

Description of Additional Supplementary Files

File name: Supplementary Data 1

Description: LC-MS data underlying the histograms in Figures 1 and 3.

File name: Supplementary Data 2

Description: Data underlying the MS/MS spectra in Figure 1.

File name: Supplementary Data 3

Description: Data underlying the experimental IR spectra in Figure 1 and 3.

File name: Supplementary Data 4

Description: Data underlying the theoretical IR spectra and coordinates of the quantum-chemically optimized structures in Figure S6.