

Supplementary Materials

$^1\text{H-NMR}$ Spectra of Labelled Opiates

$^1\text{H-NMR}$ of [*N*-Methyl- ^{13}C -O-methyl- ^{13}C]codeine ($[^{13}\text{C}_2]$ -2):

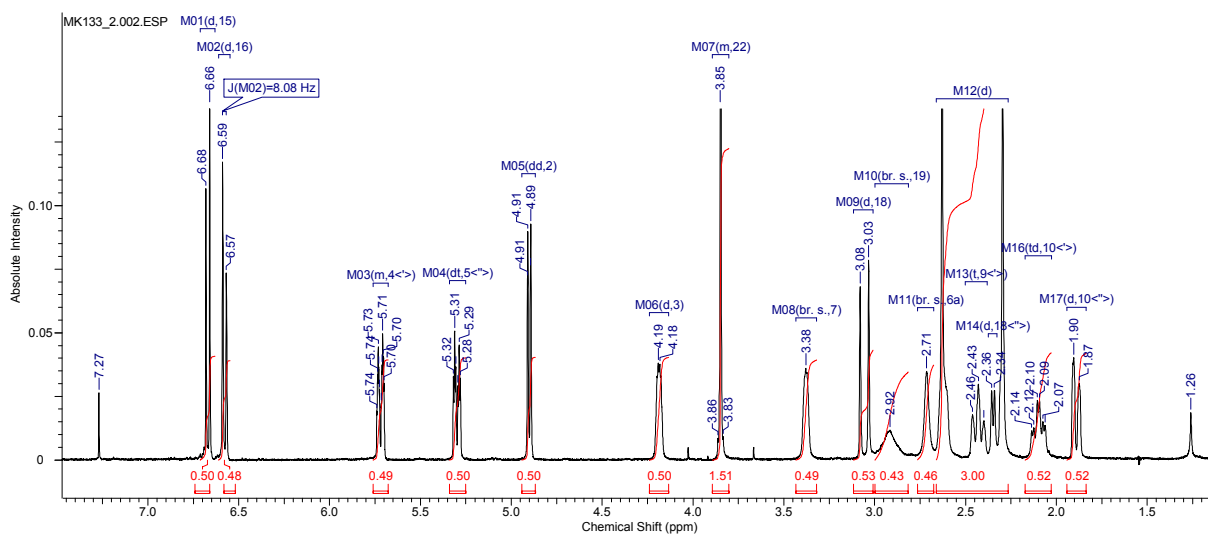


Figure S1. $^1\text{H-NMR}$ (400 MHz, CDCl_3) [*N*-methyl- ^{13}C -O-methyl- ^{13}C]codeine ($[^{13}\text{C}_2]$ -2).

$^1\text{H-NMR}$ of [Acetyl- $^{13}\text{C}_4$]heroin ($[^{13}\text{C}_4]$ -4):

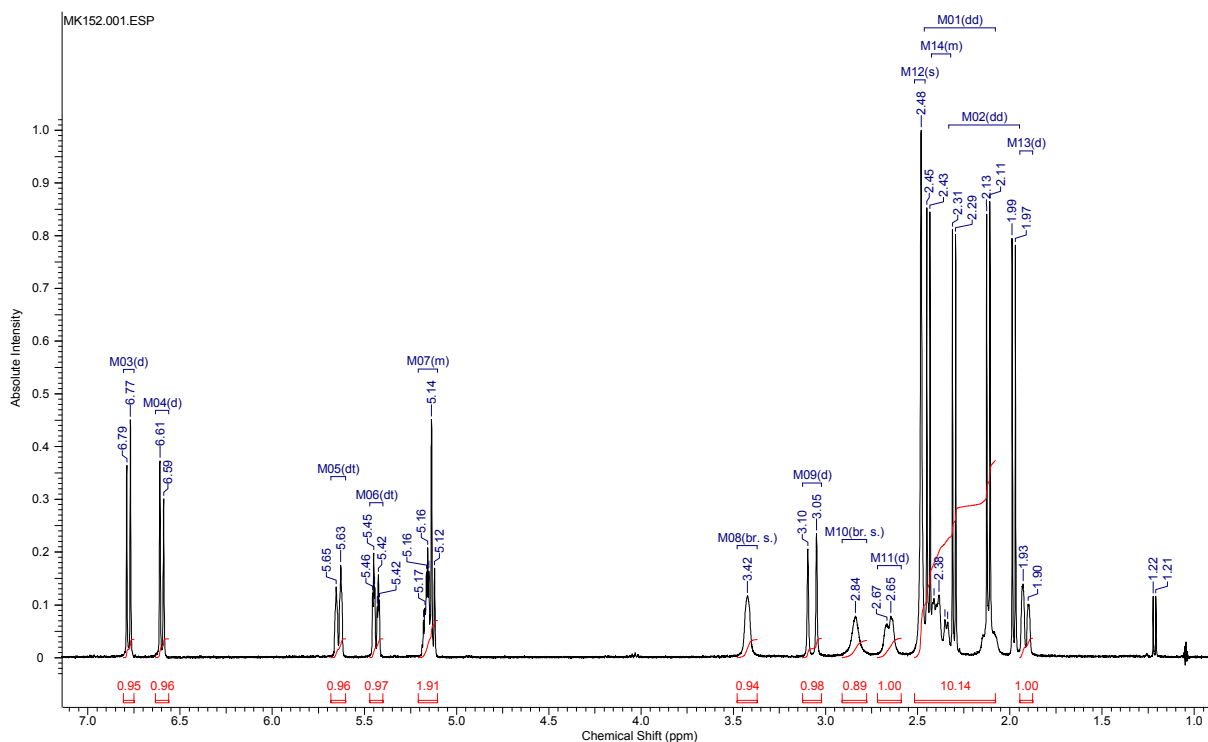


Figure S2. $^1\text{H-NMR}$ (400 MHz, CDCl_3) of [acetyl- $^{13}\text{C}_4$]heroin ($[^{13}\text{C}_4]$ -4).

$^1\text{H-NMR}$ of [Acetyl- $^{13}\text{C}_4$ -methyl- ^{13}C]heroin ($[^{13}\text{C}_5]$ -4):

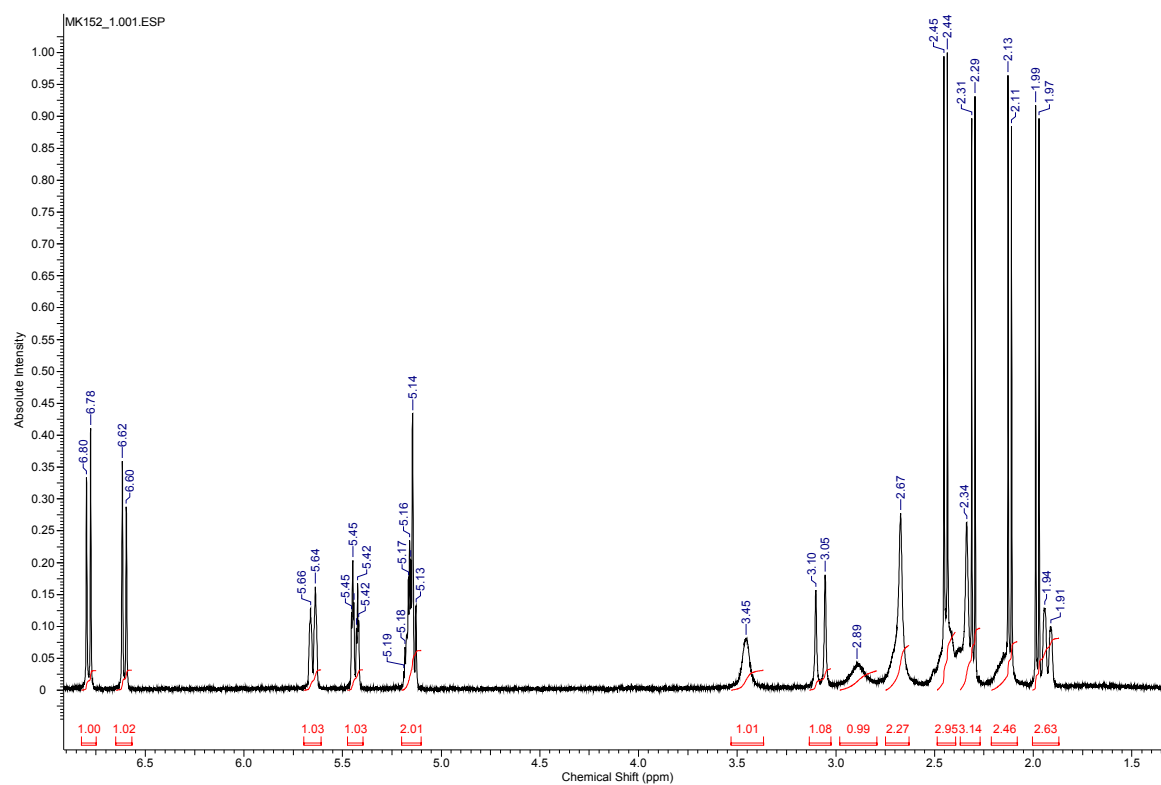


Figure S3. $^1\text{H-NMR}$ (400 MHz, CDCl_3) of [acetyl- $^{13}\text{C}_4$ -methyl- ^{13}C]heroin ($[^{13}\text{C}_5]$ -4).

$^1\text{H-NMR}$ of [Acetyl- $^{13}\text{C}_2$ -methyl- ^{13}C]6-acetylmorphine ($[^{13}\text{C}_3]$ -5):

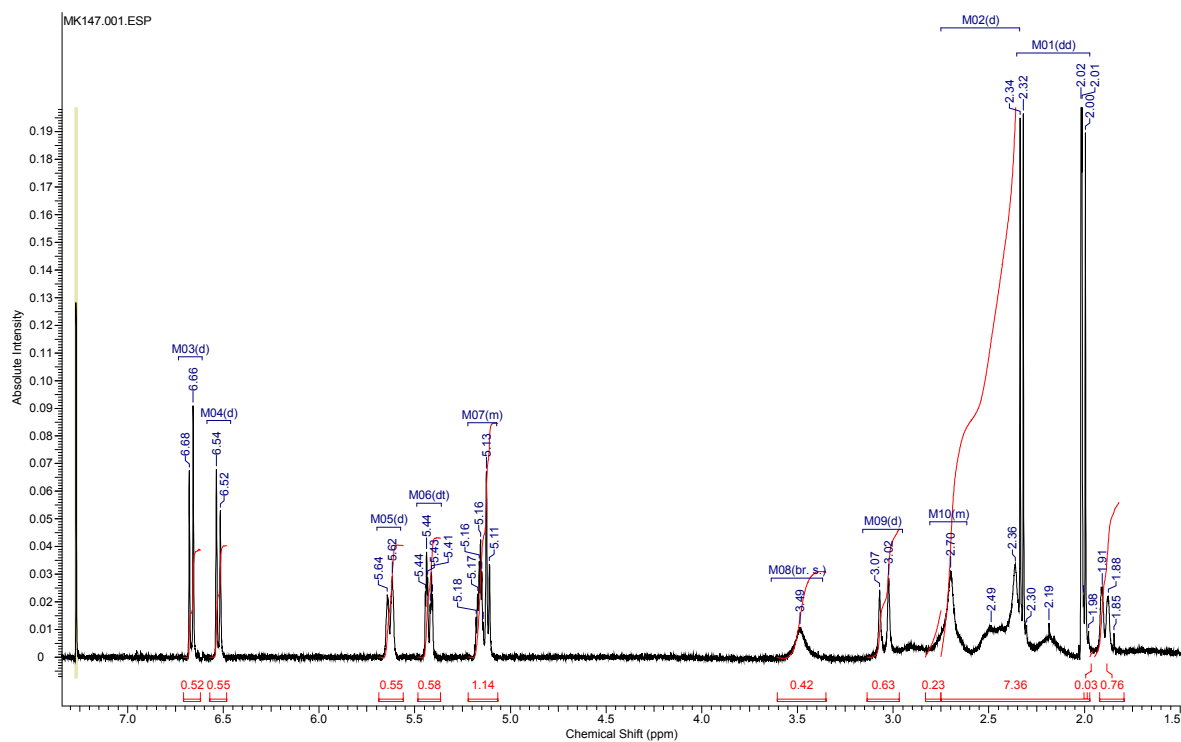
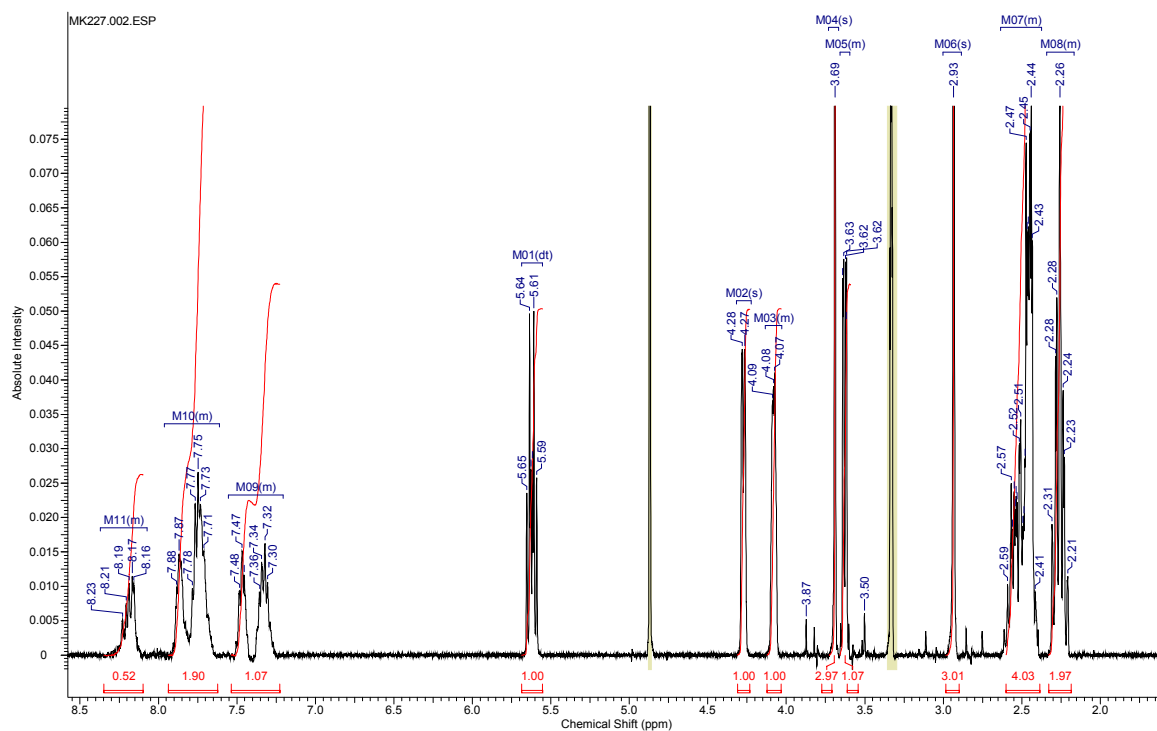
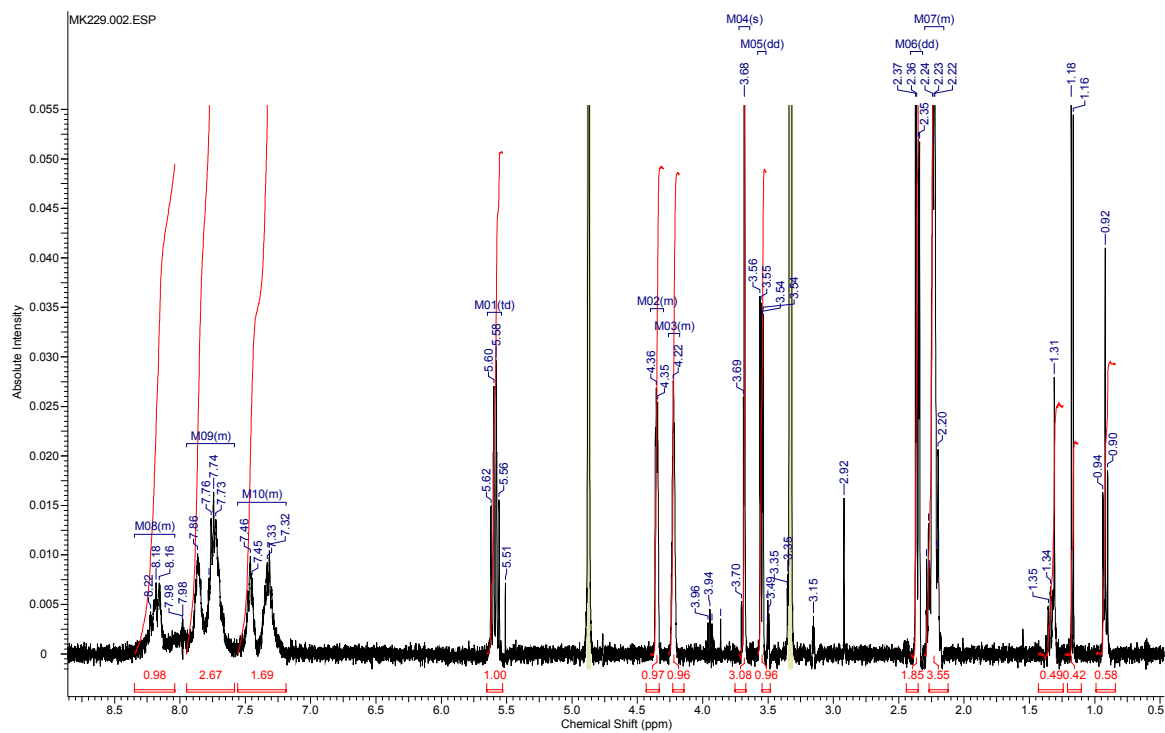


Figure S4. $^1\text{H-NMR}$ (400 MHz, CDCl_3) of [acetyl- $^{13}\text{C}_2$ -methyl- ^{13}C]6-acetylmorphine ($[^{13}\text{C}_3]$ -5).

$^1\text{H-NMR}$ of Labelled Cocaine Derivatives *$^1\text{H-NMR}$ of [Phenyl- $^{13}\text{C}_6$]cocaine ([$^{13}\text{C}_6$]-7) hydrochloride:***Figure S5.** $^1\text{H-NMR}$ (400 MHz, CD_3OD) of [phenyl- $^{13}\text{C}_6$]cocaine ([$^{13}\text{C}_6$]-7) hydrochloride. *$^1\text{H-NMR}$ of [Phenyl- $^{13}\text{C}_6$]norcocaine ([$^{13}\text{C}_6$]-8):***Figure S6.** $^1\text{H-NMR}$ (400 MHz, CD_3OD) of [phenyl- $^{13}\text{C}_6$]norcocaine ([$^{13}\text{C}_6$]-8).

$^1\text{H-NMR}$ of [Phenyl- $^{13}\text{C}_6$]benzoylecgonine ($^{13}\text{C}_6$ -9)

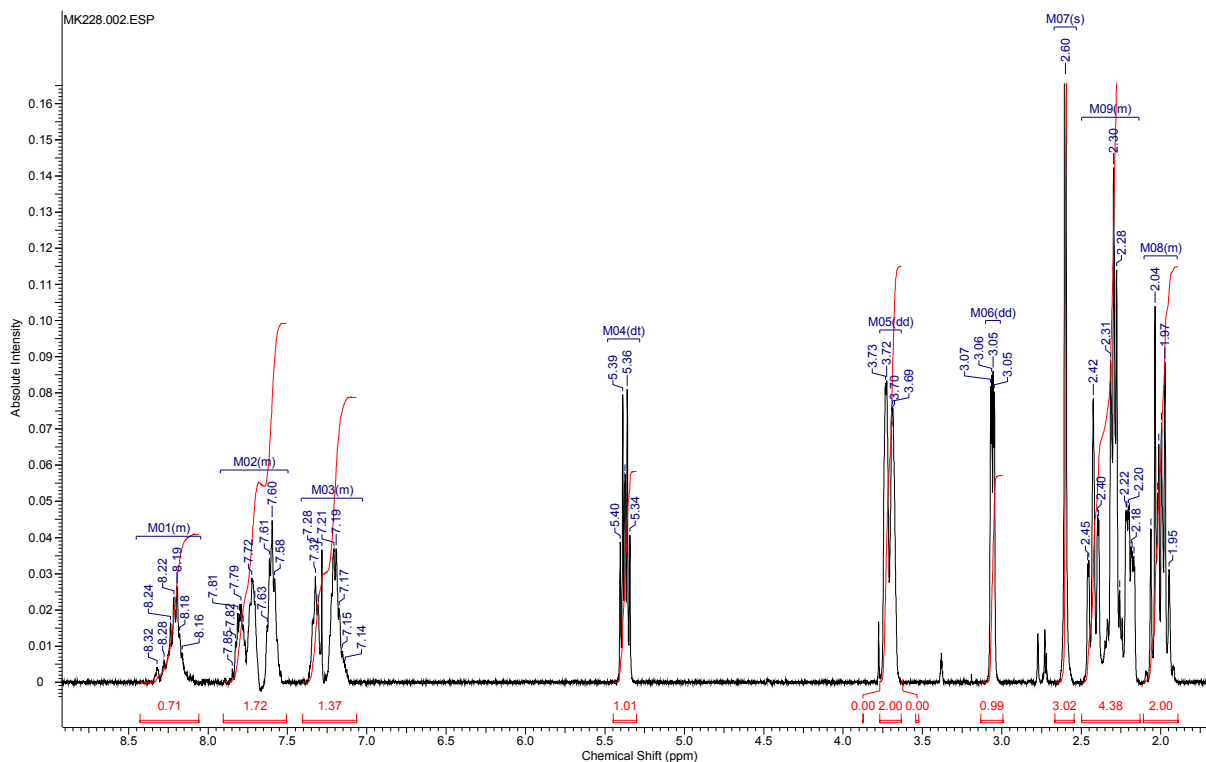


Figure S7. $^1\text{H-NMR}$ (400 MHz, CDCl_3) of [phenyl- $^{13}\text{C}_6$]benzoylecgonine ($^{13}\text{C}_6$ -9).

$^1\text{H-NMR}$ of [Phenyl- $^{13}\text{C}_6$]cocaethylene (10):

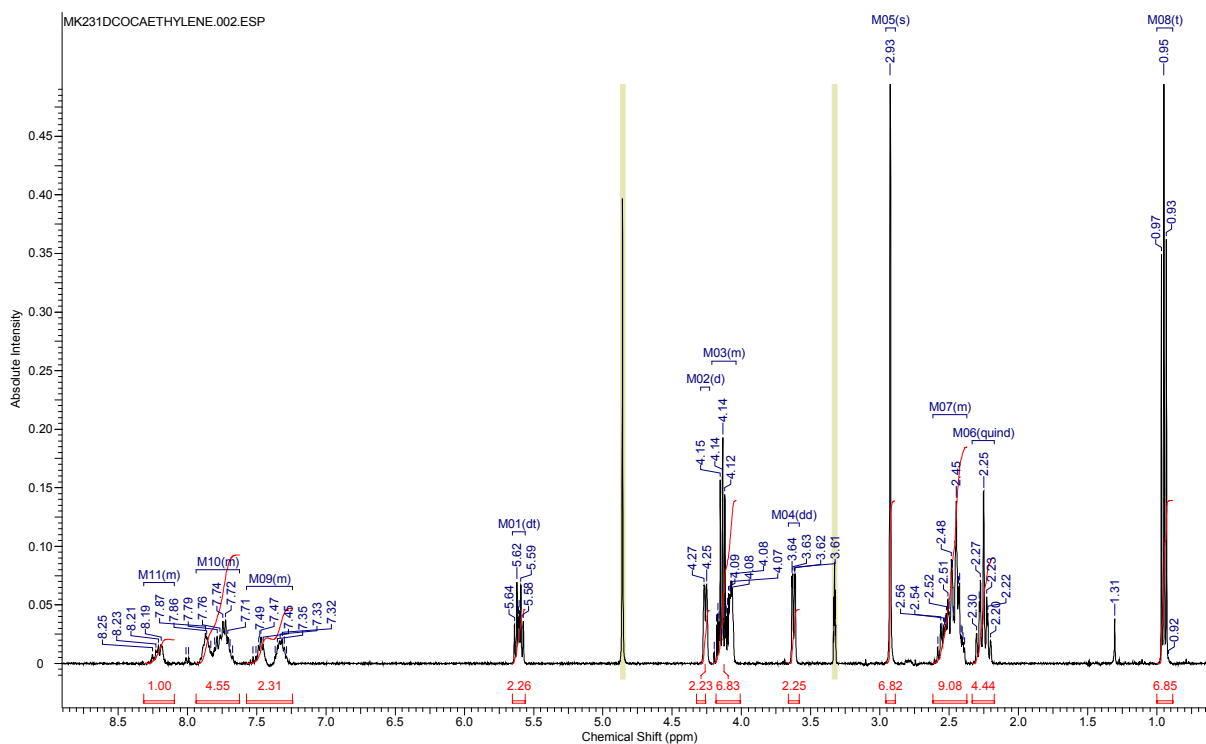


Figure S8. $^1\text{H-NMR}$ (400 MHz, CD_3OD) of [phenyl- $^{13}\text{C}_6$]cocaethylene (10).