Supplementary Materials

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

![NMR spectrum of 6-selenocaffeine](image)
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.