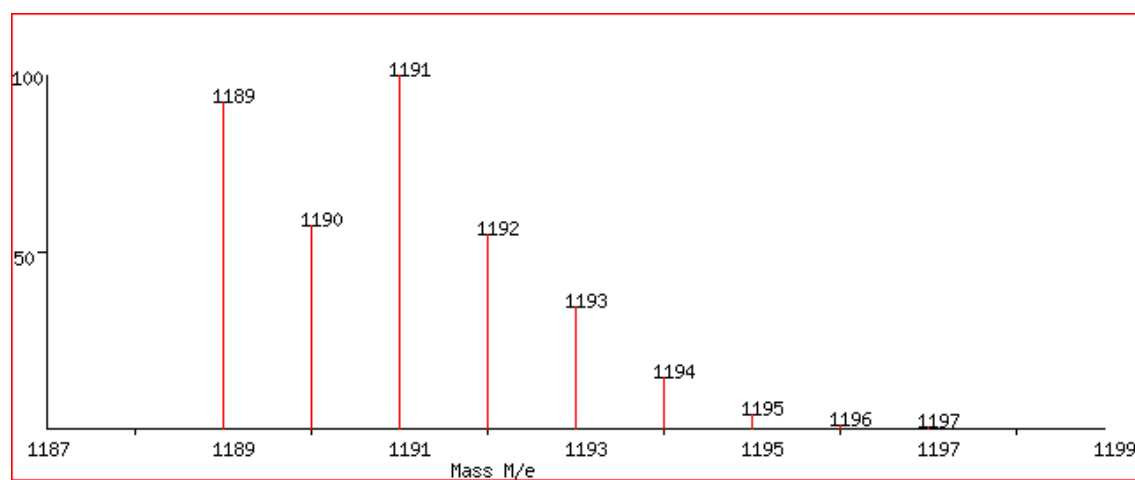
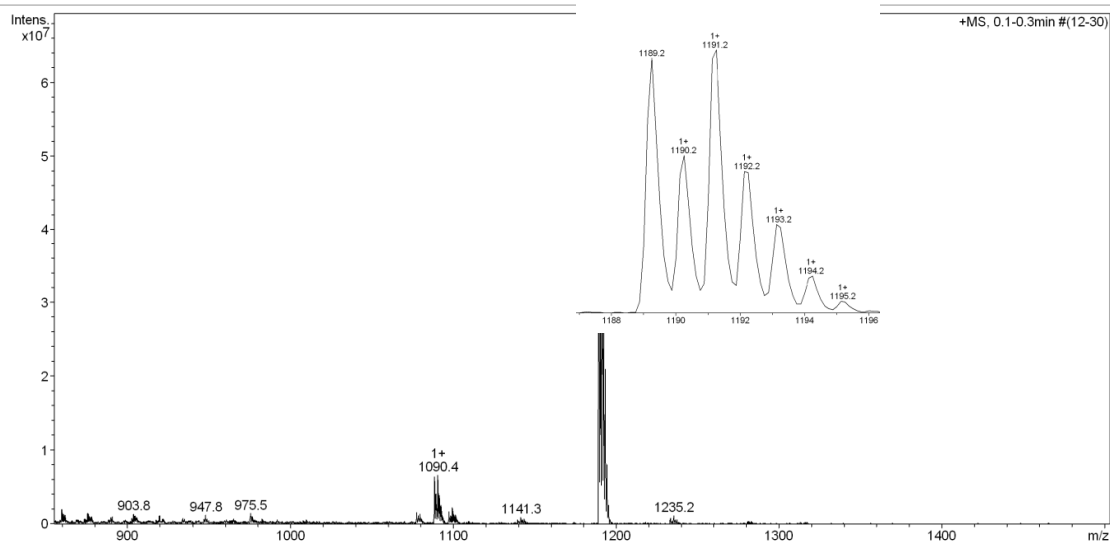
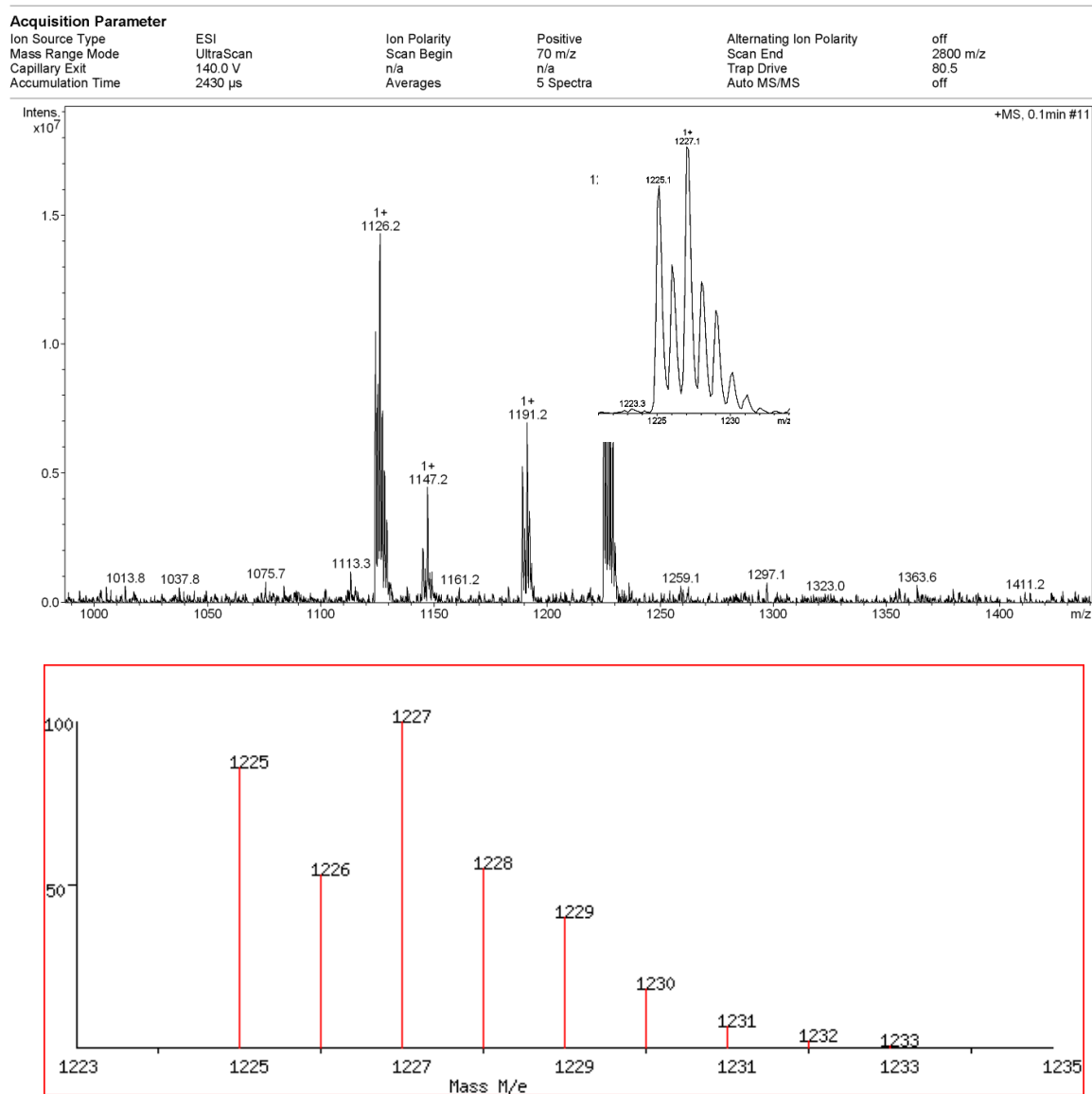


#### Acquisition Parameter

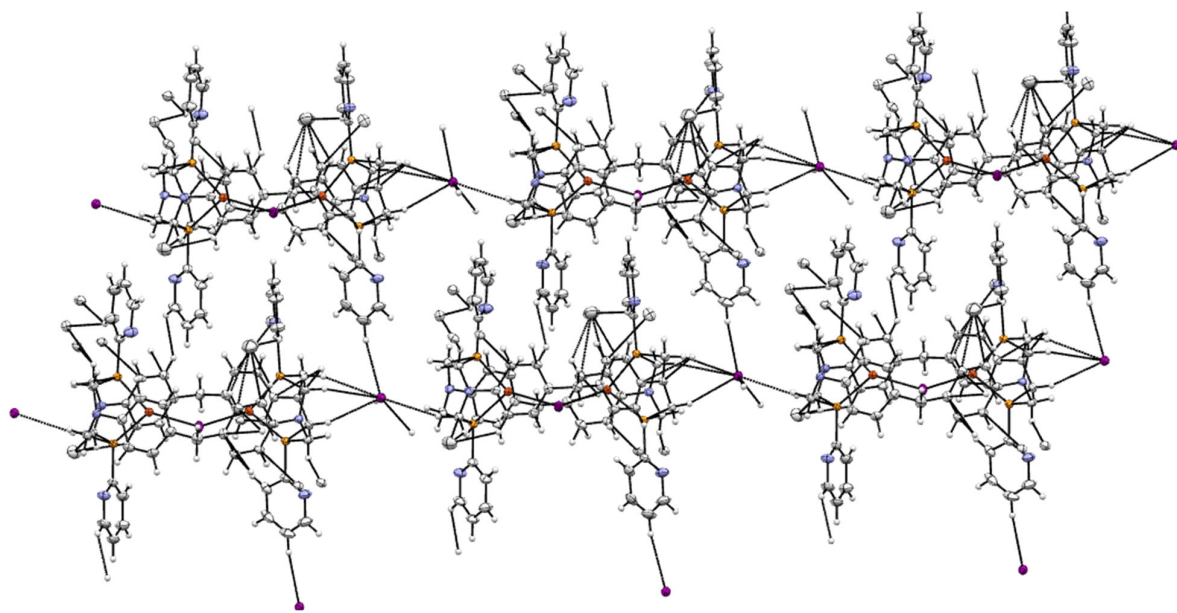
Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	UltraScan	Scan Begin	100 m/z	Scan End	2700 m/z
Capillary Exit	140.0 V	n/a	n/a	Trap Drive	73.0
Accumulation Time	315 $\mu$ s	Averages	5 Spectra	Auto MS/MS	off



**Figure S1.** Experimental ESI mass-spectrum for complex **3**. Theoretical (bottom) isotope distributions of the pick  $[M-I]^+$  (calc. by <https://www.sisweb.com/mstools/isotope.htm> (accessed on 02 December 2022)).



**Figure S2.** Experimental ESI mass-spectrum for complex **4**. Theoretical (bottom) isotope distributions of the pick  $[M-I]^+$  (calc. by <https://www.sisweb.com/mstools/isotope.htm> (accessed on 02 December 2022)).



**Figure S3.** I...H-C-Contacts forming a supramolecular chain structure of complex 3.