

**p-tert-Butyl thiocalix[4]arenes functionalized at the lower rim by amide, hydroxyl and ester groups as anion receptors**

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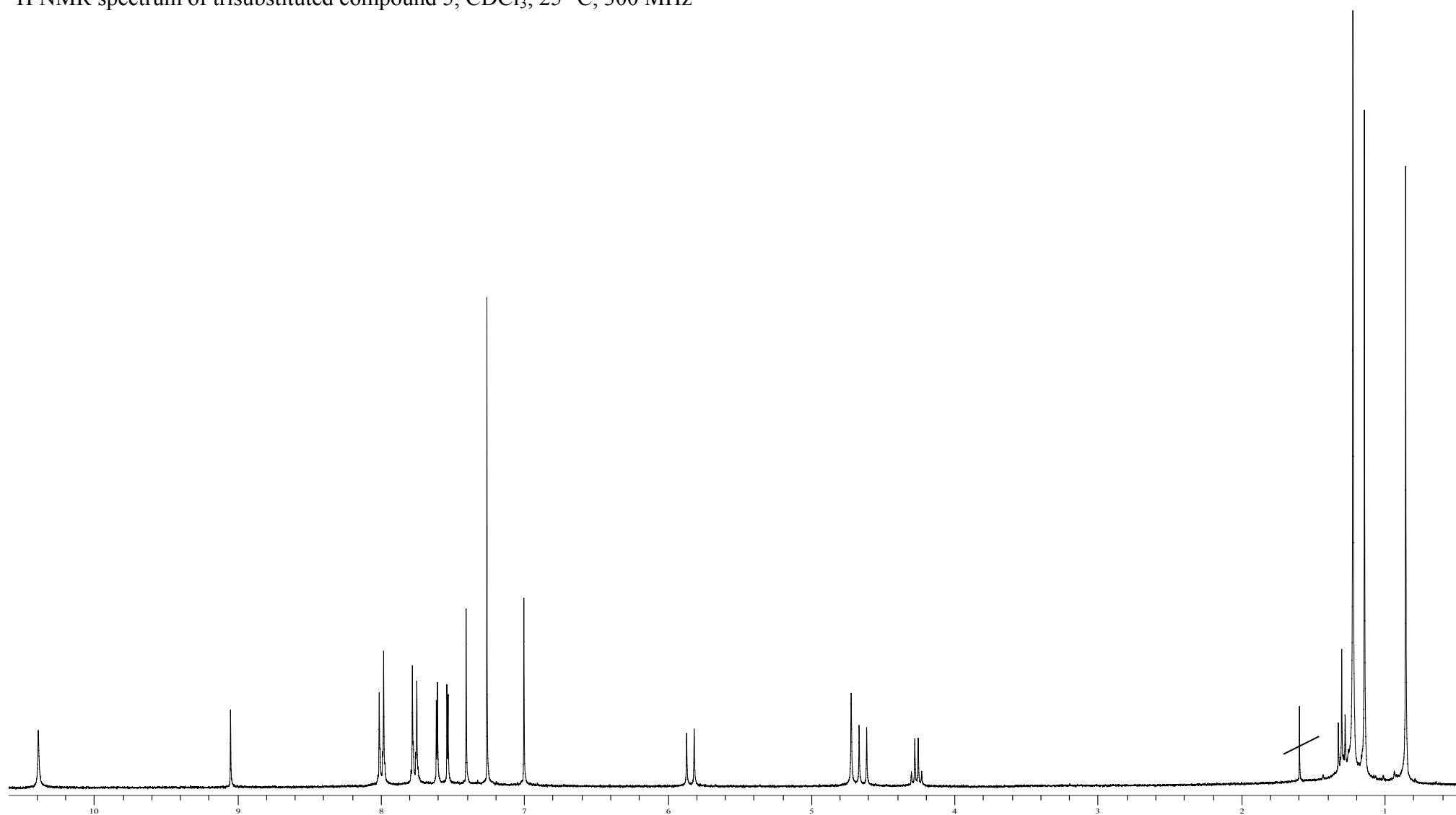
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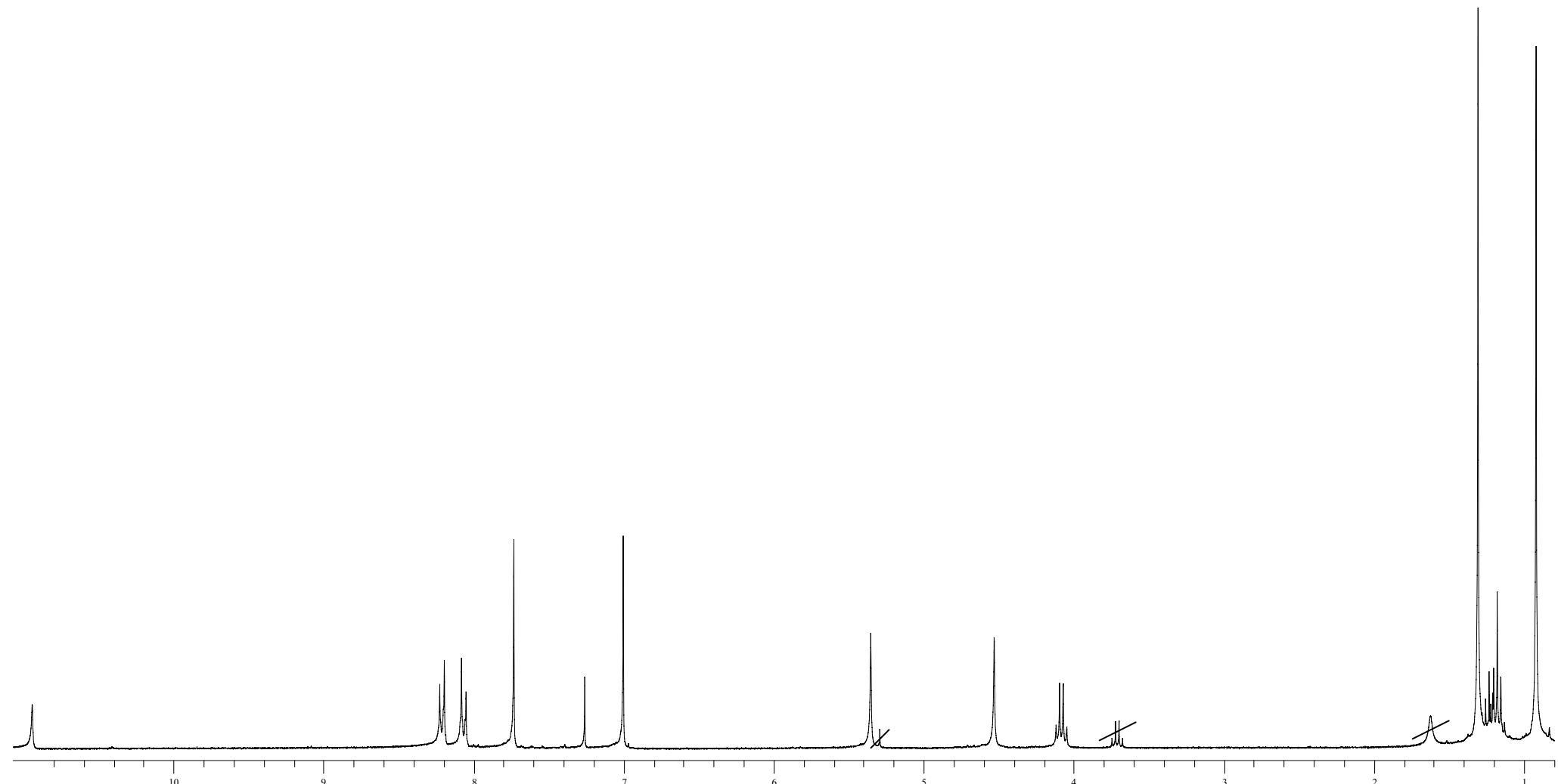
<sup>c</sup>University of Utah, Salt Lake City, Utah 84112, United States of America

**Electronic Supplementary Information**

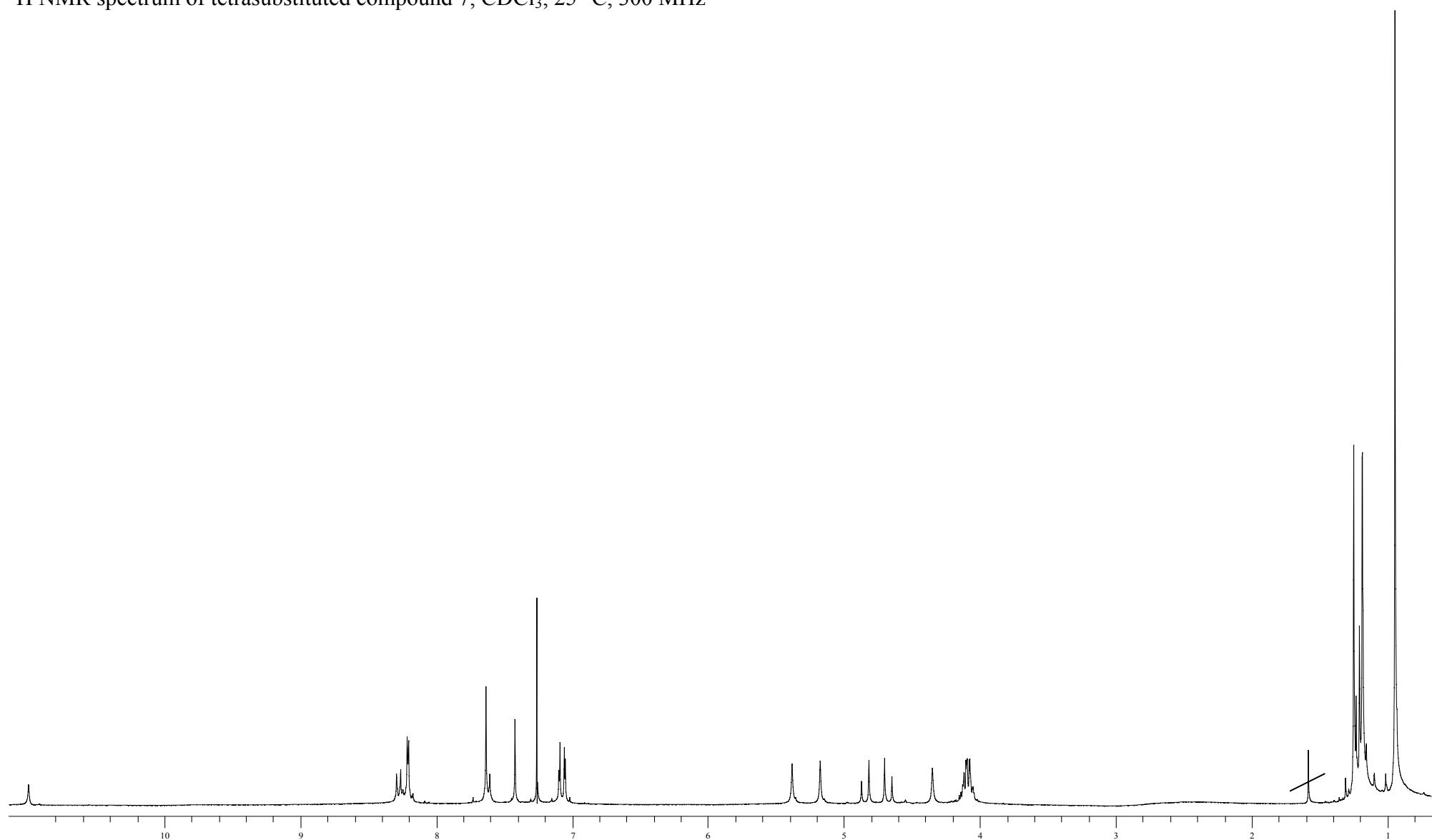
$^1\text{H}$  NMR spectrum of trisubstituted compound 5,  $\text{CDCl}_3$ , 25 °C, 300 MHz



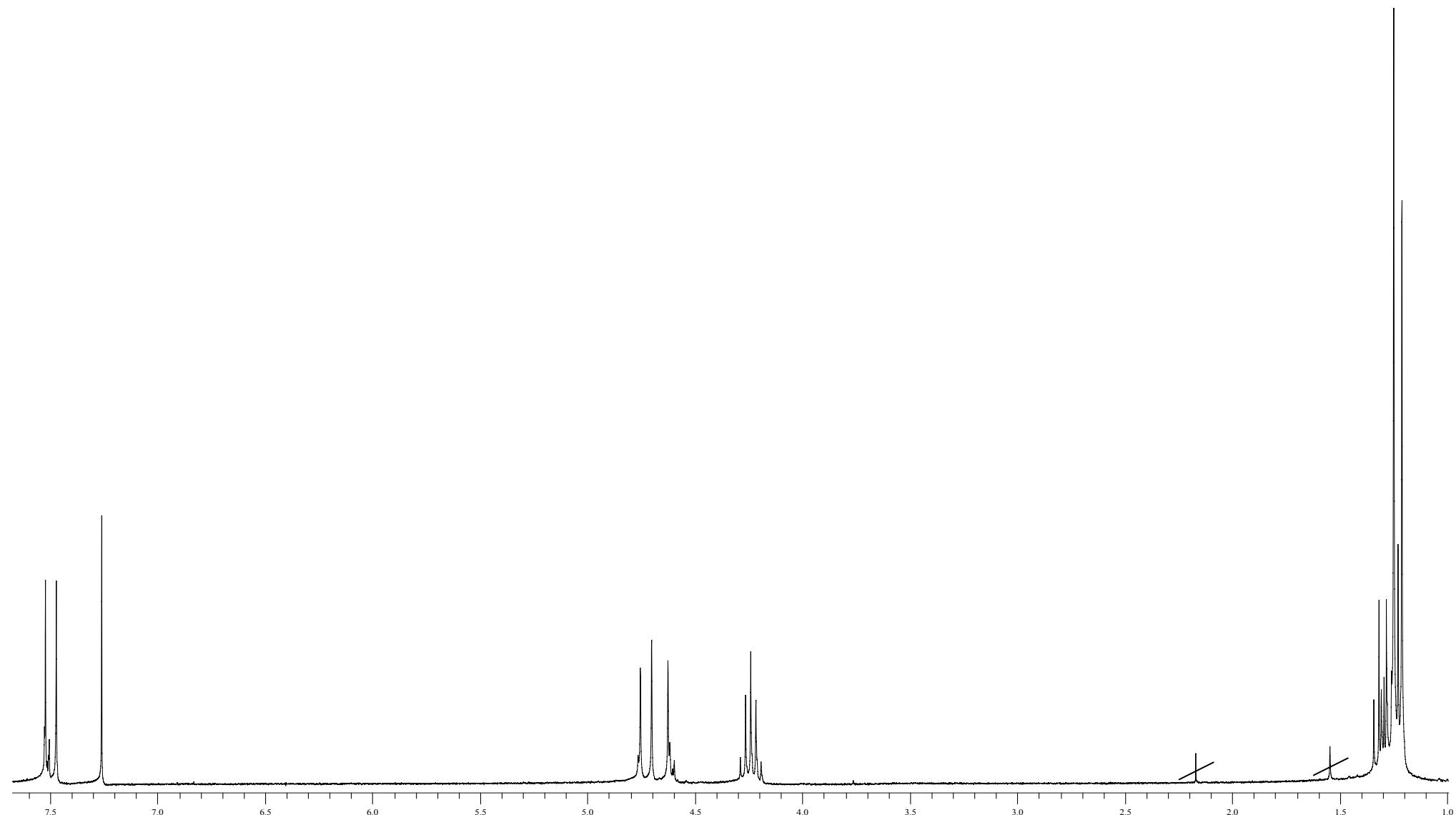
$^1\text{H}$  NMR spectrum of tetrasubstituted compound 6,  $\text{CDCl}_3$ , 25 °C, 300 MHz



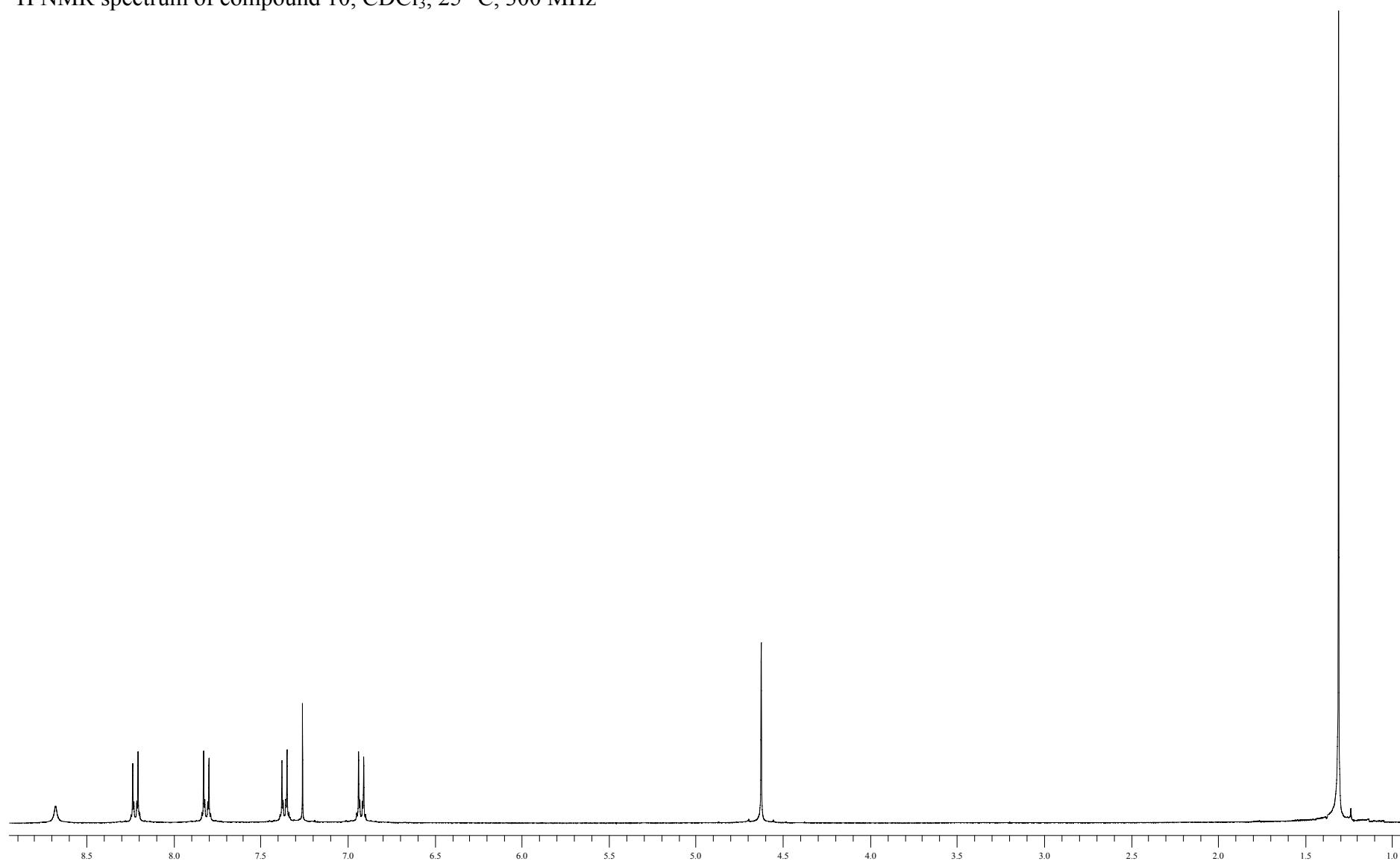
$^1\text{H}$  NMR spectrum of tetrasubstituted compound 7,  $\text{CDCl}_3$ , 25 °C, 300 MHz



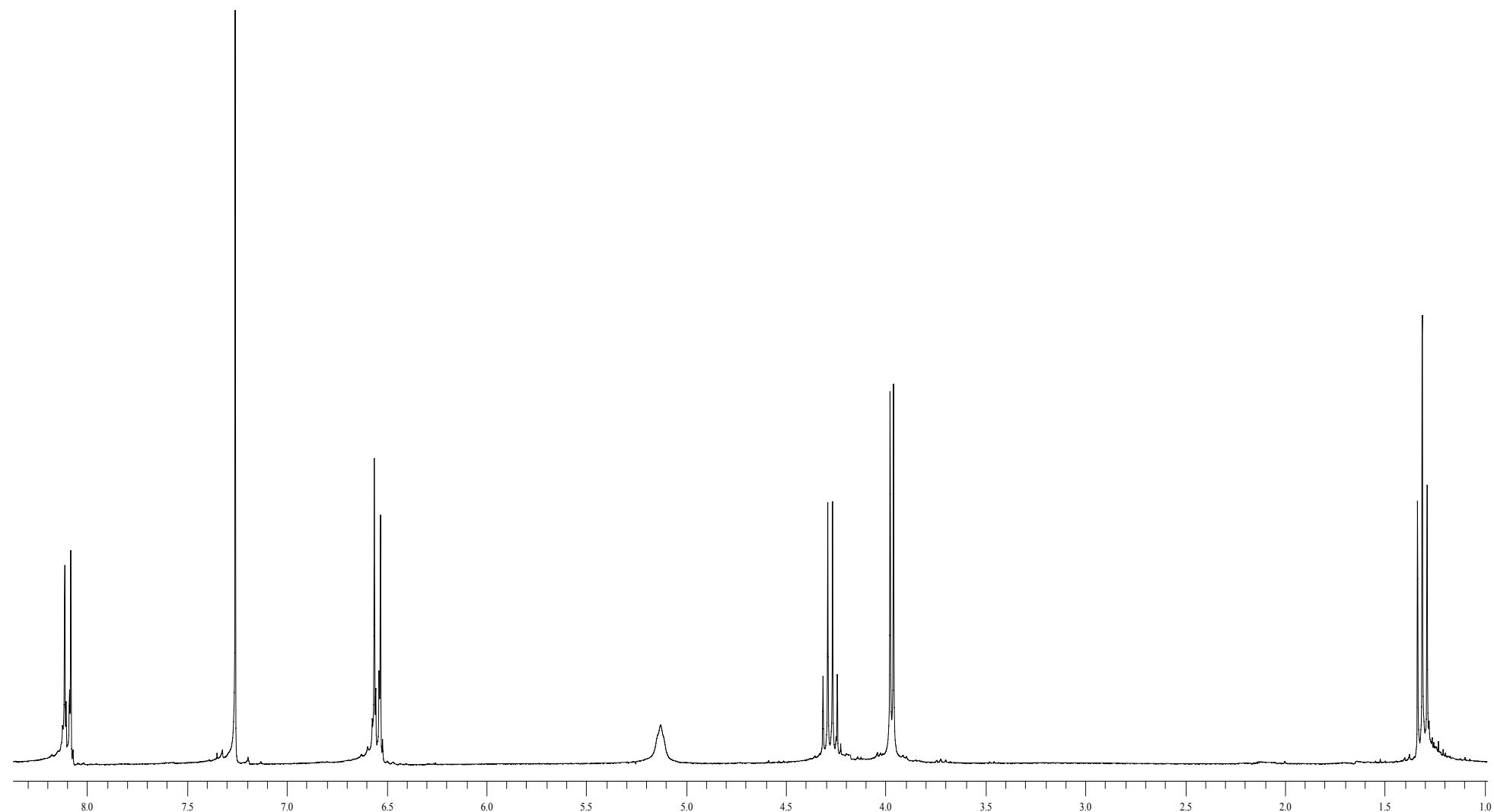
$^1\text{H}$  NMR spectrum of tetrasubstituted compound 8,  $\text{CDCl}_3$ , 25 °C, 300 MHz



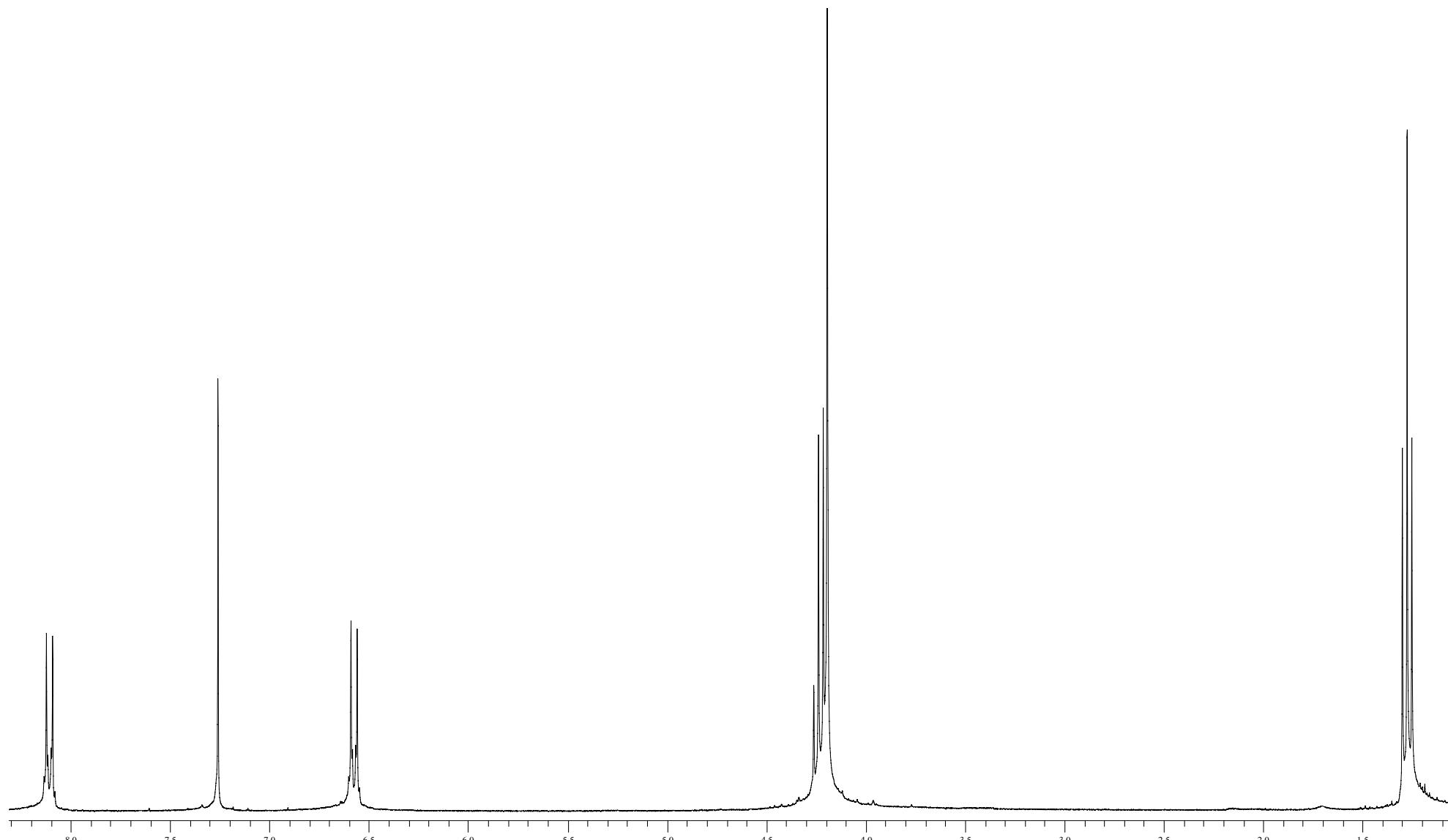
$^1\text{H}$  NMR spectrum of compound 10,  $\text{CDCl}_3$ , 25 °C, 300 MHz



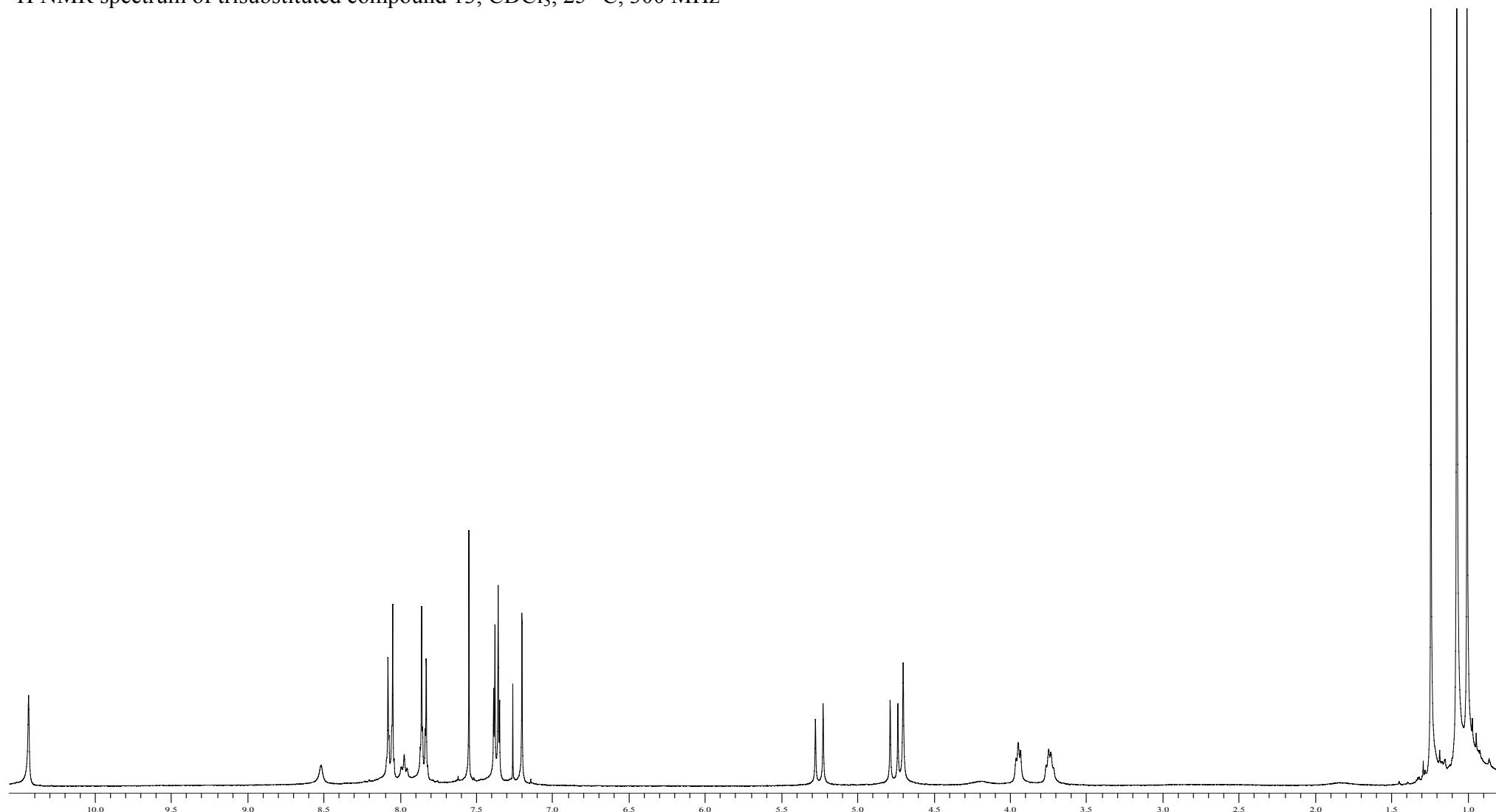
$^1\text{H}$  NMR spectrum of compound 11,  $\text{CDCl}_3$ , 25 °C, 300 MHz



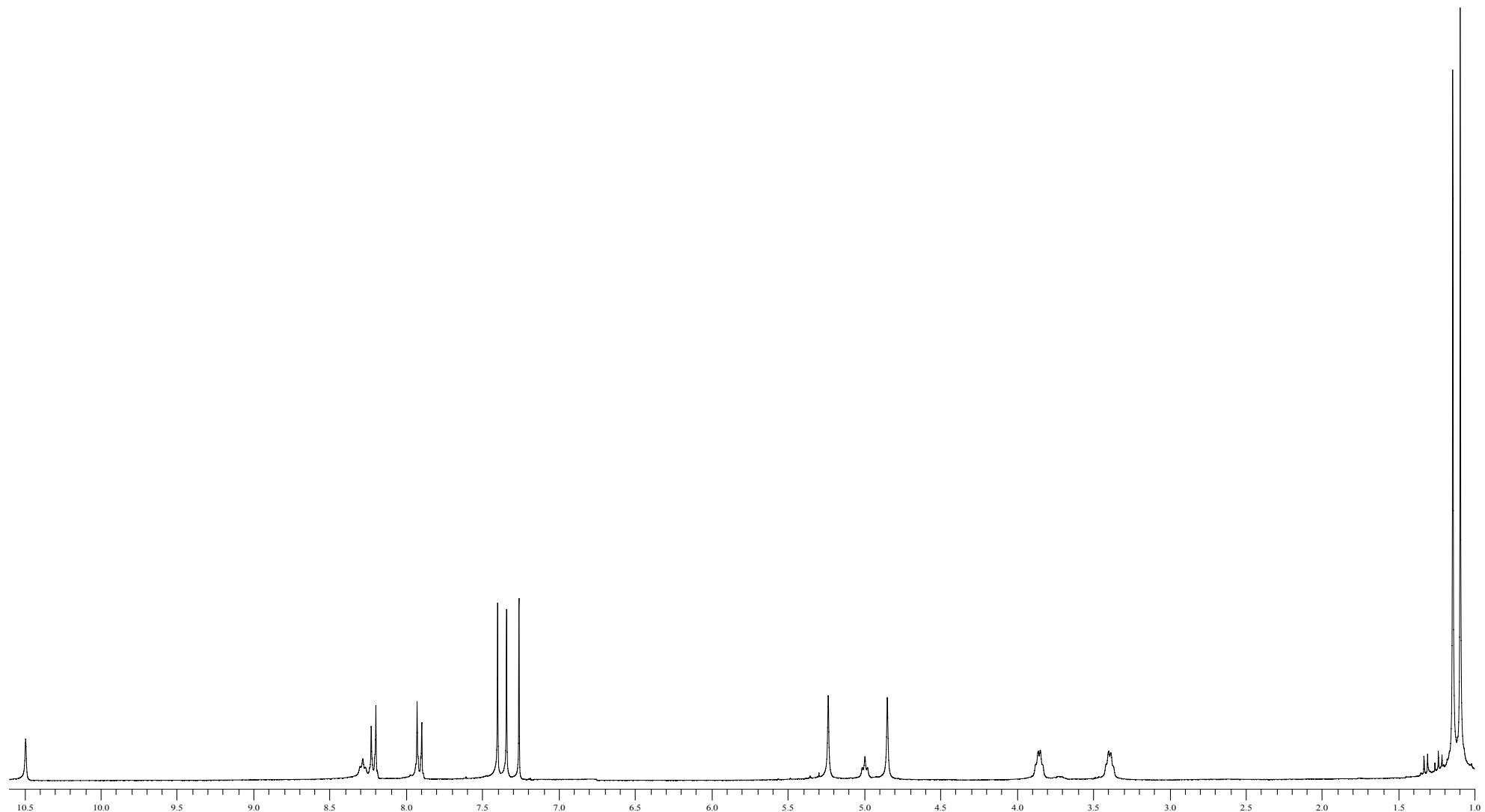
$^1\text{H}$  NMR spectrum of compound 12,  $\text{CDCl}_3$ , 25 °C, 300 MHz



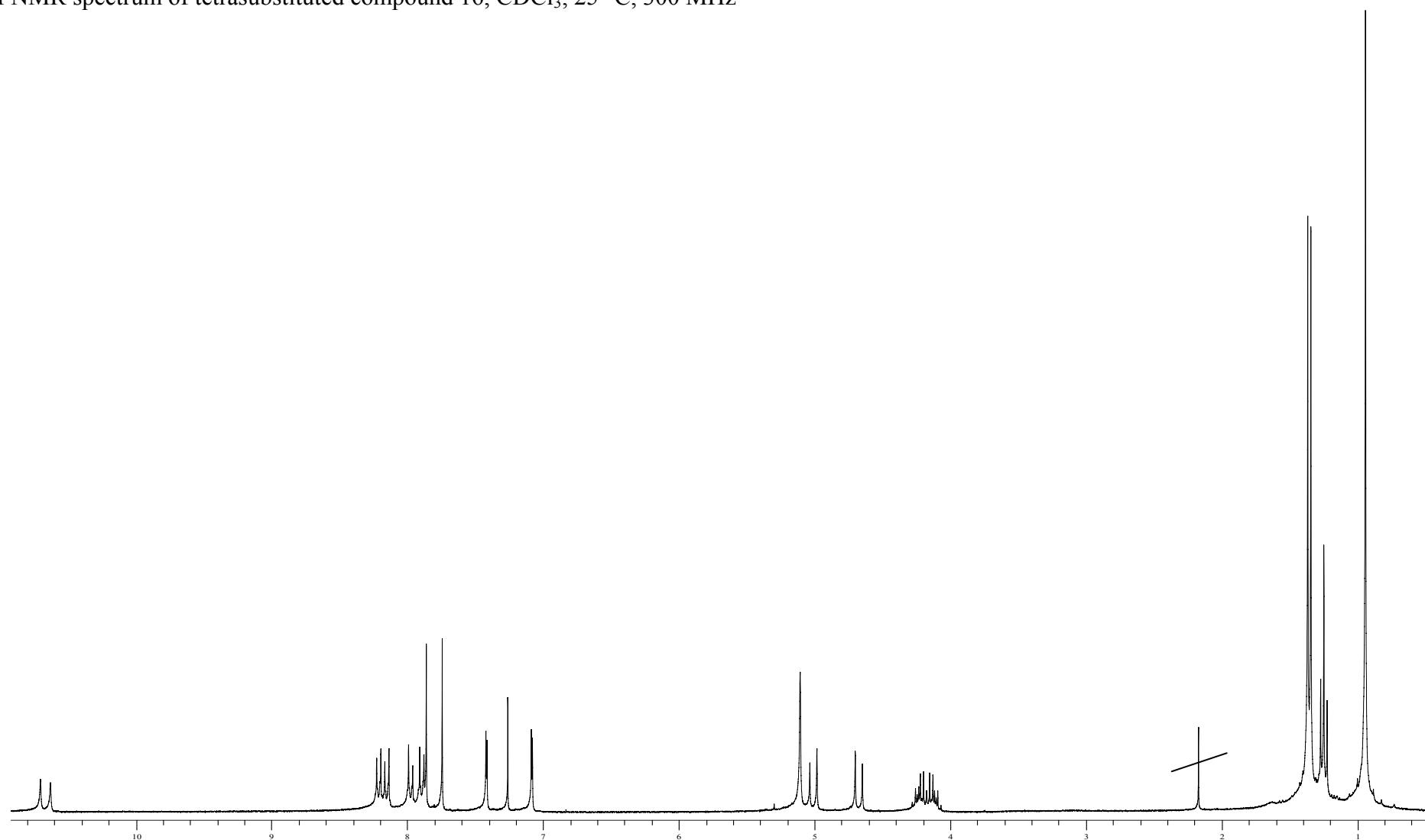
$^1\text{H}$  NMR spectrum of trisubstituted compound 13,  $\text{CDCl}_3$ , 25 °C, 300 MHz



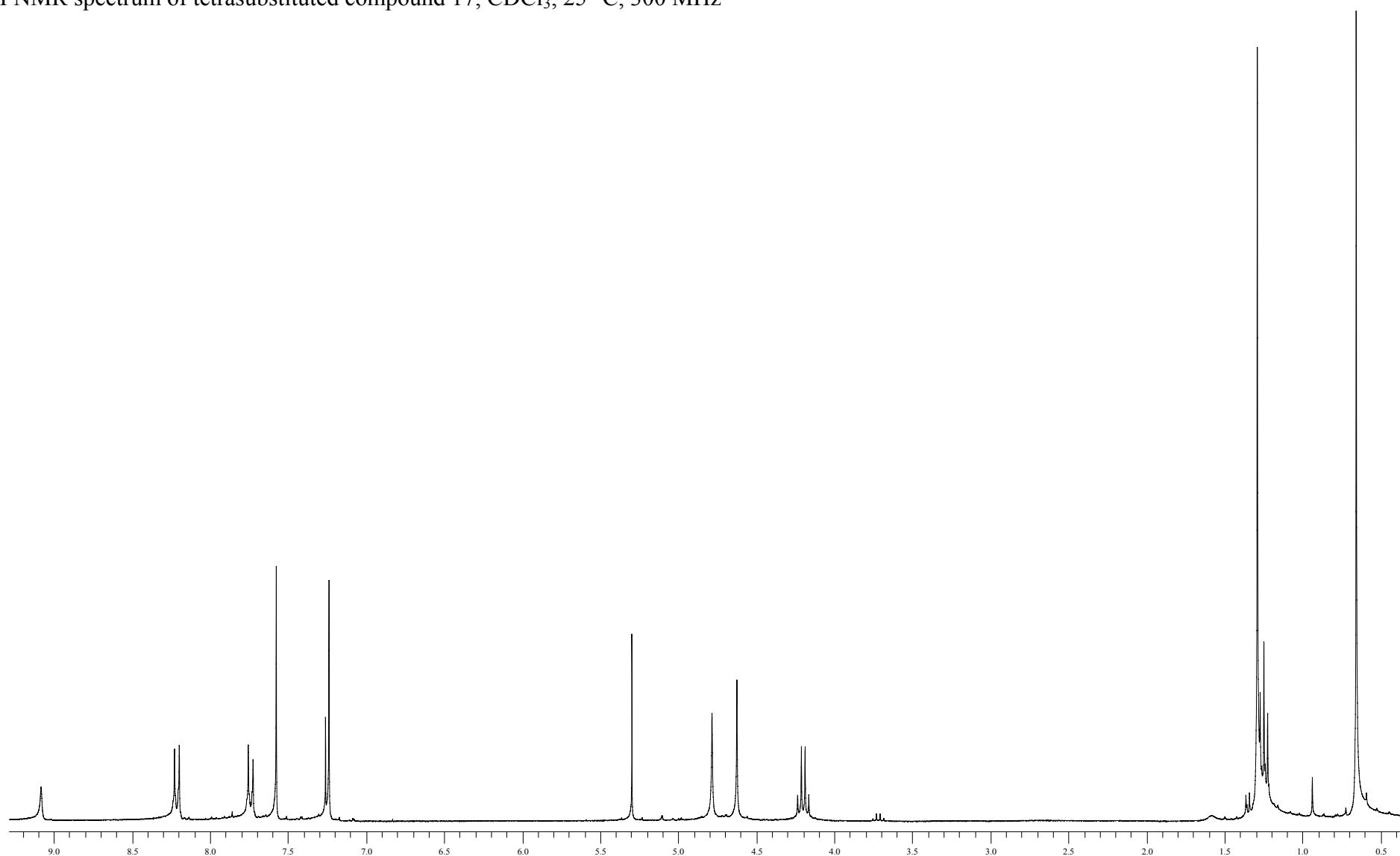
$^1\text{H}$  NMR spectrum of tetrasubstituted compound 14,  $\text{CDCl}_3$ , 25 °C, 300 MHz



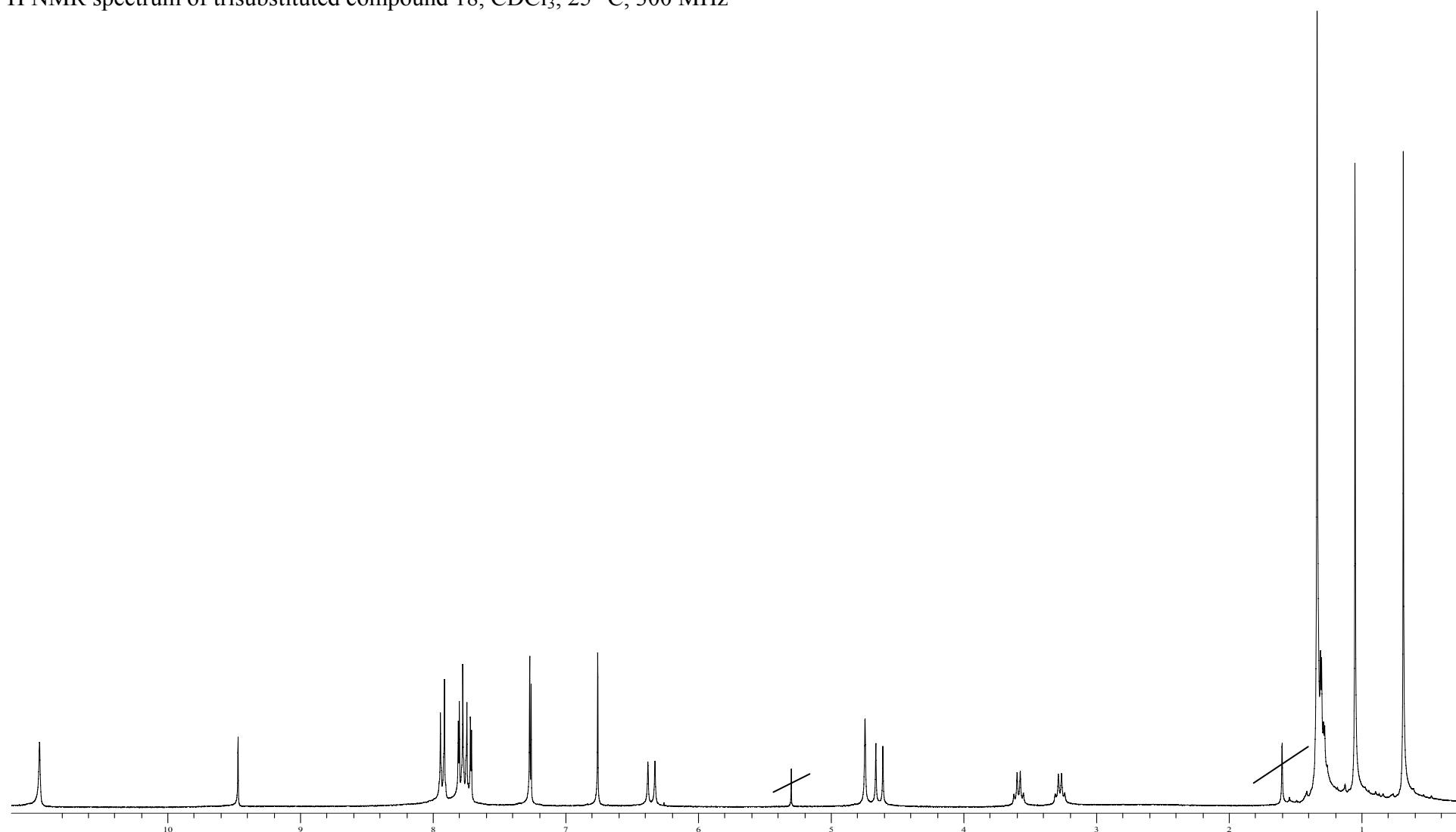
$^1\text{H}$  NMR spectrum of tetrasubstituted compound 16,  $\text{CDCl}_3$ , 25 °C, 300 MHz



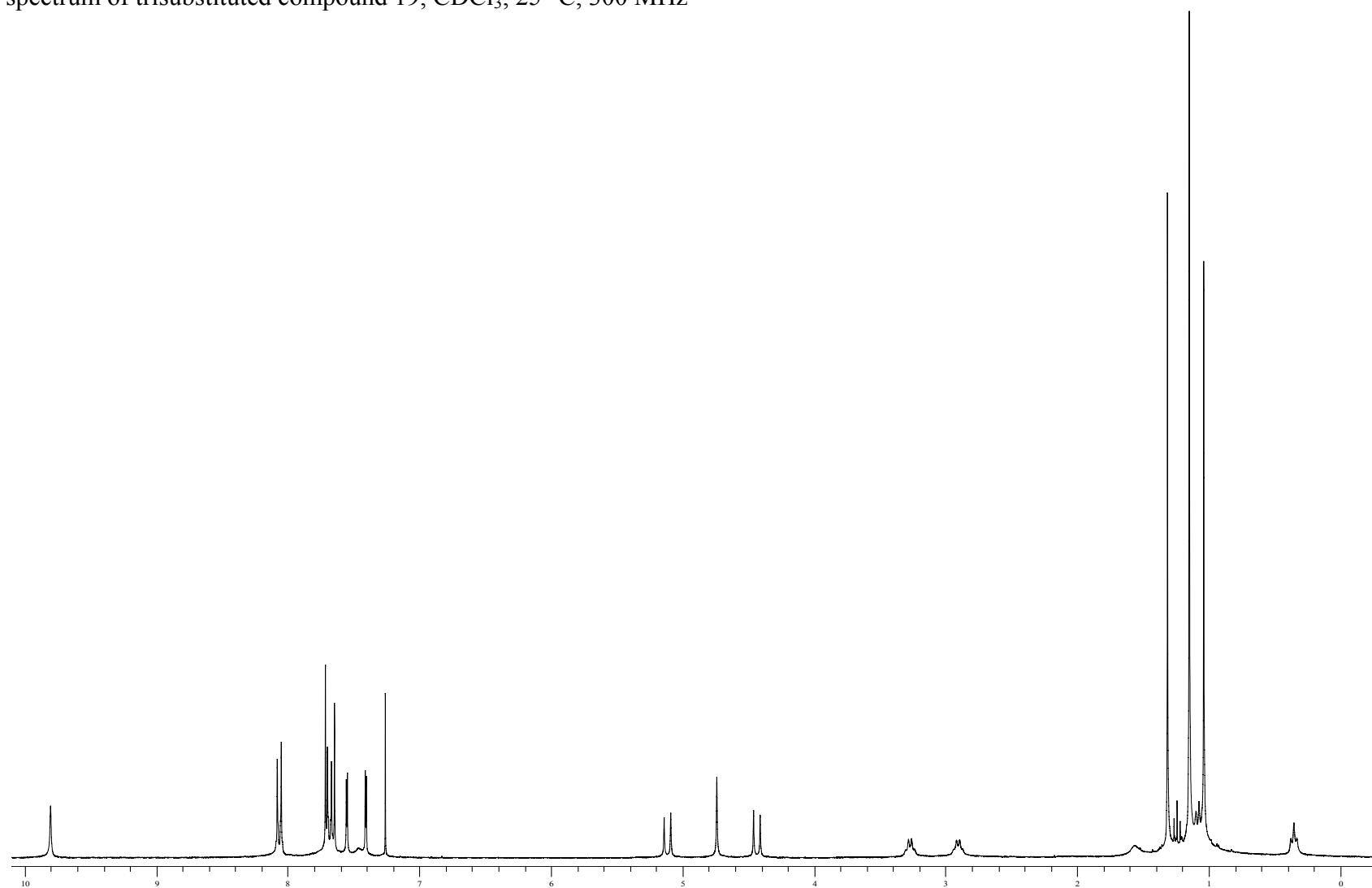
$^1\text{H}$  NMR spectrum of tetrasubstituted compound 17,  $\text{CDCl}_3$ , 25 °C, 300 MHz



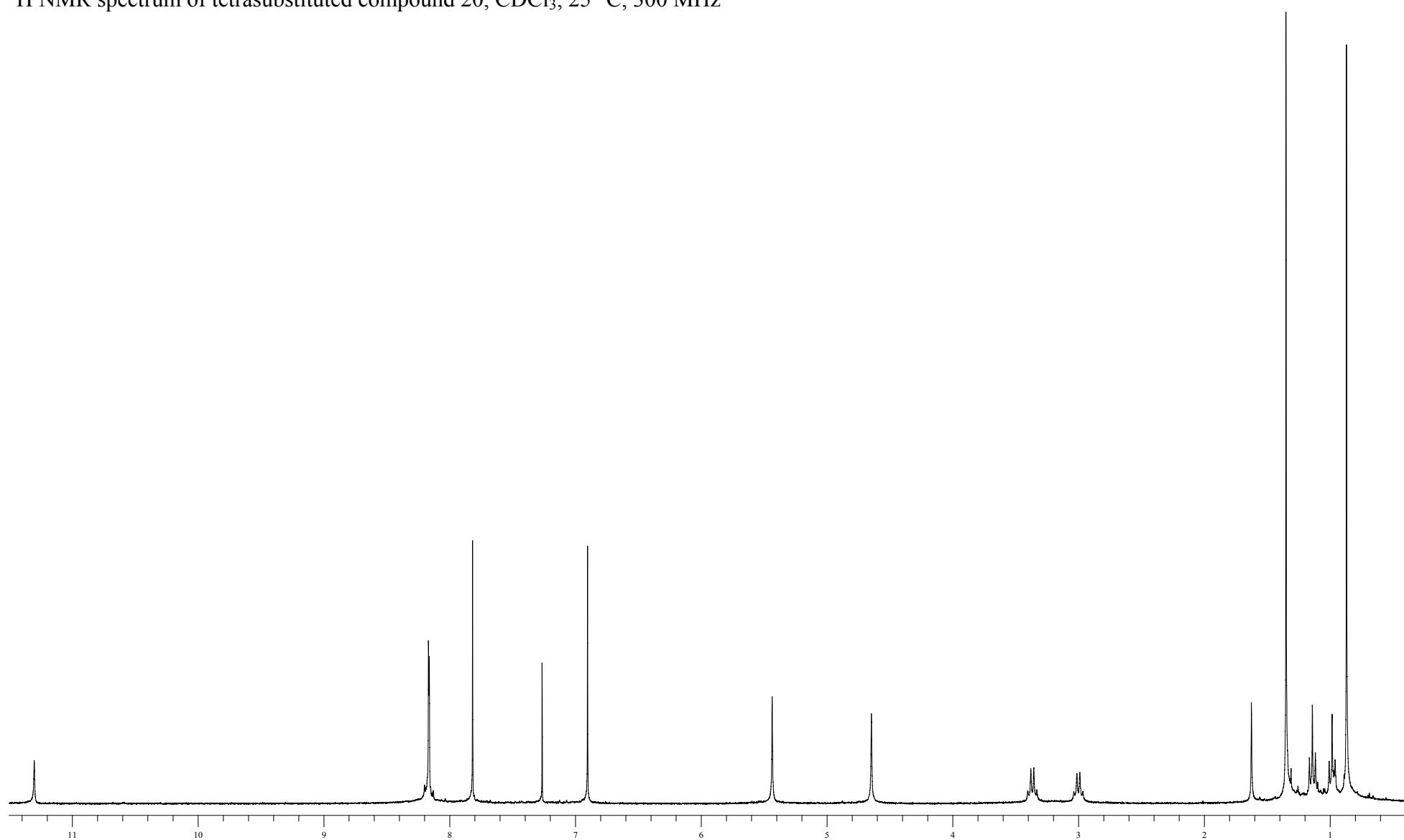
$^1\text{H}$  NMR spectrum of trisubstituted compound 18,  $\text{CDCl}_3$ , 25 °C, 300 MHz



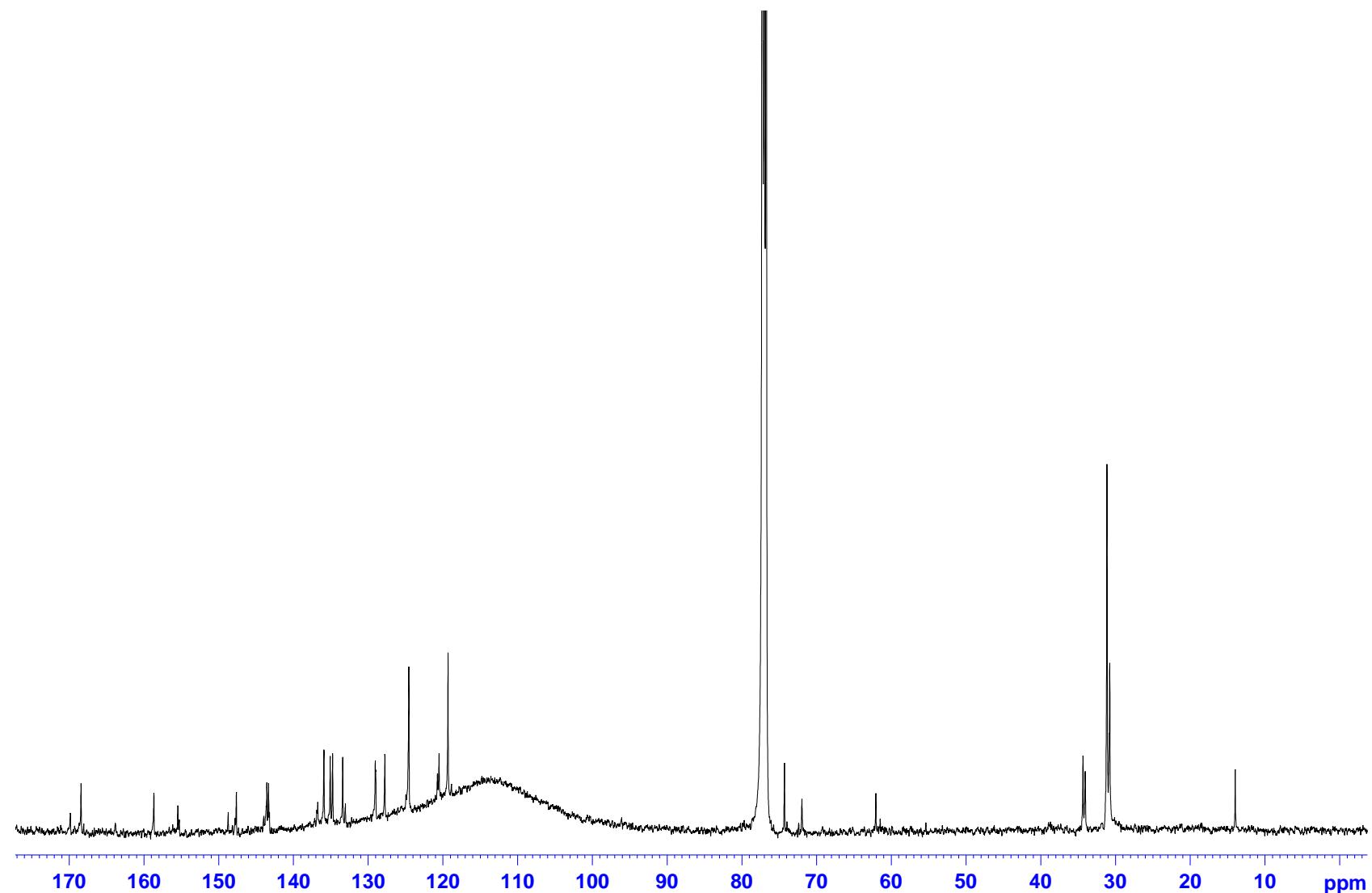
$^1\text{H}$  NMR spectrum of trisubstituted compound 19,  $\text{CDCl}_3$ , 25 °C, 300 MHz



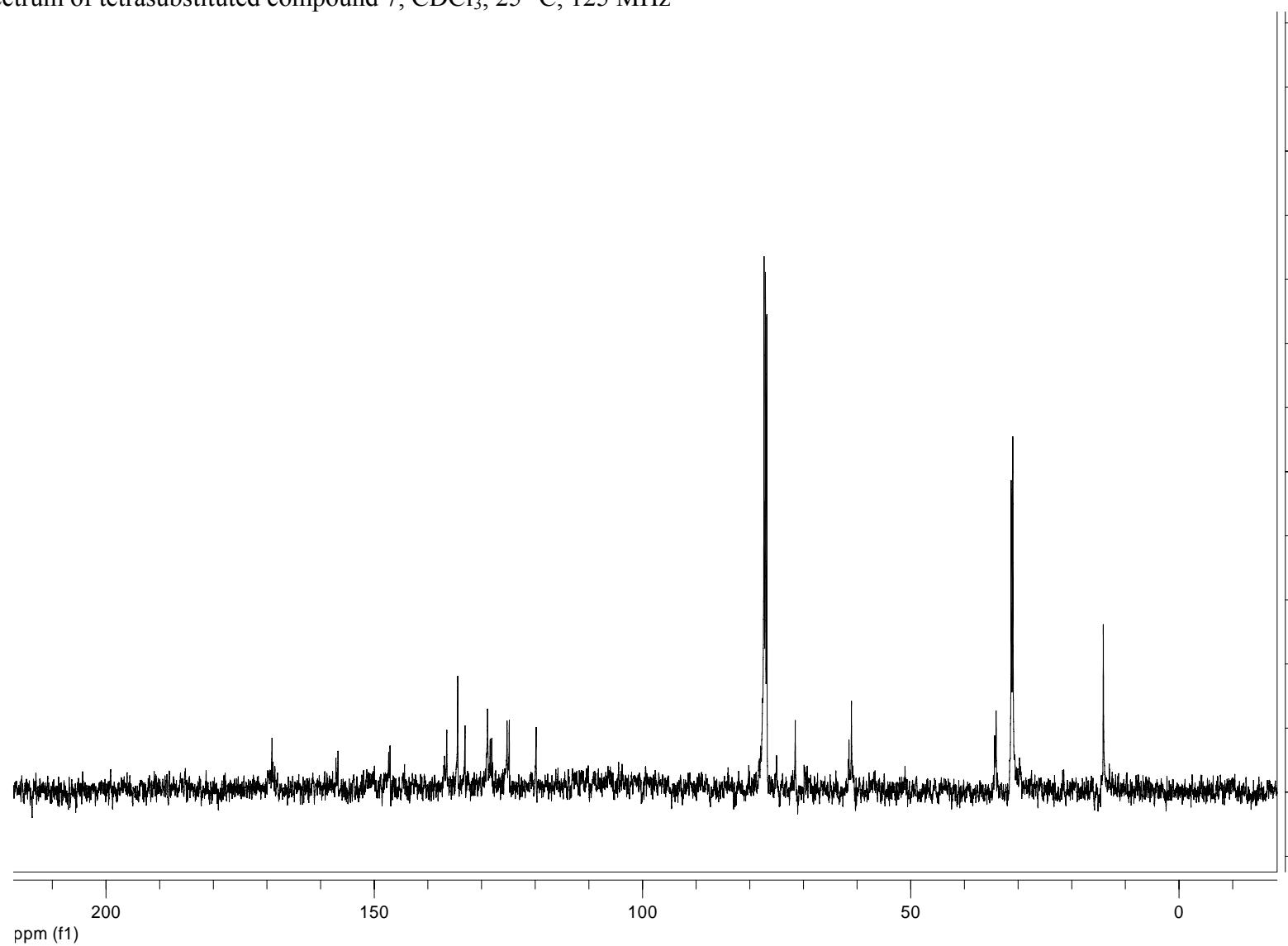
$^1\text{H}$  NMR spectrum of tetrasubstituted compound 20,  $\text{CDCl}_3$ , 25 °C, 300 MHz



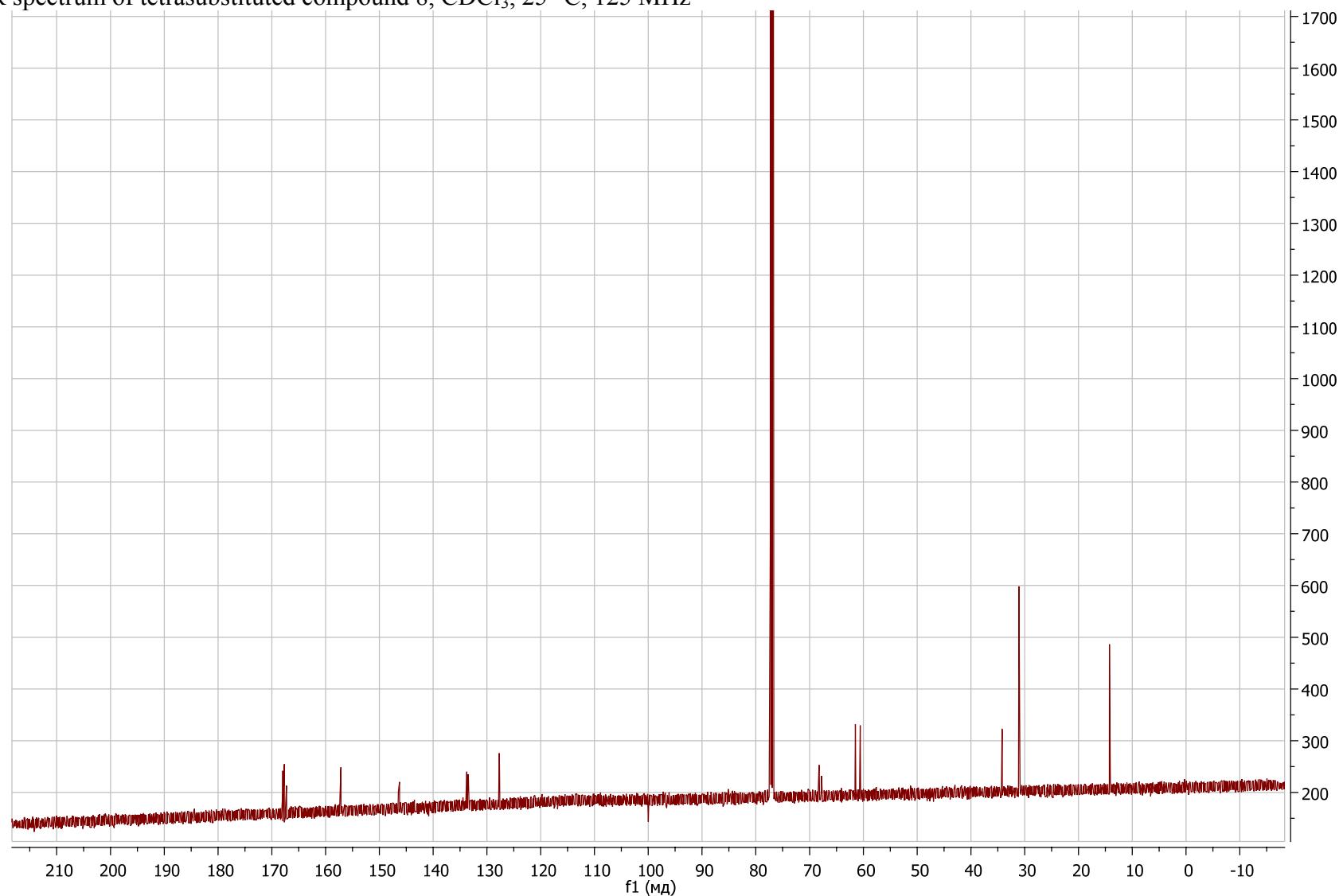
$^{13}\text{C}$  NMR spectrum of trisubstituted compound 5,  $\text{CDCl}_3$ , 25 °C, 125 MHz



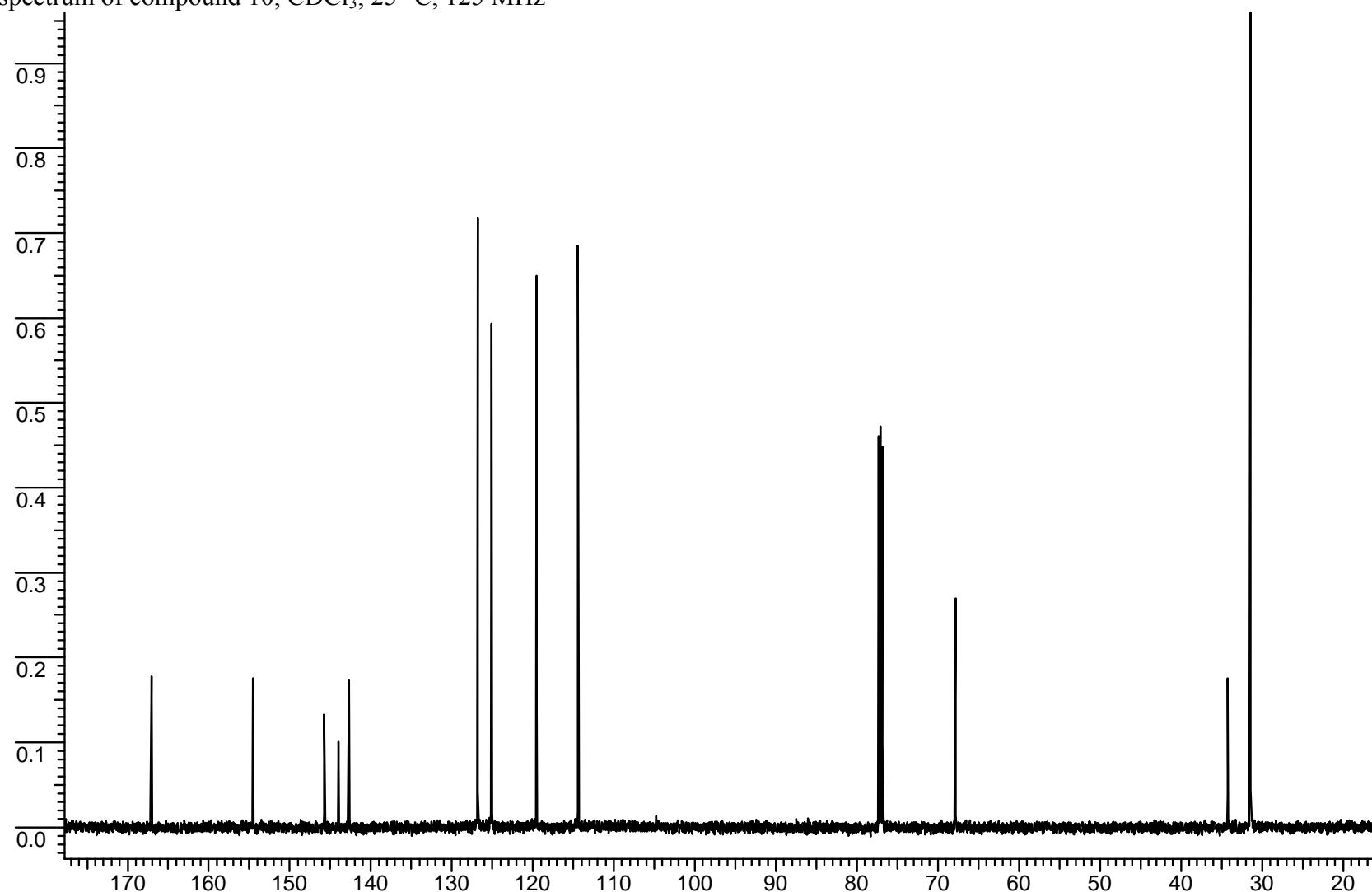
$^{13}\text{C}$  NMR spectrum of tetrasubstituted compound 7,  $\text{CDCl}_3$ , 25 °C, 125 MHz



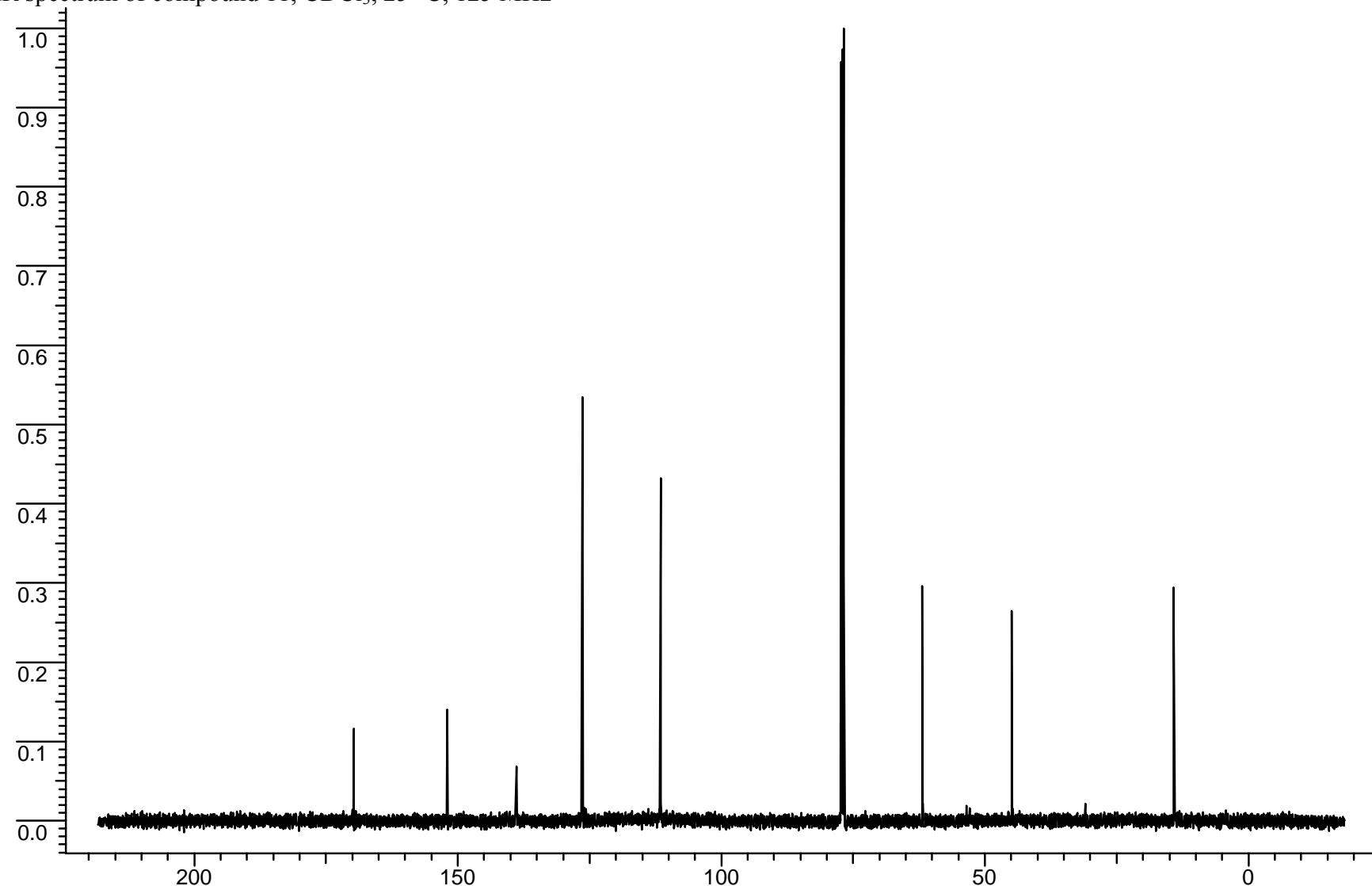
$^{13}\text{C}$  NMR spectrum of tetrasubstituted compound 8,  $\text{CDCl}_3$ , 25 °C, 125 MHz



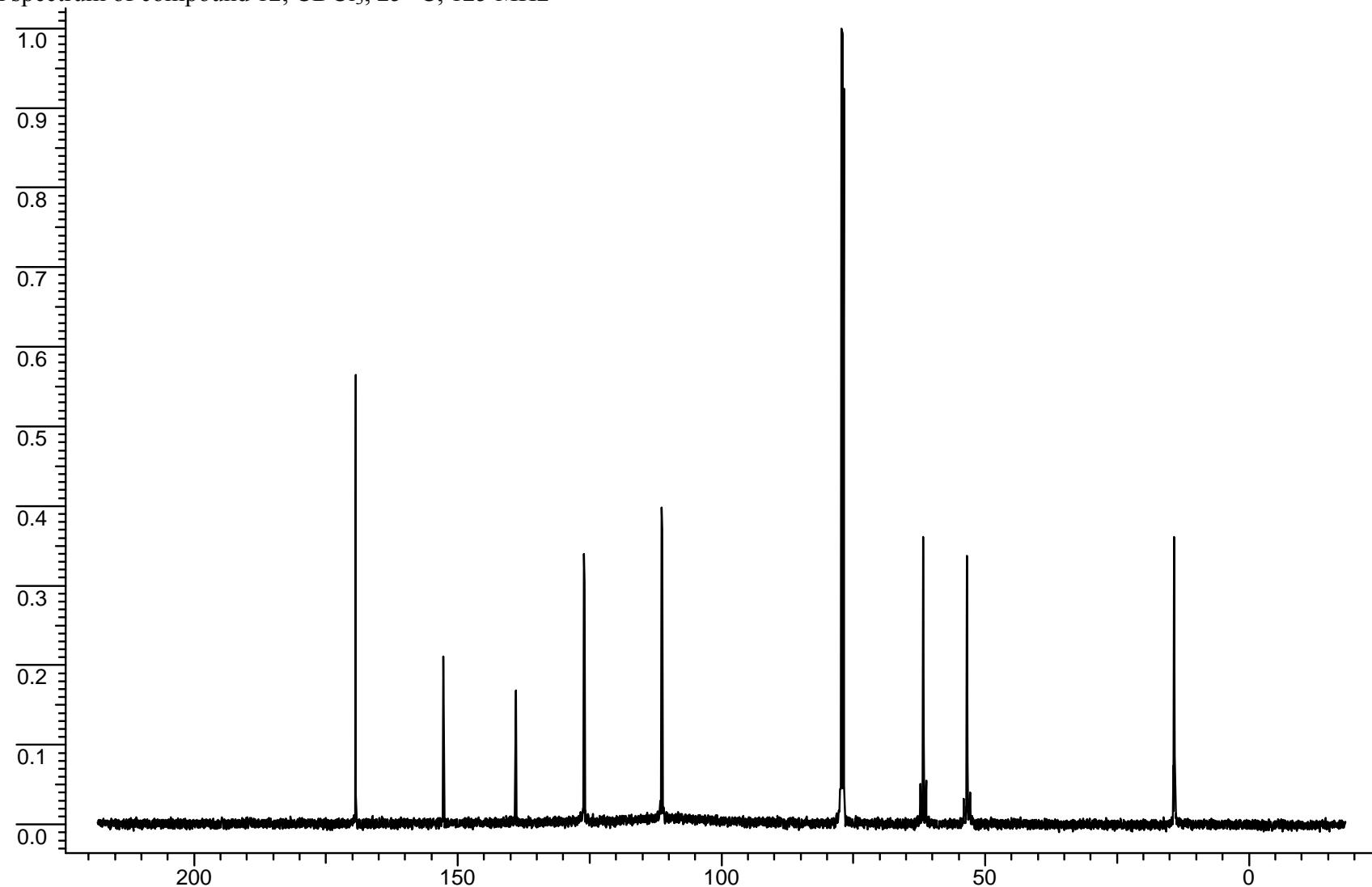
$^{13}\text{C}$  NMR spectrum of compound 10,  $\text{CDCl}_3$ , 25 °C, 125 MHz



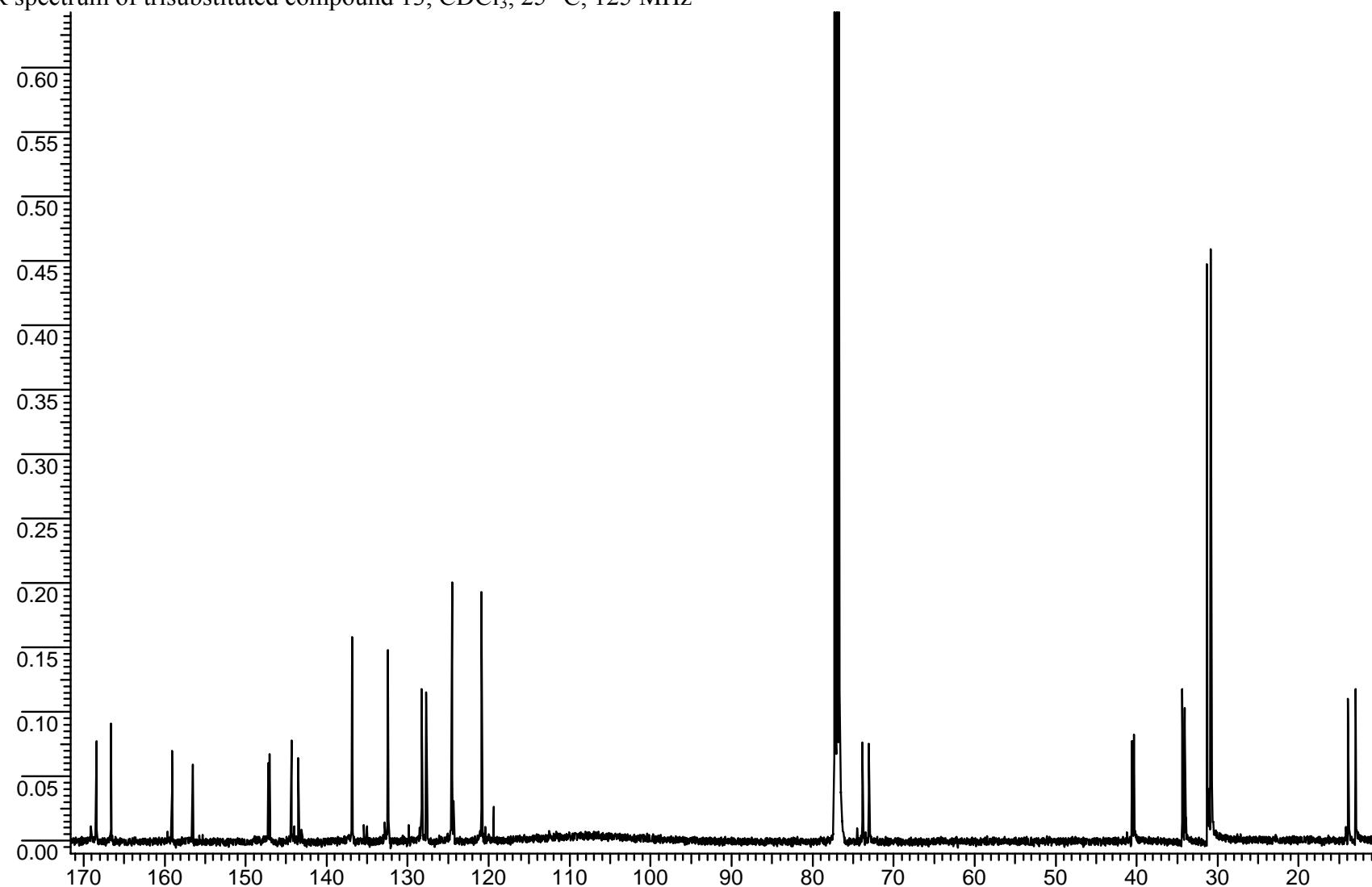
$^{13}\text{C}$  NMR spectrum of compound 11,  $\text{CDCl}_3$ , 25 °C, 125 MHz



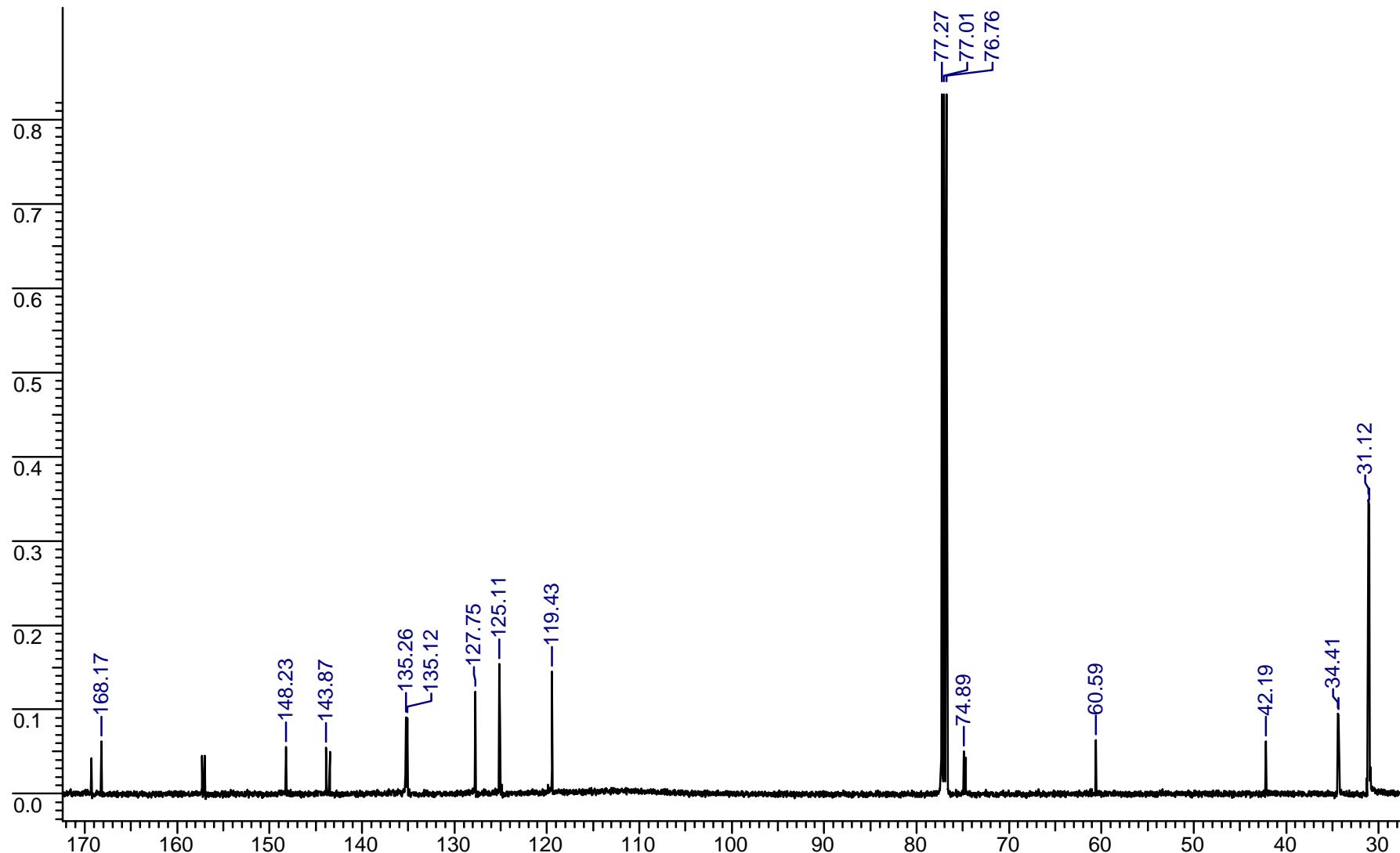
$^{13}\text{C}$  NMR spectrum of compound 12,  $\text{CDCl}_3$ , 25 °C, 125 MHz



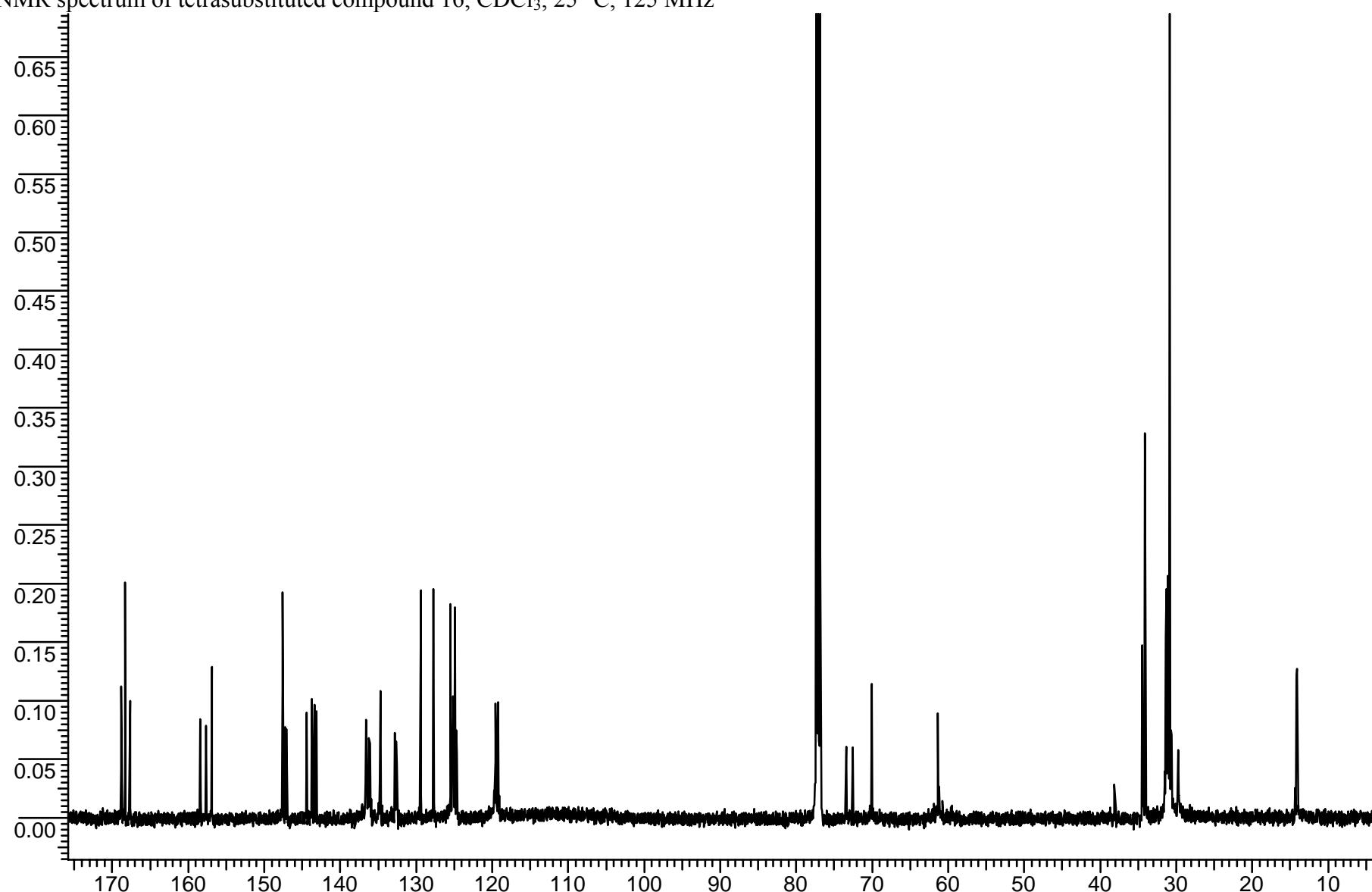
$^{13}\text{C}$  NMR spectrum of trisubstituted compound 13,  $\text{CDCl}_3$ , 25 °C, 125 MHz



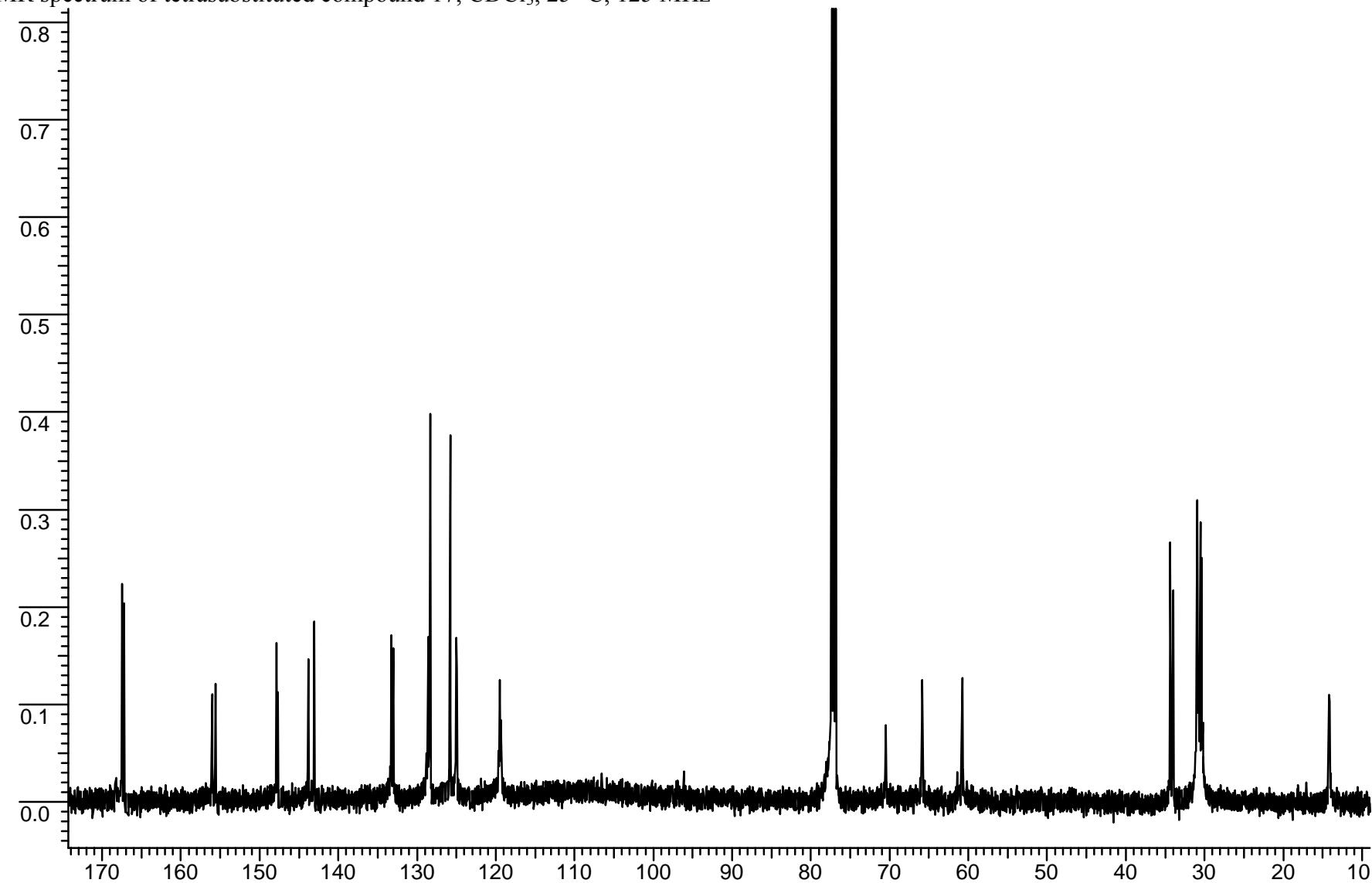
$^{13}\text{C}$  NMR spectrum of tetrasubstituted compound 14,  $\text{CDCl}_3$ , 25 °C, 125 MHz



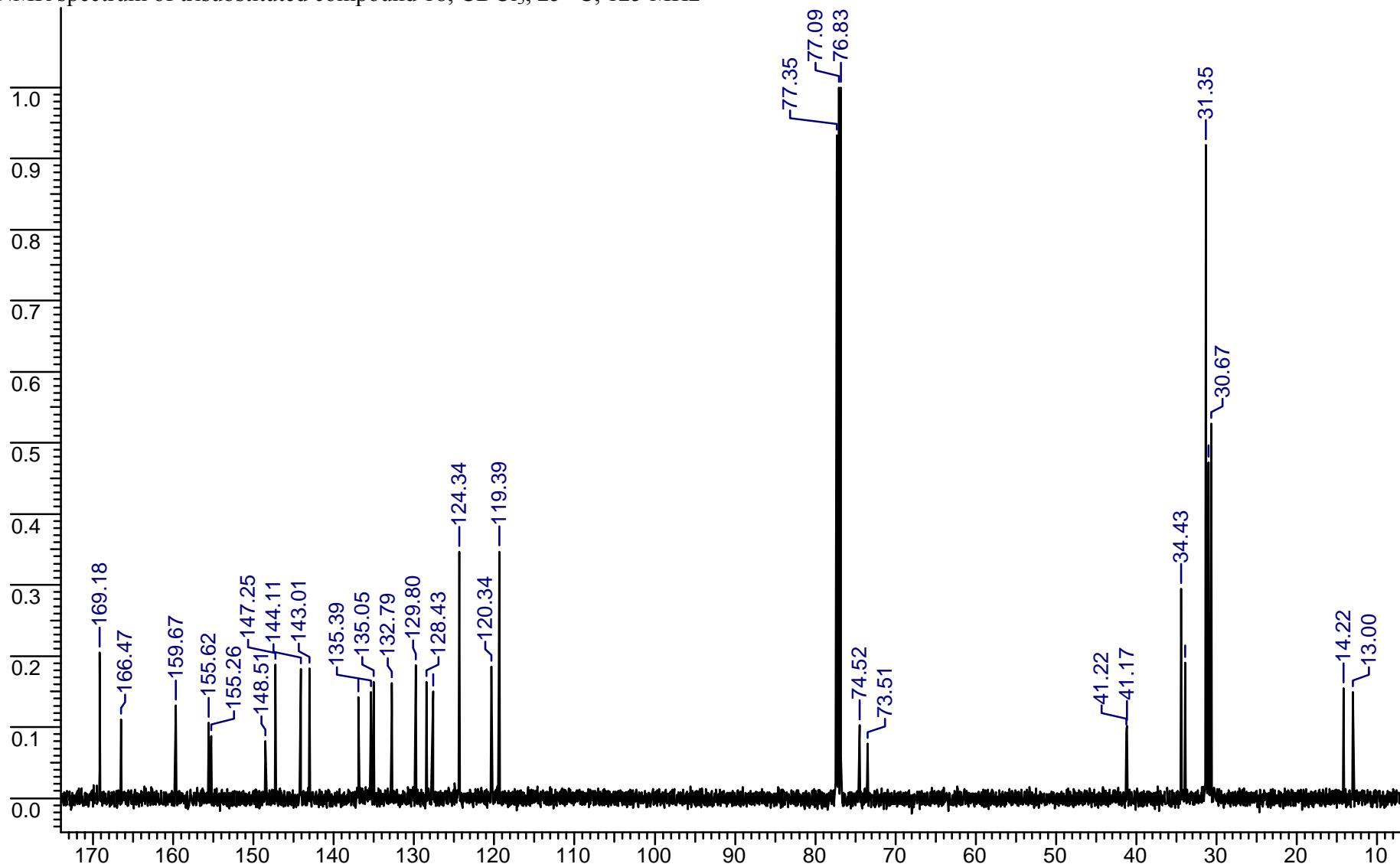
$^{13}\text{C}$  NMR spectrum of tetrasubstituted compound 16,  $\text{CDCl}_3$ , 25 °C, 125 MHz



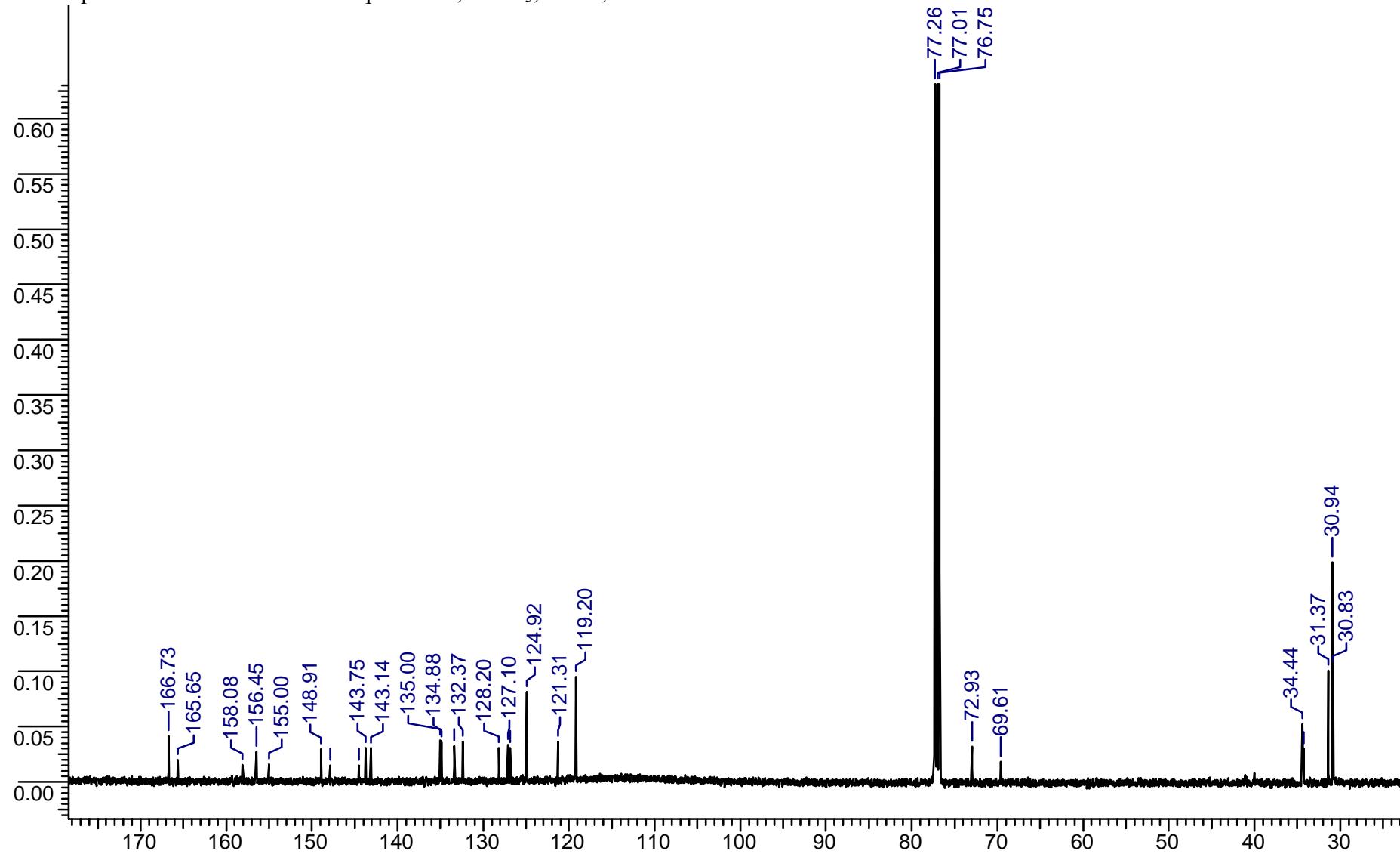
$^{13}\text{C}$  NMR spectrum of tetrasubstituted compound 17,  $\text{CDCl}_3$ , 25 °C, 125 MHz



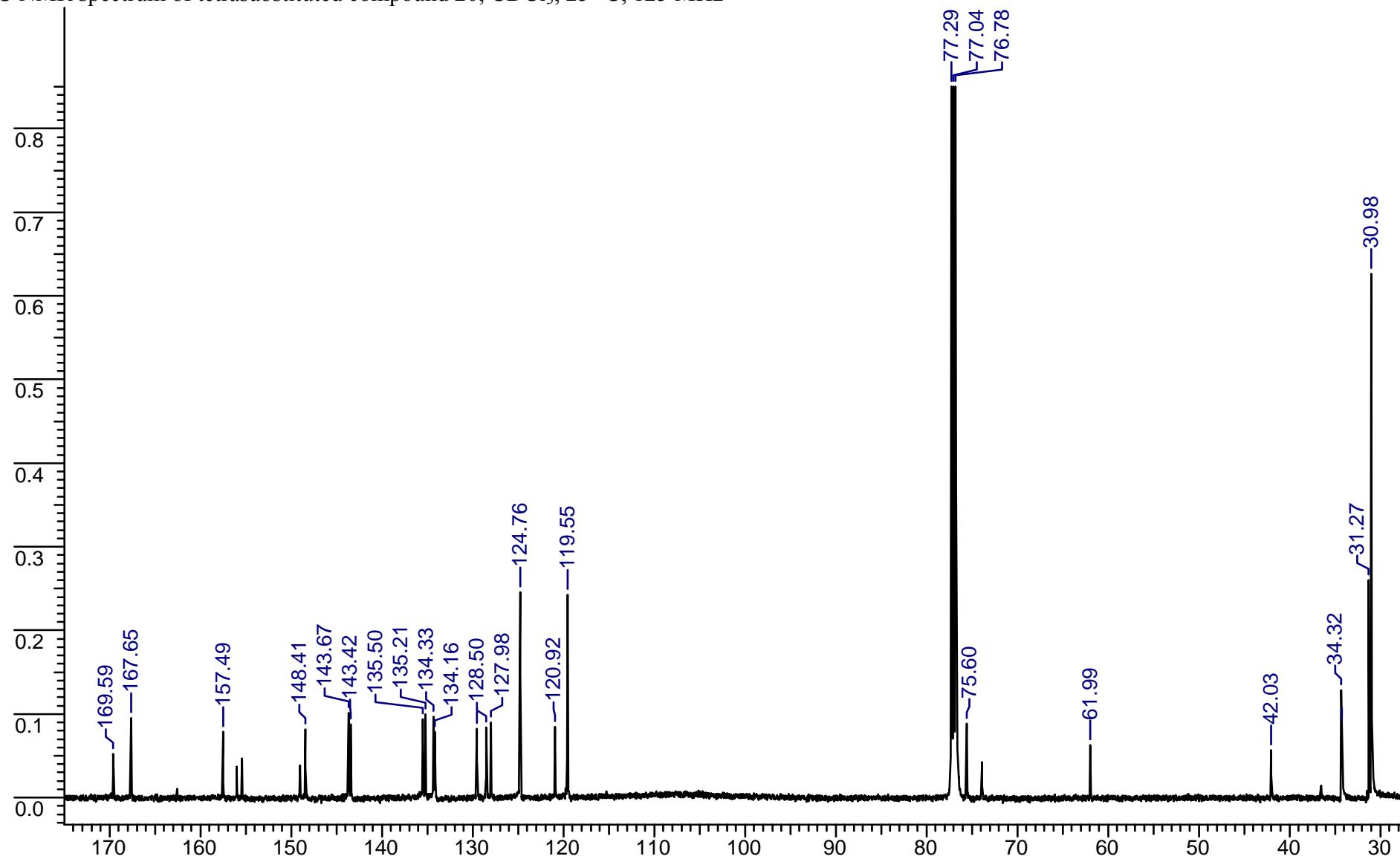
$^{13}\text{C}$  NMR spectrum of trisubstituted compound 18,  $\text{CDCl}_3$ , 25 °C, 125 MHz



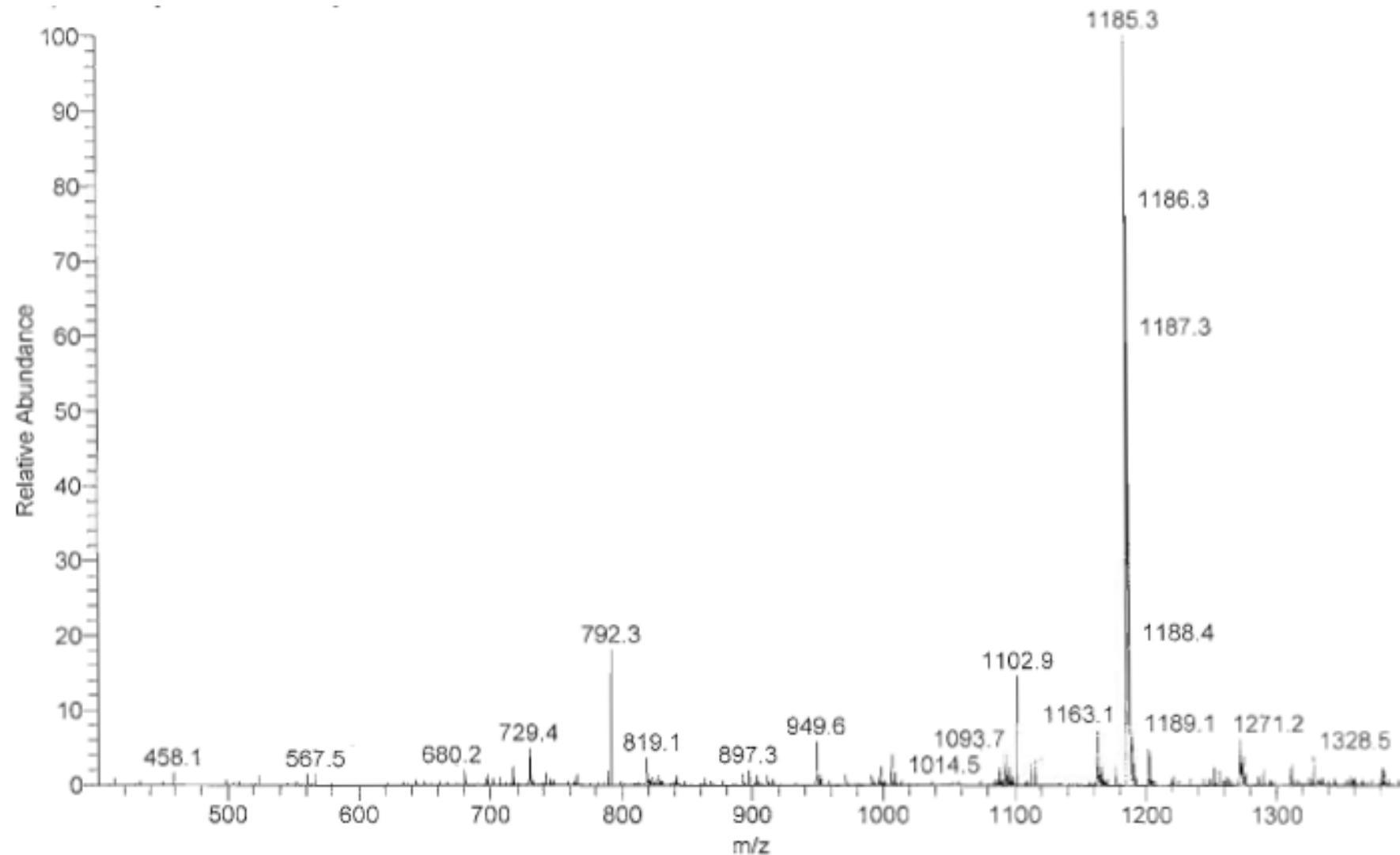
$^{13}\text{C}$  NMR spectrum of trisubstituted compound 19,  $\text{CDCl}_3$ , 25 °C, 125 MHz



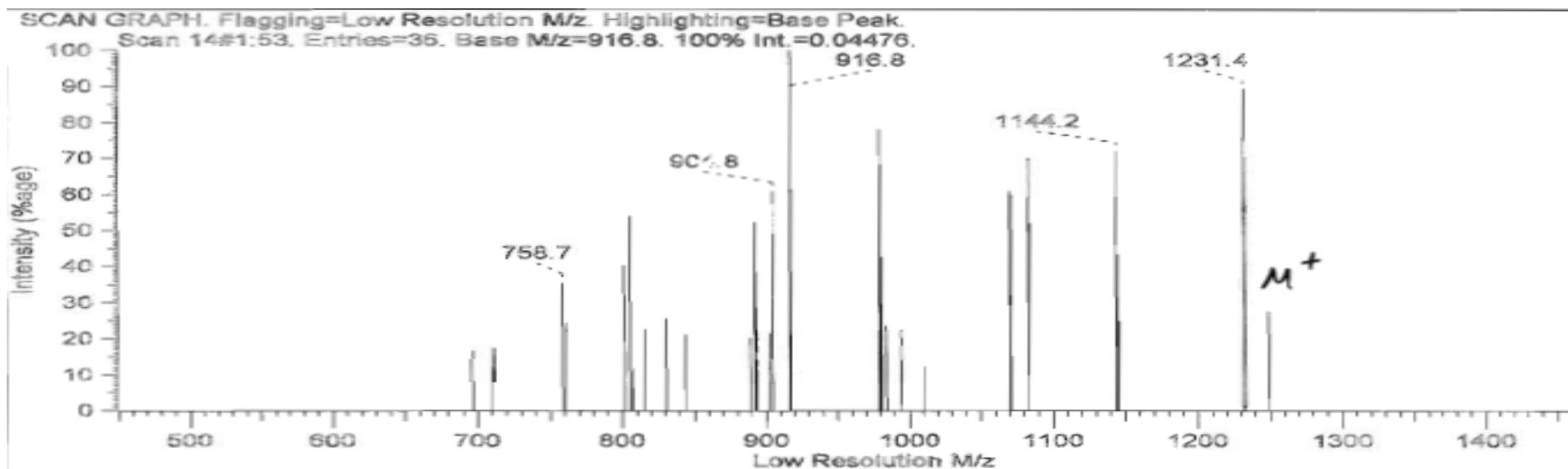
$^{13}\text{C}$  NMR spectrum of tetrasubstituted compound 20,  $\text{CDCl}_3$ , 25 °C, 125 MHz



Mass spectrum of trisubstituted compound 5



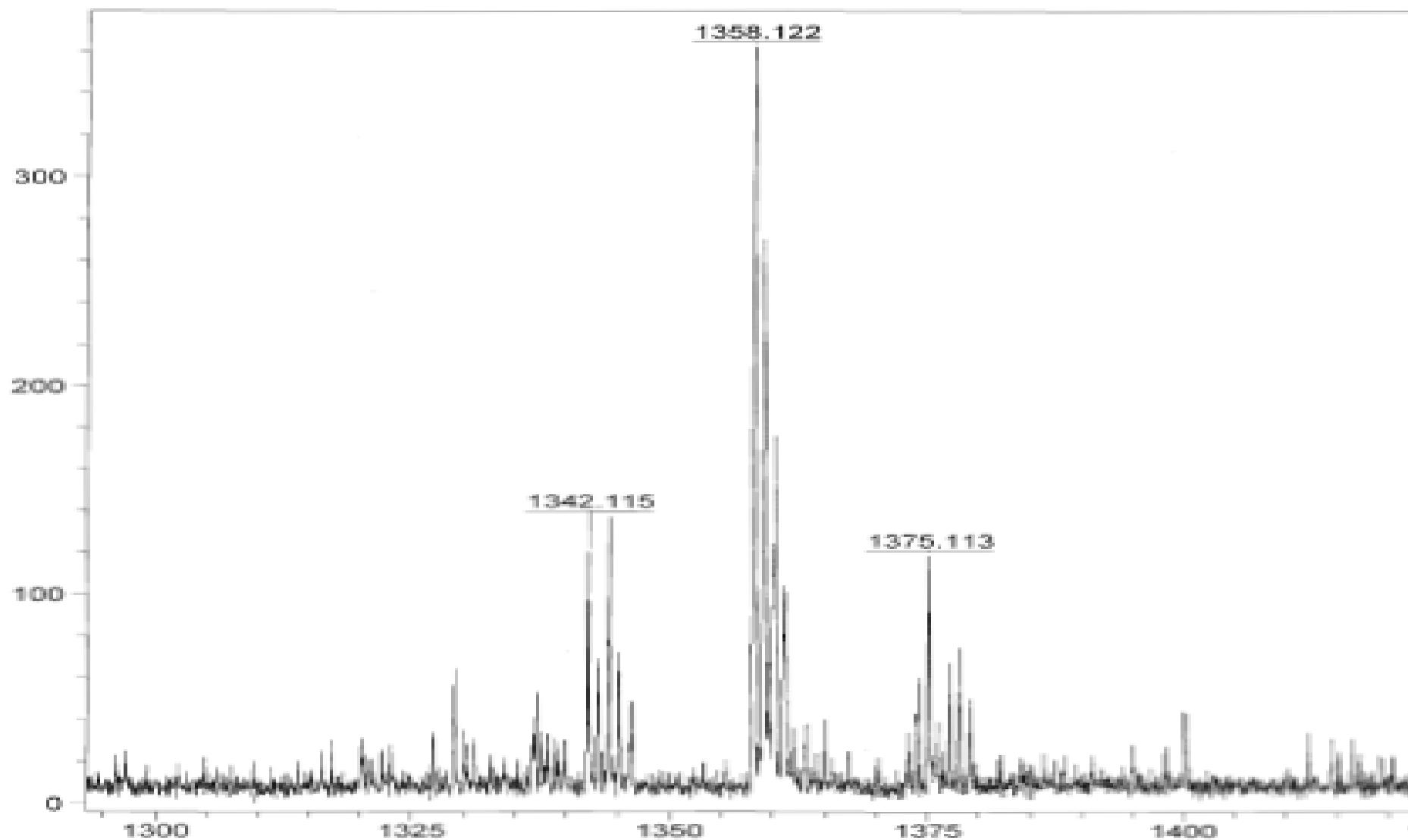
Mass spectrum of tetrasubstituted compound 6



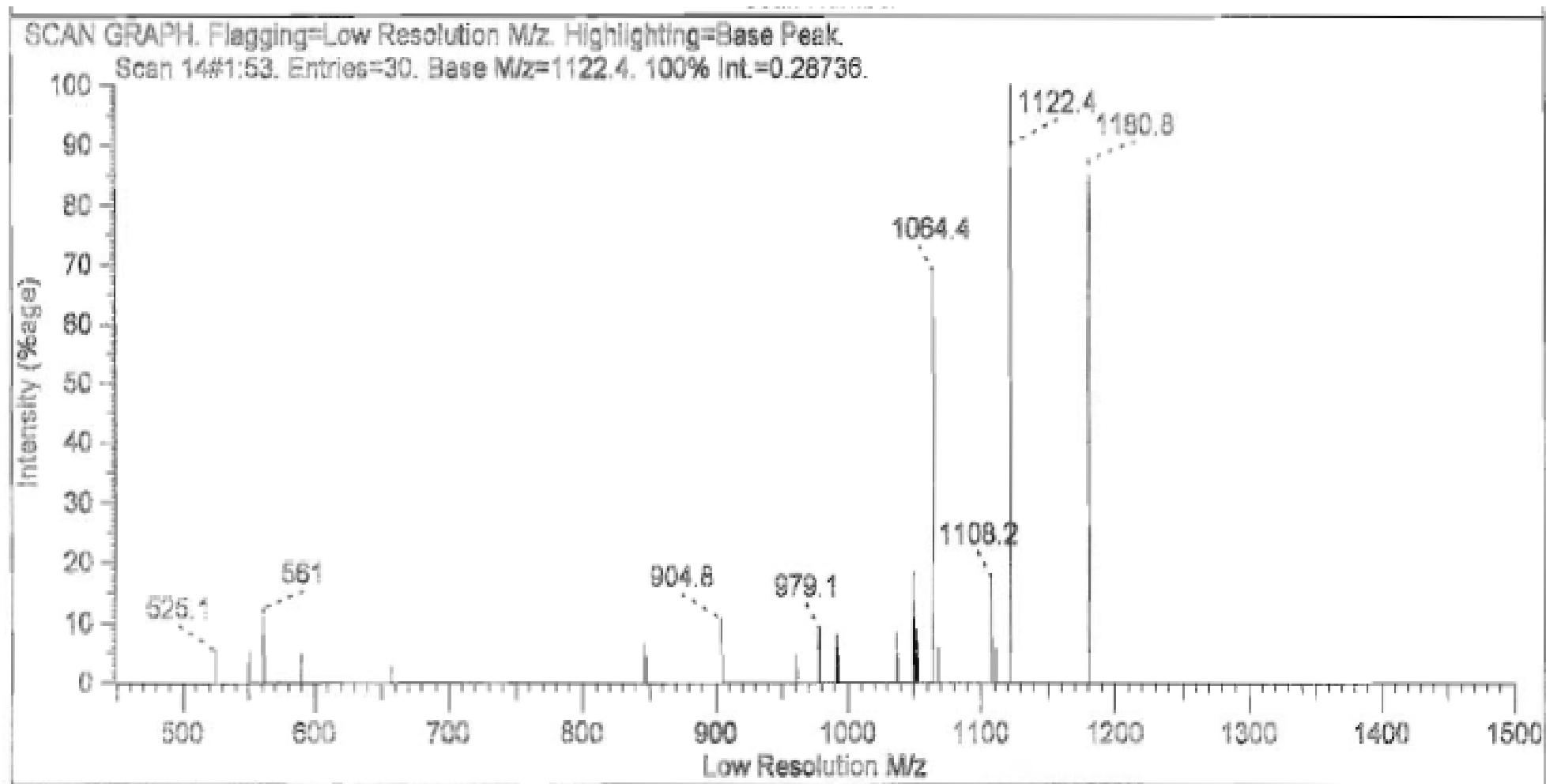
SCAN TEXT. Sorted on Low Resolution M/z (descending). Highlighting=Base Peak.  
Scan 14#1:53. Entries=36. Base M/z=916.8. 100% Int.=0.04476.

M/z	Field	%age	Width	M/z	Field	%age	Width
<i>M<sup>+</sup></i>				904.8	37472	60.68	10
1248.7	51721	24.71	14	902.8	37389	21.27	10
1248.7	51679	27.64	10	893.8	37017	28.09	11
1231.4	51054	70.46	11	892.9	36979	38.45	10
1231.4	50970	88.28	11	891.8	36935	52.14	10
1146.2	47451	24.75	11	888.8	36811	19.84	13
1145.3	47411	43.45	10	843.7	34942	21.11	12
1144.2	47369	71.94	10	830.7	34405	25.42	11
1084.0	44885	52.48	11	815.7	33790	22.45	11
1083.0	44843	70.08	11	807.6	33459	11.55	10
1071.2	44349	59.87	10	805.6	33381	53.89	12
1070.2	44307	60.72	13	801.6	33216	31.72	11
1011.2	41873	12.15	11	800.6	33176	40.26	11
995.2	41207	22.32	13	760.7	31524	24.31	11
984.1	40749	23.35	13	758.7	31442	35.37	10
981.0	40621	42.65	11	710.7	29449	17.14	10
980.1	40582	68.12	11	696.7	28876	16.55	11
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917.8	38009	61.42	10				
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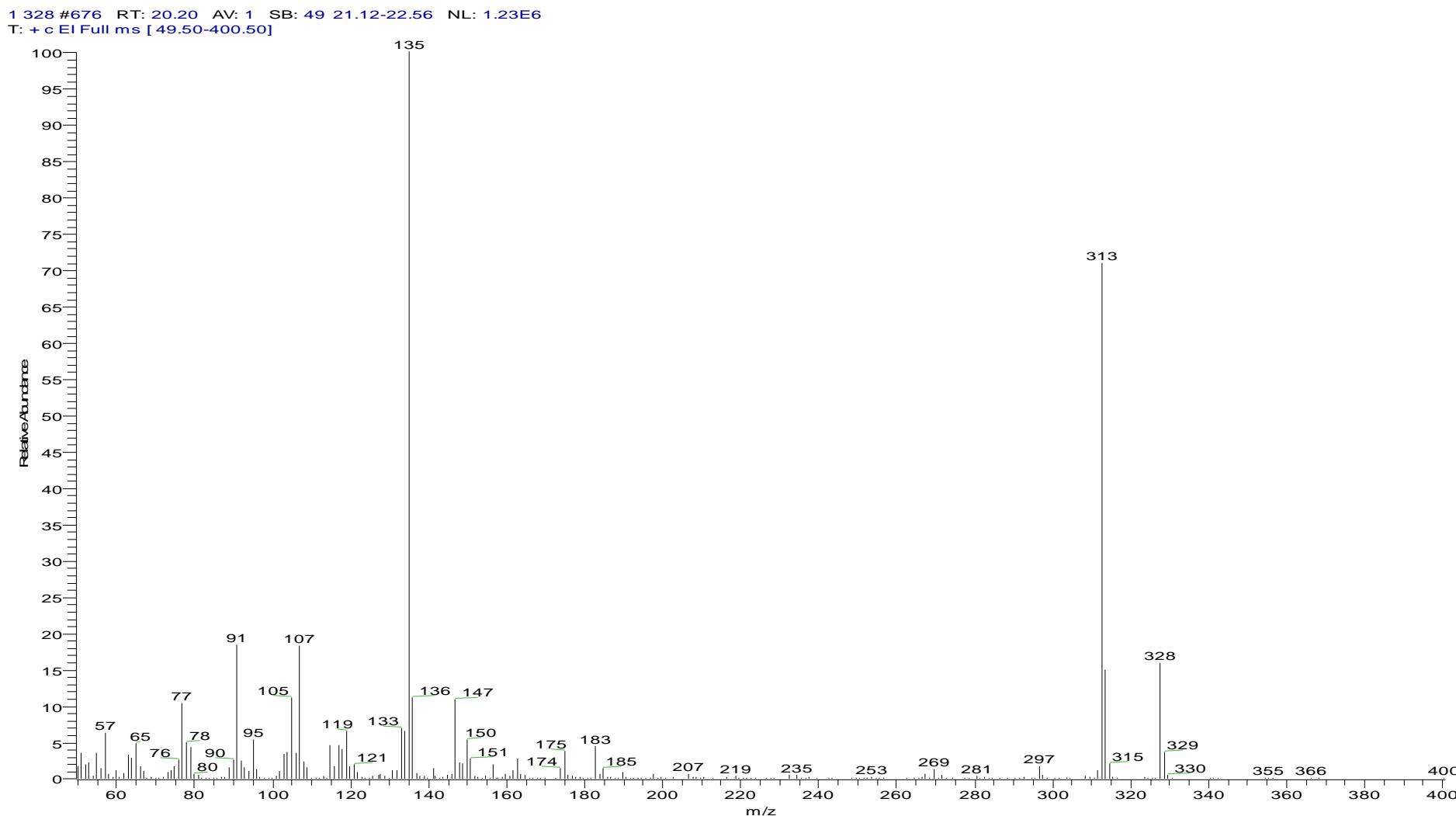
Mass spectrum of tetrasubstituted compound 7



Mass spectrum of tetrasubstituted compound 8

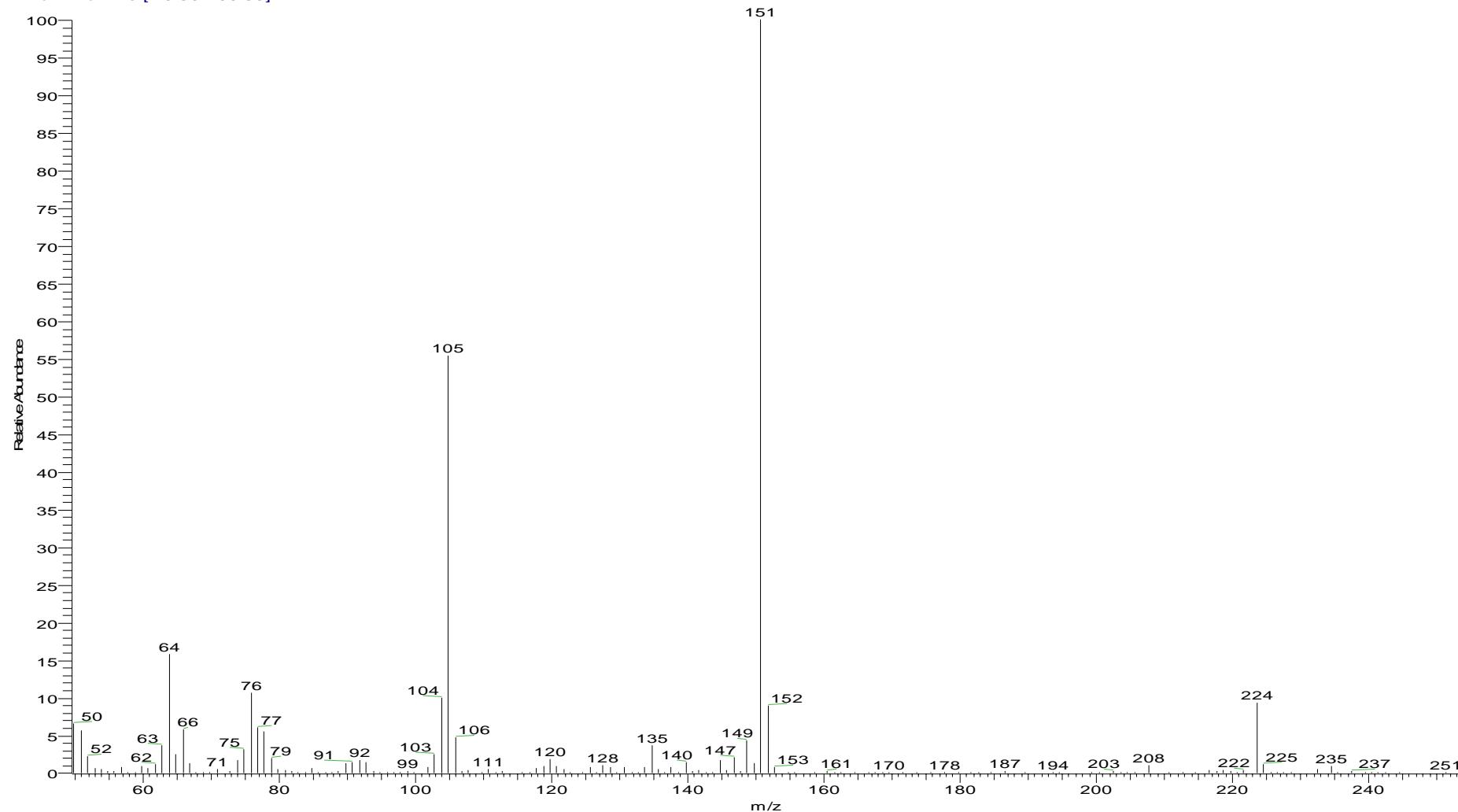


Mass spectrum of compound 10



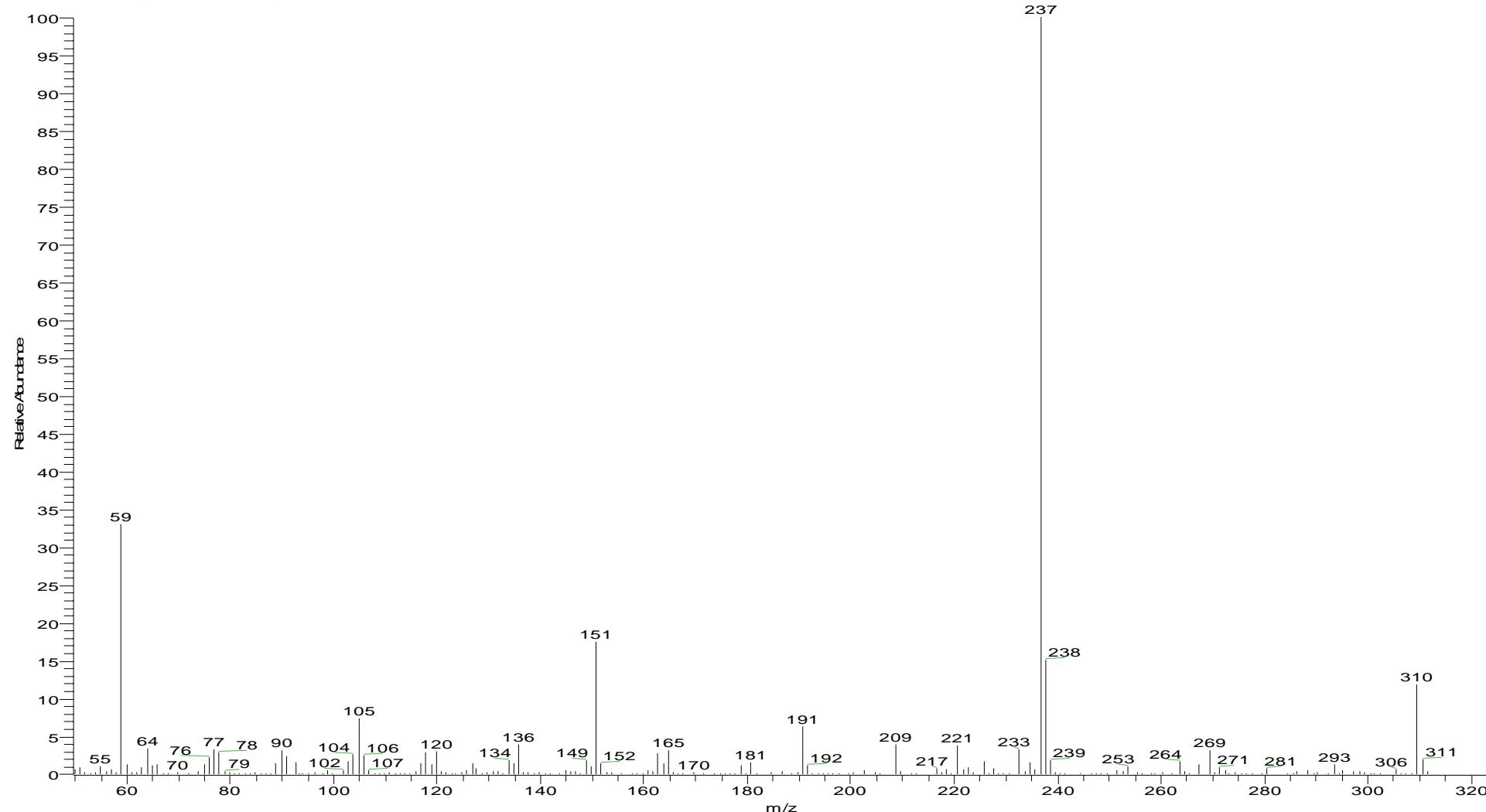
### Mass spectrum of compound 11

2 224 #421-423 RT: 12.71-12.77 AV: 3 SB: 19 13.10-13.64 NL: 3.20E5  
T: + c EI Full ms [49.50-400.50]

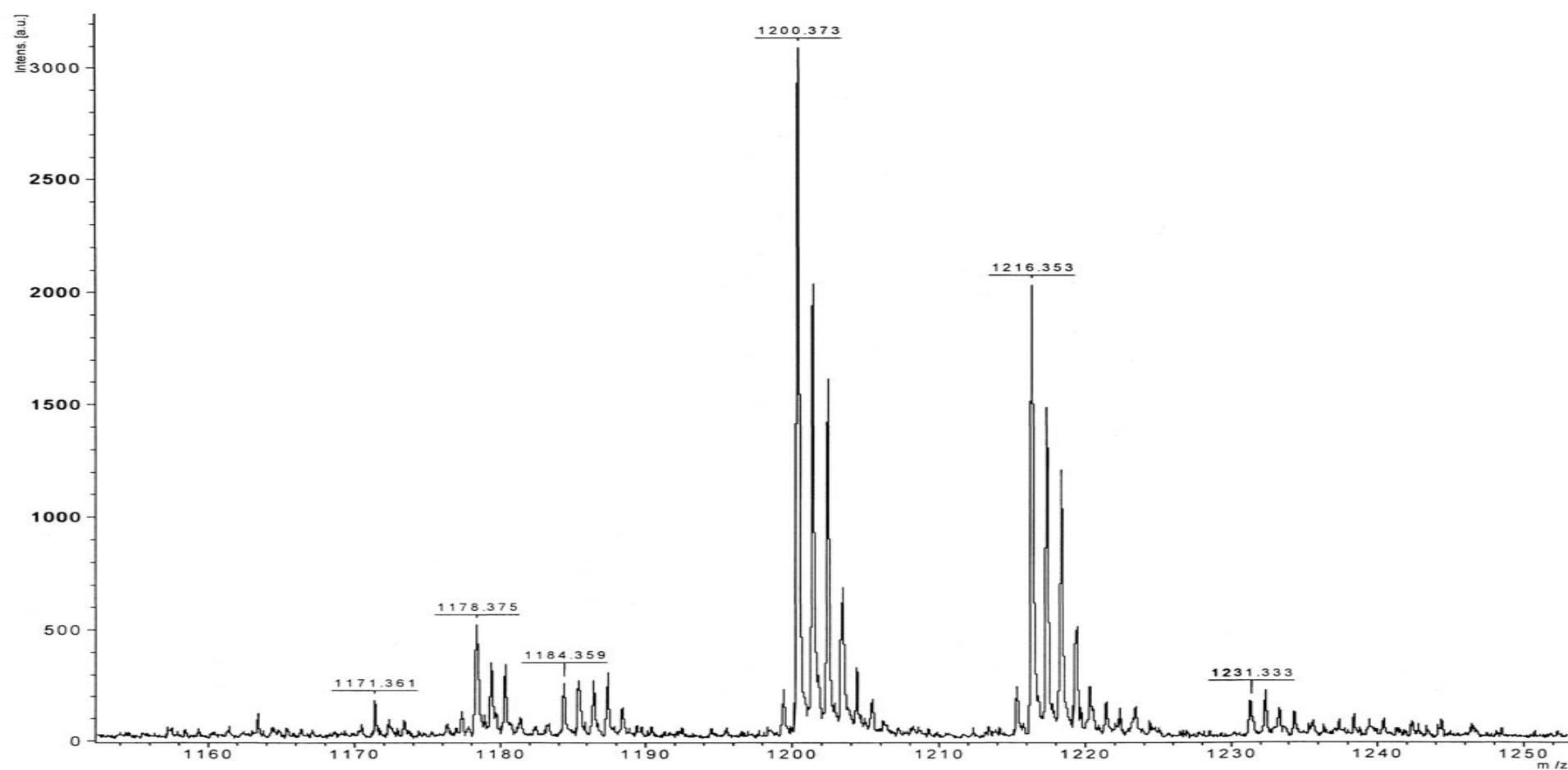


Mass spectrum of compound 12

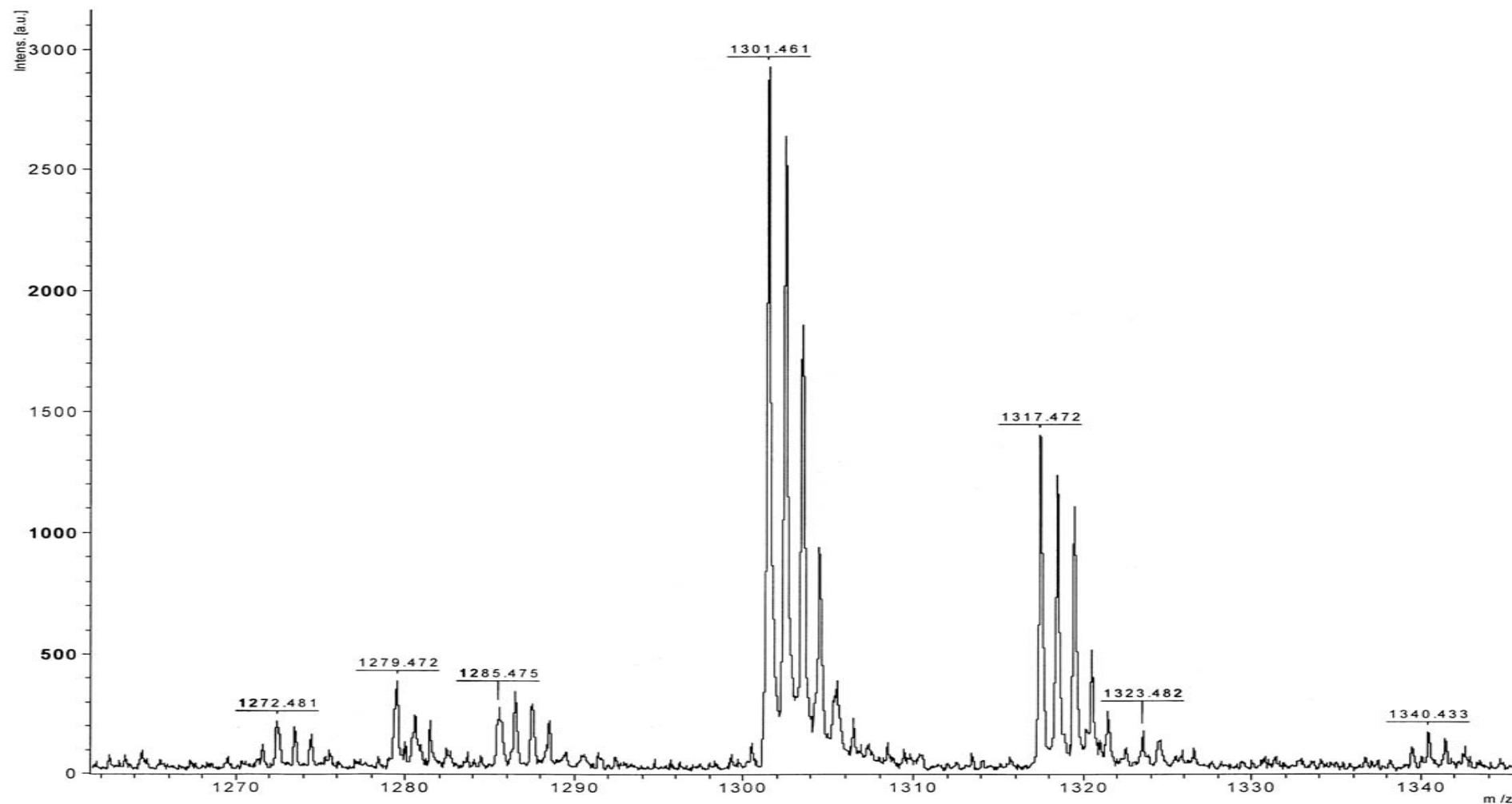
3 310 #515 RT: 15.54 AV: 1 SB: 11 15.91-16.21 NL: 7.13E5  
T: + c EI Full ms [ 49.50-400.50]



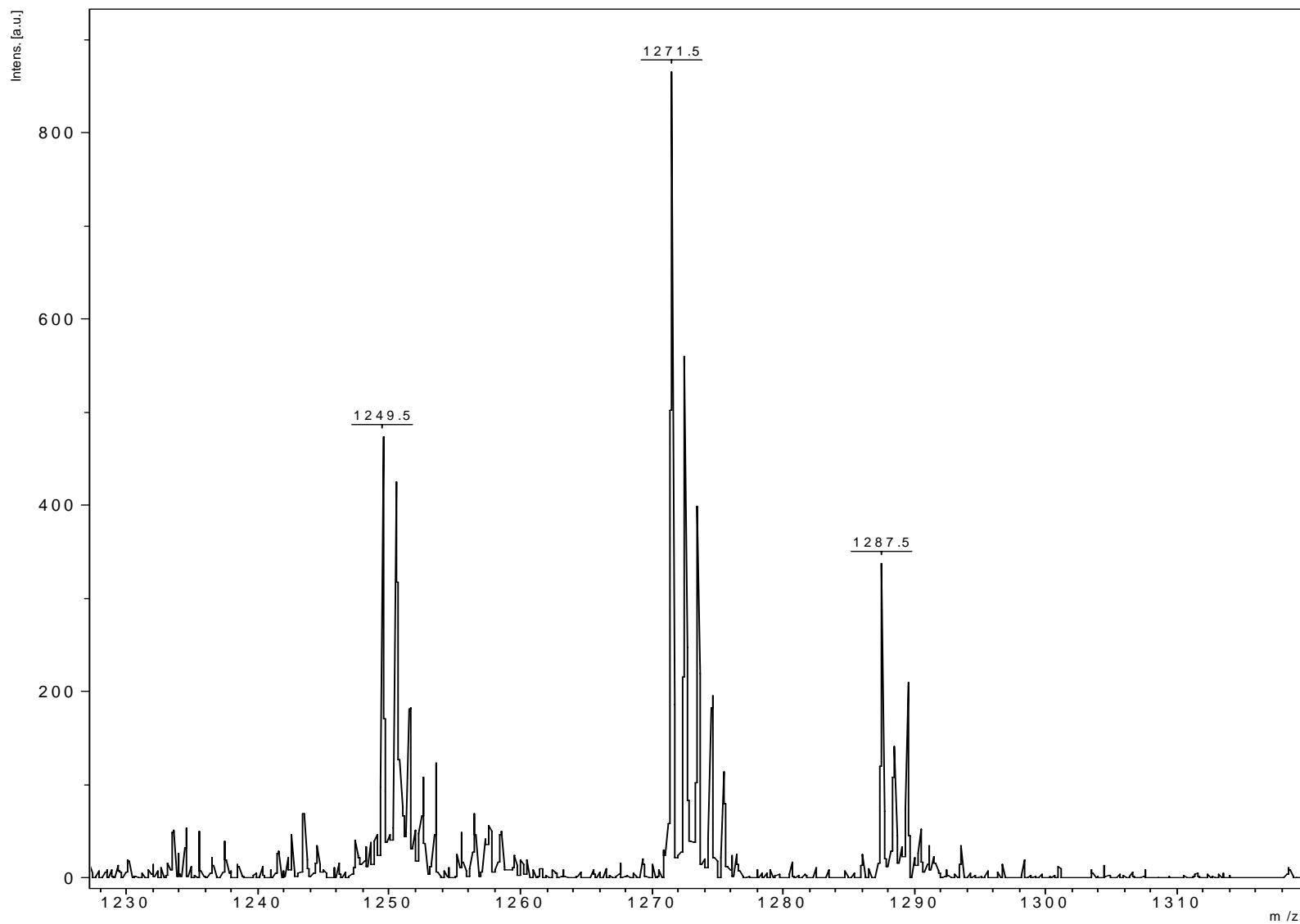
Mass spectrum of trisubstituted compound 13



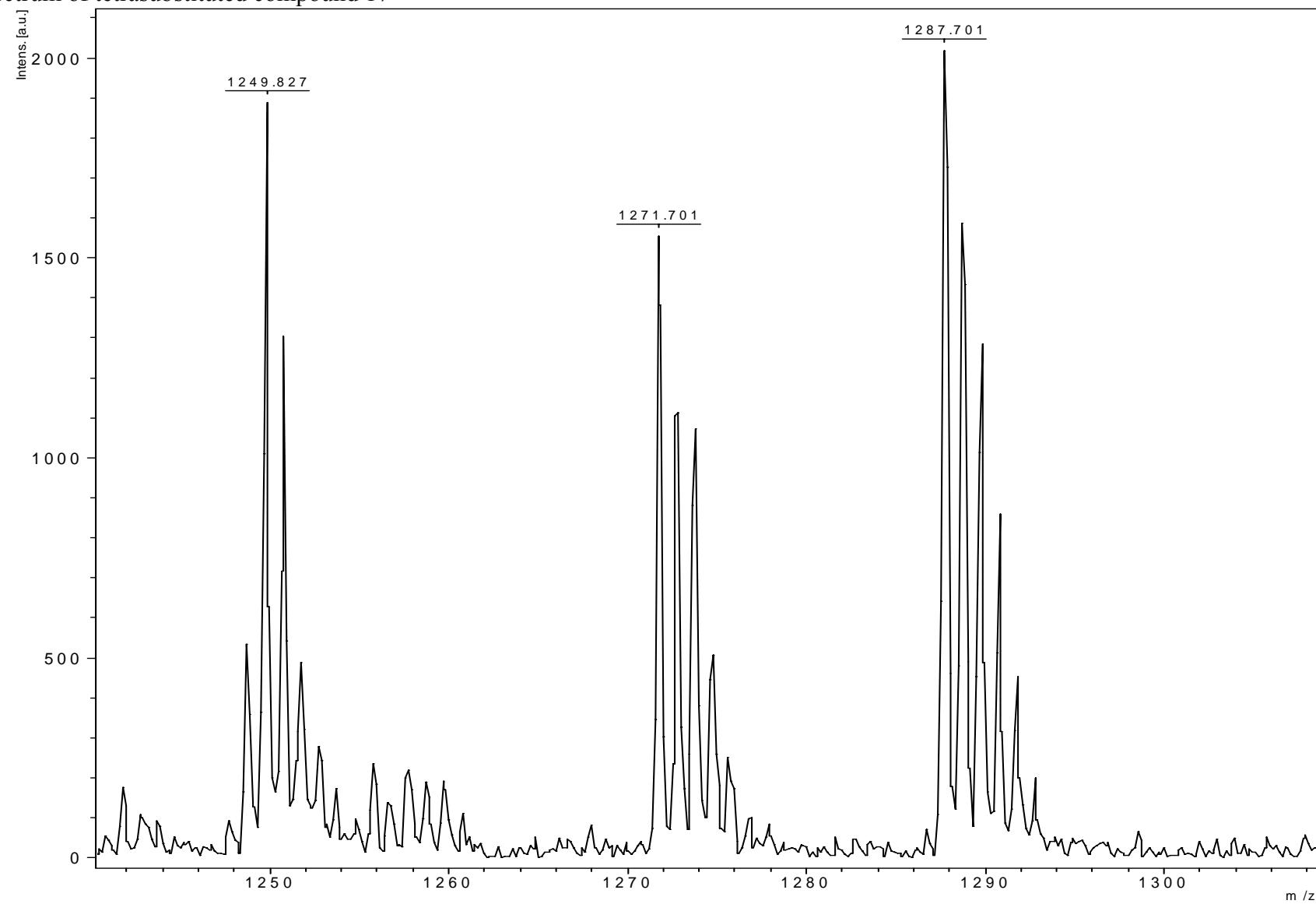
Mass spectrum of tetrasubstituted compound 14



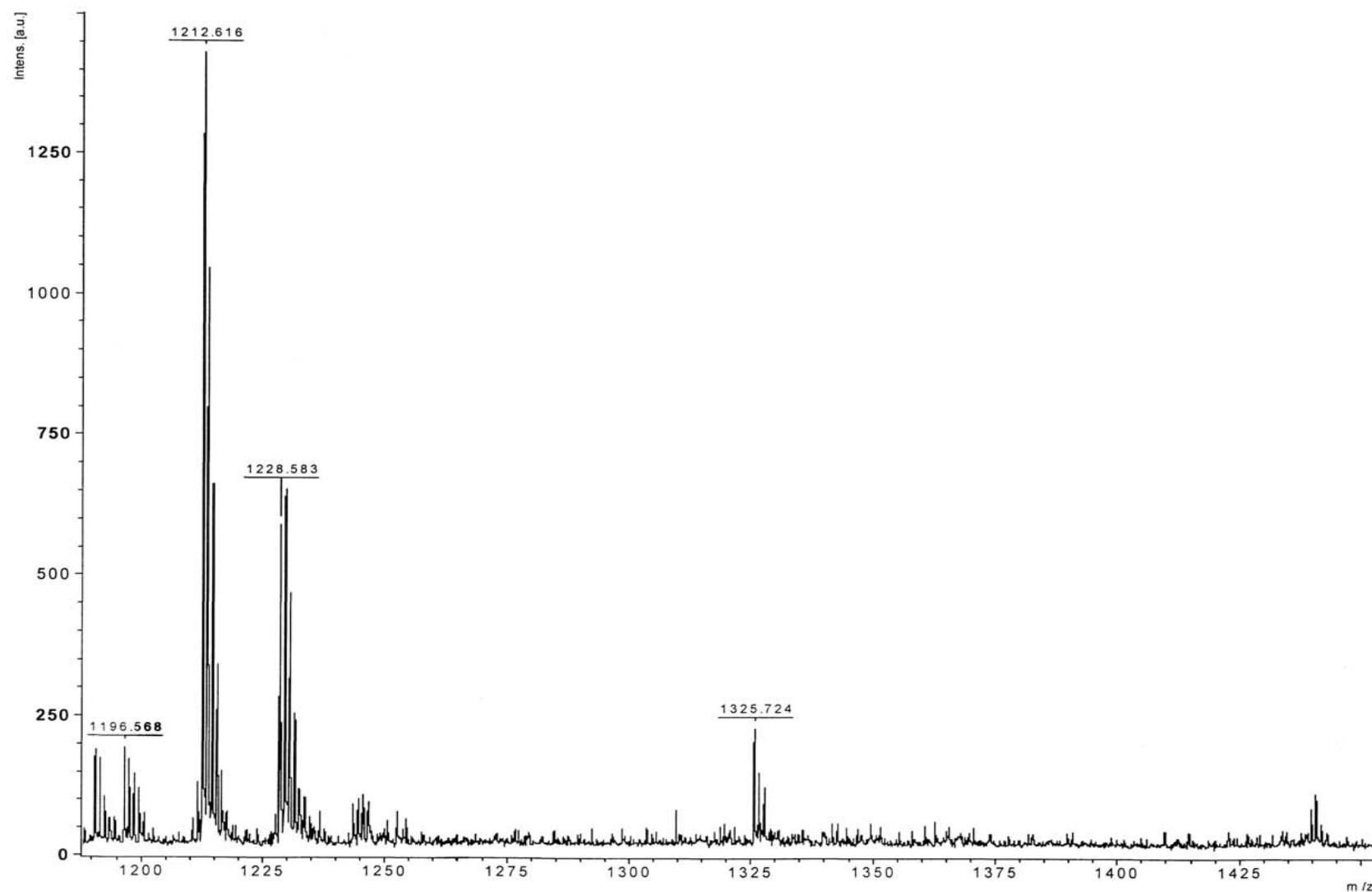
Mass spectrum of tetrasubstituted compound 16



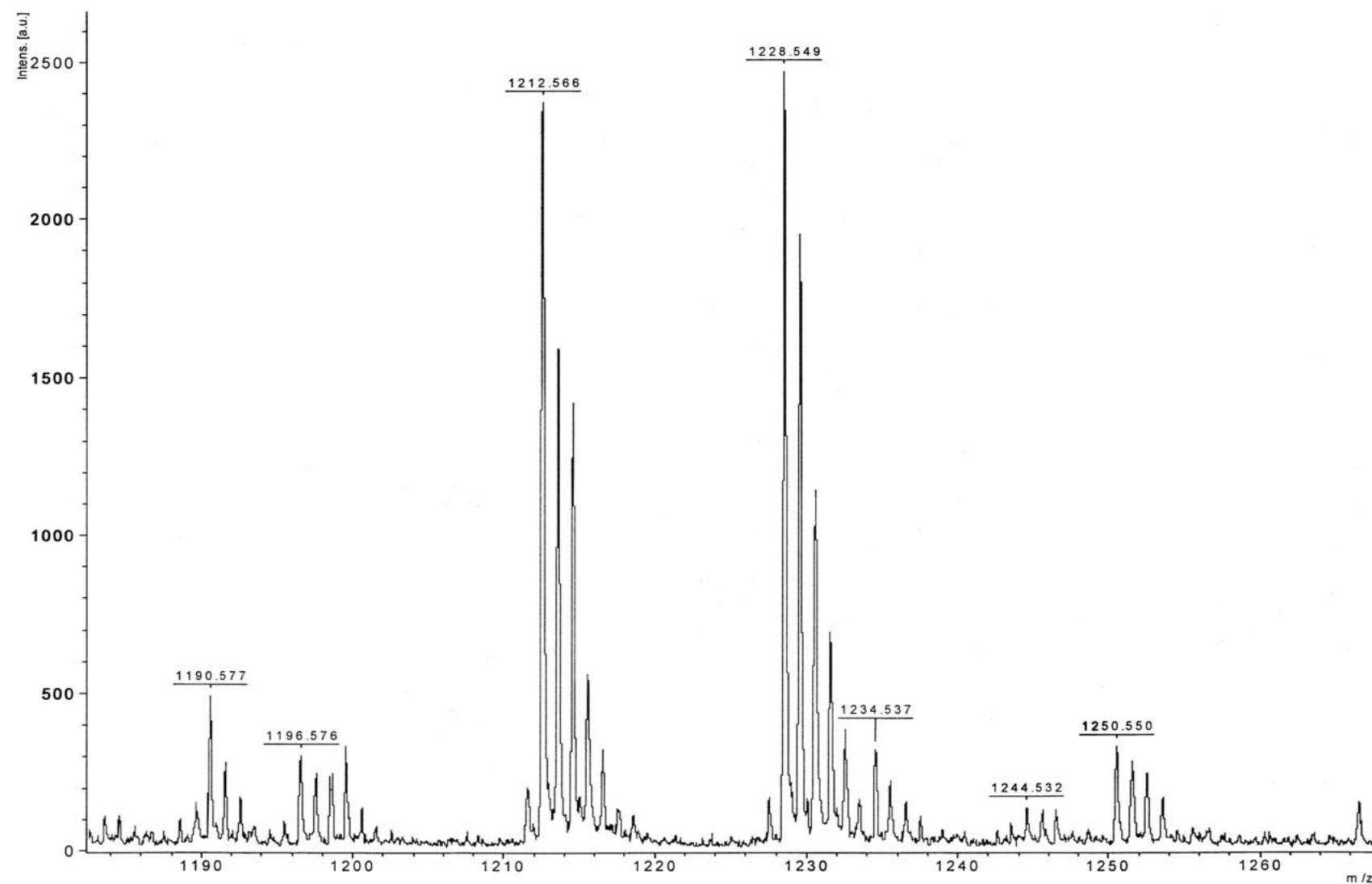
Mass spectrum of tetrasubstituted compound 17



Mass spectrum of trisubstituted compound 18



Mass spectrum of trisubstituted compound 19



Mass spectrum of tetrasubstituted compound 20

