Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

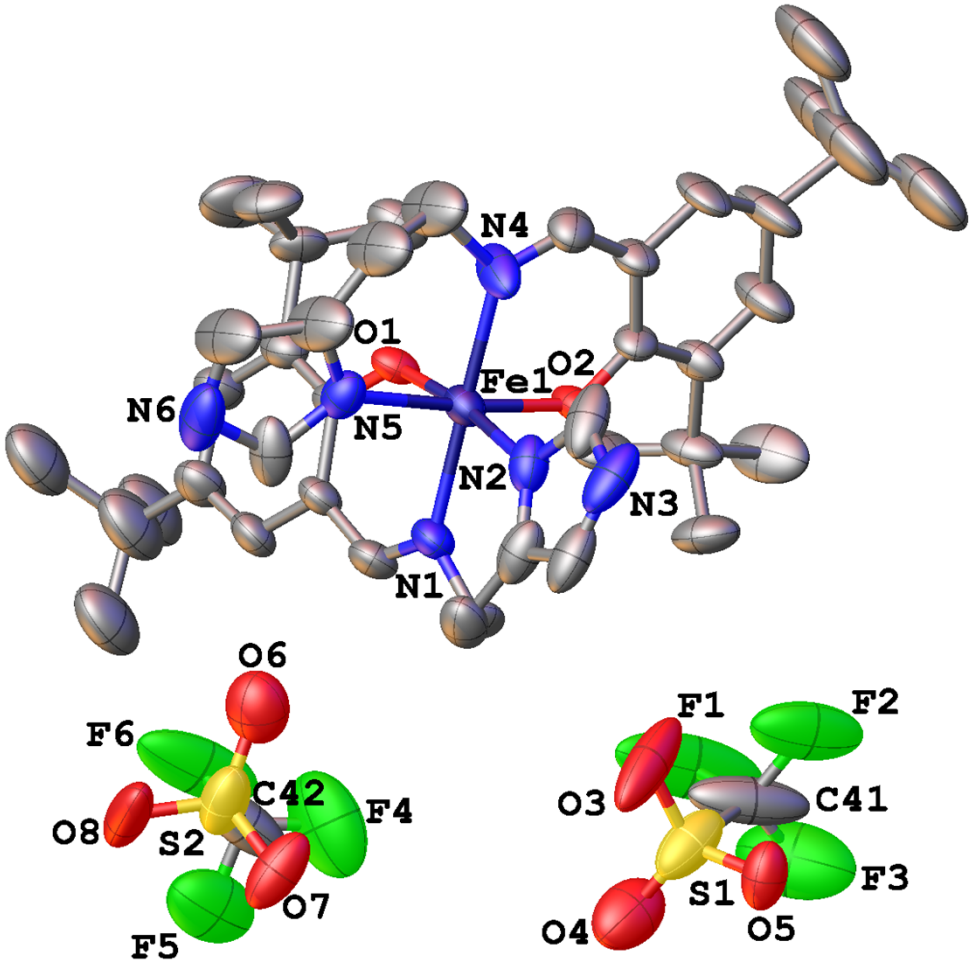


Figure S1: Molecular structure of **2**. Hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (°) are as follows: Fe1-O1, 1.907(8); Fe1-N1, 2.101(9); Fe1-N2, 2.157(11); Fe1-N4, 2.158(11); Fe1-N5, 2.171(10); Fe1-O2, 1.884(8); O3-S1, 1.433(13); C41-S1, 1.84(3); C42-S1, 1.80(3); O1-Fe1-N1, 88.6(4); O2-Fe1-N4, 86.5(3); N1-Fe1-N4, 177.9(5); N4-Fe1-O1, 94.5(4); N5-Fe1-N1, 92.4(4); N1-Fe1-N2, 86.9(4); N2-Fe1-O2, 90.3(4).

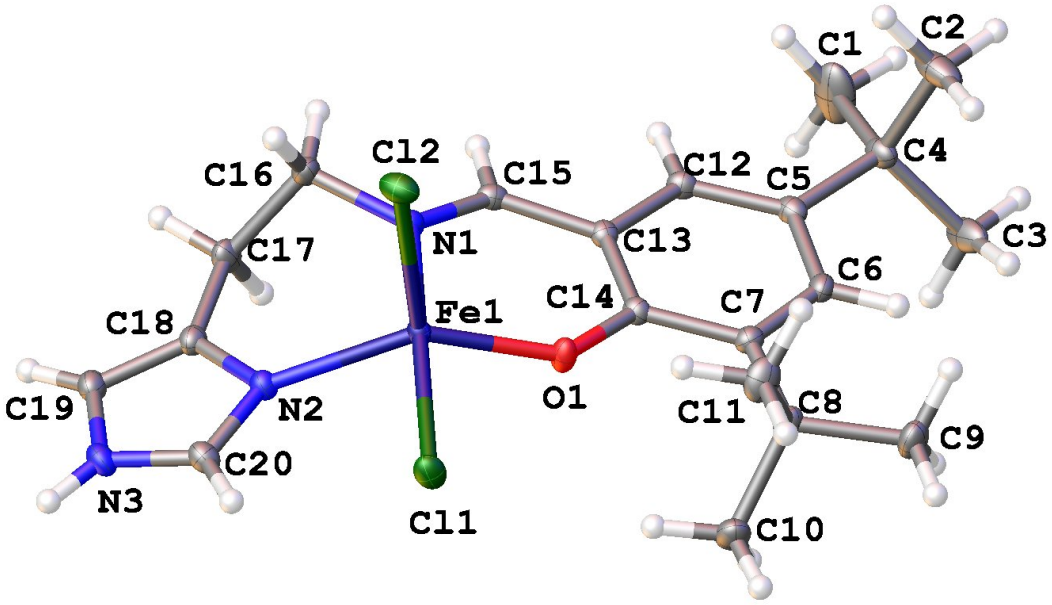


Figure S2: Molecular structure of **3**. Ellipsoids are drawn at 50 % probability level. Selected bond lengths (Å) and angles (°) are: Fe1-O1, 1.855(10); Fe1-N1, 2.123(2); Fe1-N2, 2.093(12); Fe1-Cl1, 2.312(4); Fe1-Cl2, 2.273(4); O1-Fe1-N1, 85.46(4); O1-Fe1-N2, 137.30(5); N1-Fe1-N2, 85.60(4); O1-Fe1-Cl2, 112.97(4); N1-Fe1-Cl2, 90.33(3); N2-Fe1-Cl2, 108.76(3); O1-Fe1-Cl1, 91.32(3); N1-Fe1-Cl1, 170.88(6); N2-Fe1-Cl1, 91.04(3); Cl2-Fe1-Cl1, 98.773(15).

Table S1: Crystal data collection and structural refinement parameters for **3**

Parameters	**3**
Empirical formula	$C_{20}H_{28}Cl_2FeN_3O$
Formula weight	453.2
Temperature/K	100(2)
Wavelength/Å	0.71073
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
a/ Å	7.7867(6)
b/Å	14.1036(12)
c/Å	19.9011(17)
α/°	90
b/°	90
g/°	90
Volume/Å^3	2185.5(3)
Z	4
Density (calculated)/Mg/m^3	1.377
Absorption coefficient/mm^{-1}	0.949
F(000)	948
Goodness-of-fit on F^2	1.066
Final R indices [I>2sigma(I)]	R1 = 0.0194, wR2 = 0.0495
R indices (all data)	R1 = 0.0219, wR2 = 0.0514

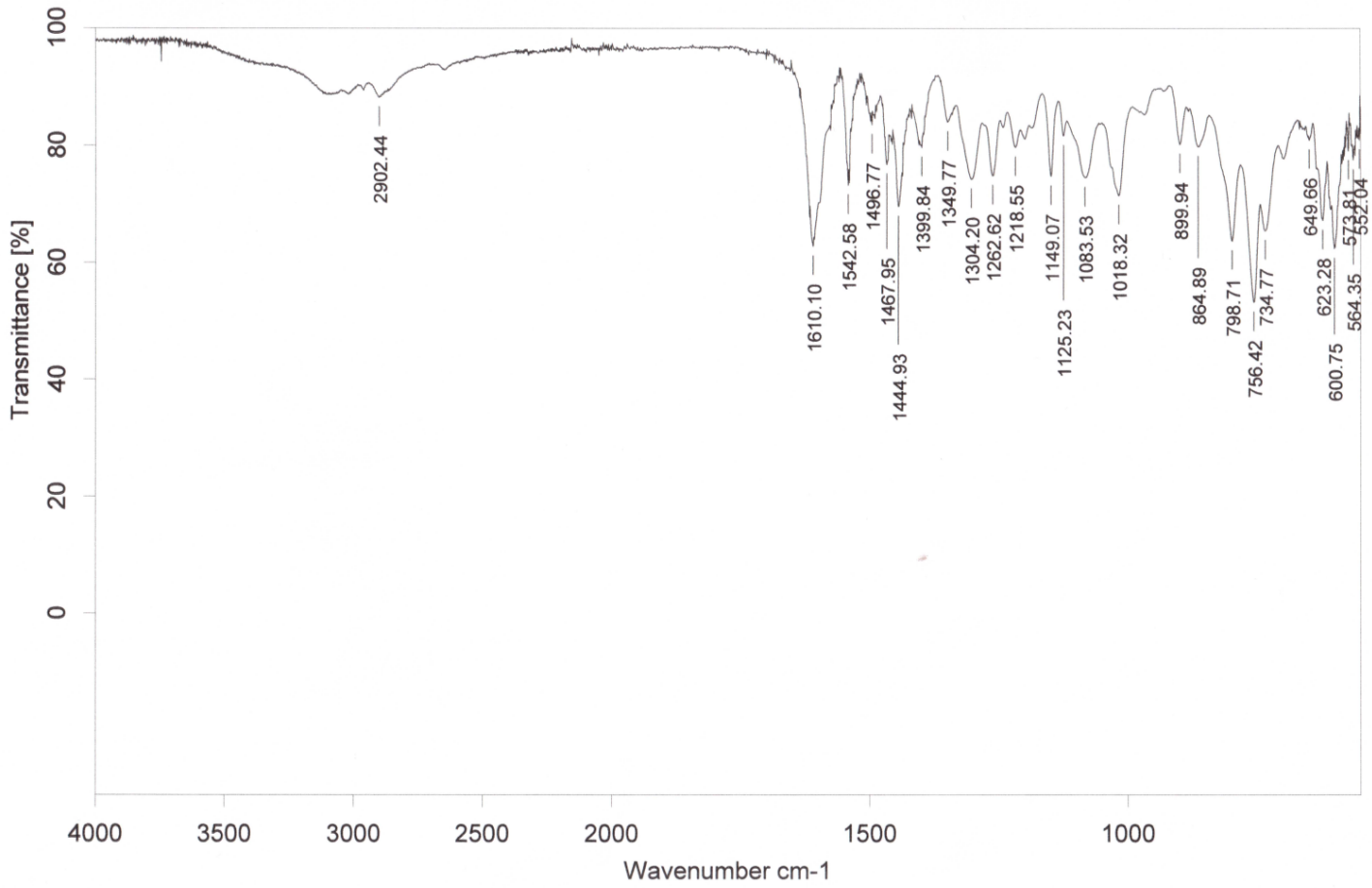


Figure S3: IR spectrum of complex **1**

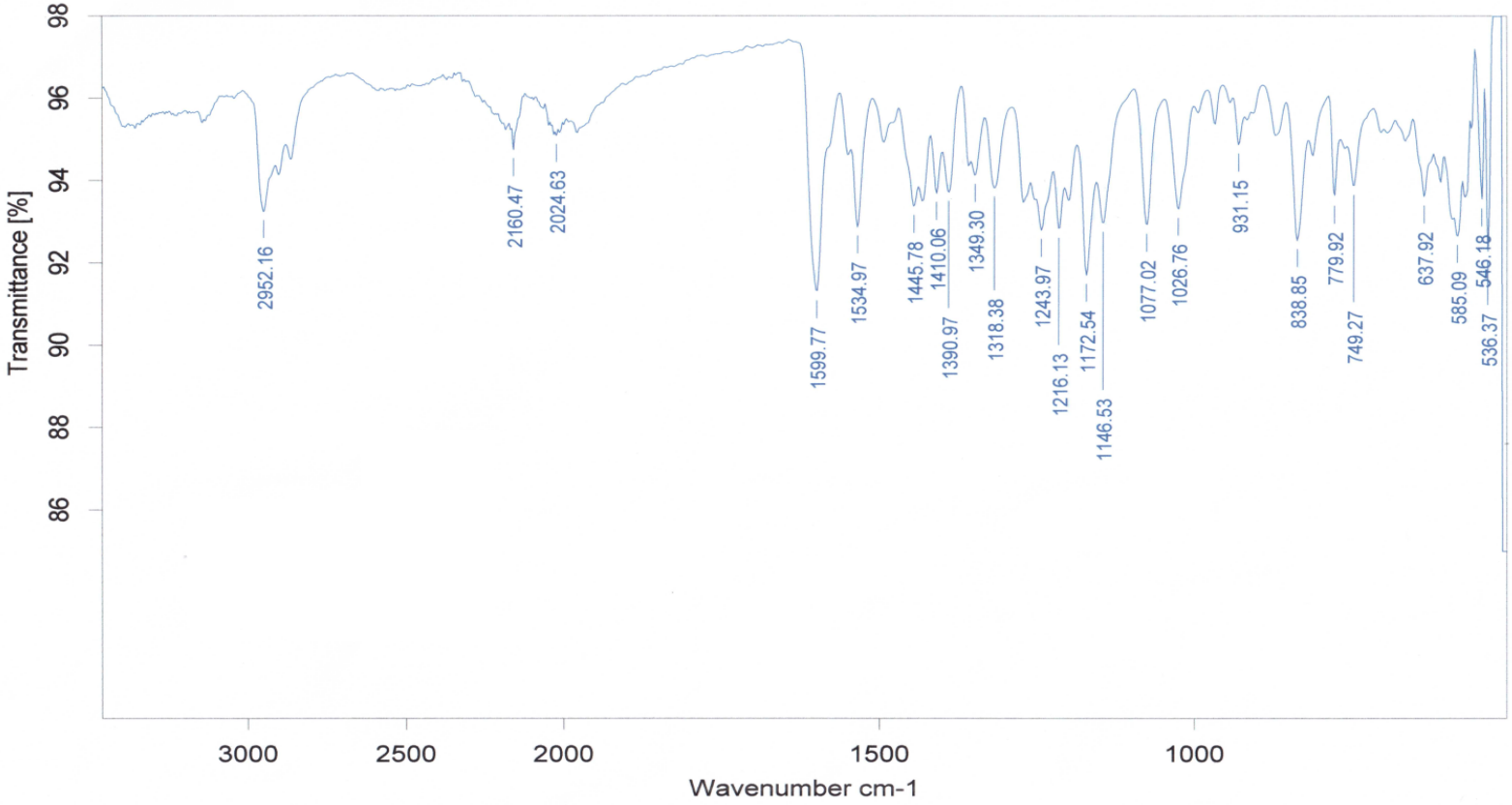


Figure S4: IR spectrum of complex **2**

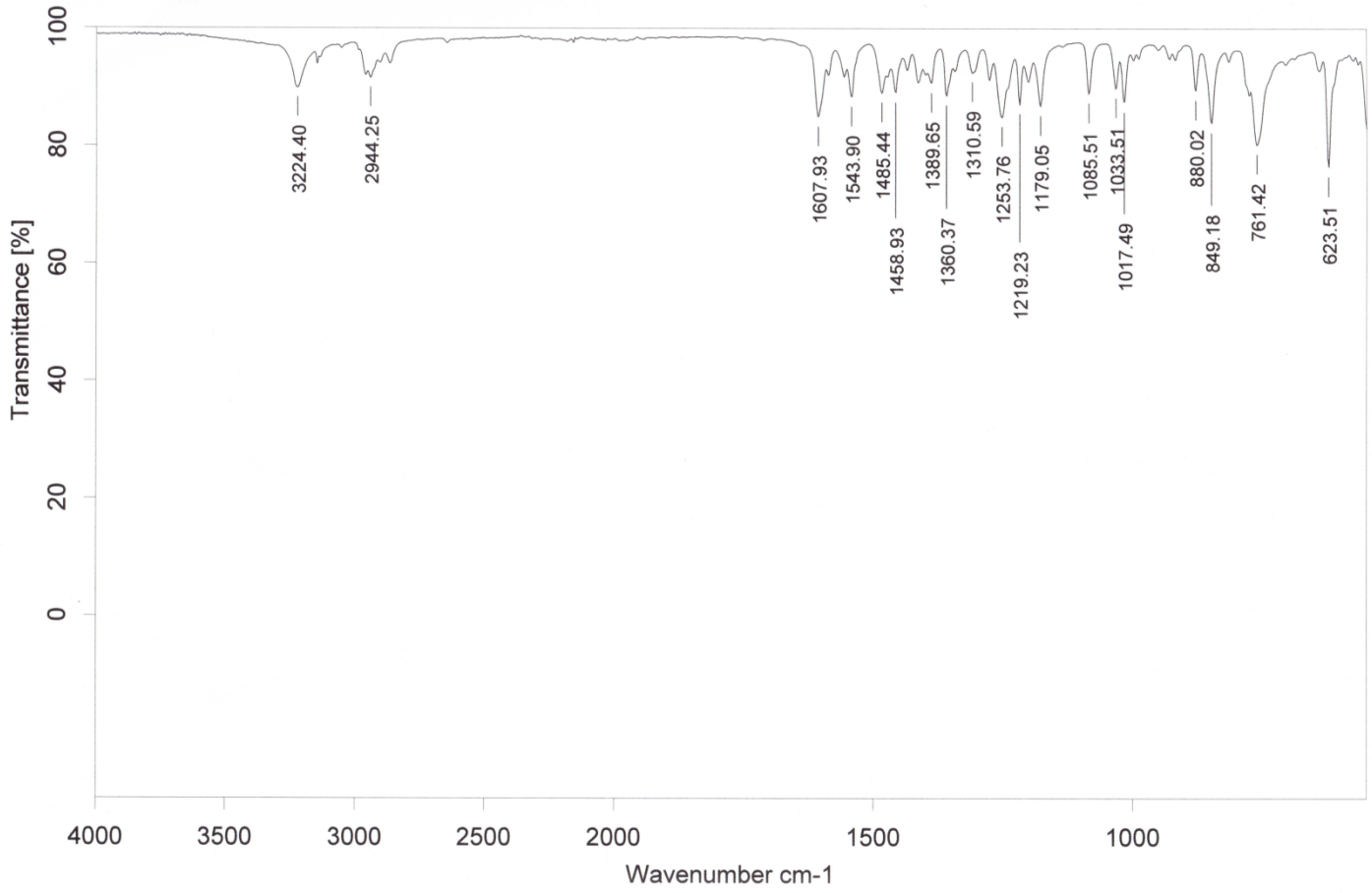


Figure S5: IR spectrum of complex **3**

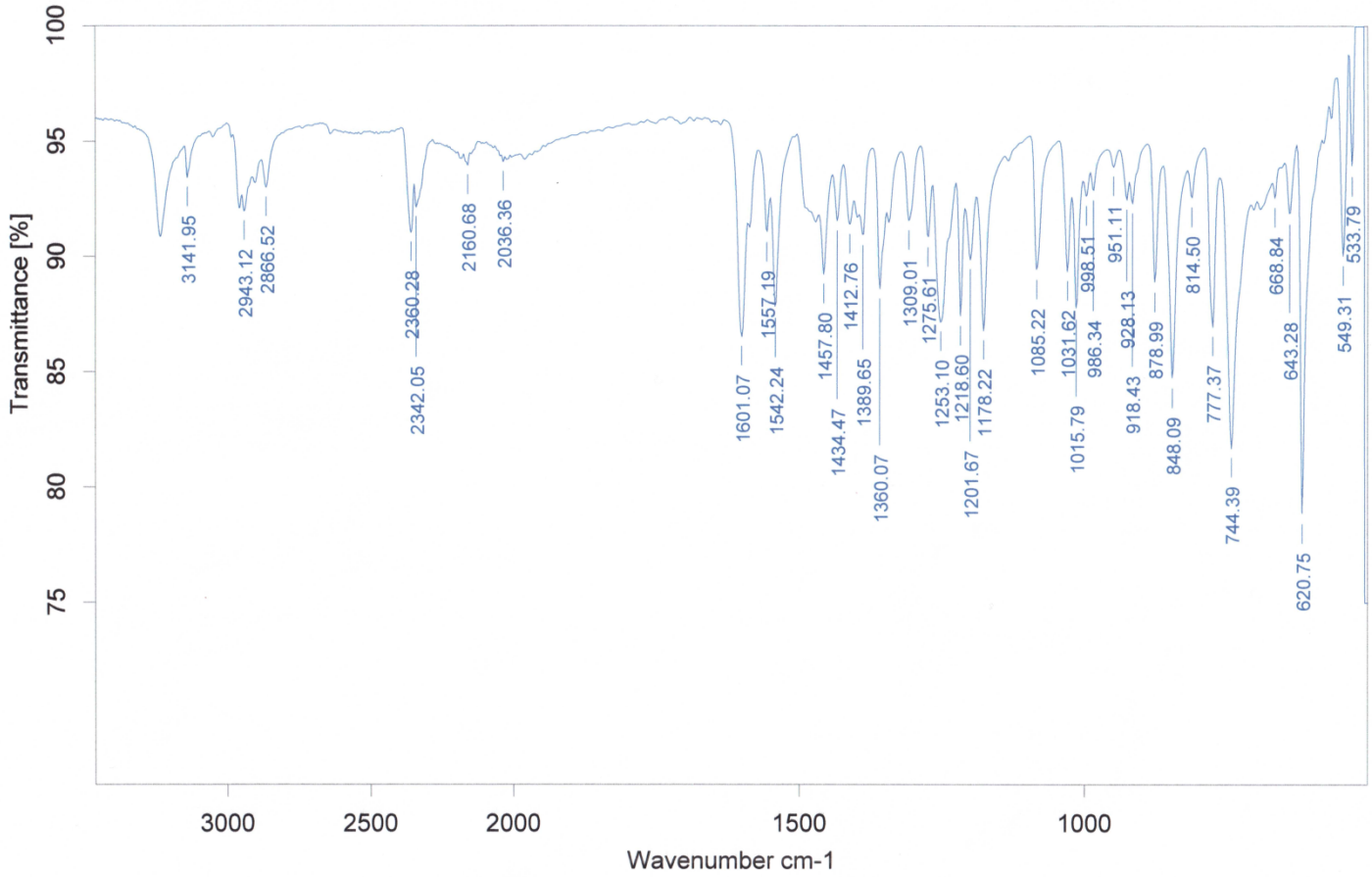


Figure S6: IR spectrum of complex **4**

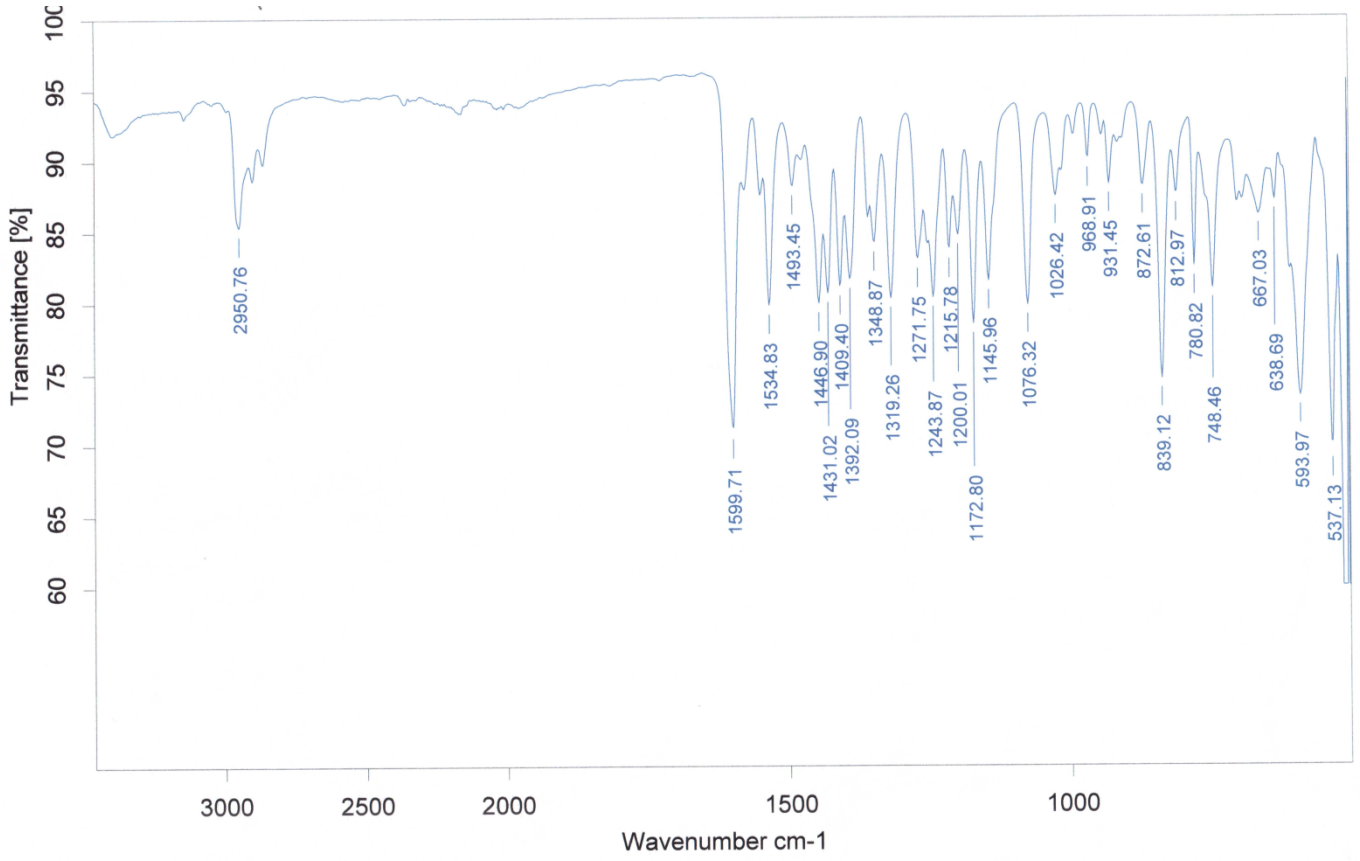


Figure S7: IR spectrum of complex **5**

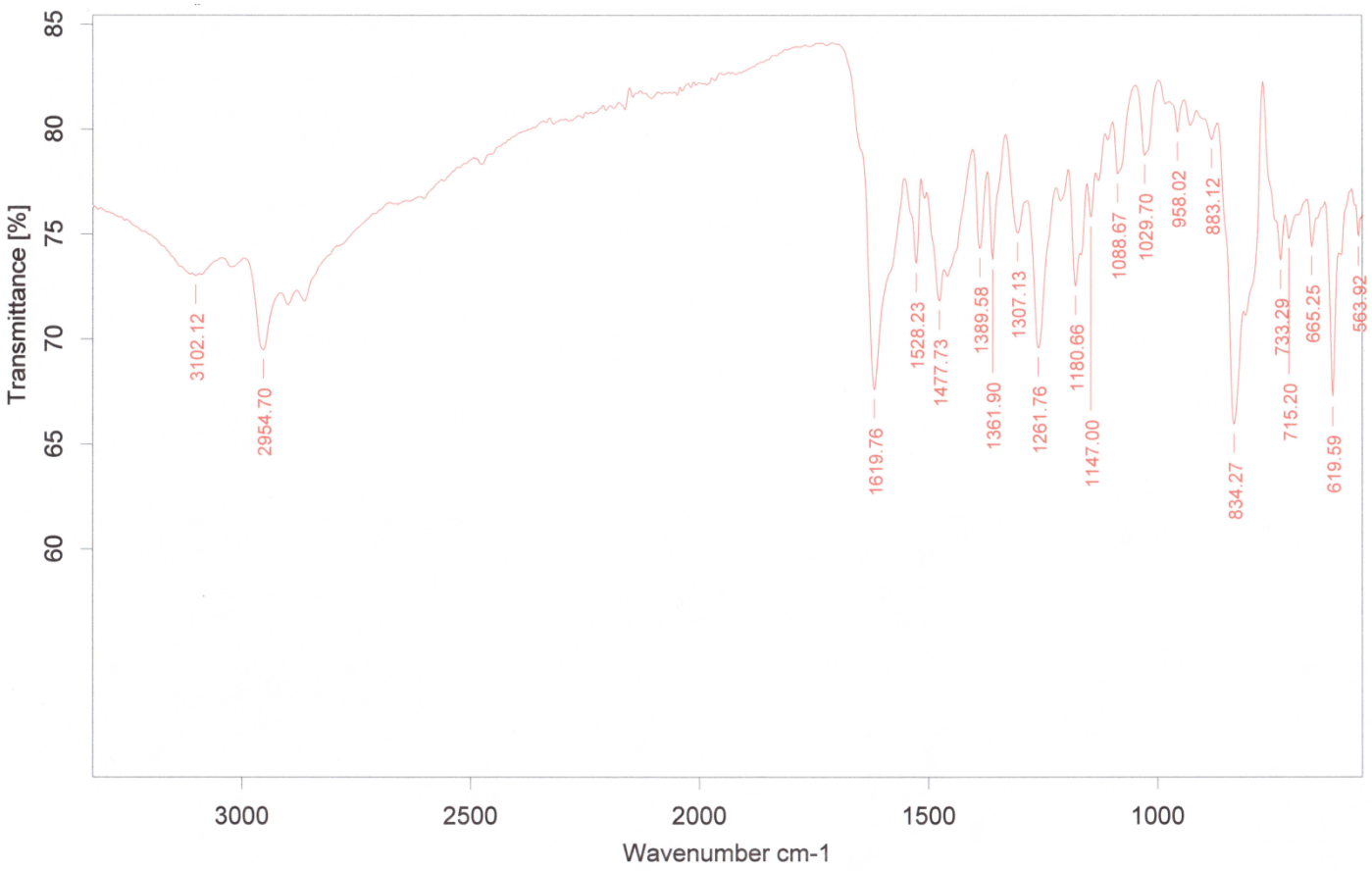


Figure S8: IR spectrum of complex **6**

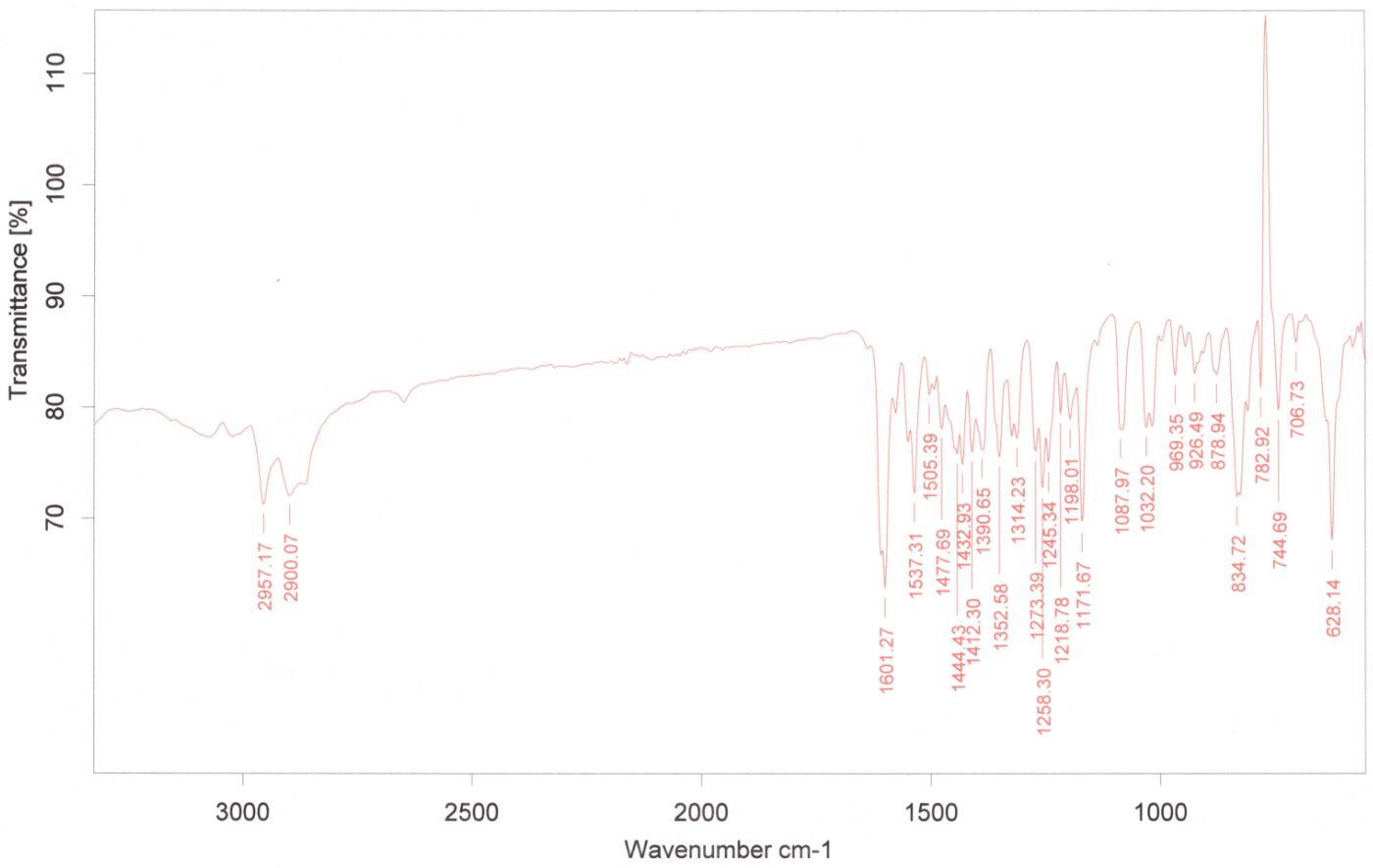


Figure S9: IR spectrum of complex **7**

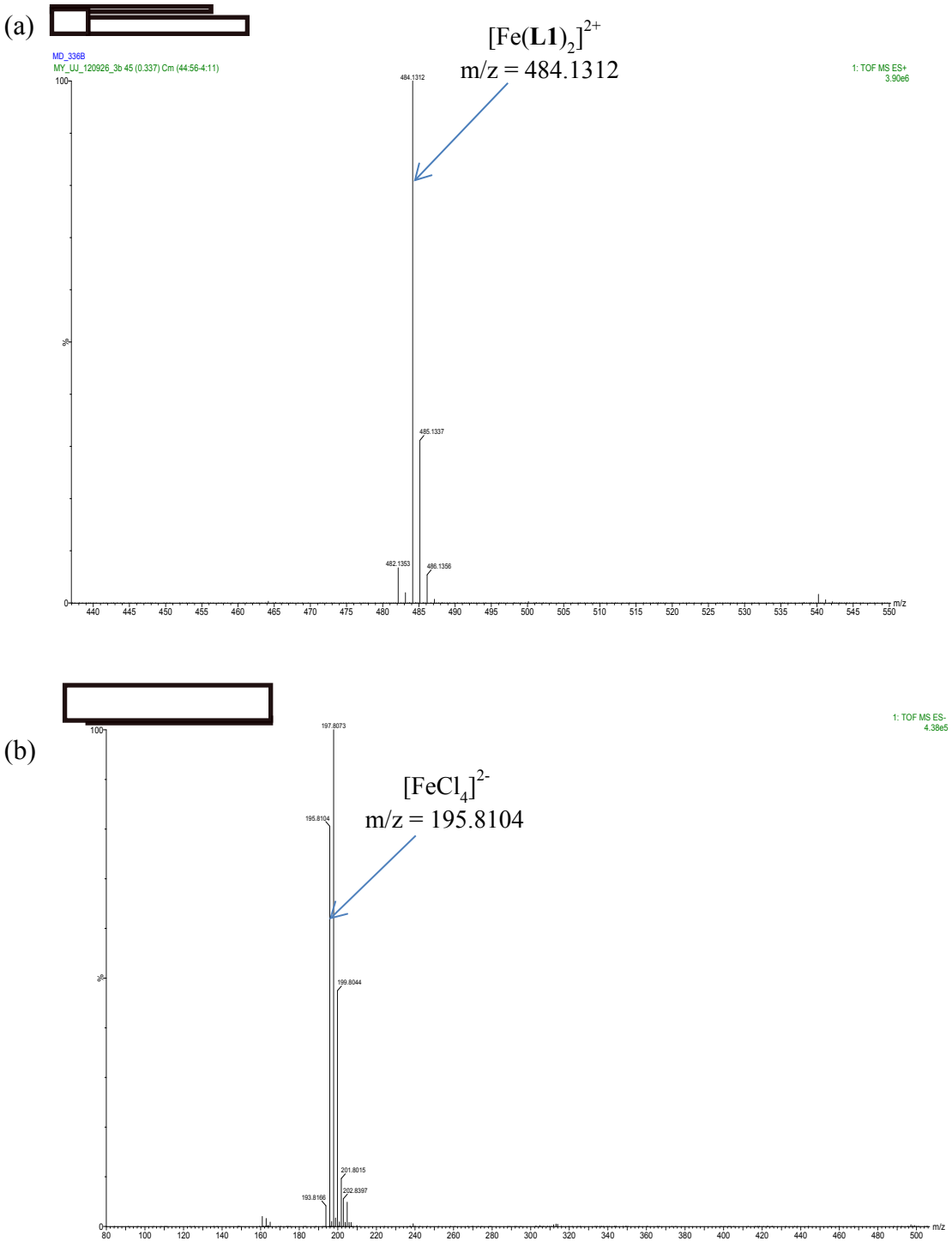
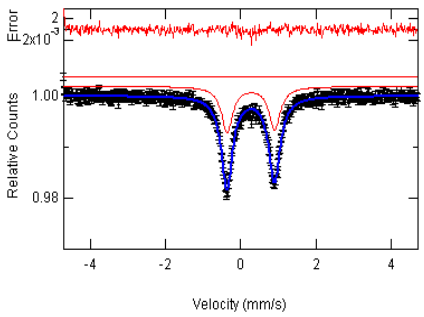
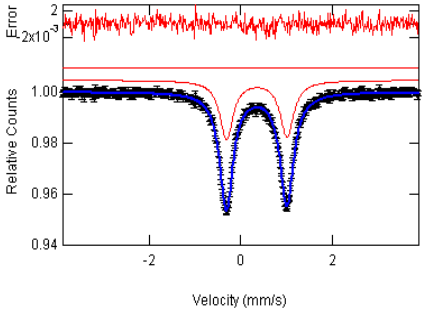


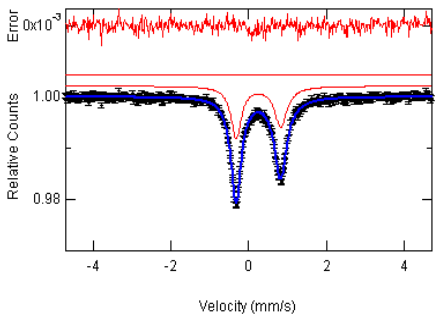
Figure S10: Positive ion (a) and negative ion (b) ESI mass spectra of complex **1** showing m/z of the bis-ligand iron(II) complex and of the anion respectively.

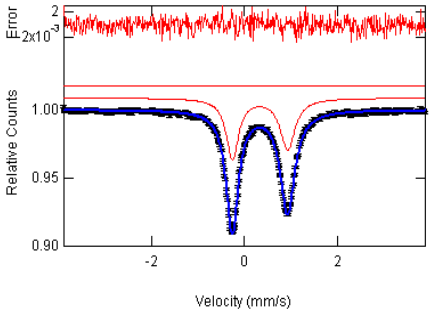




300 K 157 K

(b) Mössbauer spectra of complex **4**





300 K 157 K

(a) Mössbauer spectra of complex **3**

Figure S11: Temperature dependence of the Mössbauer spectra of (a) complex **3** and (b) complex **4**.

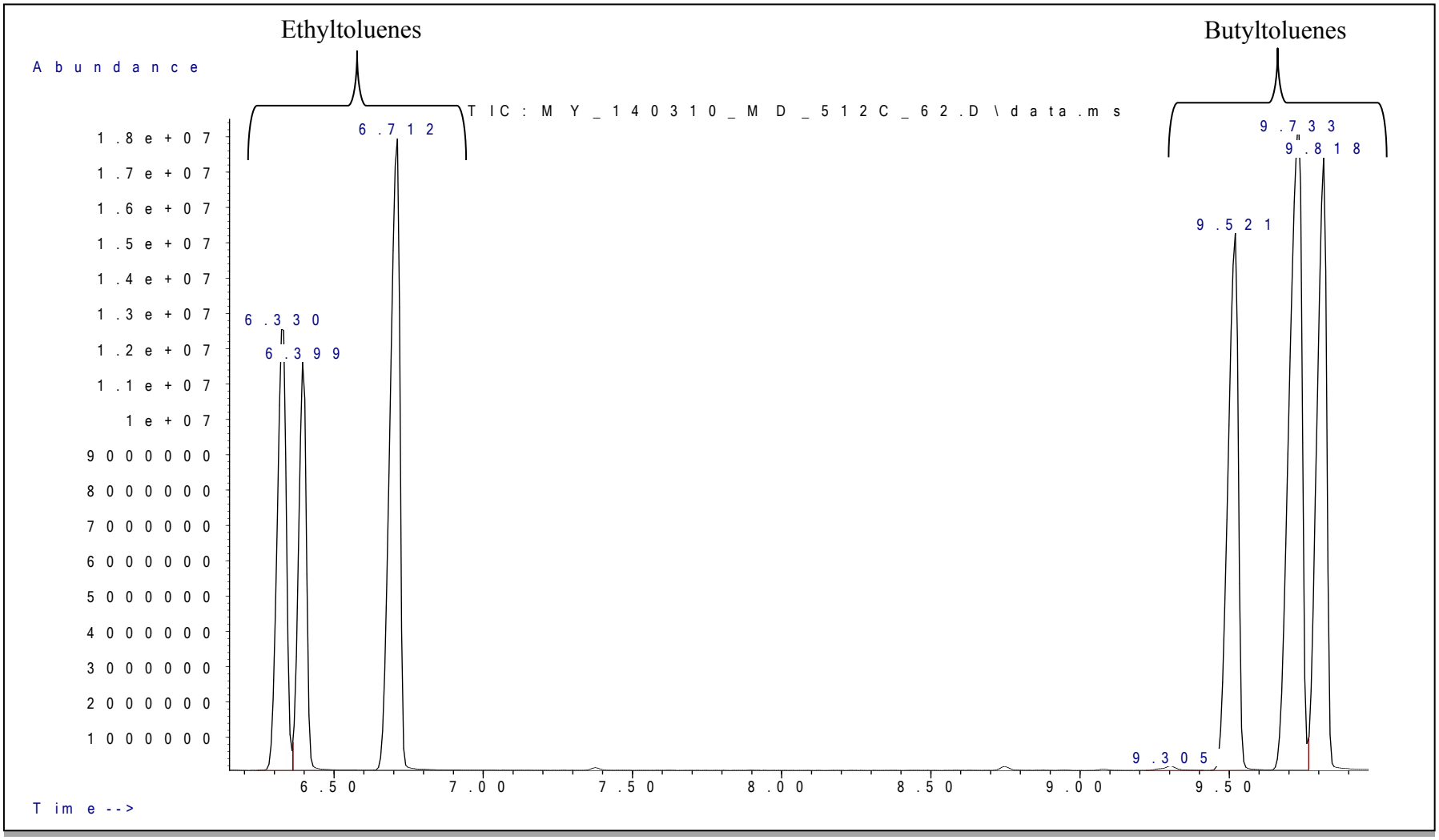


Figure S12: GC chromatogram of the mixture of alkyl-substituted toluenes obtained with **3**/$EtAlCl_2$. Signal for the solvent has been omitted for clarity.

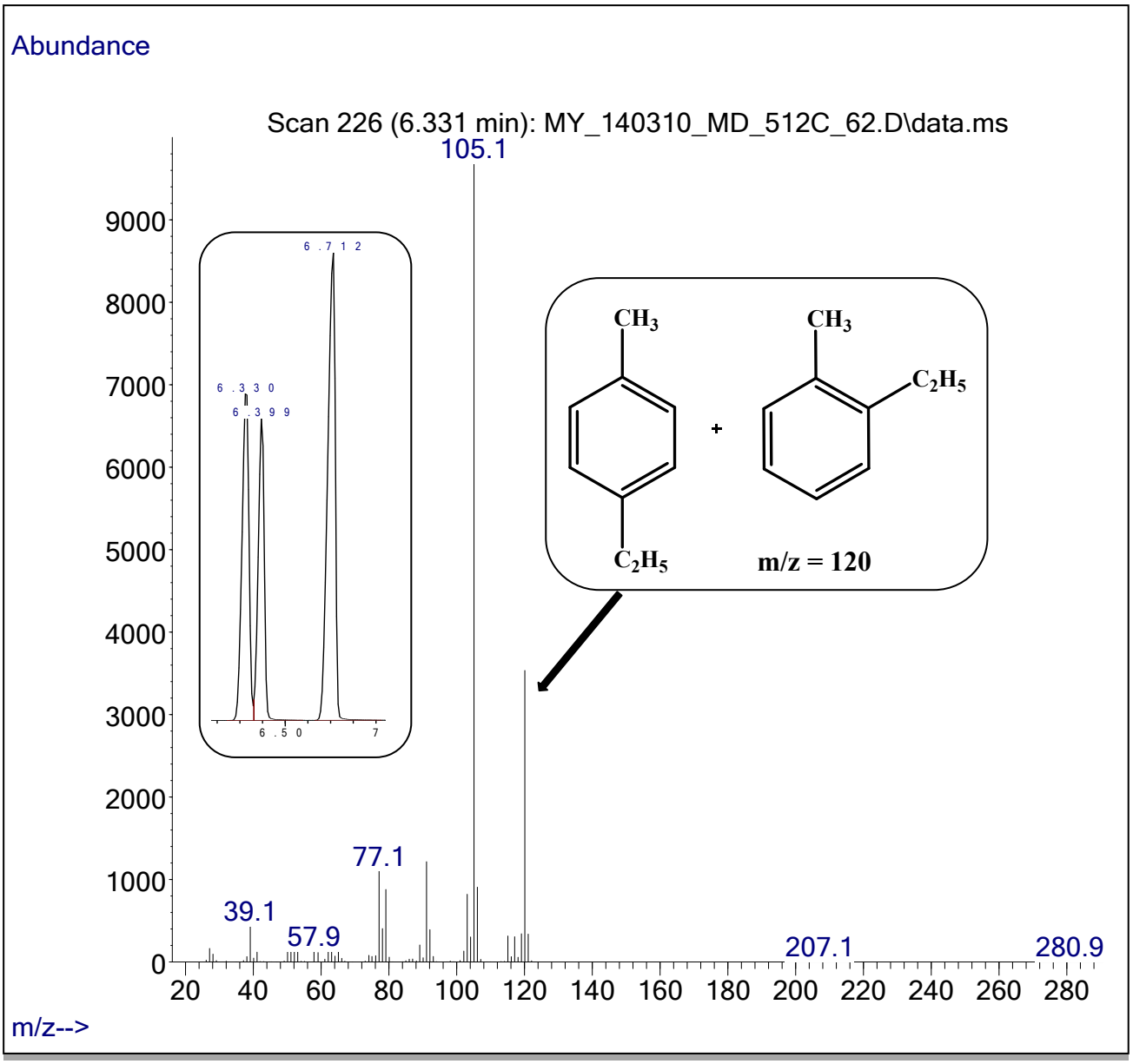


Figure S13: GC-MS spectrum of ethyltoluenes obtained with **3**/$EtAlCl_2$.

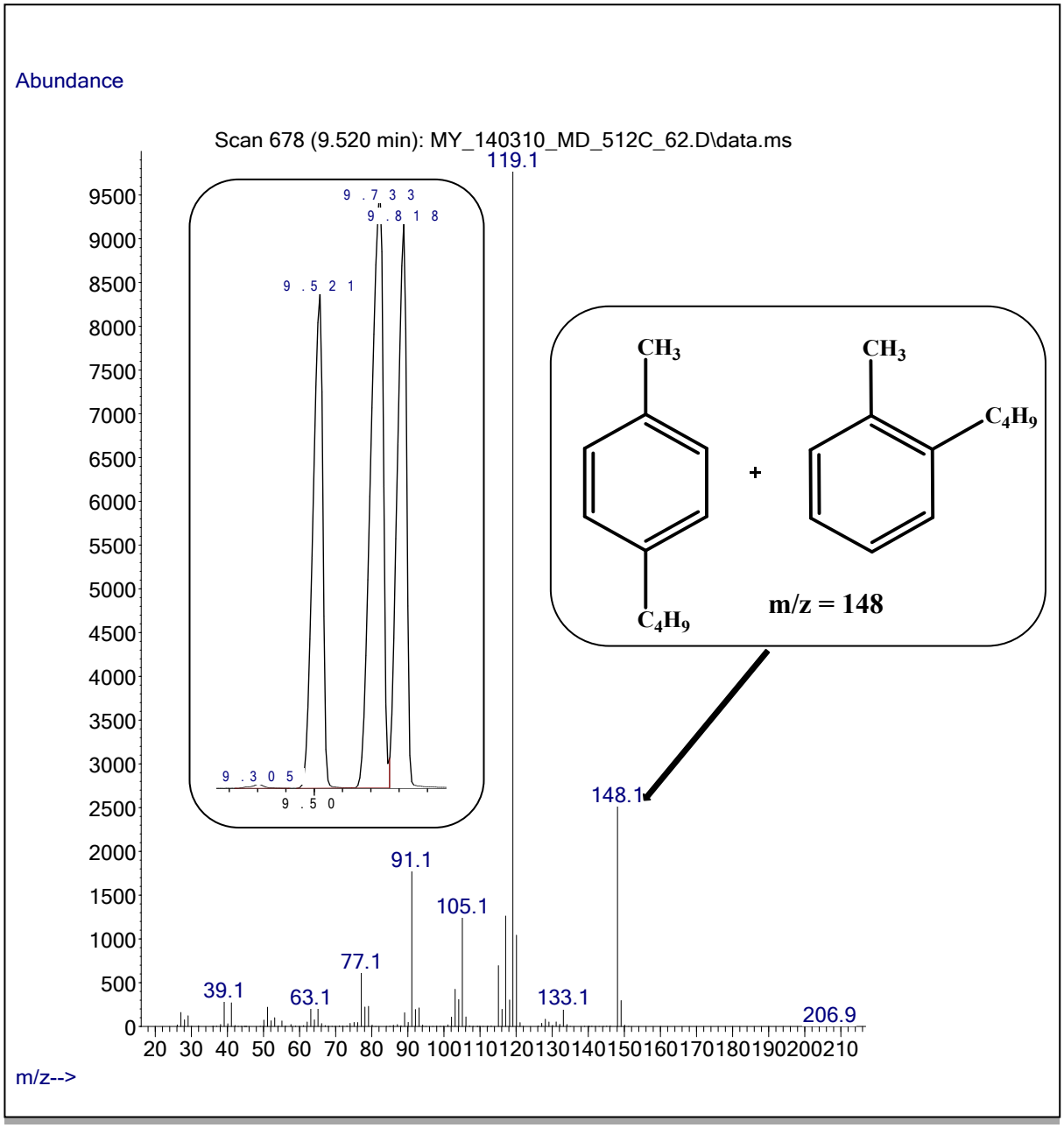


Figure S14: GC-MS spectrum of butyltoluenes obtained with **3**/$EtAlCl_2$.

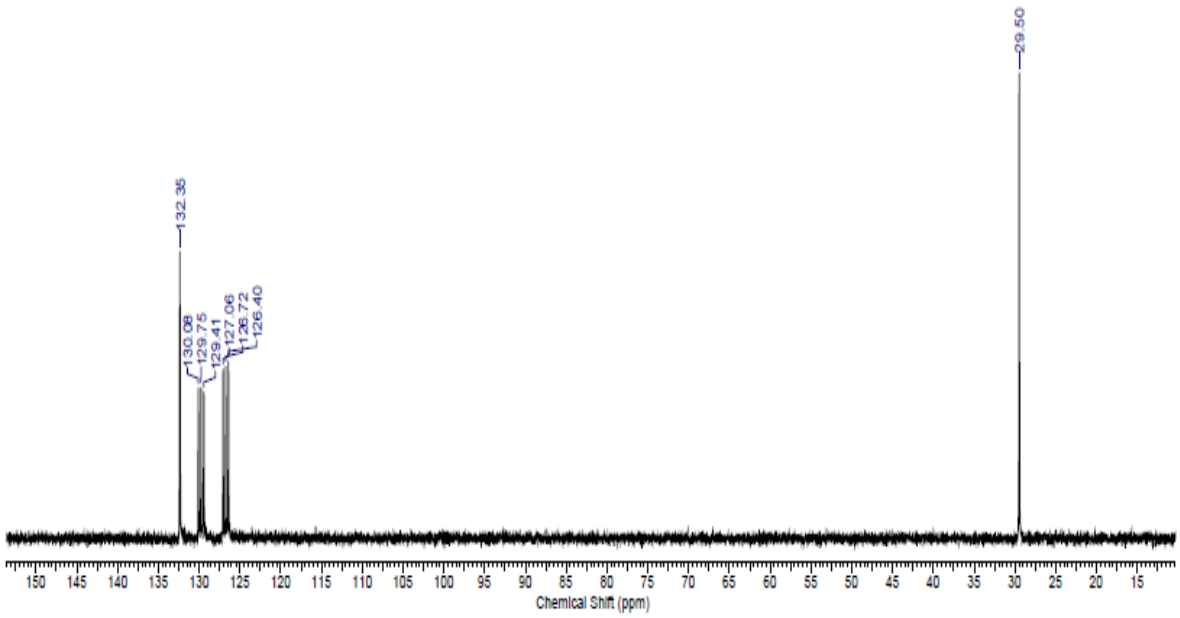


Figure S15: $^{13}C\{^{1}H\}$ NMR spectrum of the polyethylene produced by pre-catalyst **3** in toluene.

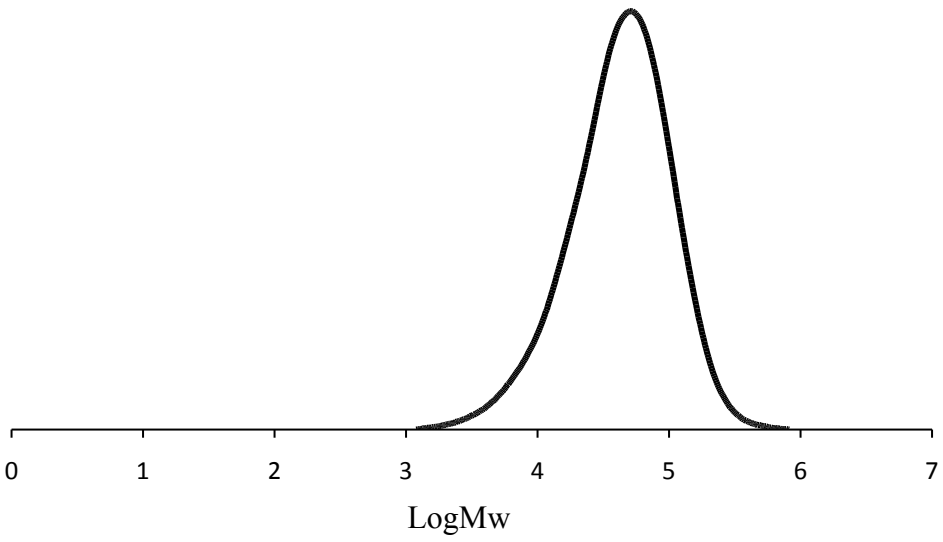


Figure S16: GPC trace of polyethylene produced by iron(III) pre-catalyst **3** in toluene.

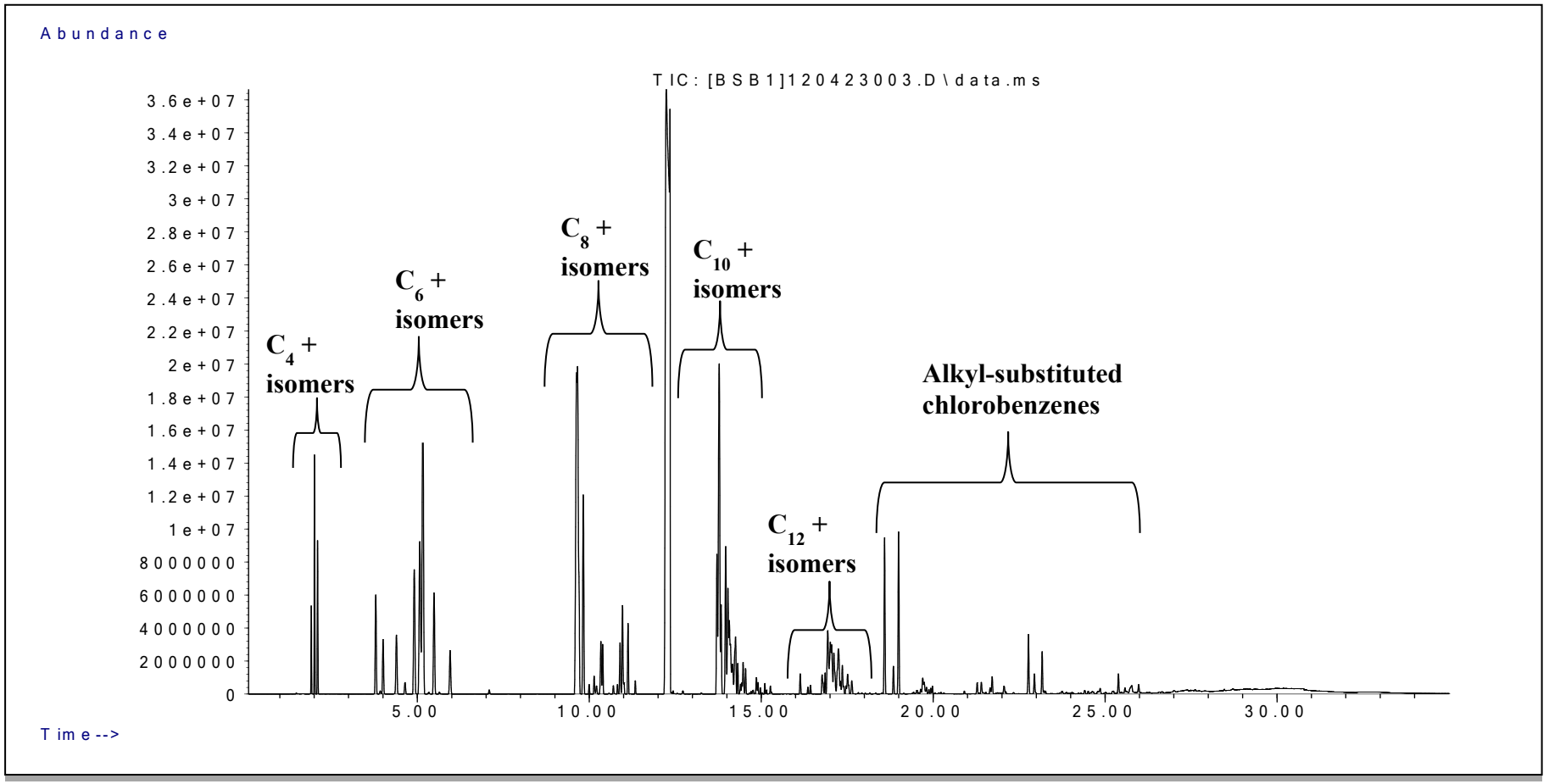


Figure S17: GC chromatogram of oligomers and alkyl-substituted chlorobenzenes obtained using **3**/$EtAlCl_2$. Signal for the solvent has been omitted for clarity.

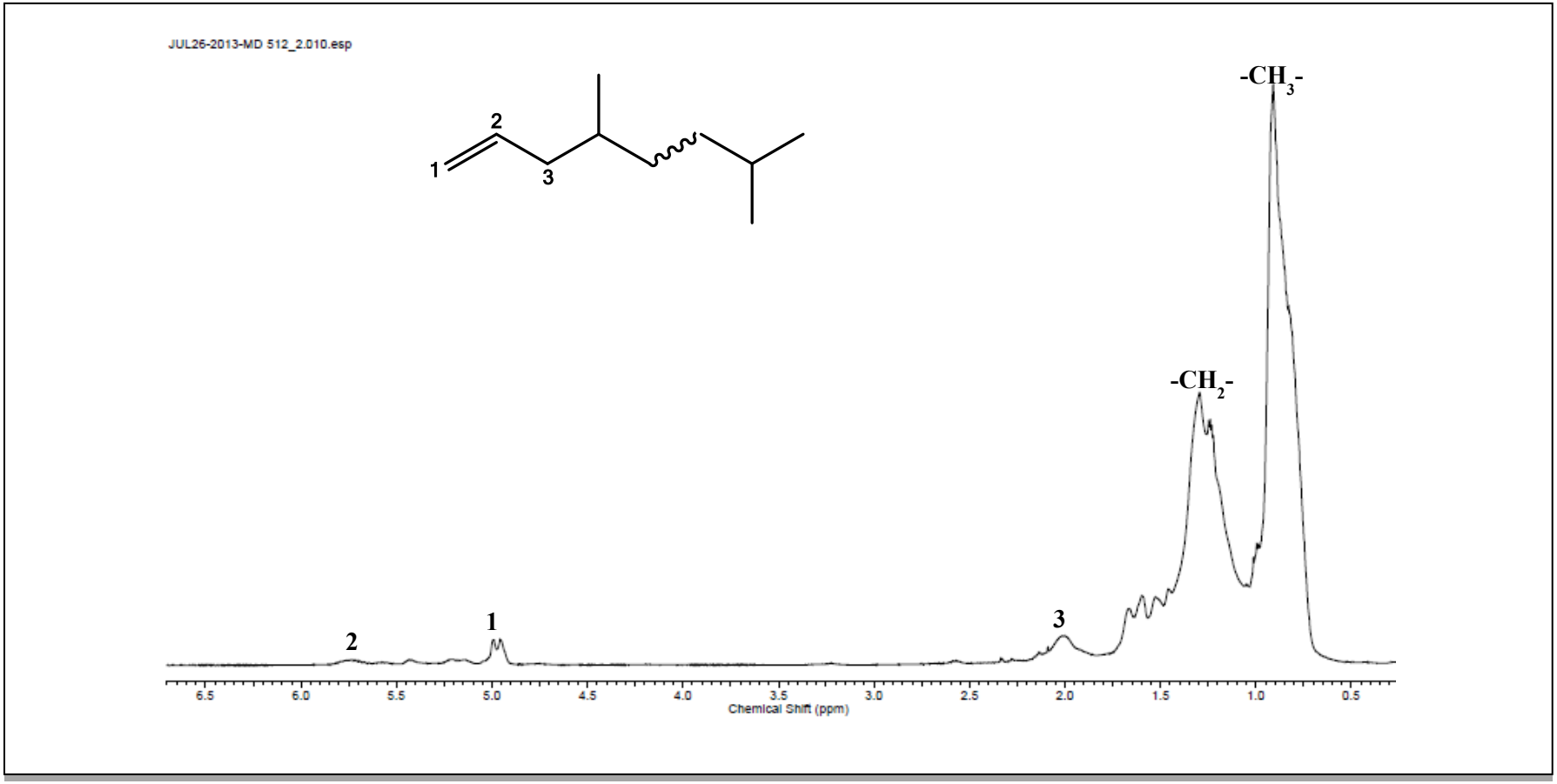


Figure S18: ^{1}H NMR spectrum of the oils obtained using **3**/$EtAlCl_2$.

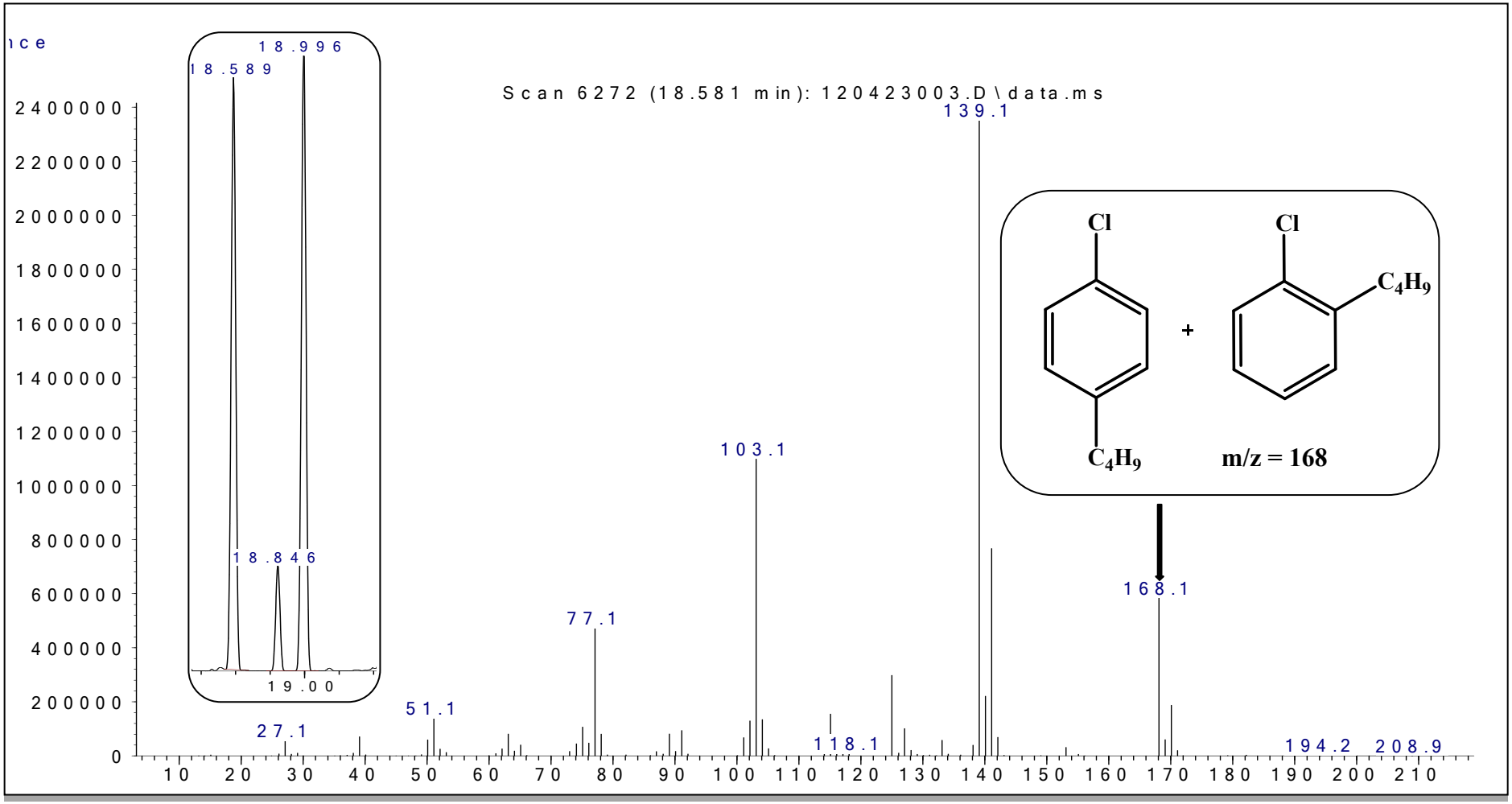


Figure S19: GC-MS spectrum of butylchlorobenzenes obtained with **3**/$EtAlCl_2$.

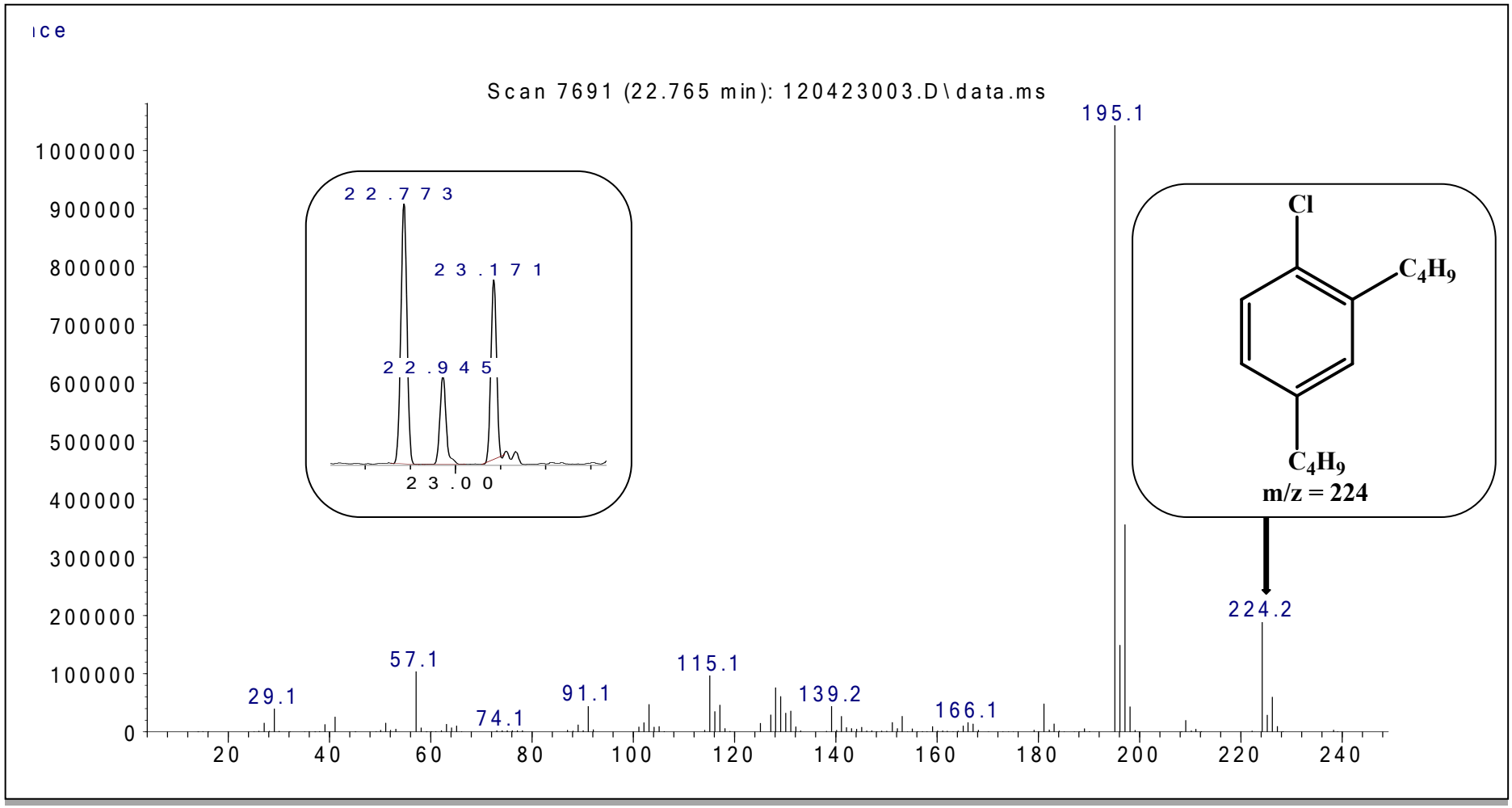


Figure S20: GC-MS spectrum of di-butylchlorobenzene obtained with **3**/$EtAlCl_2$.

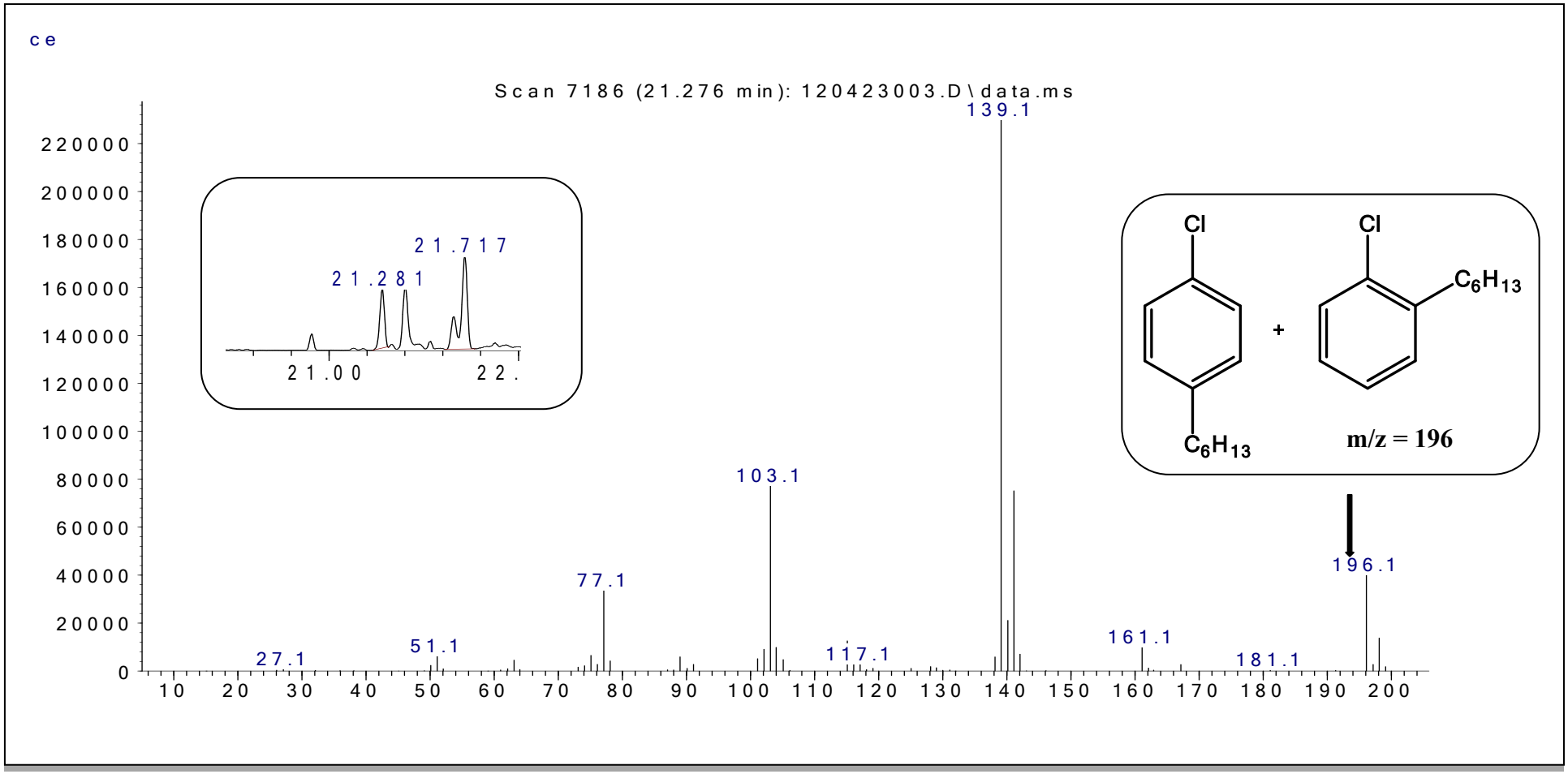


Figure S21: GC-MS spectrum of hexylchlorobenzenes obtained with **3**/$EtAlCl_2$.