

Synthesis and Biological Evaluation of Conjugates of Oleanolic Acid Derivatives-Chalcones as α -Glucosidase Inhibitors

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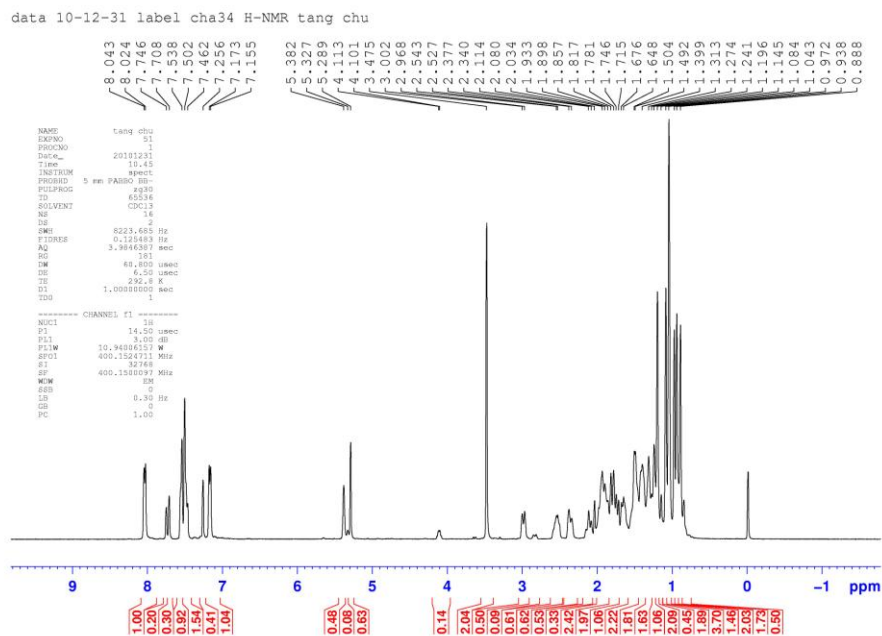
^b *College of Chemistry and Material Sciences, South Central University for Nationalities, 708 Minyuan Road, Wuhan 430074, P. R. China*

^c *College of Life Sciences, South Central University for Nationalities, 708 Minyuan Road, Wuhan 430074, P. R. China*

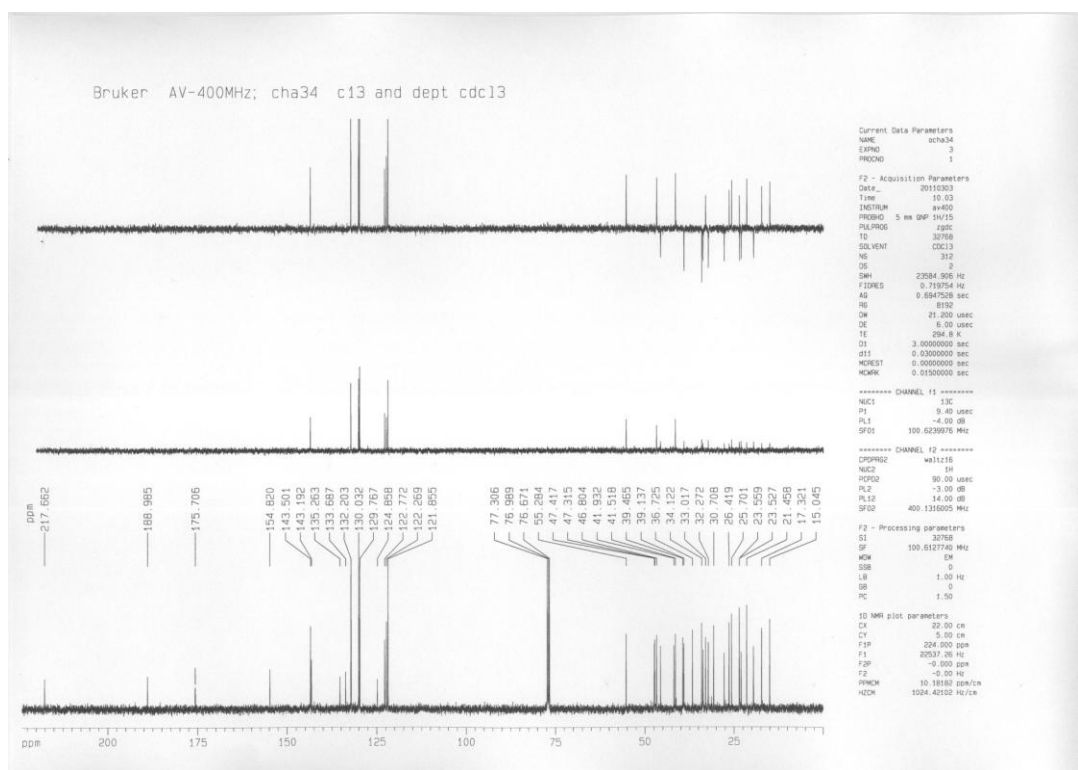
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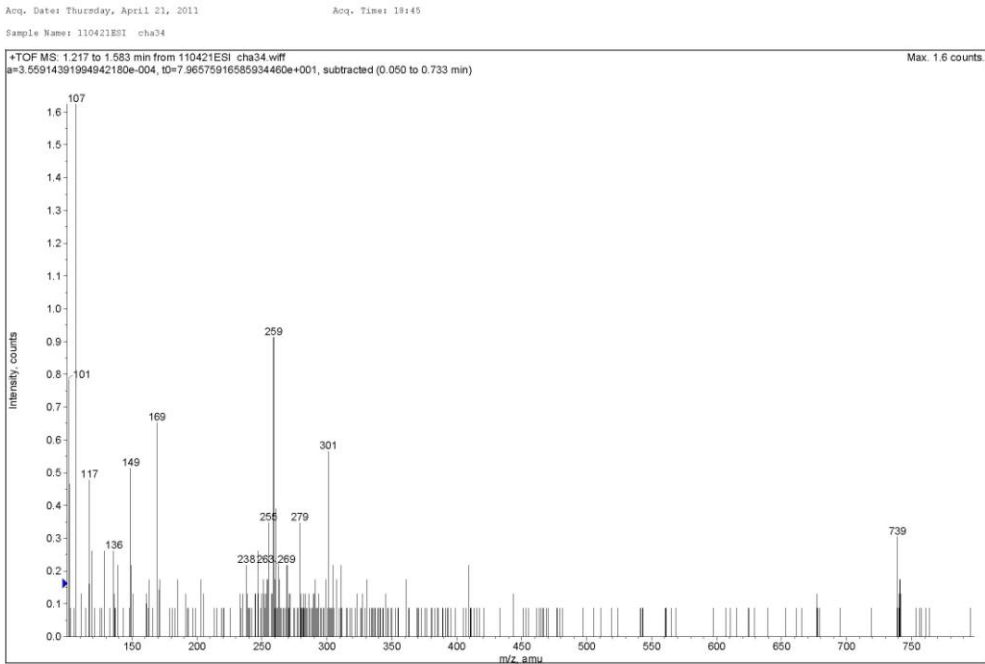
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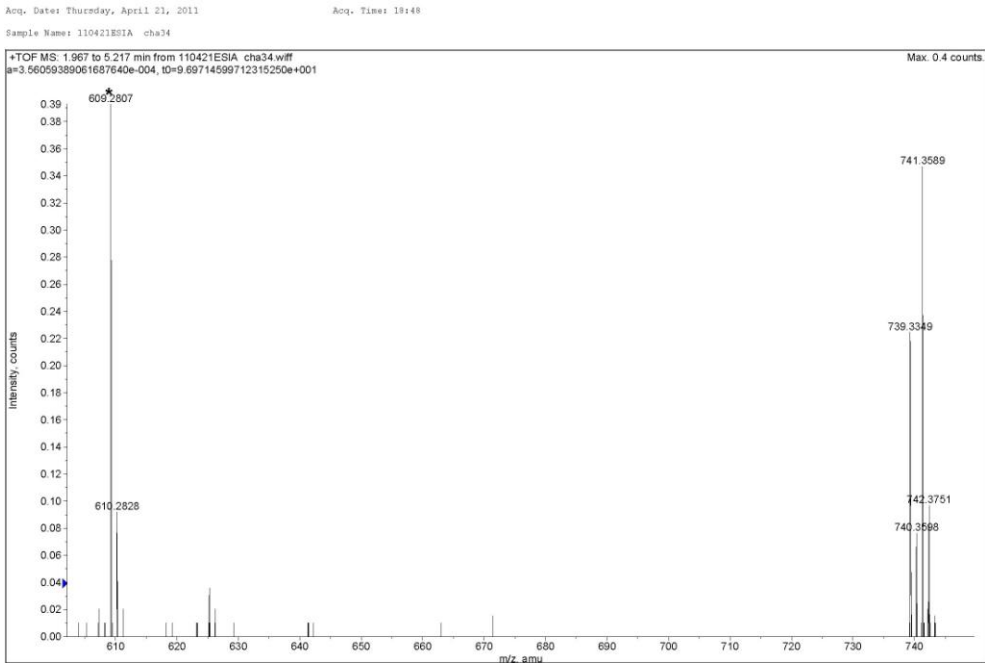
¹H NMR spectrum of compound **1a**



¹³C NMR spectrum of compound **1a**



ESI-MS spectrum of compound **1a**



Acq. Date: Thursday, April 21, 2011
Sample Name: 110421ESIA cha34

Acq. Time: 18:48

Elemental composition calculator			
Target m/z:	+739.3349	amu	
Tolerance:	+10.0000	ppm	
Result type:	Elemental		
Max num of results:	1000		
Min DBE:	-10.0000	Max DBE:	+60.0000
Electron state:	OddAndEven		
Num of charges:	0		
Add water:	N/A		
Add proton:	N/A		
File Name:	110421ESIA cha34.wiff		

	Elements	Min Number	Max Number
1	Br	1	1
2	C	0	200
3	Cl	0	0
4	F	0	0
5	H	0	400
6	K	0	0
7	N	0	0
8	Na	0	0
9	O	2	5
10	P	0	0
11	Pt	0	0

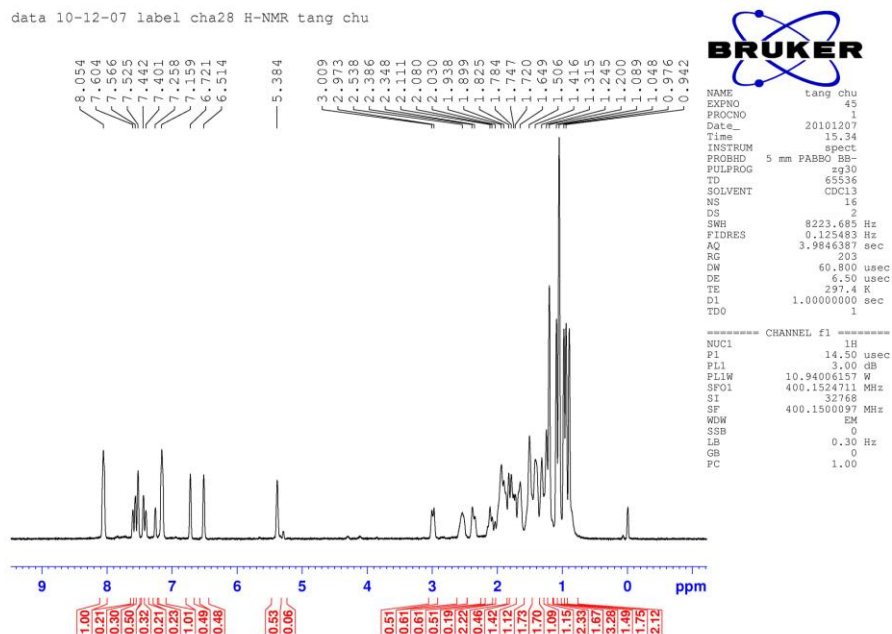
Acq. Date: Thursday, April 21, 2011
Sample Name: 110421ESIA cha34

Acq. Time: 18:48

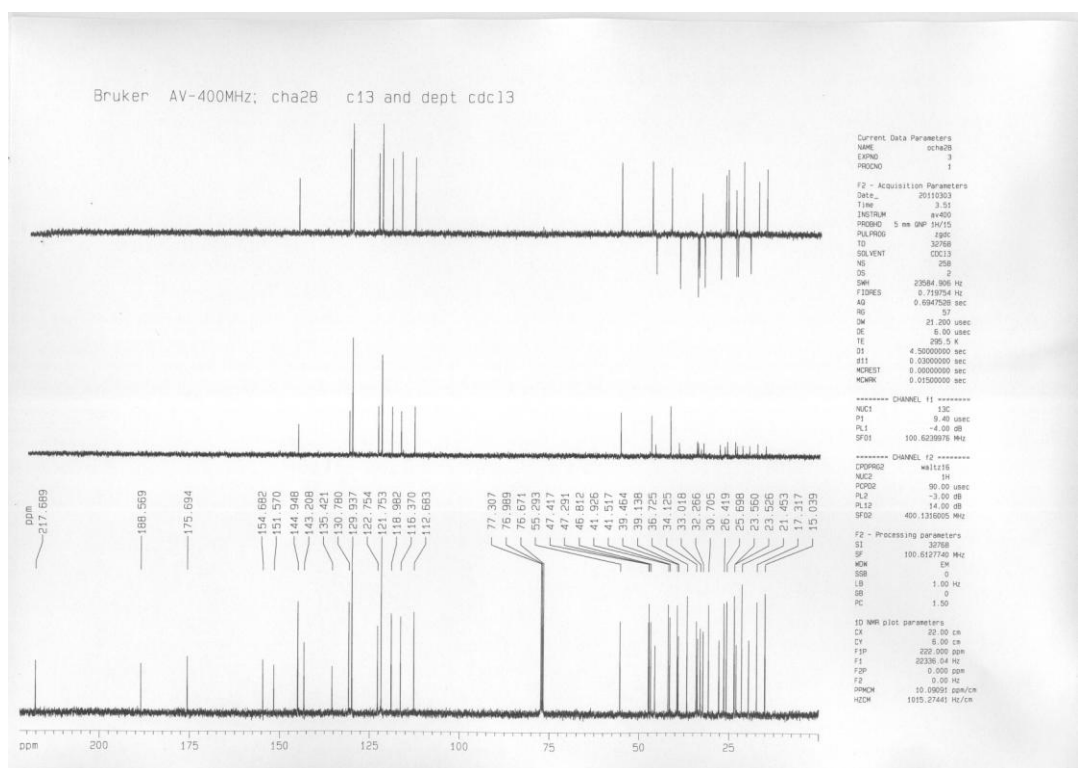
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13	Si	0	0

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C45 H56 O4 Br	739.3361	-1.2969	-1.7541	17.5

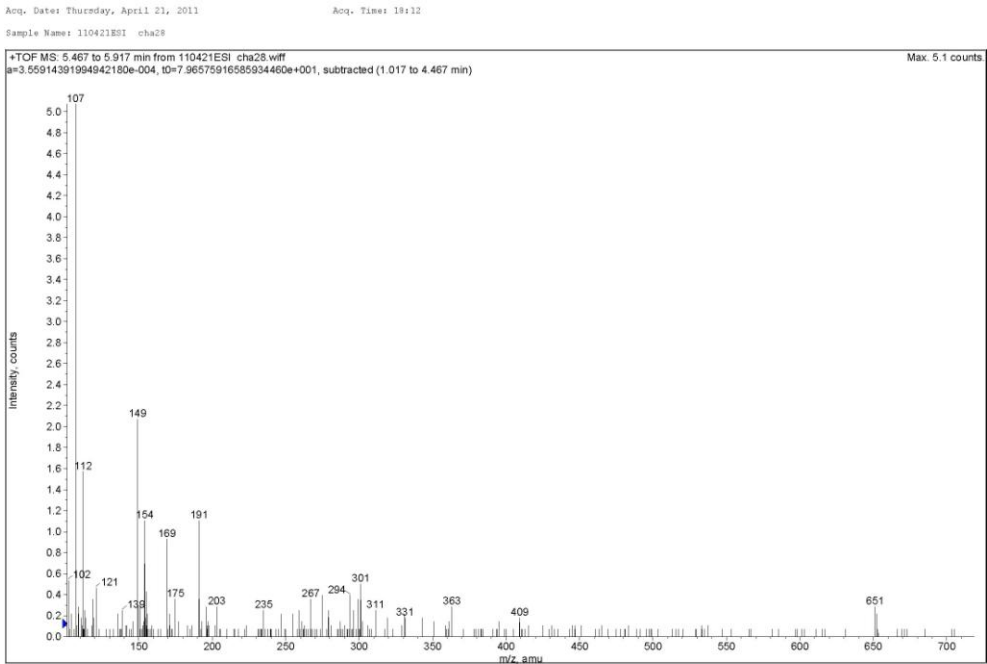
HRESIMS spectrum of compound **1a**



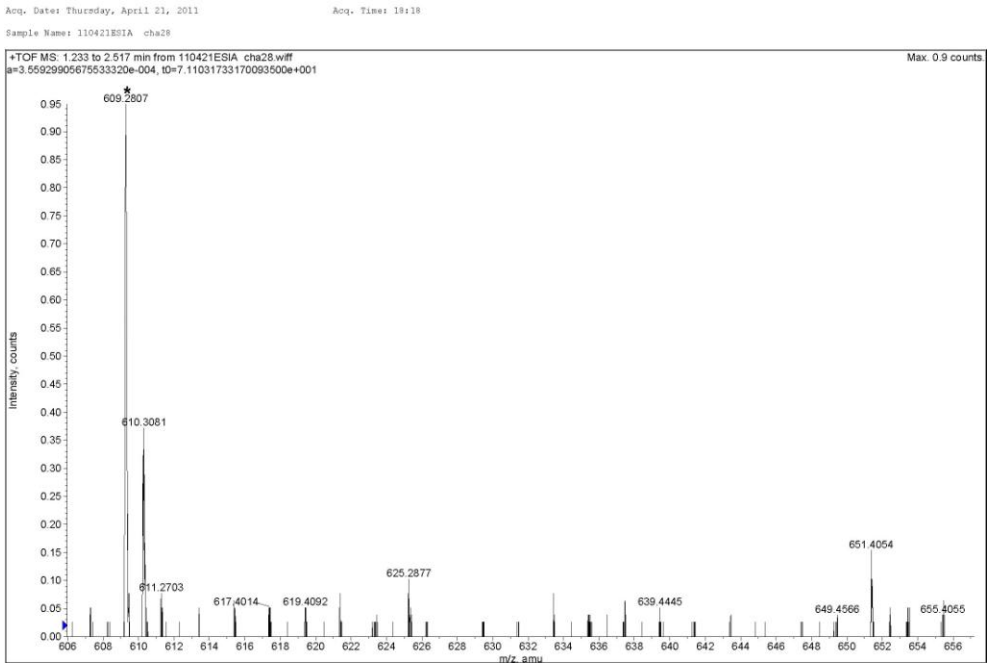
^1H NMR spectrum of compound **1b**



^{13}C NMR spectrum of compound **1b**



ESI-MS spectrum of compound **1b**



Acq. Date: Thursday, April 21, 2011
Sample Name: 110421ESIA cha28

Acq. Time: 18:18

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Target m/z:	+651.4054	amu	
Tolerance:	+10.0000	ppm	
Result type:	Elemental		
Max num of results:	1000		
Min DBE:	-10.0000	Max DBE:	+60.0000
Electron state:	OddAndEven		
Num of charges:	0		
Add water:	N/A		
Add proton:	N/A		
File Name:	110421ESIA cha28.wiff		
	Elements	Min Number	Max Number
1	Br	0	0
2	C	0	200
3	Cl	0	0
4	F	0	0
5	H	0	400
6	K	0	0
7	N	0	0
8	Na	0	0
9	O	2	5
10	P	0	0
11	Pt	0	0

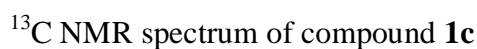
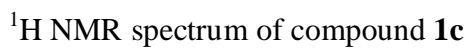
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Sample Name: 110421ESIA cha28

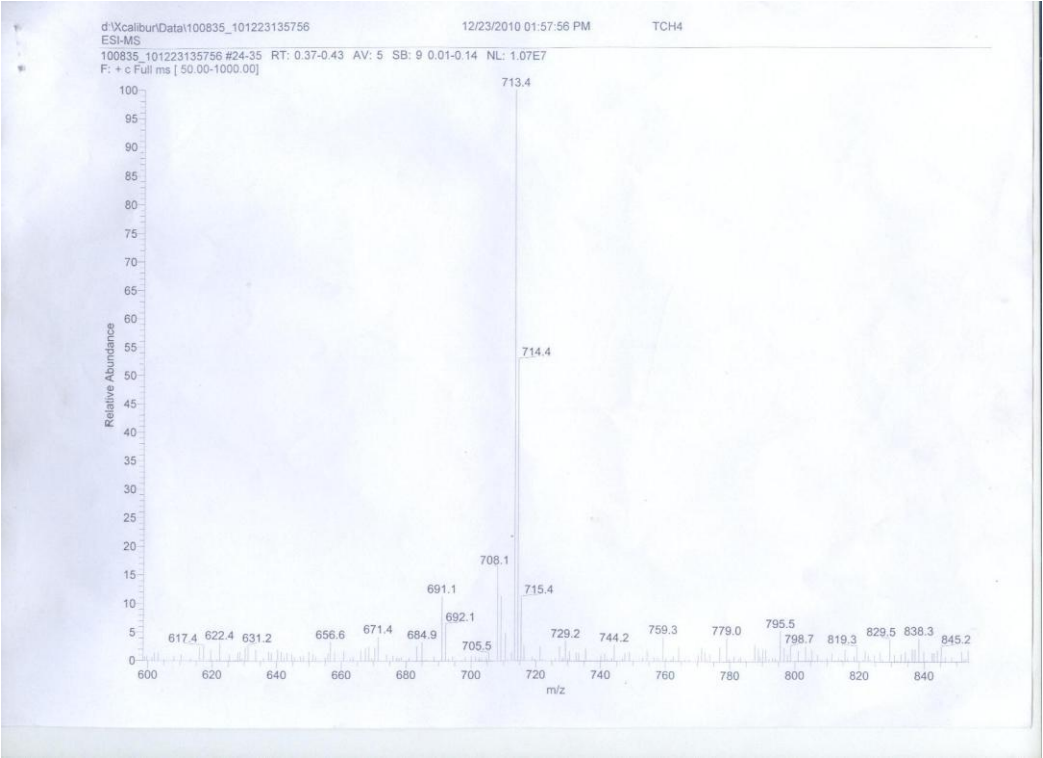
Acq. Time: 18:18

	Elements	Min Number	Max Number
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13	Si	0	0

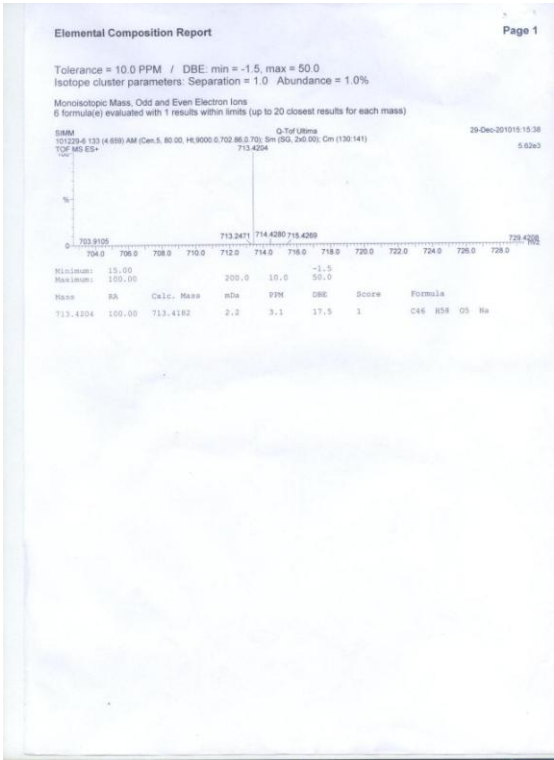
	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C43 H55 O5	651.4049	0.4496	0.6901	16.5

HRESIMS spectrum of compound **1b**

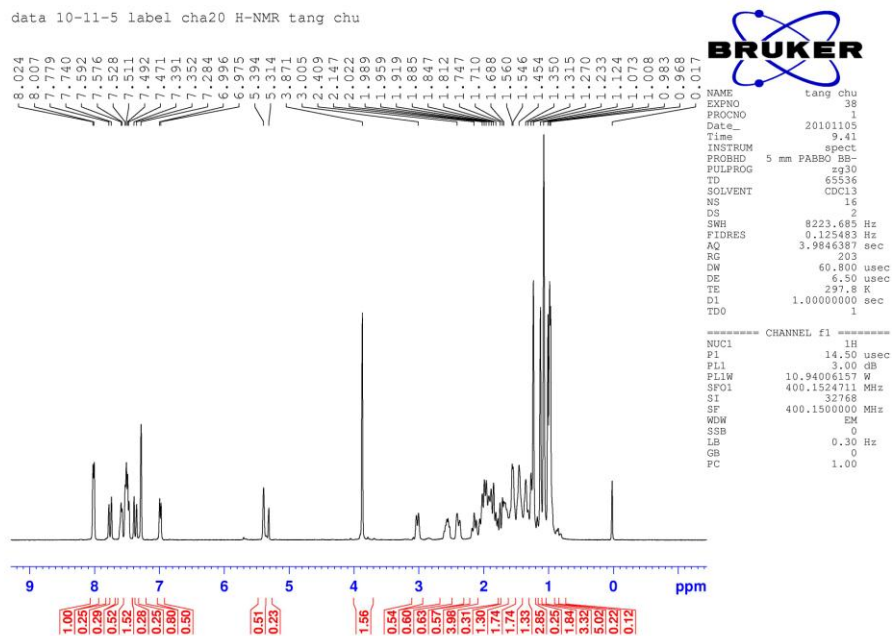




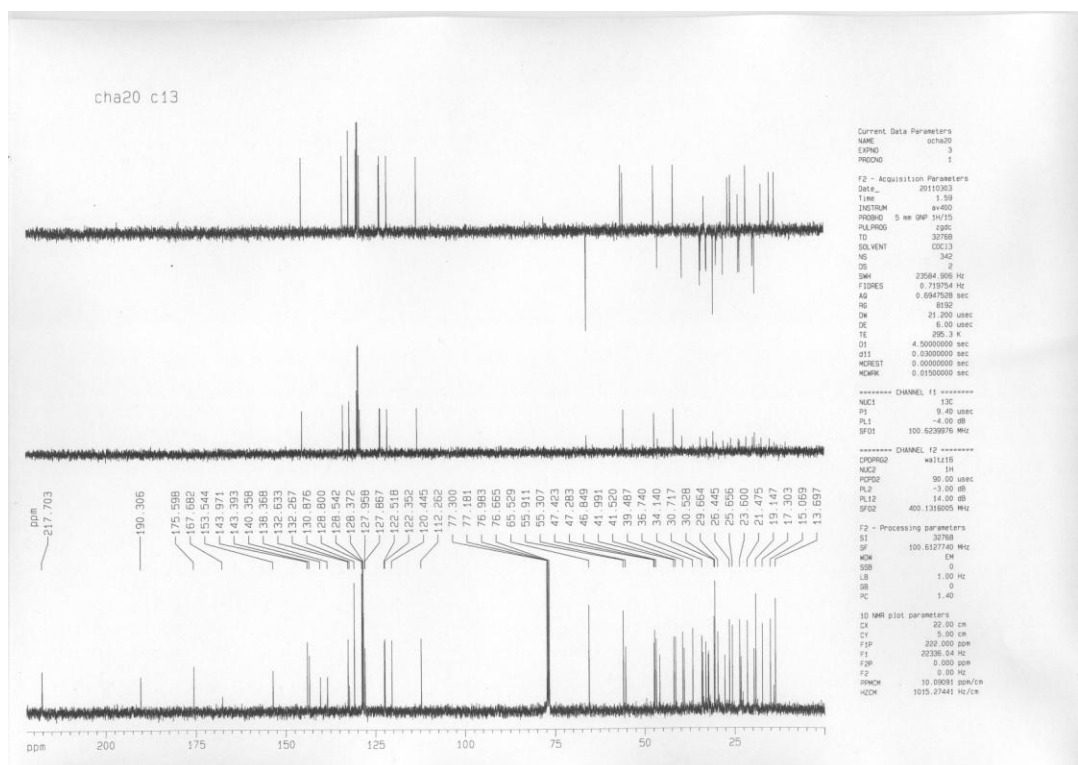
ESI-MS spectrum of compound 1c



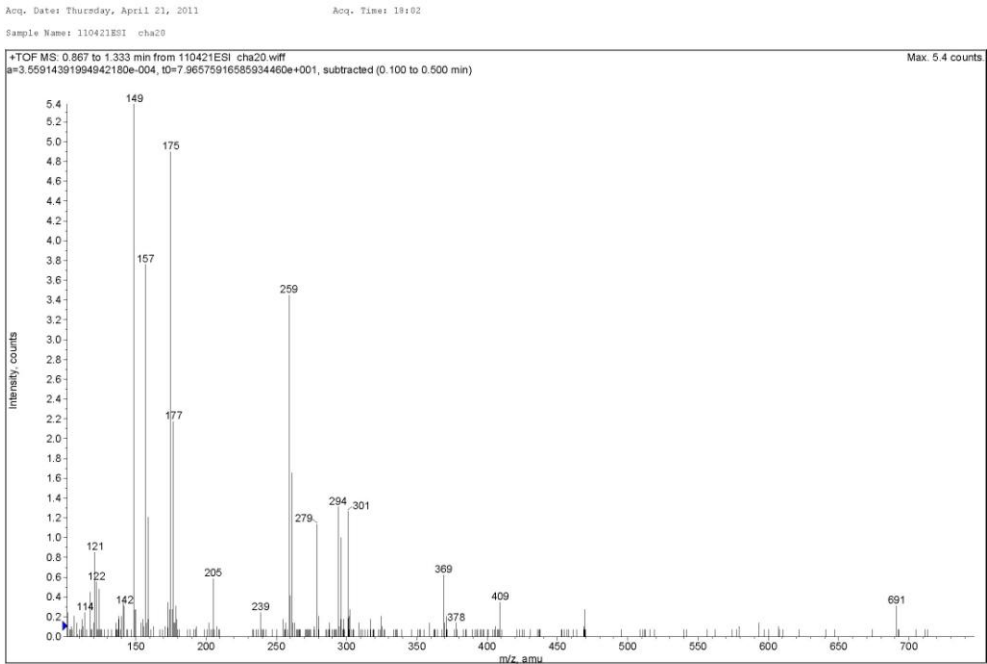
HRESIMS spectrum of compound 1c



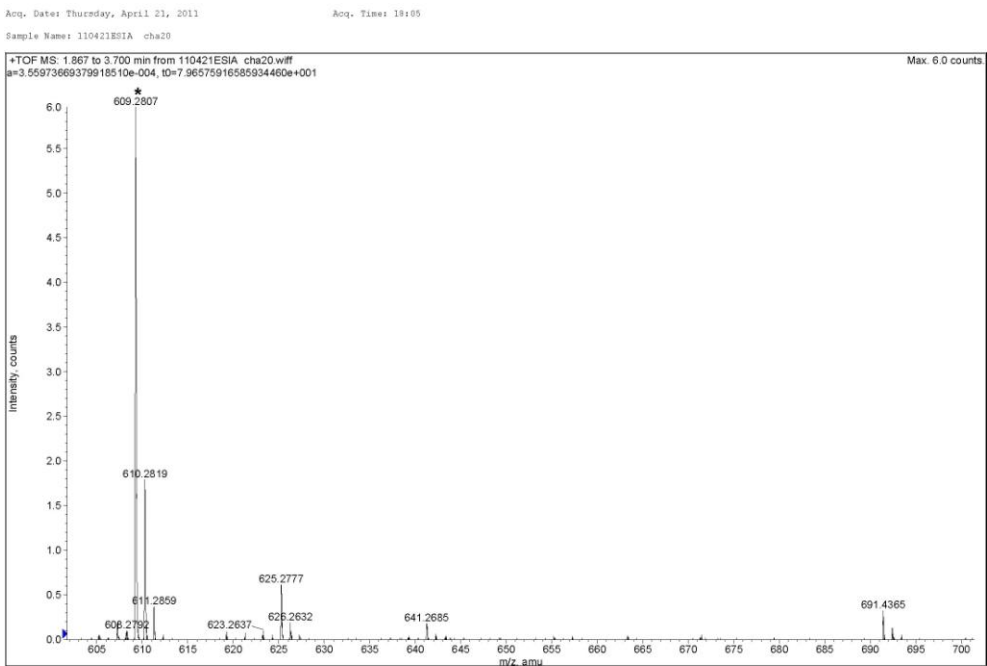
¹H NMR spectrum of compound 1d



¹³C NMR spectrum of compound 1d



ESI-MS spectrum of compound **1d**



Acq. Date: Thursday, April 21, 2011
Sample Name: 110421ESIA cha20

Acq. Time: 18:05

Elemental composition calculator

Target m/z: +691.4365 amu
Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 1000
Min DBE: -10.0000 Max DBE: +60.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 110421ESIA cha20.wiff

	Elements	Min Number	Max Number
1	Br	0	0
2	C	0	200
3	Cl	0	0
4	F	0	0
5	H	0	400
6	K	0	0
7	N	0	0
8	Na	0	0
9	O	2	5
10	P	0	0
11	Pt	0	0

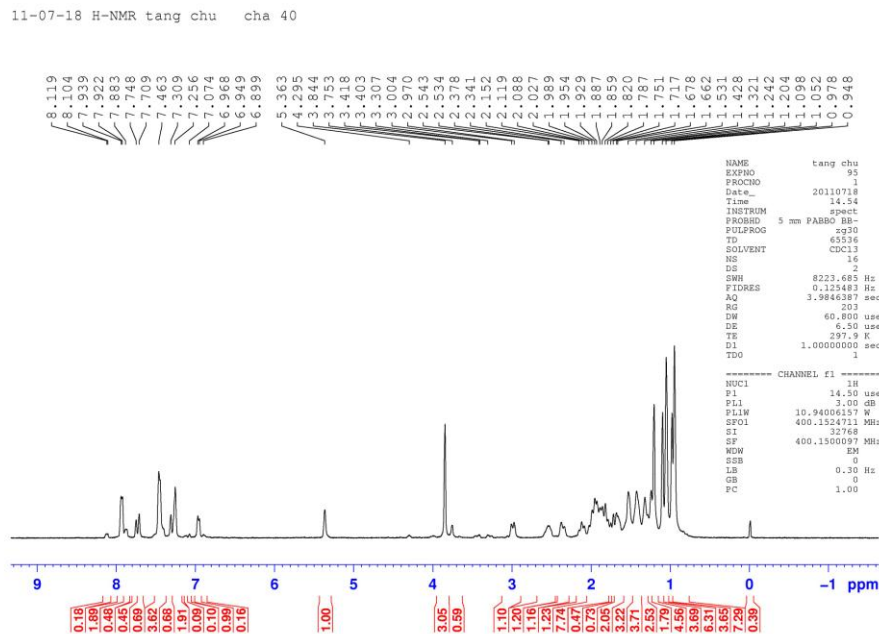
Acq. Date: Thursday, April 21, 2011
Sample Name: 110421ESIA cha20

Acq. Time: 18:05

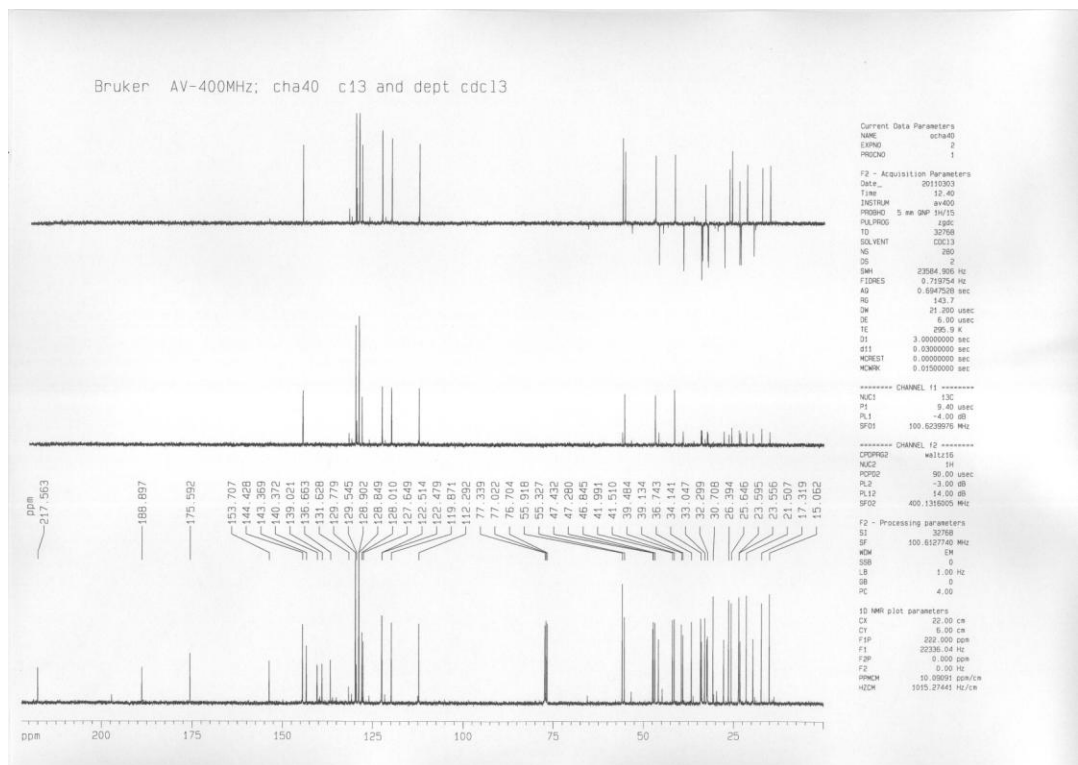
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12	S	0	0
13	Si	0	0

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1	C46 H59 O5	691.4362	0.2494	0.3607	17.5

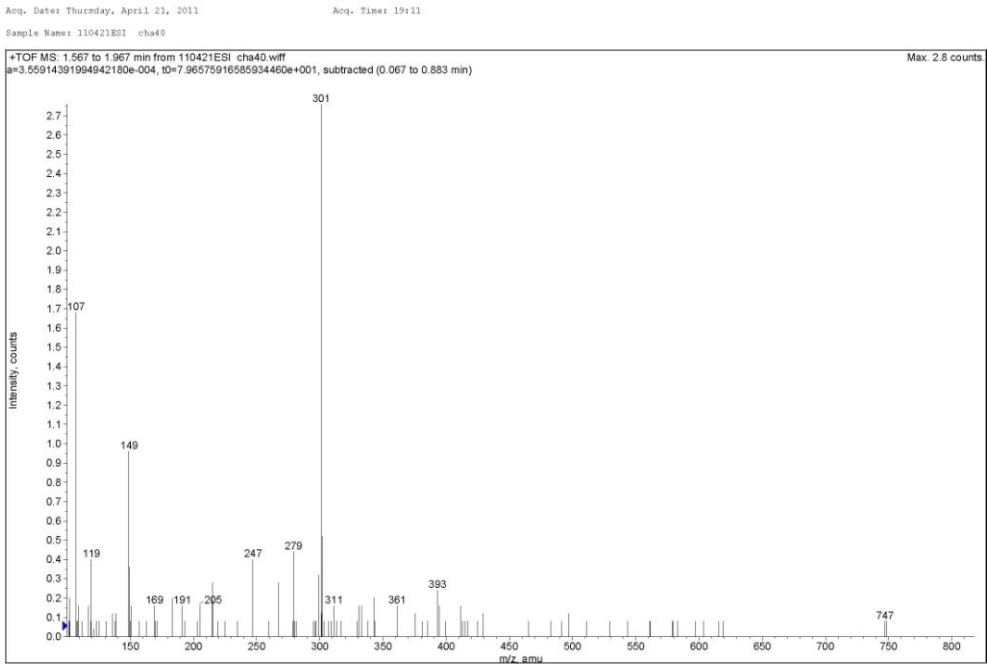
HRESIMS spectrum of compound **1d**



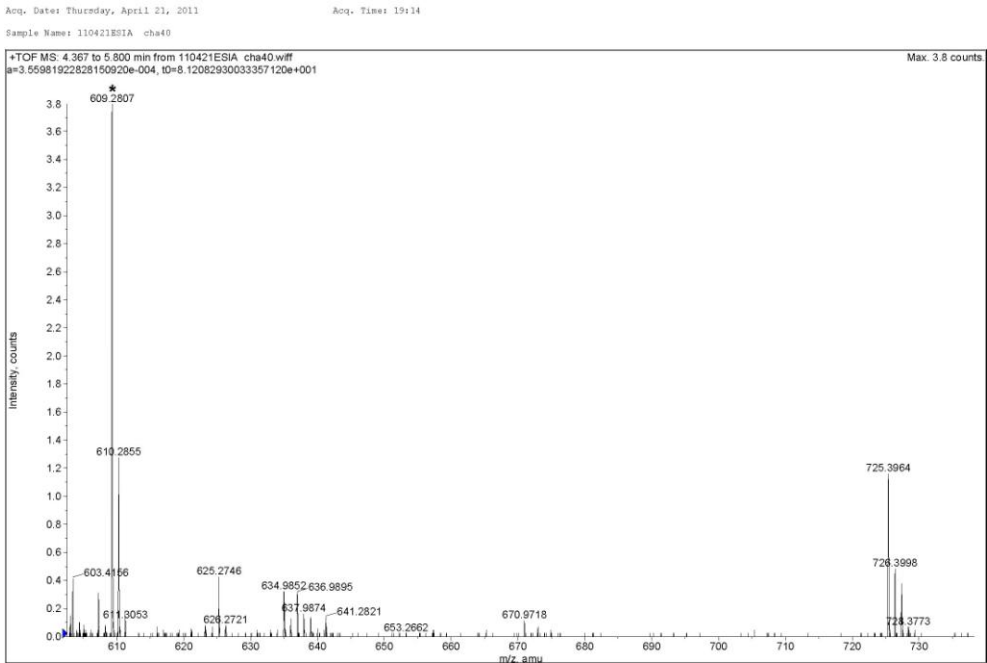
^1H NMR spectrum of compound **1e**



^{13}C NMR spectrum of compound **1e**



ESI-MS spectrum of compound **1e**



Acq. Date: Thursday, April 21, 2011 Acq. Time: 19:14
Sample Name: 110421ESIA_ cha40

	Elements	Min Number	Max Number
12	S	0	0
13	Si	0	0

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C46 H58 O5 Cl	725.3972	-0.8782	-1.2107	17.5

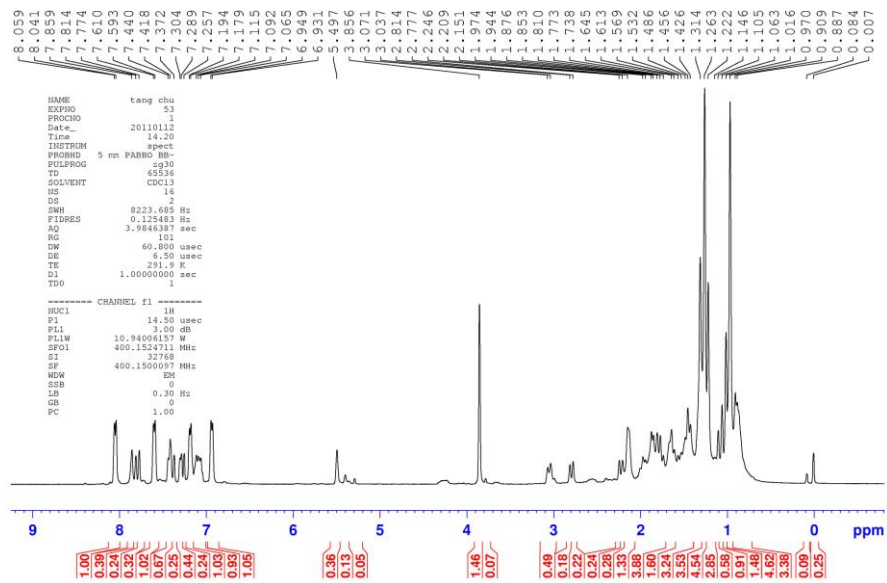
Acq. Date: Thursday, April 21, 2011 Acq. Time: 19:14
Sample Name: 110421ESIA_ cha40

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Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 1000
Min DBE: -10.0000 Max DBE: +60.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 110421ESIA_ cha40.wiff

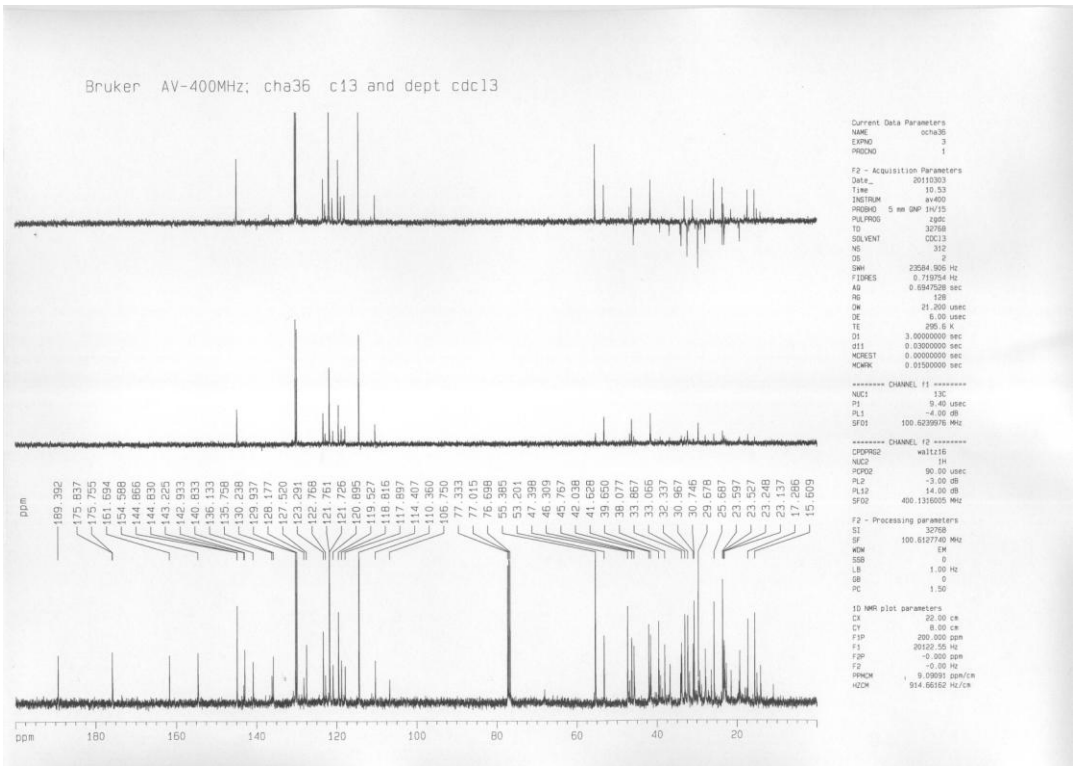
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2	C	0	200
3	Cl	1	1
4	F	0	0
5	H	0	400
6	K	0	0
7	N	0	0
8	Na	0	0
9	O	2	5
10	P	0	0
11	Pt	0	0

HRESIMS spectrum of compound **1e**

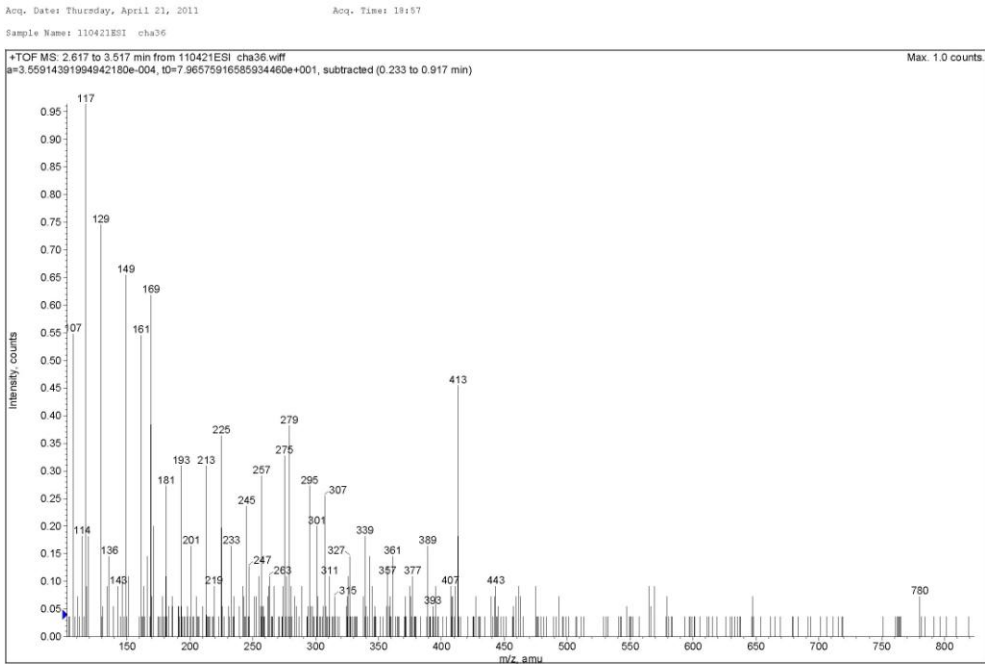
data 11-01-12 label cha36 H-NMR tang chu



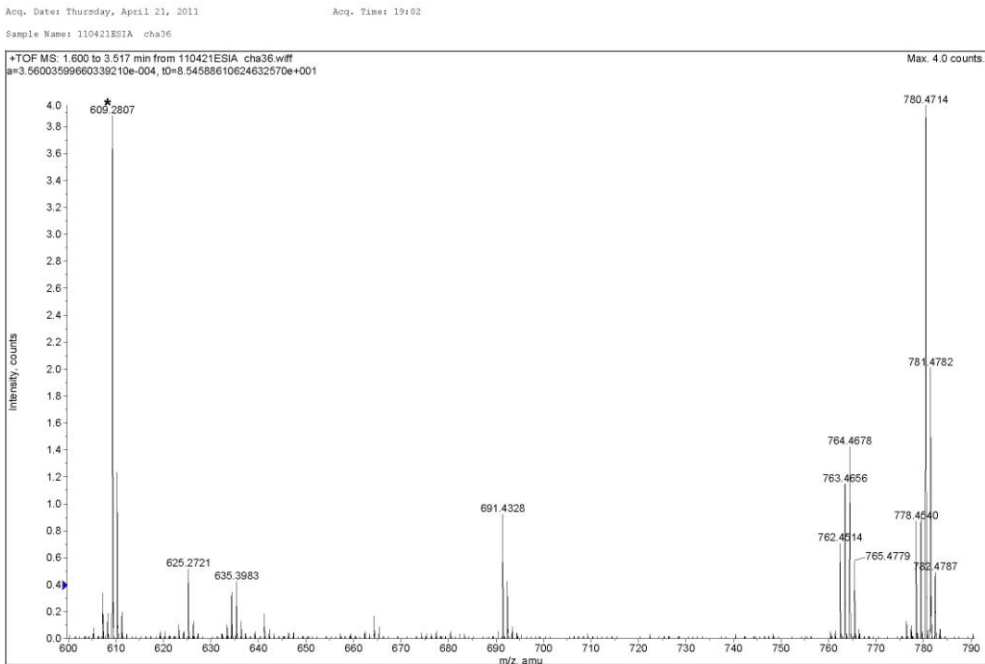
¹H NMR spectrum of compound 2a



¹³C NMR spectrum of compound 2a



ESI-MS spectrum of compound **2a**



Acq. Date: Thursday, April 21, 2011
Sample Name: 110421ESIA cha36

Acq. Time: 19:02

Elemental composition calculator			
Target m/z:	+764.4678	amu	
Tolerance:	+10.0000	ppm	
Result type:	Elemental		
Max num of results:	1000		
Min DBE:	-10.0000	Max DBE:	+60.0000
Electron state:	OddAndEven		
Num of charges:	0		
Add water:	N/A		
Add proton:	N/A		
File Name:	110421ESIA cha36.wiff		

	Elements	Min Number	Max Number
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2	C	0	200
3	Cl	0	0
4	F	0	0
5	H	0	400
6	K	0	0
7	N	1	1
8	Na	0	0
9	O	2	5
10	P	0	0
11	Pt	0	0

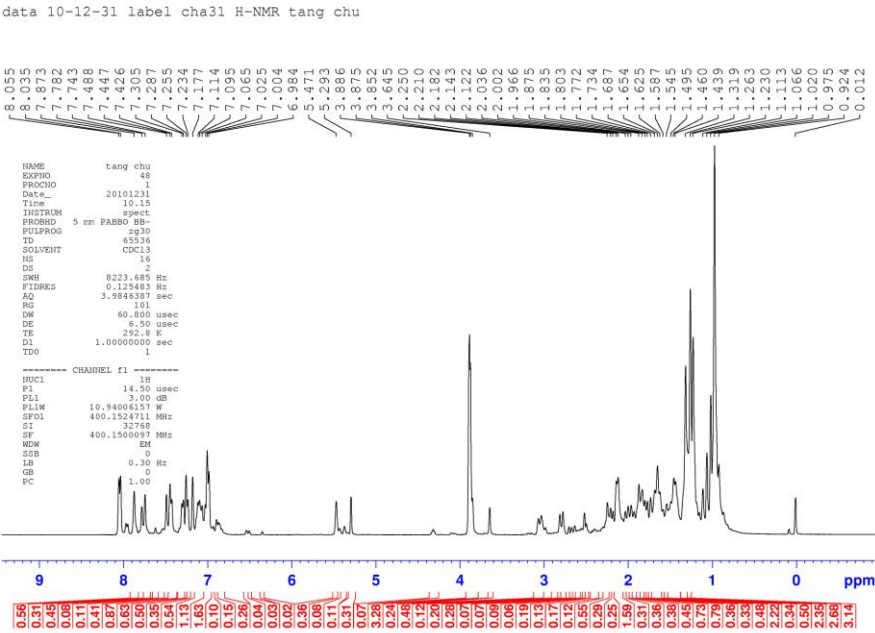
Acq. Date: Thursday, April 21, 2011
Sample Name: 110421ESIA cha36

Acq. Time: 19:02

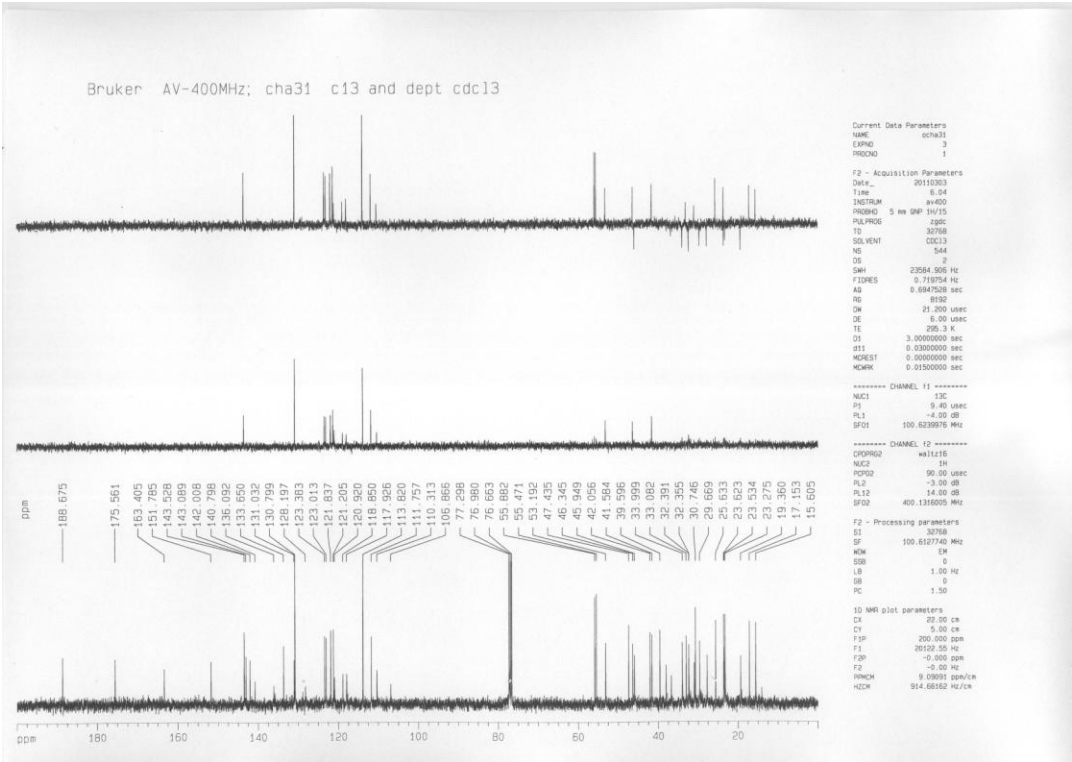
	Elements	Min Number	Max Number
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13	Si	0	0

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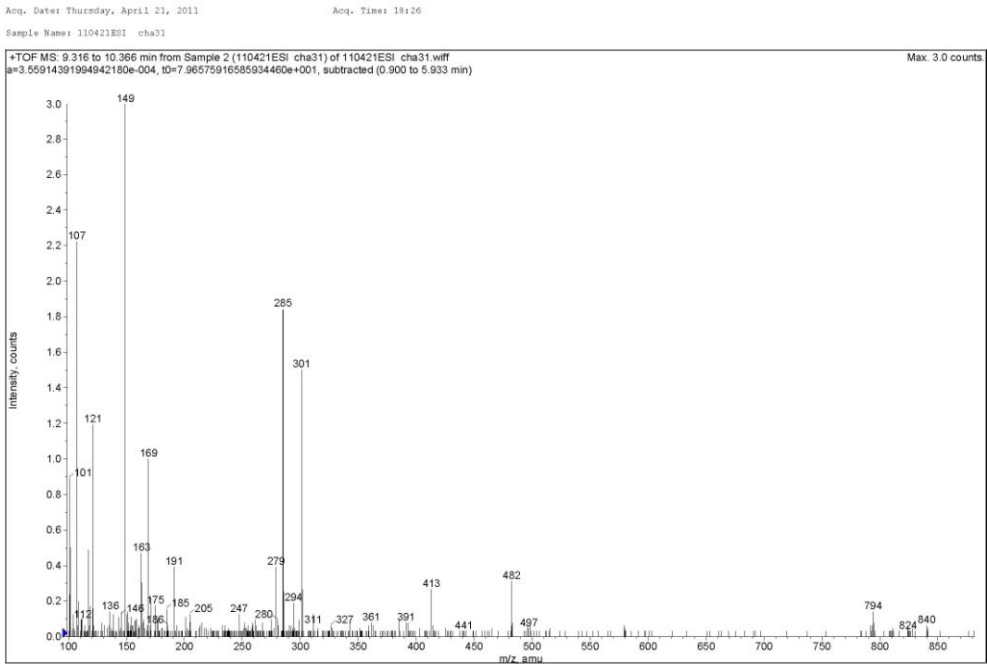
HRESIMS spectrum of compound 2a



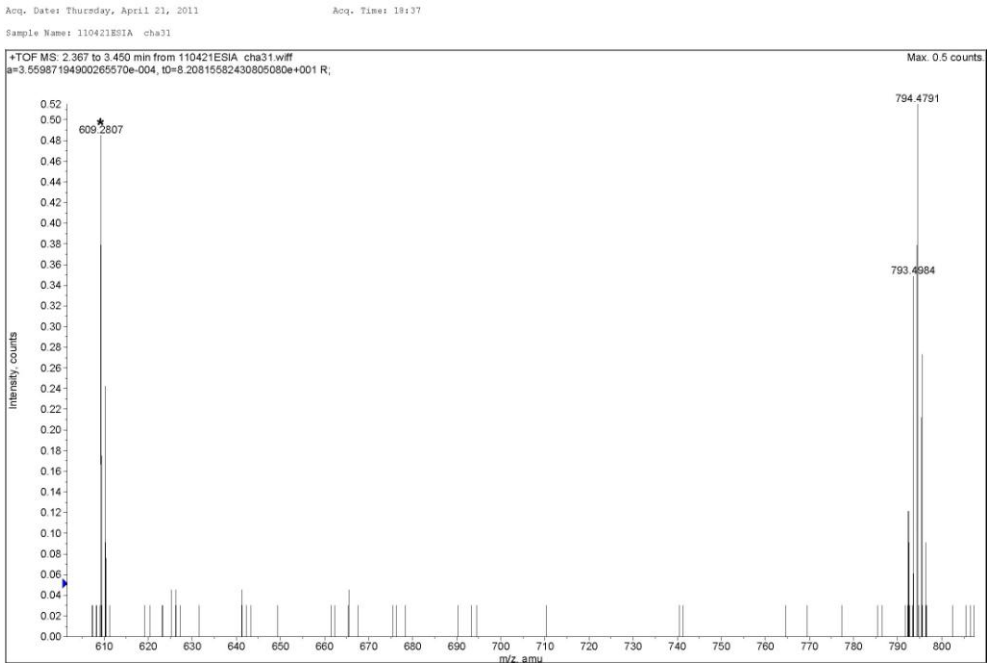
¹H NMR spectrum of compound **2b**



¹³C NMR spectrum of compound **2b**



ESI-MS spectrum of compound **2b**



Acq. Date: Thursday, April 21, 2011
Sample Name: 110421ESIA cha31

Acq. Time: 18:37

Elemental composition calculator			
Target m/z:	+794.4791	amu	
Tolerance:	+10.0000	ppm	
Result type:	Elemental		
Max num of results:	1000		
Min DBE:	-10.0000	Max DBE:	+60.0000
Electron state:	OddAndEven		
Num of charges:	0		
Add water:	N/A		
Add proton:	N/A		
File Name:	110421ESIA cha31.wiff		

	Elements	Min Number	Max Number
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2	C	0	200
3	Cl	0	0
4	F	0	0
5	H	0	400
6	K	0	0
7	N	1	1
8	Na	0	0
9	O	2	5
10	P	0	0
11	Pt	0	0

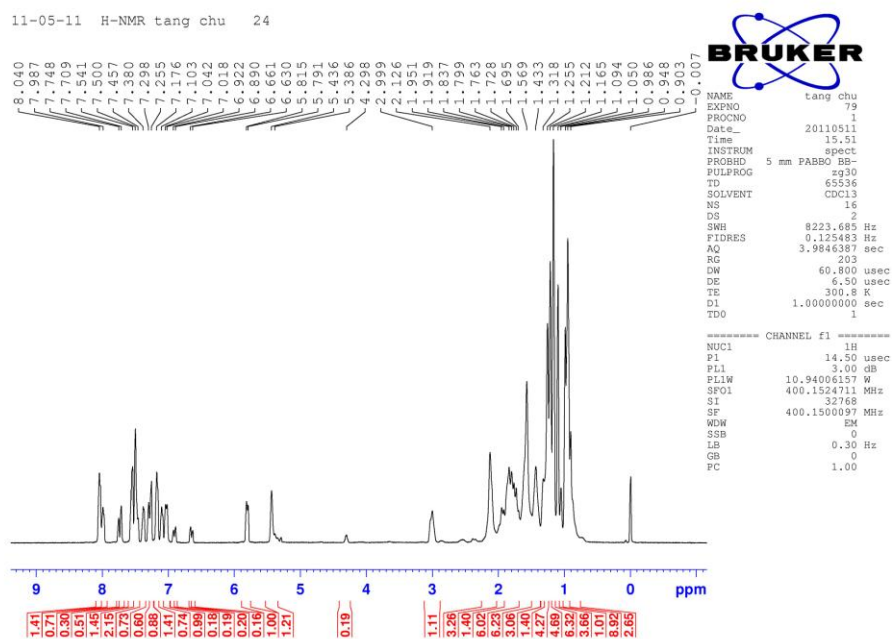
Acq. Date: Thursday, April 21, 2011
Sample Name: 110421ESIA cha31

Acq. Time: 18:37

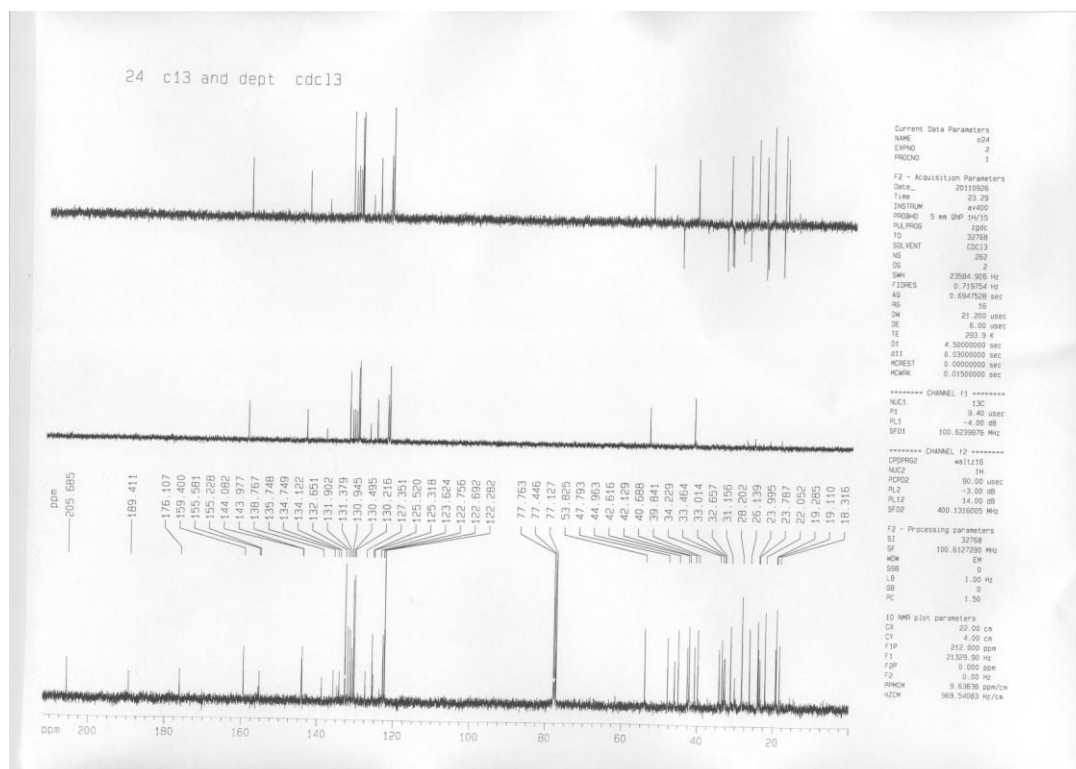
	Elements	Min Number	Max Number
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13	Si	0	0

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C53 H64 N O5	794.4784	0.6502	0.8184	22.5

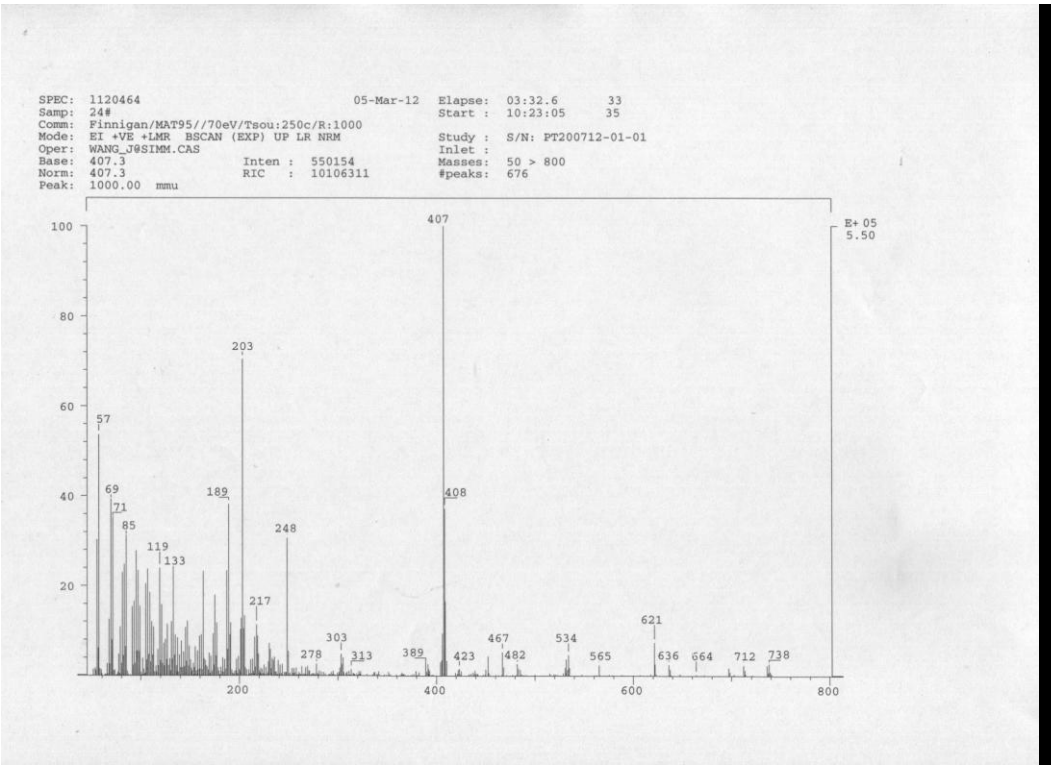
HRESIMS spectrum of compound **2b**



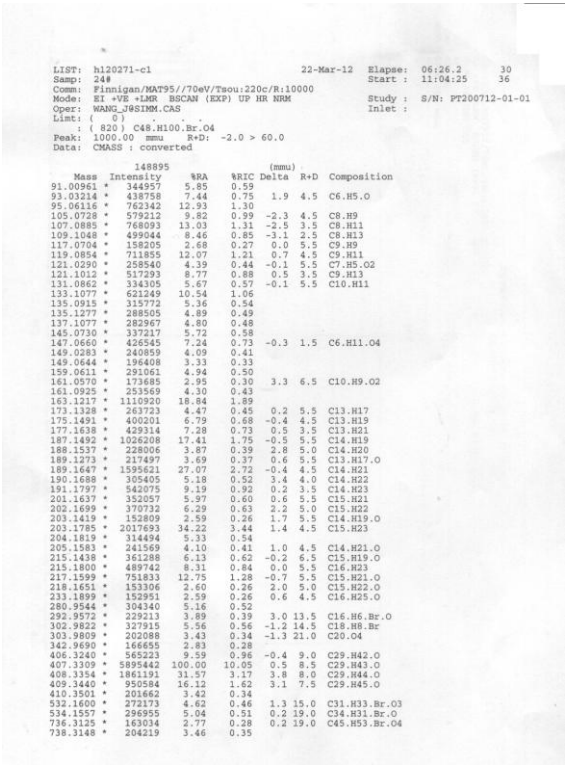
^1H NMR spectrum of compound **3a**



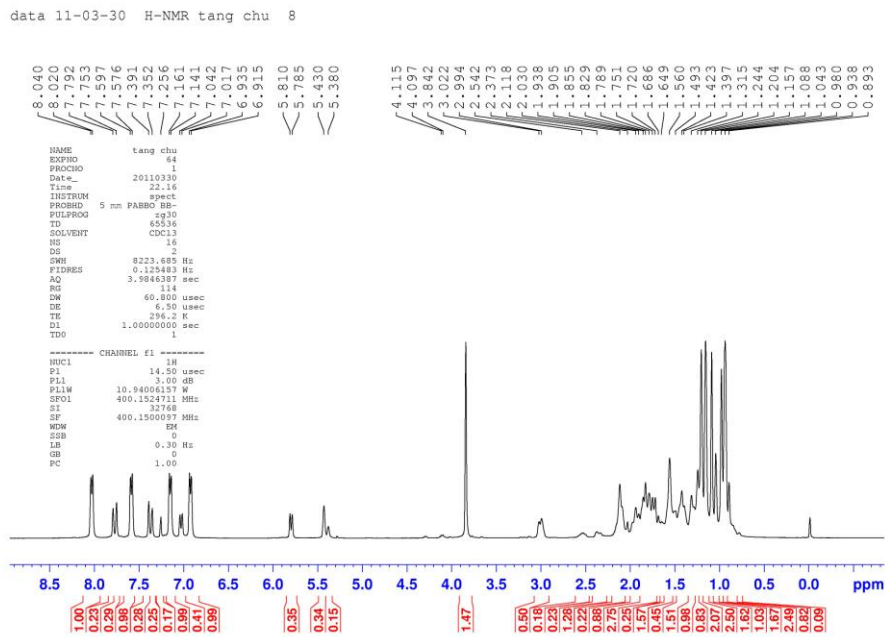
^{13}C NMR spectrum of compound **3a**



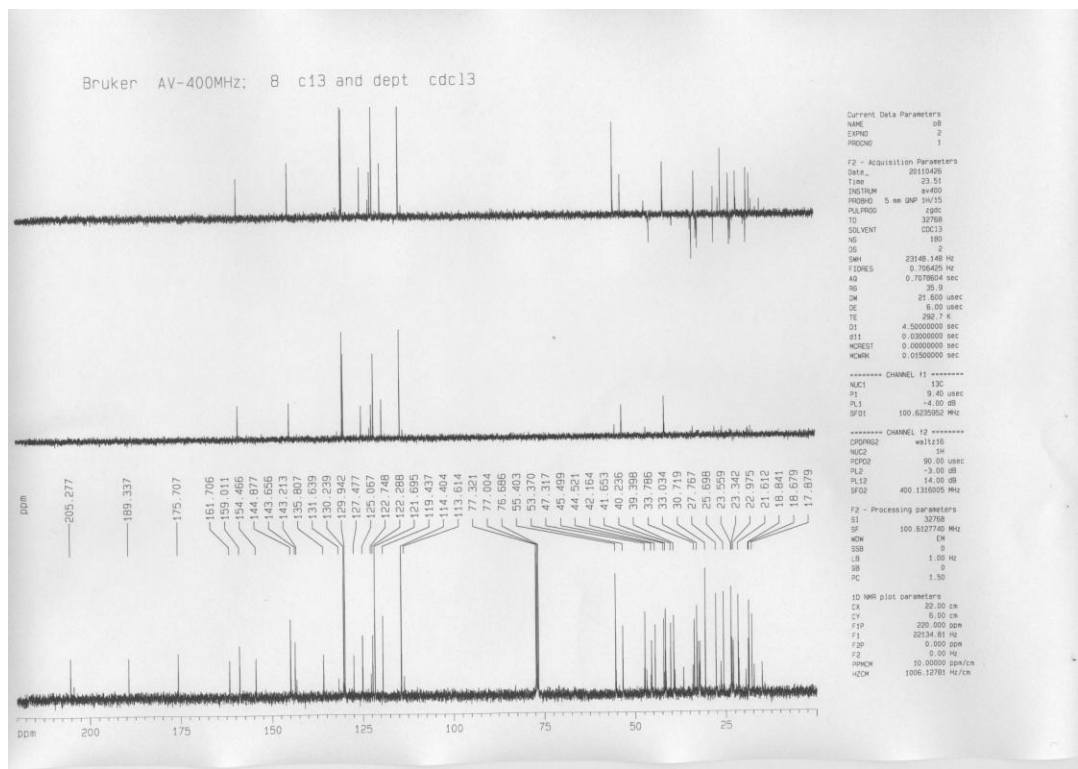
EI-MS spectrum of compound 3a



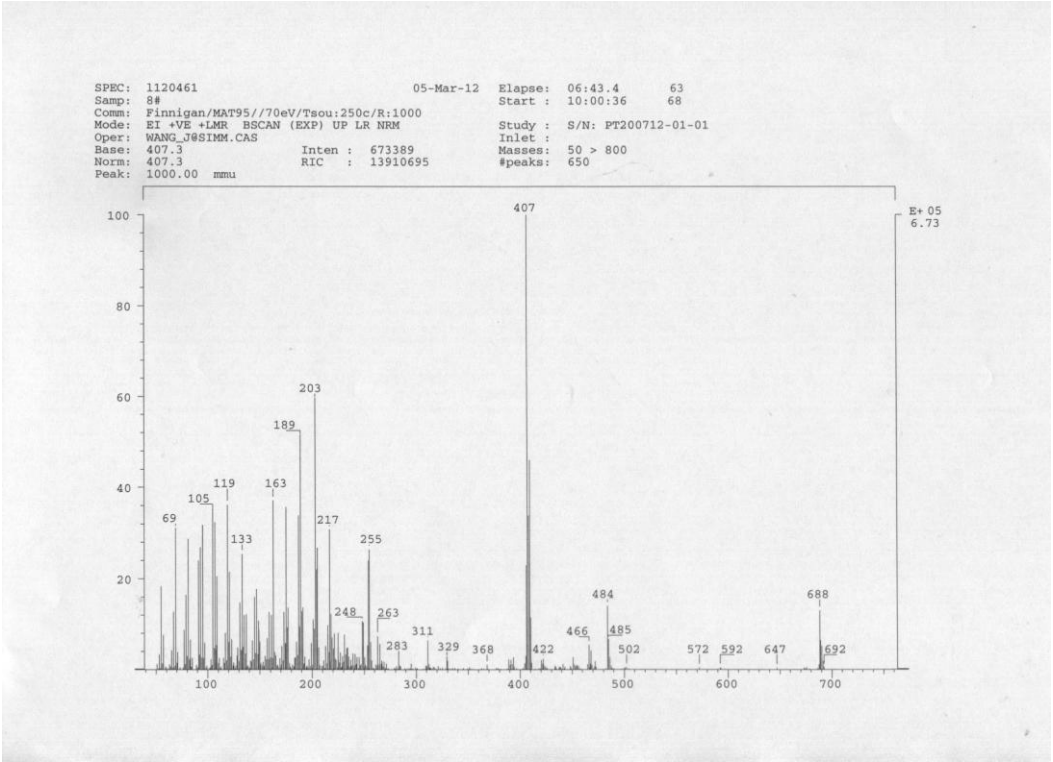
HREIMS spectrum of compound 3a



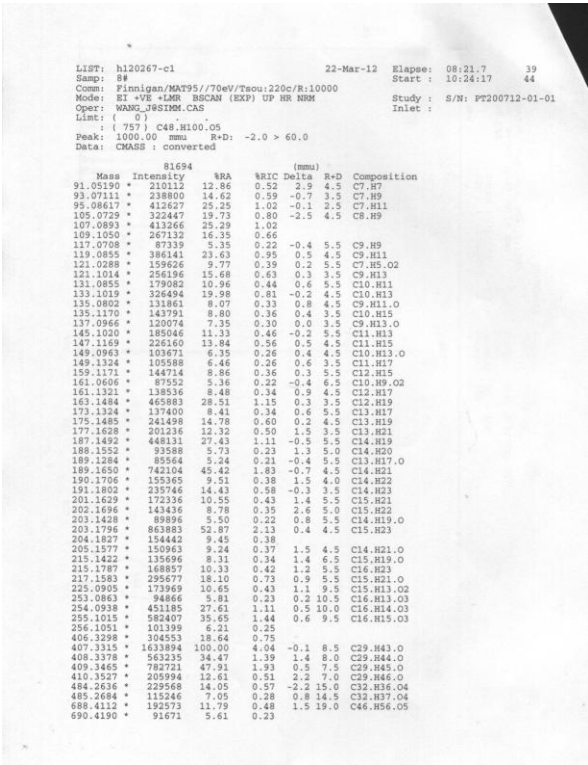
¹H NMR spectrum of compound **3b**



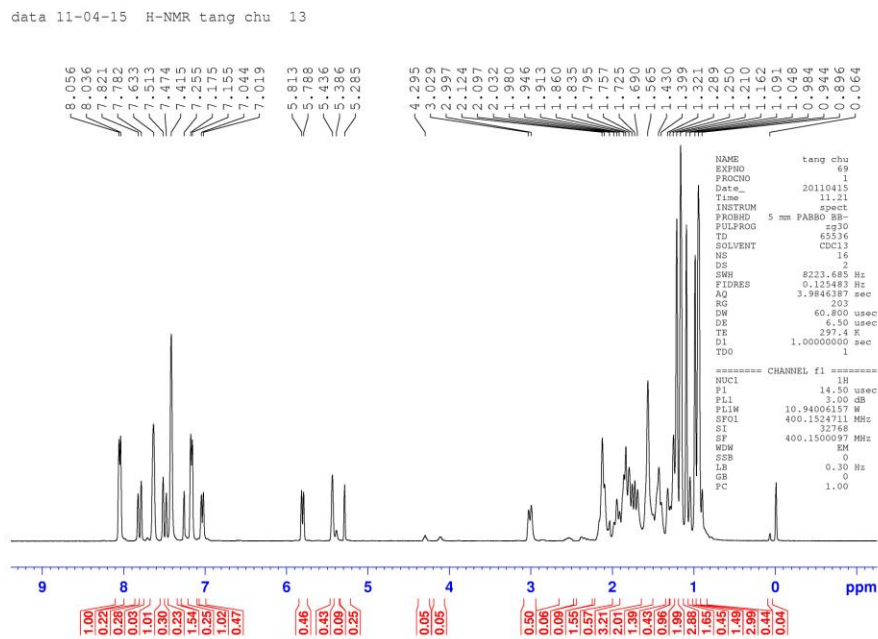
¹³C NMR spectrum of compound **3b**



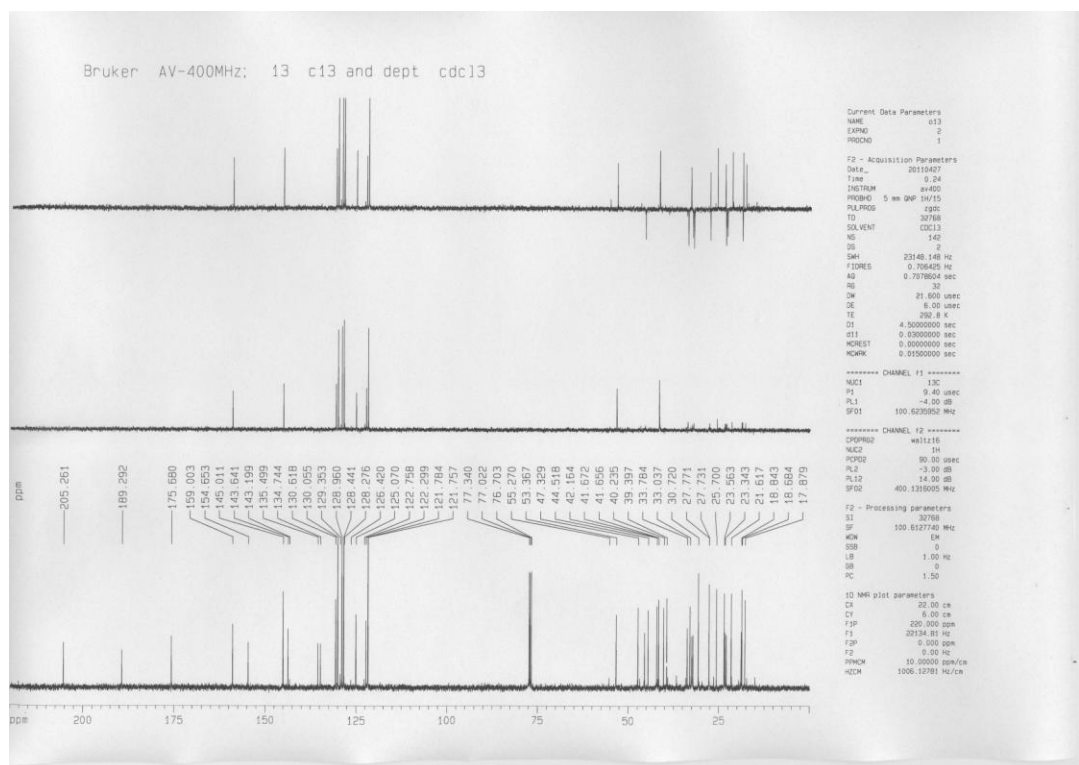
EI-MS spectrum of compound **3b**



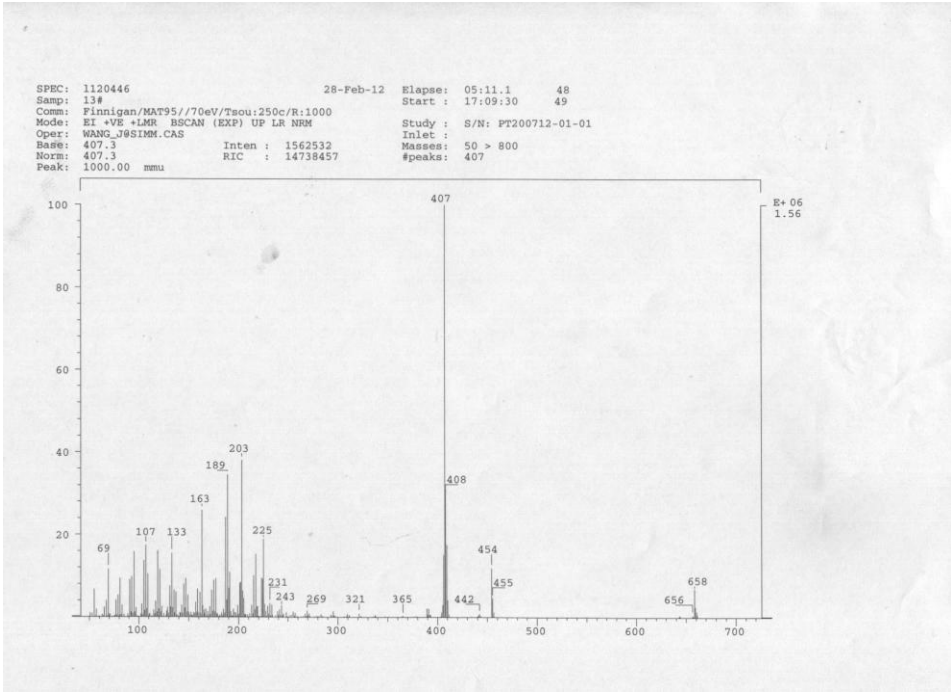
HREIMS spectrum of compound **3b**



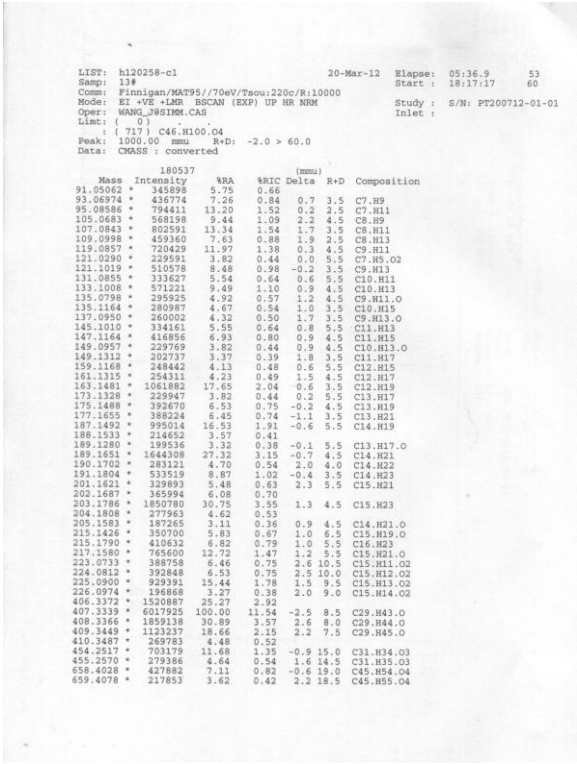
¹H NMR spectrum of compound **3c**



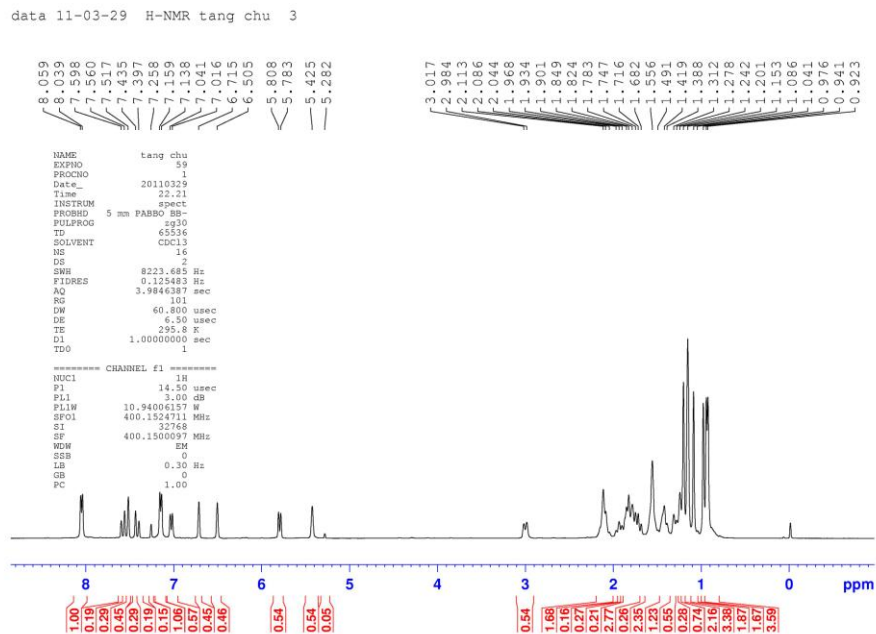
¹³C NMR spectrum of compound **3c**



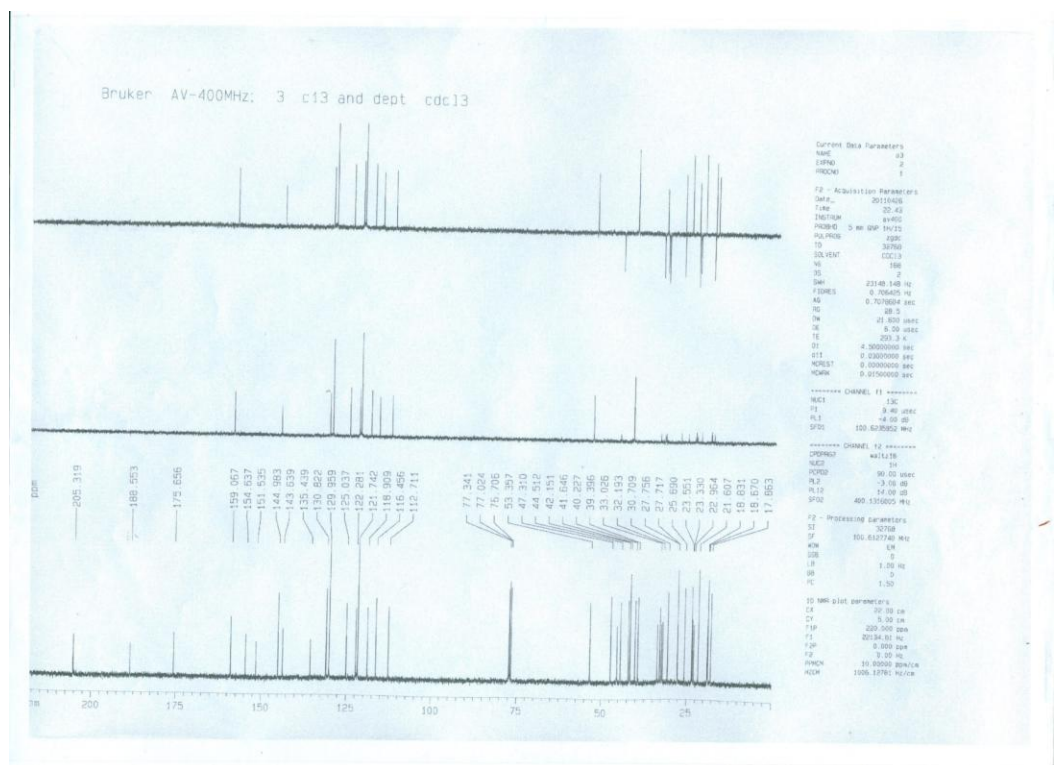
EI-MS spectrum of compound **3c**



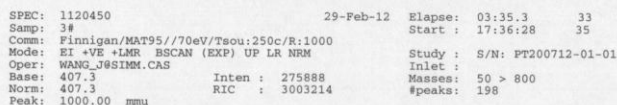
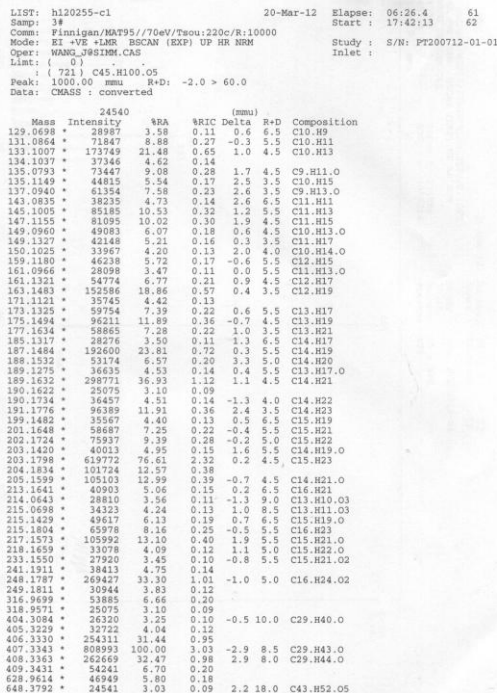
HREIMS spectrum of compound **3c**



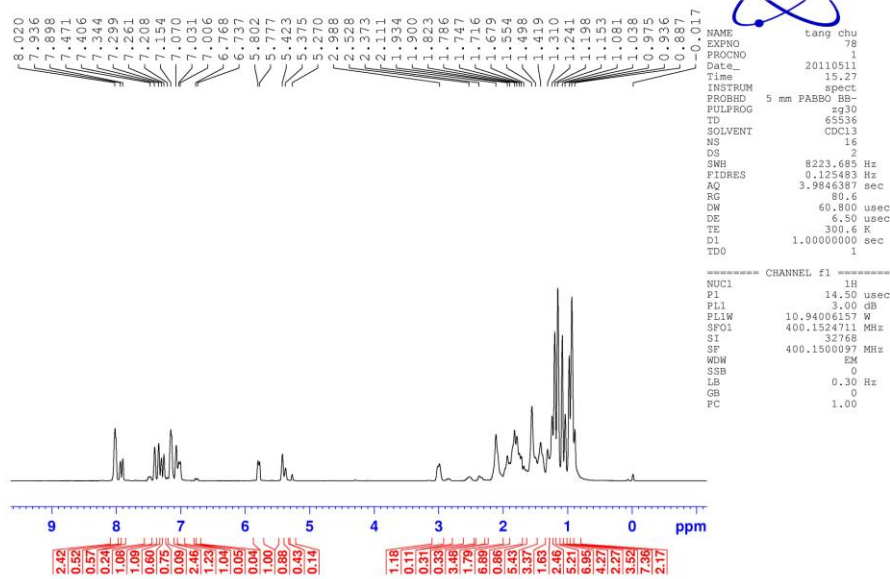
¹H NMR spectrum of compound **3d**



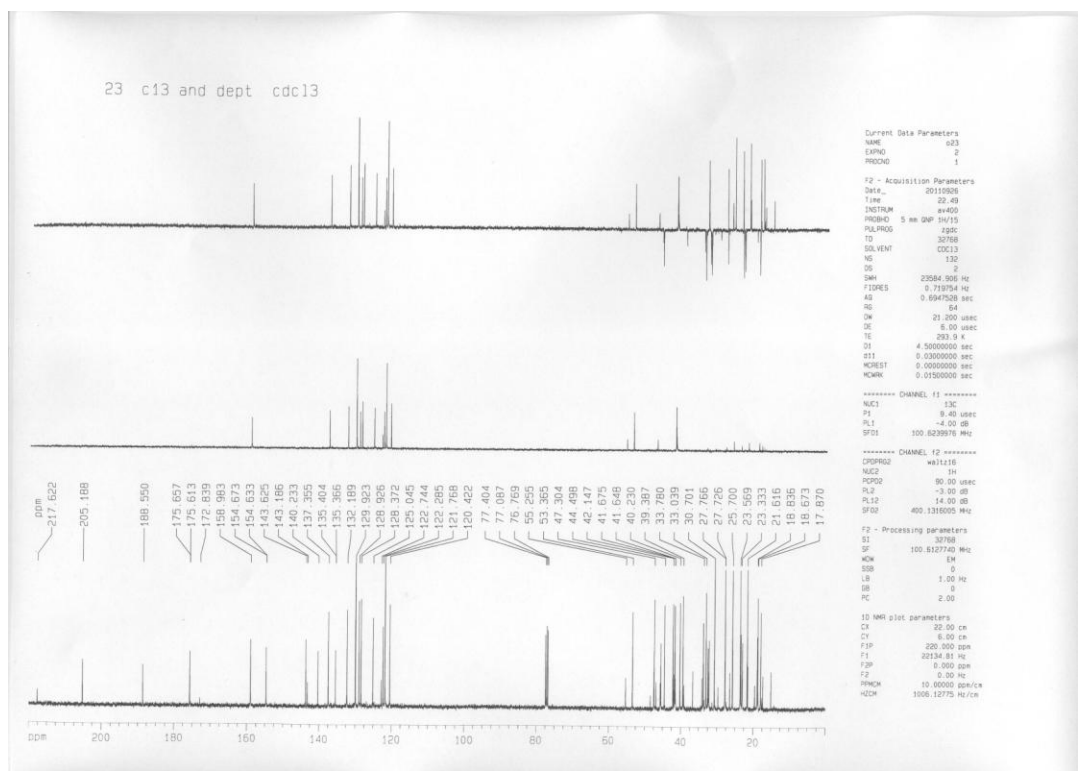
¹³C NMR spectrum of compound **3d**

EI-MS spectrum of compound **3d**HREIMS spectrum of compound **3d**

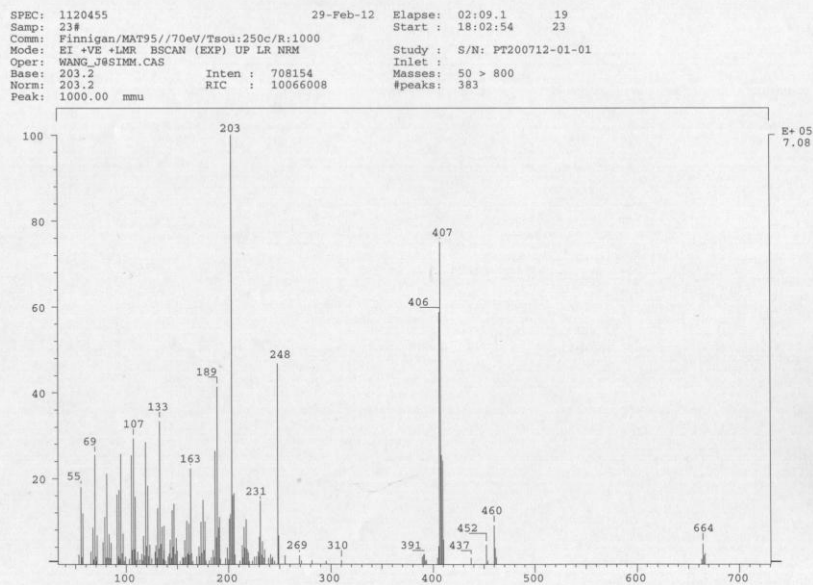
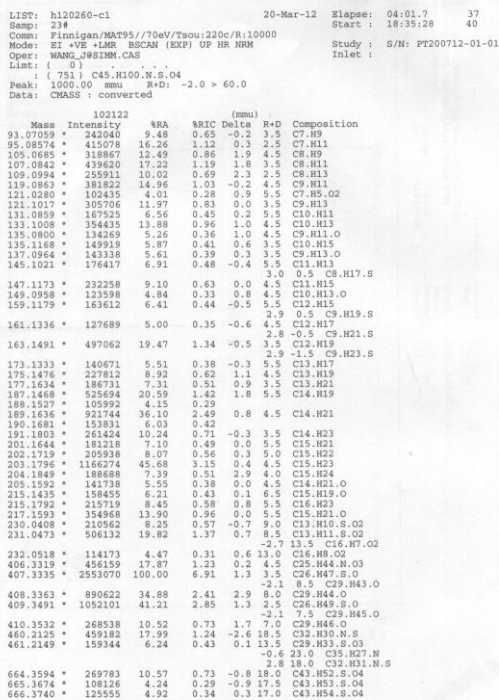
11-05-11 H-NMR tang chu 23



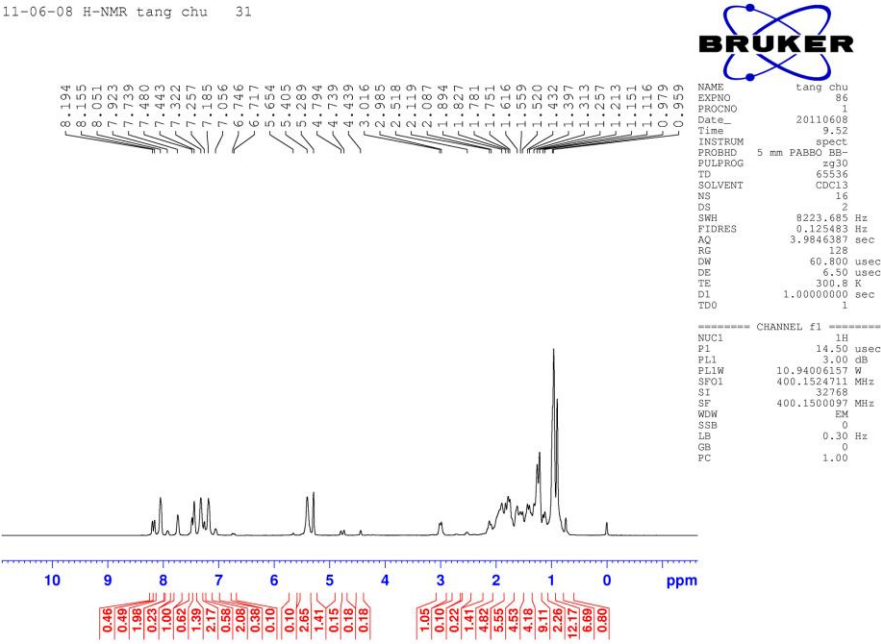
¹H NMR spectrum of compound 3e



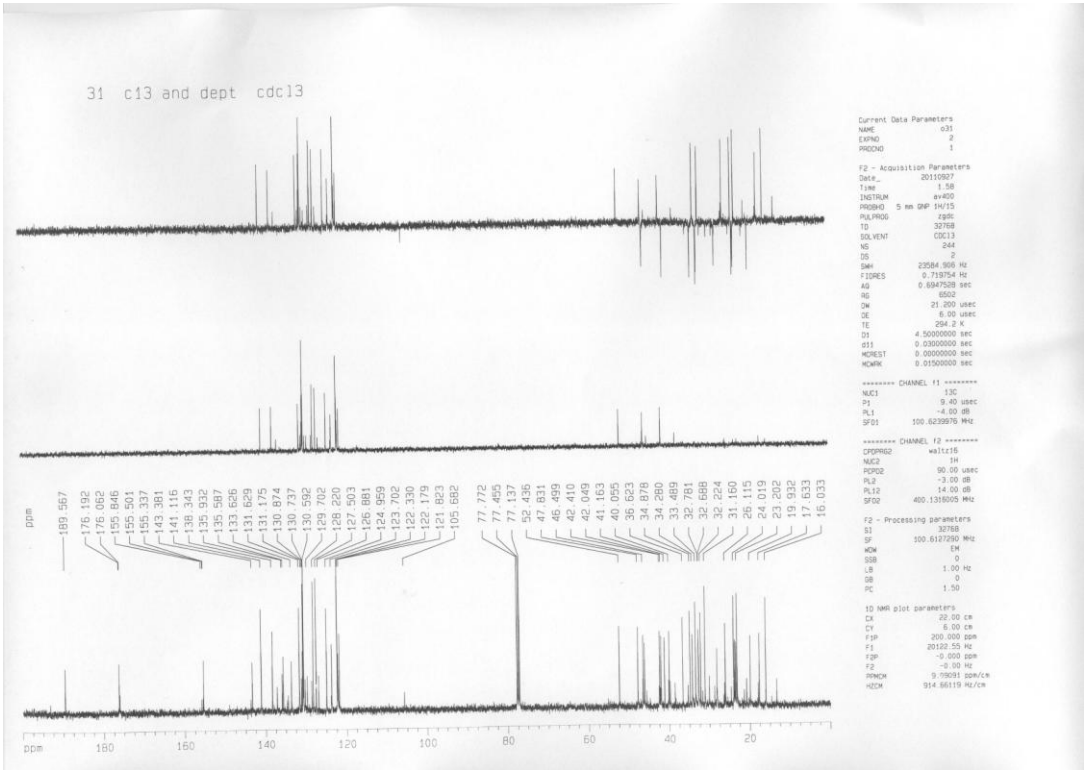
¹³C NMR spectrum of compound 3e

EI-MS spectrum of compound **3e**HREIMS spectrum of compound **3e**

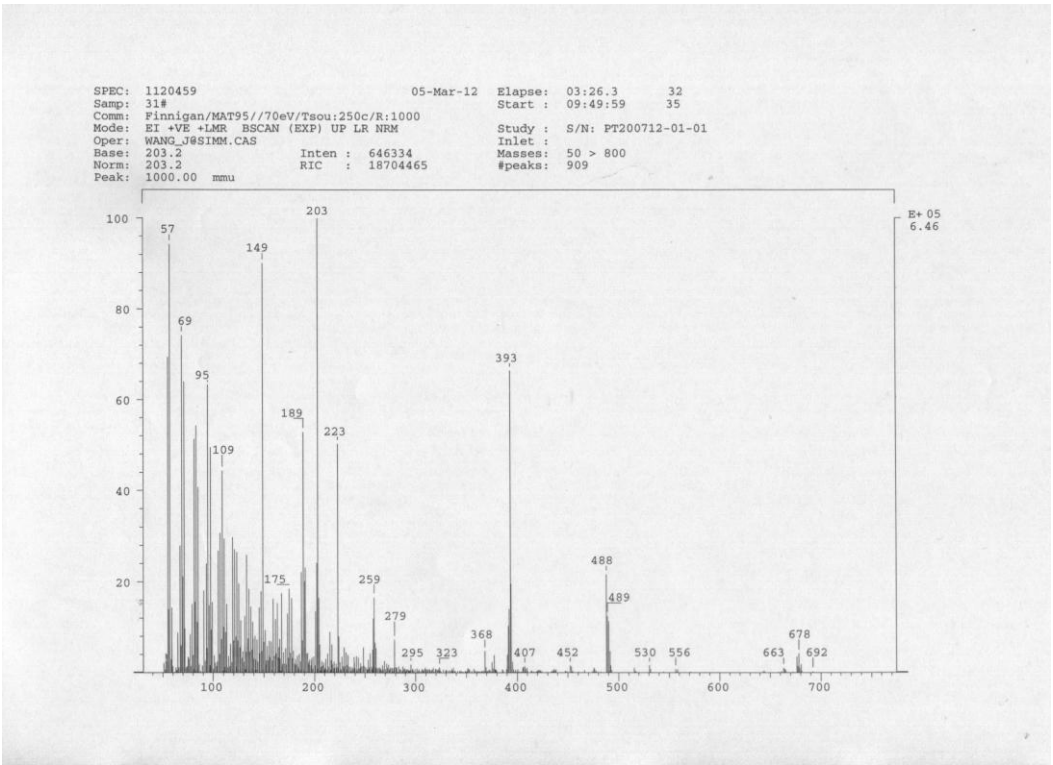
11-06-08 H-NMR tang chu 31



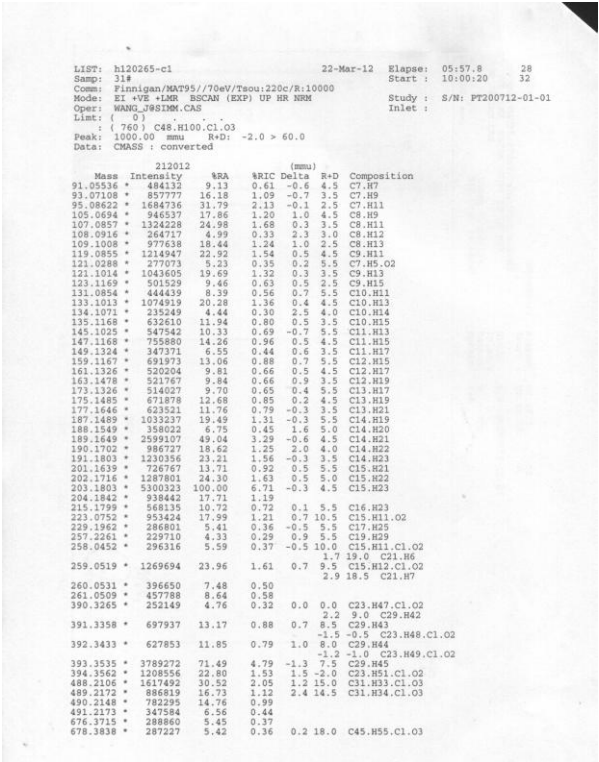
¹H NMR spectrum of compound 4a



¹³C NMR spectrum of compound 4a

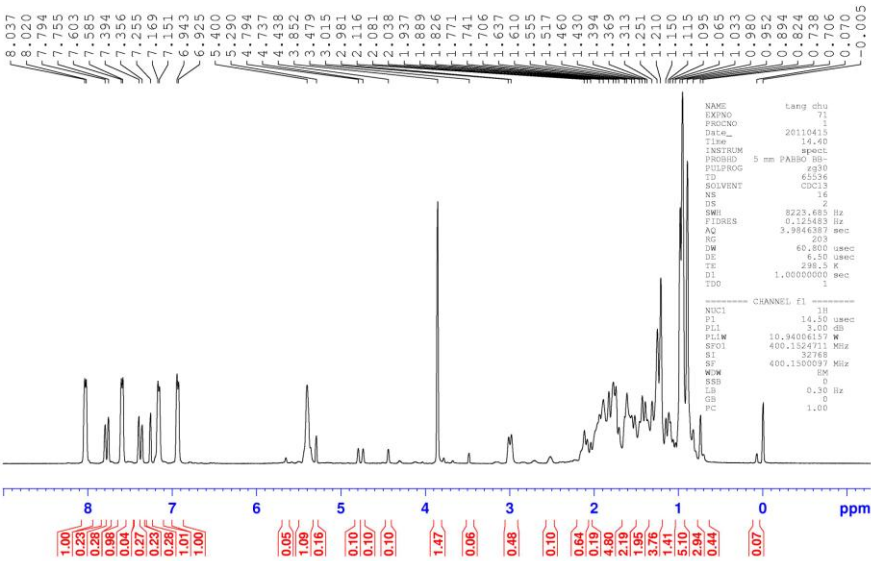


EI-MS spectrum of compound 4a

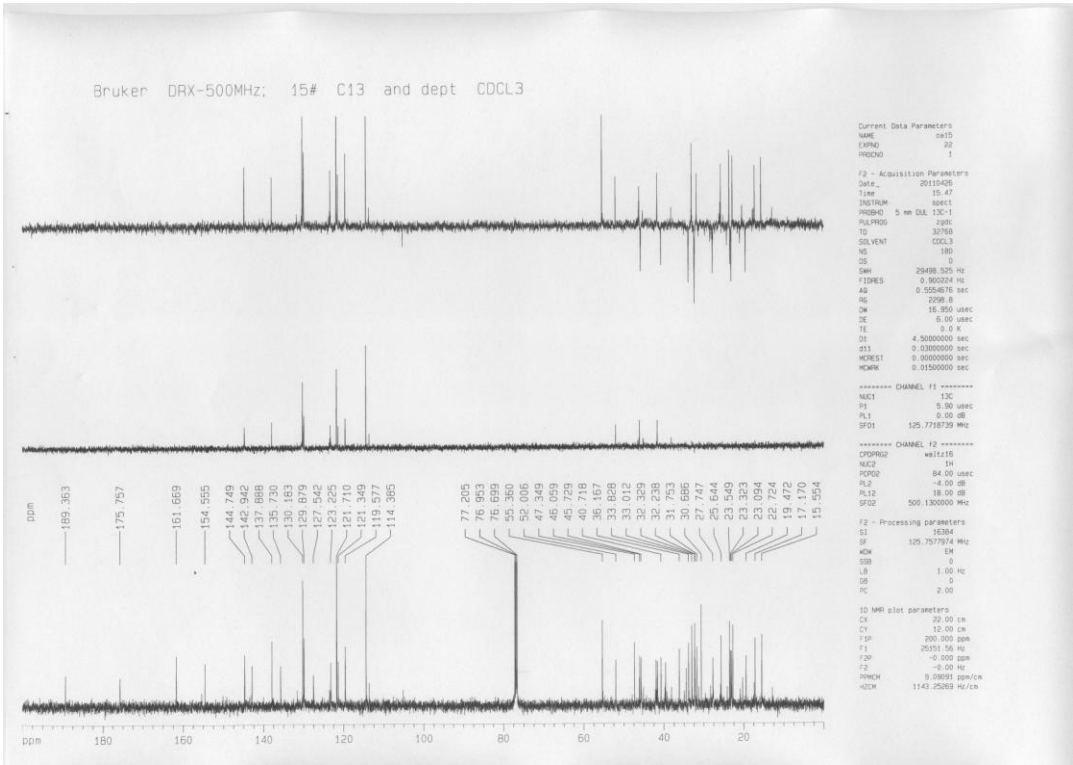


HREIMS spectrum of compound 4a

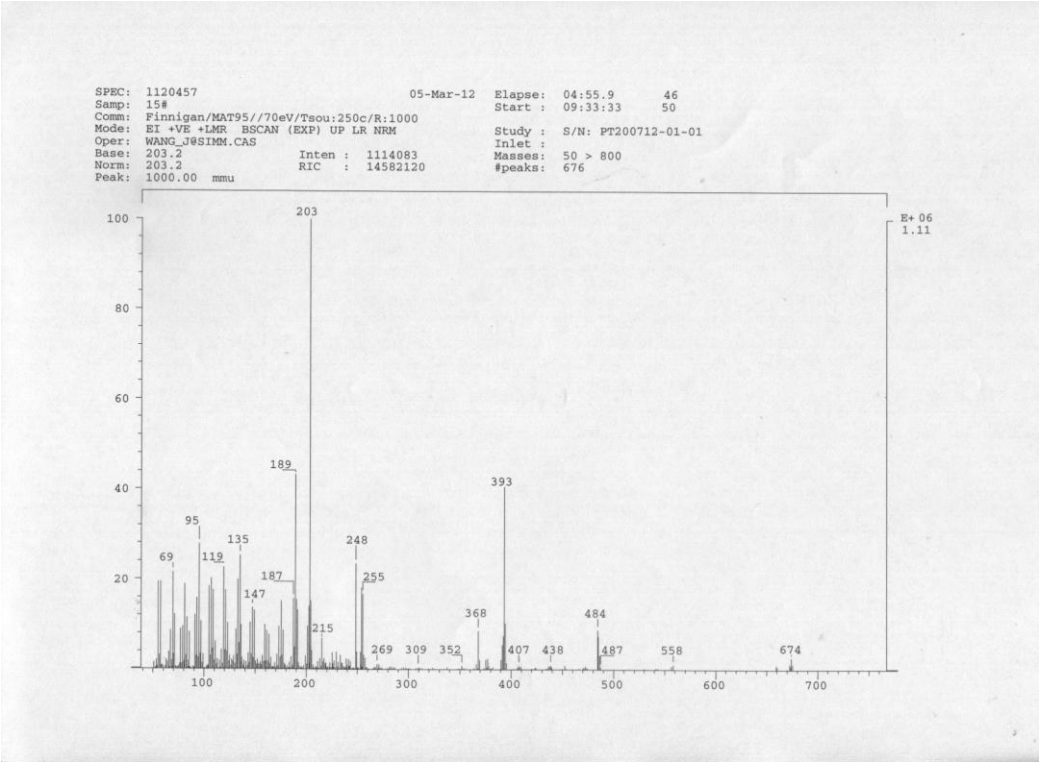
data 11-04-15 H-NMR tang chu 15



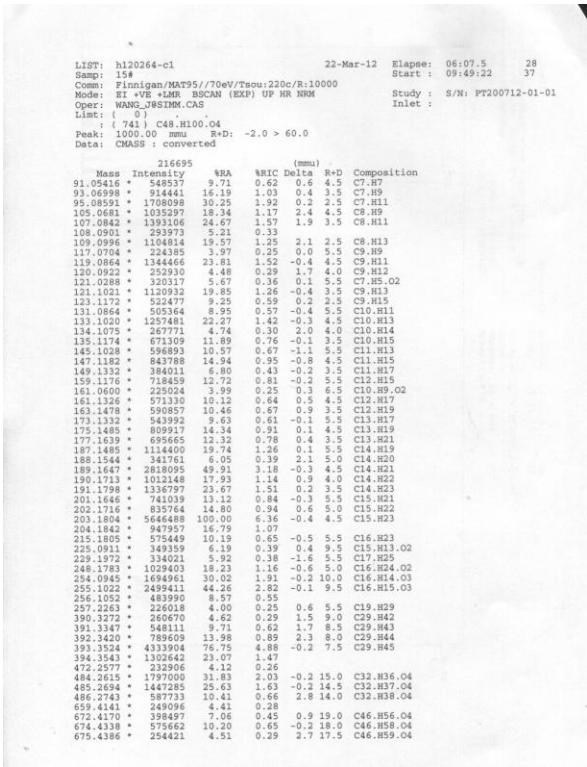
¹H NMR spectrum of compound 4b



¹³C NMR spectrum of compound 4b

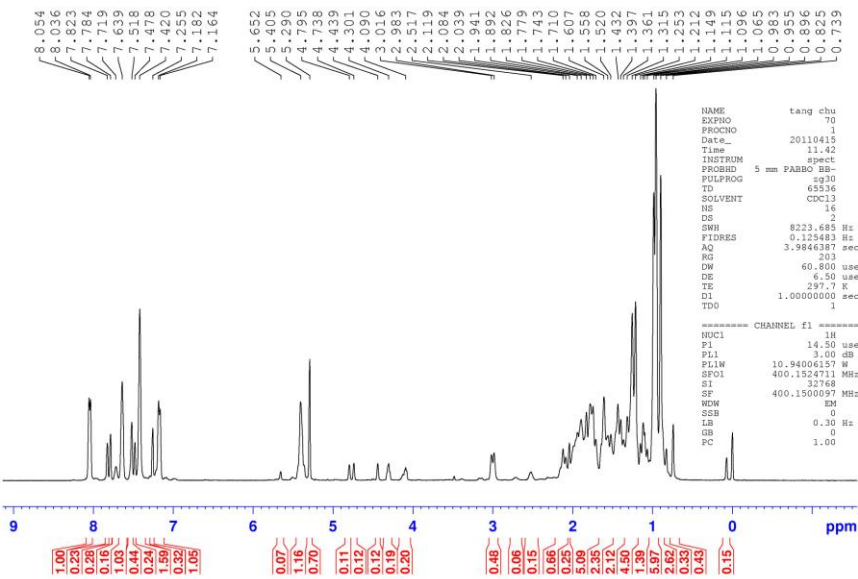


EI-MS spectrum of compound **4b**

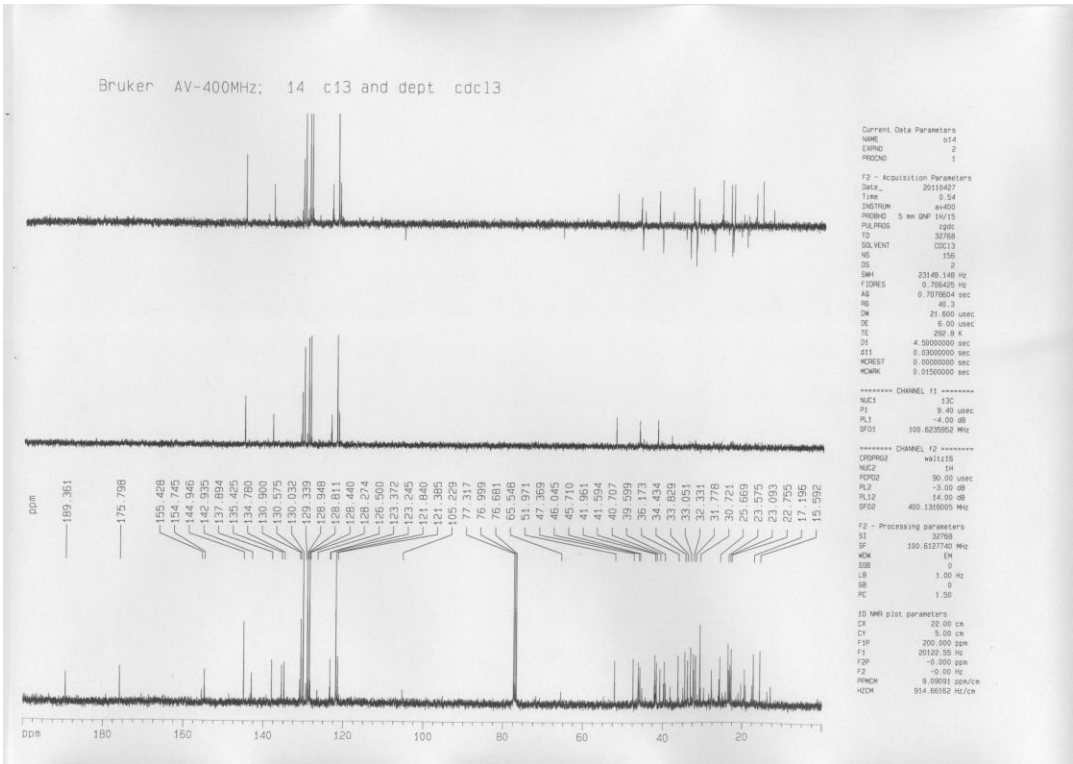


HREIMS spectrum of compound **4b**

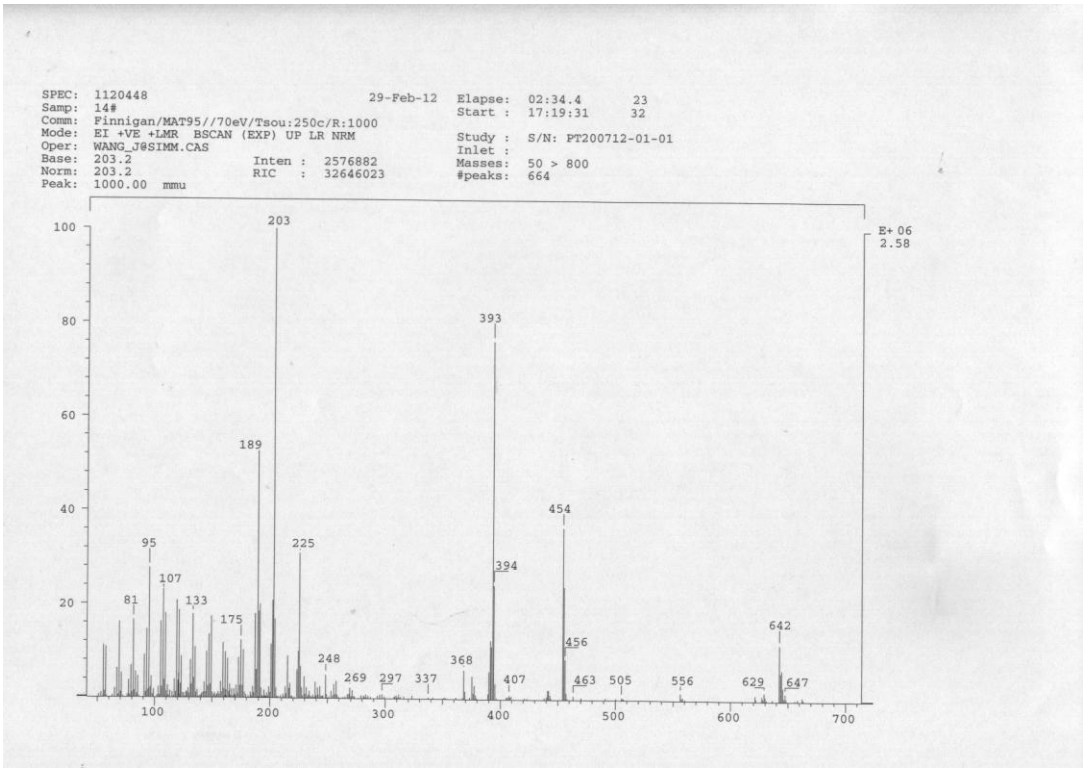
data 11-04-15 H-NMR tang chu 14



¹H NMR spectrum of compound 4c



¹³C NMR spectrum of compound 4c

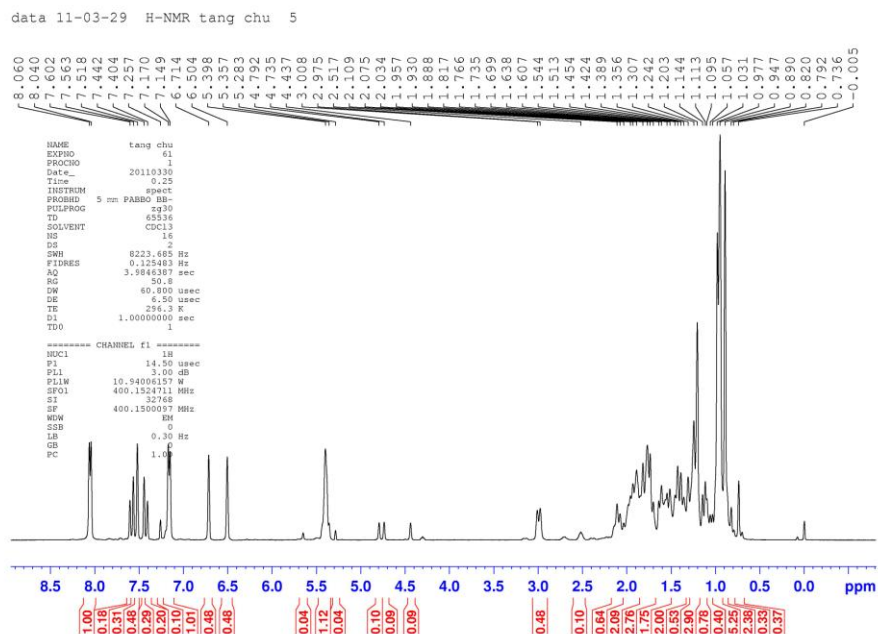


EI-MS spectrum of compound 4c

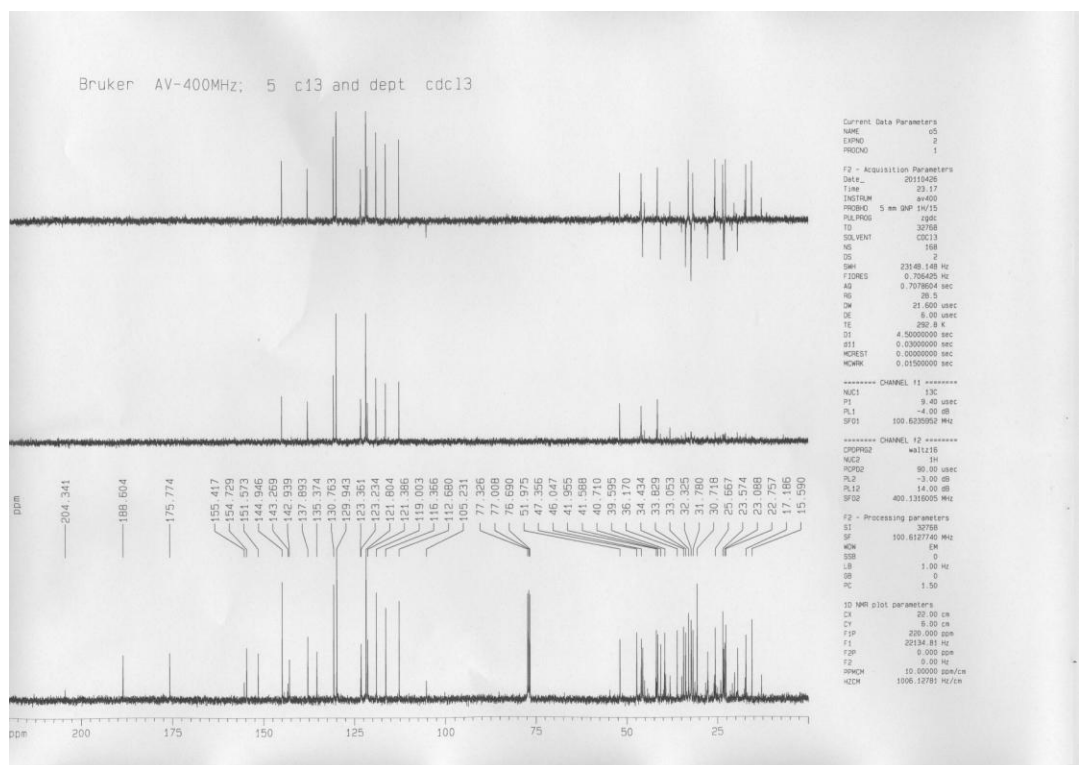
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Samp: 14# Start: 17:25:45 45
Comm: Finnigan/MAT95//70eV/Tsou:220c/R:10000
Mode: EI +VE +LMR BSCAN (EXP) UP HR NRM Study: S/N: PT200712-01-01
Oper: WANG_J08IMM.CAS Inlet: Inlet:
Limit: (0)
(705) C45.H100.04
Peak: 1000.00 mmu R=D: -2.0 > 60.0
Data: CMASS : converted

Mass	Intensity	%A	%RIC	Delta	R+D	Composition
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93.07086	413833	15.77	0.94	-0.4	3.5	C7.H9
95.08839	787297	30.00	1.79	-2.3	2.5	C7.H11
105.0273	430906	16.42	0.98			
107.0343	665832	25.37	1.51	0.1	0.5	C3.H7.O4
108.0384	118974	4.53	0.27			
109.0466	508622	19.38	1.15			
119.0863	602166	22.95	1.37	-0.2	4.5	C9.H11
120.0921	102791	3.92	0.23	1.8	4.0	C9.H12
121.0285	154365	5.88	0.35	0.4	5.3	C7.H5.O2
121.1020	491371	18.72	1.12	-0.2	3.5	C9.H13
123.1173	201670	7.68	0.46	0.1	2.5	C9.H15
131.0498	105992	4.04	0.24	-0.1	6.5	C9.H7.O
131.0859	206827	7.88	0.47	0.2	5.5	C10.H11
133.1022	523916	19.96	1.19	-0.5	4.5	C10.H13
135.1180	335761	12.79	0.76	-0.6	3.5	C10.H15
145.1025	256445	9.77	0.58	-0.7	5.5	C11.H13
147.1174	356569	13.59	0.81	-0.1	4.5	C11.H15
149.1330	174638	6.65	0.40	0.0	3.5	C11.H17
157.1023	101190	3.86	0.23	-0.6	6.5	C12.H13
159.1169	109263	11.79	0.70	0.5	5.5	C12.H15
161.1326	233503	8.90	0.53	0.4	4.5	C12.H17
163.1488	237772	9.06	0.54	-0.1	3.5	C12.H19
173.1329	248620	9.47	0.56	0.1	5.5	C13.H17
175.1482	324380	12.36	0.74	0.5	4.5	C13.H19
177.1634	320823	12.23	0.73	1.0	3.5	C13.H21
187.1469	515024	19.63	1.17	1.7	5.5	C14.H19
188.1548	184775	7.04	0.42	1.7	5.0	C14.H20
189.1635	1248436	47.57	2.83	0.9	4.5	C14.H21
190.1692	485147	18.49	1.10	2.9	4.0	C14.H22
191.1798	570332	21.73	1.29	0.1	3.5	C14.H23
201.1635	338251	12.89	0.77	0.8	5.5	C15.H21
202.1726	571577	21.78	1.30	-0.4	5.0	C15.H22
203.1802	2624206	100.00	5.96	-0.2	4.5	C15.H23
204.1861	413477	15.76	0.94	1.7	4.0	C15.H24
215.1795	285077	10.86	0.65	0.4	5.5	C16.H23
223.0745	209495	7.98	0.48	1.5	10.5	C15.H11.O2
224.0816	321178	12.24	0.73	2.1	10.0	C15.H12.O2
225.0907	1043564	39.77	2.37	0.9	9.5	C15.H13.O2
226.0949	206472	7.87	0.47			
229.1962	135869	5.18	0.31	-0.6	5.5	C17.H25
257.2251	111861	4.26	0.25	1.9	5.5	C19.H29
375.3035	114173	4.35	0.26	1.7	9.5	C28.H39
390.3285	150274	5.73	0.34	0.2	9.0	C29.H42
391.3339	422547	16.10	0.96	2.5	8.5	C29.H43
392.3407	341274	13.00	0.77			
393.3512	2012258	76.68	4.57	0.9	7.5	C29.H45
394.3551	634355	24.17	1.44			
395.3557	105814	4.03	0.24			
454.2519	1028804	39.20	2.33	-1.2	15.0	C31.H34.O3
455.2581	676325	25.77	1.53	0.6	14.5	C31.H35.O3
456.2593	201136	7.66	0.46			
642.4117	261602	9.97	0.59			
643.4126	113461	4.32	0.26	2.5	18.5	C45.H55.O3
644.4222	166813	6.36	0.38	0.7	18.0	C45.H56.O3

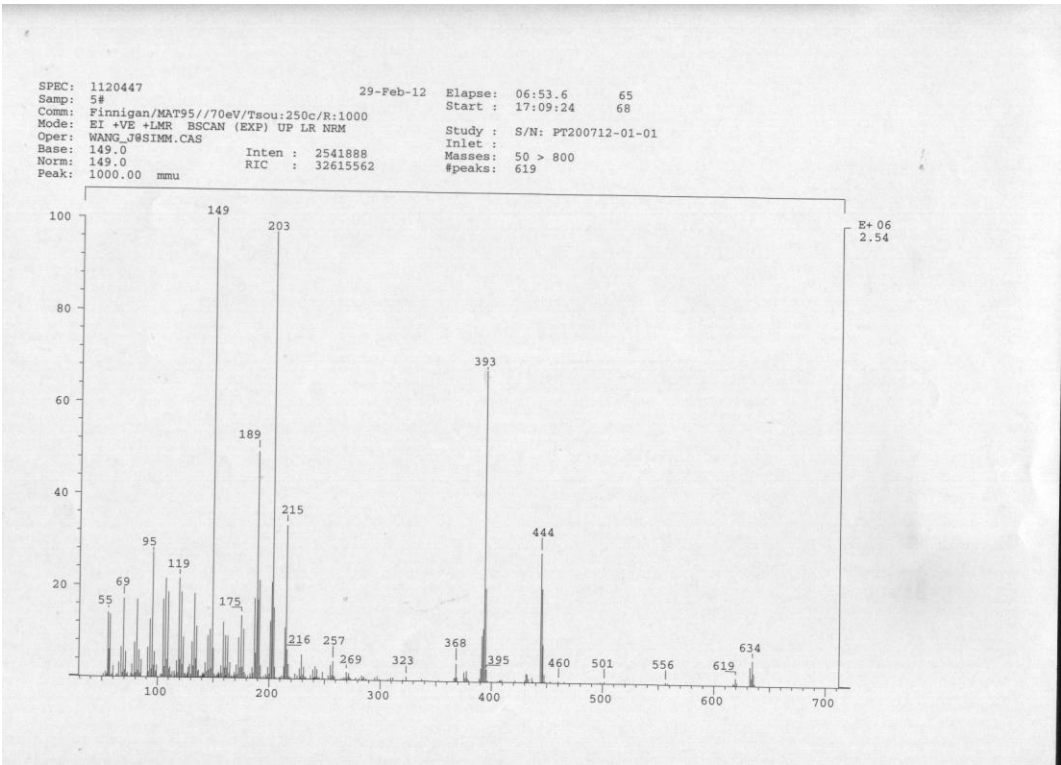
HREIMS spectrum of compound 4c



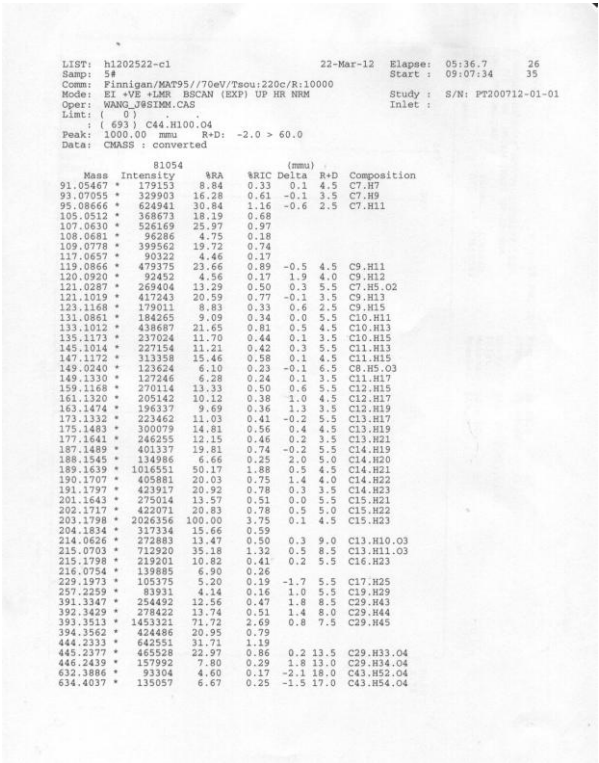
¹H NMR spectrum of compound **4d**



¹³C NMR spectrum of compound **4d**

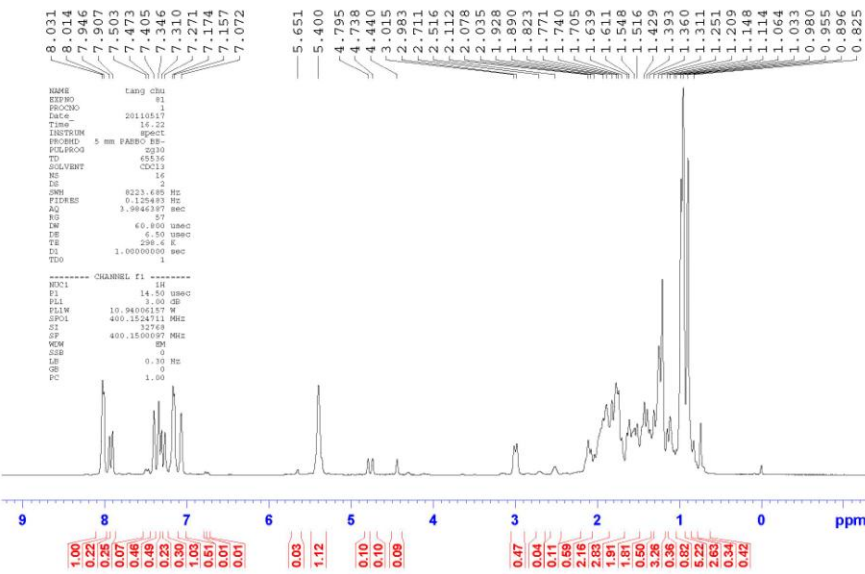


EI-MS spectrum of compound **4d**

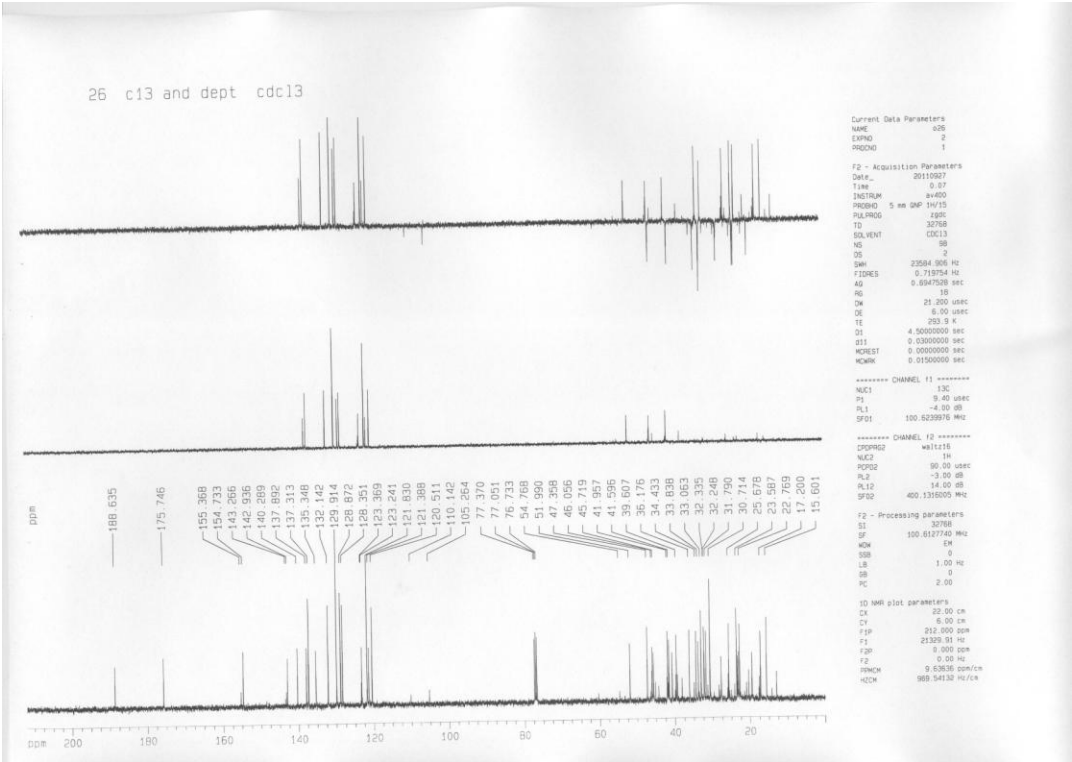


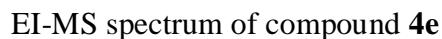
HREIMS spectrum of compound **4d**

11-05-17 H-NMR tang chu 26



¹H NMR spectrum of compound **4e**





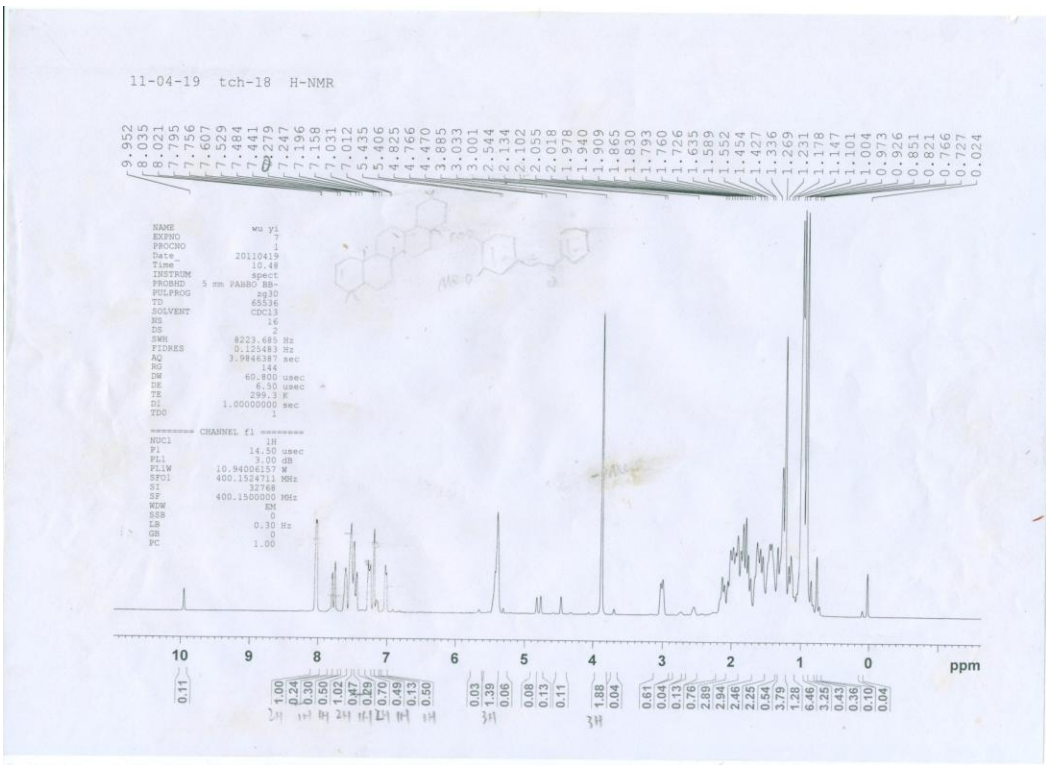
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Study: 8/31/2700712-01-01
Limit: 0
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Peak: 1000.00 mmu R.D.
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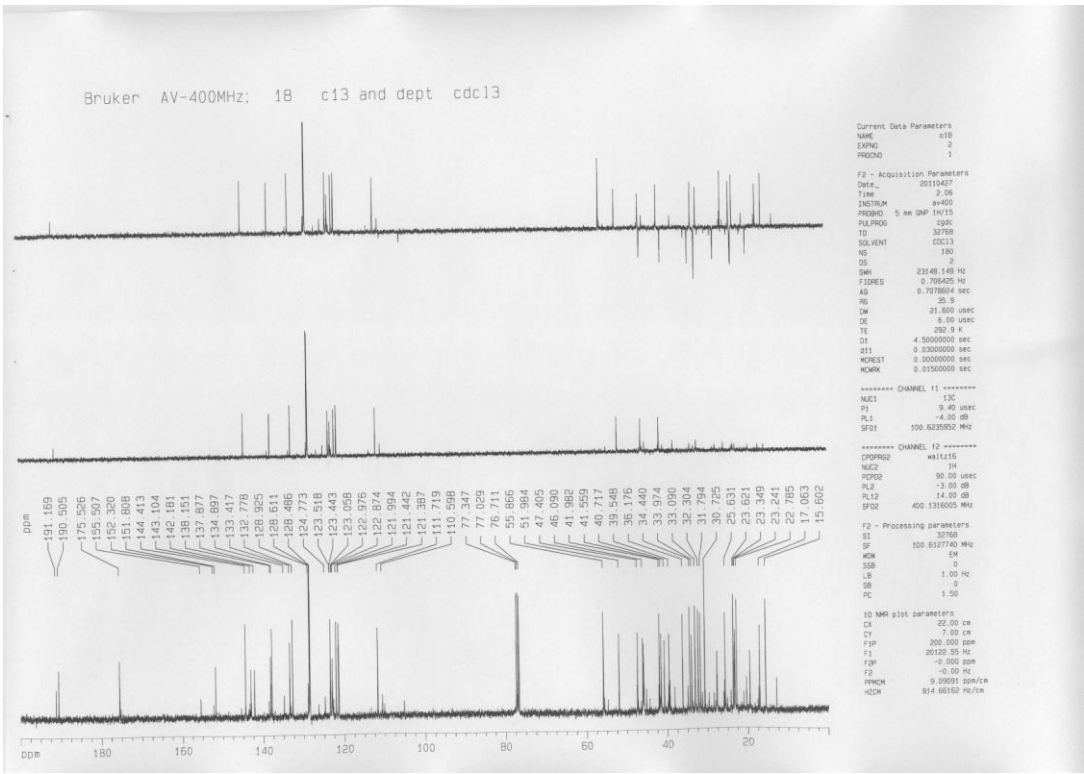
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107.09226      797790      25.11      1.71      -3.5      -1.5      C5.H13.0
109.08925      575667      18.12      1.24      -3.5      -1.5      C5.H13.0
119.08600      702645      22.12      1.01      0.4      4.5      C9.H11
121.1018      606434      19.09      1.30      -0.1      3.5      -0.5      C6.H15.S
123.1179      297516      8.09      0.55      -0.5      2.5      C9.H13
131.0885      239550      7.54      0.51      0.5      0.5      C10.H11
133.1023      629375      19.81      1.35      -0.5      4.5      C10.H13
135.1175      387335      12.19      0.83      -0.2      3.5      -2.0      C7.H17.S
135.1175      387335      12.19      0.83      -0.2      3.5      -1.0      C10.H15
145.1022      294982      9.43      0.64      -0.5      3.2      -1.5      C7.H19.S
147.1163      409921      12.90      0.88      1.1      4.5      2.0      C8.H17.S
159.1167      380755      11.98      0.82      0.7      5.5      C12.H15
161.1303      312286      9.83      0.67      -0.3      4.5      C12.H17
163.1483      275296      8.66      0.59      0.4      3.5      -0.5      C9.H21.S
173.1330      279742      8.80      0.60      0.4      3.5      C12.H19
175.1483      417568      13.14      0.90      0.4      4.5      C13.H19
177.1484      362497      11.41      0.78      0.1      3.5      C13.H21.S
187.1500      590428      18.58      1.27      -1.3      3.5      -1.5      C10.H25.S
189.1658      1510394      47.54      3.24      -1.4      4.5      C14.H21
190.1716      562152      17.69      1.21      0.5      4.0      C14.H22
191.1805      703890      22.16      1.51      -0.5      3.5      C14.H23
201.1656      429305      13.51      0.92      -1.3      5.5      C15.H22
202.1726      658007      20.71      1.41      -0.5      5.0      C15.H23
203.1806      3177110      100.00      6.82      -0.7      4.5      C15.H22
204.1850      487637      15.35      1.05      2.8      4.0      C15.H27.S
215.1974      354968      11.17      0.76      0.9      4.5      C16.H23
230.0400      417568      13.14      0.90      0.2      3.5      C16.H26.0
231.0482      1149201      36.17      2.47      -0.2      3.5      C13.H11.S-02
232.0517      271917      8.56      0.58      0.7      3.0      C16.H48.0
233.0411      410276      12.91      0.88      -0.3      3.5      C26.H47.0
392.3449      377020      11.87      0.81      -0.6      8.0      C29.H44
393.3535      2443520      76.91      5.24      -1.3      7.5      C29.H48.S
394.3558      773425      24.34      1.66      2.0      2.5      C26.H49.S
460.2808      1155959      36.38      2.48      -4.2      14.0      C29.H32.S-03
460.2808      888310      21.96      1.35      -0.9      2.5      C29.H34.S-03
462.2214      360125      11.33      0.77      1.5      13.0      C29.H34.S-03
462.2214      360125      11.33      0.77      1.5      13.0      C29.H34.S-03
500.3802      265515      8.36      0.57      -0.8      17.0      C43.H54.S-03

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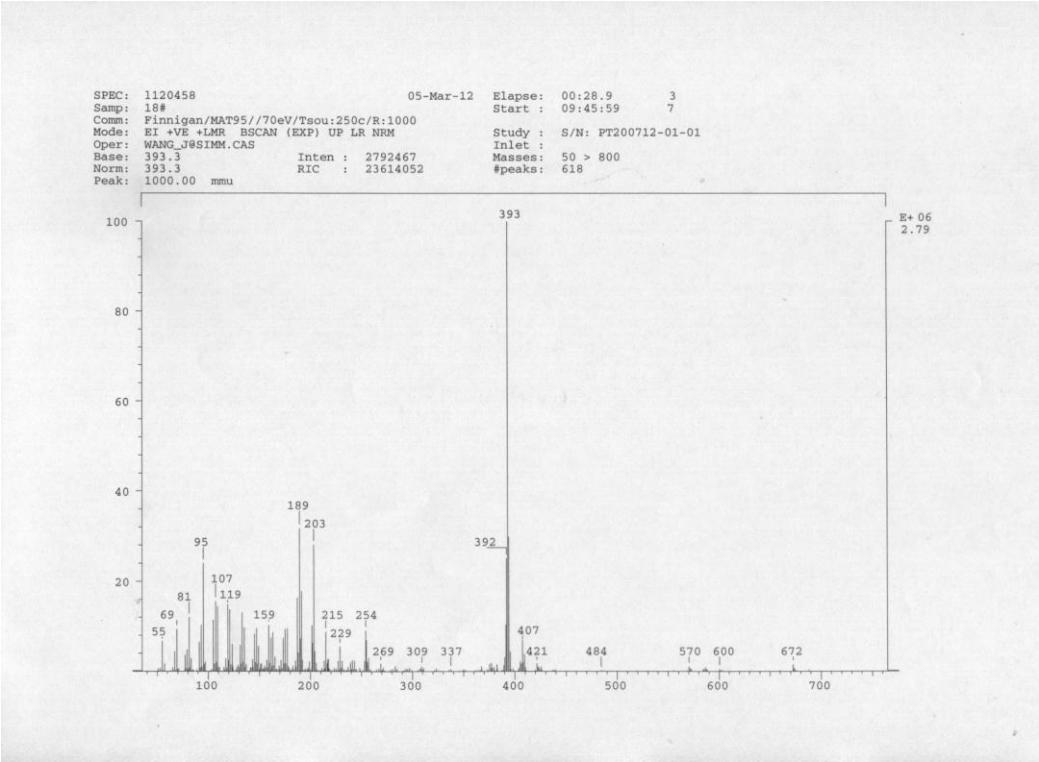
HREIMS spectrum of compound **4e**



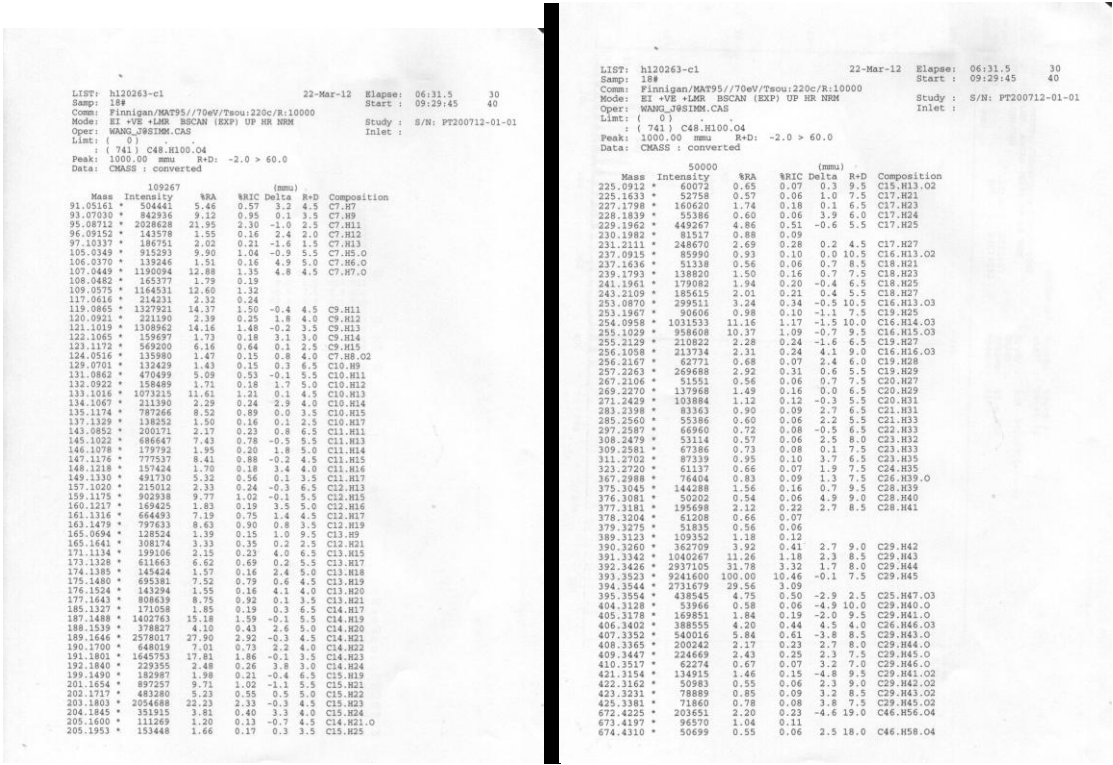
¹H NMR spectrum of compound 4f



¹³C NMR spectrum of compound 4f

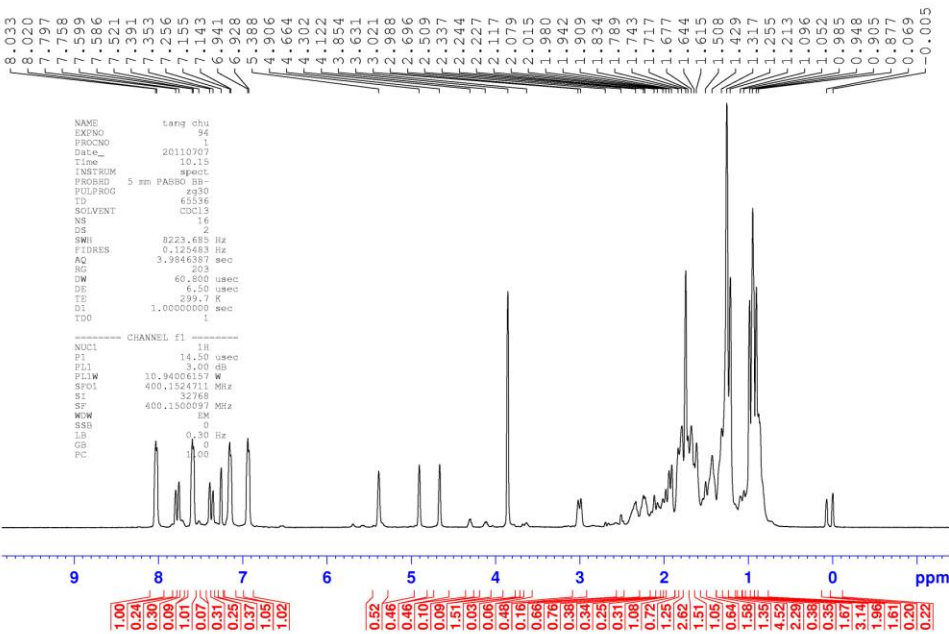


EI-MS spectrum of compound 4f

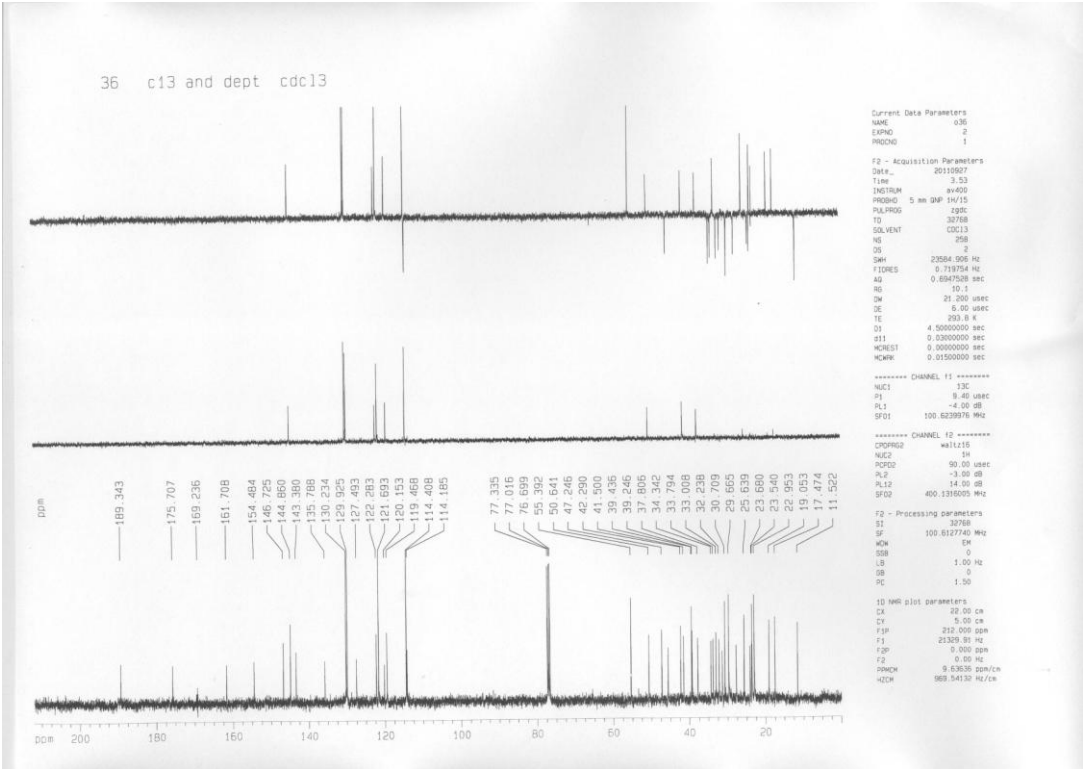


HREIMS spectrum of compound 4f

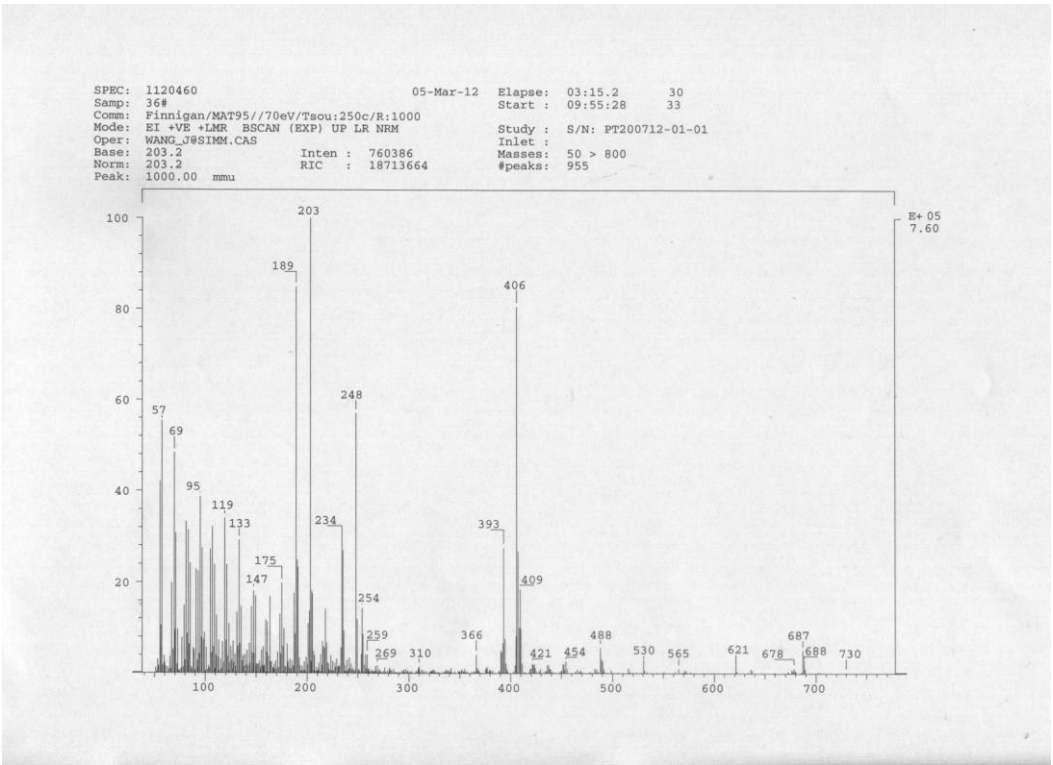
11-07-07 H-NMR tang chu 36



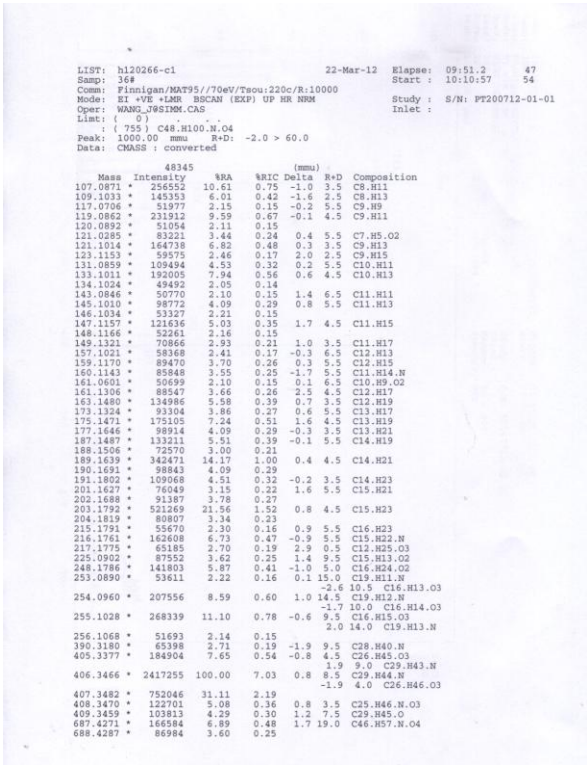
¹H NMR spectrum of compound 5a



¹³C NMR spectrum of compound 5a

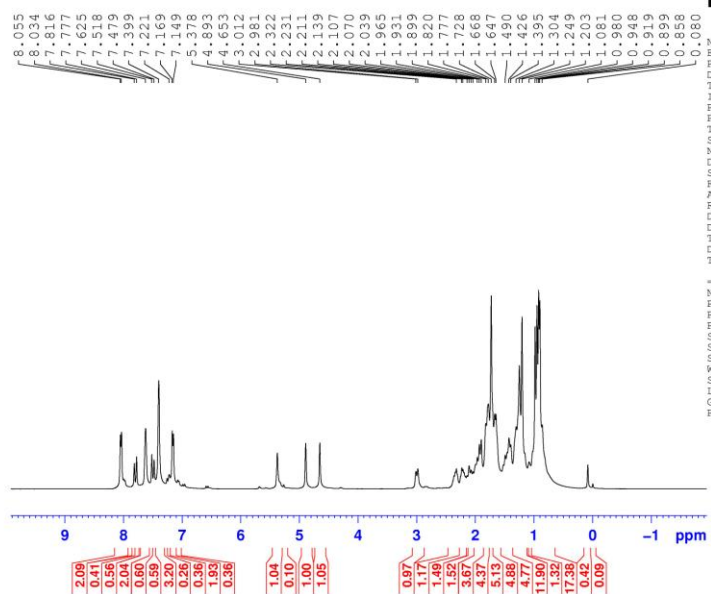


EI-MS spectrum of compound **5a**

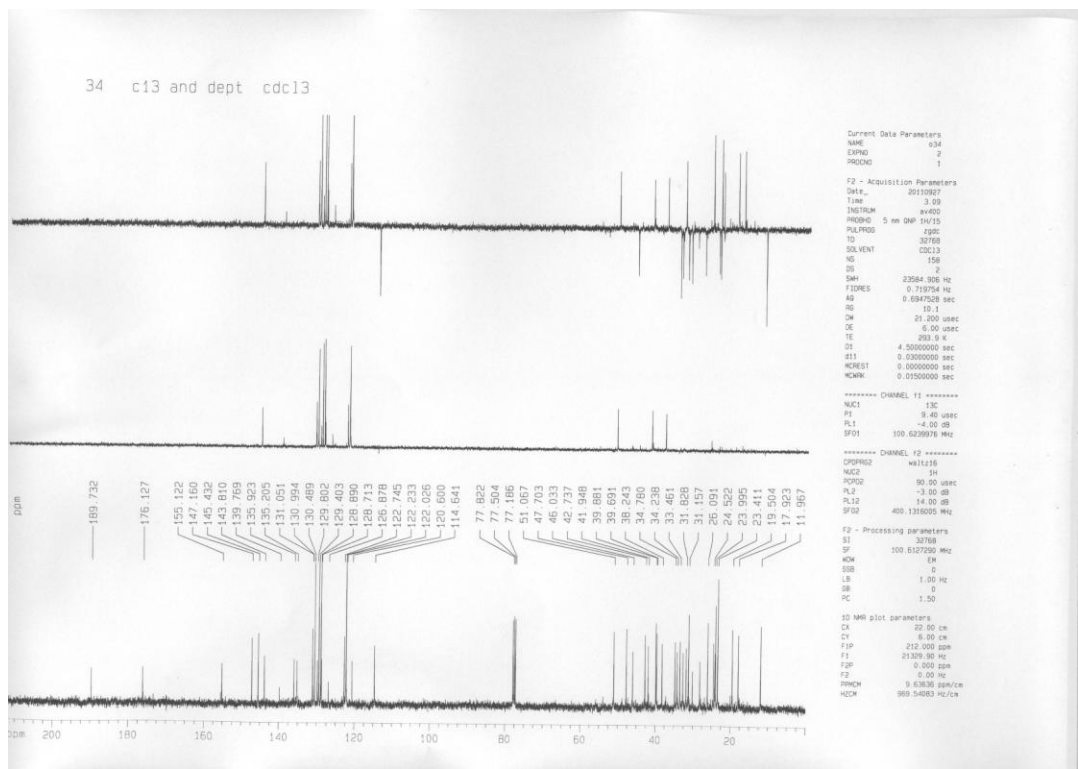


HREIMS spectrum of compound **5a**

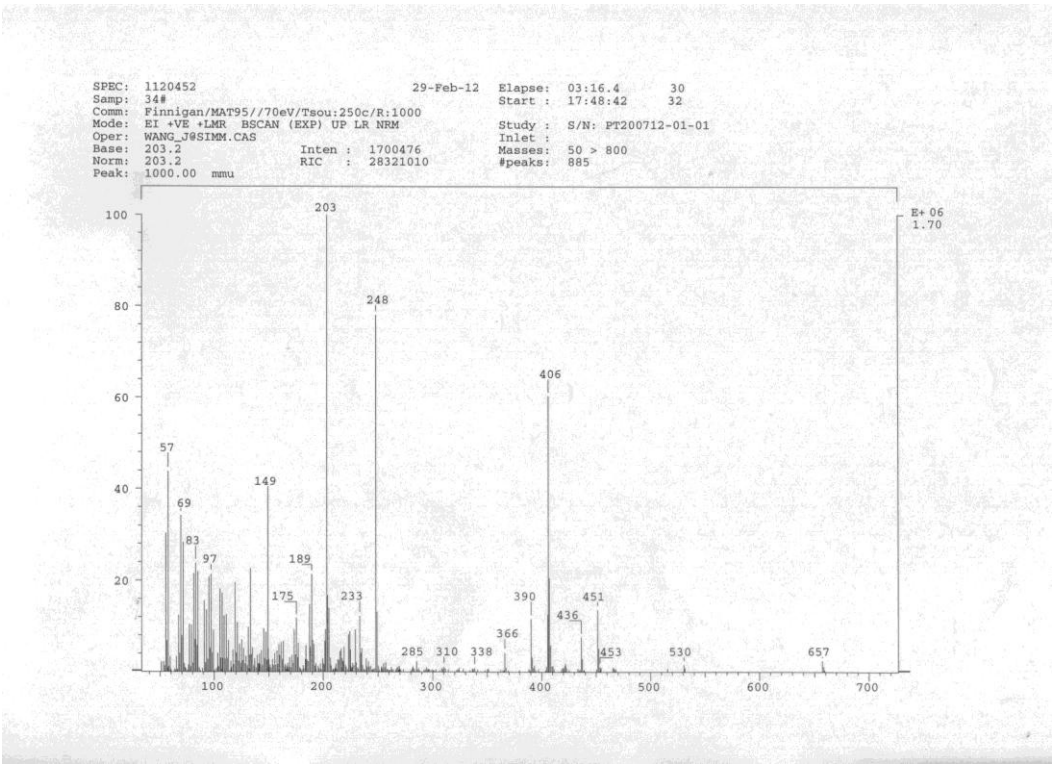
11-11-02 H-NMR tang chu 60



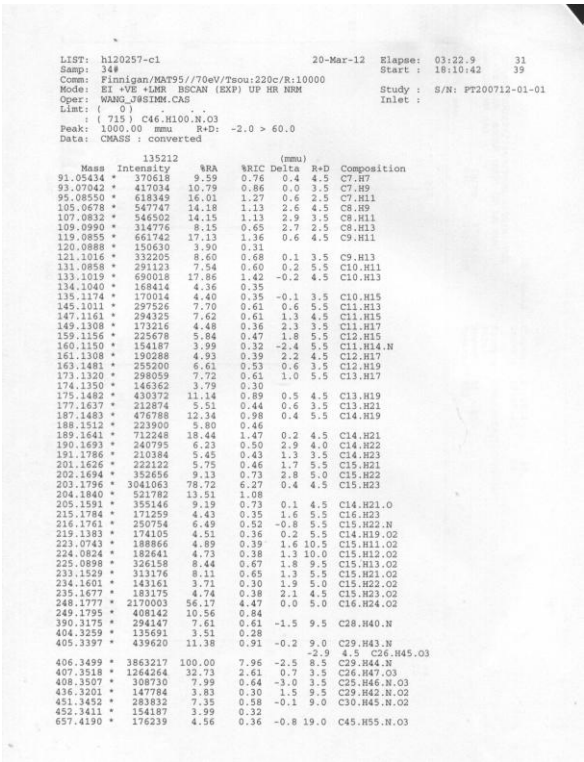
¹H NMR spectrum of compound **5b**



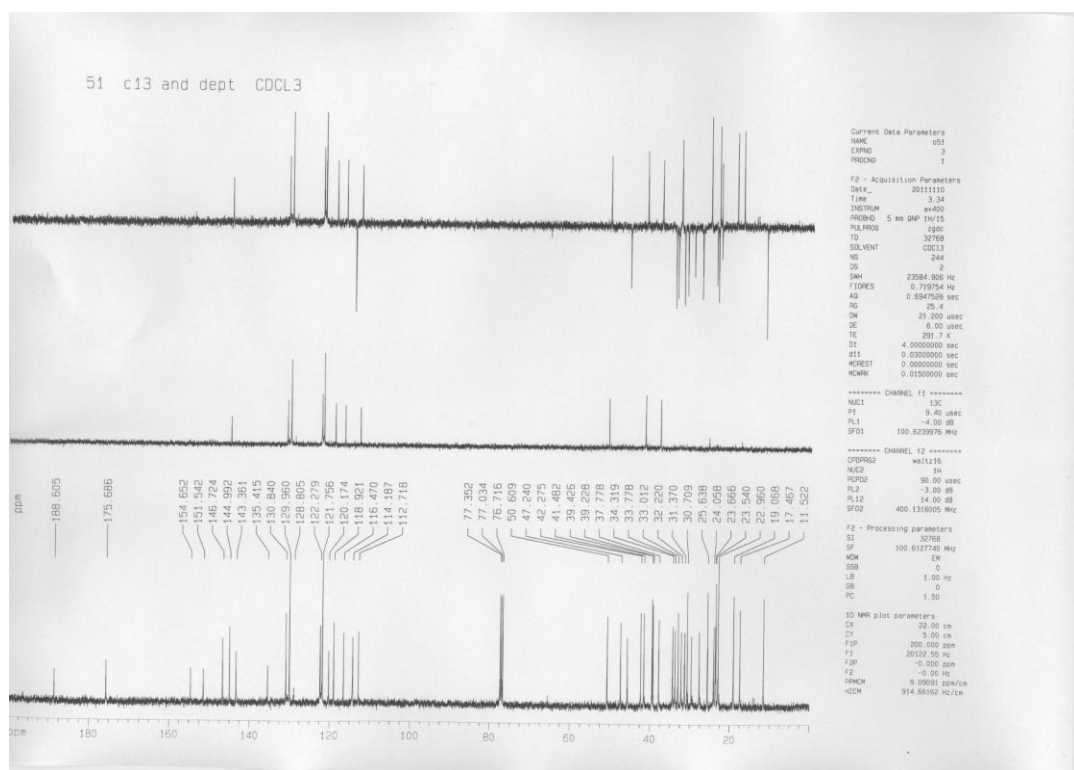
¹³C NMR spectrum of compound **5b**

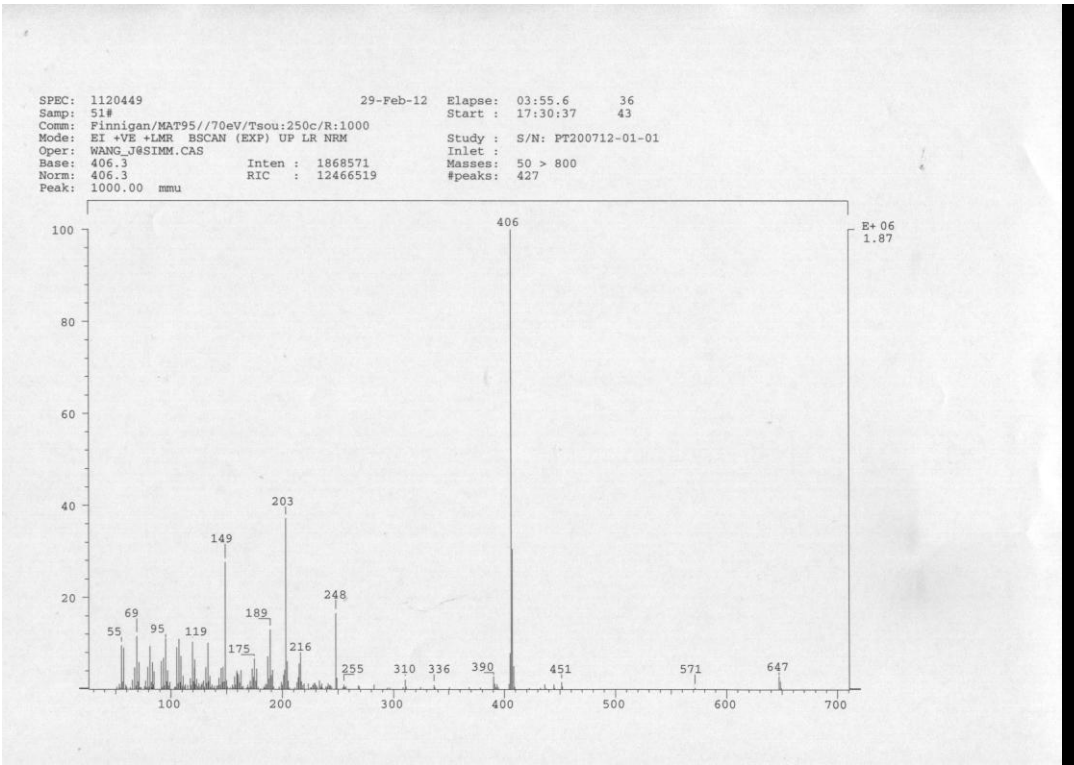


EI-MS spectrum of compound **5b**

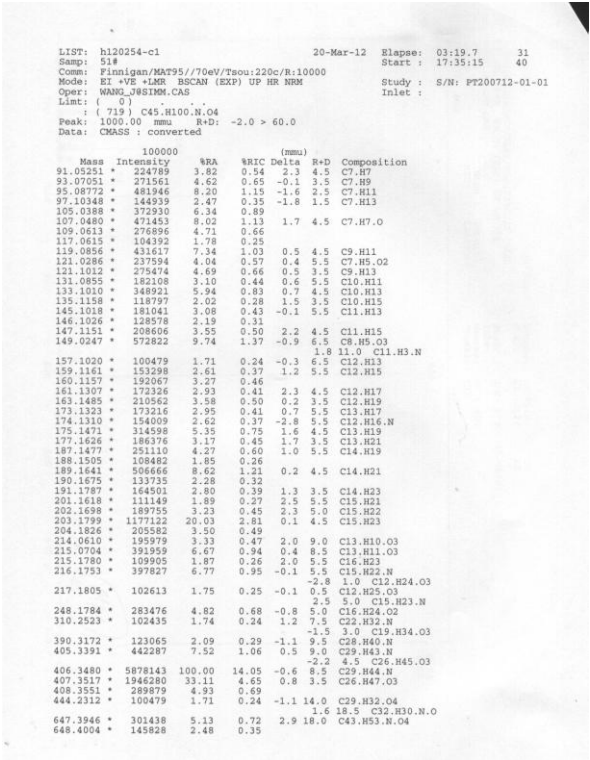


HREIMS spectrum of compound **5b**

¹H NMR spectrum of compound **5c** ^{13}C NMR spectrum of compound **5c**

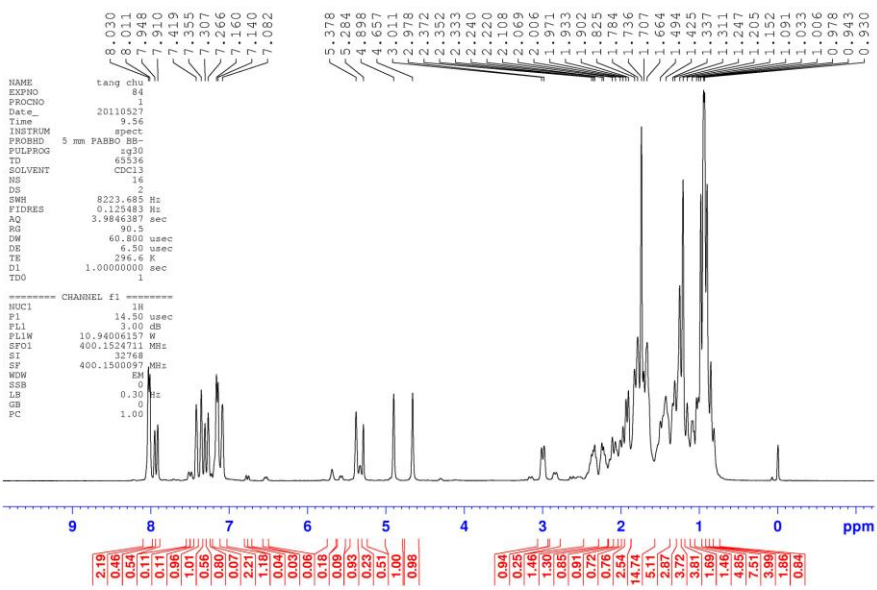


EI-MS spectrum of compound **5c**

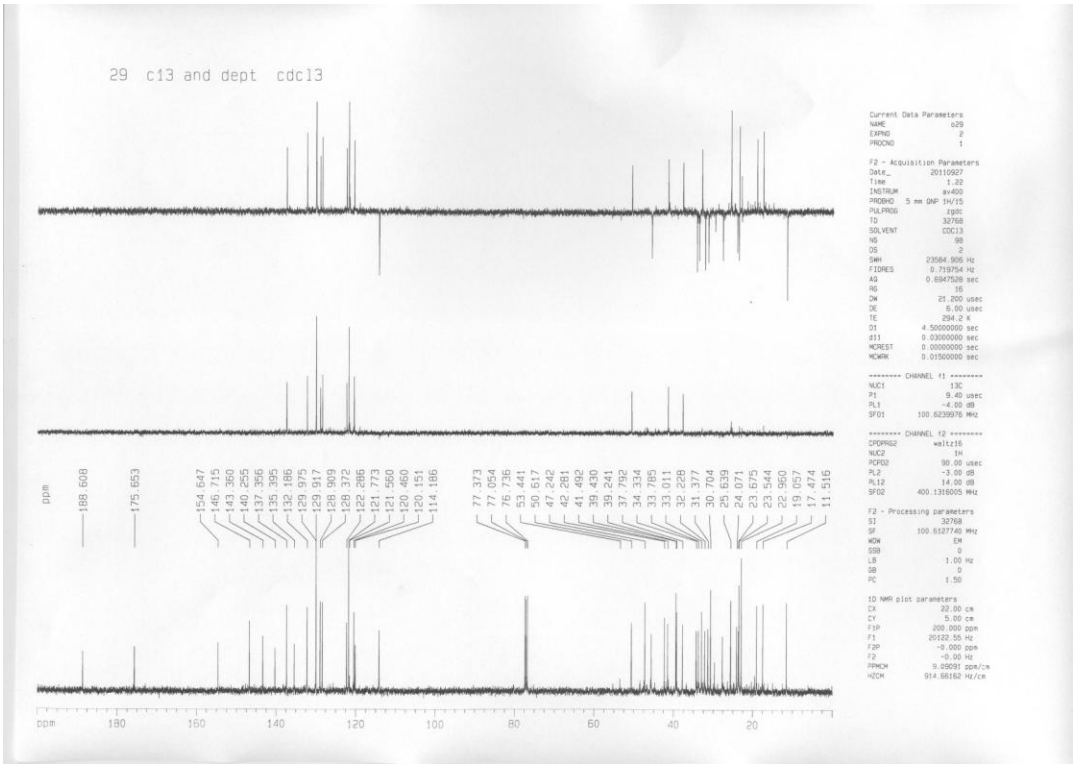


HREIMS spectrum of compound **5c**

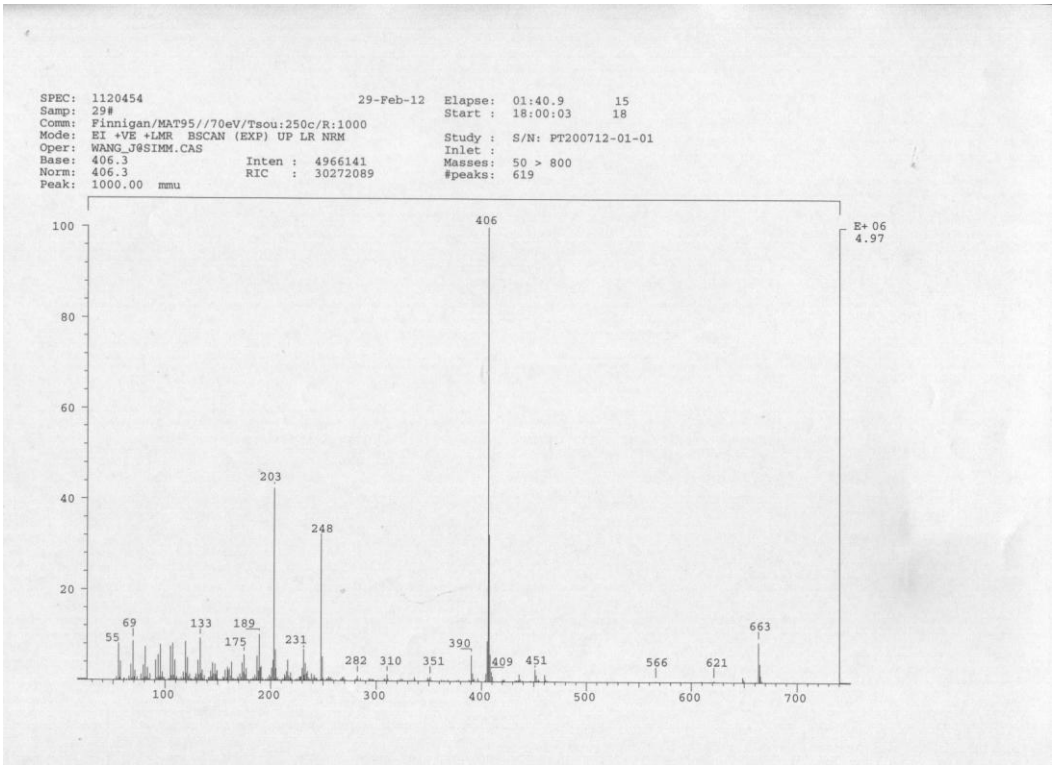
11-05-27 H-NMR tang chu 29



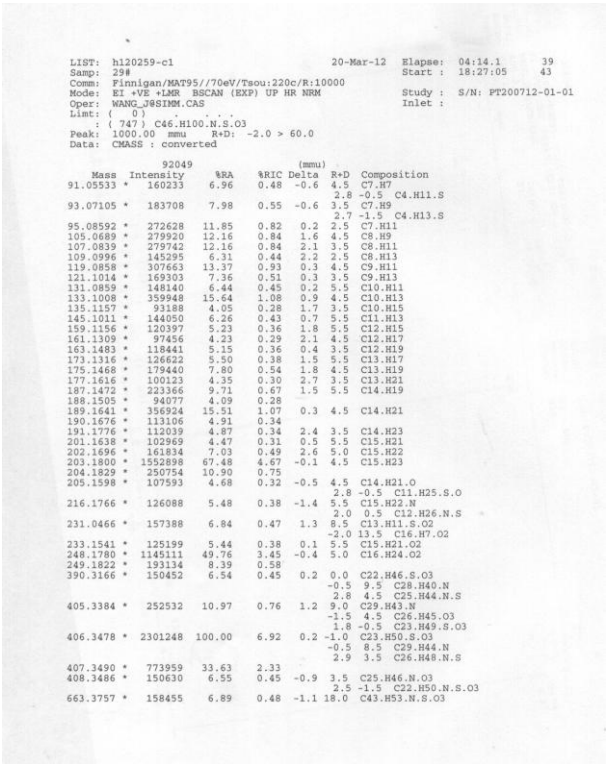
¹H NMR spectrum of compound **5d**



¹³C NMR spectrum of compound **5d**

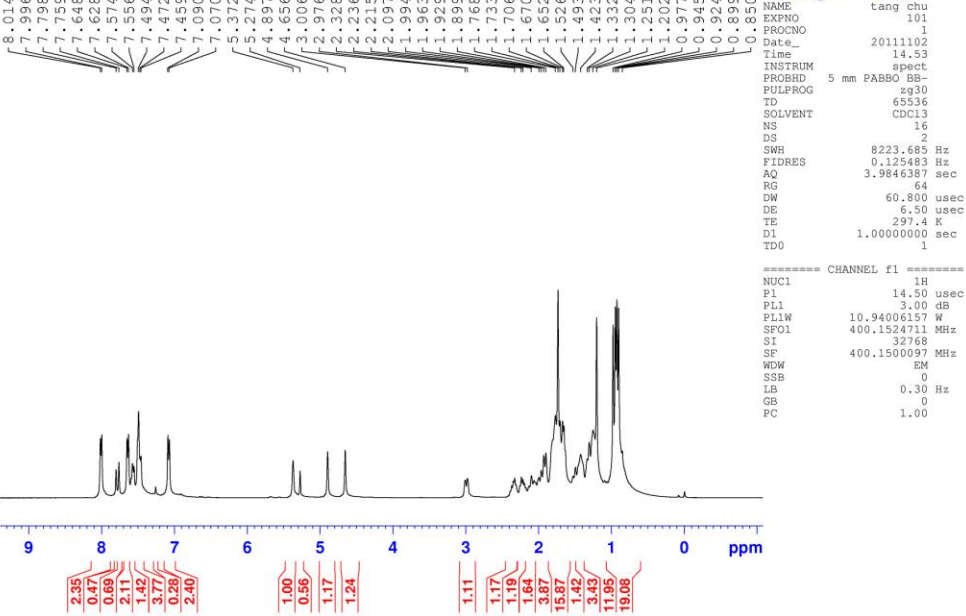


EI-MS spectrum of compound **5d**

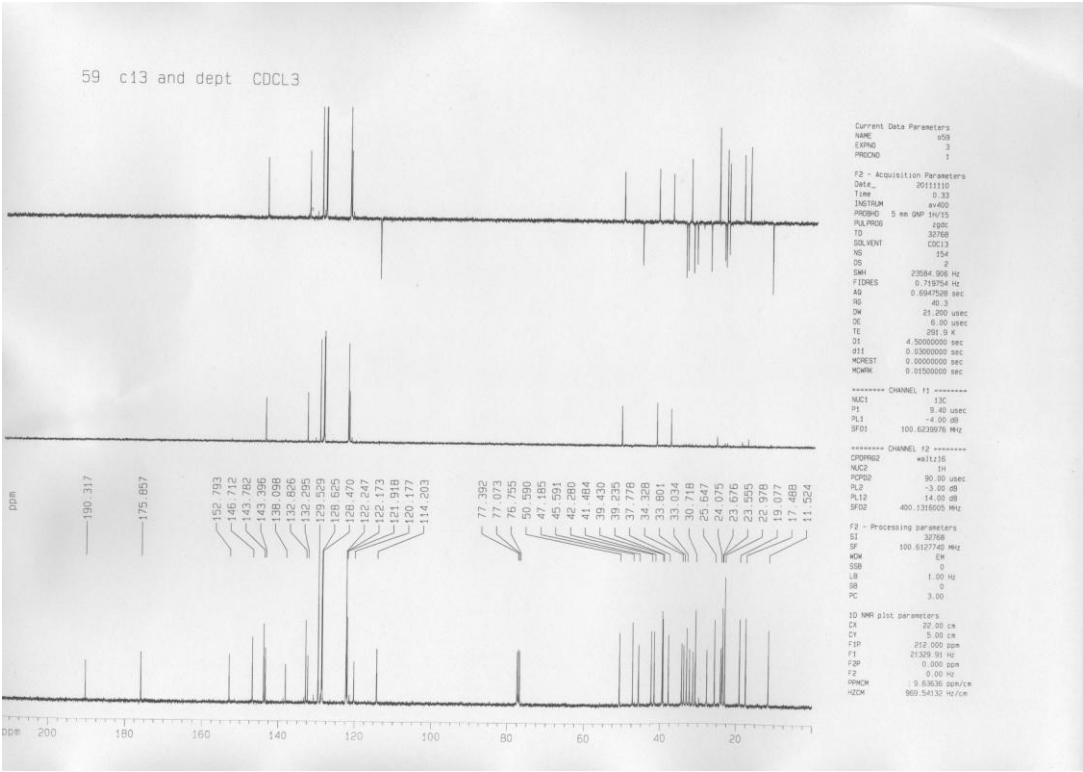


HREIMS spectrum of compound **5d**

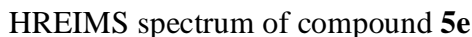
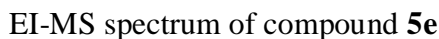
11-11-02 H-NMR tang chu 59

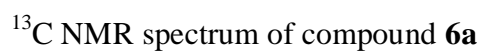
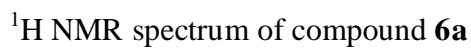


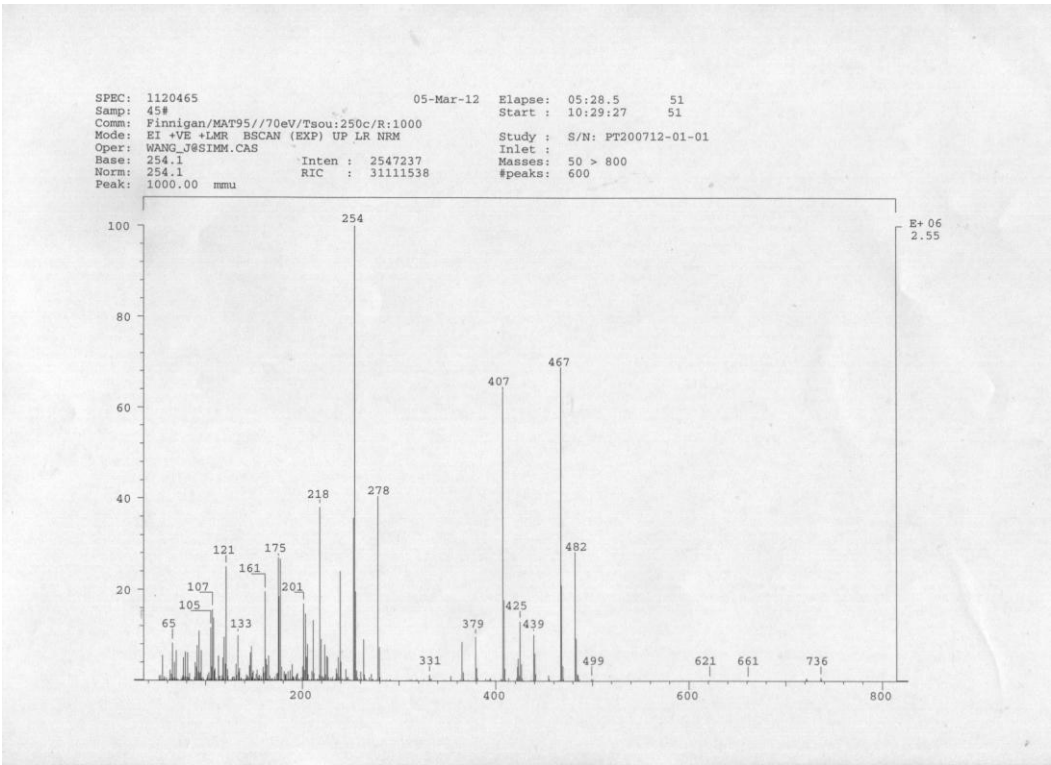
¹H NMR spectrum of compound **5e**



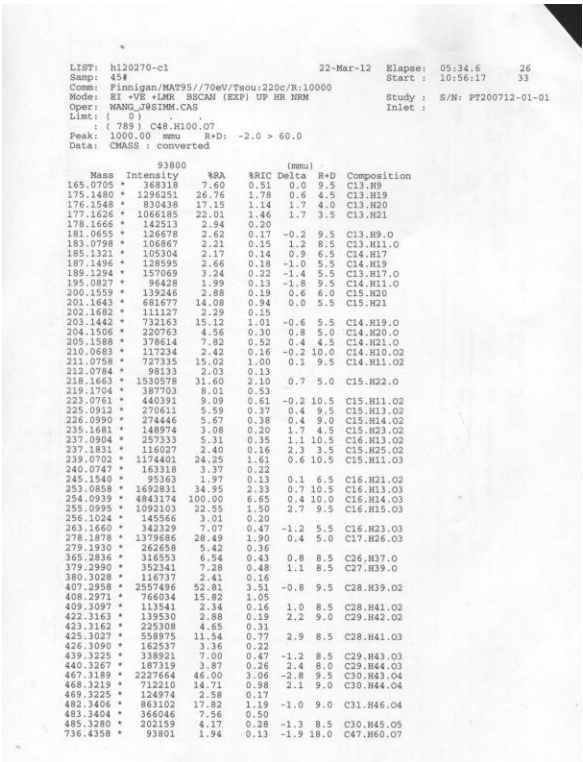
¹³C NMR spectrum of compound **5e**



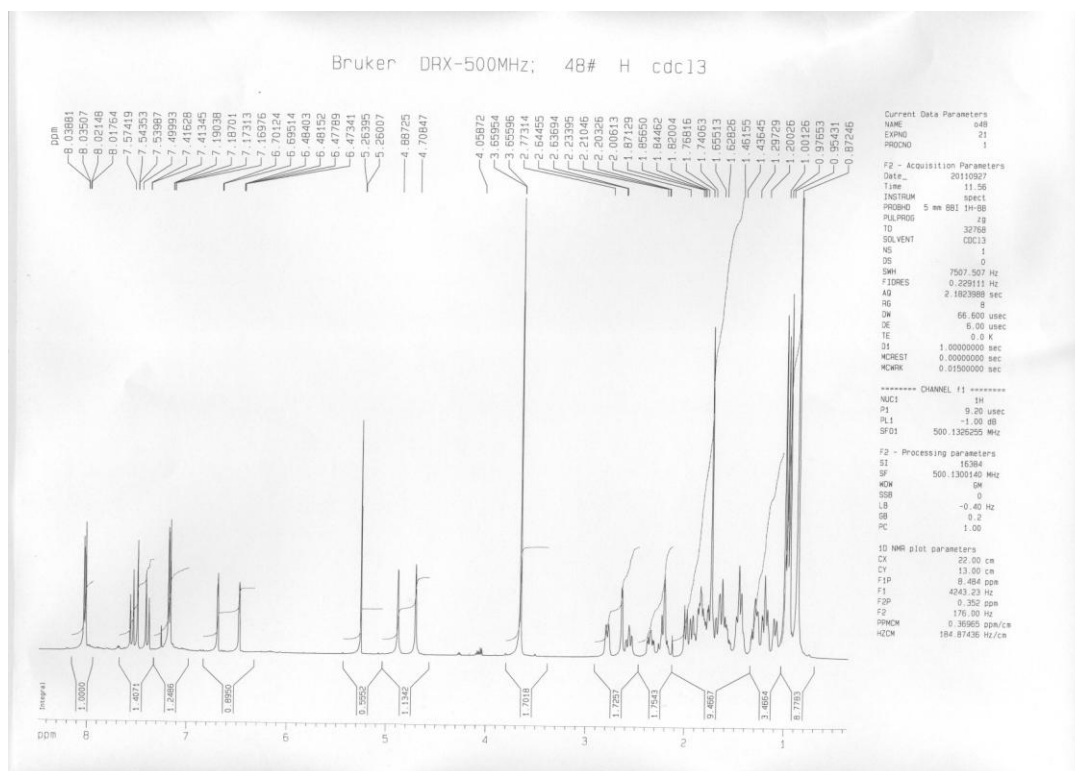




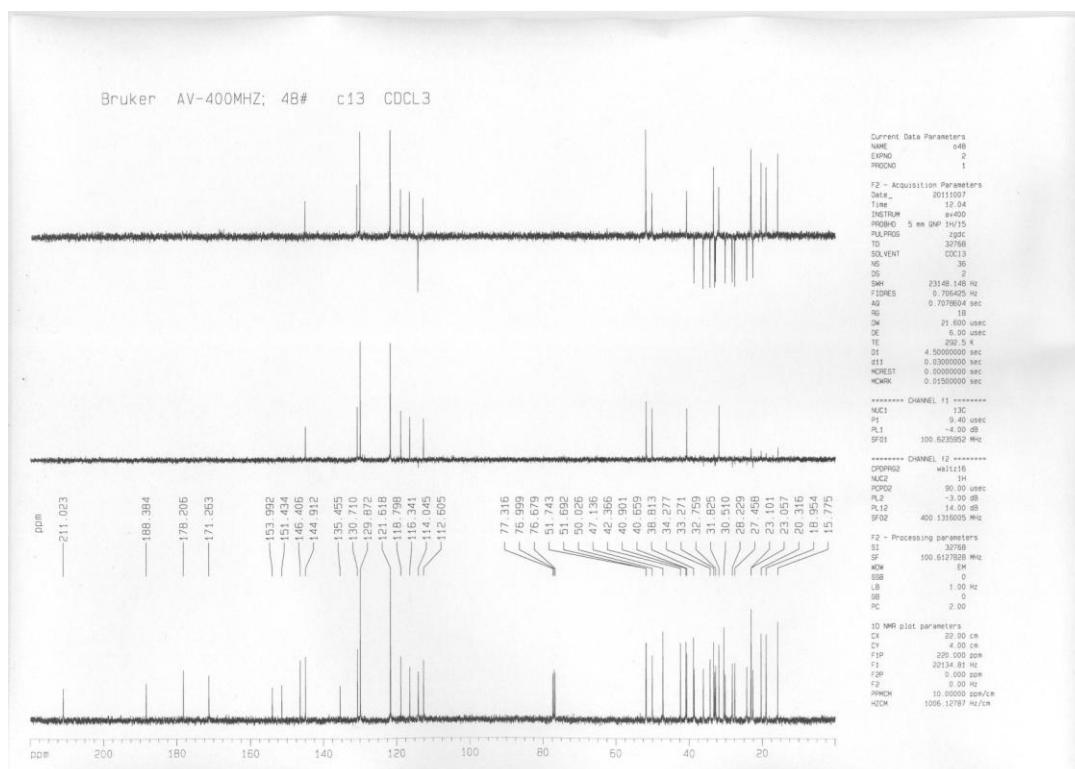
EI-MS spectrum of compound **6a**



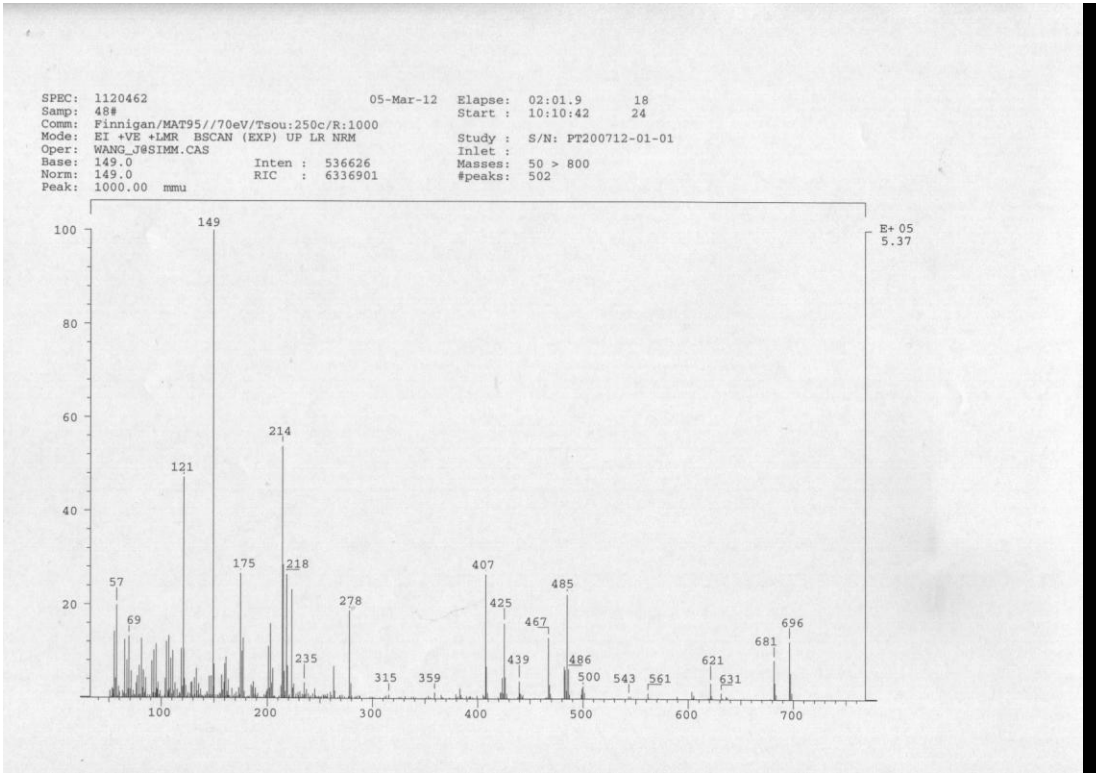
HREIMS spectrum of compound **6a**



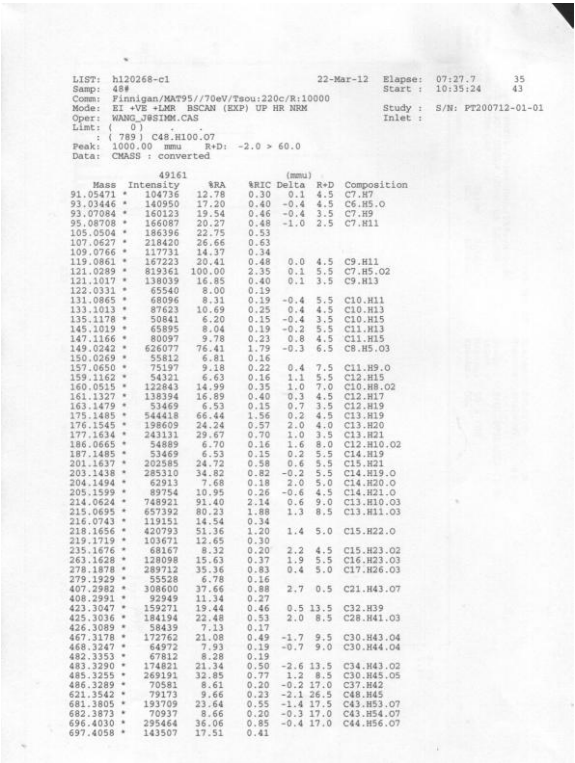
¹H NMR spectrum of compound **6b**



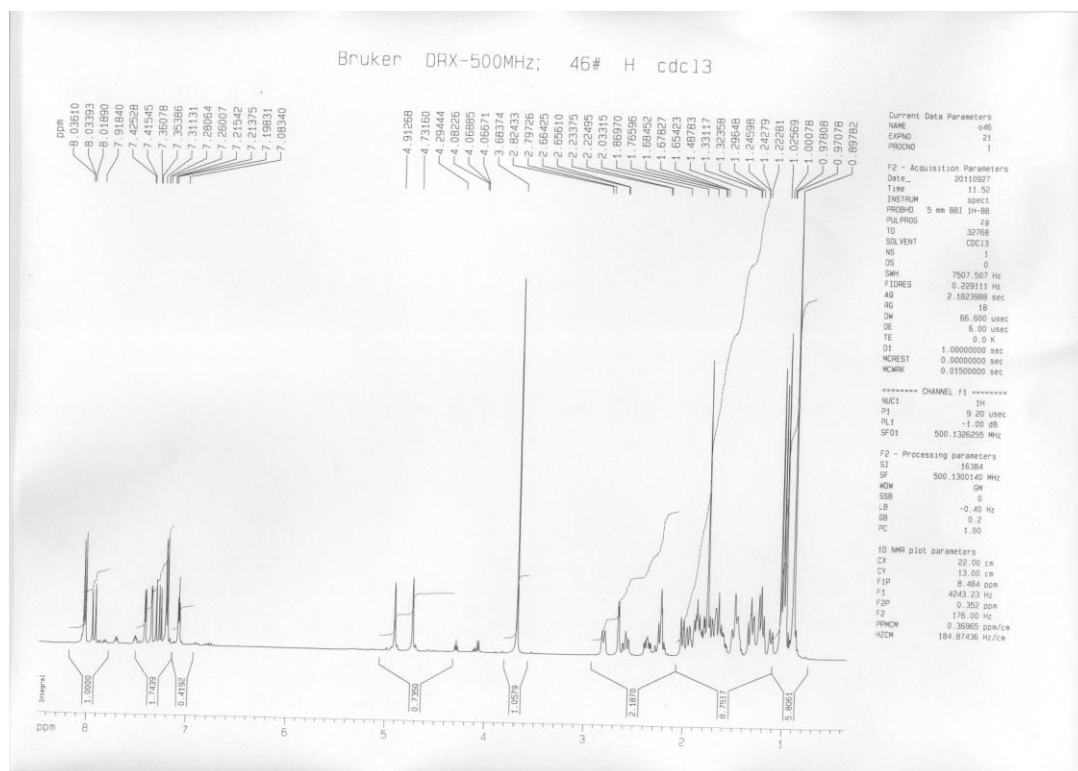
¹³C NMR spectrum of compound **6b**



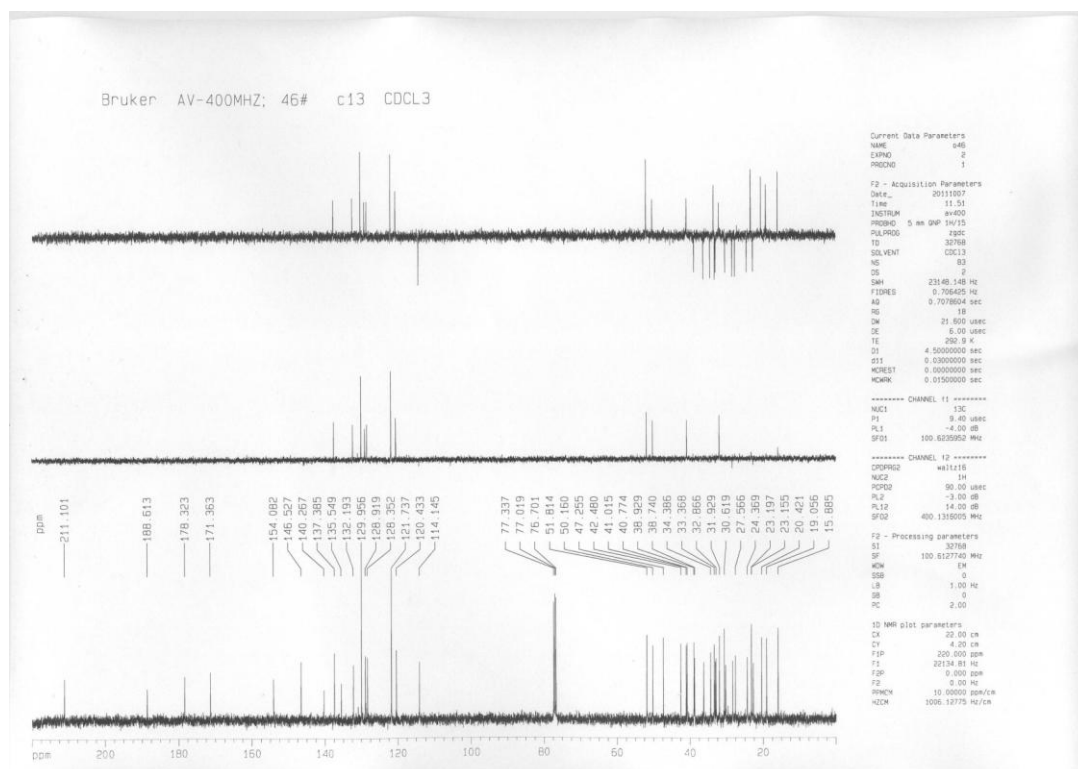
EI-MS spectrum of compound **6b**



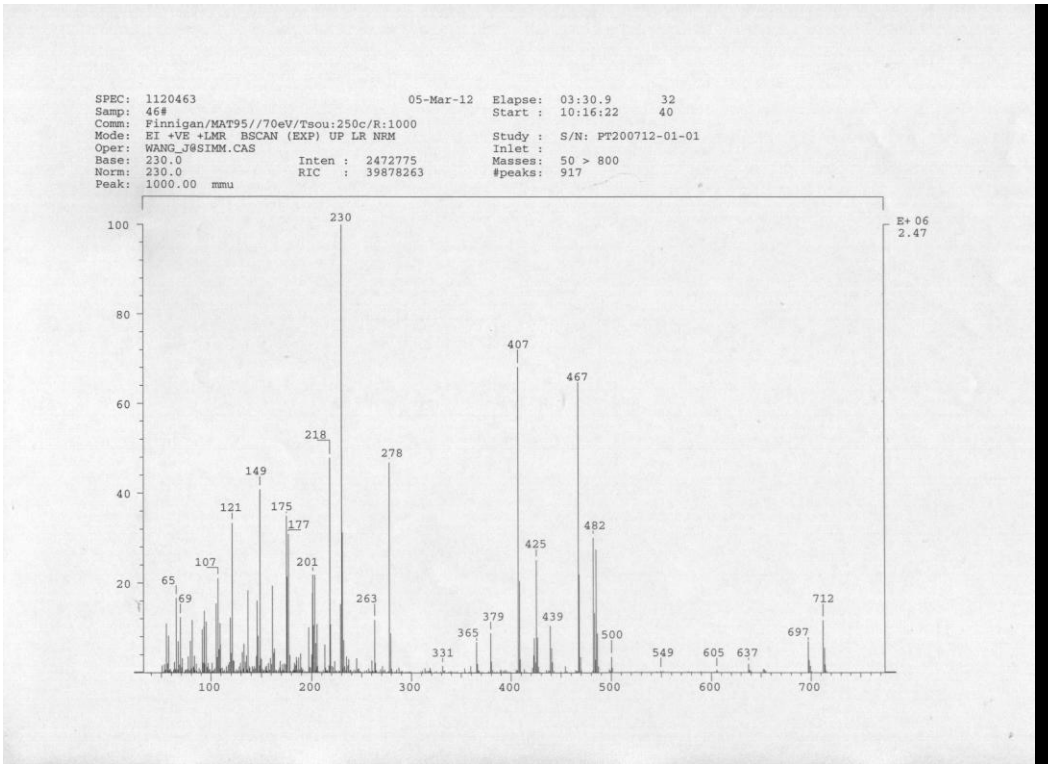
HREIMS spectrum of compound **6b**



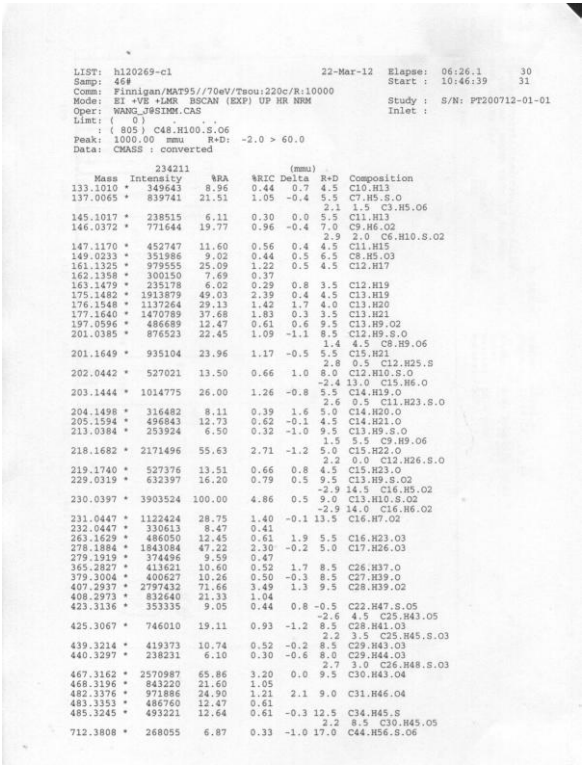
^1H NMR spectrum of compound **6c**



^{13}C NMR spectrum of compound **6c**



EI-MS spectrum of compound **6c**



HREIMS spectrum of compound **6c**