3	0.89	0.89	0.96

- Ligand 1: separated from the complex (native form, not prepared).
- Ligand 2: separated from the complex and re-prepared using appropriate procedure indicated in the section of Materials and Methods
- Ligand 3: built and prepared from the beginning.

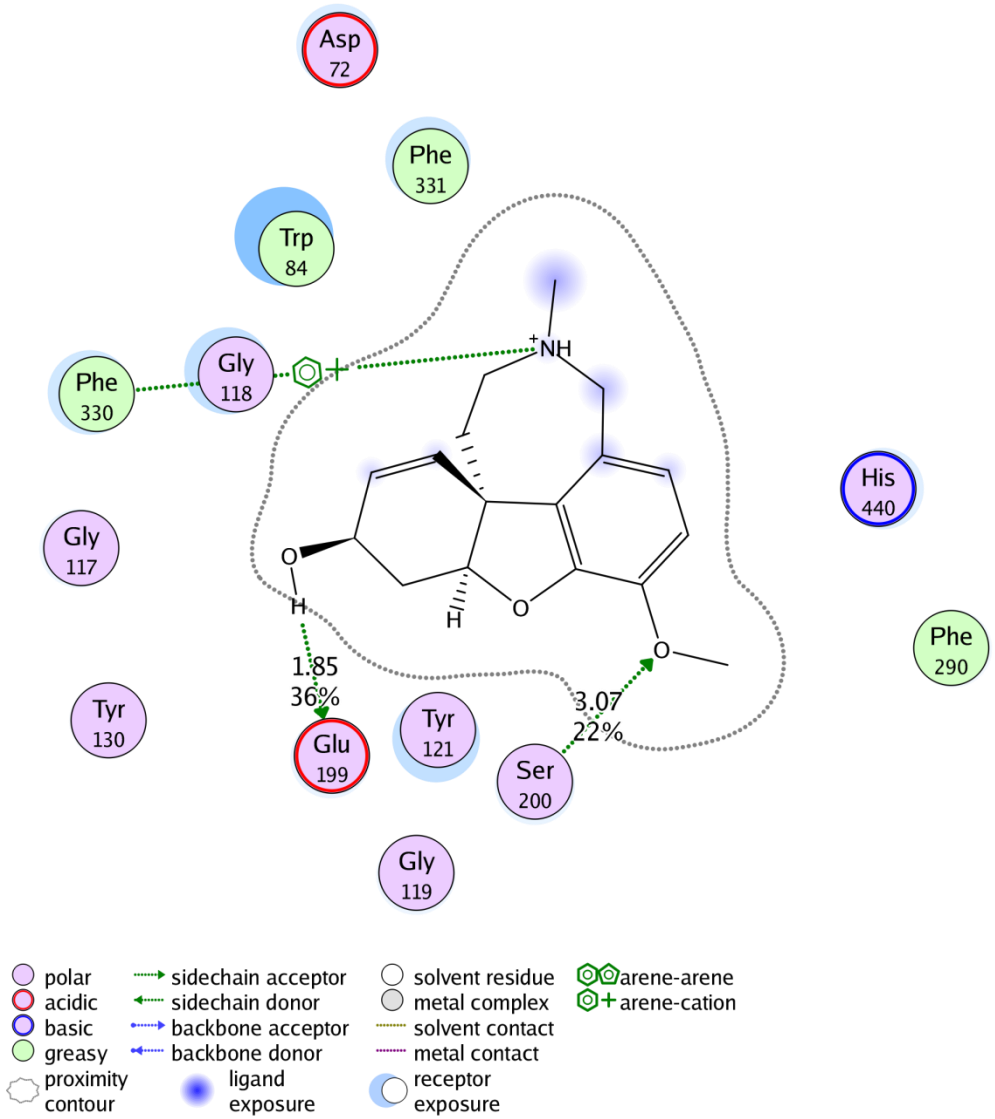


Figure S1. Interactions of co-crystallized ligand in the protein complex 1DX6 (2D)

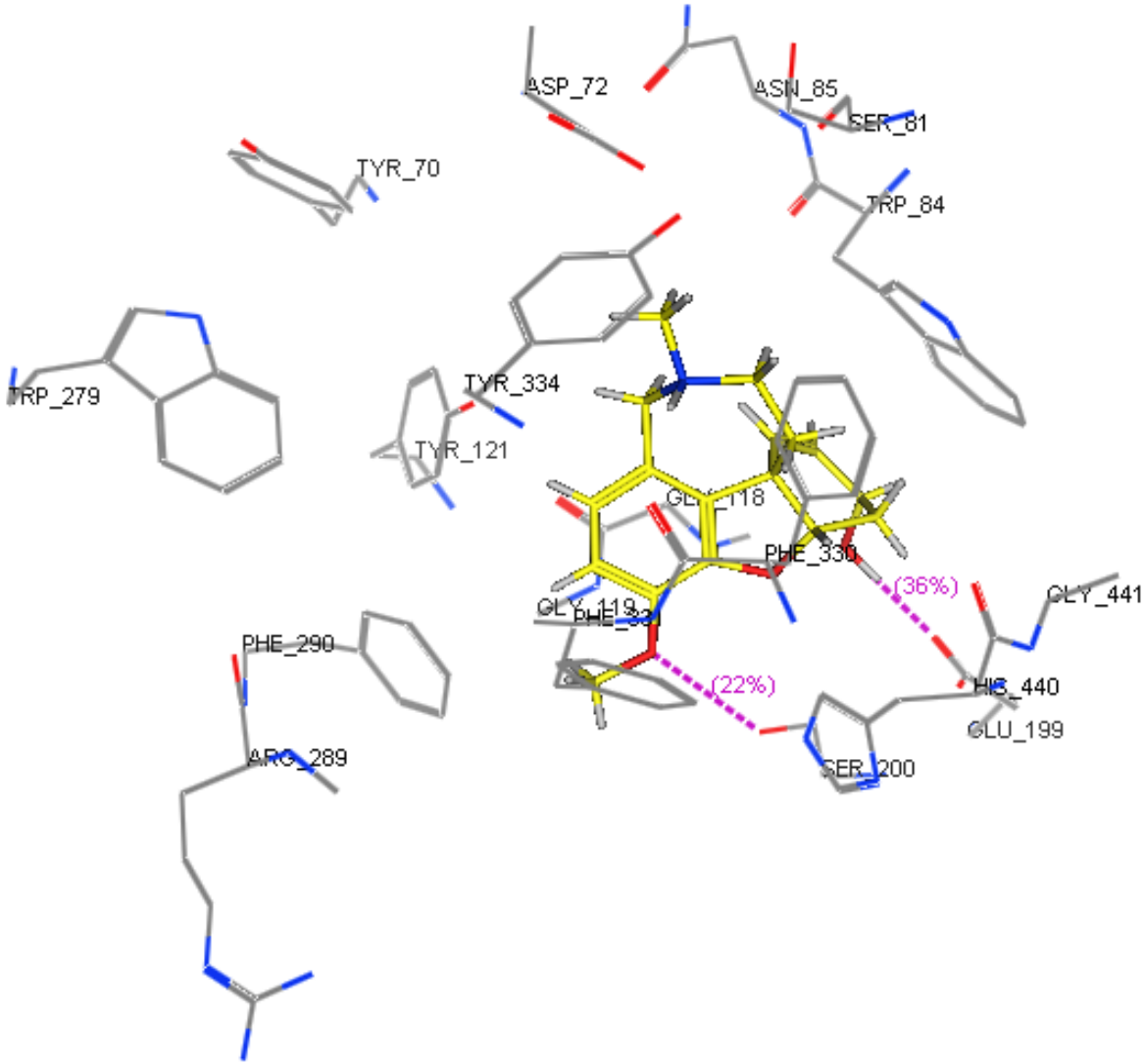


Figure S2. Interactions of co-crystallized ligand in the protein complex 1DX6 (3D)

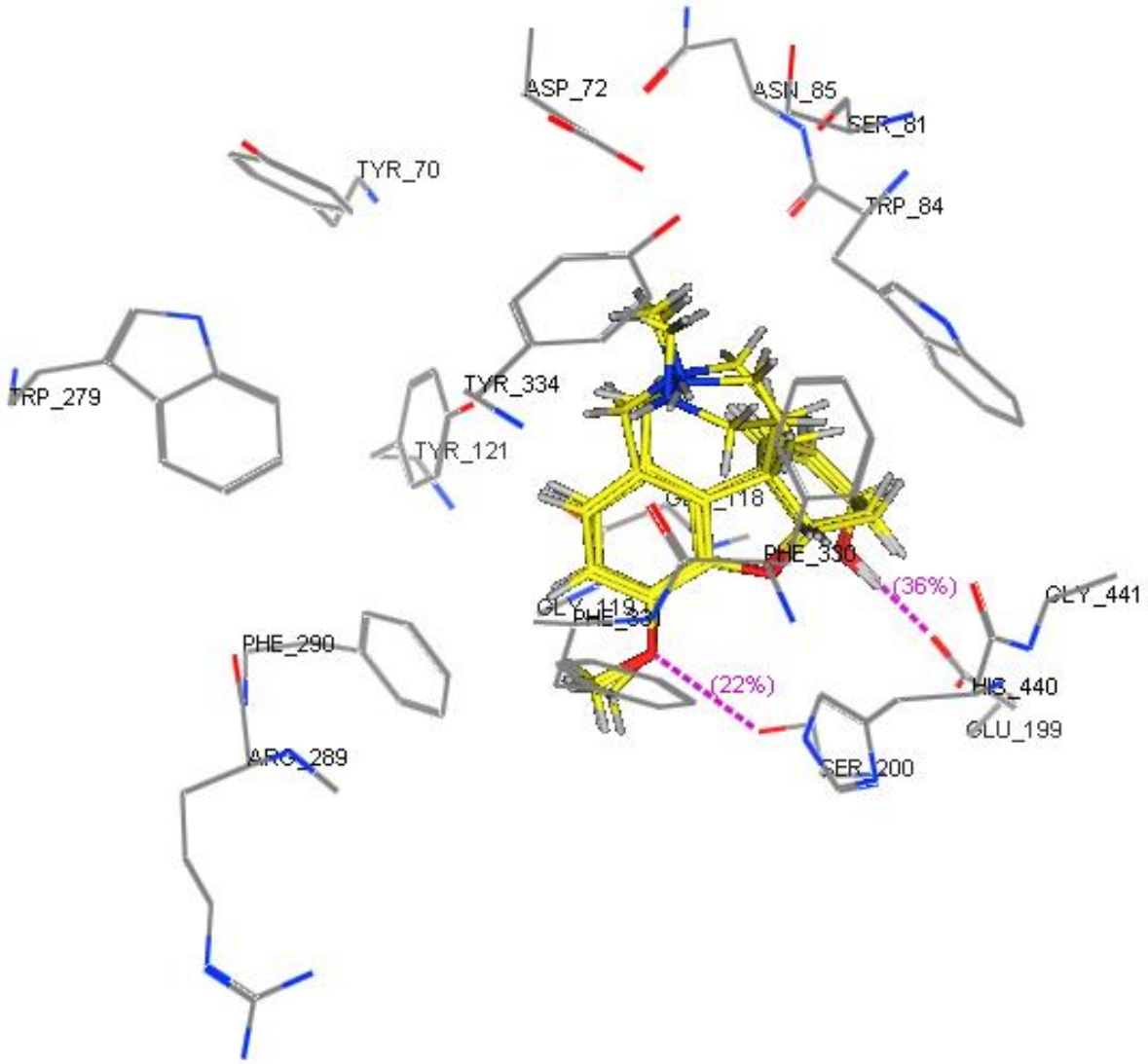


Figure S3. Alignment of re-dock ligands with the native one in the binding pocket of of 1DX6

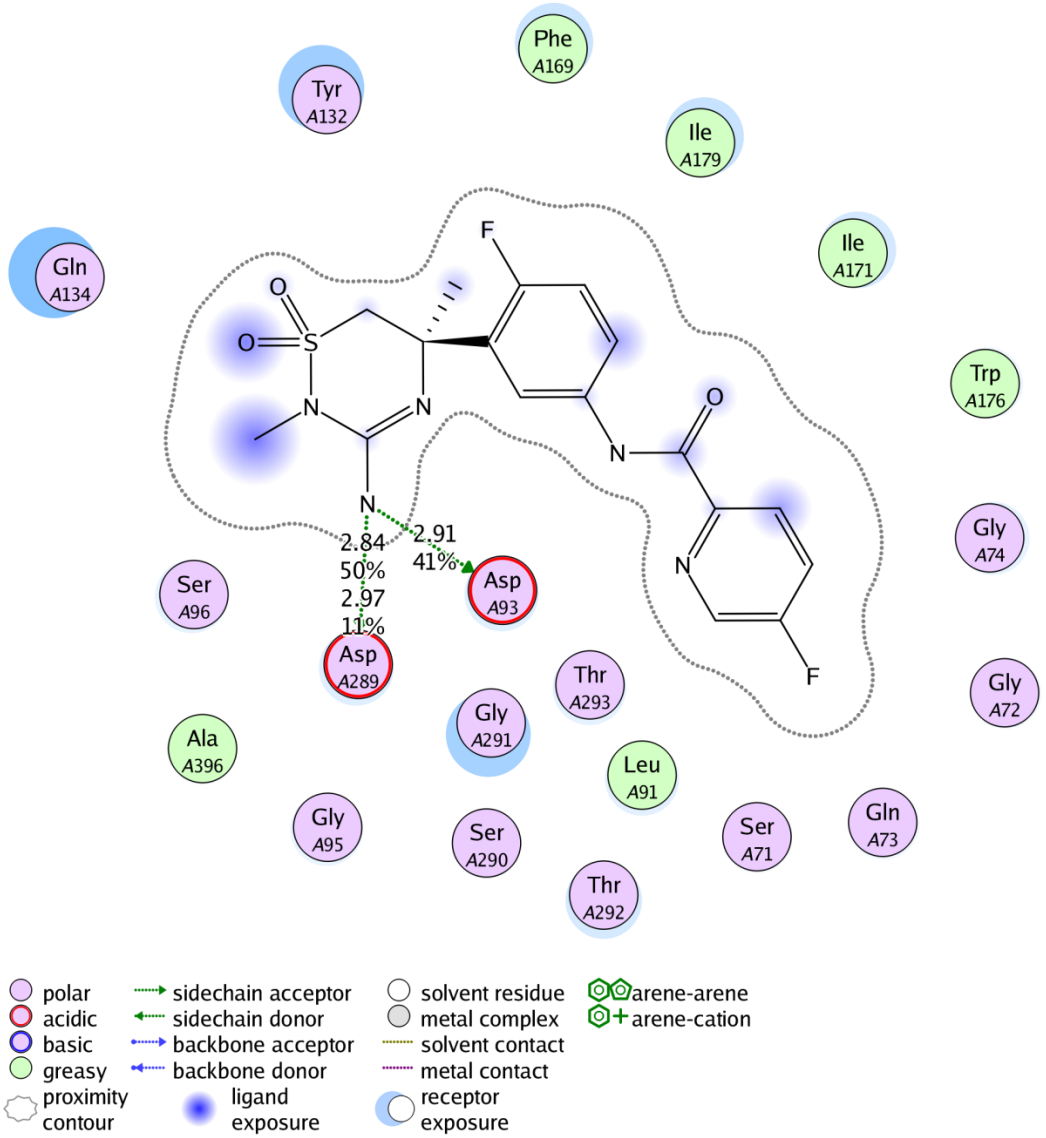


Figure S4. Interactions of co-crystallized ligand in the protein complex 5HU1-chain A (2D)

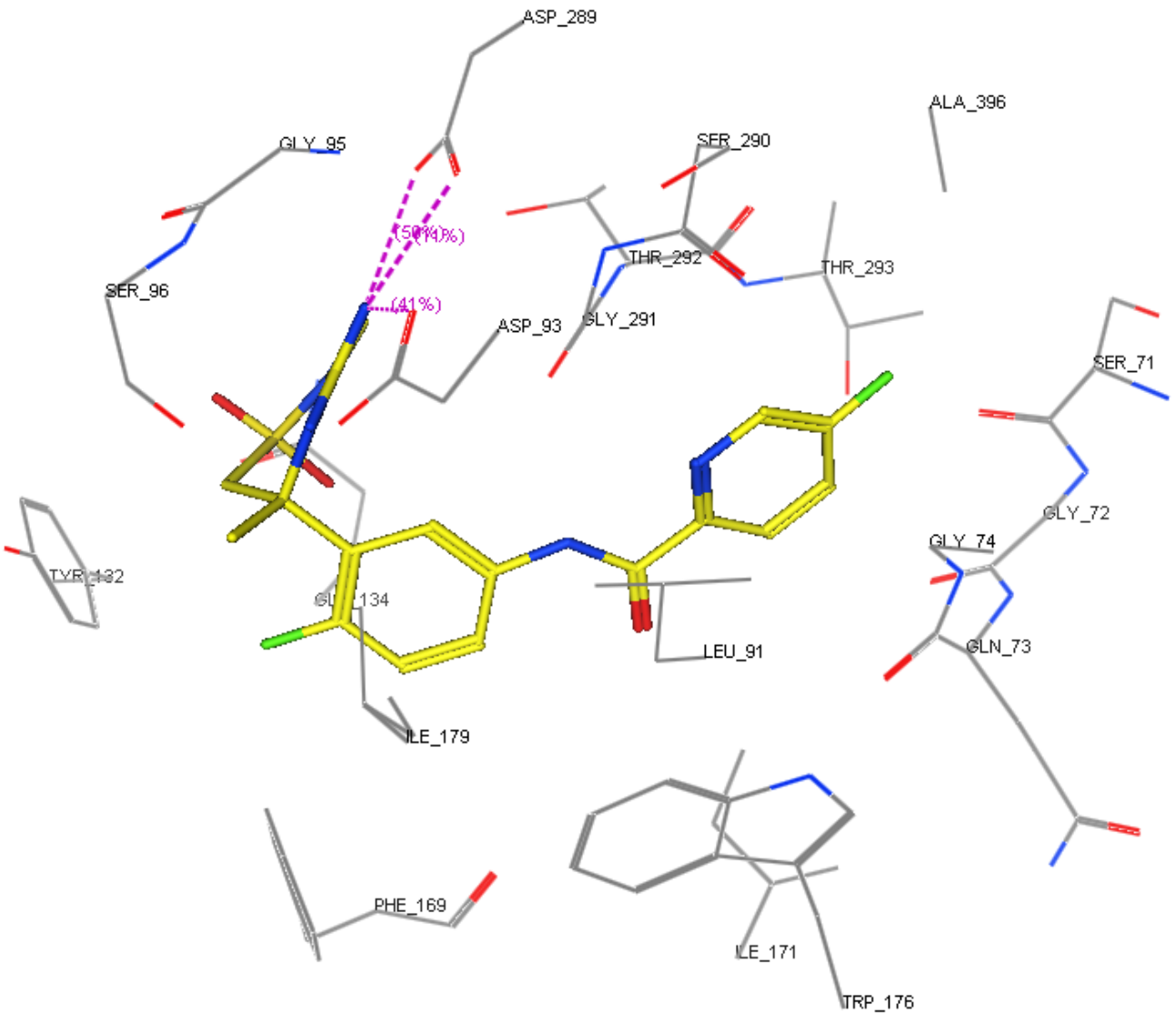


Figure S5. Interactions of co-crystallized ligand in the protein complex 5HU1-chain A (3D)

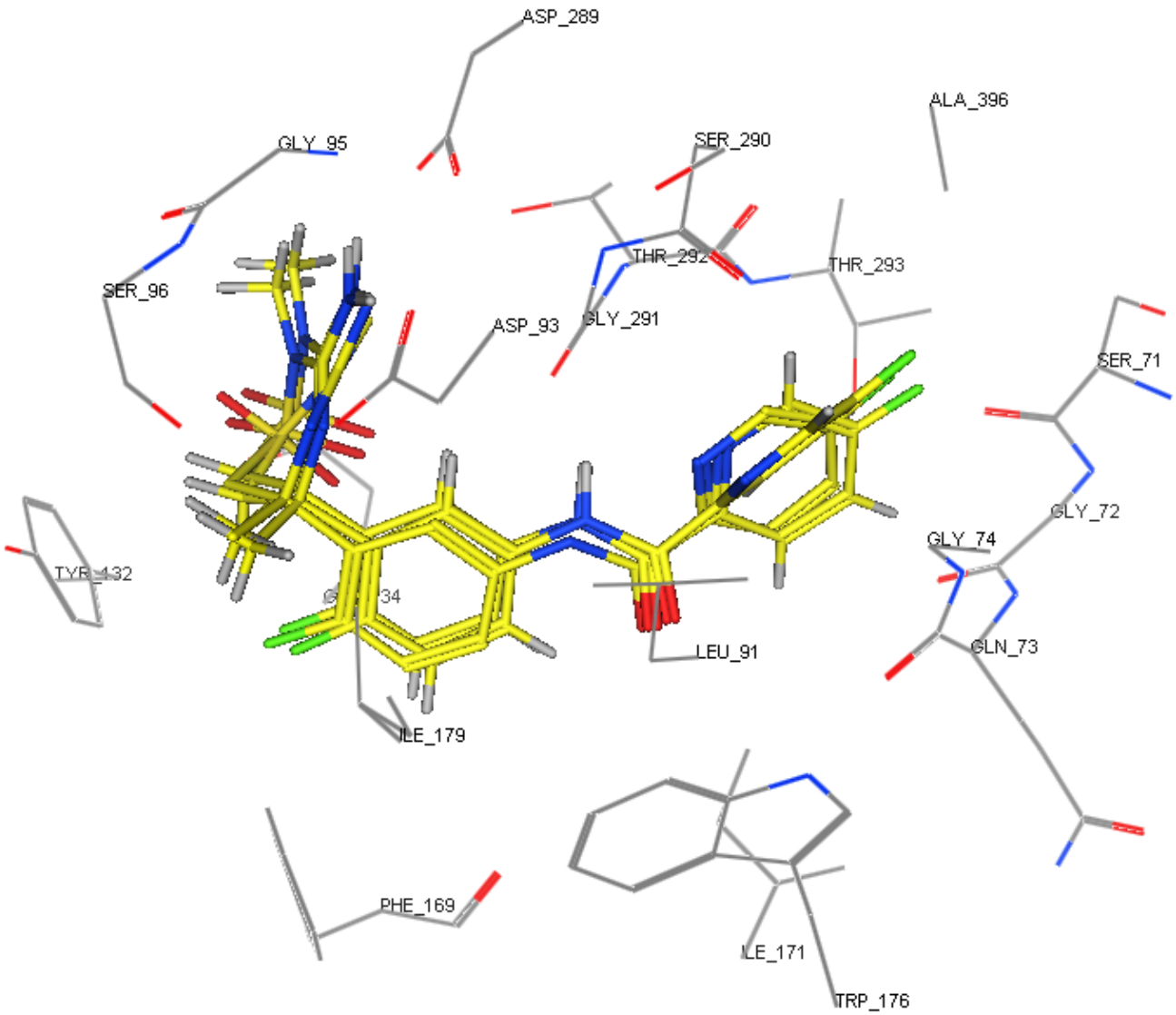


Figure S6. Alignment of re-dock ligands with the native one in the binding pocket of of 5HU1-chain A

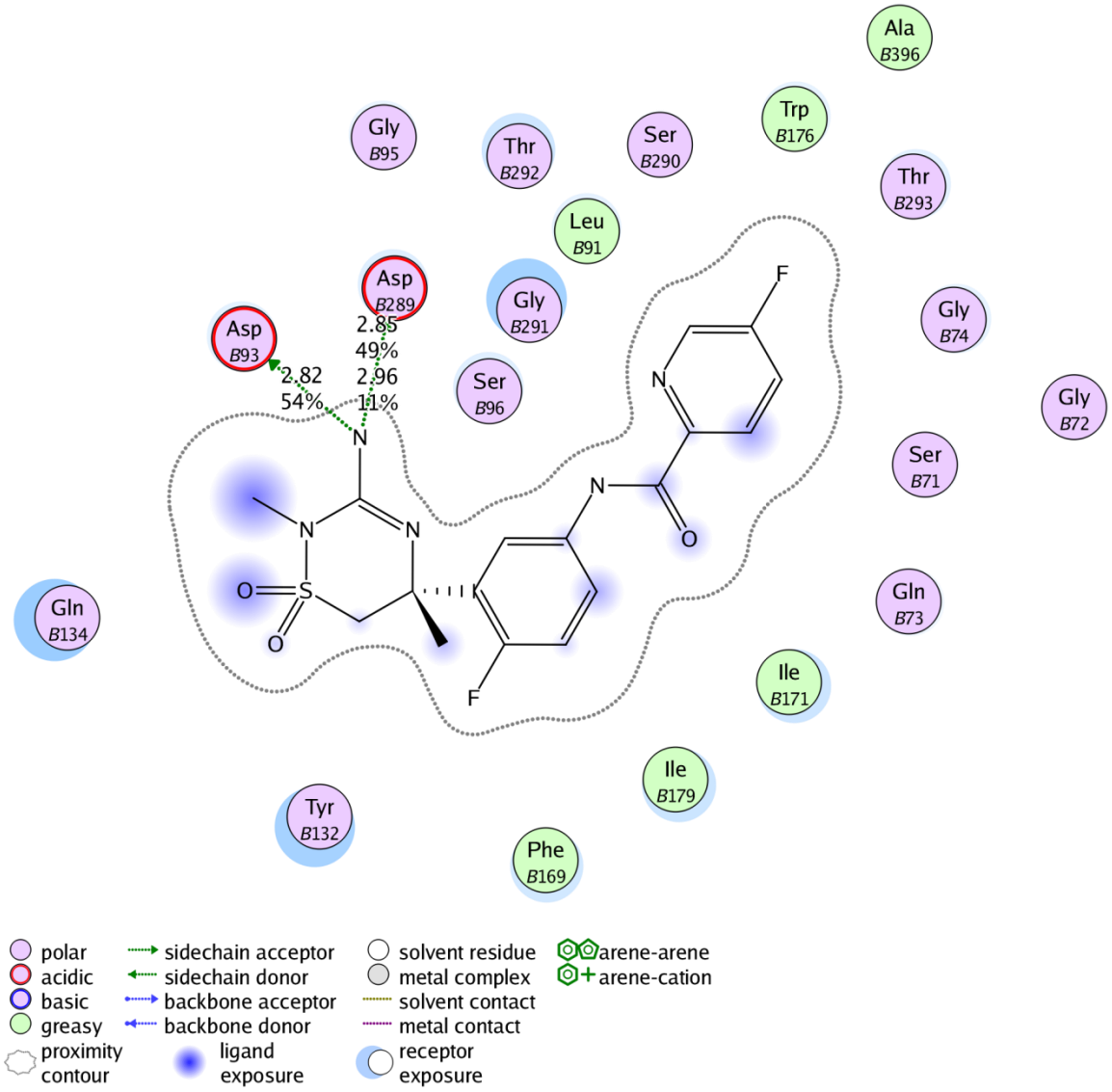


Figure S7. Interactions of co-crystallized ligand in the protein complex 5HU1-chain B (2D)

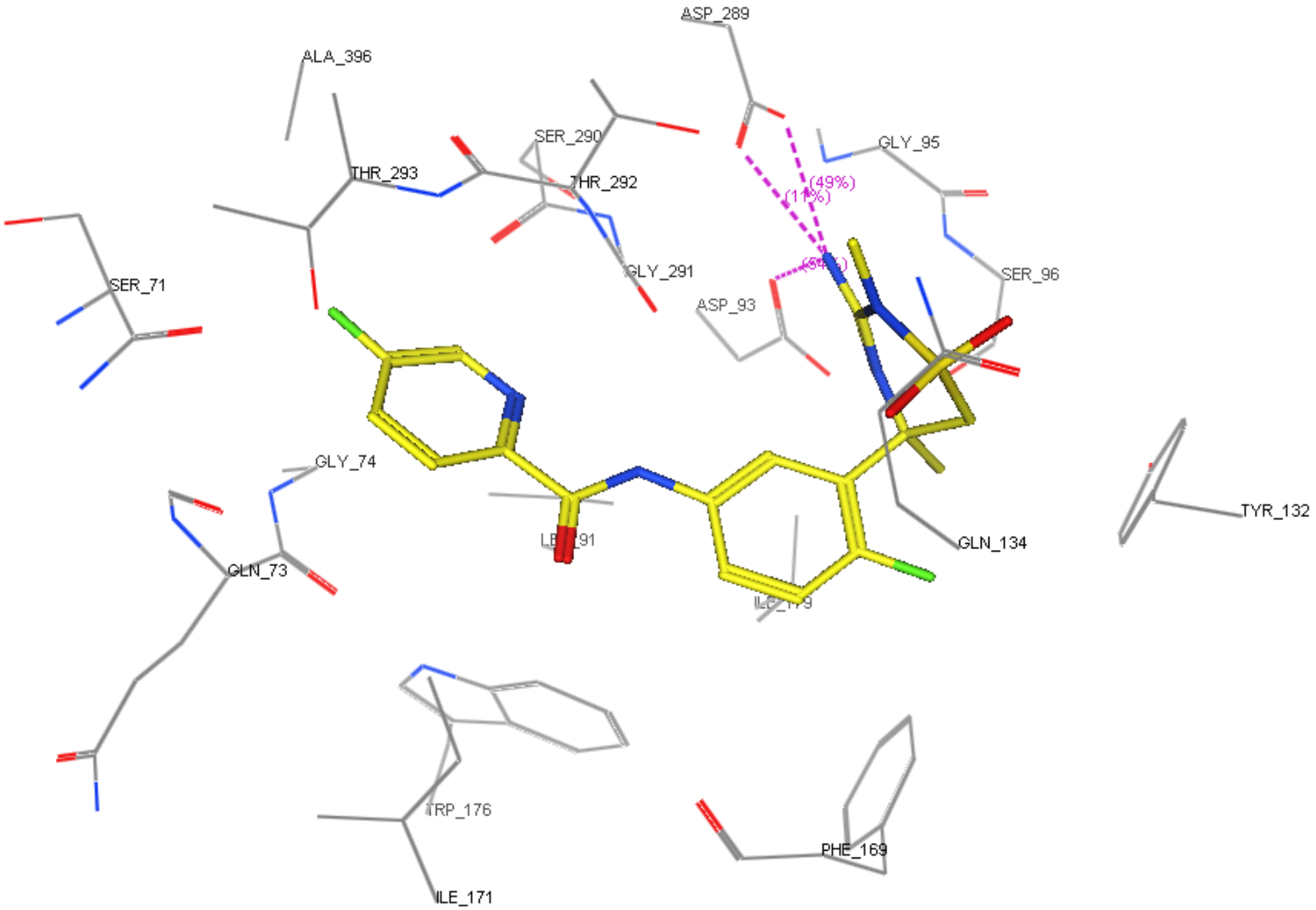


Figure S8. Interactions of co-crystallized ligand in the protein complex 5HU1-chain B (3D)

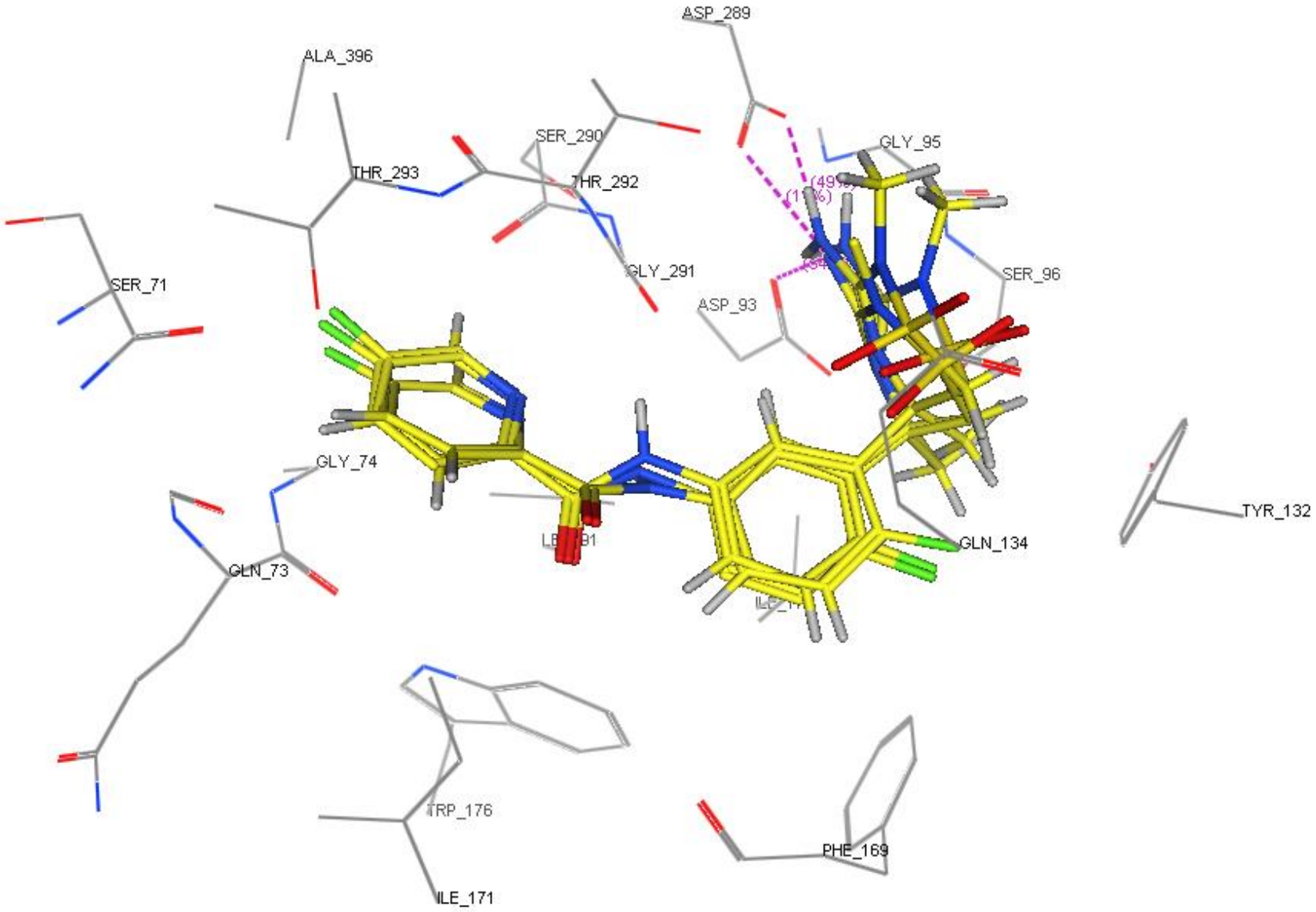


Figure S9. Alignment of re-dock ligands with the native one in the binding pocket of of 5HU1-chain B

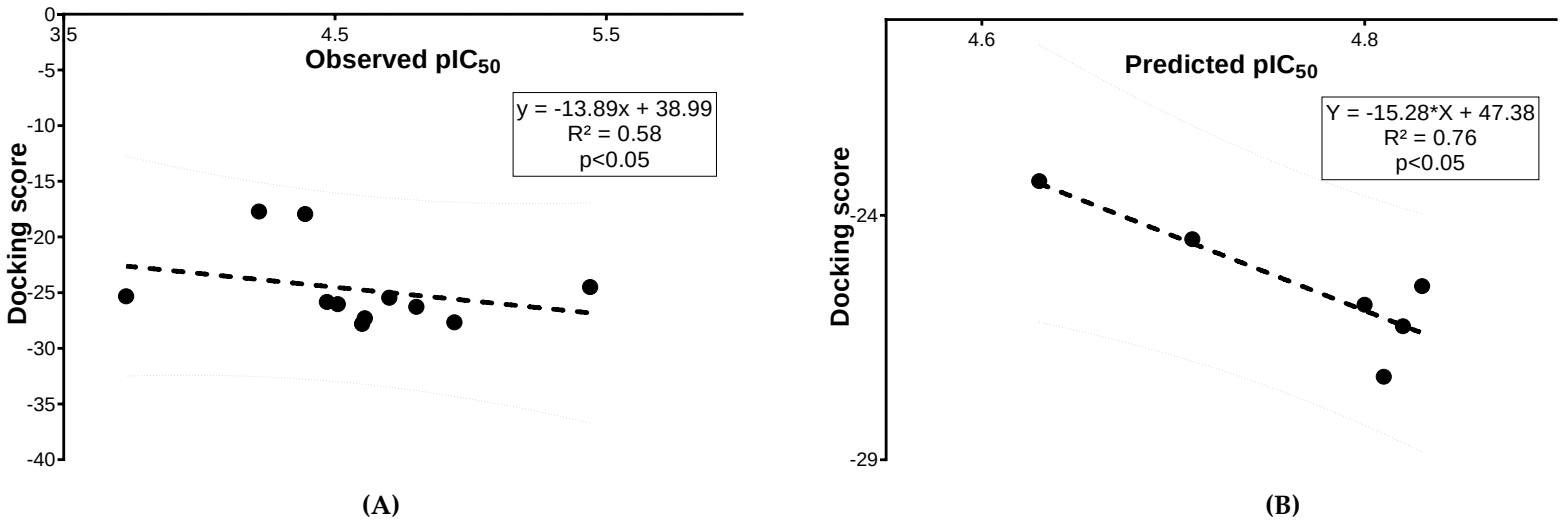
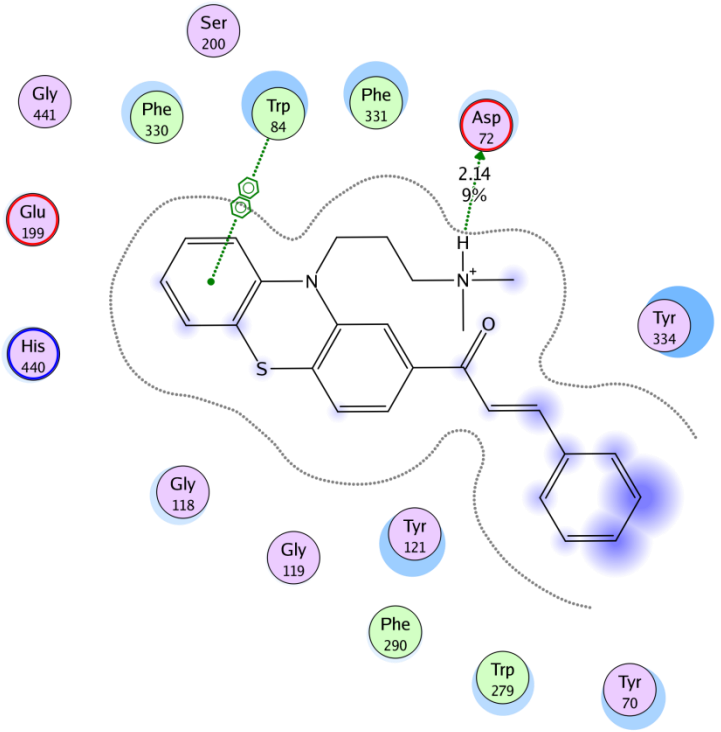
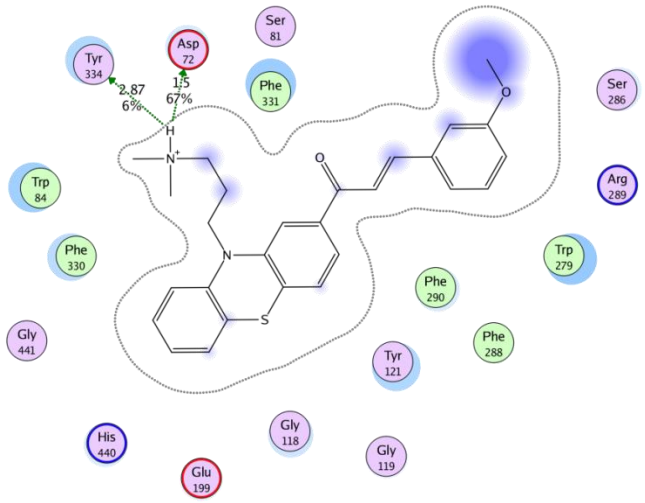
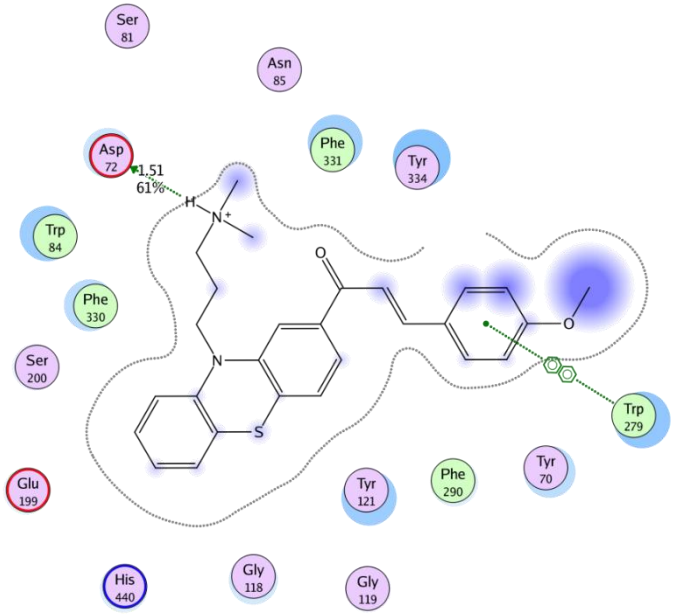
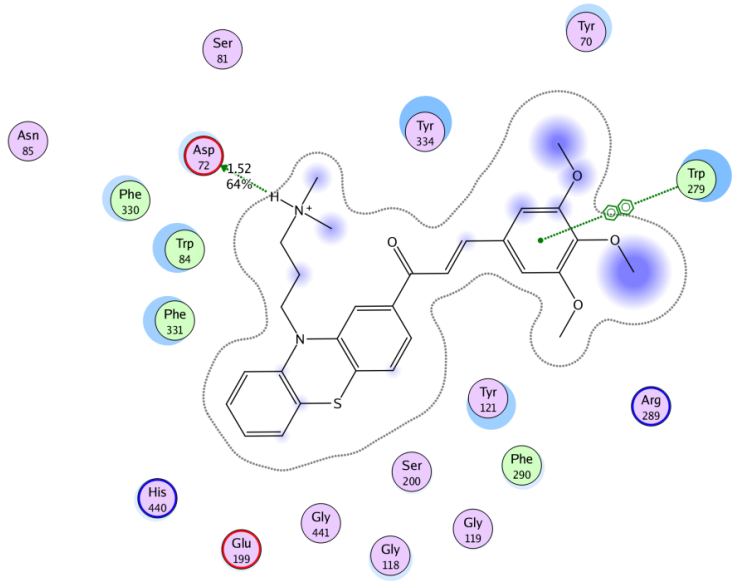
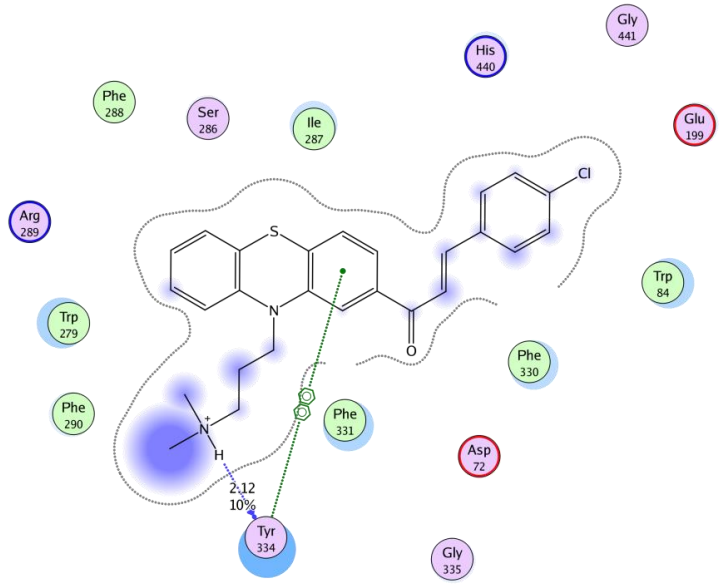


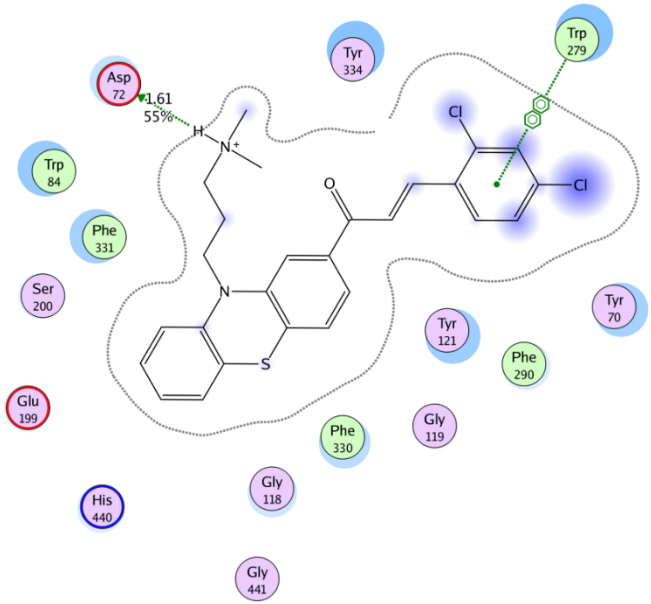
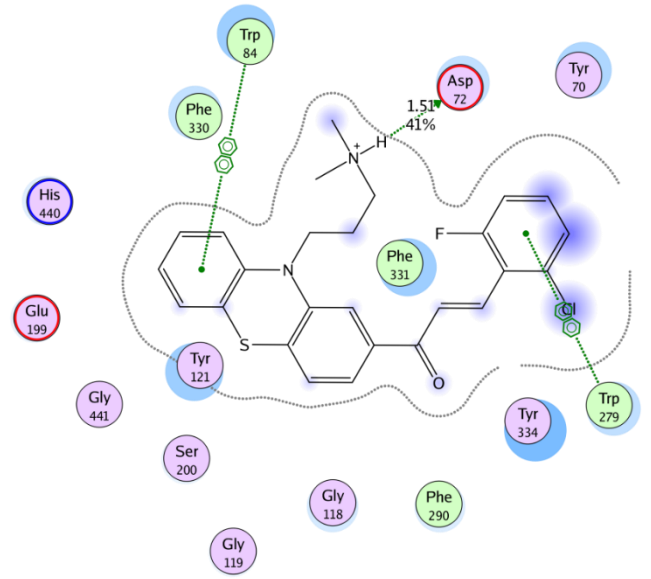
Figure S10. The linear regression between docking score and pIC_{50} on AChE of synthesized chalcone derivatives (A. observed values from **AC1-3** and **AC5-10**, B. predicted values from **AC1, AC4, AC6, AC8, AC10, AC13**)

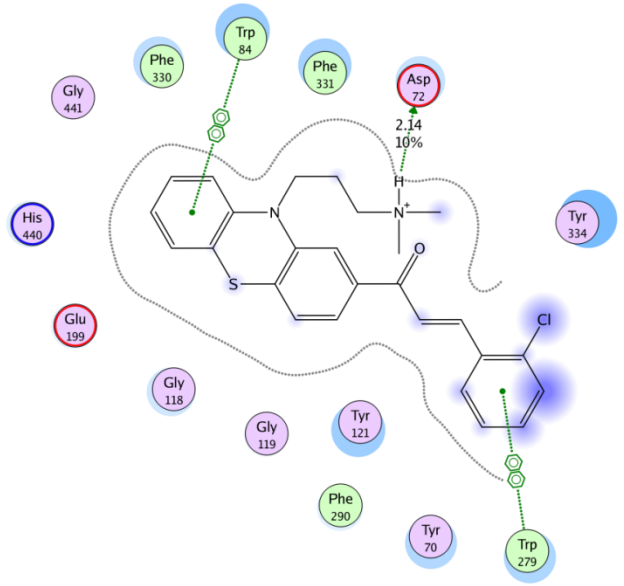
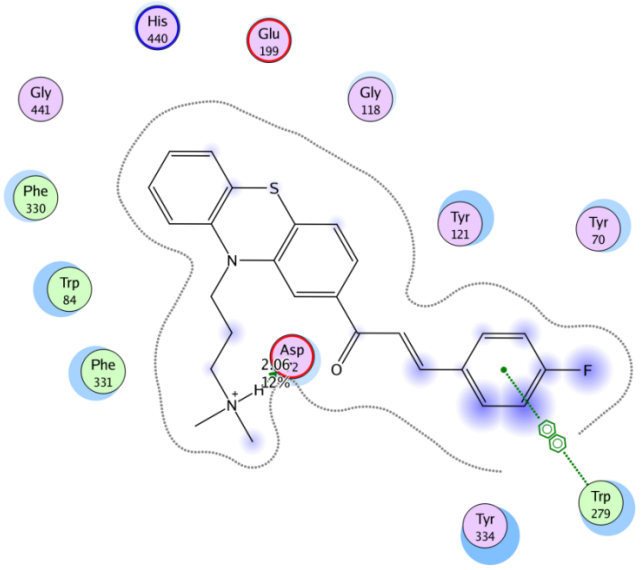
Table S2: Docking results and ligand interaction (Co-crystallized 1DX6)

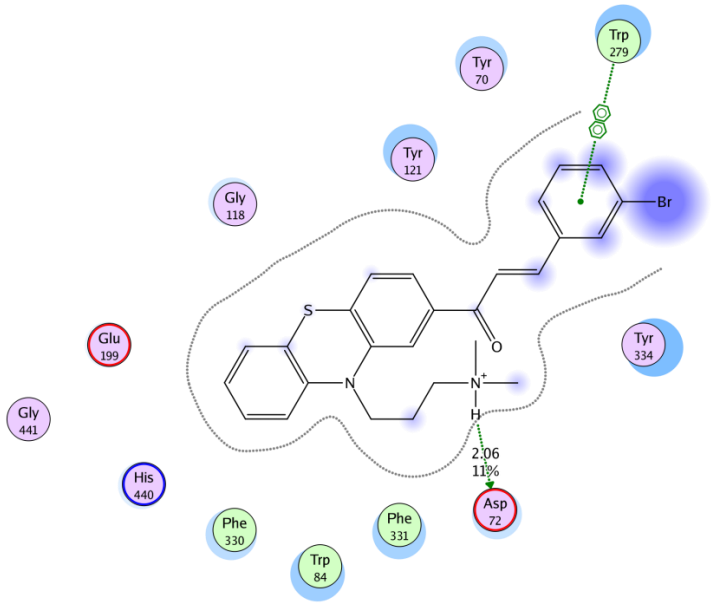
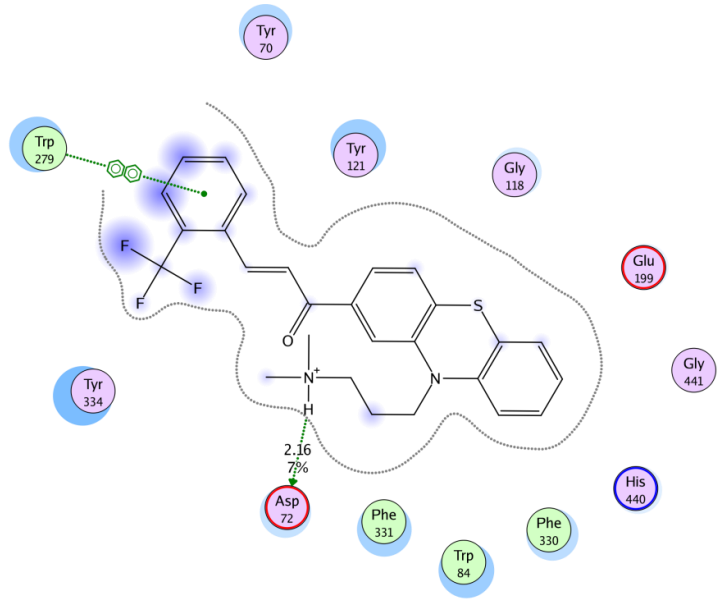
Compound	pIC_{50}		Docking score ($kJ.mol^{-1}$)	Ligand interaction
	Observed	Predicted		
AC1	4.47	4.80	-25.83	 Trp84 (arene-arene), Asp72 (hydrogen bond, score: 9%, length: 2.14 Å)

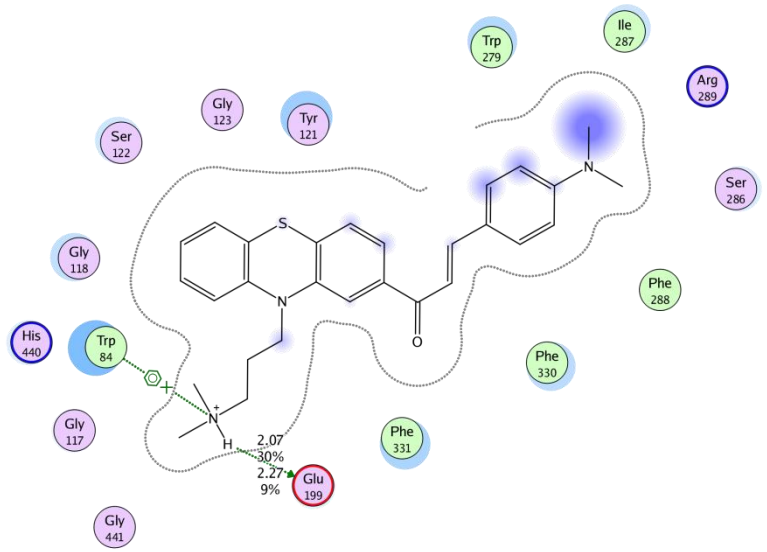
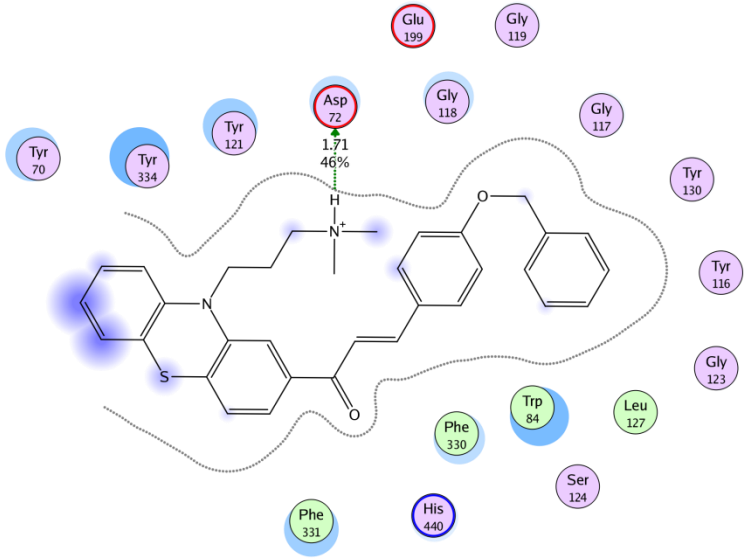
AC2	4.51	4.74	-26.03	 Tyr334 (hydrogen bond, score: 6%, length: 2.87 Å), Asp72 (hydrogen bond, score: 67%, length: 1.5 Å)
AC3	4.94	4.74	-27.67	 Trp279 (arene-arene), Asp72 (hydrogen bond, score: 61%, length: 1.51 Å)

AC4	5.44	4.71	-24.49	 Trp279 (arene-arene), Asp72 (hydrogen bond, score: 64%, length: 1.52 Å)
AC5	4.22	4.82	-17.71	 Tyr334 (arene-arene; hydrogen bond, score 10%, length: 2.12 Å)

AC6	4.70	4.83	-25.45	 Trp279 (arene-arene), Asp72 (hydrogen bond, score: 55%, length: 1.61 Å)
AC7	4.39	4.76	-17.94	 Trp279 (arene-arene), Trp84 (arene-arene), Asp72 (hydrogen bond, score: 41%, length: 1.51 Å)

AC8	4.80	4.82	-26.27	 Trp279 (arene-arene), Trp84 (arene-arene), Asp72 (hydrogen bond, score: 10%, length: 2.14 Å)
AC9	4.60	4.76	-27.80	 Trp279 (arene-arene), Asp72 (hydrogen bond, score: 12%, length: 2.06 Å)

AC10	4.61	4.81	-27.30	 Trp279 (arene-arene), Asp72 (hydrogen bond, score: 11%, length: 2.06 Å)
AC11	3.73	4.59	-25.33	 Trp279 (arene-arene), Asp72 (hydrogen bond, score: 7%, length: 2.16 Å)

AC12	5.96	4.81	-22.15	 Trp84 (arene-cation), Glu199 (hydrogens, score: 9%; 30%; length: 2.27; 2.07 Å)
AC13	4.93	4.63	-23.30	 Asp72 (hydrogen bond, score: 46%, length: 1.71 Å)

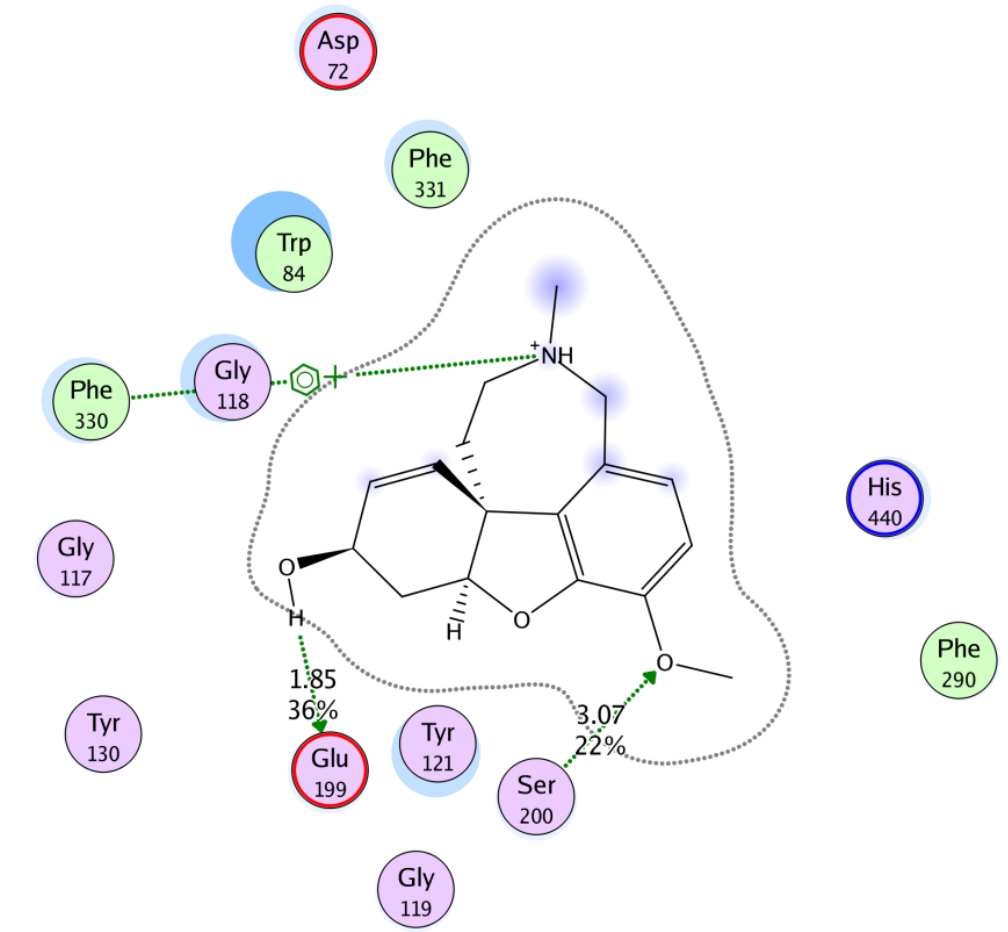
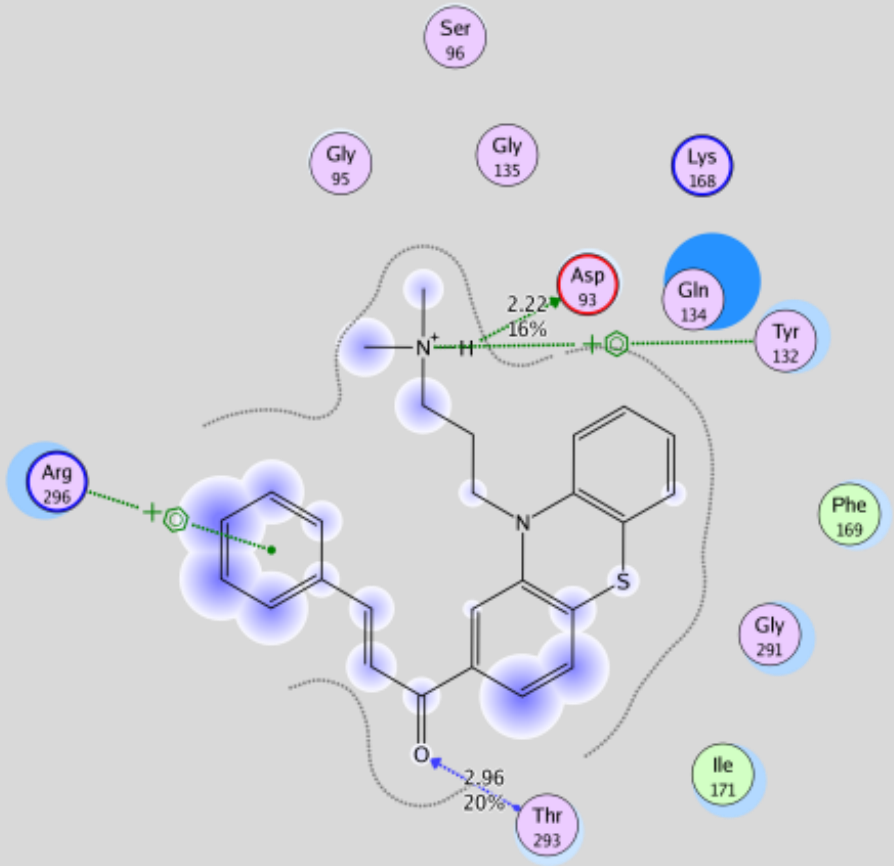
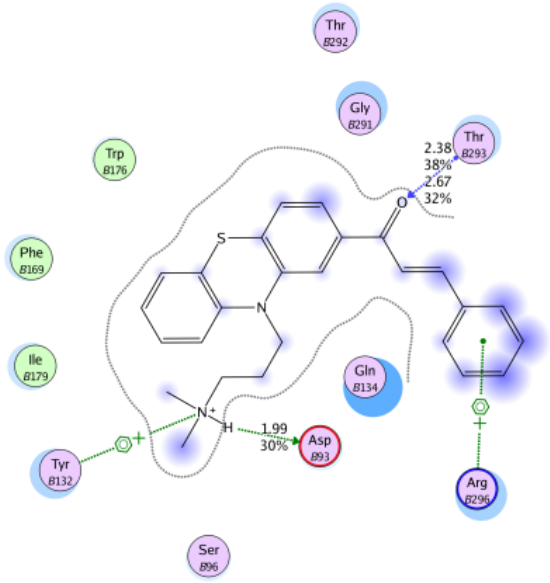
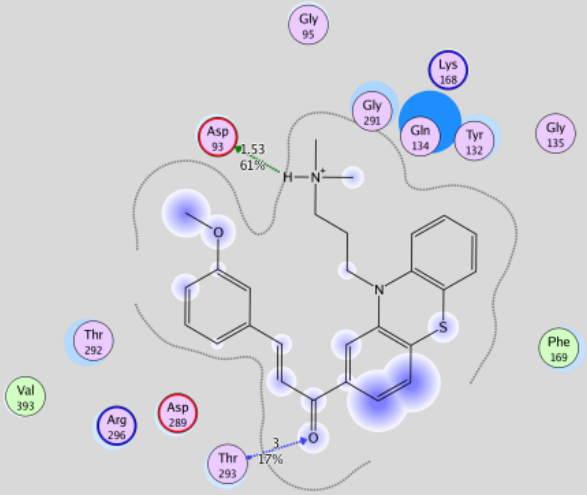
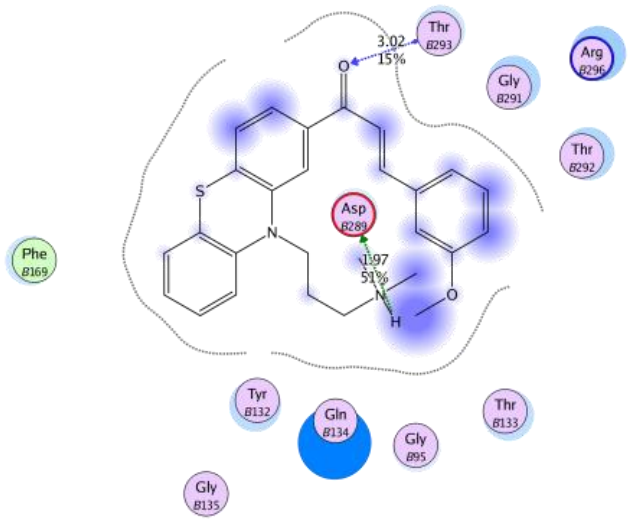
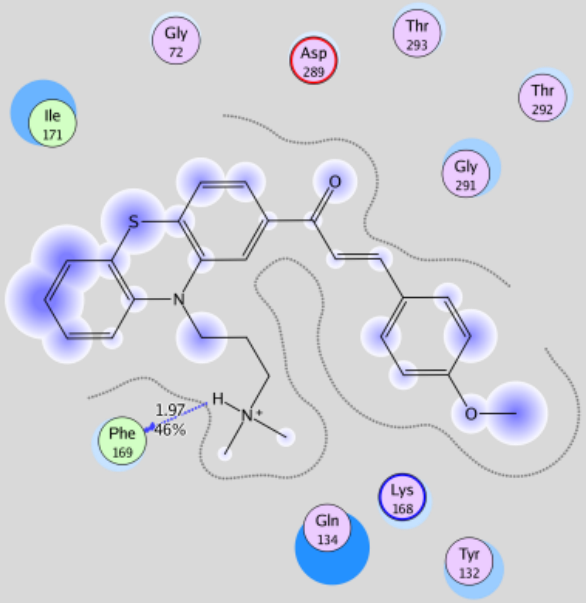
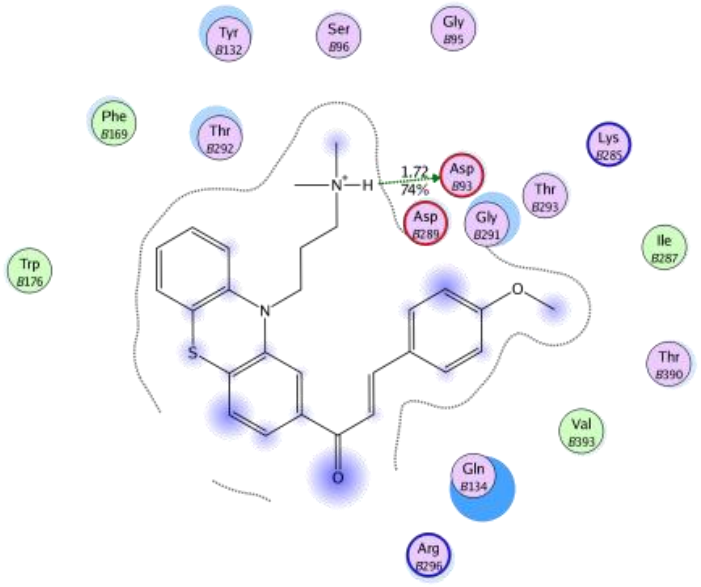
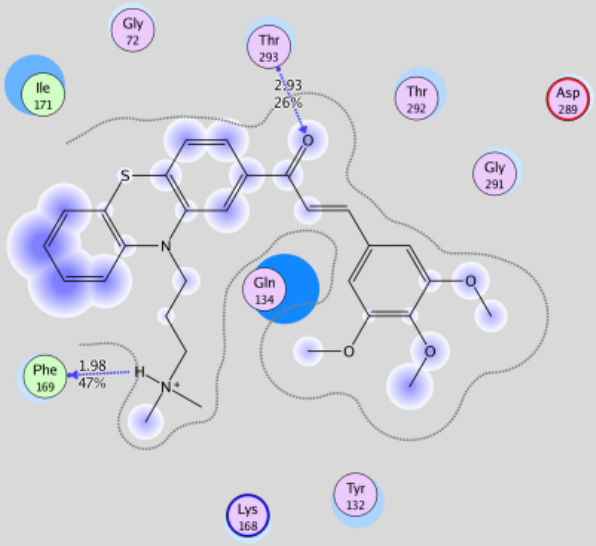
Galanthamine	5.9	5.14	-28.53	 Phe330 (arene-cation), Glu199 (hydrogen, score: 36%, length: 1.85 Å), Ser200 (hydrogen, score: 22%, length: 3.07 Å)

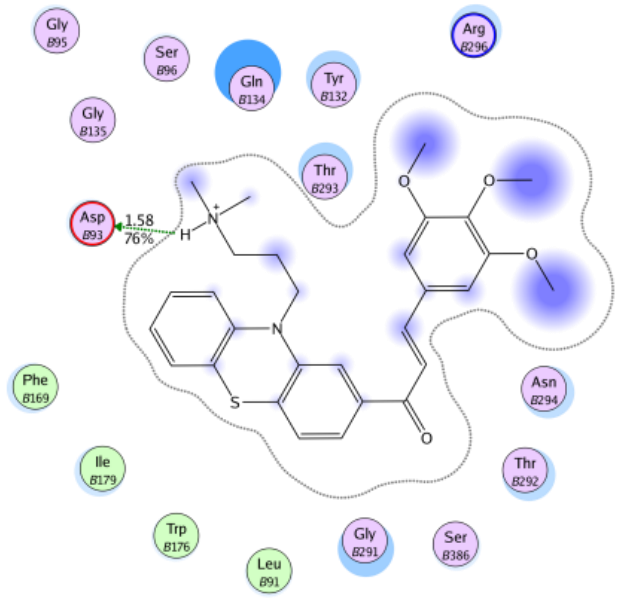
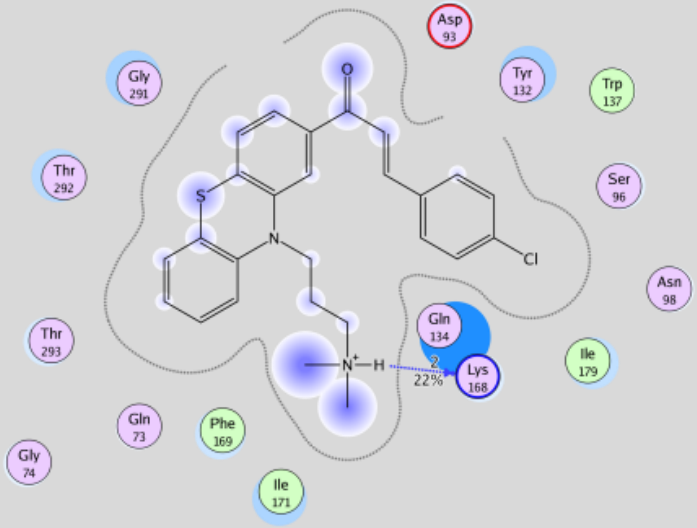
Table S3. Docking results and ligand interaction (Co-crystallized 5HU1 chain A and B)

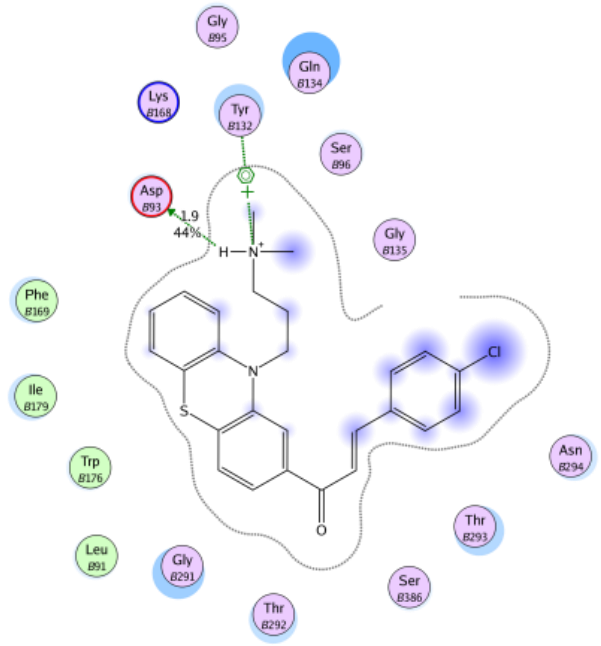
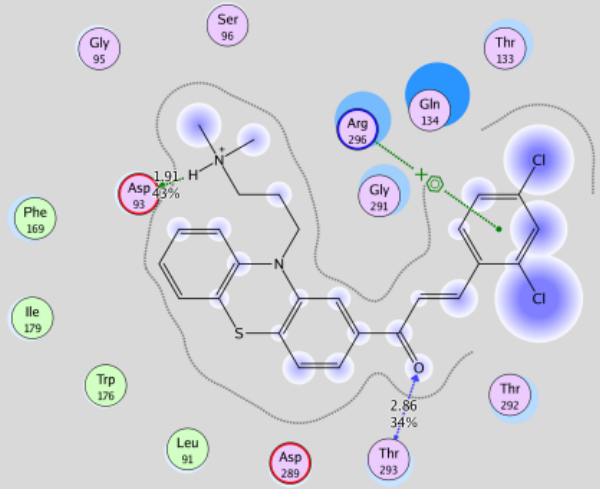
Compound	pIC_{50}		Chain	Docking score ($kJ.mol^{-1}$)	Interactions
	Observed	Predicted			
AC1	5.20	6.52	A	-17.82	 TyrA132 (arene-cation), ArgA296 (arene-cation), AspA93 (hydrogen bond, score: 16%, length 2.22 Å), ThrA293 (hydrogen bond, score: 20%, length 2.96 Å)

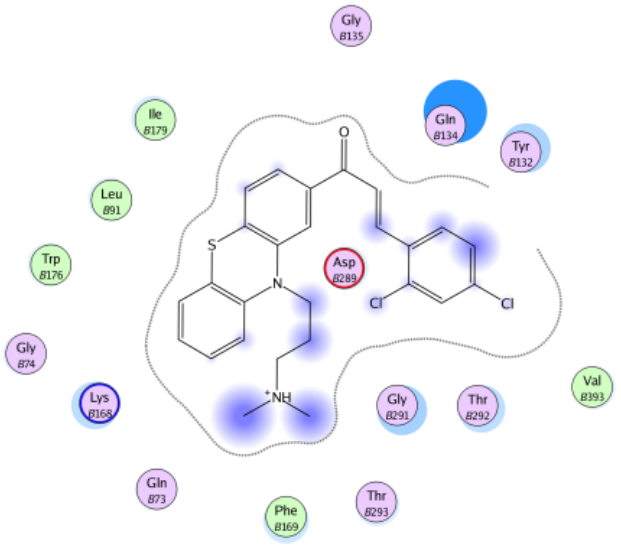
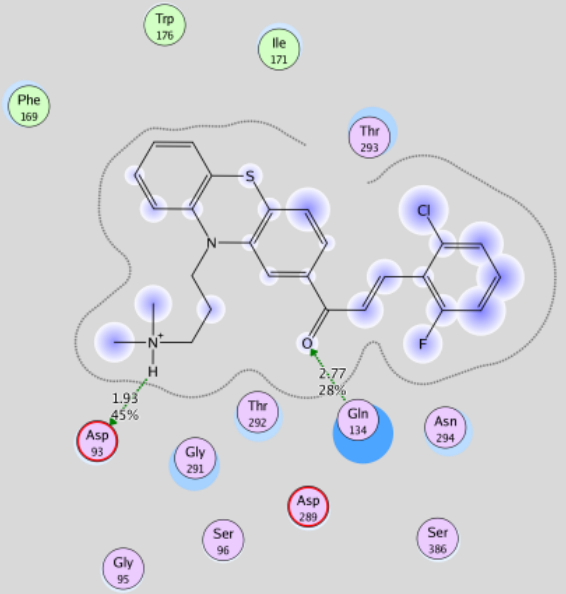
			B	-17.69	 TyrB132 (arene-cation, ArgB296 (arene-cation), AspB93 (hydrogen bond, score: 30%, length 1.99 Å), ThrB293 (hydrogen bonds, score: 32%; 38%, length: 2.67 Å; 2.38 Å)
AC2	5.52	7.38	A	-17.22	 AspA93 (hydrogen bond, score: 61%, length 1.53 Å), ThrA293 (hydrogen bond, score: 17%, length 3 Å)

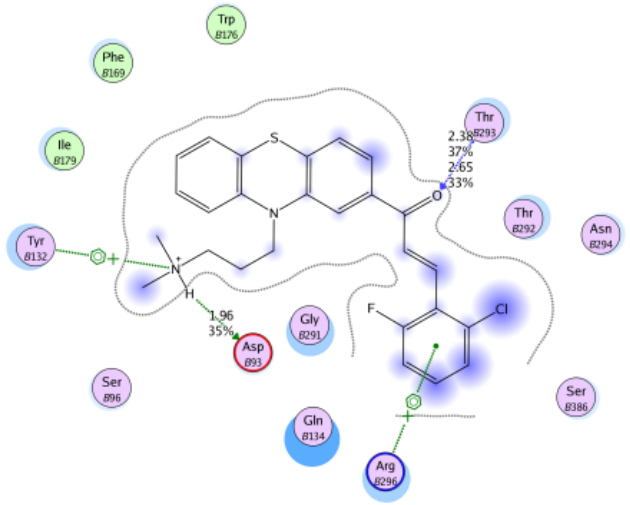
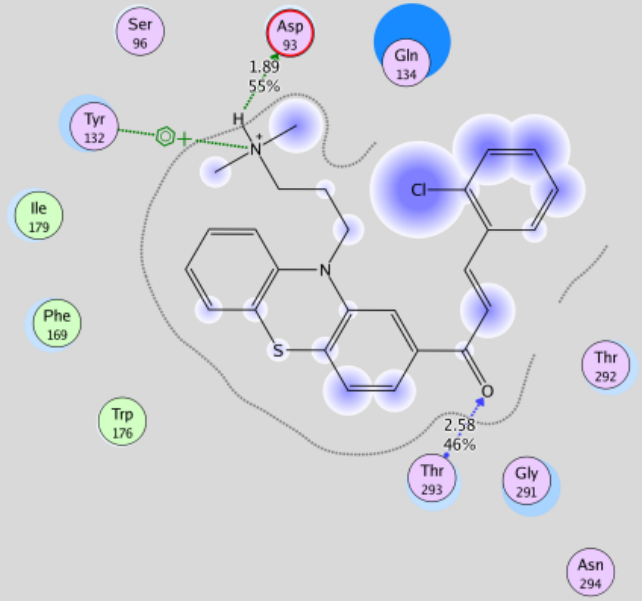
			B	-17.81	 ThrB293 (hydrogen bond, score: 15%, length 3.02 Å), AspB289 (hydrogen bond, score: 51%, length 1.97 Å)
AC3	5.35	7.37	A	-16.28	 PheA169 (hydrogen bond, score: 46%, length 1.97 Å)

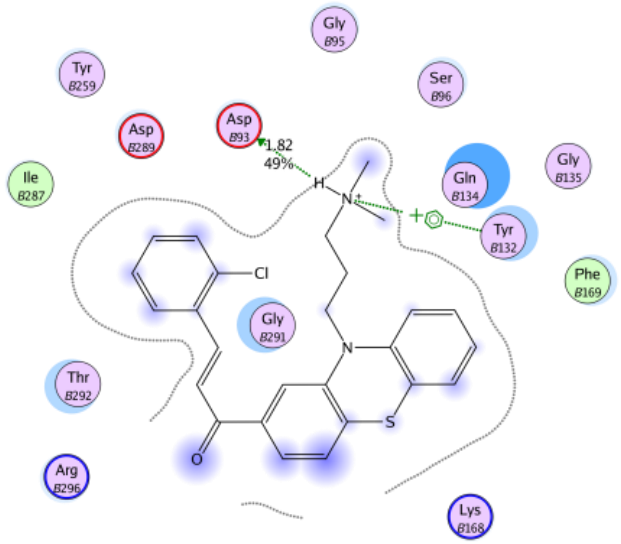
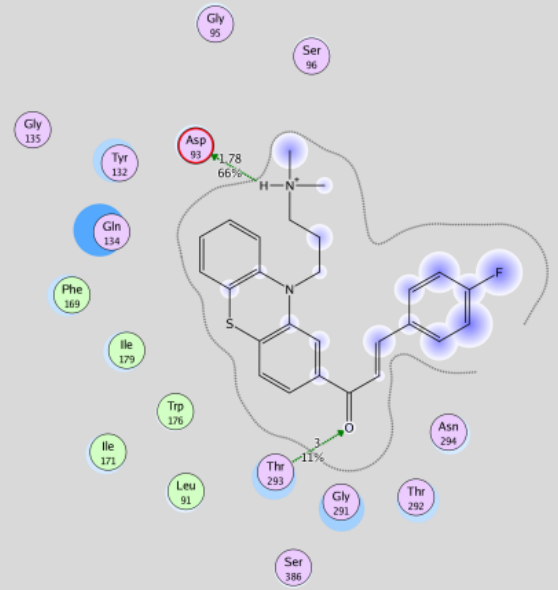
			B	-15.37	 AspB93 (hydrogen bond, score: 74%, length 1.72 Å)
AC4	6.81	8.49	A	-16.71	 ThrA293 (hydrogen bond, score: 26%, length 2.93 Å), PheA169 (hydrogen bond, score: 47%, length 1.98 Å)

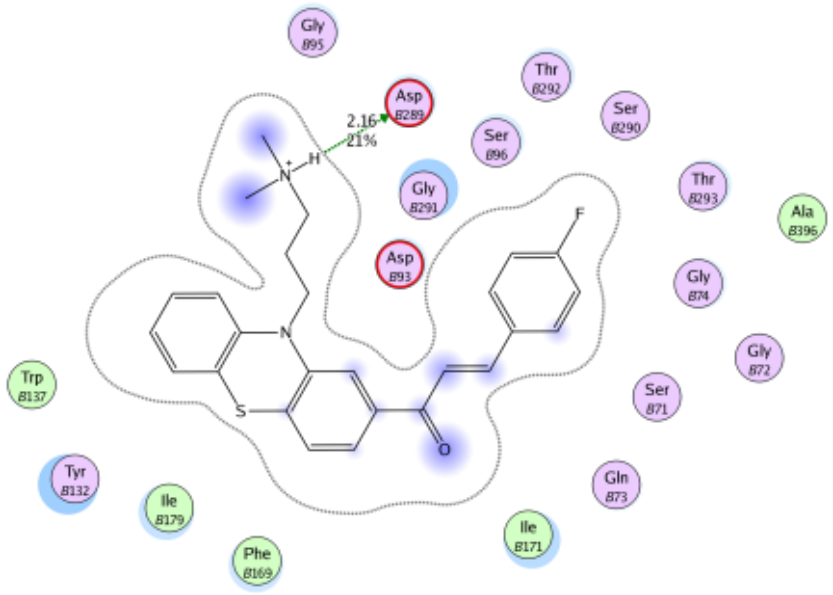
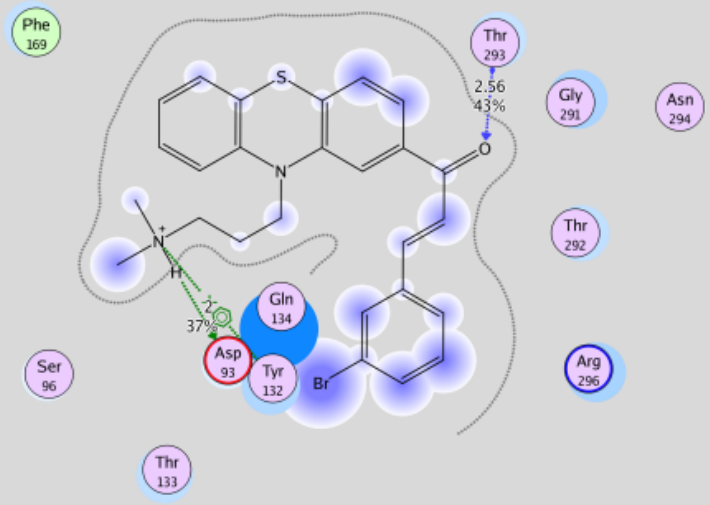
			B	-13.92	 AspB93 (hydrogen bond, score: 76%, length 1.58 Å)
AC5	5.91	7.25	A	-20.77	 LysA168 (hydrogen bond, score: 22%, length 2 Å)

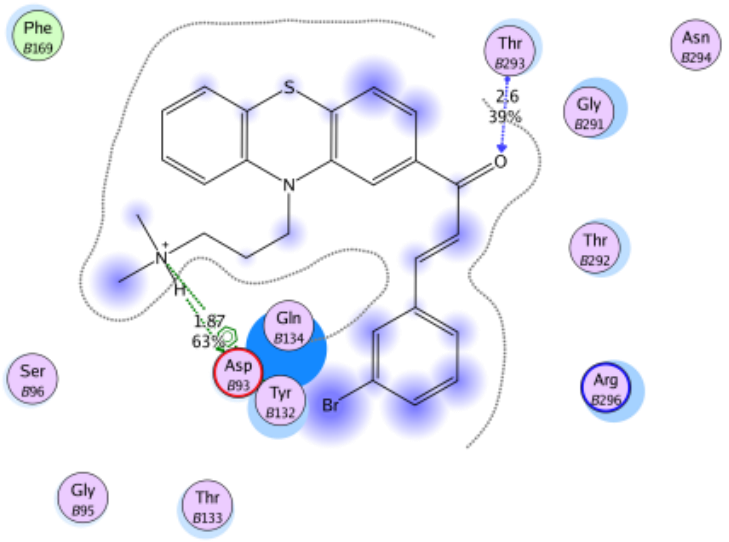
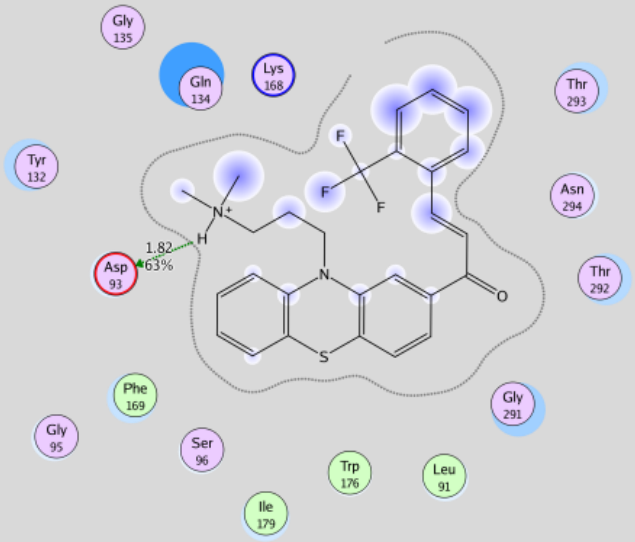
			B	-16.87	 AspB93 (hydrogen bond, score: 44%, length 1.9 Å), TyrB132 (arene-cation)
AC6	6.30	7.68	A	-18.79	 AspA93 (hydrogen bond, score: 43%, length 1.91 Å), ThrA293 (hydrogen bond, score: 34%, length 2.86 Å) ArgA296 (arene-cation)

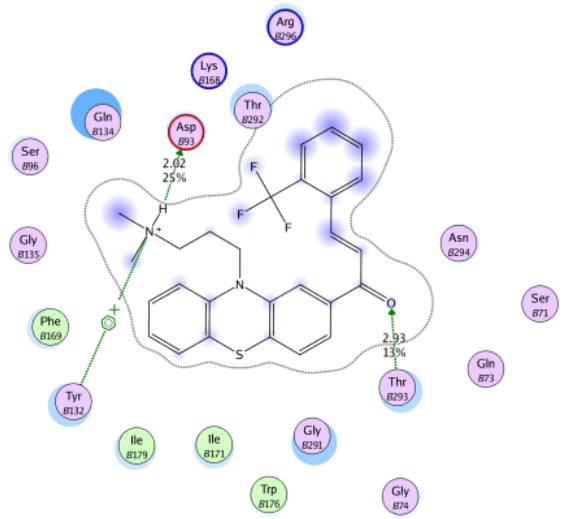
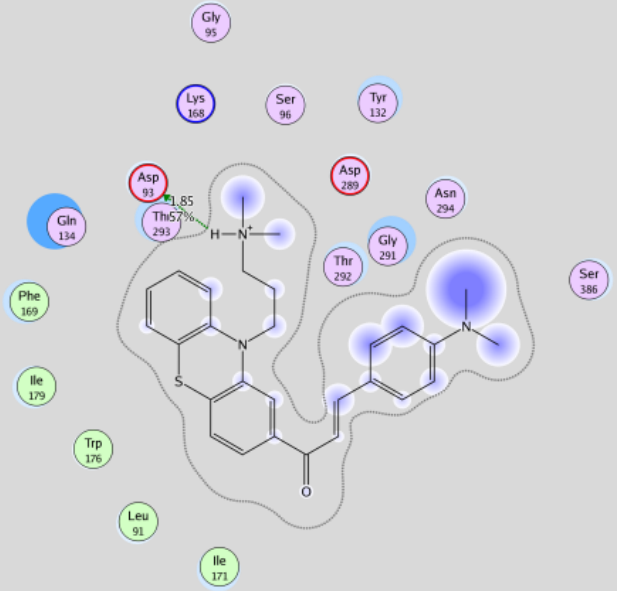
			B	-16.73	 No strong interaction
AC7	6.35	7.63	A	-19.51	 AspA93 (hydrogen bond, score: 45%, length 1.93 Å), GlnA134 (hydrogen bond, score: 28%, length 2.77 Å)

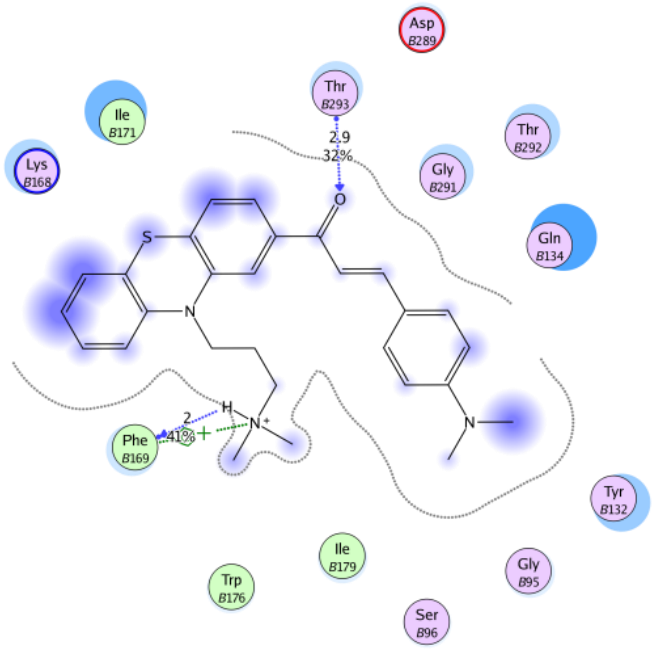
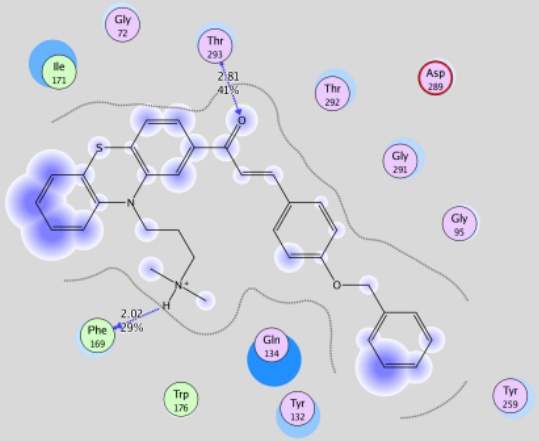
			B	-16.85	 AspB93 (hydrogen bond, score: 35%, length 1.96 Å), ThrB293 (hydrogen bonds, score: 33%; 37%, length: 2.65 Å; 2.38 Å), TyrB132 (arene-cation), ArgB296 (arene-cation)
AC8	5.53	7.15	A	-20.36	 AspA93 (hydrogen bond, score: 55%, length 1.89 Å), ThrA293 (hydrogen bond, score: 46%, length 2.58 Å), TyrA132 (arene-cation)

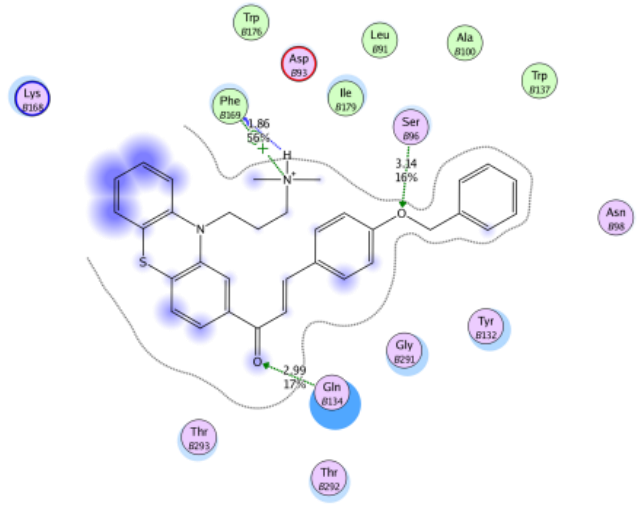
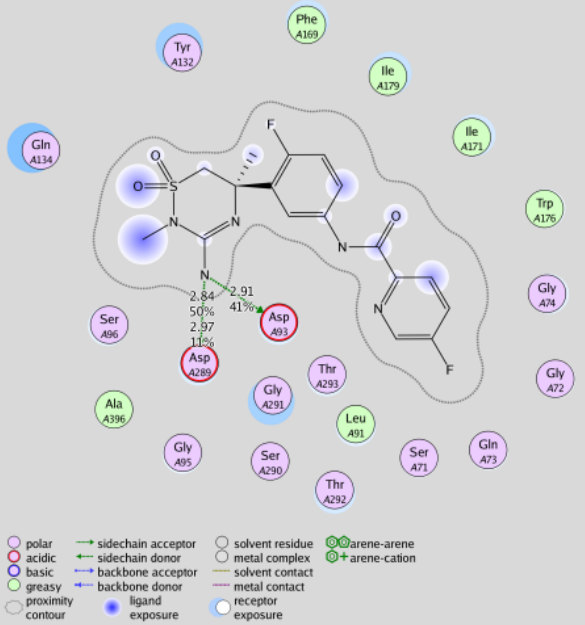
			B	-16.81	 AspB93 (hydrogen bond, score: 49%, length 1.82 Å), TyrB132 (arene-cation)
AC9	5.43	7.12	A	-20.97	 AspA93 (hydrogen bond, score: 66%, length 1.78 Å), ThrA293 (hydrogen bond, score: 11%, length 3 Å)

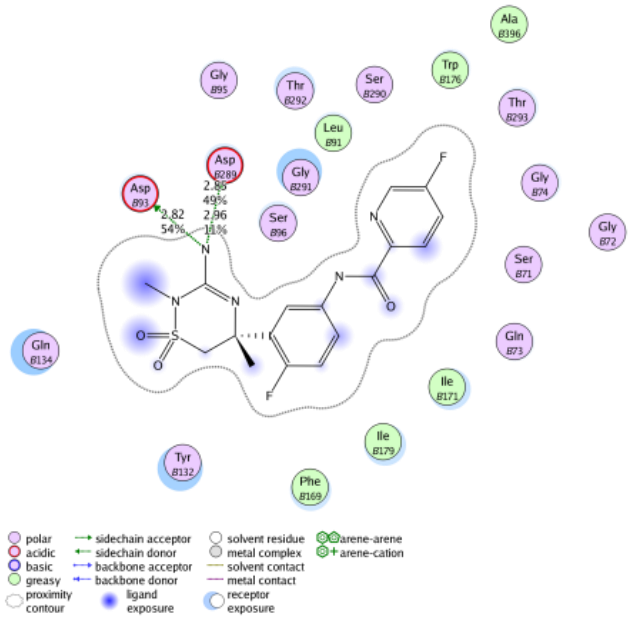
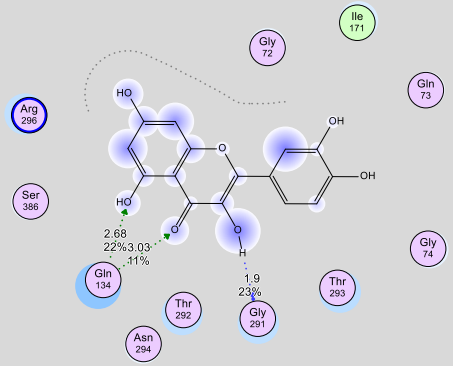
			B	-18.06	 AspB289 (hydrogen bond, score: 21%, length 2.16 Å)
AC10	5.70	7.28	A	-22.51	 AspA93 (hydrogen bond, score: 37%, length 2 Å), ThrA293 (hydrogen bond, score: 43%, length 2.56 Å), TyrA132 (arene-cation)

			B	-20.81	 AspB93 (hydrogen bond, score: 63%, length 1.87 Å), ThrB293 (hydrogen bond, score: 39%, length 2.6 Å), TyrB132 (arene-cation)
AC11	6.40	7.99	A	-19.35	 AspA93 (hydrogen bond, score: 63%, length 1.82 Å)

			B	-16.41	 AspB93 (hydrogen bond, score: 25%, length 2.02 Å), ThrB293 (hydrogen bond, score: 13%, length 2.93 Å), TyrB132 (arene-cation)
AC12	6.46	8.08	A	-18.25	 AspA93 (hydrogen bond, score: 57%, length 1.85 Å)

			B	-16.18	 PheB169 (hydrogen bond, score: 41%, length 2 Å), (arene-cation), ThrB293 (hydrogen bond, score: 32%, length 2.9 Å)
AC13	5.52	7.20	A	-11.50	 ThrA293 (hydrogen bond, score: 41%, length 2.81 Å), PheA169 (hydrogen bond, score: 29%, length 2.02 Å)

			B	-14.09	 SerB96 (hydrogen bond, score: 16%, length 3.14 Å), PheB169 (hydrogen bond, score: 56%, length 1.86 Å), (arene-cation), GlnB134 (hydrogen bond, score: 17%, length: 2.99 Å)
Verubecestat	-	7.66	A		 AspA93 (hydrogen bond, score: 41%, length 2.91Å), AspA289 (hydrogen bonds, score: 50%; 11%, length 2.84 Å, 2.97 Å)

			B		 AspB93 (hydrogen bond, score: 54%, length 2.82 Å), AspB289 (hydrogen bonds, score: 49%; 11%, length 2.85 Å, 2.96 Å)
Quercetin	5.02	5.24	A	-22.23	 GlnA134 (hydrogen bonds, score: 22%, length: 2.68 Å; score: 11%, length 3.03 Å), GlyA291 (hydrogen bond, score: 23%, length: 1.9 Å)

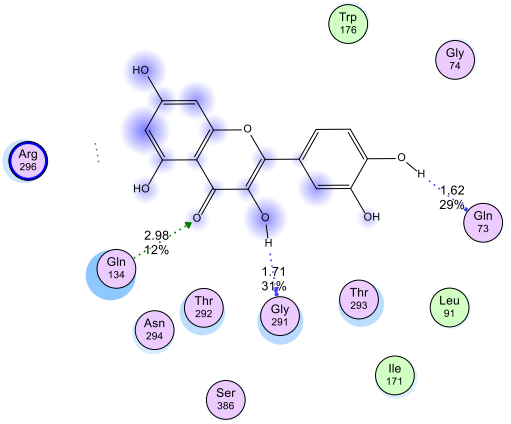
			B	-23.95	 GlnB134 (hydrogen bonds, score: 12%, length: 2.98 Å; score), GlyB291 (hydrogen bond, score: 31%, length: 1.71 Å), GlnB73 (hydrogen bond, score: 29%, length: 1.62 Å)

Table S4. Dataset of 72 compounds used in the building of 2D-QSAR model for AChE inhibitors

No.	Name	pIC50	predicted pIC50
1	CHEMBL3133246	5.45	5.21
2	CHEMBL2296124	4.33	4.26
3	CHEMBL237223	4.59	4.72
4	CHEMBL2334727	4.72	4.60
5	CHEMBL3617370	4.51	4.42
6	CHEMBL3617380	4.49	4.46
7	CHEMBL2334728	4.24	4.28
8	CHEMBL416526	4.94	4.73
9	CHEMBL2393074	4.75	4.90
10	CHEMBL2385772	4.48	4.73
11	CHEMBL253386	5.49	5.22
12	CHEMBL3617382	4.63	4.52
13	CHEMBL3125443	4.90	4.67
14	CHEMBL3617375	4.28	4.49
15	CHEMBL3127216	4.84	4.70
16	CHEMBL3617367	4.38	4.27
17	CHEMBL457684	4.78	4.48
18	CHEMBL340807	4.80	4.66
19	CHEMBL2334726	4.49	4.55
20	CHEMBL659	5.62	5.42
21	CHEMBL2334730	4.64	4.78
22	CHEMBL3133247	4.81	5.07
23	CHEMBL517342	4.19	4.38
24	CHEMBL2296125	4.46	4.37
25	CHEMBL3617393	4.47	4.24
26	CHEMBL3617388	4.45	4.47
27	CHEMBL2385773	4.83	4.61
28	CHEMBL2385777	4.34	4.58
29	CHEMBL3127219	4.92	4.75
30	CHEMBL3127043	4.98	4.97
31	CHEMBL1269160	4.57	4.42
32	CHEMBL2334725	4.70	4.76
33	CHEMBL1270150	4.73	4.81
34	CHEMBL500712	4.40	4.21
35	CHEMBL2334736	4.72	4.83
36	CHEMBL2018160	4.63	4.48
37	CHEMBL2334737	4.71	4.61
38	CHEMBL269538	4.19	4.49
39	CHEMBL3617397	4.52	4.32
40	CHEMBL2334745	4.49	4.70
41	CHEMBL2296112	4.25	4.44

42	CHEMBL3617381	4.49	4.53
43	CHEMBL3133250	4.29	4.63
44	CHEMBL12014	4.23	4.50
45	CHEMBL3617372	4.26	4.44
46	CHEMBL3133243	4.97	5.10
47	CHEMBL510090	4.72	4.82
48	CHEMBL2385771	4.30	4.56
49	CHEMBL2296117	4.18	4.13
50	CHEMBL3127217	4.99	4.86
51	CHEMBL2334738	4.69	4.66
52	CHEMBL2296113	4.21	4.40
53	CHEMBL2381433	4.58	4.53
54	CHEMBL3132866	4.98	5.01
55	CHEMBL2385768	4.75	4.66
56	CHEMBL2385780	4.88	4.68
57	CHEMBL2334739	4.52	4.35
58	CHEMBL3133245	5.36	5.17
59	CHEMBL1270255	5.01	5.24
60	CHEMBL3133248	4.66	4.90
61	CHEMBL3617362	4.22	4.42
62	CHEMBL2381434	4.67	4.49
63	CHEMBL1535235	4.61	4.53
64	CHEMBL129177	4.47	4.70
65	CHEMBL2385784	4.53	4.76
66	CHEMBL2385779	4.42	4.23
67	CHEMBL3617396	4.39	4.26
68	CHEMBL1085869	5.67	5.51
69	CHEMBL2334747	4.51	4.56
70	CHEMBL2385766	4.35	4.57
71	CHEMBL463856	4.33	4.26
72	CHEMBL2334732	4.86	4.81

Table S5. Dataset of 215 compounds used in the building of 2D-QSAR model for BACE-1 inhibitors

No.	Name	pIC50	Predicted pIC50
1	BMC-2009-3671-17	6.92	7.02
2	BMC-2004-247-8	6.46	6.57
3	BMC-2007-1023-8	8.30	7.97
4	JMC-2012-27-30	5.49	5.65
5	BMC-2004-248-21	7.17	6.96
6	BMC-2009-3675-11	7.96	8.19
7	BMC-2009-3671-20	6.82	7.33
8	BMC-2009-3677-26	7.49	7.93
9	BMC-2008-1019-14	6.26	6.86
10	BMC-2014-2038-39	7.74	7.51
11	BMC-2013-4677-30	6.83	6.54
12	BMC-2004-248-19	7.37	6.74
13	BMC-2013-4677-37	5.88	6.33
14	BMC-2013-4241-10	6.46	6.45
15	BMC-2014-2036-24	7.49	8.02
16	BMC-2013-4675-7	7.35	6.70
17	BMC-2009-3667-16	7.72	7.63
18	BMC-2014-2039-43	7.28	7.39
19	EODD-2013-723-102	6.62	6.99
20	JMC-2012-26-15	5.00	5.15
21	JMC-2012-27-37	5.70	5.84
22	EODD-2013-718-42c	8.00	8.56
23	JMC-2012-9013-24	7.11	7.90
24	BMC-2014-2041-65	6.24	6.08
25	BMC-2008-1021-30	6.48	7.12
26	BMC-2009-3672-21	8.10	7.85
27	JMC-2012-9013-26	7.58	7.52
28	EODD-2013-720-53	6.82	7.20
29	BMC-2008-1021-31	6.64	6.66
30	BMC-2008-1021-28	7.08	6.58
31	JMC-2012-27-41	6.20	6.58
32	BMC-2009-3675-7	8.40	8.17
33	BMC-2009-3673-39	7.70	7.35
34	BMC-2014-2042-71	6.62	6.31
35	EODD-2013-713-11	7.55	7.25
36	BMC-2009-3672-27	7.04	7.46
37	BMC-2014-2042-90	8.07	7.85
38	EODD-2013-719-48	8.48	8.21
39	JMC-2012-27-47	6.49	6.45
40	BMC_2014-2042-81	7.60	8.12
41	BMC-2009-3665-4	8.04	7.43
42	BMC-2009-3673-36	7.64	7.69

43	BMC-2013-4676-17	6.93	7.33
44	BMC-2014-2038-41	7.70	7.60
45	BMC-2013-4677-38	6.07	6.44
46	BMC-2009-3667-20	7.47	7.71
47	EODD-2013-720-58	7.70	7.39
48	JMC-2012-26-24b	6.20	5.74
49	BMC-2014-2036-23	7.70	7.56
50	BMC-2013-4677-53	7.05	7.14
51	BMC-2007-1023-2	6.60	7.23
52	BMC-2009-3667-17	7.64	7.27
53	BMC-2008-1020-23	6.22	6.37
54	BMC-2014-2041-66	6.15	6.14
55	BMC-2013-4241-4	5.99	6.39
56	BMC-2009-3673-34	7.85	7.19
57	BMC-2014-2036-17	7.32	7.35
58	BMC-2008-1020-18	6.12	5.95
59	BMC-2014-2038-37	4.66	5.00
60	BMC-2009-3672-24	8.30	7.96
61	BMC-2007-1024-18	7.40	7.93
62	BMC-2008-1020-24	6.80	6.66
63	JMC-2012-28-64	6.10	6.08
64	BMC-2014-2035-13	8.00	7.51
65	BMC-2014-2040-53	8.15	8.02
66	BMC-2009-3667-18a	7.58	7.41
67	BMC-2009-3666-10	7.64	8.03
68	JMC-2012-9010-17	8.10	7.96
69	BMC-2014-2036-20	7.11	7.79
70	EODD-2013-721-64	6.33	6.65
71	BMC-2013-4677-35	6.38	6.60
72	BMC-2009-3671-12	7.04	7.62
73	EODD-2013-718-44	8.70	8.08
74	EODD-2013-721-65	7.20	6.65
75	BMC-2013-4242-23	7.34	7.00
76	BMC-2013-4241-9	7.92	7.22
77	BMC-2014-2040-62	7.69	7.61
78	BMC-2007-1023-5	7.30	7.87
79	BMC-2004-247-9	6.26	6.30
80	EODD-2013-718-42b	8.04	8.33
81	BMC-2009-3676-18	8.10	7.76
82	BMC-2007-1023-6	8.22	8.01
83	BMC-2009-3668-25	8.22	7.78
84	EODD-2013-718-45	7.68	7.34
85	BMC-2004-246-4	6.72	6.46
86	BMC-2013-4241-14	7.51	7.15
87	BMC-2009-3667-19	7.55	7.59

88	BMC-2007-1025-22	8.22	7.68
89	EODD-2013-716-31	8.70	8.27
90	BMC-2014-2042-85	6.53	7.06
91	BMC-2007-1023-11	8.30	8.05
92	BMC-2009-3671-16	7.58	8.09
93	BMC-2014-2039-42	7.08	7.22
94	BMC-2009-3666-11	7.74	8.32
95	BMC-2014-2038-40	7.70	7.27
96	BMC-2004-248-13	6.68	7.04
97	BMC-2014-2039-47	7.57	7.82
98	BMC-2009-3672-25	7.22	7.43
99	BMC-2009-3677-23	7.30	7.25
100	BMC-2009-3666-7	7.20	7.33
101	JMC-2012-28-83	5.10	5.52
102	BMC-2014-2035-14	7.70	8.20
103	BMC-2007-1023-10	8.30	8.19
104	BMC-2014-2035-15	8.00	8.16
105	BMC-2014-2036-22	7.04	6.54
106	EODD-2013-718-42a	7.89	8.20
107	BMC-2014-2042-72	7.58	7.34
108	BMC-2013-4242-24	6.43	6.98
109	BMC-2009-3672-26	8.04	7.58
110	BMC-2009-3676-21	6.60	6.71
111	BMC-2009-3677-24	7.40	7.21
112	BMC-2013-4242-20	6.92	6.62
113	BMC-2009-3675-9	8.00	7.47
114	BMC-2013-4241-5	6.26	6.22
115	JMC-2012-26-19b	5.20	5.44
116	BMC-2014-2042-87	7.31	7.24
117	BMC-2014-2042-84	6.49	7.03
118	BMC-2013-4676-19	7.38	7.76
119	BMC-2013-4241-3	5.05	5.61
120	BMC-2009-3668-27	7.40	7.26
121	BMC-2009-3677-25	7.70	7.26
122	BMC-2009-3675-10	7.66	7.50
123	BMC-2007-1025-21	8.40	7.77
124	BMC-2007-1024-17	8.30	8.17
125	BMC-2004-246-5	6.89	6.25
126	BMC-2009-3676-19	7.06	7.16
127	BMC-2013-4675-4	6.24	6.39
128	BMC-2014-2041-64	6.92	6.23
129	BMC-2004-246-6	5.95	6.41
130	BMC-2013-4242-22	7.64	7.14
131	BMC-2007-1024-15	7.92	7.44
132	BMC-2013-4241-12	6.86	6.99

133	BMC-2009-3673-35	8.30	7.86
134	BMC-2008-1019-13	6.52	6.58
135	BMC-2013-4241-16	6.12	6.63
136	BMC-2014-2042-73	7.52	7.45
137	JMC-2012-27-34	5.70	5.91
138	BMC-2013-4677-36	6.65	6.43
139	BMC-2004-248-20	6.75	6.64
140	BMC-2009-3672-23	7.64	7.81
141	JMC-2012-9010-18	7.64	7.67
142	BMC-2009-3675-13	7.64	7.55
143	JMC-2012-28-65	6.30	6.03
144	BMC-2013-4241-15	7.35	7.51
145	BMC-2004-246-7	5.76	6.23
146	BMC-2013-4677-48	8.04	7.86
147	BMC-2013-4241-13	7.41	7.34
148	BMC-2013-4675-6	6.42	6.42
149	BMC-2009-3671-9	8.70	8.29
150	BMC-2009-3671-11	7.72	8.26
151	BMC-2008-1019-12	7.48	6.96
152	BMC-2008-1021-27	7.70	7.30
153	BMC-2014-2039-46	7.27	7.16
154	BMC-2014-2035-9	7.10	6.33
155	JMC-2012-9010-15	7.74	7.98
156	BMC-2007-1024-13	7.47	7.41
157	BMC-2014-2042-79	7.40	7.59
158	EODD-2013-716-32	8.40	8.23
159	BMC-2008-1021-29	7.00	7.42
160	JMC-2012-9013-25	7.48	7.95
161	BMC-2004-246-3	7.09	7.26
162	BMC-2014-2042-80	7.47	7.90
163	BMC-2004-247-10	6.46	6.20
164	JMC-2012-9013-23	7.54	8.48
165	BMC-2008-1020-26	7.85	7.24
166	BMC-2009-3667-18b	7.40	7.51
167	EODD-2013-713-12a	8.41	8.84
168	BMC-2009-3677-27	7.10	7.58
169	BMC-2004-248-14	6.68	6.49
170	BMC-2007-1024-12	6.92	6.75
171	EODD-2013-718-41	7.30	7.95
172	BMC-2009-3675-14	7.32	7.60
173	BMC-2008-1019-8	5.61	6.20
174	BMC-2008-1020-22	5.77	6.13
175	BMC-2008-1019-6	6.74	6.26
176	BMC-2009-3671-15	8.15	8.22
177	BMC-2013-4242-19	7.21	6.91

178	BMC-2014-2042-82	7.55	7.36
179	EODD-2013-721-61	6.96	7.39
180	BMC-2008-1020-16	7.40	7.28
181	BMC-2014-2042-76	8.70	8.94
182	BMC-2009-3675-5	8.30	7.93
183	BMC-2009-3675-16	7.70	7.51
184	BMC-2007-1023-9	7.96	8.00
185	BMC-2014-2042-78	7.70	7.43
186	BMC-2008-1019-7	5.95	6.35
187	BMC-2013-4675-3	6.27	6.20
188	JMC-2012-26-8b	4.60	4.57
189	EODD-2013-713-10	7.06	7.07
190	JMC-2012-26-19a	5.00	5.44
191	BMC-2014-2035-12	5.47	5.08
192	BMC-2013-4676-18	6.90	7.35
193	JMC-2012-9013-19	8.27	8.63
194	BMC-2004-248-17	7.22	6.58
195	BMC-2014-2040-54	8.22	8.06
196	BMC-2009-3671-13	7.82	7.98
197	JMC-2012-26-24a	6.00	6.04
198	BMC-2008-1020-19	7.77	7.61
199	EODD-2013-719-50	7.77	8.60
200	JMC-2012-27-54a	5.40	5.90
201	EODD-2013-717-39a	9.40	9.53
202	BMC-2007-1024-14	7.74	8.09
203	BMC-2013-4677-31	6.73	6.68
204	BMC-2009-3672-22	8.70	8.02
205	BMC-2009-3667-23	6.38	6.32
206	BMC-2013-4675-5	7.03	6.31
207	BMC-2013-4677-32	7.22	7.24
208	BMC-2014-2042-88	7.44	7.03
209	BMC-2007-1023-7	8.52	7.97
210	JMC-2012-26-8a	4.79	4.94
211	JMC-2012-9013-22	7.69	8.31
212	BMC-2013-4241-18	7.02	6.58
213	BMC-2014-2042-75	8.00	8.54
214	JMC-2012-9010-16	7.45	8.05
215	BMC-2007-1024-16	8.10	7.53

Table S6. Equations for calculation of 2D-QSAR validation metrics

These metrics were calculated according to the equations (Eq.) (1-10).

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n_{TR}}(\hat{y}_i - y_i)^2}{n}} \quad (1)$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n_{TR}}(\hat{y}_i - y_i)^2}{\sum_{i=1}^{n_{TR}}(y_i - \bar{y}_i)^2} \quad (2)$$

$$\text{RMSE}_{\text{LOO}} = \sqrt{\frac{\sum_{i=1}^{n_{TR}}(\hat{y}'_i - y_i)^2}{n}} \quad (3)$$

$$R^2_{\text{LOO}} = 1 - \frac{\sum_{i=1}^{n_{TR}}(\hat{y}'_i - y_i)^2}{\sum_{i=1}^{n_{TR}}(y_i - \bar{y}_i)^2} \quad (4)$$

$$R^2_{\text{PRED}} = 1 - \frac{\sum_{I=1}^{n_{VAL}}(y_{pred(validation)} - y_{validation})^2}{\sum_{I=1}^{n_{VAL}}(y_{validation} - \bar{y}_{training})^2} \quad (5)$$

$$r_m^2 = r^2(1 - \sqrt{r^2 - r_0^2} \quad (6)$$

$$r'^2_m = r'^2\,(1 - \sqrt{r'^2 - r'^2_0}) \quad (7)$$

$$\overline{r_m^2} = \frac{r_m^2 + r'^2_m}{2} \quad (8)$$

$$\Delta r_m^2 = |r_m^2 - r'^2_m| \quad (9)$$

$$CCC = \frac{2\sum_{i=1}^{n_{VAL}}(y_i - \overline{y})(\hat{y}_i - \overline{\hat{y}})}{\sum_{i=1}^{n_{VAL}}(y_i - \overline{y})^2 + \sum_{i=1}^{n_{VAL}}(\hat{y}_i - \overline{\hat{y}})^2 + n_{VAL}(\overline{y} - \overline{\hat{y}})^2} \quad (10)$$

In Eq. (1), (2), and (10), y_i and $\hat{y}_i$ are, respectively, the observed and predicted activity values, while $\overline{y}$ and $\overline{\hat{y}}$ are, respectively, the mean values of y_i and $\hat{y}_i$. In Eq.(3) and (4), y_i and $\hat{y}'_i$ are, respectively, the observed and predicted activity values in LOO cross-validation. Eq. (6) and (7) were utilized to calculate correlation coefficients between observed and predicted activity values of the compounds of training set with (r^2) or without intercept (r_0^2) in case of using predicted data on the y-axis and experimental data on the x-axis, while (r'^2) and (r'^2_0) are, respectively, the same coefficients in the opposite case. The most stringent validation criteria thresholds including $r^2_m \geq 0.65$; $CCC \geq 0.85$; $\overline{r^2_m} \geq 0.5$; and $\Delta r^2_m \leq 0.2$ were applied to verify the external predictivity of good models [1,2]

Table S7. Selected descriptors used for building 2D-QSAR models

Code	Category	Description
BCUT_SlogP_3	Adjacency and distance matrix	A Burden's parameter using atomic contribution to logP (using the Wildman and Crippen SlogP method [3]) instead of partial charge.
BCUT_PEOE_1	Adjacency and distance matrix	A descriptor relating topological shape and partial charges
petitjean	Adjacency and distance matrix	Value of (diameter - radius) / diameter.
reactive	Physical property	An indicator of the presence of reactive groups. A non-zero value indicates that the molecule contains a reactive group. The table of reactive groups is based on the Oprea set [4] and includes metals, phospho-, N/O/S-N/O/S single bonds, thiols, acyl halides, Michael Acceptors, azides, esters, etc.
logS	Physical property	The log of the aqueous solubility (mol/L).
PEOE_VSA-0, PEOE_VSA+1, PEOE_VSA-3, PEOE_VSA-6	Partial charge	Sum of the proximate accessible *van der Waals* surface area ($Å^2$), v_i, calculation for each atom over all the atoms *i*, such that partial charge of atom *i* is in a specified range.
SlogP_VSA2, SlogP_VSA3, SlogP_VSA5	Subdivided surface areas	Sum of the proximate accessible *van der Waals* surface area ($Å^2$), v_i, calculated for each atom over all the atoms, such that partition coefficient for atom *i* is in a specified range
SMR_VSA2	Subdivided surface areas	Sum of the proximate accessible *van der Waals* surface area ($Å^2$), v_i, calculation for each atom over all the atoms *i*, such that molar refractivity for atom *i* is in a specified range.
a_ICM	Atom counts and bond counts	The entropy of the element distribution in the molecule (including implicit hydrogens but not lone pair pseudo-atoms)
chiral_u	Atom counts and bond counts	The number of unconstrained chiral centers.
rings	Atom counts and bond counts	The number of rings
a_Nn	Atom counts and bond counts	The number of nitrogen atoms.

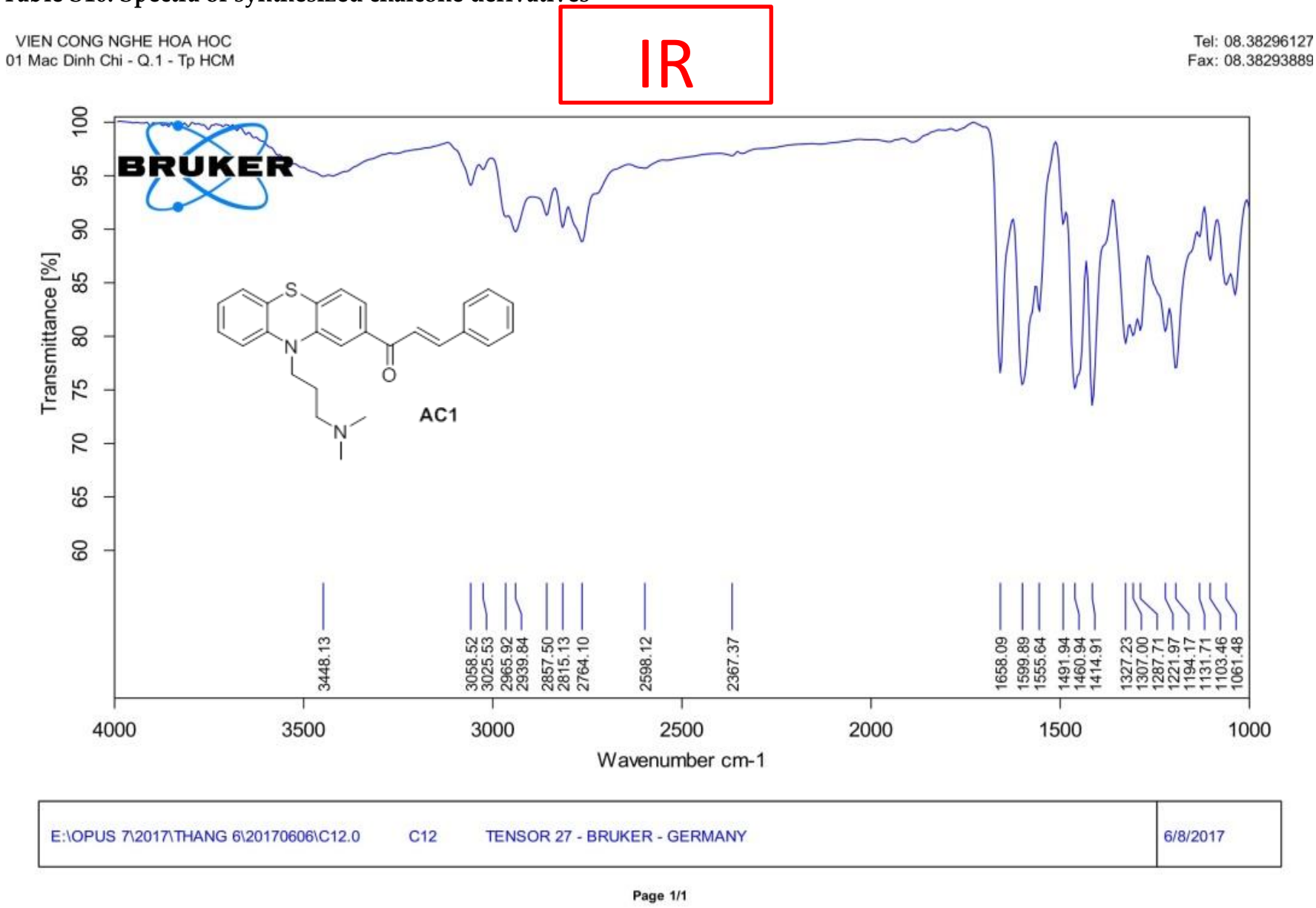
Table S8. Values of selected descriptors used in prediction of pIC_{50} of the synthesized chalcone derivatives (AChE)

Compound	BCUT_SLOGP_3	reactive	PEOE_VSA+1	PEOE_VSA-3	SlogP_VSA2	SMR_VSA2	**Predicted pIC_{50}**
AC1	2.61	1	59.72	0.00	0.00	6.23	**4.80**
AC2	2.61	1	76.70	0.00	0.00	6.23	**4.74**
AC3	2.61	1	76.70	0.00	0.00	6.23	**4.74**
AC4	2.61	1	85.31	0.00	0.00	6.23	**4.71**
AC5	2.61	1	55.45	0.00	0.00	6.23	**4.82**
AC6	2.61	1	51.18	0.00	0.00	6.23	**4.83**
AC7	2.61	1	55.70	0.00	9.12	15.35	**4.76**
AC8	2.61	1	55.45	0.00	0.00	6.23	**4.82**
AC9	2.61	1	55.45	0.00	9.12	15.35	**4.76**
AC10	2.61	1	55.45	0.00	0.00	9.28	**4.81**
AC11	2.61	1	57.66	35.73	0.00	13.99	**4.59**
AC12	2.61	1	55.45	0.00	0.00	9.35	**4.81**
AC13	2.61	1	108.72	0.00	0.00	6.23	**4.63**
Galantamine	2.77	0	114.49	0.00	12.94	0.00	**5.14**

Table S9. Values of selected descriptors used in prediction of pIC_{50} of the synthesized chalcone derivatives (BACE-1)

Compound	petitjean	BCUT_PEOE_1	a_ICM	chiral_u	rings	a_nN	PEOE_VSA-0	PEOE_VSA-6	logS	SlogP_VSA3	SlogP_VSA5	**Predicted pIC_{50}**
AC1	0.47	-0.63	1.41	0	4	2	144.11	0.00	-6.42	36.88	68.90	**6.52**
AC2	0.50	-0.61	1.46	0	4	2	168.62	2.50	-6.47	36.88	104.28	**7.38**
AC3	0.47	-0.61	1.46	0	4	2	168.62	2.50	-6.47	36.88	104.28	**7.37**
AC4	0.47	-0.59	1.52	0	4	2	168.62	7.51	-6.57	36.88	175.05	**8.49**
AC5	0.50	-0.63	1.52	0	4	2	168.62	0.00	-7.15	36.88	68.90	**7.25**
AC6	0.50	-0.64	1.59	0	4	2	180.87	0.00	-7.89	36.88	68.90	**7.68**
AC7	0.47	-0.64	1.62	0	4	2	178.67	0.00	-7.45	36.88	68.90	**7.63**
AC8	0.47	-0.64	1.52	0	4	2	168.62	0.00	-7.15	36.88	68.90	**7.15**
AC9	0.50	-0.63	1.52	0	4	2	168.62	0.00	-6.71	36.88	68.90	**7.12**
AC10	0.47	-0.63	1.52	0	4	2	168.62	0.00	-7.51	36.88	71.95	**7.28**
AC11	0.47	-0.56	1.62	0	4	2	156.36	0.00	-7.48	36.88	68.90	**7.99**
AC12	0.47	-0.58	1.42	0	4	3	215.10	0.00	-6.35	36.88	134.69	**8.08**
AC13	0.48	-0.64	1.41	0	5	2	170.83	2.50	-8.24	36.88	68.90	**7.20**
Verubecestat	0.50	-0.58	2.00	1	3	5	112.04	12.47	-3.62	17.23	49.68	**7.66**
Quercetin	0.50	-0.63	-1.52	0	3	0	61.27	41.34	-2.77	25.39	5.24	**5.24**

Table S10. Spectra of synthesized chalcone derivatives



MS

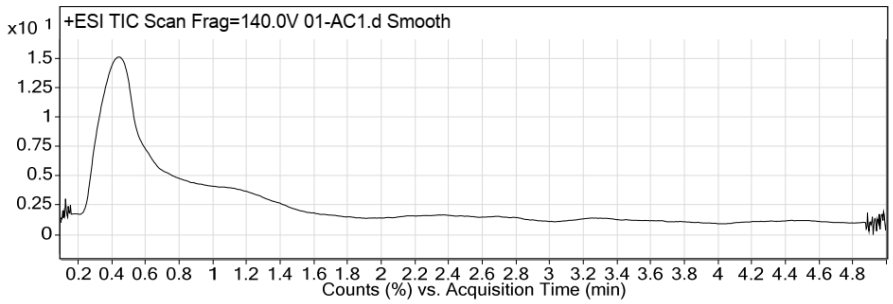
Qualitative Analysis Report

Data Filename	01-AC1.d	**Sample Name**	01-AC1
Sample Type	Sample	**Position**	P2-A9
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	22/08/2020 10:06:30 AM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

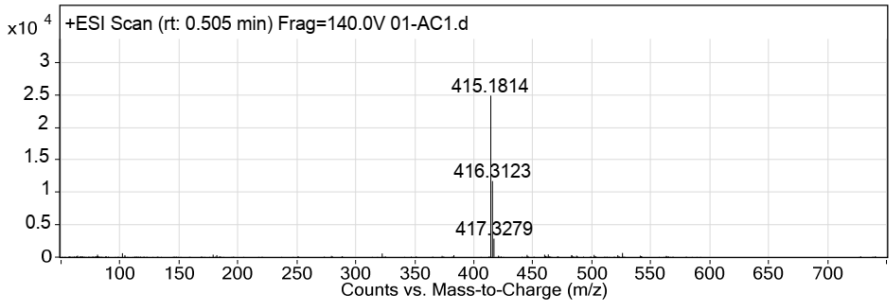
User Chromatograms

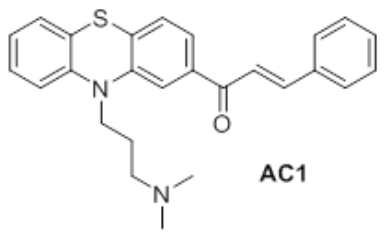
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



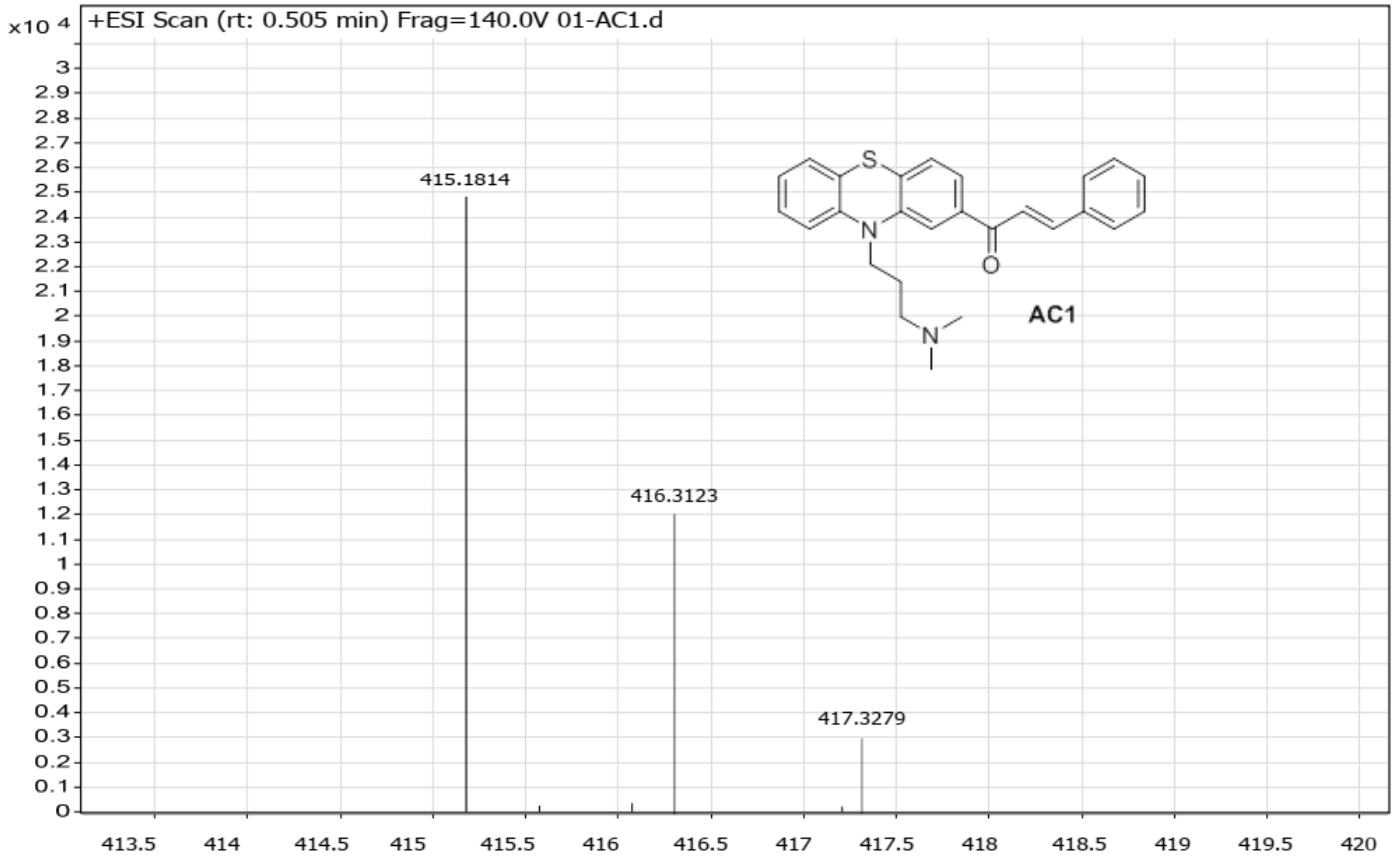


AC1

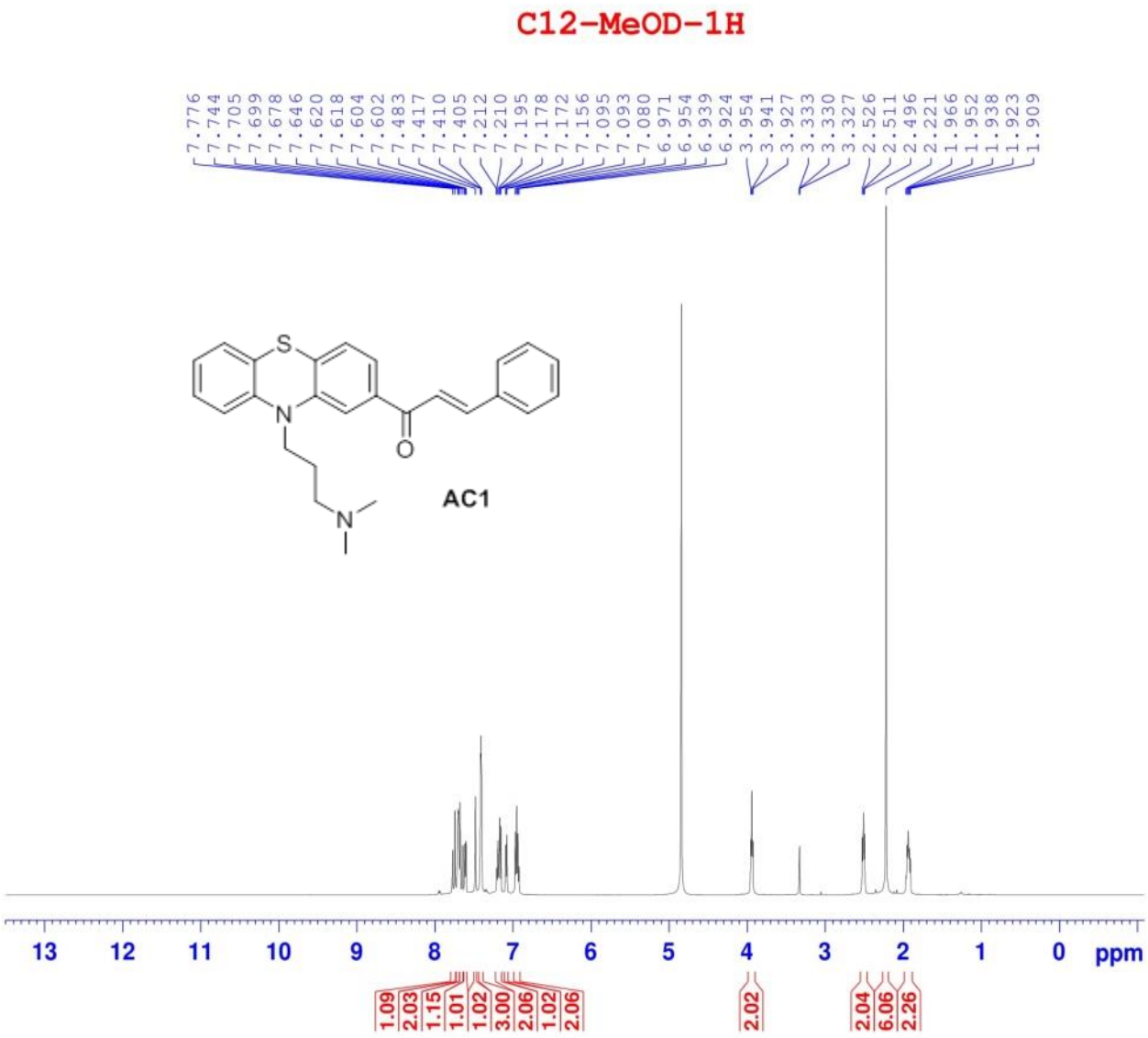
--- End Of Report ---

MS

Sample Name	01-AC1	**Position**	P2-A9	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	01-AC1.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	22/08/2020 10:06:30 AM



^{1}H-NMR



BRUKER

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PROCNO                 1

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PULPROG             zg30
TD                 65536
SOLVENT             MeOD
NS                    16
DS                     2
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FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG                 50.73
DW               50.000 usec
DE                6.50 usec
TE                303.0 K
D1           1.00000000 sec
TD0                    1

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NUC1                   1H
P1                10.00 usec
PLW1         22.00000000 W

F2 - Processing parameters
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WDW                   EM
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GB        0
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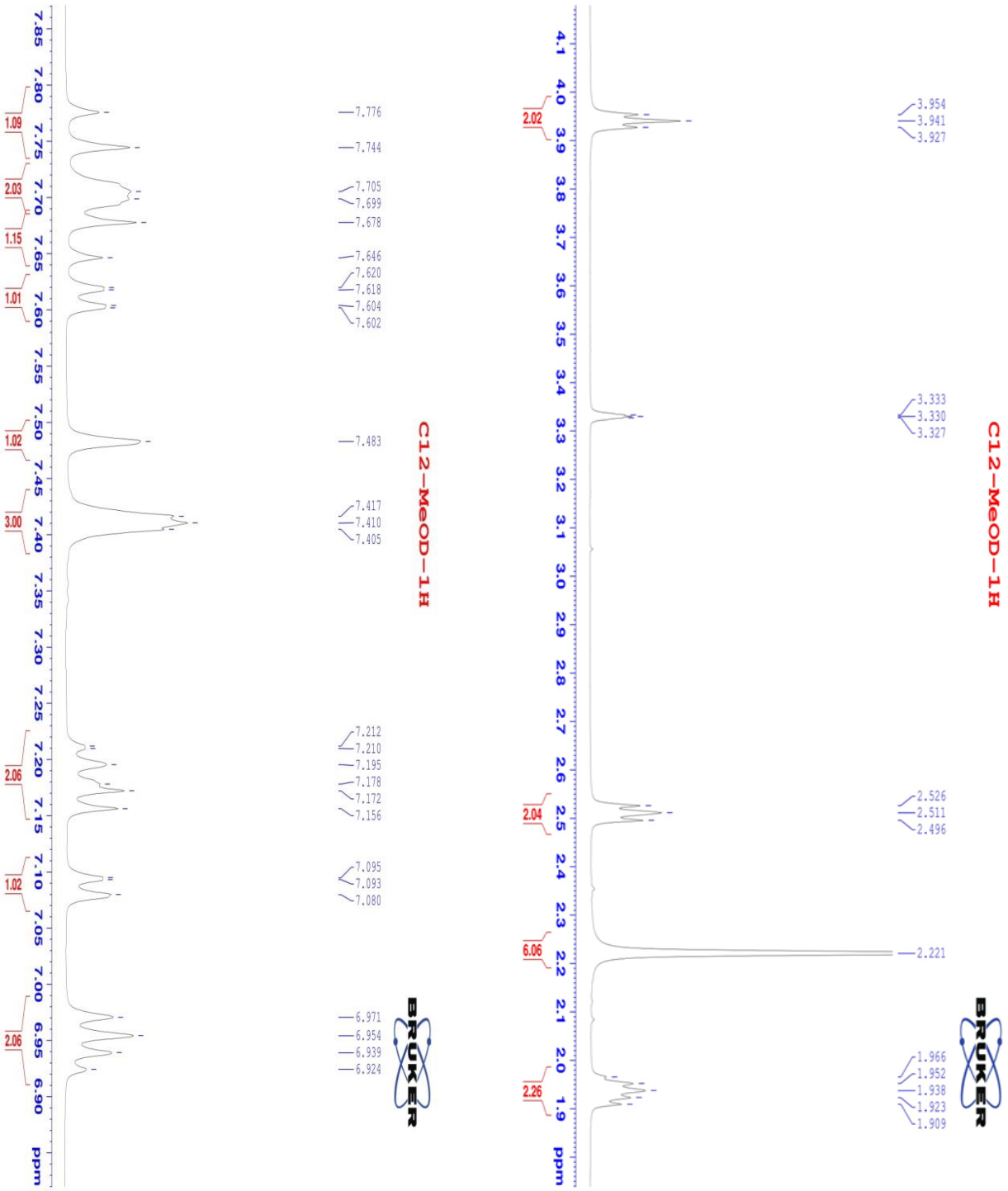
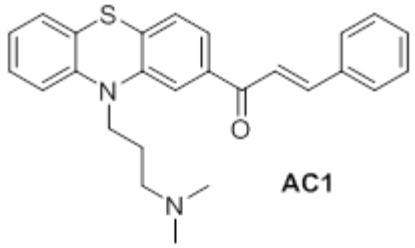
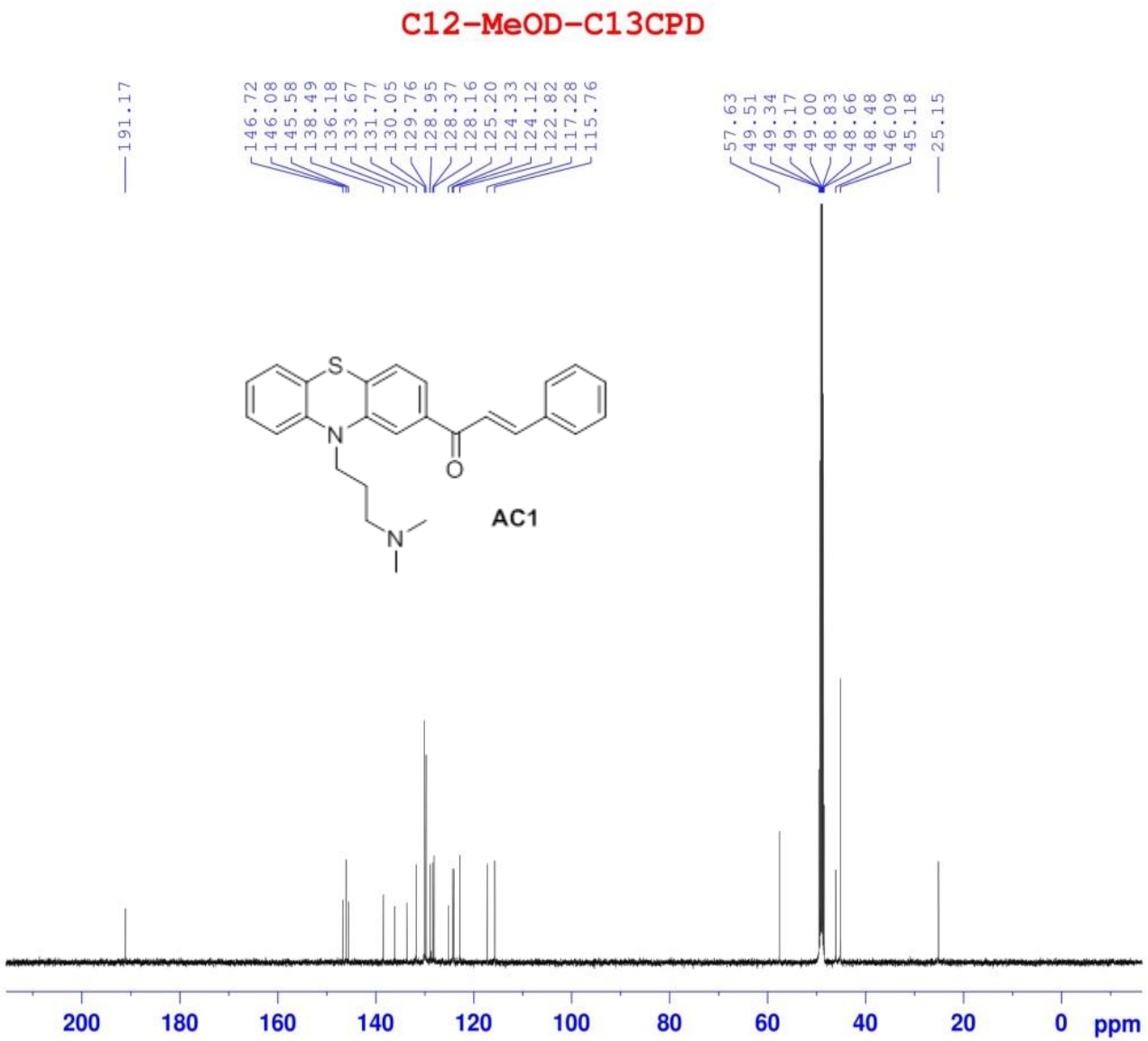
^{1}H-NMR





AC1

^{13}C-NMR



BRUKER

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EXPNO                  2
PROCNO                 1

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PULPROG          zgpg30
TD                65536
SOLVENT            MeOD
NS                  128
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG               198.57
DW               16.800 usec
DE                6.50 usec
TE               303.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
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NUC1               13C
P1               10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2        500.2020008 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2         22.00000000 W
PLW12         0.34375000 W
PLW13         0.22000000 W

F2 - Processing parameters
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SSB       0
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GB        0
PC               1.40
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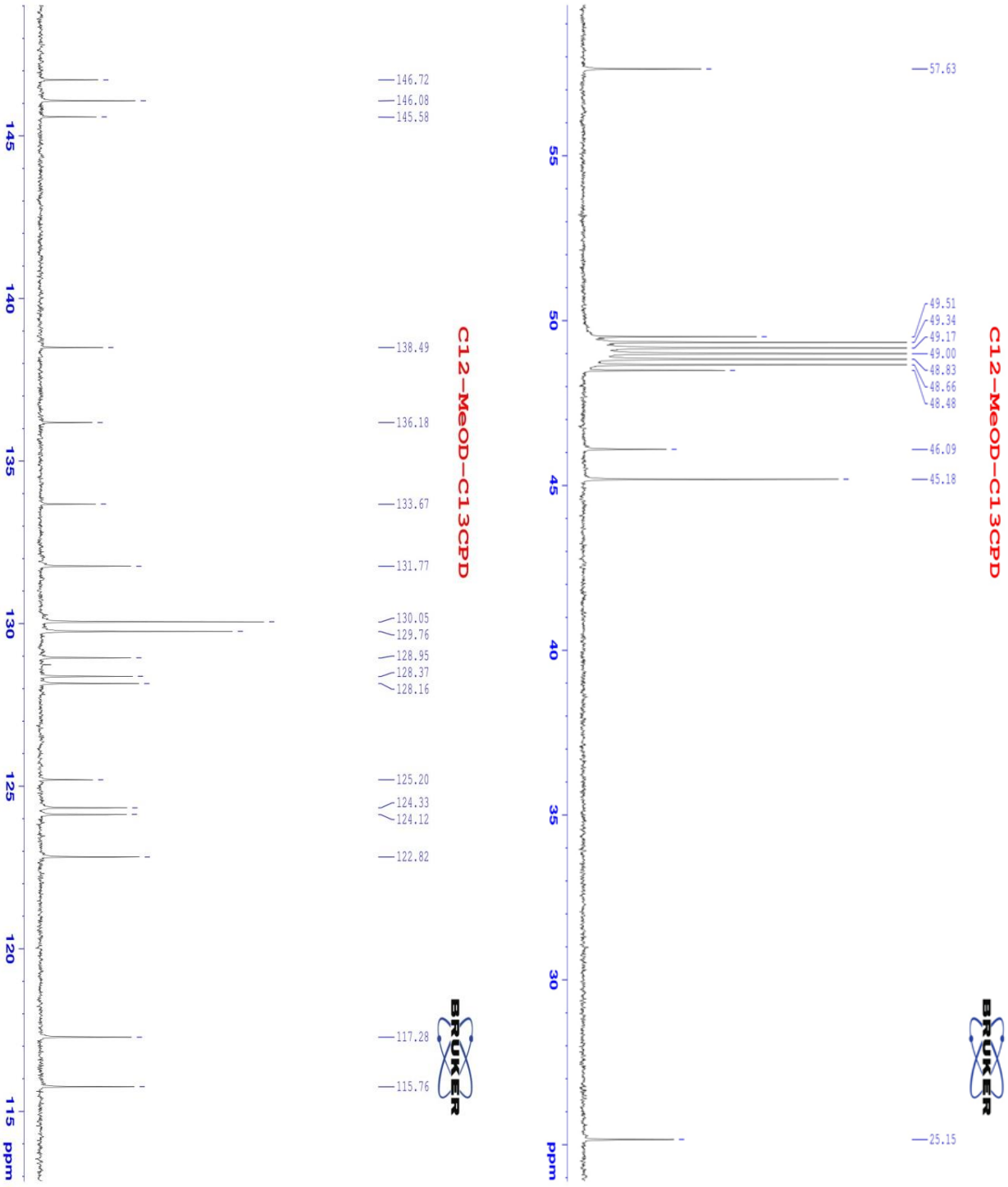
^{13}C-NMR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136.18
133.67
131.77
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128.95
128.37
128.16
125.20
124.33
124.12
122.82
117.28
115.76
C12-MeOD-C13CPD
BRUKER
57.63
49.51
49.34
49.17
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46.09
45.18
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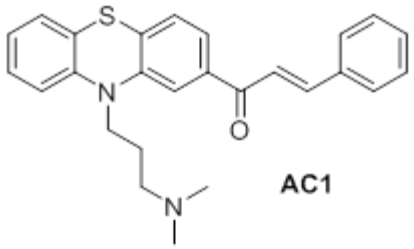
C12-MeOD-C13CPD
BRUKER
ppm
ppm

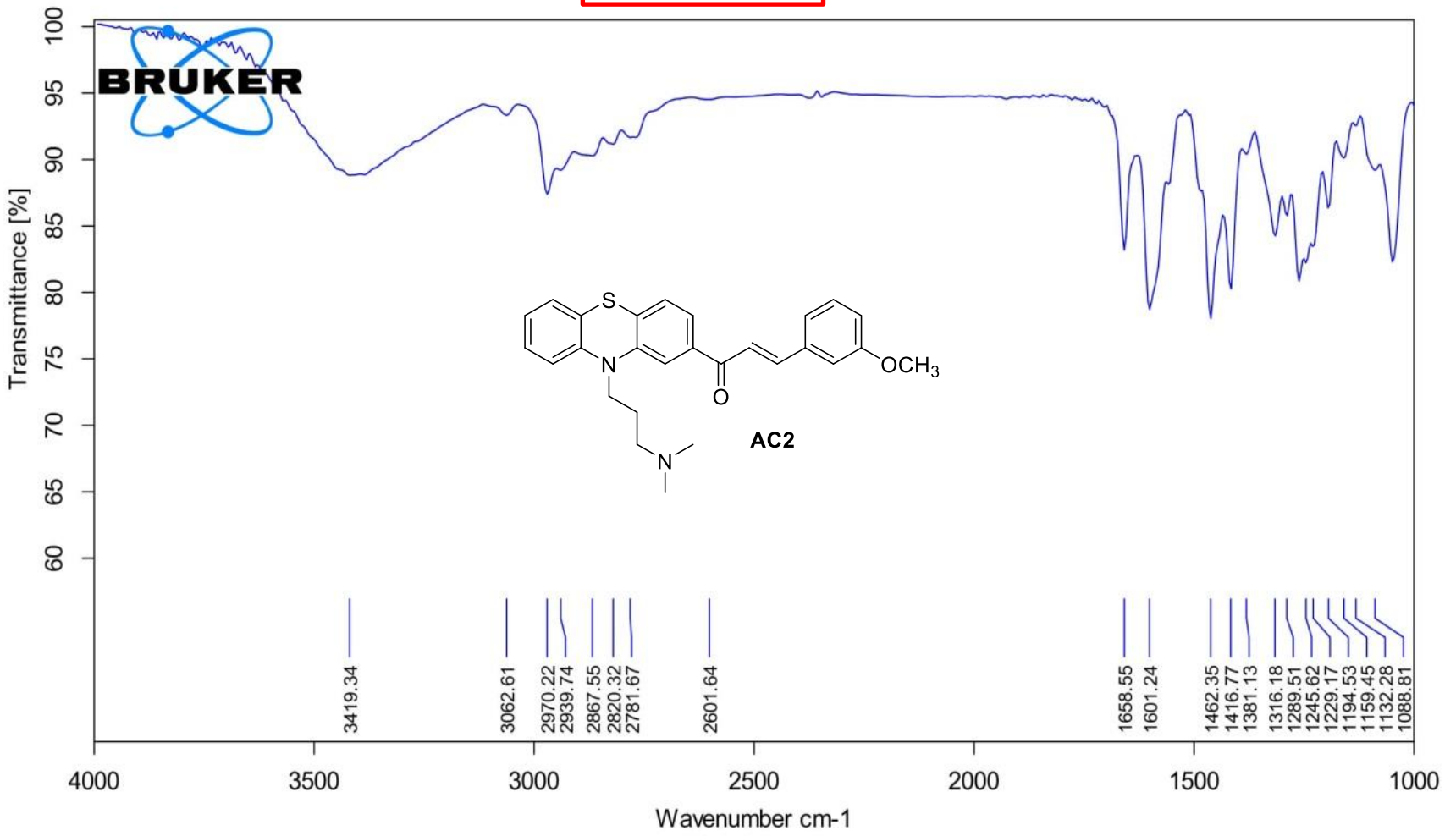

S
N
O
N

AC1

VIEN CONG NGHE HOA HOC
01 Mac Dinh Chi - Q.1 - Tp HCM

Tel: 08.38296127
Fax: 08.38293889

IR



E:\OPUS 7\2017\THANG 6\20170606\C3.0	C3	TENSOR 27 - BRUKER - GERMANY	6/6/2017

MS

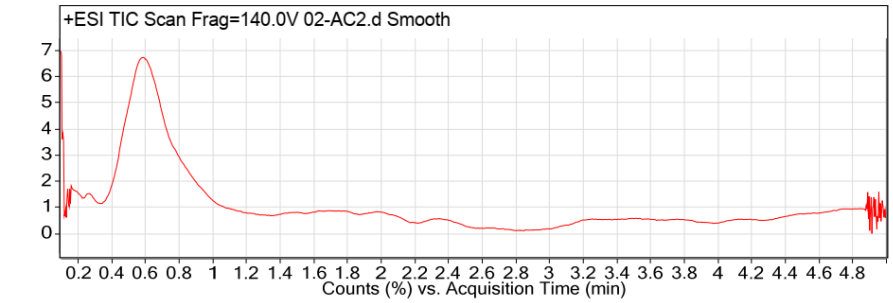
Qualitative Analysis Report

Data Filename	02-AC2.d	**Sample Name**	02-AC2
Sample Type	Sample	**Position**	P2-C6
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	22/08/2020 10:13:59 AM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Chromatograms

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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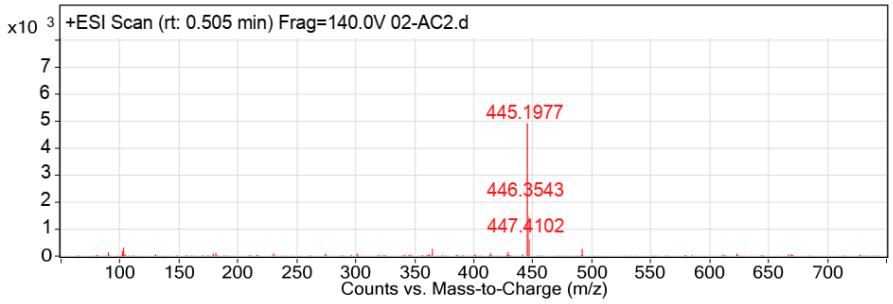

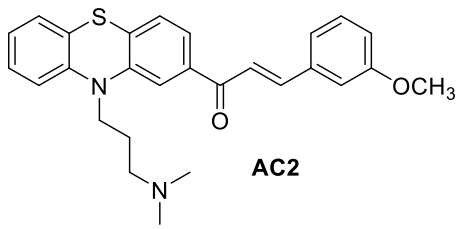

AC2

--- End Of Report ---

MS

Sample Name	02-AC2	**Position**	P2-C6	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
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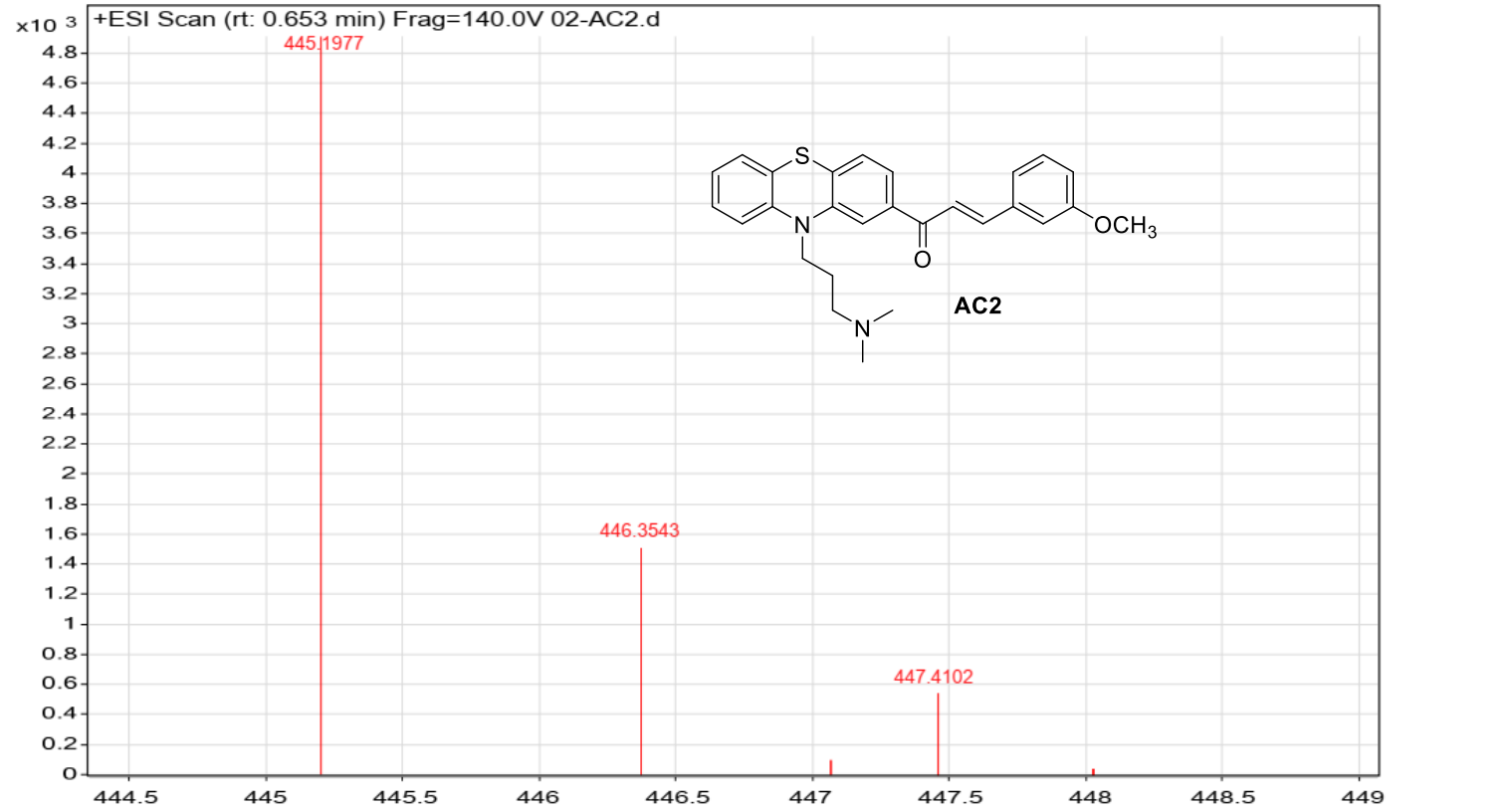
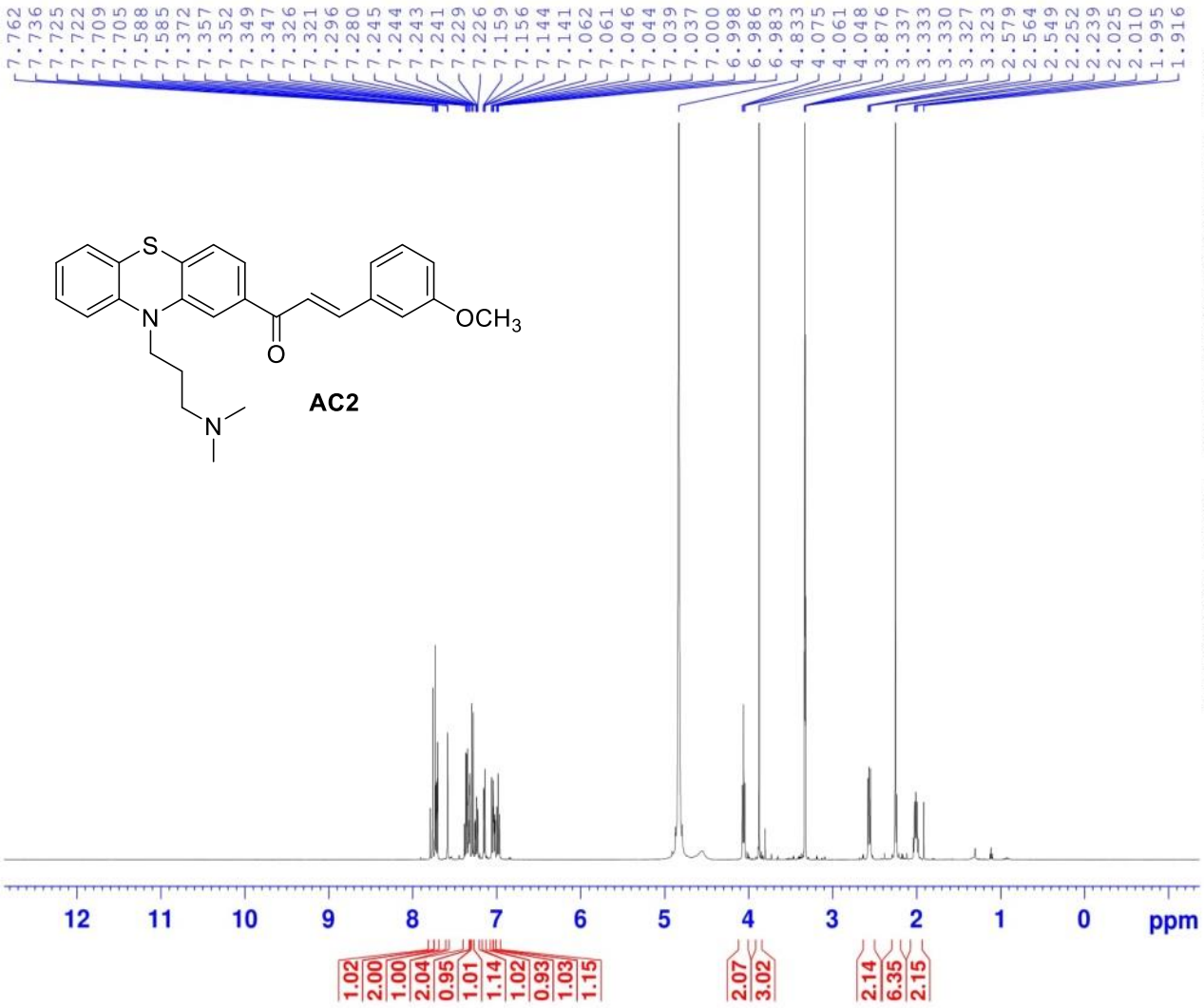


^{1}H-NMR

C3-MeOD-1H

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PROCNO                      1

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PULPROG                zg30
TD                    65536
SOLVENT                MeOD
NS                       16
DS                        2
SWH               10000.000 Hz
FIDRES                0.152588 Hz
AQ                    3.2767999 sec
RG                      127.68
DW                    50.000 usec
DE                     6.50 usec
TE                    303.0 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
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NUC1                       1H
P1                      10.00 usec
PLW1              22.00000000 W

F2 - Processing parameters
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WDW                        EM
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LB                      0.30 Hz
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PC                      1.00
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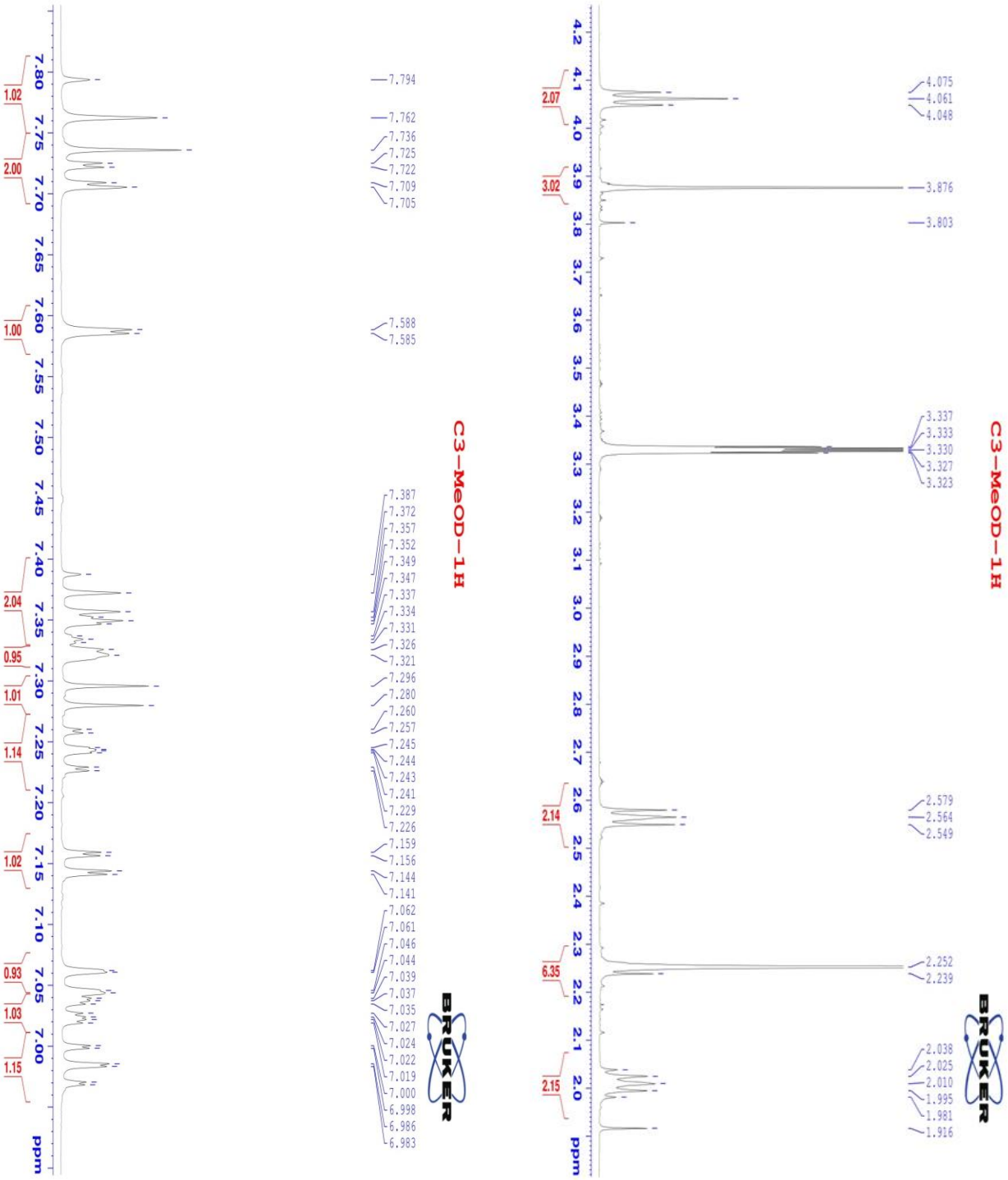
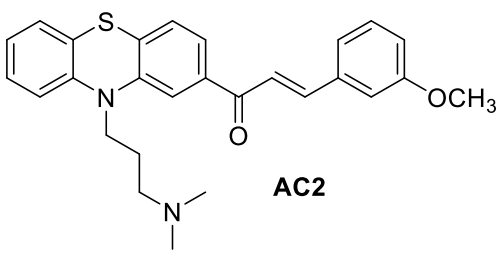
^{1}H-NMR

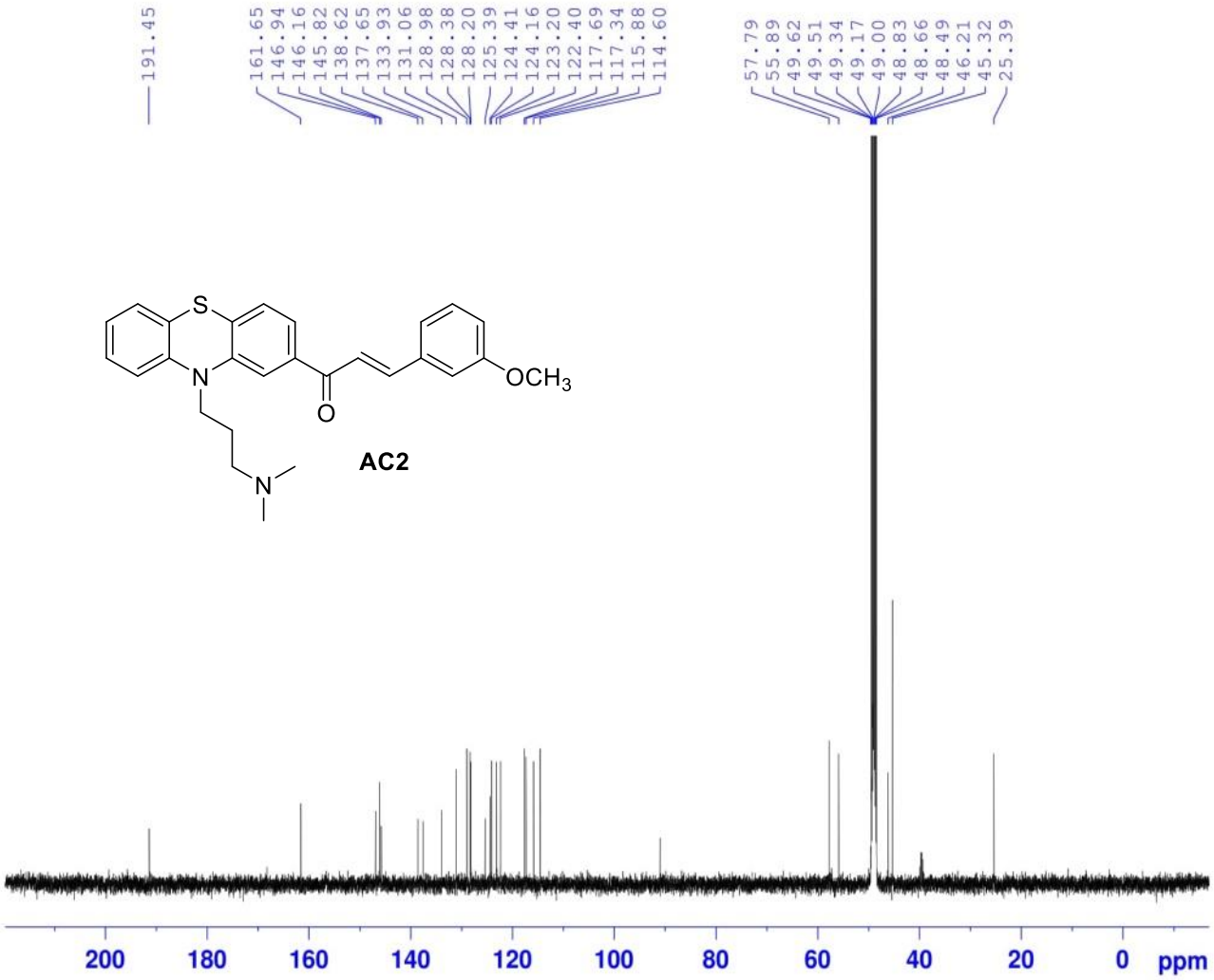




AC2

^{13}C-NMR

C3-MeOD-C13CPD

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PROCNO                     1

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TD                    65536
SOLVENT                MeOD
NS                     2048
DS                        4
SWH              29761.904 Hz
FIDRES            0.454131 Hz
AQ                1.1010048 sec
RG                   198.57
DW                   16.800 usec
DE                    6.50 usec
TE                   303.0 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1

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NUC1                    13C
P1                    10.00 usec
PLW1           88.00000000 W

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NUC2                    1H
CPDPRG[2             waltz16
PCPD2                 80.00 usec
PLW2           22.00000000 W
PLW12           0.34375000 W
PLW13           0.22000000 W

F2 - Processing parameters
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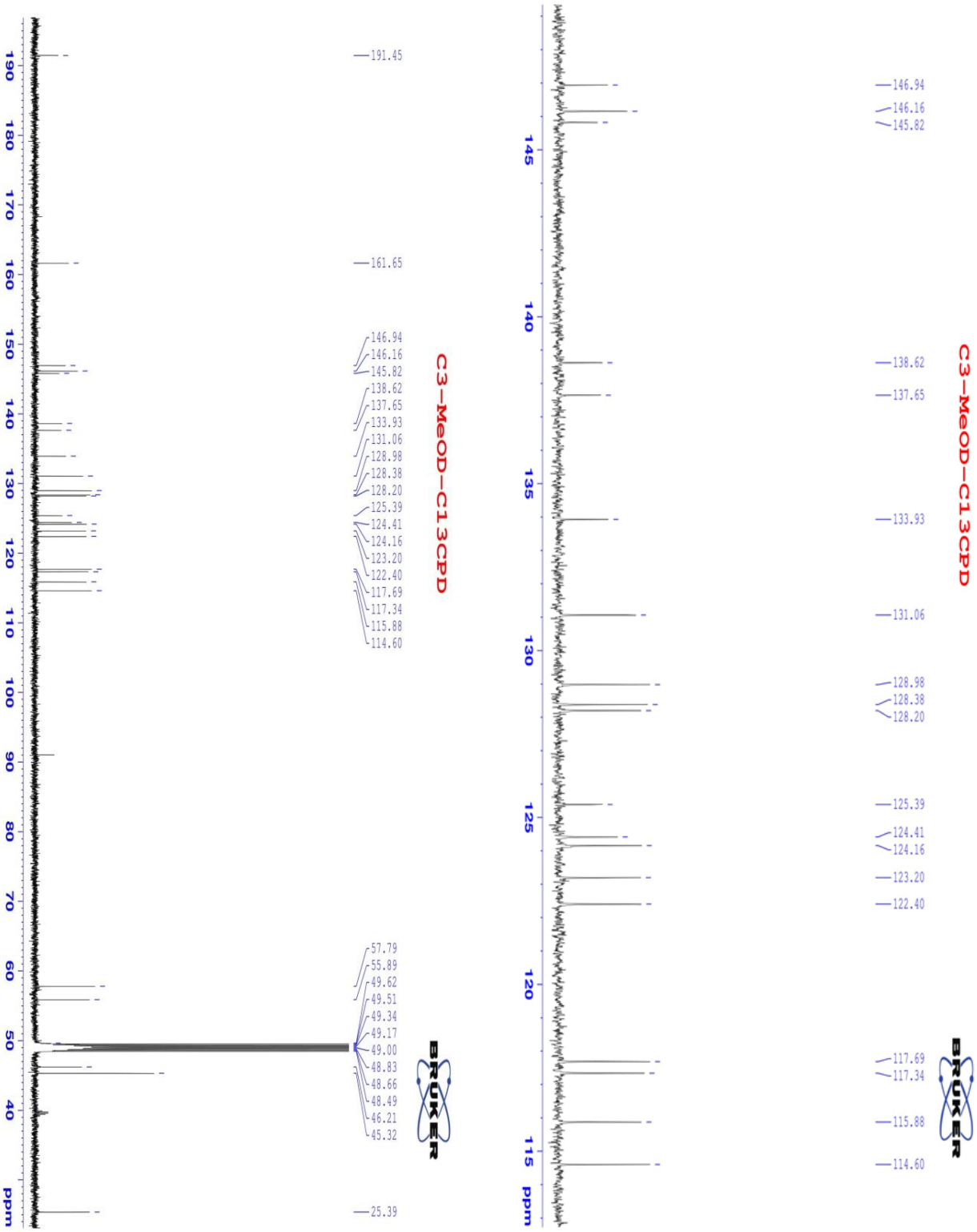
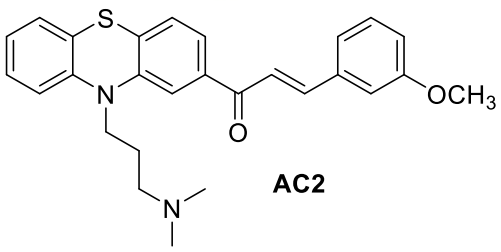
SF             125.7753900 MHz
WDW                     EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

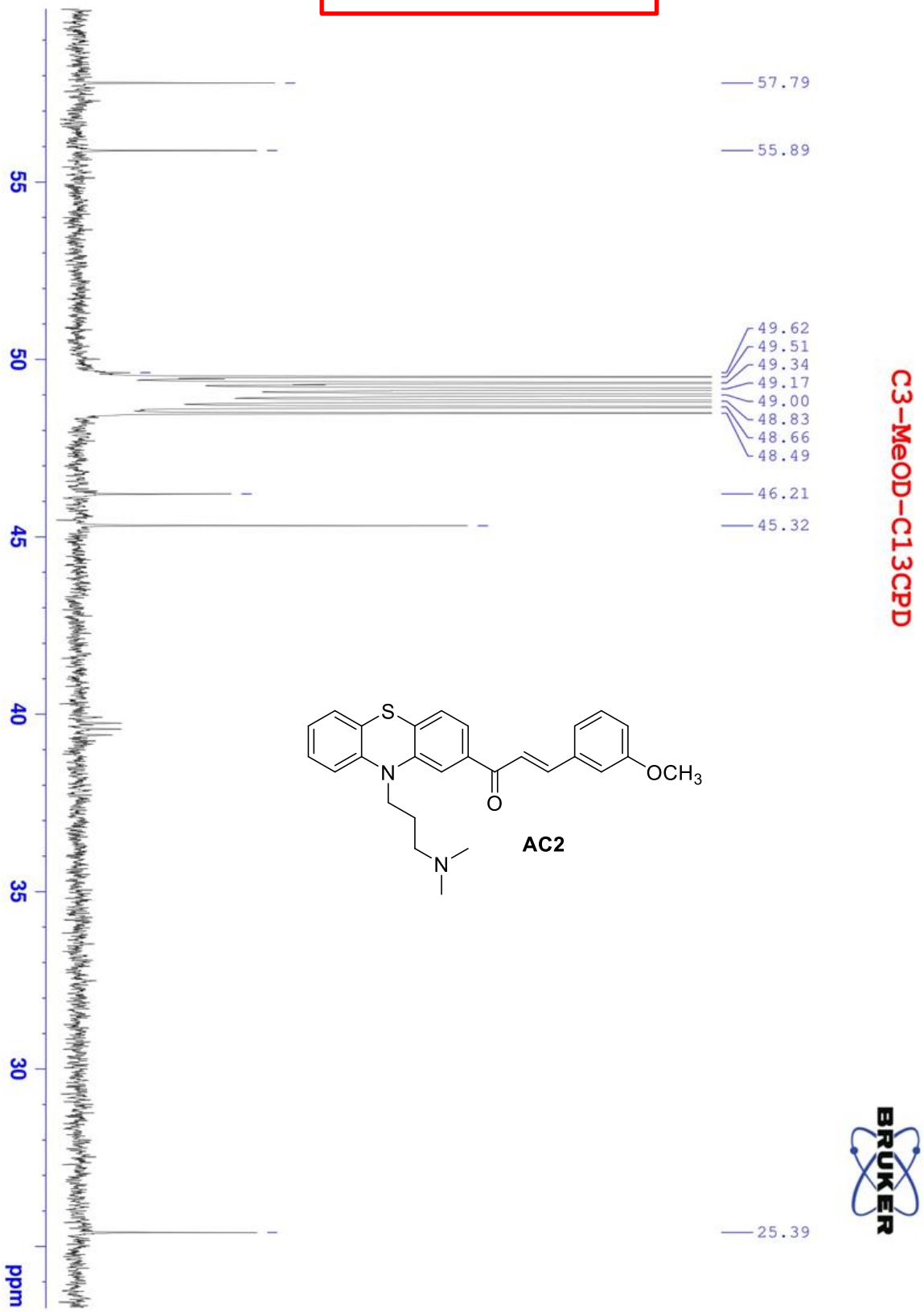
^{13}C-NMR


191.45
161.65
146.94
146.16
145.82
138.62
137.65
133.93
131.06
128.98
128.38
128.20
125.39
124.41
124.16
123.20
122.40
117.69
117.34
115.88
114.60
57.79
55.89
49.62
49.51
49.34
49.17
49.00
48.83
48.66
48.49
46.21
45.32
25.39
C3-MeOD-C13CPD
BRUKER
ppm


S
N
O
OCH3
N

AC2

^{13}C-NMR


57.79
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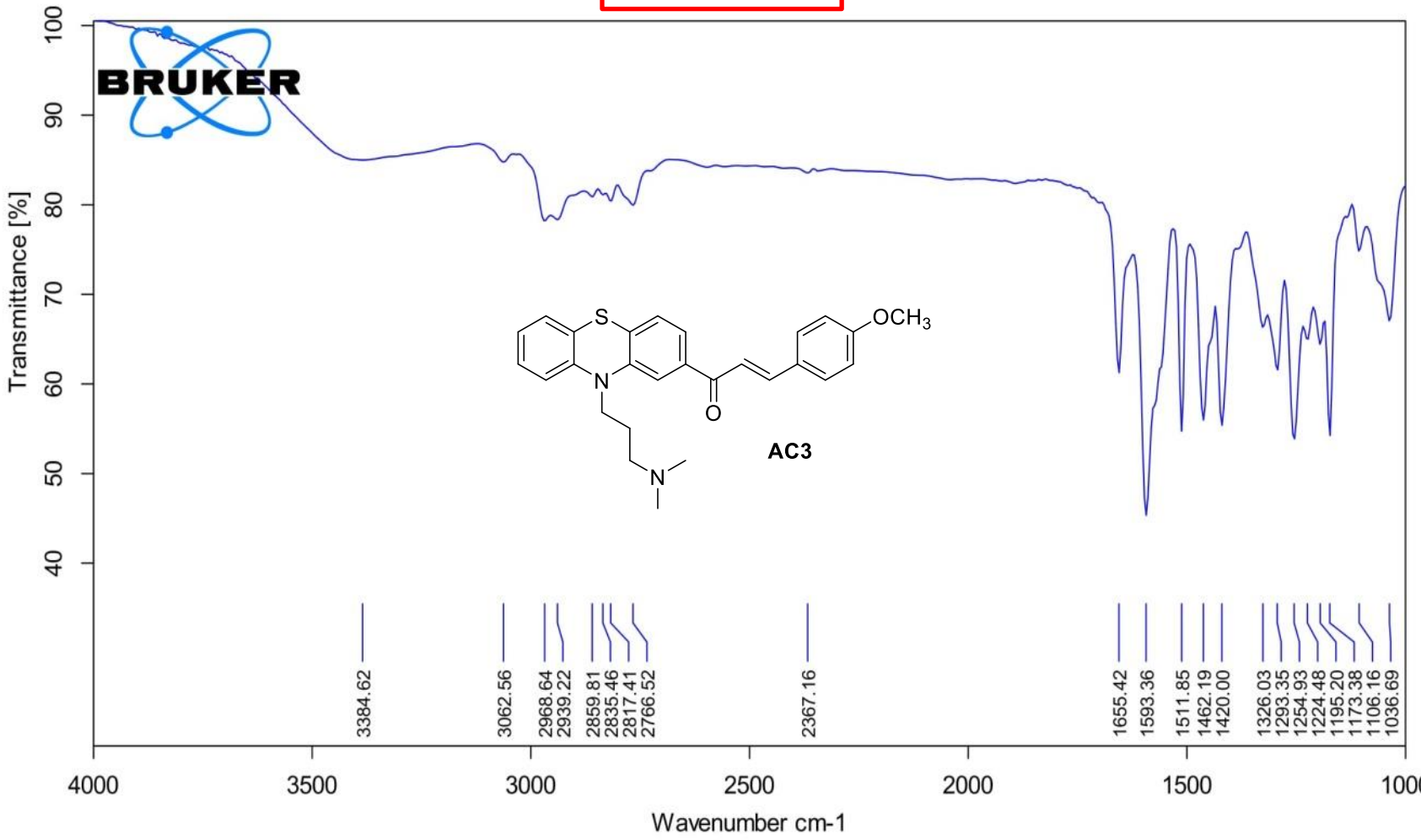
49.51
49.34
49.17
49.00
48.83
48.66
48.49
46.21
45.32
25.39
55
50
45
40
35
30
ppm
C3-MeOD-C13CPD
S
N
O
OCH3
N
AC2
BRUKER

VIEN CONG NGHE HOA HOC
01 Mac Dinh Chi - Q.1 - Tp HCM

Tel: 08.38296127
Fax: 08.38293889

IR



E:\OPUS 7\2017\THANG 6\20170606\C2.0	C2	TENSOR 27 - BRUKER - GERMANY	6/6/2017

MS

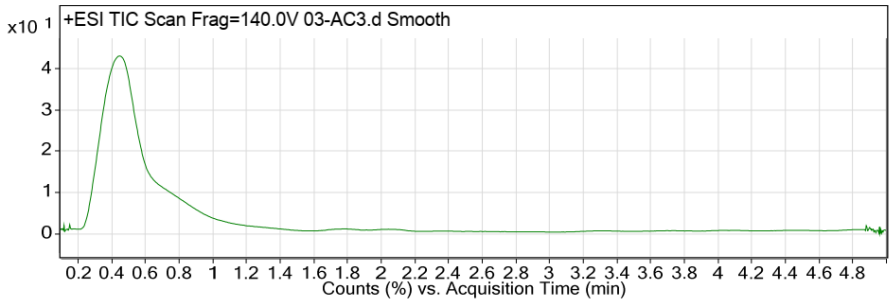
Qualitative Analysis Report

Data Filename	03-AC3.d	**Sample Name**	03-AC3
Sample Type	Sample	**Position**	P2-C4
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	22/08/2020 10:21:51 AM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

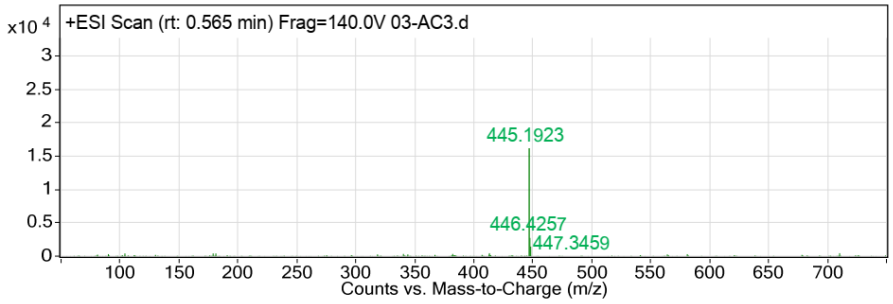
User Chromatograms

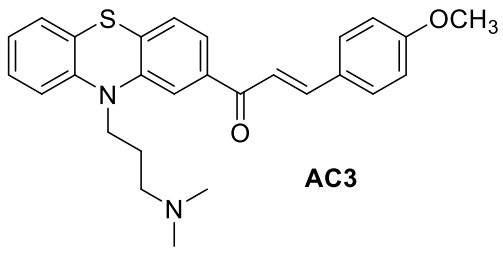
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



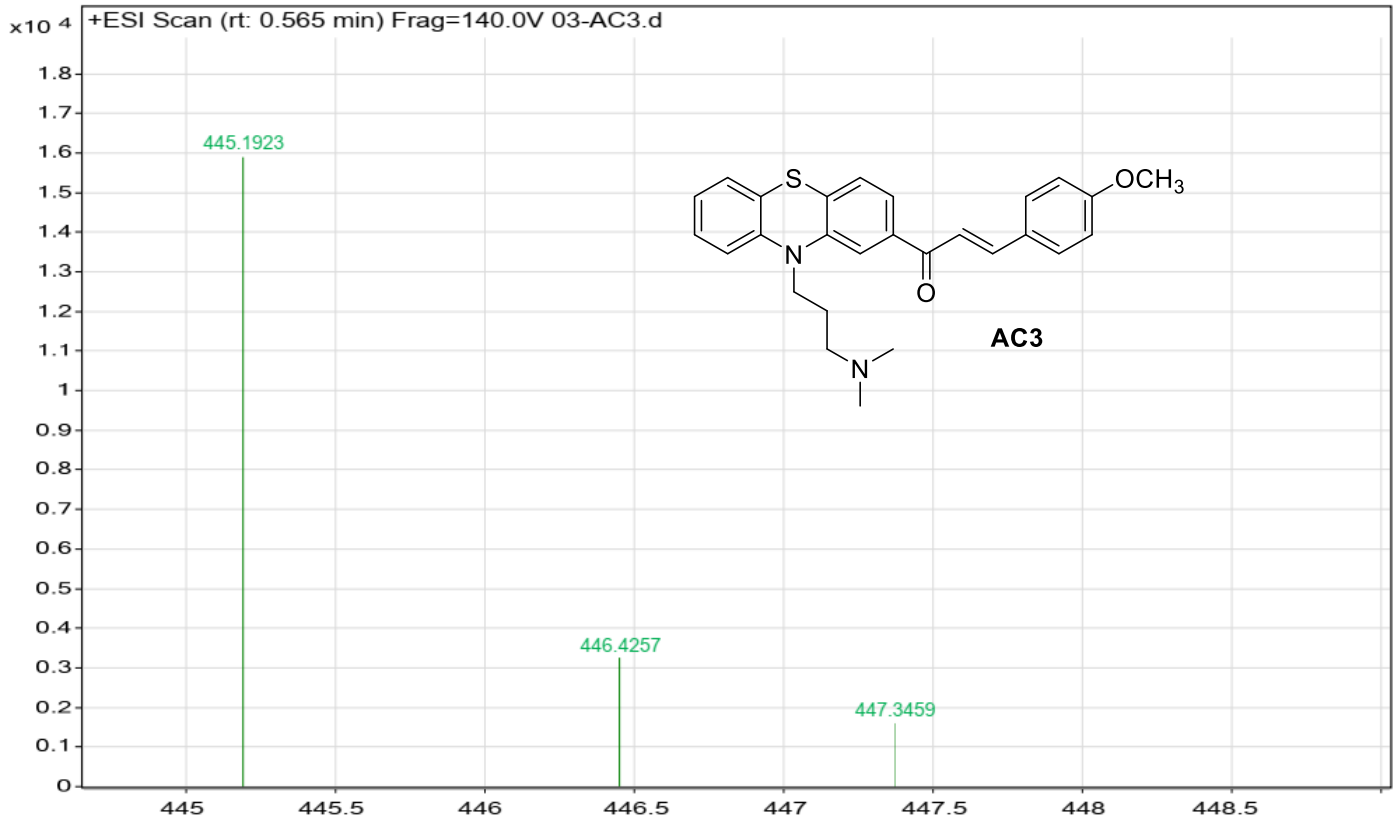


AC3

--- End Of Report ---

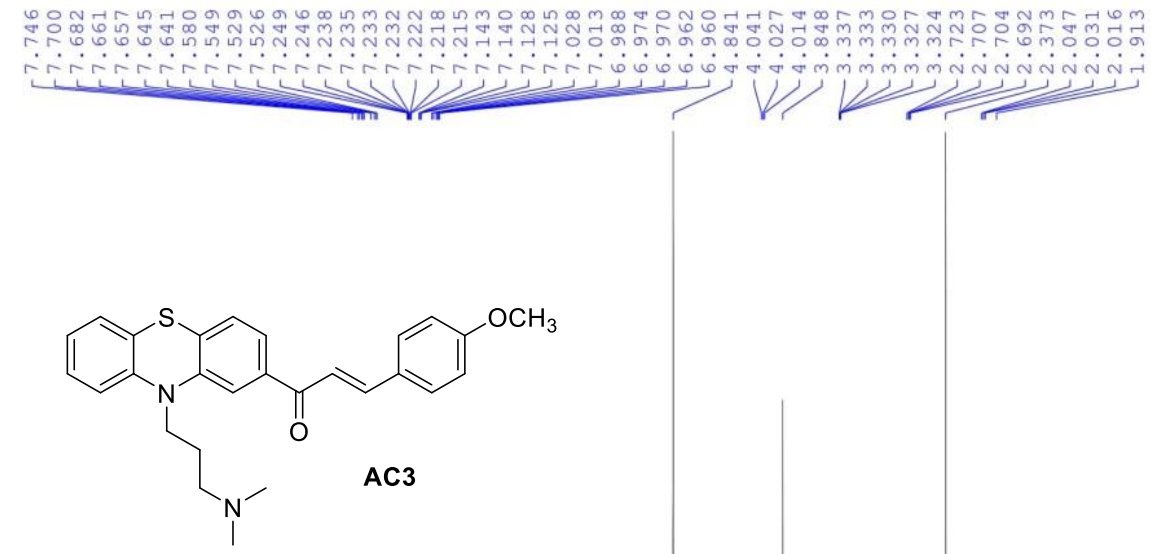
MS

Sample Name	03-AC3	**Position**	P2-C4	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	03-AC3.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	22/08/2020 10:21:51 PM

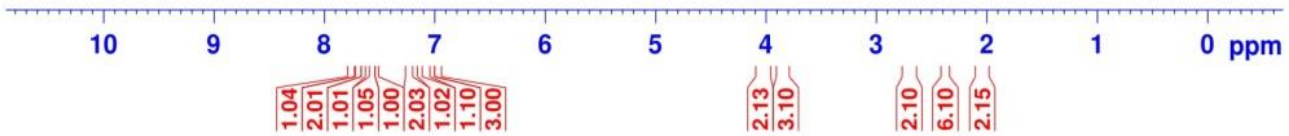


^{1}H-NMR

C2-MeOD-1H



AC3



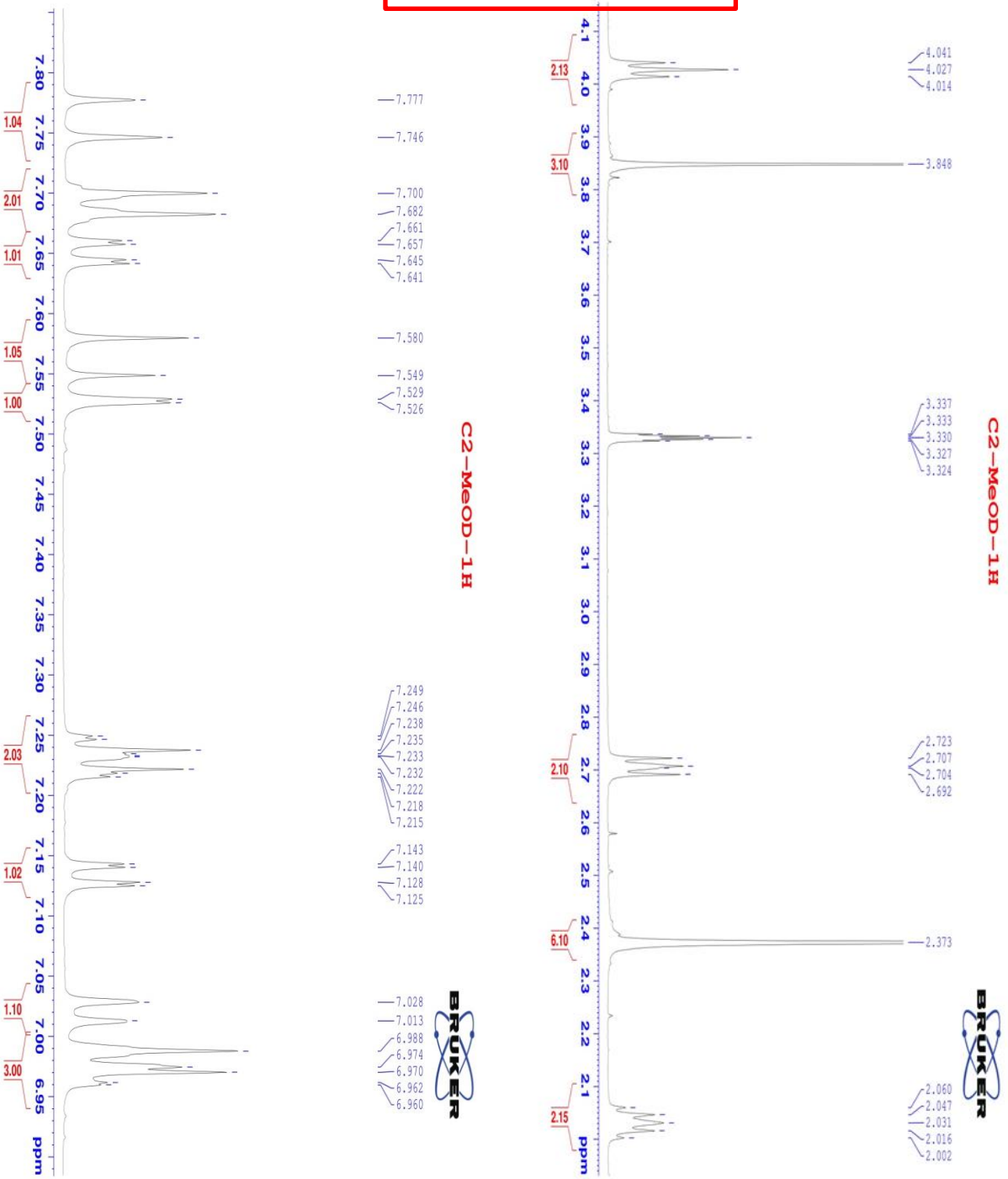

```
Current Data Parameters
NAME                  113D_C2
EXPNO                       1
PROCNO                      1

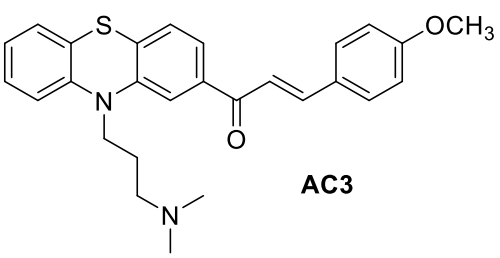
F2 - Acquisition Parameters
Date_                20170606
Time                    15.13
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                 MeOD
NS                        16
DS                         2
SWH                10000.000 Hz
FIDRES             0.152588 Hz
AQ                 3.2767999 sec
RG                     79.36
DW                    50.000 usec
DE                     6.50 usec
TE                    303.0 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1             500.2030889 MHz
NUC1                       1H
P1                     10.00 usec
PLW1            22.00000000 W

F2 - Processing parameters
SI                         65536
SF               500.2000002 MHz
WDW                        EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

^{1}H-NMR

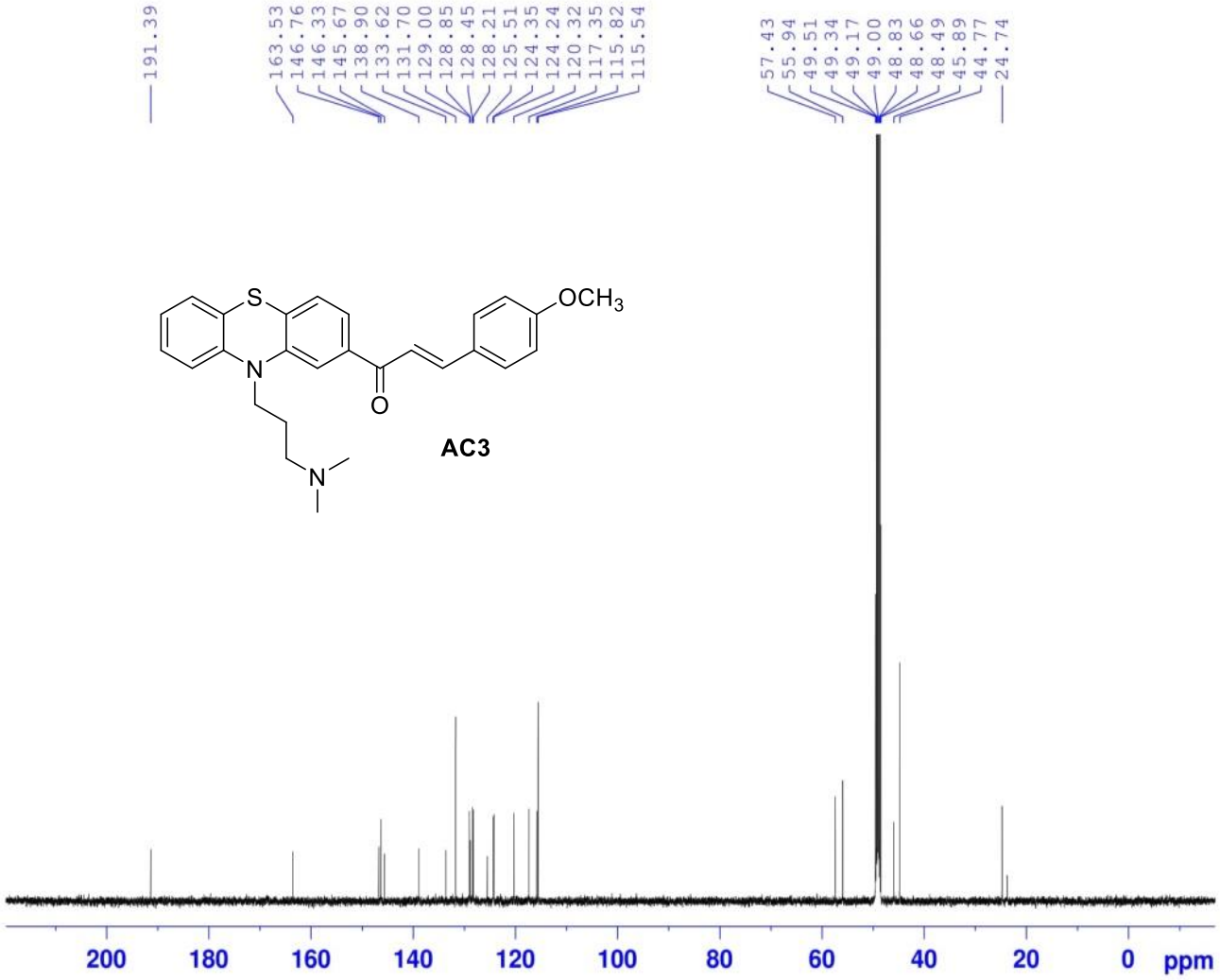




AC3

^{13}C-NMR

C2-MeOD-C13CPD




```
Current Data Parameters
NAME                 113D_C2
EXPNO                      2
PROCNO                     1

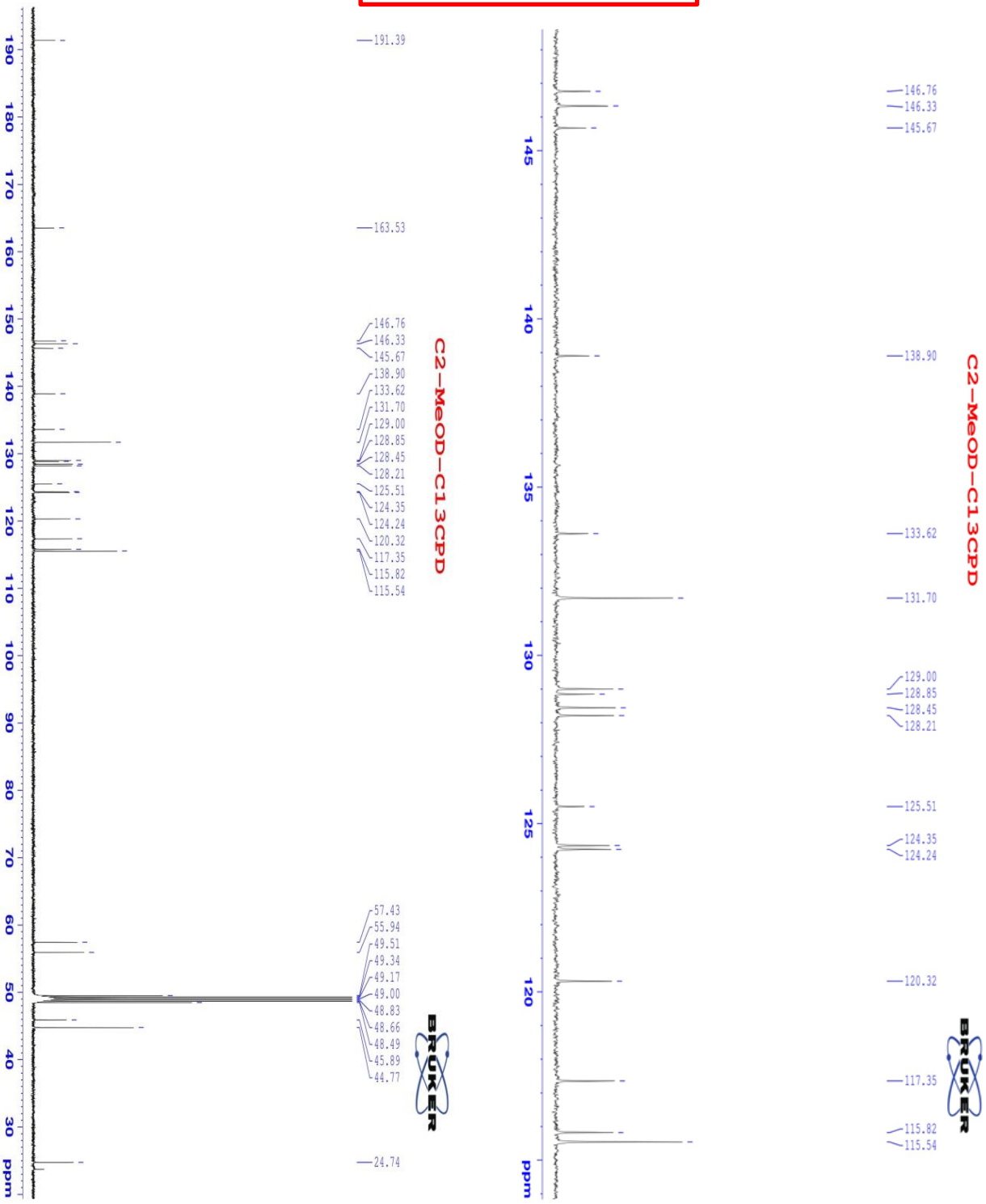
F2 - Acquisition Parameters
Date_              20170606
Time                 15.57
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT                MeOD
NS                       256
DS                         4
SWH              29761.904 Hz
FIDRES            0.454131 Hz
AQ                1.1010048 sec
RG                   198.57
DW                   16.800 usec
DE                    6.50 usec
TE                   303.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            125.7879670 MHz
NUC1                    13C
P1                    10.00 usec
PLW1           88.00000000 W

======== CHANNEL f2 ========
SFO2            500.2020008 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                 80.00 usec
PLW2           22.00000000 W
PLW12           0.34375000 W
PLW13           0.22000000 W

F2 - Processing parameters
SI                     32768
SF              125.7753900 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

^{13}C-NMR


191.39
163.53
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146.33
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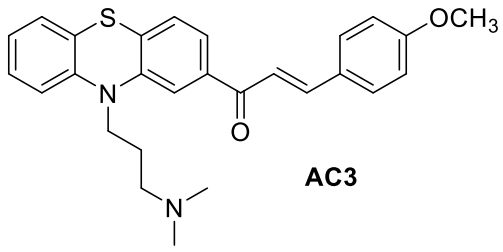
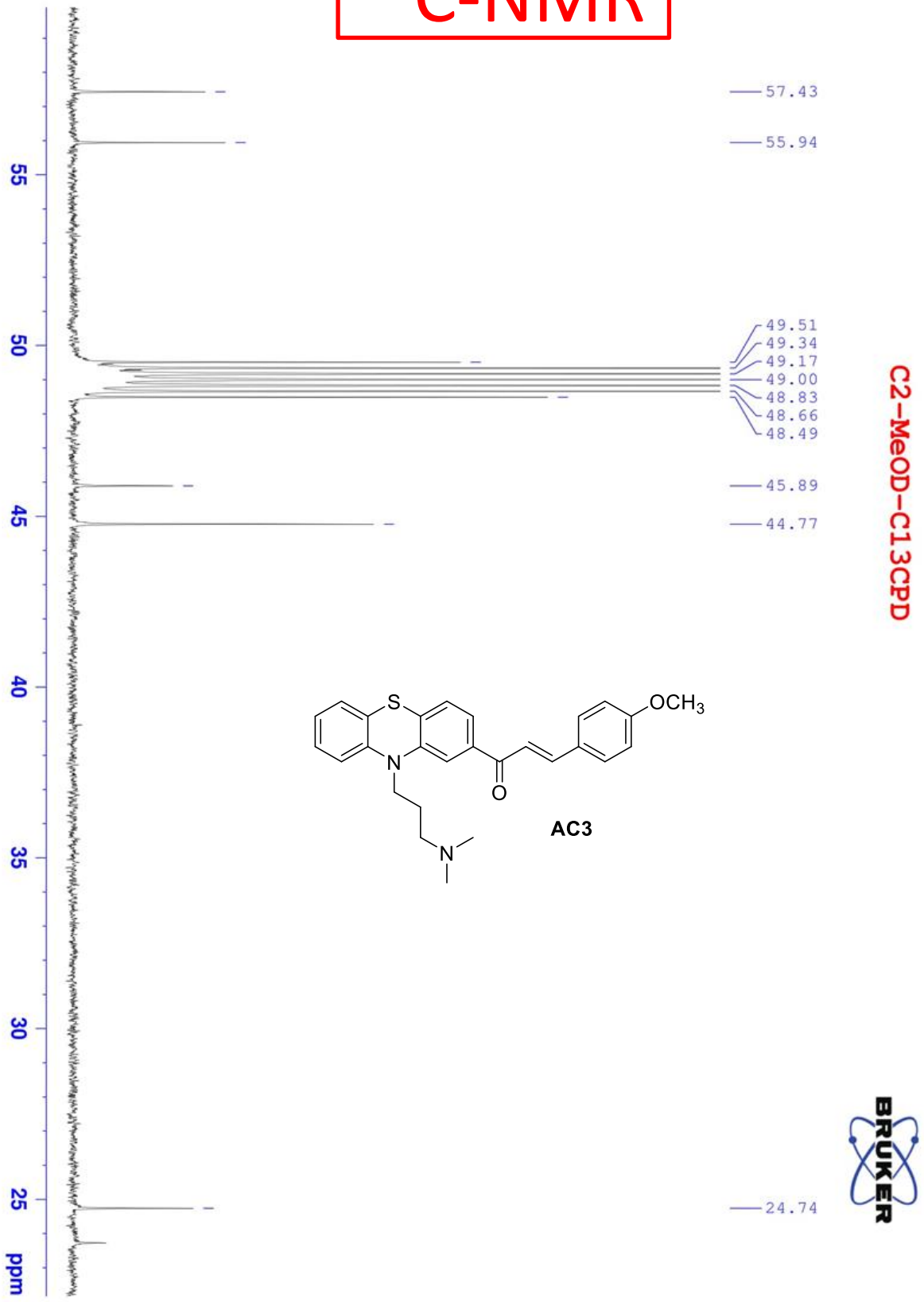
133.62
131.70
129.00
128.85
128.45
128.21
125.51
124.35
124.24
120.32
117.35
115.82
115.54
57.43
55.94
49.51
49.34
49.17
49.00
48.83
48.66
48.49
45.89
44.77
24.74
C2-MeOD-C13CPD
BRUKER
ppm


S
N
O
OCH3
N

AC3

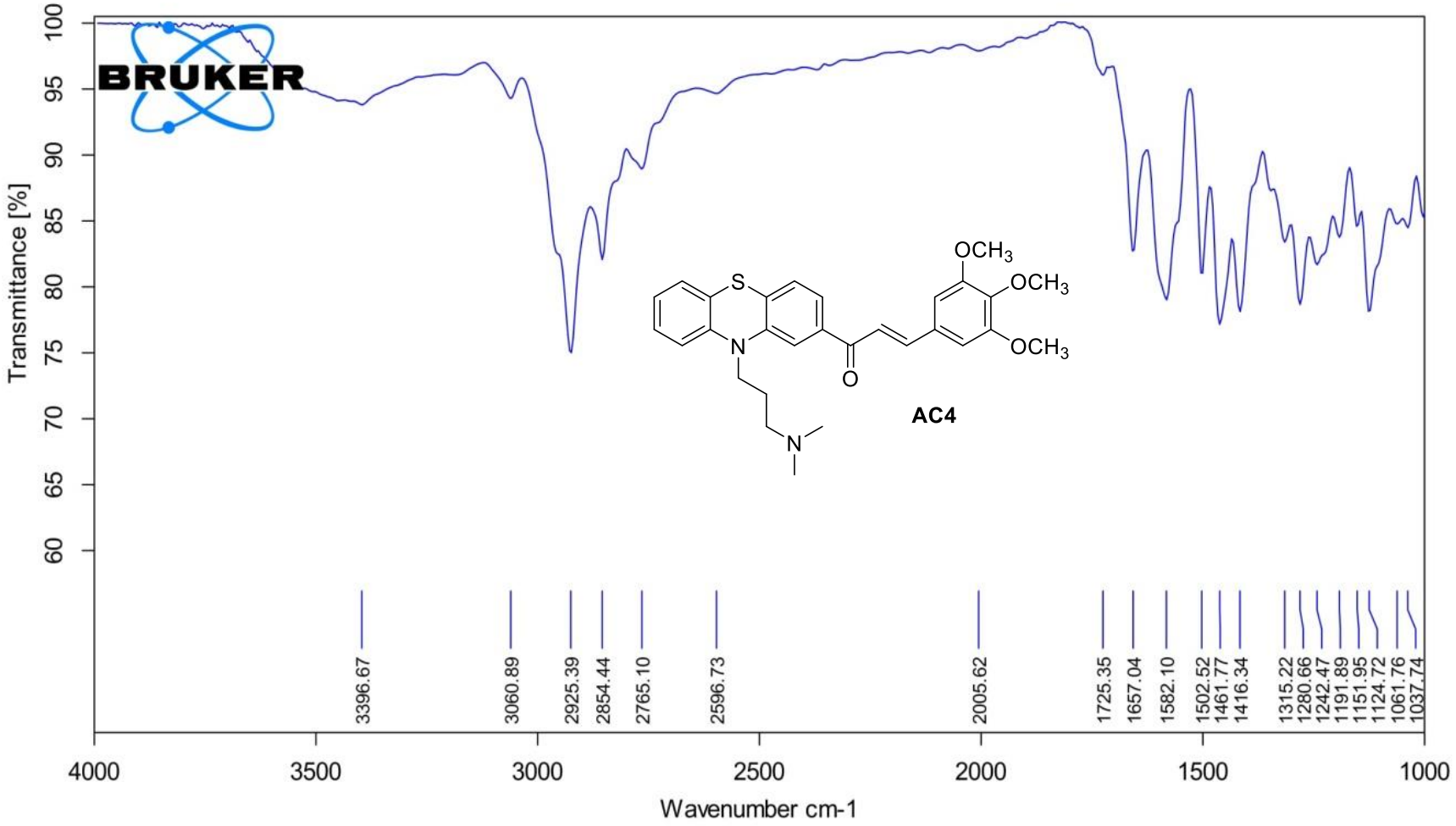
^{13}C-NMR


57.43
55.94
49.51
49.34
49.17
49.00
48.83
48.66
48.49
45.89
44.77
24.74
55
50
45
40
35
30
25
ppm
C2-MeOD-C13CPD
S
N
O
OCH3
N
AC3
BRUKER

VIEN CONG NGHE HOA HOC
01 Mac Dinh Chi - Q.1 - Tp HCM

Tel: 08.38296127
Fax: 08.38293889

IR



E:\OPUS 7\2017\THANG 6\20170606\C4.0	C4	TENSOR 27 - BRUKER - GERMANY	6/6/2017

MS

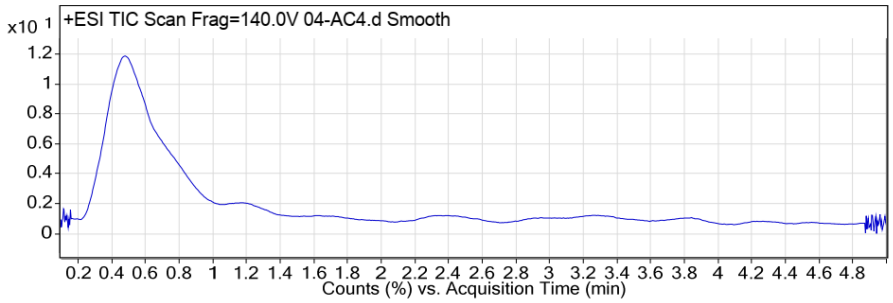
Qualitative Analysis Report

Data Filename	04-AC4.d	**Sample Name**	04-AC4
Sample Type	Sample	**Position**	P2-B5
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	22/08/2020 10:30:20 AM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

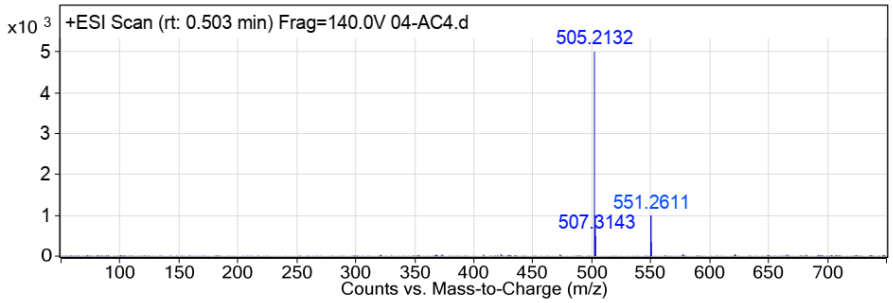
User Chromatograms

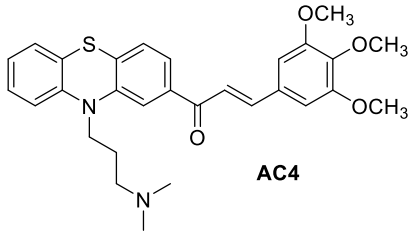
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



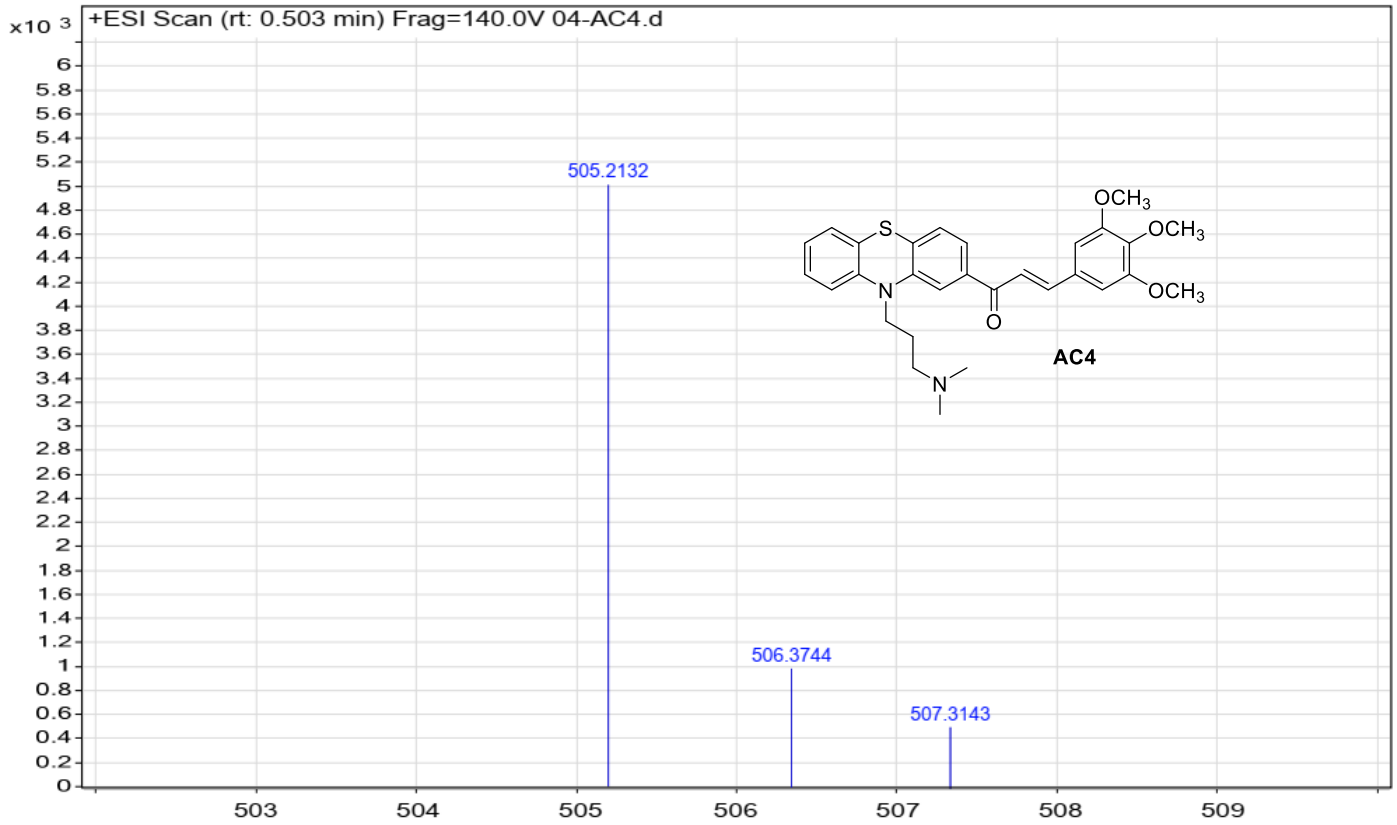


AC4

--- End Of Report ---

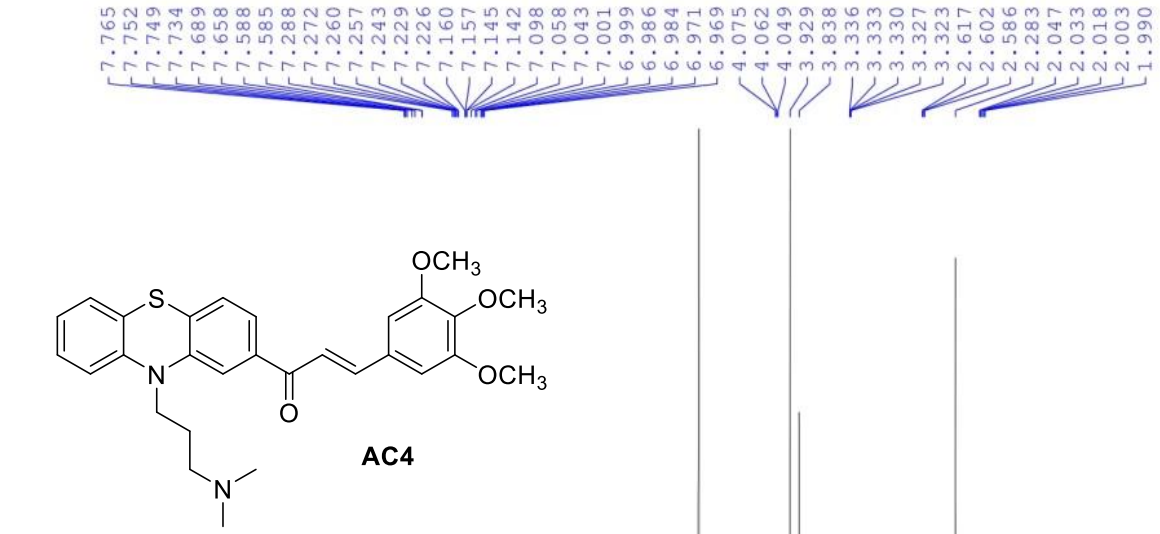
MS

Sample Name	04-AC4	**Position**	P2-B5	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	04-AC4.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	22/08/2020 10:30:20 AM

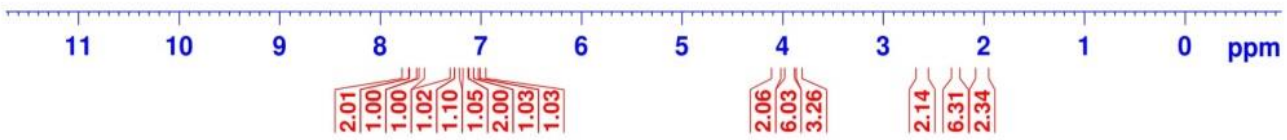


^{1}H-NMR

C4-MeOD-1H



AC4



BRUKER

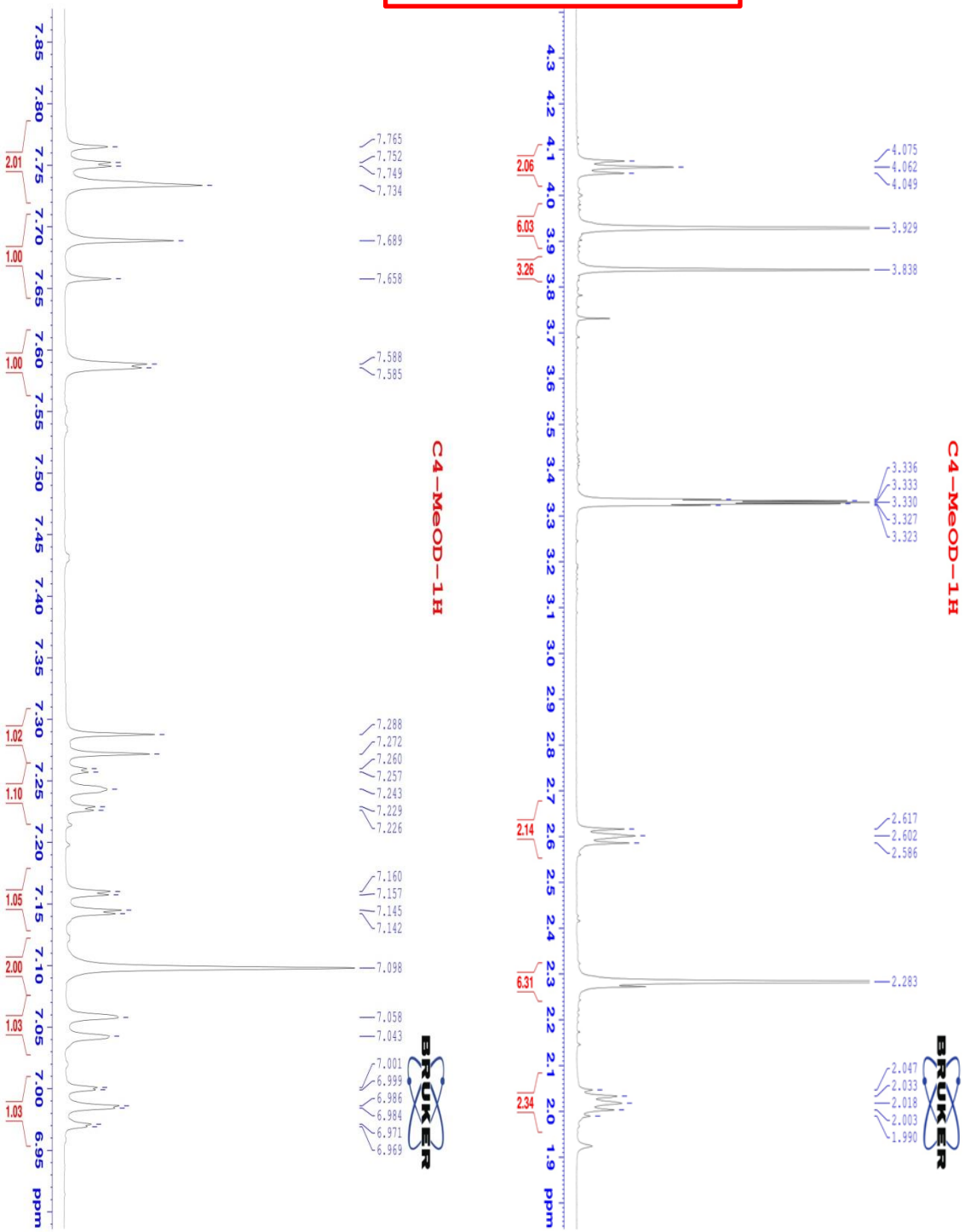
```
Current Data Parameters
NAME                  113D_C4
EXPNO                       1
PROCNO                      1

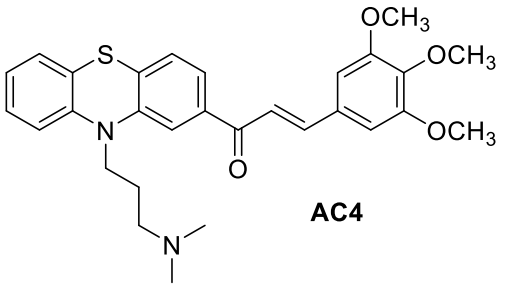
F2 - Acquisition Parameters
Date_                20170606
Time                    16.07
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                 MeOD
NS                        16
DS                         2
SWH                10000.000 Hz
FIDRES             0.152588 Hz
AQ                 3.2767999 sec
RG                    127.68
DW                    50.000 usec
DE                     6.50 usec
TE                    303.0 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1              500.2030889 MHz
NUC1                       1H
P1                      10.00 usec
PLW1             22.00000000 W

F2 - Processing parameters
SI                         65536
SF                500.2000001 MHz
WDW                        EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

^{1}H-NMR

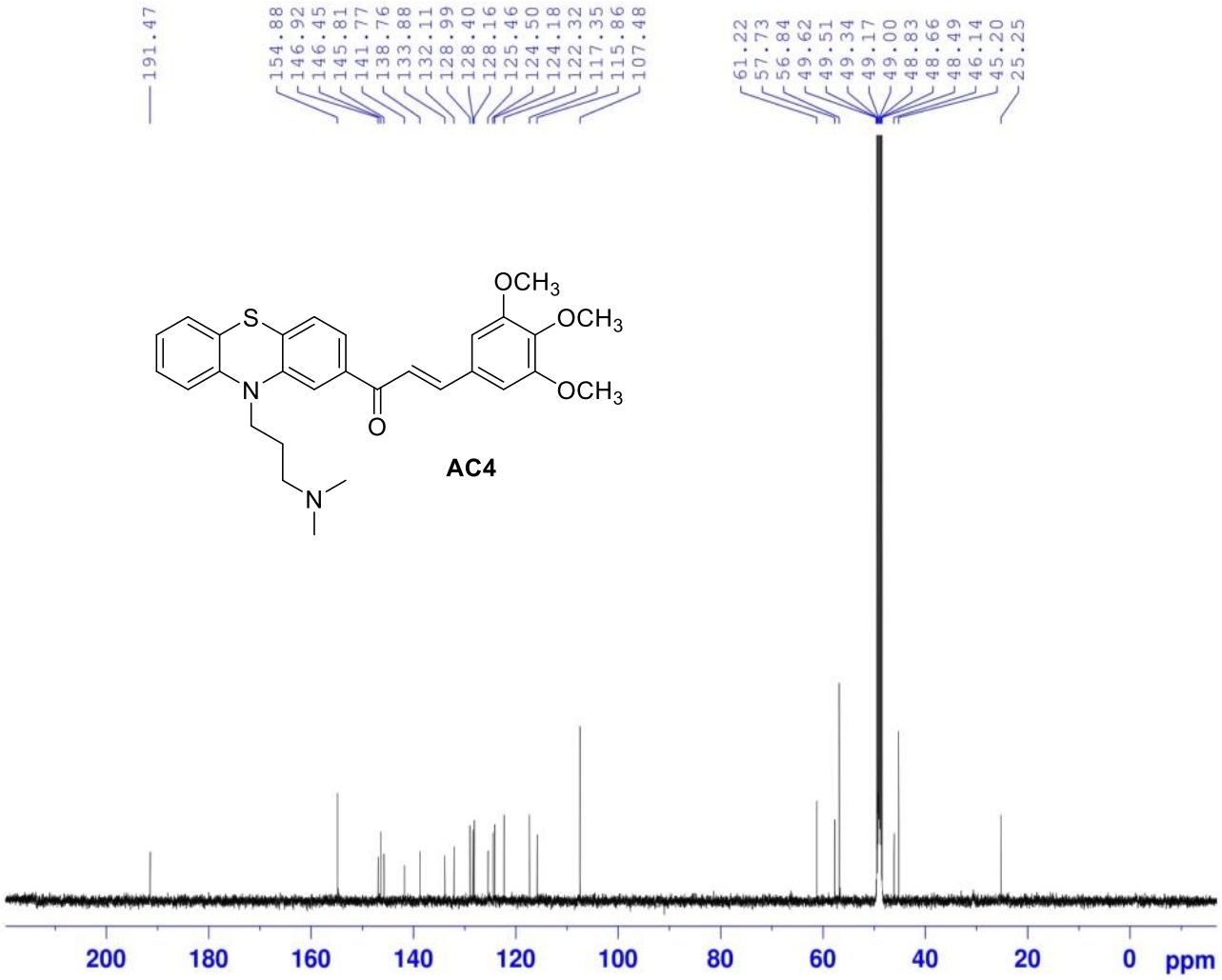




AC4

^{13}C-NMR

C4-MeOD-C13CPD



BRUKER

```
Current Data Parameters
NAME                 113D_C4
EXPNO                      2
PROCNO                     1

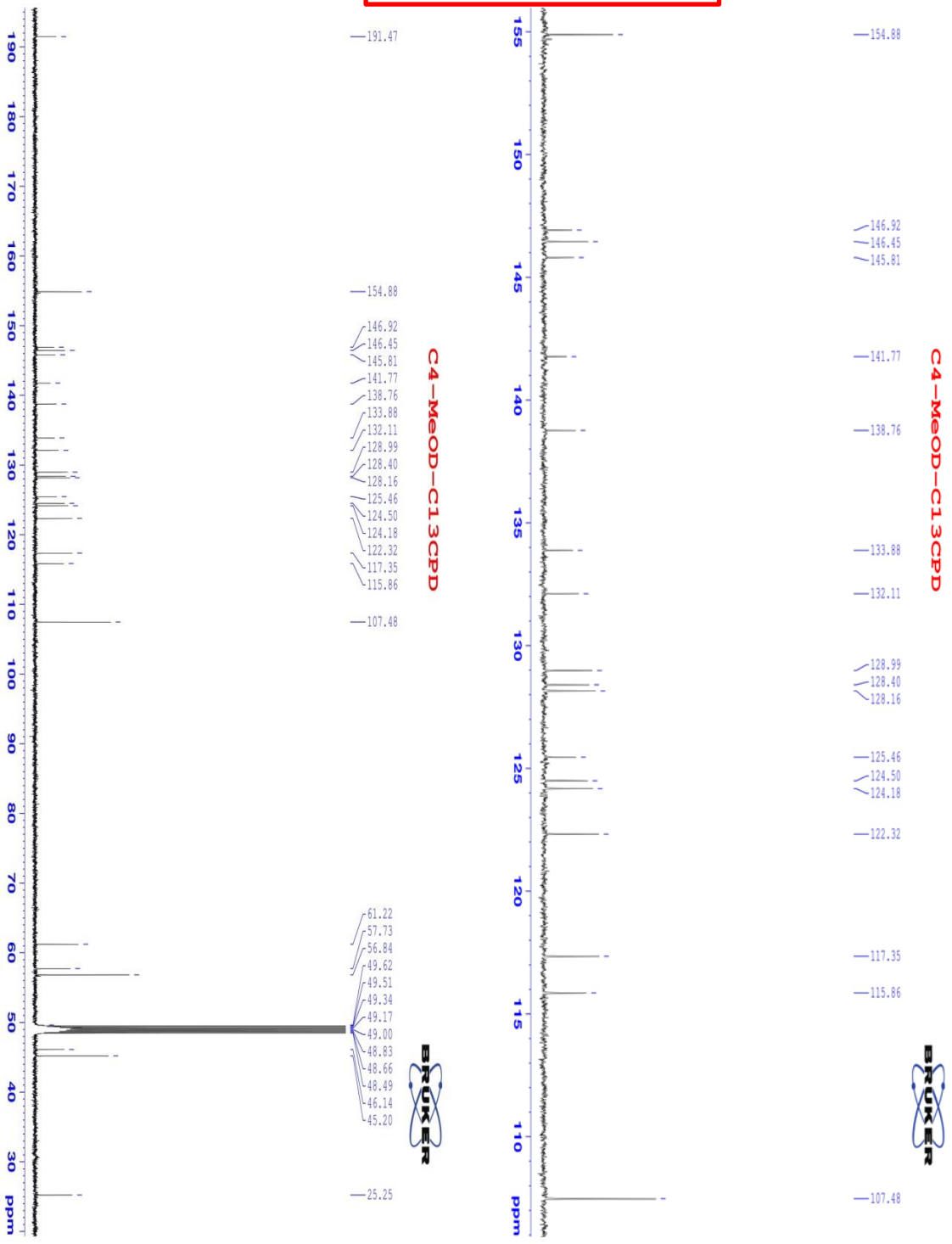
F2 - Acquisition Parameters
Date_              20170606
Time                 19.38
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG            zgpg30
TD                  65536
SOLVENT               MeOD
NS                    2048
DS                       4
SWH              29761.904 Hz
FIDRES           0.454131 Hz
AQ               1.1010048 sec
RG                  198.57
DW                  16.800 usec
DE                   6.50 usec
TE                  303.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           125.7879670 MHz
NUC1                   13C
P1                   10.00 usec
PLW1           88.00000000 W

======== CHANNEL f2 ========
SFO2           500.2020008 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                80.00 usec
PLW2           22.00000000 W
PLW12           0.34375000 W
PLW13           0.22000000 W

F2 - Processing parameters
SI                    32768
SF             125.7752144 MHz
WDW                    EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

^{13}C-NMR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154.88
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56.84
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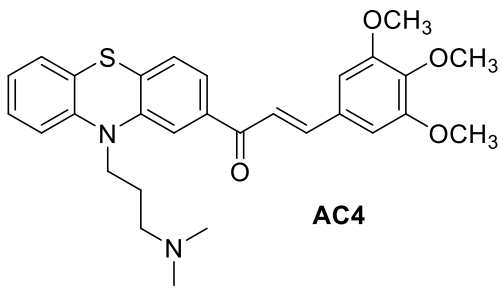
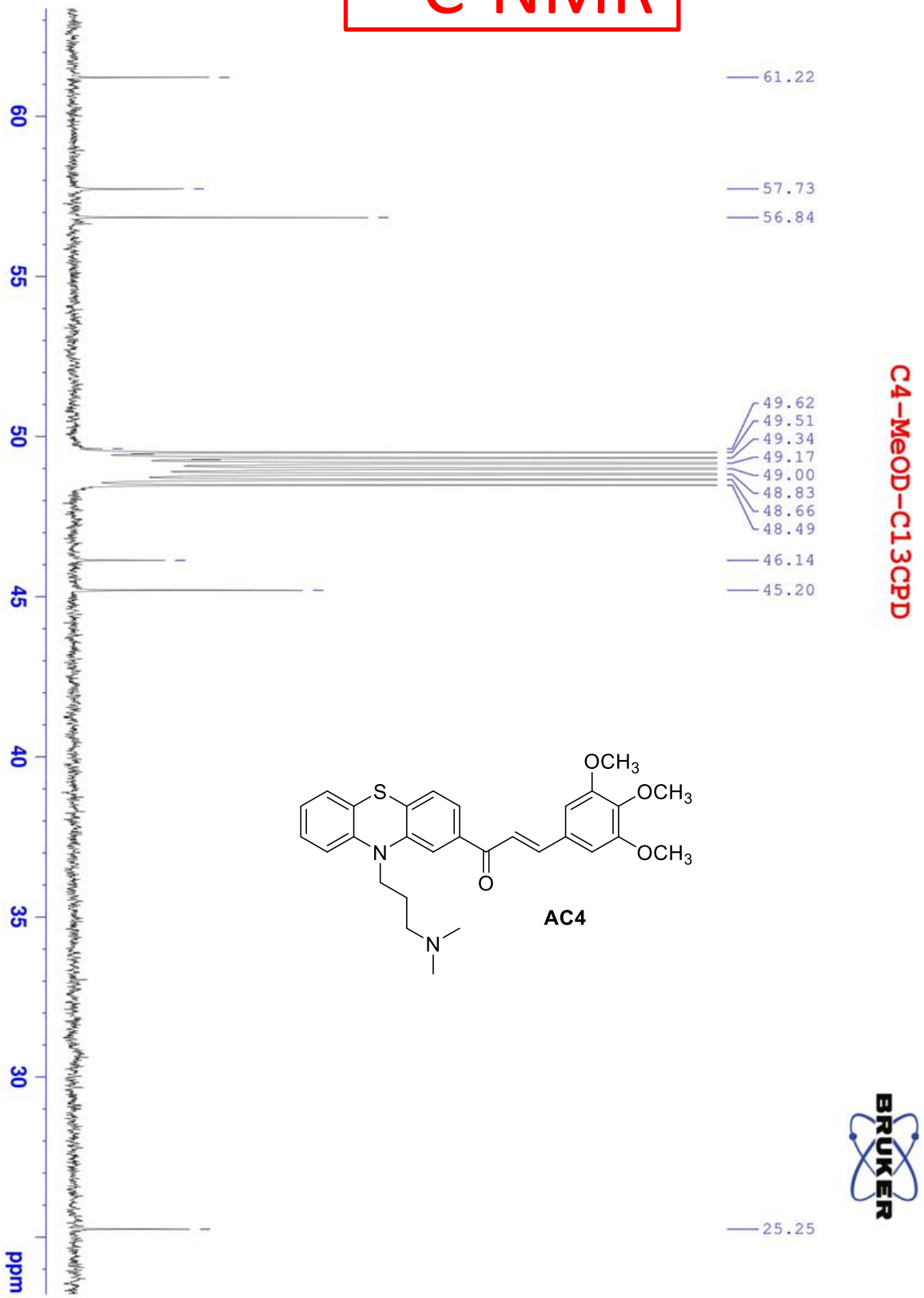
45.20
25.25
C4-MeOD-C13CPD
BRUKER
ppm


OCH3
OCH3
OCH3
S
N
O
N

AC4

^{13}C-NMR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49.00
48.83
48.66
48.49
46.14
45.20
25.25
60
55
50
45
40
35
30
ppm
C4-MeOD-C13CPD
BRUKER

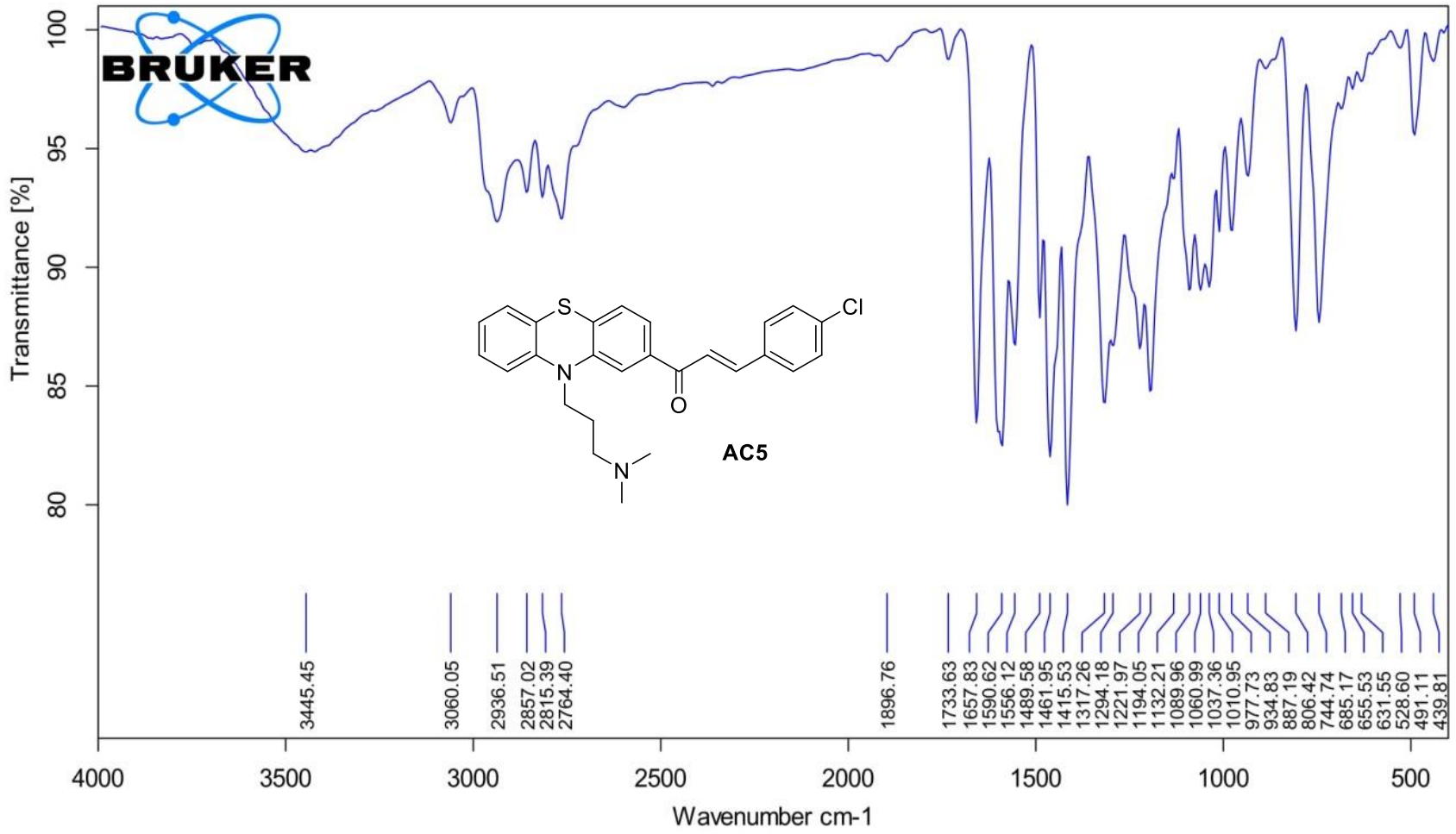
OCH3
OCH3
OCH3
S
N
O
N

AC4

VIEN CONG NGHE HOA HOC
01 Mac Dinh Chi - Q.1 - Tp HCM

Tel: 08.38296127
Fax: 08.38293889

IR



E:\OPUS 7\2017\THANG 7\20170714\C9.0	C9	TENSOR 27 - BRUKER - GERMANY	7/14/2017

MS

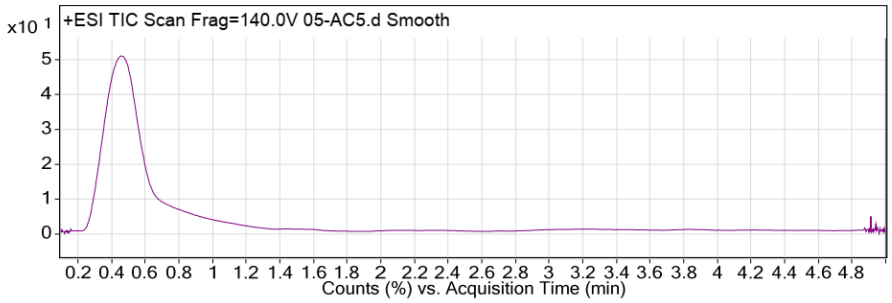
Qualitative Analysis Report

Data Filename	05-AC5.d	**Sample Name**	05-AC5
Sample Type	Sample	**Position**	P2-B4
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	22/08/2020 10:38:45 AM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

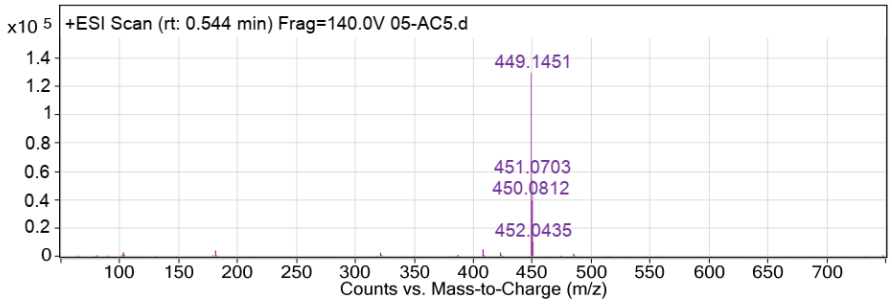
User Chromatograms

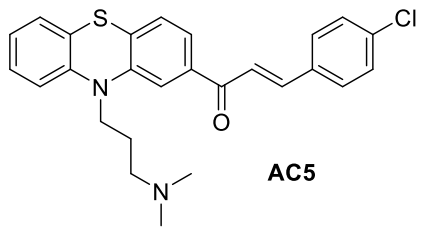
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



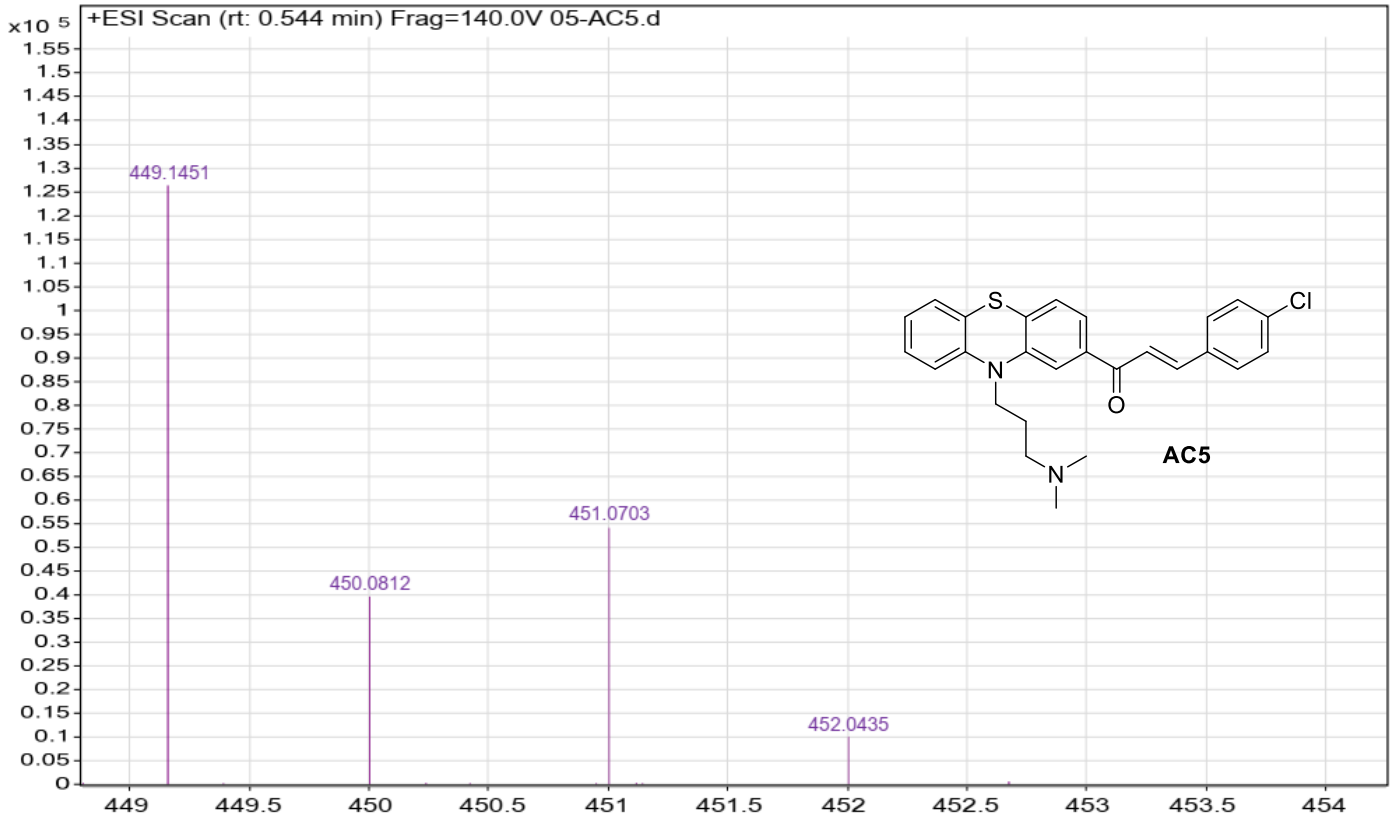


AC5

--- End Of Report ---

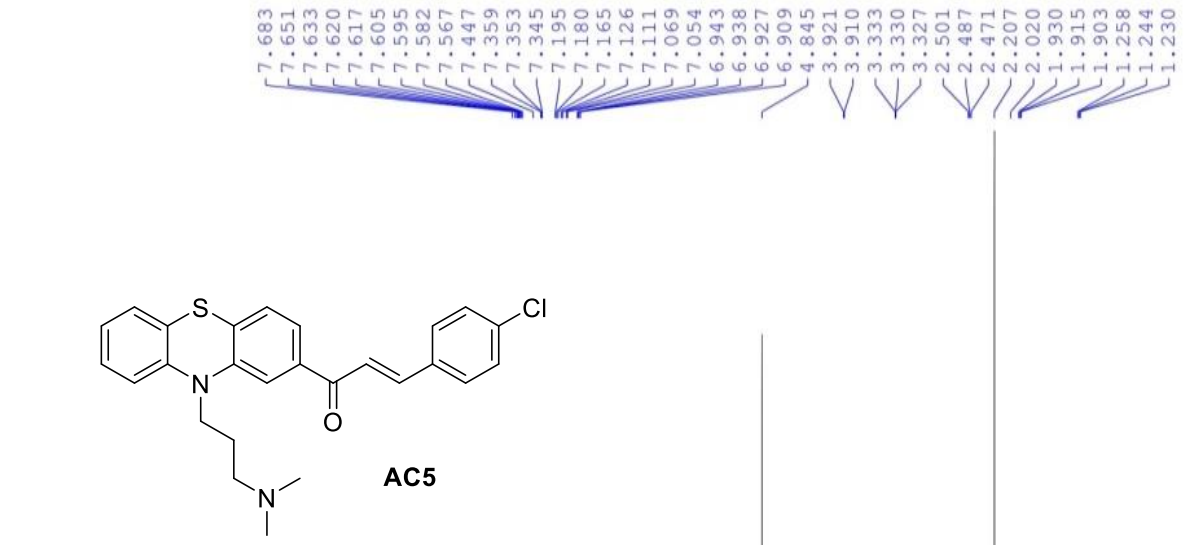
MS

Sample Name	05-AC5	**Position**	P2-B4	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	05-AC5.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	22/08/2020 10:38:45 AM

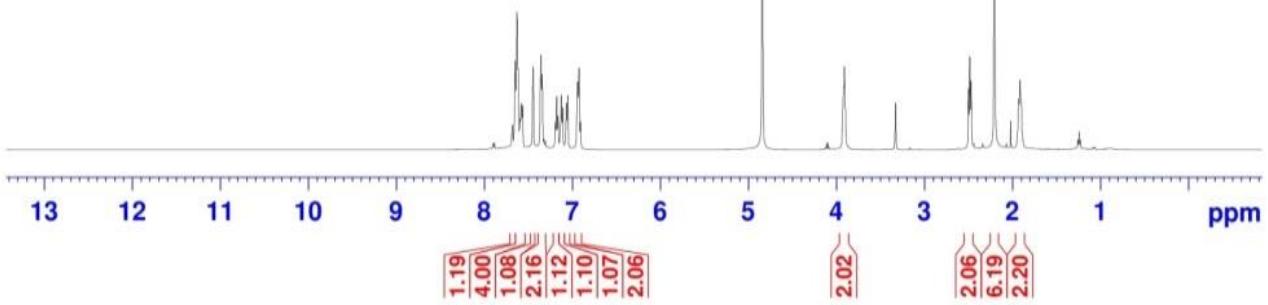


^{1}H-NMR

C9-MeOD-1H



AC5



BRUKER

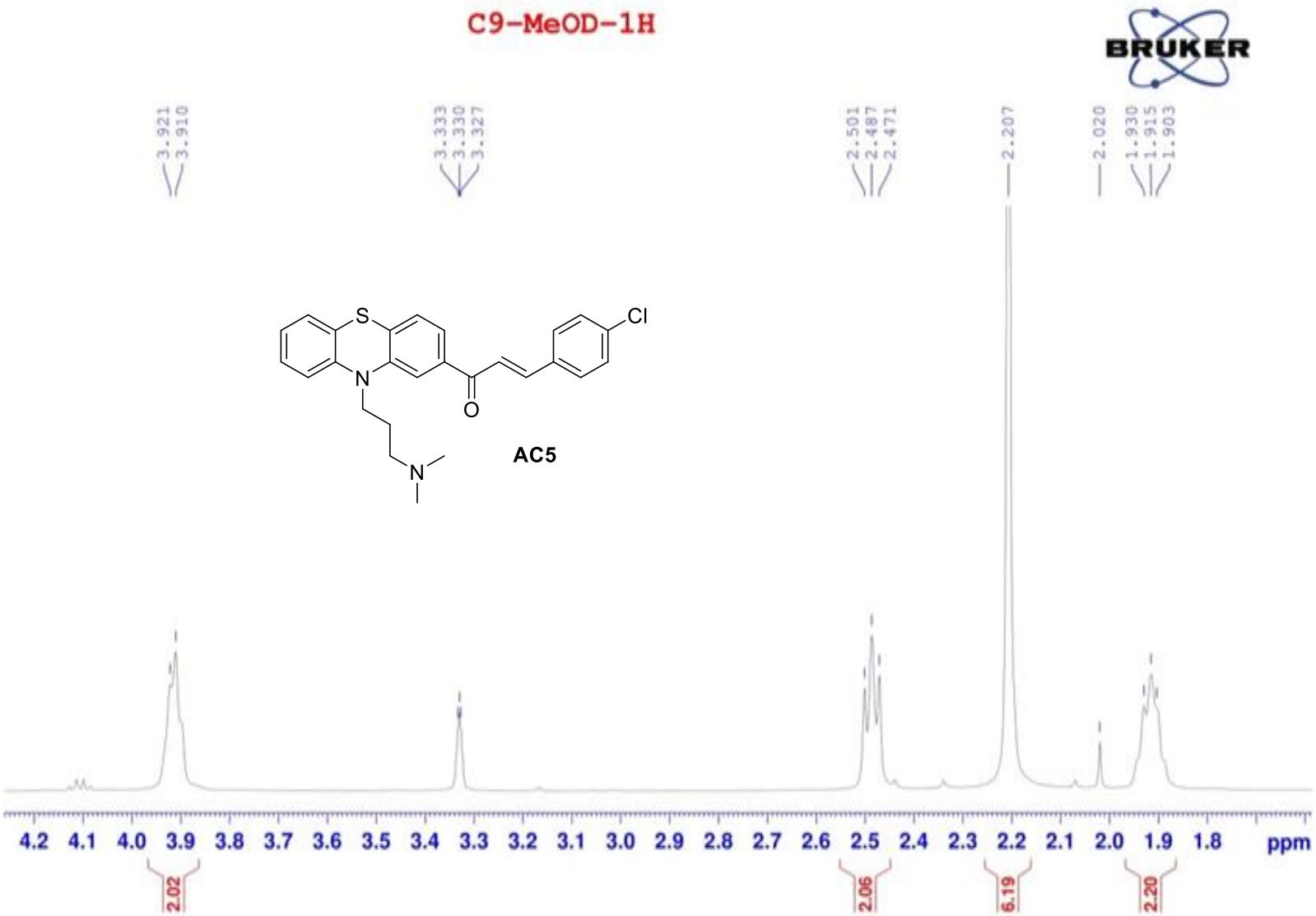
```
Current Data Parameters
NAME            113DAO_C9
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20170704
Time                11.15
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             MeOD
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ             3.2767999 sec
RG                 30.85
DW                50.000 usec
DE                 6.50 usec
TE                303.0 K
D1            1.00000000 sec
TD0                    1

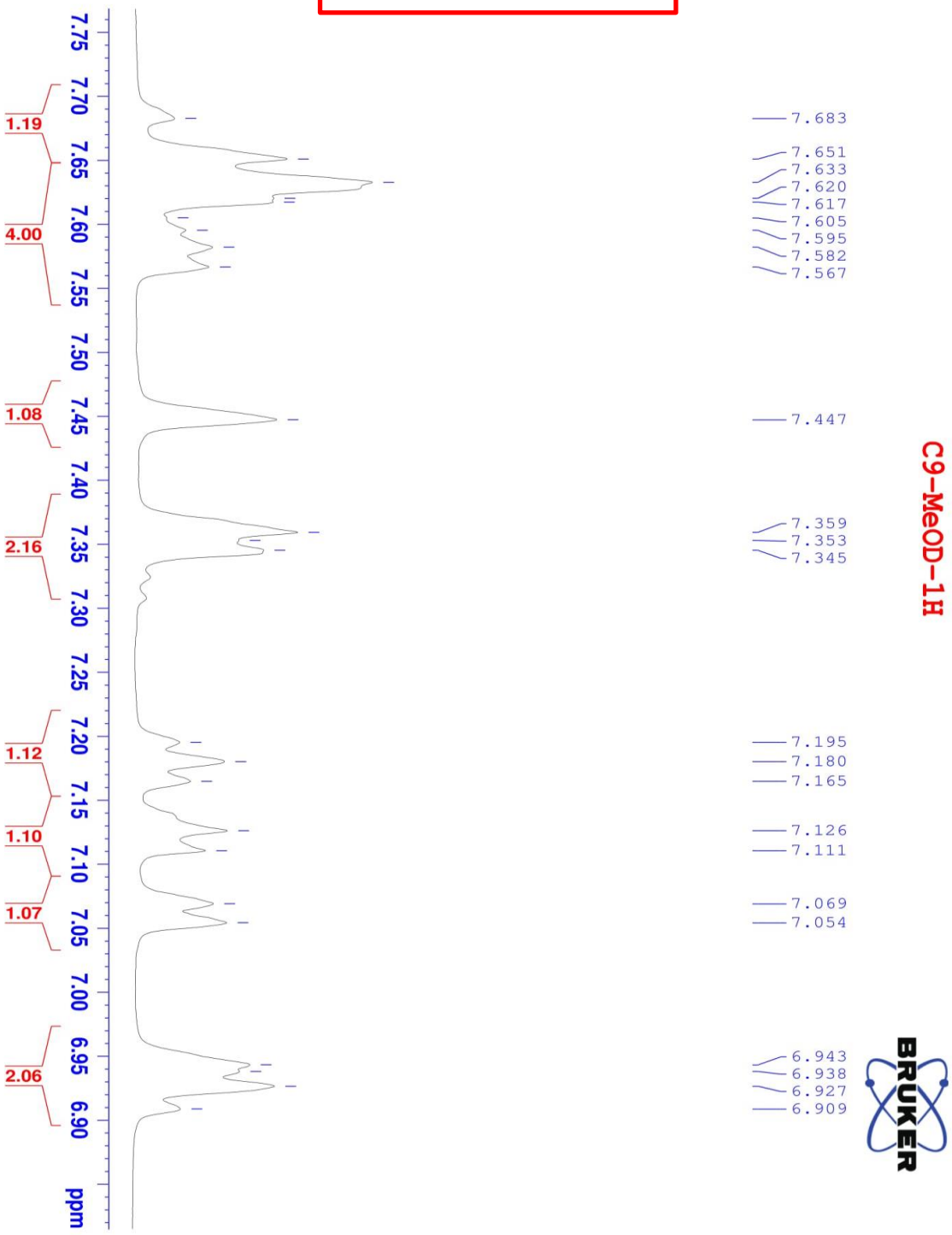
======== CHANNEL f1 ========
SFO1         500.2030889 MHz
NUC1                   1H
P1                10.00 usec
PLW1         22.00000000 W

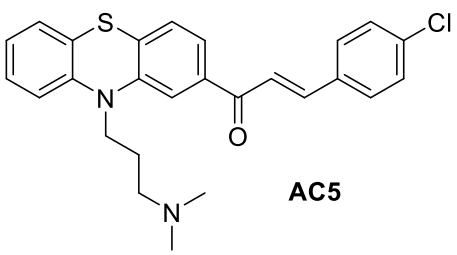
F2 - Processing parameters
SI                 65536
SF           500.2000013 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{1}H-NMR


C9-MeOD-1H
BRUKER
3.921
3.910
3.333
3.330
3.327
2.501
2.487
2.471
2.207
2.020
1.930
1.915
1.903
S
N
O
Cl
N
AC5
4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 ppm
2.02
2.06
6.19
2.20

^{1}H-NMR

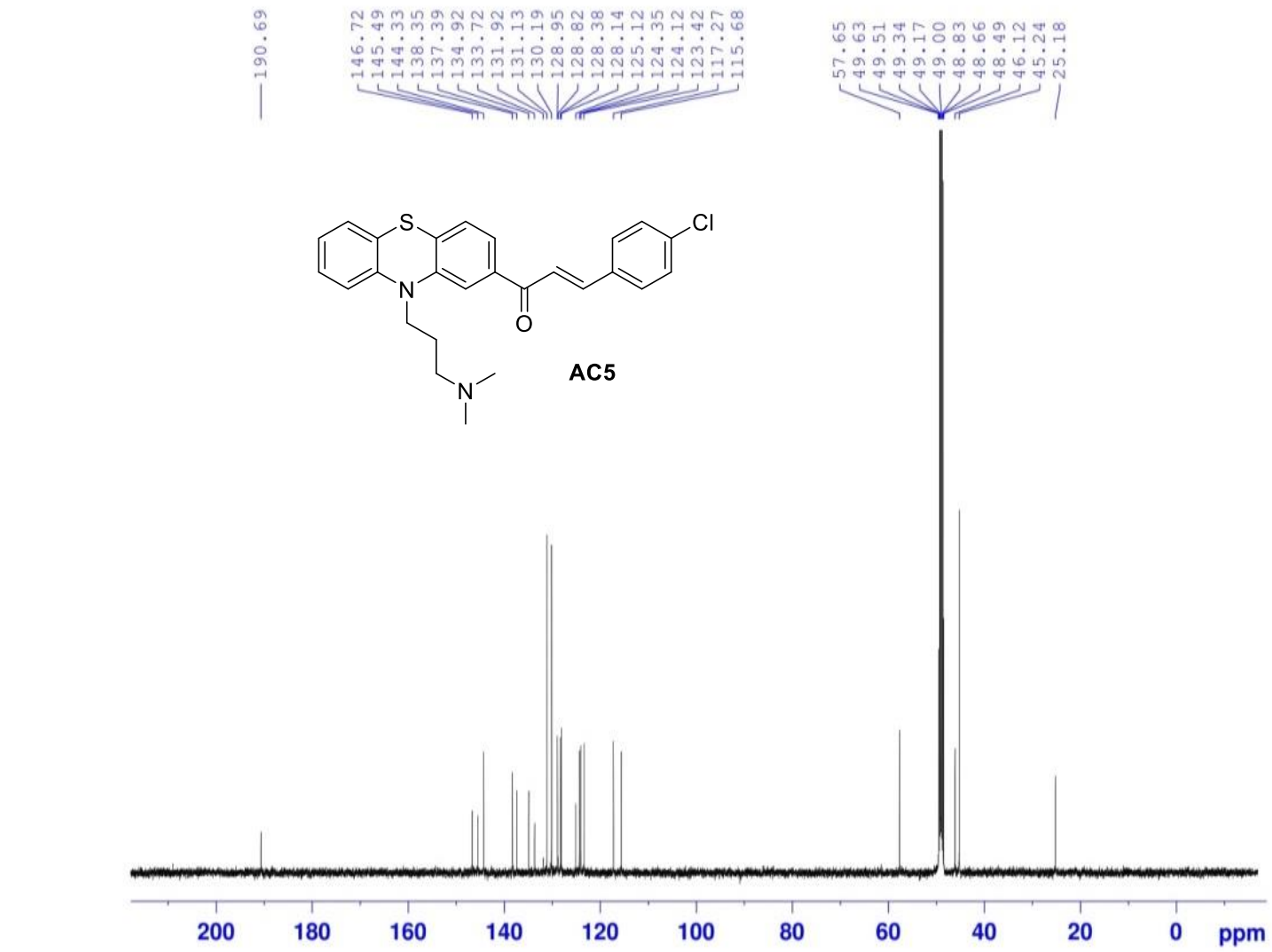

7.75
7.70
7.65
7.60
7.55
7.50
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
6.90
ppm
1.19
4.00
1.08
2.16
1.12
1.10
1.07
2.06
7.683
7.651
7.633
7.620
7.617
7.605
7.595
7.582
7.567
7.447
7.359
7.353
7.345
7.195
7.180
7.165
7.126
7.111
7.069
7.054
6.943
6.938
6.927
6.909
C9-MeOD-1H
BRUKER


S
N
O
Cl
N

AC5

^{13}C-NMR

C9-MeOD-C13CPD



BRUKER

```
Current Data Parameters
NAME                 113DAO_C9
EXPNO                        2
PROCNO                       1

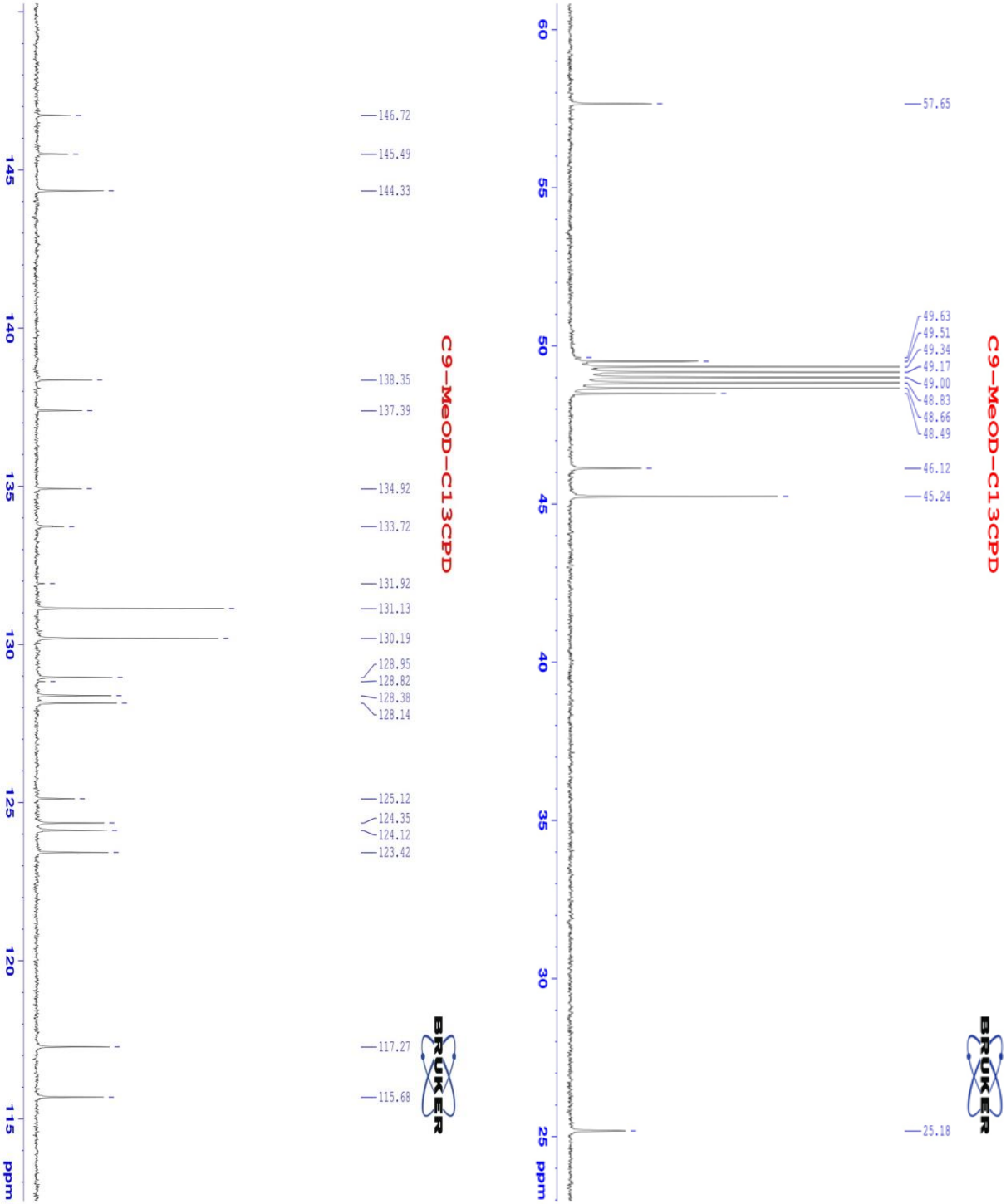
F2 - Acquisition Parameters
Date_                 20170704
Time                     16.32
INSTRUM                  spect
PROBHD     5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                   MeOD
NS                         128
DS                           4
SWH                  29761.904 Hz
FIDRES               0.454131 Hz
AQ                   1.1010048 sec
RG                      198.57
DW                      16.800 usec
DE                       6.50 usec
TE                      303.0 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          1

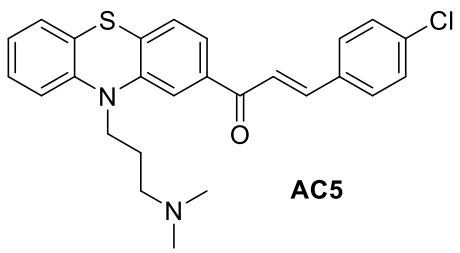
======== CHANNEL f1 ========
SFO1                125.7879670 MHz
NUC1                        13C
P1                        10.00 usec
PLW1                88.00000000 W

======== CHANNEL f2 ========
SFO2                500.2020008 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                     80.00 usec
PLW2                22.00000000 W
PLW12                0.34375000 W
PLW13                0.22000000 W

F2 - Processing parameters
SI                          32768
SF                  125.7752207 MHz
WDW                            EM
SSB                 0
LB                         1.00 Hz
GB                  0
PC                         1.40
```

^{13}C-NMR


C9-MeOD-C13CPD
146.72
145.49
144.33
138.35
137.39
134.92
133.72
131.92
131.13
130.19
128.95
128.82
128.38
128.14
125.12
124.35
124.12
123.42
117.27
115.68
57.65
49.63
49.51
49.34
49.17
49.00
48.83
48.66
48.49
46.12
45.24
25.18
ppm

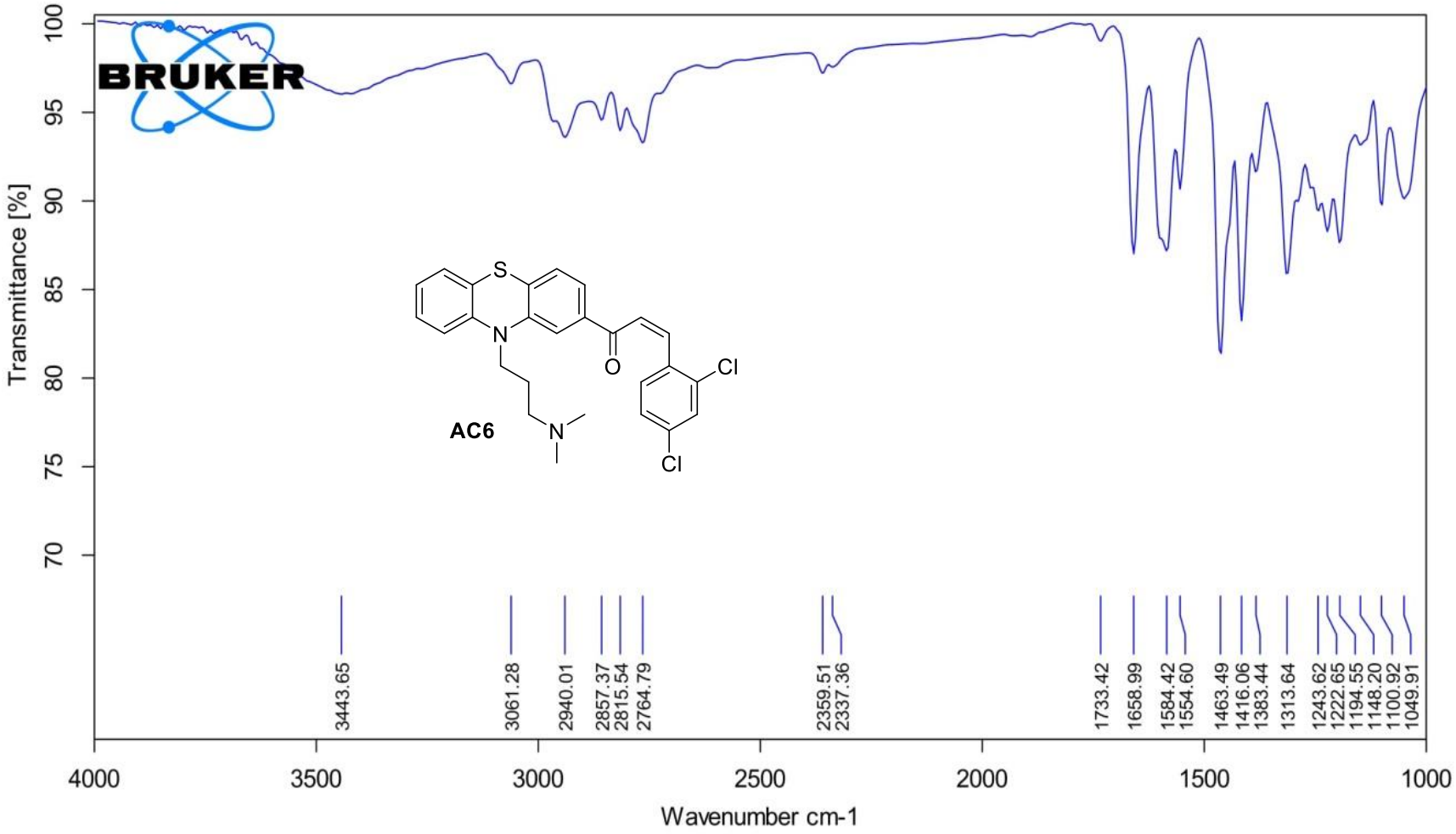

S
N
O
Cl
N

AC5

VIEN CONG NGHE HOA HOC
01 Mac Dinh Chi - Q.1 - Tp HCM

Tel: 08.38296127
Fax: 08.38293889

IR



E:\OPUS 7\2017\THANG 6\20170606\C8.0	C8	TENSOR 27 - BRUKER - GERMANY	6/8/2017

MS

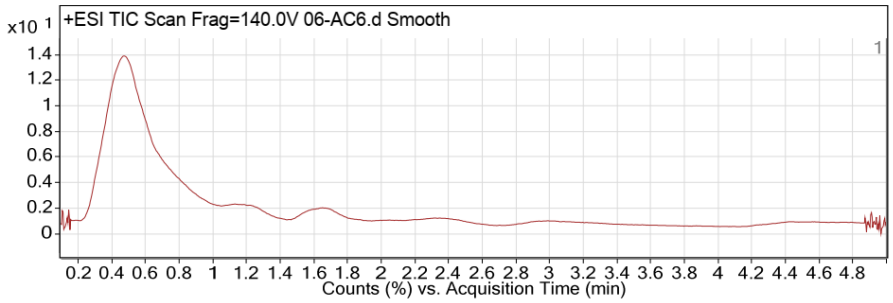
Qualitative Analysis Report

Data Filename	06-AC6.d	**Sample Name**	06-AC6
Sample Type	Sample	**Position**	P2-B3
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	22/08/2020 10:43:11 AM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

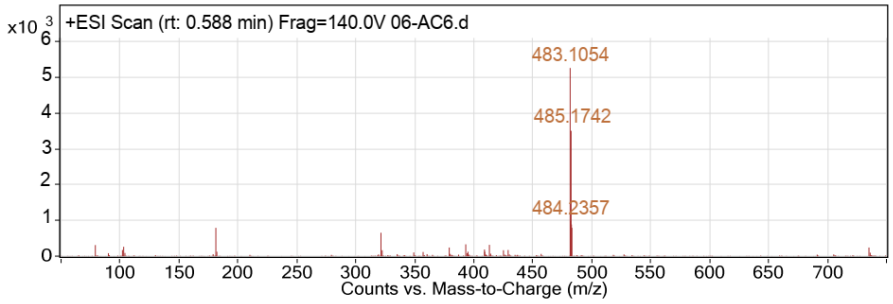
User Chromatograms

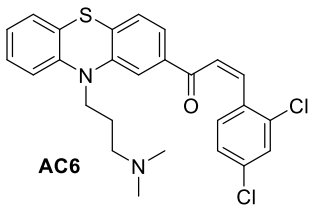
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
140	0	ESI



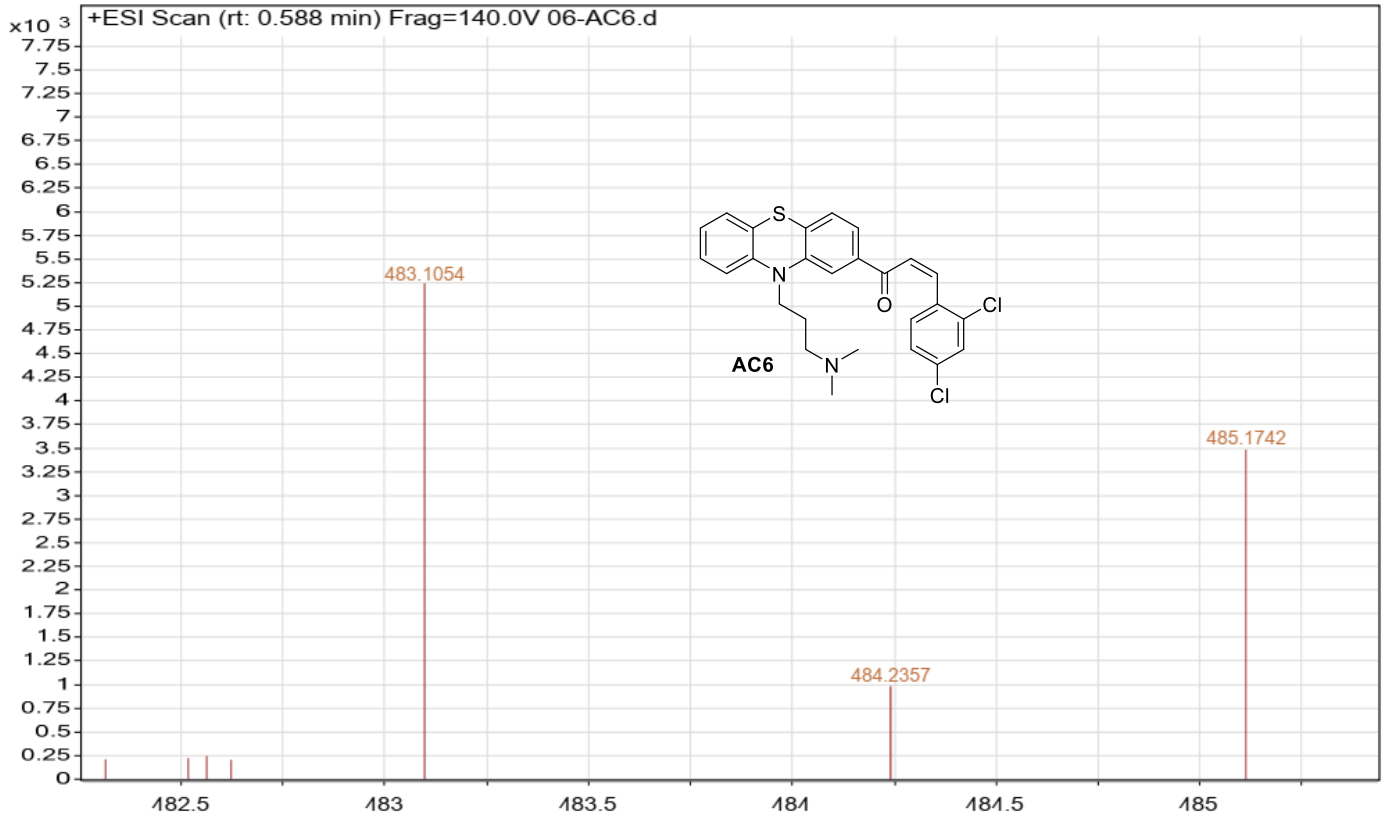


AC6

--- End Of Report ---

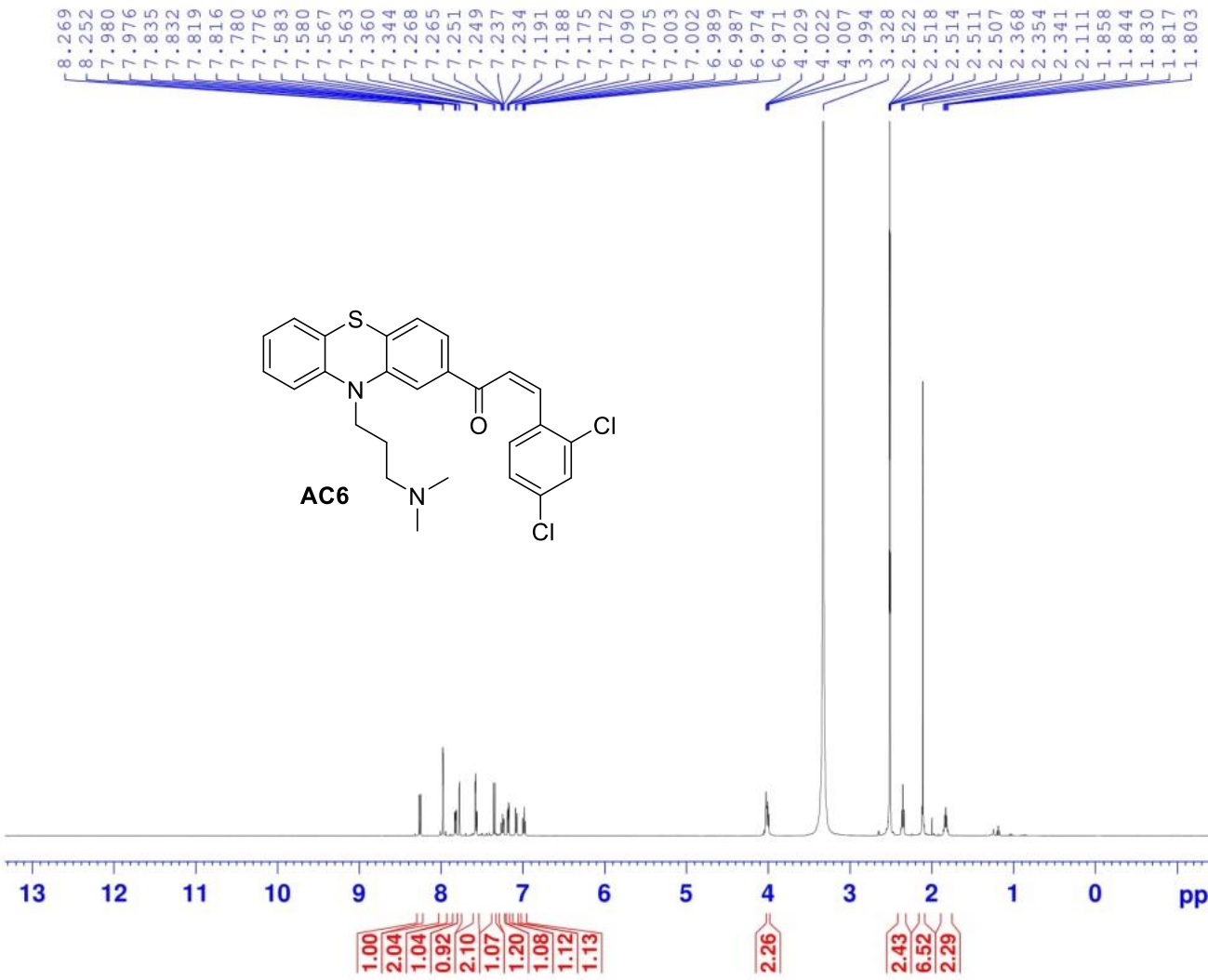
MS

Sample Name	06-AC6	**Position**	P2-B3	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	06-AC6.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	22/08/2020 10:43:11 AM



^{1}H-NMR

C8-DMSO-1H



BRUKER

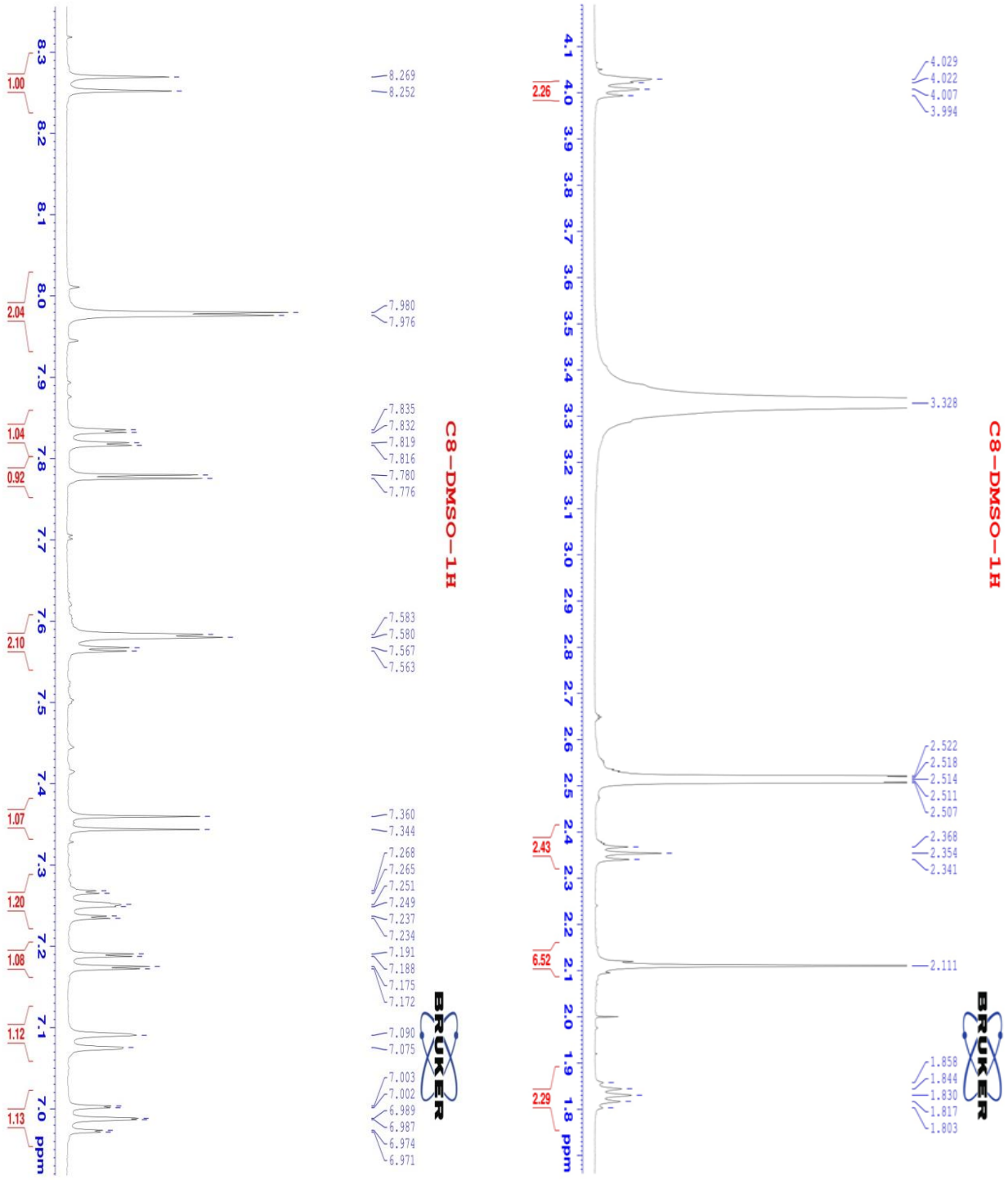
```
Current Data Parameters
NAME                  113D_C8
EXPNO                       1
PROCNO                      1

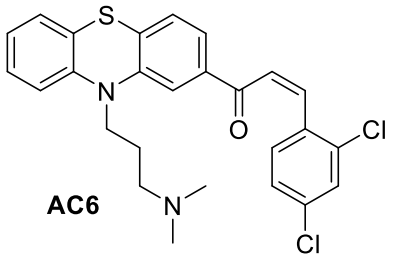
F2 - Acquisition Parameters
Date_              20170606
Time                  16.22
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ             3.2767999 sec
RG                   157.35
DW                50.000 usec
DE                 6.50 usec
TE                 303.0 K
D1             1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          500.2030889 MHz
NUC1                    1H
P1                  10.00 usec
PLW1         22.00000000 W

F2 - Processing parameters
SI                    65536
SF            500.2000000 MHz
WDW                     EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

^{1}H-NMR

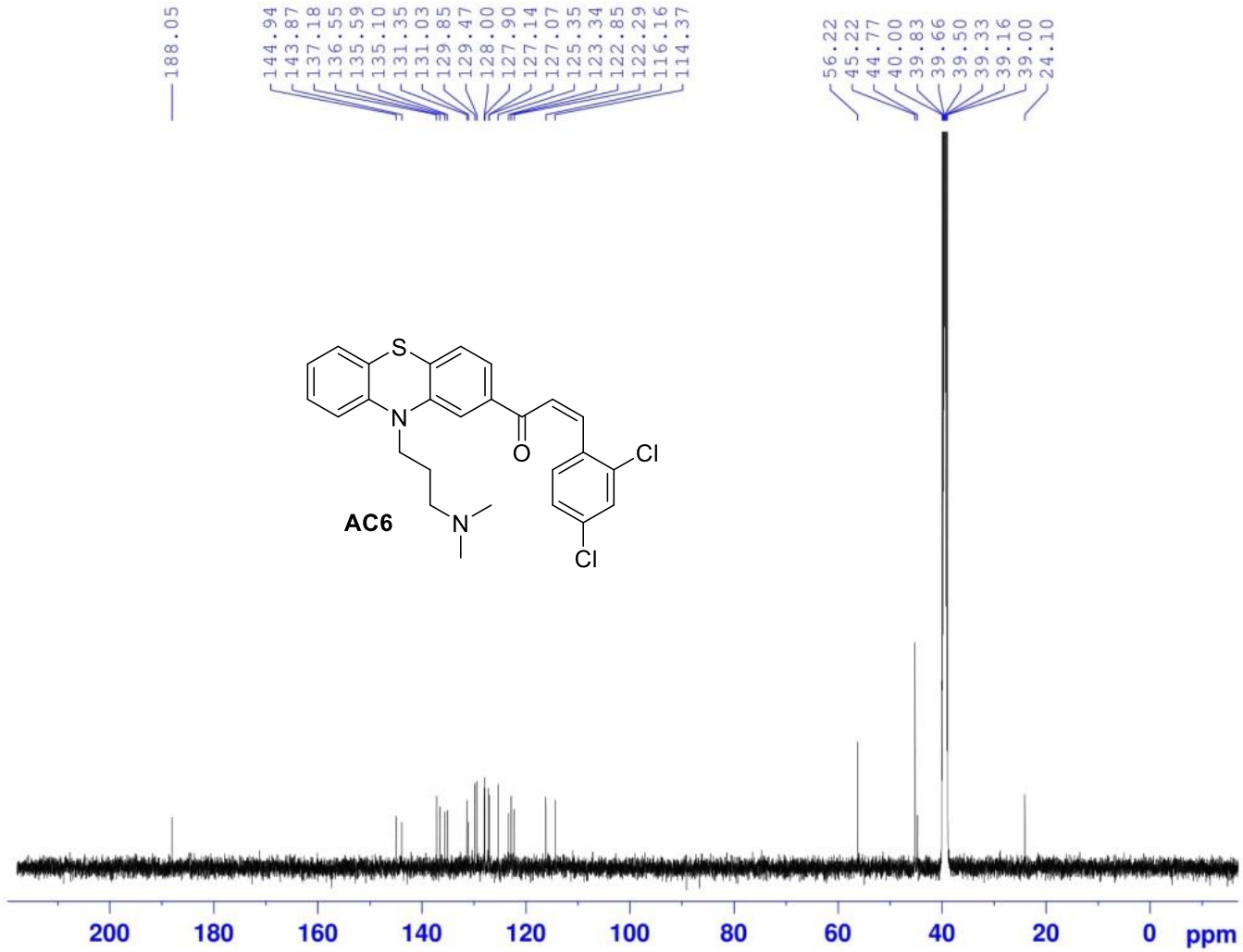




AC6

^{13}C-NMR

C8-DMSO-C13CPD




```
Current Data Parameters
NAME                  113D_C8
EXPNO                       2
PROCNO                      1

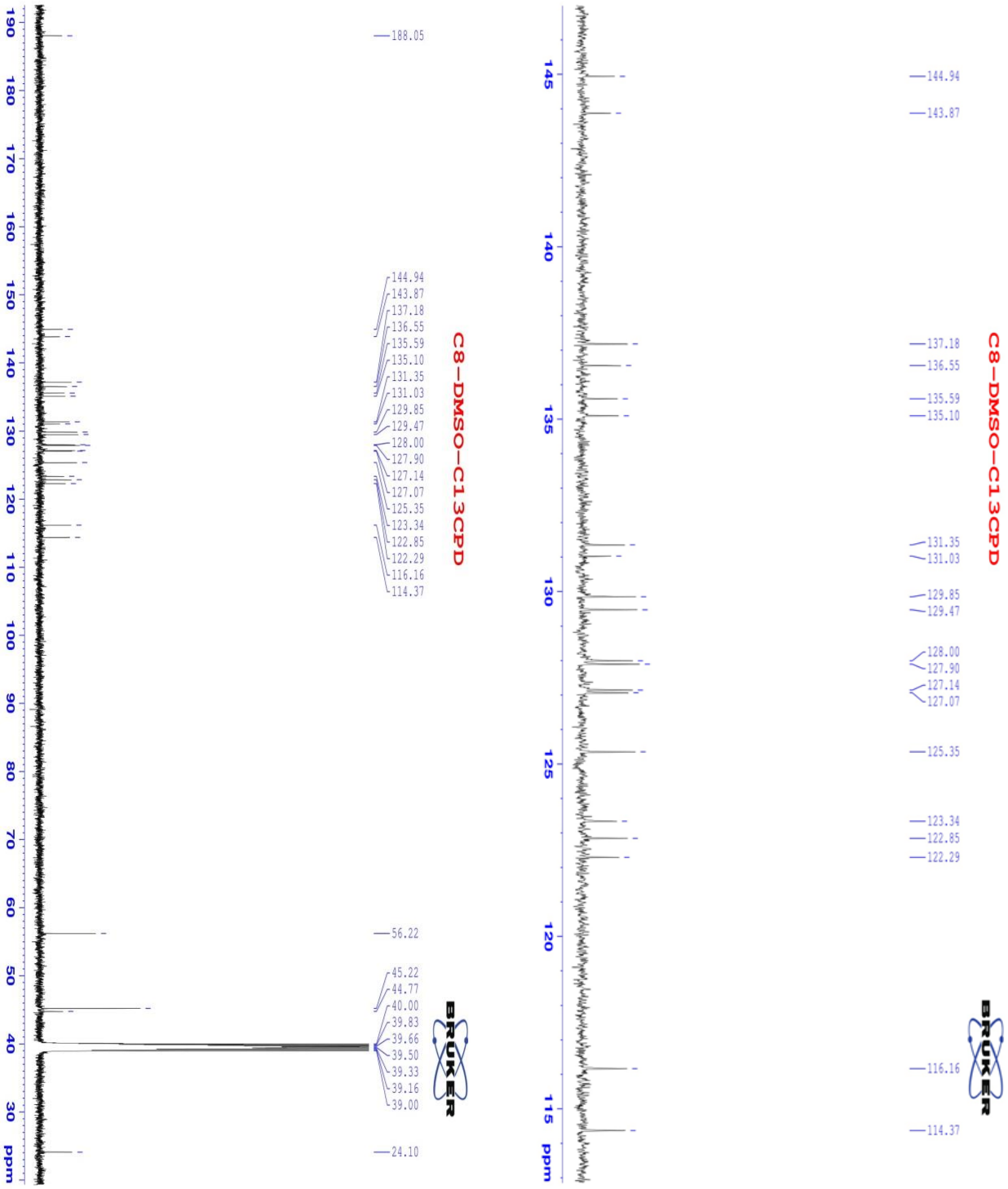
F2 - Acquisition Parameters
Date_                20170607
Time                     4.54
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                       4096
DS                          4
SWH                  29761.904 Hz
FIDRES                0.454131 Hz
AQ                    1.1010048 sec
RG                       198.57
DW                       16.800 usec
DE                        6.50 usec
TE                       303.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                         1

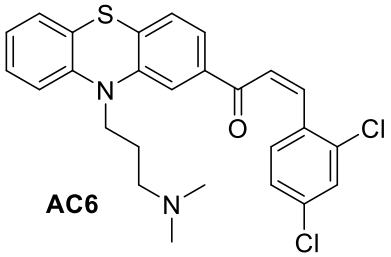
======== CHANNEL f1 ========
SFO1               125.7879670 MHz
NUC1                       13C
P1                       10.00 usec
PLW1               88.00000000 W

======== CHANNEL f2 ========
SFO2               500.2020008 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                    80.00 usec
PLW2               22.00000000 W
PLW12               0.34375000 W
PLW13               0.22000000 W

F2 - Processing parameters
SI                        32768
SF                 125.7754565 MHz
WDW                         EM
SSB                  0
LB                        1.00 Hz
GB                   0
PC                        1.40
```

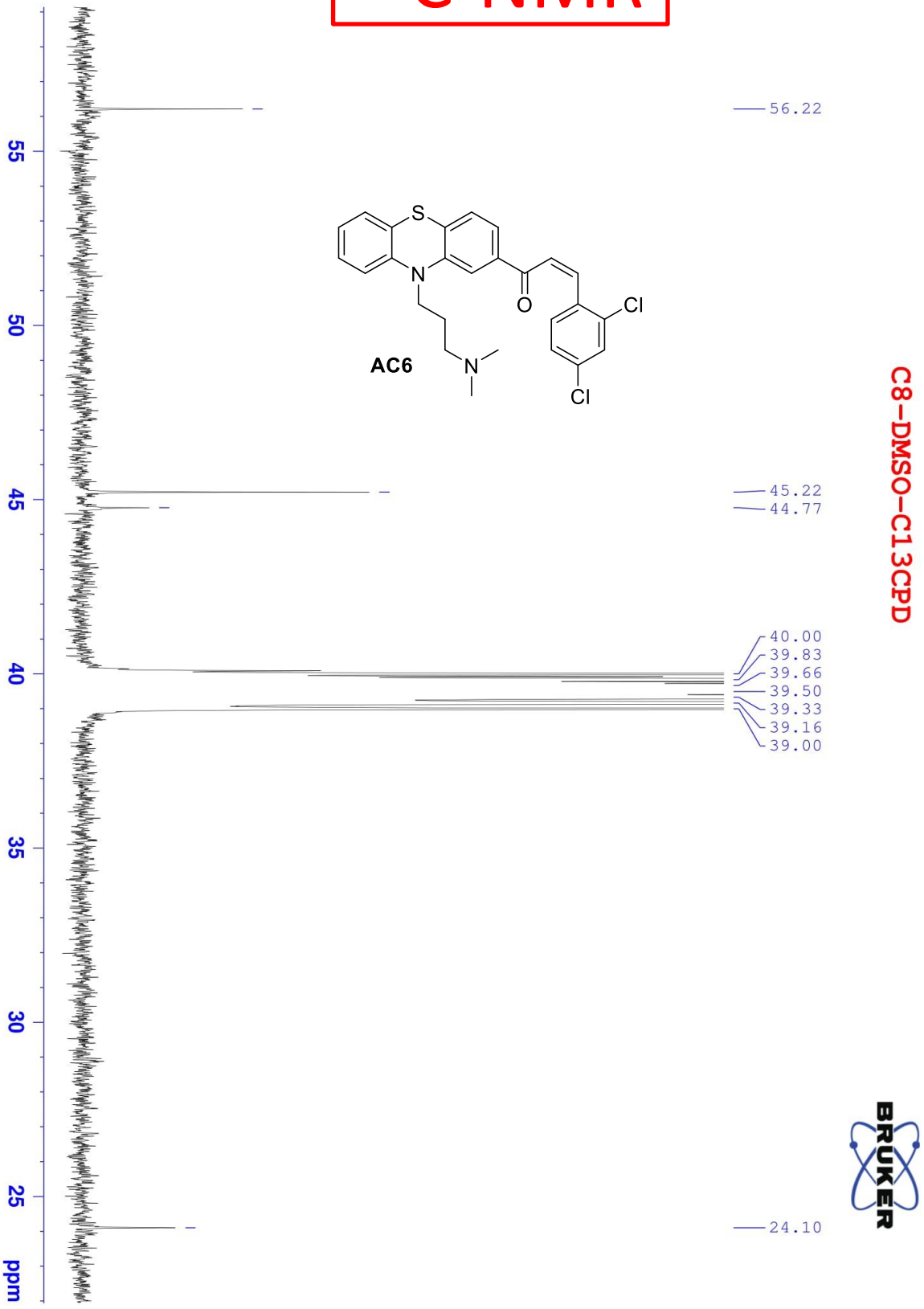
^{13}C-NMR





AC6

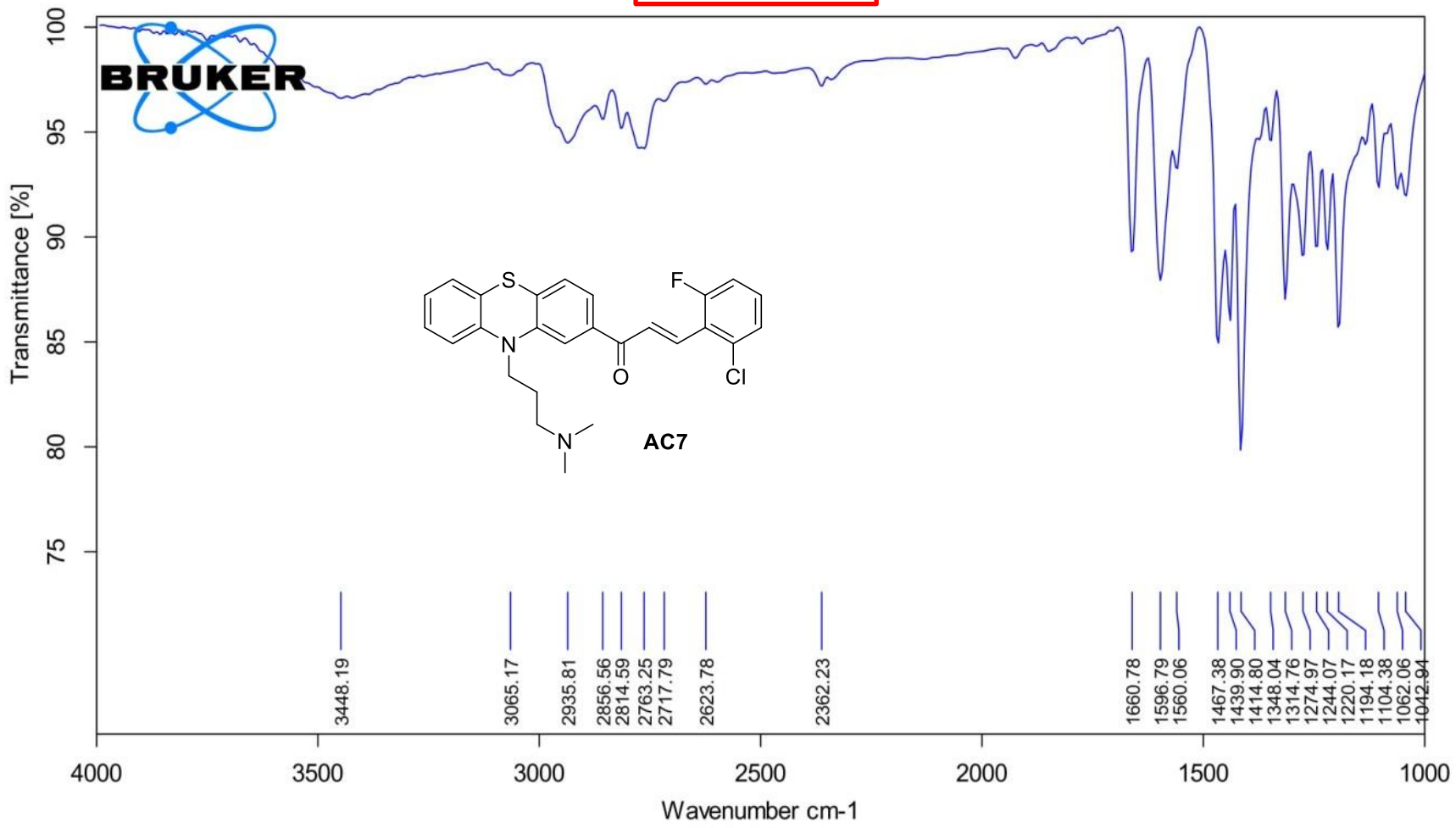
^{13}C-NMR


55
50
45
40
35
30
25
ppm
56.22
45.22
44.77
40.00
39.83
39.66
39.50
39.33
39.16
39.00
24.10
S
N
O
Cl
Cl
N
AC6
C8-DMSO-C13CPD
BRUKER

VIEN CONG NGHE HOA HOC
01 Mac Dinh Chi - Q.1 - Tp HCM

Tel: 08.38296127
Fax: 08.38293889

IR



E:\OPUS 7\2017\THANG 6\20170606\C6.0	C6	TENSOR 27 - BRUKER - GERMANY	6/8/2017

MS

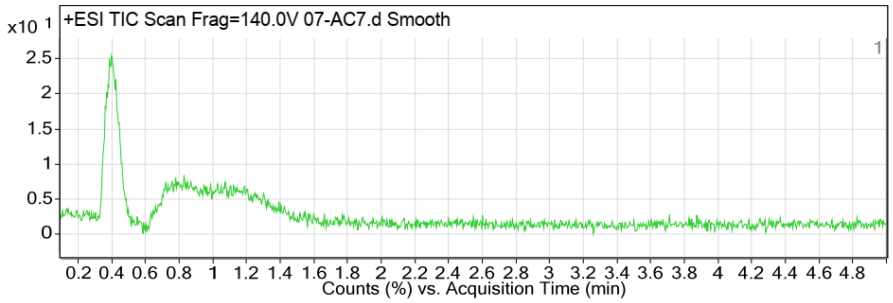
Qualitative Analysis Report

Data Filename	07-AC7.d	**Sample Name**	07-AC7
Sample Type	Sample	**Position**	P2-B7
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	22/08/2020 10:55:28 AM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

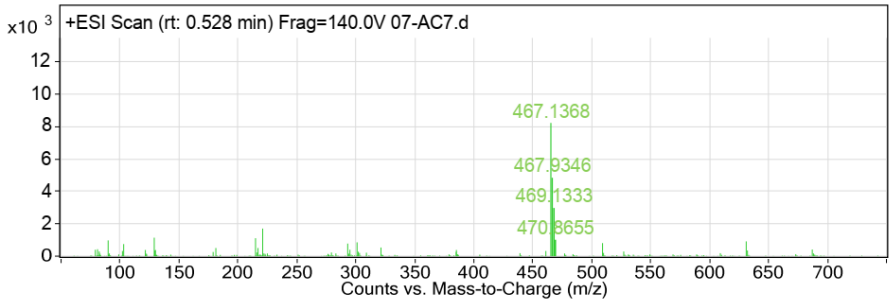
User Chromatograms

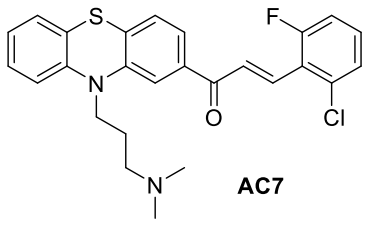
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



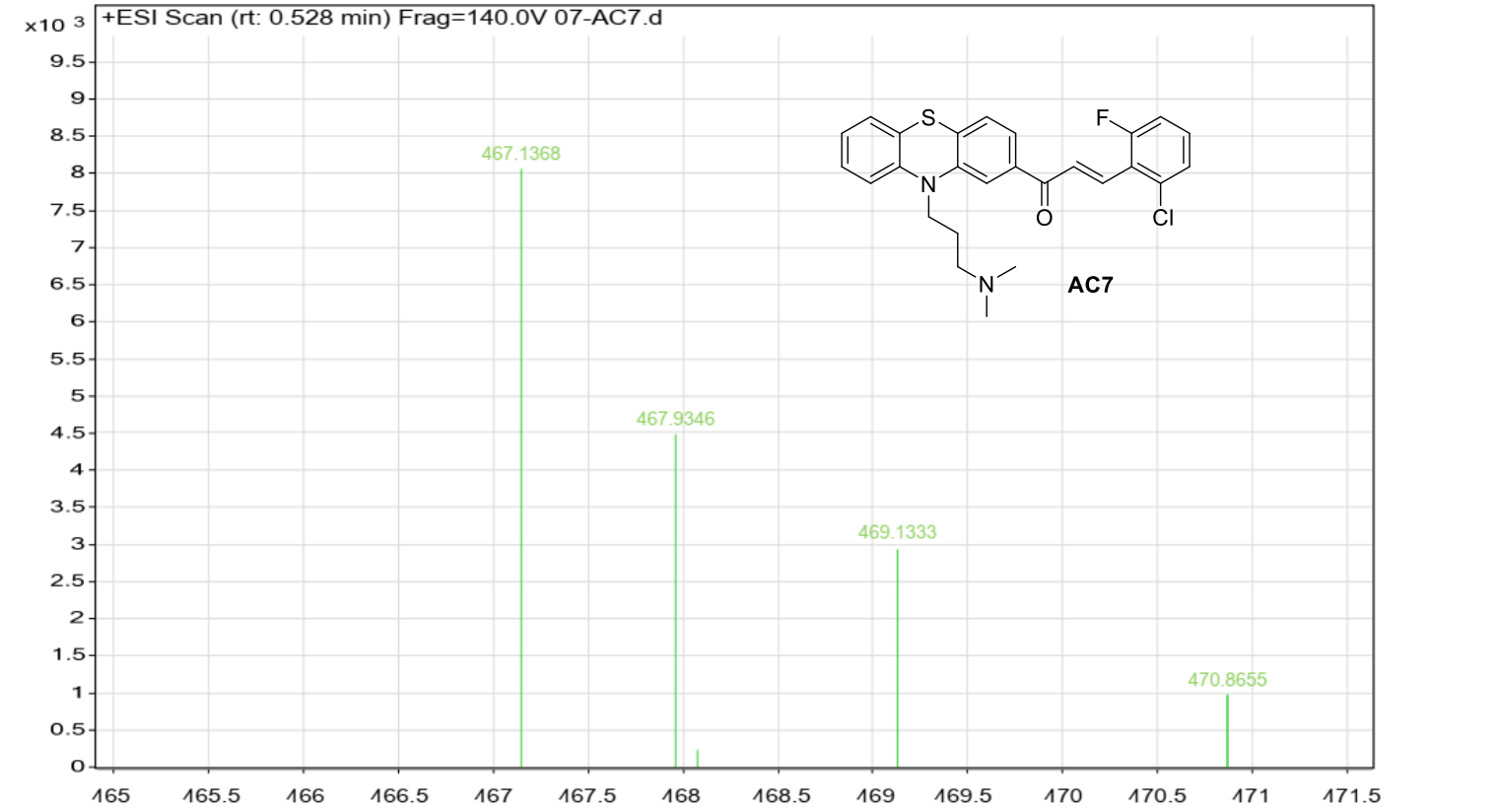


AC7

--- End Of Report ---

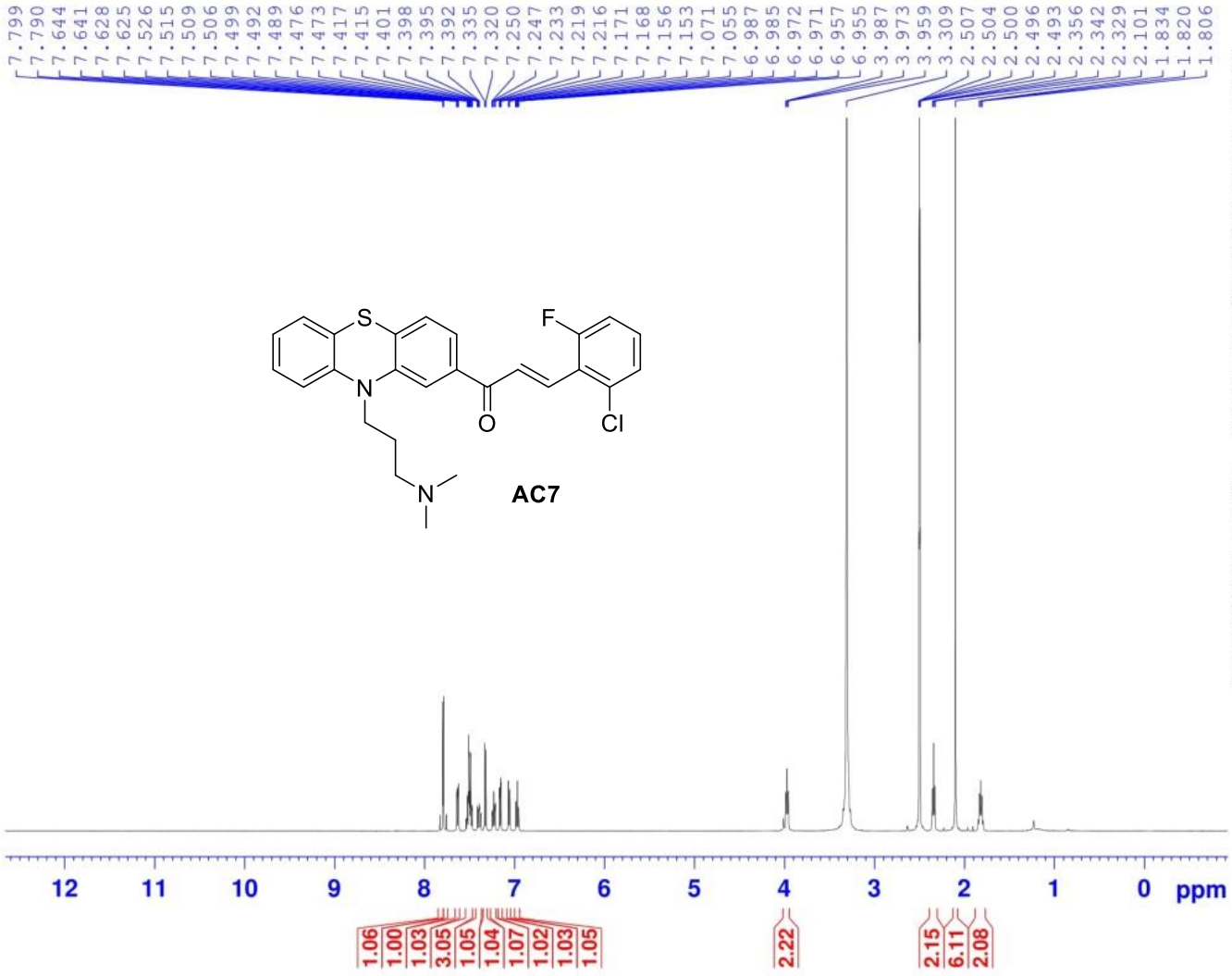
MS

Sample Name	07-AC7	**Position**	P2-B7	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	07-AC7.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	22/08/2020 10:55:28 AM



^{1}H-NMR

C6-DMSO-1H



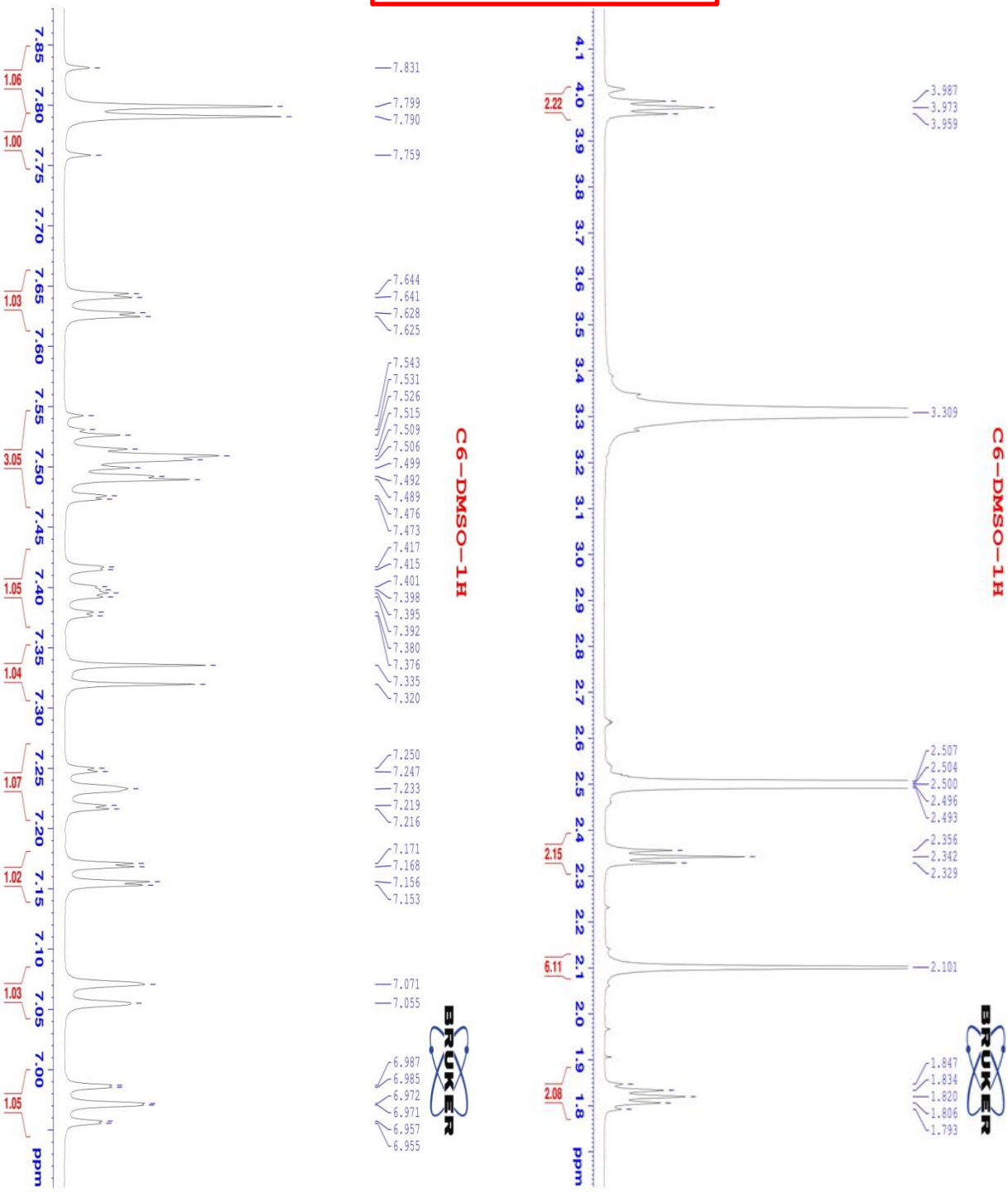

```
Current Data Parameters
NAME                  113D_C6
EXPNO                       1
PROCNO                      1

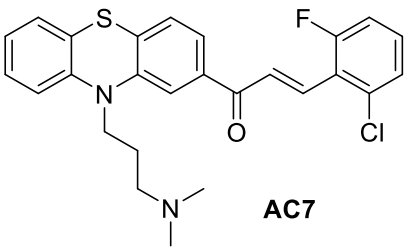
F2 - Acquisition Parameters
Date_               20170606
Time                   16.18
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH              10000.000 Hz
FIDRES           0.152588 Hz
AQ               3.2767999 sec
RG                    157.35
DW                  50.000 usec
DE                   6.50 usec
TE                   303.0 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            500.2030889 MHz
NUC1                    1H
P1                   10.00 usec
PLW1           22.00000000 W

F2 - Processing parameters
SI                    65536
SF              500.2000052 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

^{1}H-NMR

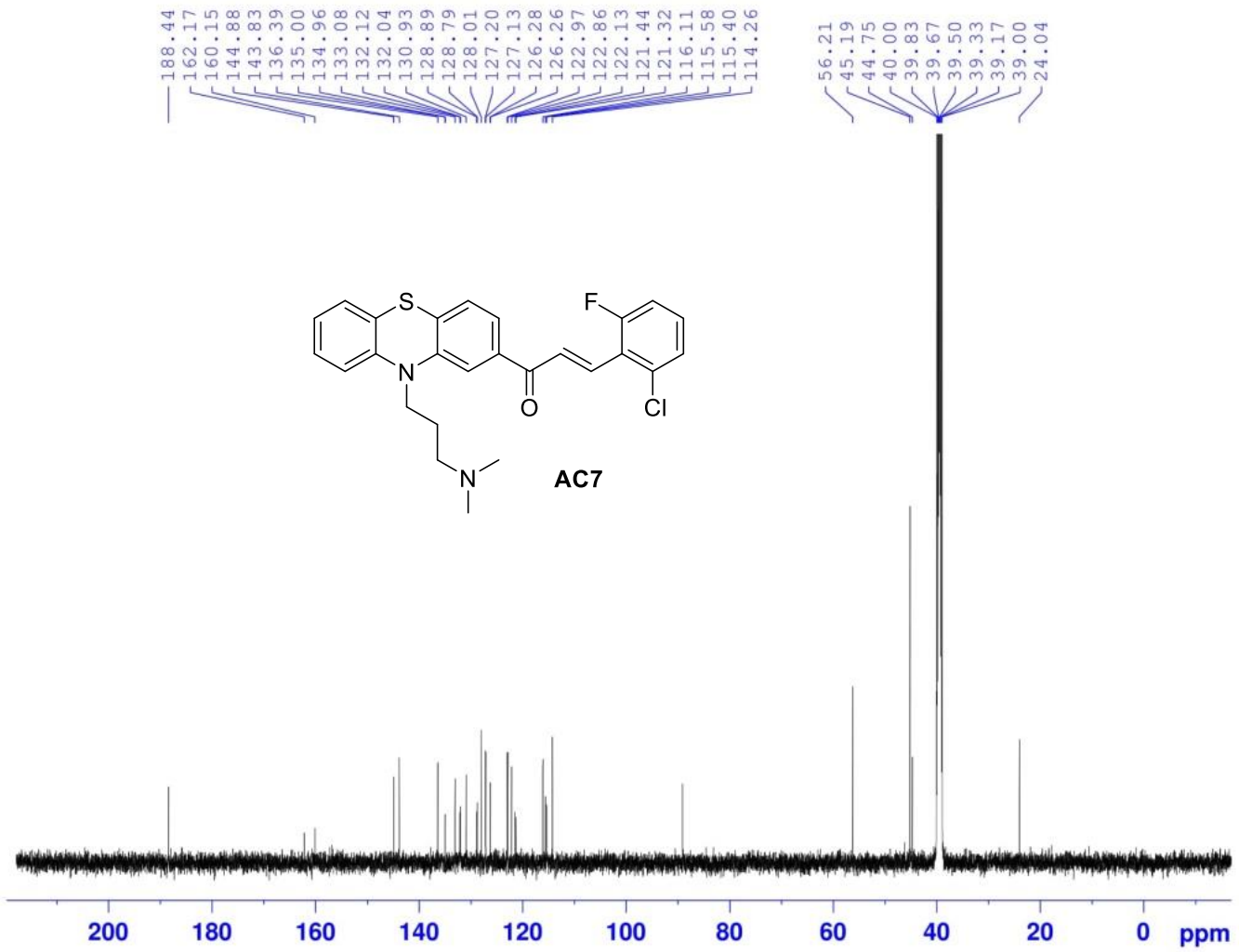




AC7

^{13}C-NMR

C6-DMSO-C13CPD



BRUKER

```
Current Data Parameters
NAME                  113D_C6
EXPNO                       2
PROCNO                      1

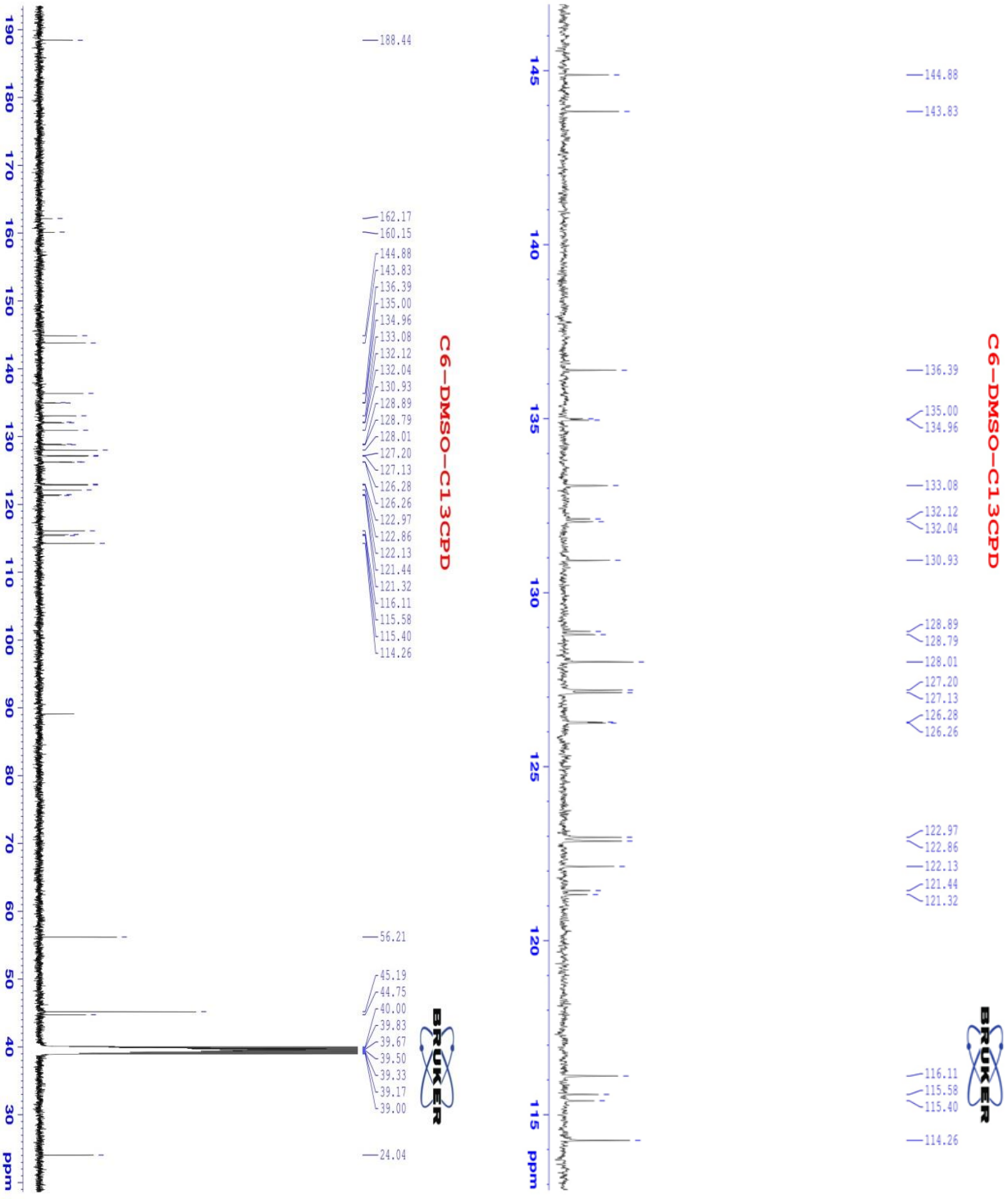
F2 - Acquisition Parameters
Date_                20170607
Time                     1.15
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                       3072
DS                          4
SWH                29761.904 Hz
FIDRES             0.454131 Hz
AQ                 1.1010048 sec
RG                     198.57
DW                     16.800 usec
DE                      6.50 usec
TE                     303.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

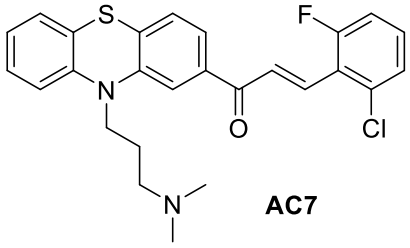
======== CHANNEL f1 ========
SFO1             125.7879670 MHz
NUC1                     13C
P1                     10.00 usec
PLW1              88.00000000 W

======== CHANNEL f2 ========
SFO2             500.2020008 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                  80.00 usec
PLW2              22.00000000 W
PLW12              0.34375000 W
PLW13              0.22000000 W

F2 - Processing parameters
SI                       32768
SF               125.7754563 MHz
WDW                         EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

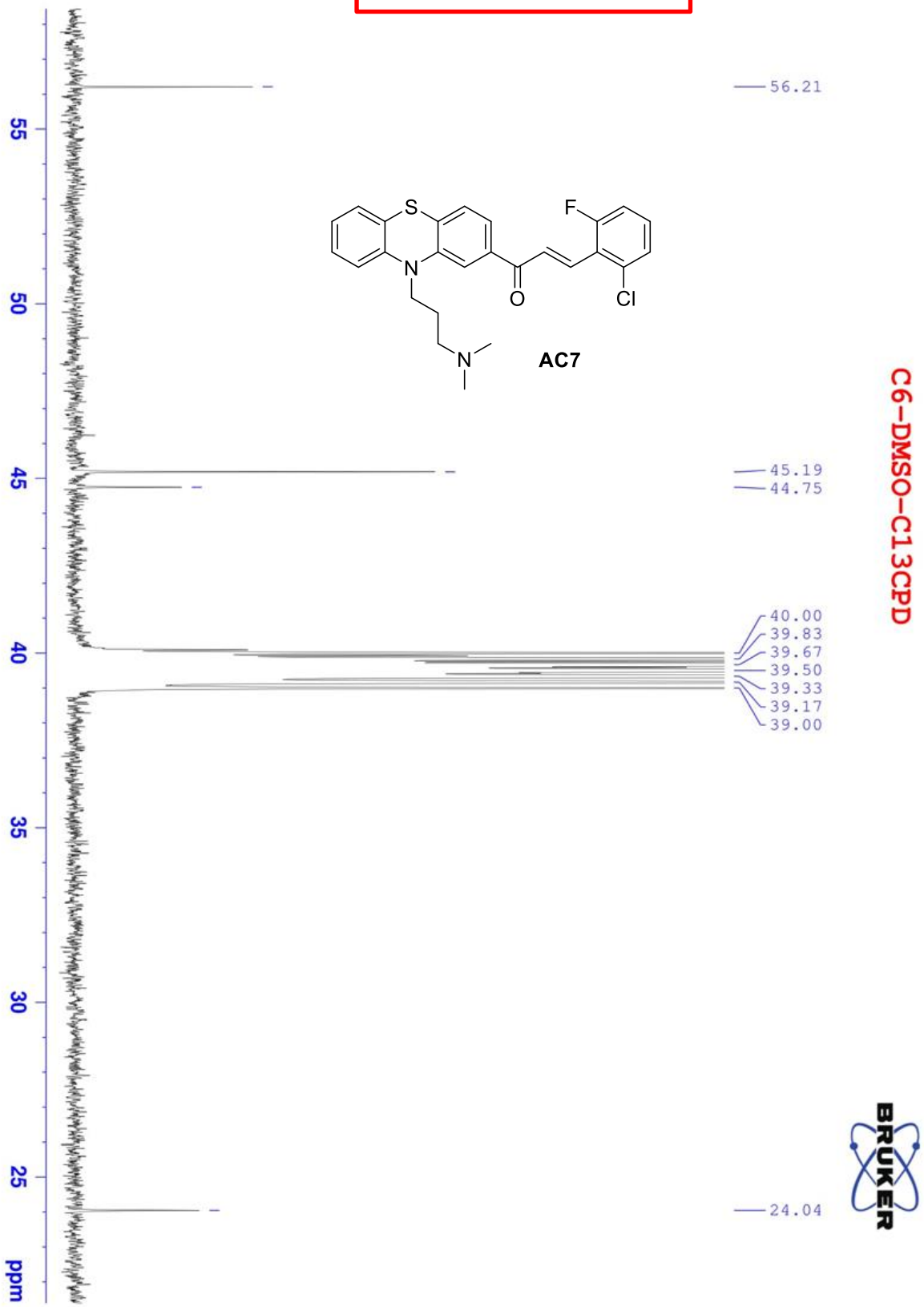
^{13}C-NMR


188.44
162.17
160.15
144.88
143.83
136.39
135.00
134.96
133.08
132.12
132.04
130.93
128.89
128.79
128.01
127.20
127.13
126.28
126.26
122.97
122.86
122.13
121.44
121.32
116.11
115.58
115.40
114.26
56.21
45.19
44.75
40.00
39.83
39.67
39.50
39.33
39.17
39.00
24.04
C6-DMSO-C13CPD
BRUKER
ppm


S
F
N
O
Cl
N

AC7

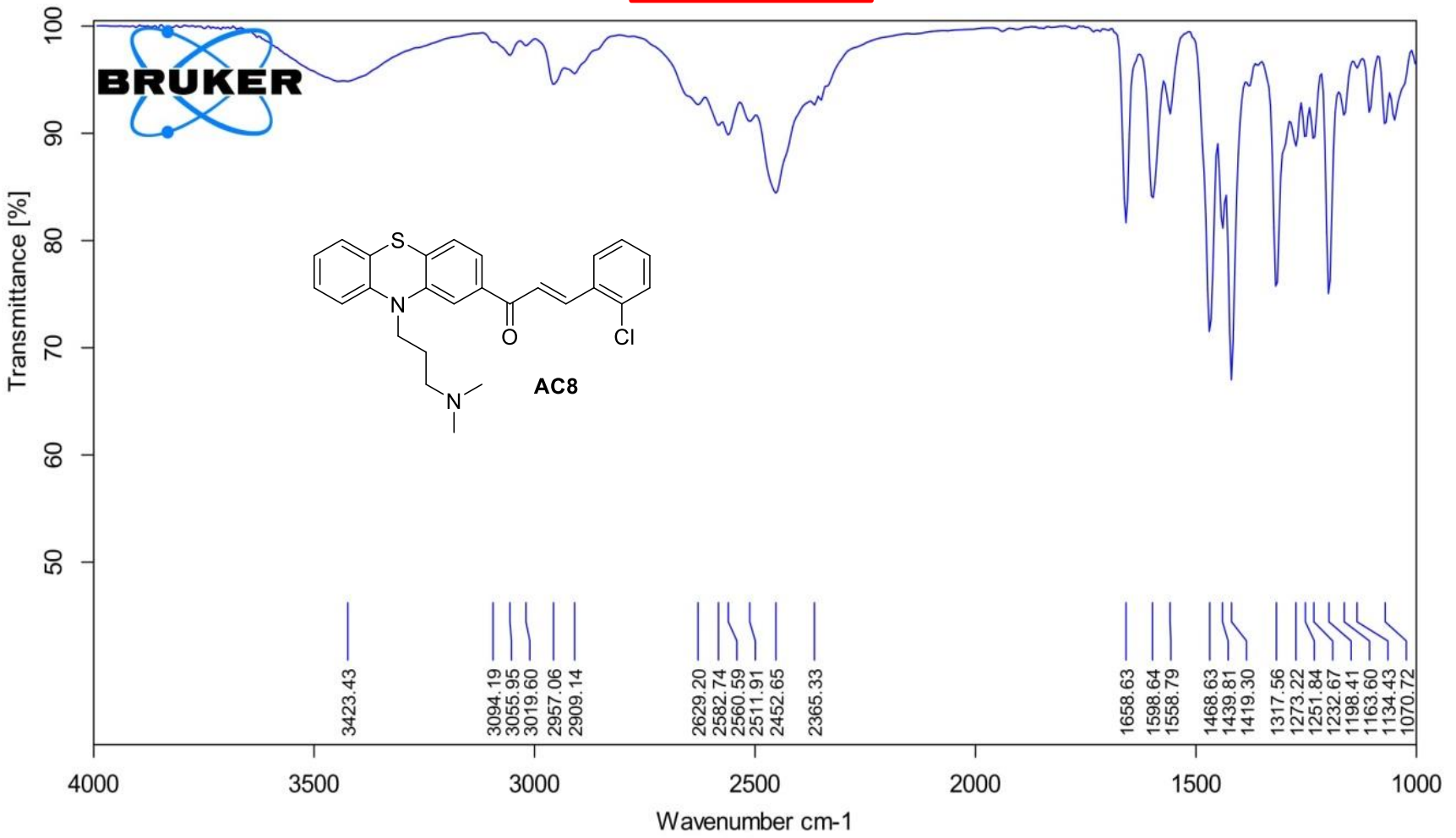
^{13}C-NMR


55
50
45
40
35
30
25
ppm
56.21
45.19
44.75
40.00
39.83
39.67
39.50
39.33
39.17
39.00
24.04
S
F
N
O
Cl
N
AC7
C6-DMSO-C13CPD
BRUKER

VIEN CONG NGHE HOA HOC
01 Mac Dinh Chi - Q.1 - Tp HCM

Tel: 08.38296127
Fax: 08.38293889

IR



E:\OPUS 7\2017\THANG 6\20170606\C1.0	C1	TENSOR 27 - BRUKER - GERMANY	6/6/2017

MS

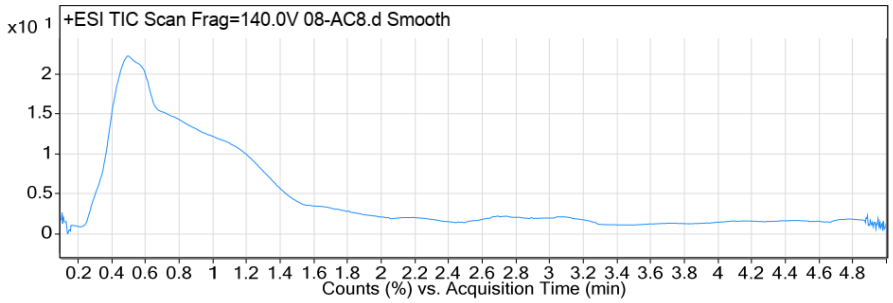
Qualitative Analysis Report

Data Filename	08-AC8.d	**Sample Name**	08-AC8
Sample Type	Sample	**Position**	P2-C5
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	22/08/2020 11:14:25 AM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

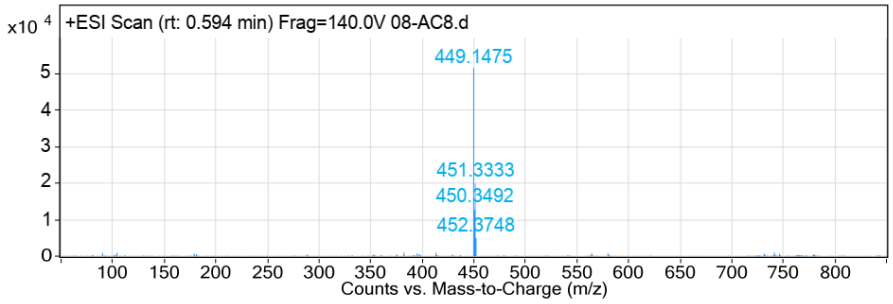
User Chromatograms

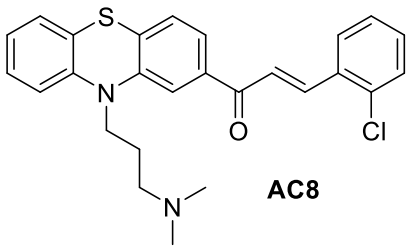
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



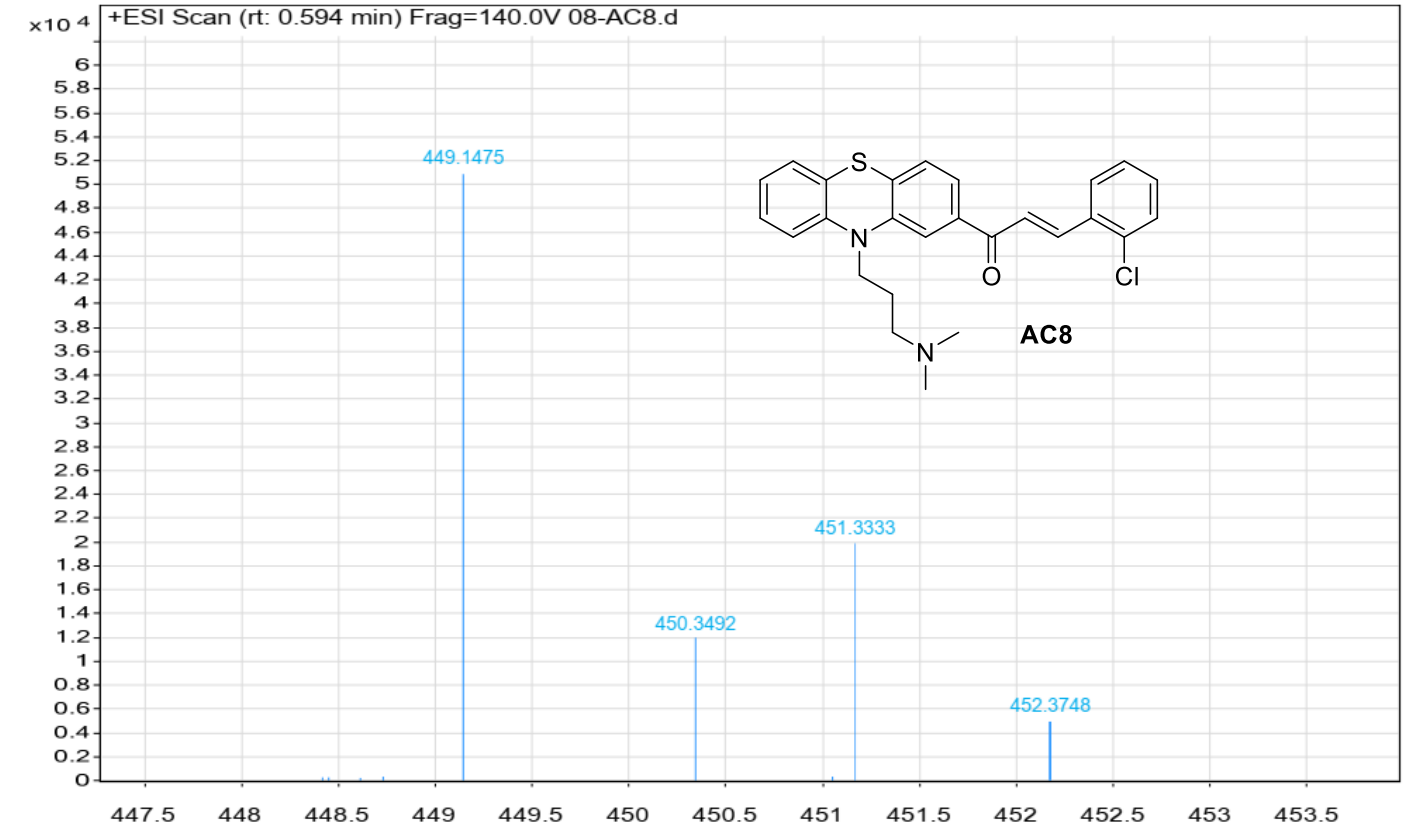


AC8

--- End Of Report ---

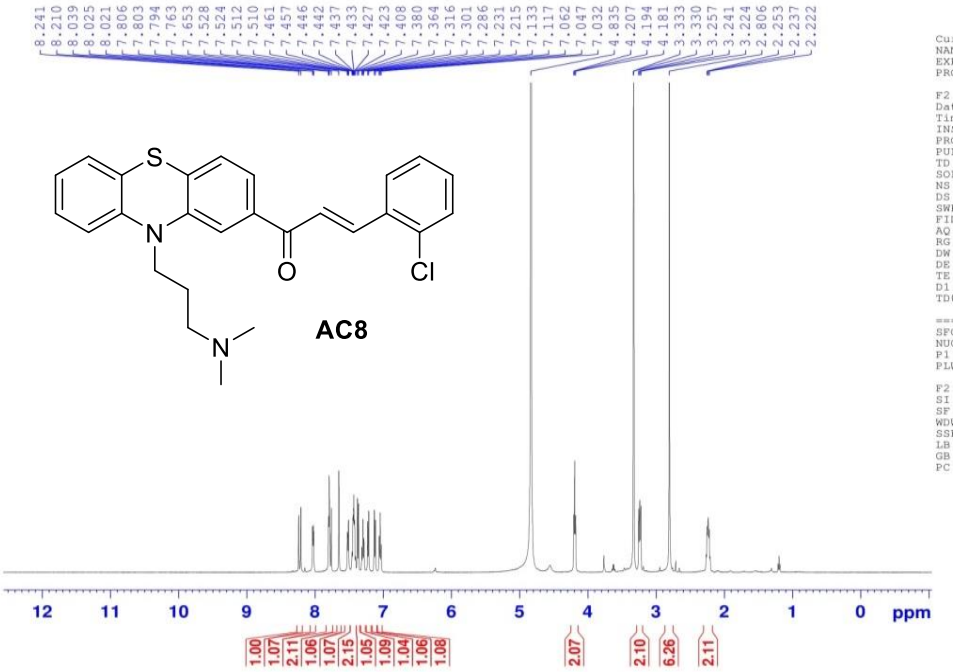
MS

Sample Name	08-AC8	**Position**	P2-C5	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	08-AC8.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	22/08/2020 11:14:25 AM



^{1}H-NMR

C1-MeOD-1H



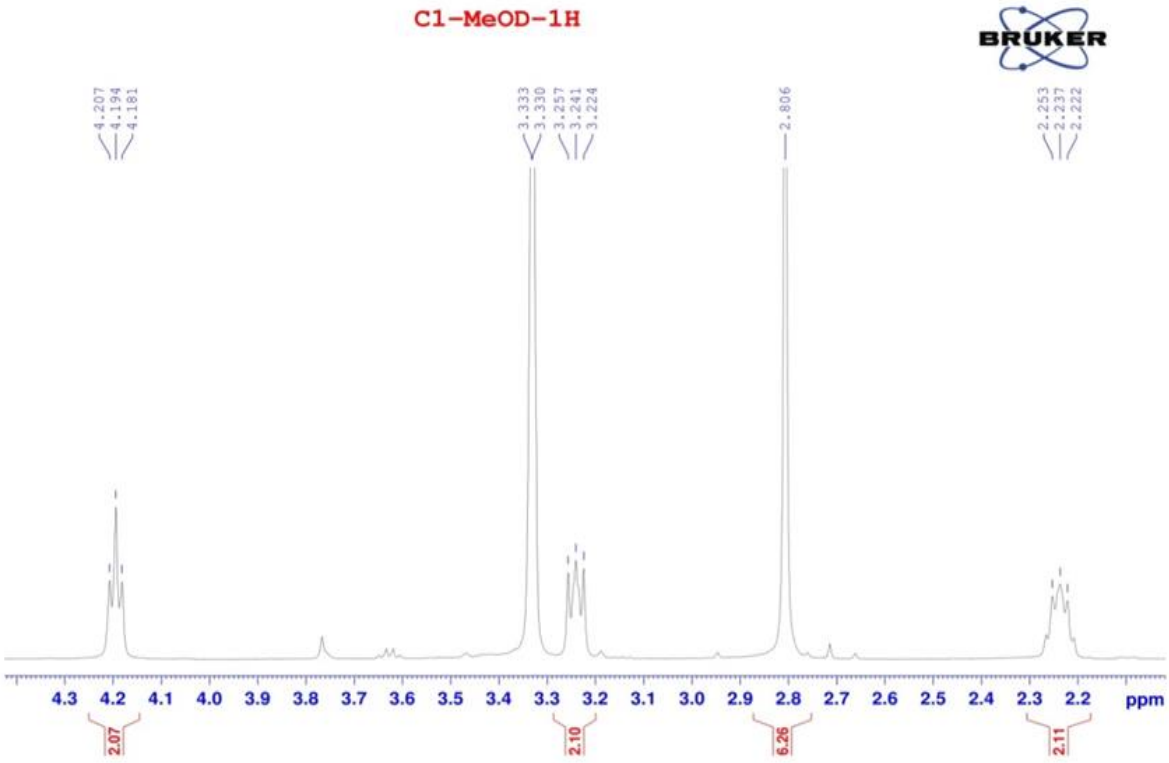
BRUKER

```
Current Data Parameters
NAME                  113D_C1
EXPNO                       1
PROCNO                      1

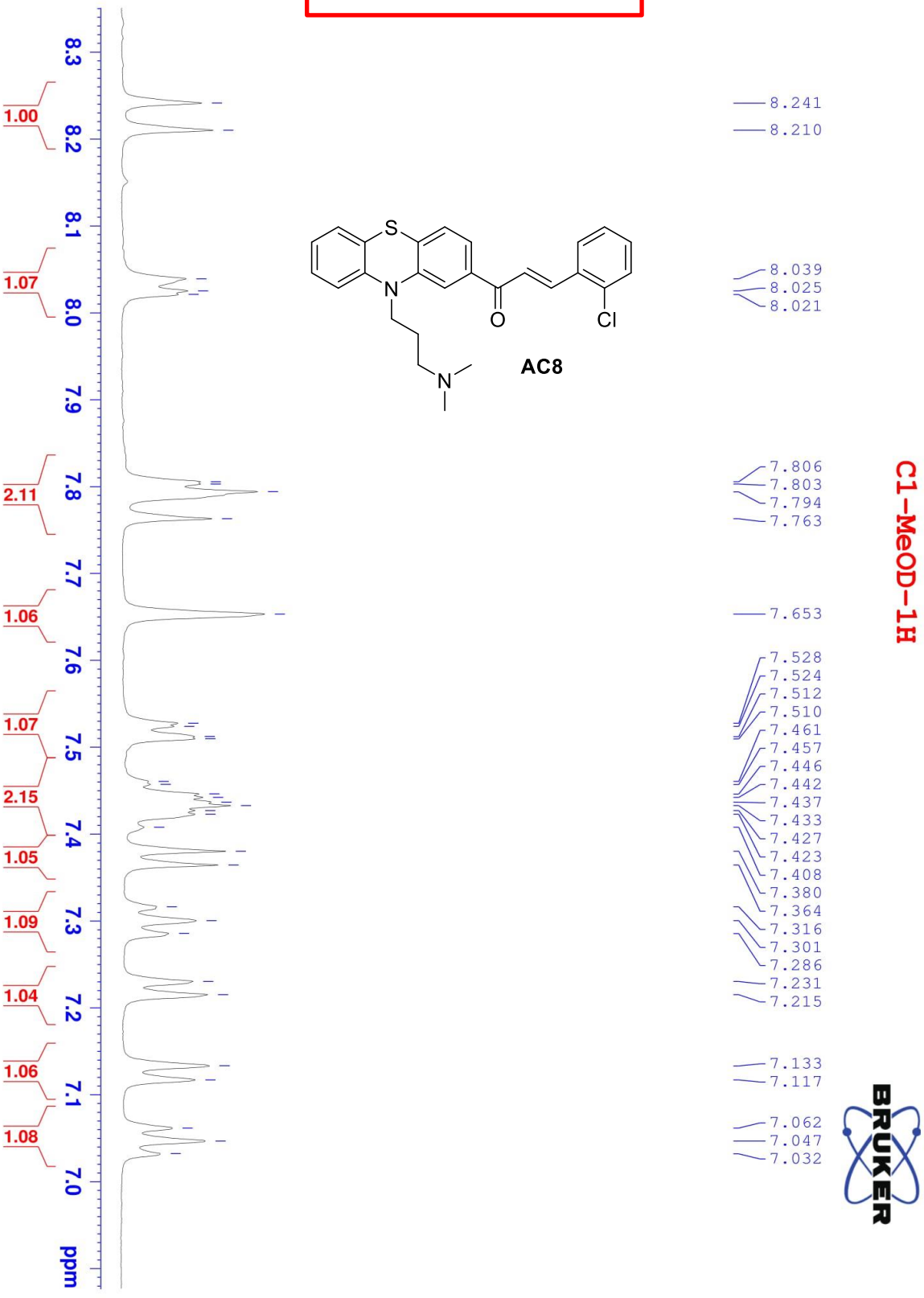
F2 - Acquisition Parameters
Date_               20170606
Time                   15.08
INSTRUM                apect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT                MeOD
NS                       16
DS                        2
SWH               10000.000 Hz
FIDRES                0.152588 Hz
AQ                 3.2767999 sec
RG                    157.35
DW                    50.000 usec
DE                     6.50 usec
TE                    303.0 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1              500.2030889 MHz
NUC1                       1H
P1                     10.00 usec
PLW1              22.00000000 W

F2 - Processing parameters
SI                        65536
SF                500.2000008 MHz
WDW                         EM
SSB                0
LB                     0.30 Hz
GB                 0
PC                     1.00
```

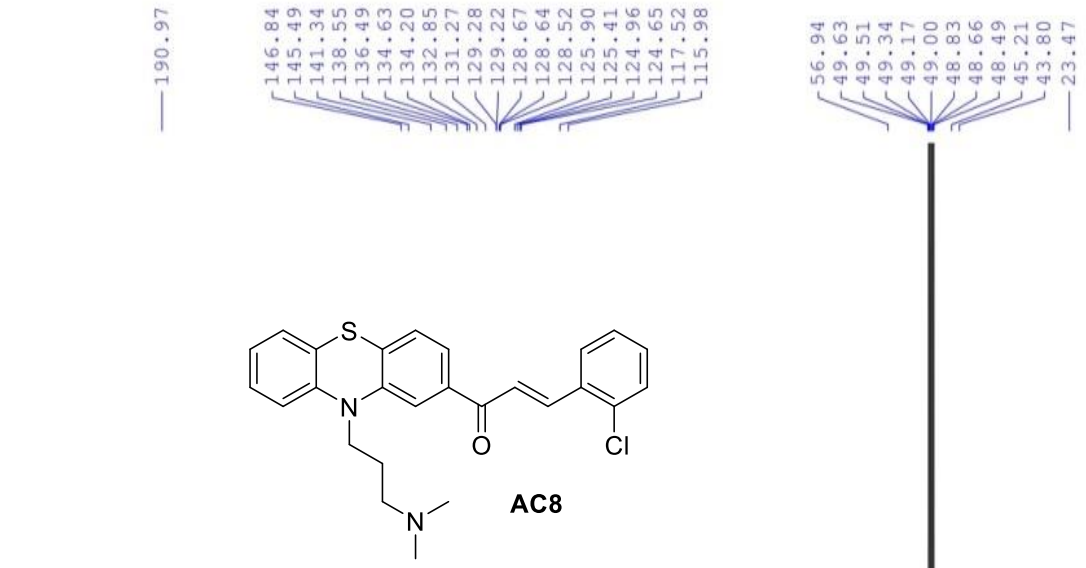

C1-MeOD-1H
BRUKER
4.207
4.194
4.181
3.333
3.330
3.257
3.241
3.224
2.806
2.253
2.237
2.222
4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 ppm
2.07
2.10
6.26
2.11

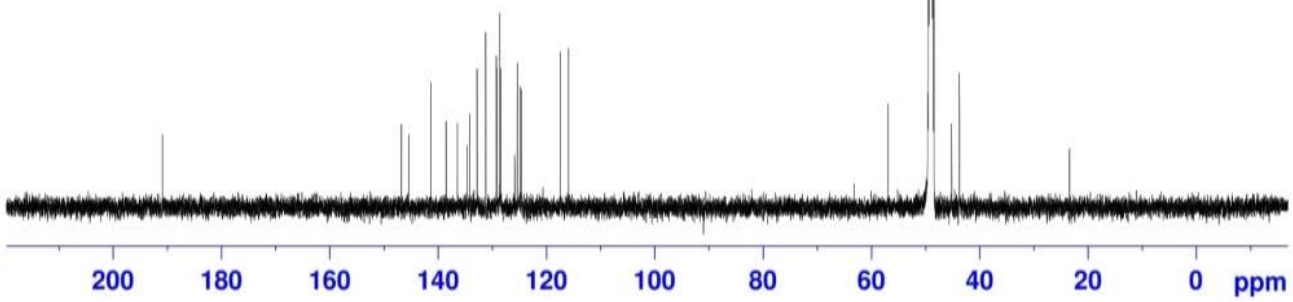
^{1}H-NMR


8.241
8.210
8.039
8.025
8.021
7.806
7.803
7.794
7.763
7.653
7.528
7.524
7.512
7.510
7.461
7.457
7.446
7.442
7.437
7.433
7.427
7.423
7.408
7.380
7.364
7.316
7.301
7.286
7.231
7.215
7.133
7.117
7.062
7.047
7.032
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
ppm
1.00
1.07
2.11
1.06
1.07
2.15
1.05
1.09
1.04
1.06
1.08
S
N
O
Cl
N
AC8
C1-MeOD-1H
BRUKER

^{13}C-NMR

C1-MeOD-C13CPD






```
Current Data Parameters
NAME                  113D_C1
EXPNO                       2
PROCNO                      1

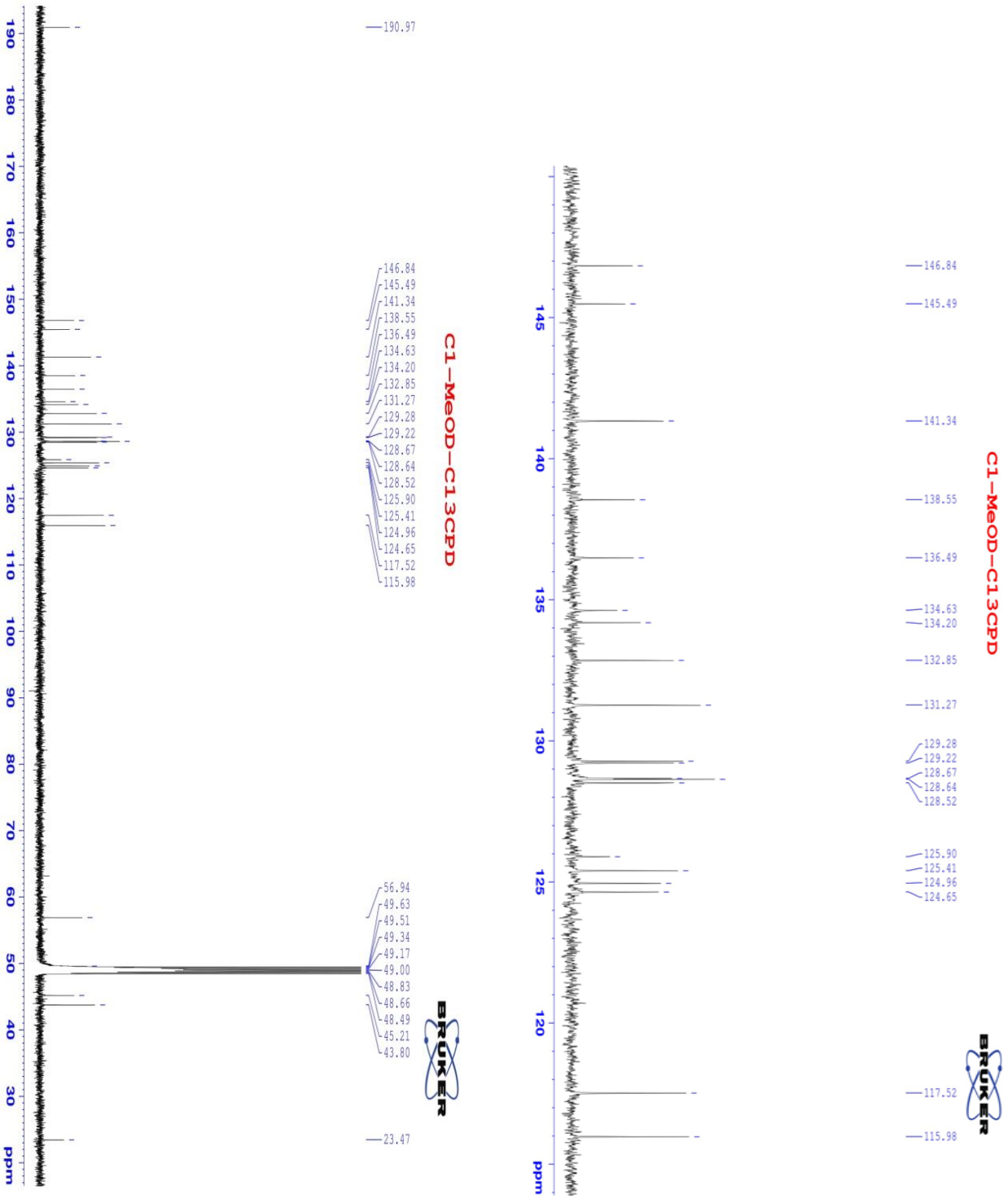
F2 - Acquisition Parameters
Date_                20170607
Time                     7.46
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg30
TD                      65536
SOLVENT                  MeOD
NS                       2048
DS                          4
SWH                29761.904 Hz
FIDRES             0.454131 Hz
AQ                 1.1010048 sec
RG                     198.57
DW                     16.800 usec
DE                      6.50 usec
TE                     303.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

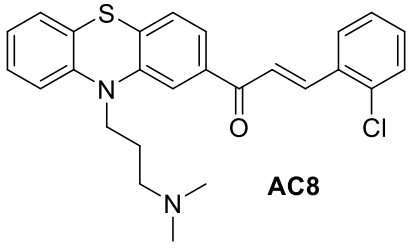
======== CHANNEL f1 ========
SFO1            125.7879670 MHz
NUC1                     13C
P1                     10.00 usec
PLW1            88.00000000 W

======== CHANNEL f2 ========
SFO2            500.2020008 MHz
NUC2                     1H
CPDPRG[2             waltz16
PCPD2                  80.00 usec
PLW2            22.00000000 W
PLW12            0.34375000 W
PLW13            0.22000000 W

F2 - Processing parameters
SI                       32768
SF              125.7752134 MHz
WDW                         EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

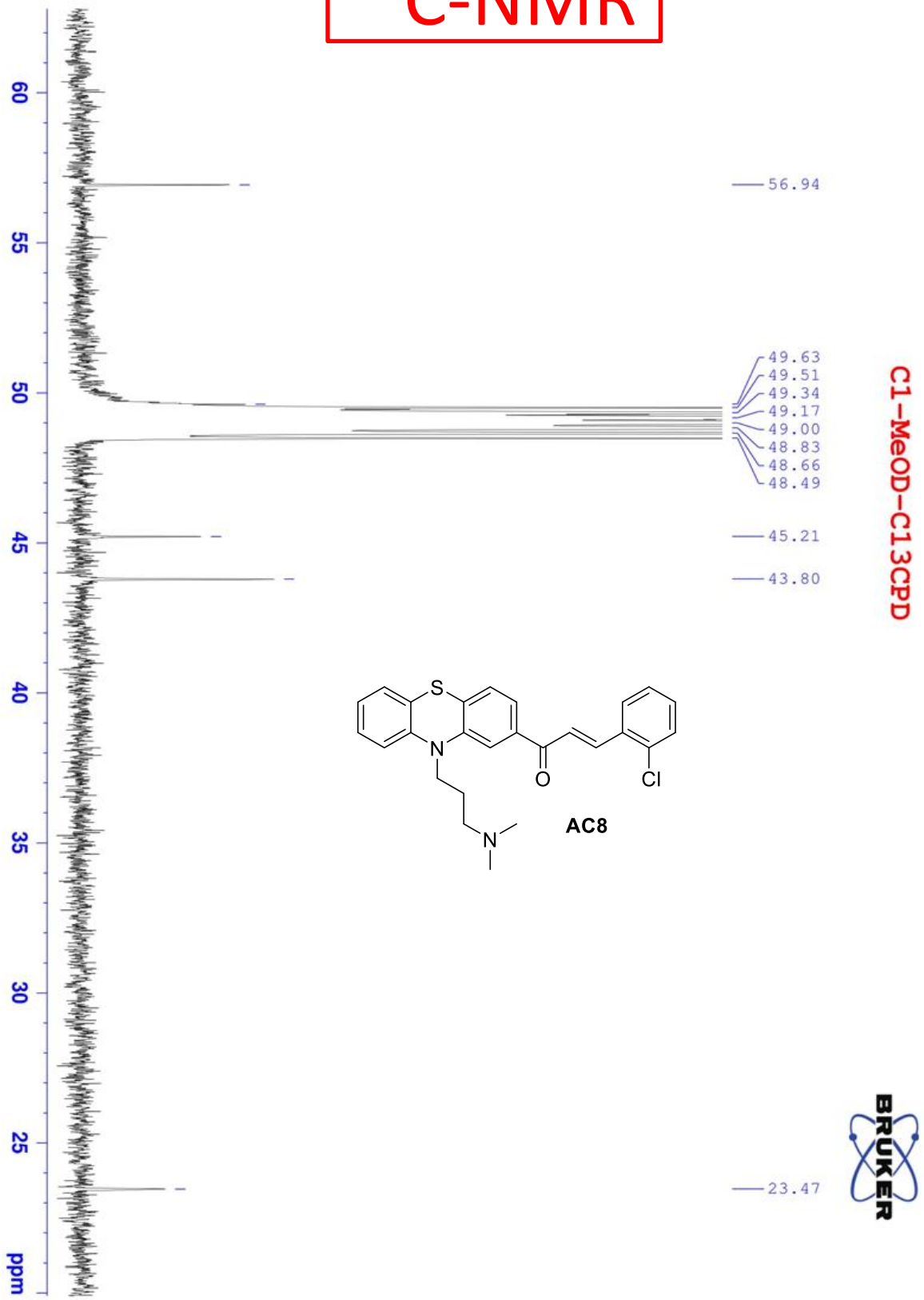
^{13}C-NMR


190.97
146.84
145.49
141.34
138.55
136.49
134.63
134.20
132.85
131.27
129.28
129.22
128.67
128.64
128.52
125.90
125.41
124.96
124.65
117.52
115.98
56.94
49.63
49.51
49.34
49.17
49.00
48.83
48.66
48.49
45.21
43.80
23.47
C1-MeOD-C13CPD
BRUKER
ppm


S
N
O
Cl
N

AC8

^{13}C-NMR


60
55
50
45
40
35
30
25
ppm
56.94
49.63
49.51
49.34
49.17
49.00
48.83
48.66
48.49
45.21
43.80
23.47
C1-MeOD-C13CPD
S
N
O
Cl
N
AC8
BRUKER

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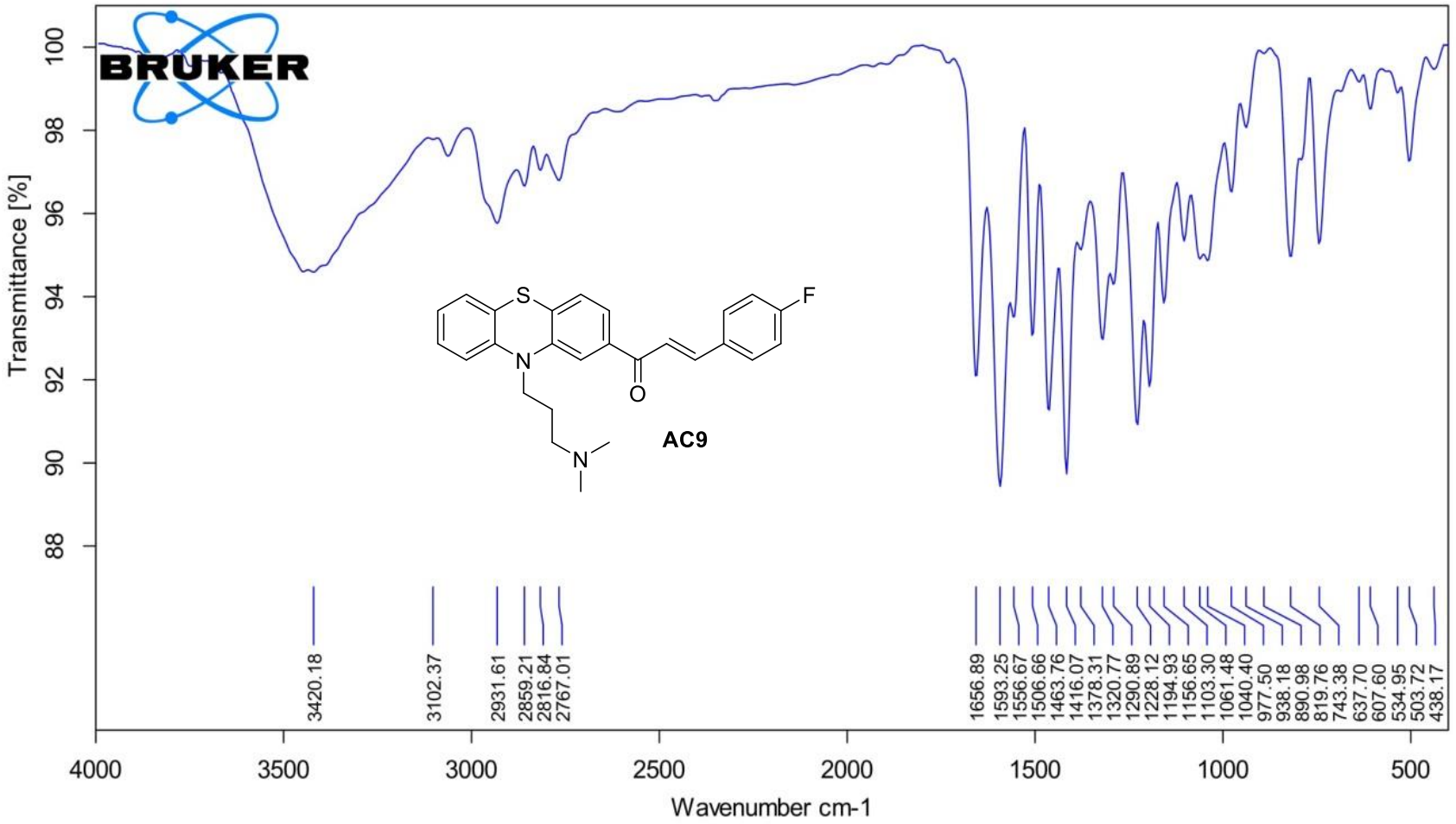
Tel: 08.38296127
Fax: 08.38293889

IR



E:\OPUS 7\2017\THANG 7\20170714\C11.0	C11	TENSOR 27 - BRUKER - GERMANY	7/14/2017

MS

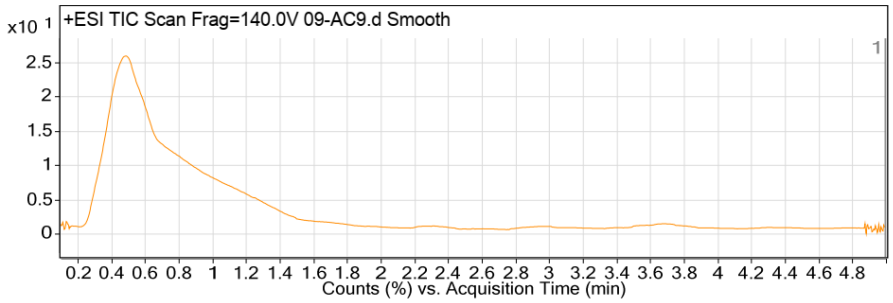
Qualitative Analysis Report

Data Filename	09-AC9.d	**Sample Name**	09-AC9
Sample Type	Sample	**Position**	P2-B2
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	22/08/2020 11:22:38 AM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

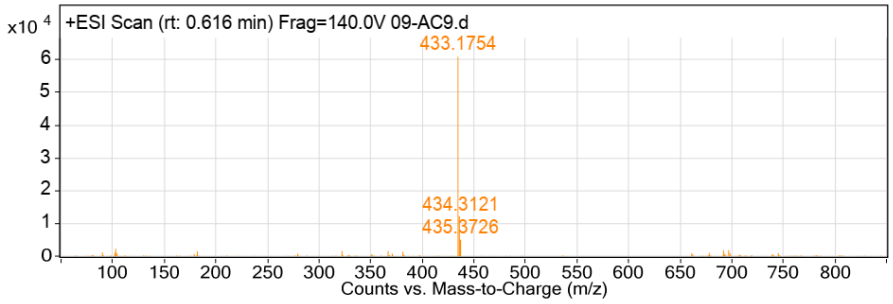
User Chromatograms

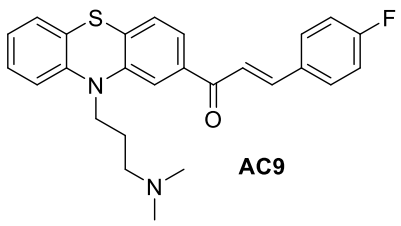
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI





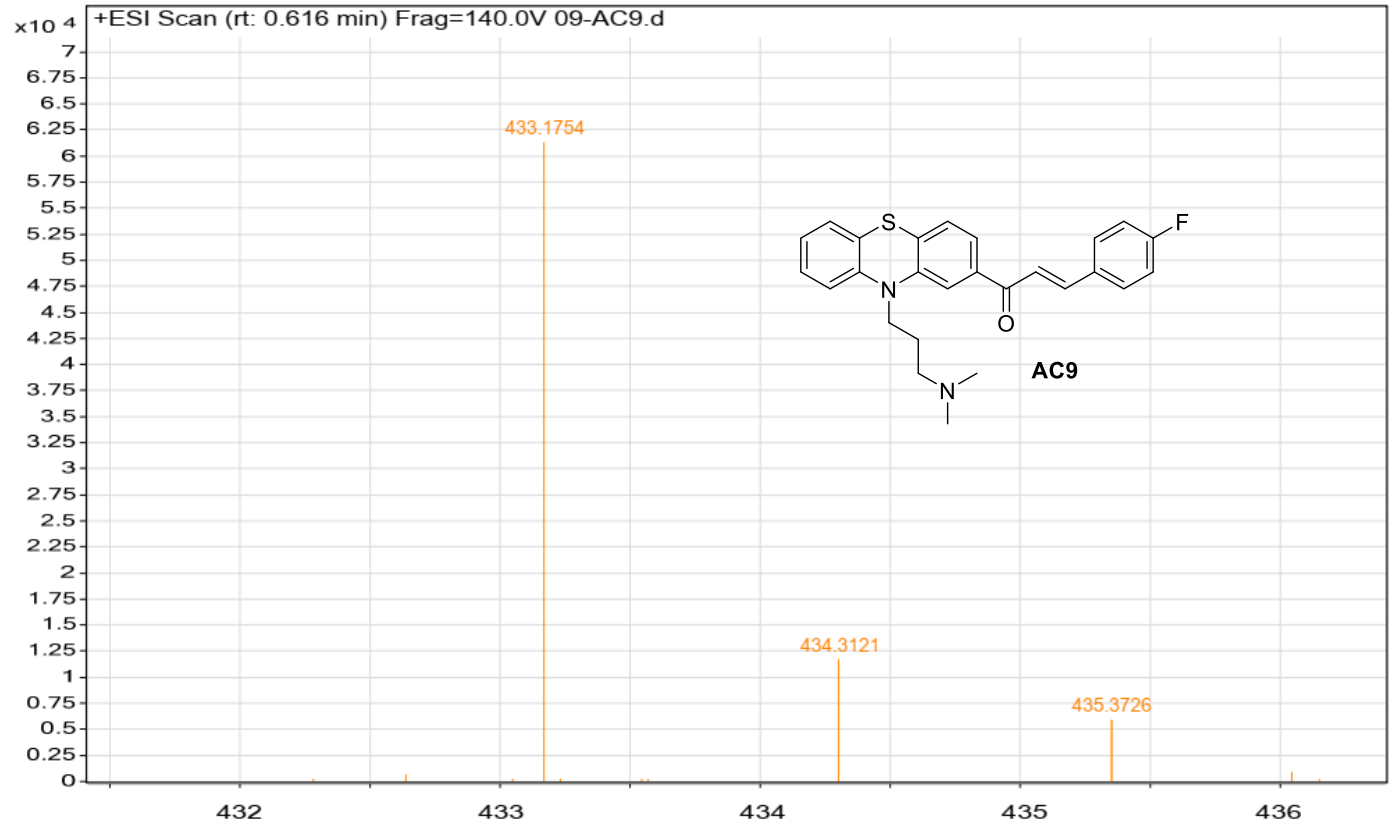
AC9

--- End Of Report ---

MS

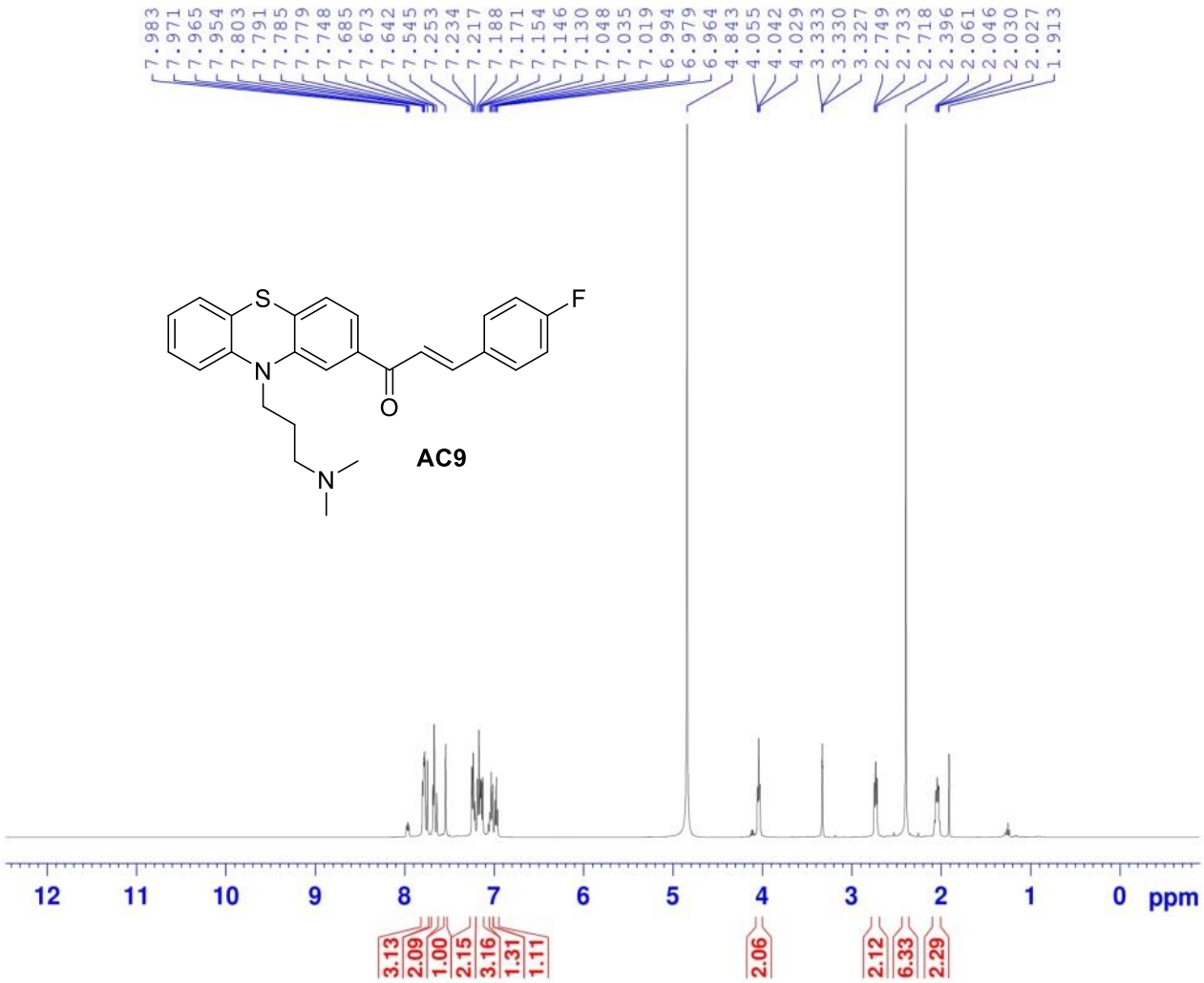
+ESI Scan (rt: 0.616 min) Frag=140.0V BDE 4.d

Sample Name	09-AC9	**Position**	P2-B2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	09-AC9.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	22/08/2020 11:22:38 AM



^{1}H-NMR

C11-MeOD-1H



BRUKER

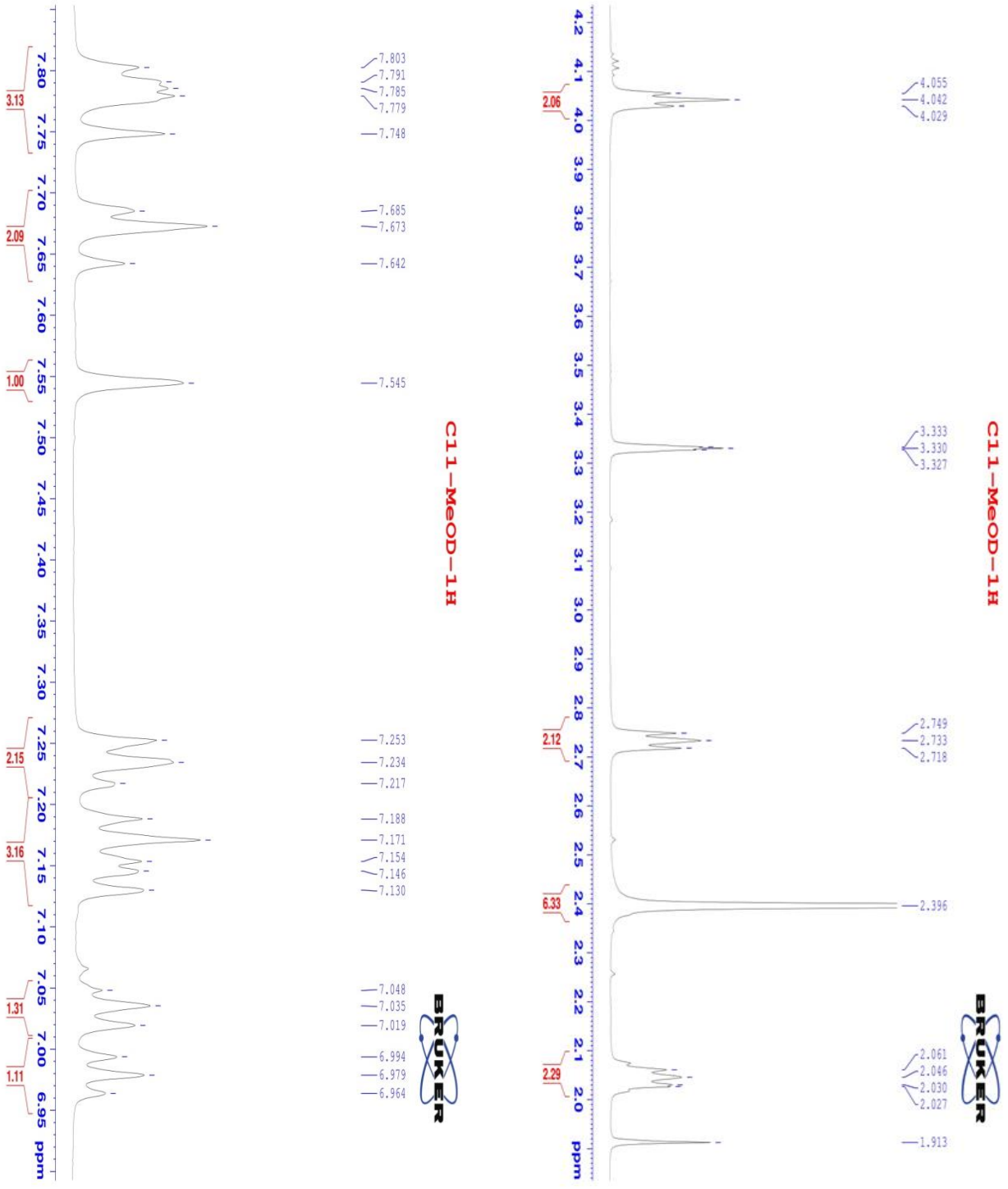
```
Current Data Parameters
NAME          114DAO_C11
EXPNO                  1
PROCNO                 1

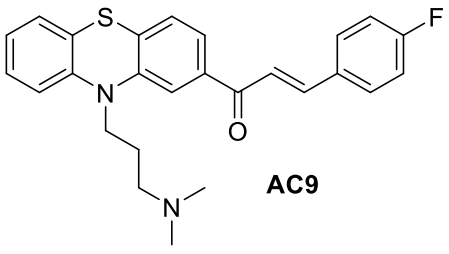
F2 - Acquisition Parameters
Date_           20170704
Time               11.25
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             MeOD
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES             0.152588 Hz
AQ             3.2767999 sec
RG                 79.36
DW                 50.000 usec
DE                  6.50 usec
TE                 303.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          500.2030889 MHz
NUC1                  1H
P1                 10.00 usec
PLW1          22.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.2000016 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{1}H-NMR

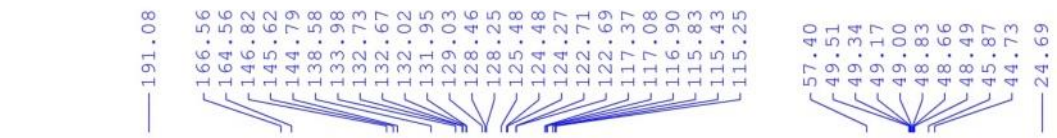


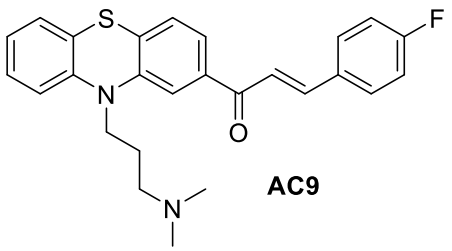


AC9

^{13}C-NMR

C11-MeOD-C13CPD





AC9

BRUKER

```
Current Data Parameters
NAME          113DAO_C11
EXPNO                  2
PROCNO                 1

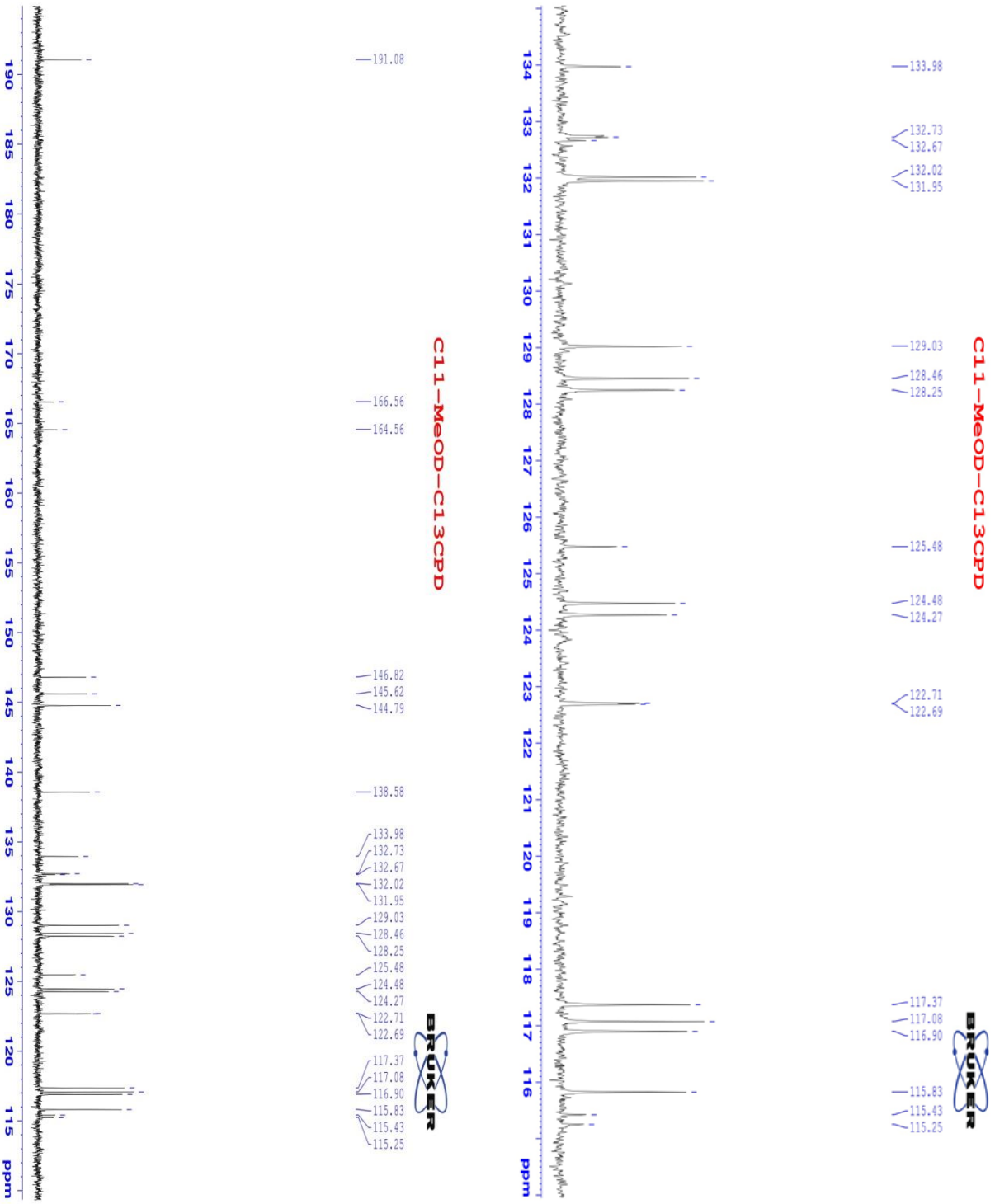
F2 - Acquisition Parameters
Date_           20170705
Time              14.39
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT            MeOD
NS                  128
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                198.57
DW               16.800 usec
DE                6.50 usec
TE               303.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         125.7879670 MHz
NUC1                13C
P1                10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.2020008 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         22.00000000 W
PLW12         0.34375000 W
PLW13         0.22000000 W

F2 - Processing parameters
SI                 32768
SF           125.7752168 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

^{13}C-NMR


C11-MeOD-C13CPD
191.08
166.56
164.56
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145.62
144.79
138.58
133.98
132.73
132.67
132.02
131.95
129.03
128.46
128.25
125.48
124.48
124.27
122.71
122.69
117.37
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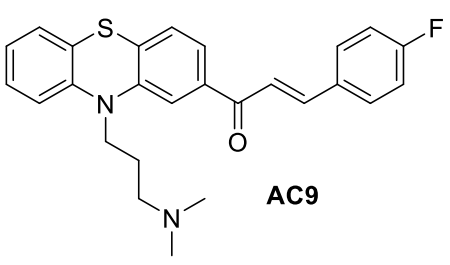
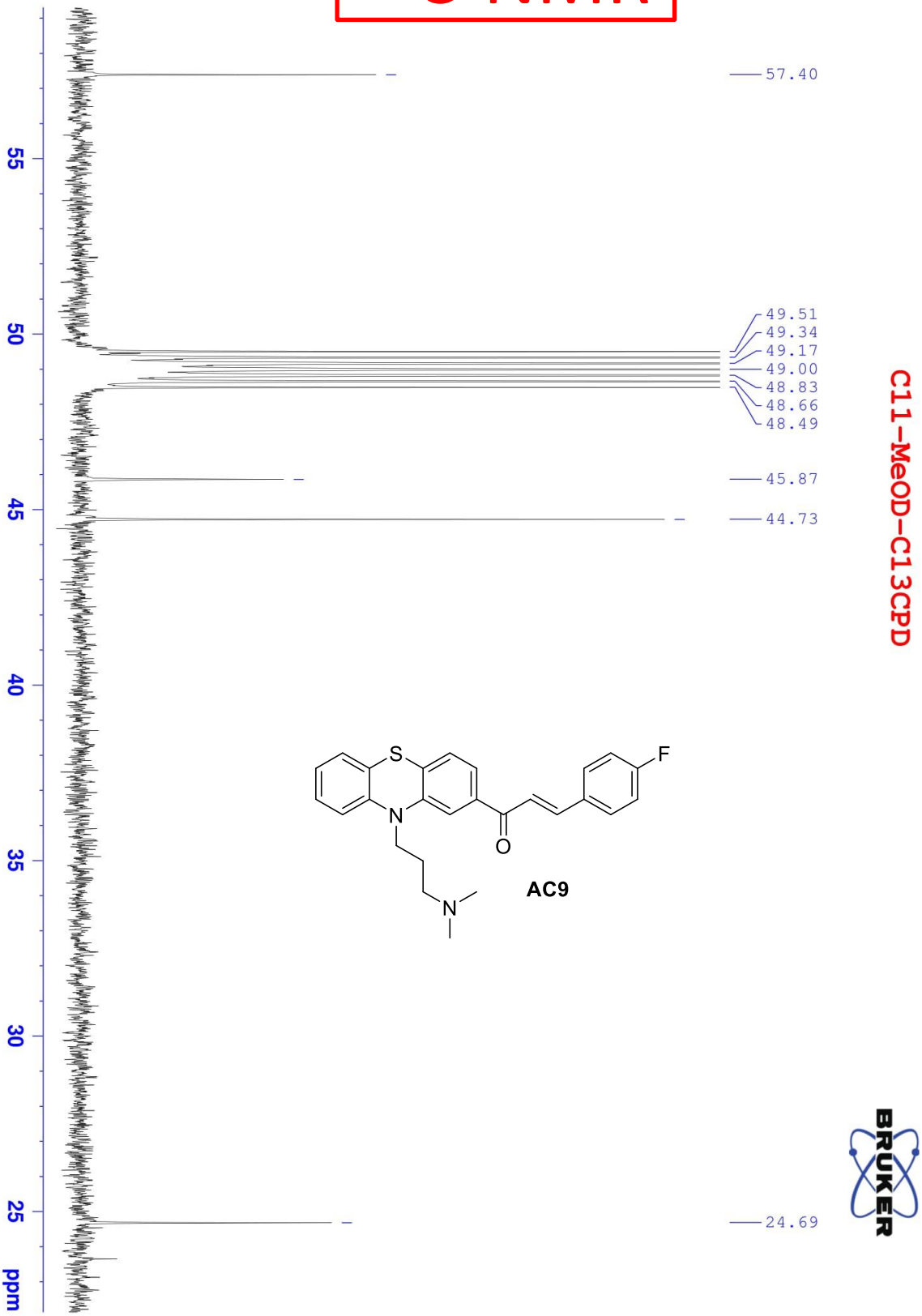
116.90
115.83
115.43
115.25
BRUKER
ppm


S
N
O
F
N

AC9

^{13}C-NMR


57.40
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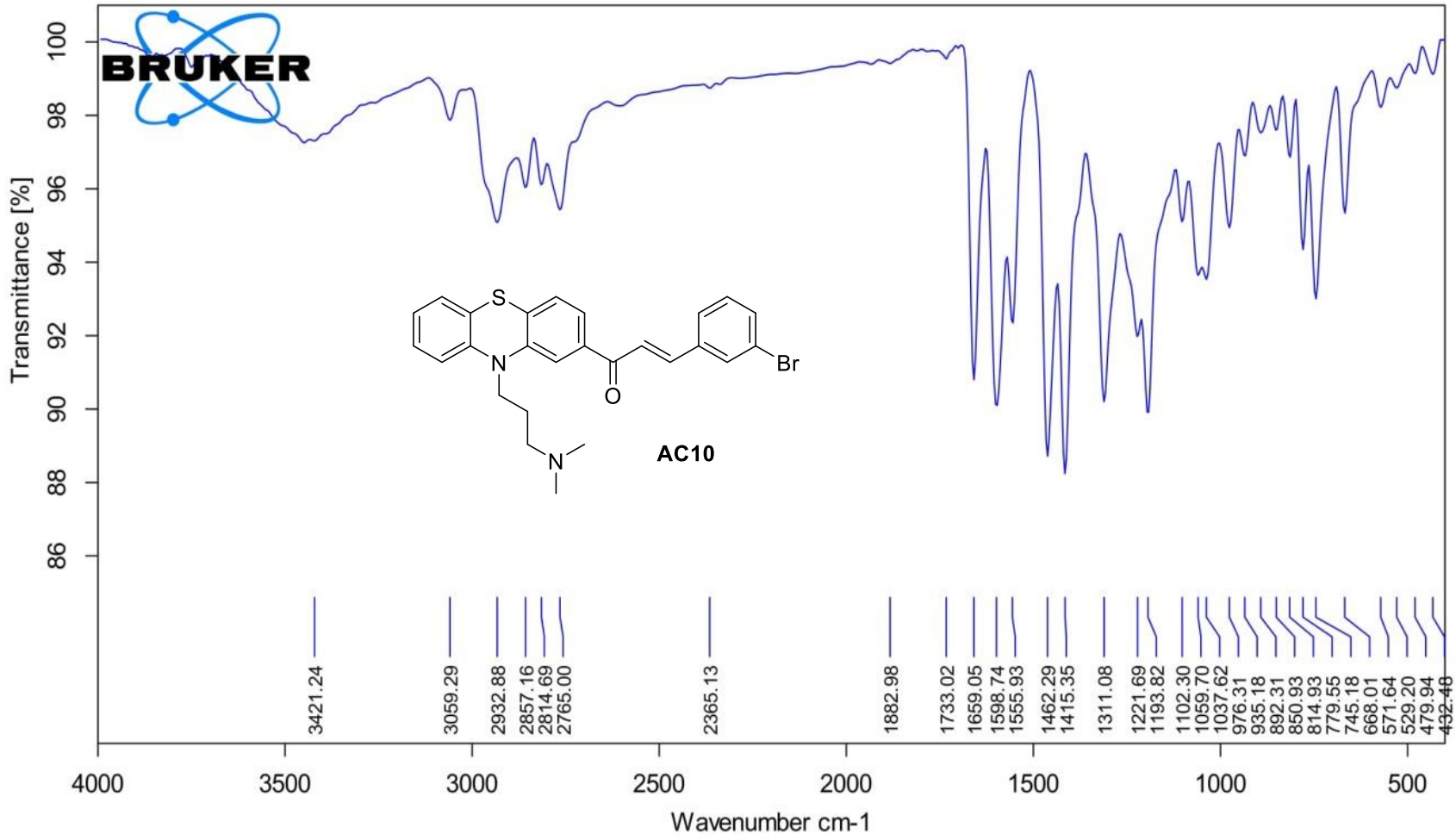
49.00
48.83
48.66
48.49
45.87
44.73
24.69
55
50
45
40
35
30
25
ppm
C11-MeOD-C13CPD
S
N
F
O
N
AC9
BRUKER

VIEN CONG NGHE HOA HOC
01 Mac Dinh Chi - Q.1 - Tp HCM

Tel: 08.38296127
Fax: 08.38293889

IR



E:\OPUS 7\2017\THANG 7\20170714\C14.0	C14	TENSOR 27 - BRUKER - GERMANY	7/14/2017

MS

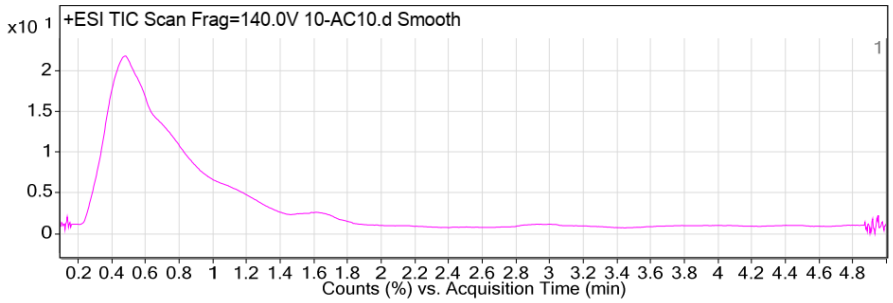
Qualitative Analysis Report

Data Filename	10-AC10.d	**Sample Name**	10-AC10
Sample Type	Sample	**Position**	P2-C1
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	22/08/2020 11:30:09 AM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

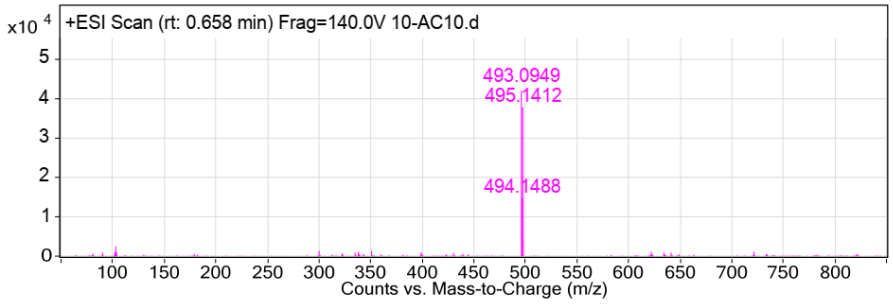
User Chromatograms

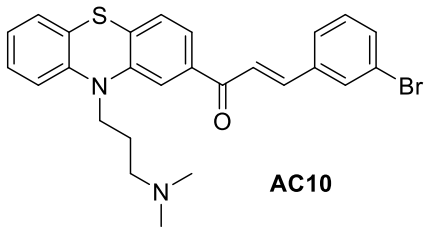
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



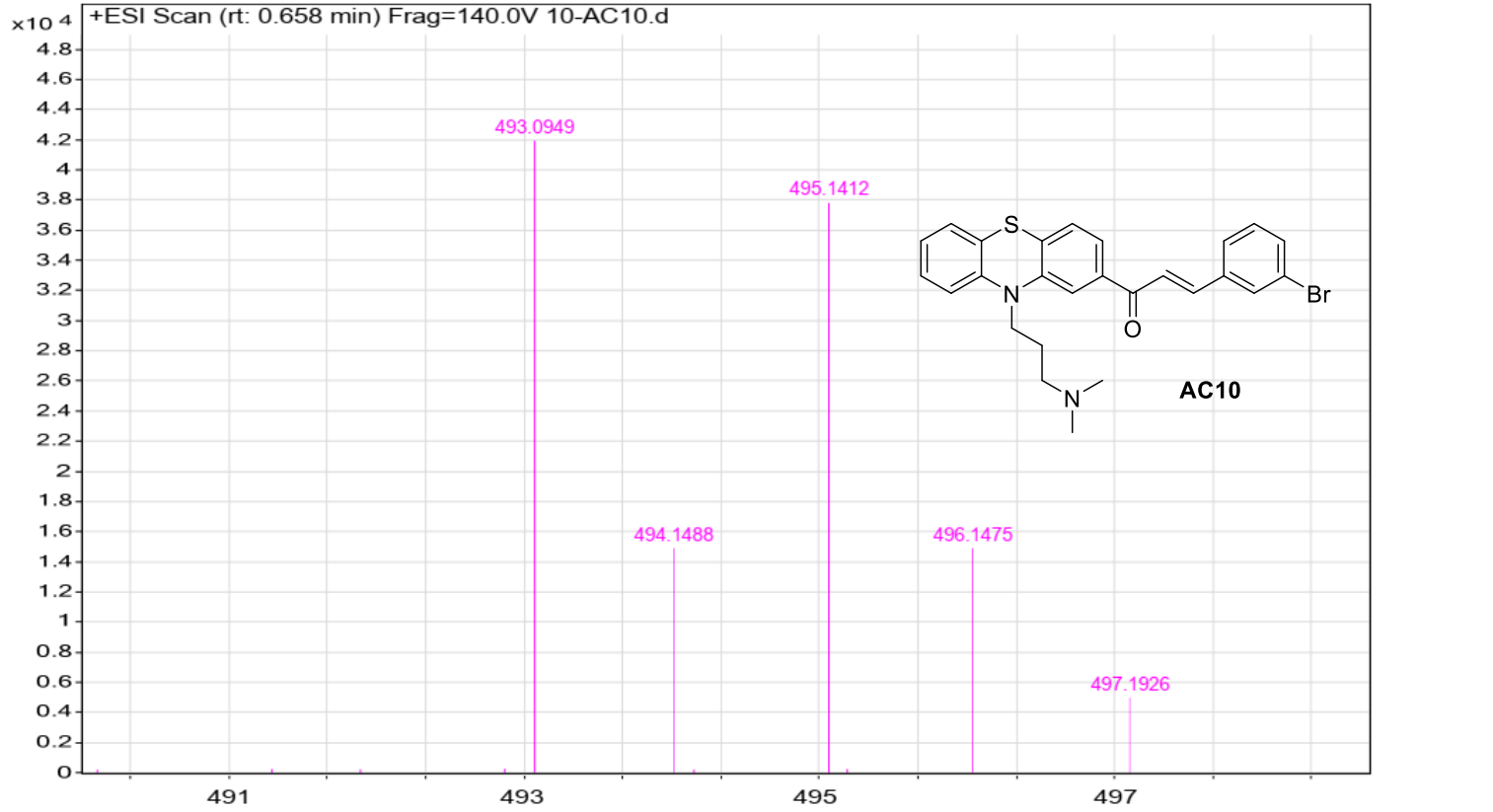


AC10

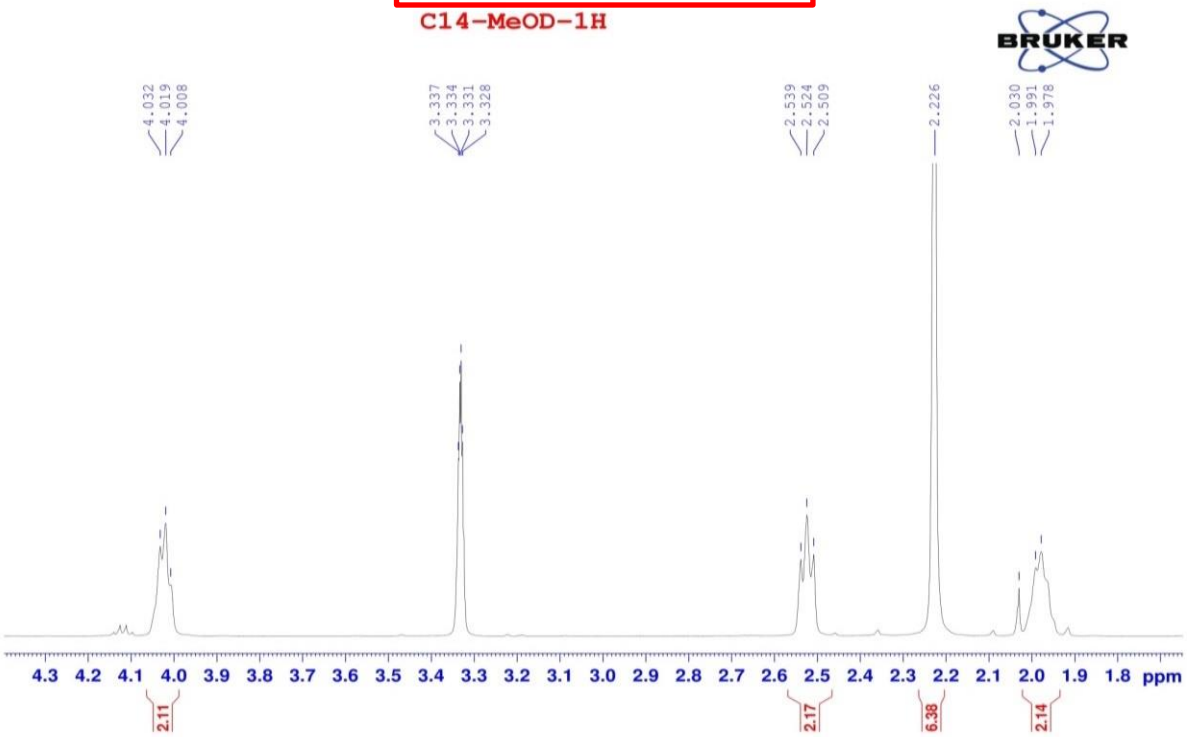
--- End Of Report ---

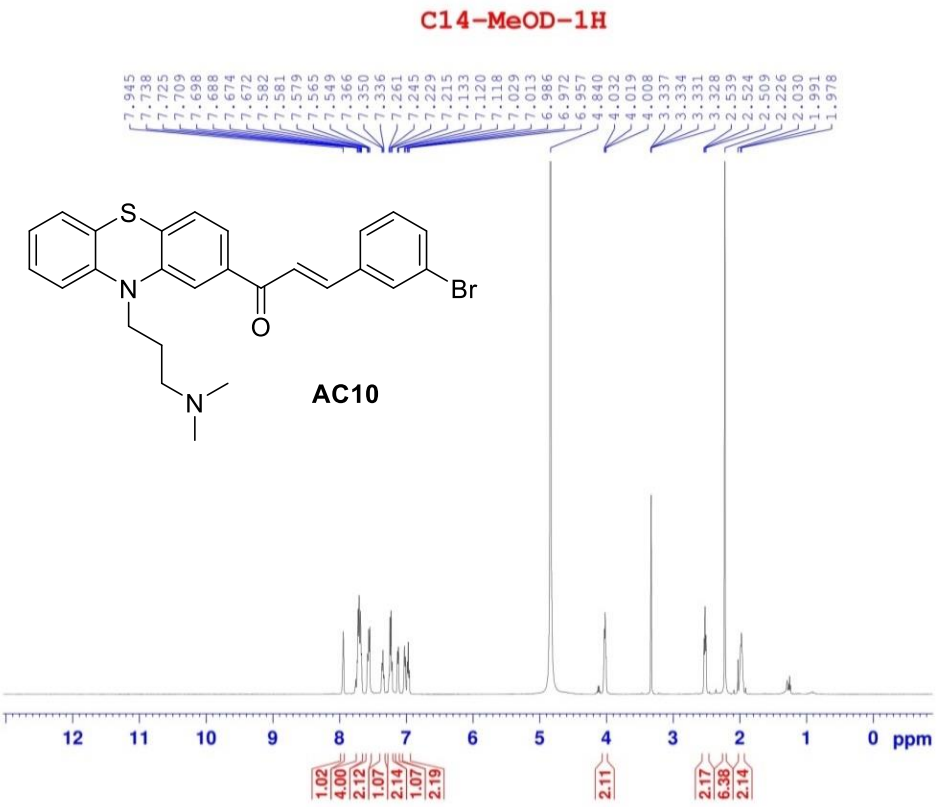
MS

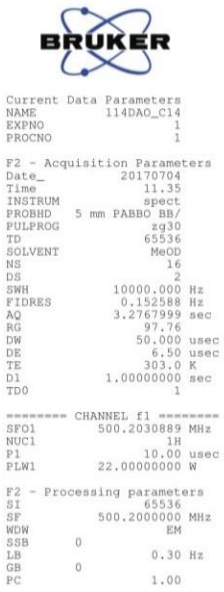
Sample Name	10-AC10	**Position**	P2-C1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	10-AC10.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	22/08/2020 11:30:09 AM



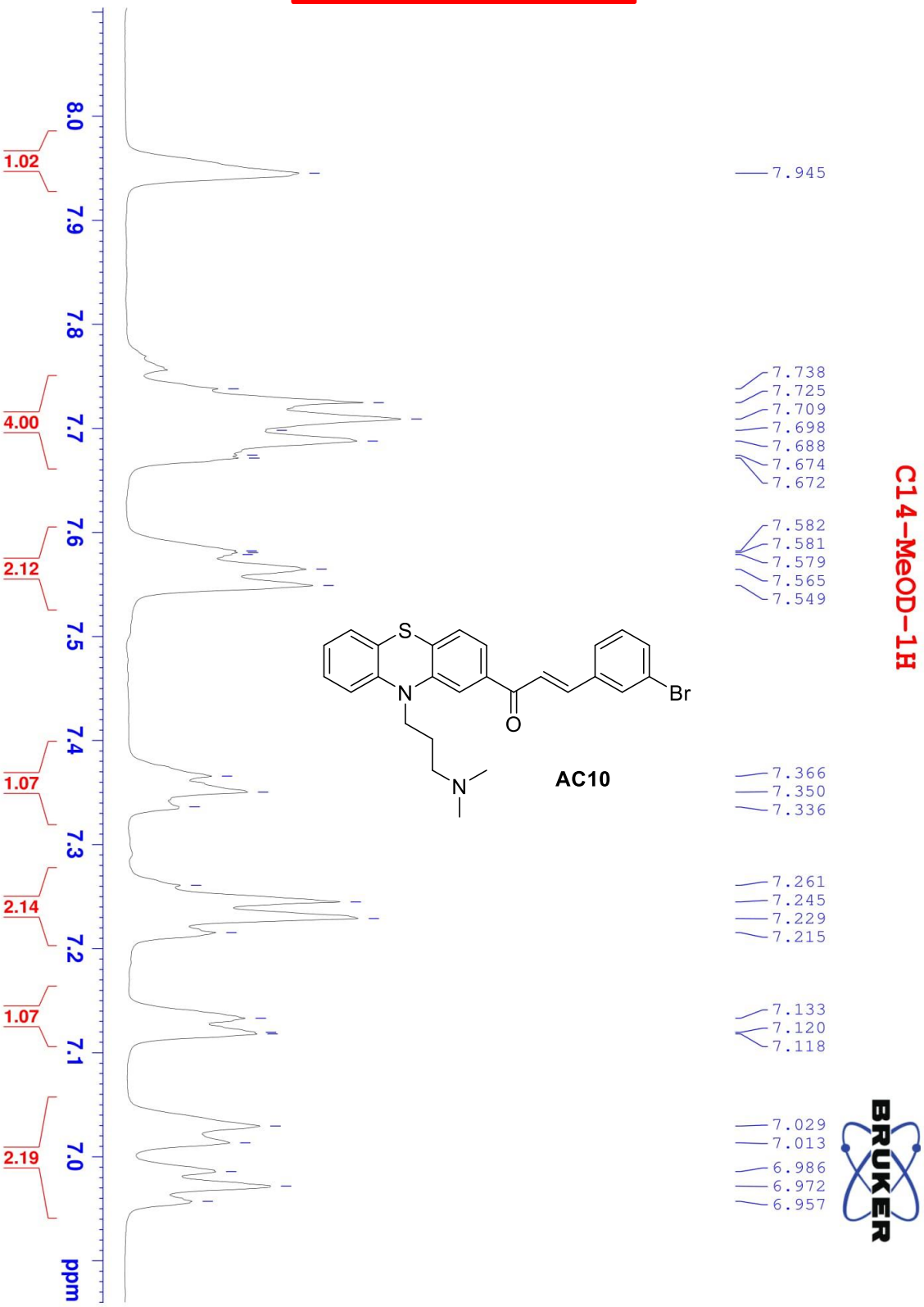
^{1}H-NMR


C14-MeOD-1H
BRUKER
4.032
4.019
4.008
3.337
3.334
3.331
3.328
2.539
2.524
2.509
2.226
2.030
1.991
1.978
4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 ppm
2.11
2.17
6.38
2.14


C14-MeOD-1H
7.945
7.738
7.725
7.709
7.698
7.688
7.674
7.672
7.582
7.581
7.579
7.565
7.549
7.366
7.350
7.336
7.261
7.245
7.229
7.215
7.133
7.120
7.118
7.029
7.013
6.986
6.972
6.957
4.840
4.032
4.019
4.008
3.337
3.334
3.331
3.328
2.539
2.524
2.509
2.226
2.030
1.991
1.978
S
N
O
Br
N
AC10
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.02
4.00
2.12
1.07
2.14
1.07
2.19
2.11
2.17
6.38
2.14

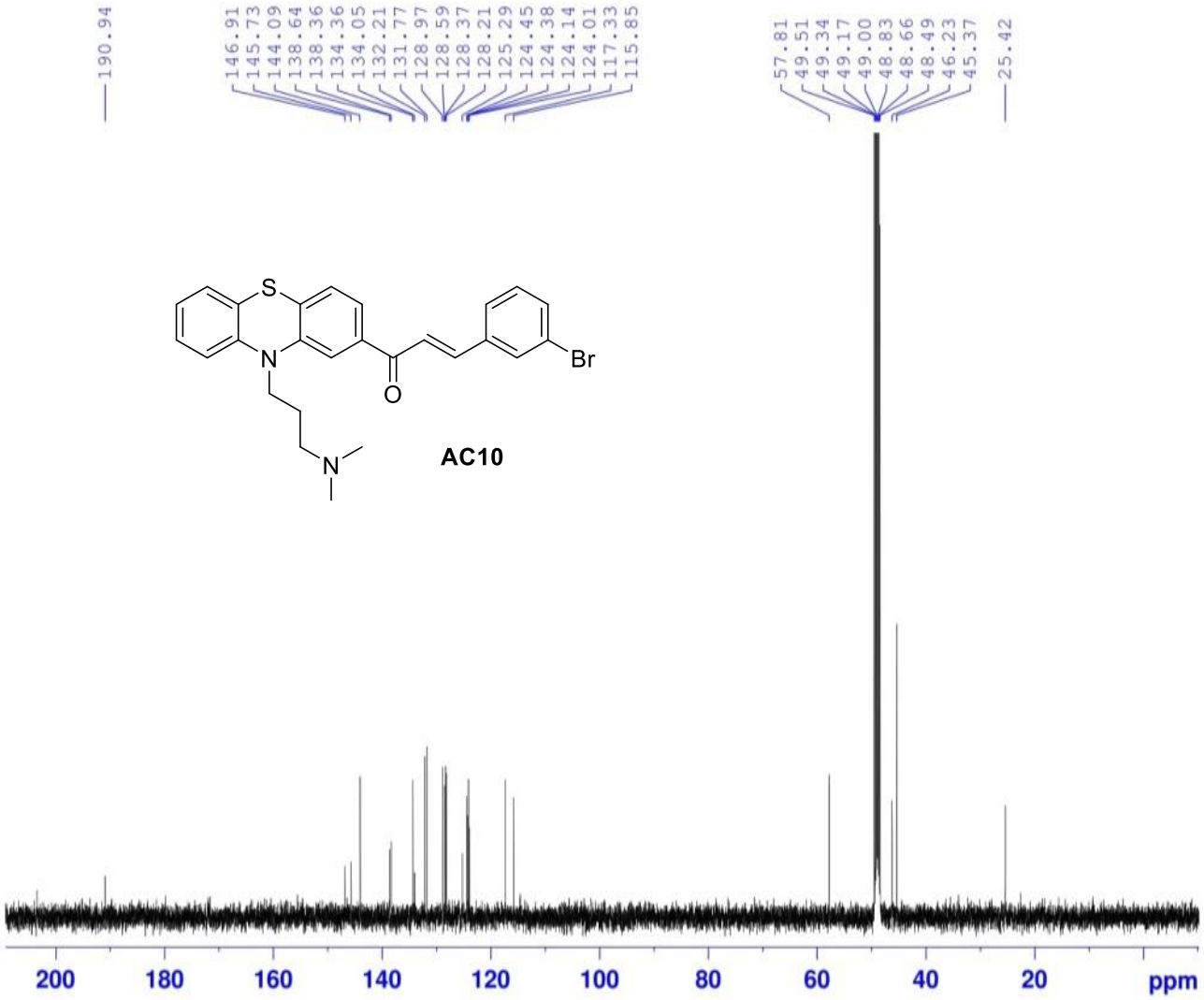

BRUKER
Current Data Parameters
NAME 114DAO_C14
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170704
Time 11.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 97.76
DW 50.000 usec
DE 6.50 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.2030889 MHz
NUC1 1H
P1 10.00 usec
PLW1 22.00000000 W
F2 - Processing parameters
SI 65536
SF 500.2000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{1}H-NMR


8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
ppm
1.02
4.00
2.12
1.07
2.14
1.07
2.19
7.945
7.738
7.725
7.709
7.698
7.688
7.674
7.672
7.582
7.581
7.579
7.565
7.549
7.366
7.350
7.336
7.261
7.245
7.229
7.215
7.133
7.120
7.118
7.029
7.013
6.986
6.972
6.957
S
N
O
Br
N
AC10
C14-MeOD-1H
BRUKER

^{13}C-NMR

C14-MeOD-C13CPD



AC10

BRUKER

```
Current Data Parameters
NAME          114DAO_C14
EXPNO                  2
PROCNO                 1

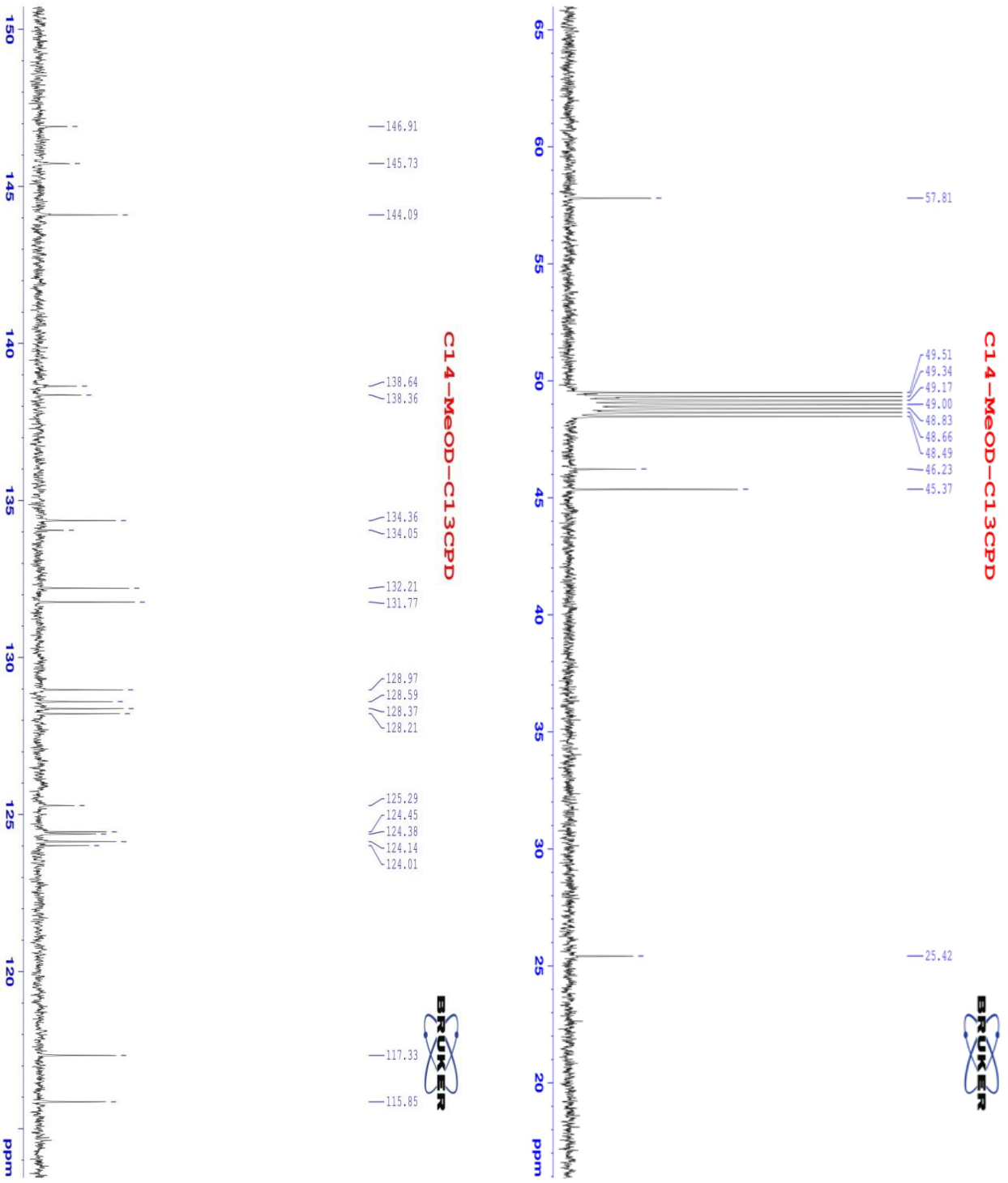
F2 - Acquisition Parameters
Date_          20170705
Time              15.02
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT            MeOD
NS                  256
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                198.57
DW                16.800 usec
DE                 6.50 usec
TE                303.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

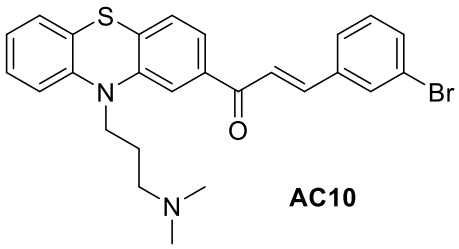
======== CHANNEL f1 ========
SFO1         125.7879670 MHz
NUC1                 13C
P1                 10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.2020008 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2         22.00000000 W
PLW12         0.34375000 W
PLW13         0.22000000 W

F2 - Processing parameters
SI                 32768
SF           125.7752156 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

^{13}C-NMR


150
145
140
135
130
125
120
ppm
146.91
145.73
144.09
138.64
138.36
134.36
134.05
132.21
131.77
128.97
128.59
128.37
128.21
125.29
124.45
124.38
124.14
124.01
117.33
115.85
C14-MeOD-C13CPD
BRUKER
65
60
55
50
45
40
35
30
25
20
ppm
57.81
49.51
49.34
49.17
49.00
48.83
48.66
48.49
46.23
45.37
25.42
C14-MeOD-C13CPD
BRUKER

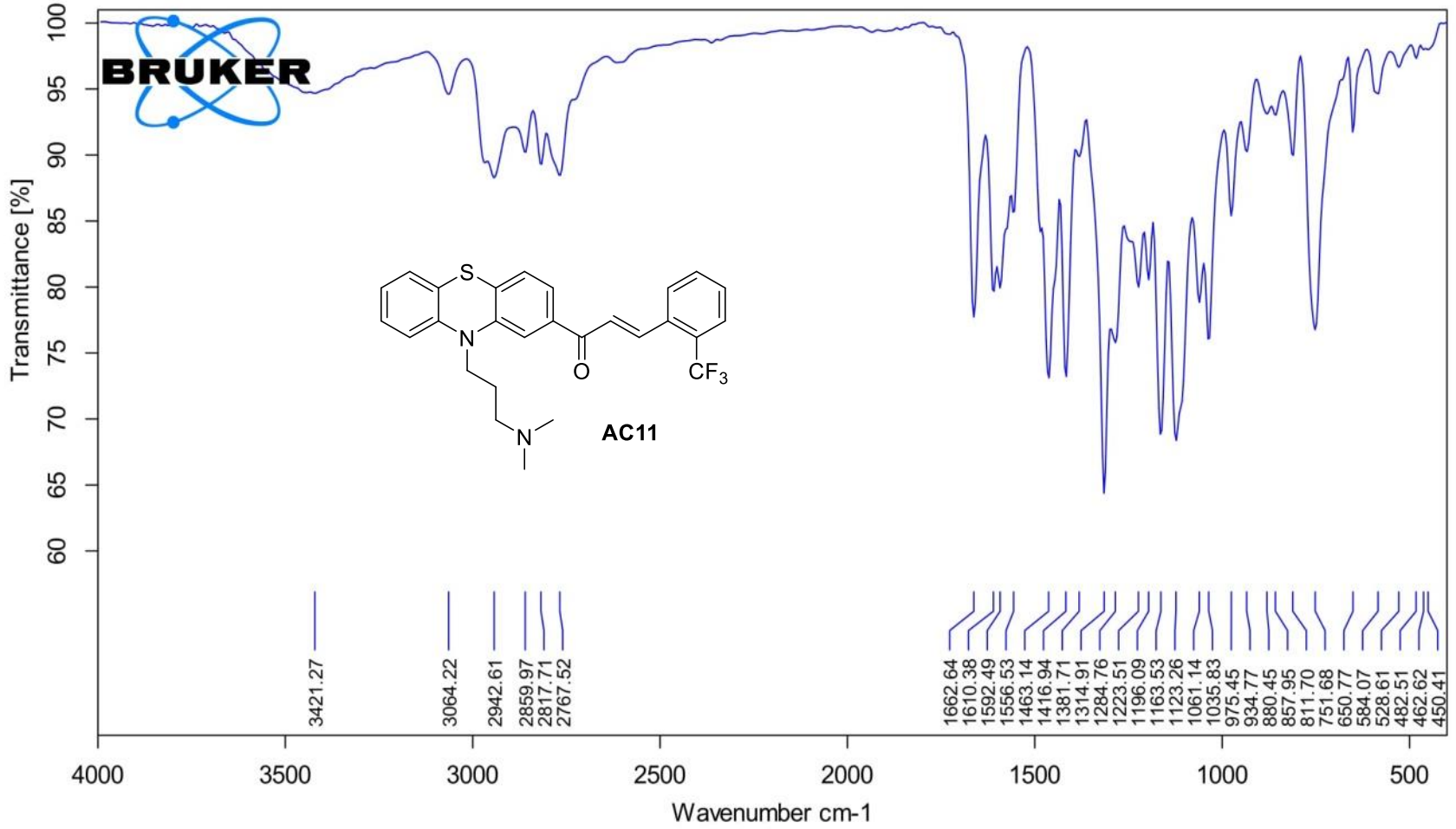

S
N
O
Br
N

AC10

VIEN CONG NGHE HOA HOC
01 Mac Dinh Chi - Q.1 - Tp HCM

IR

Tel: 08.38296127
Fax: 08.38293889



E:\OPUS 7\2017\THANG 7\20170714\C15.0	C15	TENSOR 27 - BRUKER - GERMANY	7/14/2017

MS

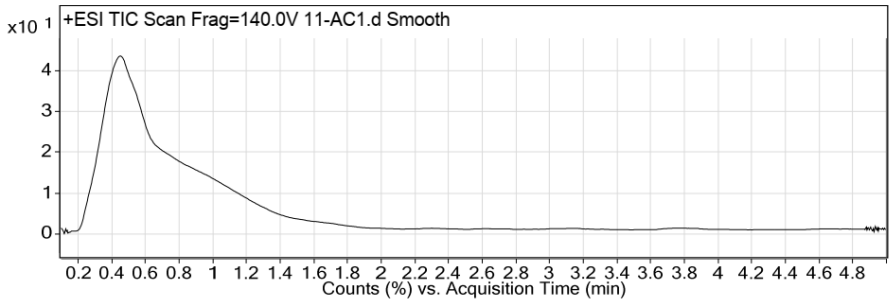
Qualitative Analysis Report

Data Filename	11-AC11.d	**Sample Name**	11-AC11
Sample Type	Sample	**Position**	P2-B1
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	22/08/2020 11:40:04 AM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

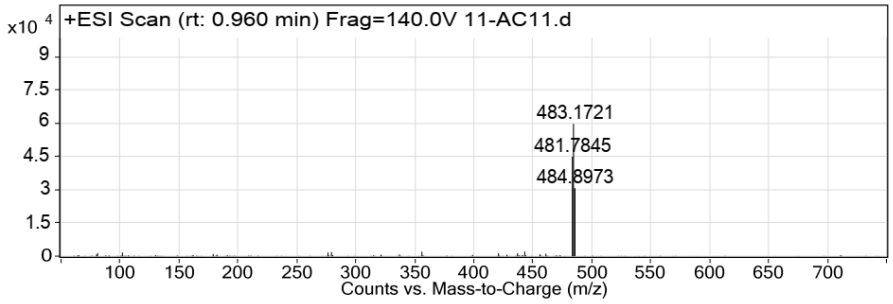
User Chromatograms

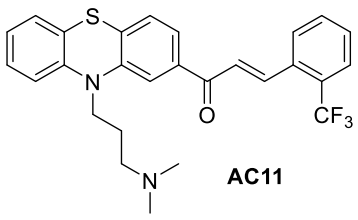
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage	**Collision Energy**	**Ionization Mode**
140	0	ESI



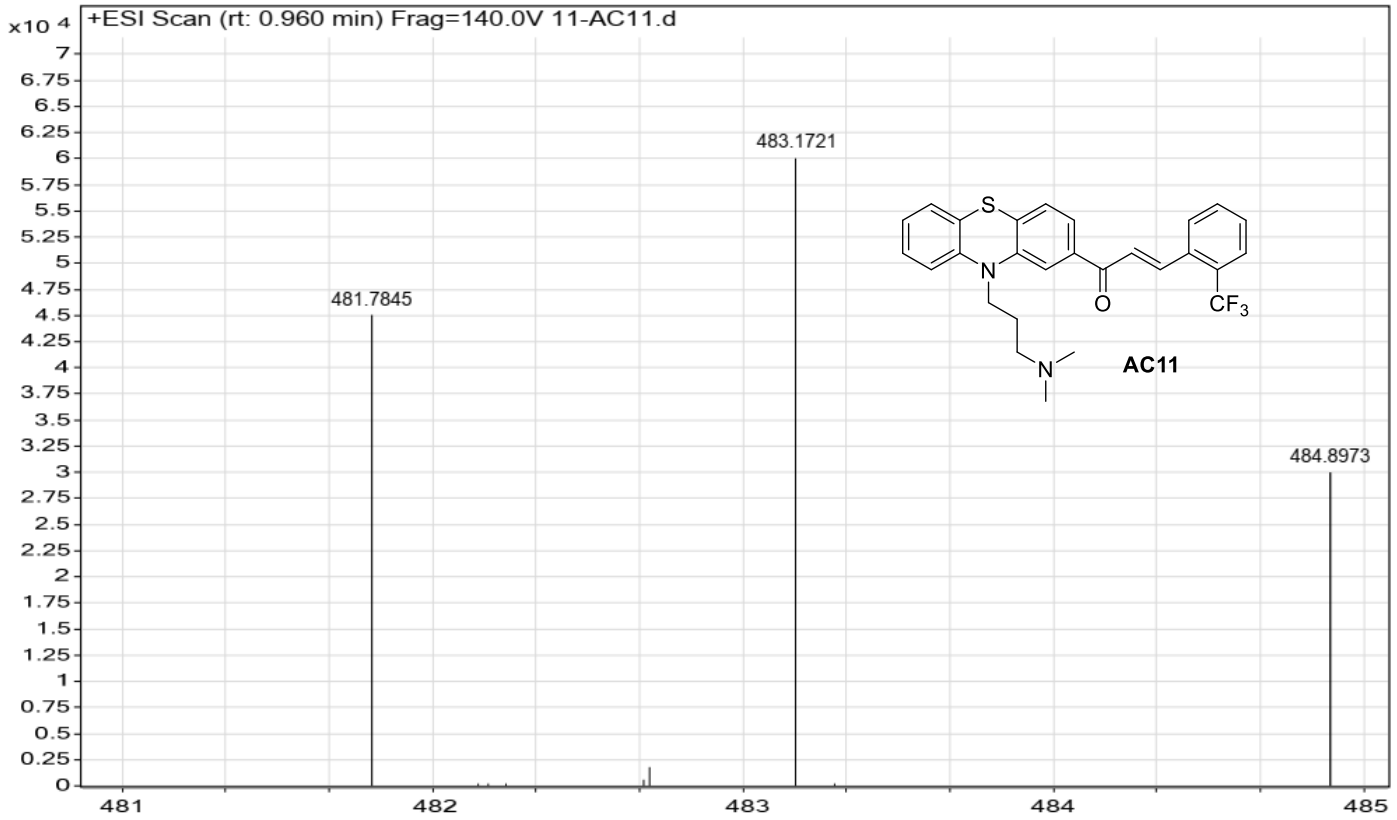


AC11

--- End Of Report ---

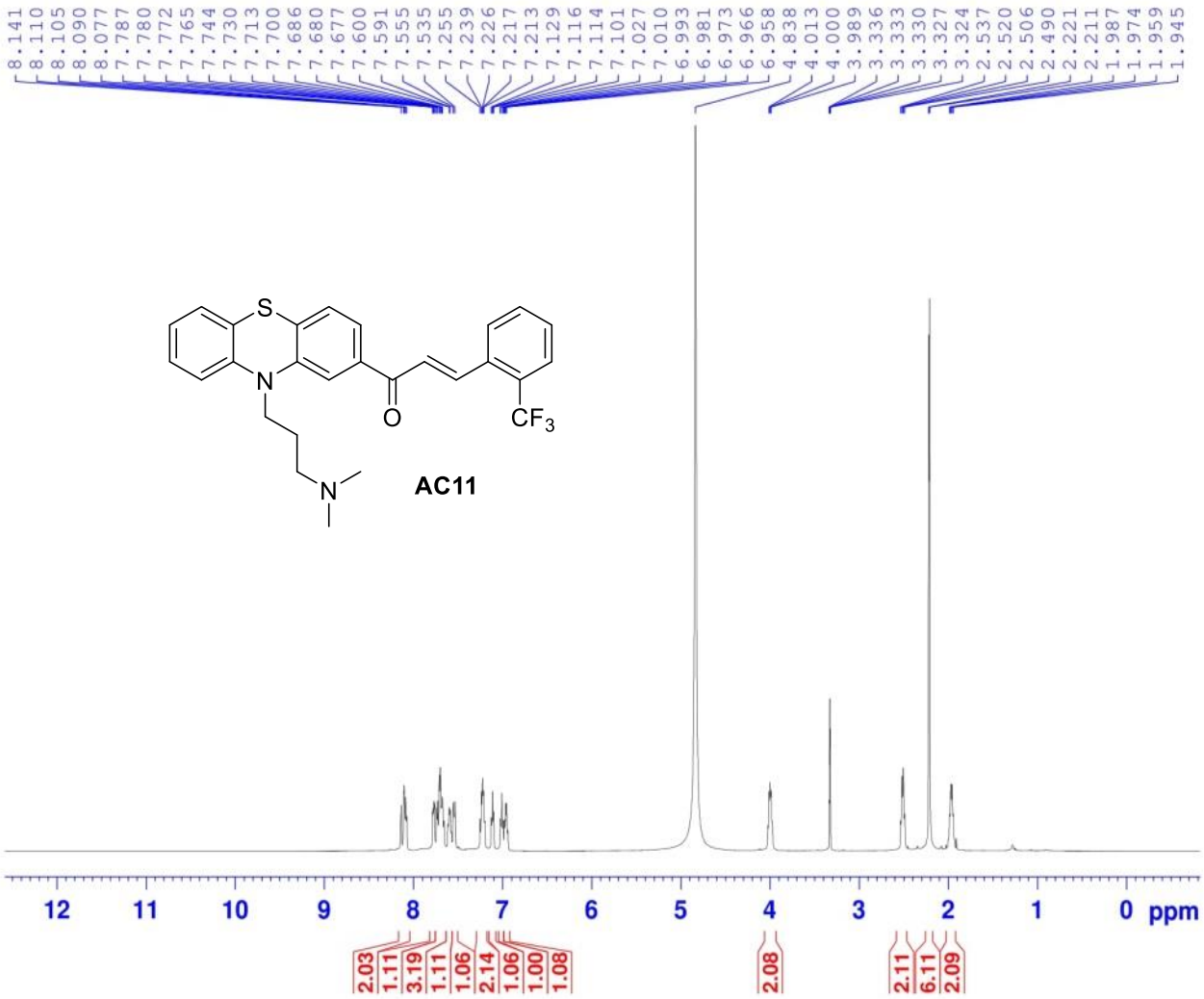
MS

Sample Name	11-AC11	**Position**	P2-B1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	11-AC11.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	22/08/2020 11:40:04 AM



^{1}H-NMR

C15-MeOD-1H



BRUKER

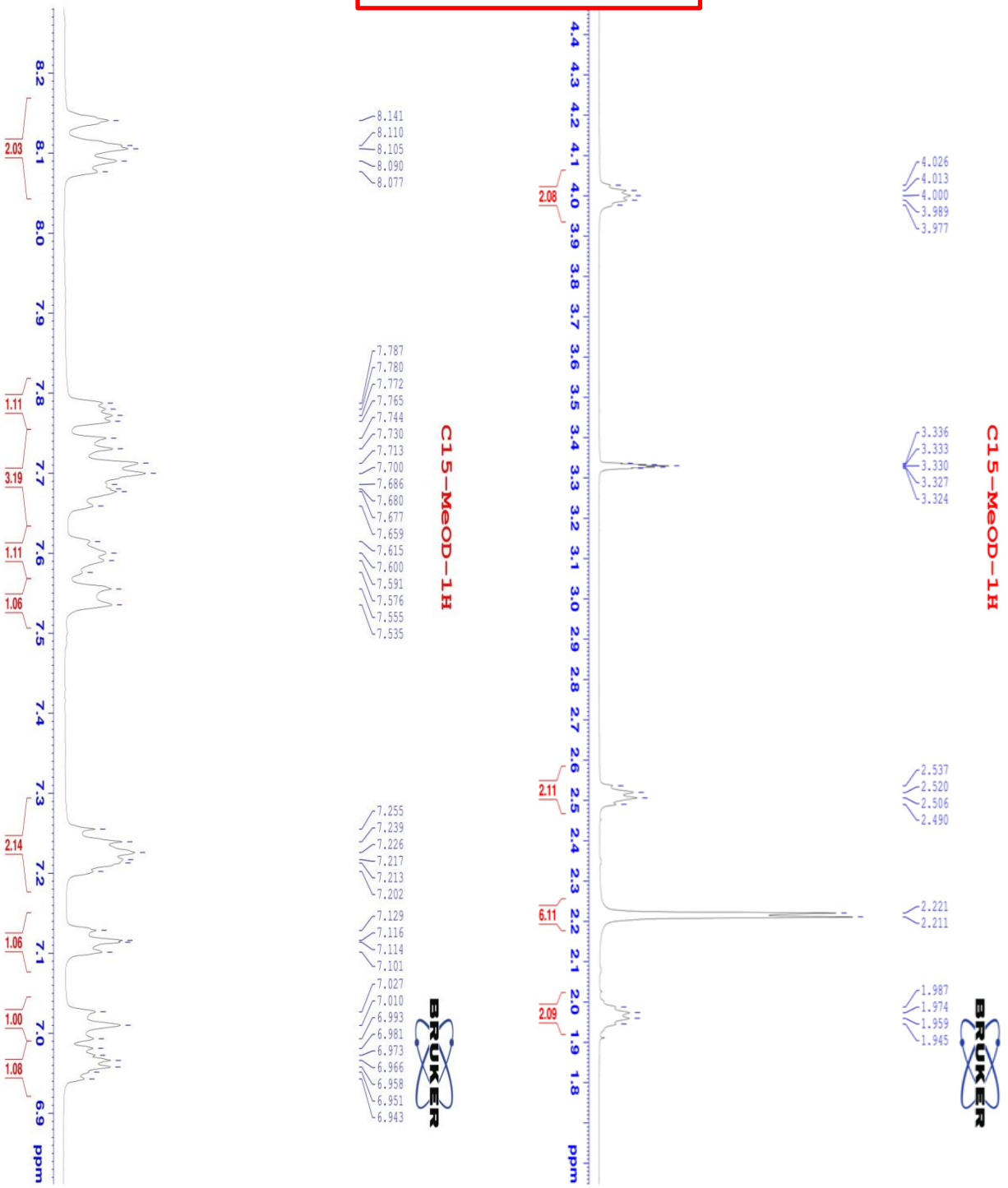
```
Current Data Parameters
NAME          113DAO_C15
EXPNO                  1
PROCNO                 1

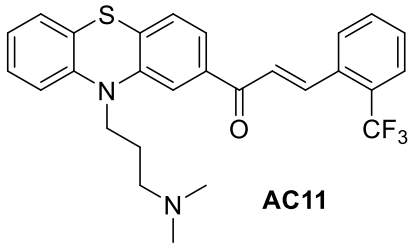
F2 - Acquisition Parameters
Date_           20170705
Time               15.07
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             MeOD
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES             0.152588 Hz
AQ             3.2767999 sec
RG                 79.36
DW                 50.000 usec
DE                  6.50 usec
TE                303.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          500.2030889 MHz
NUC1                   1H
P1                 10.00 usec
PLW1          22.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.2000011 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{1}H-NMR

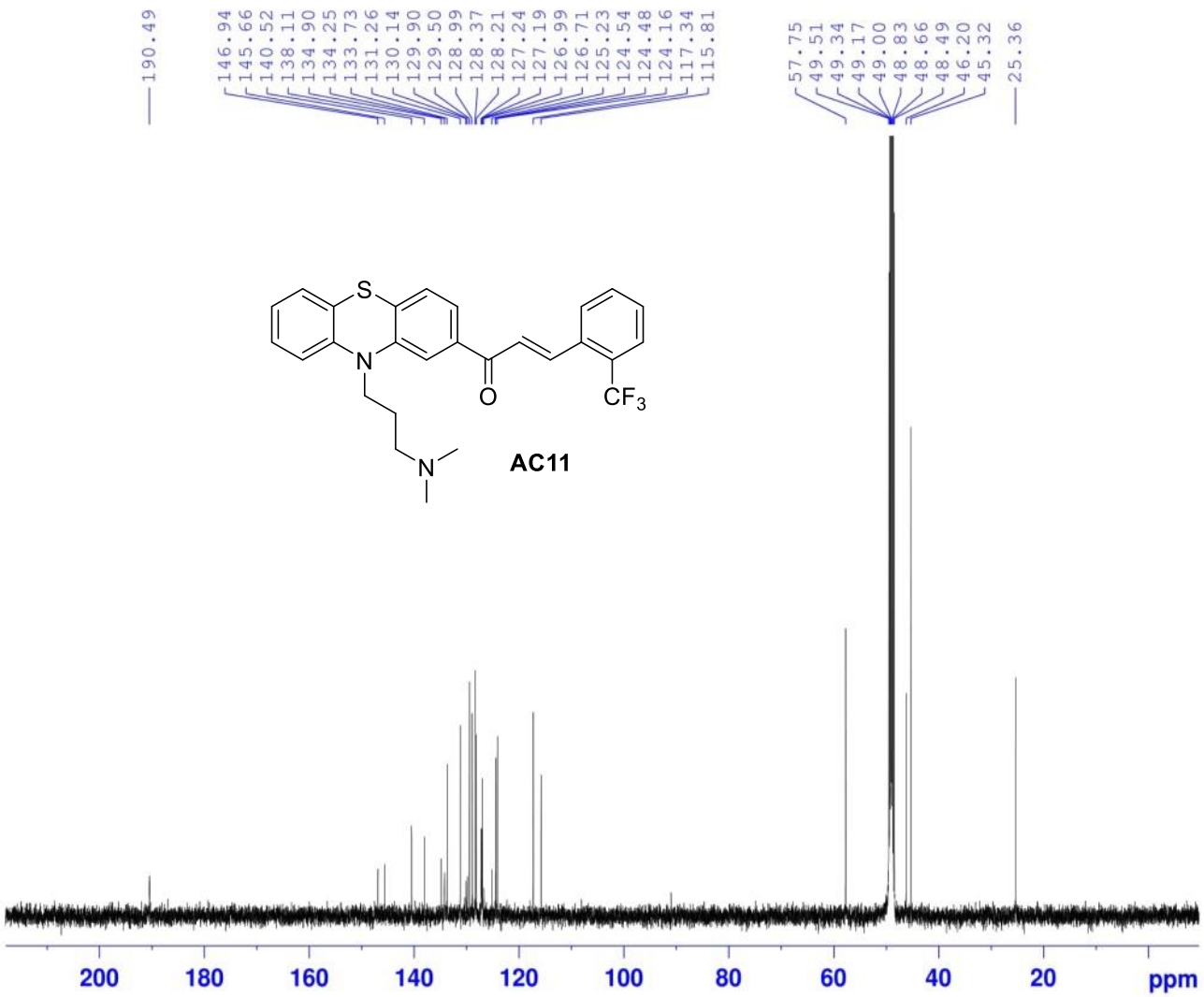




AC11

^{13}C-NMR

C15-MeOD-C13CPD



BRUKER

```
Current Data Parameters
NAME          113DAO_C15
EXPNO                  2
PROCNO                 1

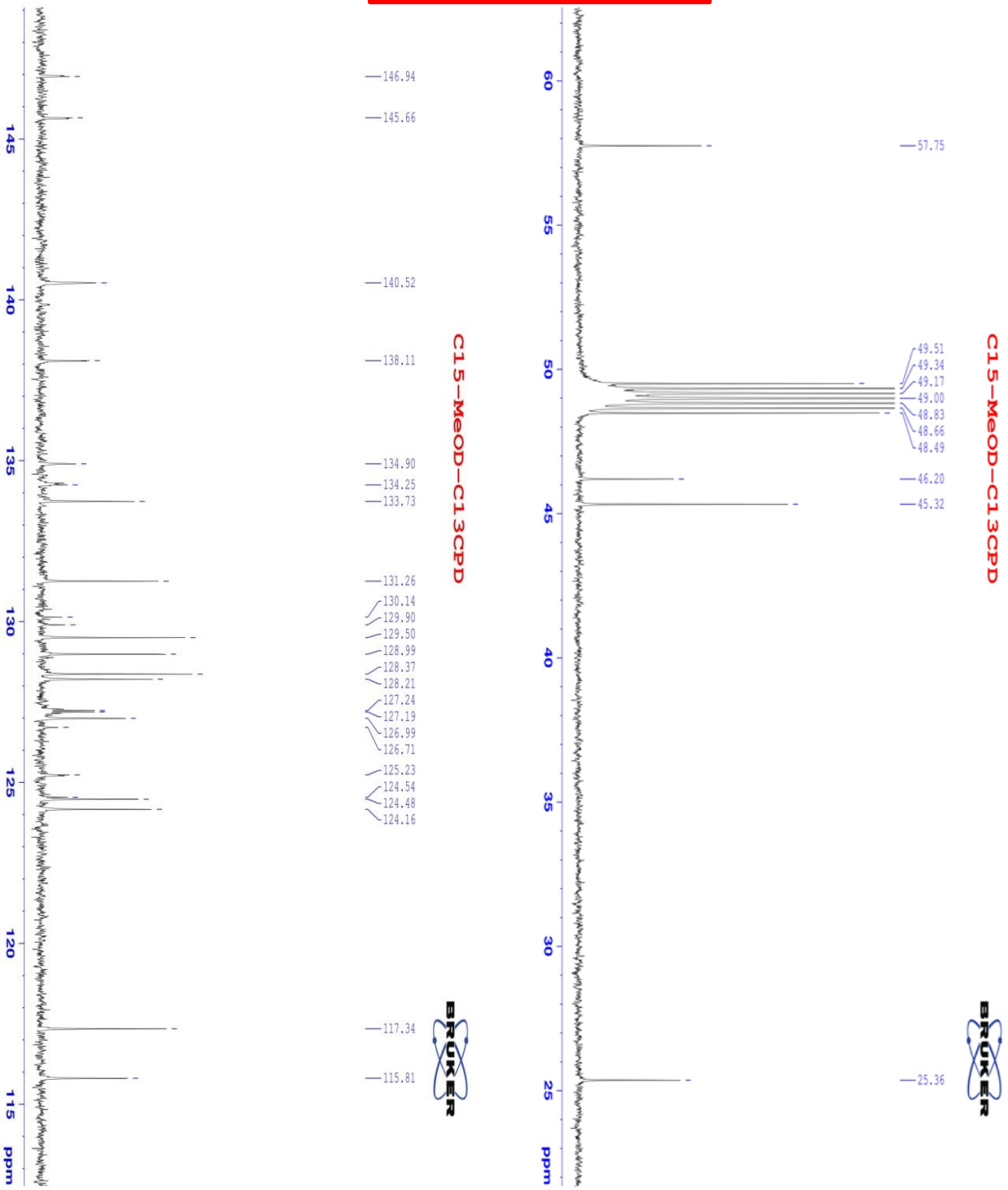
F2 - Acquisition Parameters
Date_           20170705
Time               15.23
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT             MeOD
NS                   256
DS                     4
SWH            29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                198.57
DW                16.800 usec
DE                 6.50 usec
TE                303.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

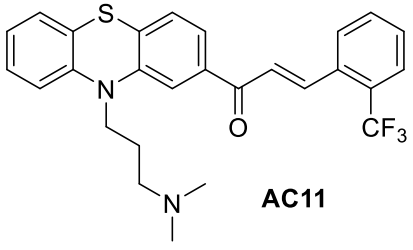
======== CHANNEL f1 ========
SFO1         125.7879670 MHz
NUC1                 13C
P1                10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.2020008 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2         22.00000000 W
PLW12         0.34375000 W
PLW13         0.22000000 W

F2 - Processing parameters
SI                  32768
SF           125.7752168 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

^{13}C-NMR


146.94
145.66
140.52
138.11
134.90
134.25
133.73
131.26
130.14
129.90
129.50
128.99
128.37
128.21
127.24
127.19
126.99
126.71
125.23
124.54
124.48
124.16
117.34
115.81
C15-MeOD-C13CPD
BRUKER
57.75
49.51
49.34
49.17
49.00
48.83
48.66
48.49
46.20
45.32
25.36
C15-MeOD-C13CPD
BRUKER
ppm

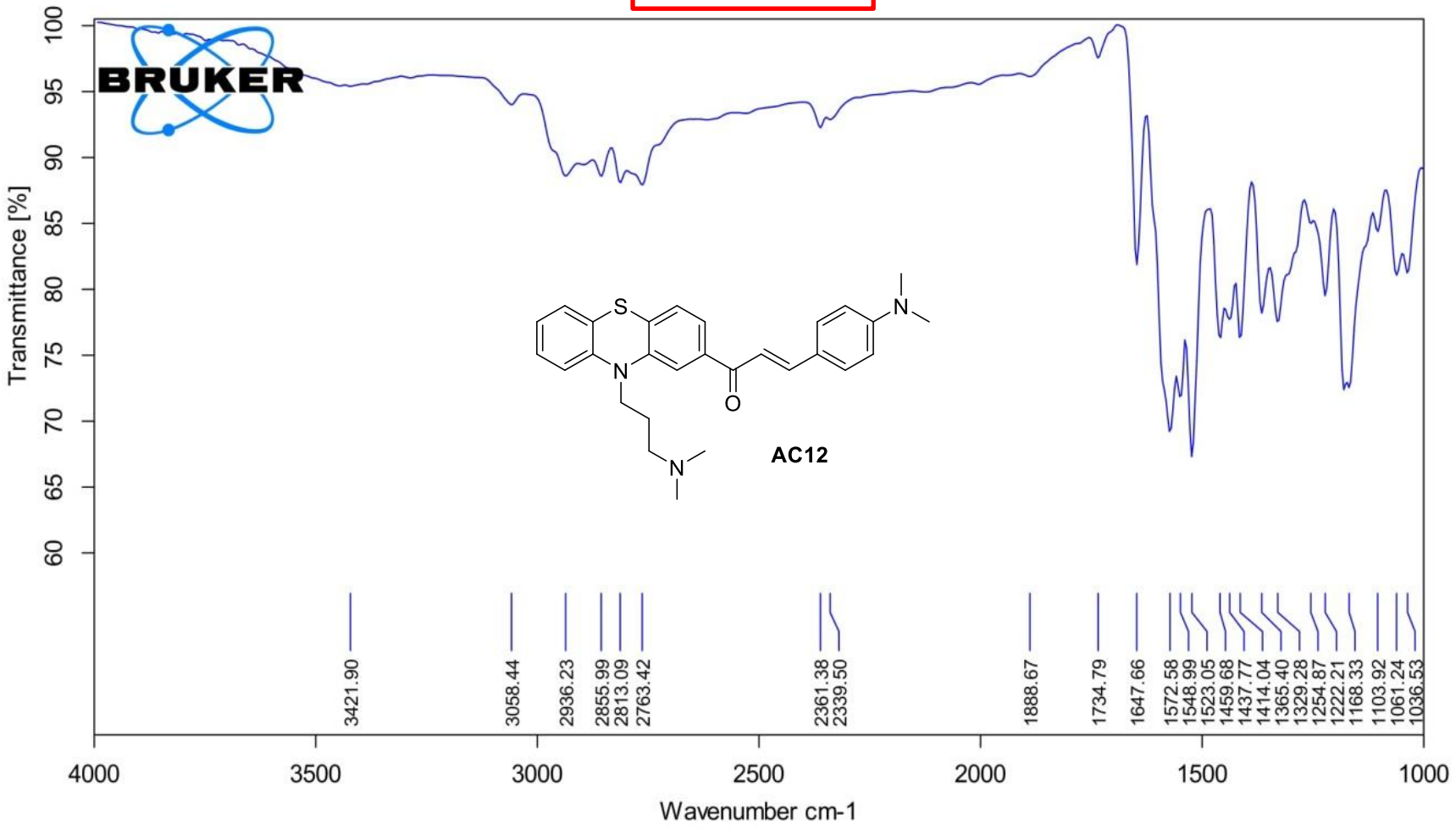

S
N
O
CF3
N

AC11

VIEN CONG NGHE HOA HOC
01 Mac Dinh Chi - Q.1 - Tp HCM

Tel: 08.38296127
Fax: 08.38293889

IR



E:\OPUS 7\2017\THANG 6\20170606\C7.0	C7	TENSOR 27 - BRUKER - GERMANY	6/8/2017

MS

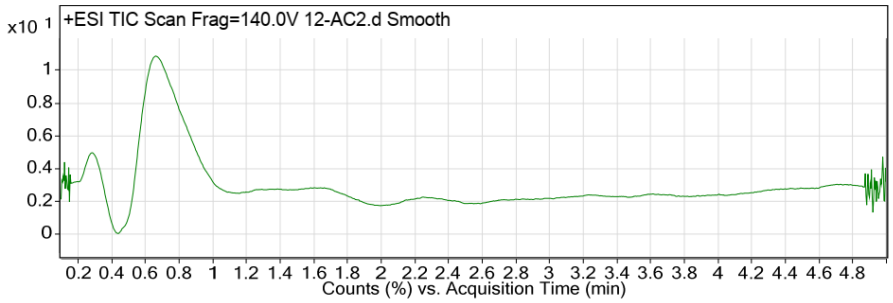
Qualitative Analysis Report

Data Filename	12-AC12.d	**Sample Name**	12-AC12
Sample Type	Sample	**Position**	P2-B9
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	22/08/2020 11:50:36 AM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

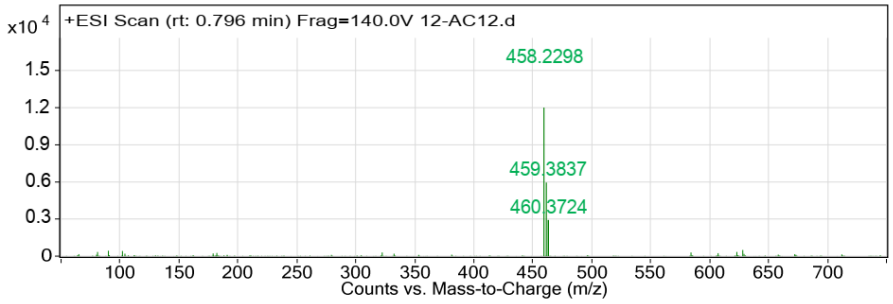
User Chromatograms

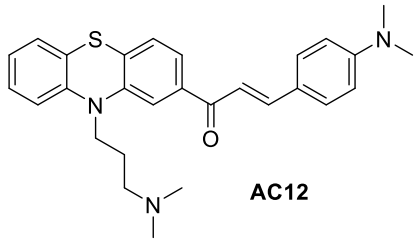
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage	**Collision Energy**	**Ionization Mode**
140	0	ESI



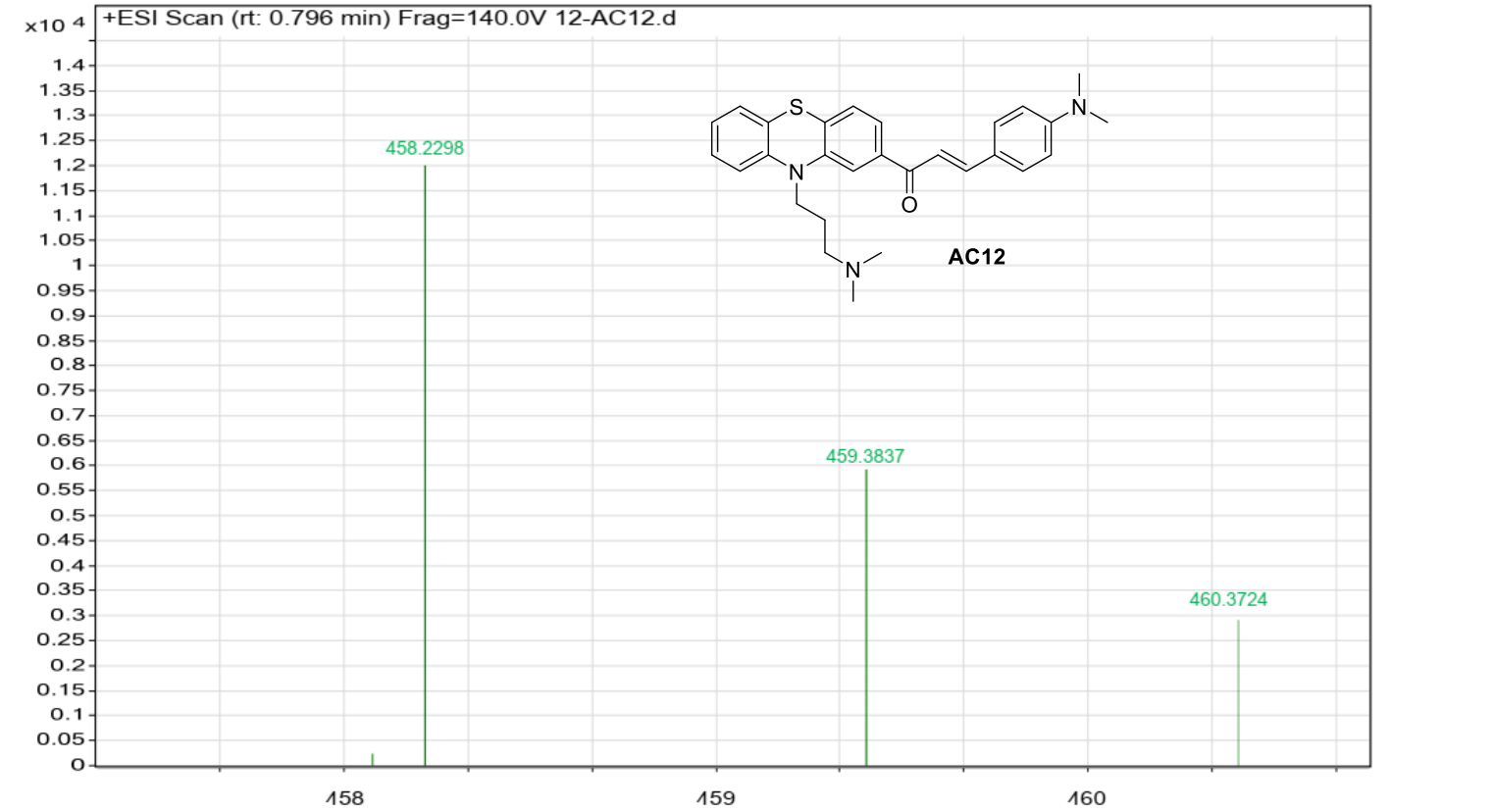


AC12

--- End Of Report ---

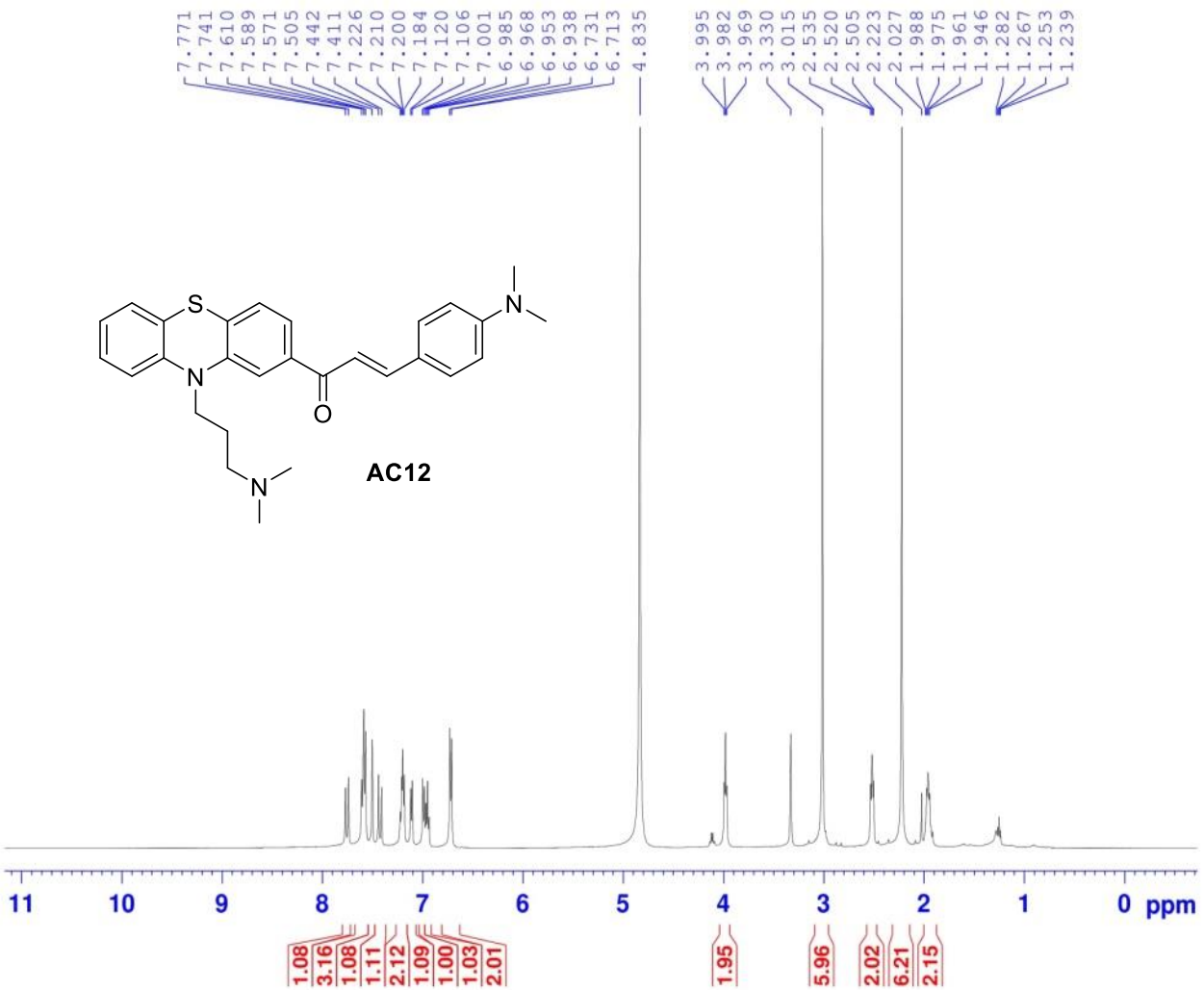
MS

Sample Name	12-AC12	**Position**	P2-B9	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	12-AC12.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	22/08/2020 11:50:36 AM



^{1}H-NMR

C7-MeOD-1H



BRUKER

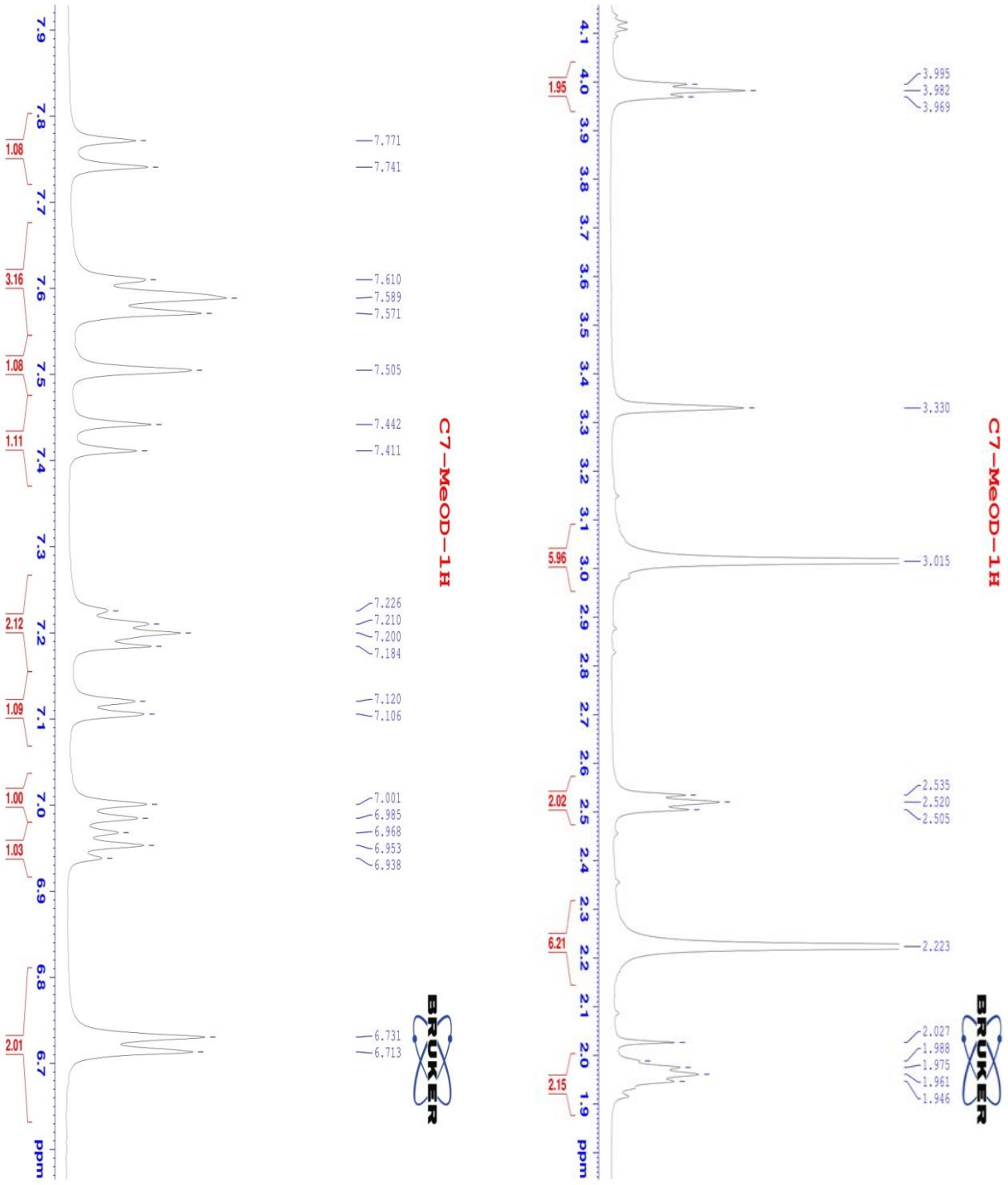
```
Current Data Parameters
NAME                 113DAO_C7
EXPNO                        1
PROCNO                       1

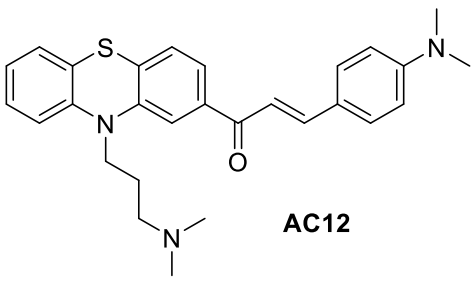
F2 - Acquisition Parameters
Date_                 20170704
Time                     16.50
INSTRUM                  spect
PROBHD     5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                  MeOD
NS                         16
DS                          2
SWH                 10000.000 Hz
FIDRES                0.152588 Hz
AQ                    3.2767999 sec
RG                       79.36
DW                      50.000 usec
DE                       6.50 usec
TE                      303.0 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1                500.2030889 MHz
NUC1                        1H
P1                       10.00 usec
PLW1               22.00000000 W

F2 - Processing parameters
SI                      65536
SF                  500.2000020 MHz
WDW                        EM
SSB                 0
LB                       0.30 Hz
GB                  0
PC                       1.00
```

^{1}H-NMR

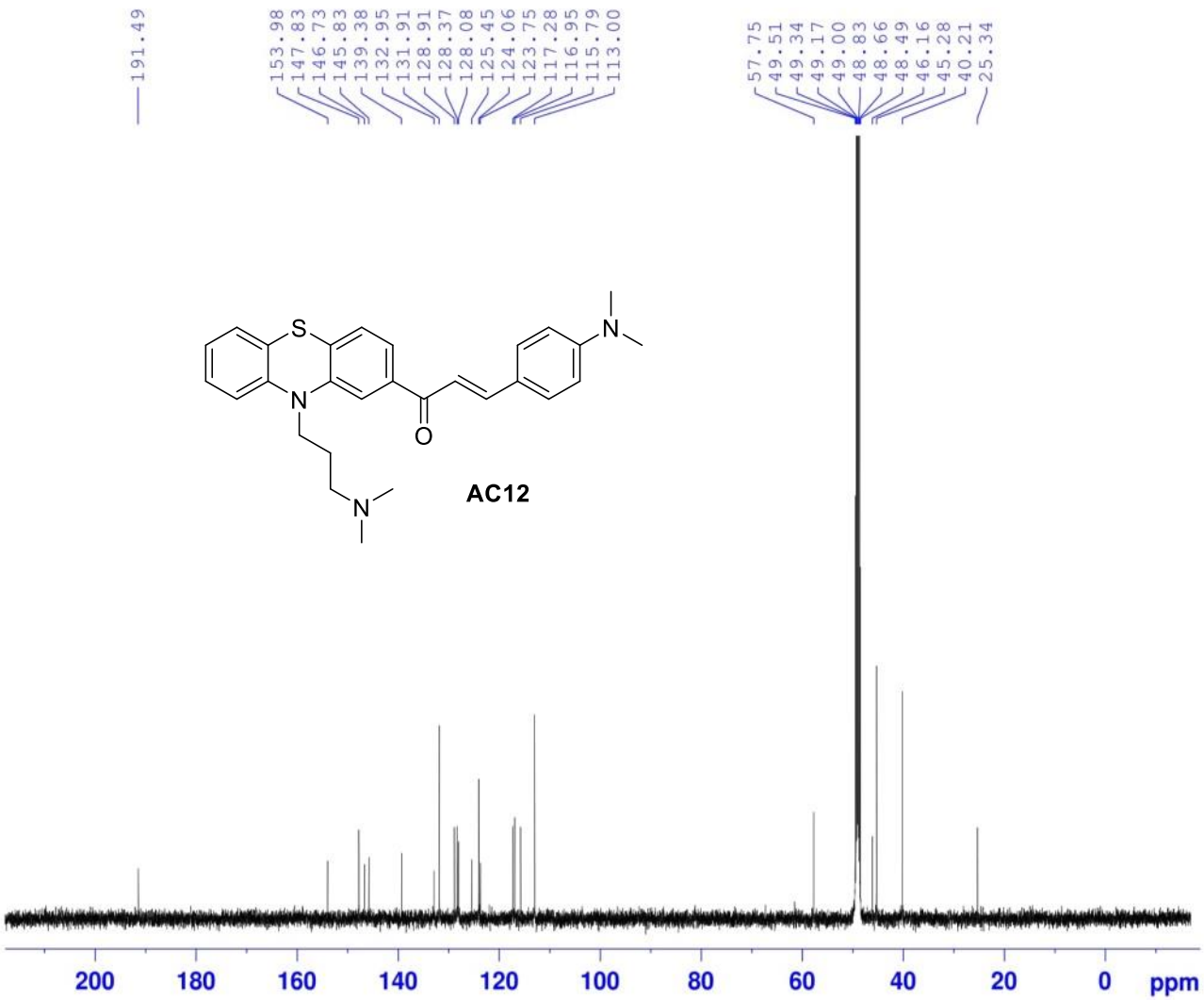




AC12

^{13}C-NMR

C7-MeOD-C13CPD



BRUKER

```
Current Data Parameters
NAME                 113DAO_C7
EXPNO                        2
PROCNO                       1

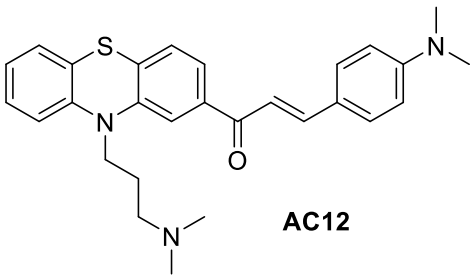
F2 - Acquisition Parameters
Date_                 20170704
Time                     17.00
INSTRUM                  spect
PROBHD     5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                   MeOD
NS                         128
DS                           4
SWH                29761.904 Hz
FIDRES              0.454131 Hz
AQ                  1.1010048 sec
RG                     198.57
DW                     16.800 usec
DE                      6.50 usec
TE                     303.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1             125.7879670 MHz
NUC1                      13C
P1                     10.00 usec
PLW1              88.00000000 W

======== CHANNEL f2 ========
SFO2             500.2020008 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                  80.00 usec
PLW2              22.00000000 W
PLW12              0.34375000 W
PLW13              0.22000000 W

F2 - Processing parameters
SI                       32768
SF               125.7752164 MHz
WDW                         EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

^{13}C-NMR


S
N
N
O
N

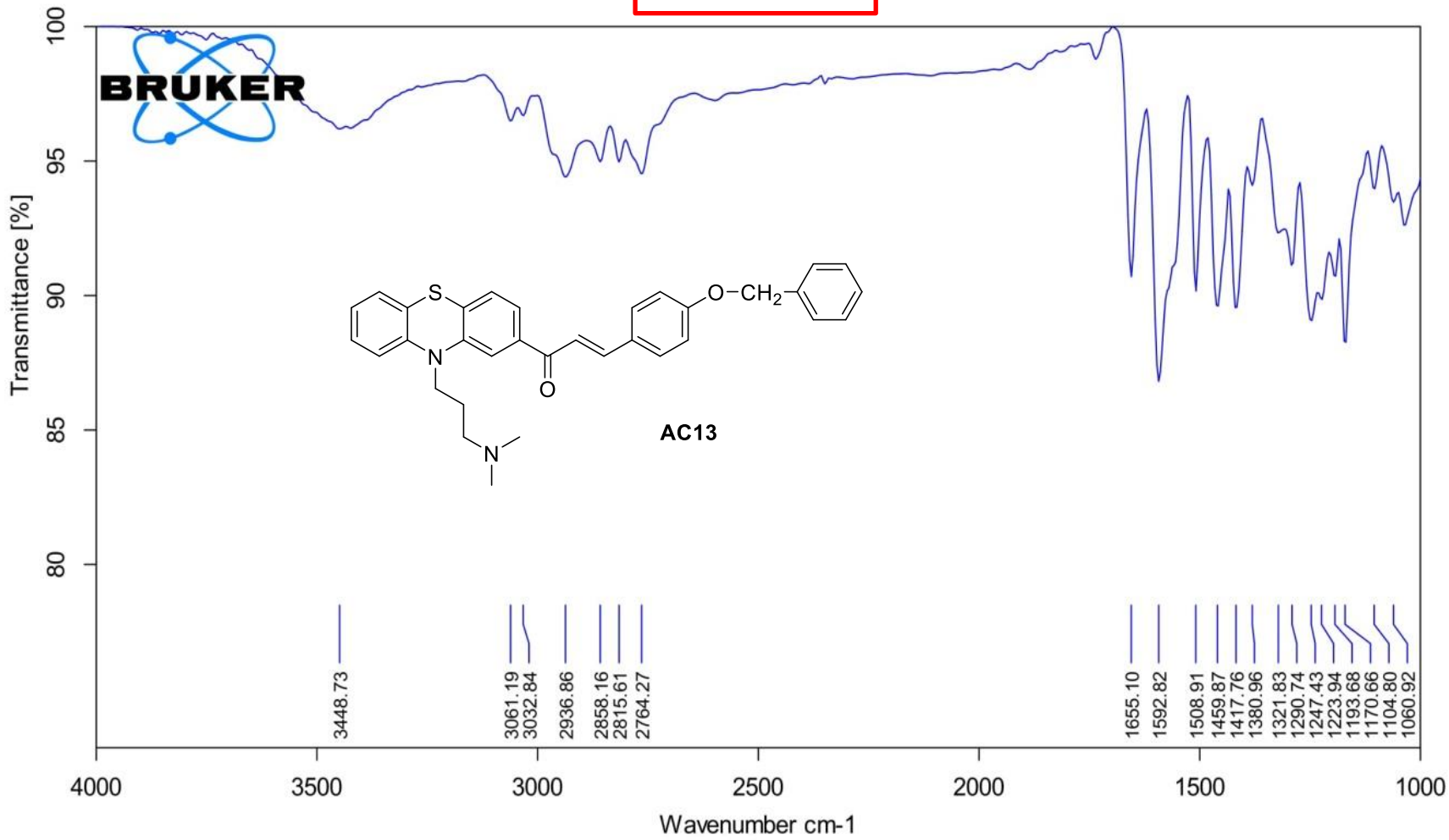
AC12

155
150
145
140
135
130
125
120
115
ppm
153.98
147.83
146.73
145.83
139.38
132.95
131.91
128.91
128.37
128.08
125.45
124.06
123.75
117.28
116.95
115.79
113.00
C7-MeOD-C13CPD
BRUKER

VIEN CONG NGHE HOA HOC
01 Mac Dinh Chi - Q.1 - Tp HCM

Tel: 08.38296127
Fax: 08.38293889

IR



E:\OPUS 7\2017\THANG 6\20170606\C5.0	C5	TENSOR 27 - BRUKER - GERMANY	6/6/2017

MS

Qualitative Analysis Report

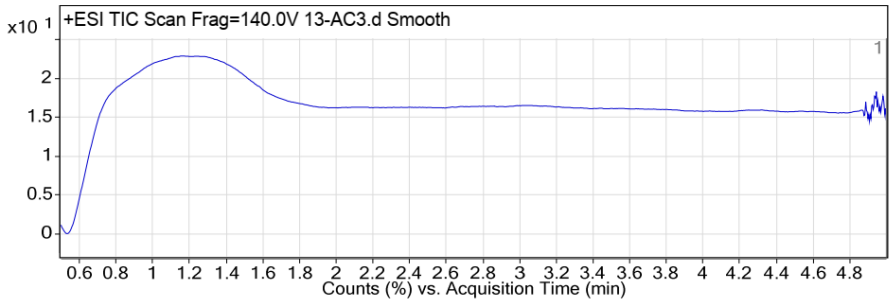
Data Filename	13-AC13.d	**Sample Name**	13-AC13
Sample Type	Sample	**Position**	P2-C2
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	22/08/2020 12:00:43 PM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

+ESI TIC Scan Frag=140.0V BTBZ 9.d Smooth

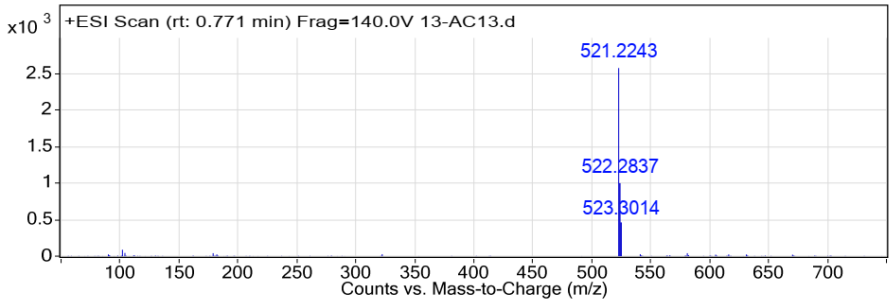
User Chromatograms

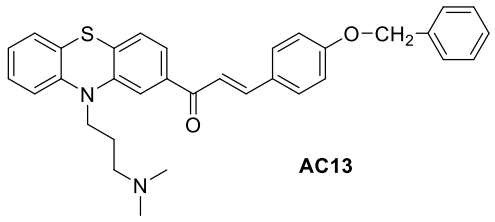
Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage	**Collision Energy**	**Ionization Mode**
140	0	ESI



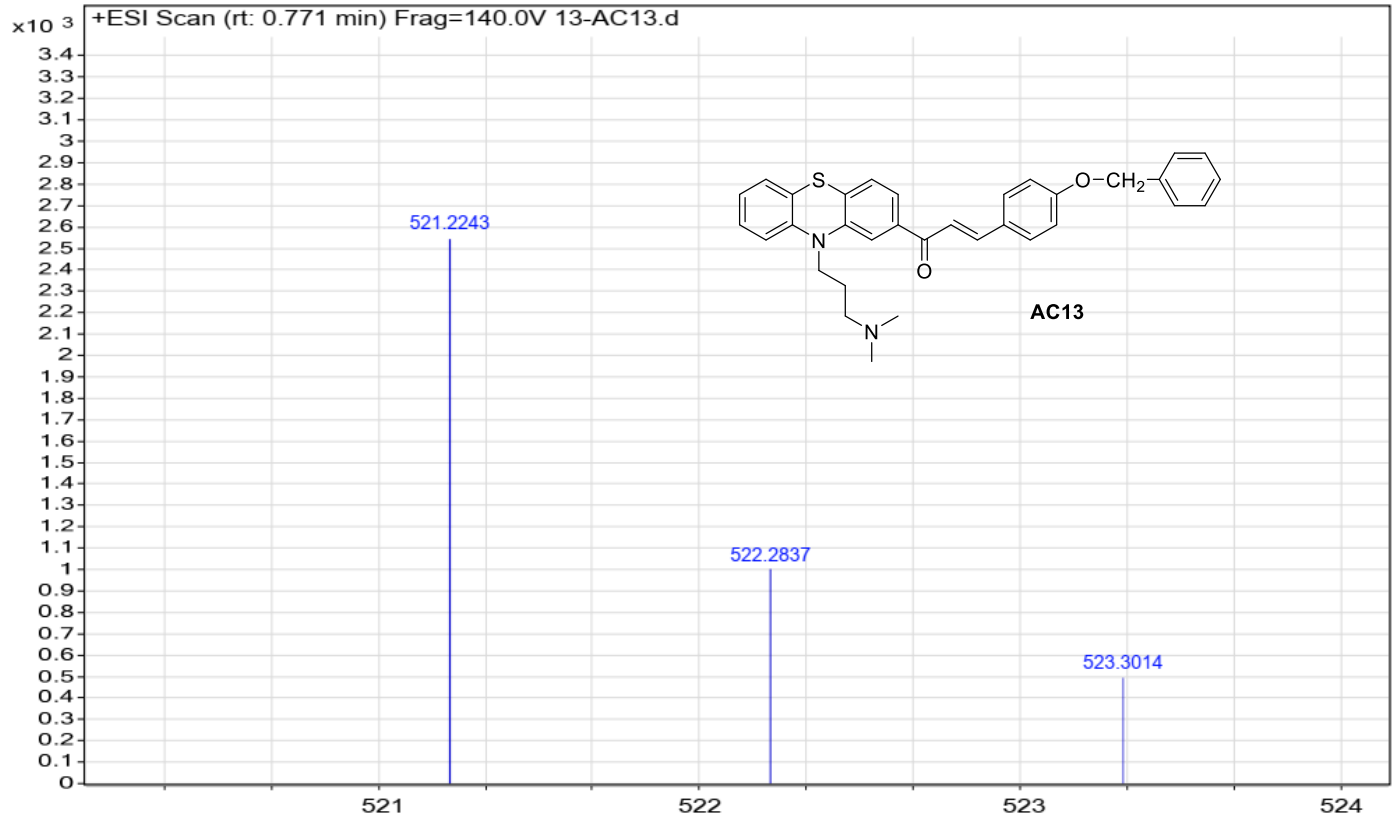


AC13

--- End Of Report ---

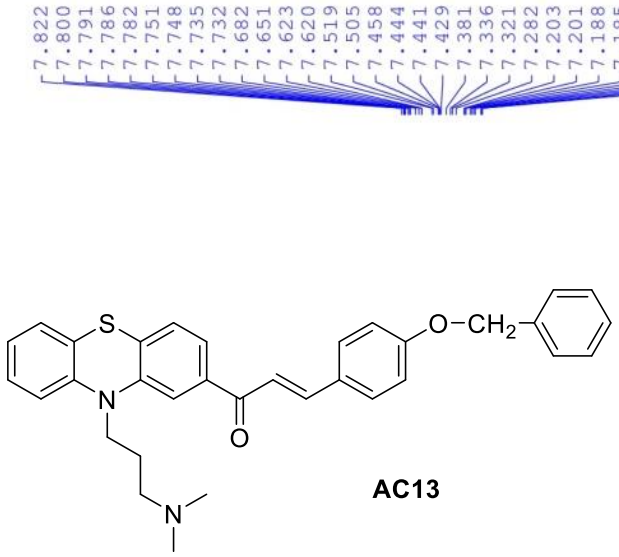
MS

Sample Name	13-AC13	**Position**	P2-C2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	13-AC13.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	22/08/2020 12:00:43 PM



^{1}H-NMR

C5-MeOD+DMSO-1H



AC13

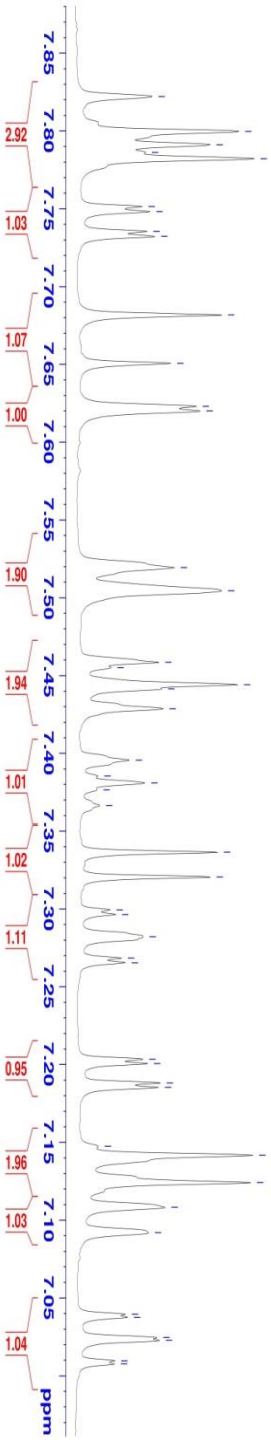

```
Current Data Parameters
NAME                  113D_C5
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20170607
Time                    10.47
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                 MeOD
NS                        16
DS                         2
SWH                10000.000 Hz
FIDRES             0.152588 Hz
AQ                 3.2767999 sec
RG                    111.09
DW                    50.000 usec
DE                     6.50 usec
TE                    303.0 K
D1                 1.00000000 sec
TD0                        1

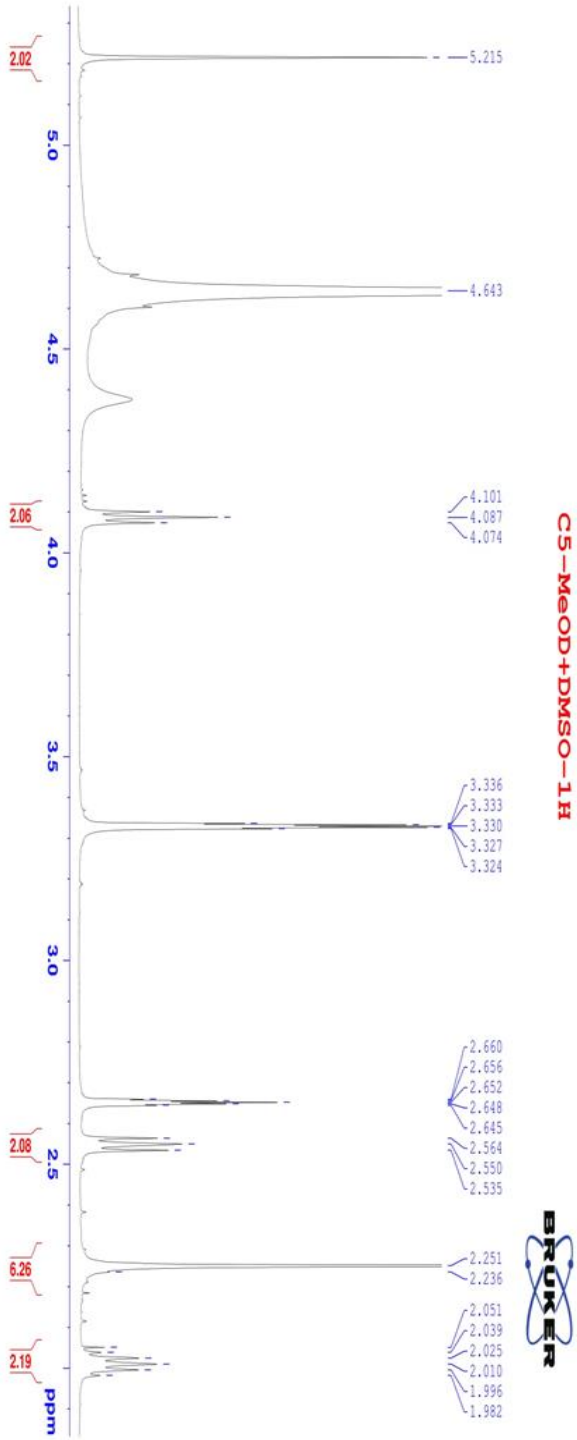
======== CHANNEL f1 ========
SFO1             500.2030889 MHz
NUC1                       1H
P1                    10.00 usec
PLW1            22.00000000 W

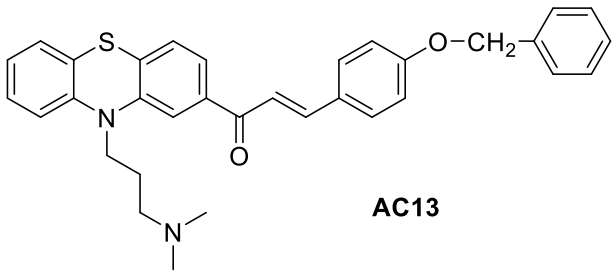
F2 - Processing parameters
SI                     65536
SF               500.2000003 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

^{1}H-NMR


7.85
7.80
7.75
7.70
7.65
7.60
7.55
7.50
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
ppm
2.92
1.03
1.07
1.00
1.90
1.94
1.01
1.02
1.11
0.95
1.96
1.03
1.04


7.822
7.800
7.791
7.786
7.782
7.751
7.748
7.735
7.732
7.682
7.651
7.623
7.620
7.519
7.505
7.458
7.455
7.444
7.441
7.429
7.396
7.385
7.381
7.377
7.366
7.336
7.321
7.299
7.296
7.282
7.268
7.265
7.203
7.201
7.188
7.185
7.147
7.142
7.124
7.108
7.092
7.040
7.037
7.024
7.023
7.010
7.008
C5—MeOD+DMSO—1H
BRUKER

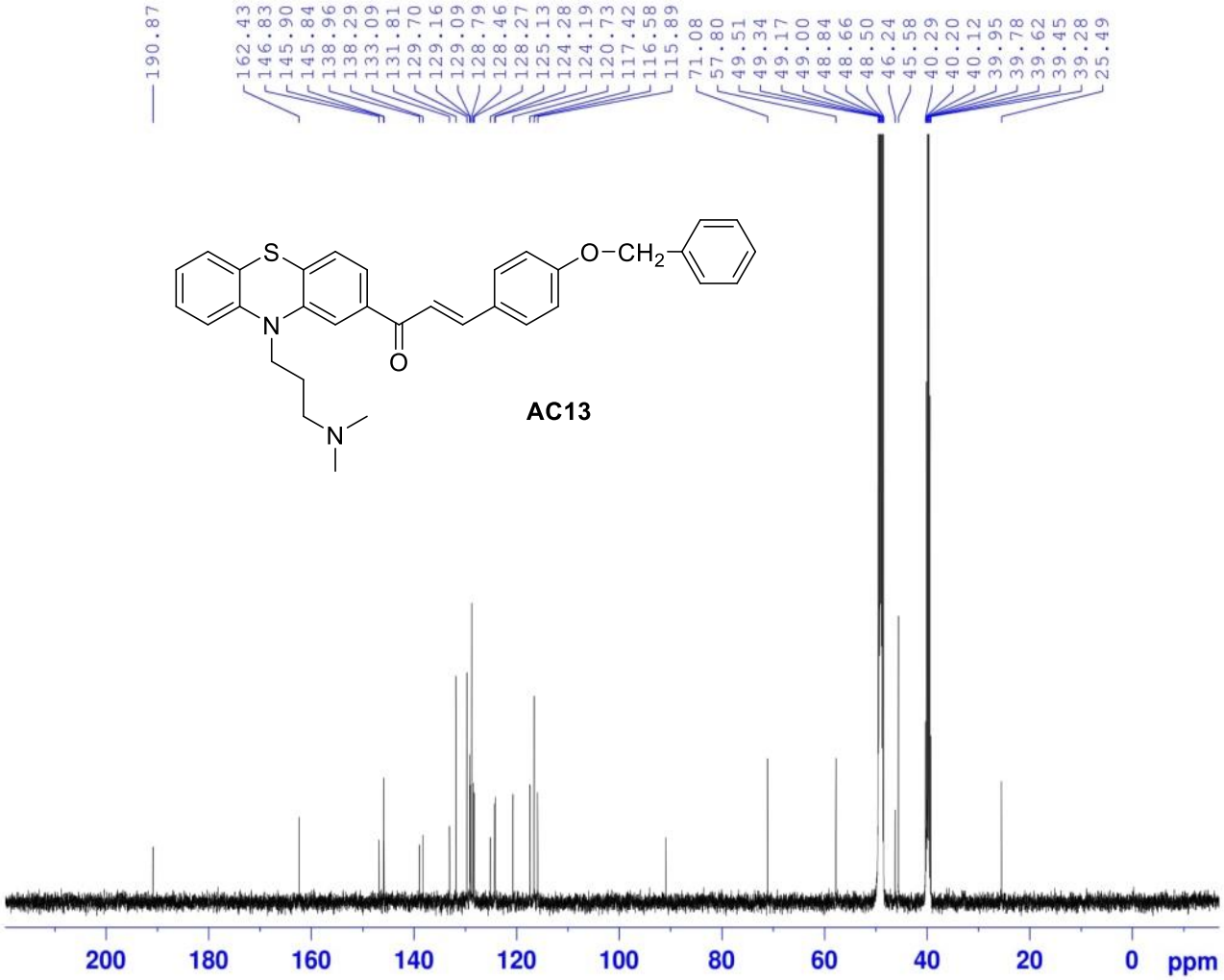

5.0
4.5
4.0
3.5
3.0
2.5
ppm
2.02
2.06
6.26
2.08
2.19
5.215
4.643
4.101
4.087
4.074
3.336
3.333
3.330
3.327
3.324
2.660
2.656
2.652
2.648
2.645
2.564
2.550
2.535
2.251
2.236
2.051
2.039
2.025
2.010
1.996
1.982
C5—MeOD+DMSO—1H
BRUKER


S
N
O
O—CH2
N

AC13

^{13}C-NMR

C5-MeOD+DMSO-C13CPD




```
Current Data Parameters
NAME                  113D_C5
EXPNO                       2
PROCNO                      1

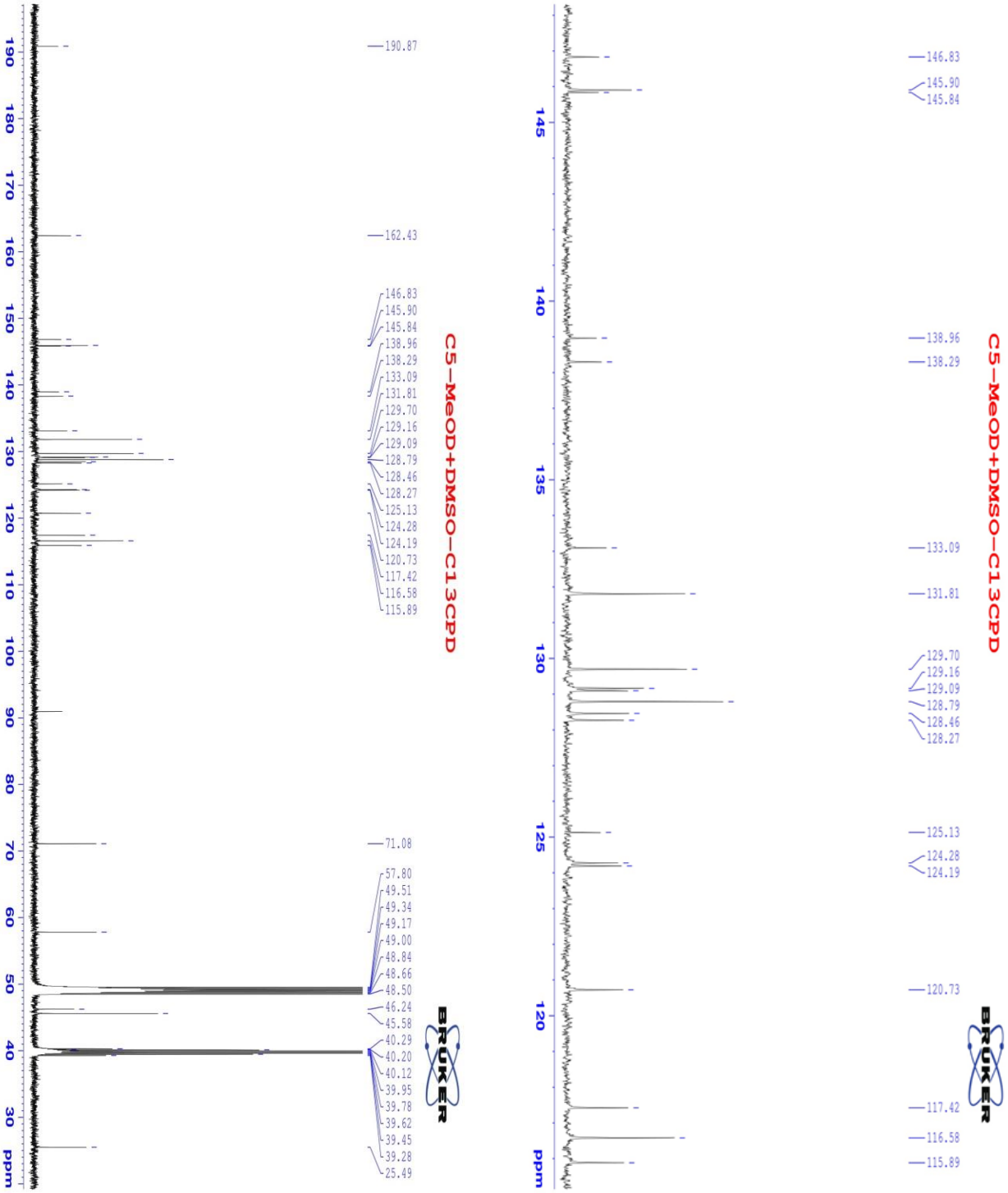
F2 - Acquisition Parameters
Date_                20170607
Time                    13.48
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                   MeOD
NS                        2048
DS                           4
SWH                  29761.904 Hz
FIDRES               0.454131 Hz
AQ                   1.1010048 sec
RG                      198.57
DW                      16.800 usec
DE                       6.50 usec
TE                      303.0 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          1

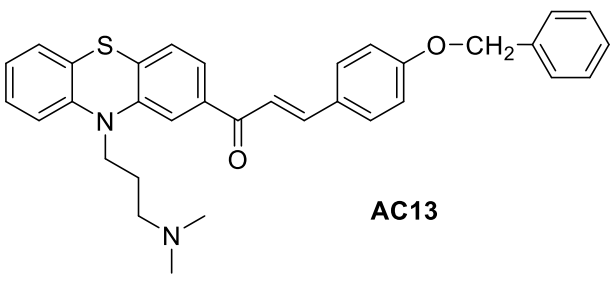
======== CHANNEL f1 ========
SFO1               125.7879670 MHz
NUC1                       13C
P1                       10.00 usec
PLW1                88.00000000 W

======== CHANNEL f2 ========
SFO2               500.2020008 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                    80.00 usec
PLW2                22.00000000 W
PLW12                0.34375000 W
PLW13                0.22000000 W

F2 - Processing parameters
SI                         32768
SF                 125.7753900 MHz
WDW                           EM
SSB                 0
LB                        1.00 Hz
GB                  0
PC                        1.40
```

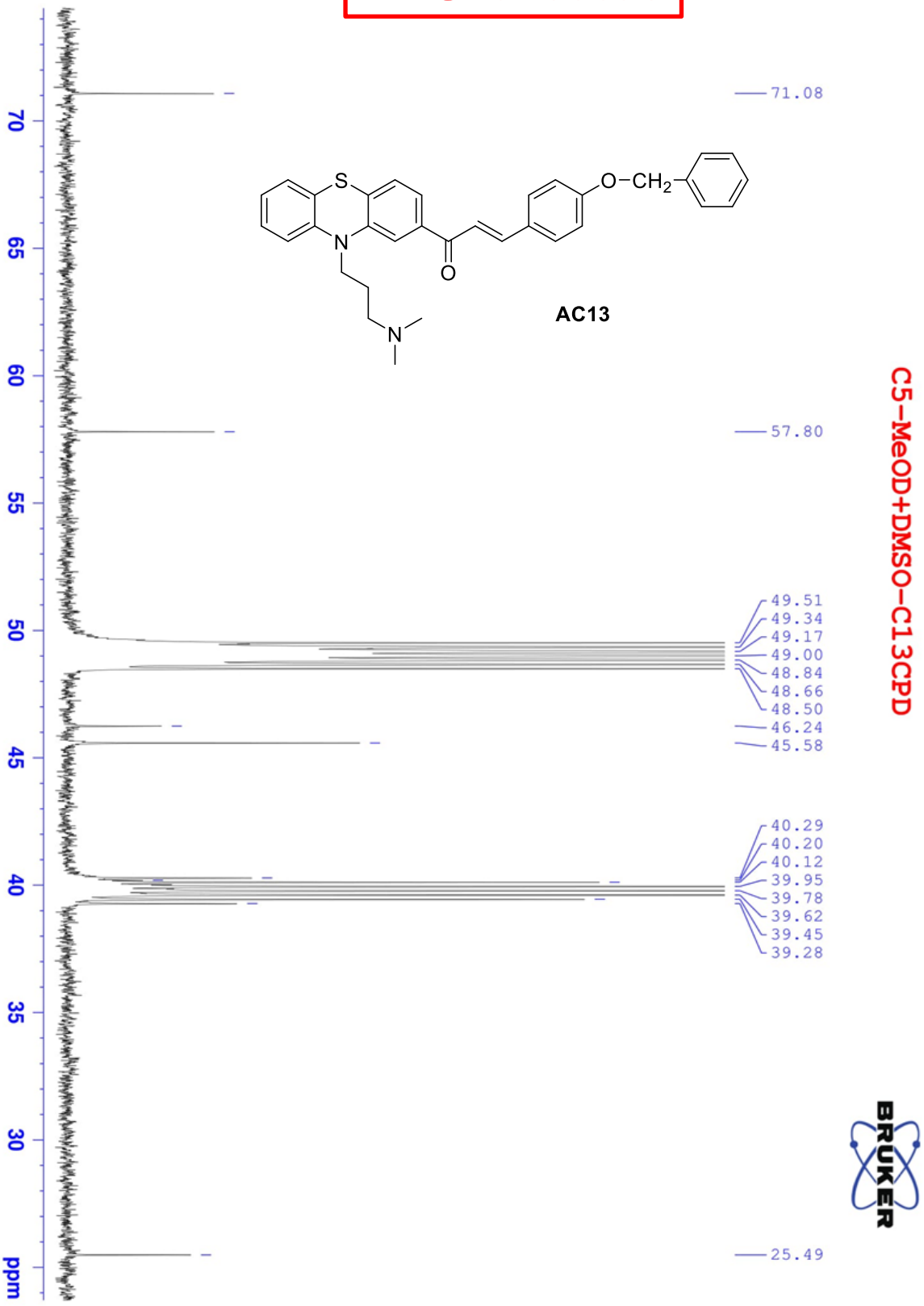
^{13}C-NMR


190.87
162.43
146.83
145.90
145.84
138.96
138.29
133.09
131.81
129.70
129.16
129.09
128.79
128.46
128.27
125.13
124.28
124.19
120.73
117.42
116.58
115.89
71.08
57.80
49.51
49.34
49.17
49.00
48.84
48.66
48.50
46.24
45.58
40.29
40.20
40.12
39.95
39.78
39.62
39.45
39.28
25.49
C5-MeOD+DMSO-C13CPD
BRUKER
ppm


S
N
O
O-CH2
N

AC13

^{13}C-NMR


71.08
57.80
49.51
49.34
49.17
49.00
48.84
48.66
48.50
46.24
45.58
40.29
40.20
40.12
39.95
39.78
39.62
39.45
39.28
25.49
70
65
60
55
50
45
40
35
30
ppm
S
N
O
O−CH2
N
AC13
C5−MeOD+DMSO−C13CPD
BRUKER

Reference

1. Thai, K.-M.; Bui, Q.-H.; Tran, T.-D.; Huynh, T.-N.-P. QSAR modeling on benzo[c]phenanthridine analogues as topoisomerase I inhibitors and anti-cancer agents. *Molecules* **2012**, *17*, 5690-5712, doi:10.3390/molecules17055690.
2. Chirico, N.; Gramatica, P. Real external predictivity of QSAR models: how to evaluate it? Comparison of different validation criteria and proposal of using the concordance correlation coefficient. *J Chem Inf Model* **2011**, *51*, 2320-2335, doi:10.1021/ci200211n.
3. Wildman, S.A.; Crippen, G.M. Prediction of Physicochemical Parameters by Atomic Contributions. *J Chem Inf Comput Sci* **1999**, *39*, 868-873, doi:10.1021/ci990307l.
4. Oprea, T.I. Property distribution of drug-related chemical databases. *Journal of computer-aided molecular design* **2000**, *14*, 251-264, doi:10.1023/a:1008130001697.