

Supplementary Materials

Figure S1. ^1H -NMR spectrum of 6-selenocaffeine, recorded in DMSO-d_6 .

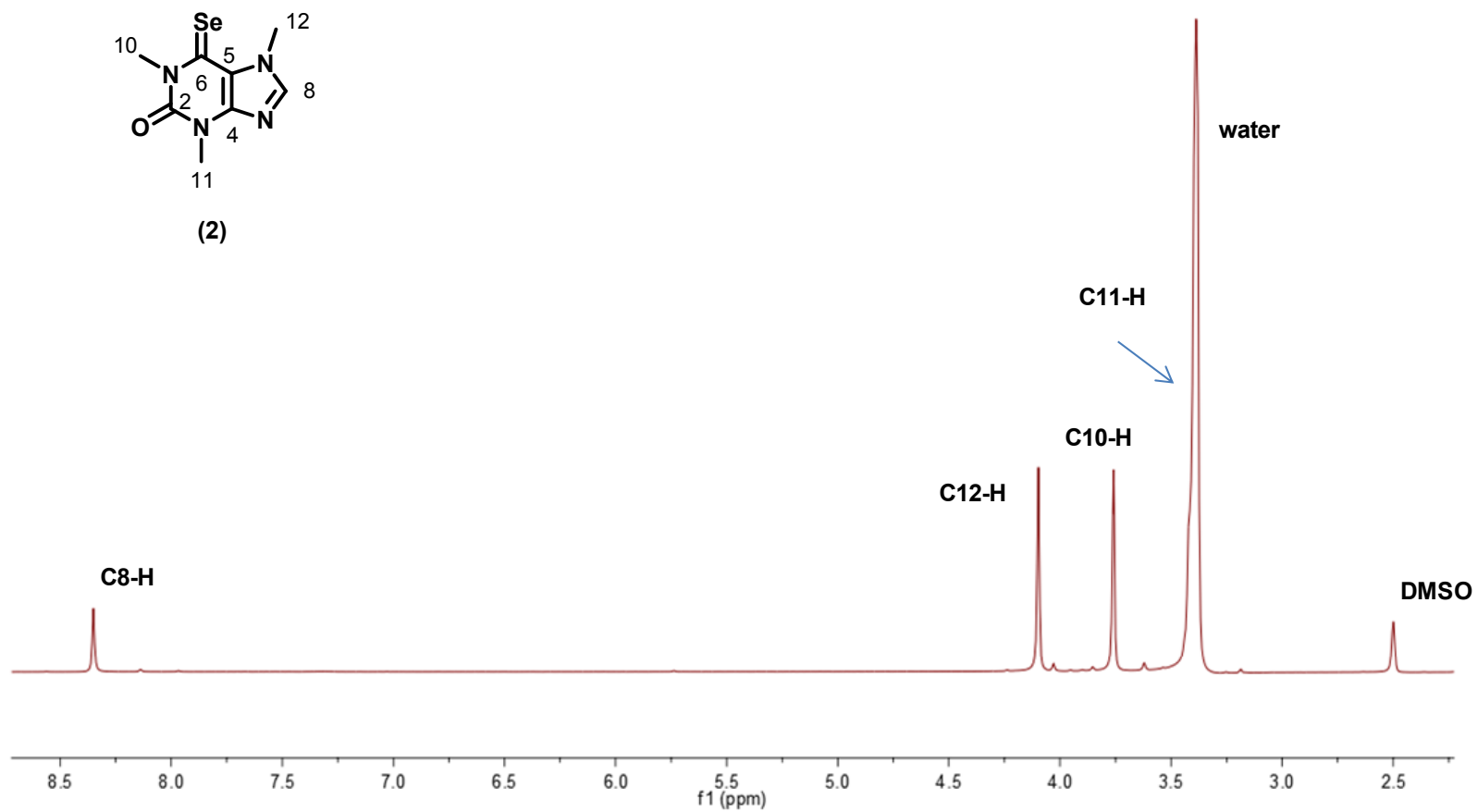


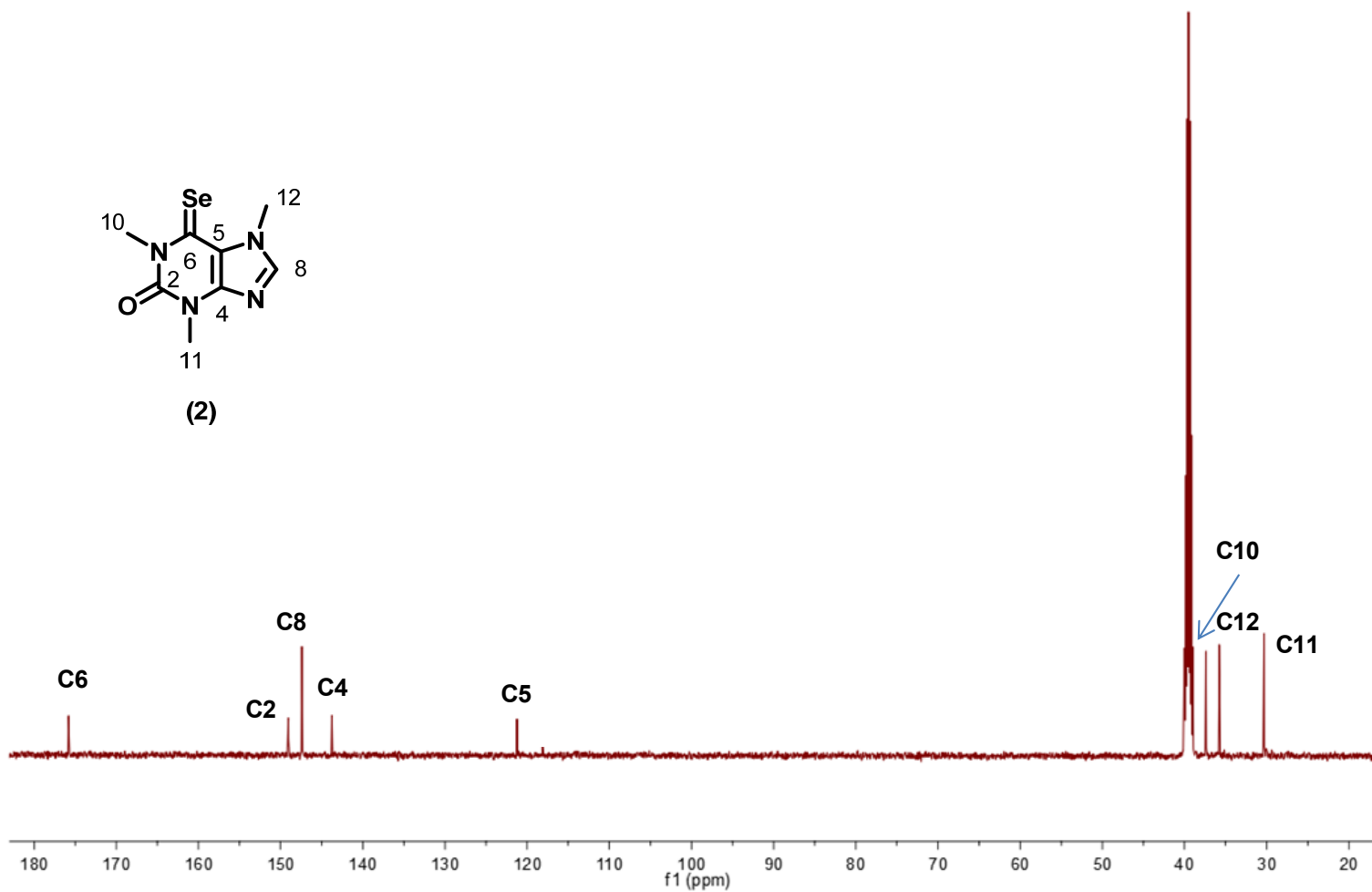
Figure S2. ^{13}C -NMR spectrum of 6-selenocaffeine, recorded in DMSO-d_6 .

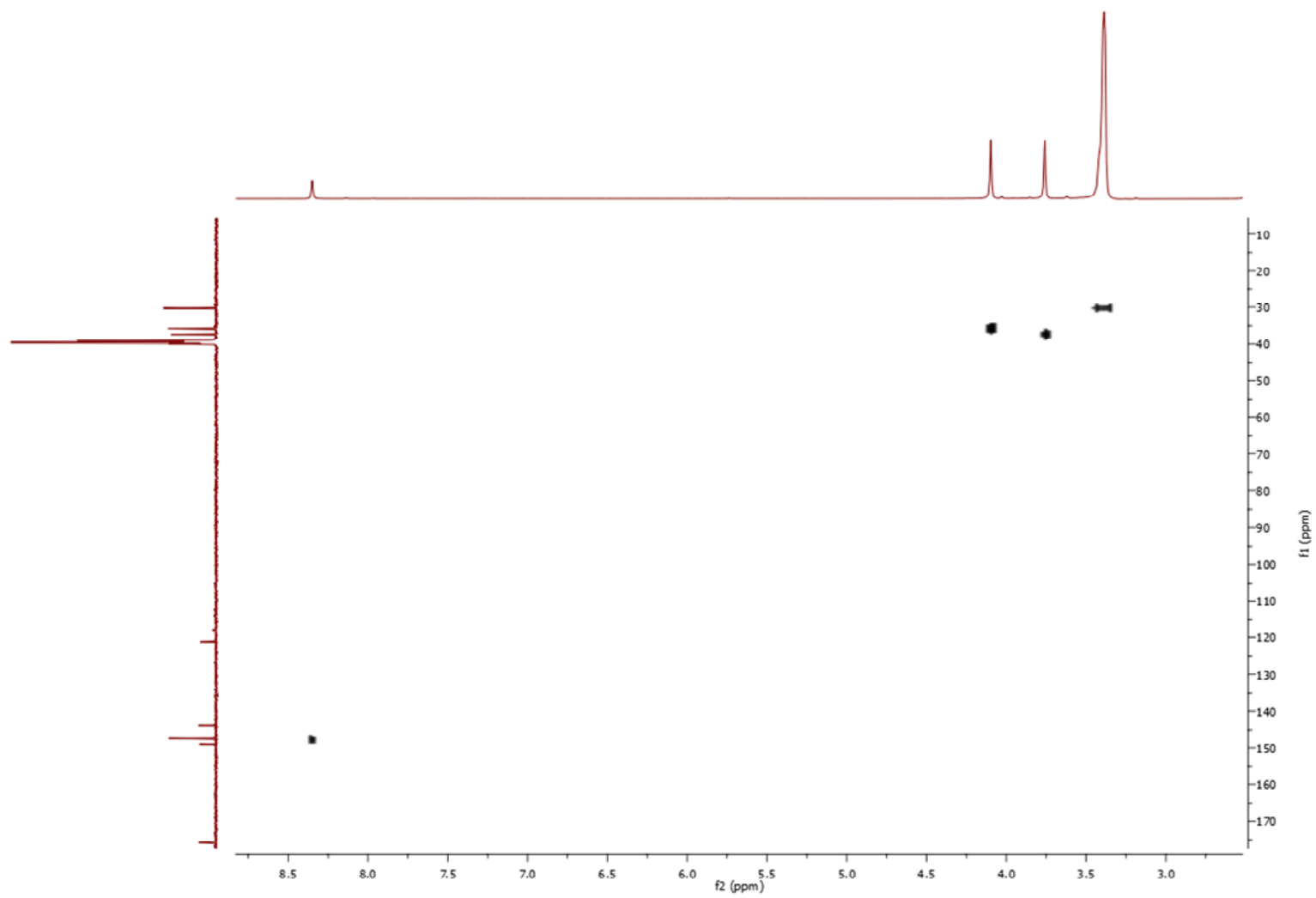
Figure S3. HSQC spectrum of 6-selenocaffeine, recorded in DMSO-d₆.

Figure S4. ^{77}Se -NMR spectrum of 6-selenocaffeine, recorded in DMSO- d_6 .

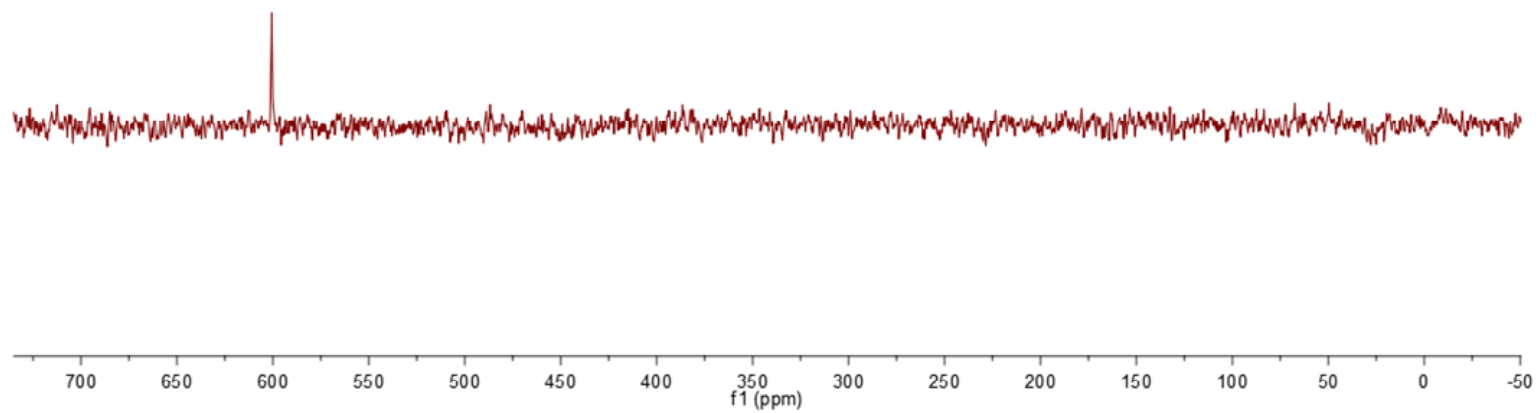


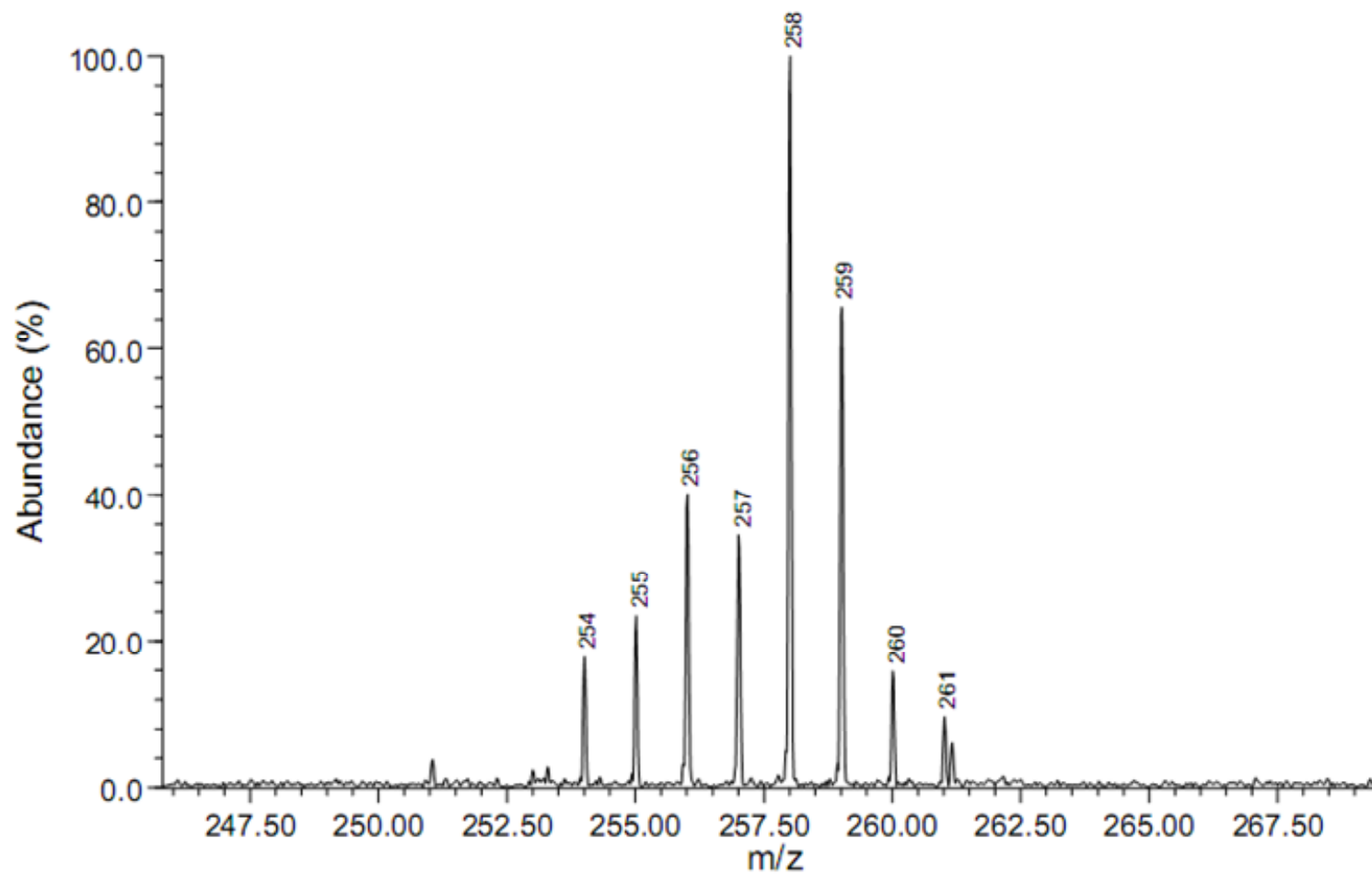
Figure S5. Mass spectrum HRMS (EI) of 6-selenocaffeine.

Figure S6. HPLC-DAD chromatogram of 6-selenocaffeine.

