Electronic Supplementary Information for

Amphiphilic Palladium NHC-complexes with Chelating Bis-NHC Ligands Based on Imidazole-4,5-dicarboxylic Acid: Synthesis and Catalysis in water.

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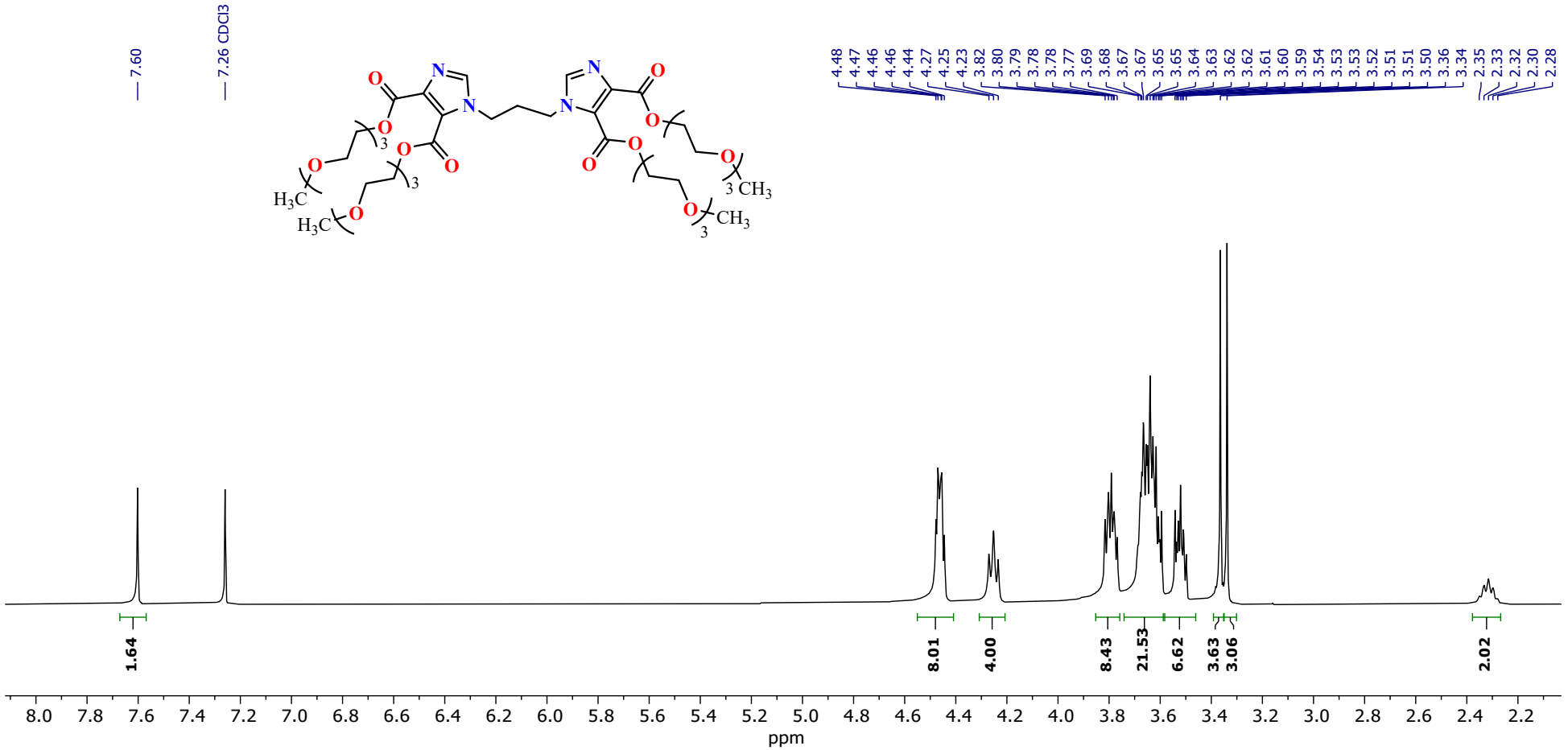


Figure S1. NMR ^{1}H spectrum (400 MHz, $CDCl_3$, 25 ^{o}C) of imidazole **2**

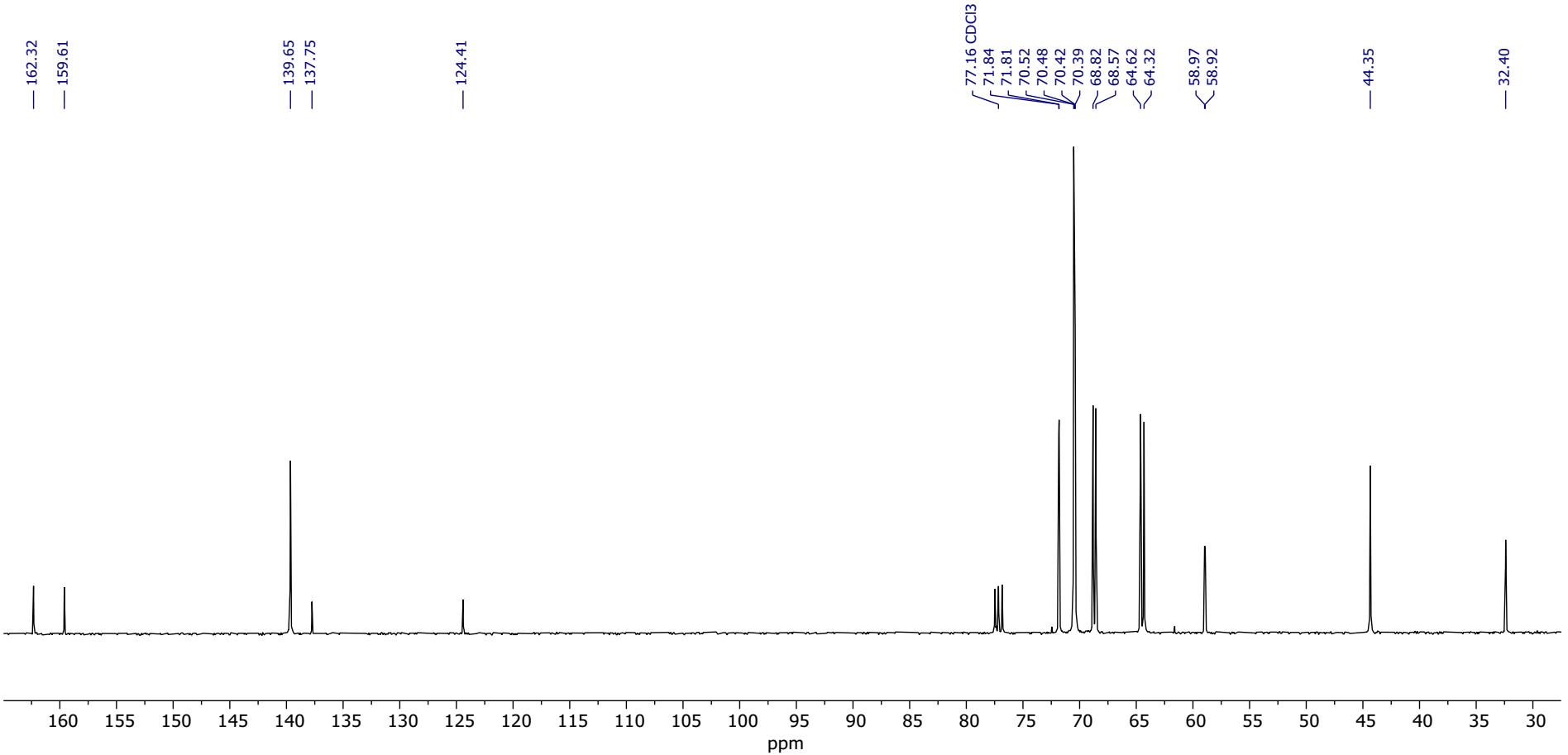


Figure S2. NMR ^{13}C spectrum (100.6 MHz, $CDCl_3$, 25 ^{o}C) of imidazole **2**

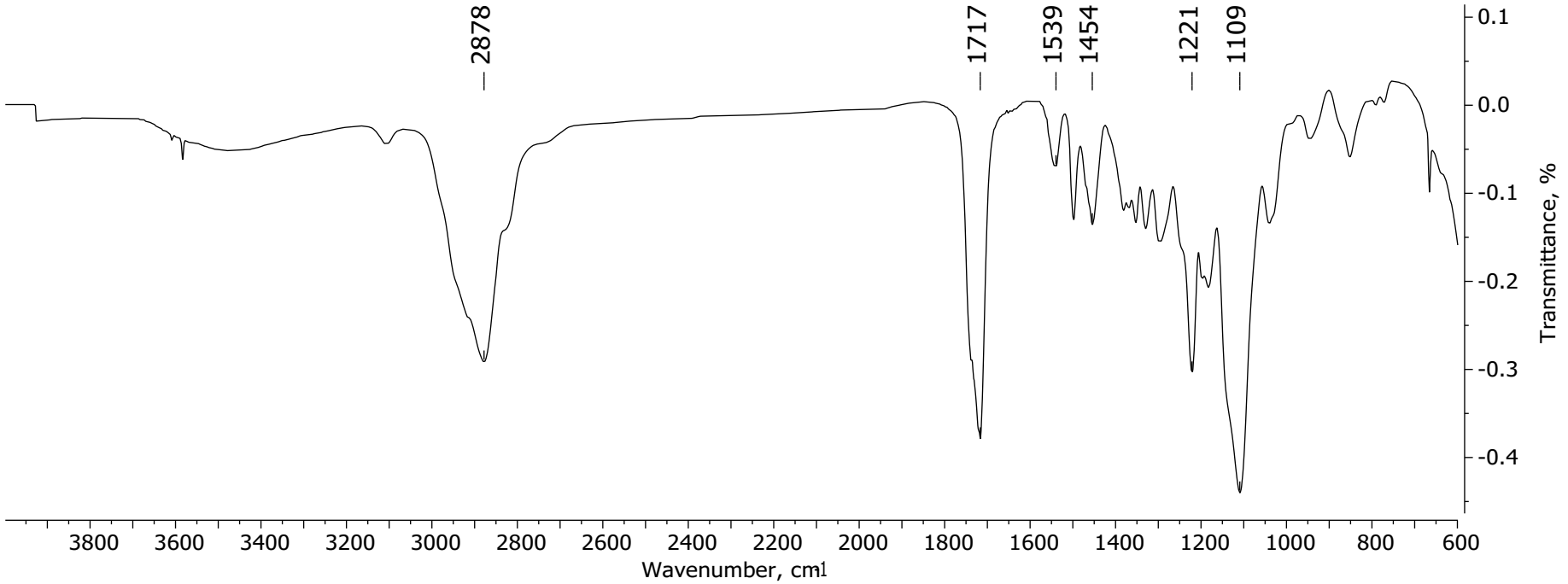


Figure S3. FT-IR spectrum of imidazole **2**

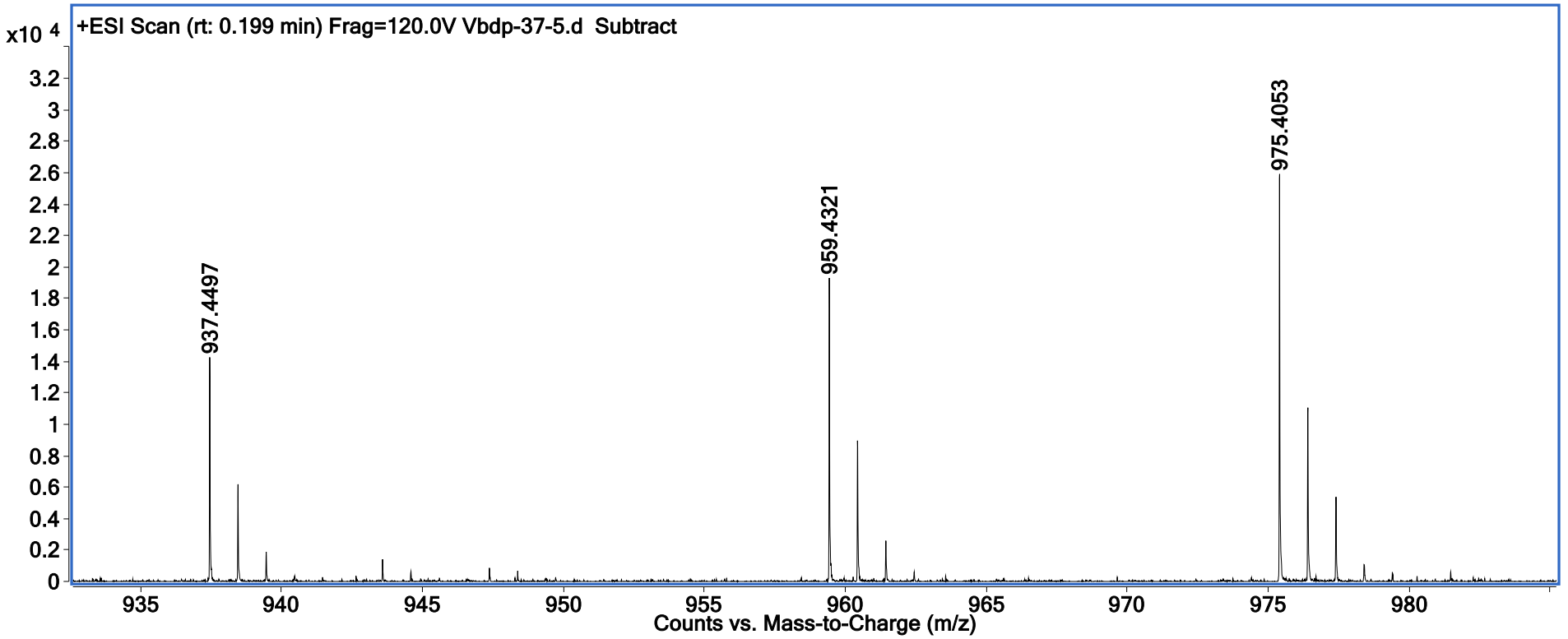
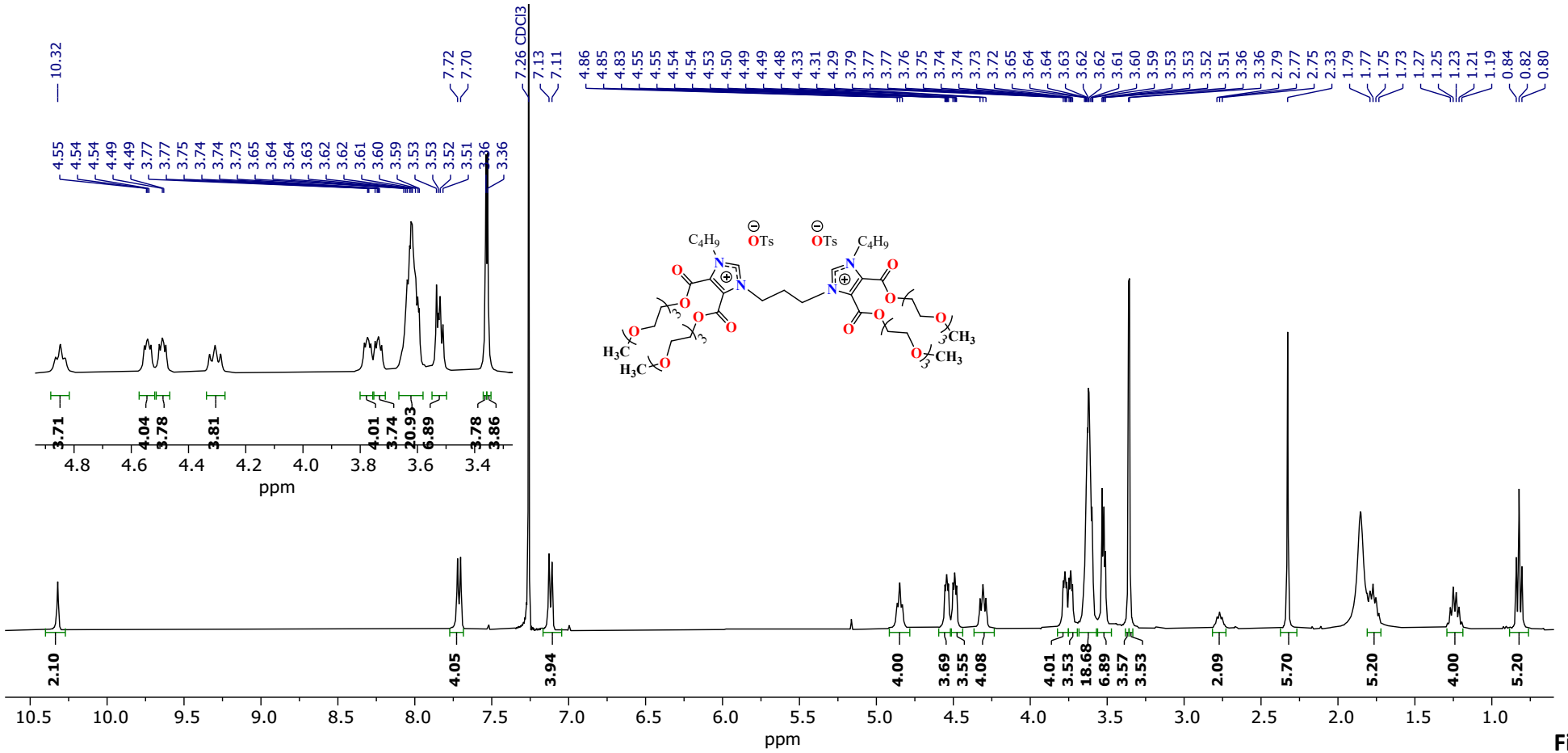


Figure S4. HR-ESI mass-spectrum of imidazole **2**



Fi gure S5. NMR ^{1}H spectrum (400 MHz, $CDCl_3$, 25 °C) of bis-imidazolium salt **4**

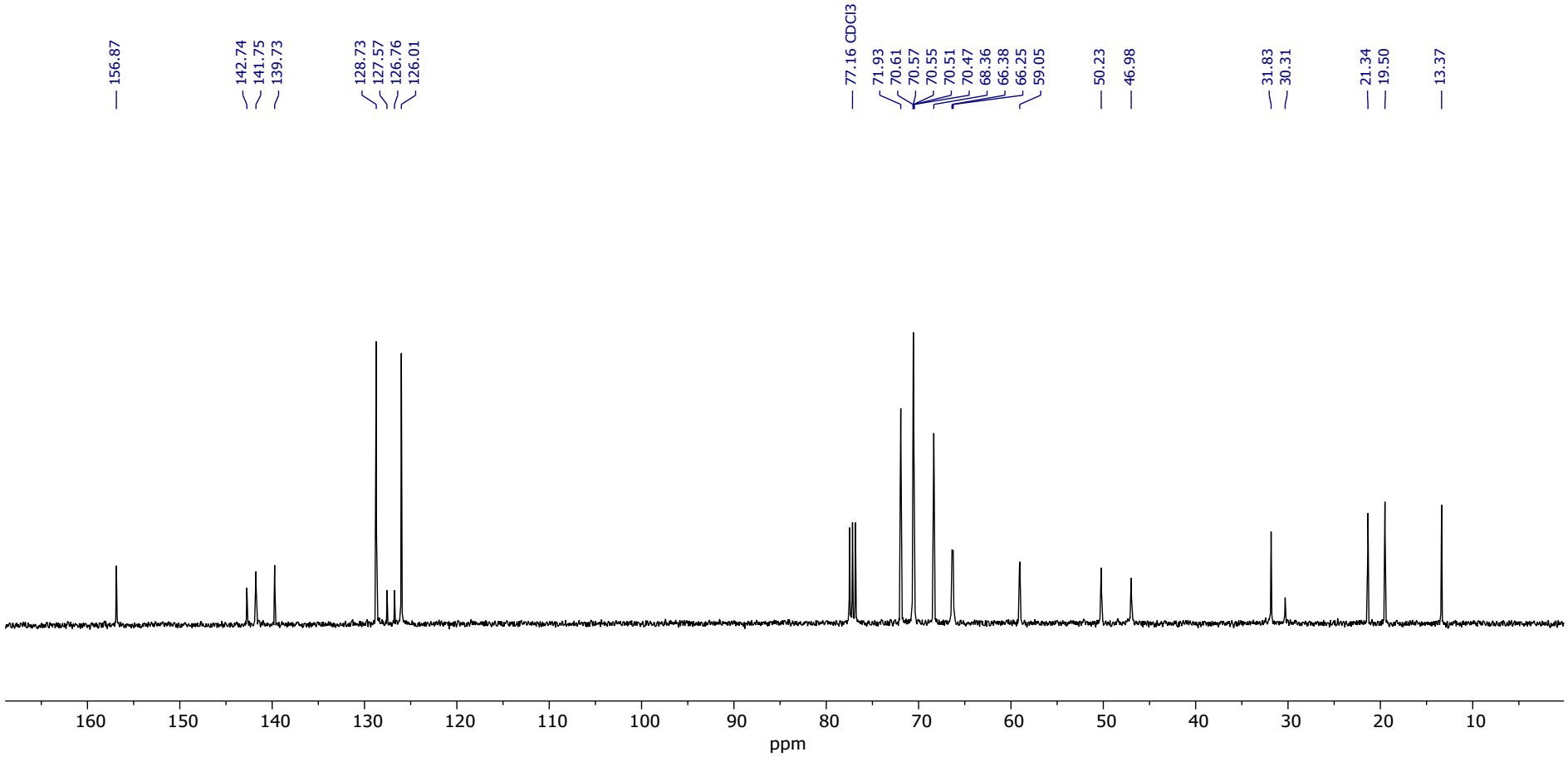


Figure S6. NMR ^{13}C spectrum (100.6 MHz, $CDCl_3$, 25 ^oC) of bis-imidazolium salt **4**

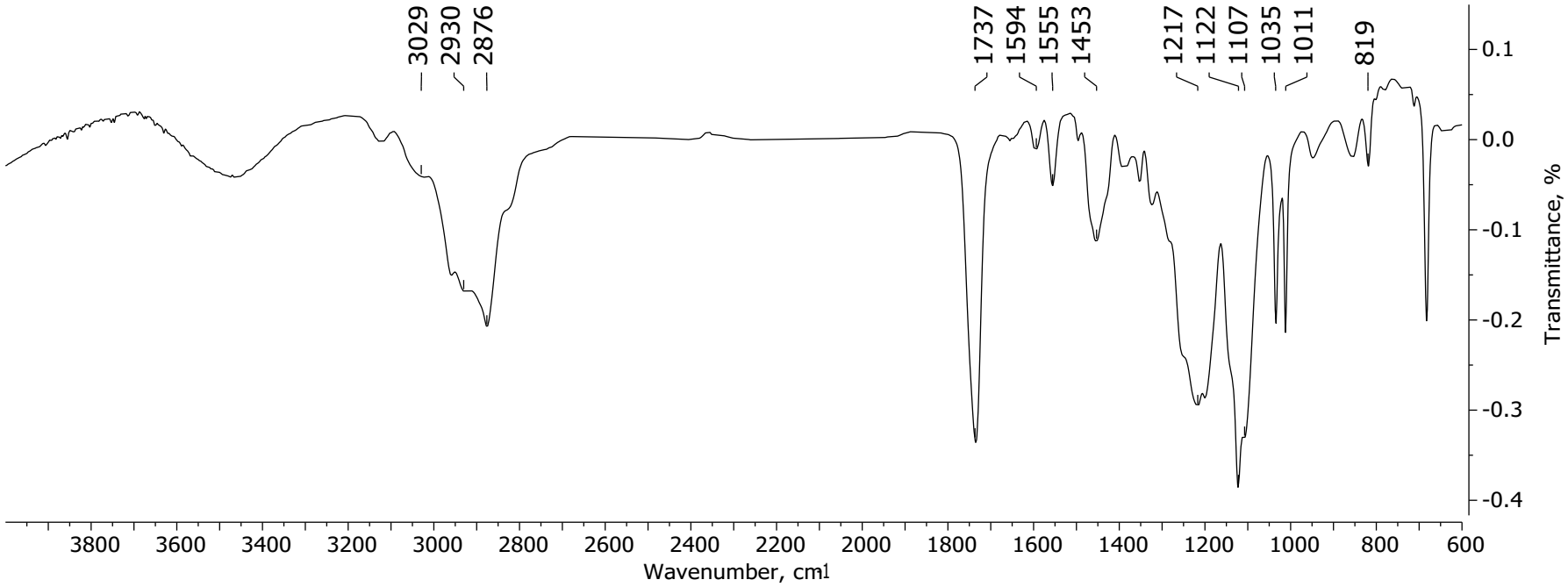


Figure S7. FT-IR spectrum of bis-imidazolium salt **4**

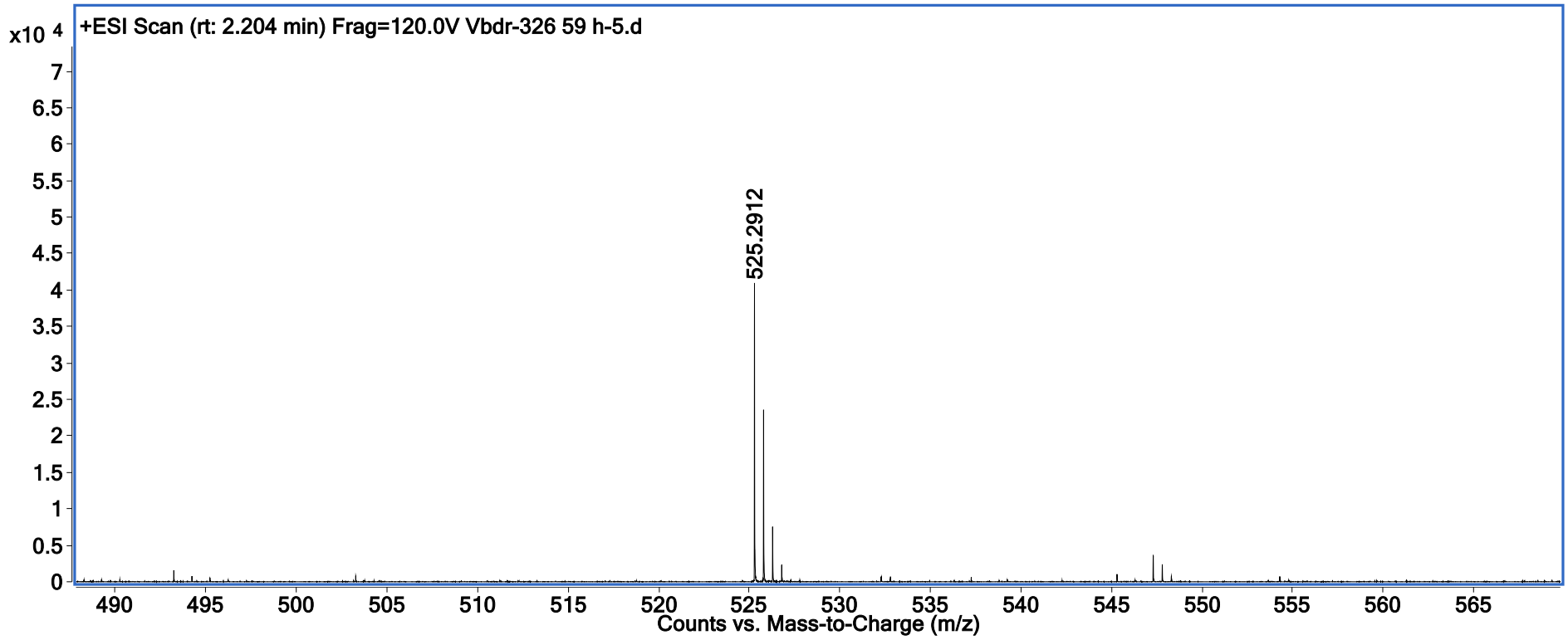


Figure S8. HR-ESI mass-spectrum of bis-imidazolium salt **4**

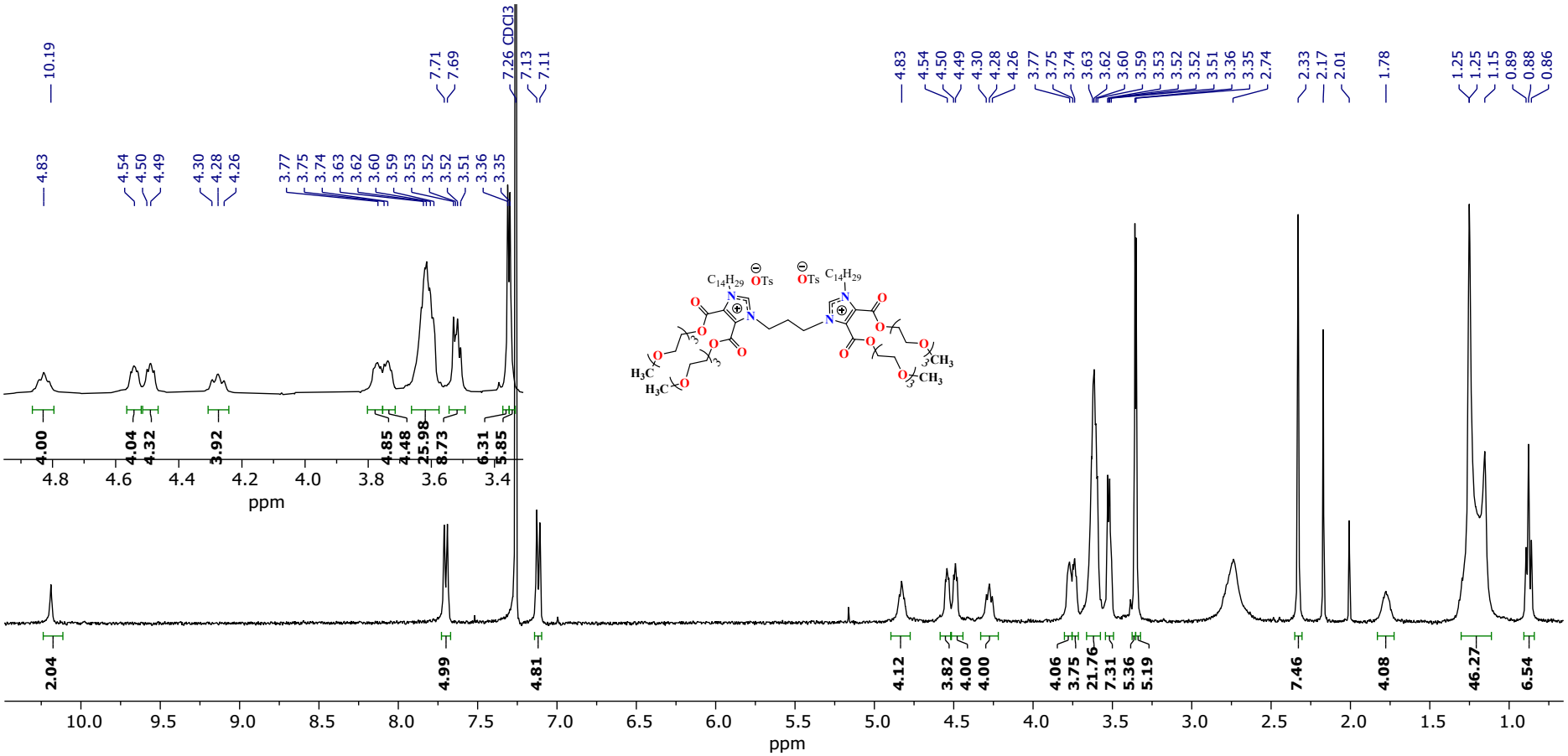


Figure S9. NMR ^{1}H spectrum (400 MHz, $CDCl_3$, 25 ^{o}C) of bis-imidazolium salt **5**

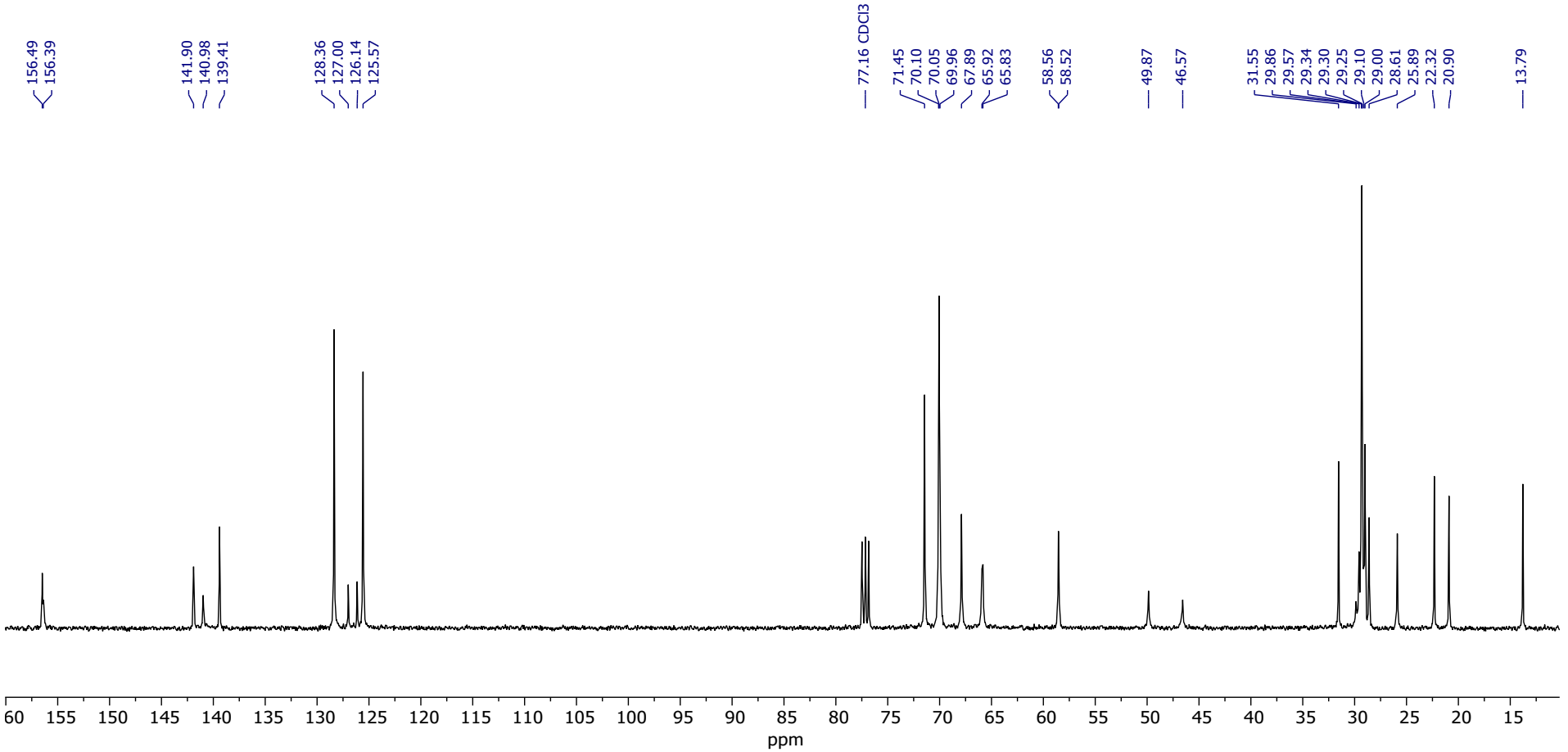


Figure S10. NMR ^{13}C spectrum (100.6 MHz, $CDCl_3$, 25 ^oC) of bis-imidazolium salt **5**

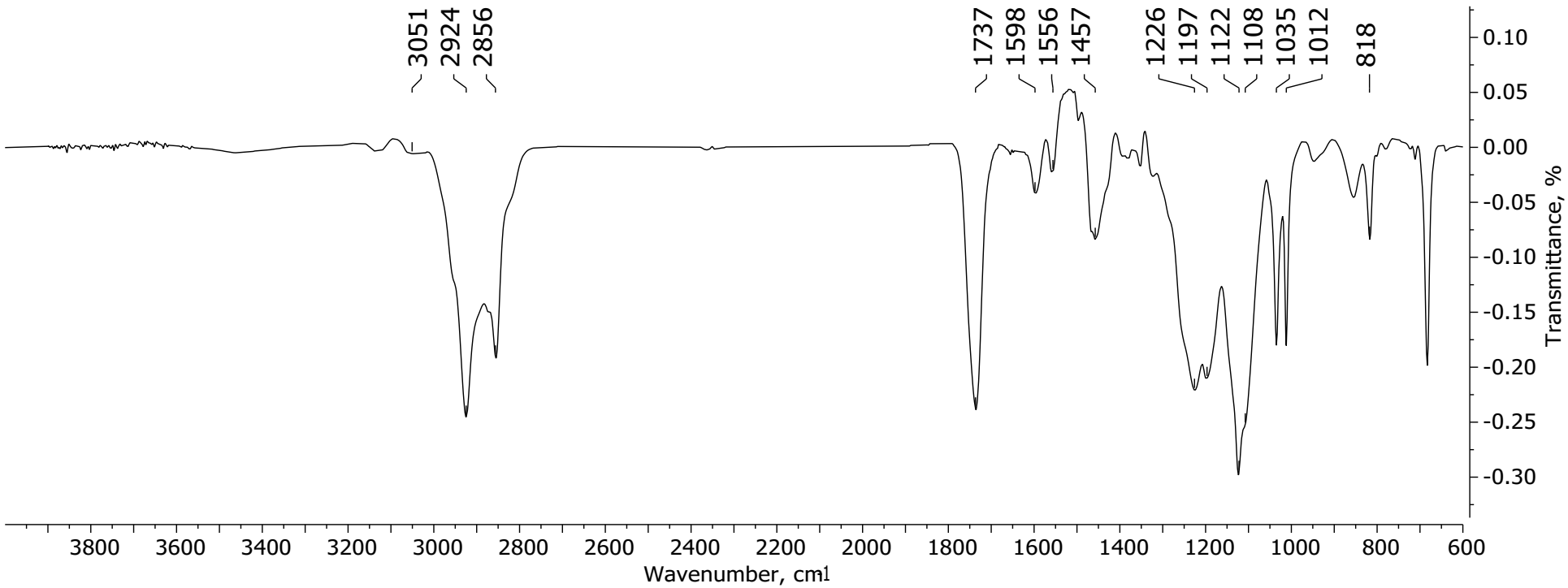


Figure S11. FT-IR spectrum of bis-imidazolium salt **5**

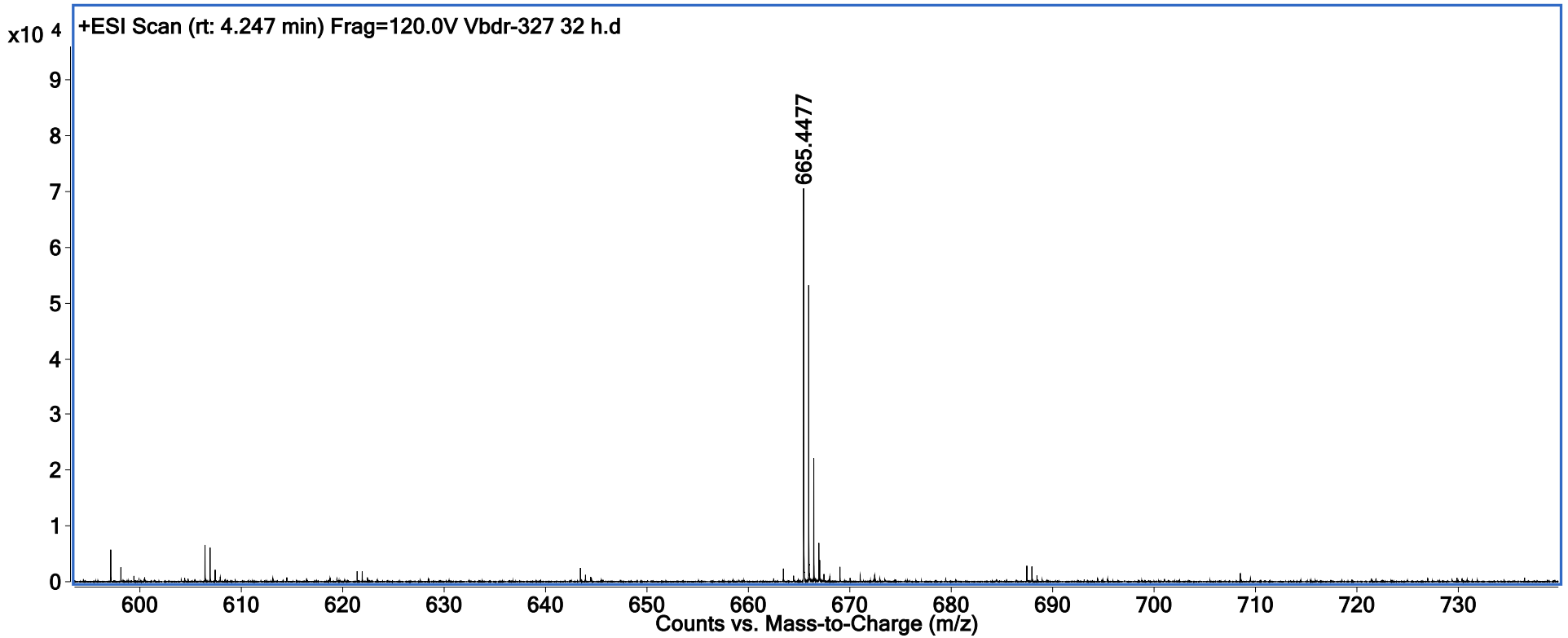


Figure S12. HR-ESI mass-spectrum of bis-imidazolium salt **5**

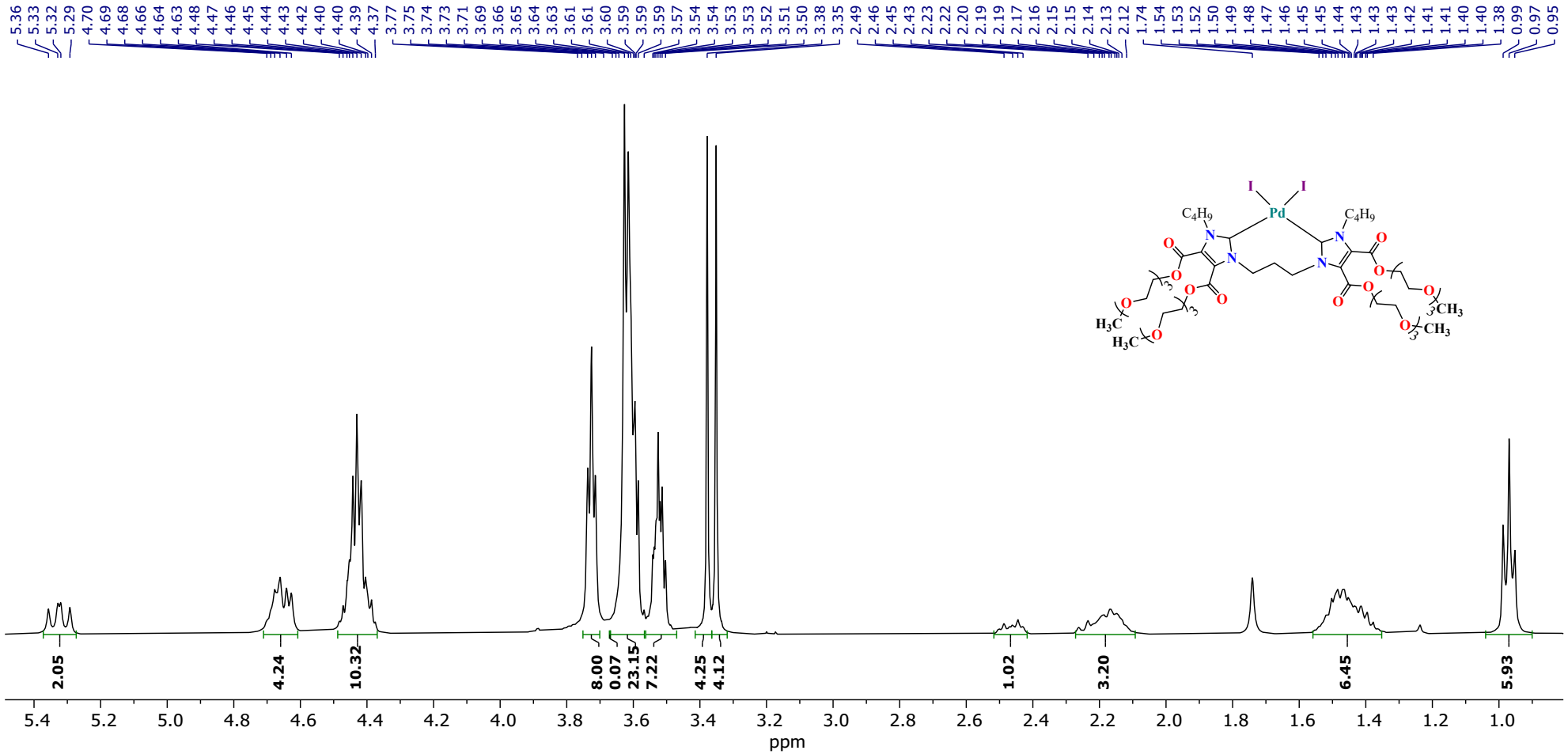


Figure S13. NMR ^{1}H spectrum (400 MHz, $CDCl_3$, 25 ^{o}C) of complex **6**

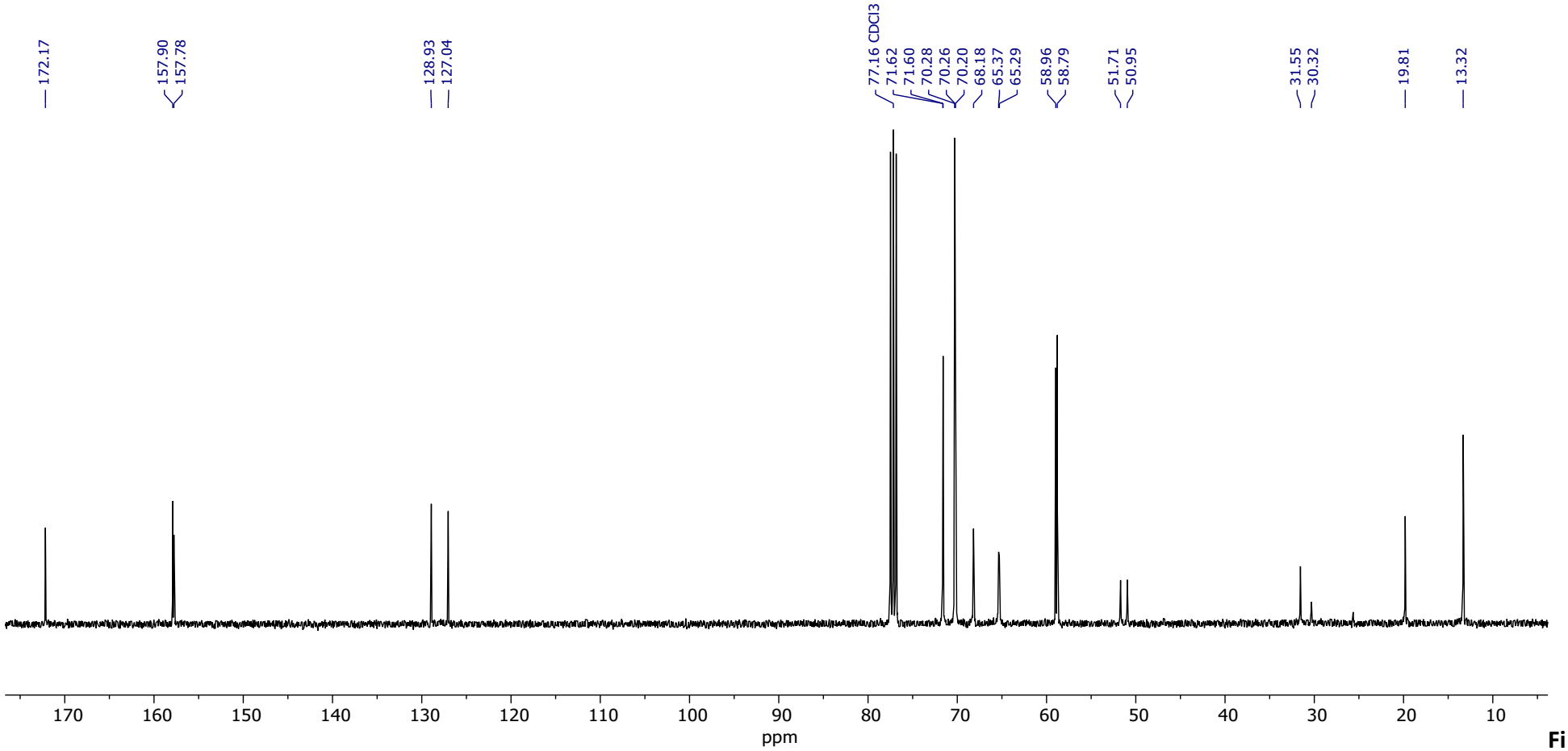


Figure S14. NMR ^{13}C spectrum (100.6 MHz, $CDCl_3$, 25 ^{o}C) of complex **6**

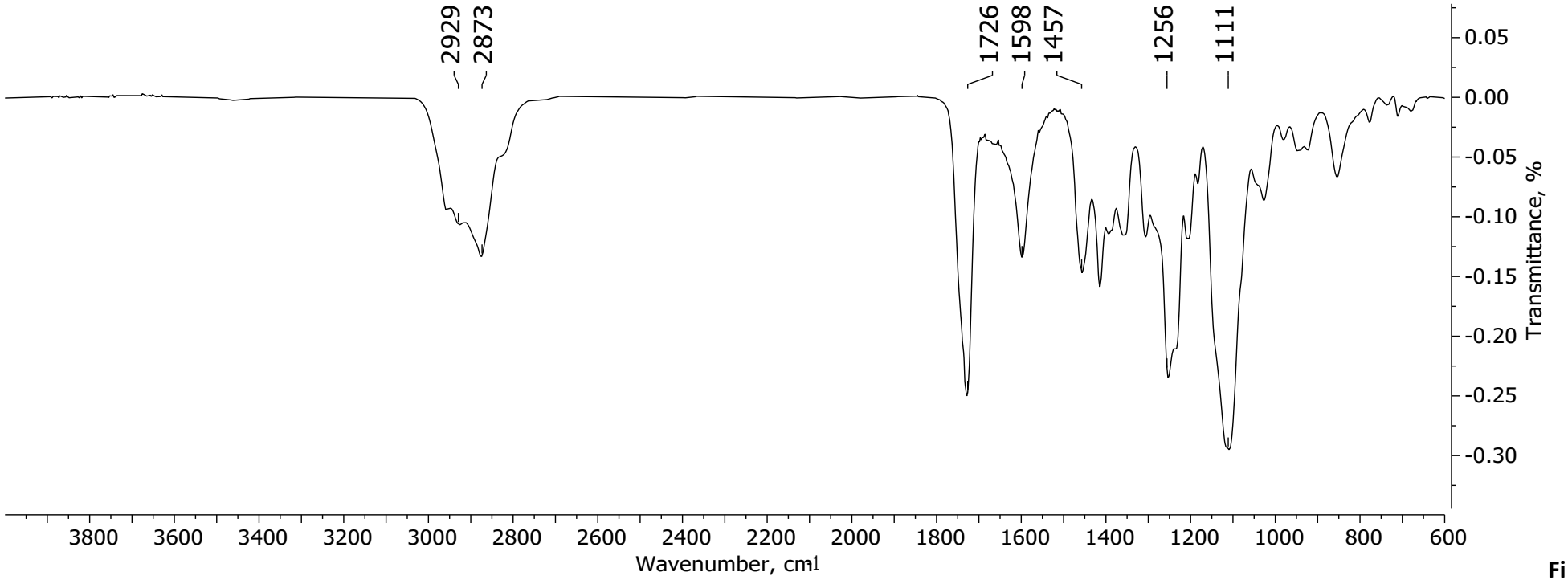


Figure S15. FT-IR spectrum of complex **6**

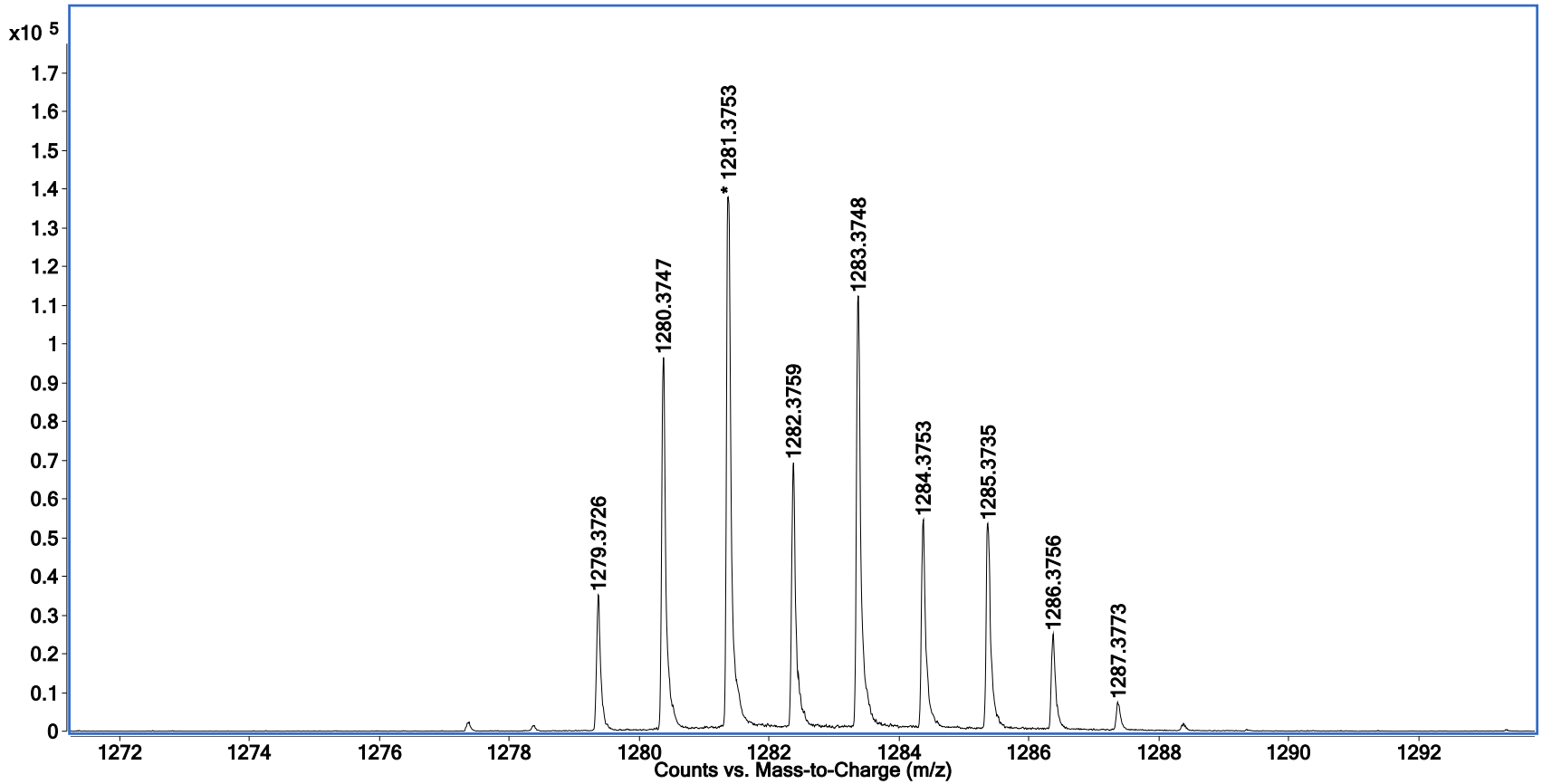


Figure S16. HR-ESI mass-spectrum of complex **6**

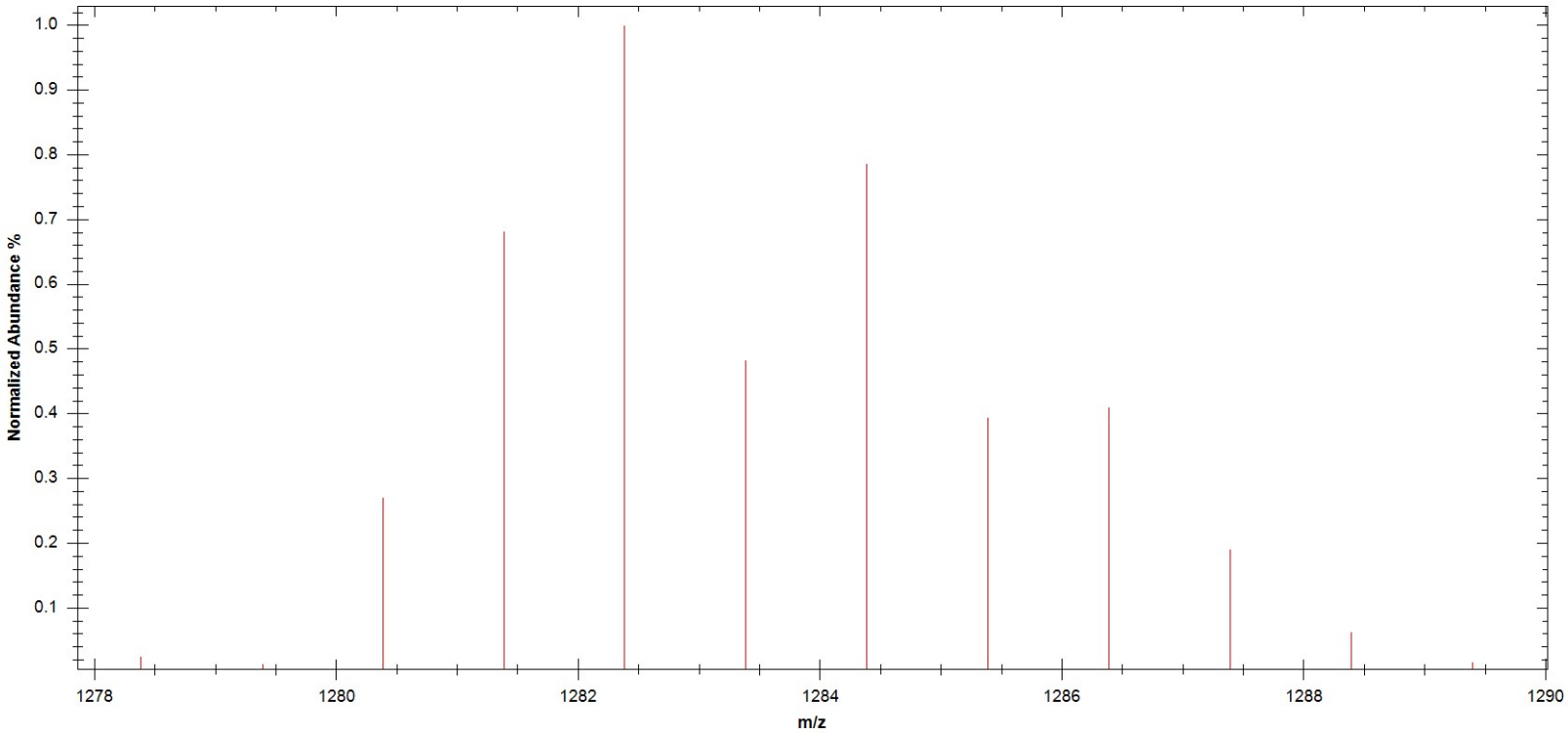


Figure S17. Calculated isotopic distribution for complex **6** ($[M\text{-}I]^+$, $C_{49}H_{84}IN_4O_{20}Pd^+$)

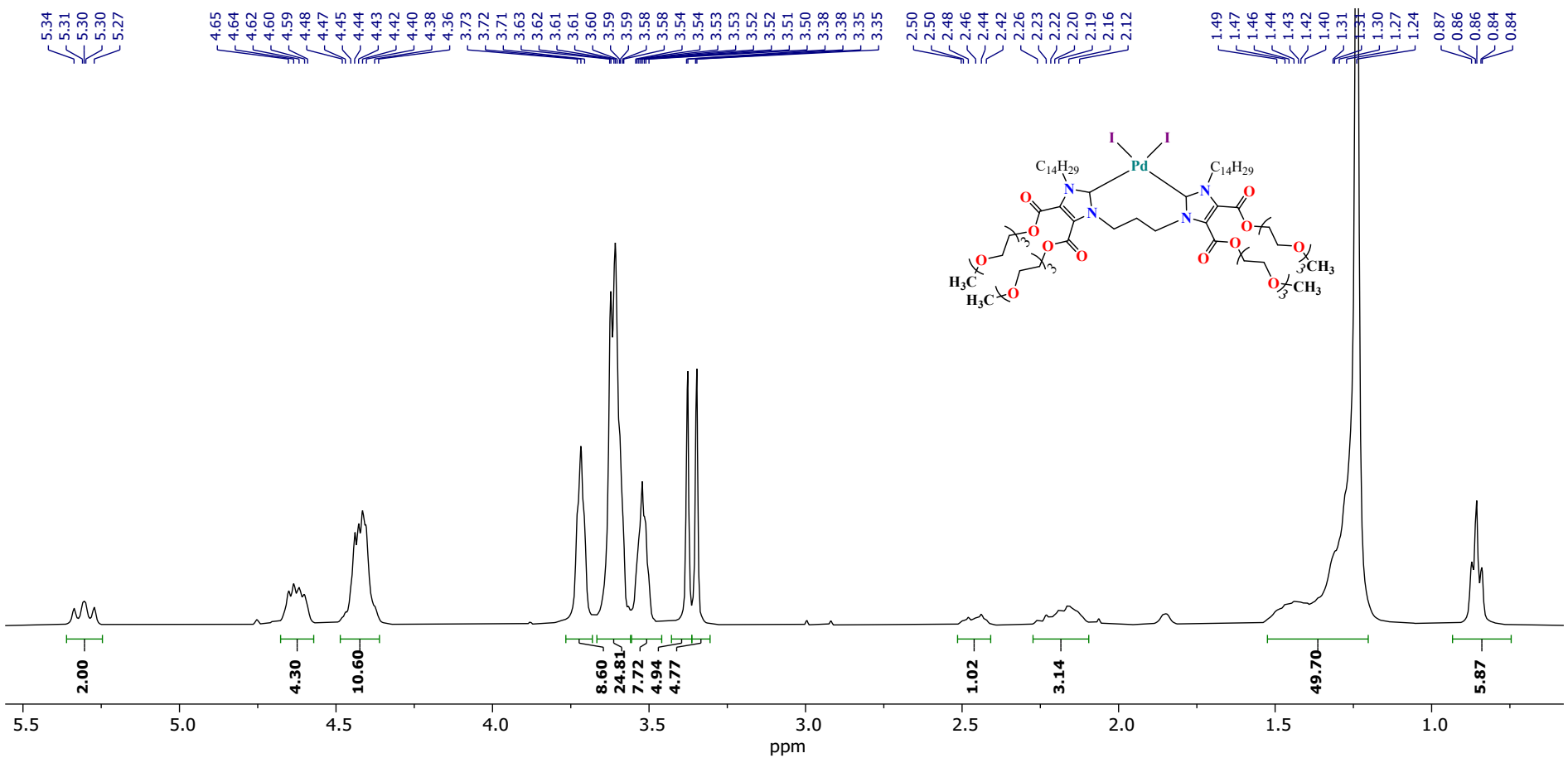


Figure S18. NMR ^{1}H spectrum (400 MHz, $CDCl_3$, 25 ^{o}C) of complex **7**

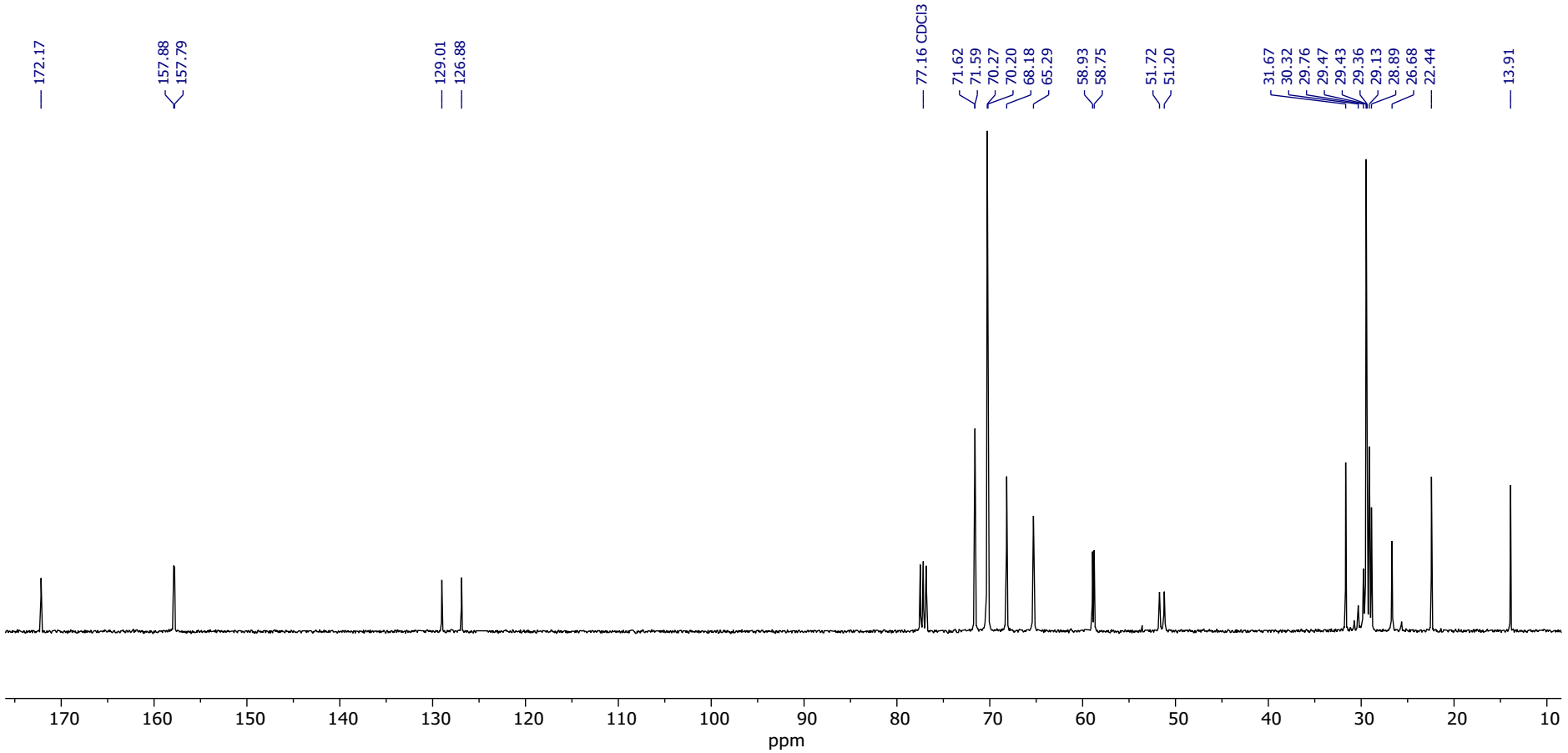


Figure S19. NMR ^{13}C spectrum (100.6 MHz, $CDCl_3$, 25 ^{o}C) of complex **7**

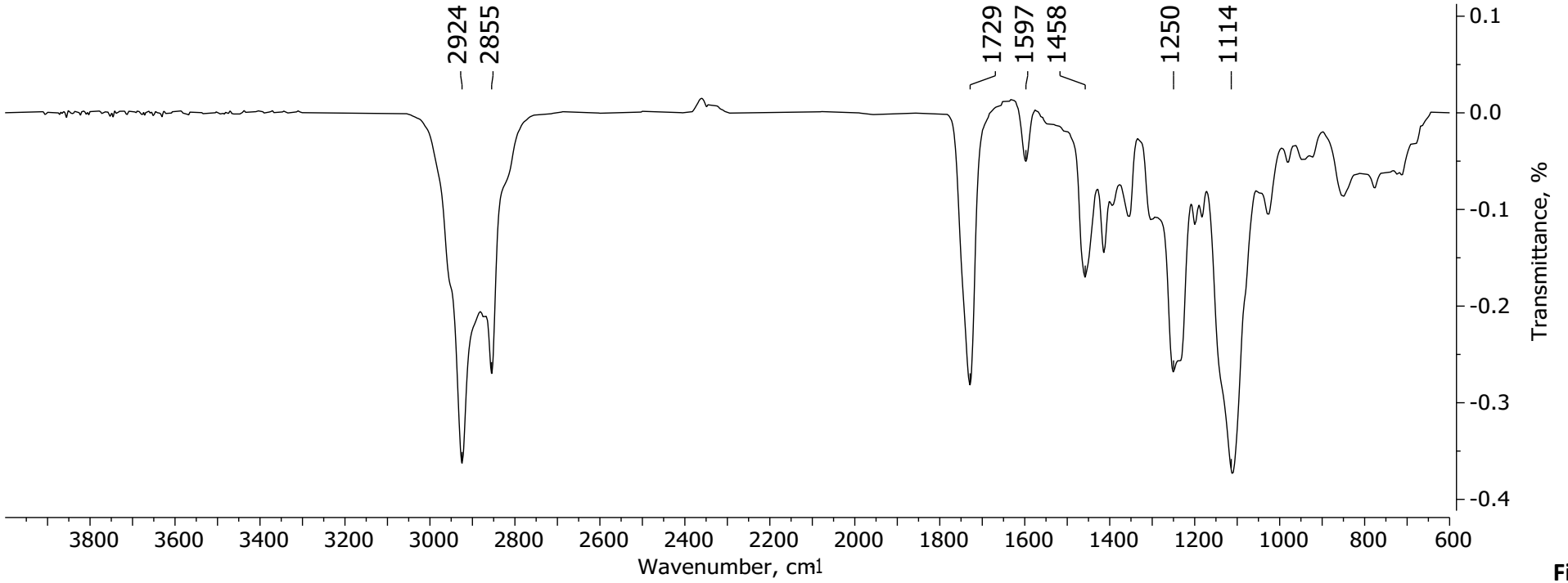


Figure S20. FT-IR spectrum of complex **7**

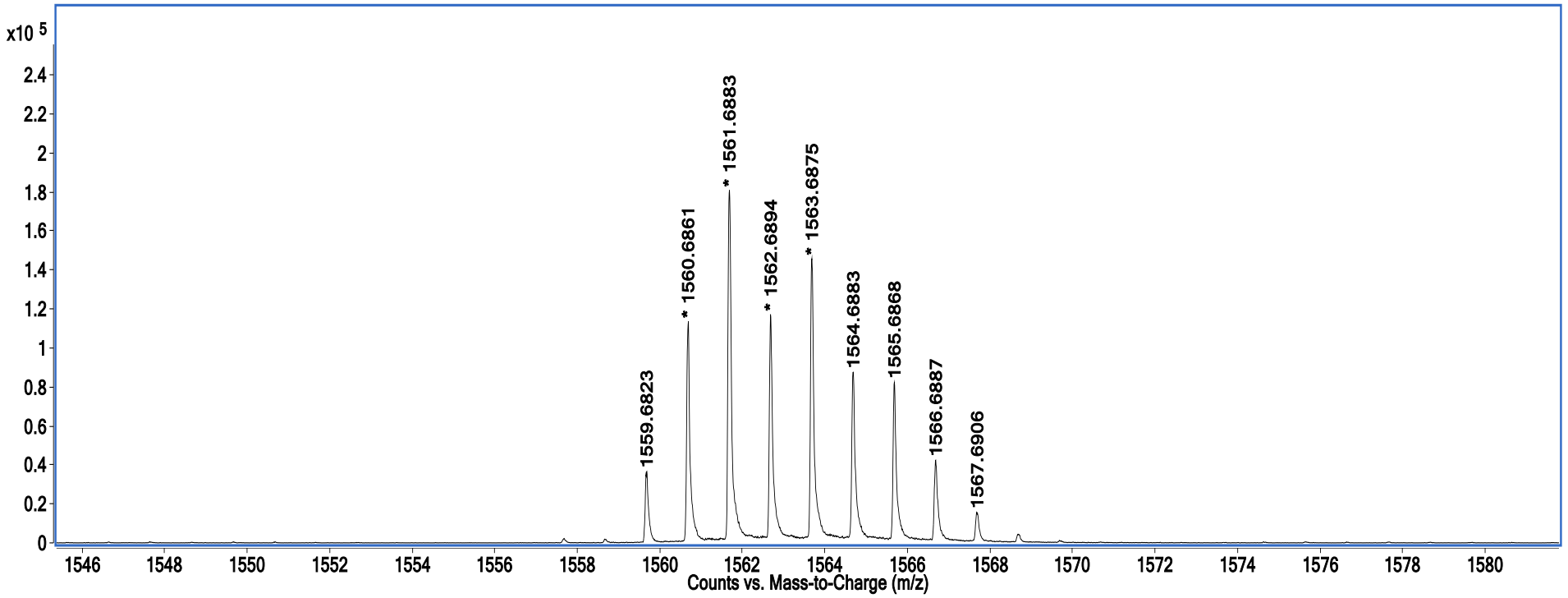


Figure S17. HR-ESI mass-spectrum of complex **7**

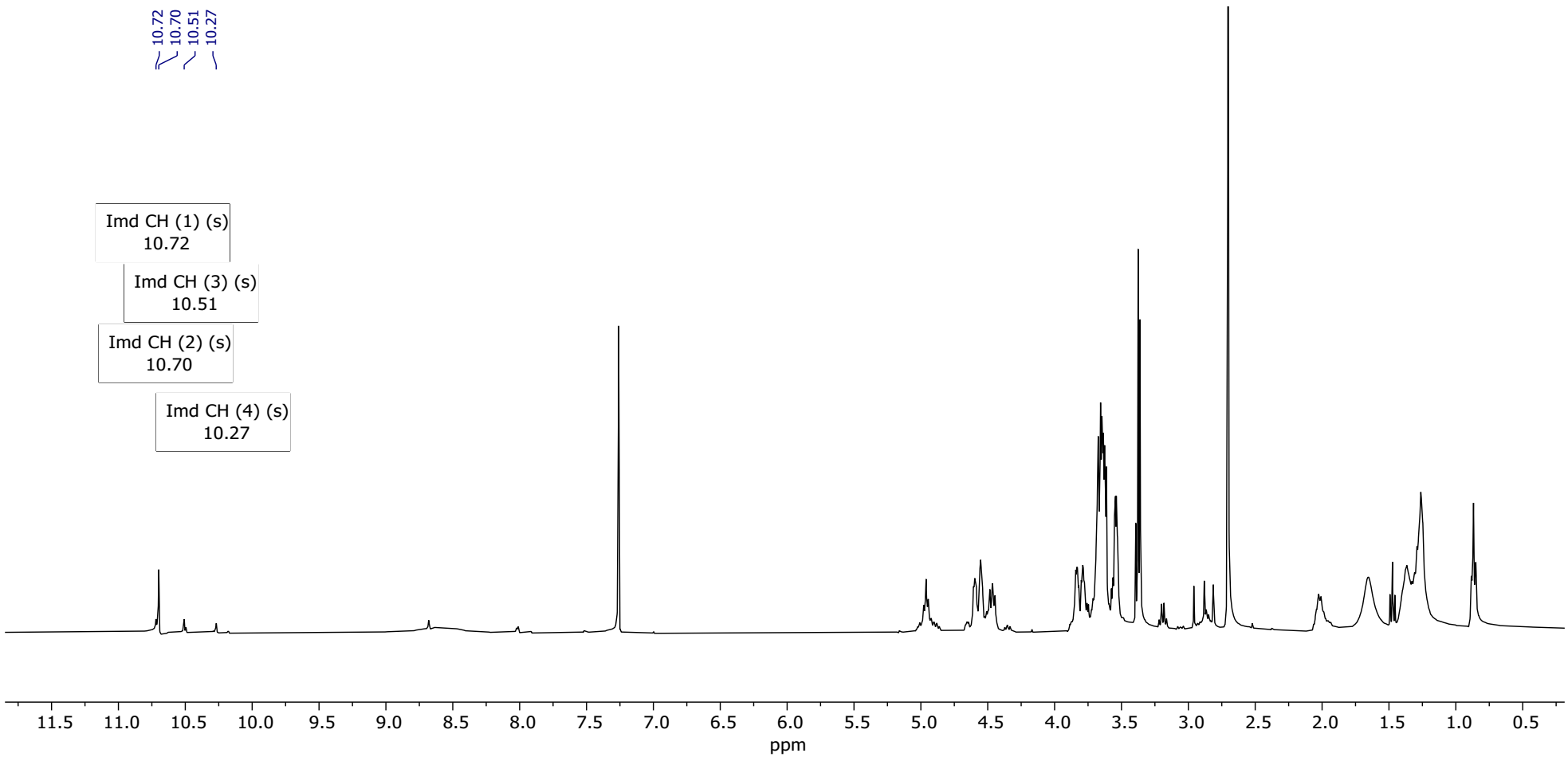

10.72
10.70
10.51
10.27
Imd CH (1) (s)
10.72
Imd CH (3) (s)
10.51
Imd CH (2) (s)
10.70
Imd CH (4) (s)
10.27
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

Figure S18. NMR ^{1}H spectrum (400 MHz, $CDCl_3$, 25 ^{o}C) of the reaction mixture of bis-imidazolium salt **2** with 1-iodooctane after 150 h reaction time (60^{o}C in DMF).

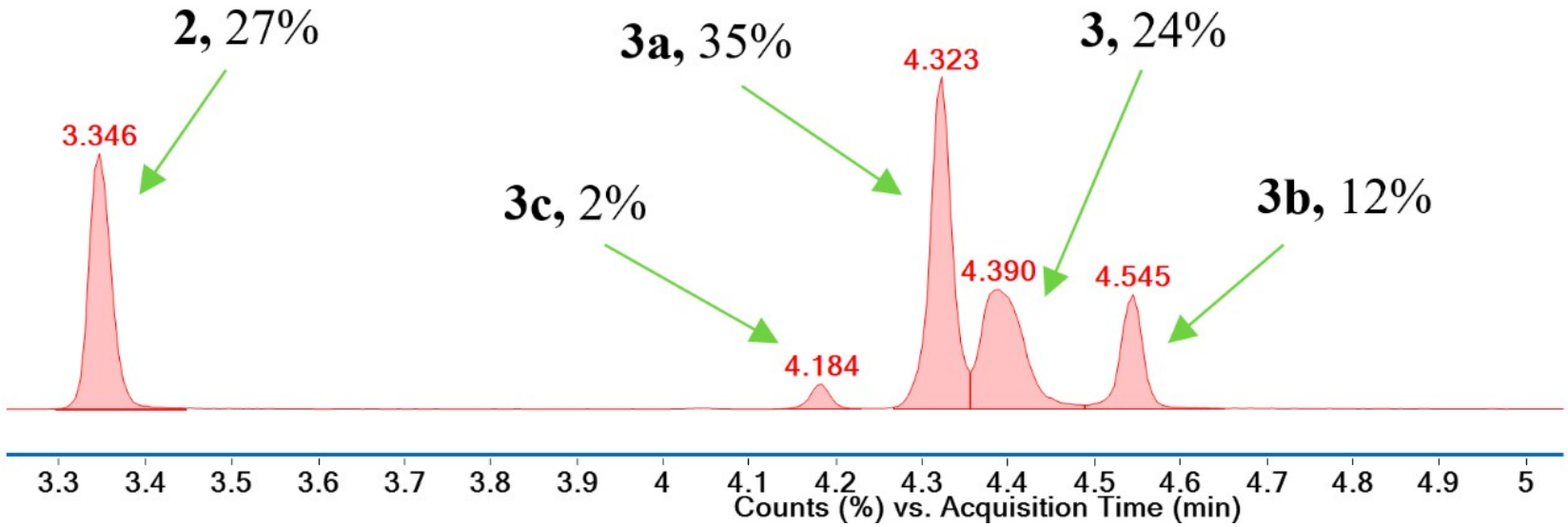
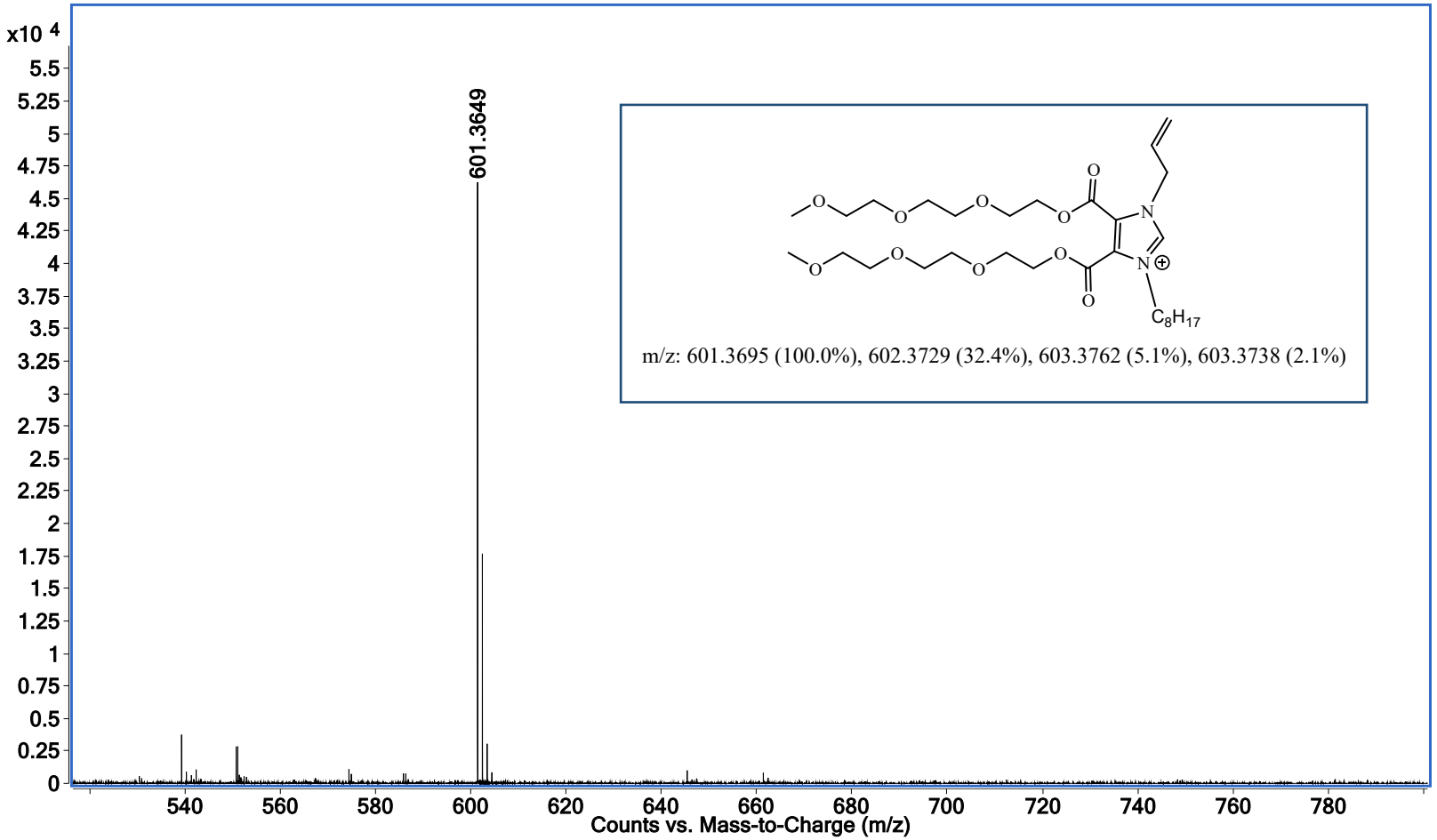
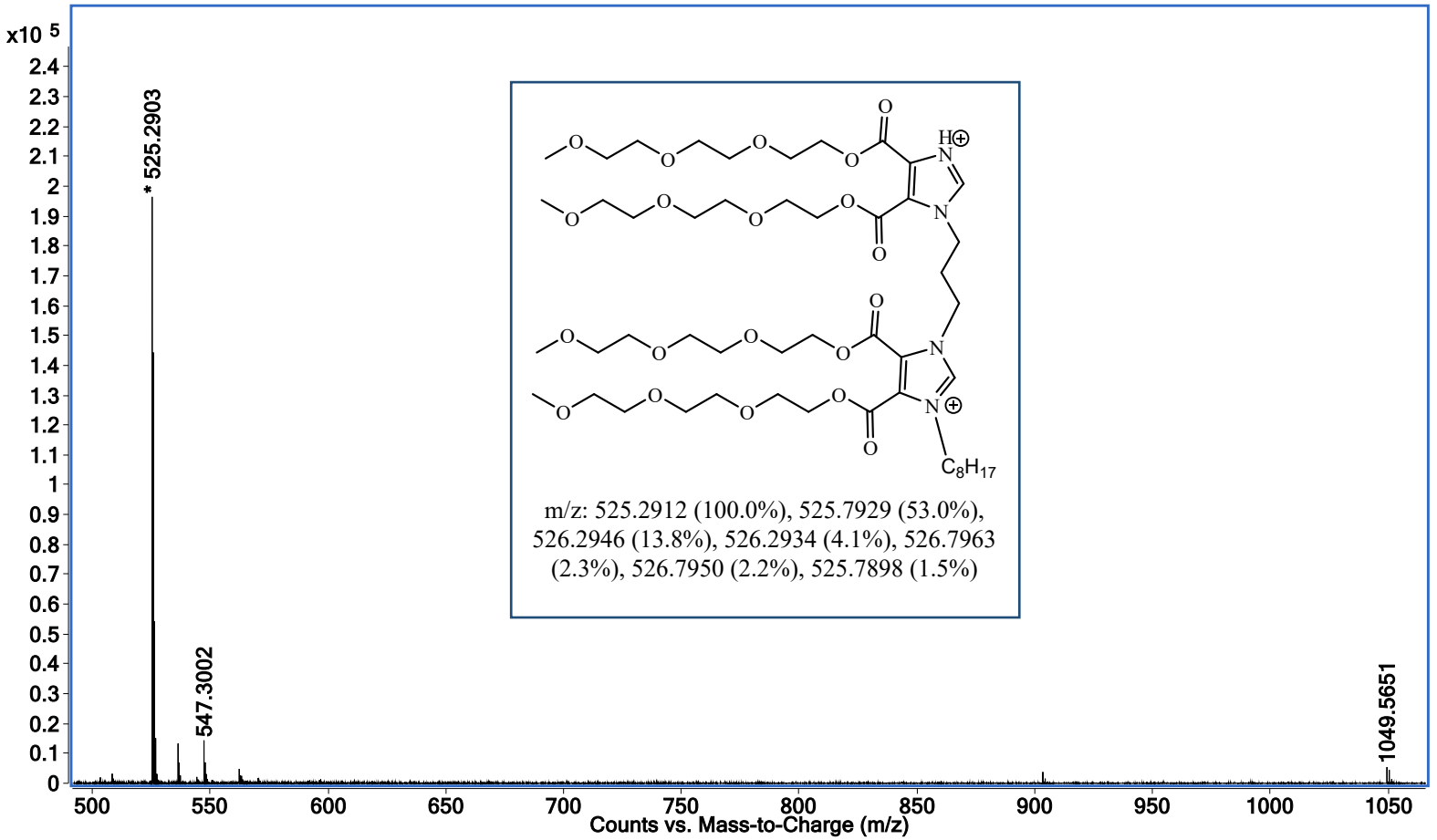
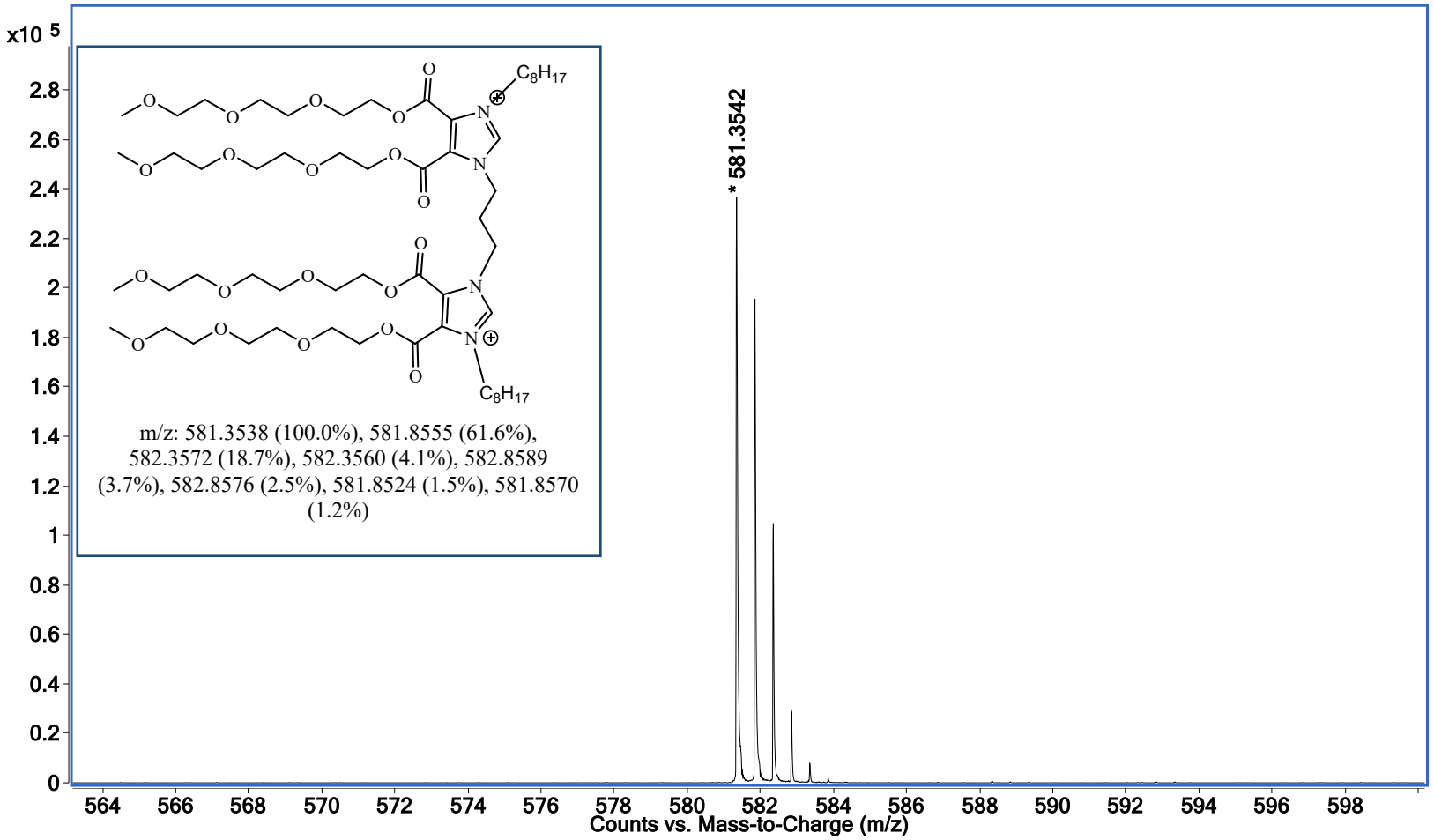


Figure S19. LC-MS data of the reaction mixture of bis-imidazolium salt **2** with 1-iodooctane after 30 h of stirring at 90^{o}C.


x10 4
5.5
5.25
5
4.75
4.5
4.25
4
3.75
3.5
3.25
3
2.75
2.5
2.25
2
1.75
1.5
1.25
1
0.75
0.5
0.25
0
601.3649
540
560
580
600
620
640
660
680
700
720
740
760
780
Counts vs. Mass-to-Charge (m/z)
m/z: 601.3695 (100.0%), 602.3729 (32.4%), 603.3762 (5.1%), 603.3738 (2.1%)


x10 5
2.4
2.3
2.2
2.1
2
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
* 525.2903
547.3002
1049.5651
500
550
600
650
700
750
800
850
900
950
1000
1050
Counts vs. Mass-to-Charge (m/z)
m/z: 525.2912 (100.0%), 525.7929 (53.0%), 526.2946 (13.8%), 526.2934 (4.1%), 526.7963 (2.3%), 526.7950 (2.2%), 525.7898 (1.5%)


x10 5
2.8
2.6
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
* 581.3542
m/z: 581.3538 (100.0%), 581.8555 (61.6%), 582.3572 (18.7%), 582.3560 (4.1%), 582.8589 (3.7%), 582.8576 (2.5%), 581.8524 (1.5%), 581.8570 (1.2%)
564 566 568 570 572 574 576 578 580 582 584 586 588 590 592 594 596 598
Counts vs. Mass-to-Charge (m/z)

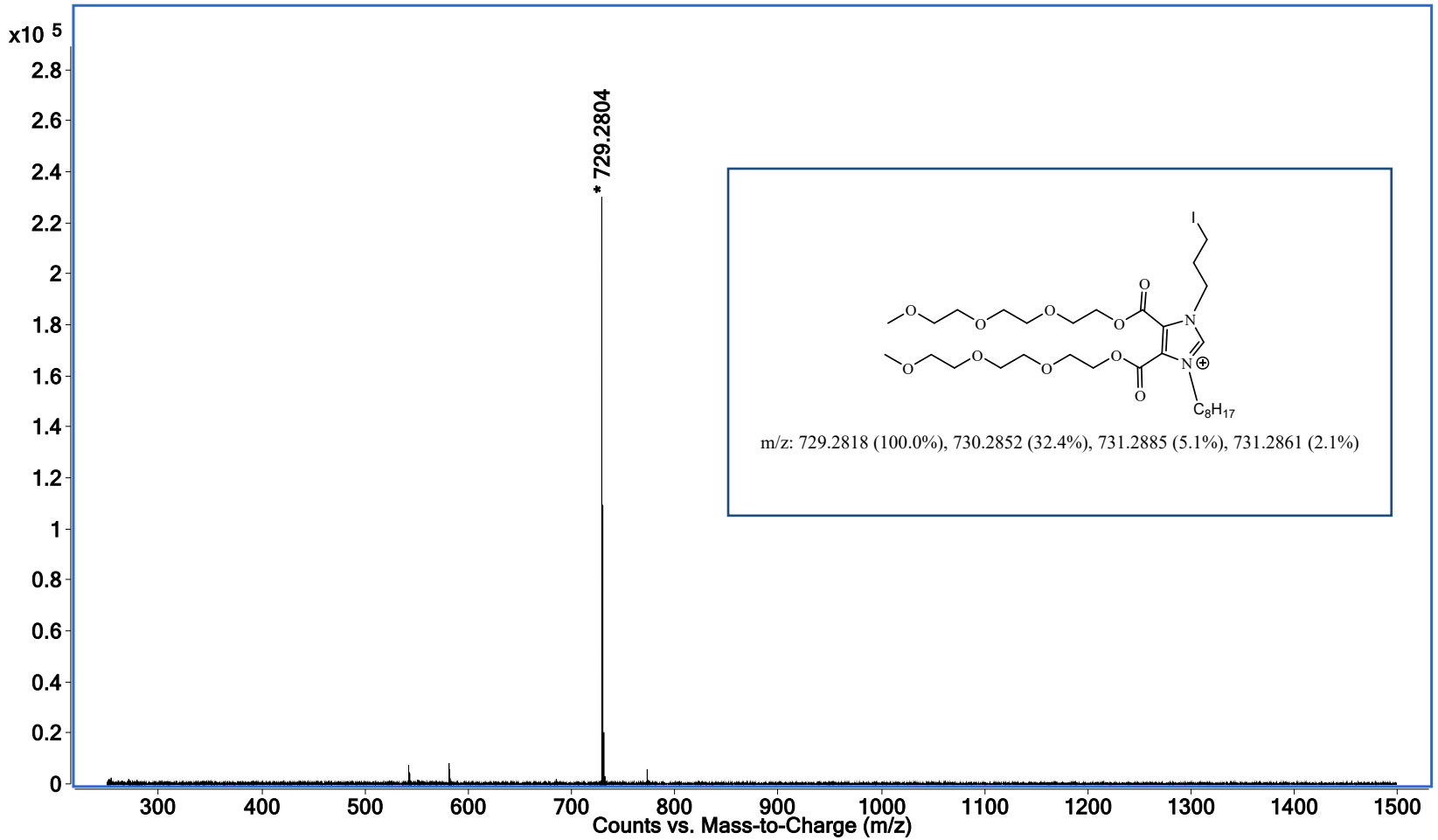


Figure S20. ESI-MS spectra of **3** and **3a-c**.

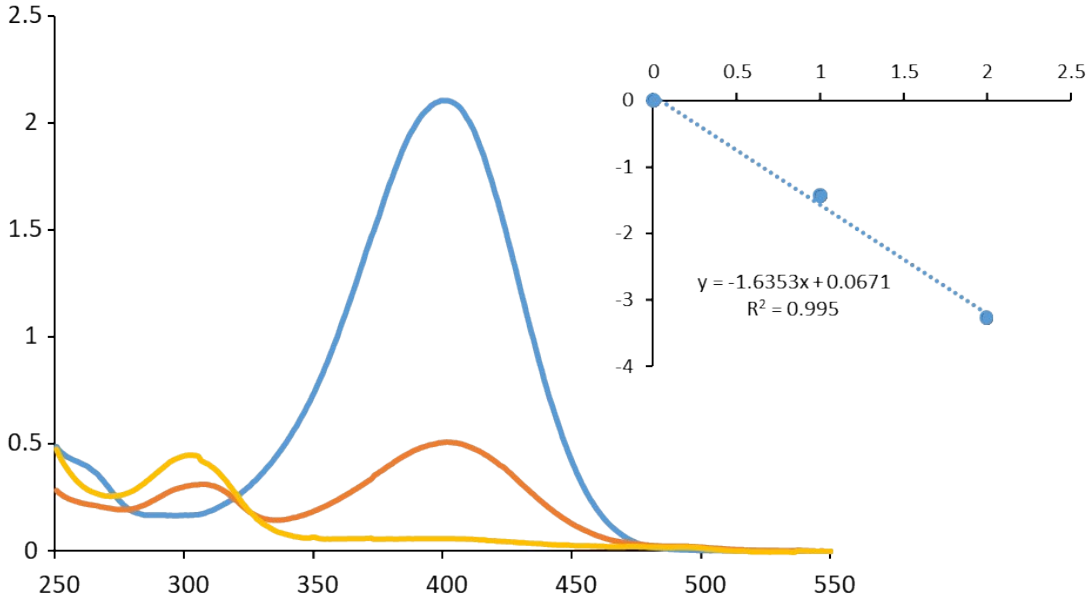


Figure S21. UV-visible spectra and $\ln(C_t/C_0)$ time dependence of a mixture of *p*-nitrophenol and sodium borohydride in the presence of **6**; water-THF, where THF is 0.4 vol.%, C(*p*-nitrophenol)=0.1 mM, C($NaBH_4$)=5 mM, C(**6**)=0.002 mM (0.2 mol%), l=1cm.

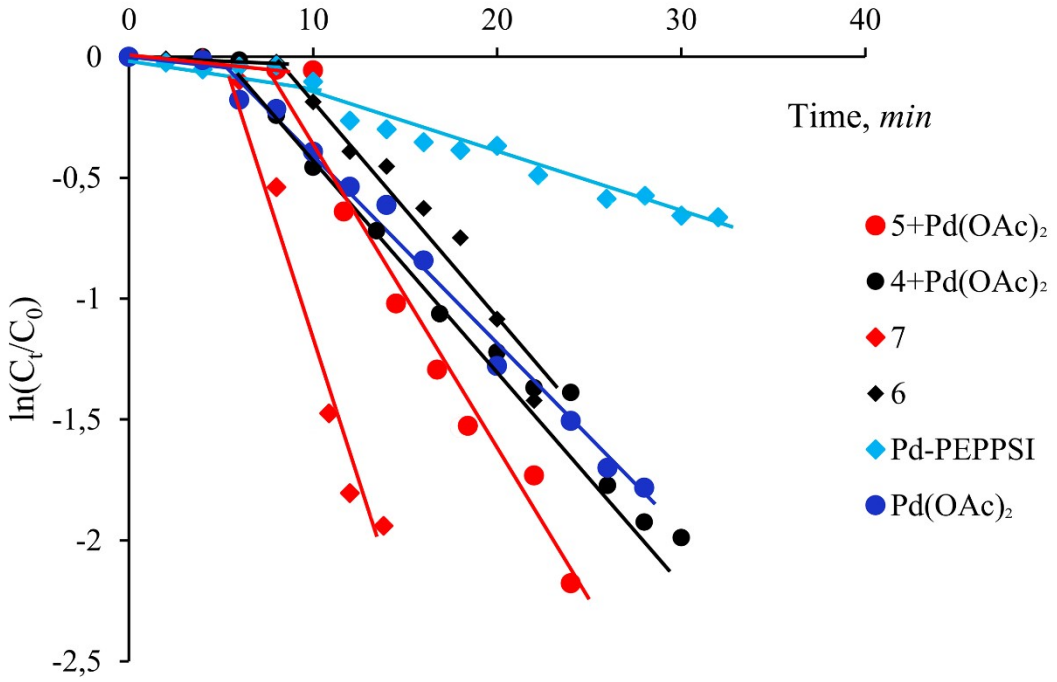


Figure S22. Time dependence of $\ln(C_t/C_0)$ of a mixture of *p*-ethylnitrobenzene and sodium borohydride in the presence of **6**, **7**, **4**+$Pd(OAc)_2$, **5**+$Pd(OAc)_2$, $Pd(OAc)_2$ or Pd-PEPPSI; water with 0.2 vol% THF, C(*p*-ethylnitrobenzene) = 0.1 mM, C($NaBH_4$)=5 mM, C(**4**) = C(**5**) = C(**6**) = C(**7**) = C($Pd(OAc)_2$) = C(Pd-PEPPSI) = 0.002 mM (0.2 mol%), l = 1cm.

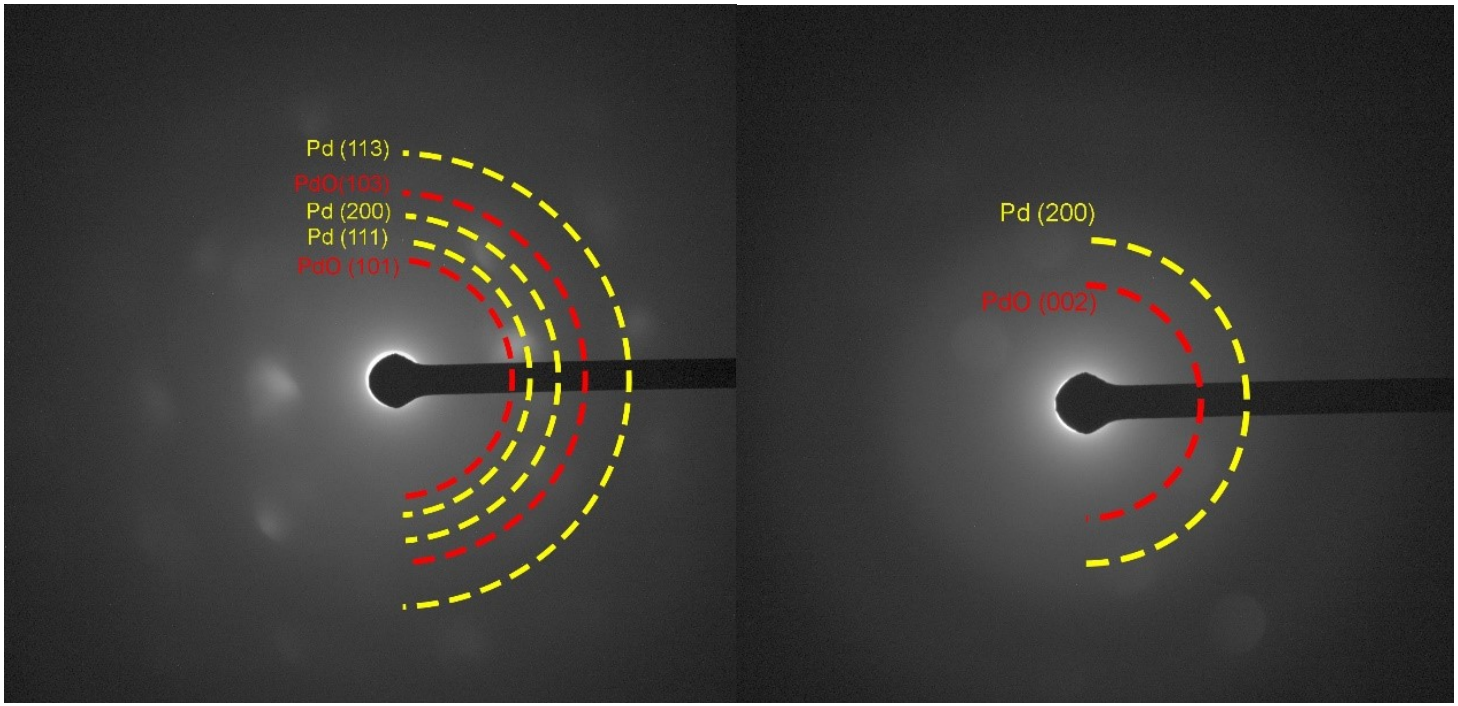


Figure S22. SAED images of compound A **4**+ $Pd(OAc)_2$ and B **5**+ $Pd(OAc)_2$.

Table S1. Interplanar distances d (hkl) measured on the complex *in situ* and possible correlation to fcc Pd and tetragonal PdO

4 + $Pd(OAc)_2$			**5** + $Pd(OAc)_2$		
d (hkl) Expt.	Lattice plane	d (hkl) Theor	d (hkl) Expt.	Lattice plane	d (hkl) Theor
2.62	PdO (101)	2.63	2.67	PdO (002)	2.665
1.52	PdO (103)	1.53			
2.23	Pd (111)	2.24	1.93	Pd(200)	1.94
1.93	Pd (200)	1.94			
1.18	Pd (113)	1.17			