Discovery of novel celastrol derivatives as Hsp90-Cdc37 interaction disruptors with antitumour activity

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Contents:

1. Spectral data.

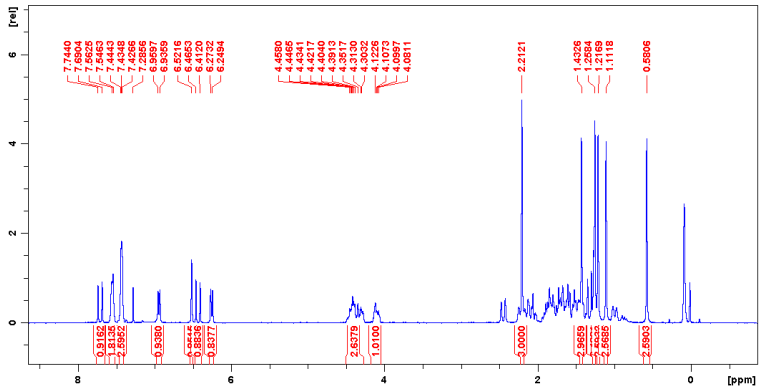


Fig. S1 ^{1}H NMR spectrum of **1** (300 MHz in $CDCl_3$)

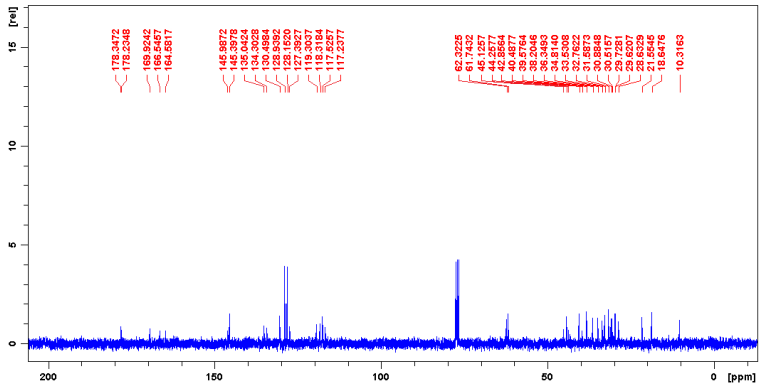
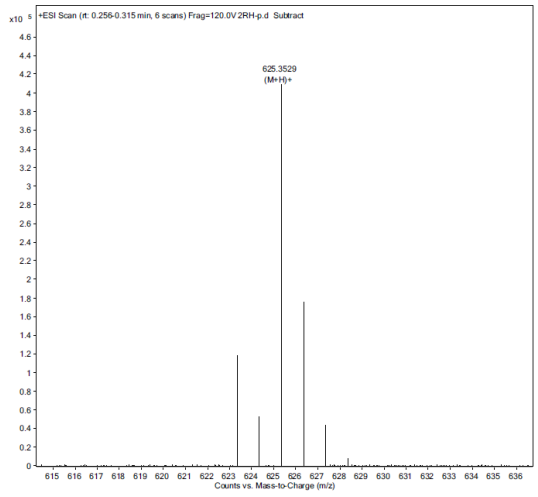


Fig. S2 ^{13}C NMR spectrum of **1** (75 MHz in $CDCl_3$)



Spectrum Identification Results: + Scan (rt: 0.256-0.315 min) Sub - 2RH-p.d (2RH-p.d)

Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C40 H48 O6	(M+H)+	625.3529	99.38	-0.54	0.54	-0.34	99.38	624.3456	624.3451	17

Fig. S3 ESI/HREMS spectrum of **1**

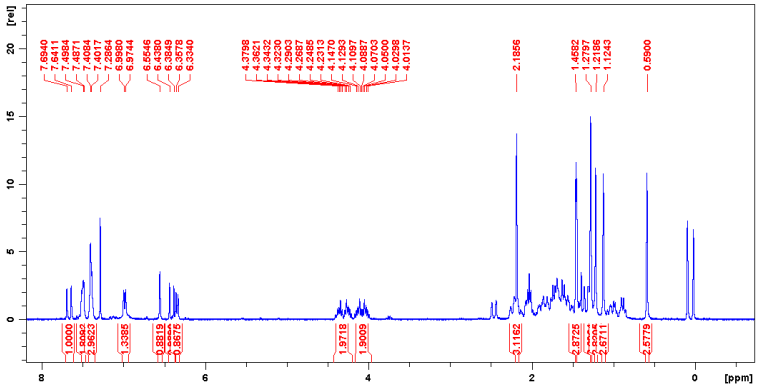


Fig. S4. ^{1}H NMR spectrum of **2** (300 MHz in $CDCl_3$)

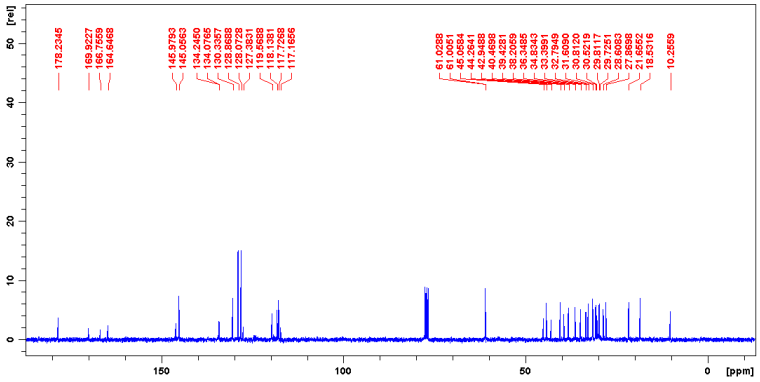
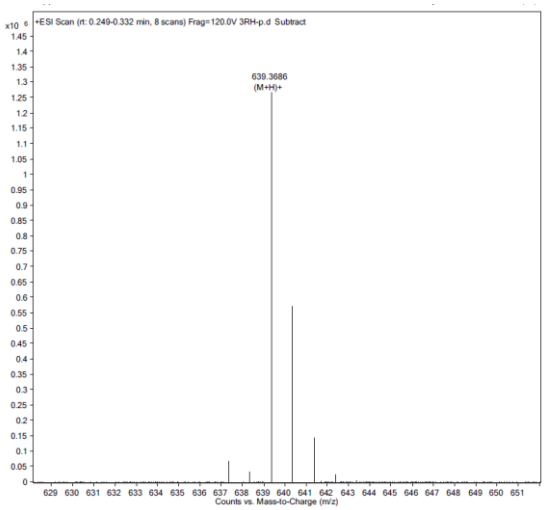


Fig. S5. ^{13}C NMR spectrum of **2** (75 MHz in $CDCl_3$)



Spectrum Identification Results: + Scan (rt: 0.249-0.332 min) Sub - 3RH-p.d (3RH-p.d)

Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C41 H50 O6	(M+H)+	639.3686	98.65	-1.29	1.29	-0.82	98.65	638.3616	638.3607	17

Fig. S6 ESI/HRMS spectrum of **2**

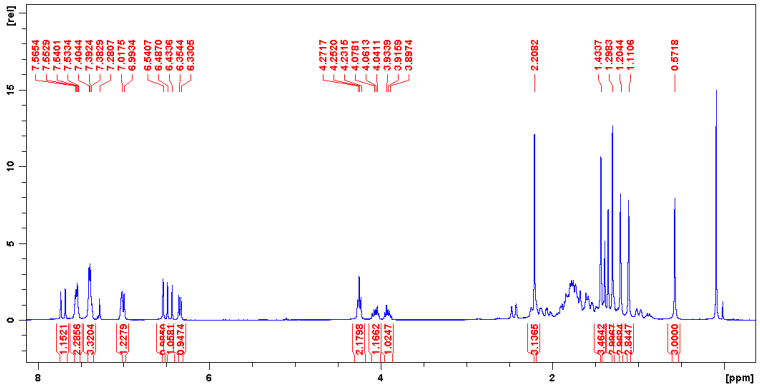


Fig. S7 ^{1}H NMR spectrum of **3** (300 MHz in $CDCl_3$)

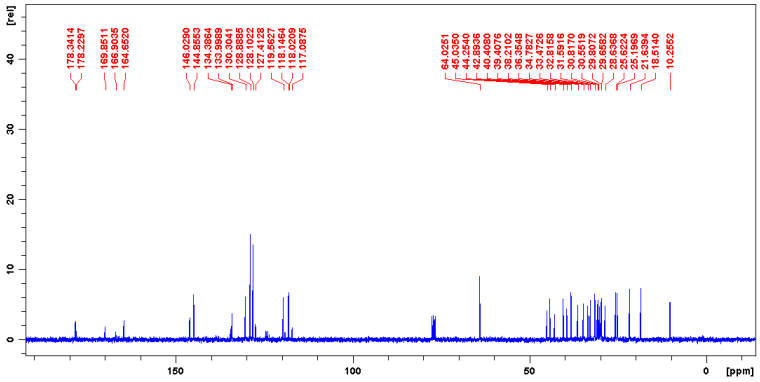
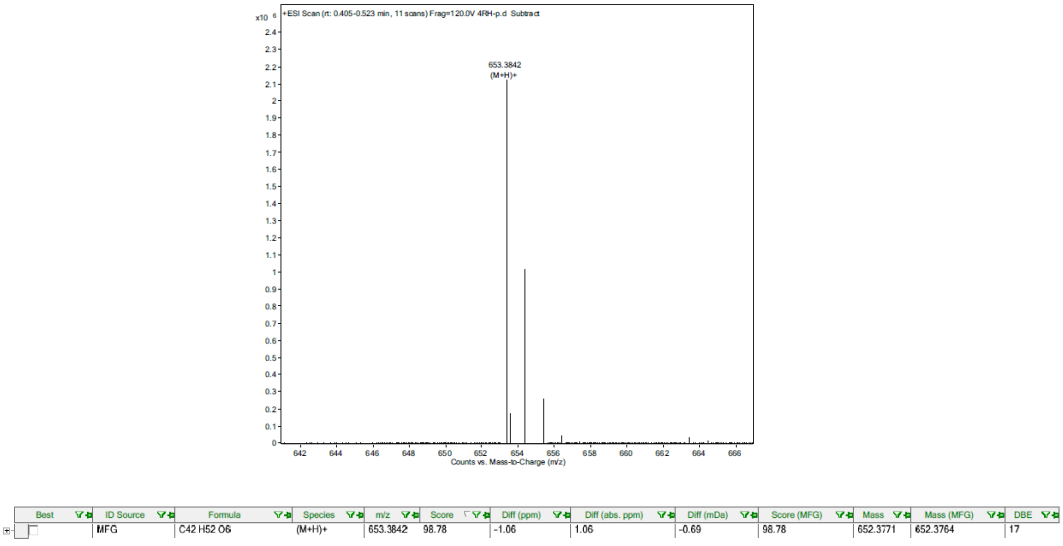


Fig. S8 ^{13}C NMR spectrum of **3** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C42 H52 O6	(M+H)+	653.3842	98.78	-1.06	1.06	-0.69	98.78	652.3771	652.3764	17

Fig. S9 ESI/HRMS spectrum of **3**

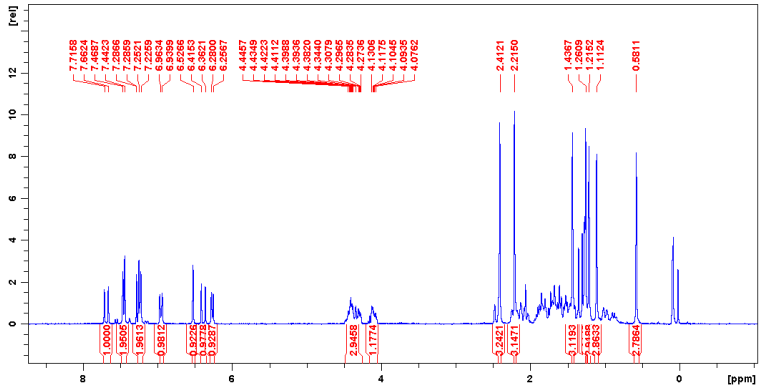


Fig. S10 ^{1}H NMR spectrum of **4** (300 MHz in $CDCl_3$)

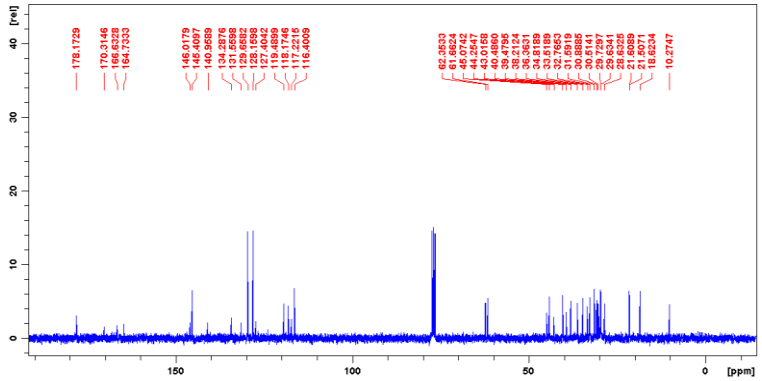
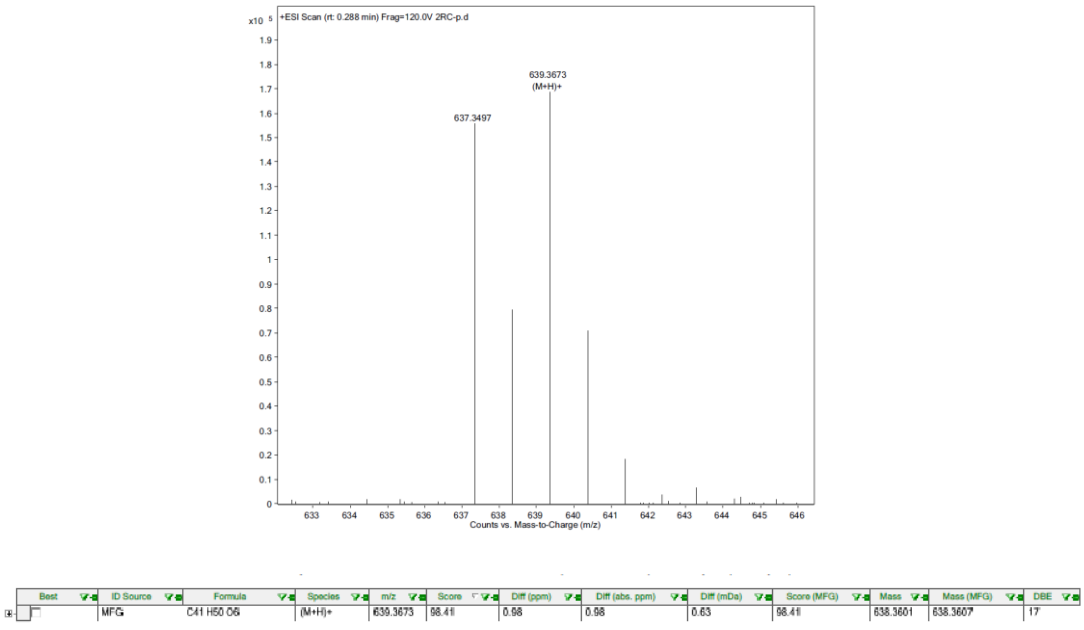


Fig. S11 ^{13}C NMR spectrum of **4** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C41 H50 O6	(M+H)+	639.3673	98.41	0.98	0.98	0.63	98.41	638.3601	638.3607	17

Fig. S12 ESI/HRMS spectrum of **4**

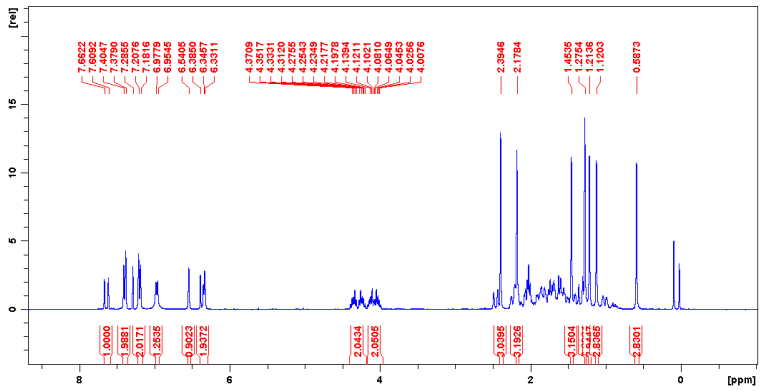


Fig. S13 ^{1}H NMR spectrum of **5** (300 MHz in $CDCl_3$)

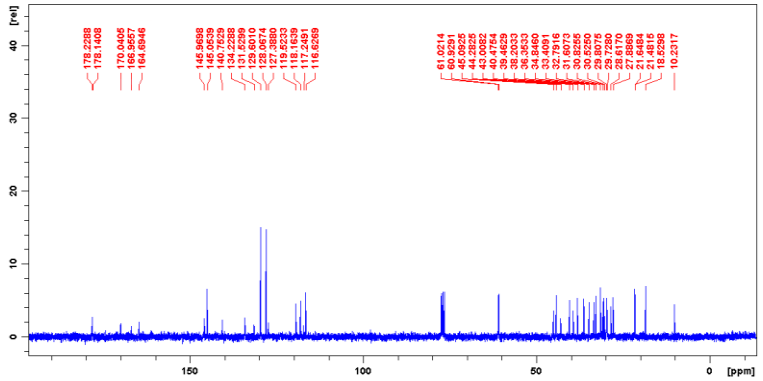
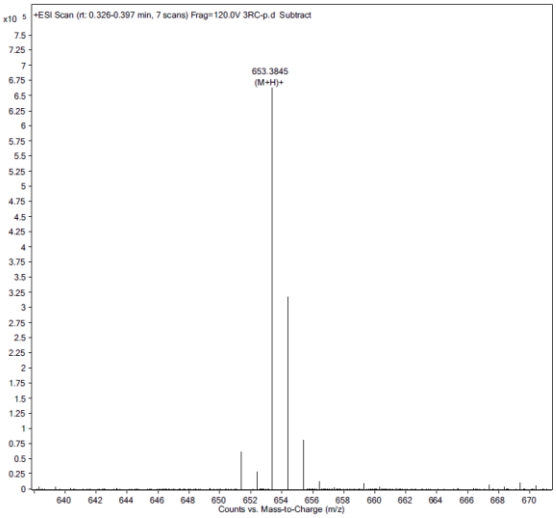


Fig. S14 ^{13}C NMR spectrum of **5** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C42 H52 O6	(M+H)+	653.3845	95.18	0.02	0.02	0.02	95.18	652.3764	652.3764	17

Fig. S15 ESI/HREMS spectrum of **5**

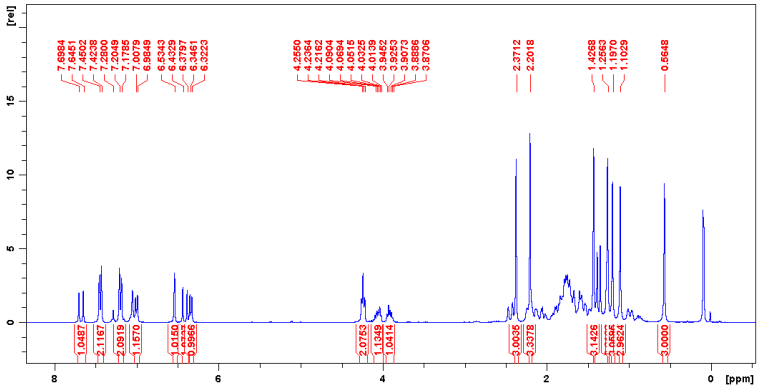


Fig. S16 ^{1}H NMR spectrum of **6** (300 MHz in $CDCl_3$)

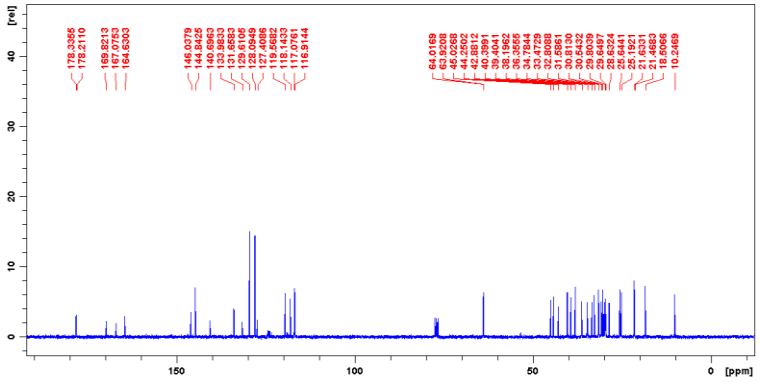
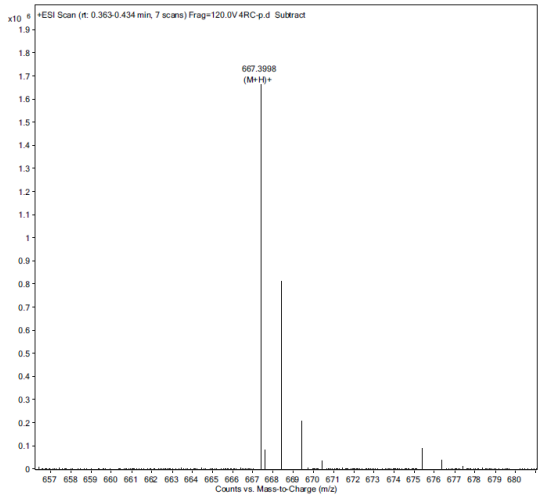


Fig. S17 ^{13}C NMR spectrum of **6** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C43 H54 O6	(M+H)+	667.3998	98.59	-1.07	1.07	-0.71	98.59	666.3928	666.392	17

Fig. S18 ESI/HREMS spectrum of **6**

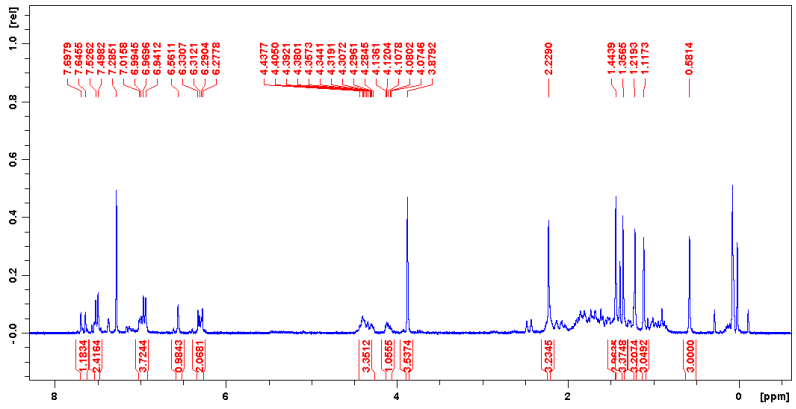


Fig. S19 ^{1}H NMR spectrum of **7** (300 MHz in $CDCl_3$)

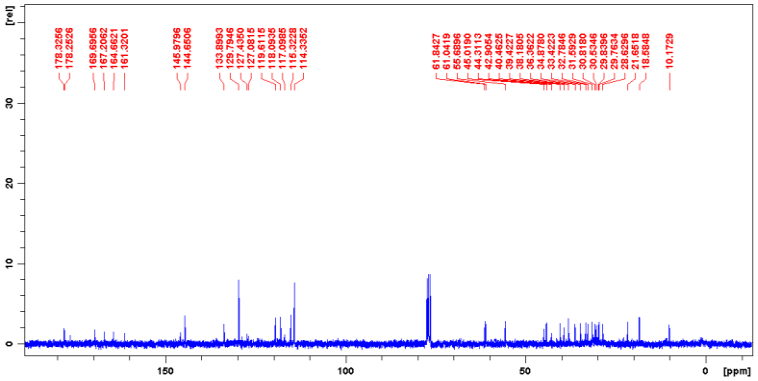
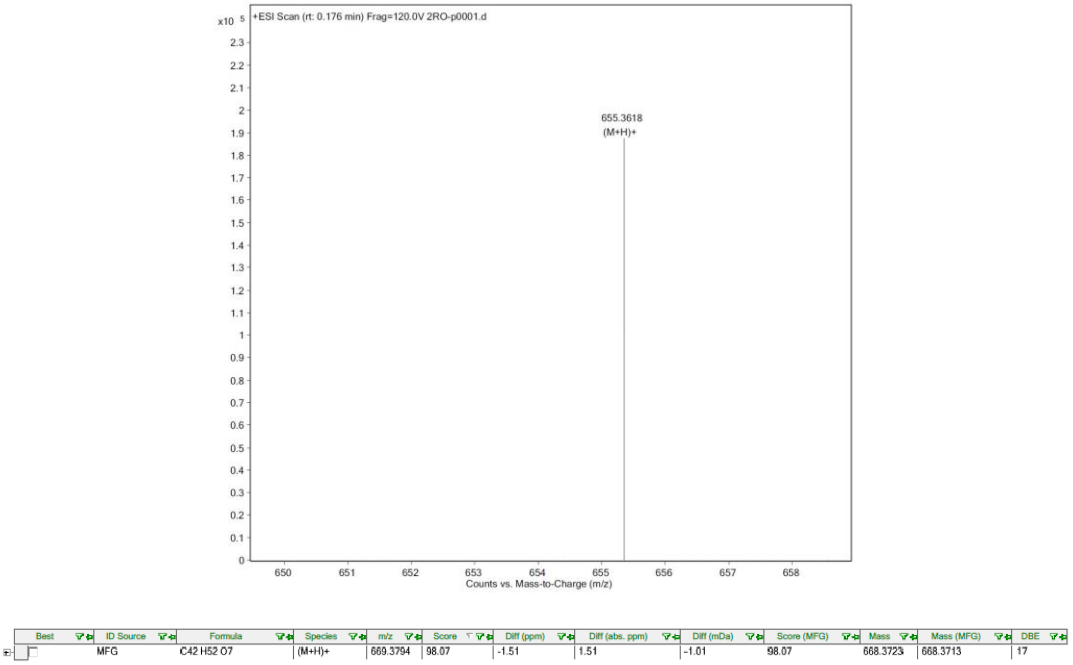


Fig. S20 ^{13}C NMR spectrum of **7** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C42 H52 O7	(M+H)+	669.3794	98.07	-1.51	1.51	-1.01	98.07	668.3723	668.3713	17

Fig. S21 ESI/HRMS spectrum of **7**

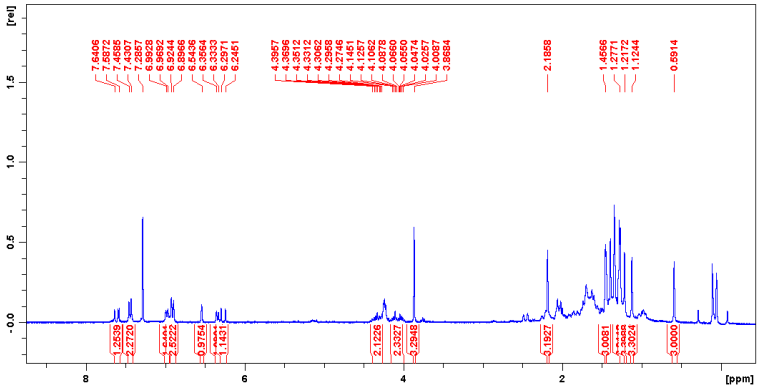


Fig. S22 ^{1}H NMR spectrum of **8** (300 MHz in $CDCl_3$)

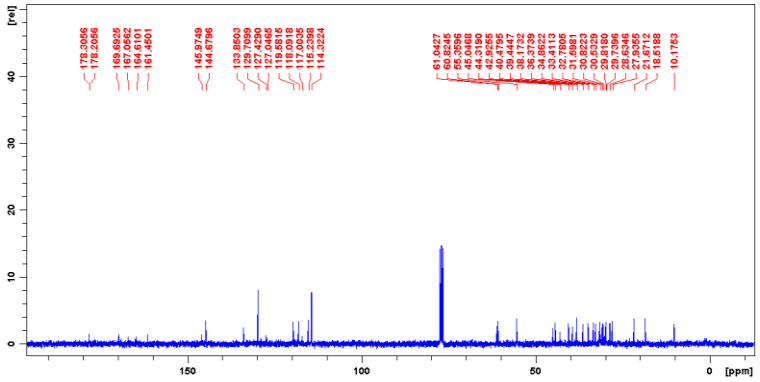
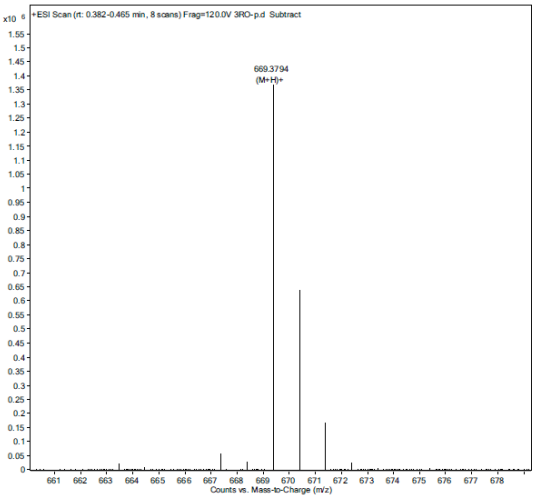


Fig. S23 ^{13}C NMR spectrum of **8** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C42 H52 O7	(M+H)+	669.3794	98.07	-1.51	1.51	-1.01	98.07	668.3723	668.3713	17

Fig. S24 ESI/HRMS spectrum of **8**

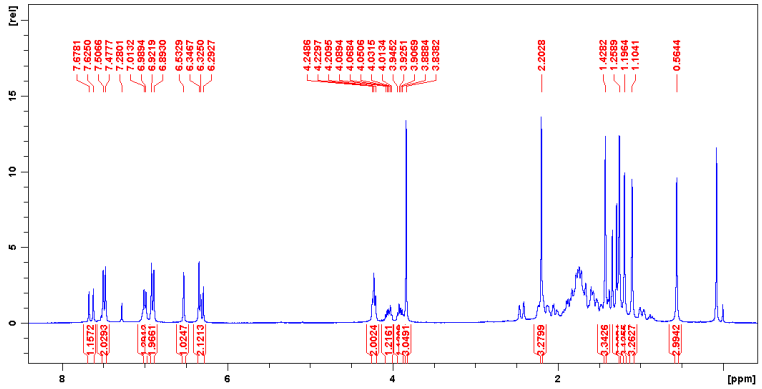


Fig. S25 ^{1}H NMR spectrum of **9** (300 MHz in $CDCl_3$)

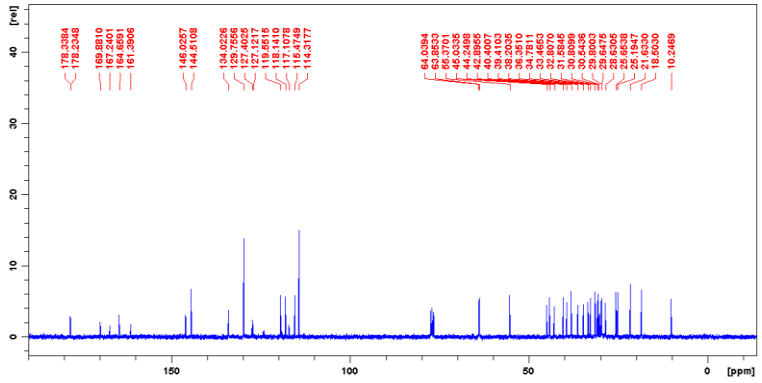
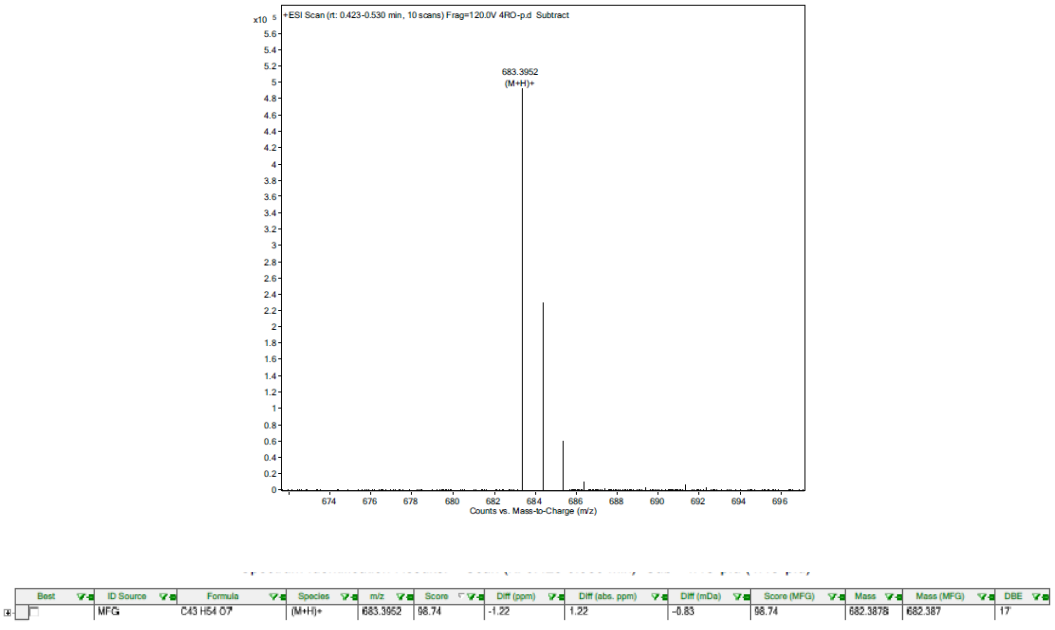


Fig. S26 ^{13}C NMR spectrum of **9** (75 MHz in DMSO-d_6)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C43 H54 O7	(M+H)+	683.3952	98.74	-1.22	1.22	-0.83	98.74	682.3878	682.387	17

Fig. S27 ESI/HRMS spectrum of **9**

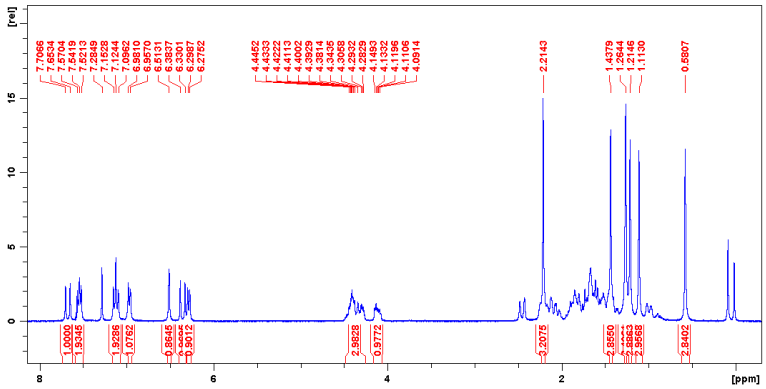


Fig. S28 ^{1}H NMR spectrum of **10** (300 MHz in $CDCl_3$)

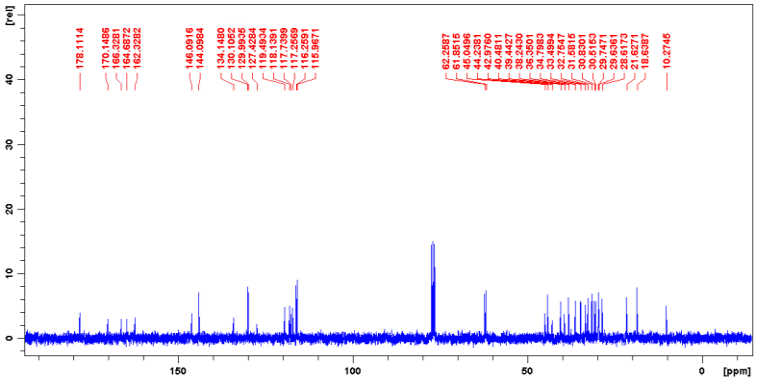
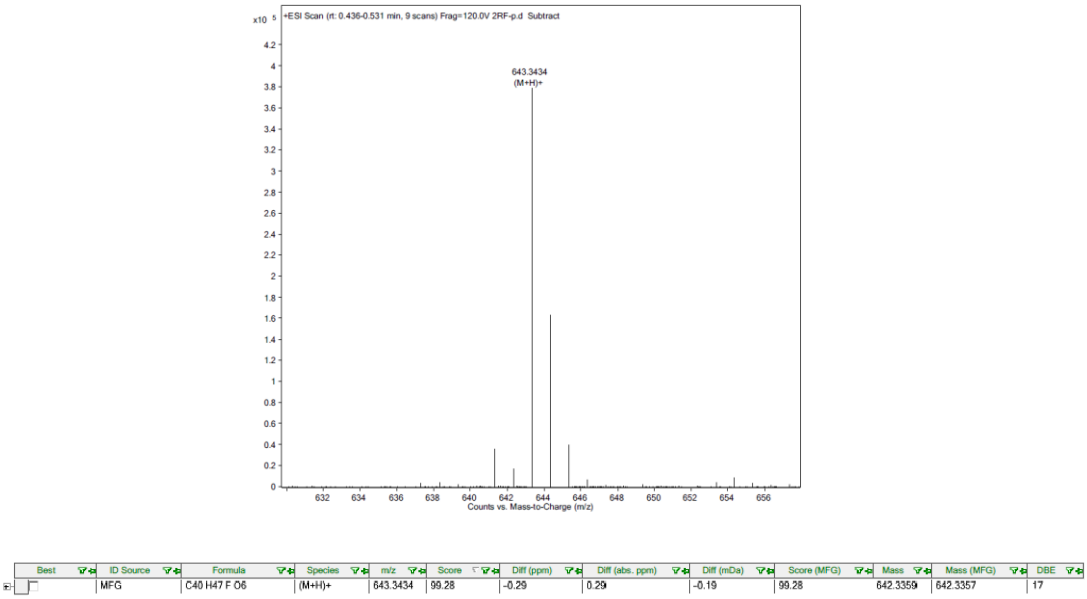


Fig. S29 ^{13}C NMR spectrum of **10** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C40 H47 F O6	(M+H)+	643.3434	99.28	-0.29	0.29	-0.19	99.28	642.3359	642.3357	17

Fig. S30 ESI/HRMS spectrum of **10**

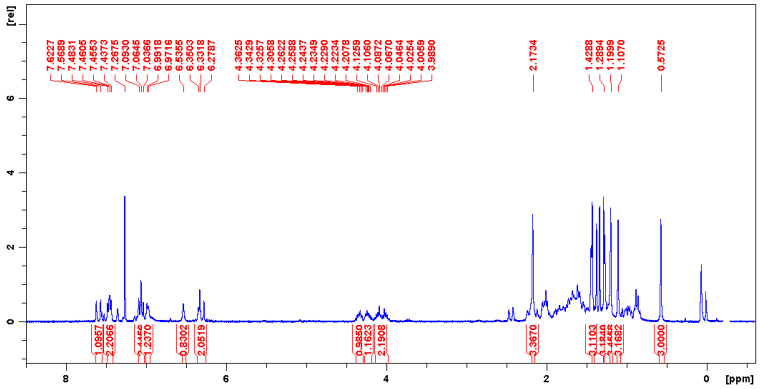


Fig. S31 ^{1}H NMR spectrum of **11** (300 MHz in $CDCl_3$)

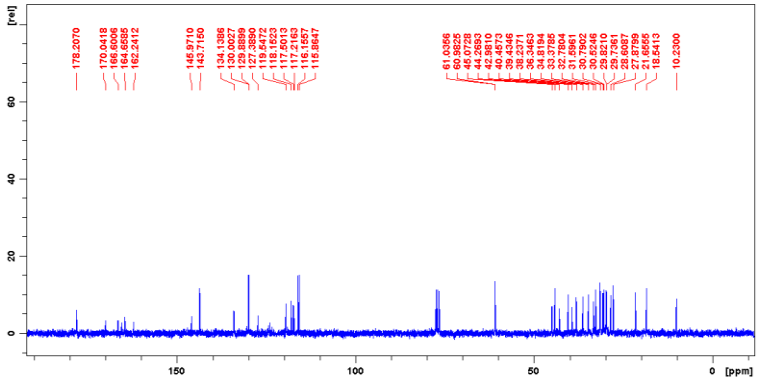
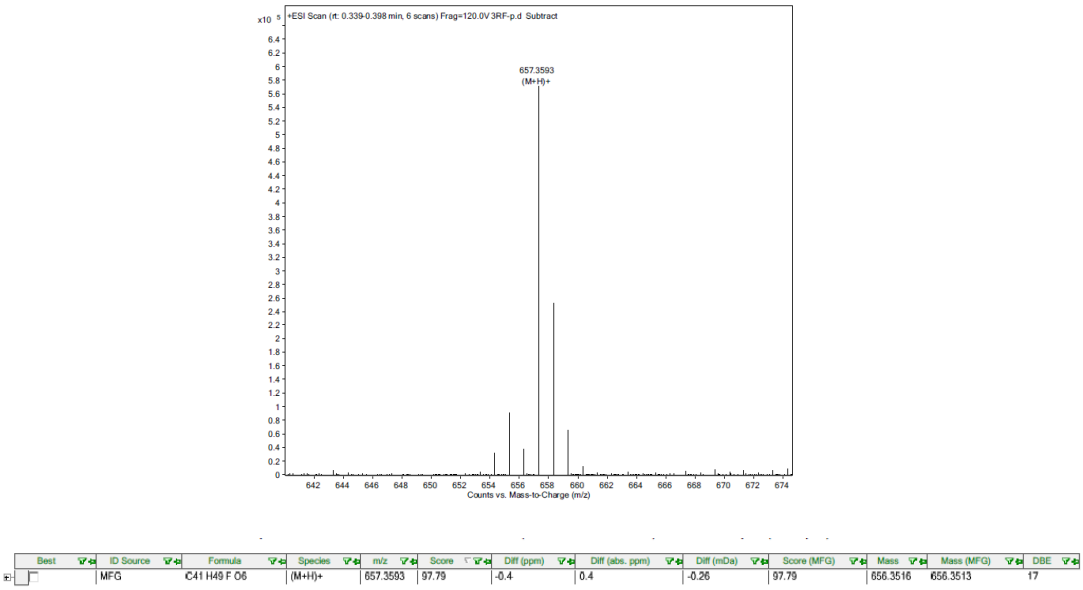


Fig. S32 ^{13}C NMR spectrum of **11** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C41 H49 F O6	(M+H)+	657.3593	97.79	-0.4	0.4	-0.26	97.79	656.3516	656.3513	17

Fig. S33 ESI/HRMS spectrum of **11**

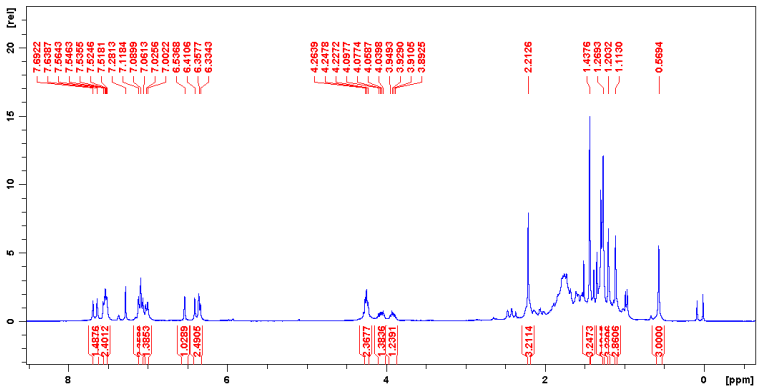


Fig. S34. ^{1}H NMR spectrum of **12** (300 MHz in $CDCl_3$)

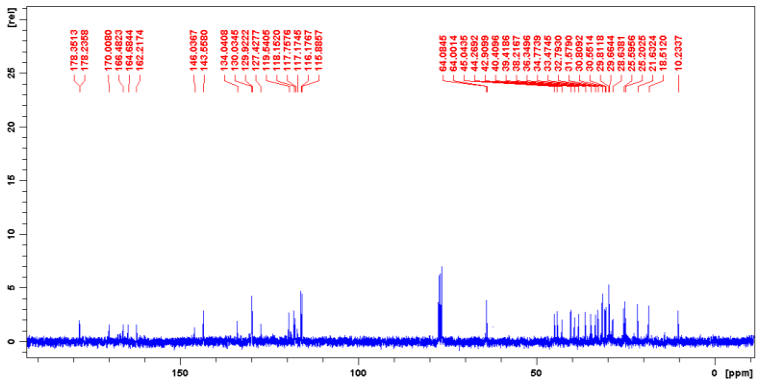
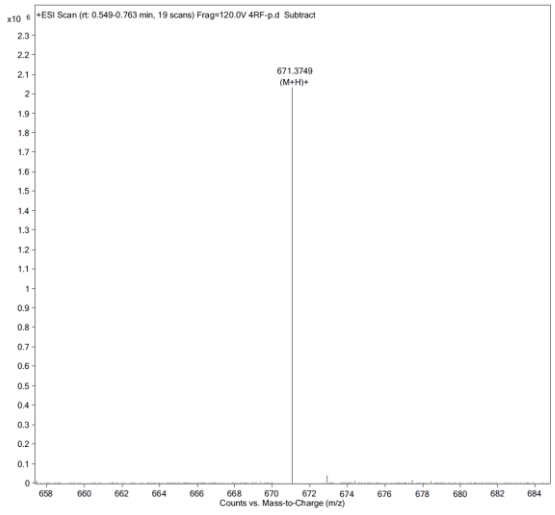


Fig. S35. ^{13}C NMR spectrum of **12** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C42 H52 F O6	(M+H)+	671.3749	99.18	-0.77	0.77	-0.56	69.18	670.3643	670.3638	17

Fig. S36 ESI/HRMS spectrum of **12**

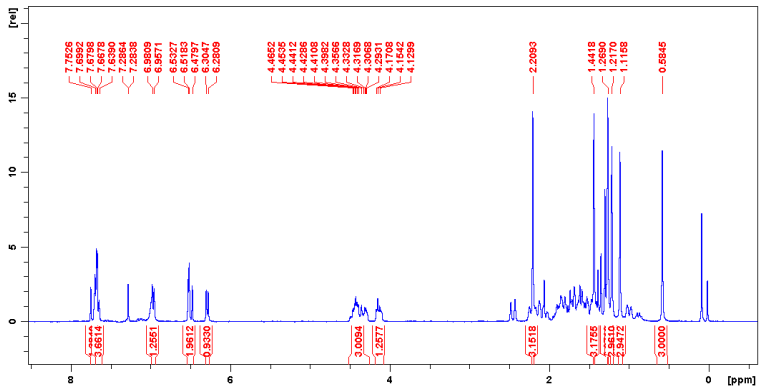


Fig. S37 ^{1}H NMR spectrum of **13** (300 MHz in $CDCl_3$)

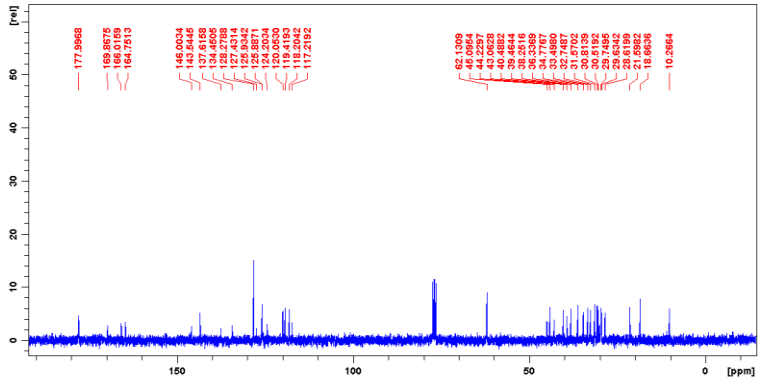
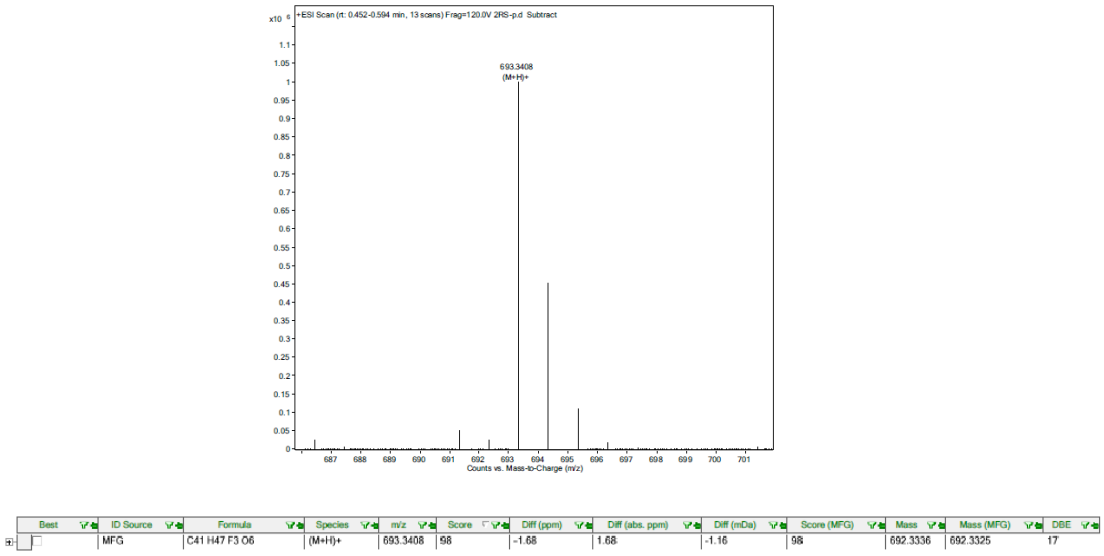


Fig. S38 ^{13}C NMR spectrum of **13** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C41 H47 F3 O6	(M+H)+	693.3408	98	-1.68	1.68	-1.16	98	692.3336	692.3325	17

Fig. S39 ESI/HRMS spectrum of **13**

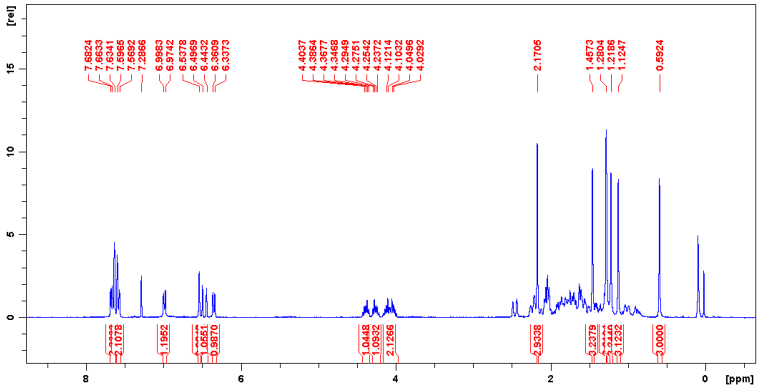


Fig. S40 ^{1}H NMR spectrum of **14** (300 MHz in $CDCl_3$)

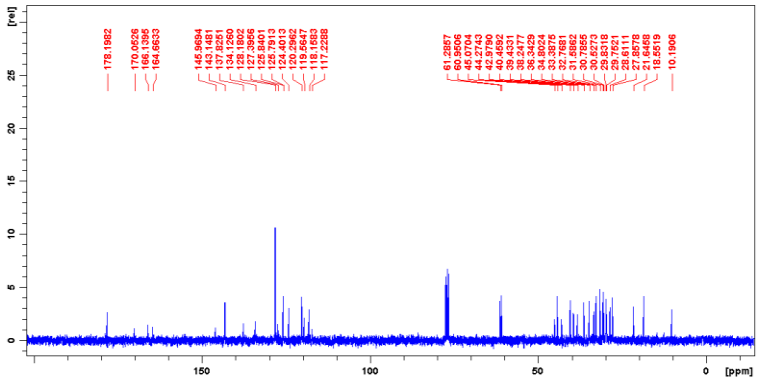
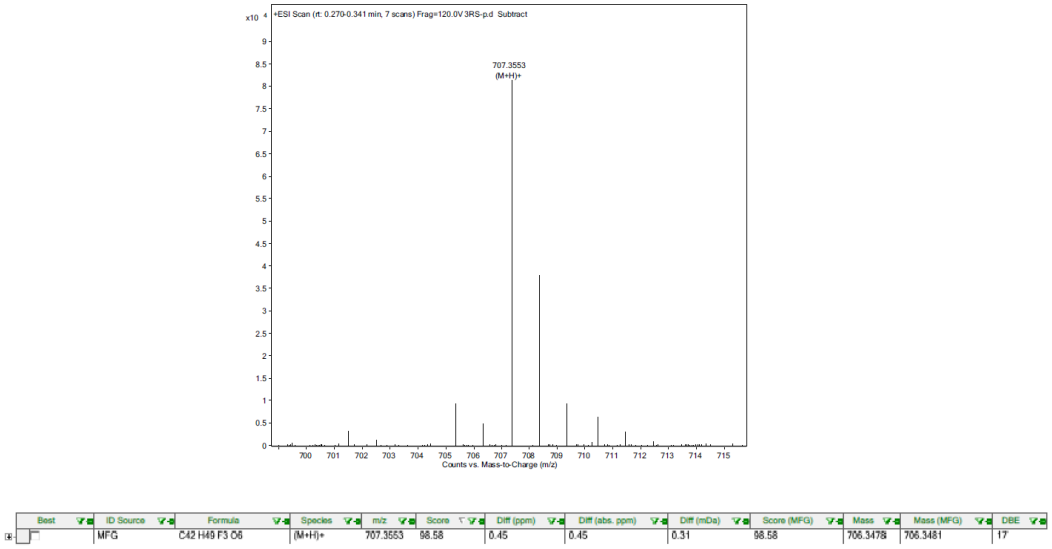


Fig. S41 ^{13}C NMR spectrum of **14** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C42 H49 F3 O6	(M+H)+	707.3553	98.58	0.45	0.45	0.31	98.58	706.3478	706.3481	17

Fig. S42 ESI/HRMS spectrum of **14**

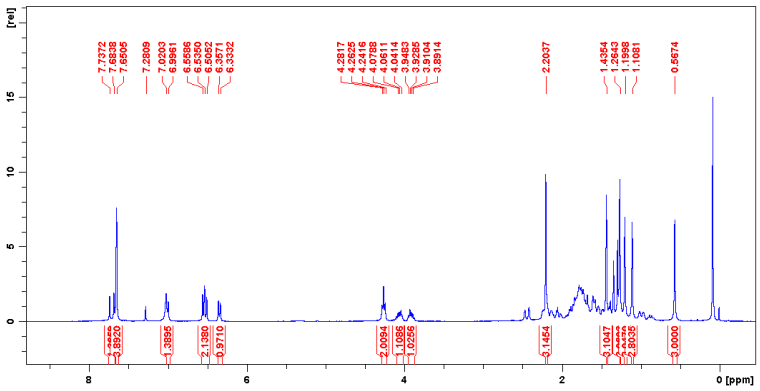


Fig. S43 ^{1}H NMR spectrum of **15** (300 MHz in $CDCl_3$)

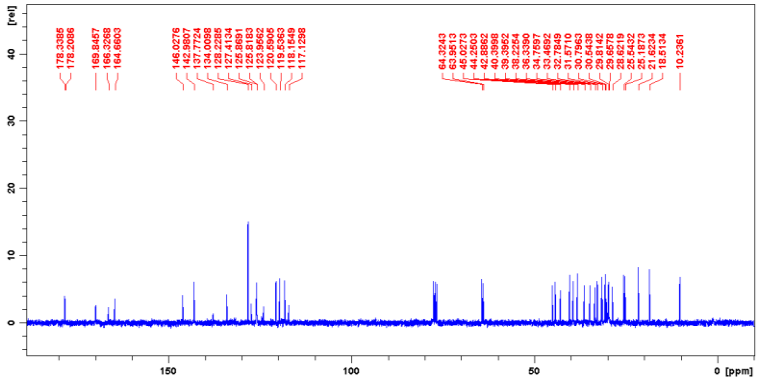
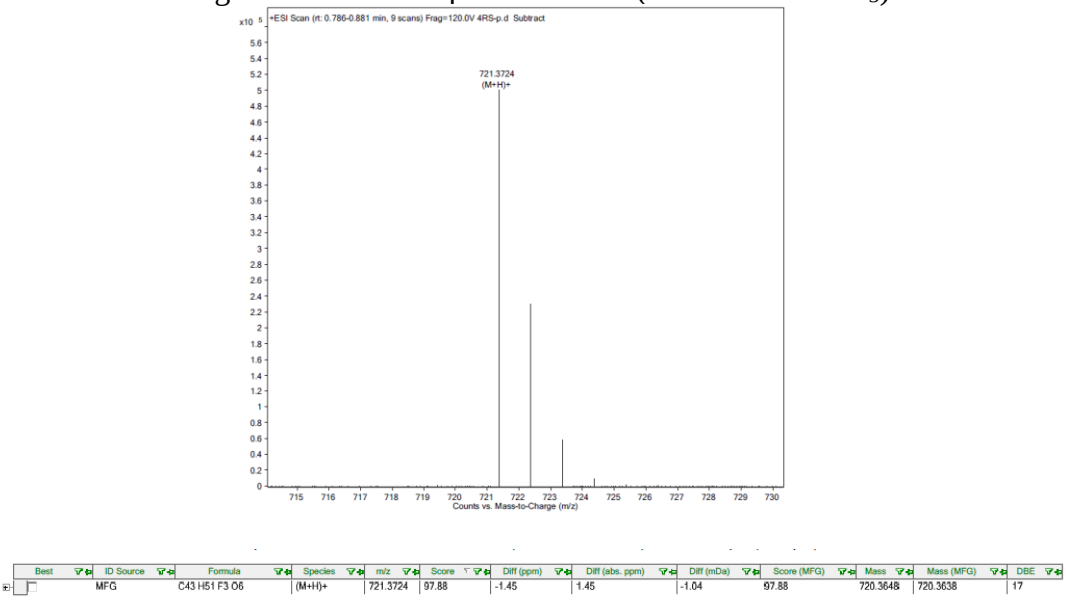


Fig. S44 ^{13}C NMR spectrum of **15** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C43 H51 F3 O6	(M+H)+	721.3724	97.88	-1.45	1.45	-1.04	97.88	720.3648	720.3638	17

Fig. S45 ESI/HRMS spectrum of **15**

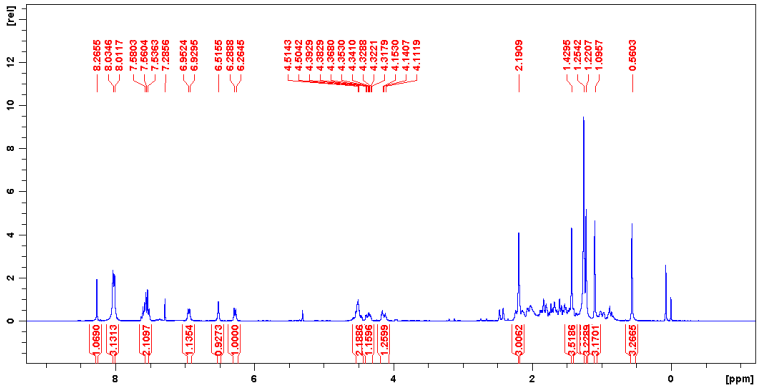


Fig. S46 ^{1}H NMR spectrum of **16** (300 MHz in $CDCl_3$)

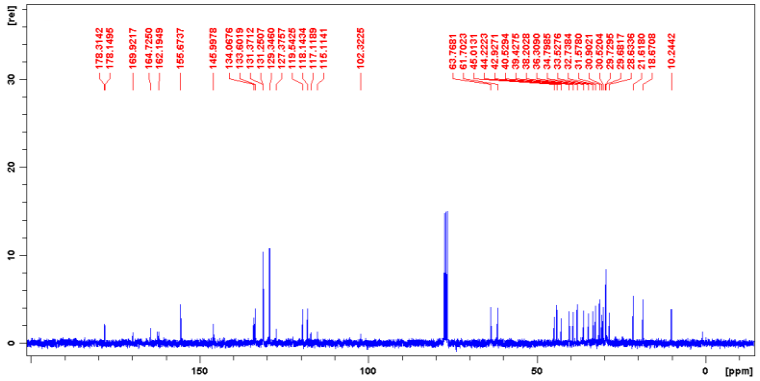
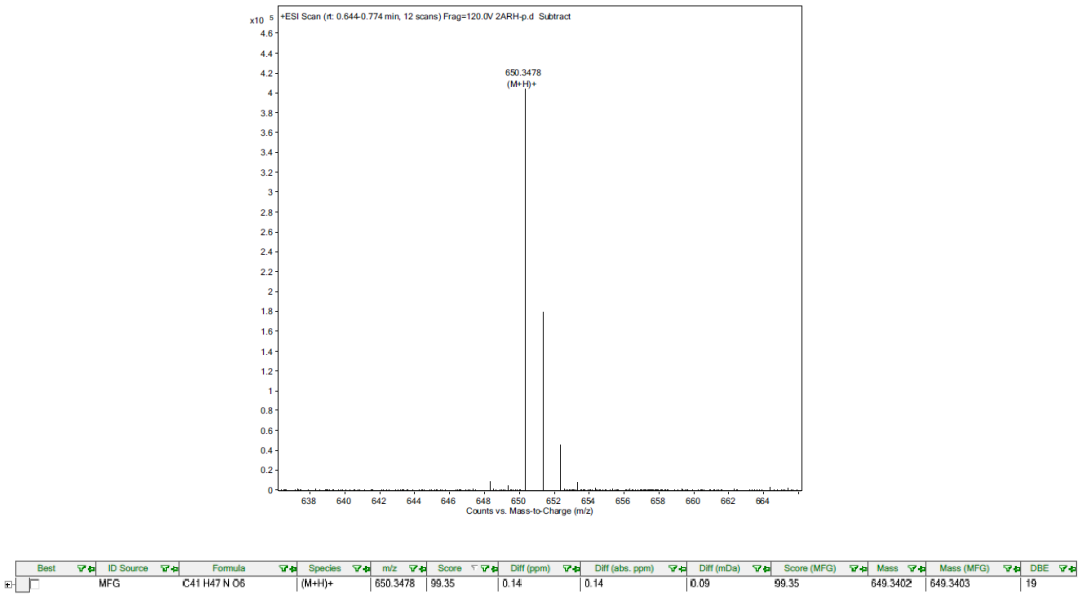


Fig. S47 ^{13}C NMR spectrum of **16** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C41 H47 N O6	(M+H)+	650.3478	99.35	0.14	0.14	0.09	99.35	649.3402	649.3403	19

Fig. S48 ESI/HRMS spectrum of **16**

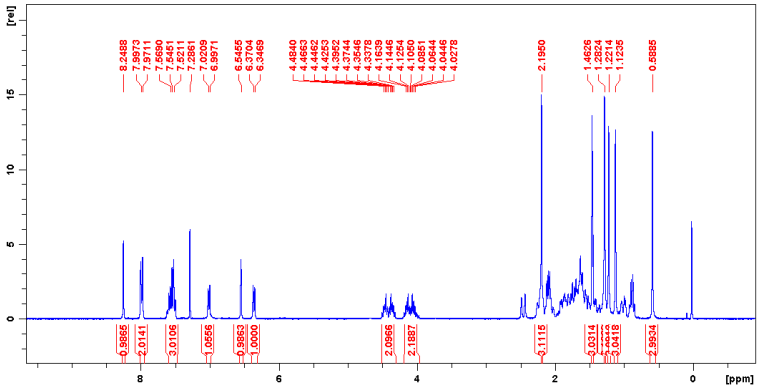


Fig. S49 ^{1}H NMR spectrum of **17** (300 MHz in $CDCl_3$)

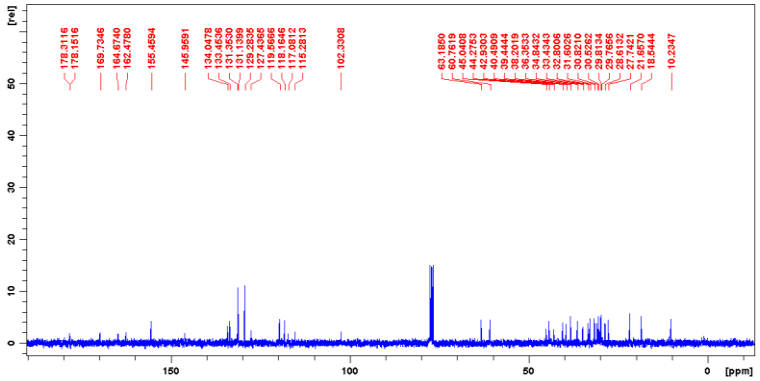
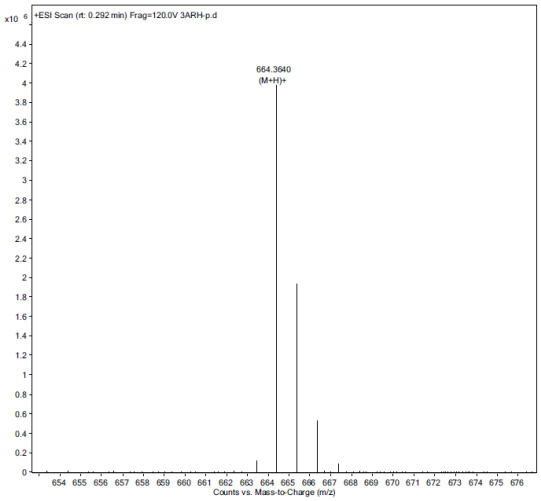


Fig. S50 ^{13}C NMR spectrum of **17** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C42 H49 N O6	(M+H)+	664.3640	98.8	-0.87	0.87	-0.58	98.8	663.3566	663.356	19

Fig. S51 ESI/HRMS spectrum of **17**

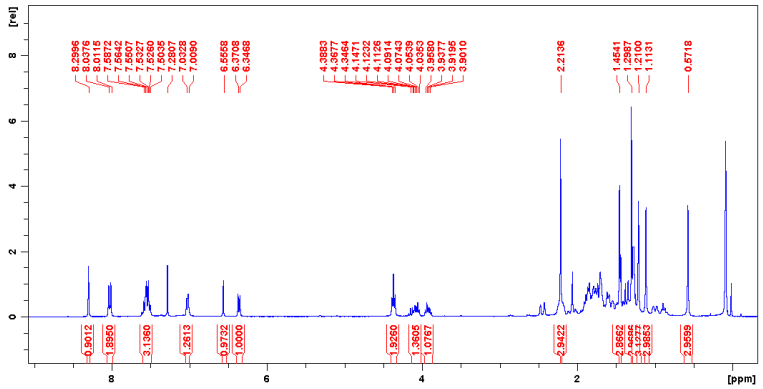


Fig. S52 ^{1}H NMR spectrum of **18** (300 MHz in $CDCl_3$)

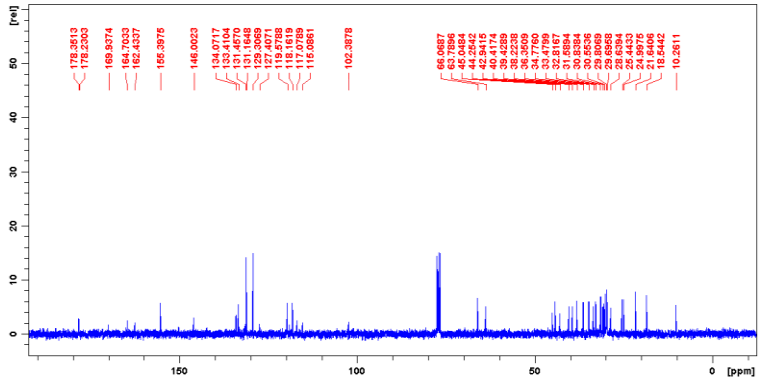
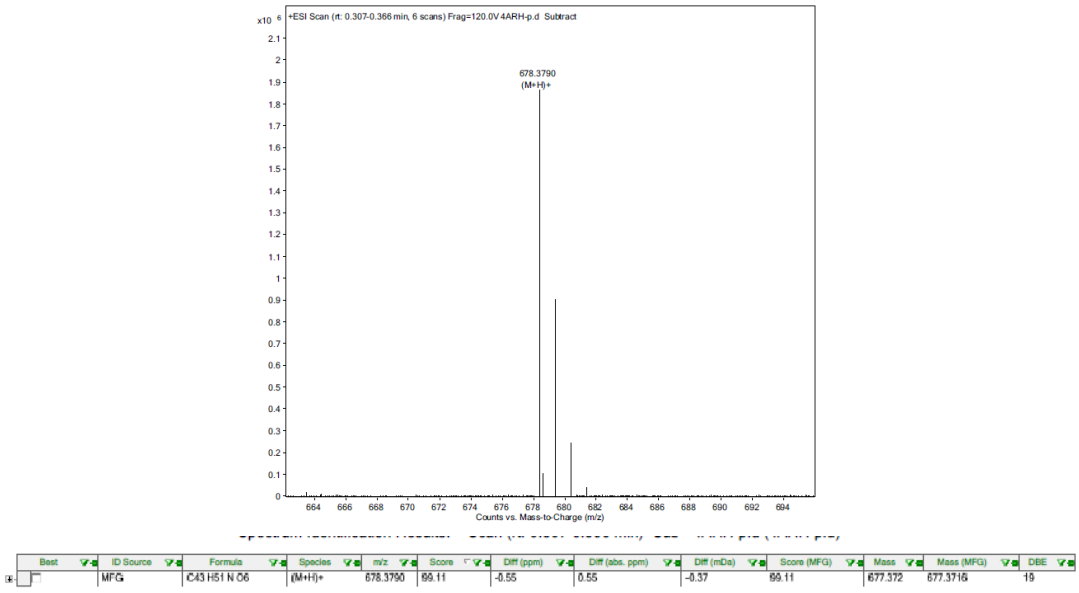


Fig. S53 ^{13}C NMR spectrum of **18** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C43 H51 N O6	(M+H)+	678.3790	99.11	-0.55	0.55	-0.37	99.11	677.372	677.3716	19

Fig. S54 ESI/HRMS spectrum of **18**

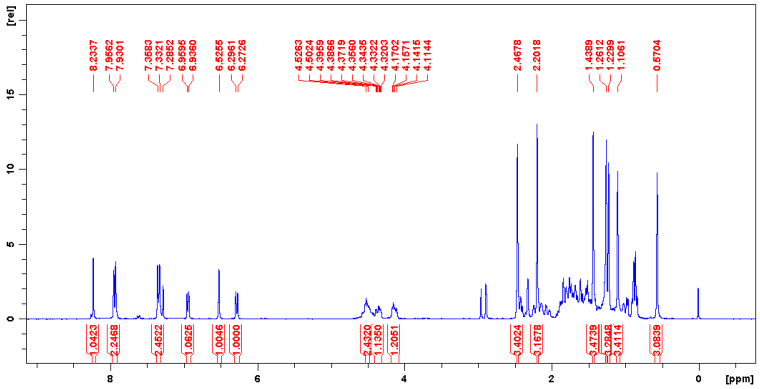


Fig. S55 ^{1}H NMR spectrum of **19** (300 MHz in $CDCl_3$)

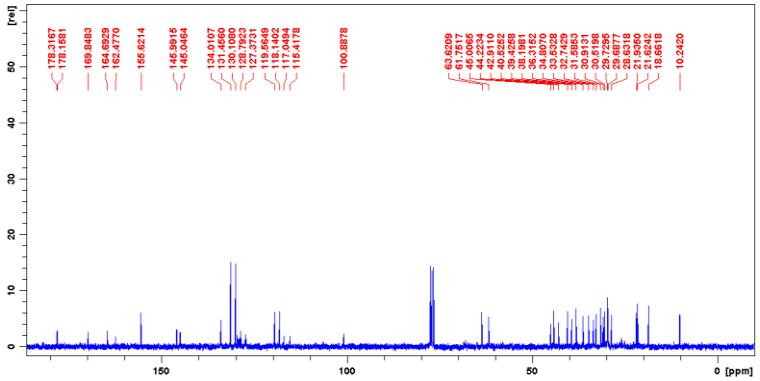
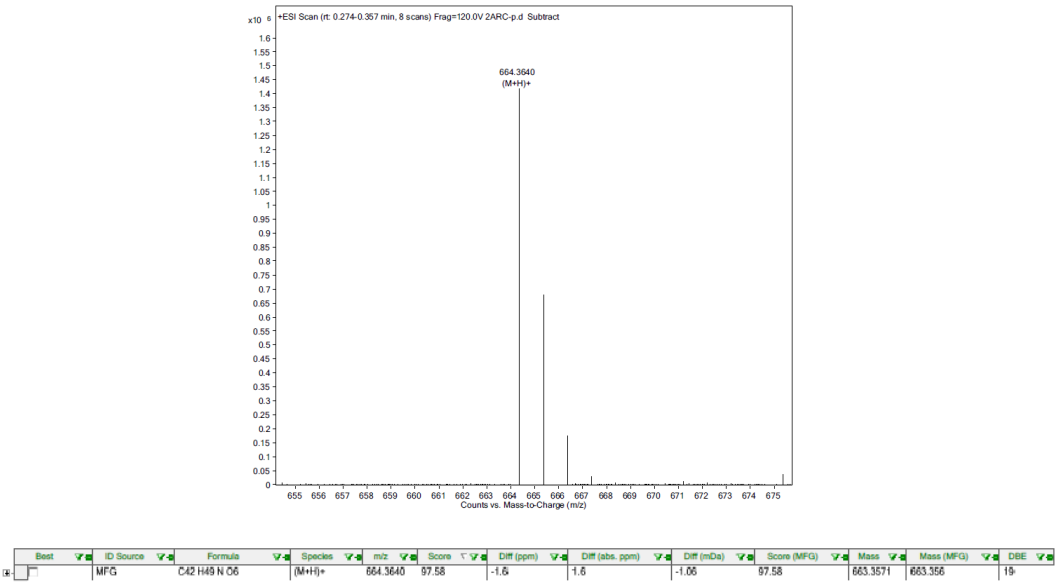


Fig. S56 ^{13}C NMR spectrum of **19** (75 MHz in DMSO-d_6)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C42 H49 N O6	(M+H)+	664.3640	97.58	-1.6	1.6	-1.06	97.58	663.3571	663.356	19

Fig. S57 ESI/HRMS spectrum of **19**

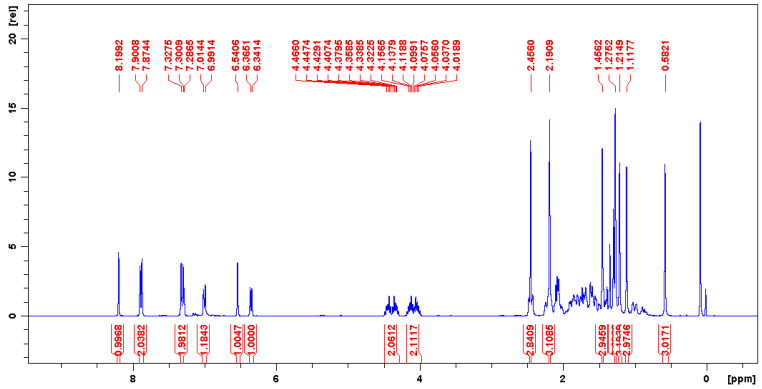


Fig. S58 ^{1}H NMR spectrum of **20** (300 MHz in $CDCl_3$)

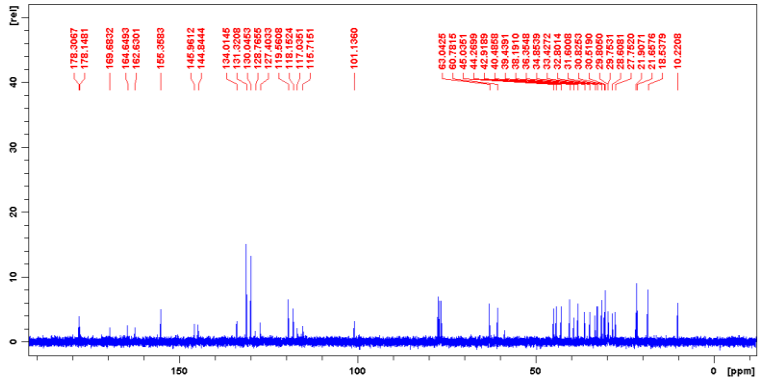
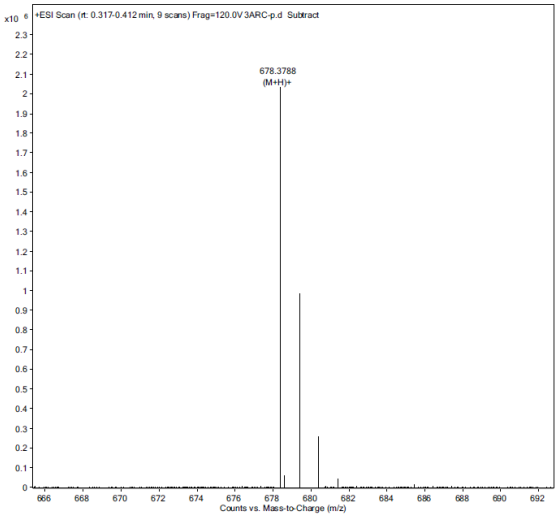


Fig. S59 ^{13}C NMR spectrum of **20** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C43 H51 N O6	(M+H)+	678.3788	99.4	-0.3	0.3	-0.2	99.4	677.3716	677.3716	19

Fig. S60 ESI/HRMS spectrum of **20**

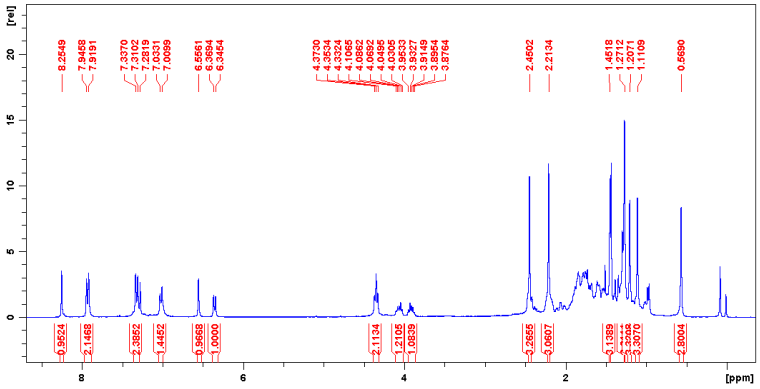


Fig. S61 ^{1}H NMR spectrum of **21** (300 MHz in $CDCl_3$)

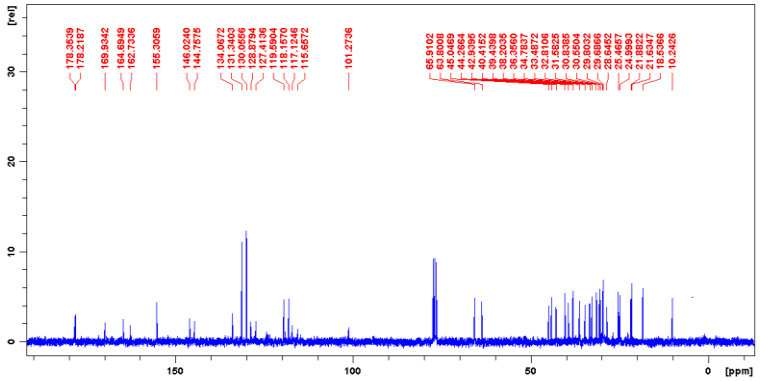


Fig. S62 ^{13}C NMR spectrum of **21** (75 MHz in $CDCl_3$)

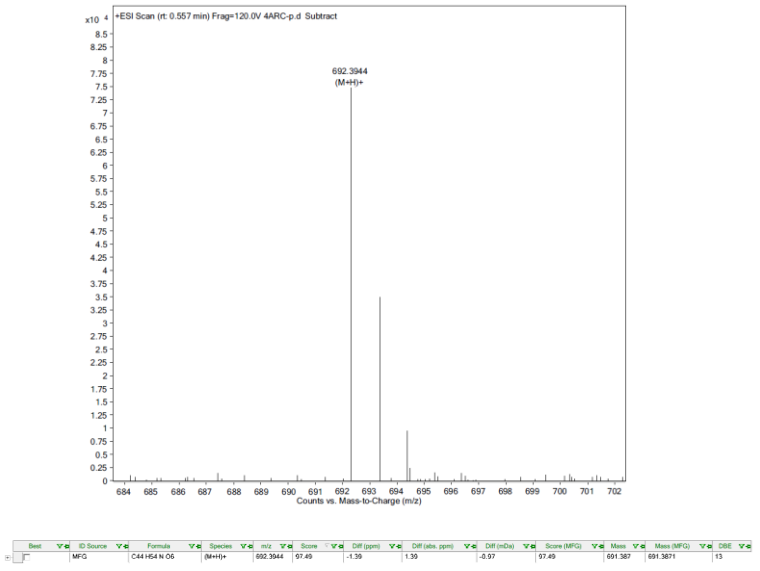


Fig. S63 ESI/HRMS spectrum of **21**

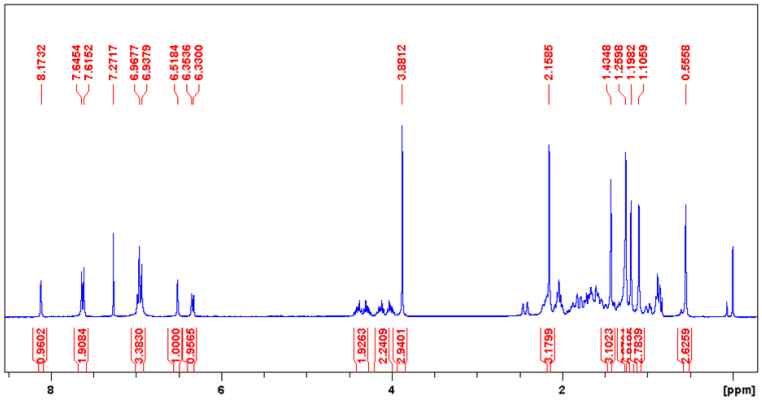


Fig. S64. ^{1}H NMR spectrum of **22** (300 MHz in $CDCl_3$)

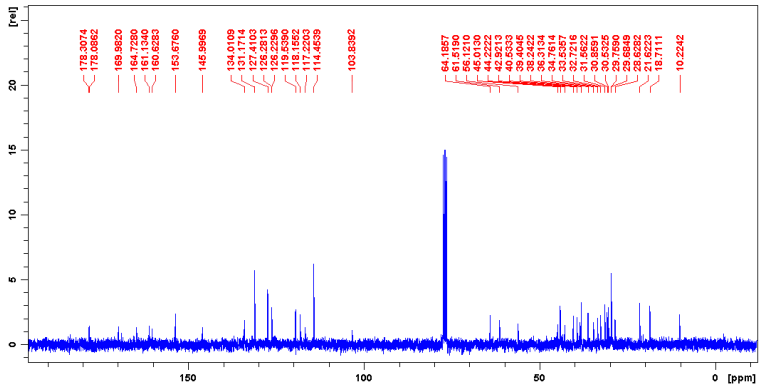
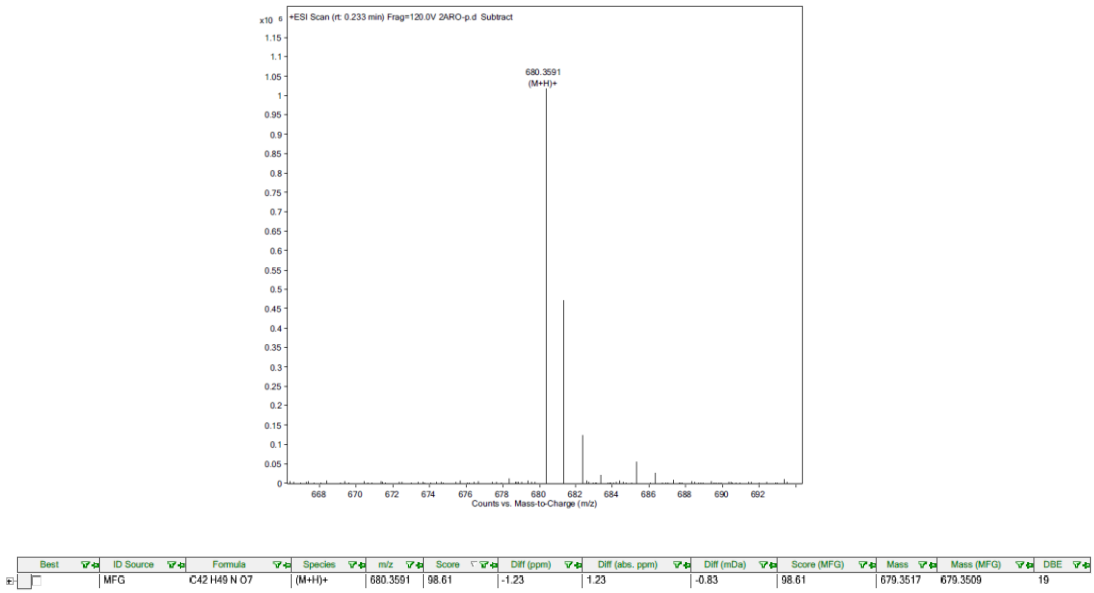


Fig. S65. ^{13}C NMR spectrum of **22** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C42 H49 N O7	(M+H)+	680.3591	98.61	-1.23	1.23	-0.83	98.61	679.3517	679.3509	19

Fig. S66 ESI/HRMS spectrum of **22**

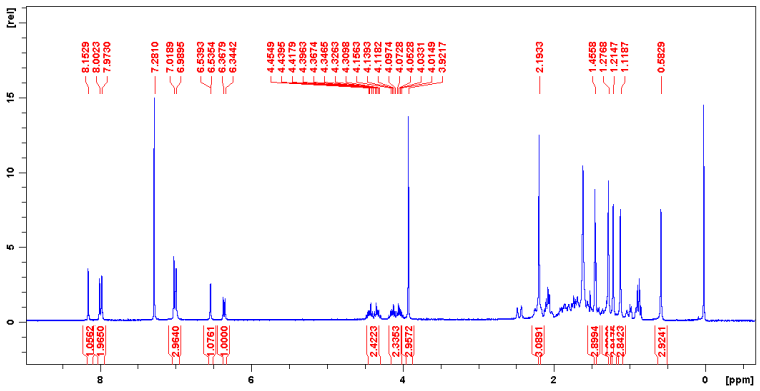


Fig. S67 ^{1}H NMR spectrum of **23** (300 MHz in $CDCl_3$)

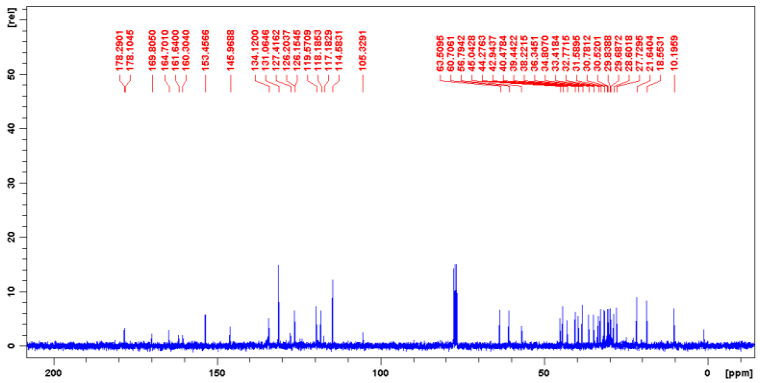
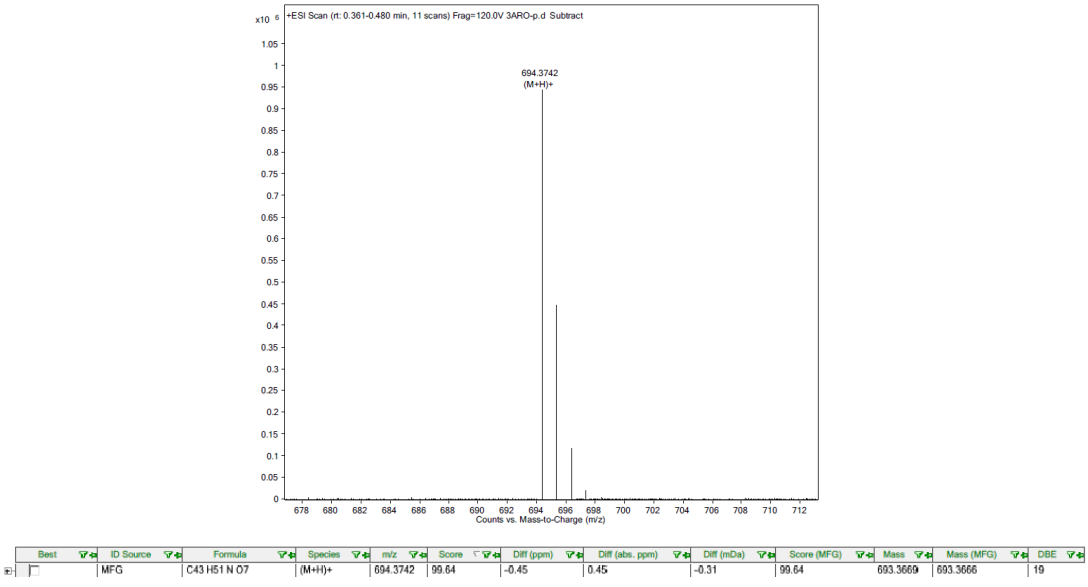


Fig. S68 ^{13}C NMR spectrum of **23** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C43 H51 N O7	(M+H)+	694.3742	99.64	-0.45	0.45	-0.31	99.64	693.3669	693.3666	19

Fig. S69 ESI/HRMS spectrum of **23**

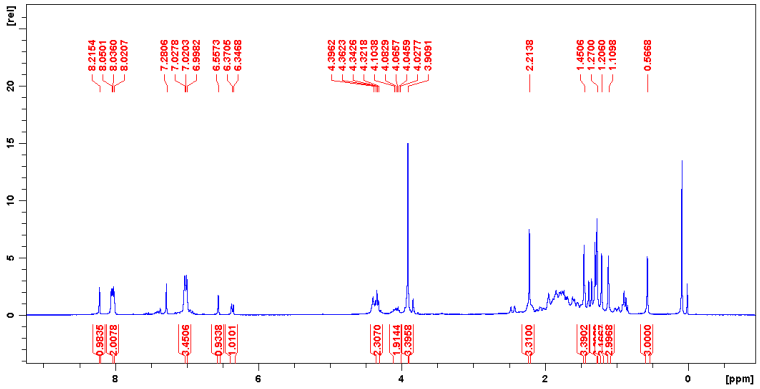


Fig. S70 ^{1}H NMR spectrum of **24** (300 MHz in $CDCl_3$)

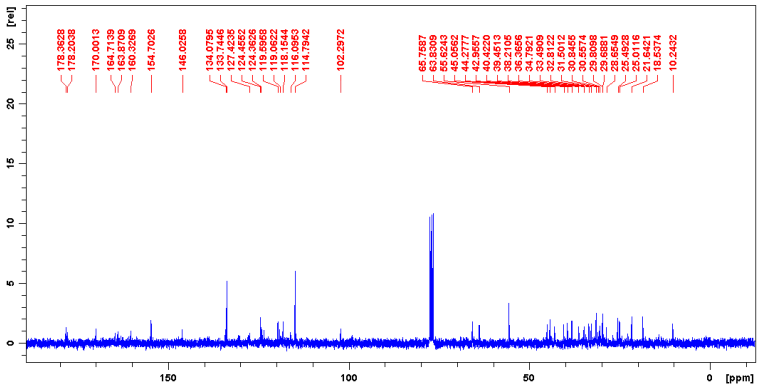
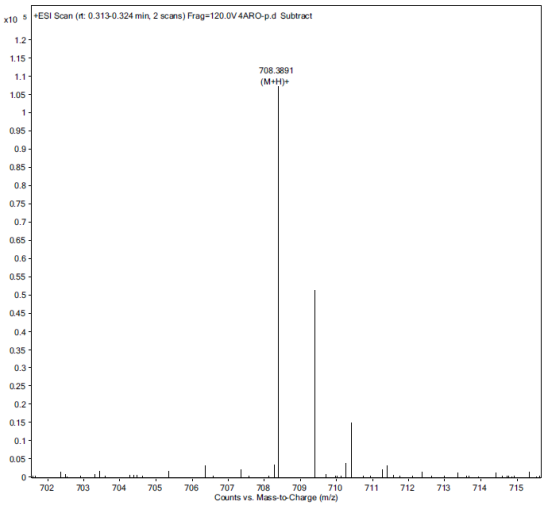


Fig. S71 ^{13}C NMR spectrum of **24** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C44 H53 N O7	(M+H)+	708.3891	92.11	-0.49	0.49	-0.34	92.11	707.3825	707.3822	19

Fig. S72 ESI/HRMS spectrum of **24**

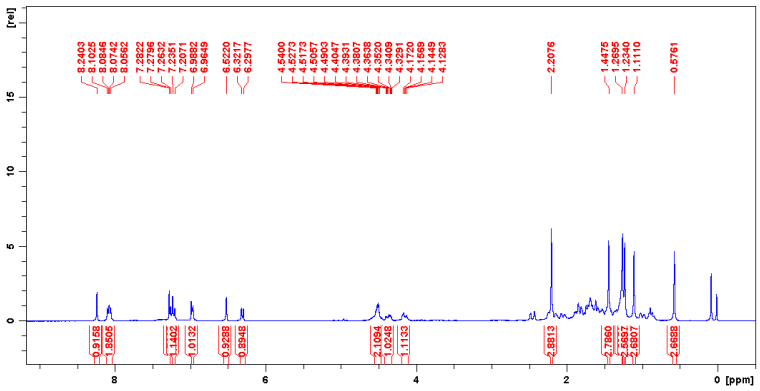


Fig. S73 ^{1}H NMR spectrum of **25** (300 MHz in $CDCl_3$)

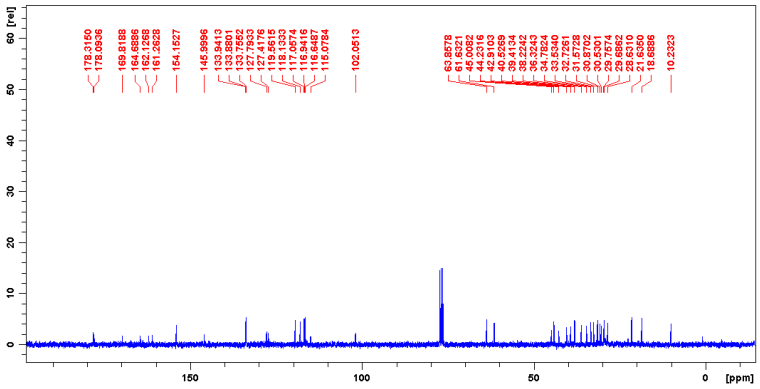
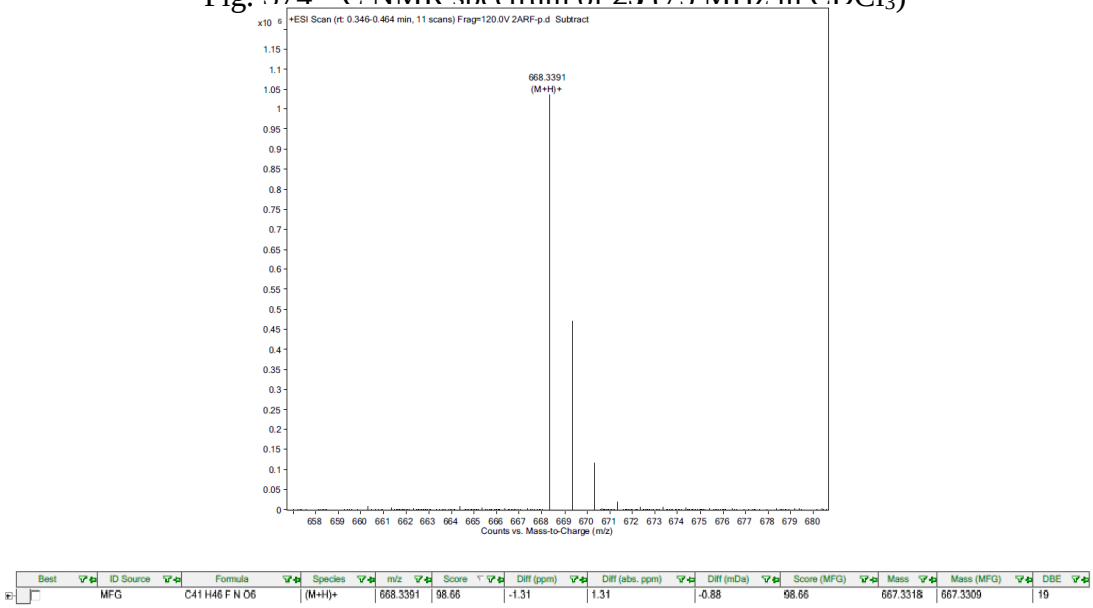


Fig. S74 ^{13}C NMR spectrum of **25** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C41 H46 F N O6	(M+H)+	668.3391	98.66	-1.31	1.31	-0.88	98.66	667.3318	667.3309	19

Fig. S75 ESI/HRMS spectrum of **25**

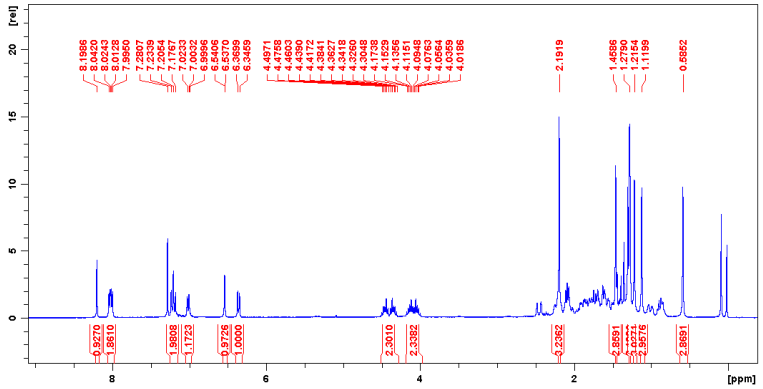


Fig. S76 ^{1}H NMR spectrum of **26** (300 MHz in $CDCl_3$)

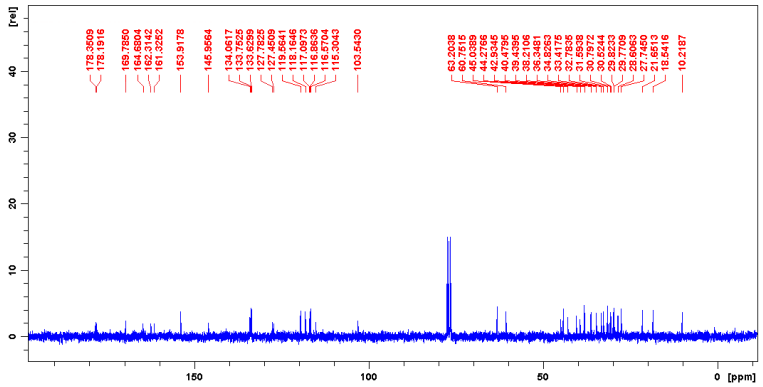
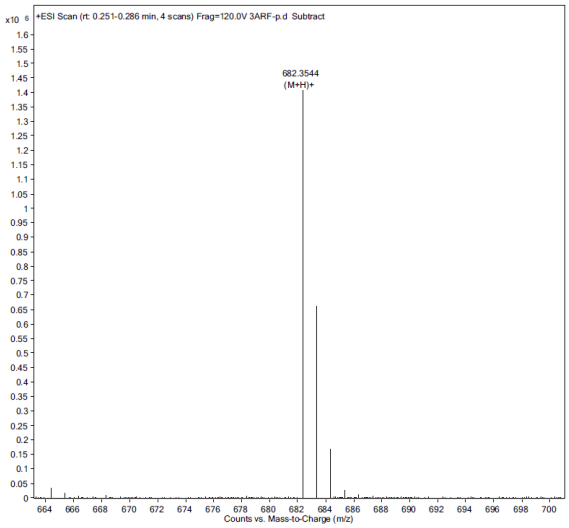


Fig. S77 ^{13}C NMR spectrum of **26** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C42 H48 F N O6	(M+H)+	682.3544	98.41	-1.26	1.26	-0.86	98.41	681.3474	681.3466	19

Fig. S78 ESI/HRMS spectrum of **26**

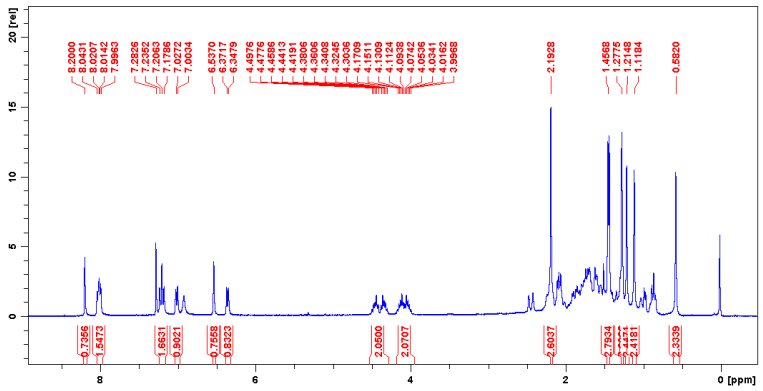


Fig. S79 ^{1}H NMR spectrum of **27** (300 MHz in $CDCl_3$)

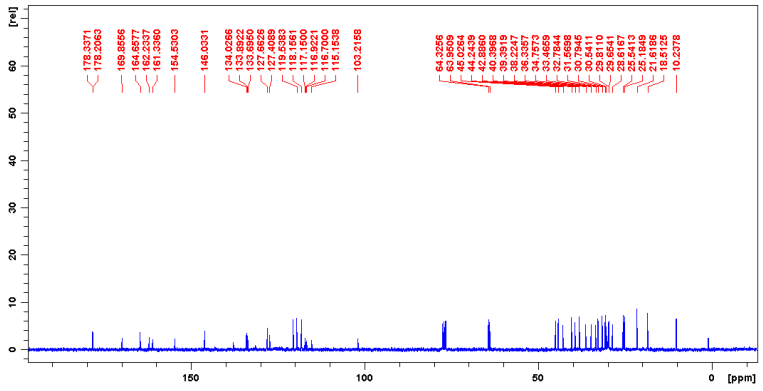


Fig. S80 ^{13}C NMR spectrum of **27** (75 MHz in $CDCl_3$)

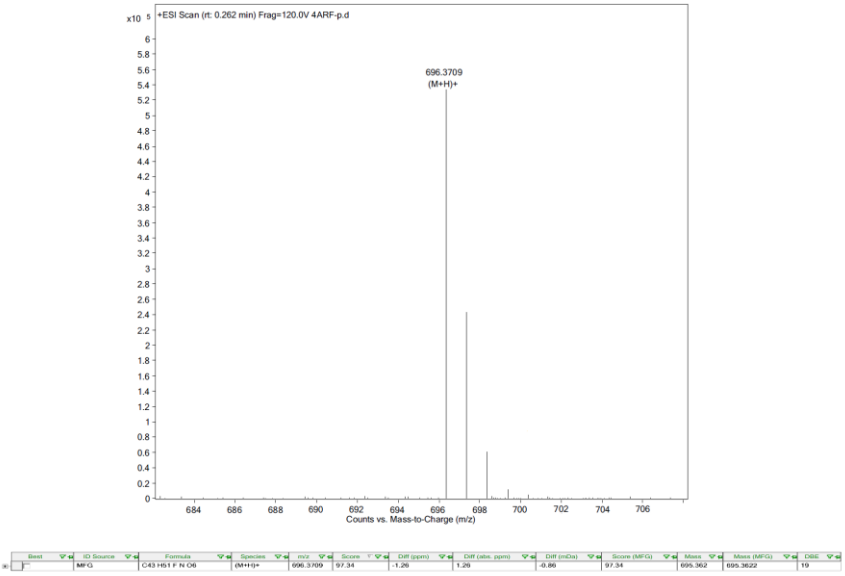


Fig. S81 ESI/HRMS spectrum of **27**

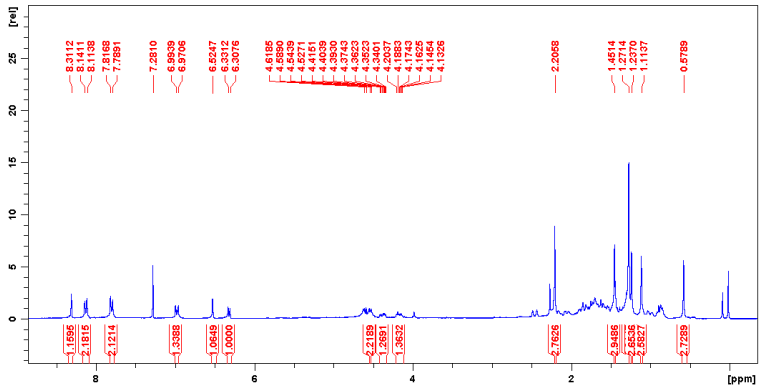


Fig. S82 ^{1}H NMR spectrum of **28** (300 MHz in $CDCl_3$)

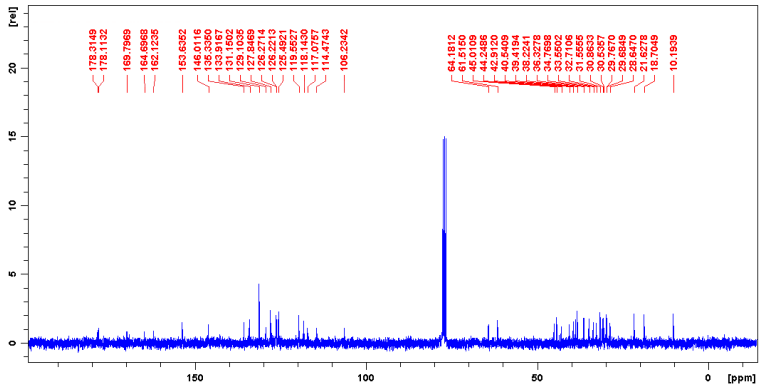
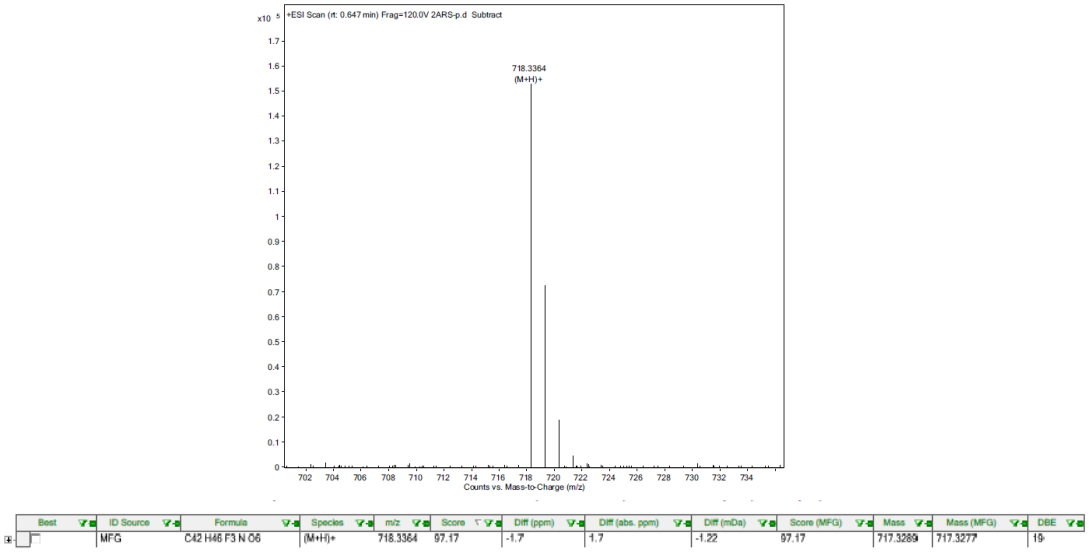


Fig. S83 ^{13}C NMR spectrum of **28** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C42 H46 F3 N O6	(M+H)+	718.3364	97.17	-1.7	1.7	-1.22	97.17	717.3289	717.3277	19

Fig. S84 ESI/HRMS spectrum of **28**

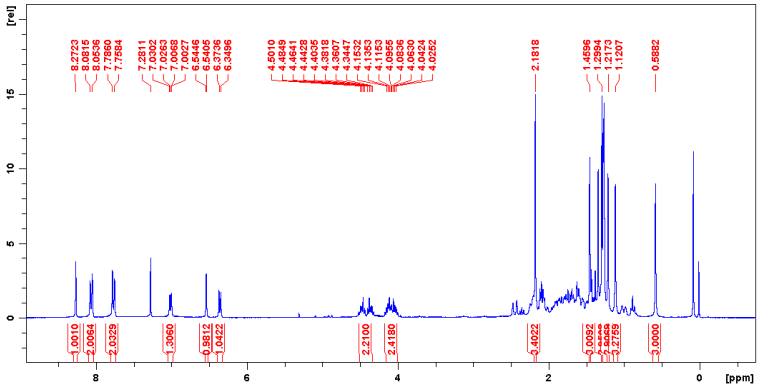


Fig. S85 ^{1}H NMR spectrum of **29** (300 MHz in $CDCl_3$)

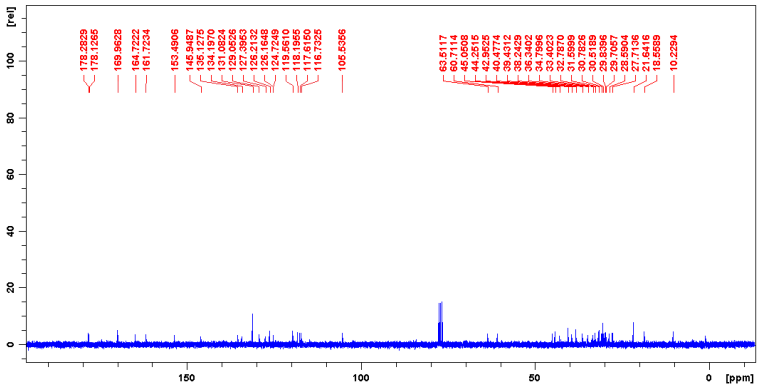
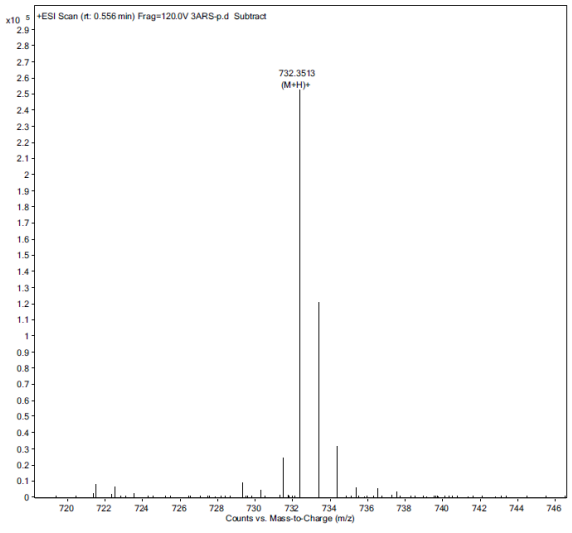


Fig. S86 ^{13}C NMR spectrum of **29** (75 MHz in DMSO-d_6)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C43 H48 F3 N O6	(M+H)+	732.3513	99.3	-0.36	0.36	-0.26	99.3	731.3436	731.3434	19

Fig. S87 ESI/HRMS spectrum of **29**

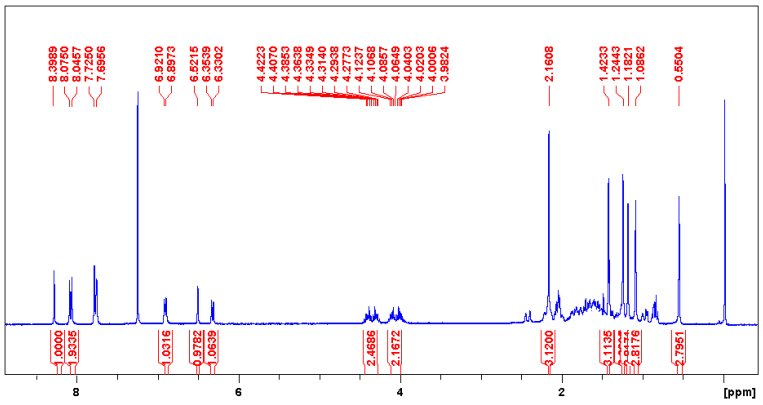


Fig. S88 ^{1}H NMR spectrum of **30** (300 MHz in $CDCl_3$)

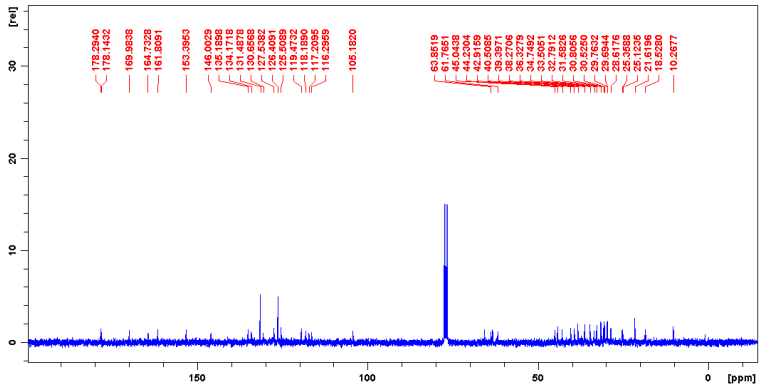
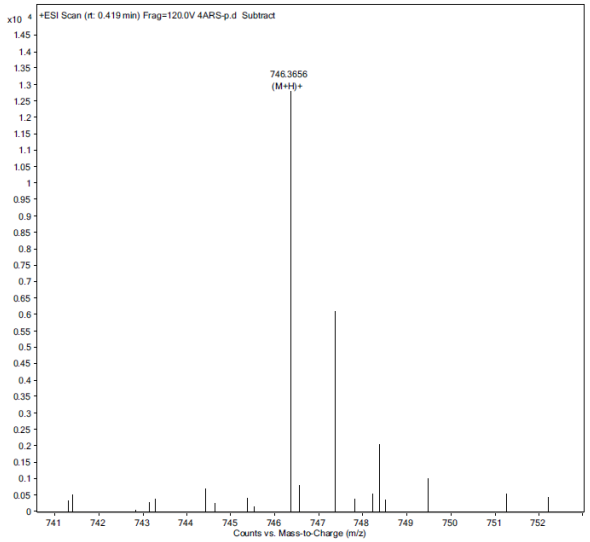


Fig. S89 ^{13}C NMR spectrum of **30** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C44 H50 F3 N O6	(M+H)+	746.3656	90.73	-0.12	0.12	-0.09	90.73	745.3591	745.359	19

Fig. S90 ESI/HRMS spectrum of **30**

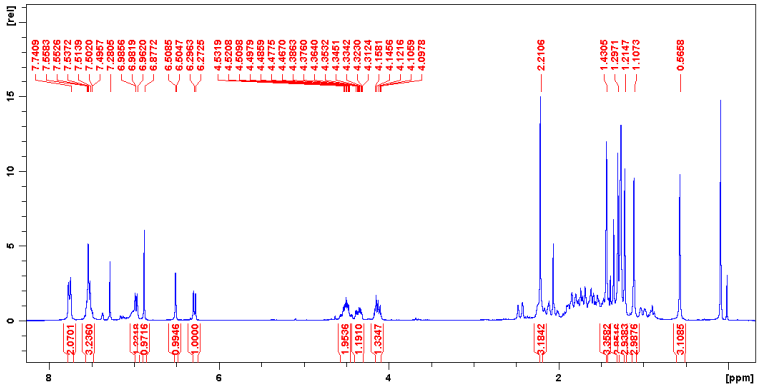


Fig. S91 ^{1}H NMR spectrum of **31** (300 MHz in $CDCl_3$)

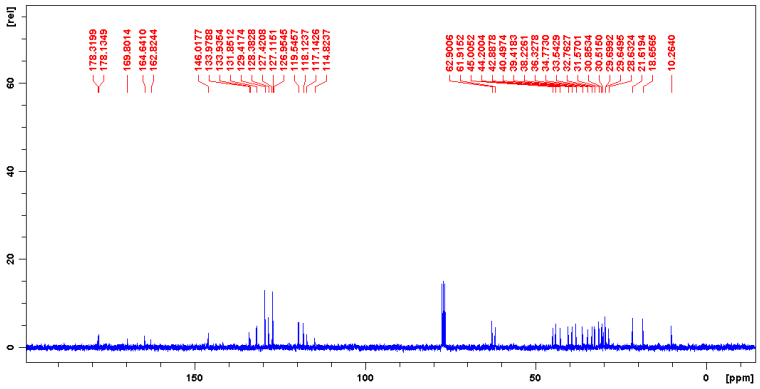
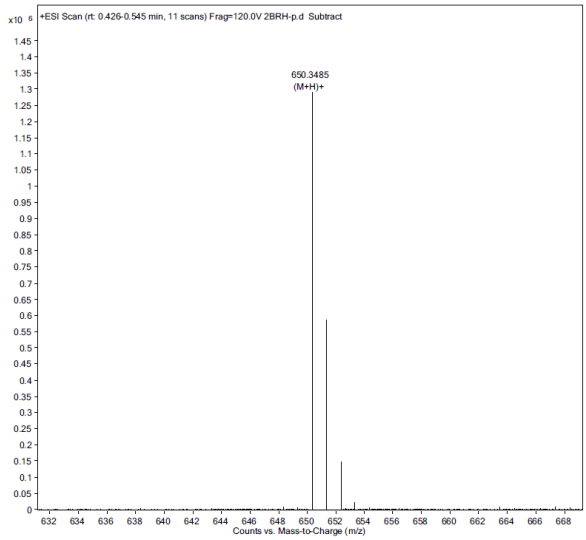


Fig. S92 ^{13}C NMR spectrum of **31** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C41 H47 N O6	(M+H)+	650.3485	98.34	-1.5	1.5	-0.97	98.34	649.3413	649.3403	19

Fig. S93 ESI/HRMS spectrum of **31**

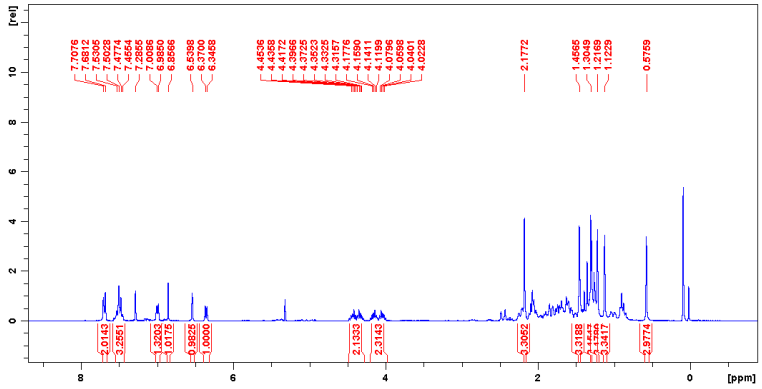


Fig. S94. ^{1}H NMR spectrum of **32** (300 MHz in $CDCl_3$)

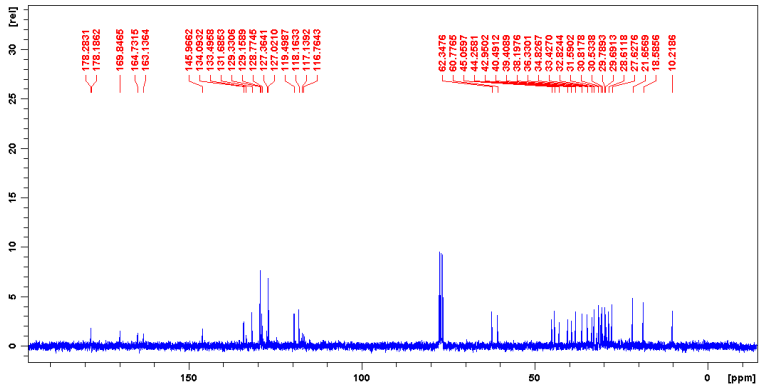
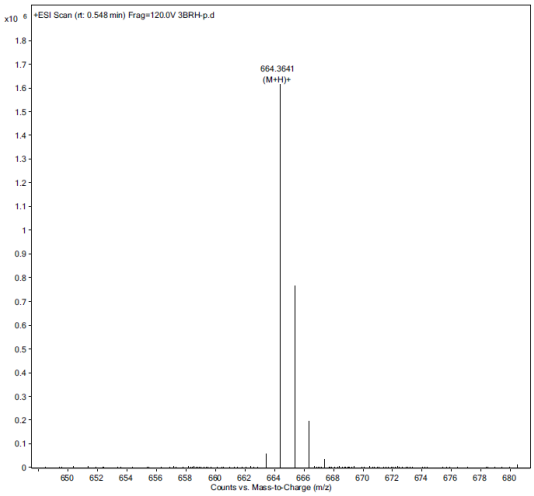


Fig. S95. ^{13}C NMR spectrum of **32** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C42 H49 N O8	(M+H)+	664.3641	98.59	-1.37	1.37	-0.91	98.59	663.3569	663.356	19

Fig. S96 ESI/HRMS spectrum of **32**

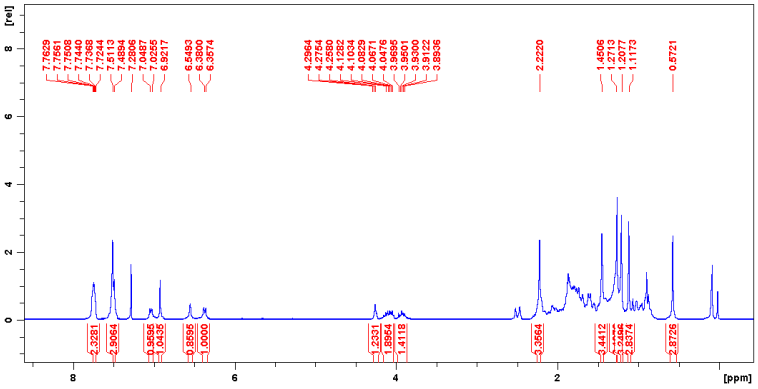


Fig. S97 ^{1}H NMR spectrum of **33** (300 MHz in $CDCl_3$)

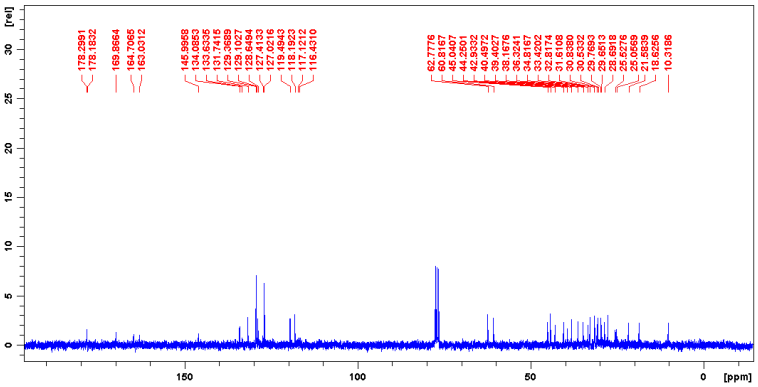
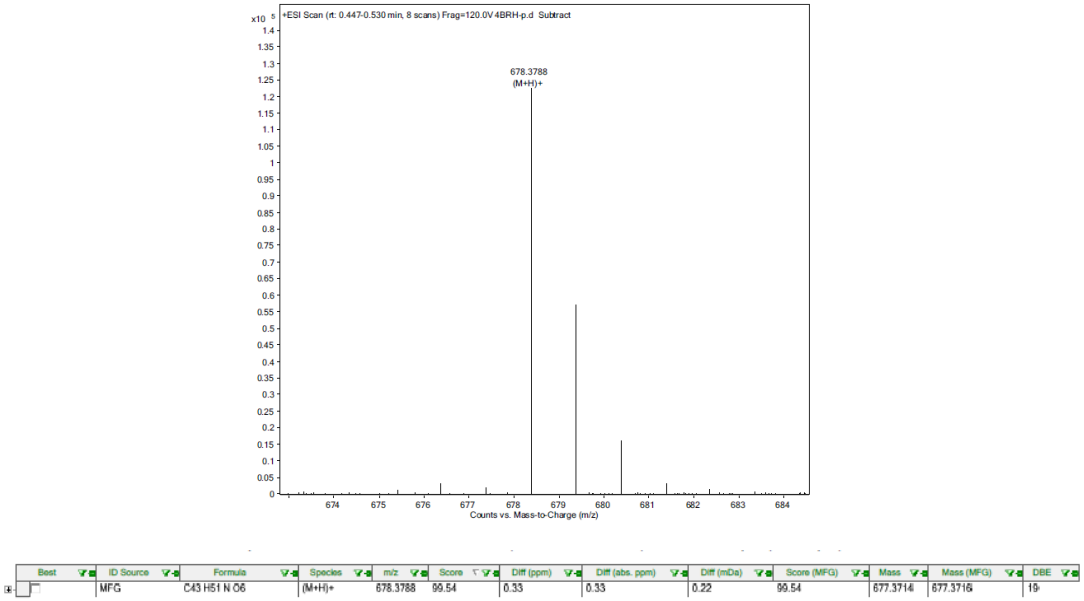


Fig. S98 ^{13}C NMR spectrum of **33** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C43 H51 N O6	(M+H)+	678.3788	99.54	0.33	0.33	0.22	99.54	677.3714	677.3716	19

Fig. S99 ESI/HRMS spectrum of **33**

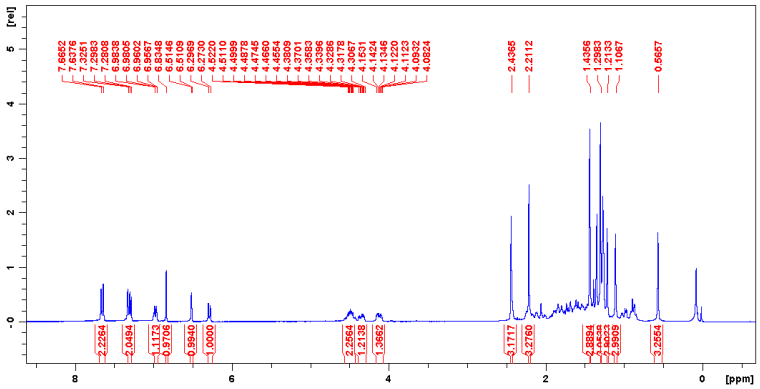


Fig. S100 ^{1}H NMR spectrum of **34** (300 MHz in $CDCl_3$)

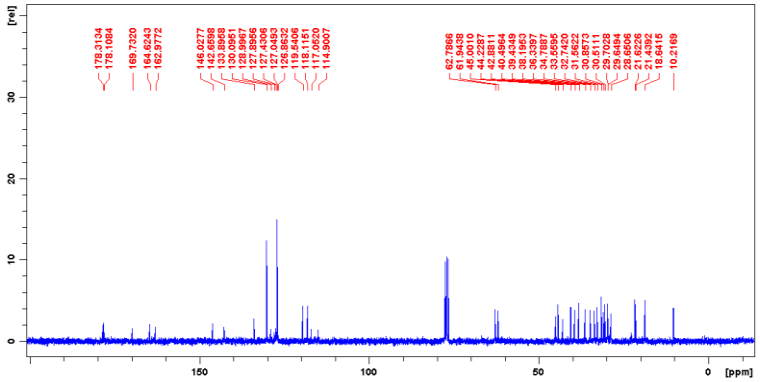
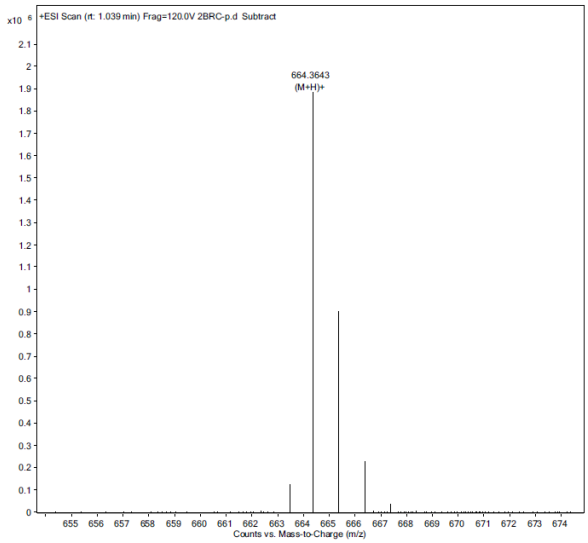


Fig. S101 ^{13}C NMR spectrum of **34** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C42 H49 N O6	(M+H)+	664.3643	97.72	-1.73	1.73	-1.15	97.72	663.3571	663.356	19

Fig. S102 ESI/HRMS spectrum of **34**

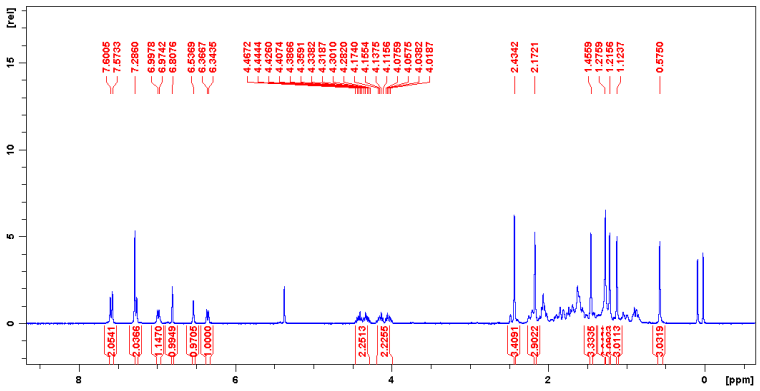


Fig. S103 ^{1}H NMR spectrum of **35** (300 MHz in $CDCl_3$)

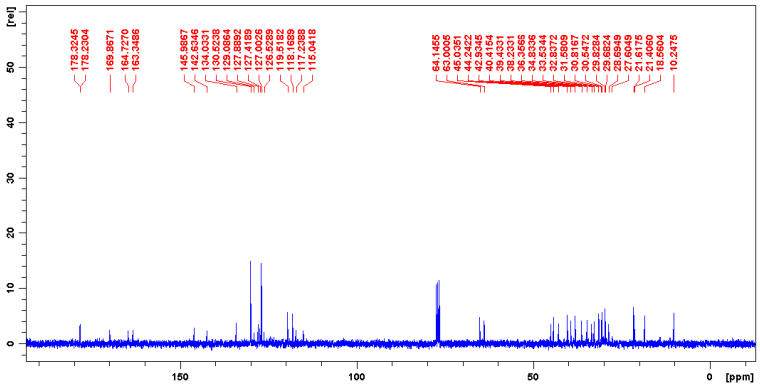
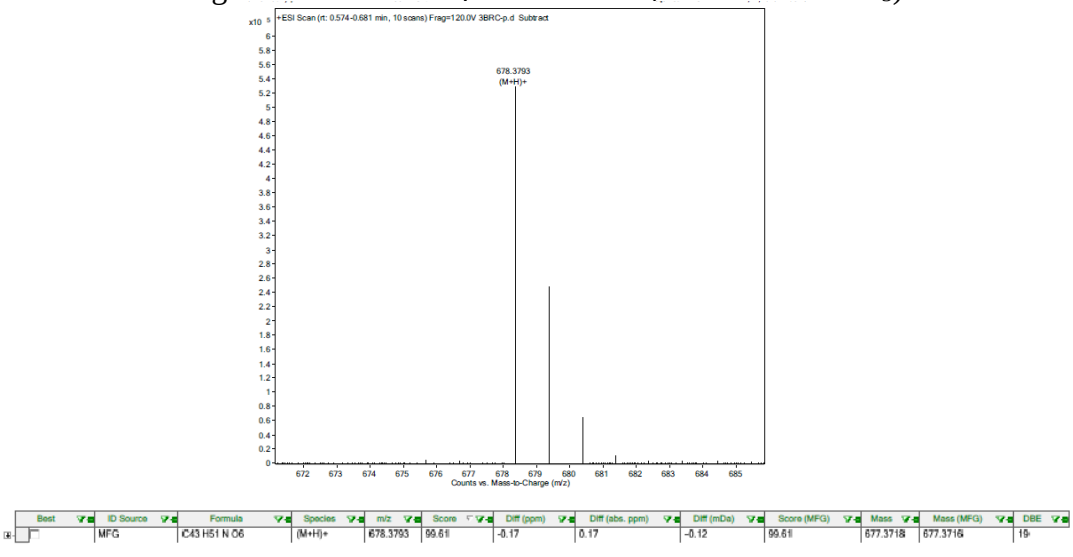


Fig. S104 ^{13}C NMR spectrum of **35** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C43 H51 N O6	(M+H)+	678.3793	99.61	-0.17	0.17	-0.12	99.61	677.3718	677.3716	19

Fig. S105 ESI/HRMS spectrum of **35**

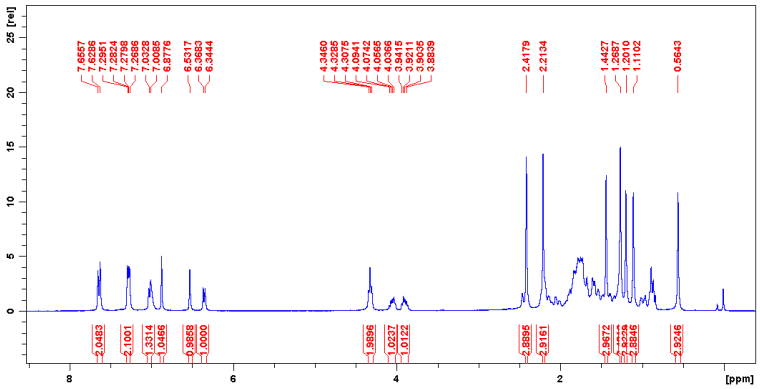


Fig. S106 ^{1}H NMR spectrum of **36** (300 MHz in $CDCl_3$)

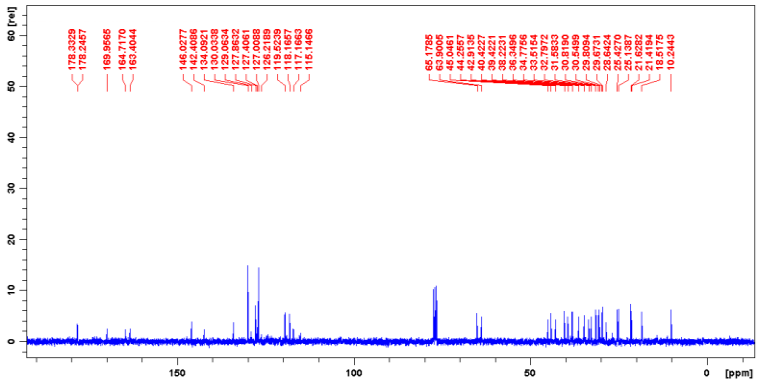
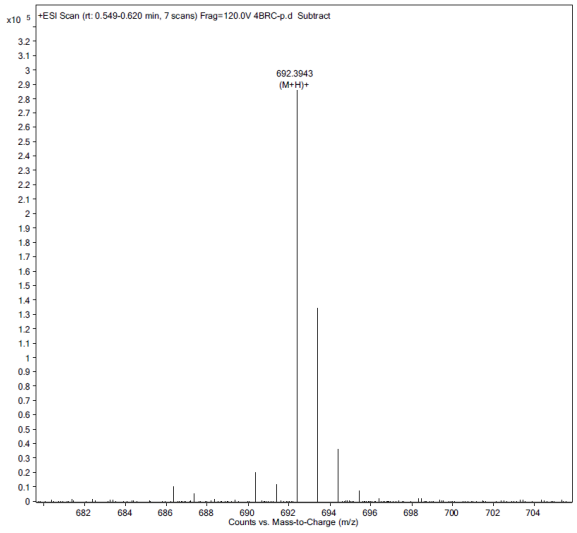


Fig. S107 ^{13}C NMR spectrum of **36** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C44 H53 N O5	(M+H)+	692.3943	99.24	0.71	0.71	0.49	99.24	691.3868	691.3873	19

Fig. S108 ESI/HRMS spectrum of **36**

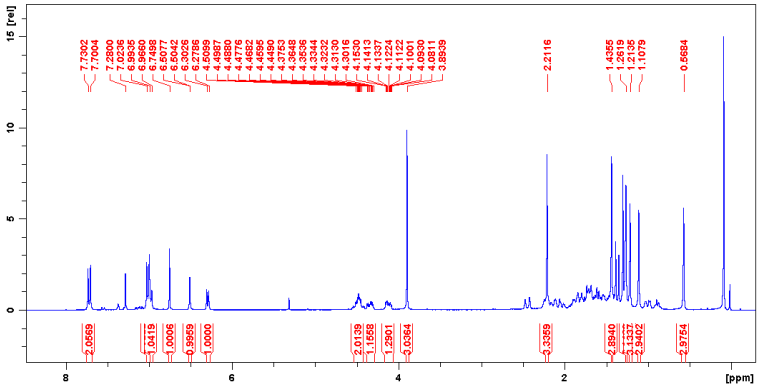


Fig. S109 ^{1}H NMR spectrum of **37** (300 MHz in $CDCl_3$)

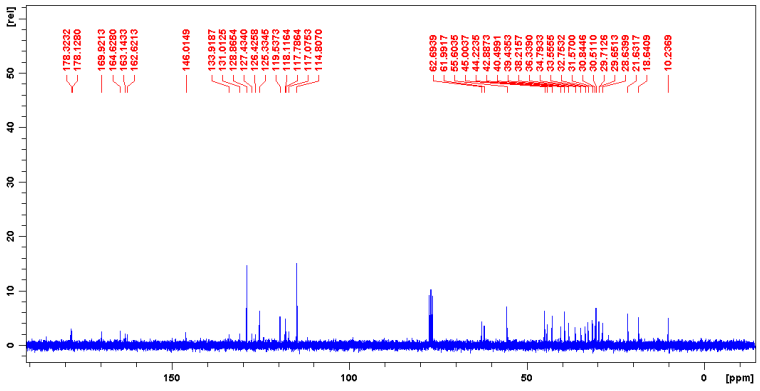
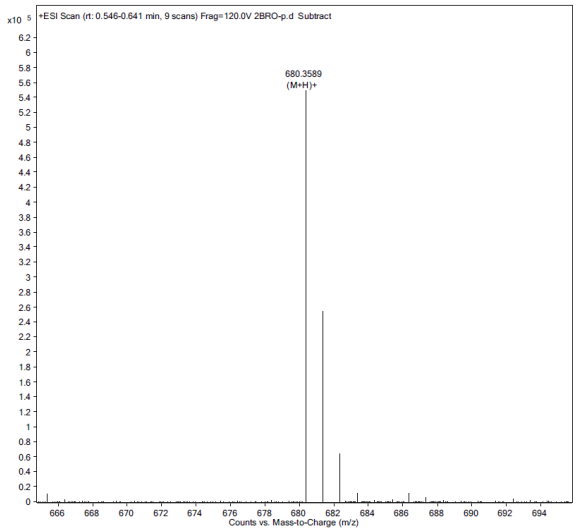


Fig. S110 ^{13}C NMR spectrum of **37** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C42 H49 N O7	(M+H)+	680.3589	99.09	-0.65	0.65	-0.44	99.09	679.3513	679.3509	19

Fig. S111 ESI/HRMS spectrum of **37**

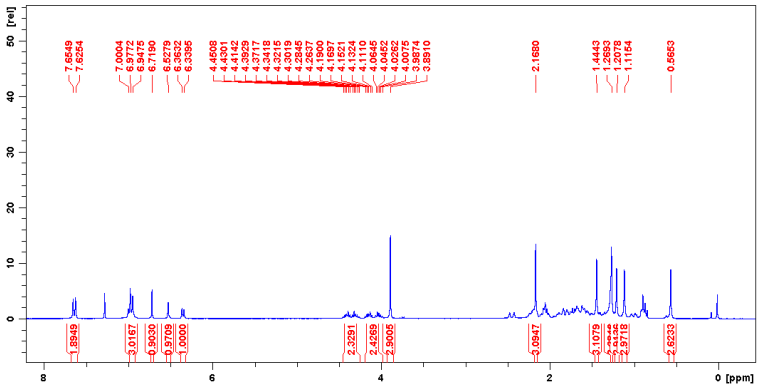


Fig. S112 ^{1}H NMR spectrum of **38** (300 MHz in $CDCl_3$)

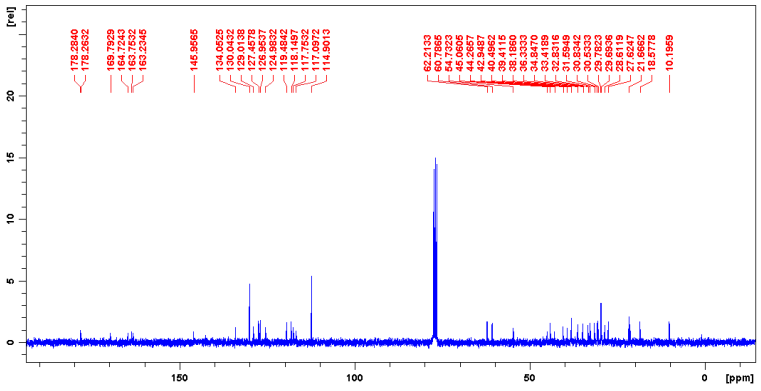


Fig. S113 ^{13}C NMR spectrum of **38** (75 MHz in $CDCl_3$)

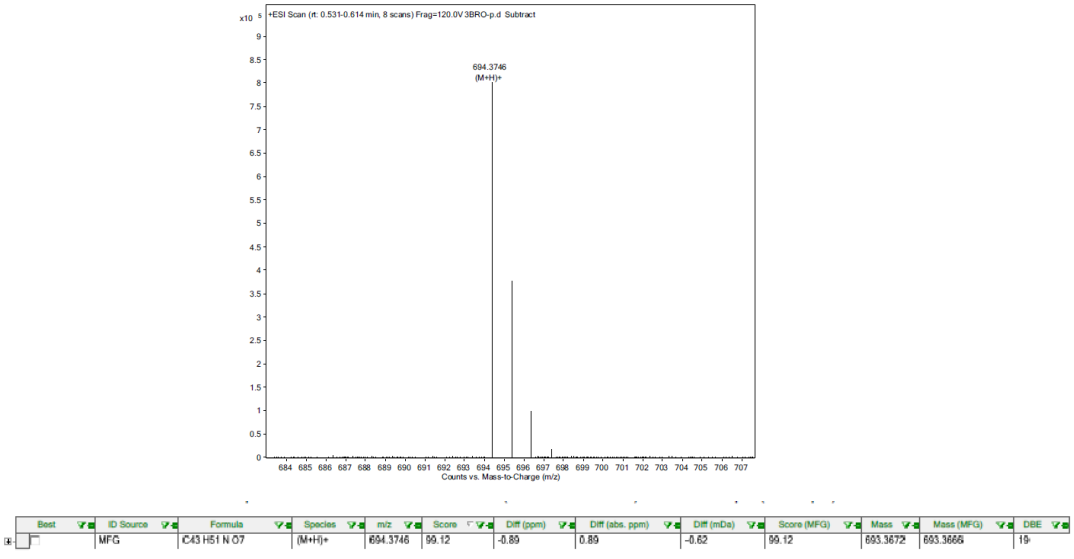


Fig. S114 ESI/HRMS spectrum of **38**

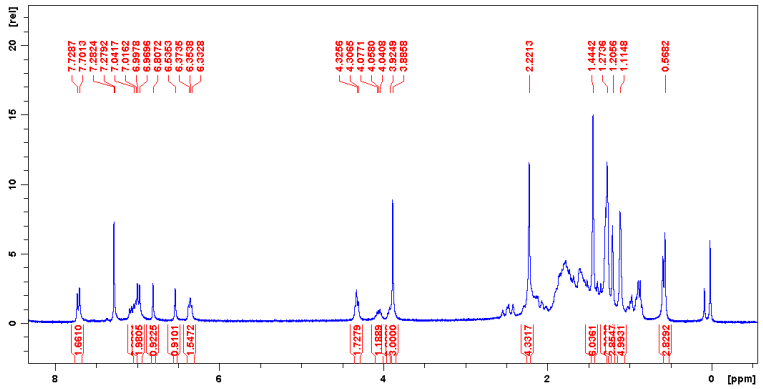


Fig. S115 ^{1}H NMR spectrum of **39** (300 MHz in $CDCl_3$)

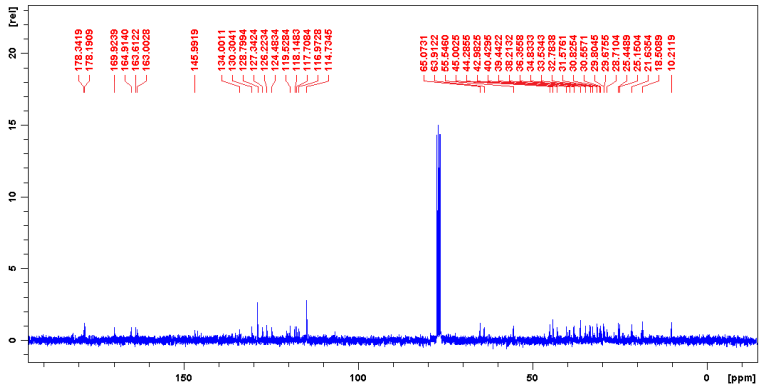
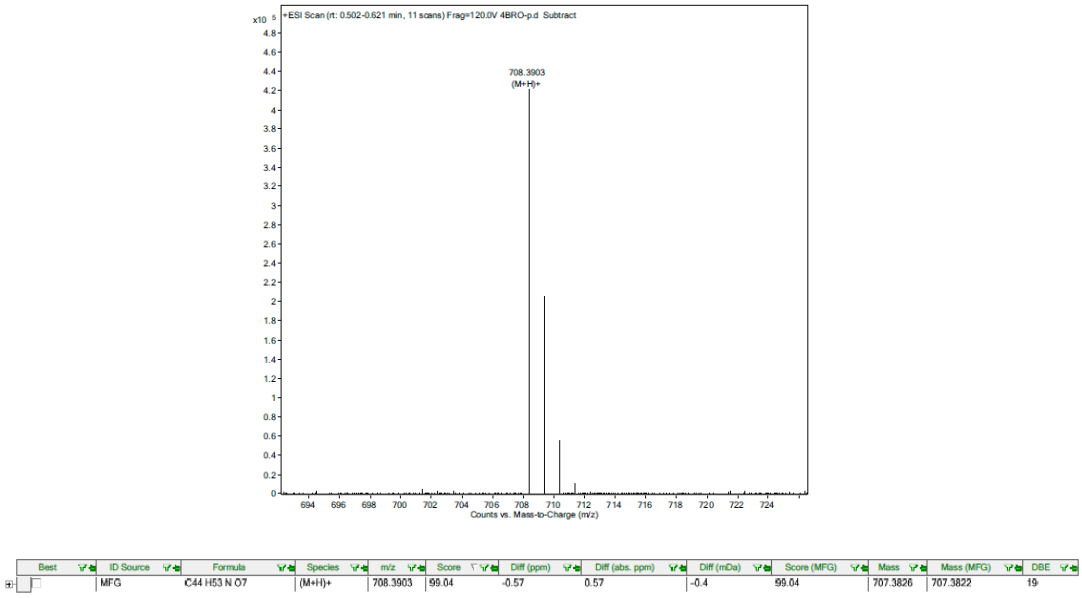


Fig. S116 ^{13}C NMR spectrum of **39** (75 MHz in DMSO-d_6)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C44 H53 N O7	(M+H)+	708.3903	99.04	-0.57	0.57	-0.4	99.04	707.3826	707.3822	19

Fig. S117 ESI/HRMS spectrum of **39**

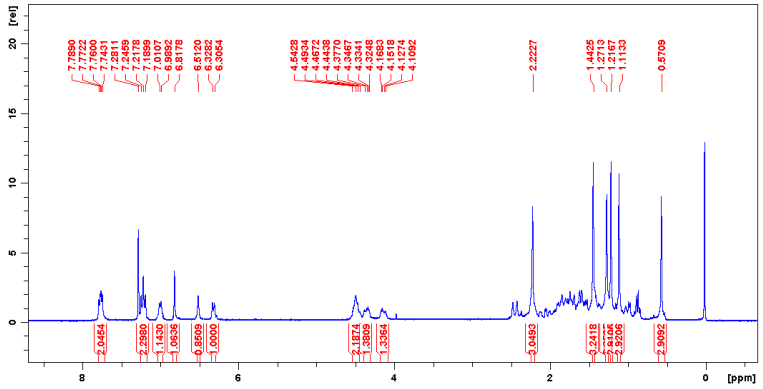


Fig. S118 ^{1}H NMR spectrum of **40** (300 MHz in $CDCl_3$)

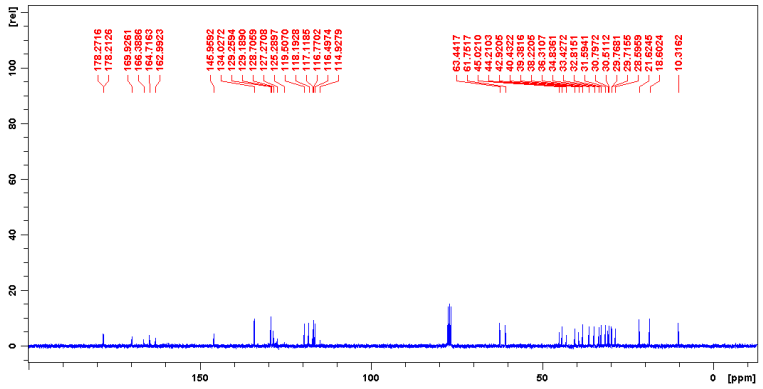
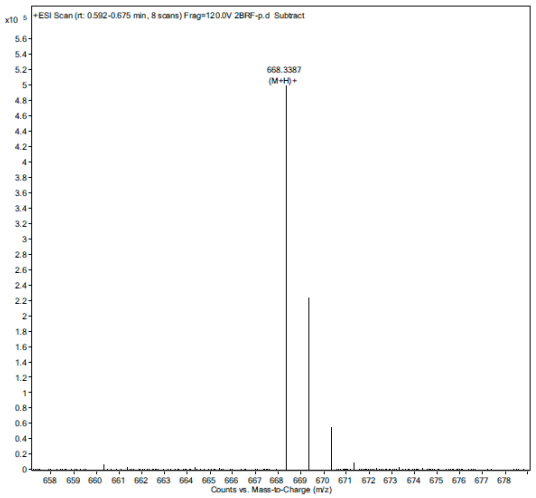


Fig. S119 ^{13}C NMR spectrum of **40** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C41 H46 F N O6	(M+H)+	668.3387	99.33	-0.5	0.5	-0.33	99.33	667.3312	667.3309	19

Fig. S120 ESI/HRMS spectrum of **40**

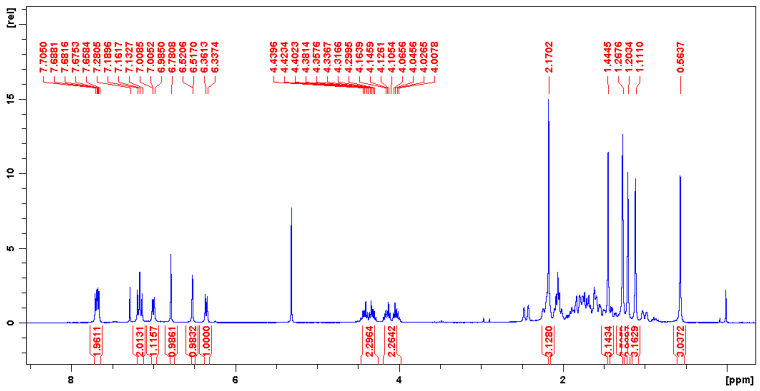


Fig. S121 ^{1}H NMR spectrum of **41** (300 MHz in $CDCl_3$)

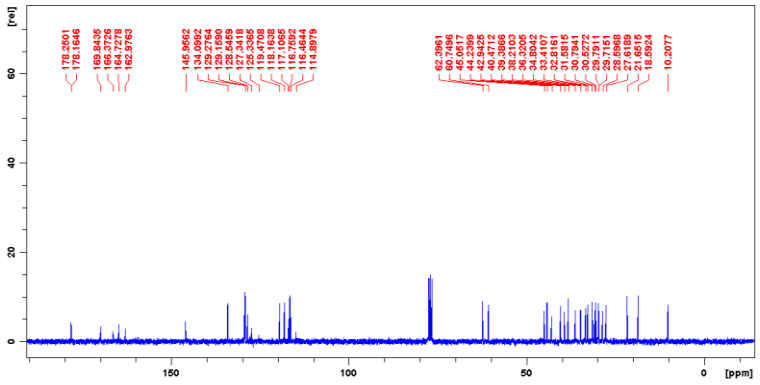
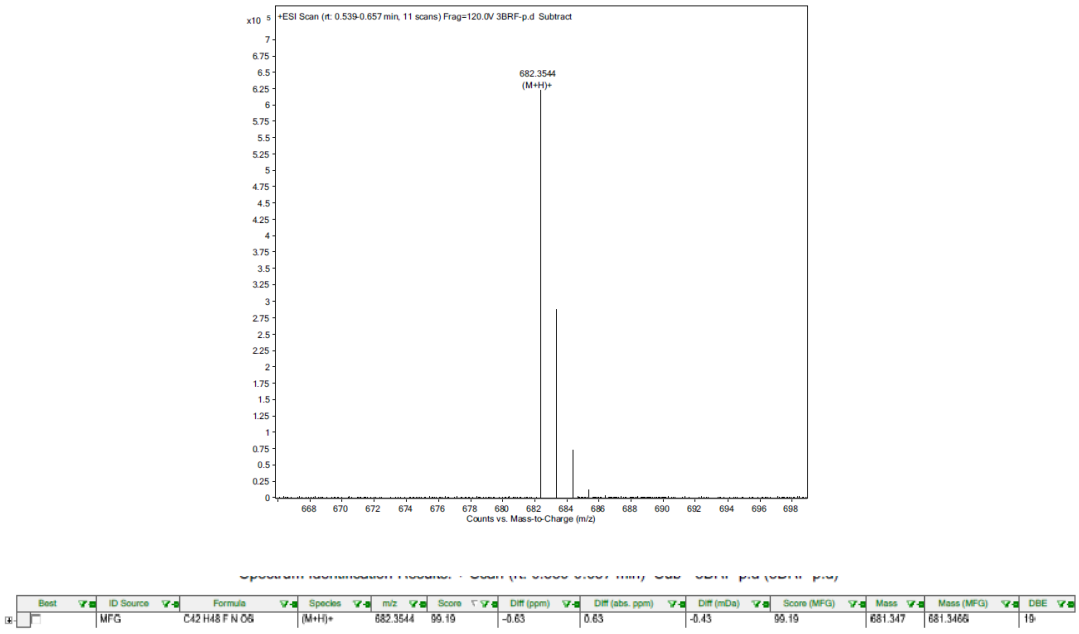


Fig. S122 ^{13}C NMR spectrum of **41** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C42 H48 F N O5	(M+H)+	682.3544	99.19	-0.63	0.63	-0.43	99.19	681.347	681.3466	19

Fig. S123 ESI/HRMS spectrum of **41**

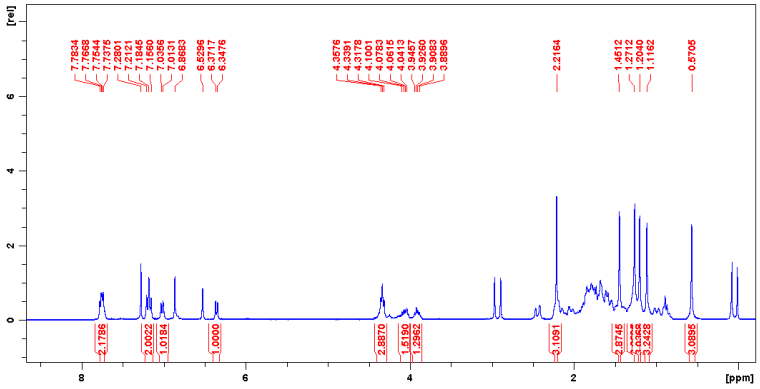


Fig. S124. ^{1}H NMR spectrum of **42** (300 MHz in $CDCl_3$)

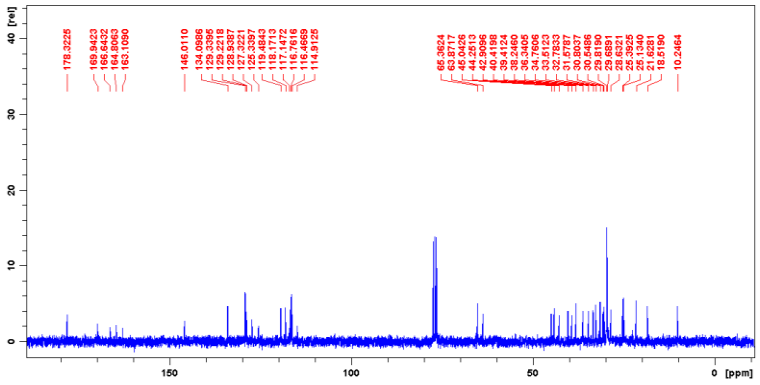
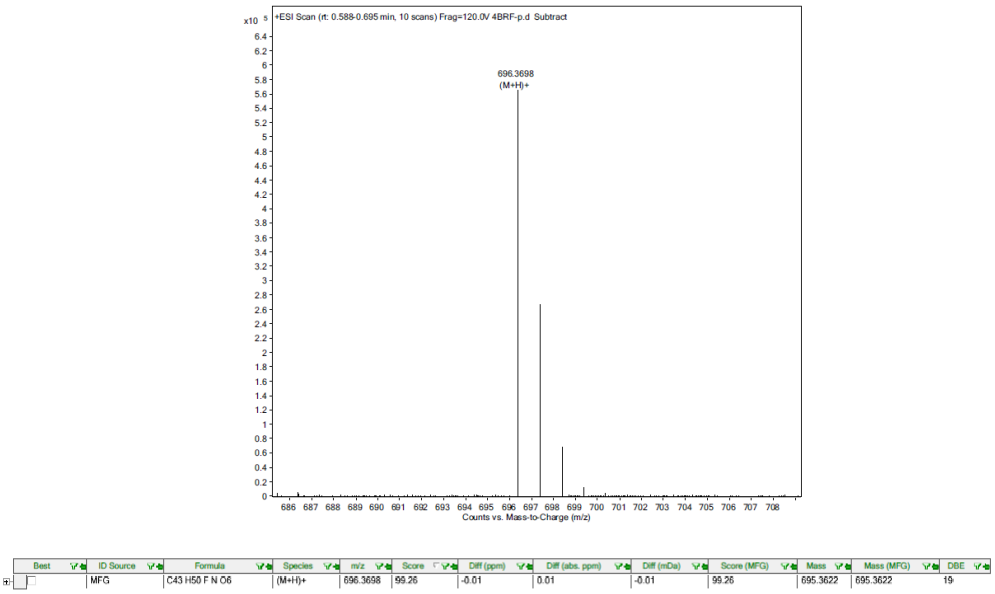


Fig. S125. ^{13}C NMR spectrum of **42** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C43 H50 F N O6	(M+H)+	696.3698	99.26	-0.01	0.01	-0.01	99.26	695.3622	695.3622	19

Fig. S126 ESI/HRMS spectrum of **42**

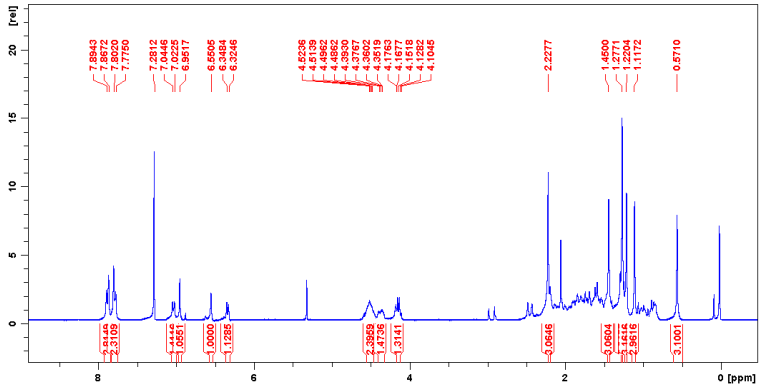


Fig. S127 ^{1}H NMR spectrum of **43** (300 MHz in $CDCl_3$)

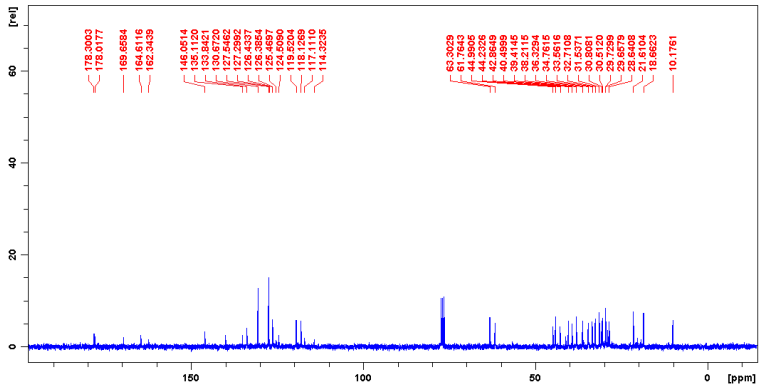
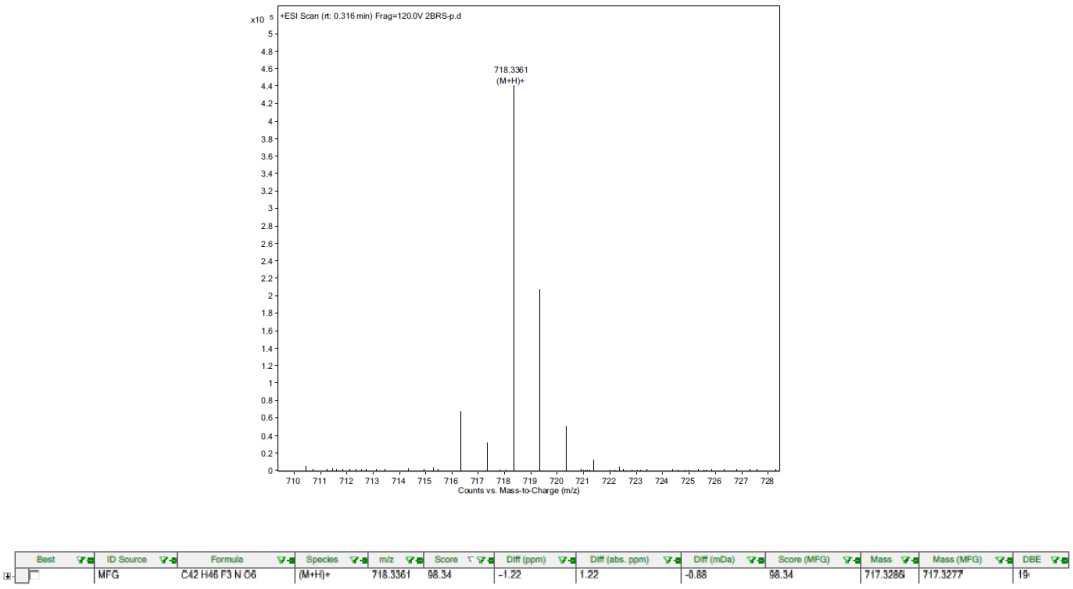


Fig. S128 ^{13}C NMR spectrum of **43** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C42 H46 F3 N O6	(M+H)+	718.3361	98.34	-1.22	1.22	-0.88	98.34	717.3288	717.3277	19

Fig. S129 ESI/HRMS spectrum of **43**

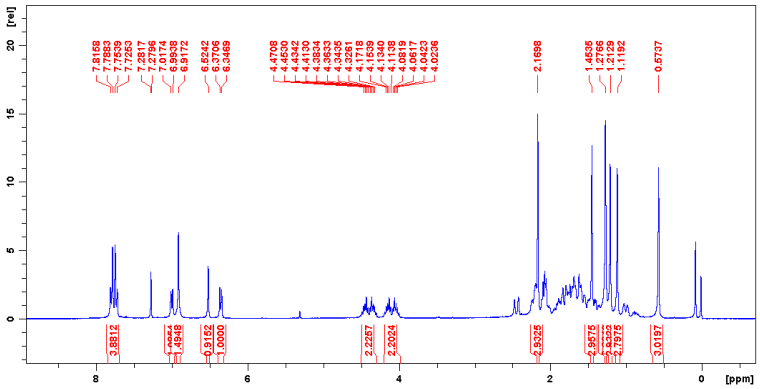


Fig. S130 ^{1}H NMR spectrum of **44** (300 MHz in $CDCl_3$)

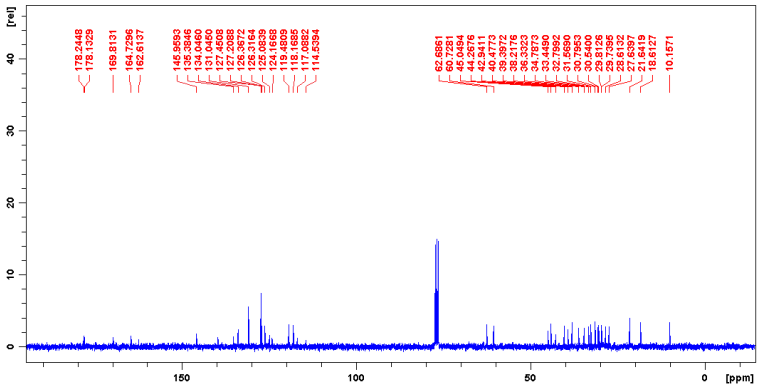
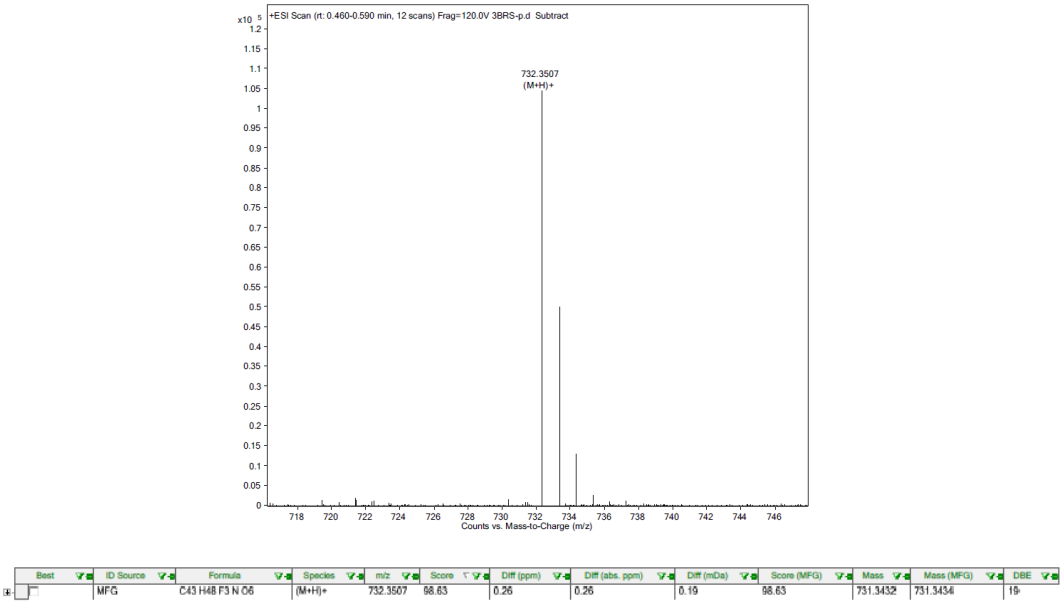


Fig. S131 ^{13}C NMR spectrum of **44** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C43 H48 F3 N O6	(M+H)+	732.3507	98.63	0.26	0.26	0.19	98.63	731.3432	731.3434	19

Fig. S132 ESI/HRMS spectrum of **44**

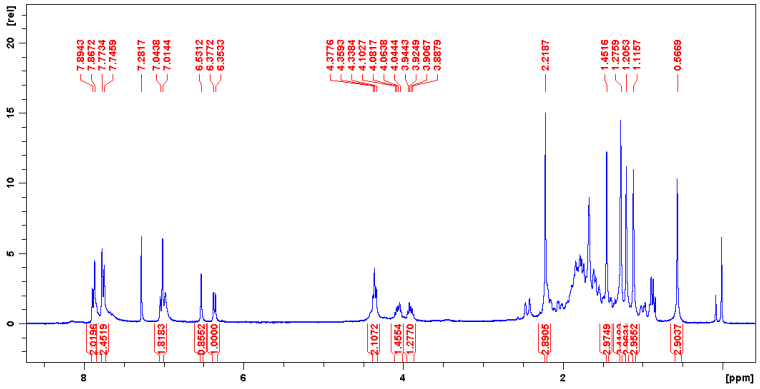


Fig. S133 ^{1}H NMR spectrum of **45** (300 MHz in $CDCl_3$)

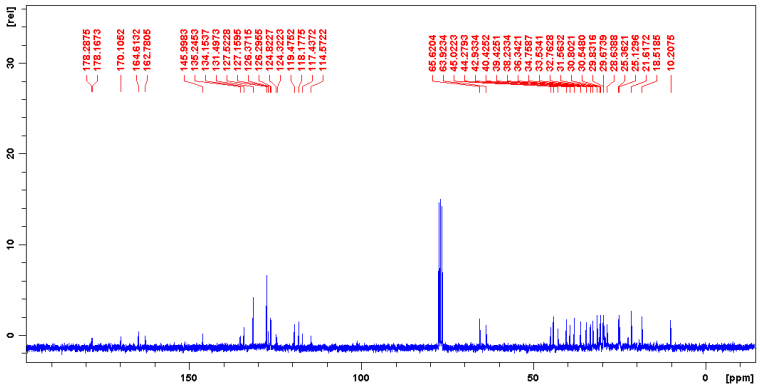
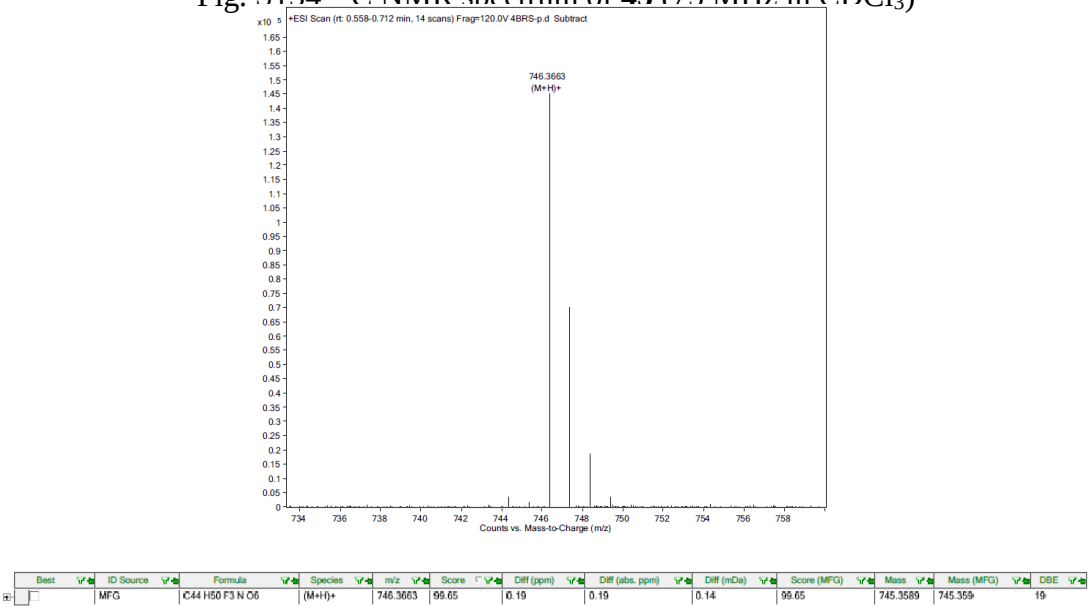


Fig. S134 ^{13}C NMR spectrum of **45** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C44 H50 F3 N O6	(M+H)+	746.3663	99.65	0.19	0.19	0.14	99.65	745.3589	745.359	19

Fig. S135 ESI/HRMS spectrum of **45**

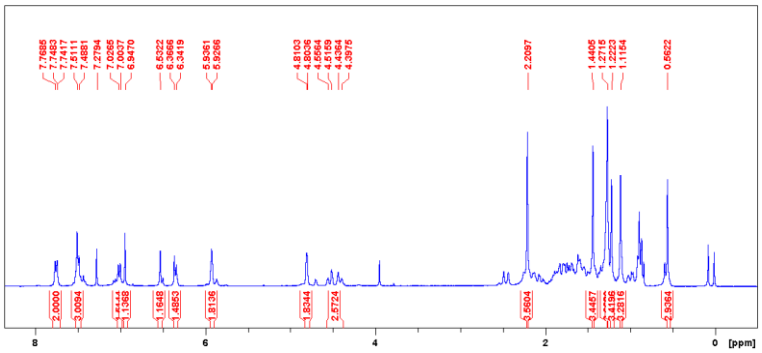


Fig. S136 ^{1}H NMR spectrum of **46** (300 MHz in $CDCl_3$)

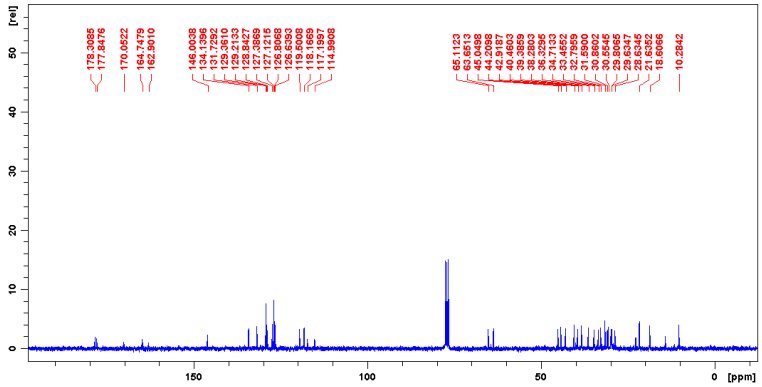
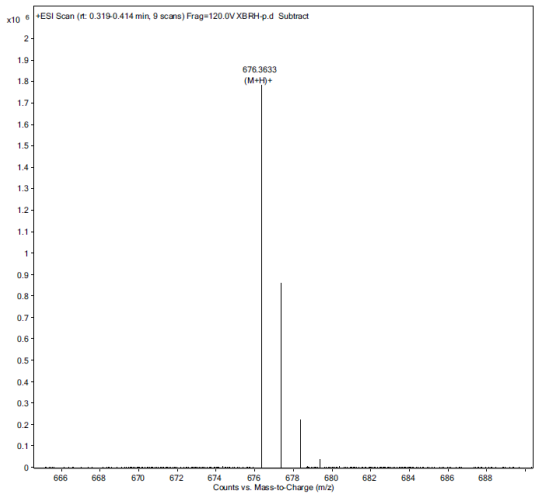


Fig. S137 ^{13}C NMR spectrum of **46** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C43 H49 N O6	(M+H)+	676.3633	99.4	-0.46	0.46	-0.31	99.4	675.3563	675.356	20

Fig. S138 ESI/HRMS spectrum of **46**

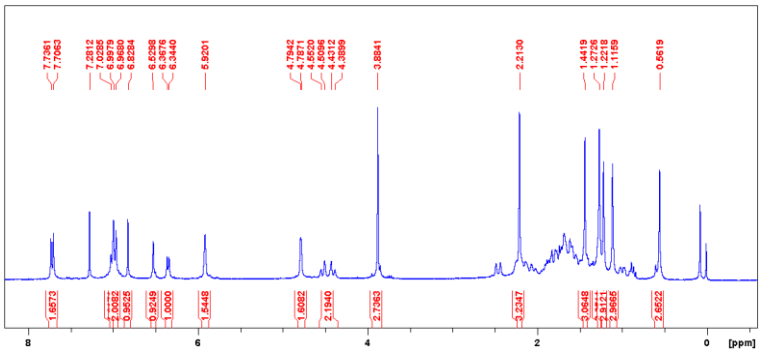


Fig. S139 ^{1}H NMR spectrum of **47** (300 MHz in $CDCl_3$)

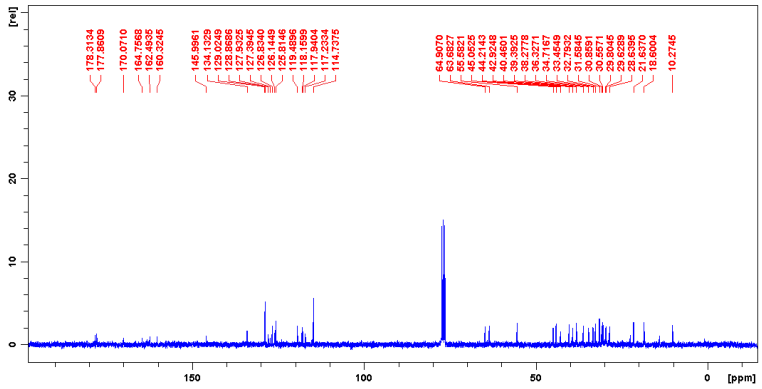
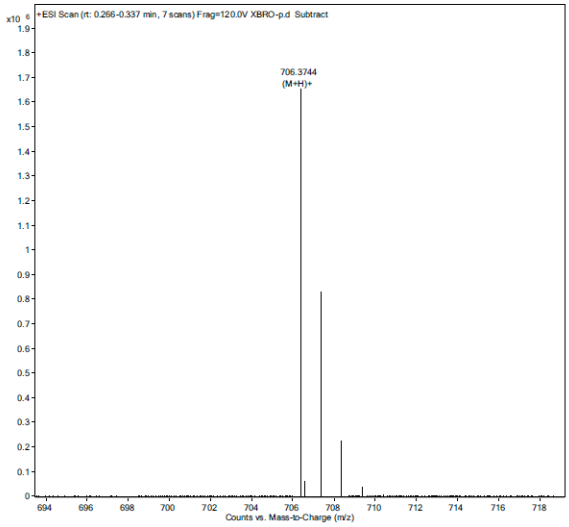


Fig. S140 ^{13}C NMR spectrum of **47** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C44 H51 N O7	(M+H)+	706.3744	98.49	-1.16	1.16	-0.82	98.49	705.3674	705.3666	20

Fig. S141 ESI/HRMS spectrum of **47**

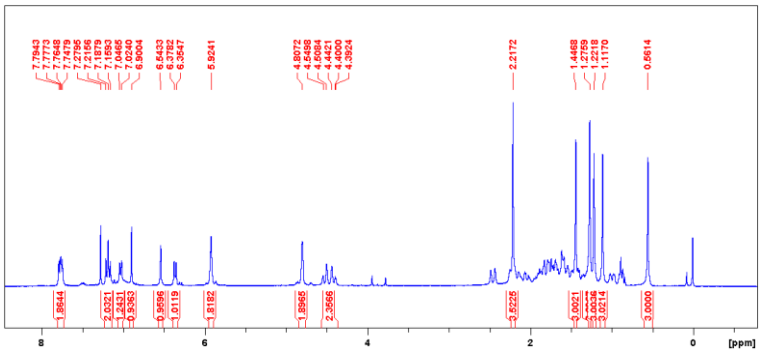


Fig. S142 ^{1}H NMR spectrum of **48** (300 MHz in $CDCl_3$)

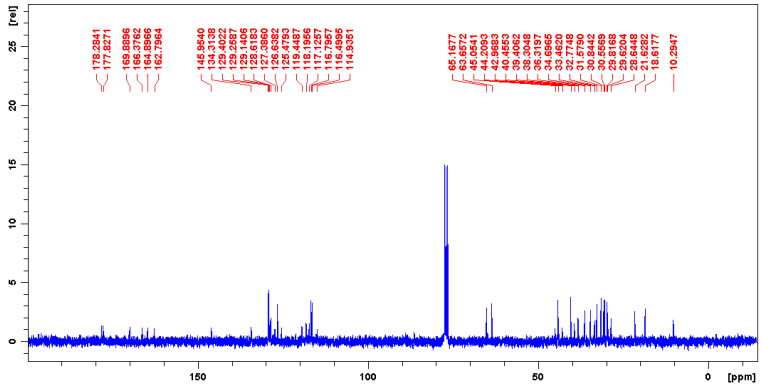
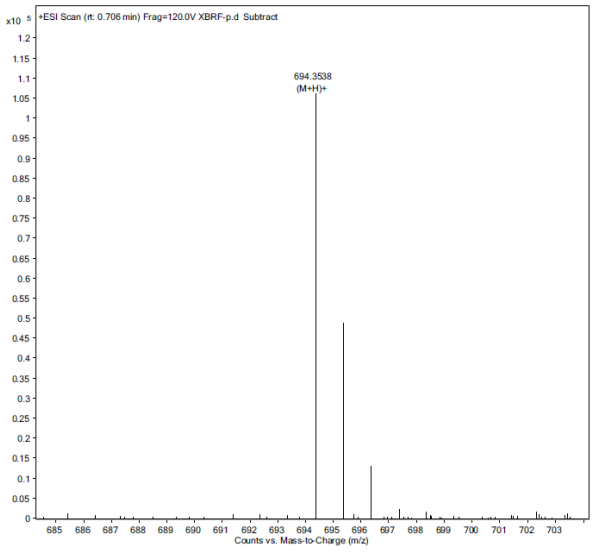


Fig. S143 ^{13}C NMR spectrum of **48** (75 MHz in $CDCl_3$)



Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	Score (MFG)	Mass	Mass (MFG)	DBE
	MFG	C43 H48 F N O6	(M+H)+	694.3538	99.51	-0.21	0.21	-0.15	99.51	693.3467	693.3466	20

Fig. S144 ESI/HRMS spectrum of **48**

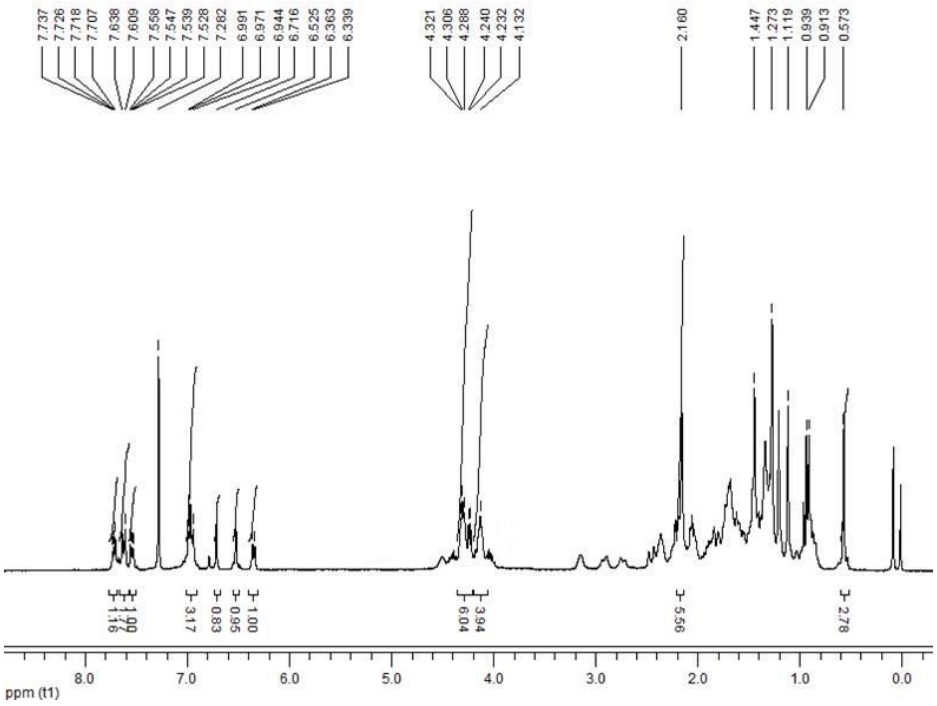


Fig. S145 ^{1}H NMR spectrum of **41-Bio** (300 MHz in $CDCl_3$)

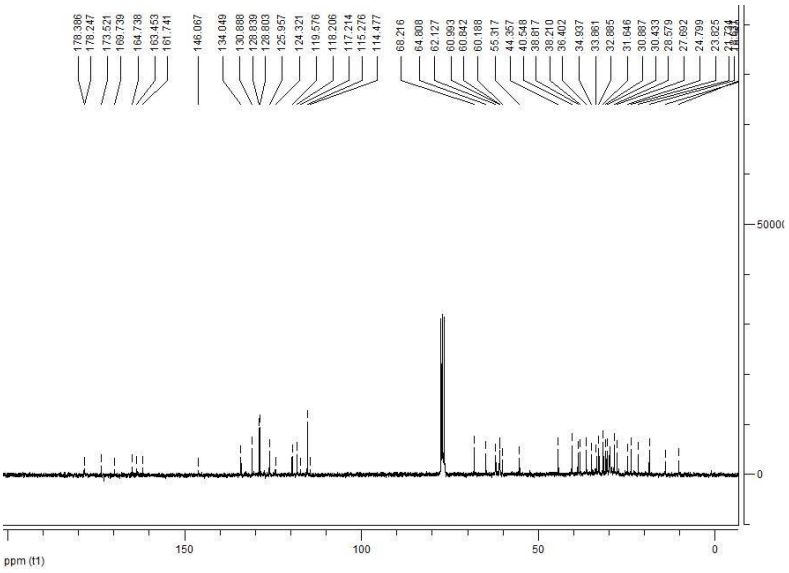


Fig. S146 ^{13}C NMR spectrum of **41-Bio** (75 MHz in $CDCl_3$)

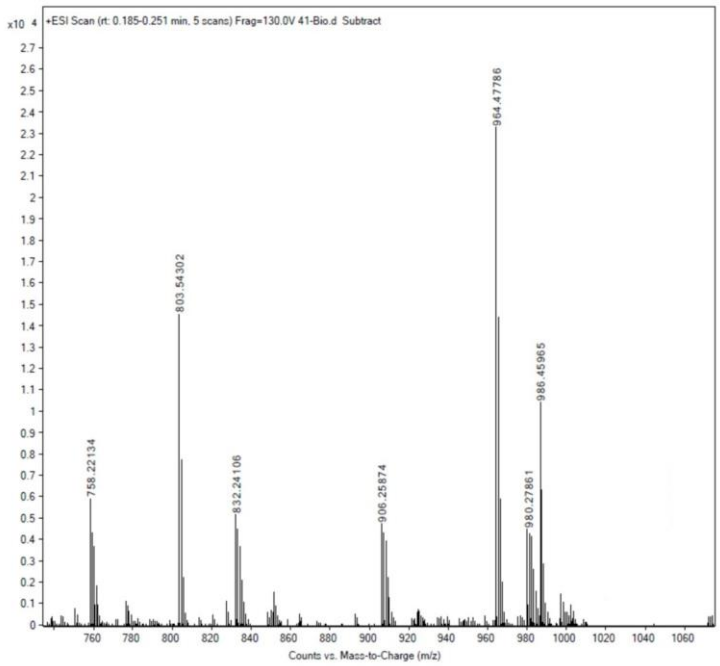


Fig. S144 ESI/HRMS spectrum of **41-Bio**

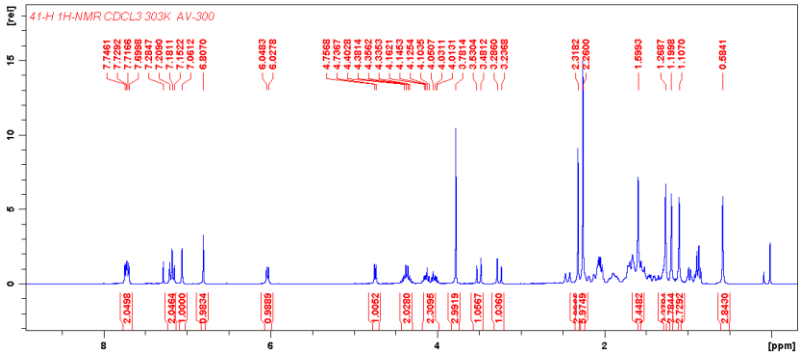


Fig. S145 ^{1}H NMR spectrum of **41-H**

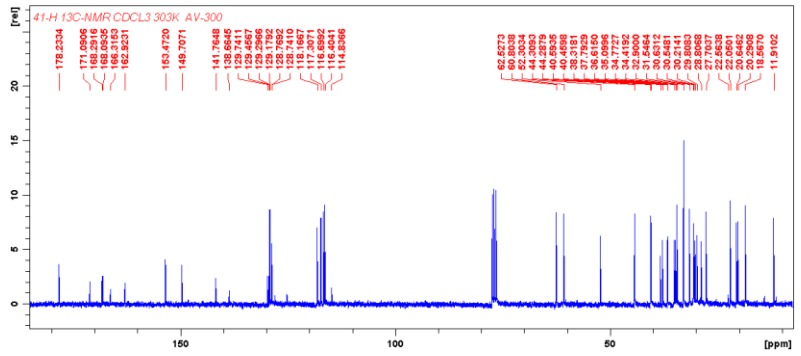


Fig. S146 ^{13}C NMR spectrum of **41-H** (75 MHz in $CDCl_3$)

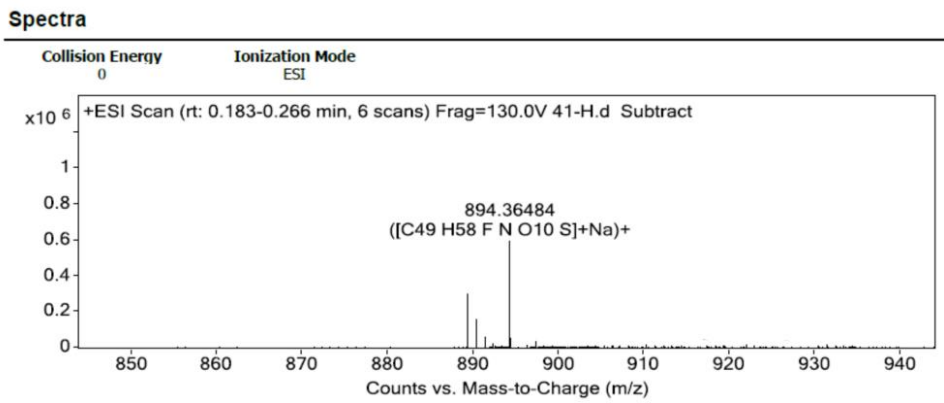


Fig. S147 ESI/HRMS spectrum of **41-H**

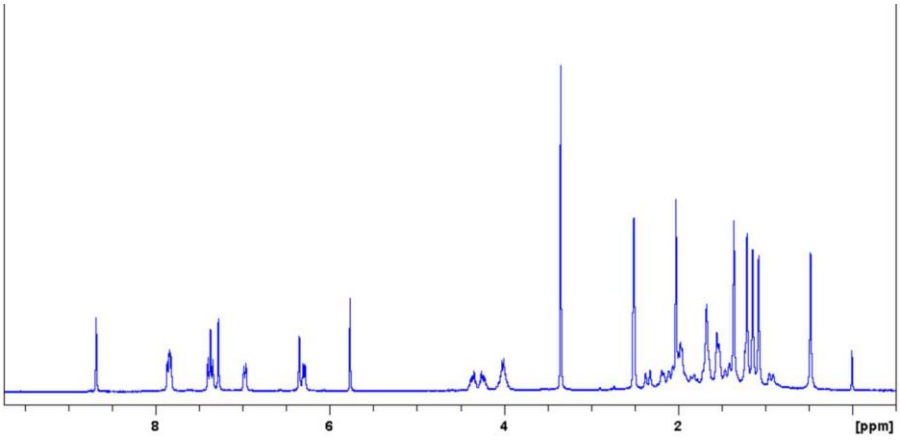


Fig. S148 ^{1}H NMR spectrum of **41** (75 MHz in DMSO-d_6)

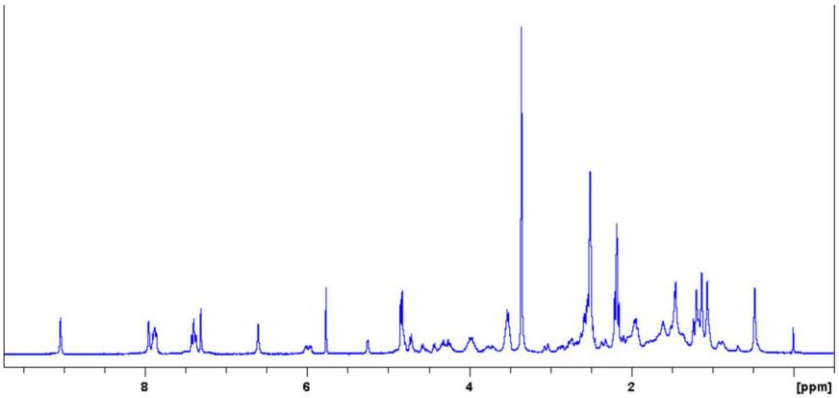
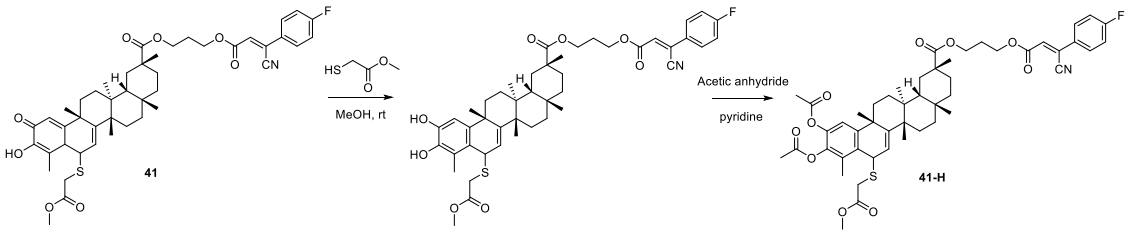


Fig. S149 ^{1}H NMR spectrum of **41** with DTT (75 MHz in DMSO-d_6)

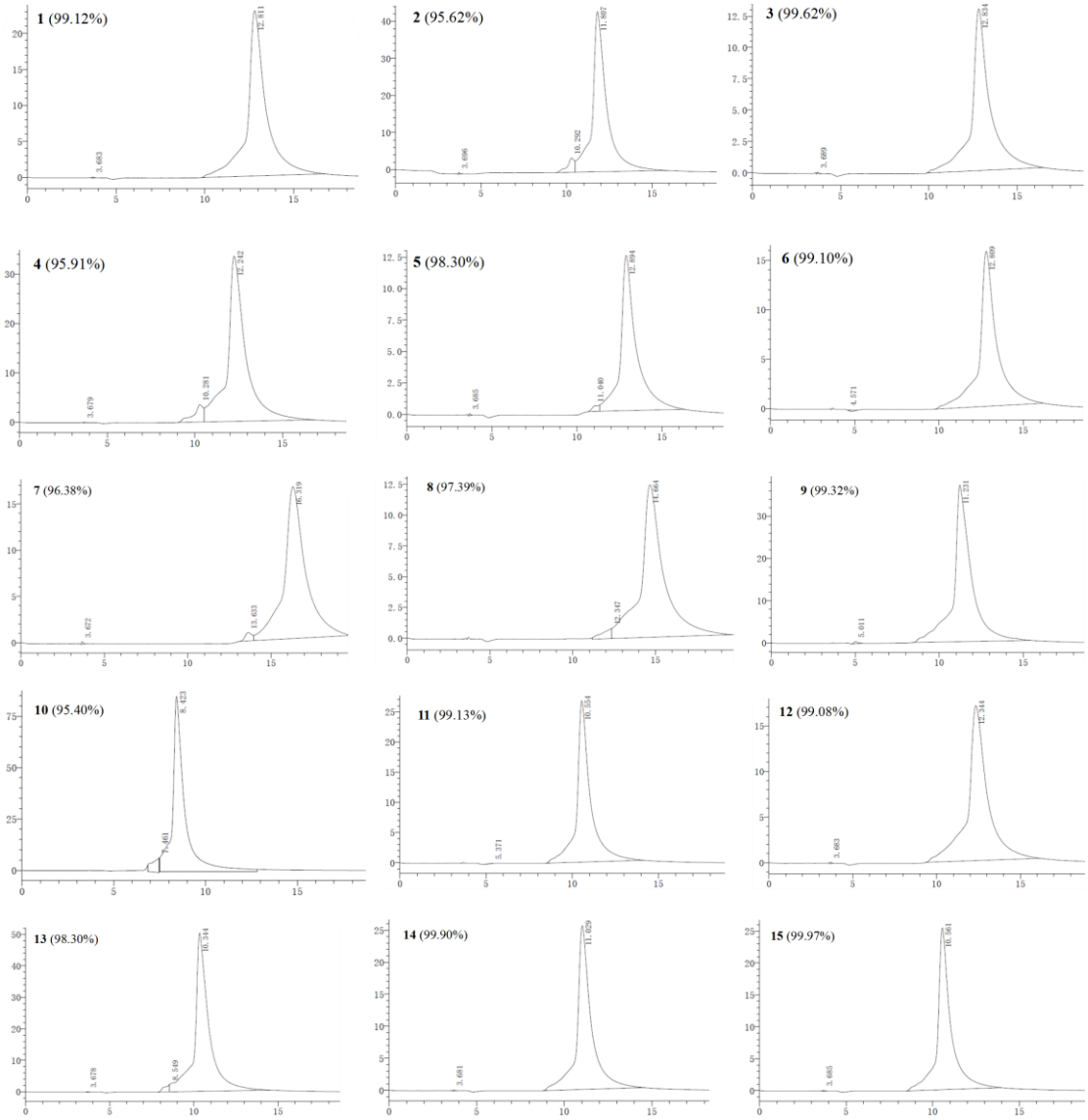
2. The synthetic route of compound **41-H**



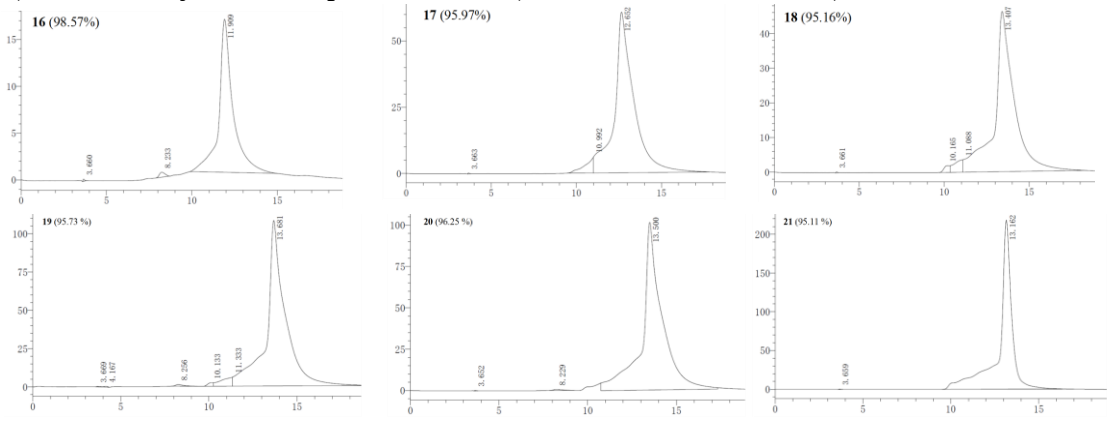
Scheme S1. Reagents and Conditions: (a) sulfhydryl group, MeOH, rt, 15 min; (b) Acetic anhydride, pyridine, rt, 12 h.

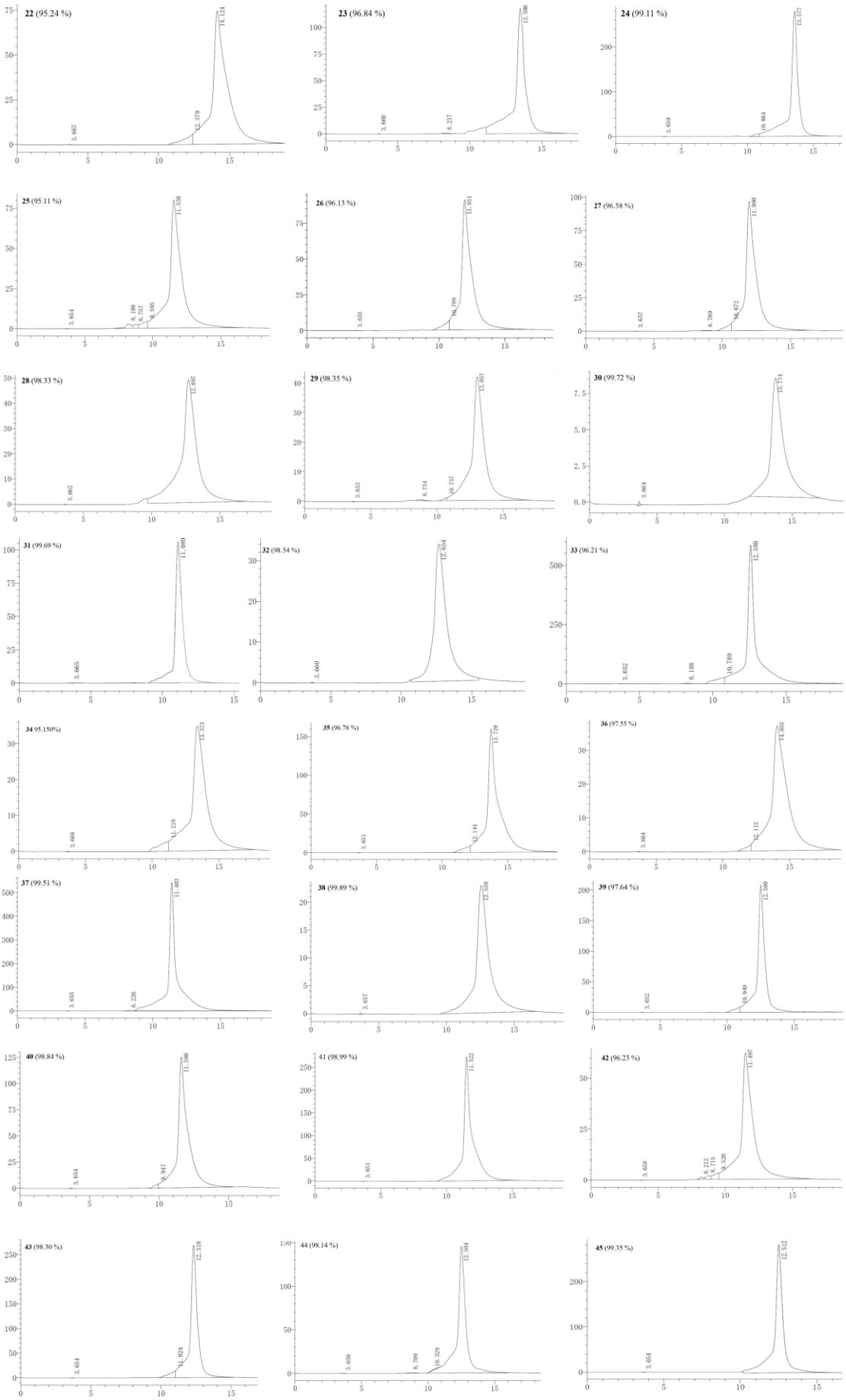
3. HPLC analysis of target compounds

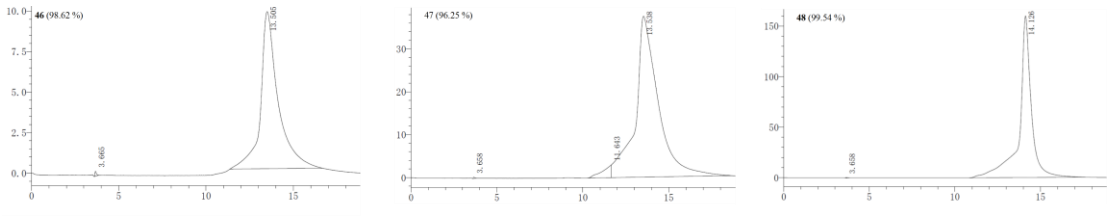
1) HPLC analysis of compounds **1-15** (0.8 ml/min, 97% MeOH)



2) HPLC analysis of compounds **16-48** (0.8 ml/min, 94% MeOH)




22 (95.24 %)
23 (96.84 %)
24 (99.11 %)
25 (95.11 %)
26 (96.13 %)
27 (96.58 %)
28 (98.33 %)
29 (98.35 %)
30 (99.72 %)
31 (99.69 %)
32 (98.54 %)
33 (96.21 %)
34 95.150%)
35 (96.78 %)
36 (97.55 %)
37 (99.51 %)
38 (99.89 %)
39 (97.64 %)
40 (98.84 %)
41 (98.99 %)
42 (96.23 %)
43 (98.30 %)
44 (98.14 %)
45 (99.35 %)



3) HPLC analysis of compounds **41-H** (0.8 ml/min, 94% MeOH)