SEMI-SYNTHETIC CHASMANTHININE ANALOGUES WITH ANTIFEEDANT EFFECTS AGAINST *SPODOPTERA EXIGUA*

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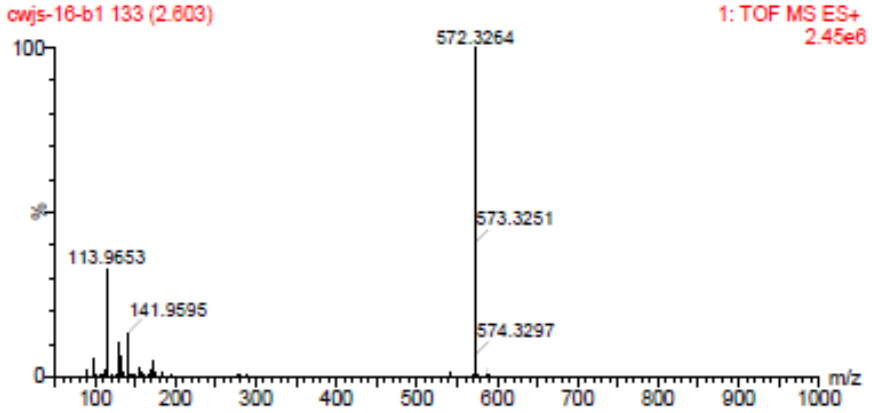
[‡]These authors contributed equally to this work and should be considered co-first authors.

Contents

Figure S1. HR-ESI-MS spectrum for compound **a**.



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

90 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 15-40 H: 30-50 N: 1-5 O: 1-10

Minimum:						-1.5
Maximum:		5.0	10.0		50.0	
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	572.3237	2.7	4.7	15.5		C33 H42 N5 O4
	572.3296	-3.2	-5.6	6.5		C26 H46 N5 O9
	572.3223	4.1	7.2	10.5		C32 H46 N O8

Figure S2. ^{1}H NMR spectrum for compound **a** in $CDCl_3$ (400Hz).

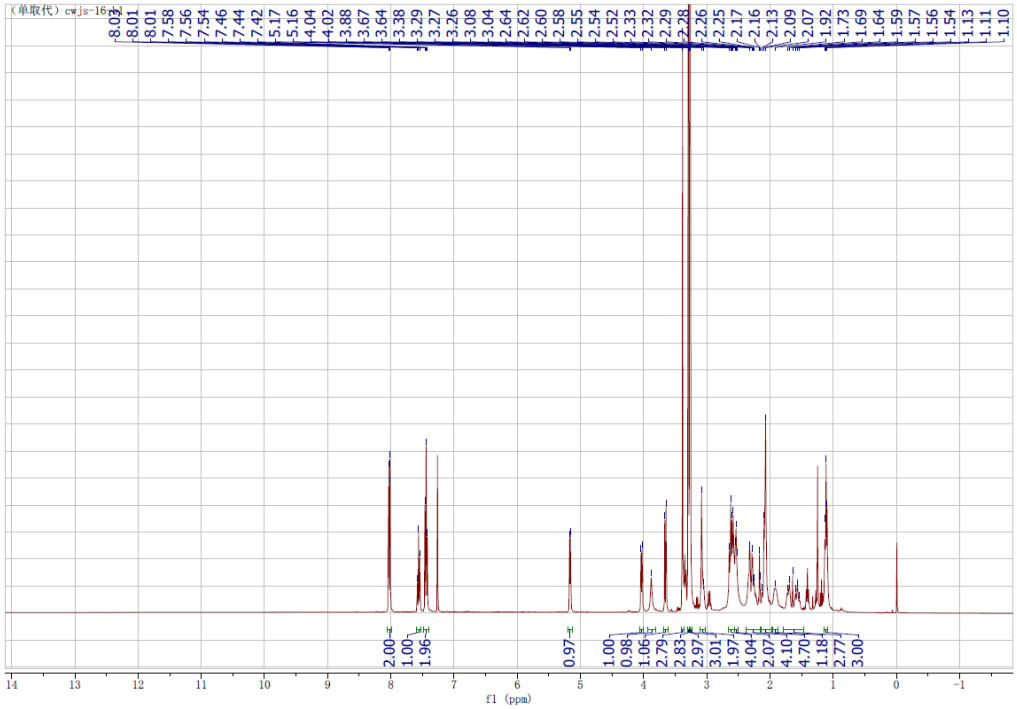


Figure S3. ^{13}C NMR spectrum for compound **a** in $CDCl_3$ (100Hz).

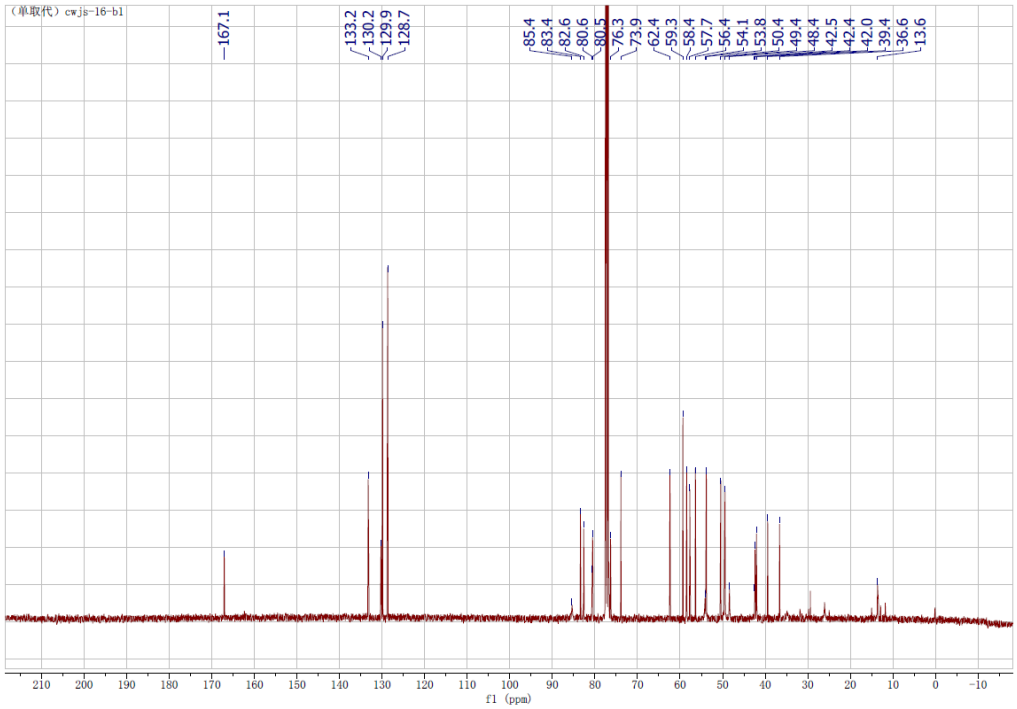


Figure S4. DEPT ($\theta = 135^{\circ}$) spectrum for compound **a** in $CDCl_3$.

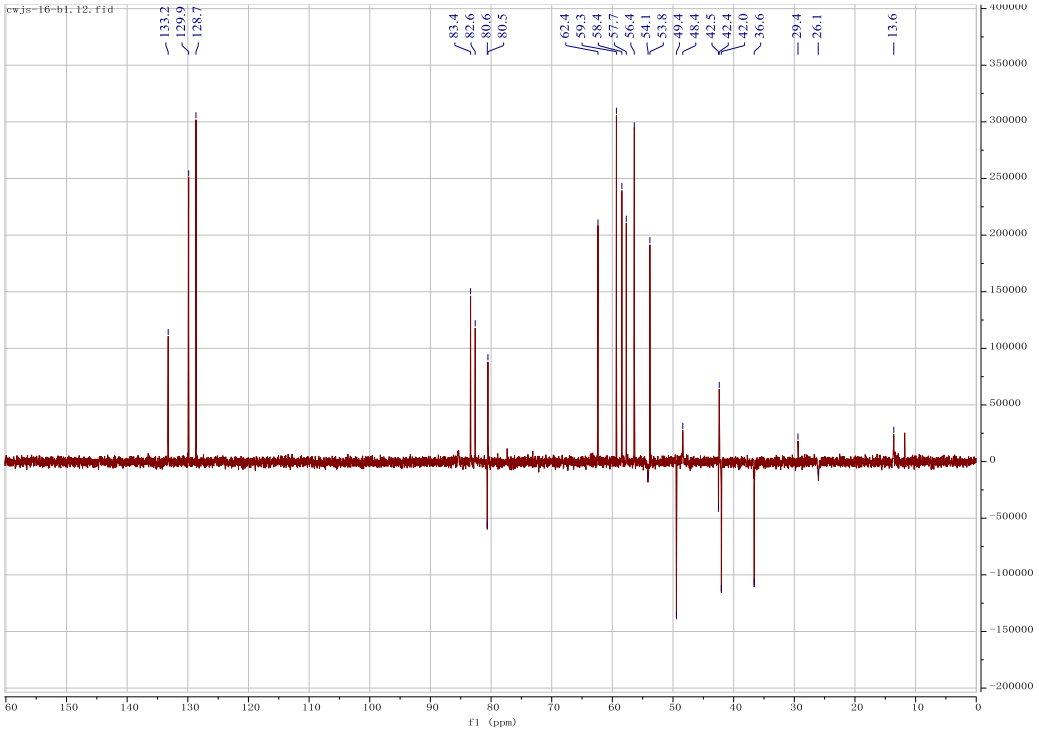


Figure S5. HR-ESI-MS spectrum for compound **b.**

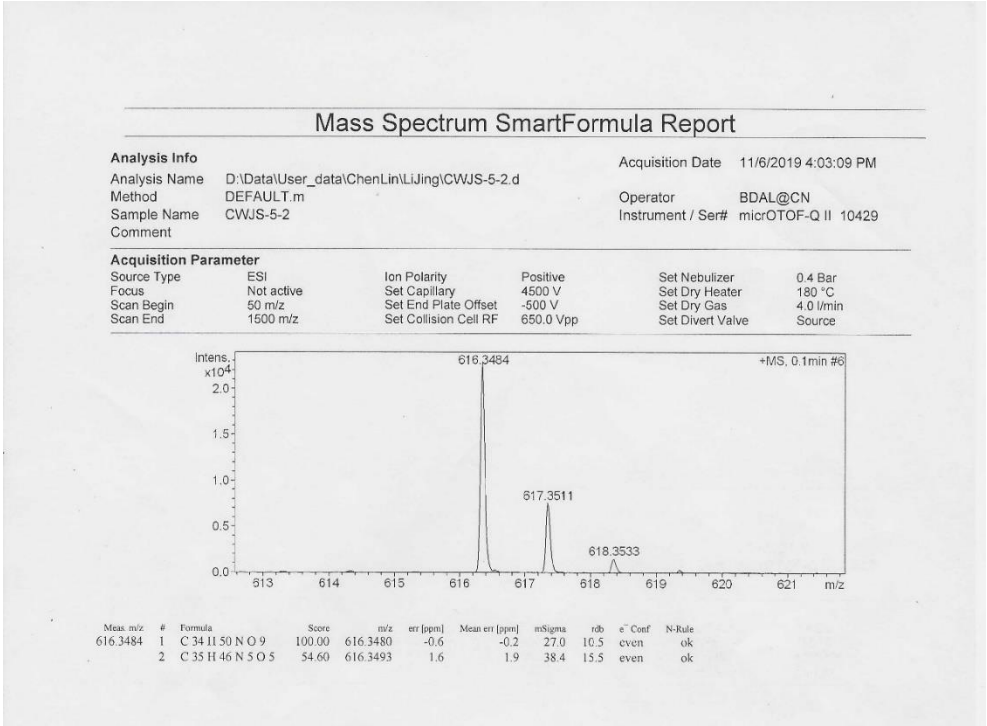


Figure S6. ^{1}H NMR spectrum for compound **b** in $CDCl_3$ (400Hz).

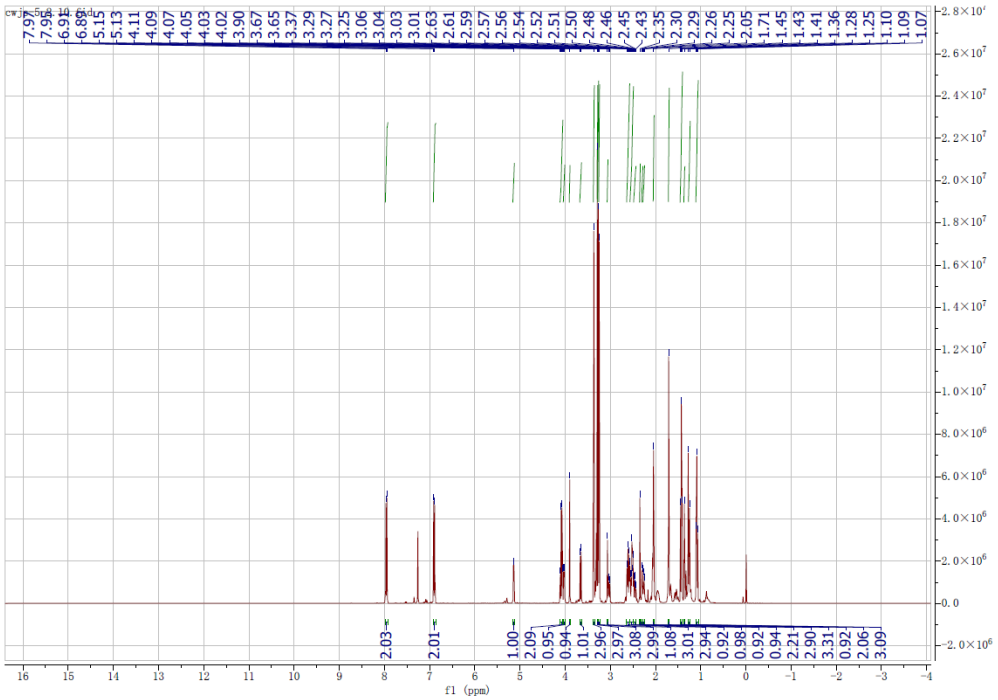


Figure S7. ^{13}C NMR spectrum for compound **b** in $CDCl_3$ (100Hz).

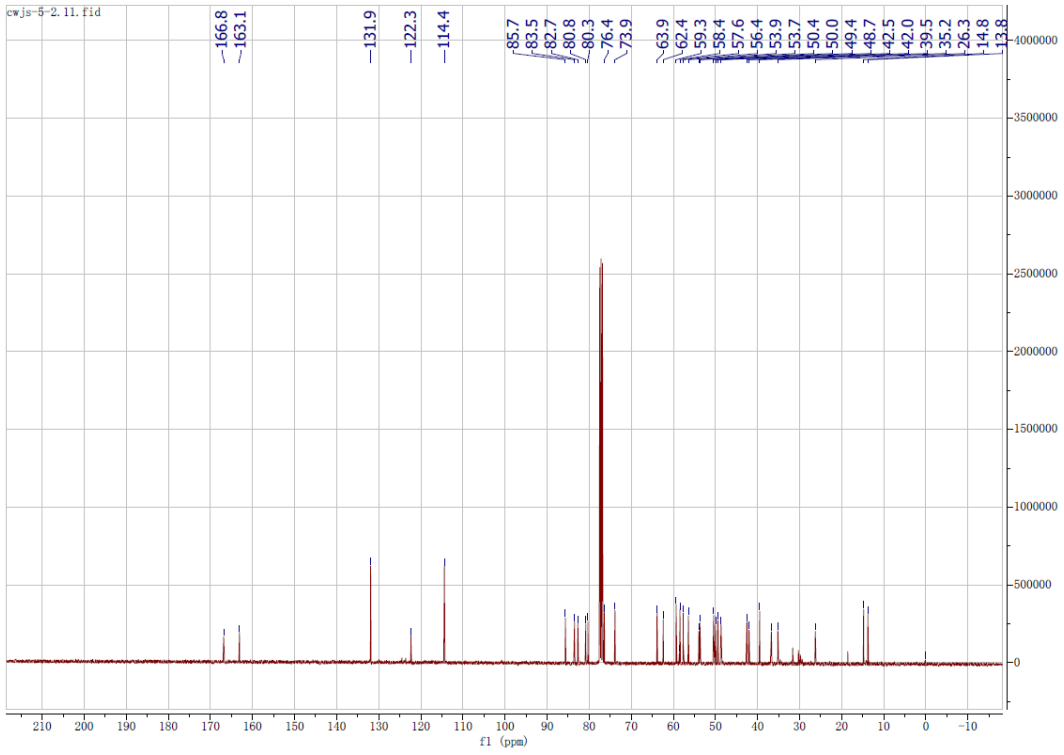


Figure S8. DEPT ($\theta = 135^{\circ}$) spectrum for compound **b** in $CDCl_3$.

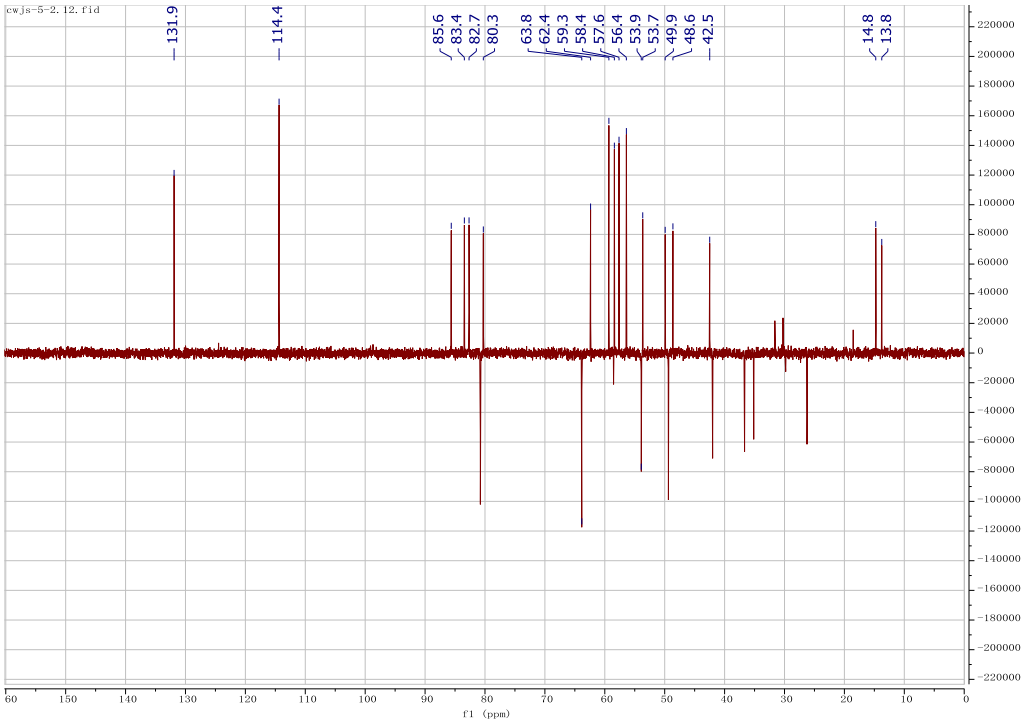


Figure S9. HR-ESI-MS spectrum for compoud **c**.

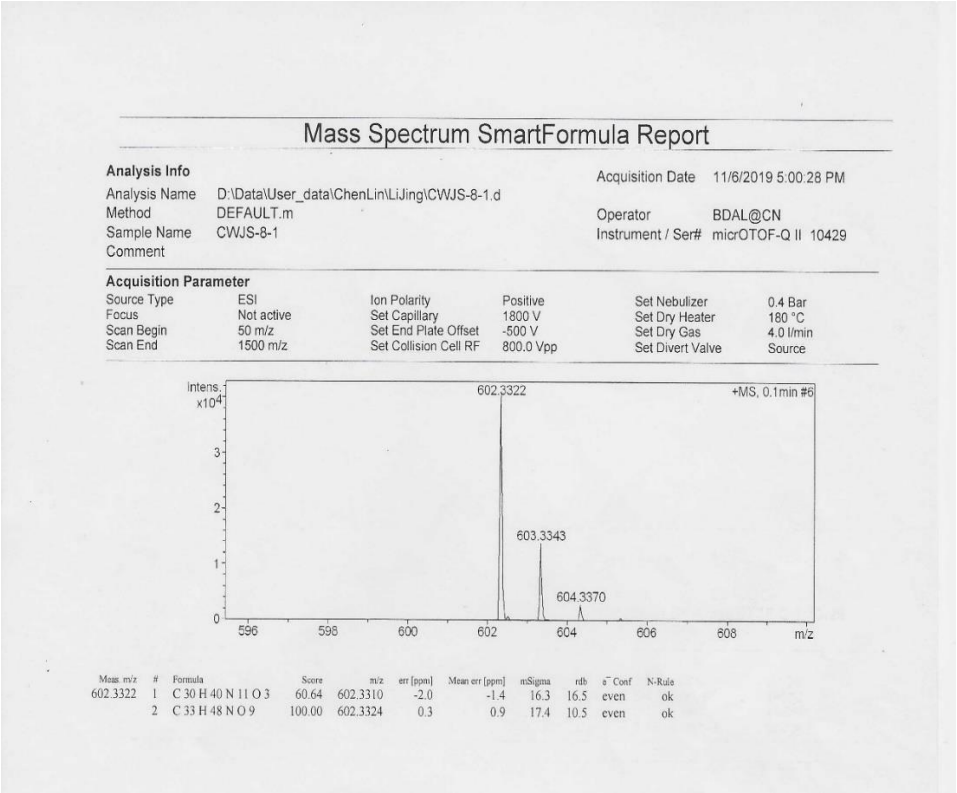


Figure S10. ^{1}H NMR spectrum for compoud **c** in $CDCl_3$ (400Hz).

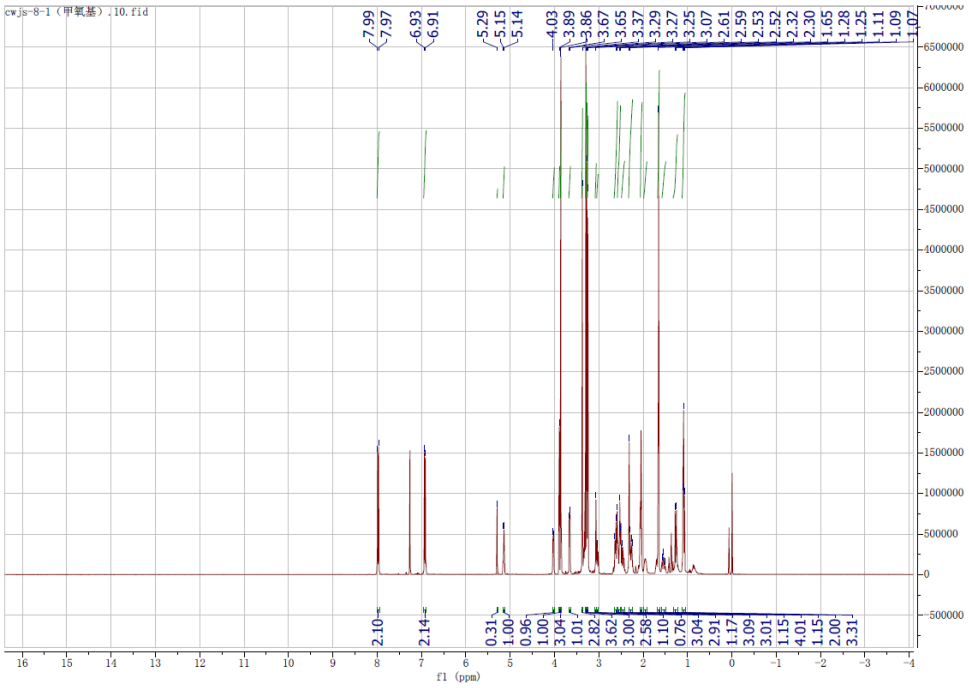


Figure S11. ^{13}C NMR spectrum for compoud **c** in $CDCl_3$ (100Hz).

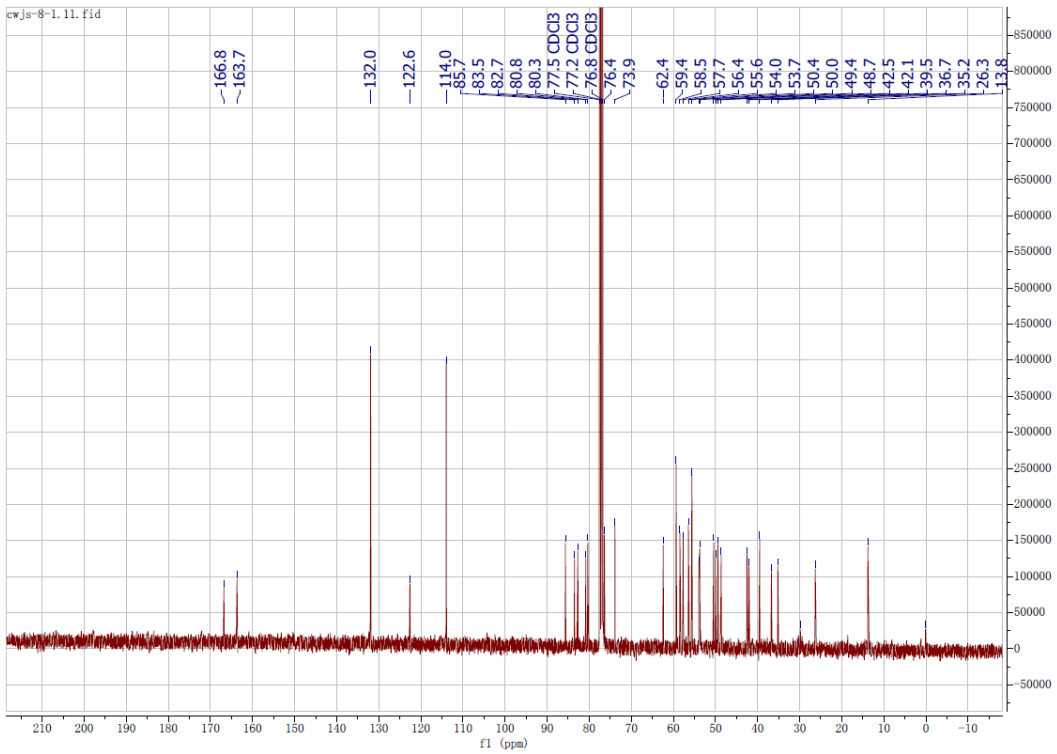


Figure S12. DEPT (θ = 135°) spectrum for compound **c** in $CDCl_3$.

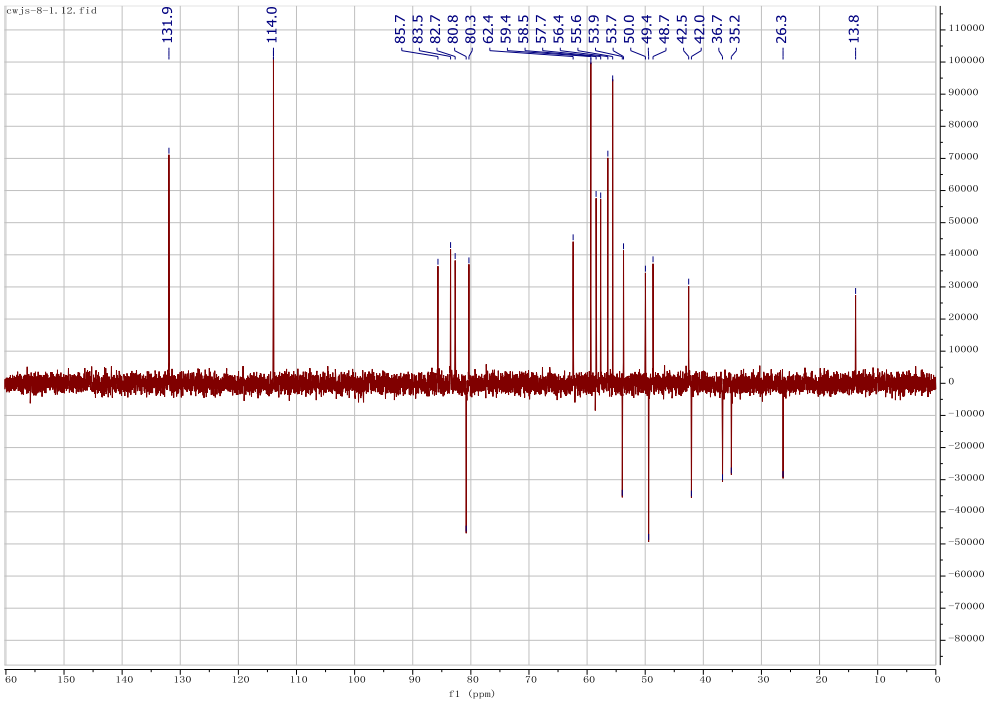
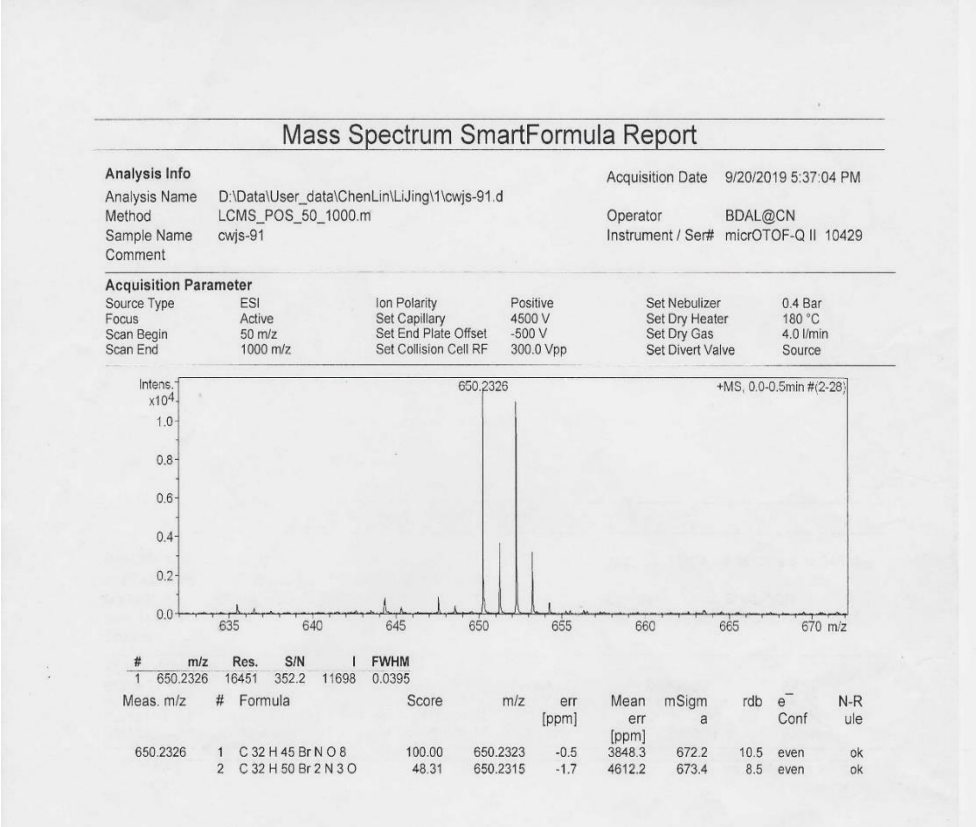


Figure S13. HR-ESI-MS spectrum for compoud **d**.



Mass Spectrum SmartFormula Report

Analysis Info

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Sample Name	cwjs-91	Instrument / Ser#	micrOTOF-Q II 10429
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

#	m/z	Res.	S/N	I	FWHM
1	650.2326	16451	352.2	11698	0.0395

Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
650.2326	1	C 32 H 45 Br N O 8	100.00	650.2323	-0.5	3848.3	672.2	10.5	even	ok
	2	C 32 H 50 Br 2 N 3 O	48.31	650.2315	-1.7	4612.2	673.4	8.5	even	ok

Figure S14. ^{1}H NMR spectrum for compoud **d** in $CDCl_3$ (400Hz).

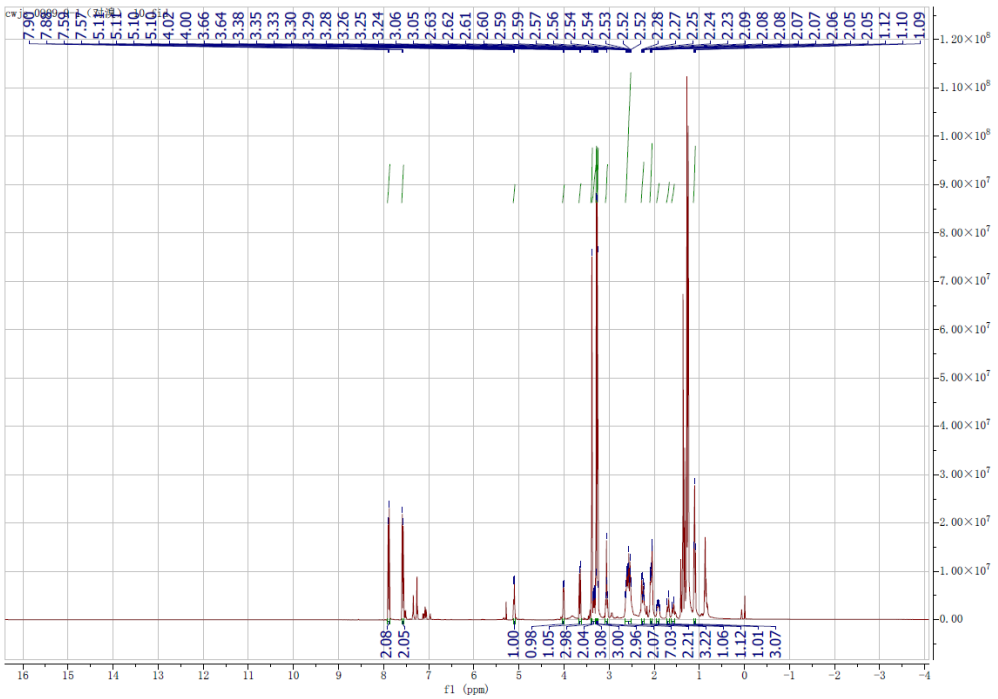


Figure S15. ^{13}C NMR spectrum for compoud **d** in $CDCl_3$ (100Hz).

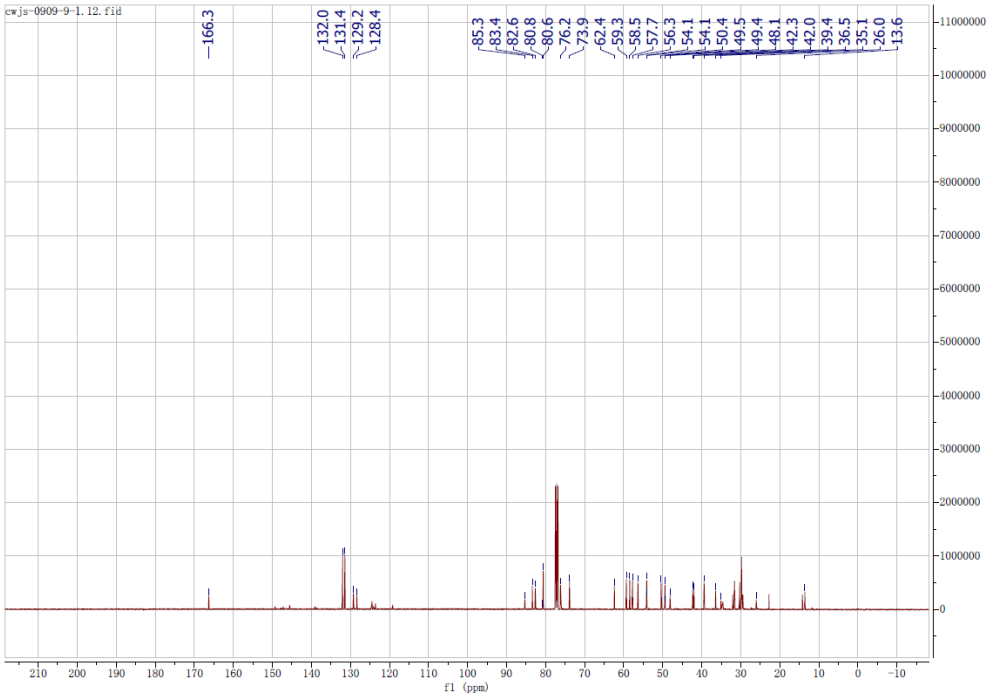


Figure S16. DEPT (θ = 135°) spectrum for compound **d** in $CDCl_3$.

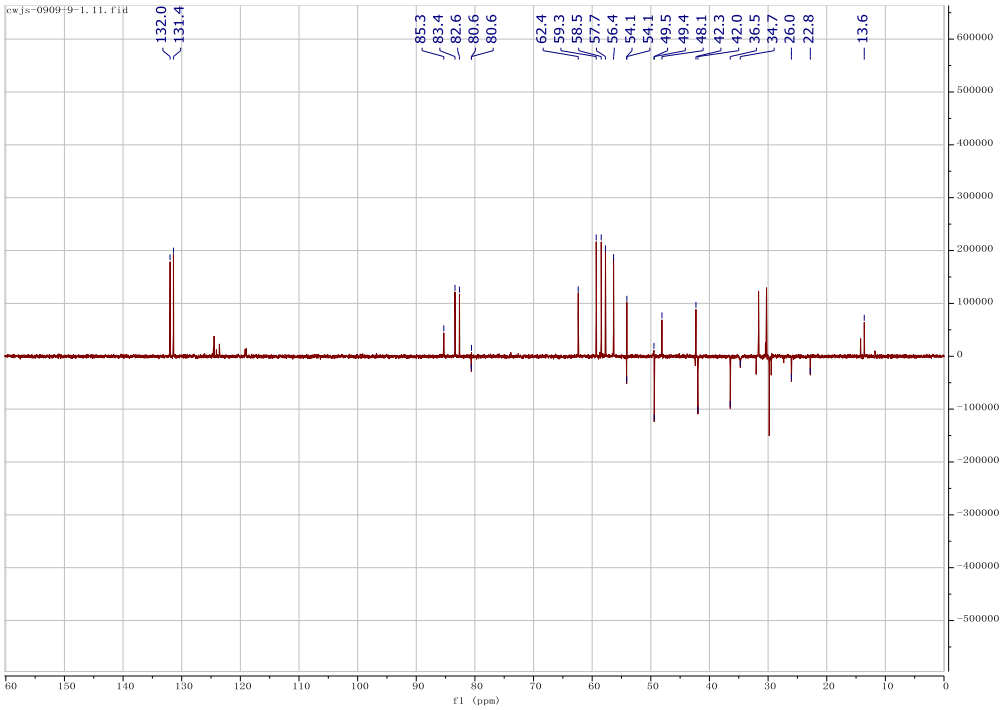
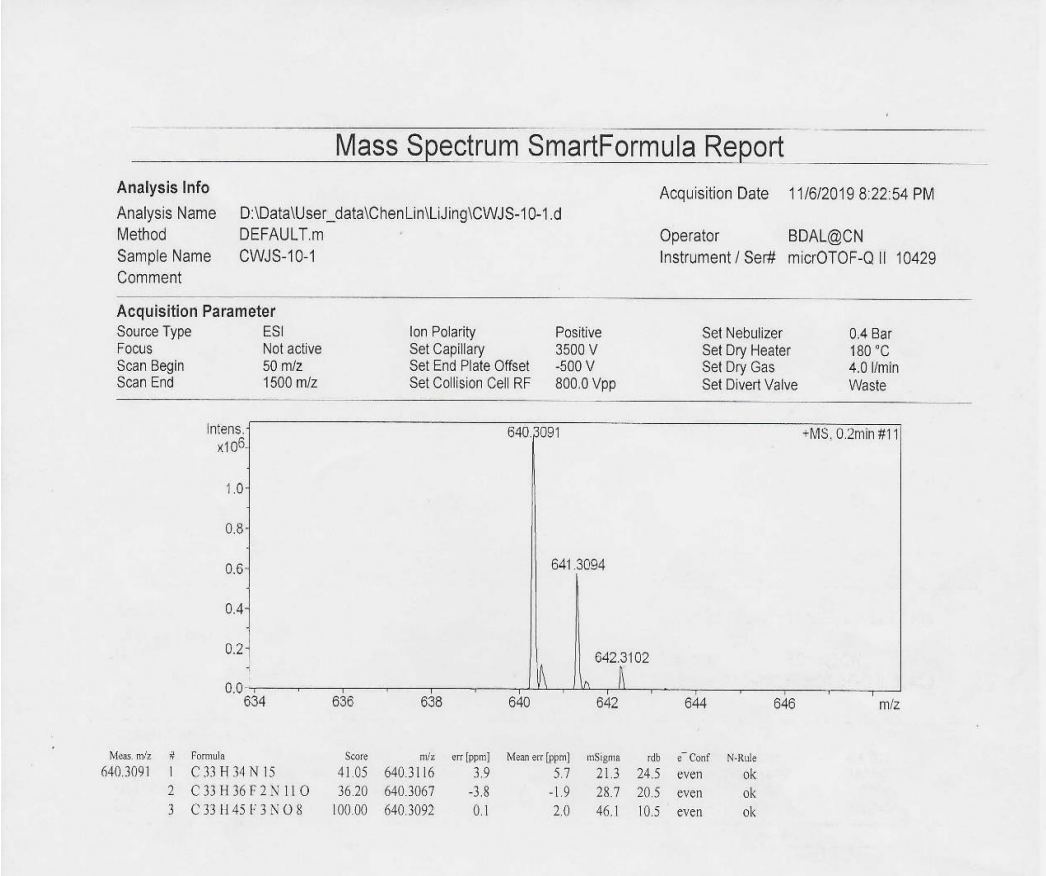


Figure S17. HR-ESI-MS spectrum for compoud **e**.



Mass Spectrum SmartFormula Report

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Sample Name	CWJS-10-1	Instrument / Ser#	micrOTOF-Q II 10429
Comment			

Acquisition Parameter

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Focus	Not active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	800.0 Vpp	Set Divert Valve	Waste

Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
640.3091	1	C 33 H 34 N 15	41.05	640.3116	3.9	5.7	21.3	24.5	even	ok
	2	C 33 H 36 F 2 N 11 O	36.20	640.3067	-3.8	-1.9	28.7	20.5	even	ok
	3	C 33 H 45 F 3 N O 8	100.00	640.3092	0.1	2.0	46.1	10.5	even	ok

Figure S18. ^{1}H NMR spectrum for compoud **e** in $CDCl_3$ (400Hz).

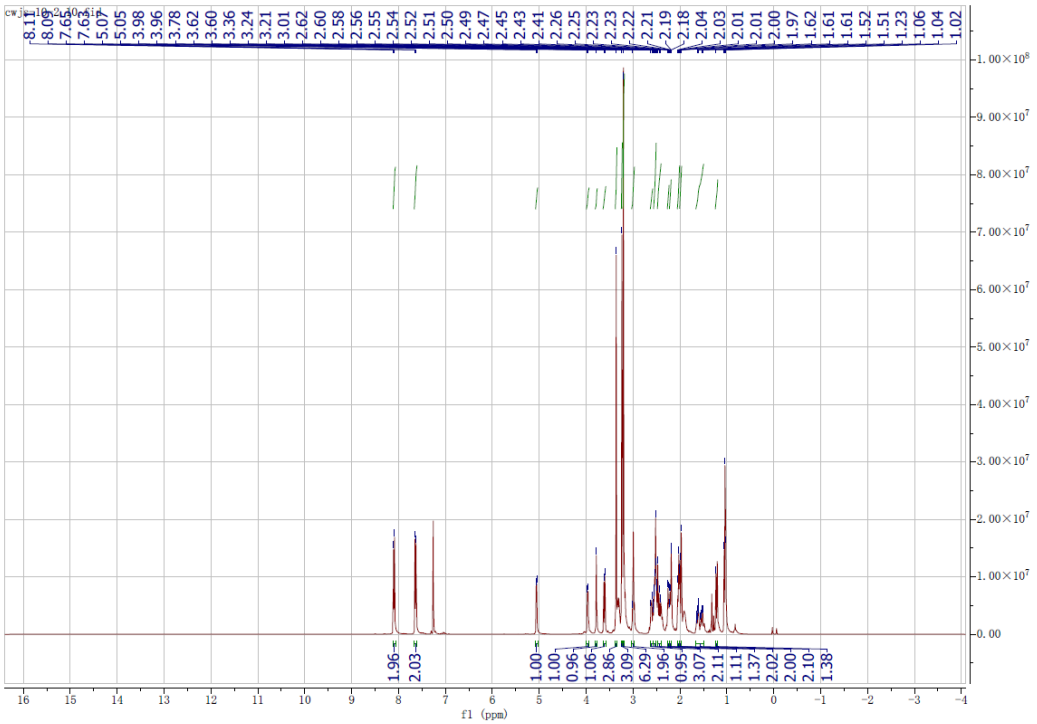


Figure S19. ^{13}C NMR spectrum for compoud **e** in $CDCl_3$ (100Hz).

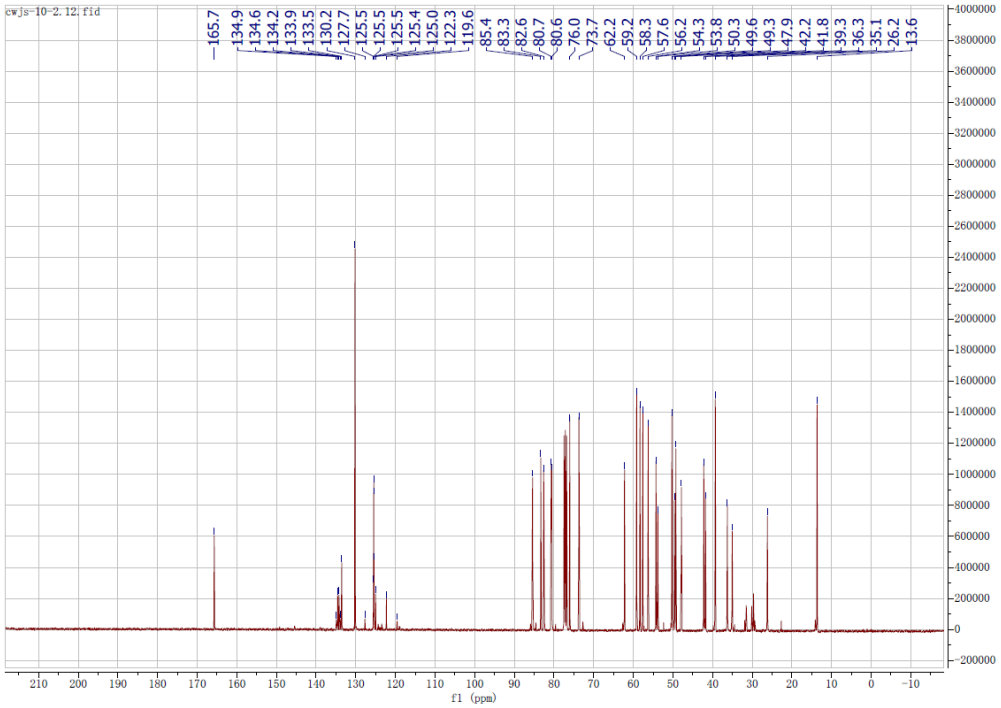


Figure S20. DEPT (θ = 135°) spectrum for compound **e** in $CDCl_3$.

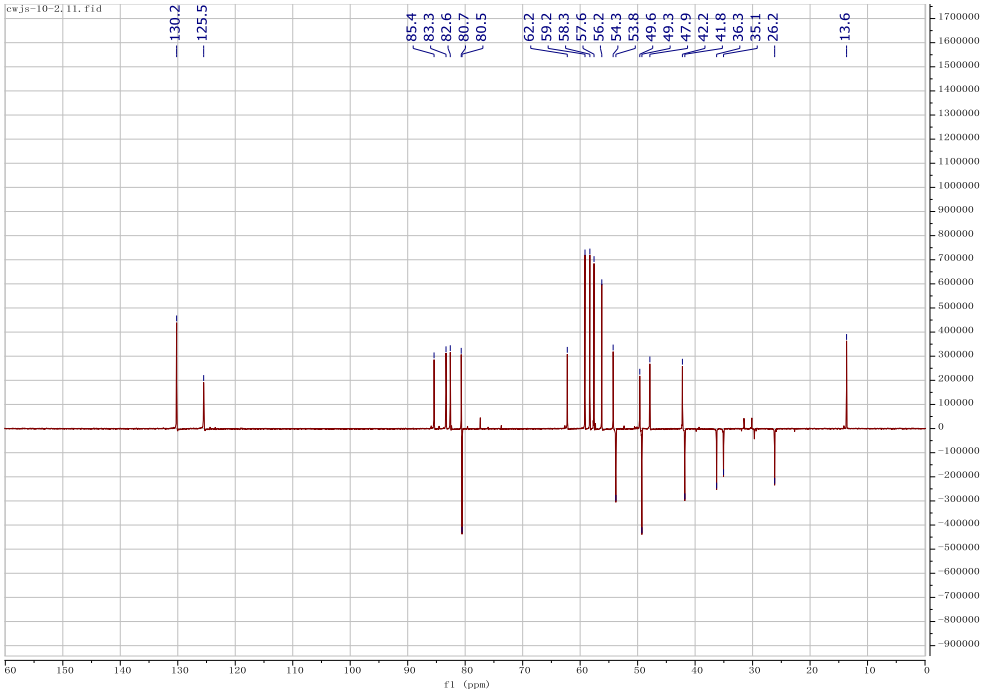
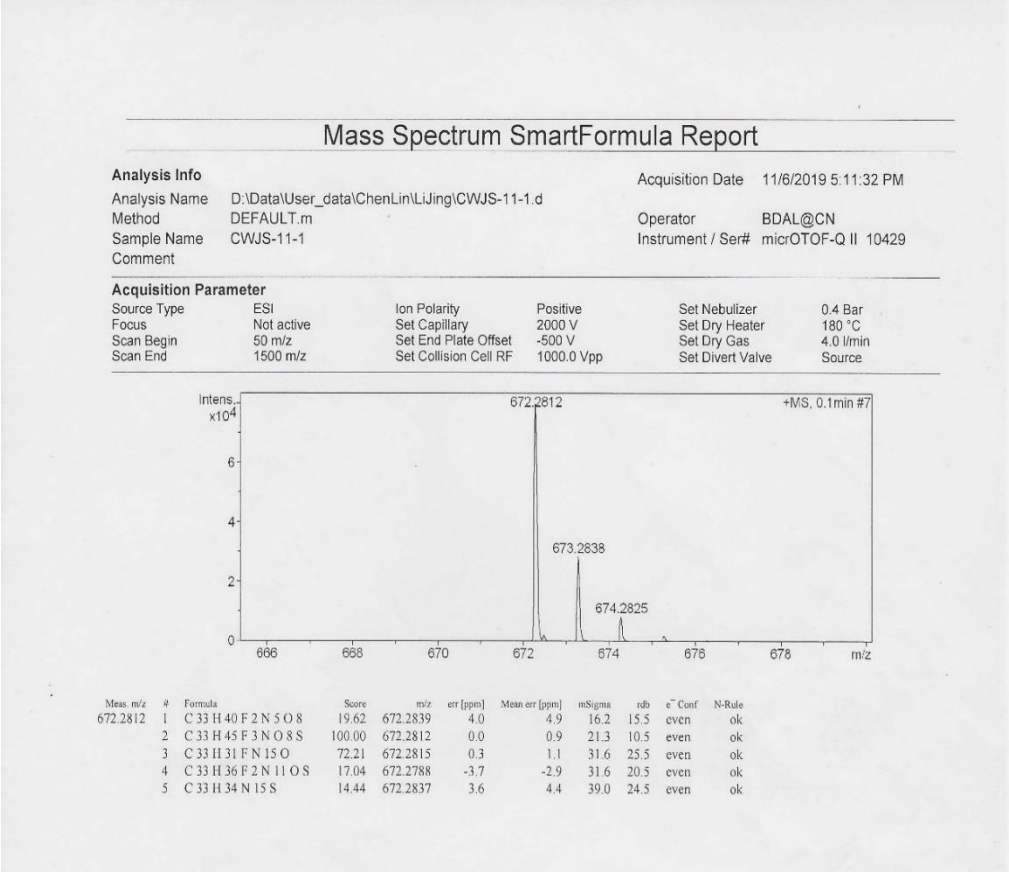


Figure S21. HR-ESI-MS spectrum for compoud **f.**



Mass Spectrum SmartFormula Report

Analysis Info

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Sample Name	CWJS-11-1	Instrument / Ser#	micrOTOF-Q II 10429
Comment			

Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	1000.0 Vpp	Set Divert Valve	Source

Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
672.2812	1	C 33 H 40 F 2 N 5 O 8	19.62	672.2839	4.0	4.9	16.2	15.5	even	ok
	2	C 33 H 45 F 3 N O 8 S	100.00	672.2812	0.0	0.9	21.3	10.5	even	ok
	3	C 33 H 31 F N 15 O	72.21	672.2815	0.3	1.1	31.6	25.5	even	ok
	4	C 33 H 36 F 2 N 11 O S	17.04	672.2788	-3.7	-2.9	31.6	20.5	even	ok
	5	C 33 H 34 N 15 S	14.44	672.2837	3.6	4.4	39.0	24.5	even	ok

Figure S22. ^{1}H NMR spectrum for compoud **f** in $CDCl_3$ (400Hz).

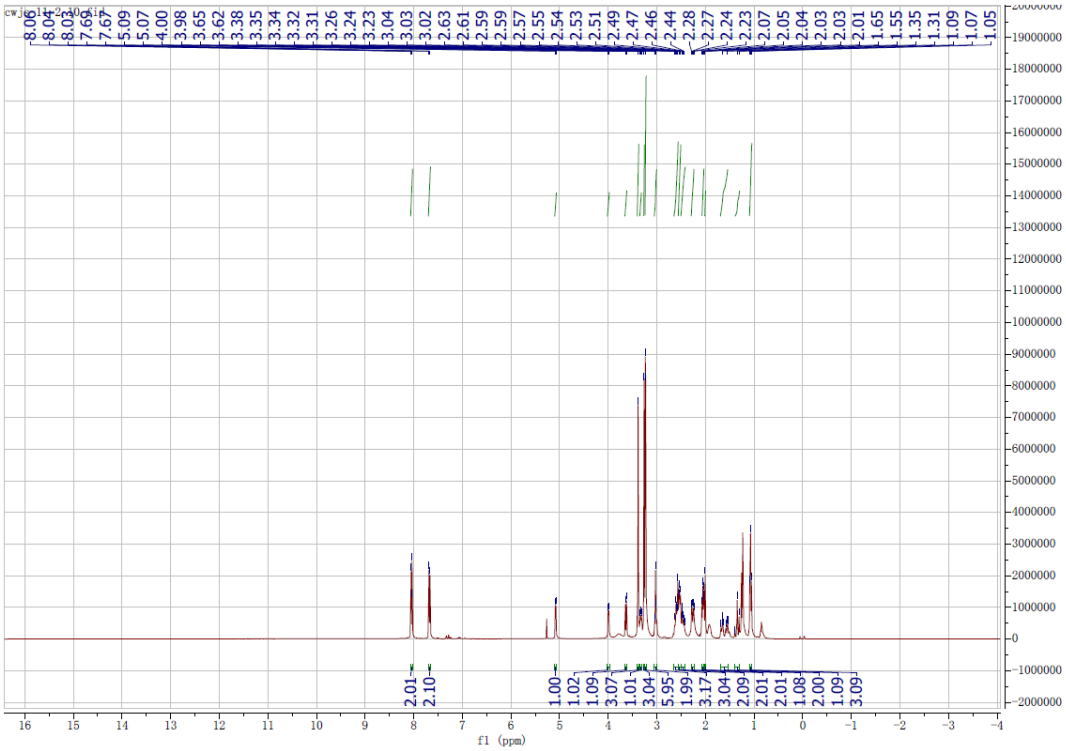


Figure S23. ^{13}C NMR spectrum for compoud **f** in $CDCl_3$ (100Hz).

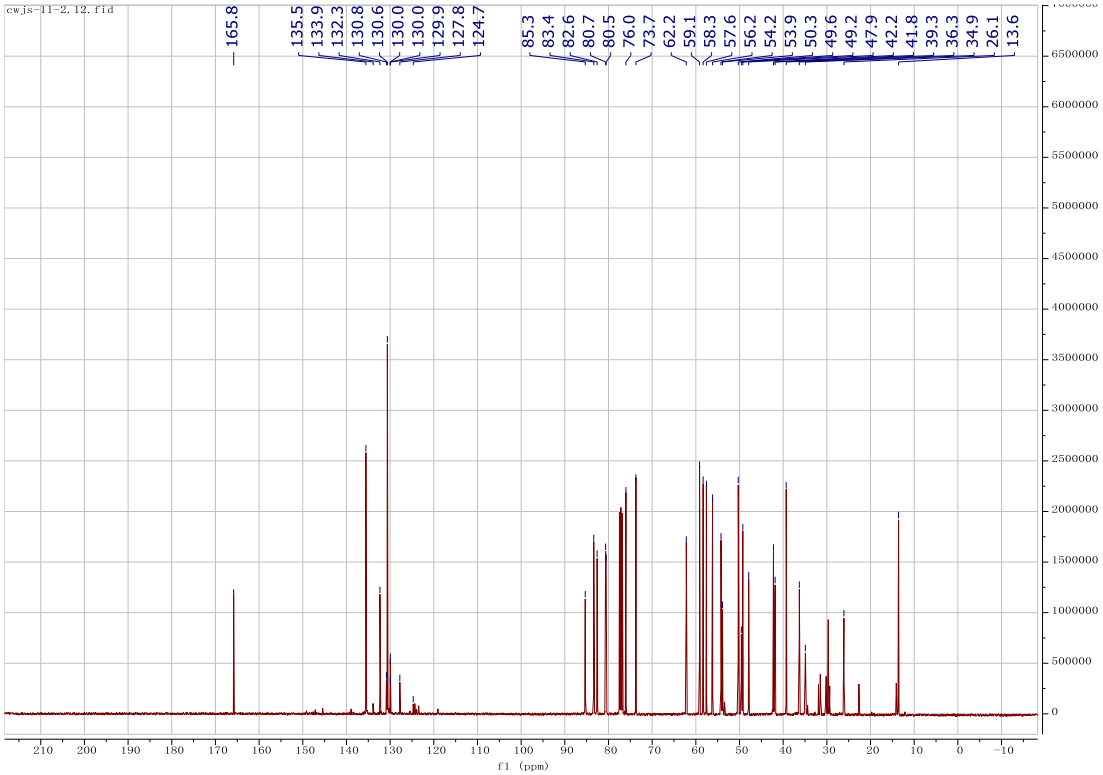


Figure S24. DEPT (θ = 135°) spectrum for compound **f** in $CDCl_3$.

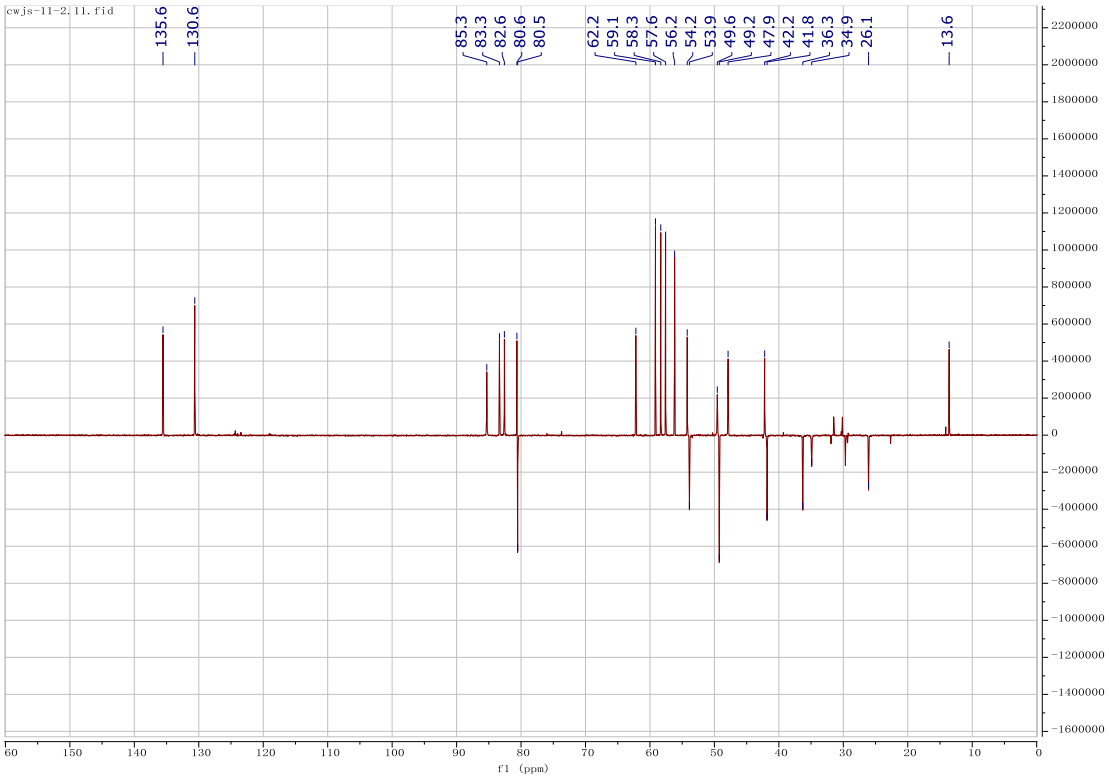
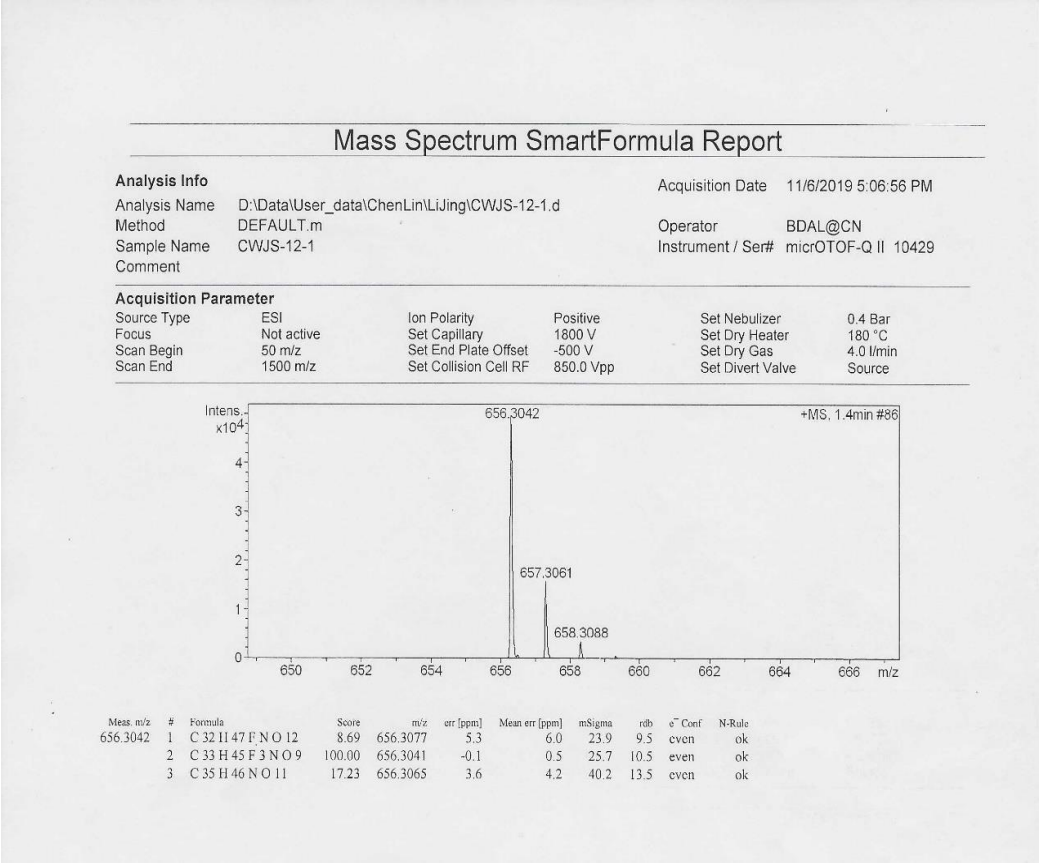


Figure S25. HR-ESI-MS spectrum for compoud **g.**



Mass Spectrum SmartFormula Report

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Comment		Instrument / Ser#	micrOTOF-Q II 10429

Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	850.0 Vpp	Set Divert Valve	Source

Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
656.3042	1	C 32 H 47 F N O 12	8.69	656.3077	5.3	6.0	23.9	9.5	even	ok
	2	C 33 H 45 F 3 N O 9	100.00	656.3041	-0.1	0.5	25.7	10.5	even	ok
	3	C 35 H 46 N O 11	17.23	656.3065	3.6	4.2	40.2	13.5	even	ok

Figure S26. ^{1}H NMR spectrum for compoud **g** in $CDCl_3$ (400Hz).

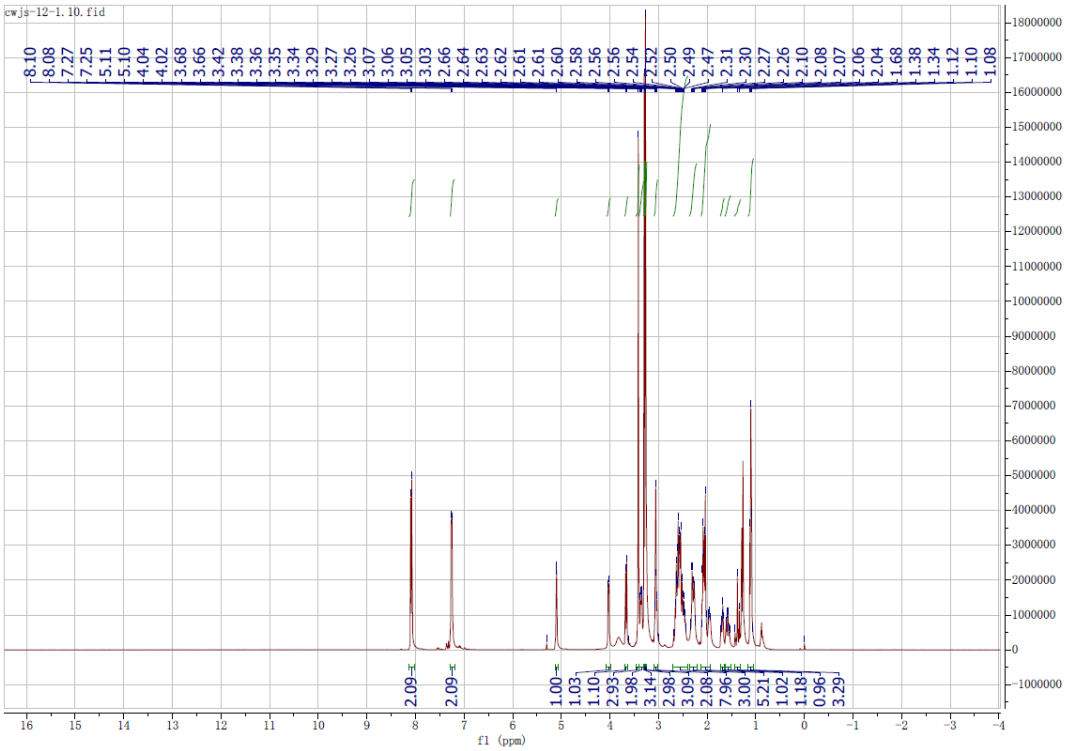


Figure S27. ^{13}C NMR spectrum for compoud **g** in $CDCl_3$ (100Hz).

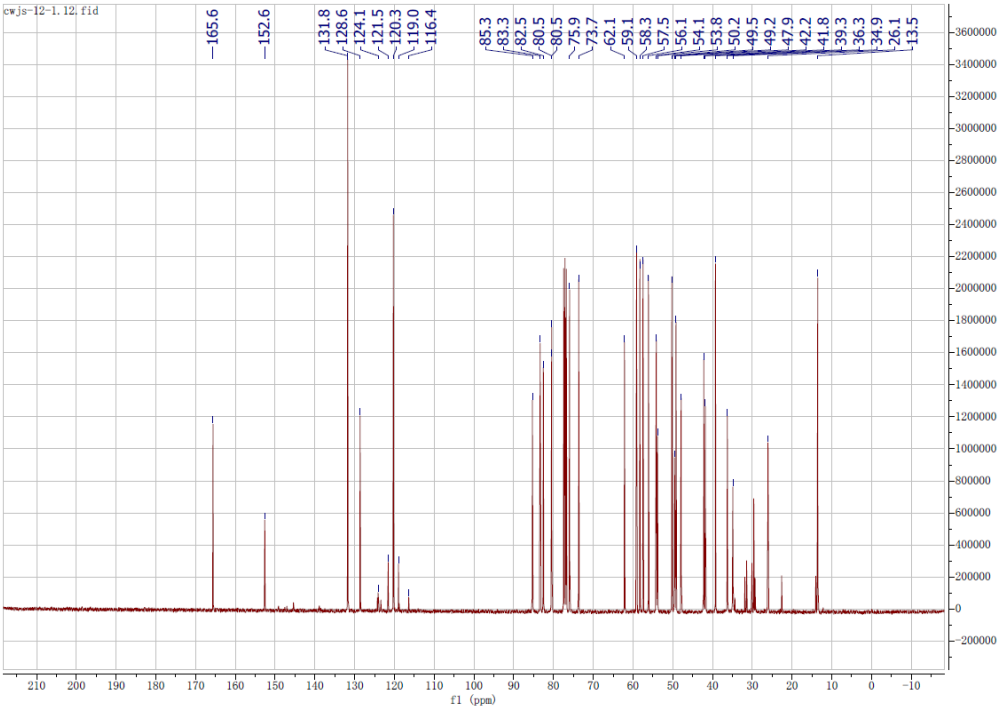


Figure S28. DEPT (θ = 135°) spectrum for compound **g** in $CDCl_3$.

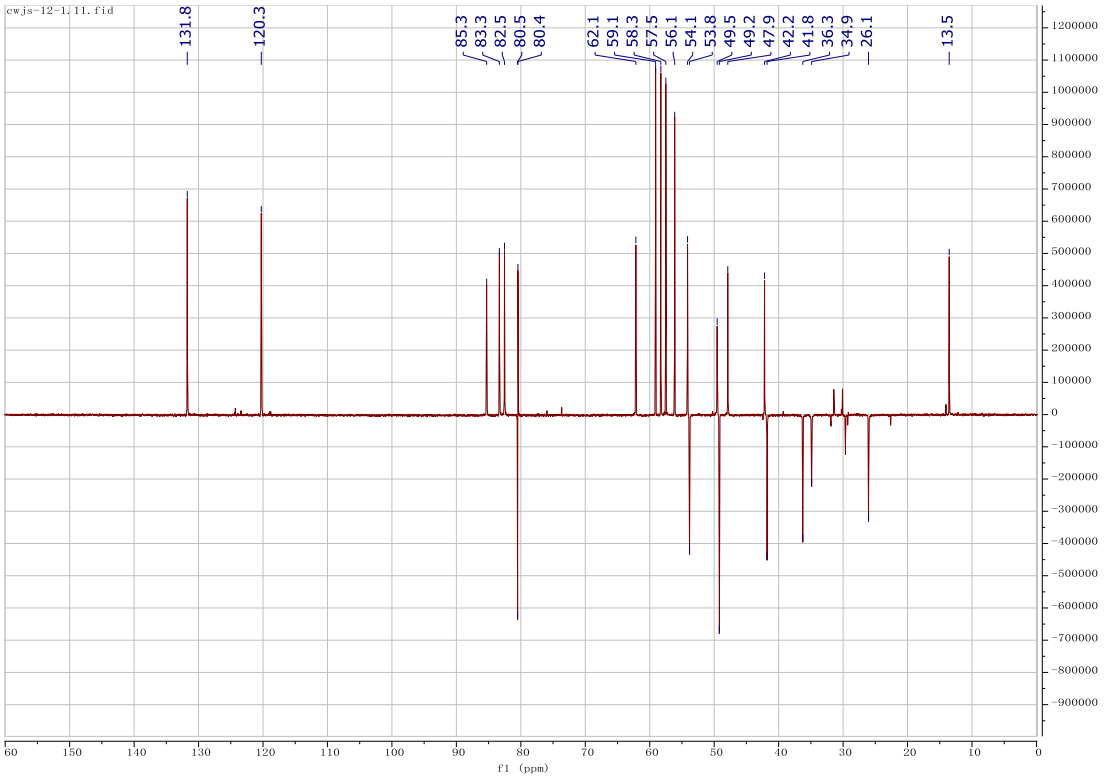


Figure S29. HR-ESI-MS spectrum for compoud **h**.

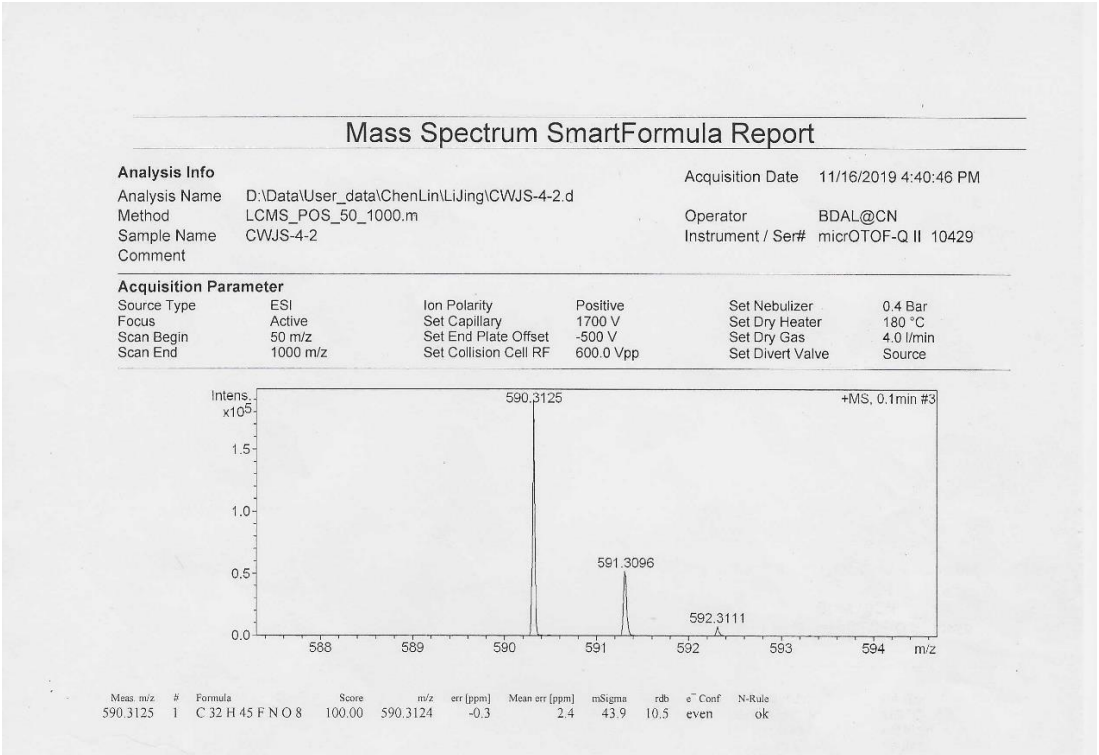


Figure S30. ^{1}H NMR spectrum for compoud **h** in $CDCl_3$ (400Hz).

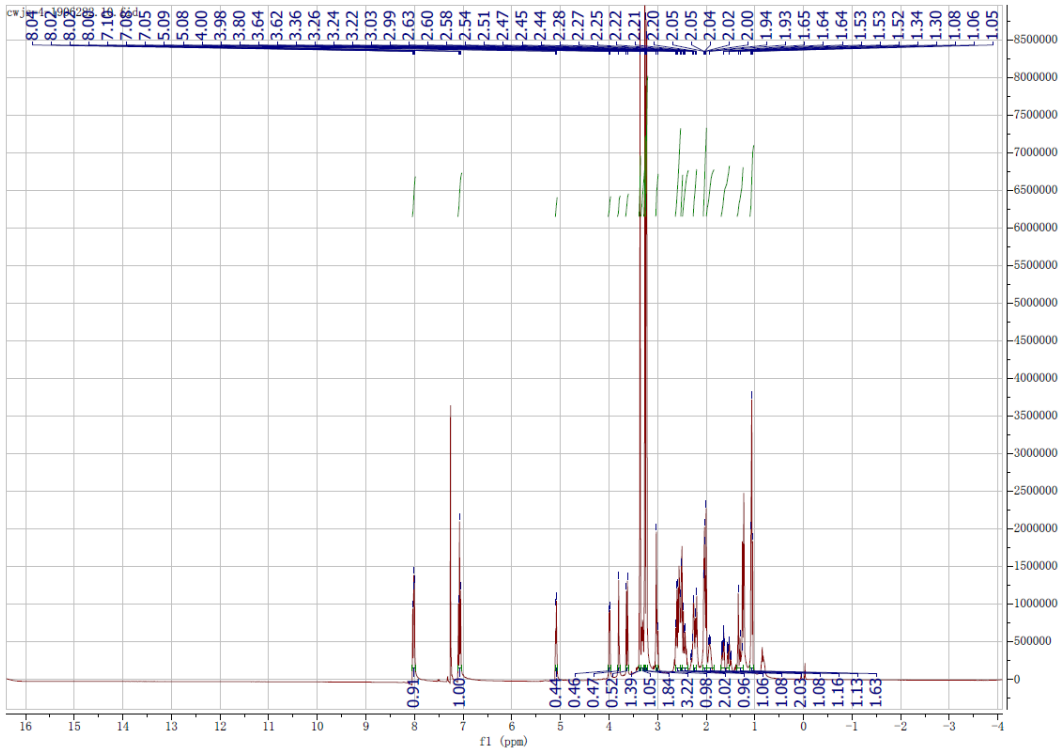


Figure S31. ^{13}C NMR spectrum for compoud **h** in $CDCl_3$ (100Hz).

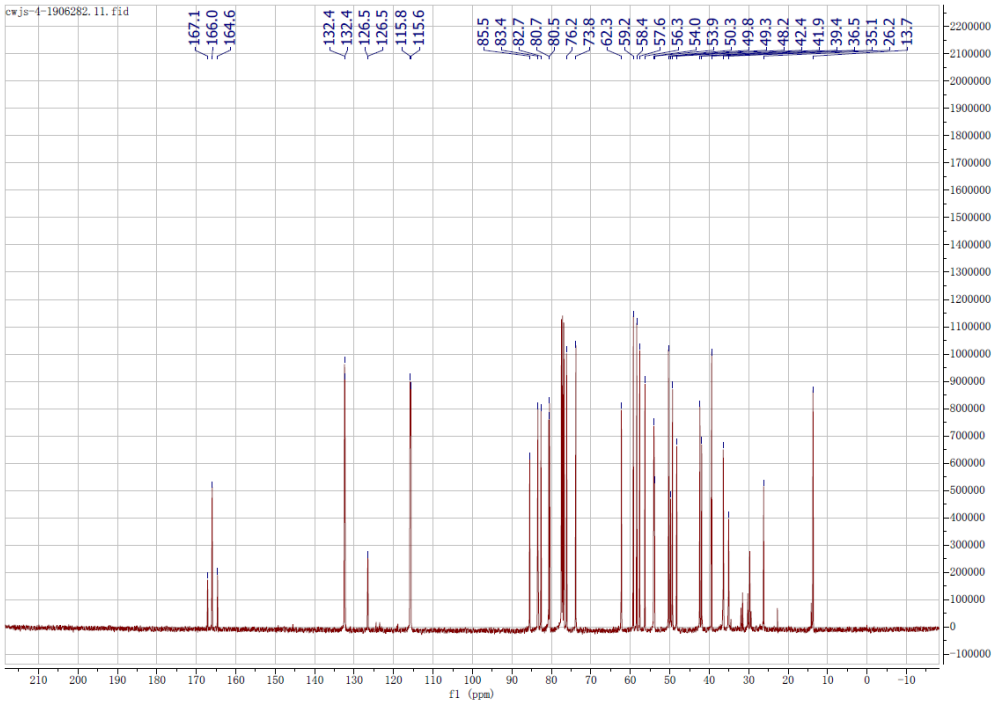


Figure S32. DEPT (θ = 135°) spectrum for compound **h** in $CDCl_3$.

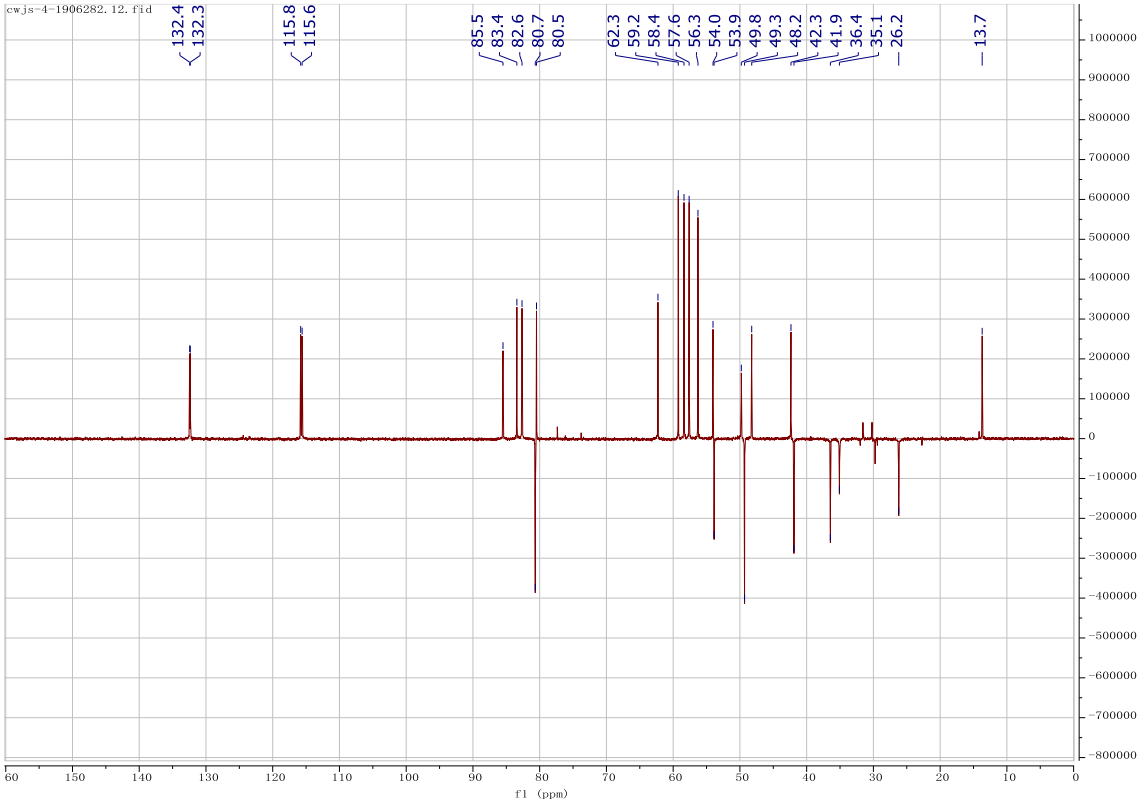
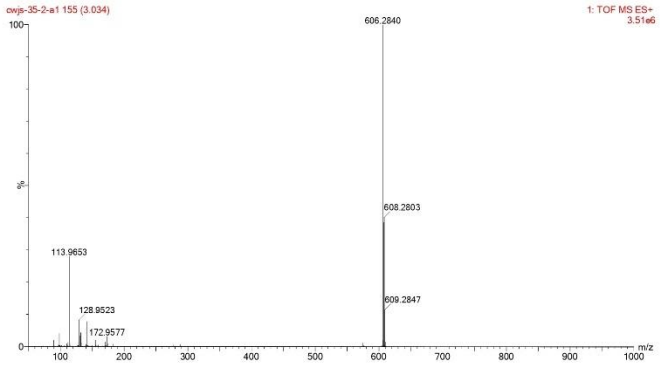


Figure S33. HR-ESI-MS spectrum for compoud **i**.



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

235 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 20-40 H: 30-70 N: 1-5 O: 1-15 Cl: 1-1

Minimum:					-1.5
Maximum:		5.0	10.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
606.2840	606.2834	0.6	1.0	10.5	C32 H45 N O8 Cl
	606.2847	-0.7	-1.2	15.5	C33 H41 N5 O4 Cl
	606.2887	-4.7	-7.8	19.5	C38 H41 N3 O2 Cl
	606.2793	4.7	7.8	6.5	C27 H45 N3 O10 Cl

Figure S34. ^{1}H NMR spectrum for compoud **i** in $CDCl_3$ (400Hz).

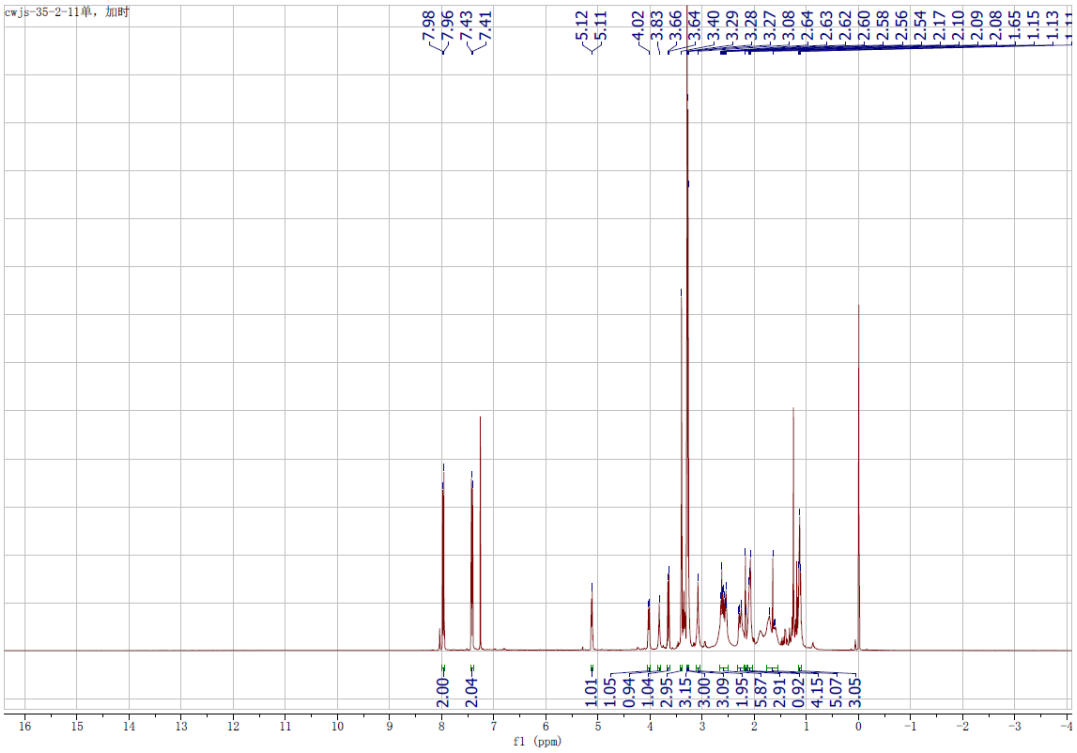


Figure S35. ^{13}C NMR spectrum for compoud **i** in $CDCl_3$ (100Hz).

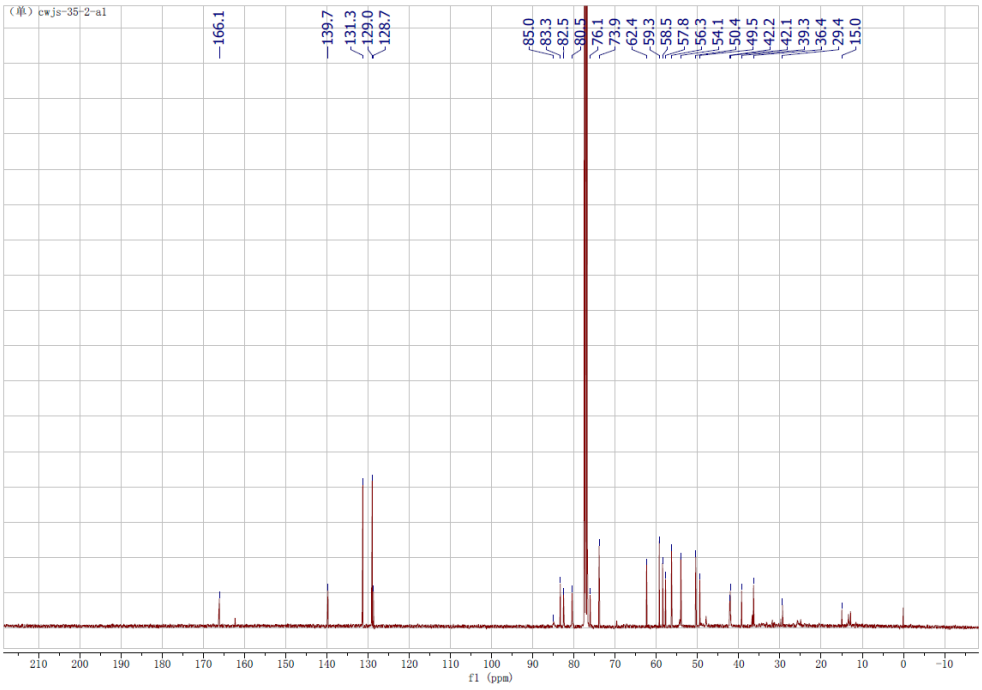


Figure S36. DEPT (θ = 135°) spectrum for compound **i** in $CDCl_3$.

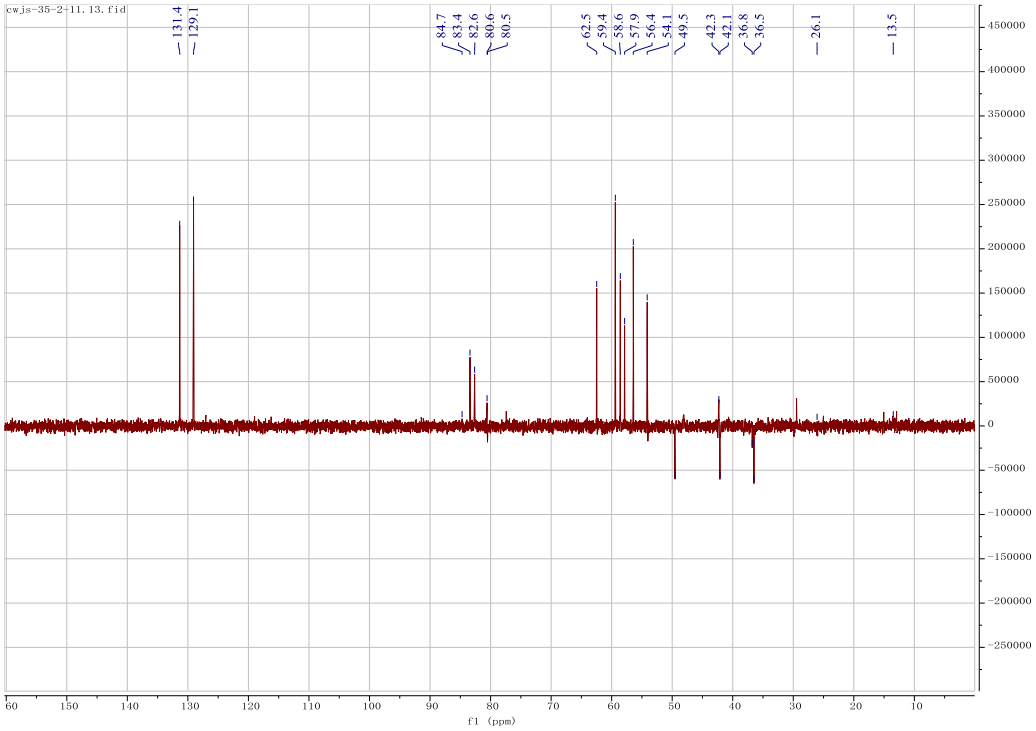
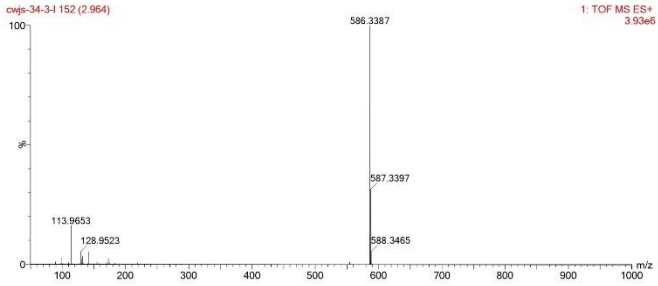


Figure S37. HR-ESI-MS spectrum for compoud **j**.



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

246 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 20-40 H: 30-70 N: 1-5 O: 1-15

Minimum:				-1.5	
Maximum:		5.0	10.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
586.3387	586.3393	-0.6	-1.0	15.5	C34 H44 N5 O4
	586.3380	0.7	1.2	10.5	C33 H48 N O8
	586.3434	-4.7	-8.0	19.5	C39 H44 N3 O2
	586.3340	4.7	8.0	6.5	C28 H48 N3 O10

Figure S38. ^{1}H NMR spectrum for compoud **j** in $CDCl_3$ (400Hz).

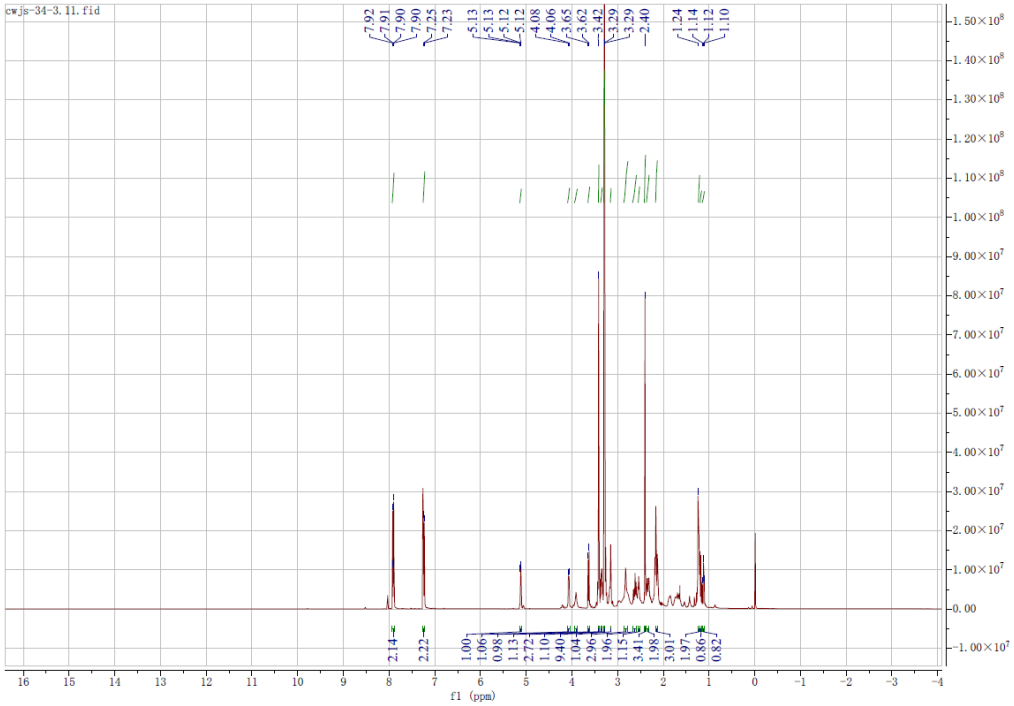


Figure S39. ^{13}C NMR spectrum for compoud **j** in $CDCl_3$ (100Hz).

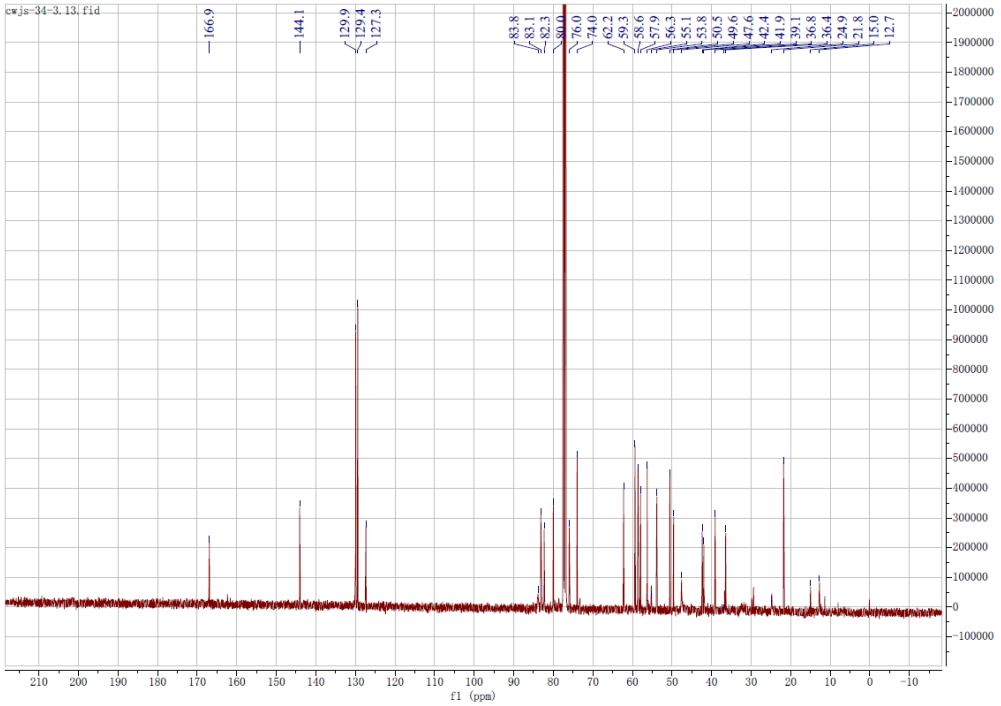


Figure S40. DEPT (θ = 135°) spectrum for compound **j** in $CDCl_3$.

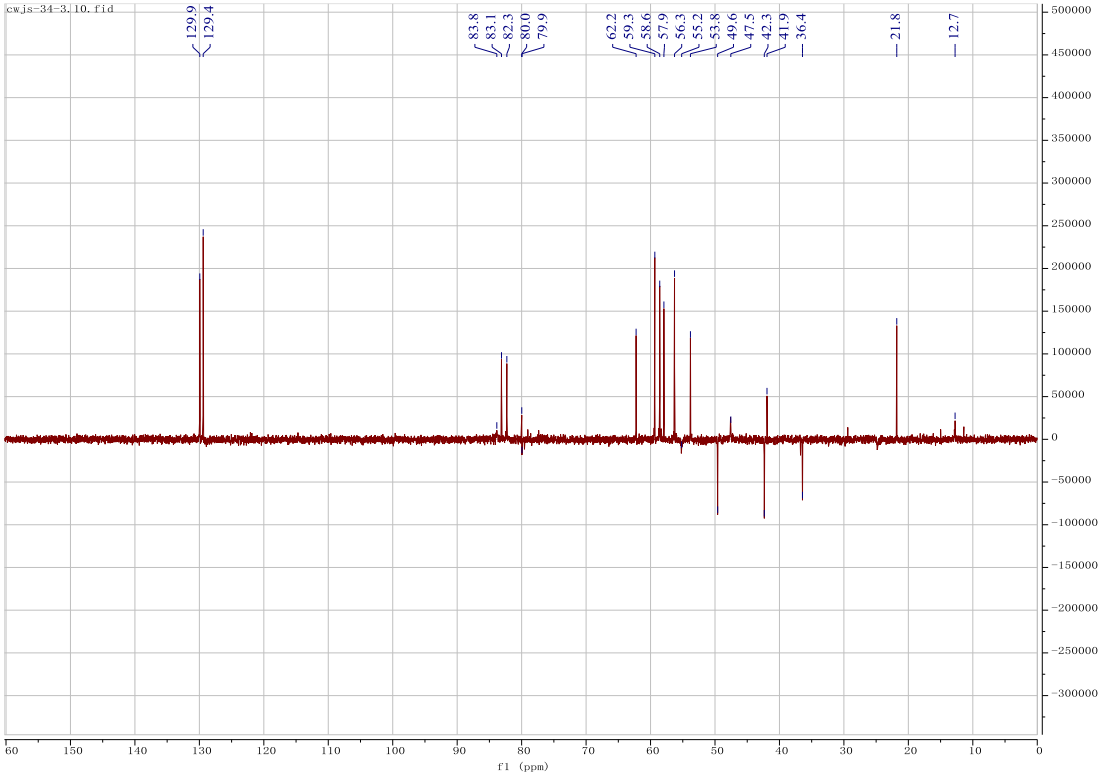


Figure S41. HR-ESI-MS spectrum for compoud **k**.

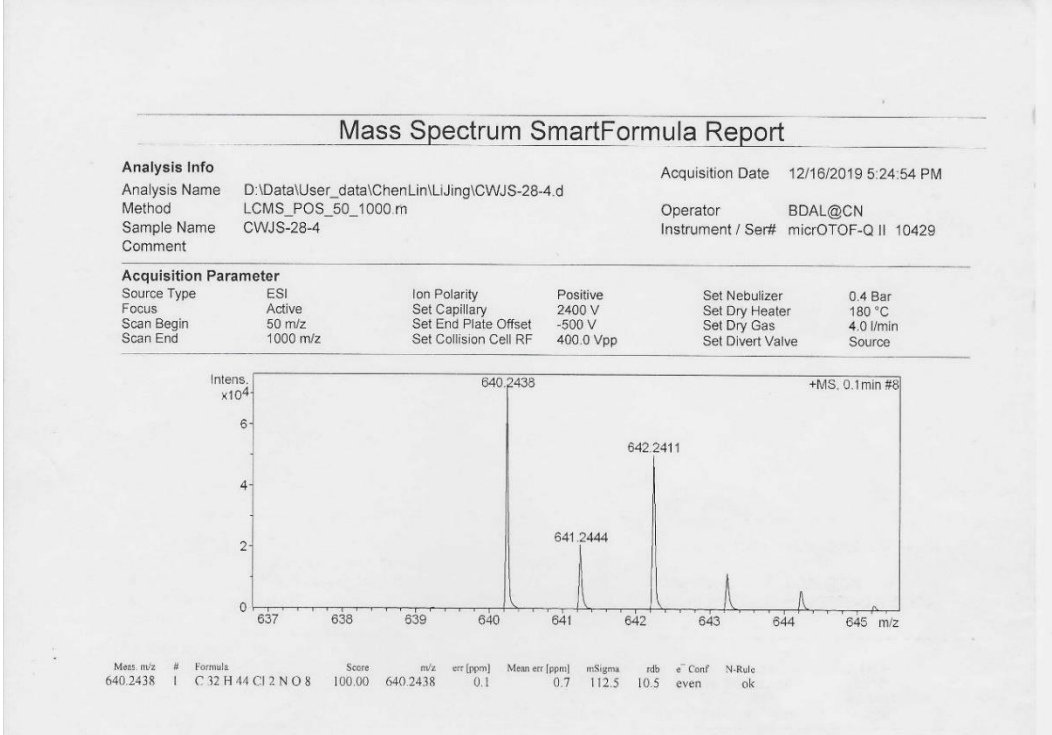


Figure S42. ^{1}H NMR spectrum for compoud **k** in $CDCl_3$ （400Hz).

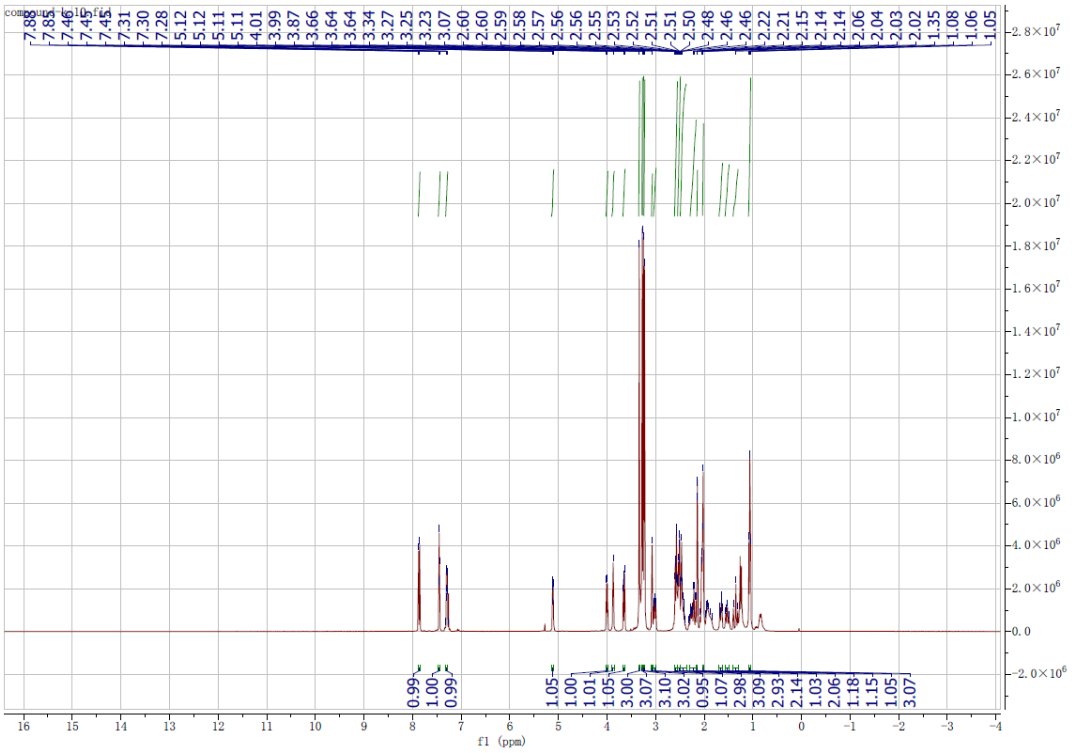


Figure S43. ^{13}C NMR spectrum for compoud **k** in $CDCl_3$ (150Hz).

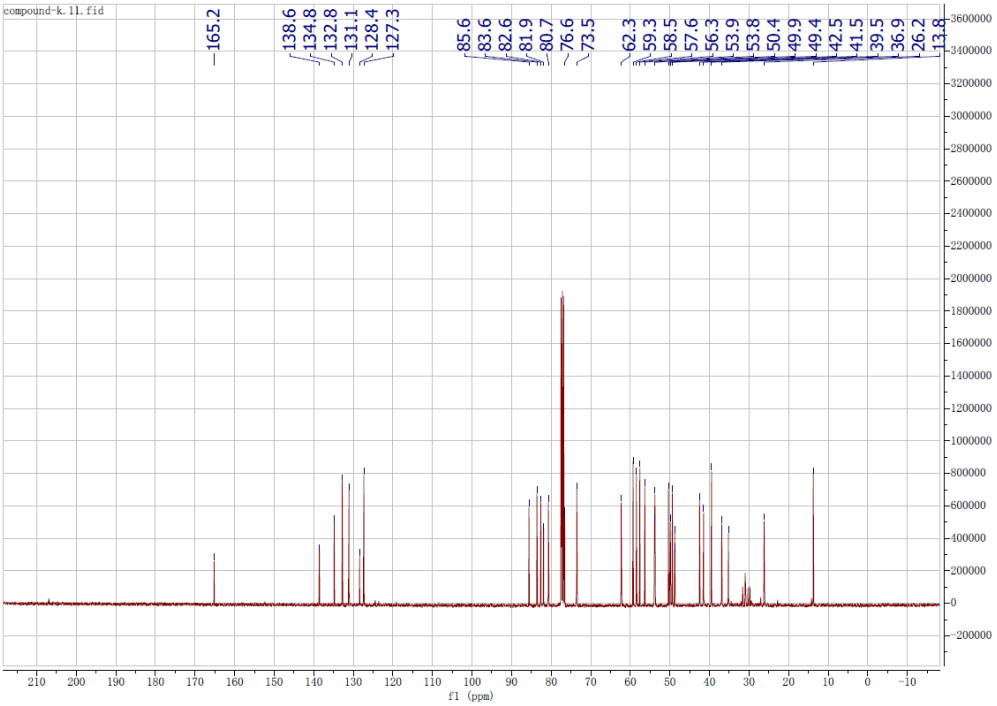
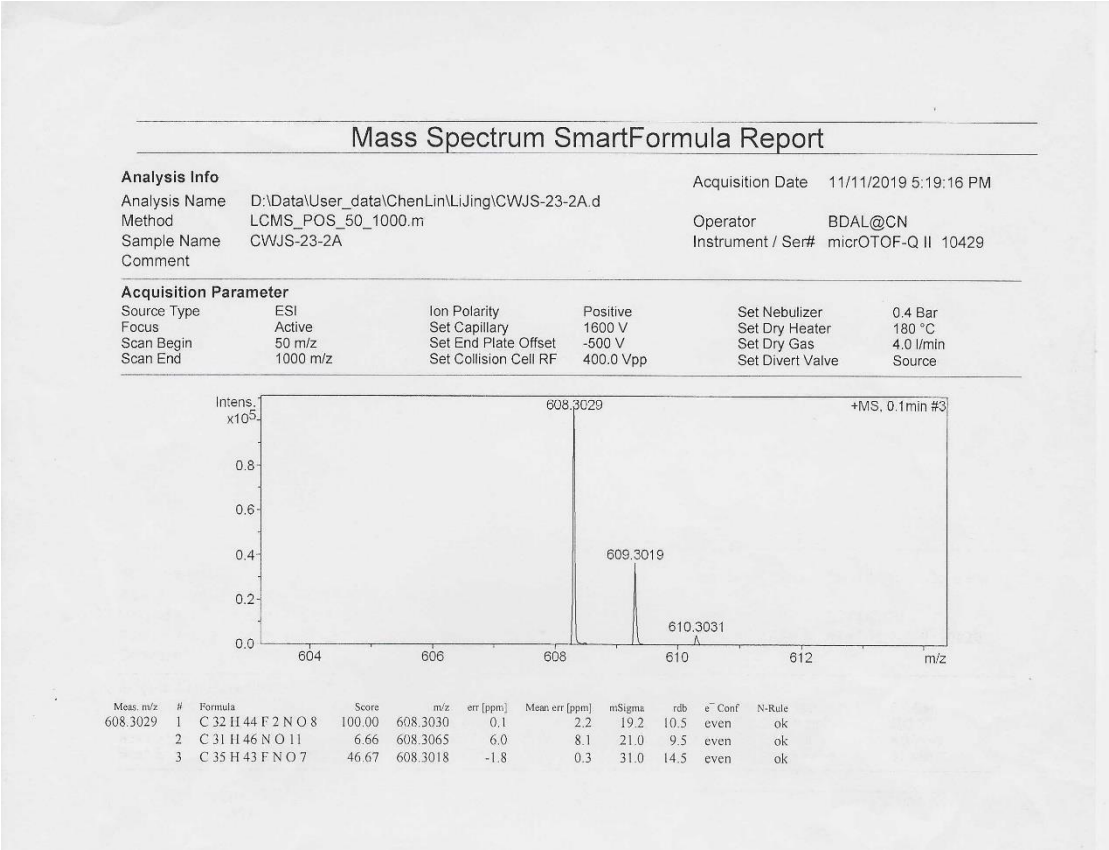


Figure S44. HR-ESI-MS spectrum for compoud **l**.



Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\User_data\ChenLin\LiJing\CWJS-23-2A.d	Acquisition Date	11/11/2019 5:19:16 PM
Method	LCMS_POS_50_1000.m	Operator	BDAL@CN
Sample Name	CWJS-23-2A	Instrument / Ser#	micrOTOF-Q II 10429
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	1600 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Source

Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
608.3029	1	C 32 H 44 F 2 N O 8	100.00	608.3030	0.1	2.2	19.2	10.5	even	ok
	2	C 31 H 46 N O 11	6.66	608.3065	6.0	8.1	21.0	9.5	even	ok
	3	C 35 H 43 F N O 7	46.67	608.3018	-1.8	0.3	31.0	14.5	even	ok

Figure S45. ^{1}H NMR spectrum for compoud **l** in $CDCl_3$ (400Hz).

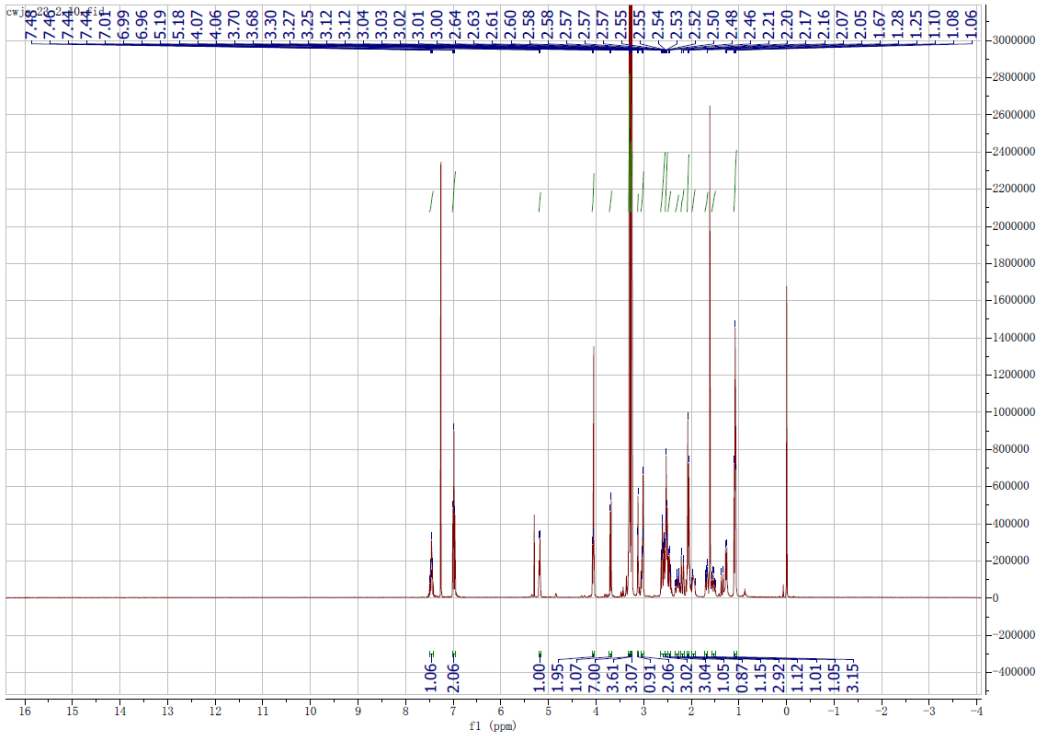


Figure S46. ^{13}C NMR spectrum for compoud **l** in $CDCl_3$ (100Hz).

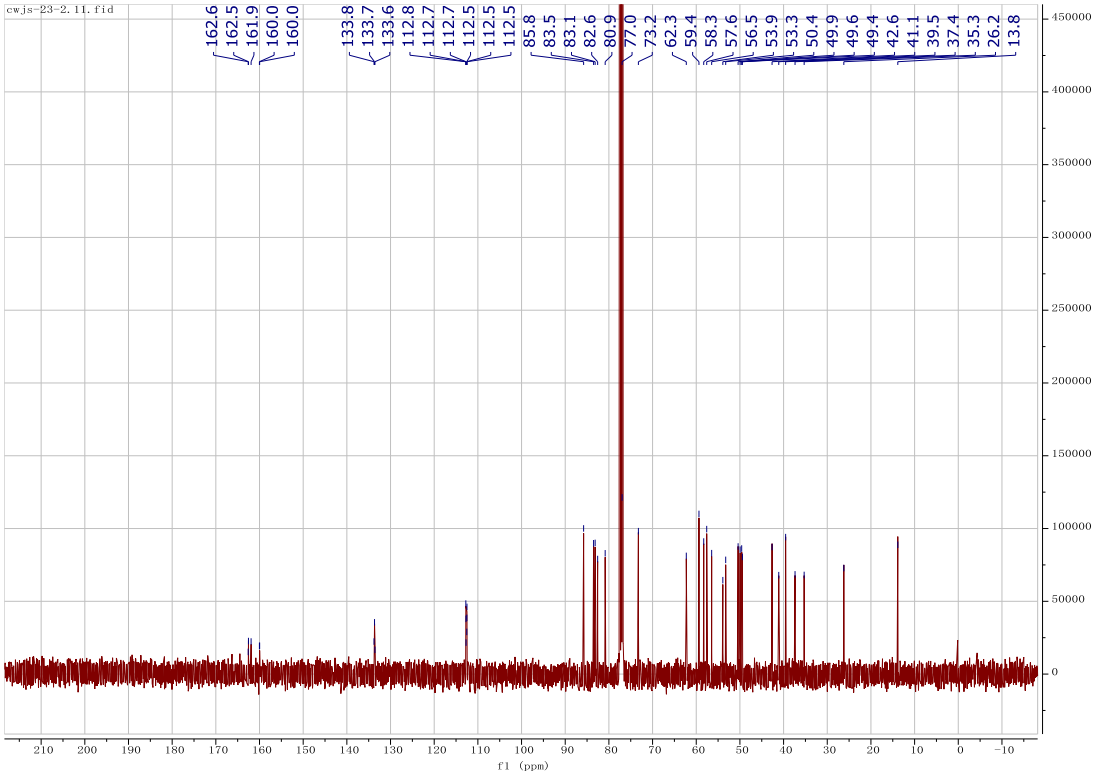


Figure S47. DEPT (θ = 135°) spectrum for compound **l** in $CDCl_3$.

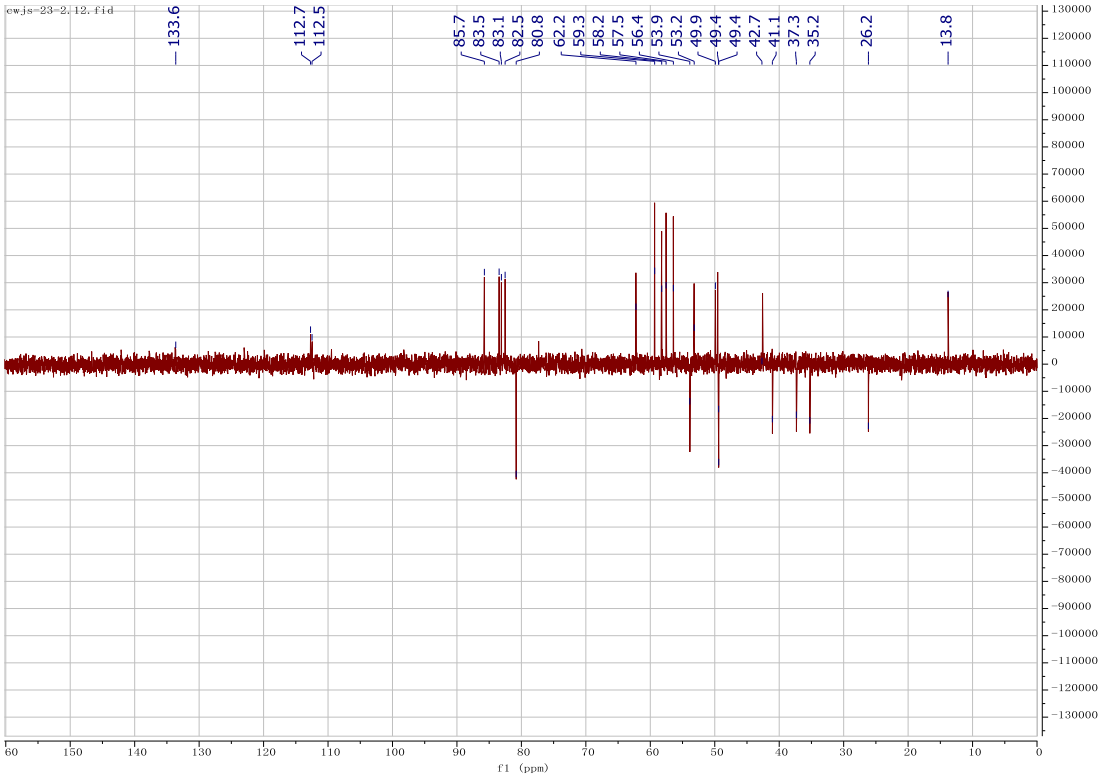
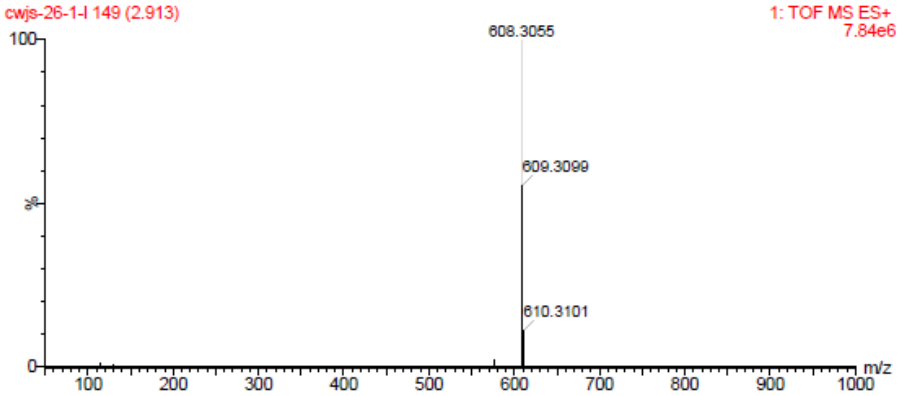


Figure S48. HR-ESI-MS spectrum for compoud **m**.



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

244 formula(e) evaluated with 4 results within limits (up to 50 closest results for each r

Elements Used:

C: 20-40 H: 30-70 N: 1-5 O: 1-15 F: 2-2

Minimum:					-1.5
Maximum:		5.0	10.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
608.3055	608.3048	0.7	1.2	15.5	C33 H40 N5 O4 F2
	608.3035	2.0	3.3	10.5	C32 H44 N O8 F2
	608.3089	-3.4	-5.6	19.5	C38 H40 N3 O2 F2
	608.3094	-3.9	-6.4	1.5	C25 H48 N O13 F2

Figure S49. ^{1}H NMR spectrum for compoud **m** in $CDCl_3$ (400Hz).

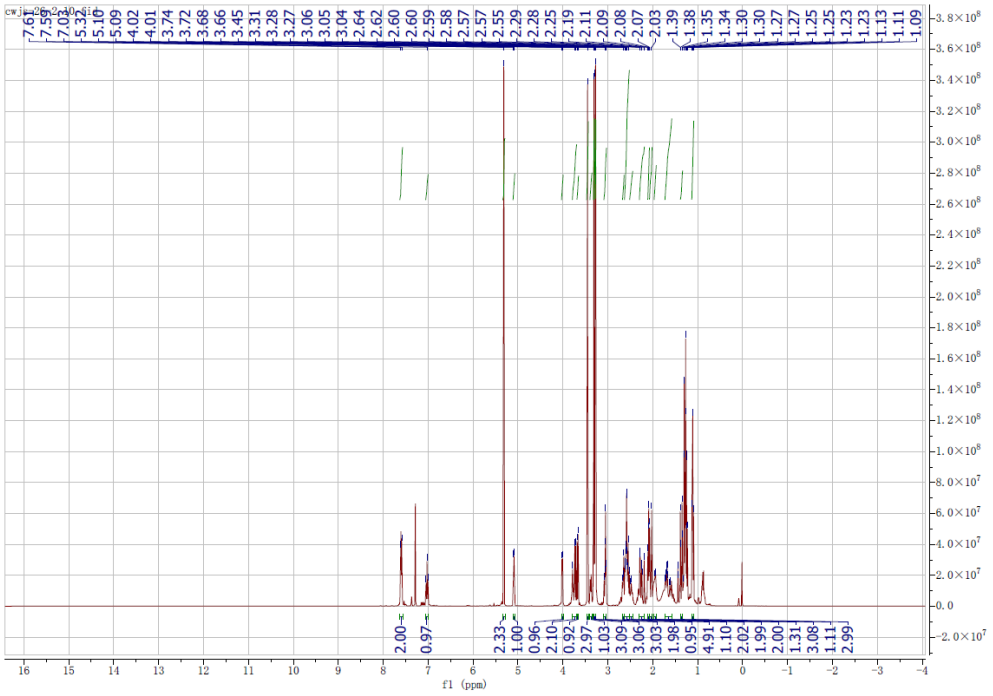


Figure S50. ^{13}C NMR spectrum for compoud **m** in $CDCl_3$ (100Hz).

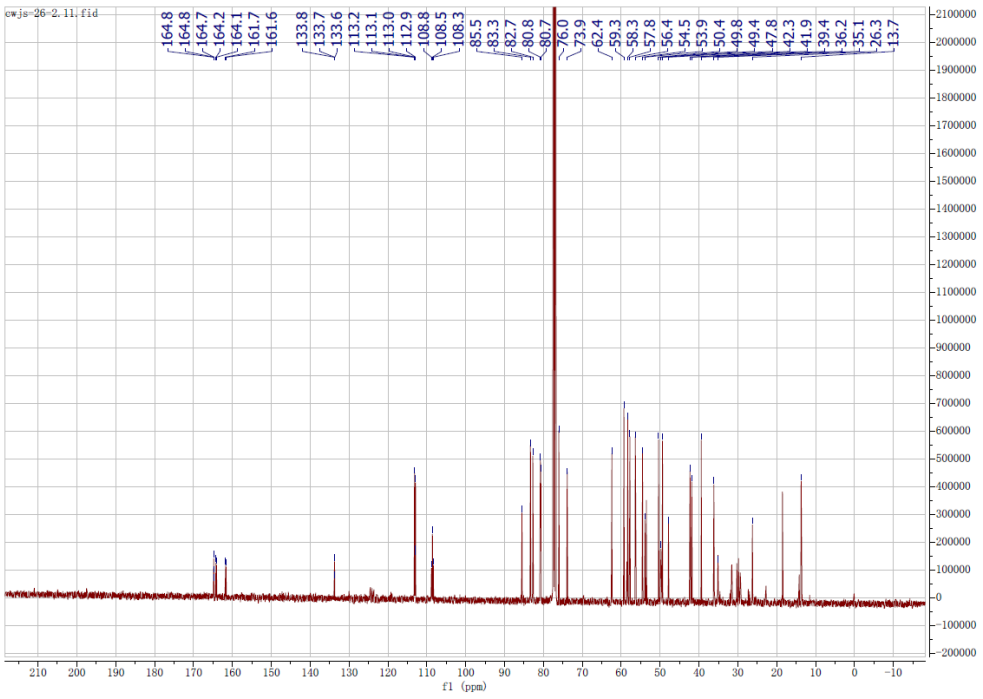


Figure S51. DEPT (θ = 135°) spectrum for compound **m** in $CDCl_3$.

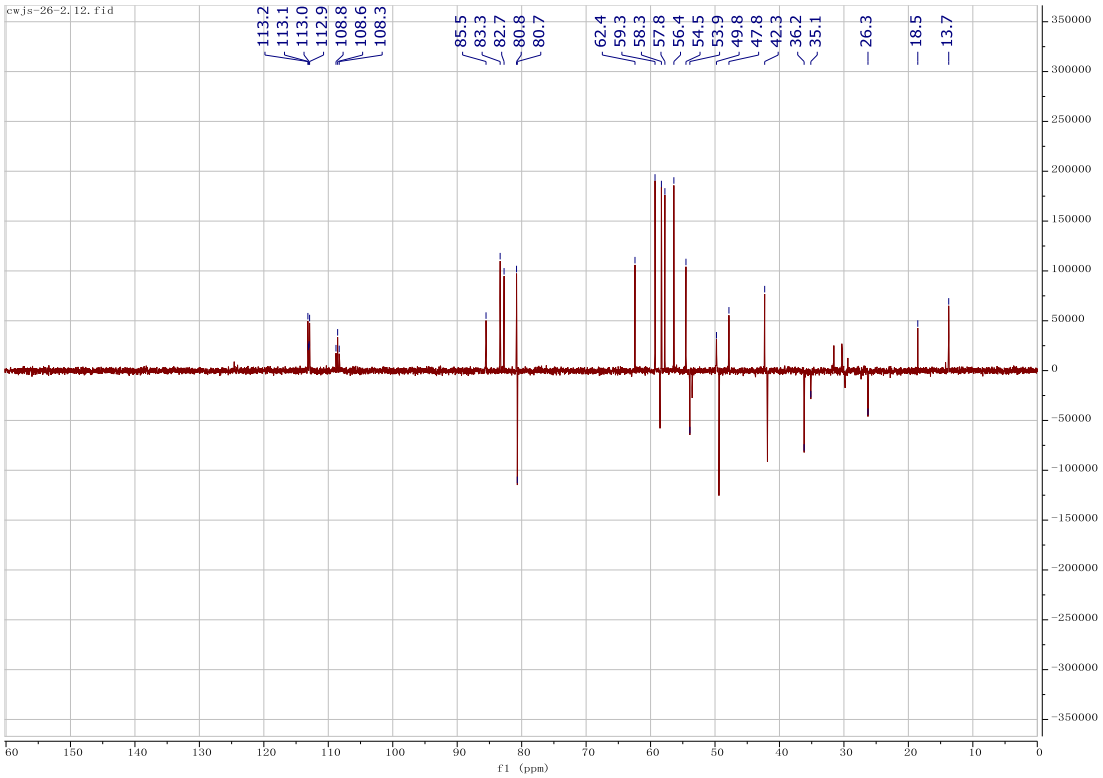
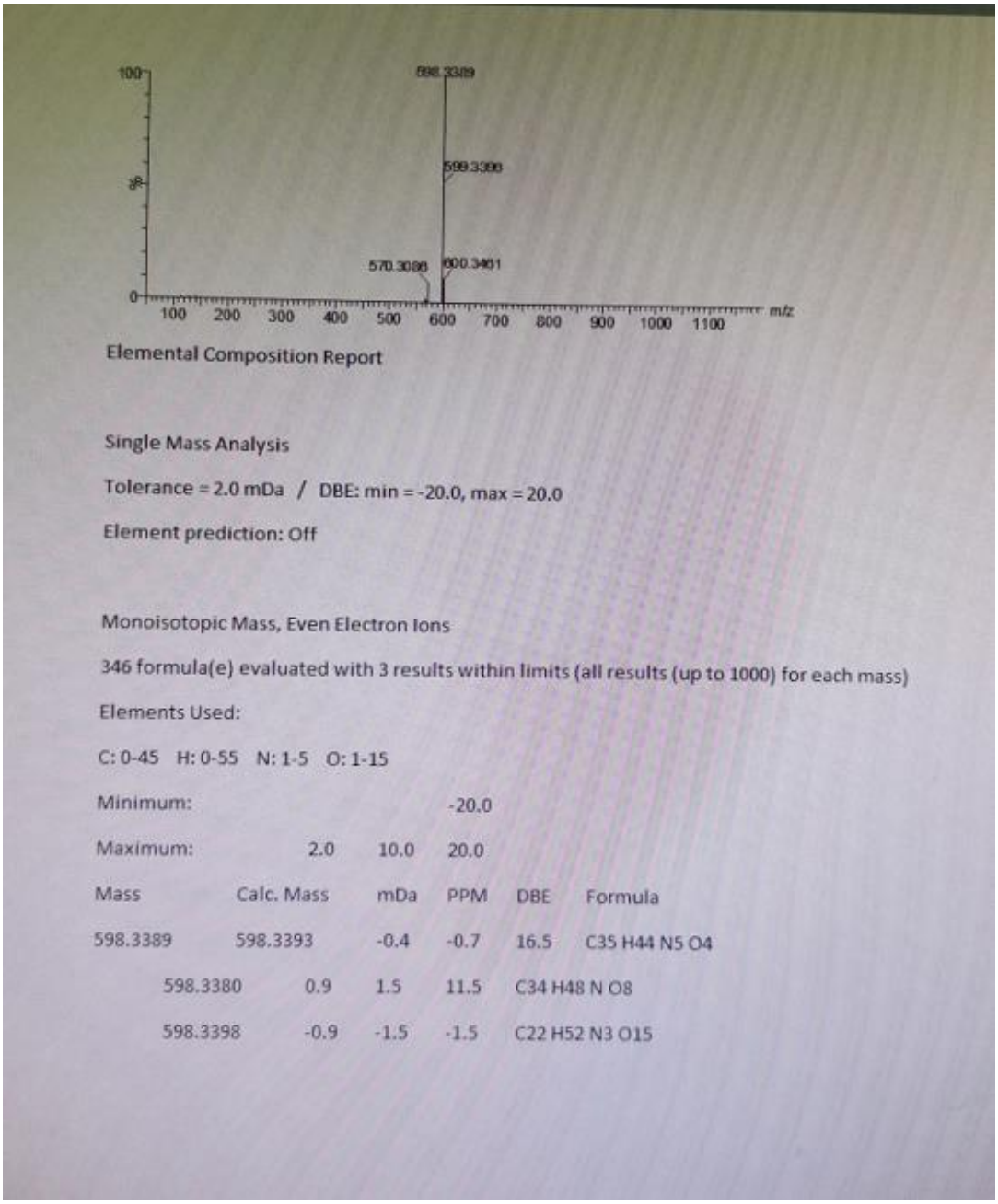


Figure S52. HR-ESI-MS spectrum for compoud **n.**



Elemental Composition Report

Single Mass Analysis

Tolerance = 2.0 mDa / DBE: min = -20.0, max = 20.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

346 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-45 H: 0-55 N: 1-5 O: 1-15

Minimum:			-20.0		
Maximum:	2.0	10.0	20.0		
Mass	Calc. Mass	mDa	PPM	DBE	Formula
598.3389	598.3393	-0.4	-0.7	16.5	C35 H44 N5 O4
	598.3380	0.9	1.5	11.5	C34 H48 N O8
	598.3398	-0.9	-1.5	-1.5	C22 H52 N3 O15

Figure S53. ^{1}H NMR spectrum for compoud **n** in $CDCl_3$ (400Hz).

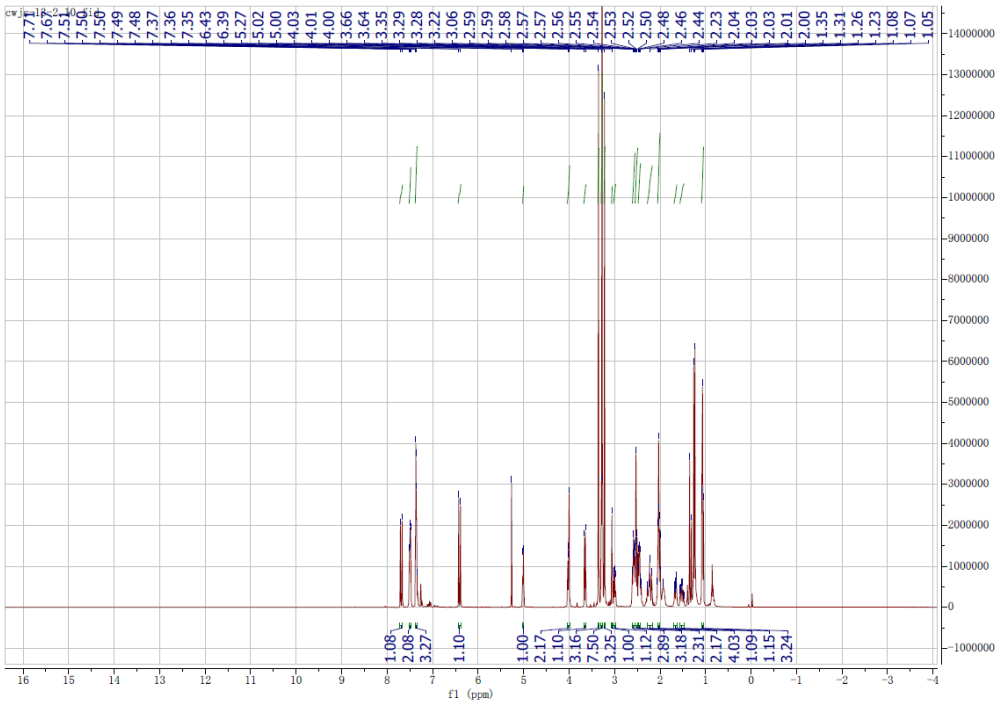


Figure S54. ^{13}C NMR spectrum for compoud **n** in $CDCl_3$ (100Hz).

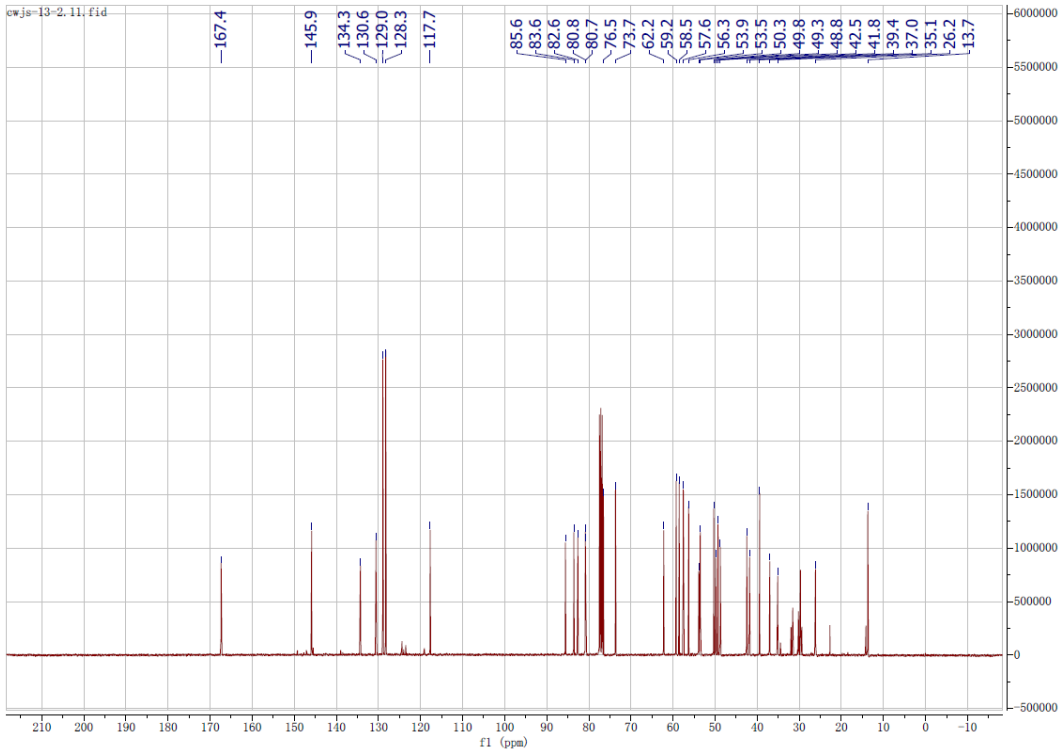


Figure S55. DEPT (θ = 135°) spectrum for compound **n** in $CDCl_3$.

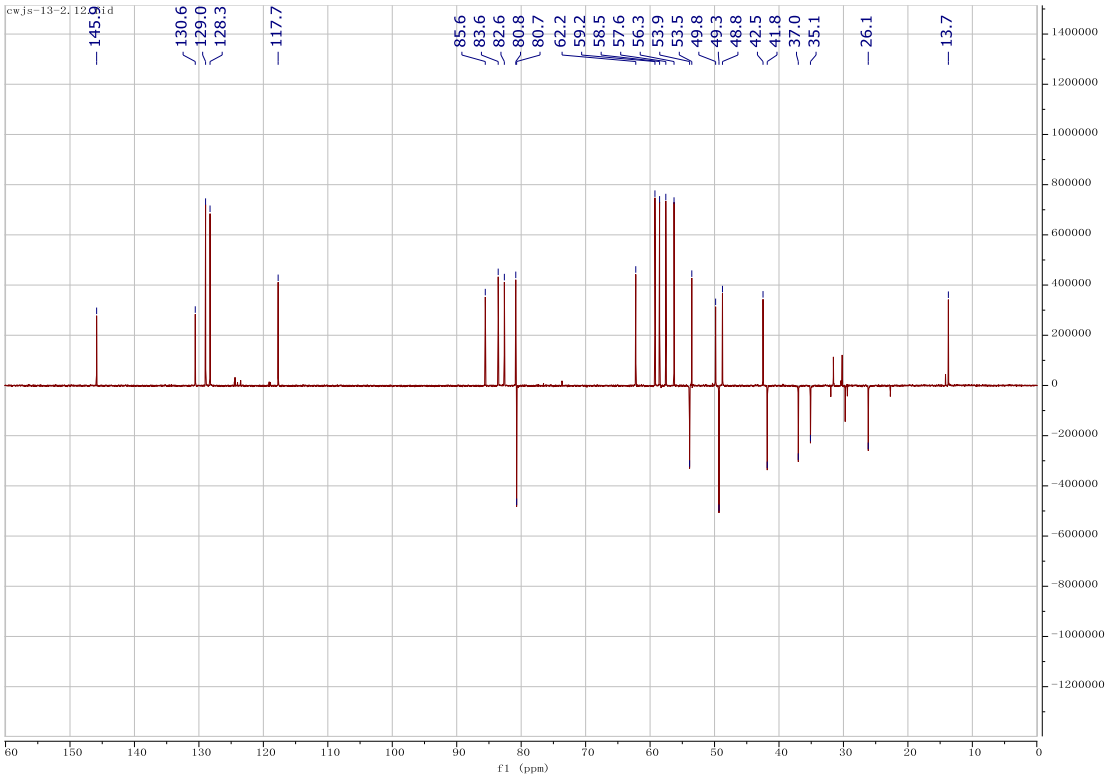
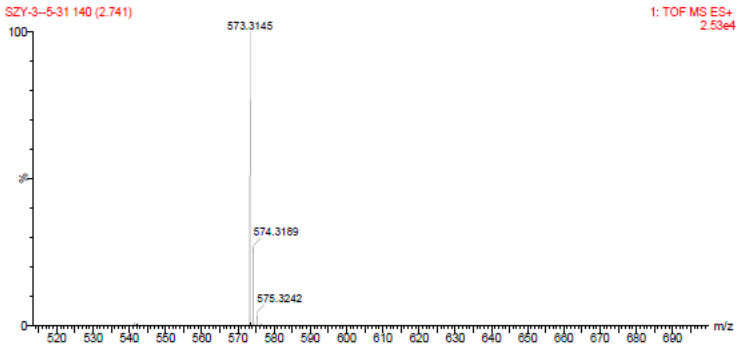


Figure S56. HR-ESI-MS spectrum for compoud **o.**



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

68 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 25-35 H: 20-50 N: 1-5 O: 5-10

Minimum:					-1.5	
Maximum:		5.0	10.0		50.0	
Mass	Calc. Mass	mDa		PPM	DBE	Formula
573.3145	573.3136	0.9	1.6	6.5	C26 H45 N4 O10	
	573.3176	-3.1	-5.4	10.5	C31 H45 N2 O8	

Figure S57. ^{1}H NMR spectrum for compoud **o** in $CDCl_3$ (400Hz).

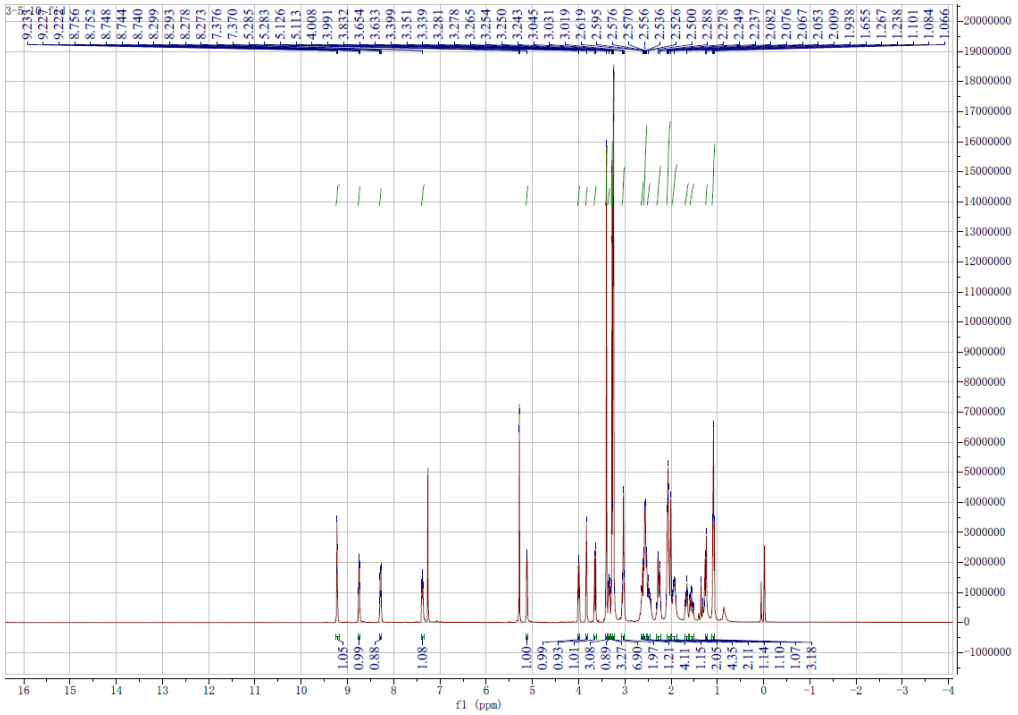


Figure S58. ^{13}C NMR spectrum for compoud **o** in $CDCl_3$ (100Hz).

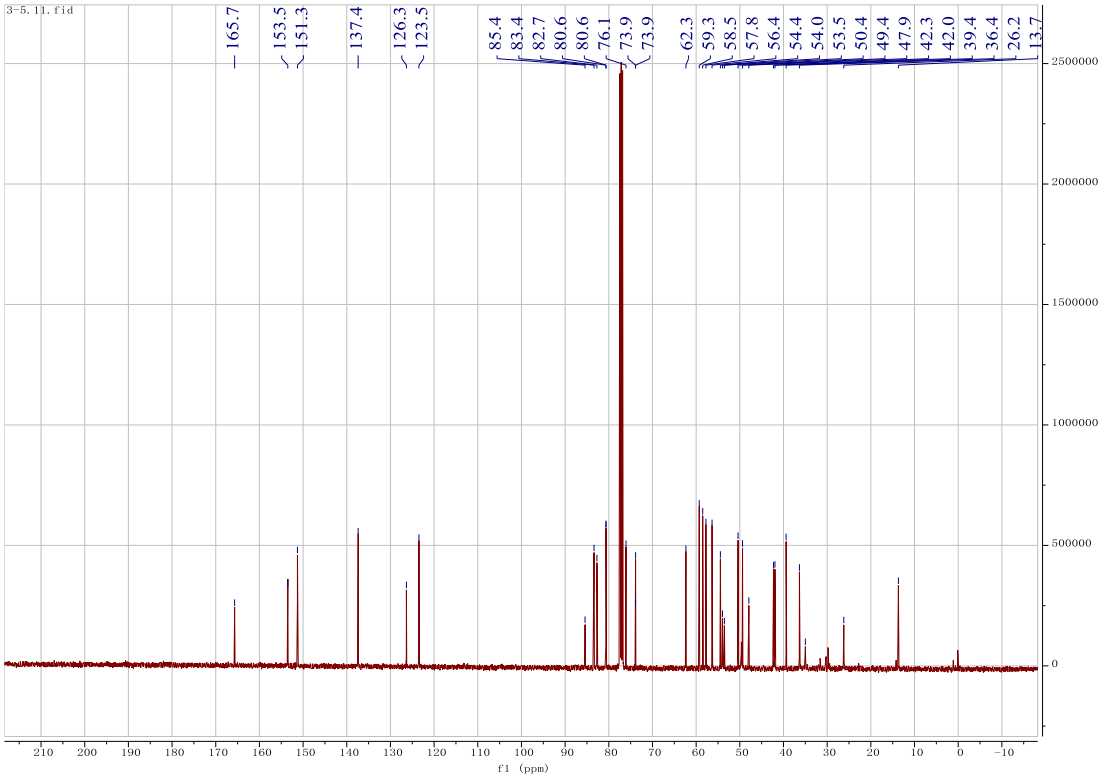


Figure S59. DEPT (θ = 135°) spectrum for compound **o** in $CDCl_3$.

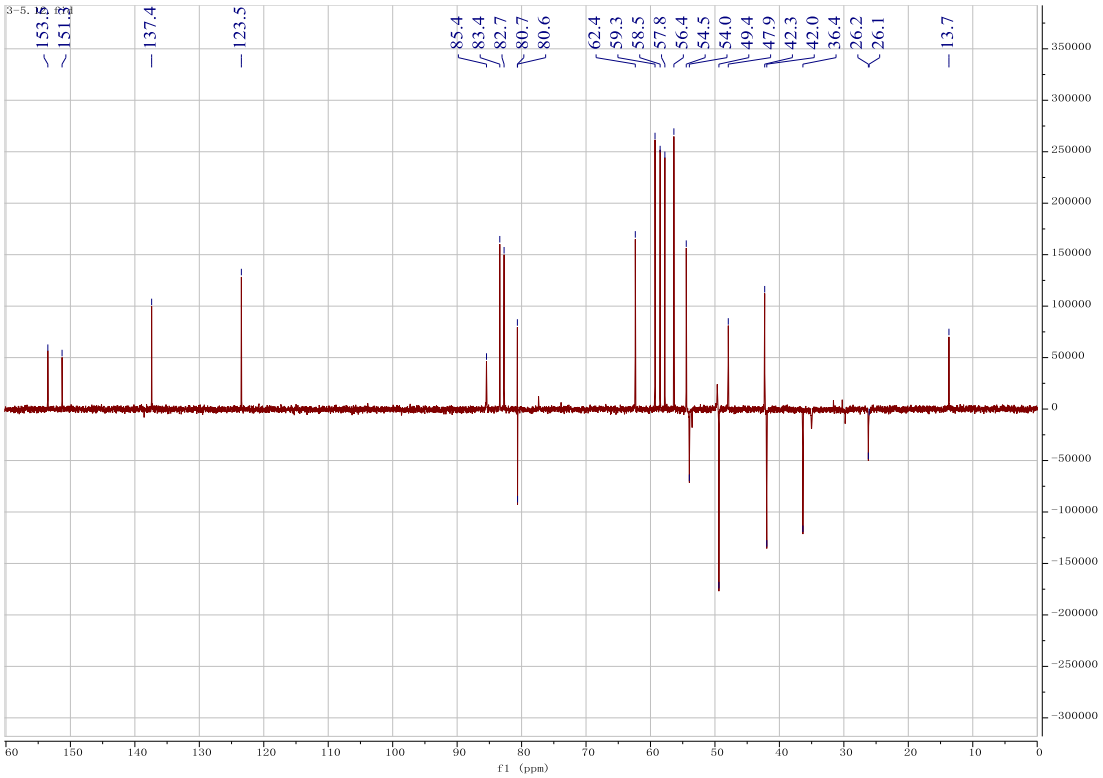
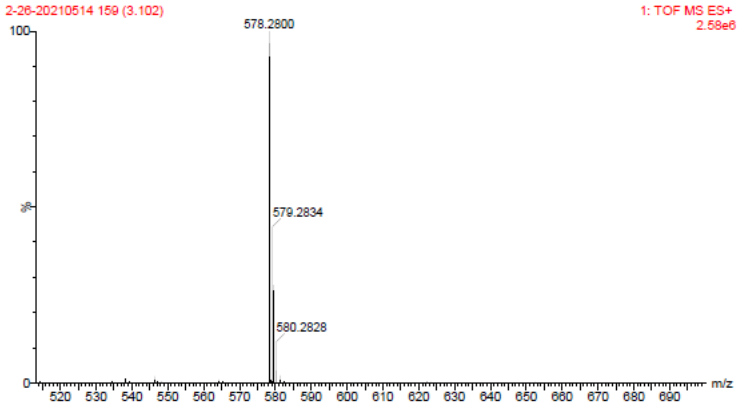


Figure S60. HR-ESI-MS spectrum for compoud **p**.



Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

106 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 25-35 H: 20-50 N: 1-1 O: 5-10 S: 0-3

Minimum:	80.00					-1.5
Maximum:	100.00		5.0	10.0	50.0	
Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
578.2800	100.00	578.2788	1.2	2.1	9.5	C30 H44 N O8 S

Figure S61. ^{1}H NMR spectrum for compoud **p** in $CDCl_3$ (400Hz).

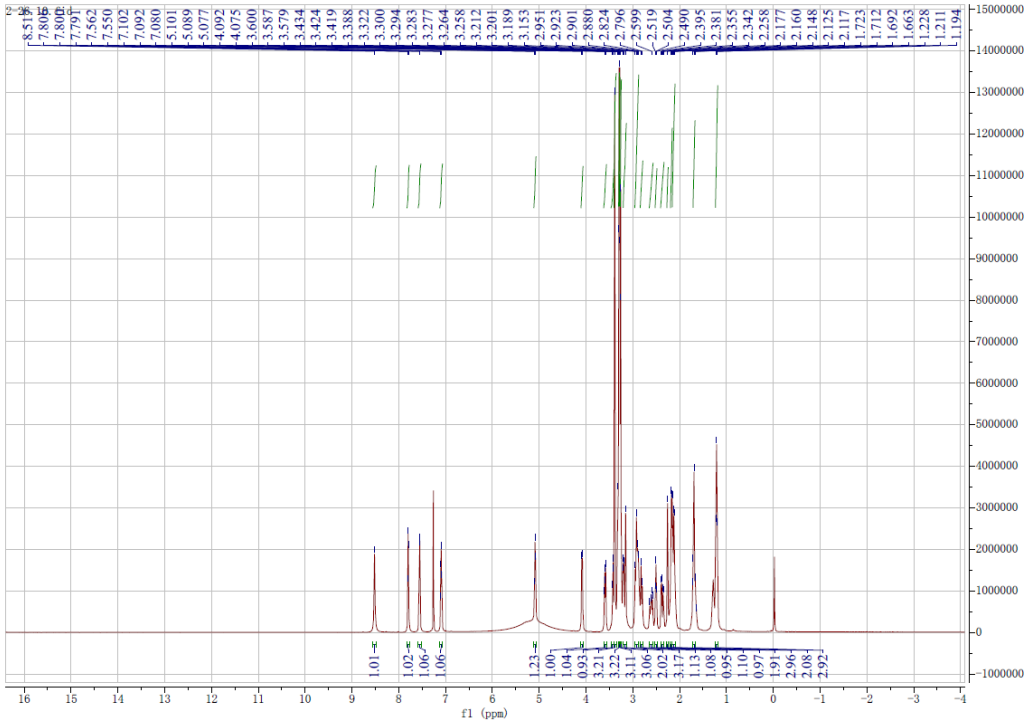


Figure S62. ^{13}C NMR spectrum for compoud **p** in $CDCl_3$ (100Hz).

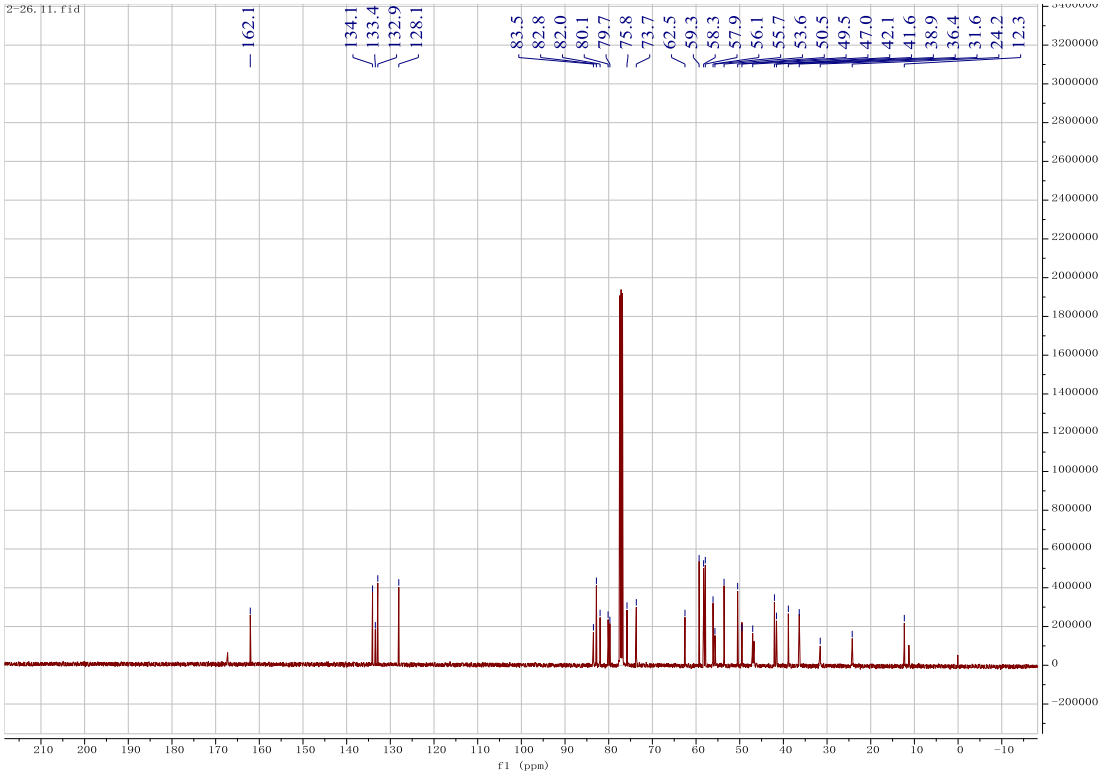


Figure S63. DEPT (θ = 135°) spectrum for compound **p** in $CDCl_3$.

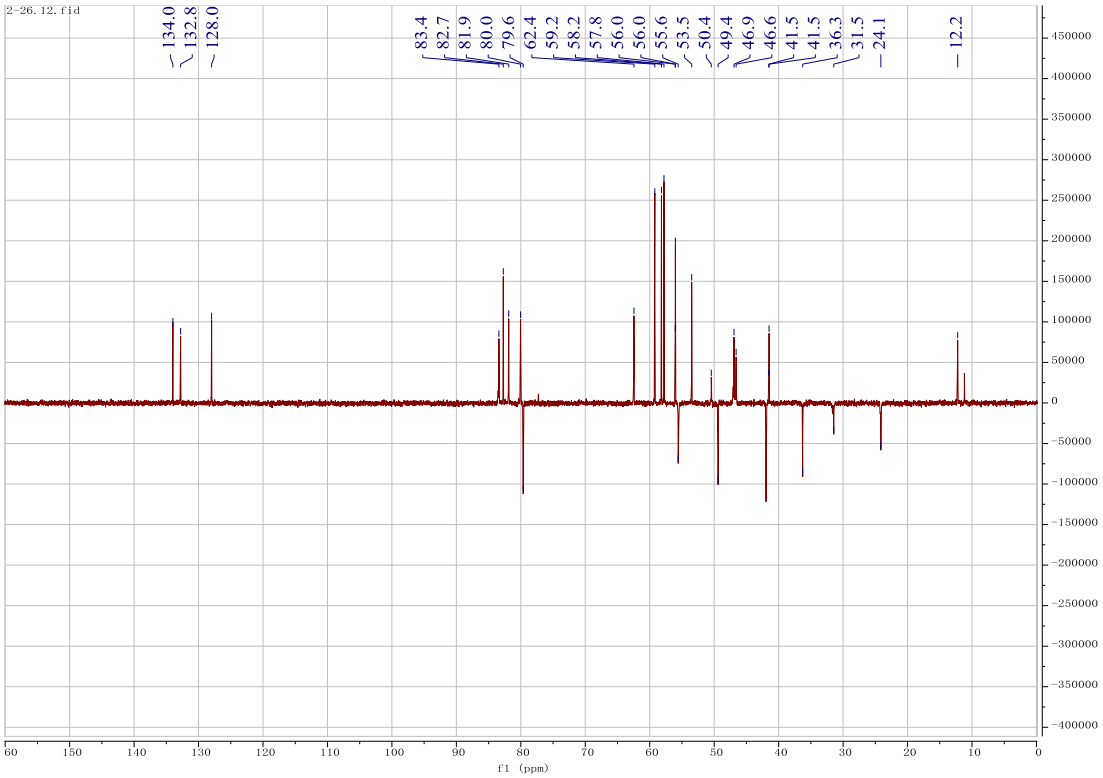
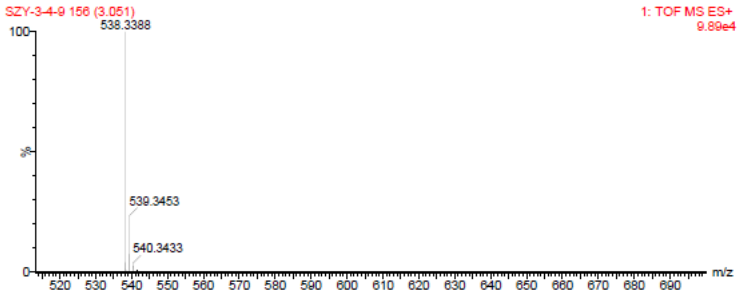


Figure S64. HR-ESI-MS spectrum for compoud **q**.



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

159 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 20-35 H: 30-60 N: 1-5 O: 1-15

Minimum:					-1.5	
Maximum:		5.0	10.0		50.0	
Mass	Calc. Mass	mDa		PPM	DBE	Formula
538.3388	538.3393	-0.5	-0.9	11.5		C30 H44 N5 O4
	538.3380	0.8	1.5	6.5		C29 H48 N O8
	538.3434	-4.6	-8.5	15.5		C35 H44 N3 O2
	538.3340	4.8	8.9	2.5		C24 H48 N3 O10

Figure S65. ^{1}H NMR spectrum for compoud **q** in $CDCl_3$ (400Hz).

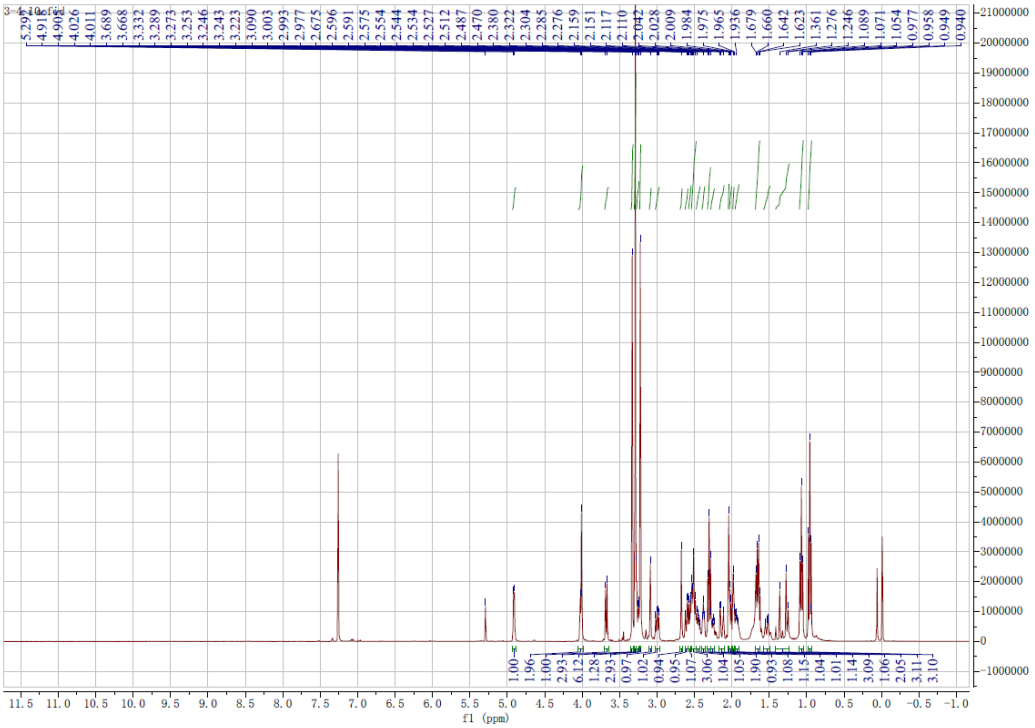


Figure S66. ^{13}C NMR spectrum for compoud **q** in $CDCl_3$ (100Hz).

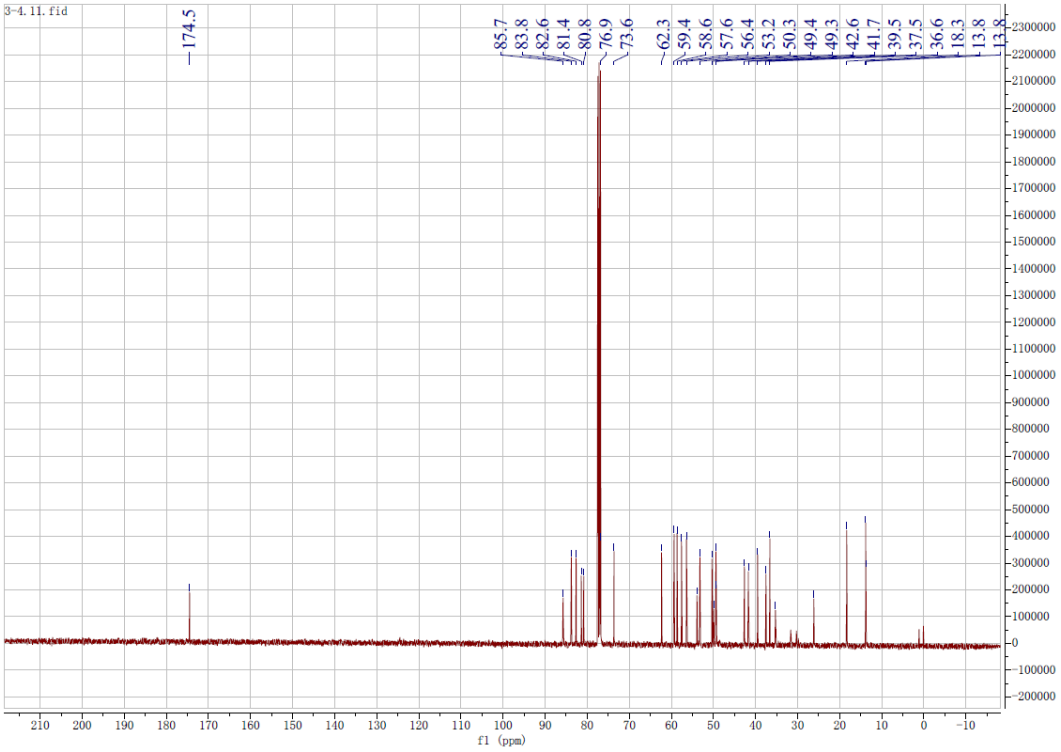


Figure S67. DEPT ($\theta = 135^{\circ}$) spectrum for compound **q** in $CDCl_3$.

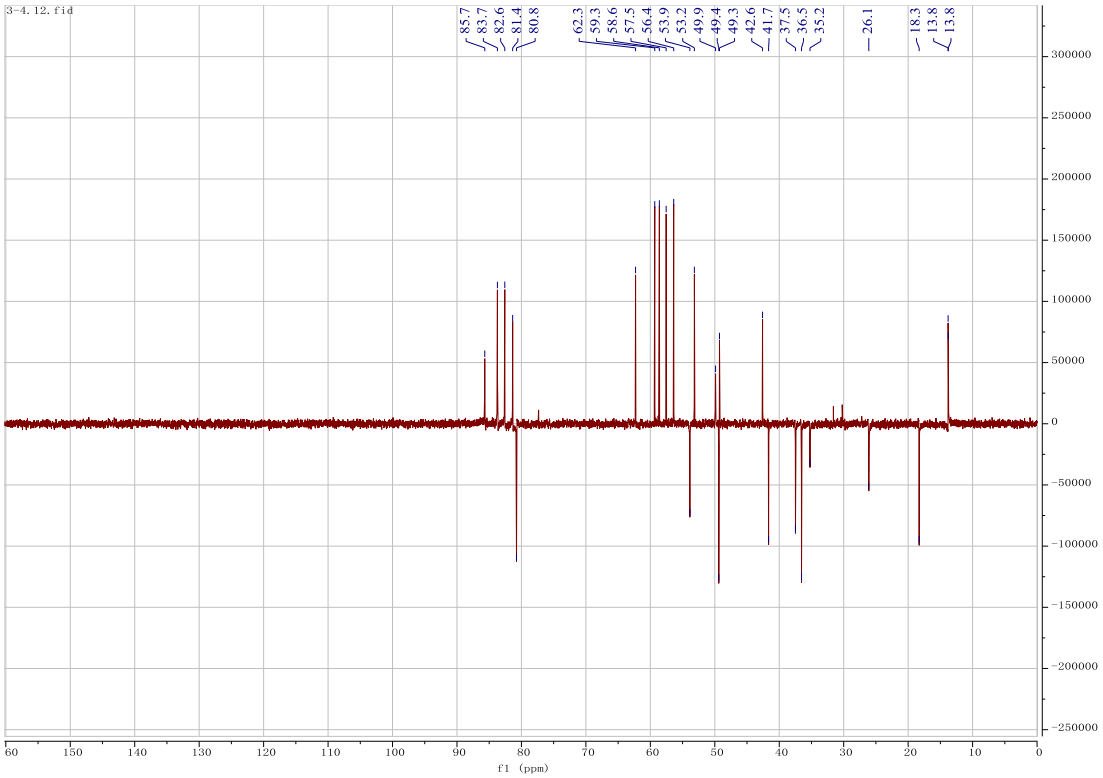
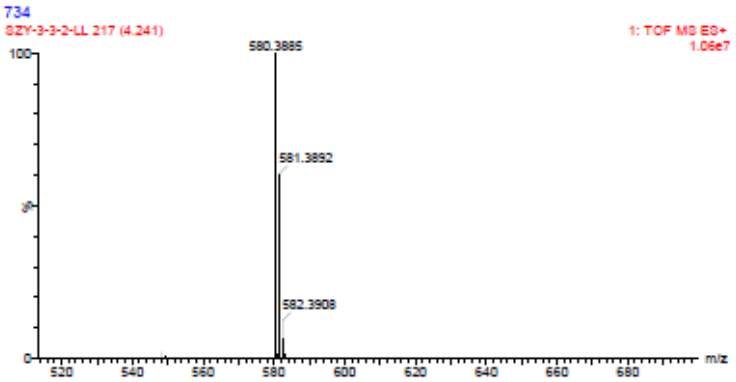


Figure S68. HR-ESI-MS spectrum for compoud **r.**



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

205 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 20-40 H: 20-70 N: 1-5 O: 1-10

Minimum:					-1.5	
Maximum:		5.0	10.0		50.0	
Mass	Calc. Mass	mDa		PPM	DBE	Formula
580.3885	580.3903	-1.8	-3.1	15.5		C38 H50 N3 O2
	580.3863	2.2	3.8	11.5		C33 H50 N5 O4
	580.3849	3.6	6.2	6.5		C32 H54 N O8
	580.3922	-3.7	-6.4	2.5		C26 H54 N5 O9

Figure S69. ^{1}H NMR spectrum for compoud **r** in $CDCl_3$ (400Hz).

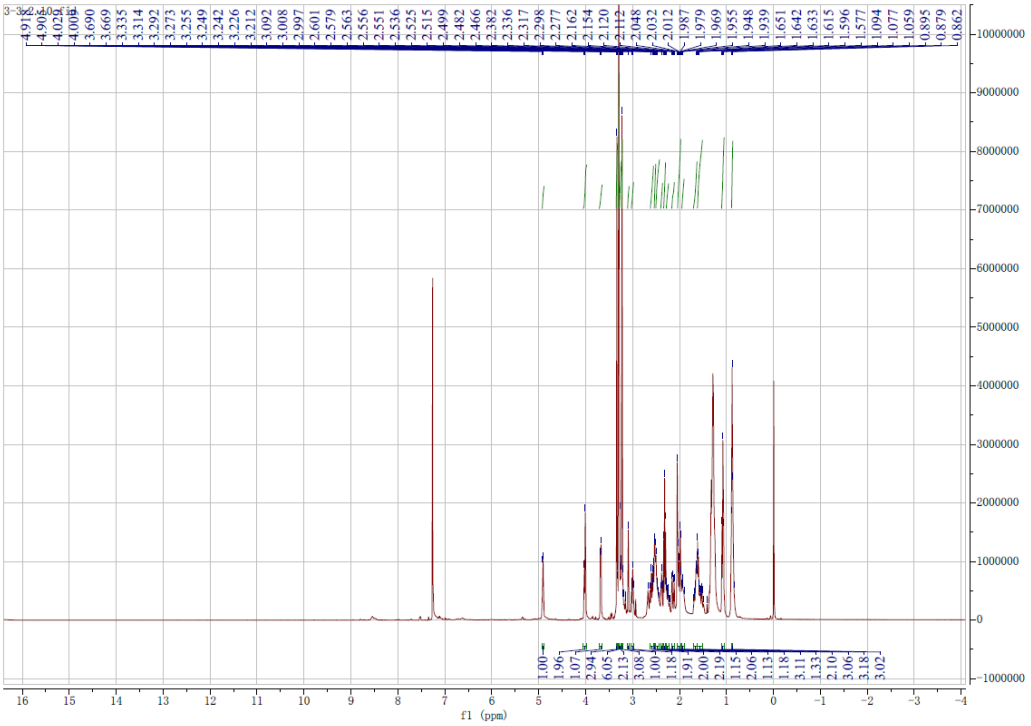


Figure S70. ^{13}C NMR spectrum for compoud **r** in $CDCl_3$ (100Hz).

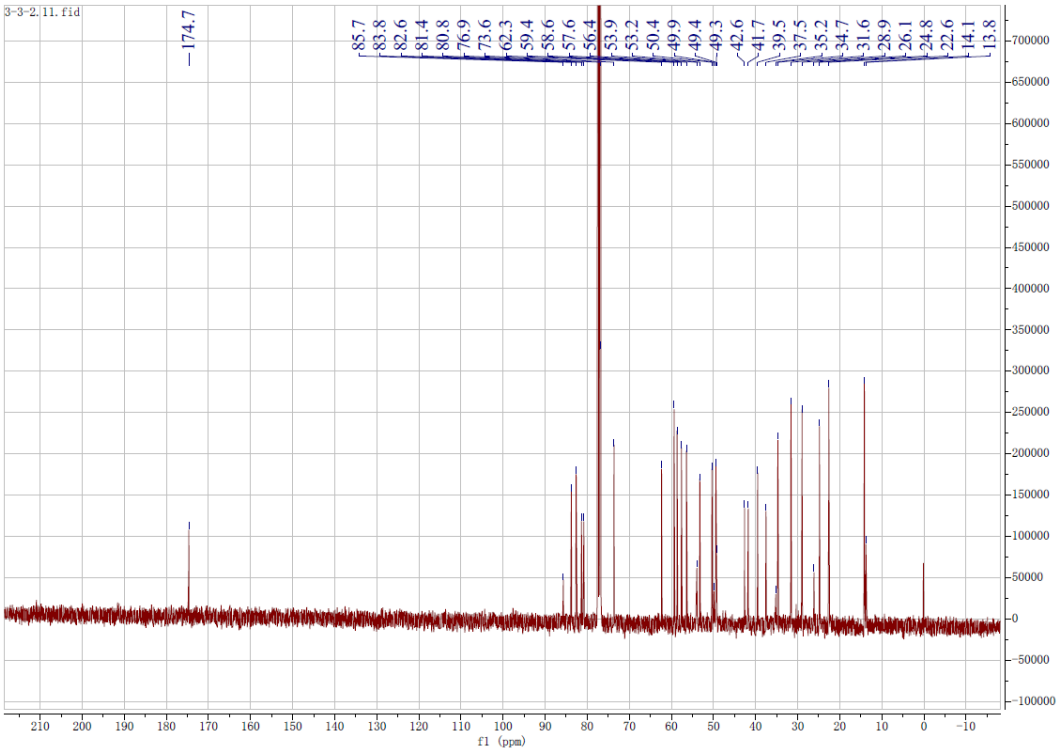


Figure S71. DEPT (θ = 135°) spectrum for compound **r** in $CDCl_3$.

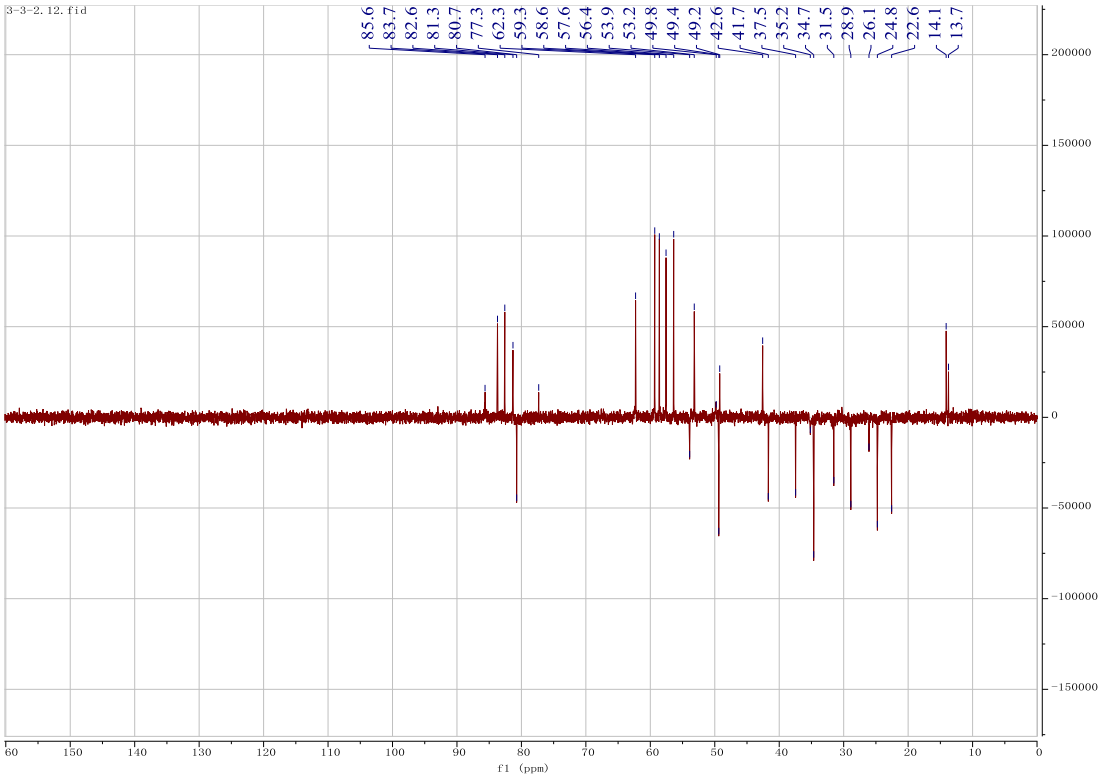
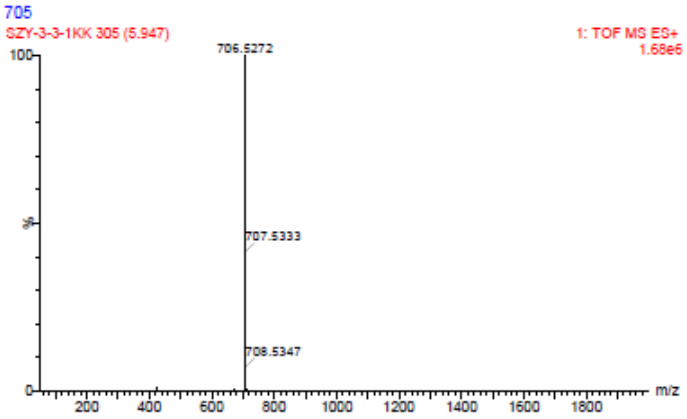


Figure S72. HR-ESI-MS spectrum for compoud **s**.



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

361 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 1-50 H: 1-100 N: 1-5 O: 1-10

Minimum:					-1.5	
Maximum:		5.0	10.0		50.0	
Mass	Calc. Mass	mDa		PPM	DBE	Formula
706.5272	706.5271	0.1	0.1	11.5		C42 H68 N5 O4
	706.5258	1.4	2.0	6.5		C41 H72 N O8
	706.5312	-4.0	-5.7	15.5		C47 H68 N3 O2

Figure S73. ^{1}H NMR spectrum for compoud **s** in $CDCl_3$ (400Hz).

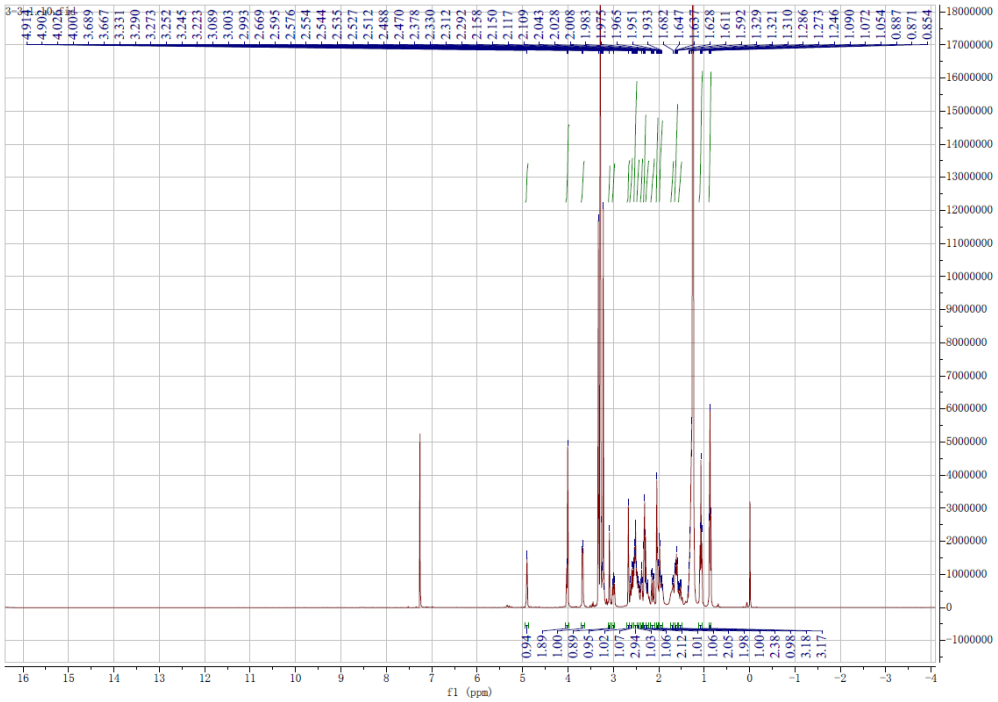


Figure S74. ^{13}C NMR spectrum for compoud **s** in $CDCl_3$ (100Hz).

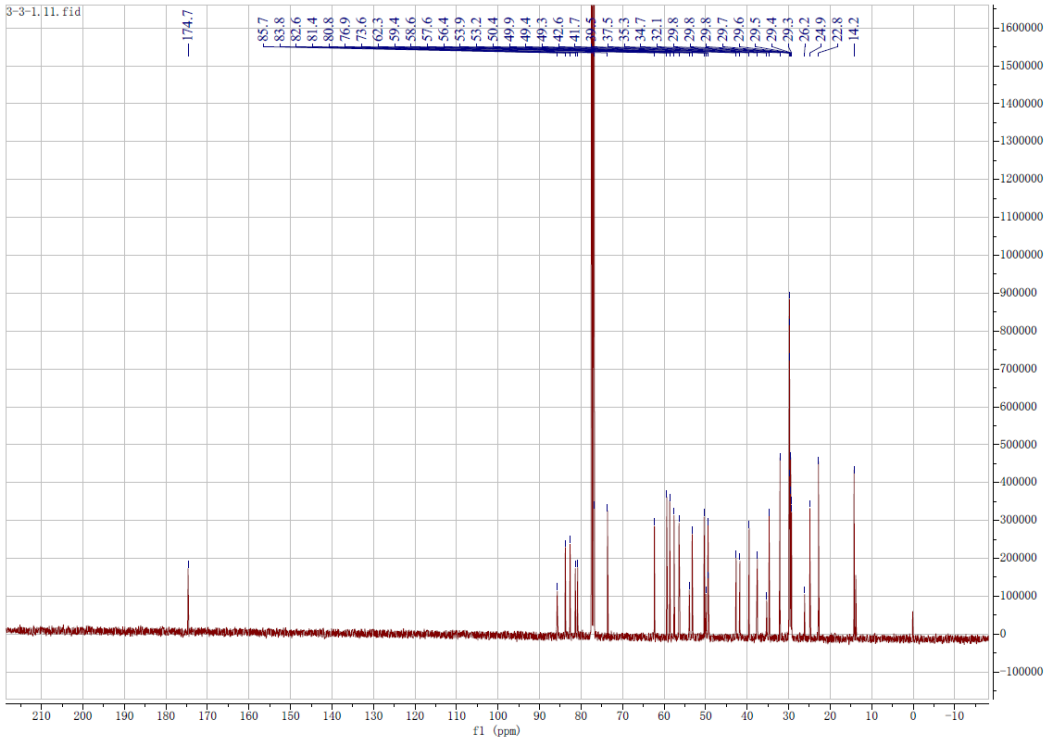


Figure S75. DEPT (θ = 135°) spectrum for compound **s** in $CDCl_3$.