

Supplementary Materials

Design, Synthesis, and Biological Evaluation of Pyridazinones Containing the (2-Fluorophenyl) Piperazine Moiety as selective MAO-B Inhibitors

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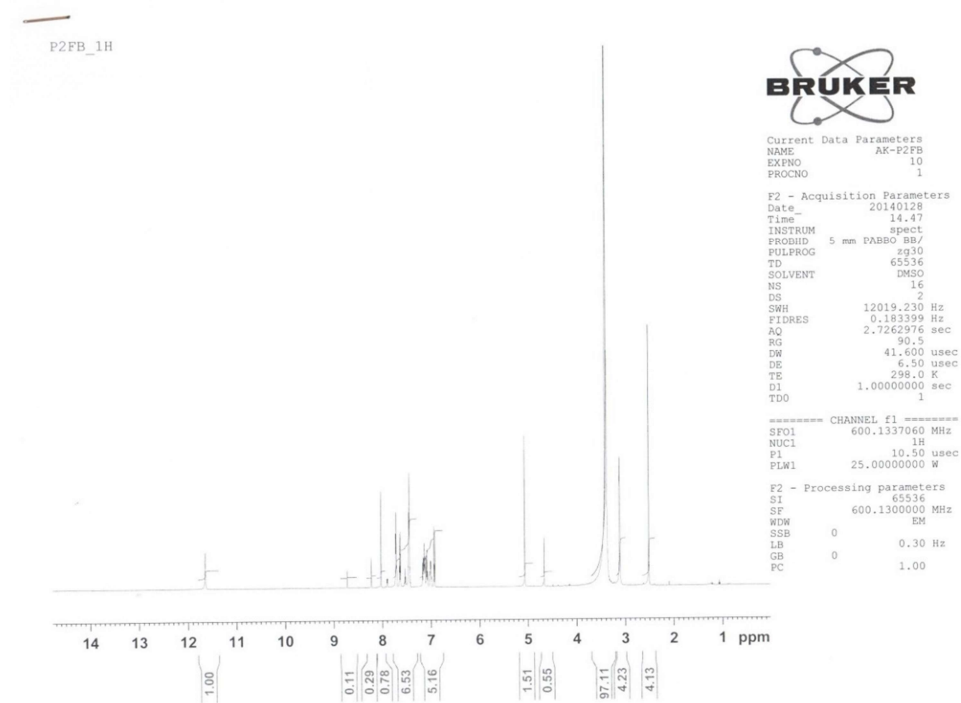
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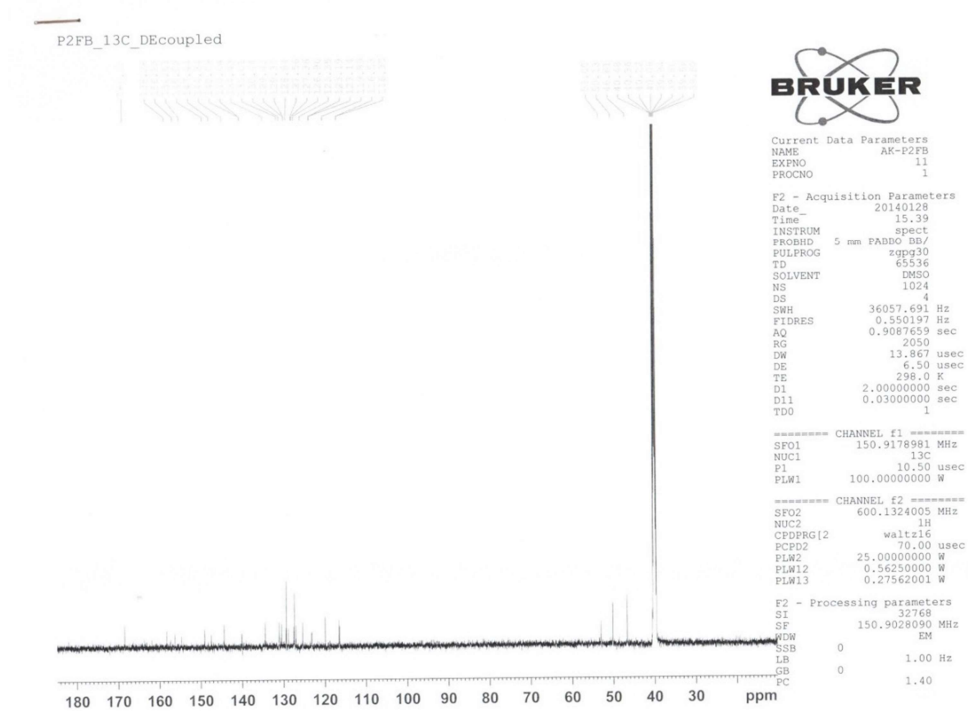
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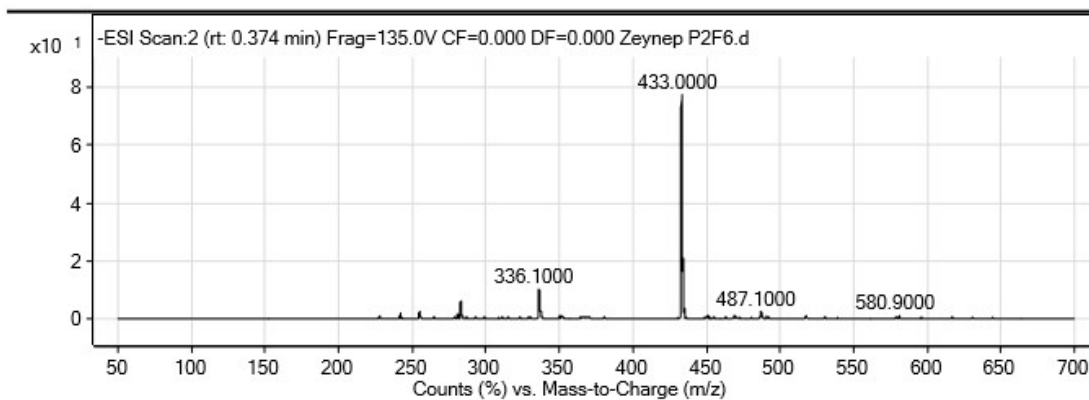
Data 1. ¹H-NMR spectrum of compound T1



Data 2. ¹³C-NMR spectrum of compound T1



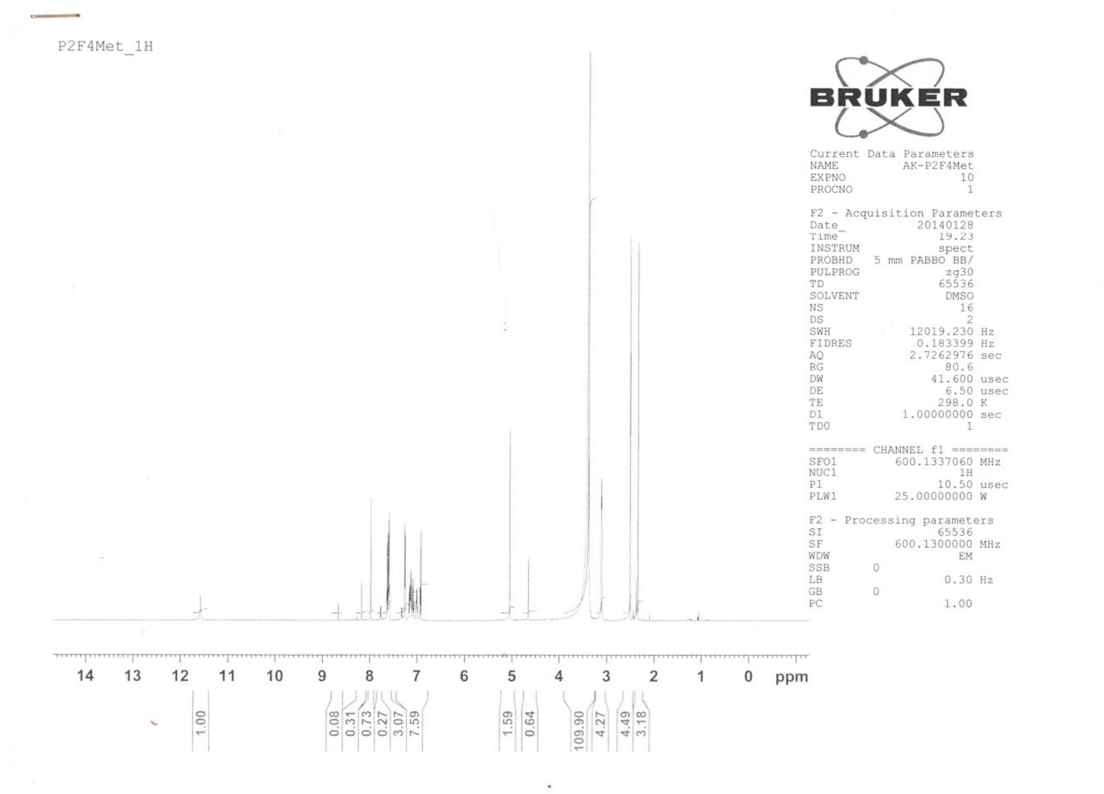
Data 3. HRMS spectrum of compound T1



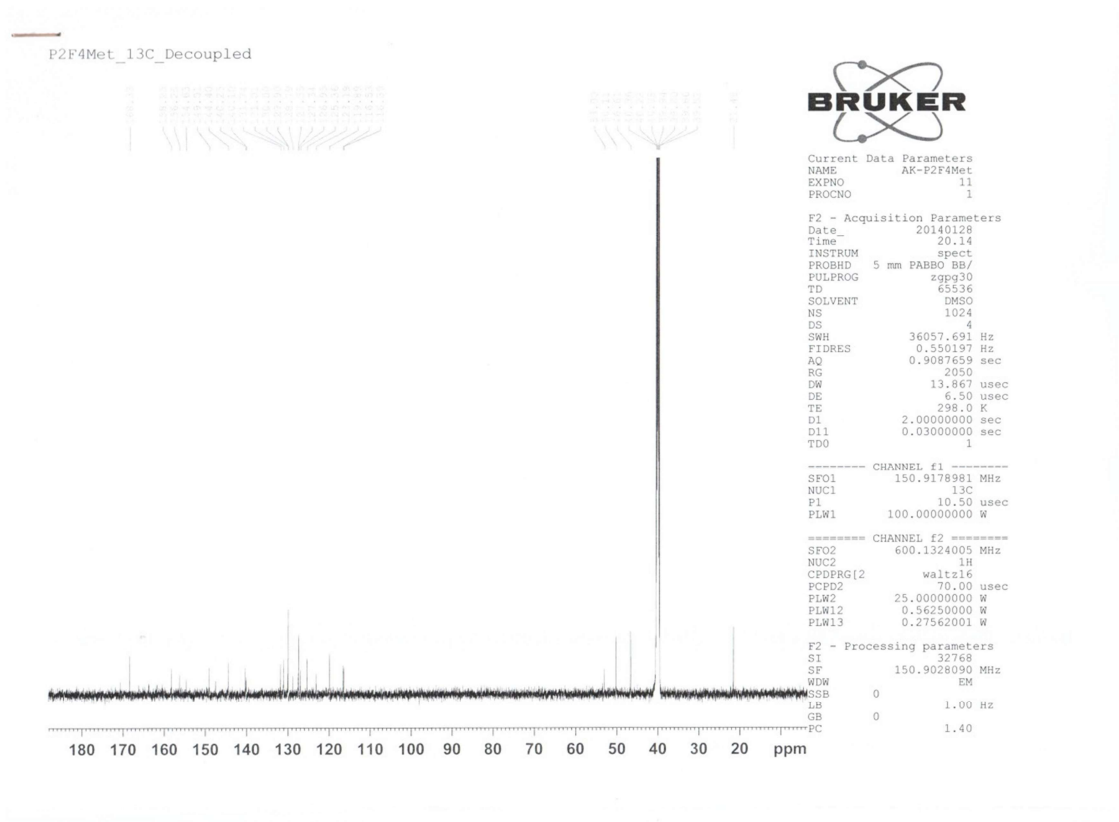
Peak List

m/z	z	Abund
241.9		2196.5
255.1	1	3057.06
280.8		1658.48
283.1		7019.18
336.1	1	11244.46
337.1	1	3218.38
433	1	85811.05
434	1	22975.82
435	1	3972.78

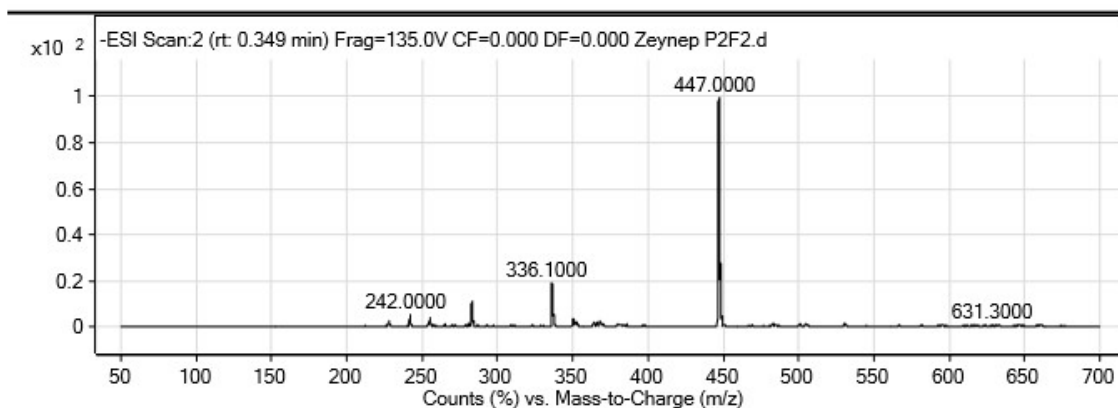
Data 4. ¹H-NMR spectrum of compound T2



Data 5. ¹³C-NMR spectrum of compound T2



Data 6. HRMS spectrum of compound T2

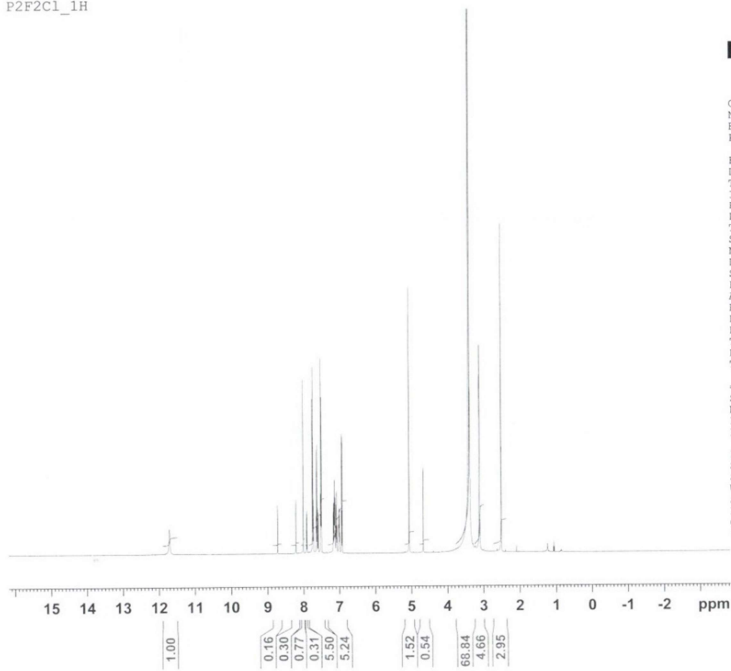


Peak List

m/z	z	Abund
228.1		2618.28
242		5255.52
255.1		3681.6
283		10534.4
336.1		18198.36
337.2	1	4868.92
350.1		3531.82
447	1	93741.25
448	1	25748.56
449	1	4422.98

Data 7. ¹H-NMR spectrum of compound T3

P2F2C1_1H



Current Data Parameters
NAME AK-P2F2C1
EXPNO 10
PROCNO 1

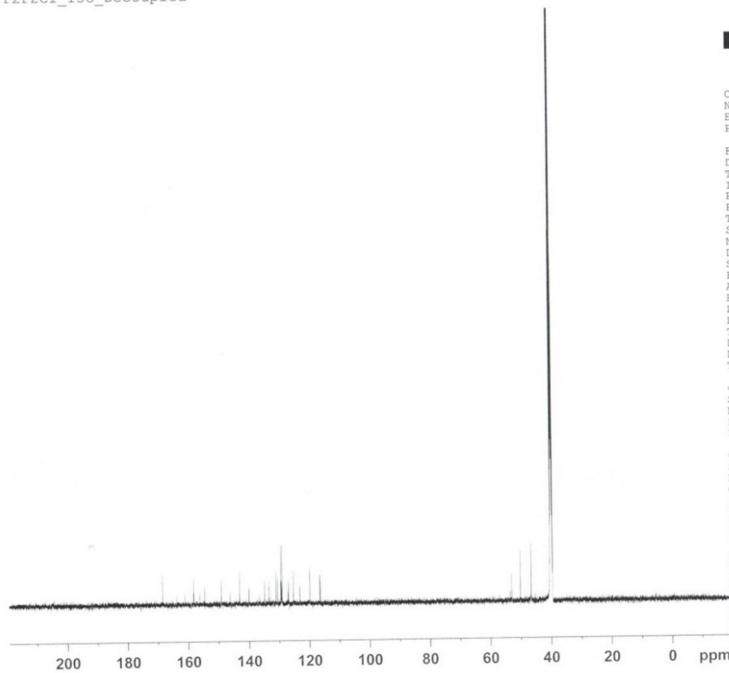
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Date_ 20140128
Time 15.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 80.6
DW 41.600 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 10.50 usec
PLW1 25.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Data 8. ¹³C-NMR spectrum of compound T3

P2F2C1_13C_Decoupled



Current Data Parameters
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EXPNO 11
PROCNO 1

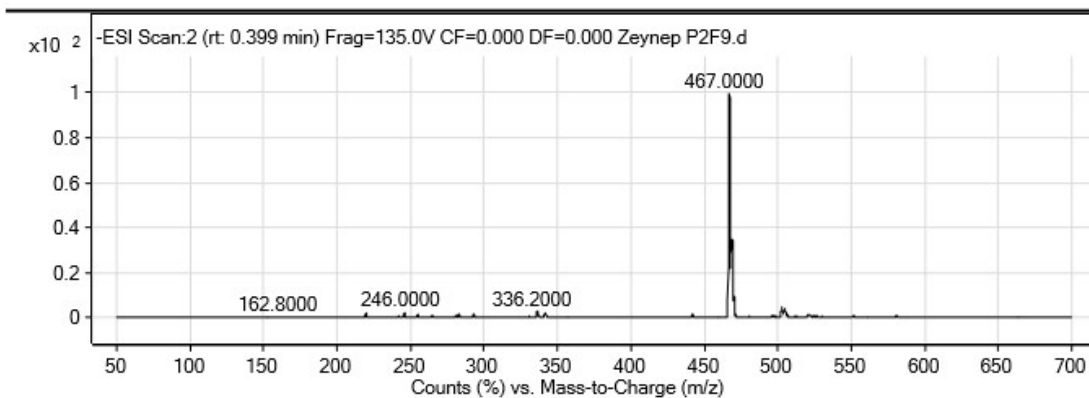
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 150.9178981 MHz
NUC1 13C
P1 10.50 usec
PLW1 100.00000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 25.00000000 W
PLW12 0.56250000 W
PLW13 0.27562001 W

F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

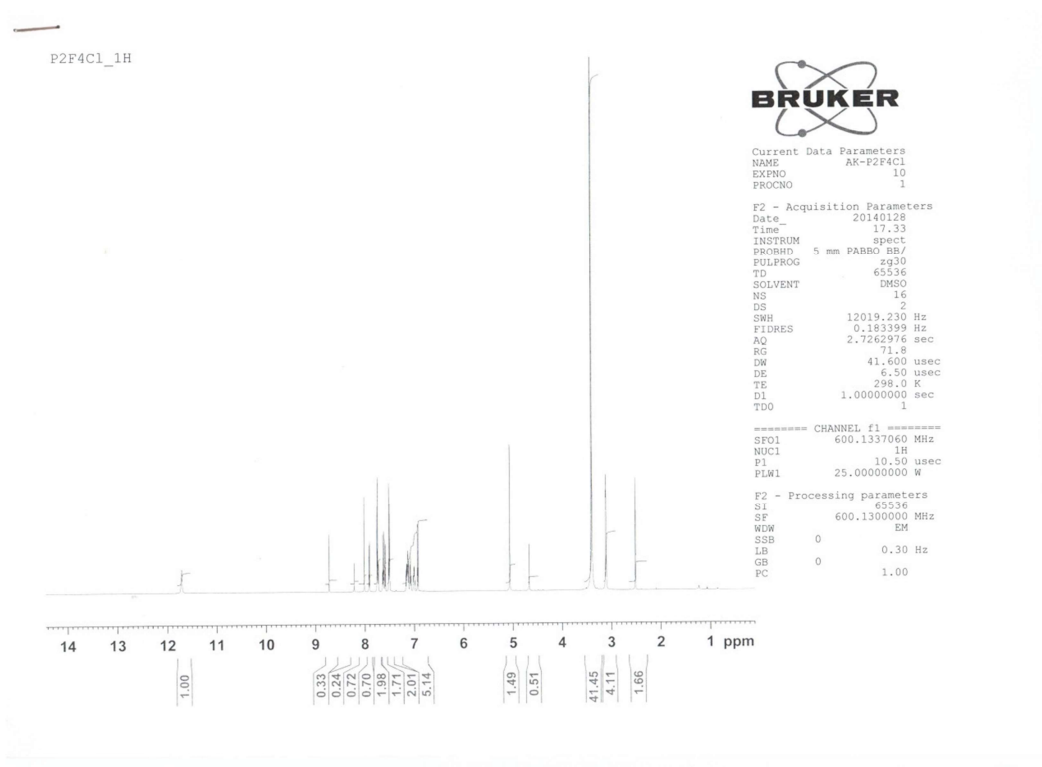
Data 9. HRMS spectrum of compound T3



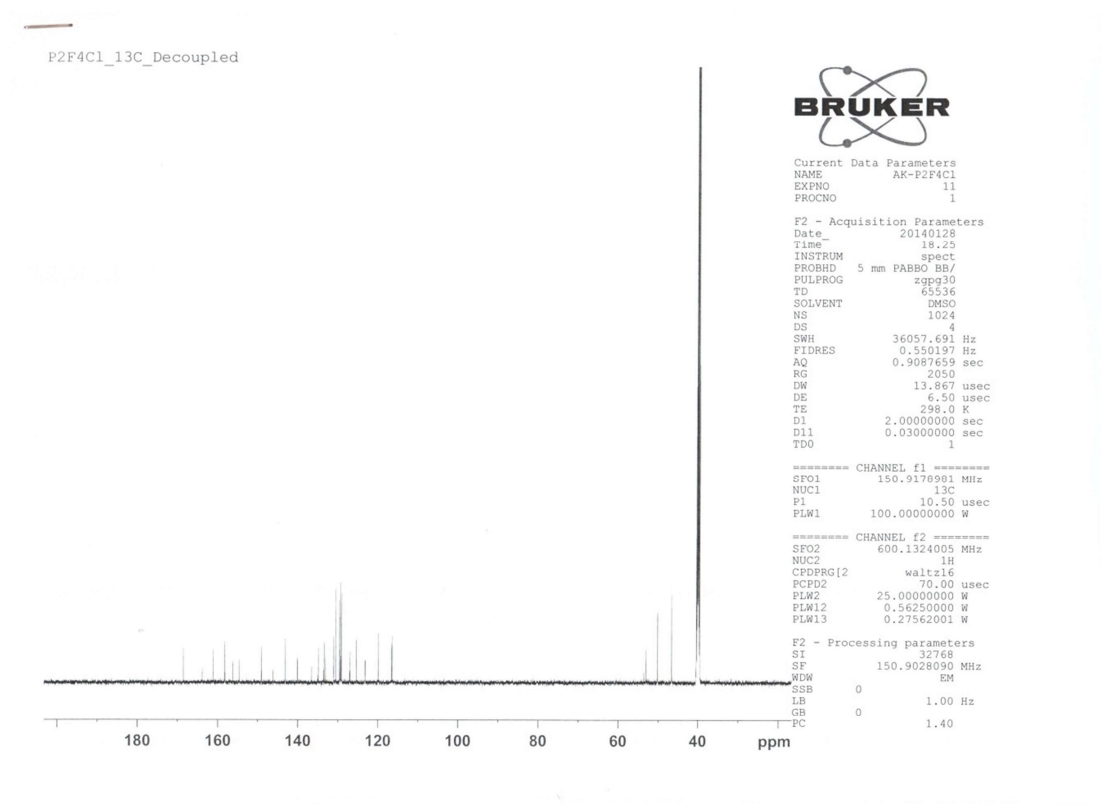
Peak List

m/z	z	Abund
220	1	2460.52
246		2666.44
336.2		3515.12
341.6	2	2662.1
467		118998.15
468.3		40049.68
469	1	41925.7
470	1	11476.82

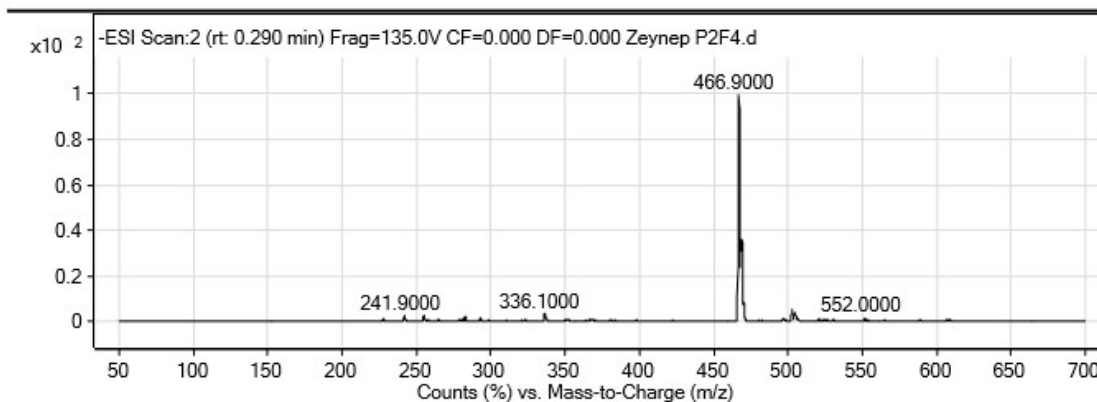
Data 10. ¹H-NMR spectrum of compound T4



Data 11. ¹³C-NMR spectrum of compound T4



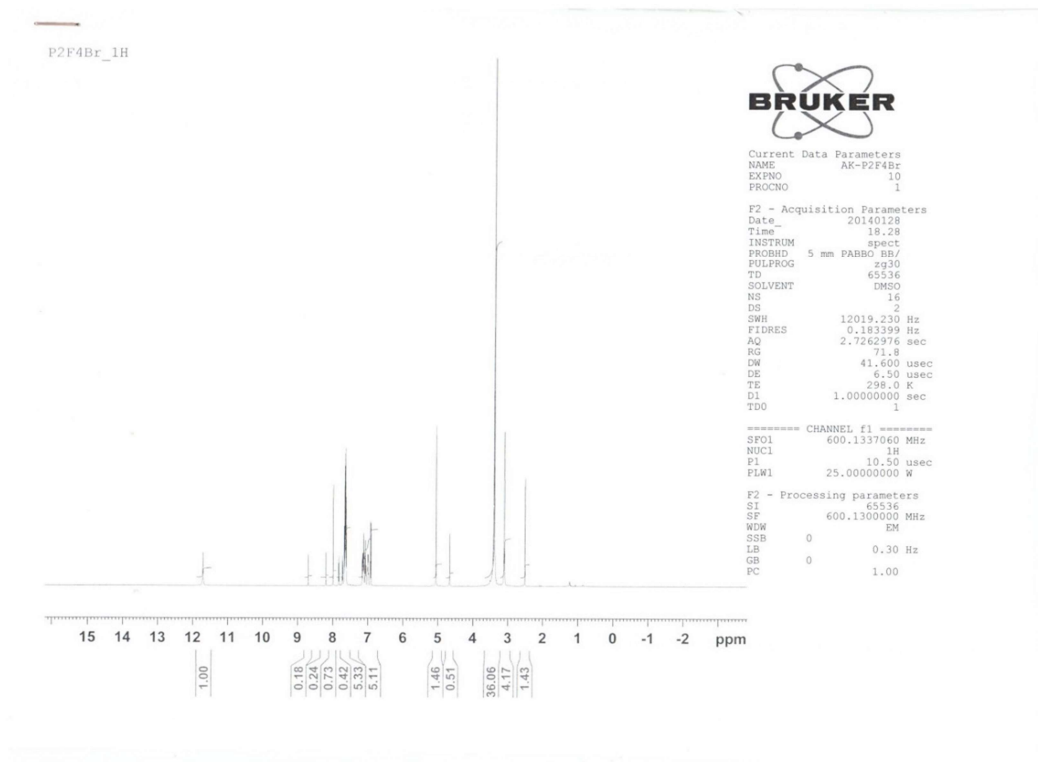
Data 12. HRMS spectrum of compound T4



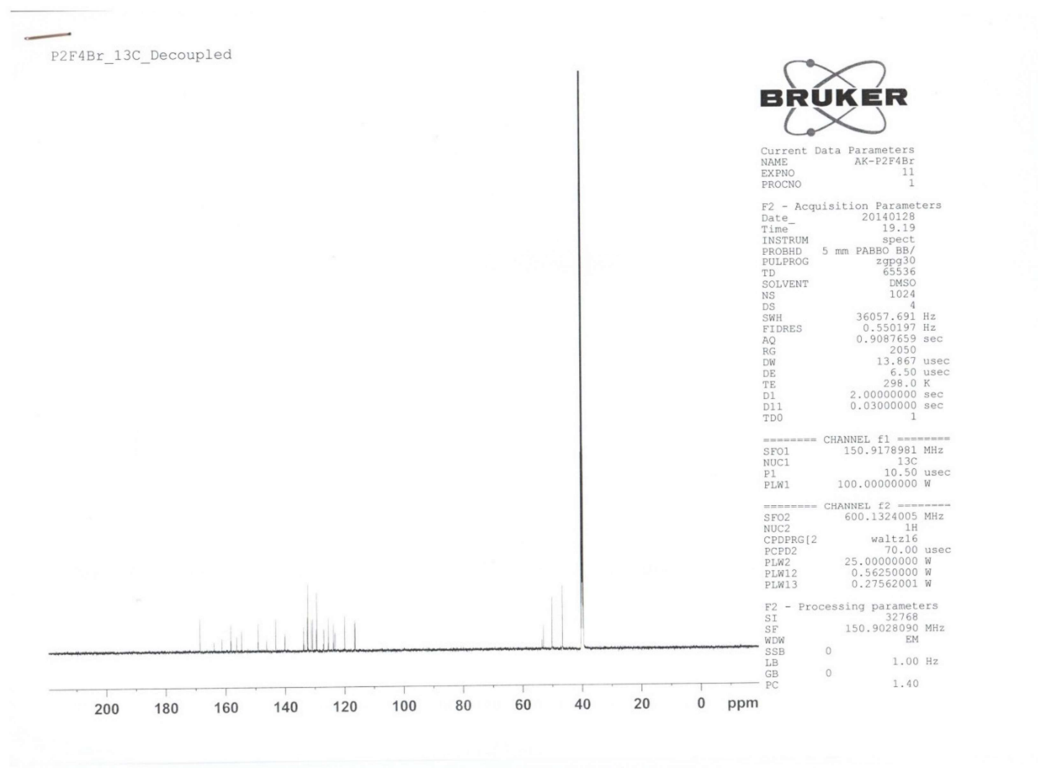
Peak List

m/z	z	Abund
241.9		3589.42
254.7	2	2865.68
255.1		3232.08
336.1	1	4549.26
466.9		121424.79
468.2		43604.76
468.9	1	43965.76
469.9	1	10811.56

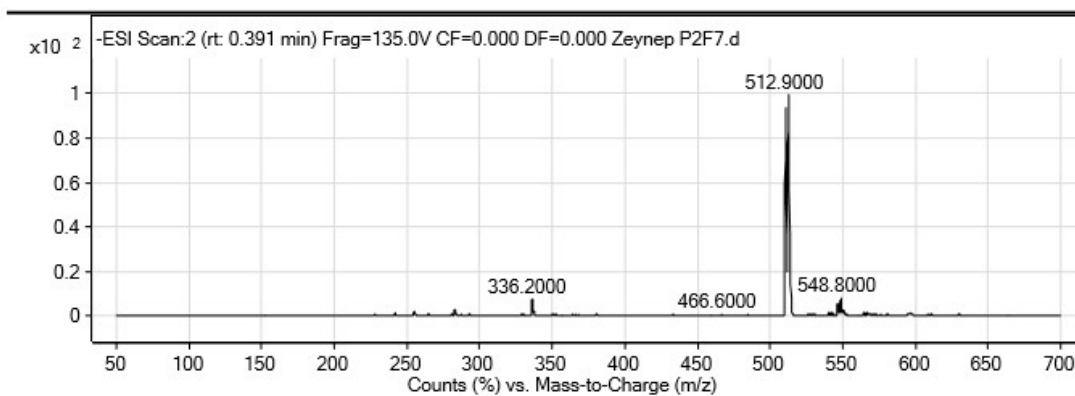
Data 13. ¹H-NMR spectrum of compound T5



Data 14. ¹³C-NMR spectrum of compound T5



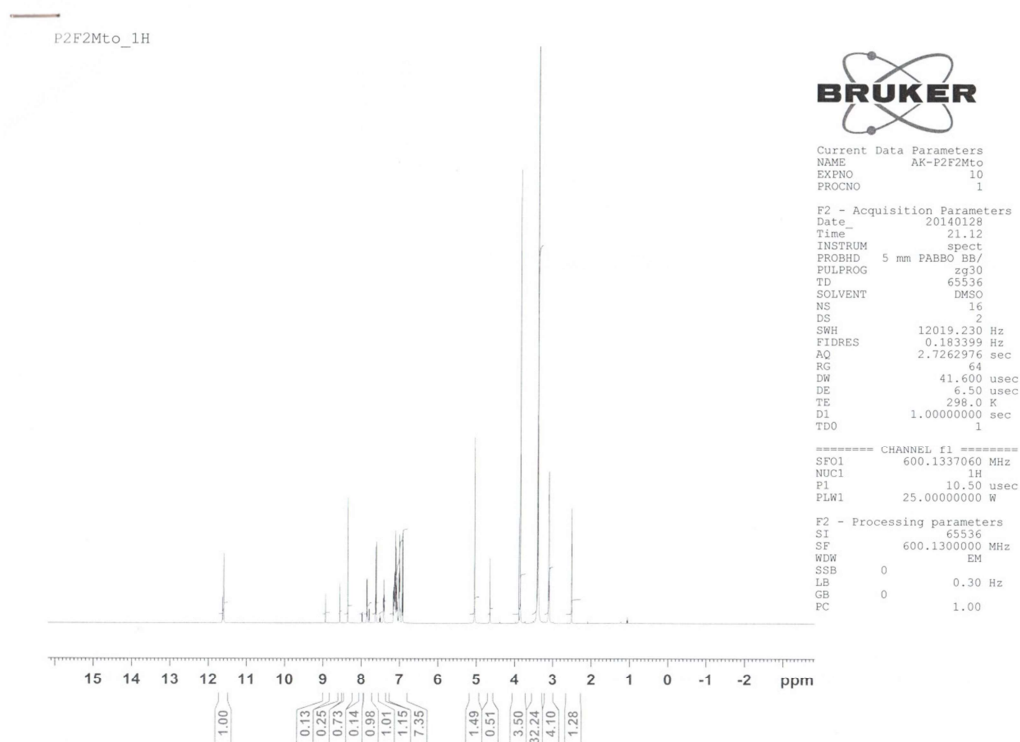
Data 15. HRMS spectrum of compound T5



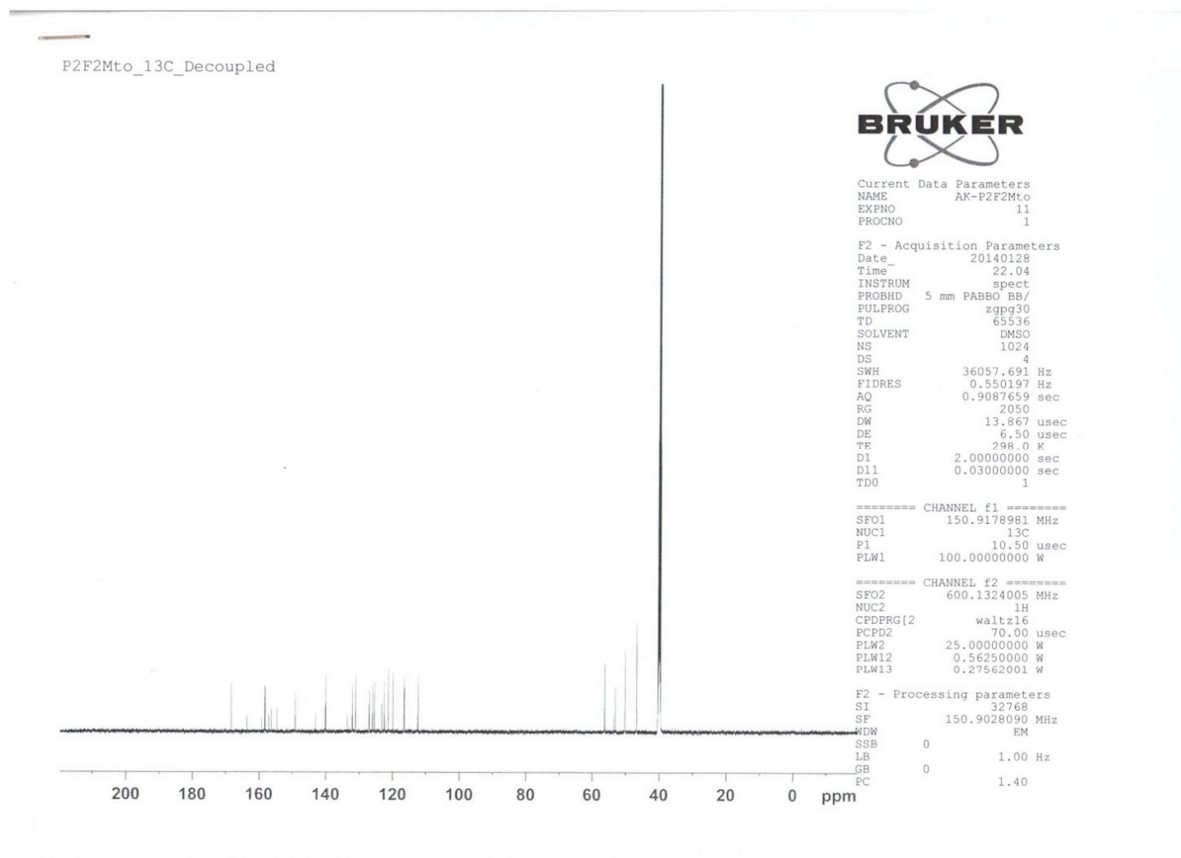
Peak List

m/z	z	Abund
283.1		2781.52
336.2	1	7290.16
510.9		93370.91
512.9	1	99546.02
513.9	1	25357.88
514.9	1	4260.32

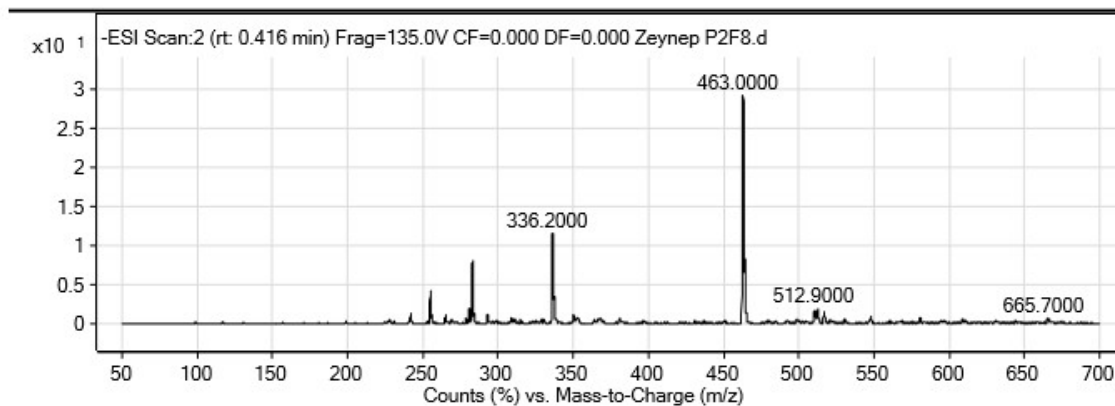
Data 16. ¹H-NMR spectrum of compound T6



Data 17. ¹³C-NMR spectrum of compound T6



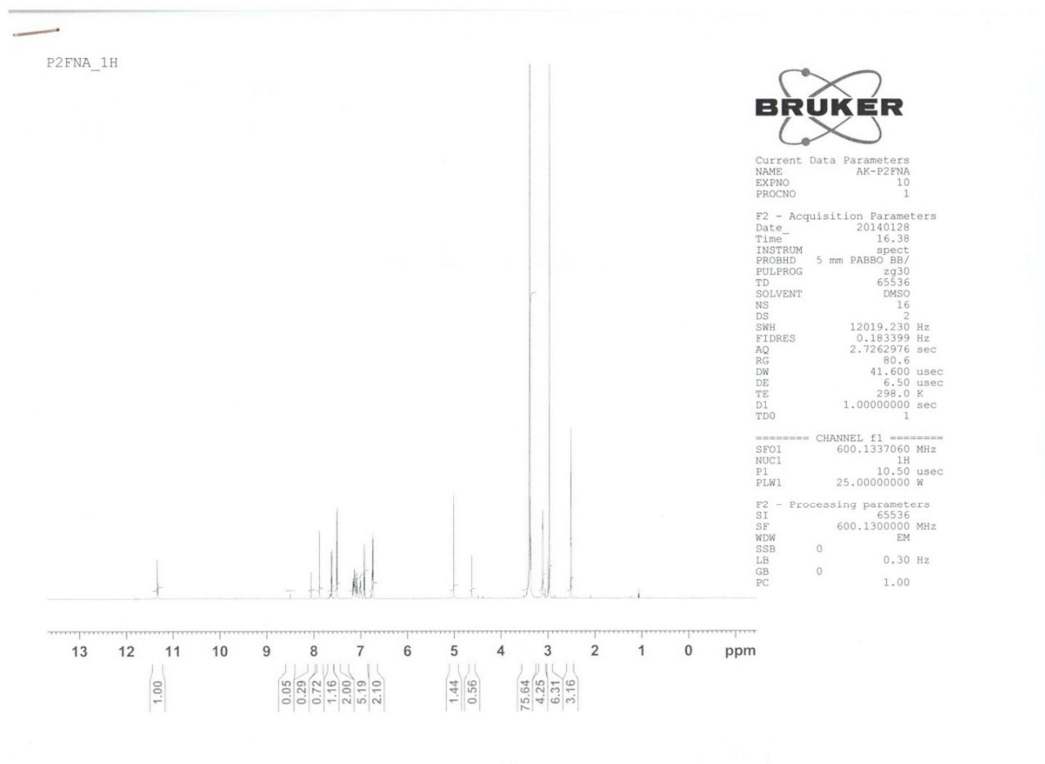
Data 18. HRMS spectrum of compound T6



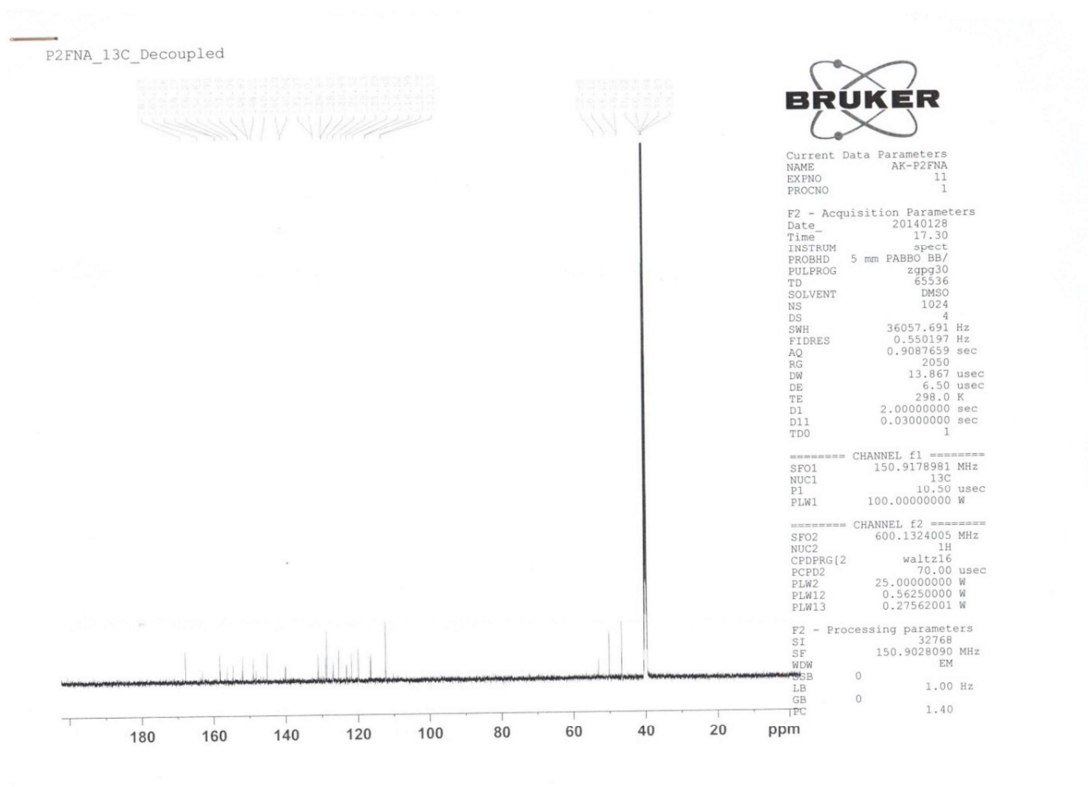
Peak List

m/z	Abund
255.1	4895.28
281	2339.54
283	9136.32
336.2	13092.22
337.1	3950.88
463	32864.1
464.1	9337.26

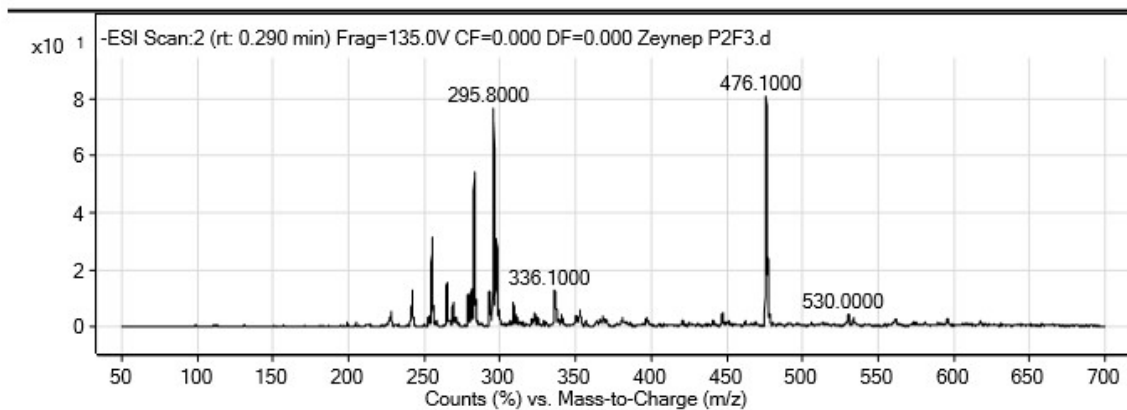
Data 19. ¹H-NMR spectrum of compound T7



Data 20. ^{13}C -NMR spectrum of compound T7



Data 21. HRMS spectrum of compound T7

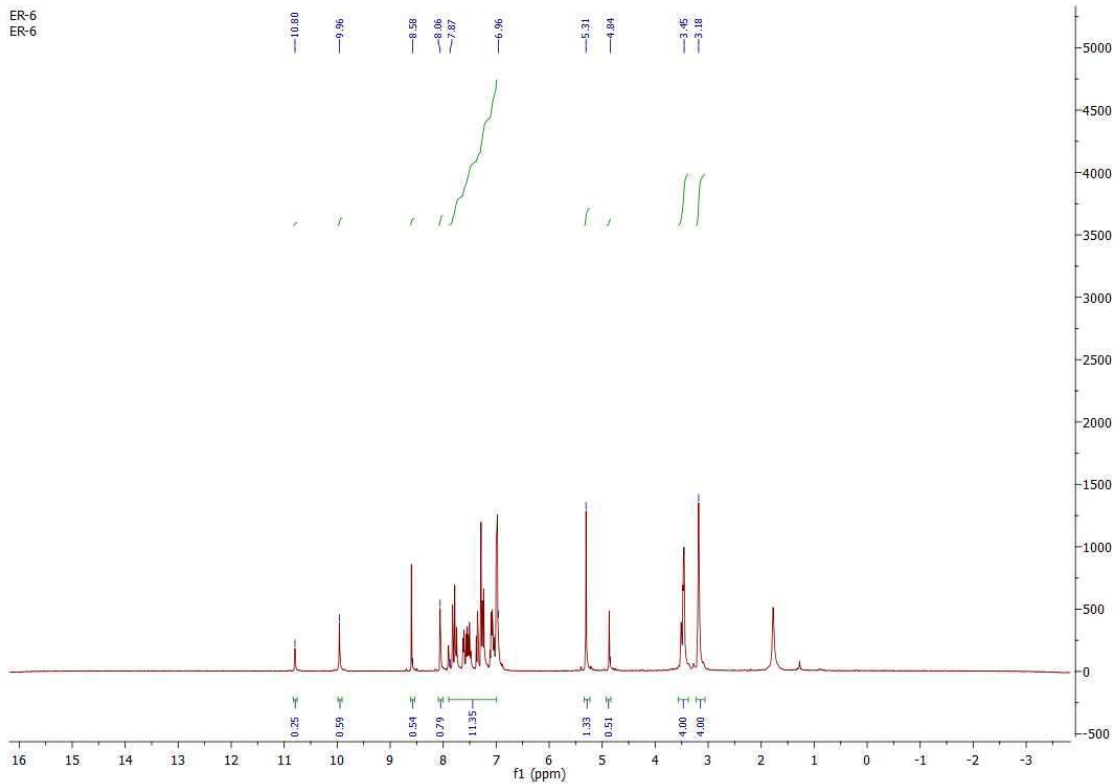


Peak List

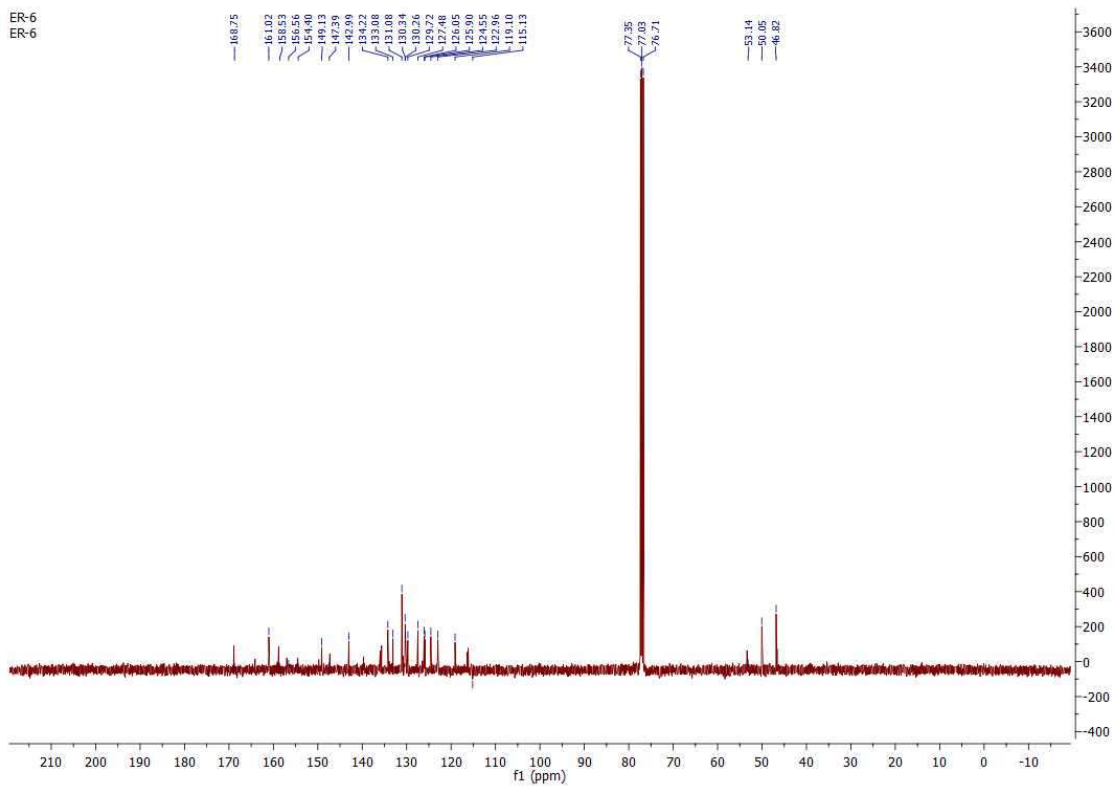
m/z	z	Abund
242.1		4177.8
255.1	1	9973.54
264.9	1	4965.84
281.1		4239.44
283	1	17355.72
295.8		24492.76
297.7	2	9943.44
336.1		4078.94
476.1	1	25842.92
477.1	1	7893.2

<New compounds>

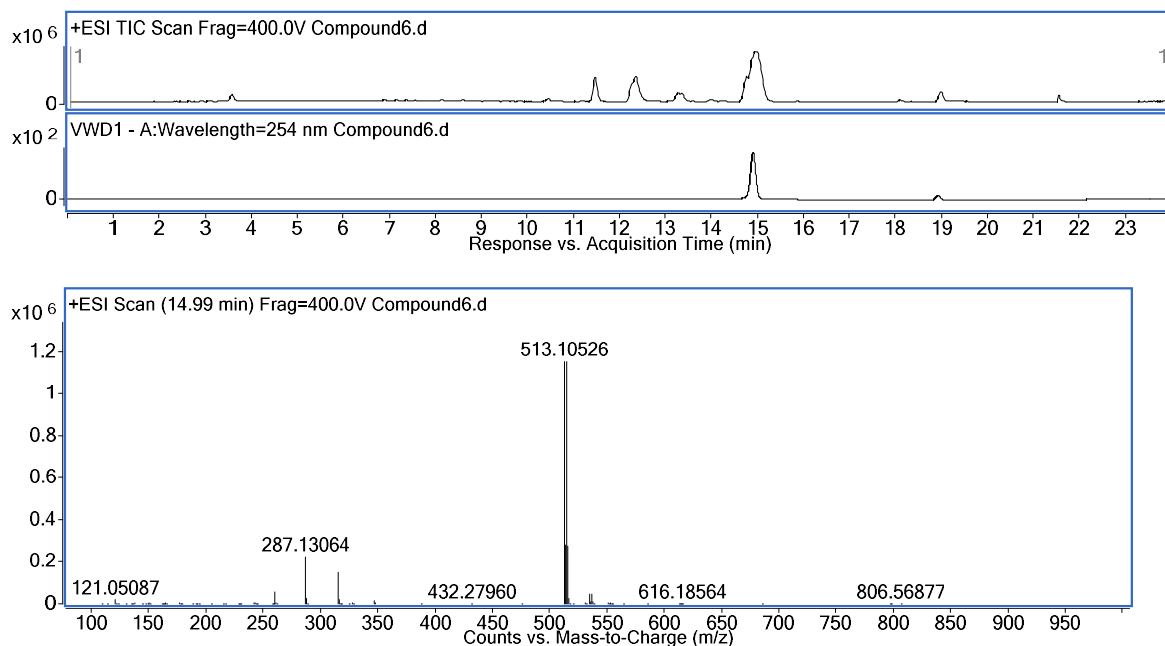
Data 1. ¹H-NMR spectrum of compound T8



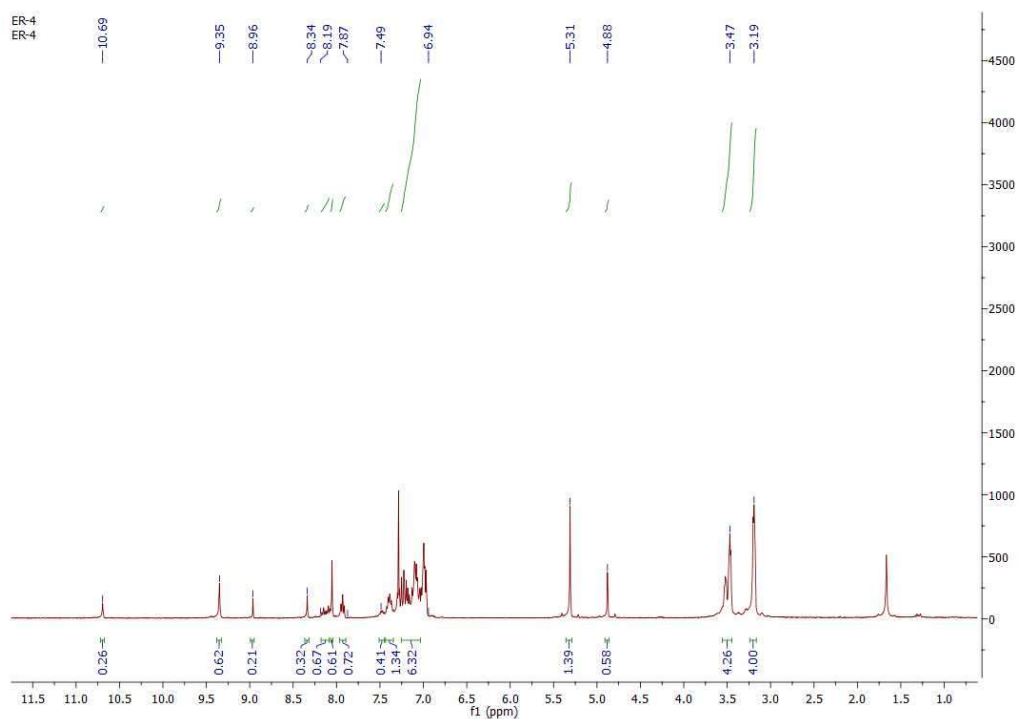
Data 2. ¹³C-NMR spectrum of compound T8



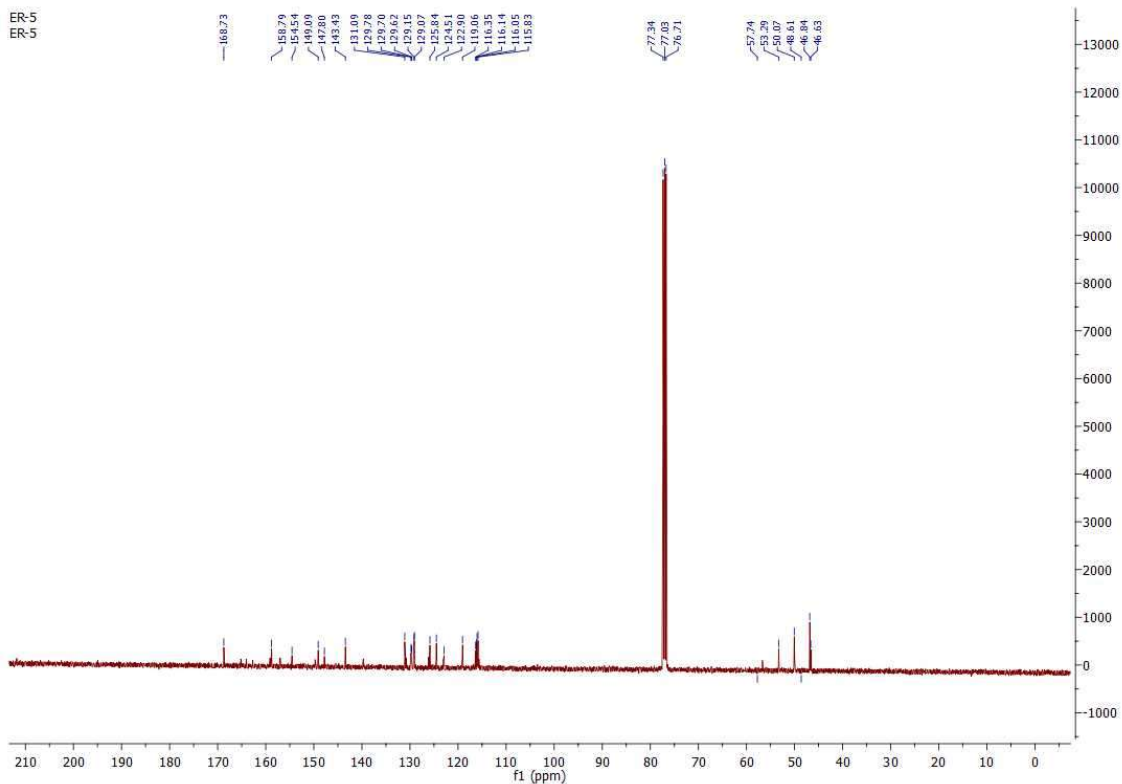
Data 3. HRMS spectrum of compound T8



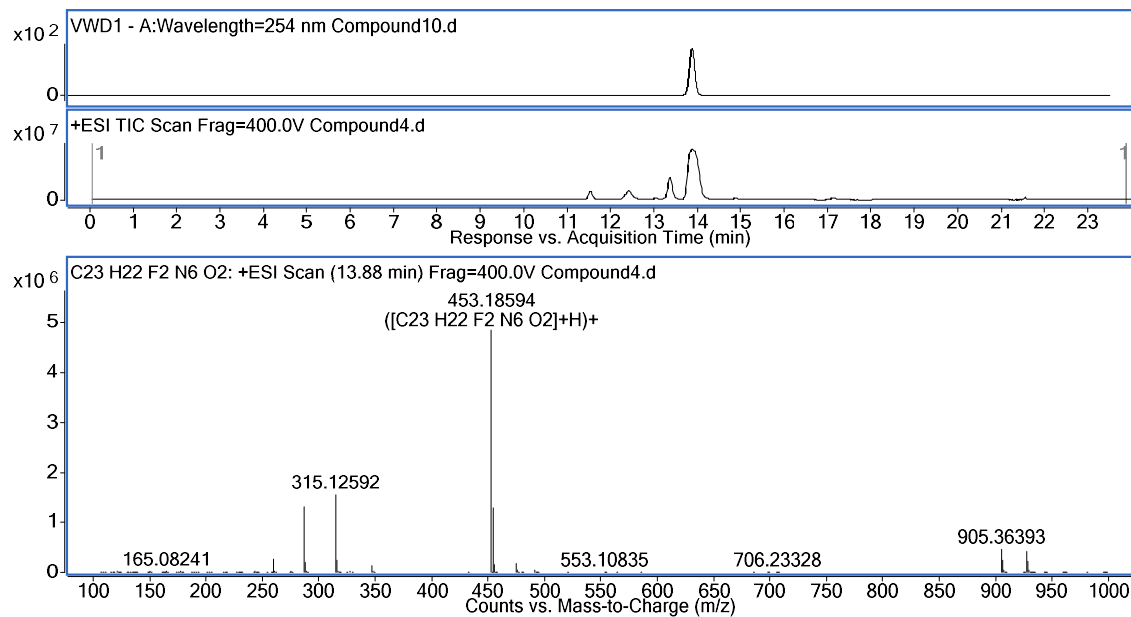
Data 4. ¹H-NMR spectrum of compound T9



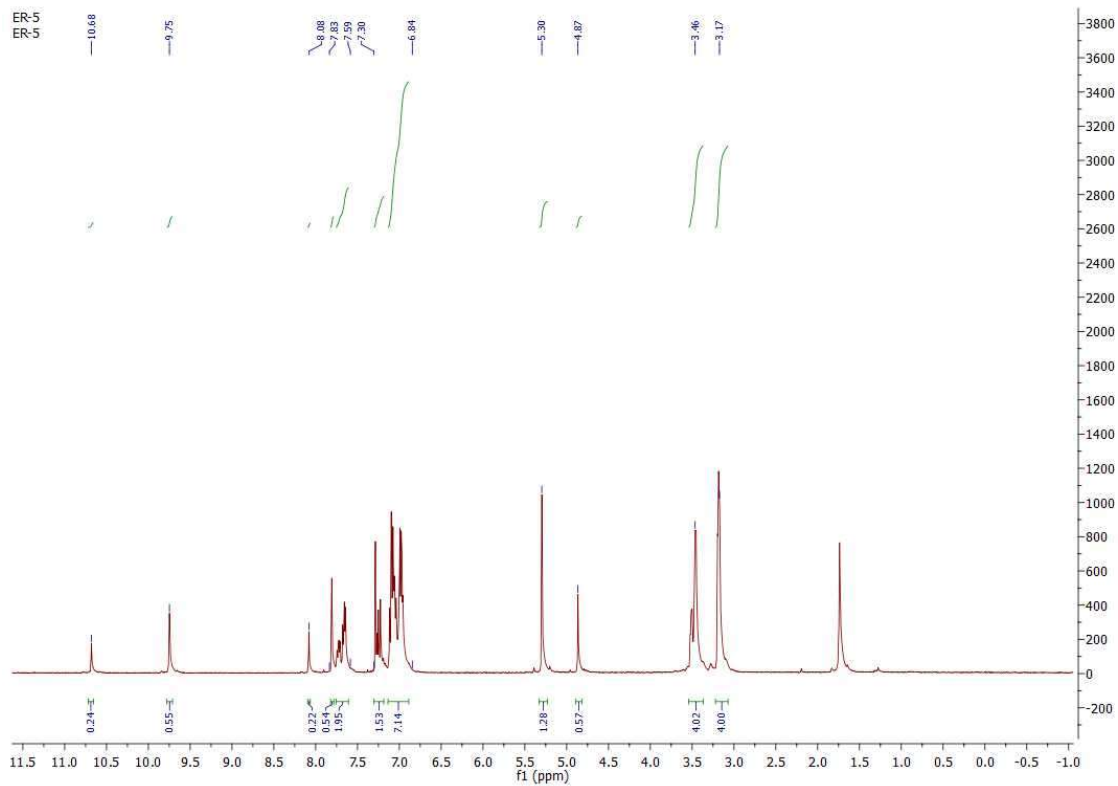
Data 5. ¹³C-NMR spectrum of compound T9



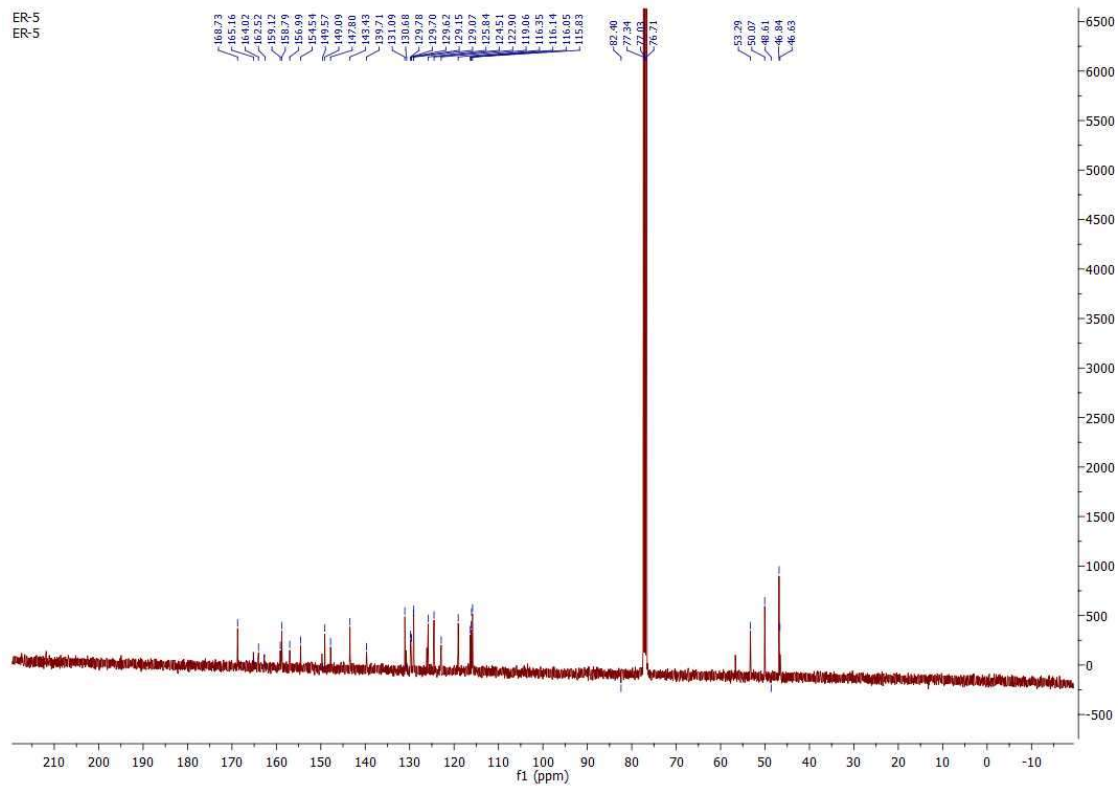
Data 6. HRMS spectrum of compound T9



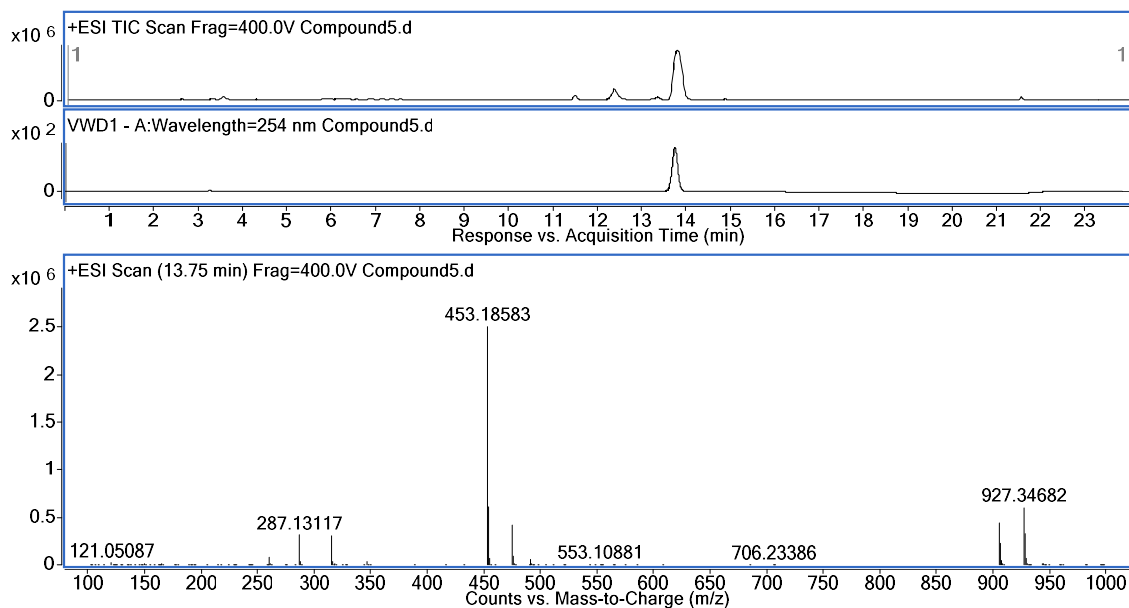
Data 7. ¹H-NMR spectrum of compound T10



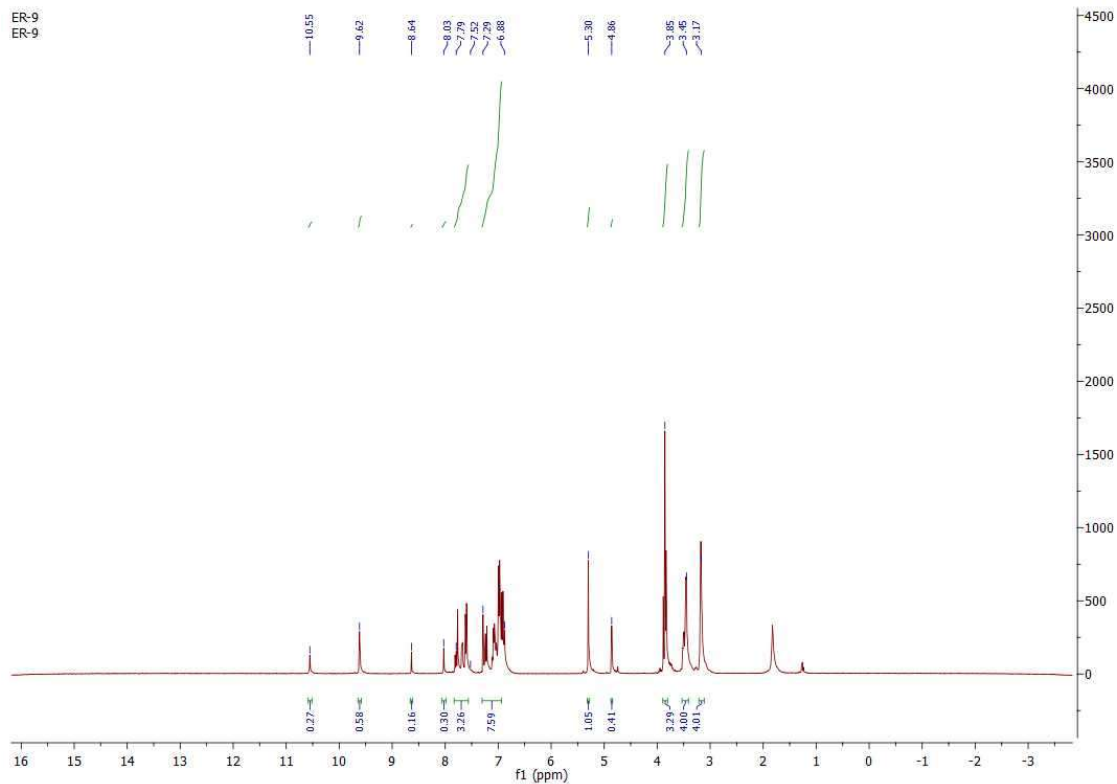
Data 8. ¹³C-NMR spectrum of compound T10



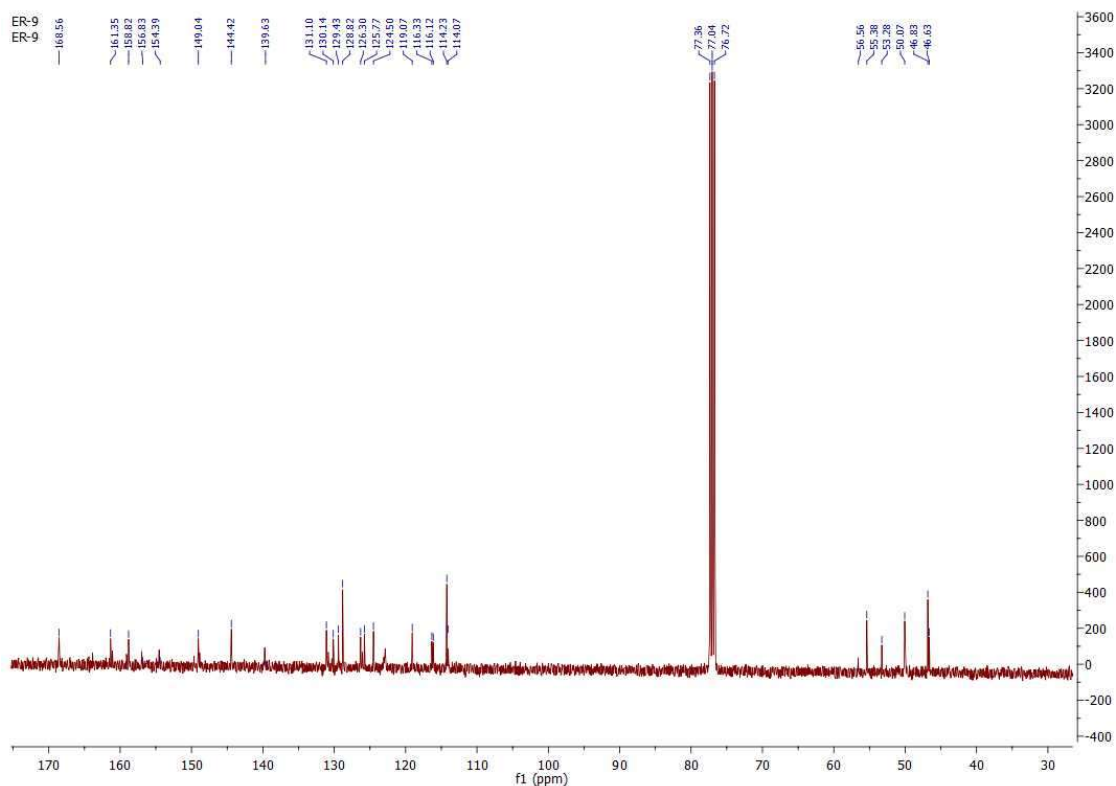
Data 9. HRMS spectrum of compound T10



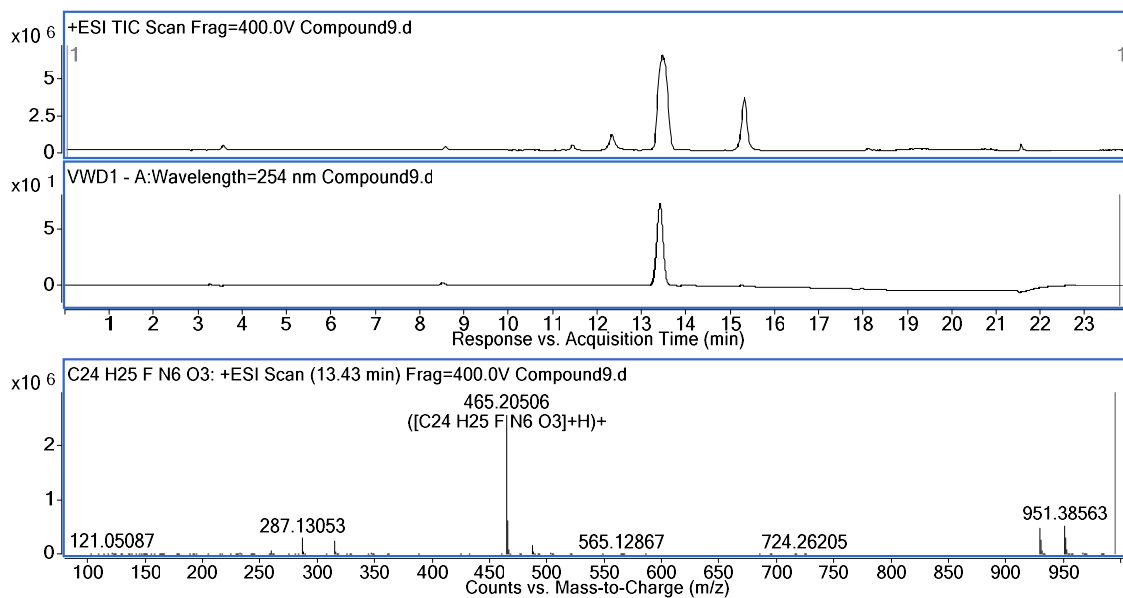
Data 10. ¹H-NMR spectrum of compound T11



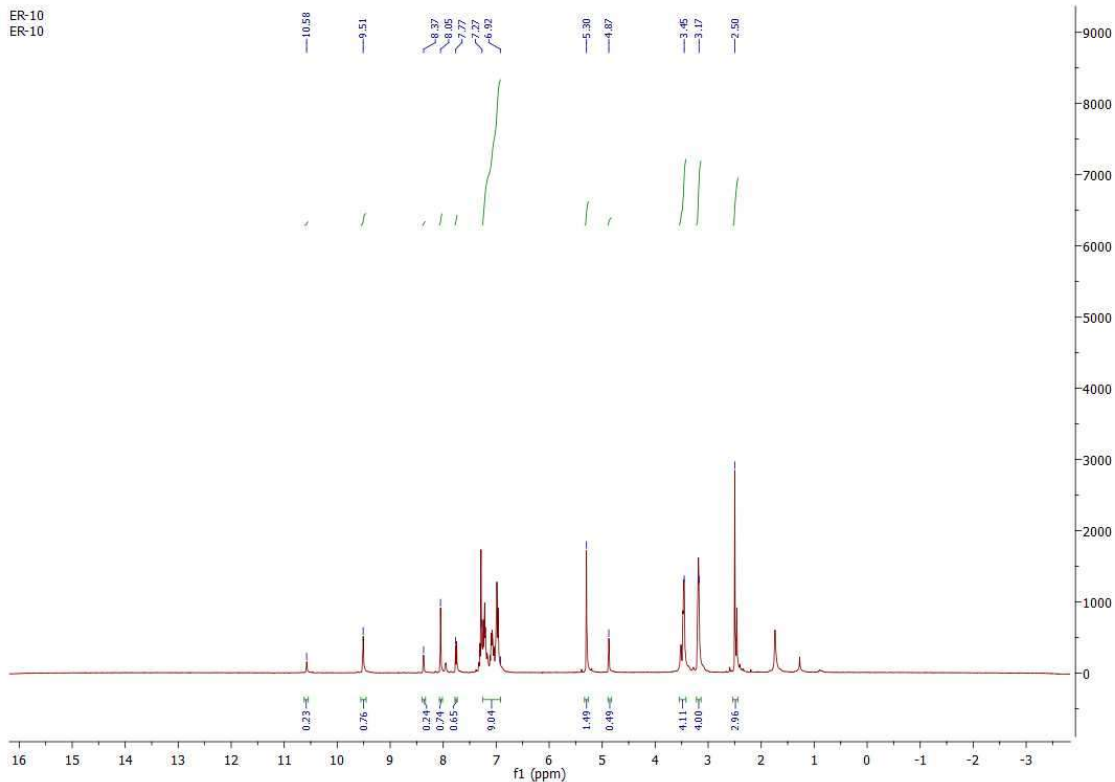
Data 11. ¹³C-NMR spectrum of compound T11



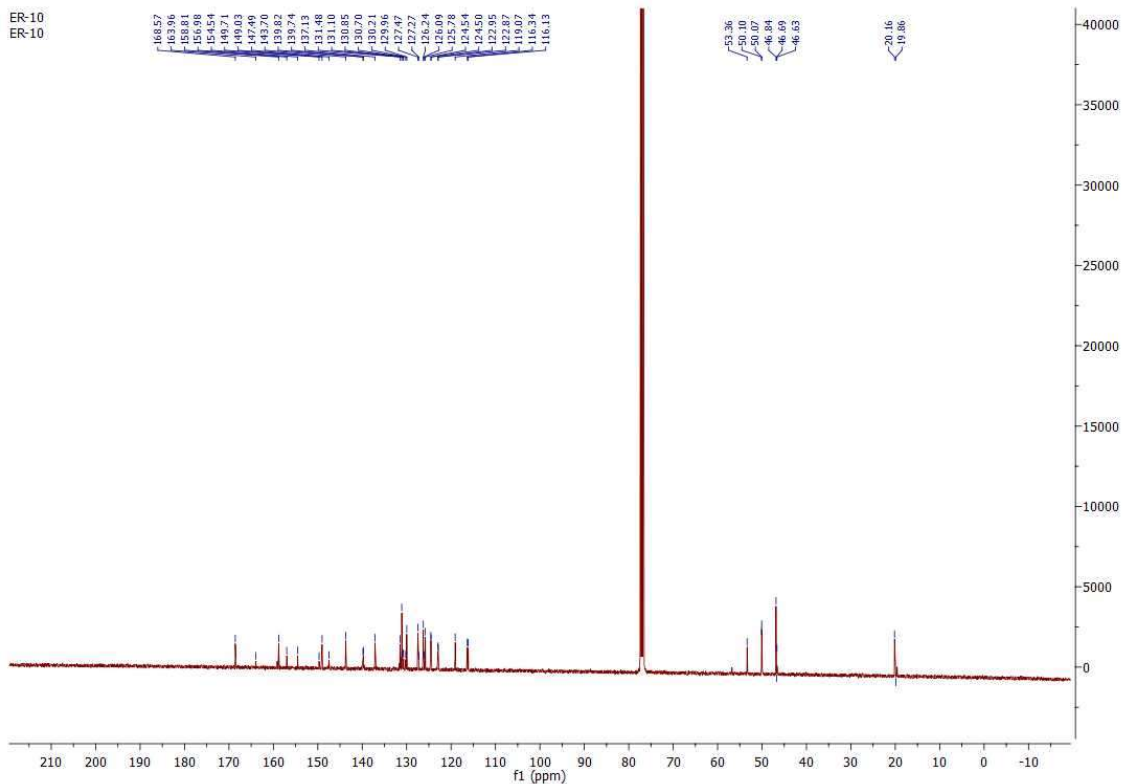
Data 12. HRMS spectrum of compound T11



Data 13. ¹H-NMR spectrum of compound T12



Data 14. ¹³C-NMR spectrum of compound T12



Data 15. HRMS spectrum of compound T12

