Supplementary Materials

Enantioselectivity of Pentedrone and Methylone on Metabolic Profiling in 2D and 3D Human Hepatocyte-like Cells

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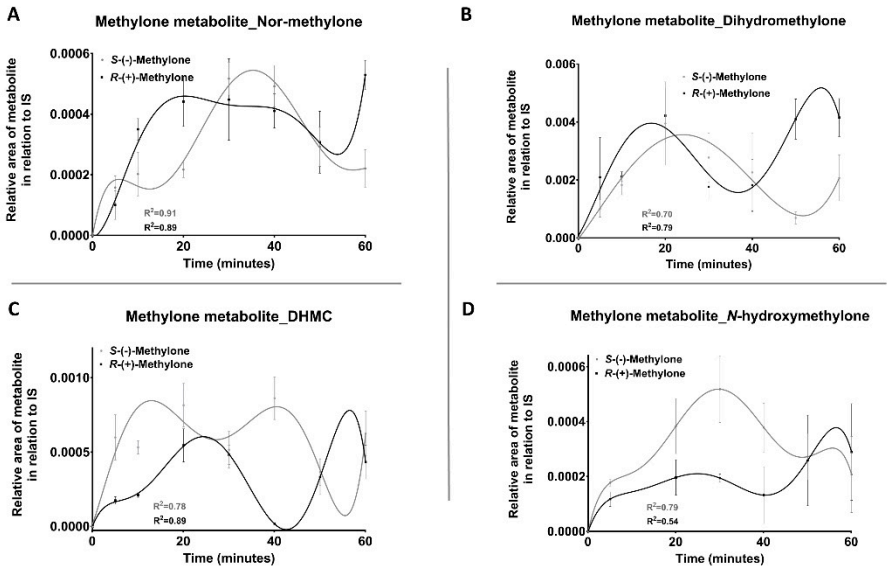

Figure S1. Methylone metabolites (nor-methylone, DHMC, *N*-hydroxymethylone and dihydromethylone) produced over the time after incubation with microsomes (1 mg/mL). Data is presented as average ± SD (n=2). Polynomial regression was used to fit the curves (Nor-methylone, DHMC and *N*-hydroxymethylone: Centered sixth order; Dihydromethylone: Centered fifth order).

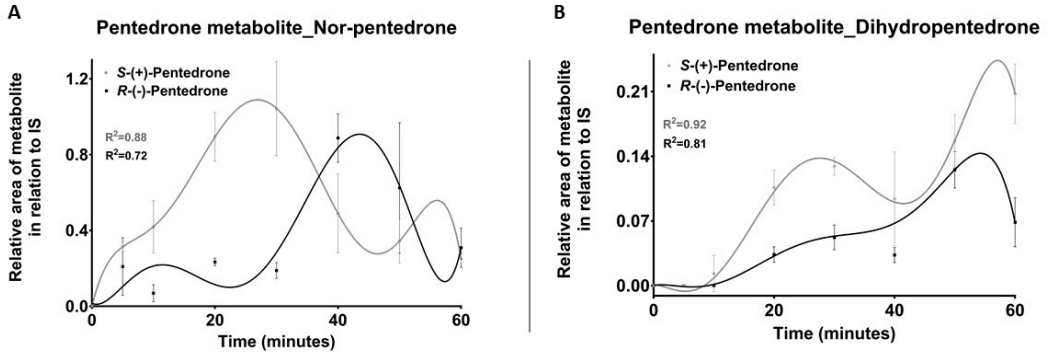

Figure S2. Pentedrone metabolites (nor-pentedrone and dihydropentedrone) produced over the time after incubation with microsomes (1 mg/mL). Data is presented as average ± SD (n=2). Centered sixth order polynomial regression were used to fit the curves.

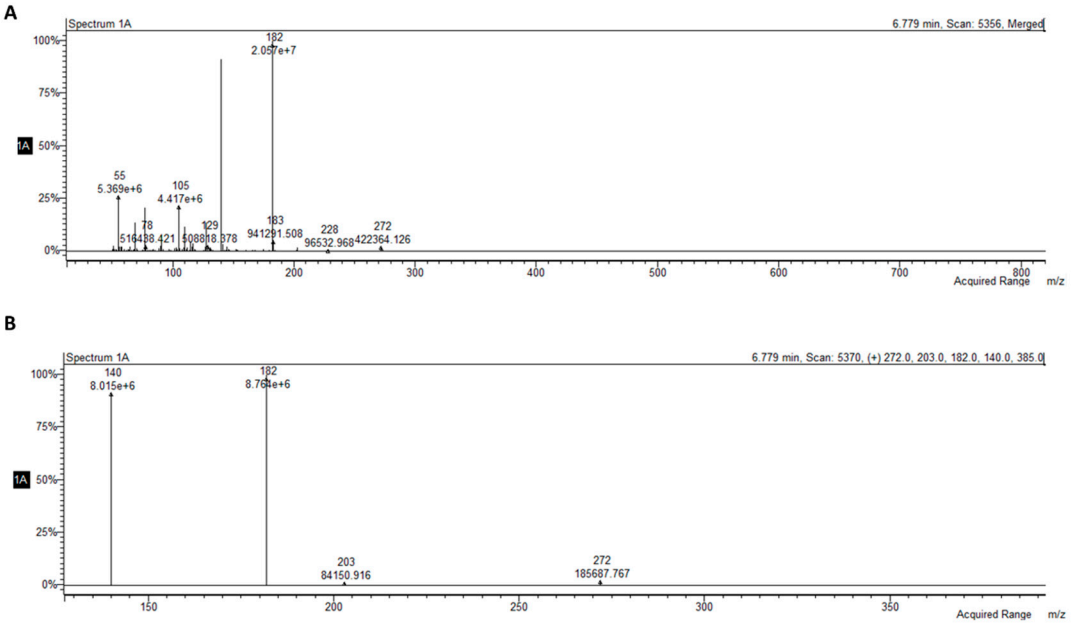

Figure S3. GC-MS spectrum of dihydropentedrone in (**A**) Full Scan and (**B**) SIM mode.

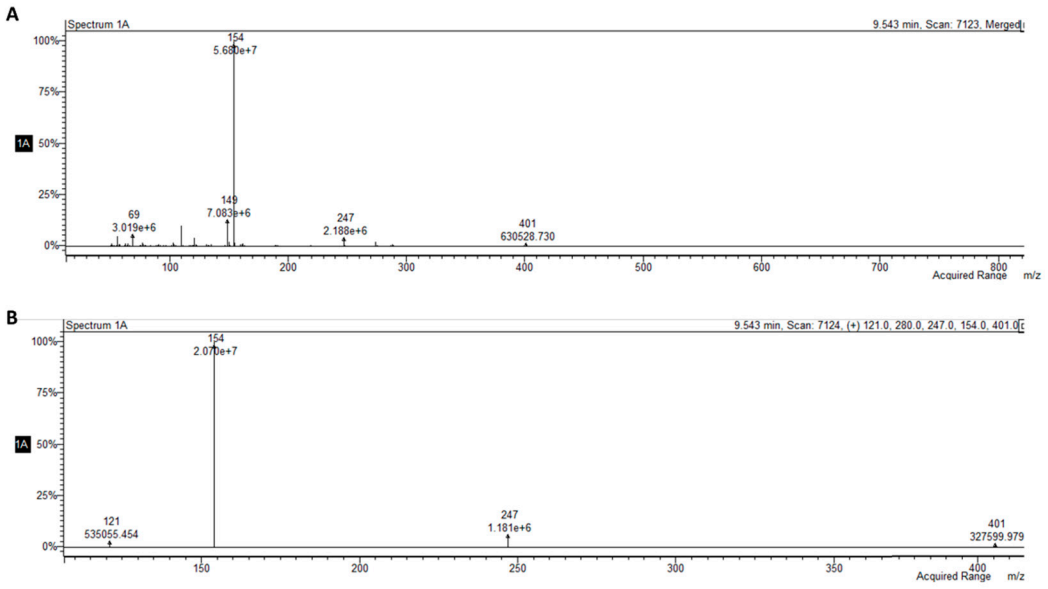

Figure S4. GC-MS spectrum of dihydromethylone in (**A**) Full Scan and (**B**) SIM mode.

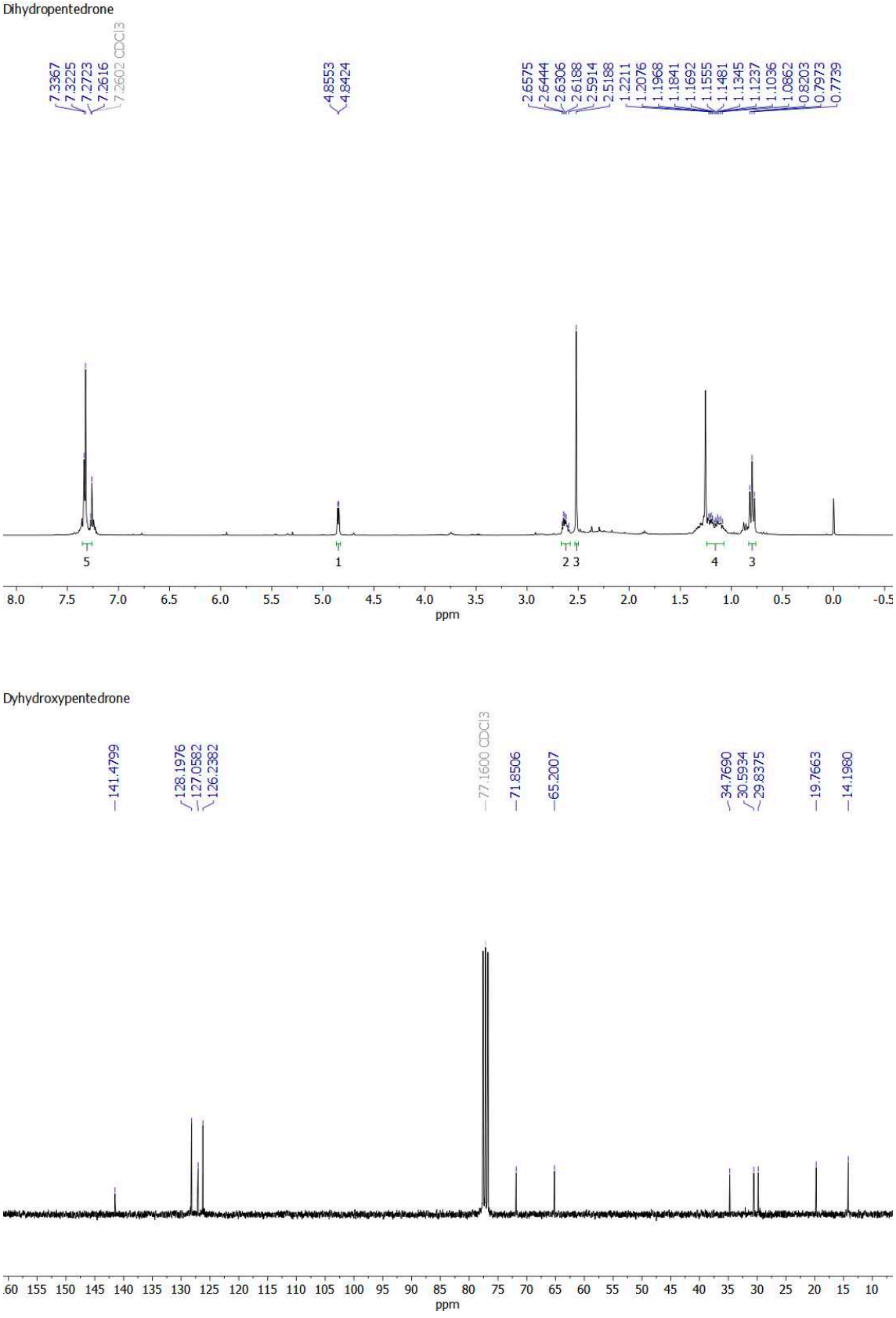

Figure S5. ^{1}H NMR (300.13 MHz, $CDCl_3$) and ^{13}C NMR (75.48 MHz, DMSO-d_6) for dihydromethylone.

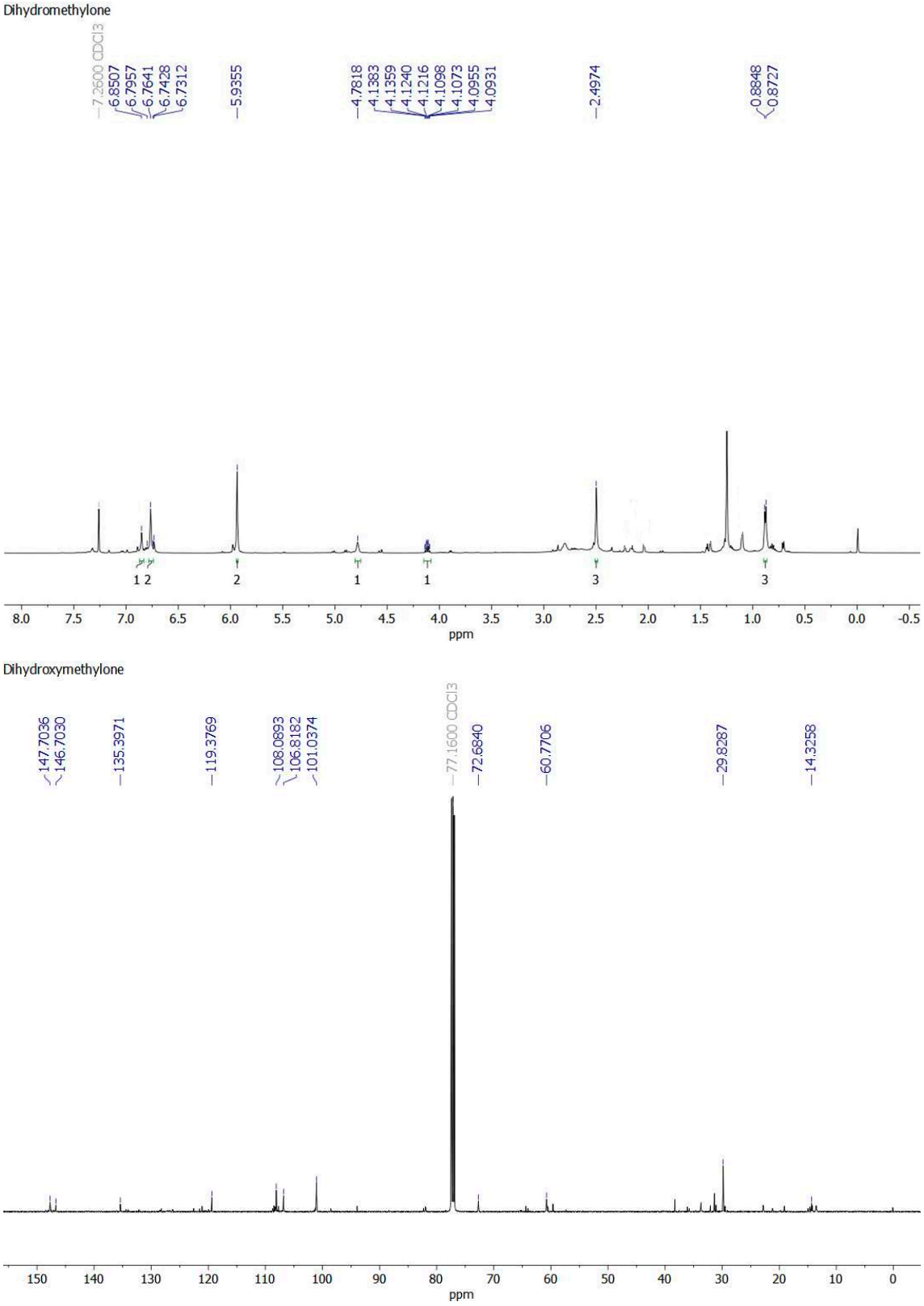

Figure S6. ^{1}H NMR (300.13 MHz, $CDCl_3$) and ^{13}C NMR (75.48 MHz, DMSO-d_6) for dihydropentedrone.