Electronic Supplementary Material (ESI) for New Journal of Chemistry

A tetraamido isophthaloyl-based macrocyclic calcium chloride and strontium chloride tritopic receptor

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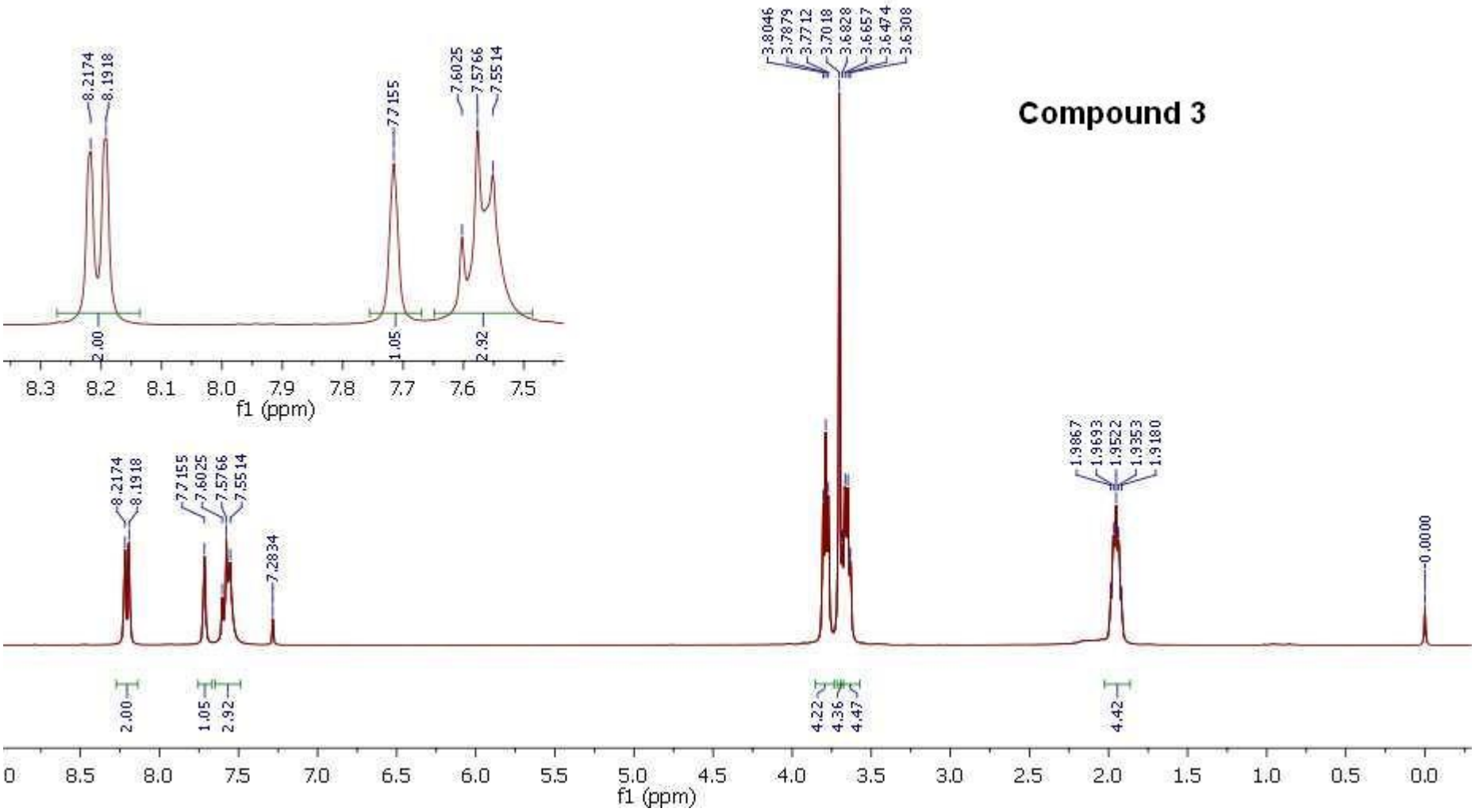
^{1}H- and ^{13}C-NMR spectra were conducted using either a 300 or 500 MHz Bruker instrument as noted in the Experimental section of the paper.

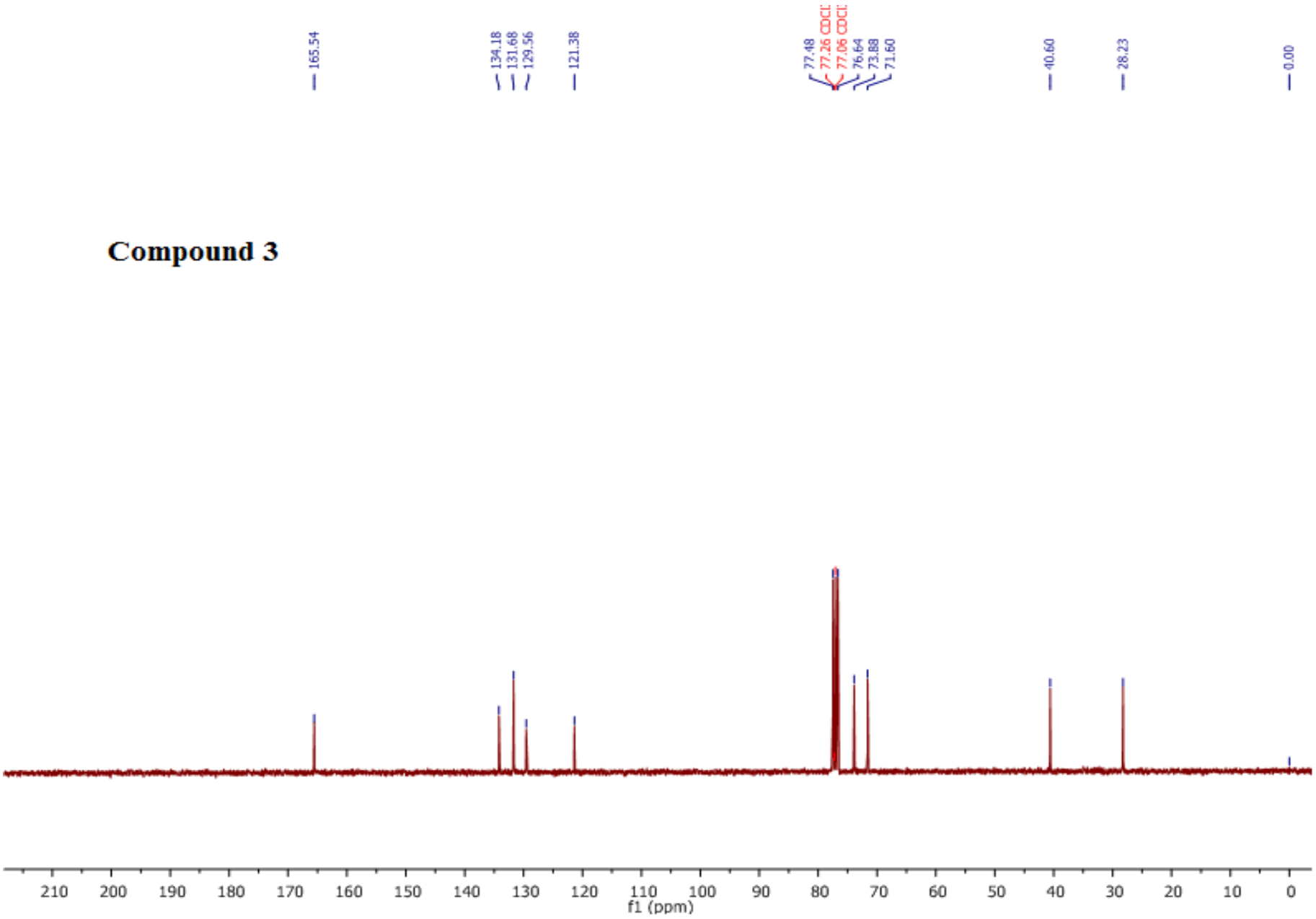
^{1}H NMR titration experiments were conducted using a 300 MHz Bruker instrument.

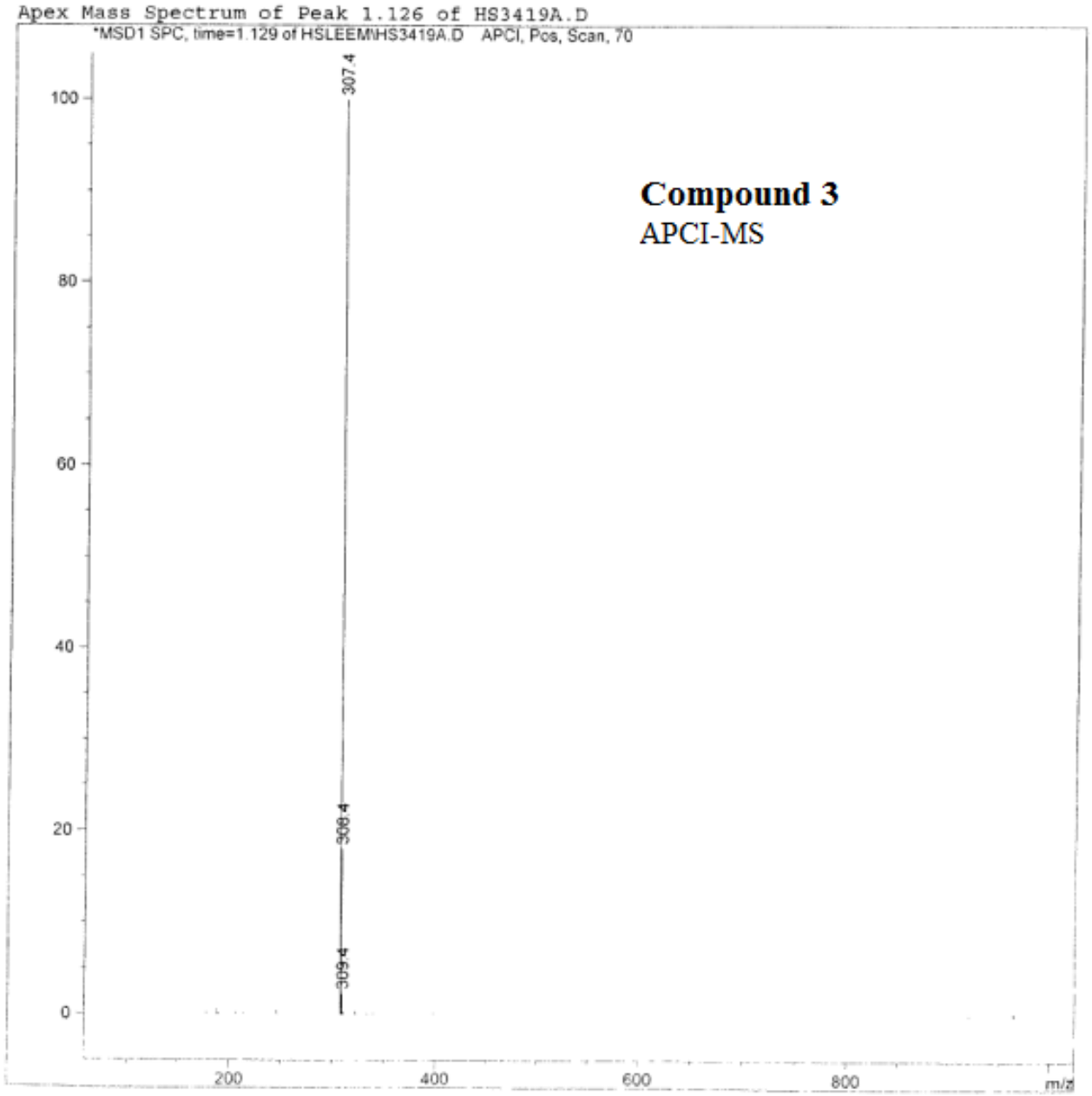
Mass spectra for all new compounds were conducted using an Agilent 1100 series SL LC/MSD (Trap) in the APCI mode in chloroform or as otherwise noted.

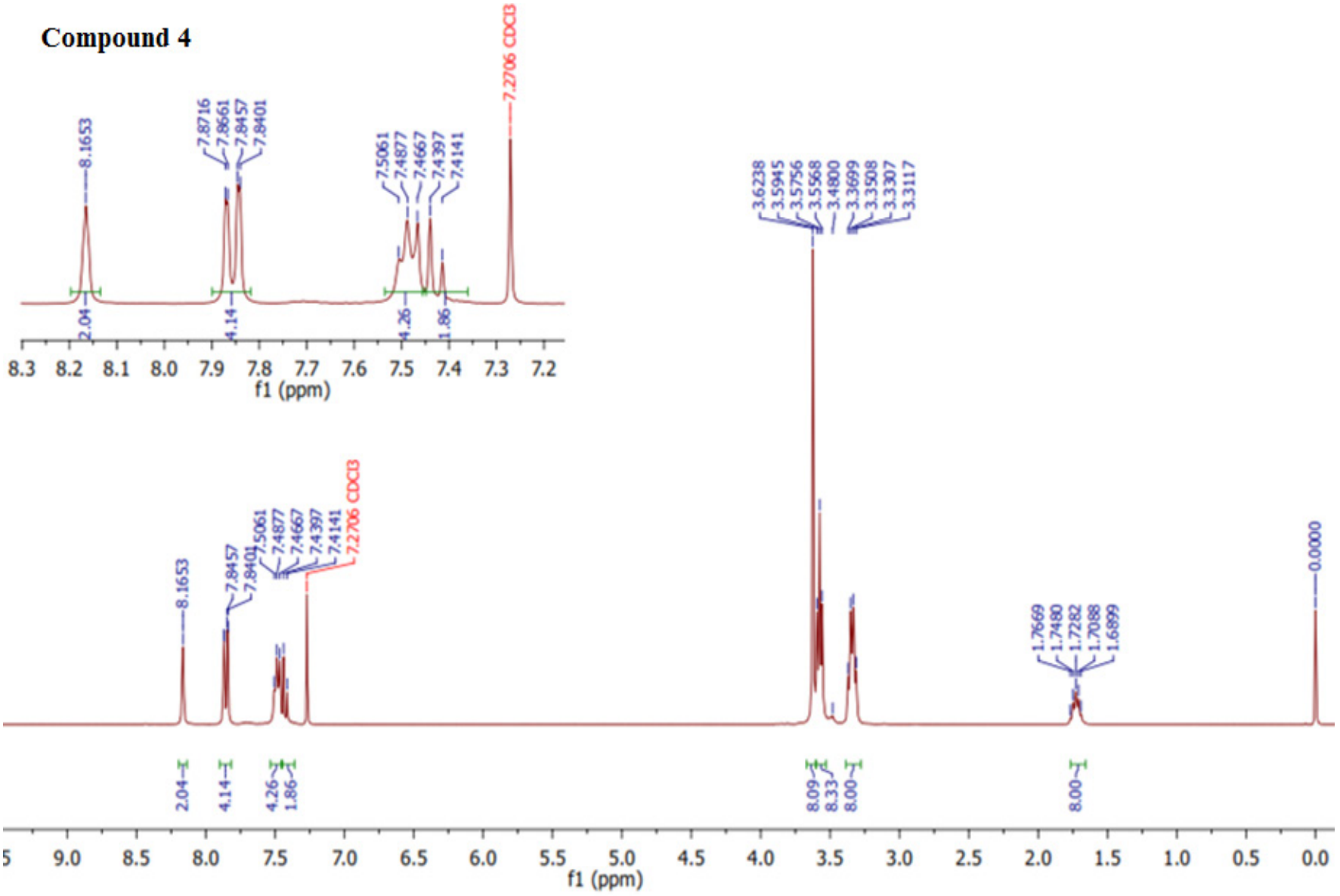
Mass spectra for all titration experiments were conducted using an Agilent 1100 series SL LC/MSD (Trap) in the ESI mode with the following method parameters: Nebulizer (50 psi), dry gas (11 l/min), dry temperature (250 ^{O}C), for compound stability (50%), and trap drive level (100%).

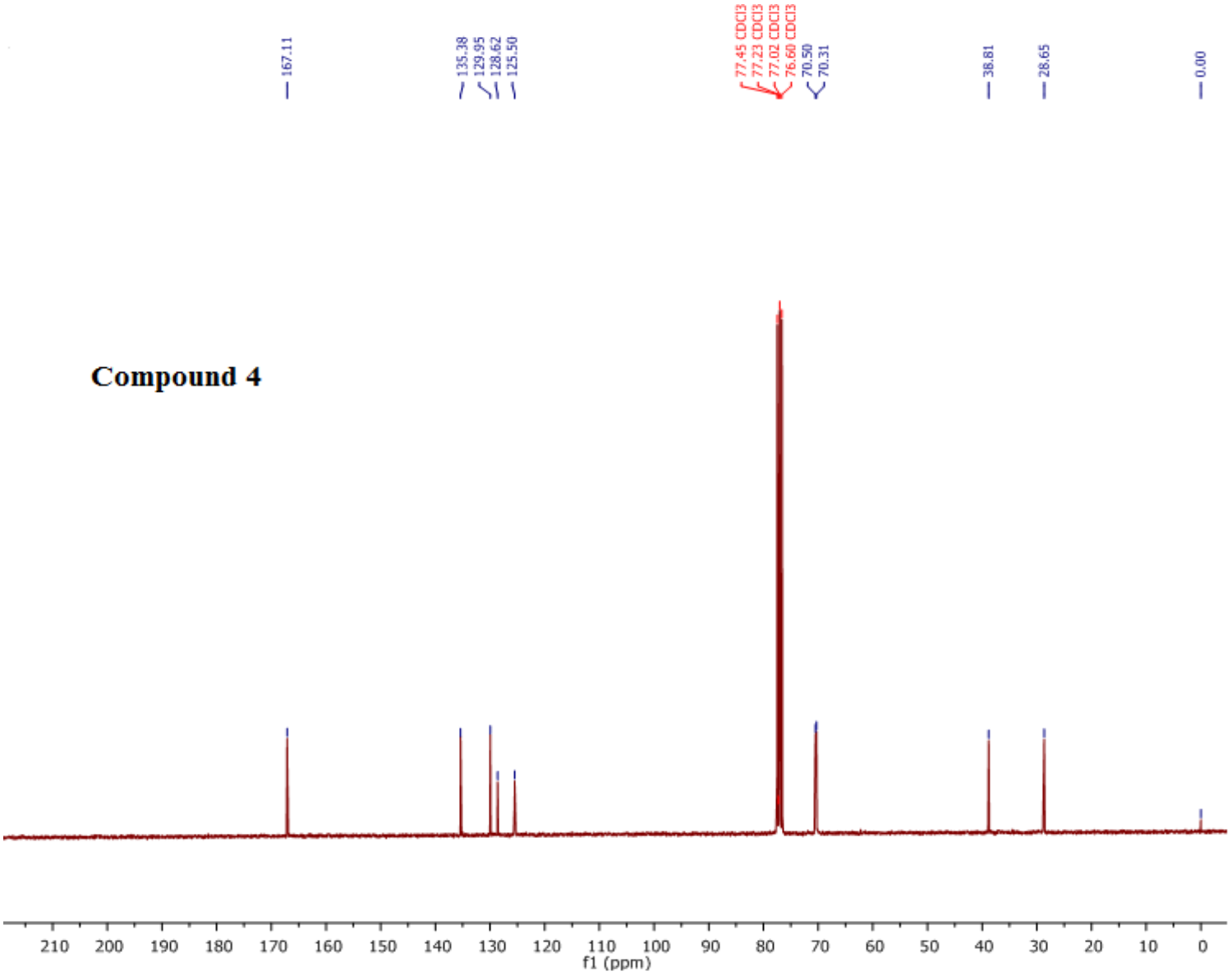


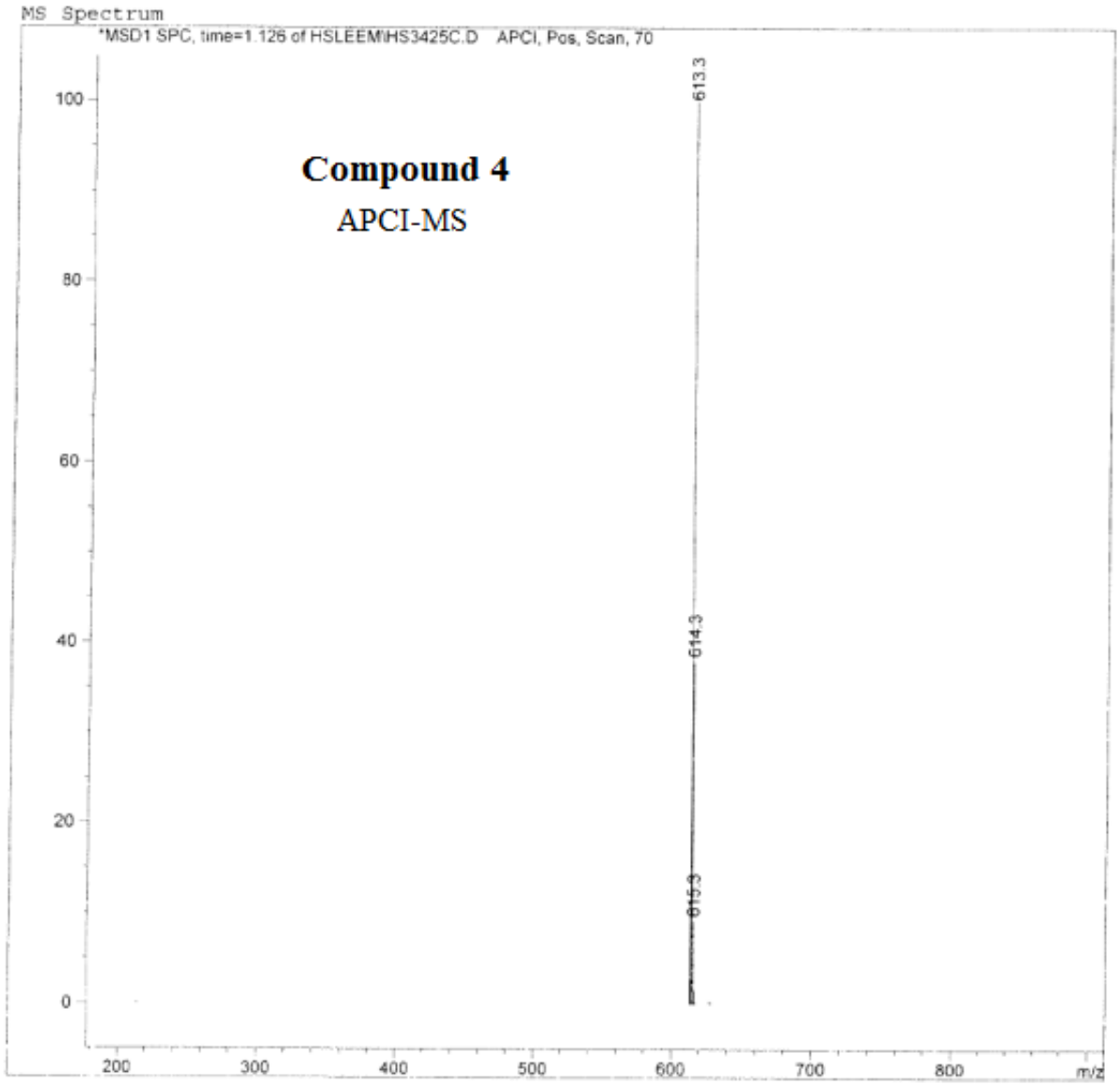
Compound 3

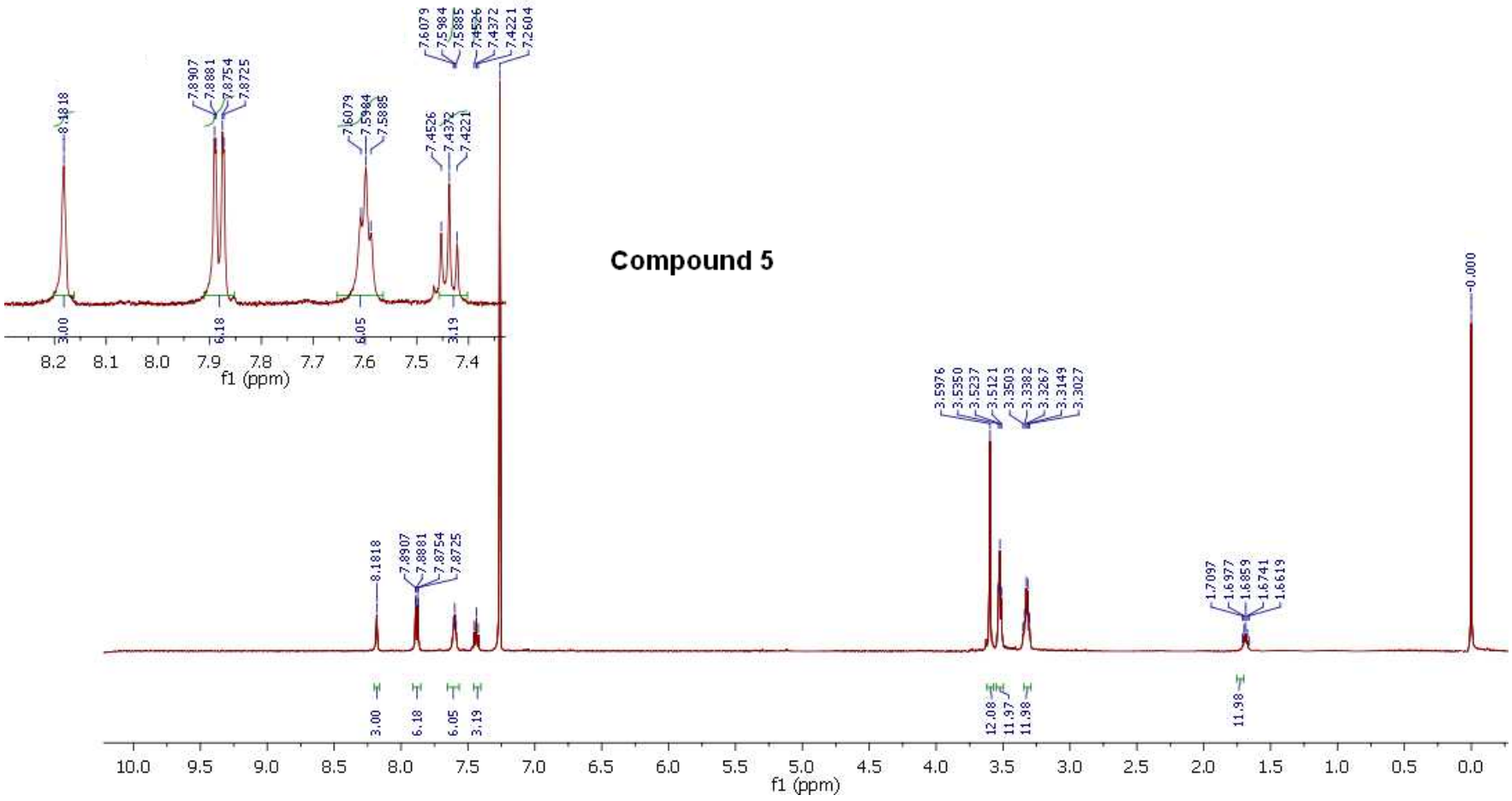


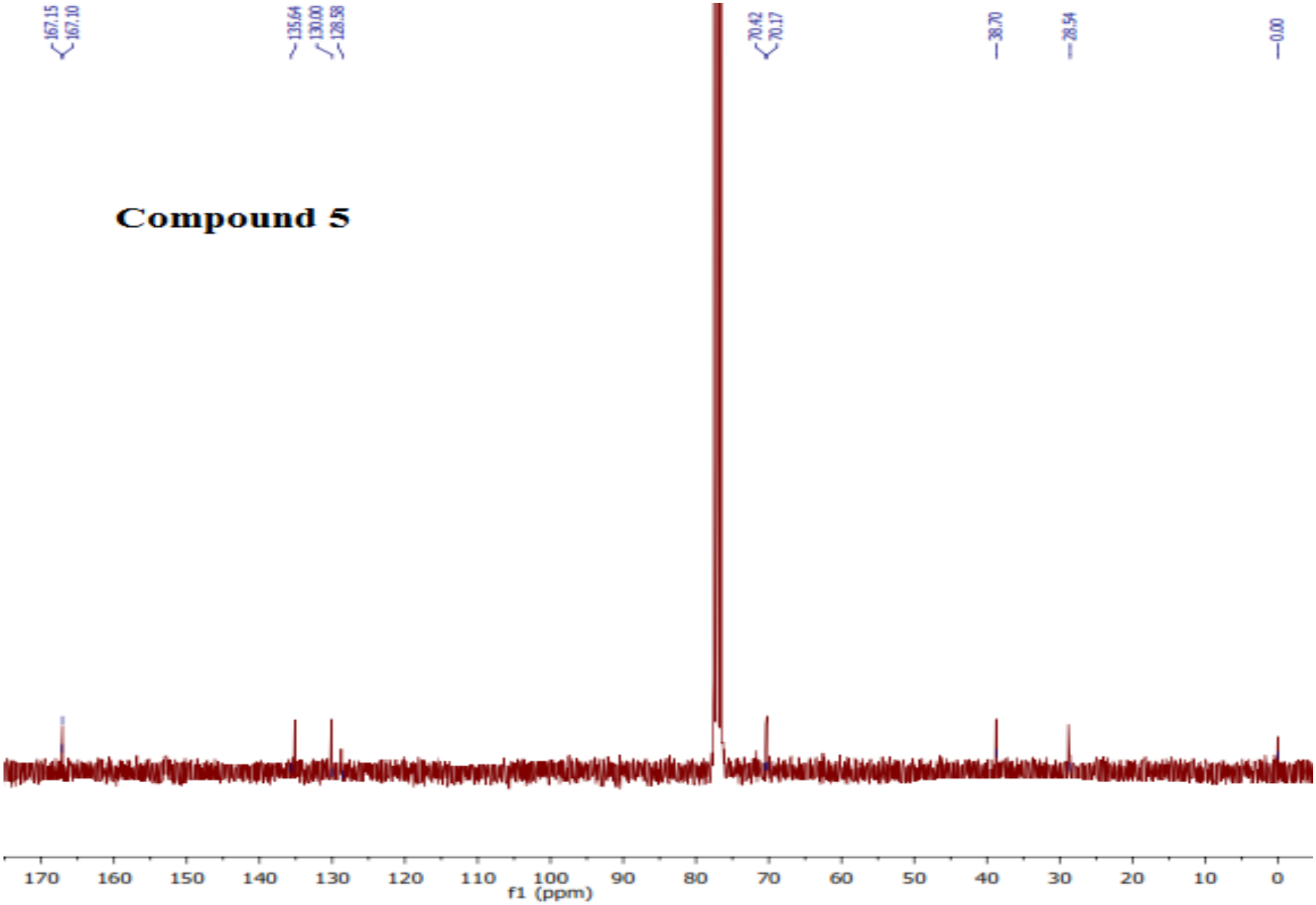


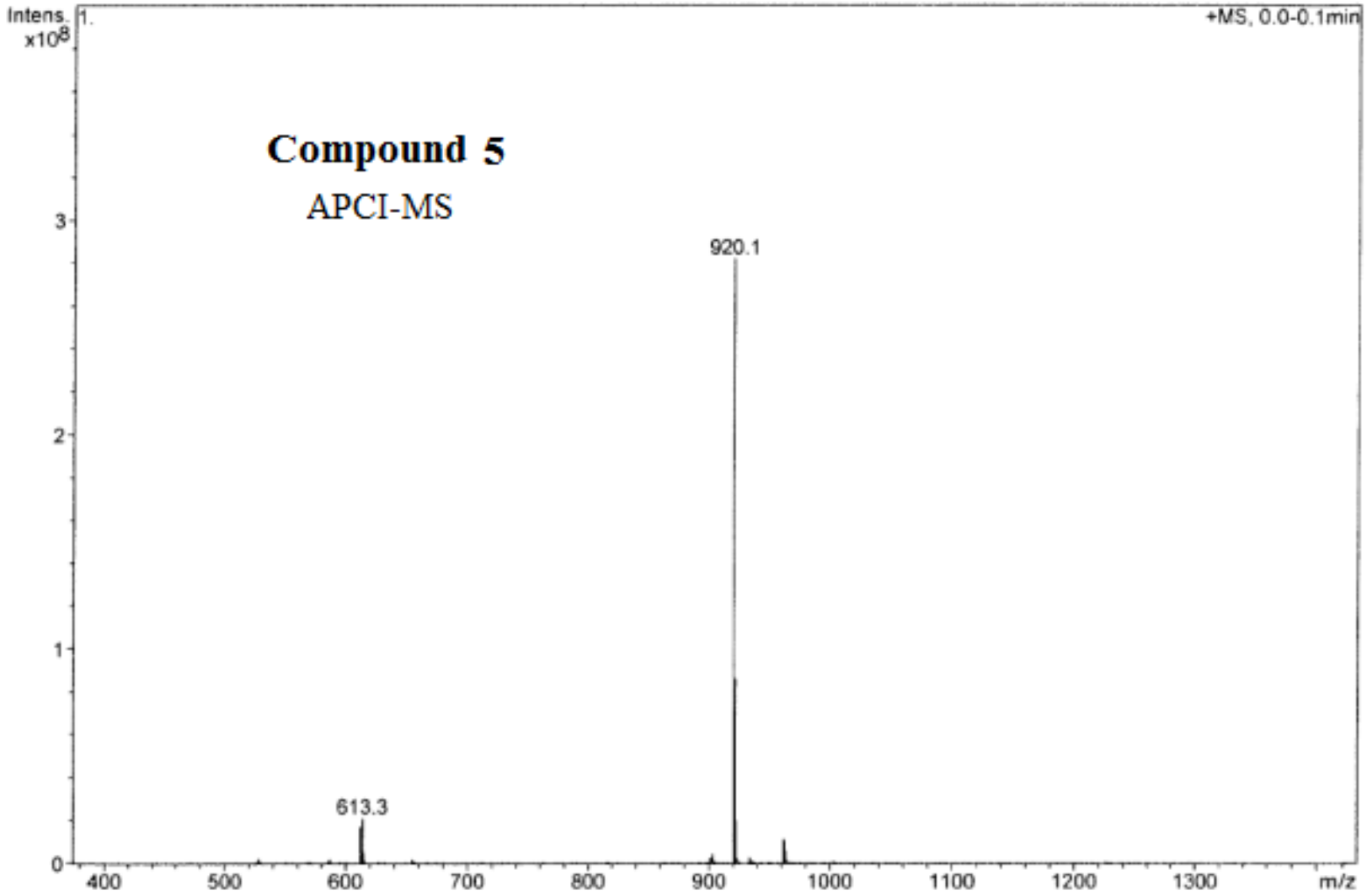


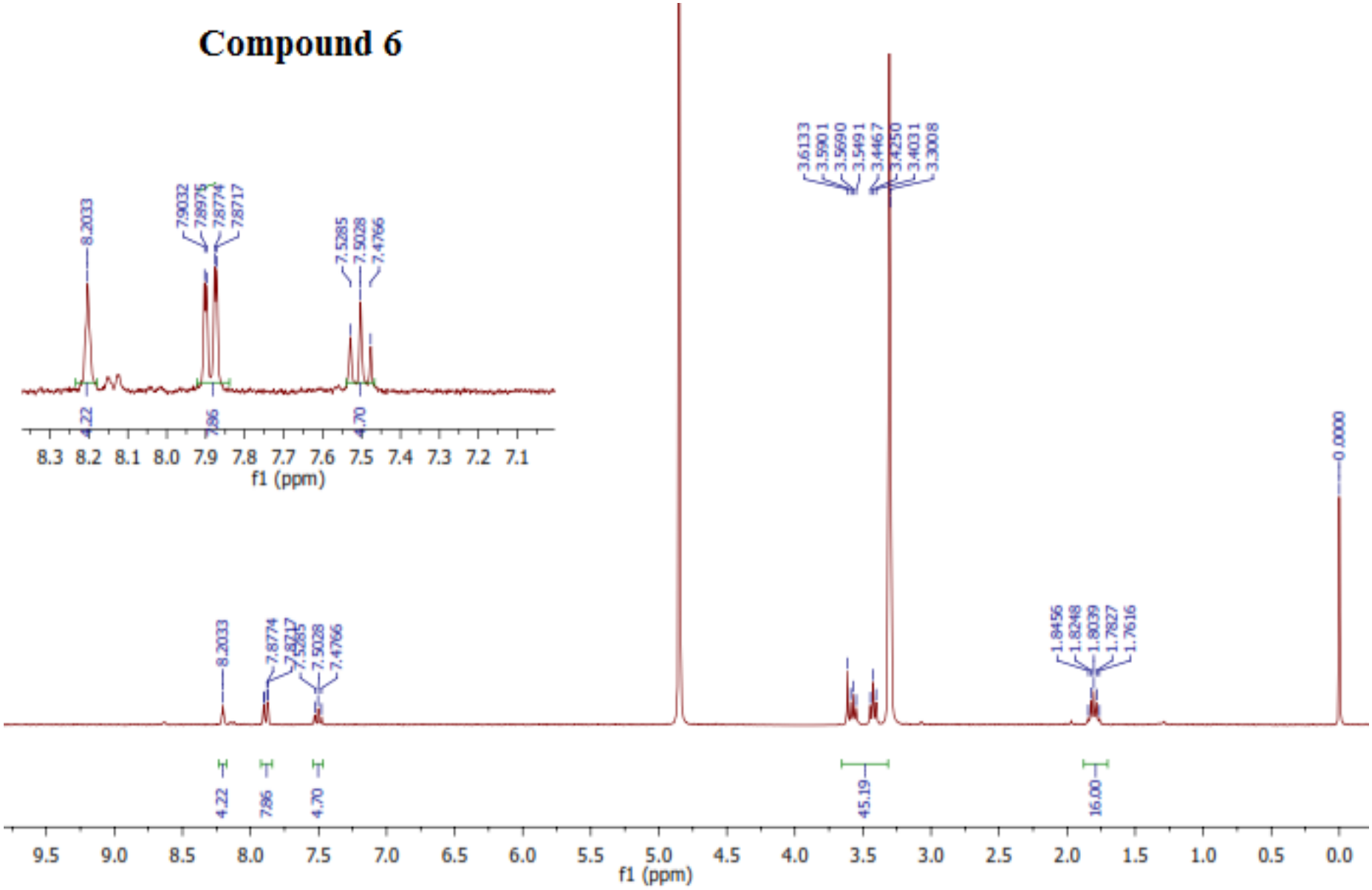


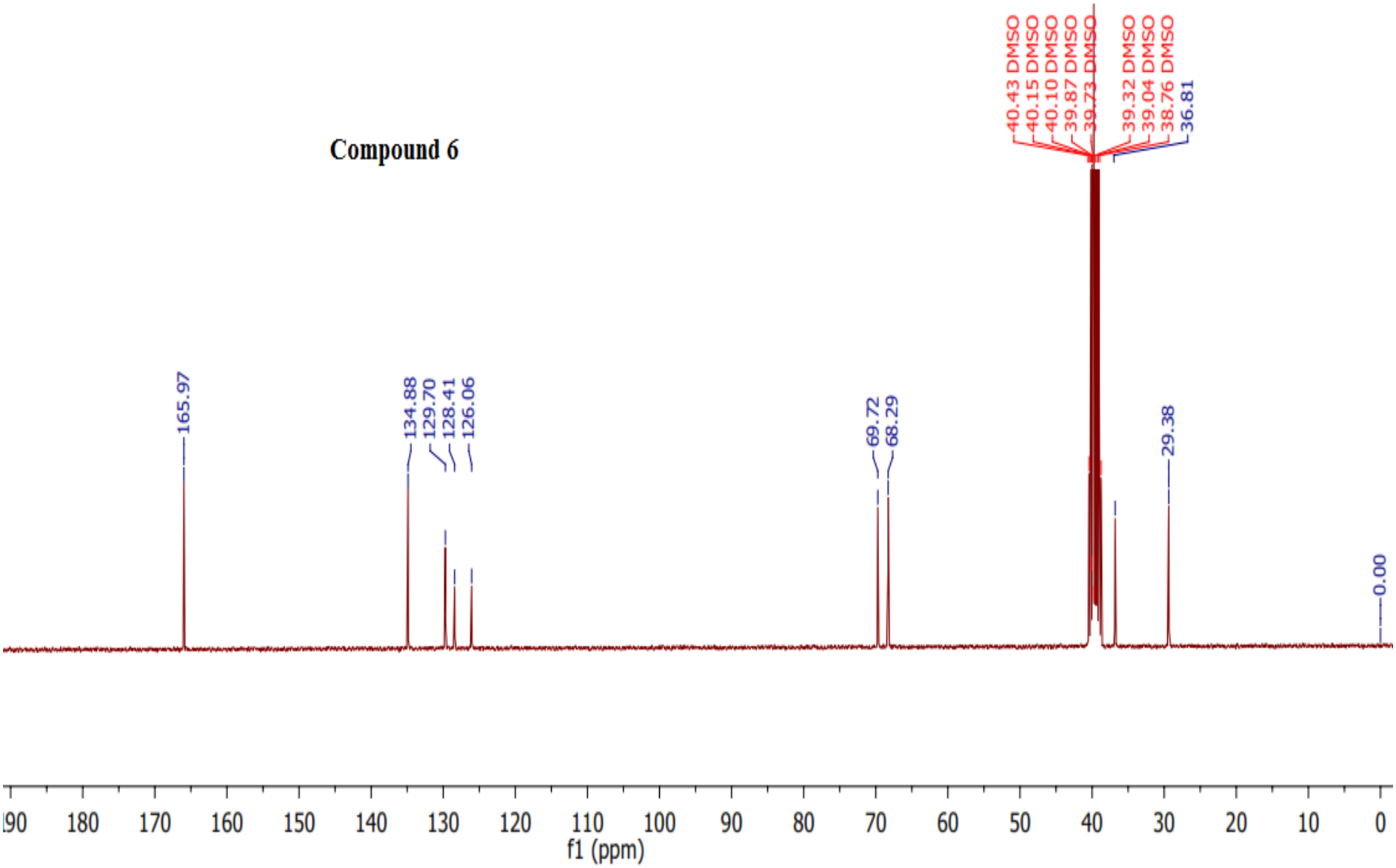


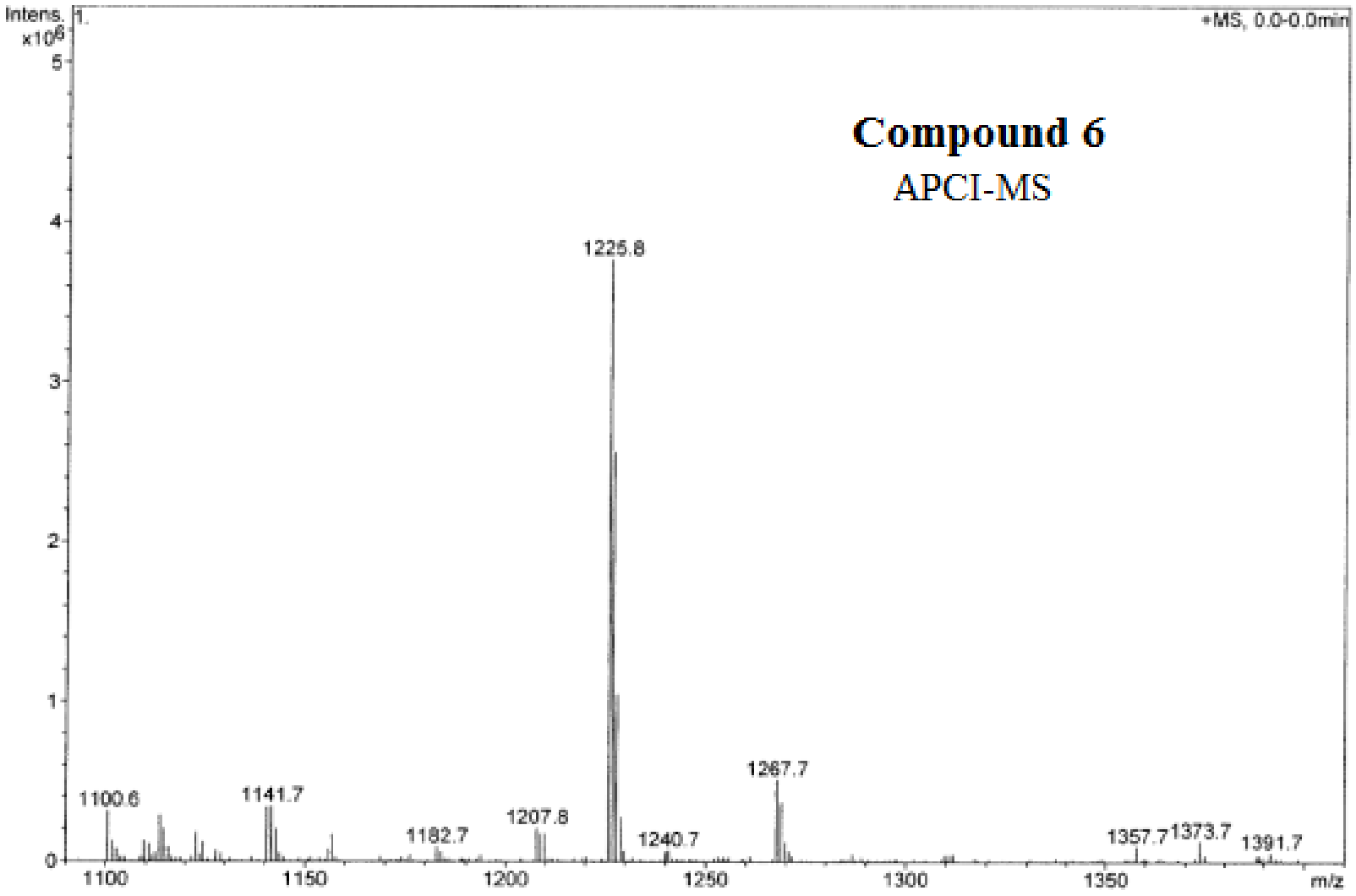


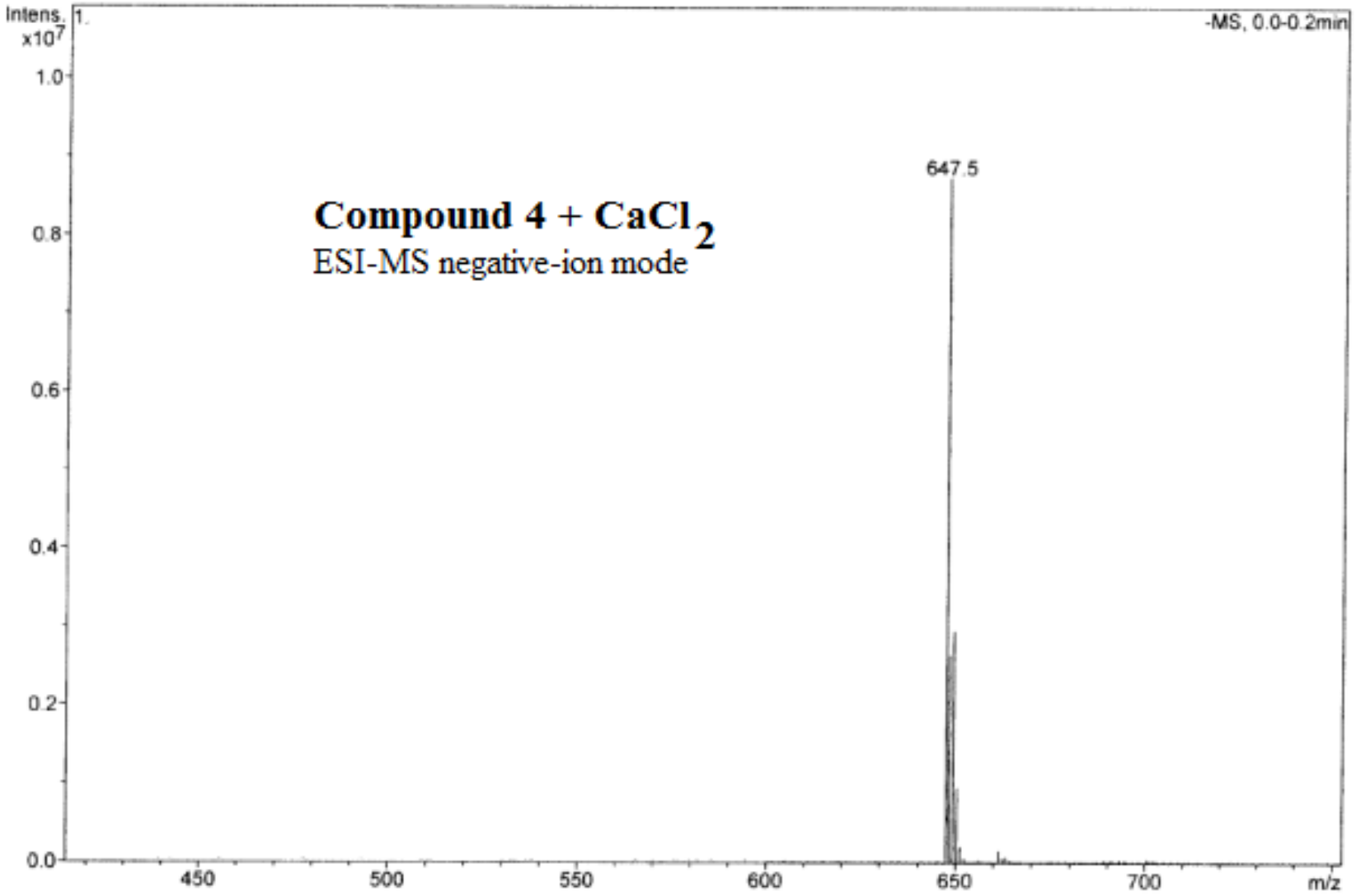


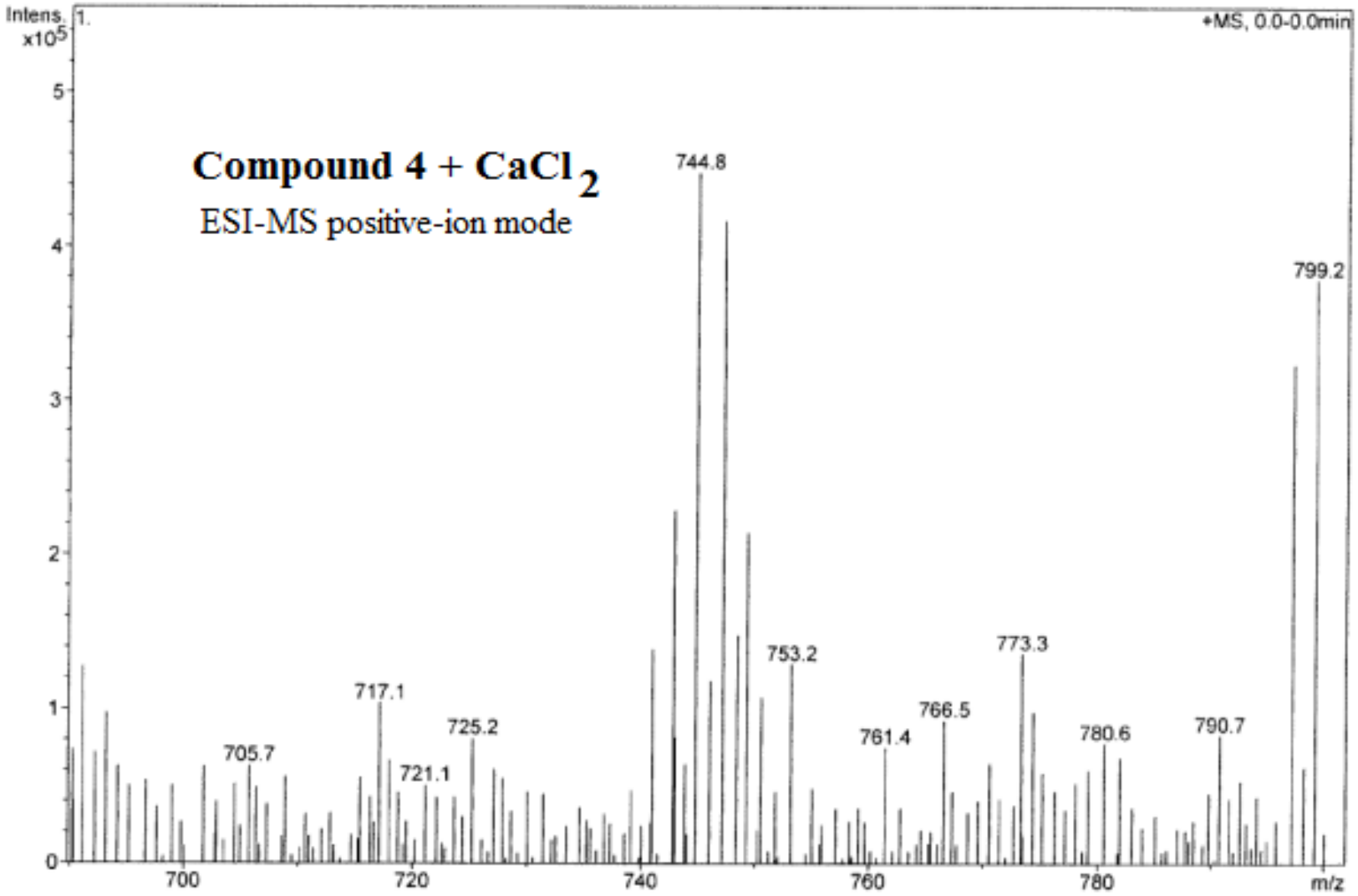


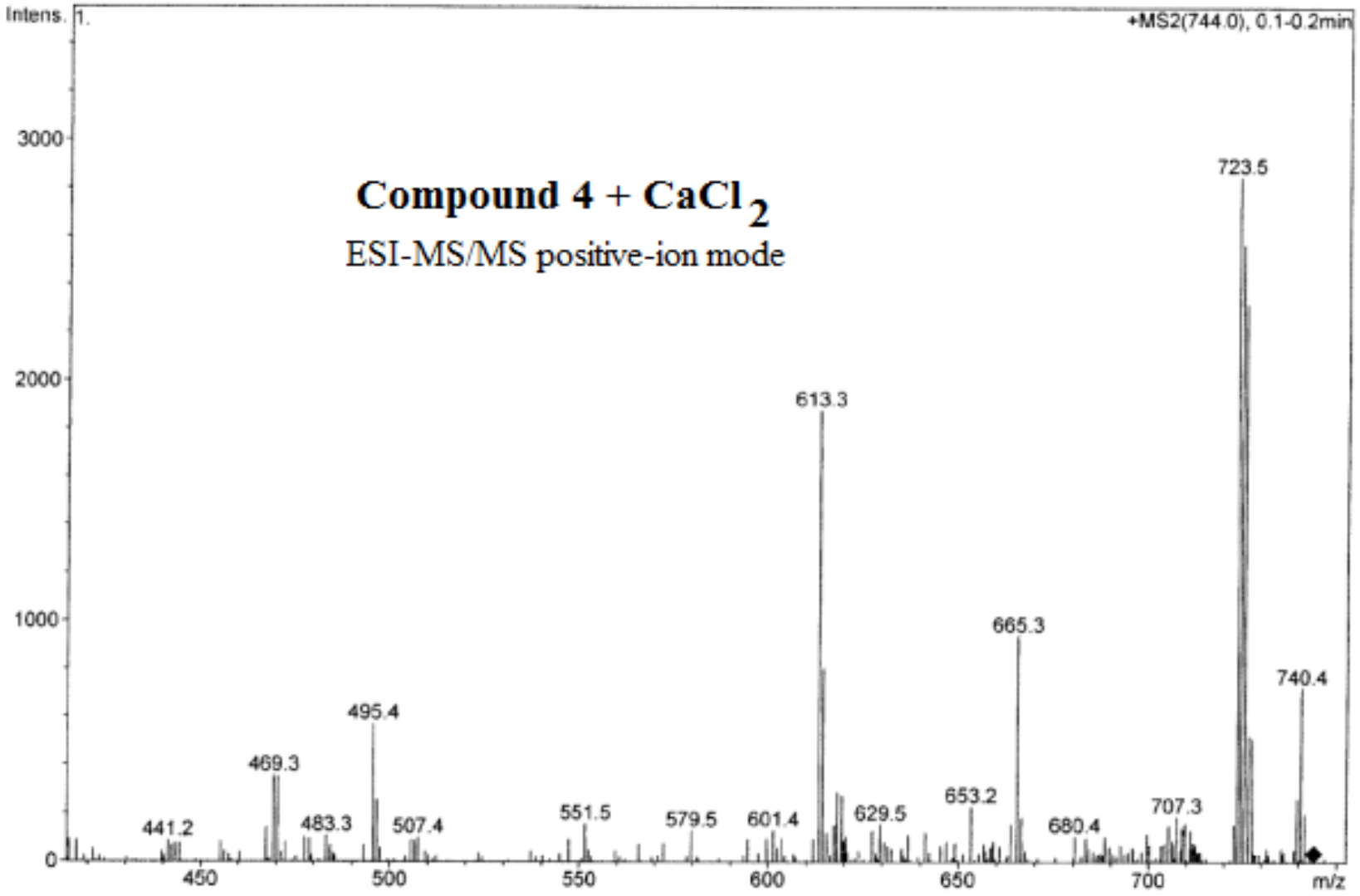


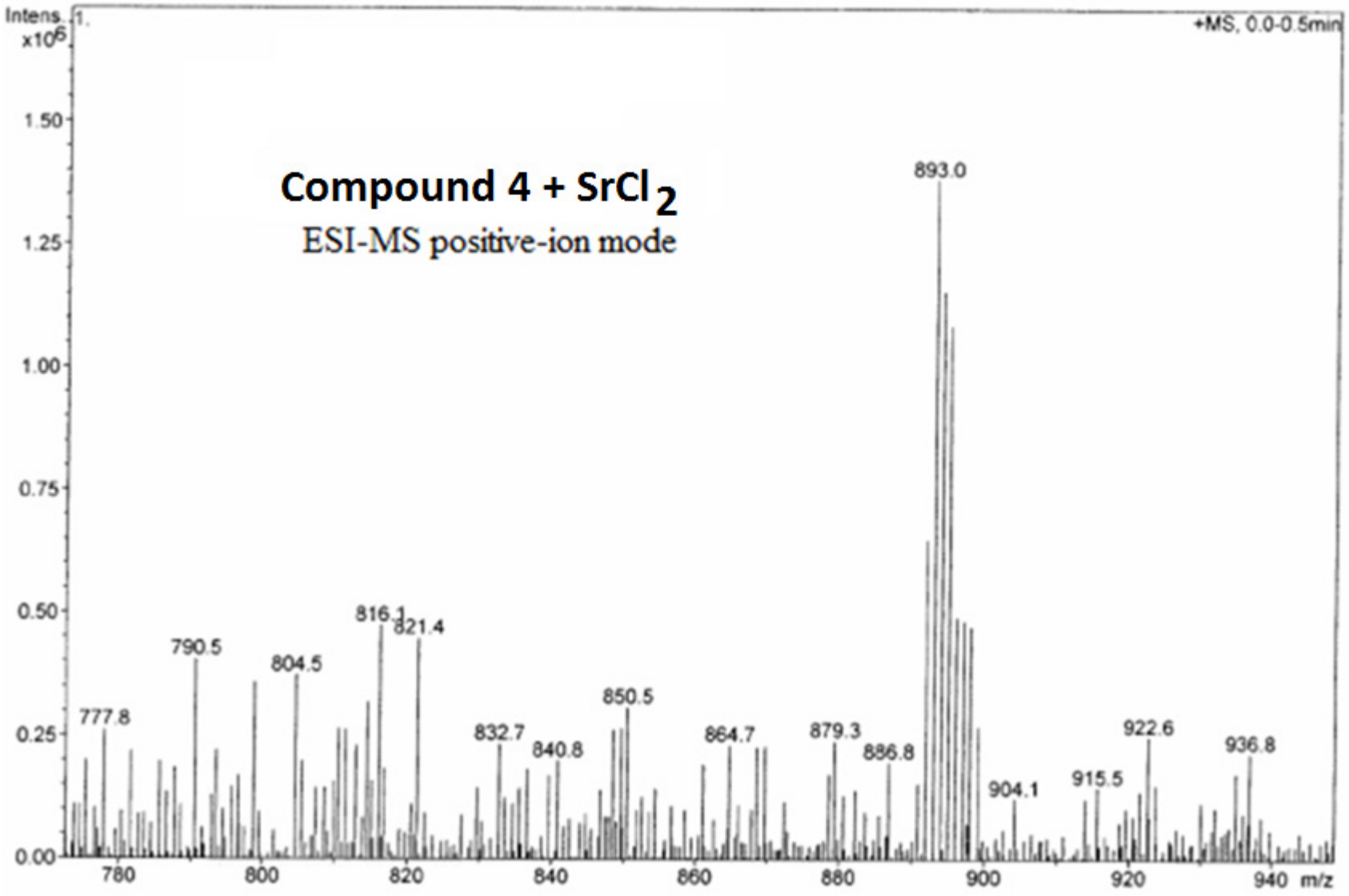


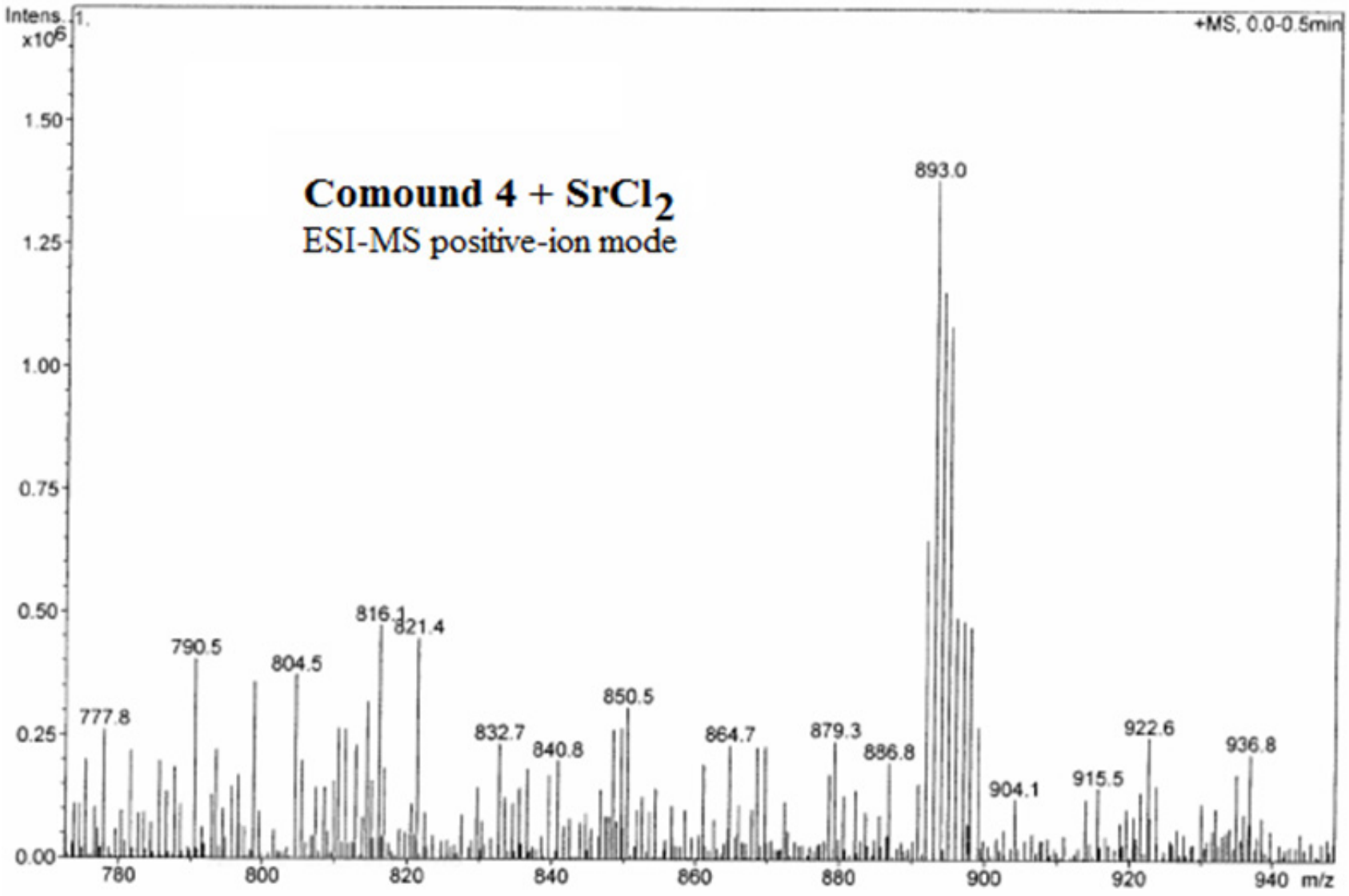


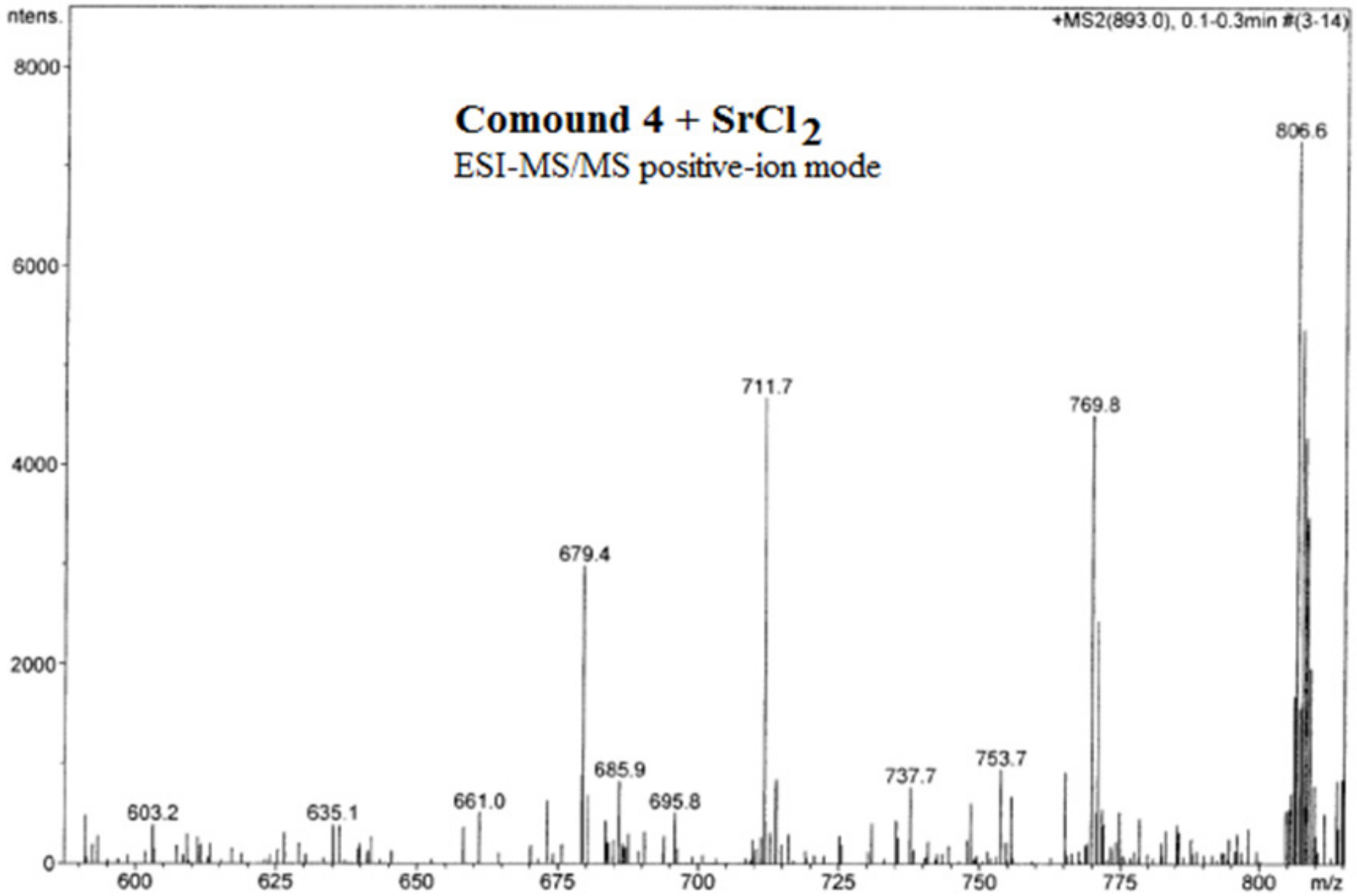


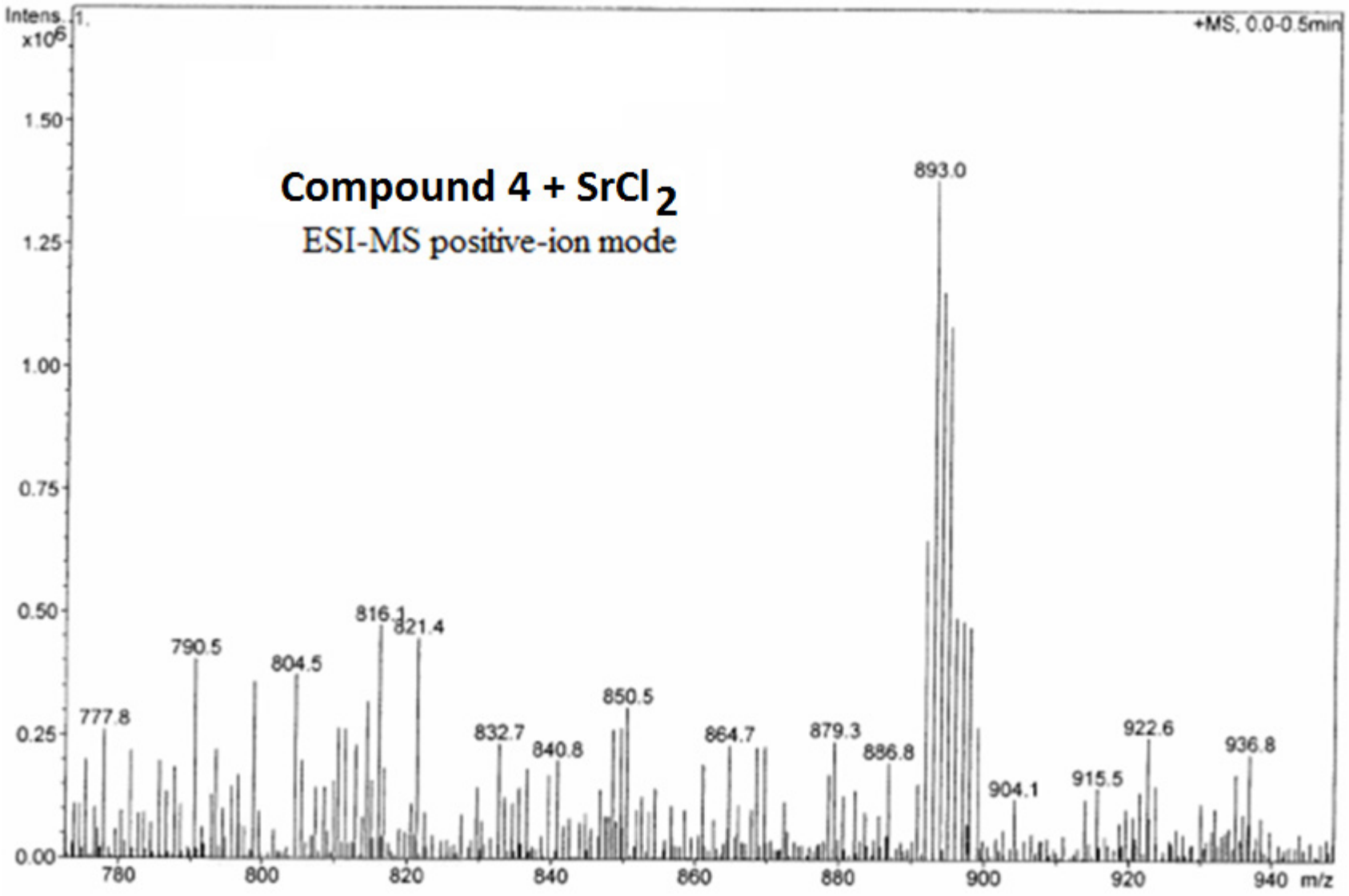


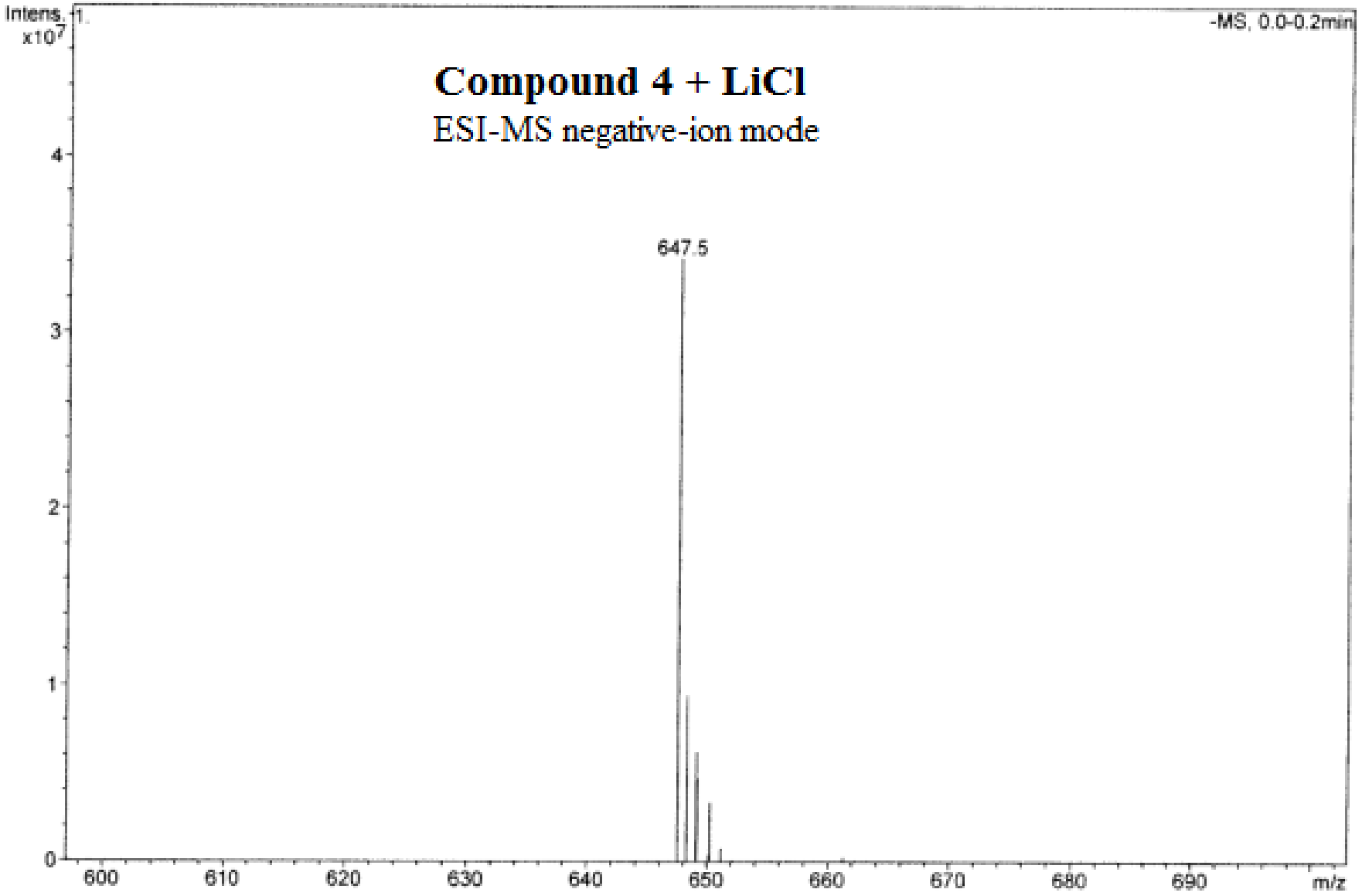


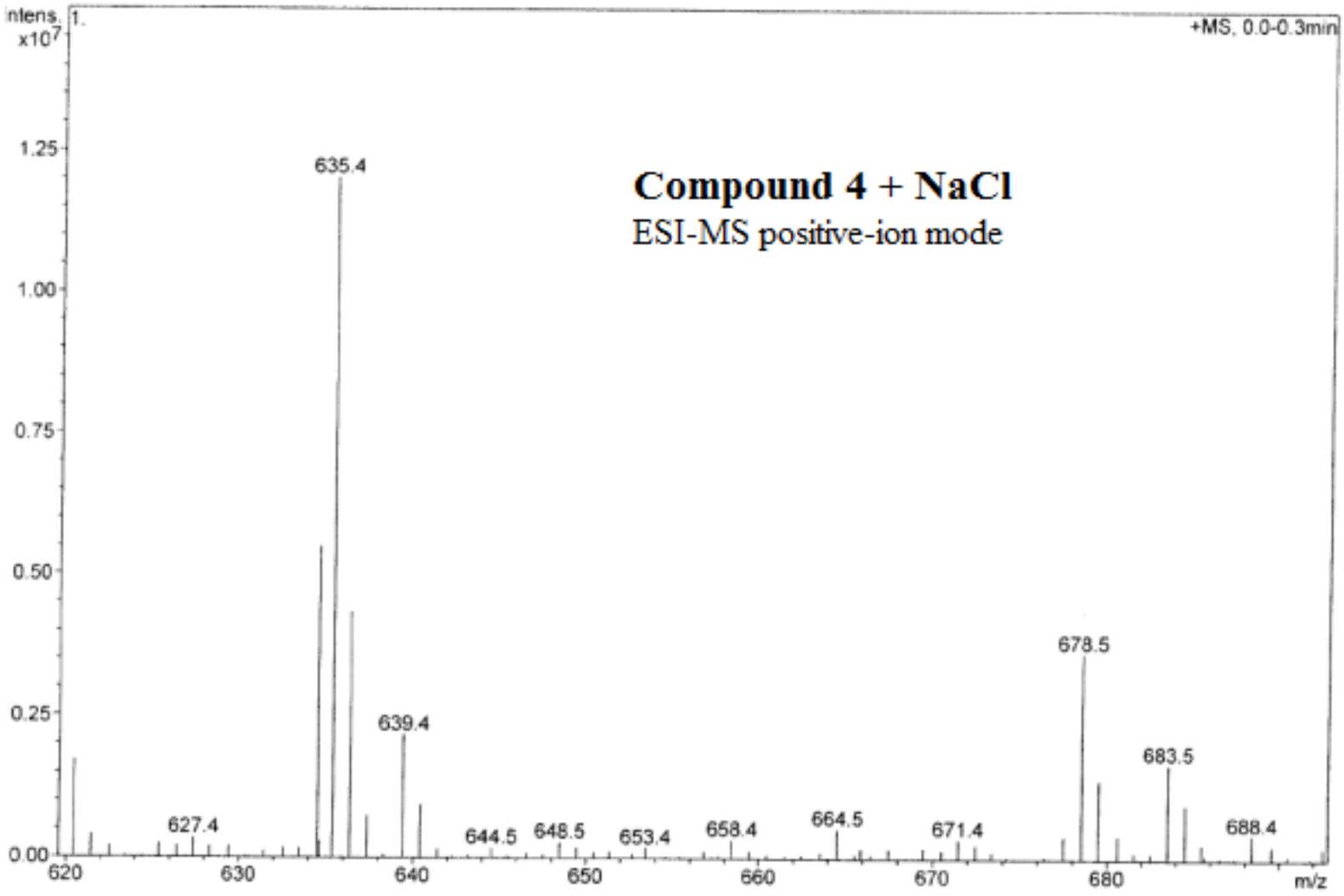


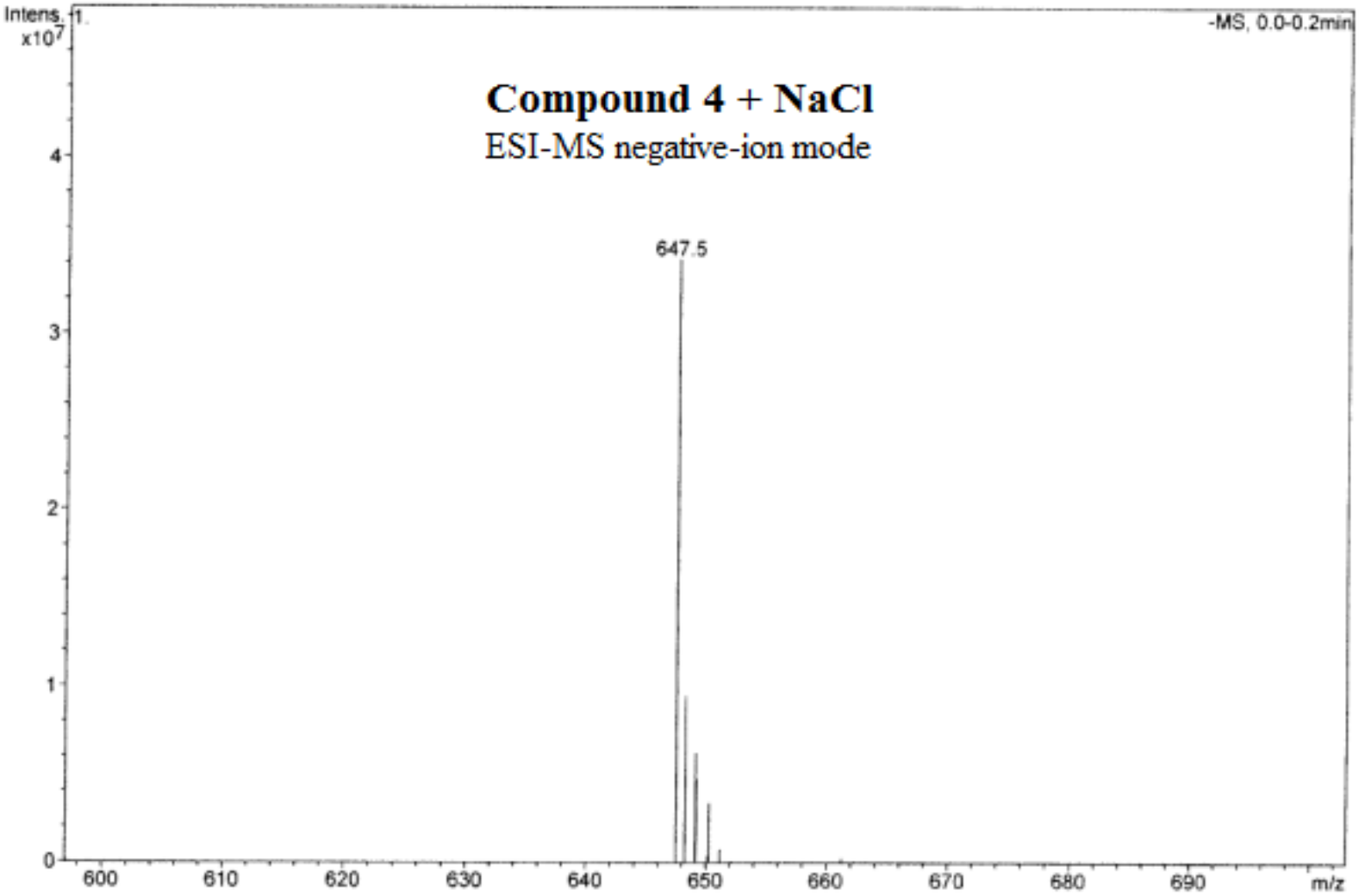


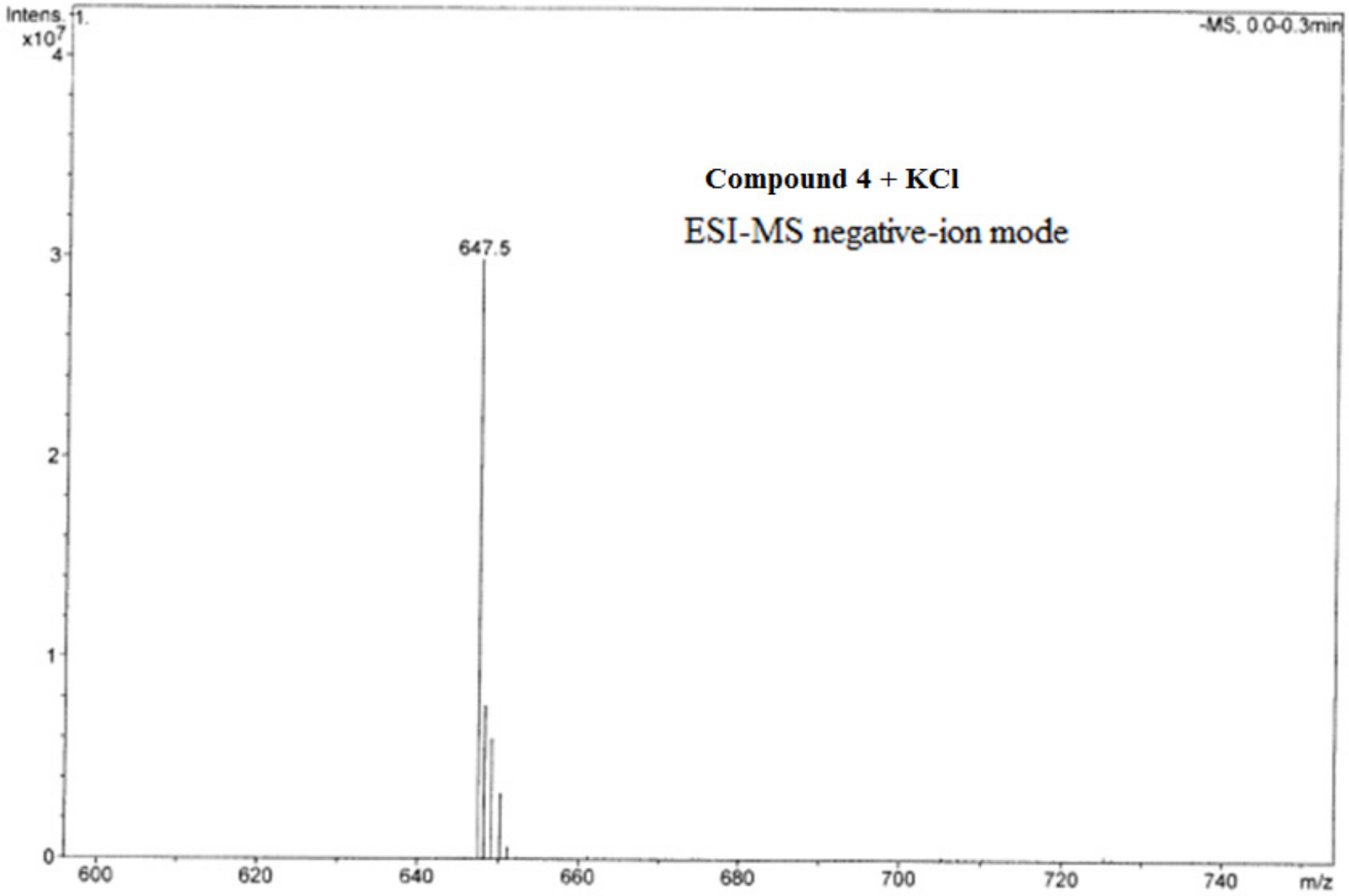


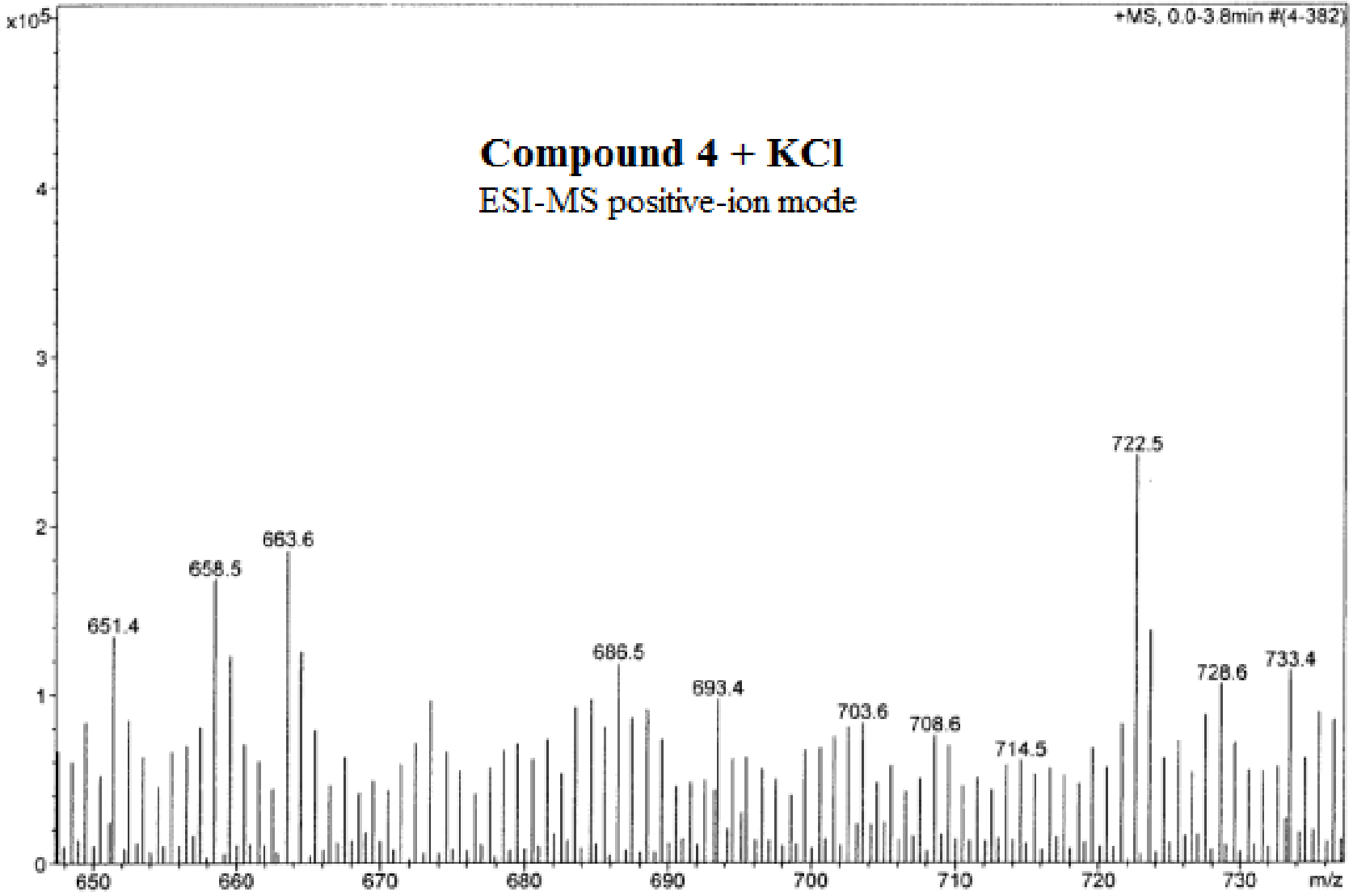


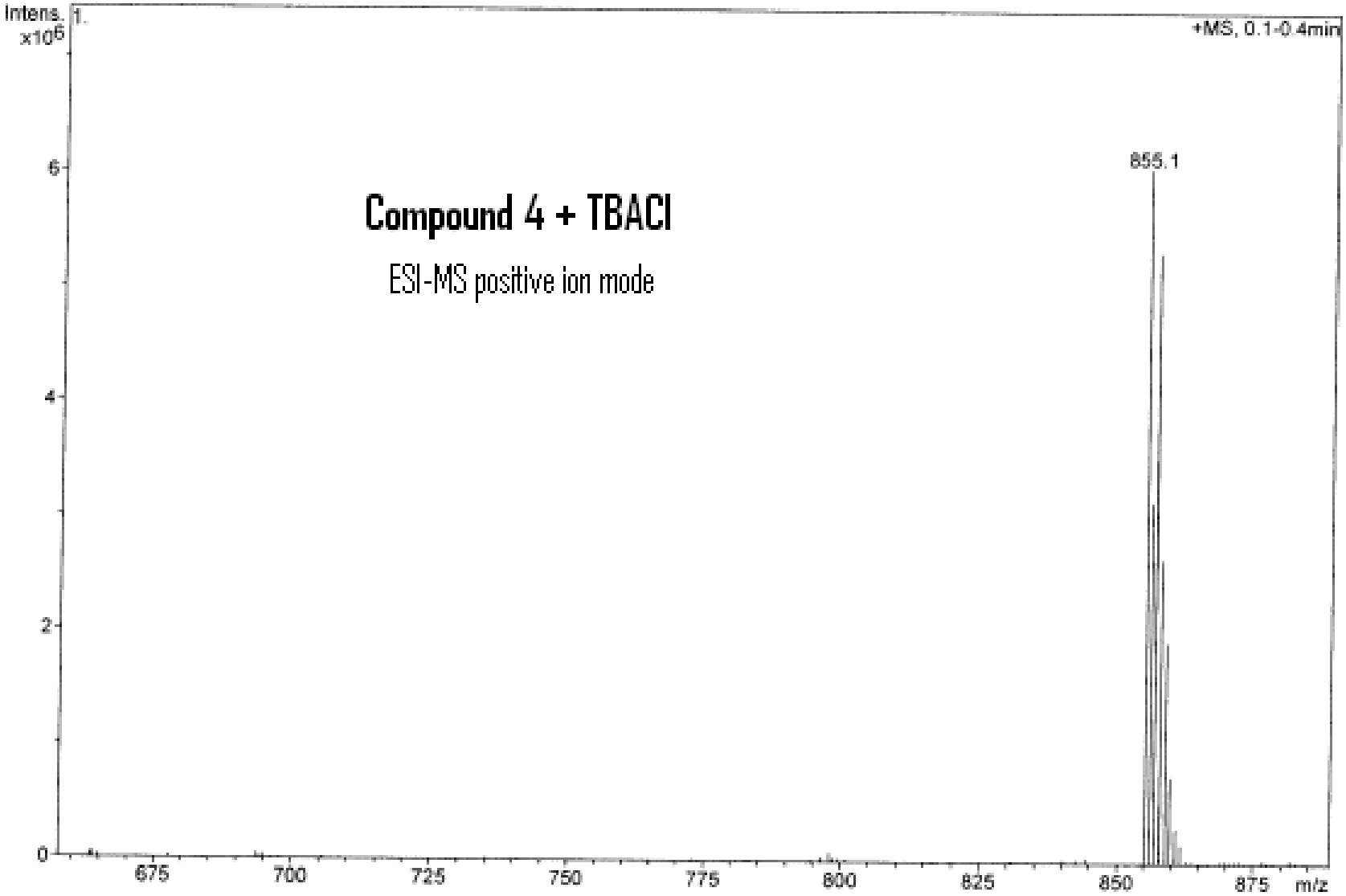


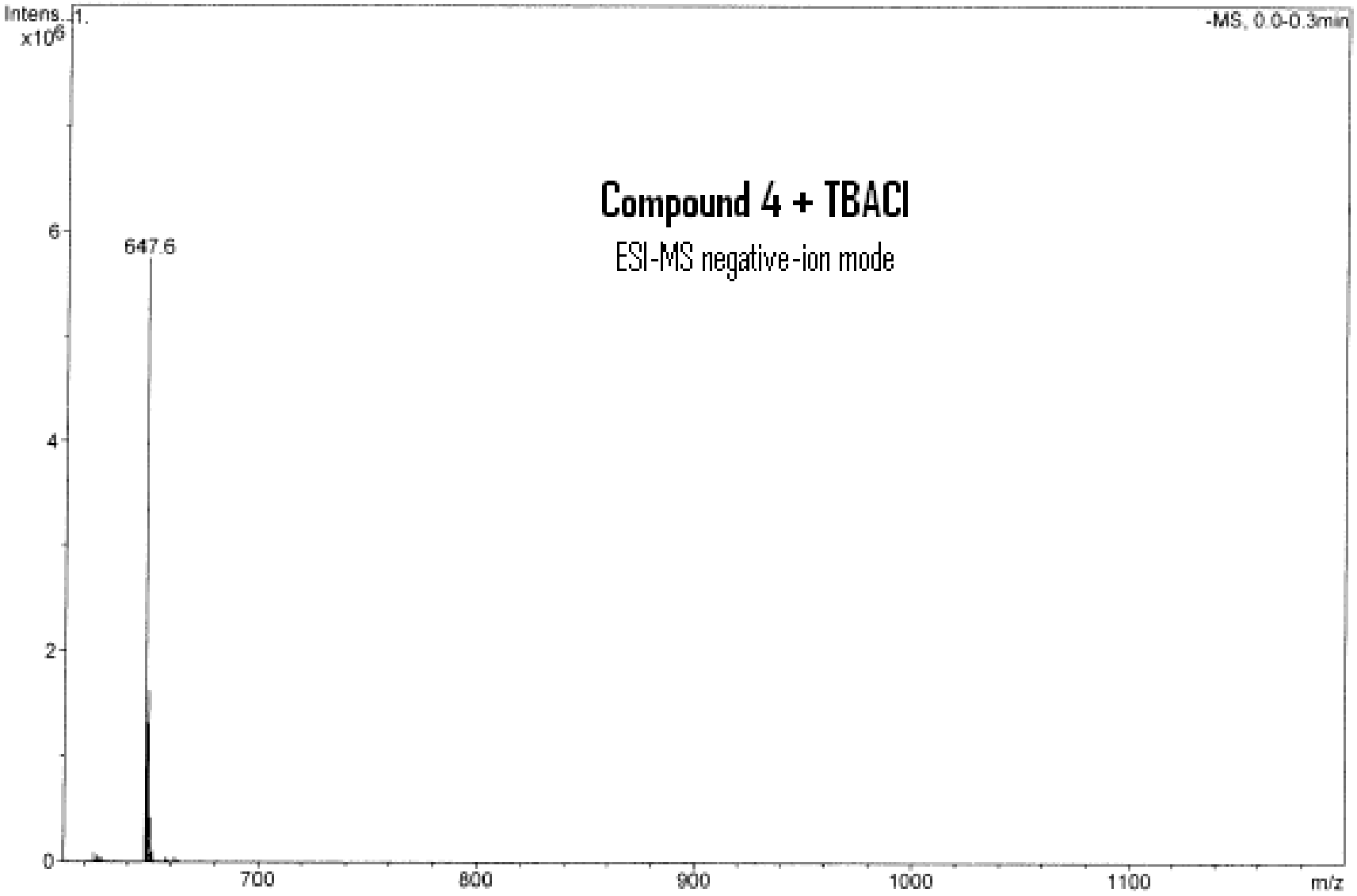


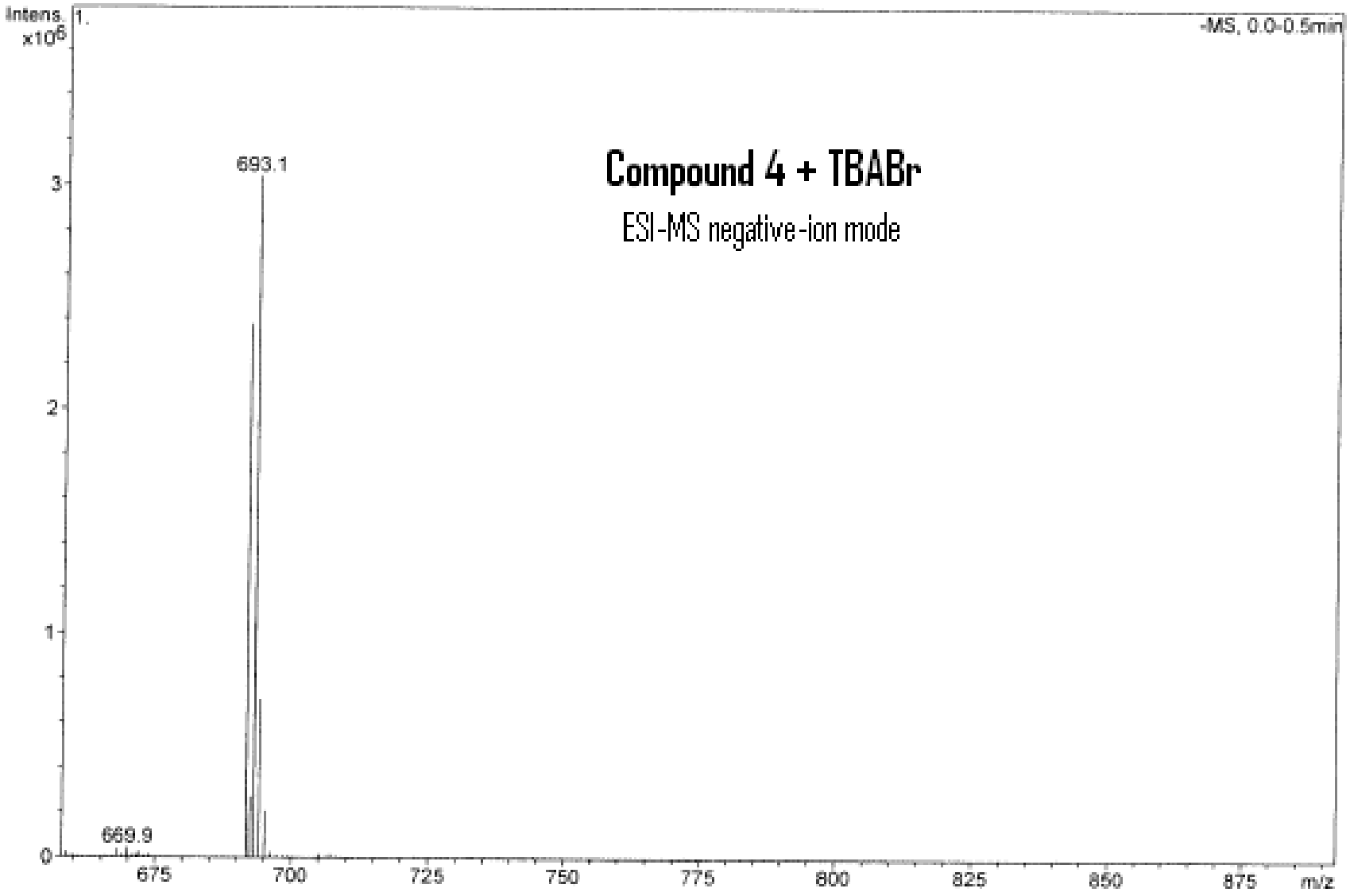


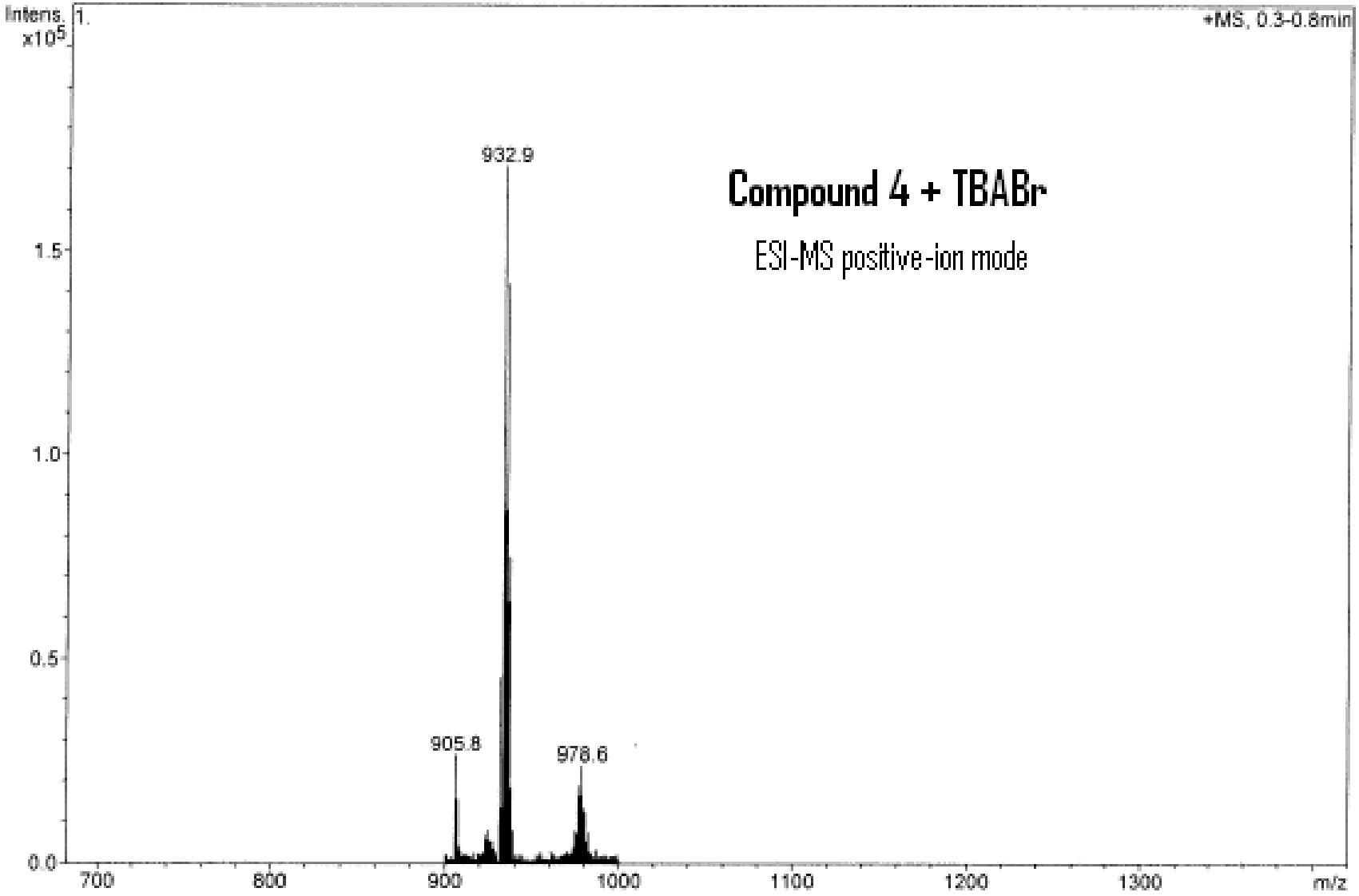


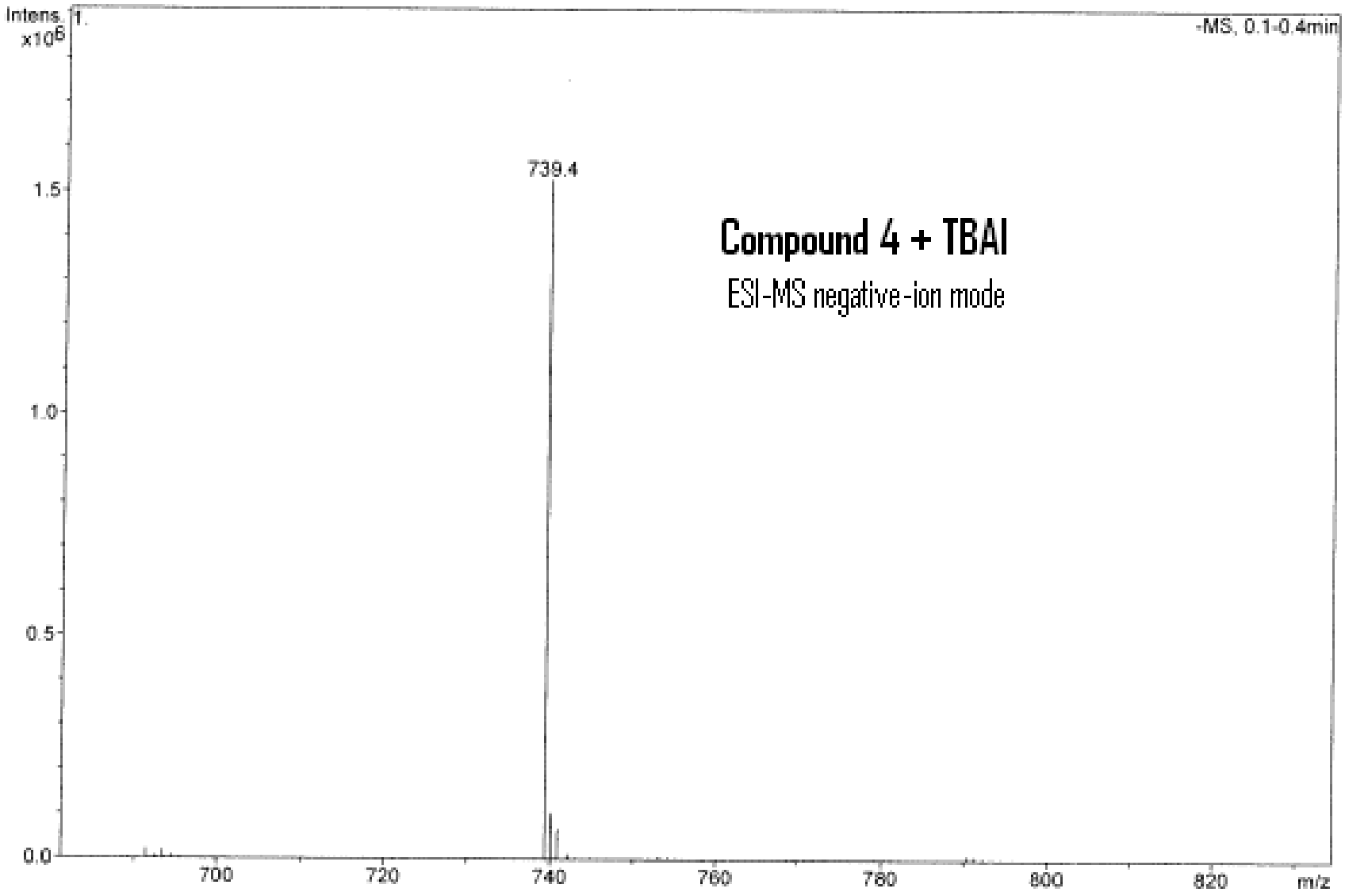


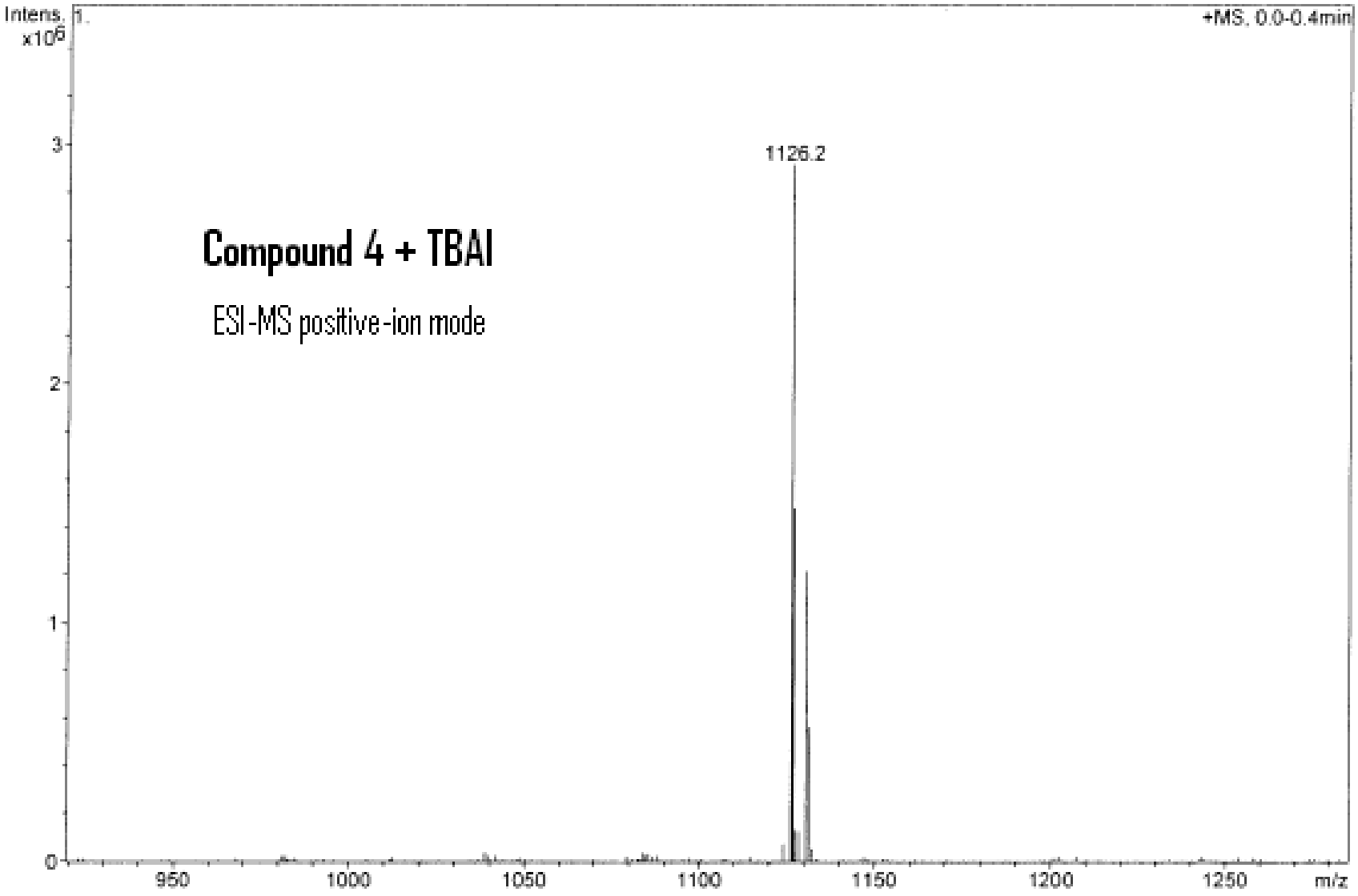


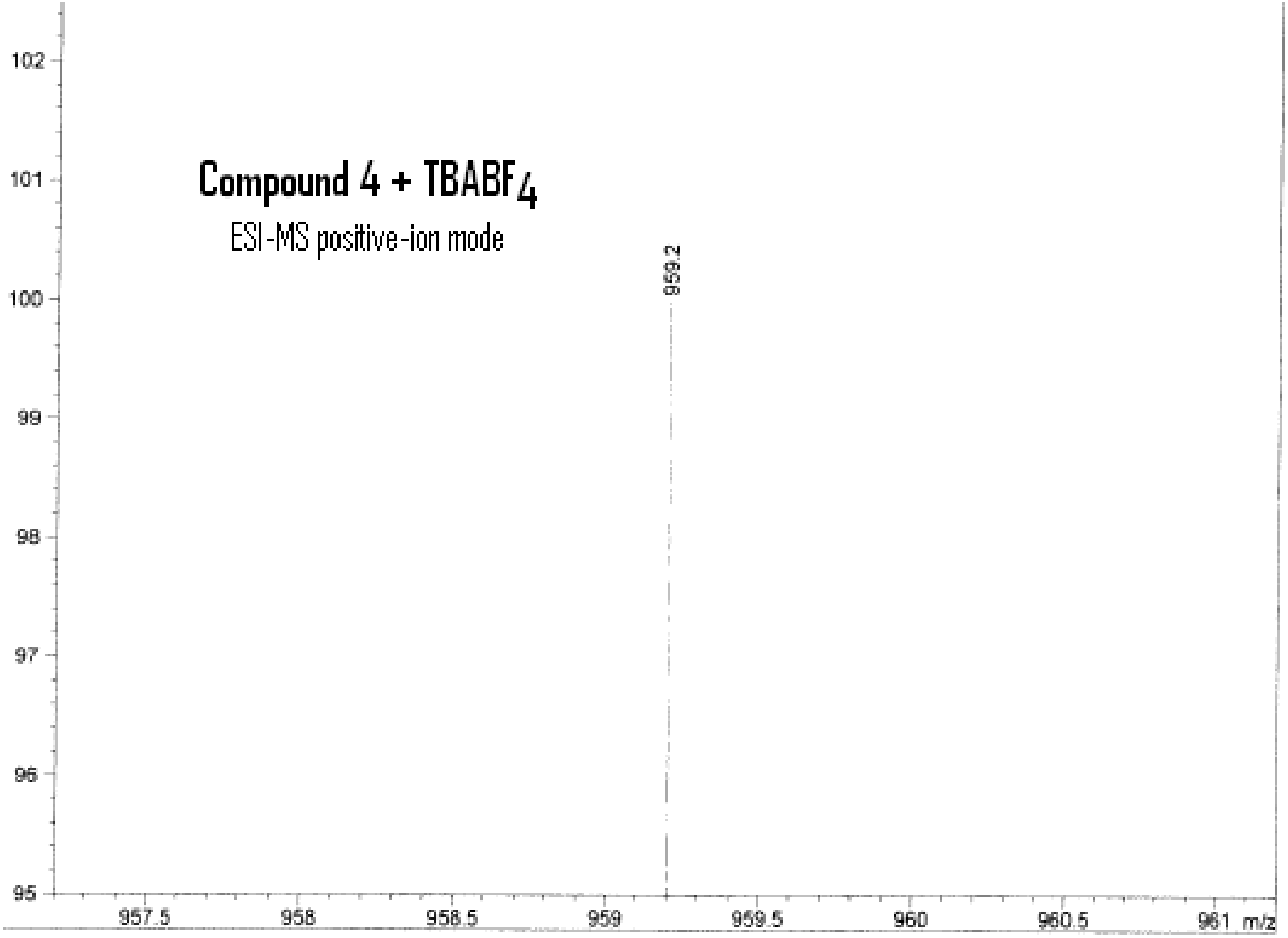


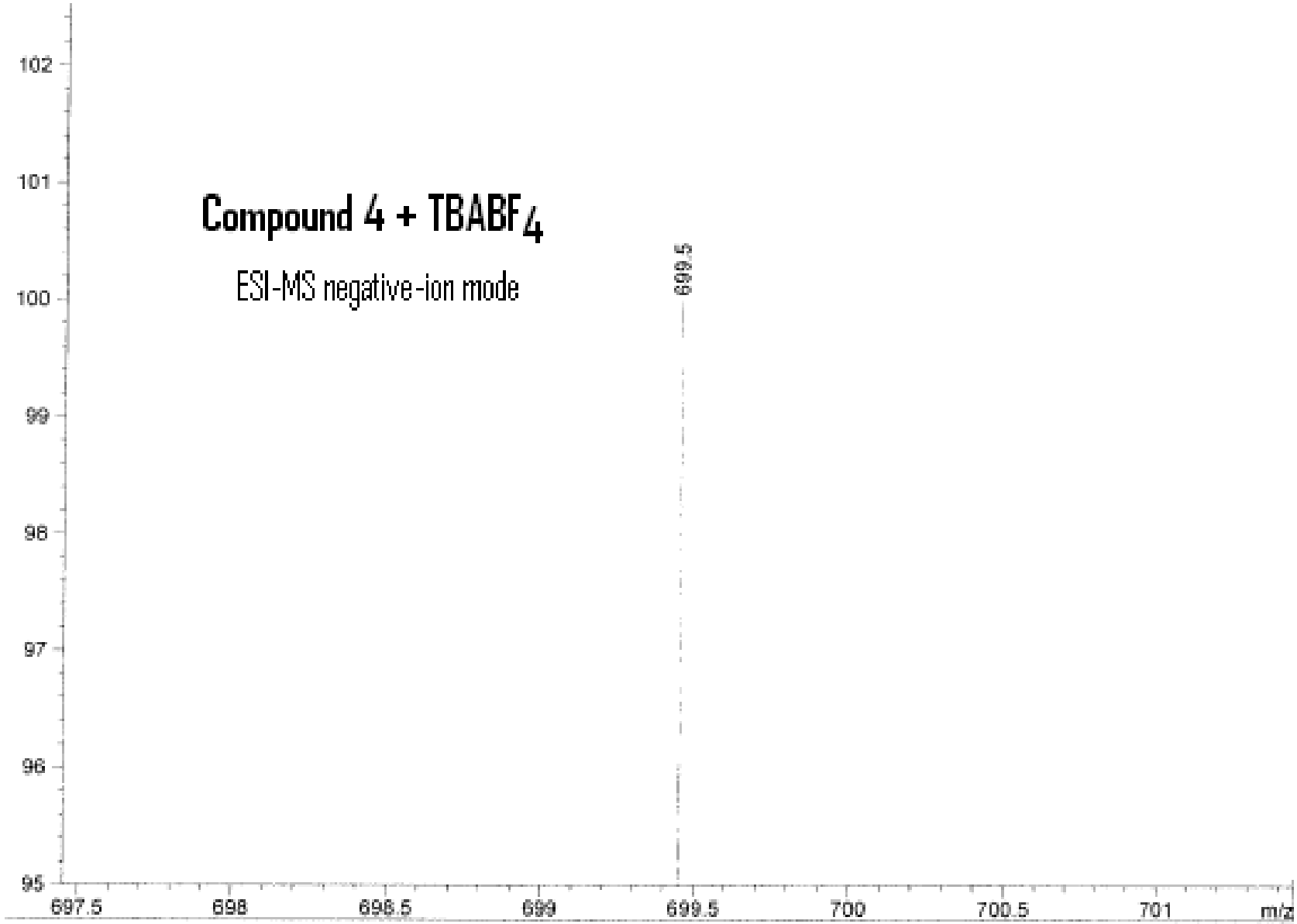


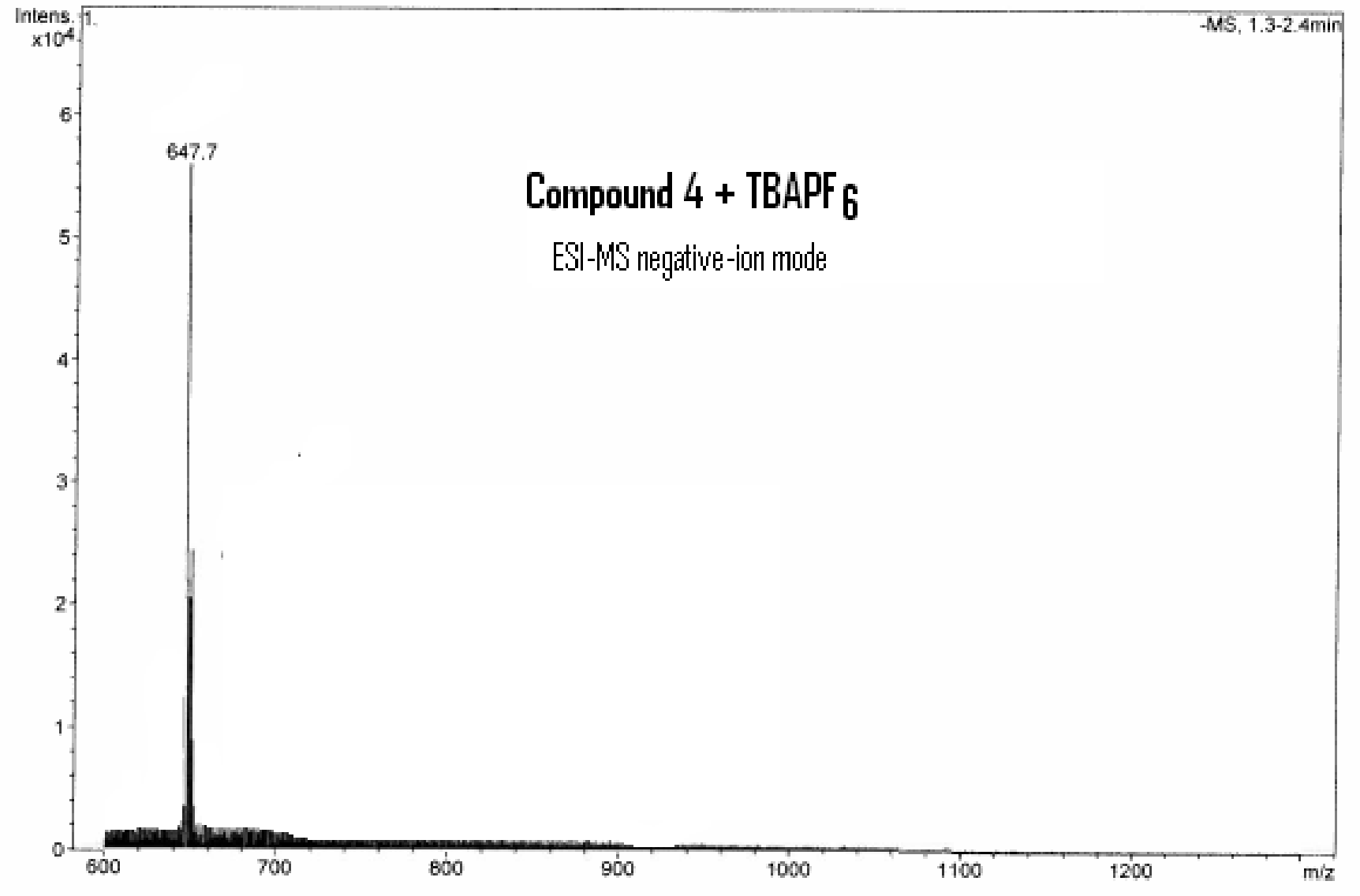


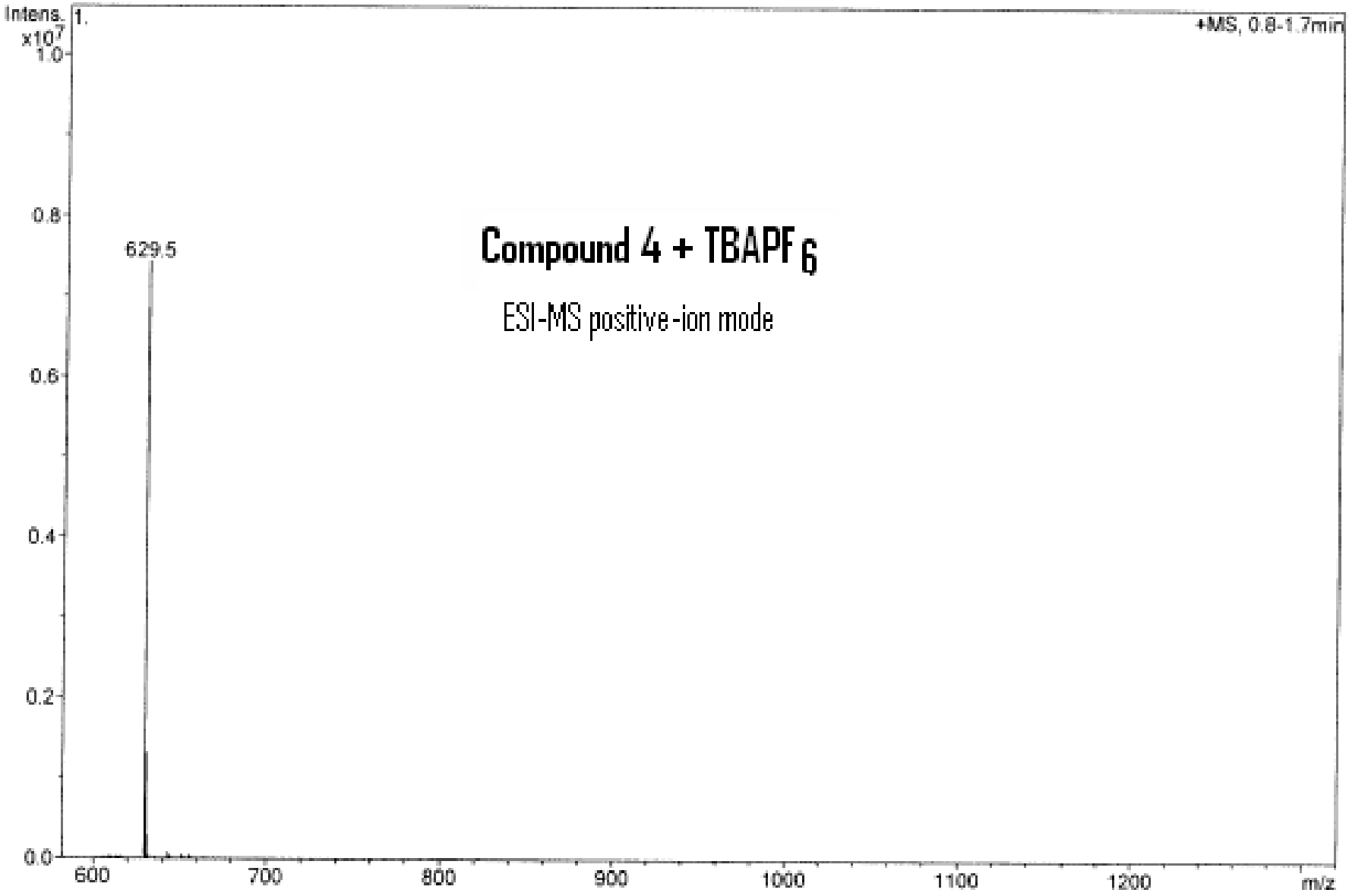










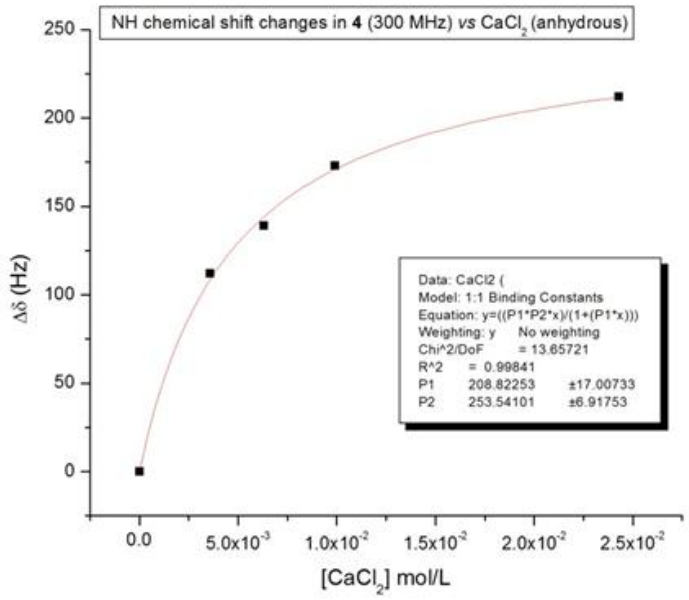


Compound 4 + $TBAPF_6$

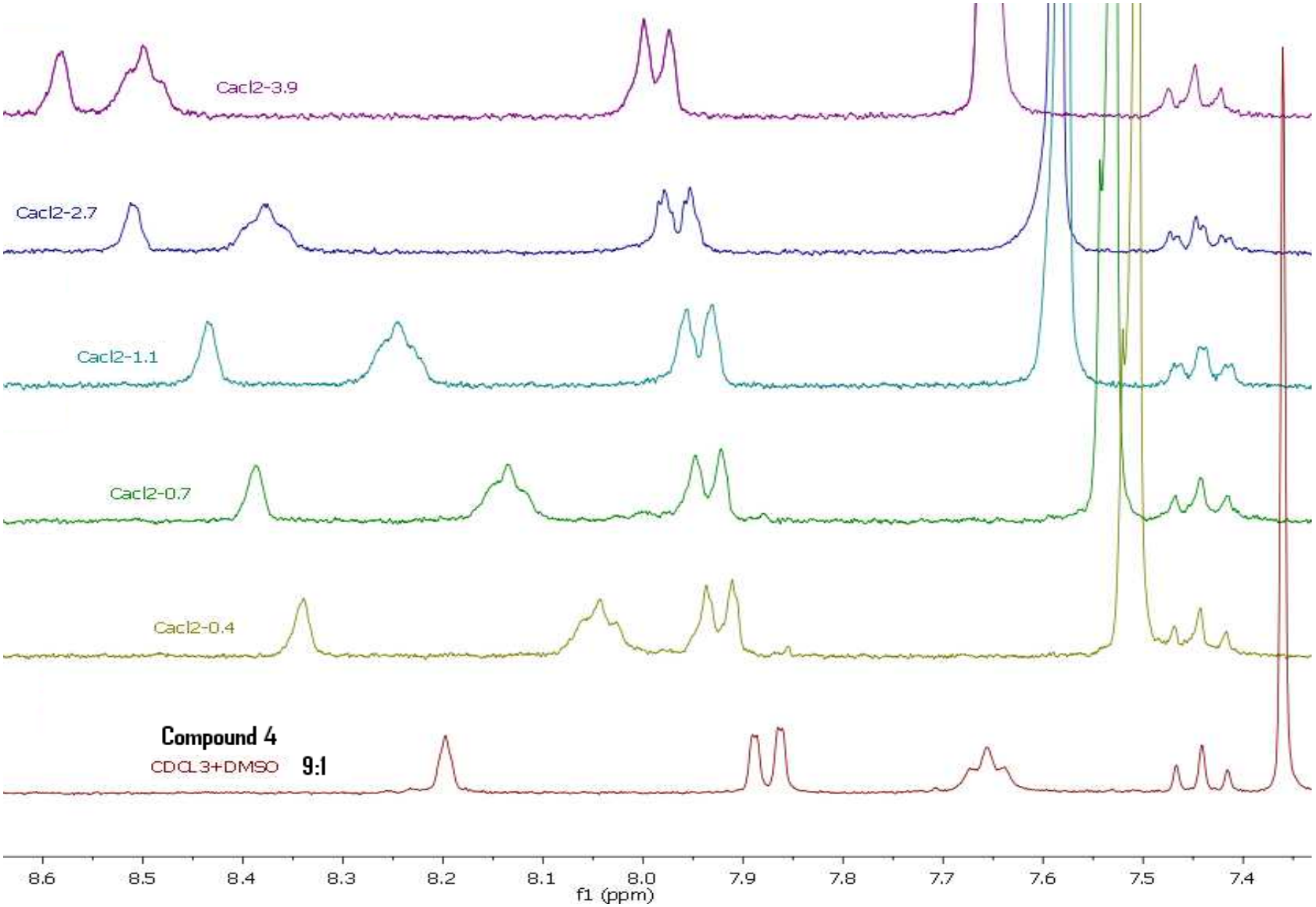
ESI-MS positive-ion mode

^{1}H NMR titration spectral data for compound 4 vs $CaCl_2$ (anhydrous)

ENTRY	g	Moles guest	[guest]	Moles host	H/G ratio:	G/H ratio	δ	Δδ	δ	Δδ
	0	0.00E+00	**0.00E+00**				8.21	0	7.67	**0**
1	**4.00E-04**	3.60E-06	**3.60E-03**	9.12E-07	**0.25**	4	8.339	38.7	8.042	**112**
2	**7.00E-04**	6.31E-06	**6.31E-03**	9.12E-07	**0.14**	7	8.386	52.8	8.134	**139**
3	**1.10E-03**	9.91E-06	**9.91E-03**	9.12E-07	**0.09**	11	8.435	67.5	8.245	**173**
4	**2.70E-03**	2.43E-05	**2.43E-02**	9.12E-07	**0.04**	27	8.51	90	8.378	**212**
5	**3.90E-03**	3.51E-05	**3.51E-02**	9.12E-07	0.03	39	8.585	112.5	8.497	**248**

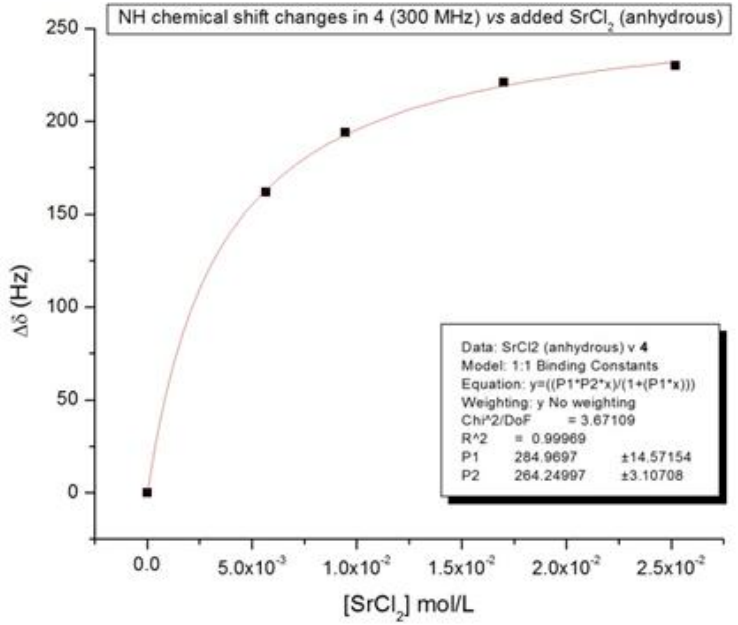


^{1}H NMR titration curves for compound 4 vs $CaCl_2$:

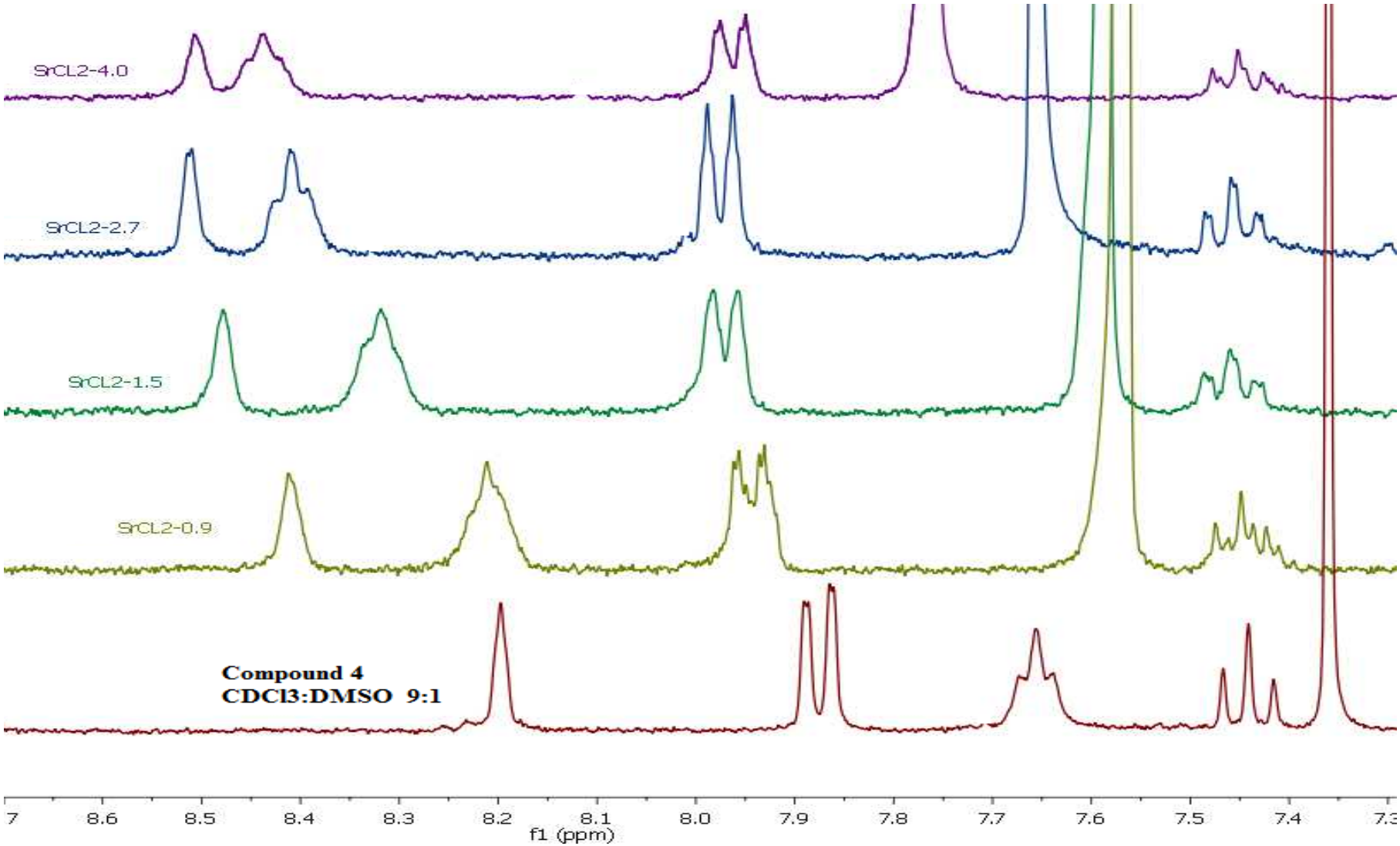


^{1}H NMR titration spectral data for compound 4 vs $SrCl_2$ (anhydrous):

ENTRY	g	Moles guest	[guest]	Moles host	H/G ratio:	G/H ratio	Singlet δ	Singlet Δδ	NH δ	NH Δδ
	0	0.00E+00	**0.00E+00**				8.210	0	7.670	**0**
1	**9.00E-04**	5.68E-06	**5.68E-03**	1.06E-06	**0.19**	5	8.412	60.6	8.211	**162**
2	**1.50E-03**	9.46E-06	**9.46E-03**	1.06E-06	**0.11**	9	8.479	80.7	8.318	**194**
3	**2.70E-03**	1.70E-05	**1.70E-02**	1.06E-06	**0.06**	16	8.513	90.9	8.408	**221**
4	**4.00E-03**	2.52E-05	**2.52E-02**	1.06E-06	**0.042**	24	8.506	88.8	8.437	**230**

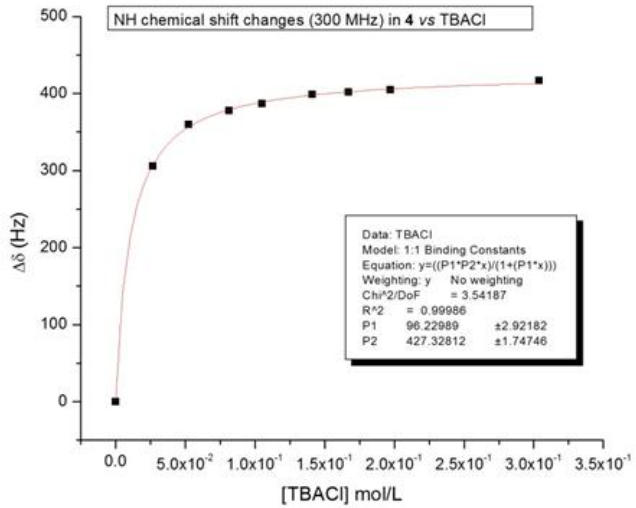


^{1}H NMR titration spectra for compound 4 vs $SrCl_2$ (anhydrous):

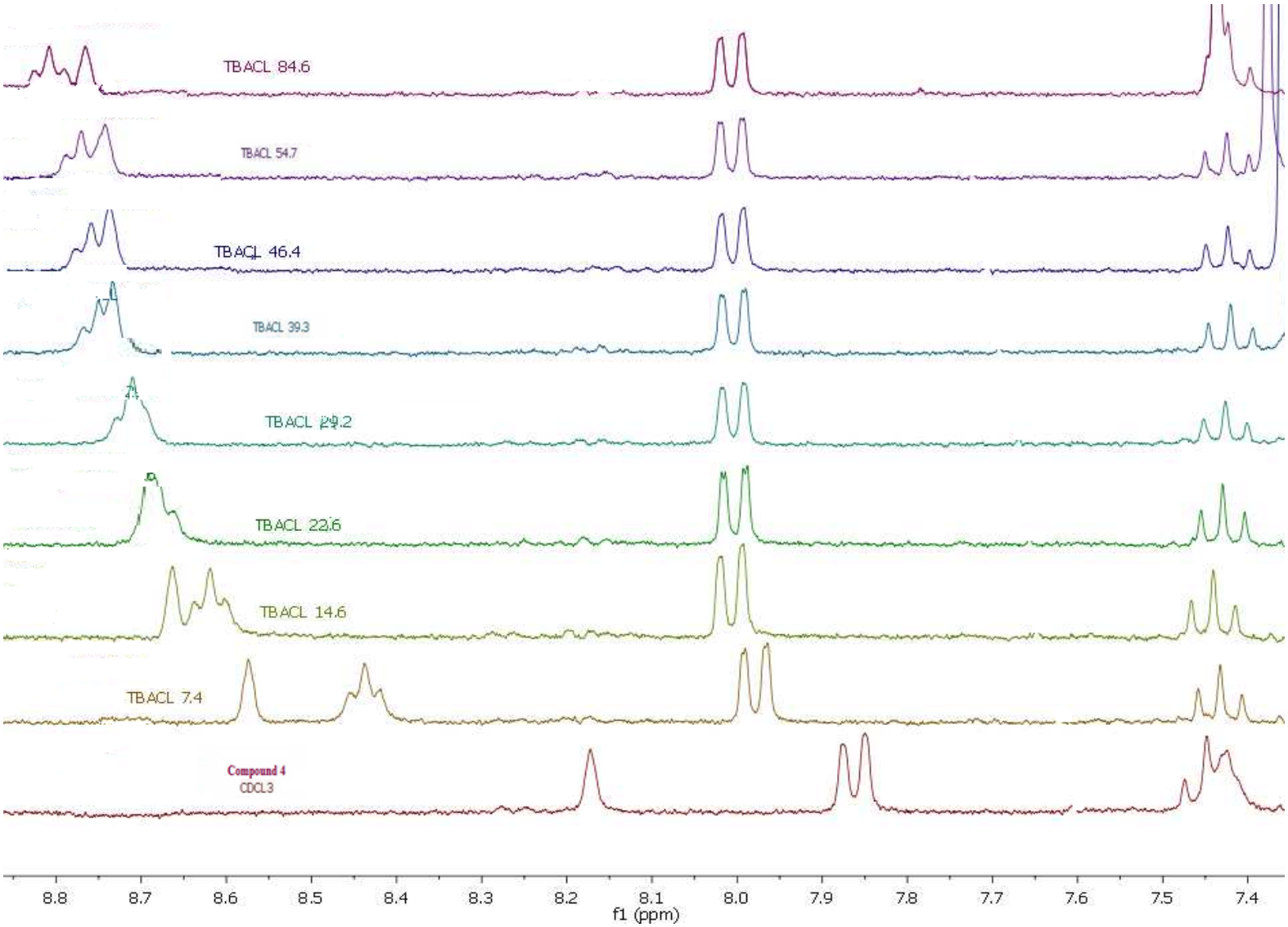


^{1}H NMR titration spectral data for compound 4 vs TBACl:

	0	0.00E+00					8.19	0	7.42	0
1	**7.40E-03**	2.66E-05	**2.66E-02**	1.70E-06	**0.06**	16	8.57	114	8.44	**306**
2	**1.46E-02**	5.25E-05	**5.25E-02**	1.70E-06	**0.03**	31	8.66	141	8.62	**360**
3	**2.26E-02**	8.13E-05	**8.13E-02**	1.70E-06	**0.02**	48	8.69	150	8.68	**378**
4	**2.92E-02**	1.05E-04	**1.05E-01**	1.70E-06	**0.02**	62	8.7	153	8.71	**387**
5	**3.93E-02**	1.41E-04	**1.41E-01**	1.70E-06	**0.012**	83	8.73	162	8.75	**399**
6	**4.64E-02**	1.67E-04	**1.67E-01**	1.70E-06	**0.010**	98	8.74	165	8.76	**402**
7	**5.47E-02**	1.97E-04	**1.97E-01**	1.70E-06	**0.009**	116	8.74	165	8.77	**405**
8	**8.46E-02**	3.04E-04	**3.04E-01**	1.70E-06	**0.006**	179	8.77	174	8.81	**417**

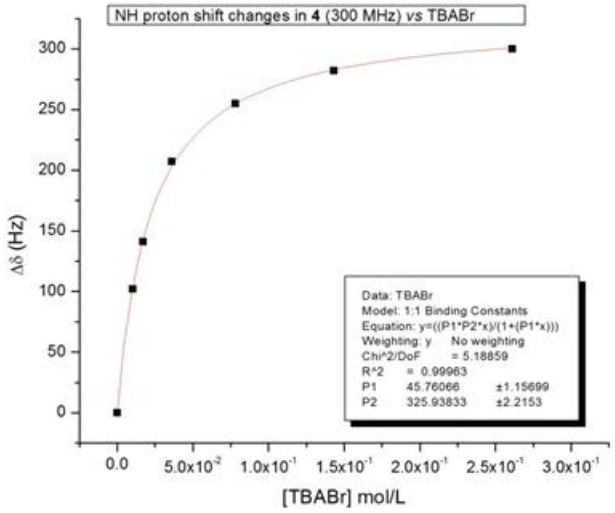


^{1}H NMR titration spectra for compound 4 vs TBACl :

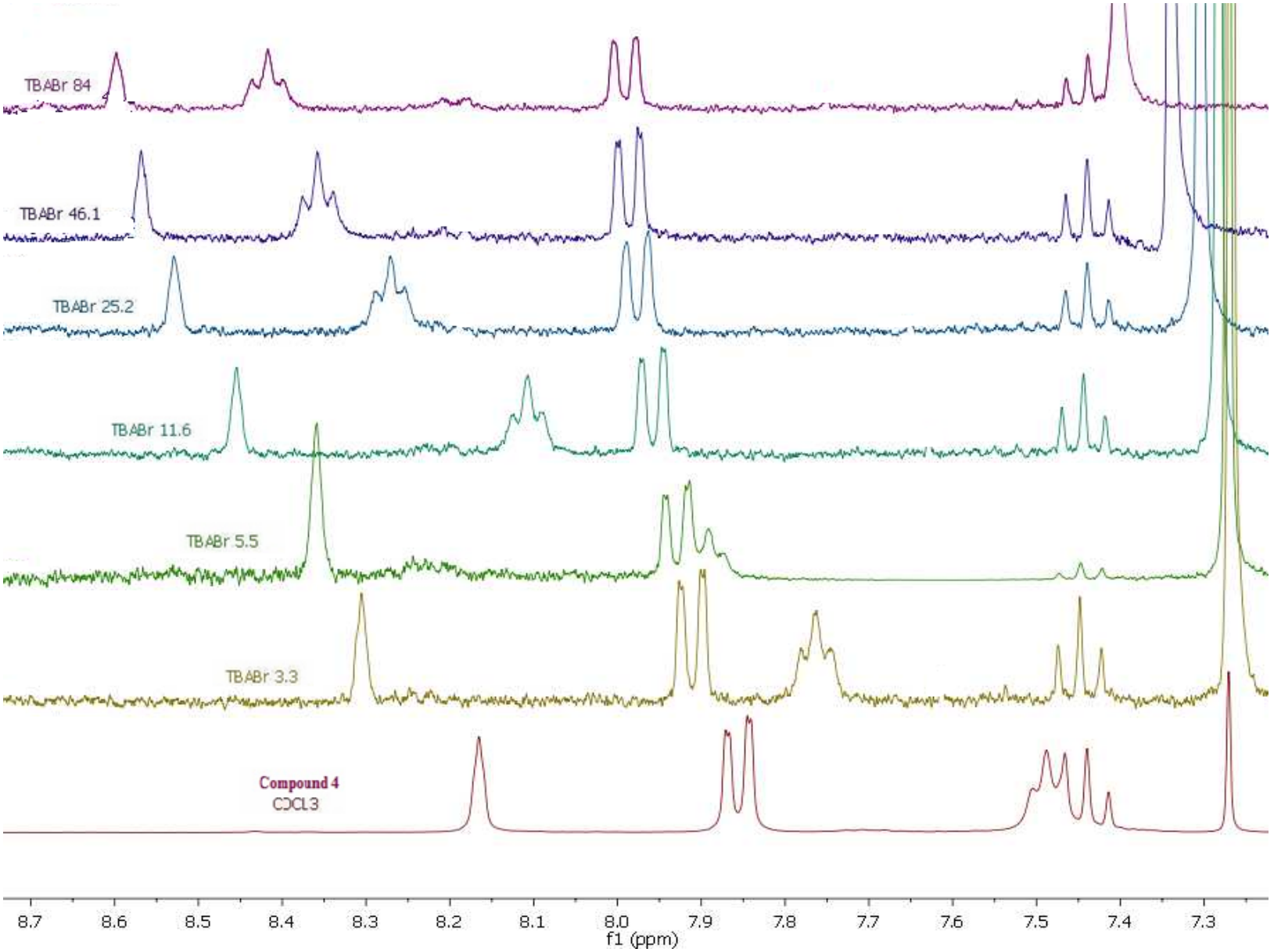


^{1}H NMR titration spectral data for compound 4 vs TBABr:

							Singlet		NH	
ENTRY	**g**	**Moles guest**	**[guest]**	**Moles host**	**H/G ratio:**	**G/H ratio**	**δ**	**Δδ**	**δ**	**Δδ**
	0	0.00E+00					8.19	0	7.42	0
1	**3.30E-03**	1.02E-05	**1.02E-02**	9.35E-07	**0.09**	11	8.31	36	7.76	**102**
2	**5.50E-03**	1.71E-05	**1.71E-02**	9.35E-07	**0.05**	18	8.36	51	7.89	**141**
3	**1.16E-02**	3.60E-05	**3.60E-02**	9.35E-07	**0.03**	38	8.45	78	8.11	**207**
4	**2.52E-02**	7.82E-05	**7.82E-02**	9.35E-07	**0.01**	84	8.53	102	8.27	**255**
5	**4.61E-02**	1.43E-04	**1.43E-01**	9.35E-07	**0.007**	153	8.57	114	8.36	**282**
6	**8.40E-02**	2.61E-04	**2.61E-01**	9.35E-07	**0.004**	279	8.6	123	8.42	**300**

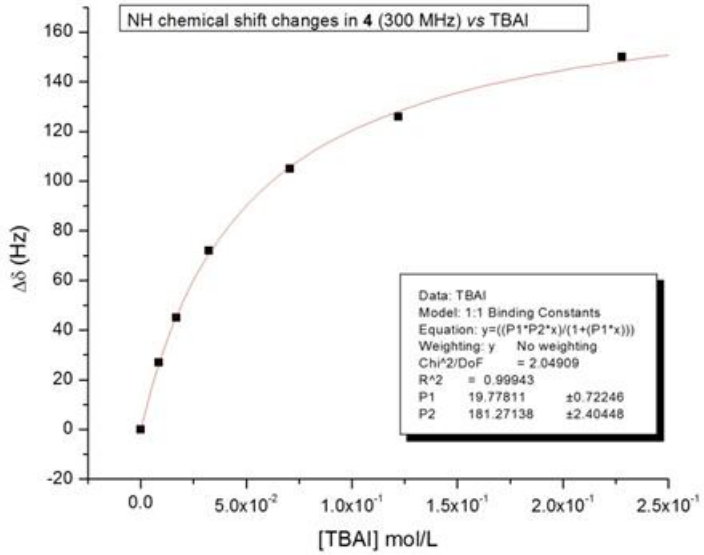


^{1}H NMR titration spectra for compound 4" vs TBABr :

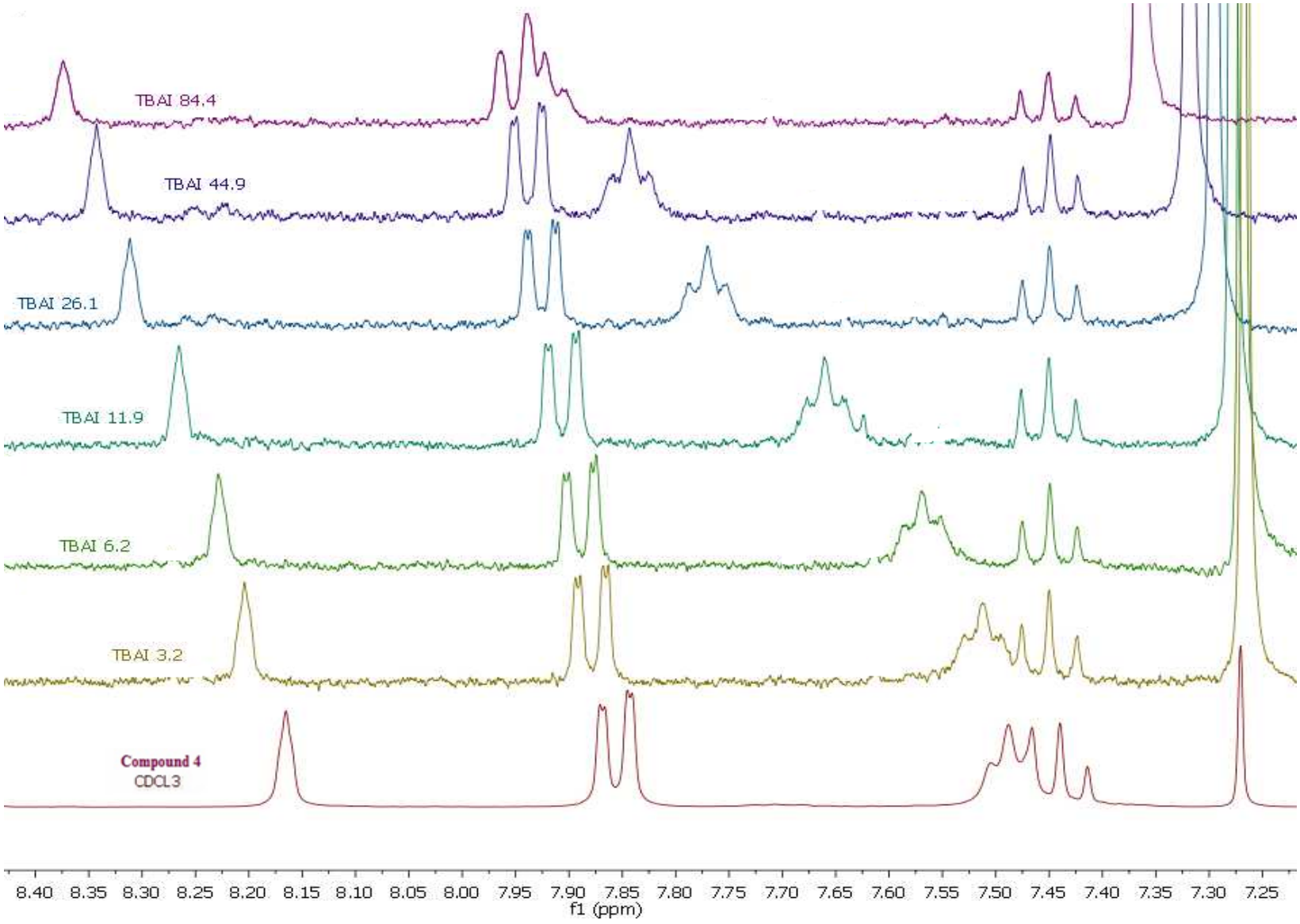


^{1}H NMR titration spectral data for compound 4 vs TBAI:

							Singlet		NH	
ENTRY	**g**	**Moles guest**	**[guest]**	**Moles host**	**H/G ratio:**	**G/H ratio**	**δ**	**Δδ**	**δ**	**Δδ**
	0	0.00E+00					8.19	0	7.42	**0**
1	**3.20E-03**	8.66E-06	**8.66E-03**	9.35E-07	**0.11**	9	8.2	3	7.51	**27**
2	**6.20E-03**	1.68E-05	**1.68E-02**	9.35E-07	**0.06**	18	8.23	12	7.57	**45**
3	**1.19E-02**	3.22E-05	**3.22E-02**	9.35E-07	**0.03**	34	8.27	24	7.66	**72**
4	**2.61E-02**	7.07E-05	**7.07E-02**	9.35E-07	**0.01**	76	8.31	36	7.77	**105**
5	**4.49E-02**	1.22E-04	**1.22E-01**	9.35E-07	**0.008**	130	8.34	45	7.84	**126**
6	**8.44E-02**	2.28E-04	**2.28E-01**	9.35E-07	**0.004**	244	8.37	54	7.92	**150**

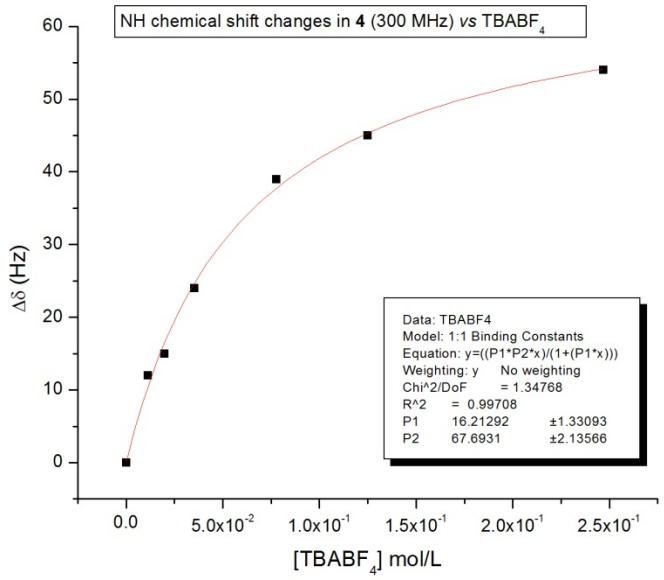


^{1}H NMR titration spectra for compound 4 vs TBAI :



^{1}H NMR titration spectral data for compound 4 vs $TBABF_4$:

							Singlet		NH	
ENTRY	**g**	Moles guest	**[guest]**	**Moles host**	**H/G ratio:**	G/H ratio	δ	Δδ	δ	Δδ
	0	0.00E+00					8.19	0	7.42	**0**
1	**3.70E-03**	1.12E-05	**1.12E-02**	9.35E-07	**0.08**	12	8.18	-3	7.46	**12**
2	**6.50E-03**	1.98E-05	**1.98E-02**	9.35E-07	**0.05**	21	8.18	-3	7.47	**15**
3	**1.16E-02**	3.53E-05	**3.53E-02**	9.35E-07	**0.03**	38	8.18	-3	7.5	**24**
4	**2.56E-02**	7.78E-05	**7.78E-02**	9.35E-07	**0.01**	83	8.19	0	7.55	**39**
5	**4.12E-02**	1.25E-04	**1.25E-01**	9.35E-07	**0.007**	134	8.19	0	7.57	**45**
6	**8.11E-02**	2.47E-04	**2.47E-01**	9.35E-07	**0.004**	264	8.2	3	7.6	**54**



^{1}H NMR titration spectra for compound "4" vs $TBABF_4$: