Isolation and Structural Determination of Non-Racemic Tertiary Cathinone Derivatives

Electronic Supplementary Information

MengJie Zhou,[a] Samira Bouazzaoui,[a] Louise E. Jones,[a] Peter Goodrich,[a] Steven J. E. Bell,[a] Gary N. Sheldrake,[a] Peter N. Horton, [b] Simon J. Coles,[b] and Nicholas C. Fletcher*[a,]

a: School of Chemistry and Chemical Engineering, Queen's University of Belfast, David Keir Building, Belfast, Northern Ireland, BT9 5AG, UK.
b: University of Southampton, Chemistry Department, EPSRC National, Crystallography Service, Southampton, SO17 1BJ, UK.
c: Department of Chemistry, Lancaster University, Bailrigg, Lancaster, LA1 4YB, UK
Email: n.fletcher@lancaster.ac.uk

Contents:

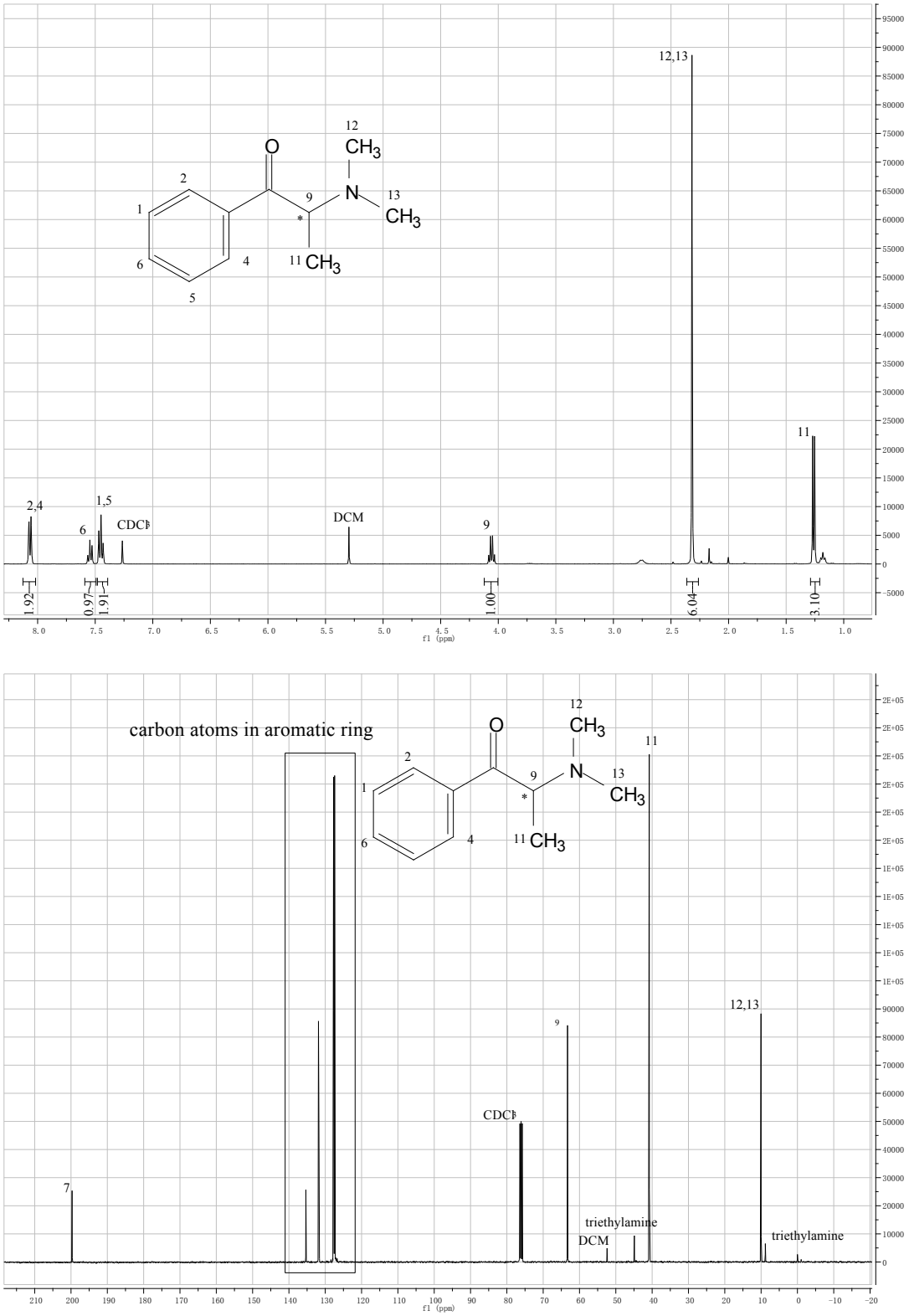


Figure S1 (a) ^{1}H NMR and (b) ^{13}C NMR spectra of (±)-*N,N*-dimethylcathinone (1) ($CDCl_3$, 20 °C).

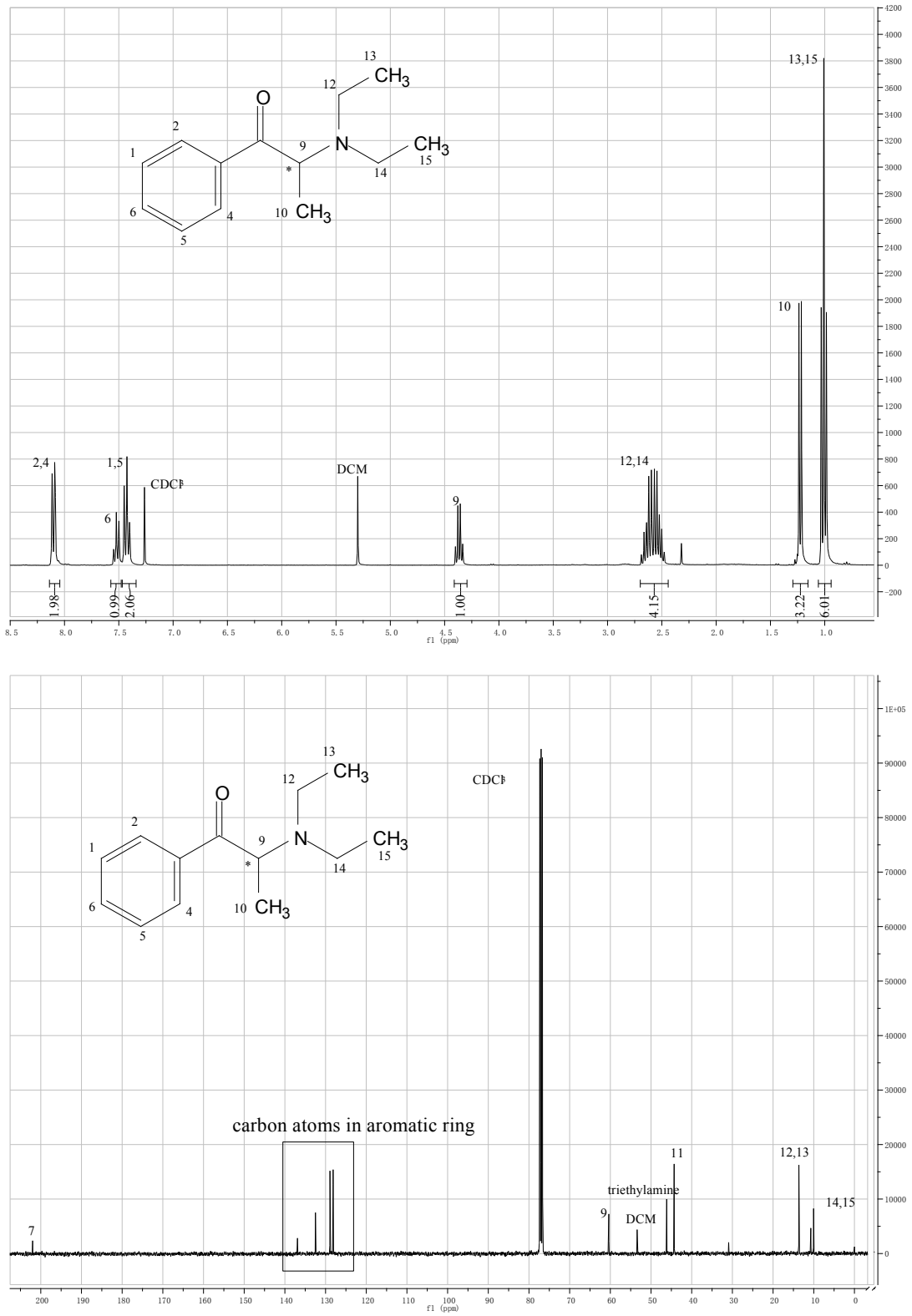


Figure S2 (a) ^{1}H NMR and (b) ^{13}C NMR spectra of (±)-*N,N*-diethylcathinone (2) ($CDCl_3$, 20 °C).

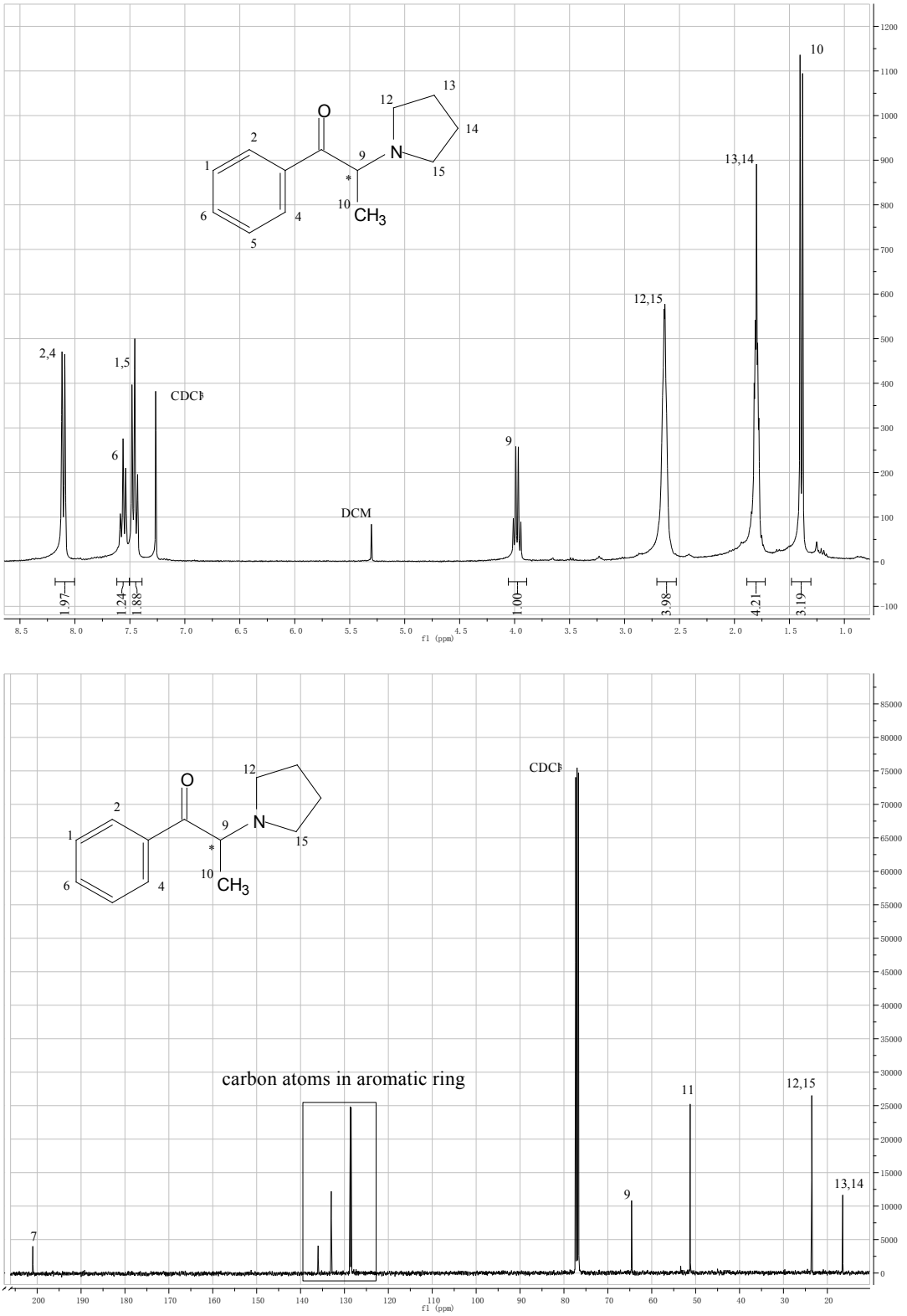


Figure S3 (a) ^{1}H NMR and (b) ^{13}C NMR spectra of (±)-2-(1-pyrrolidinyl)-propiophenone (3) ($CDCl_3$, 20 ^{o}C).

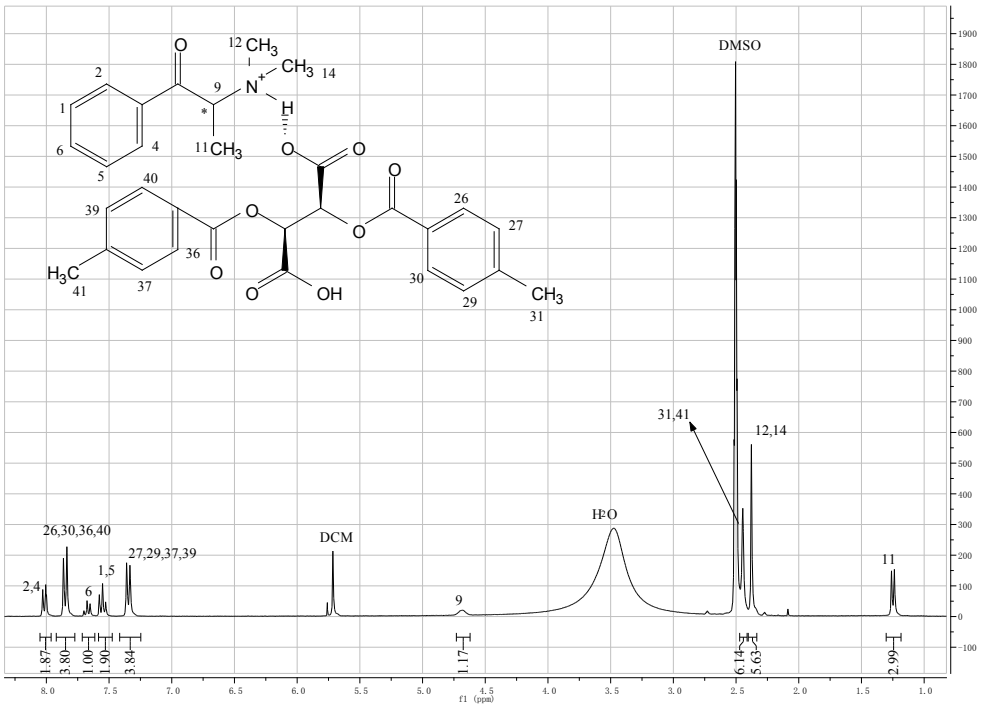


Figure S4 ^{1}H NMR spectrum of (±)-*N,N*-dimethylcathinone *D*-DTT salt (**1**-*D*-DTT) (DMSO-D_6, 20 °C).

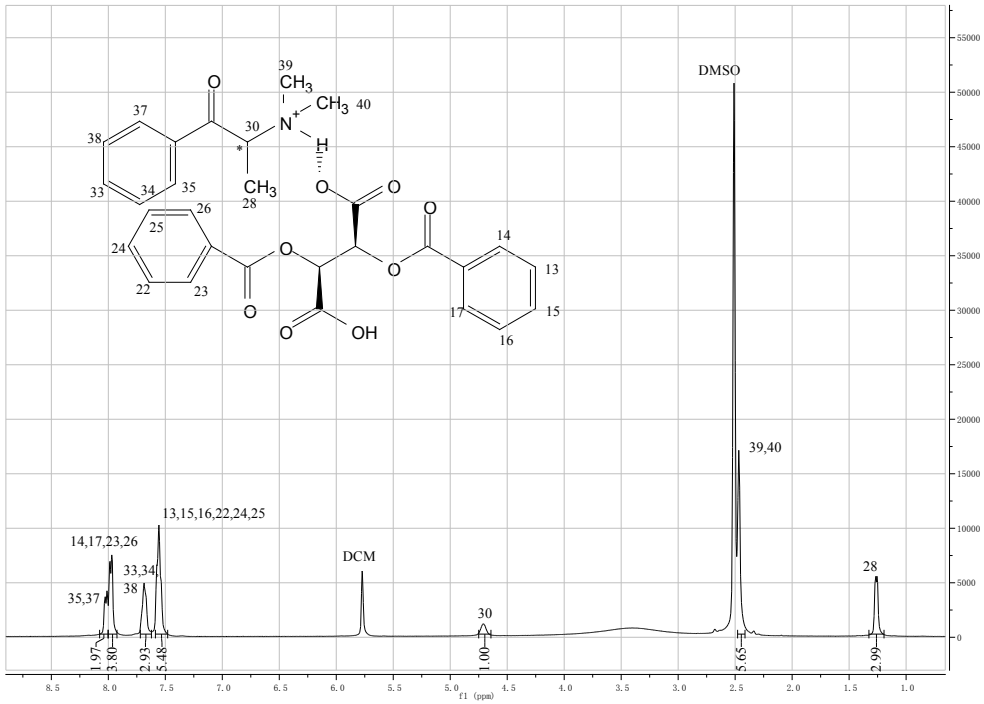


Figure S5 ^{1}H NMR spectrum of (±)-*N,N*-dimethylcathinone *D*-DBT salt (**1**-*D*-DBT) (DMSO-D_6, 20 °C).

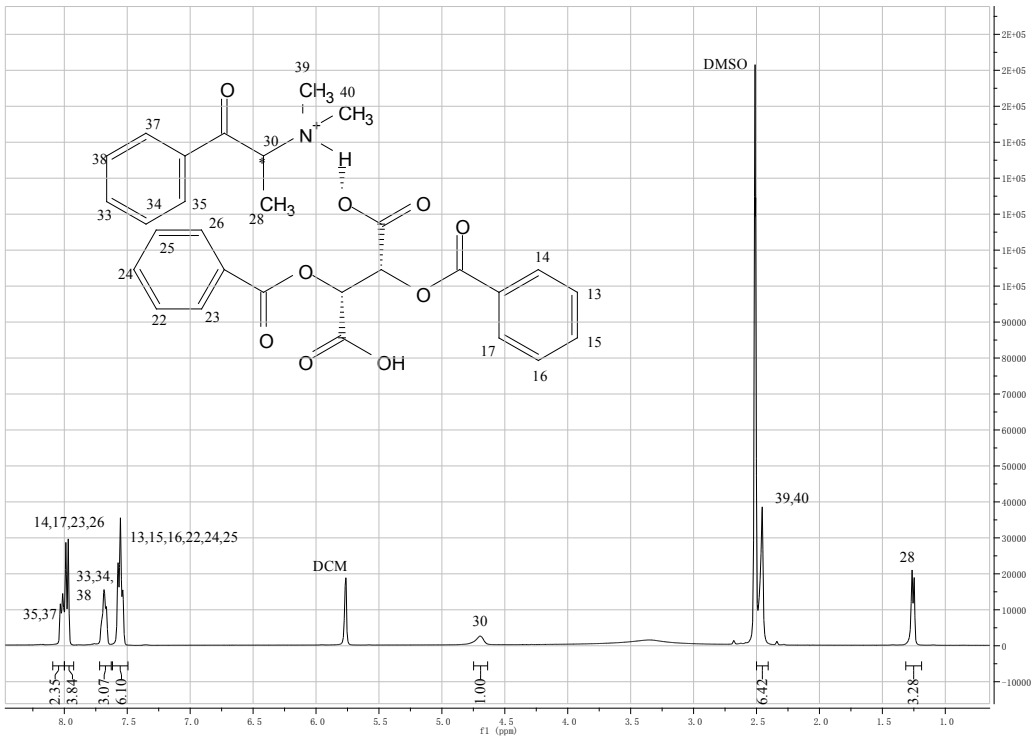


Figure S6 ^{1}H NMR spectrum of (±)-*N,N*-dimethylcathinone *L*-DBT salt (**1**-*L*-DBT) (DMSO-D_6, 20 °C).

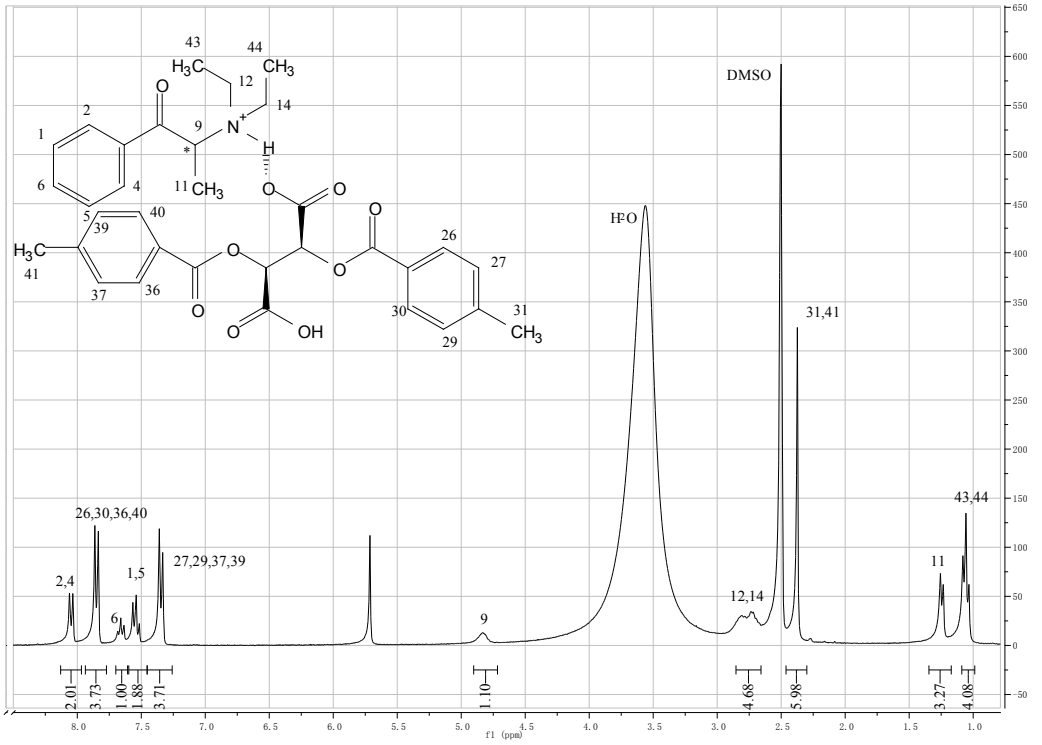


Figure S7 ^{1}H NMR spectrum of (±)-*N,N*-diethylcathinone *D*-DTT salt (**2**-*D*-DTT) (DMSO-D_6, 20 °C).

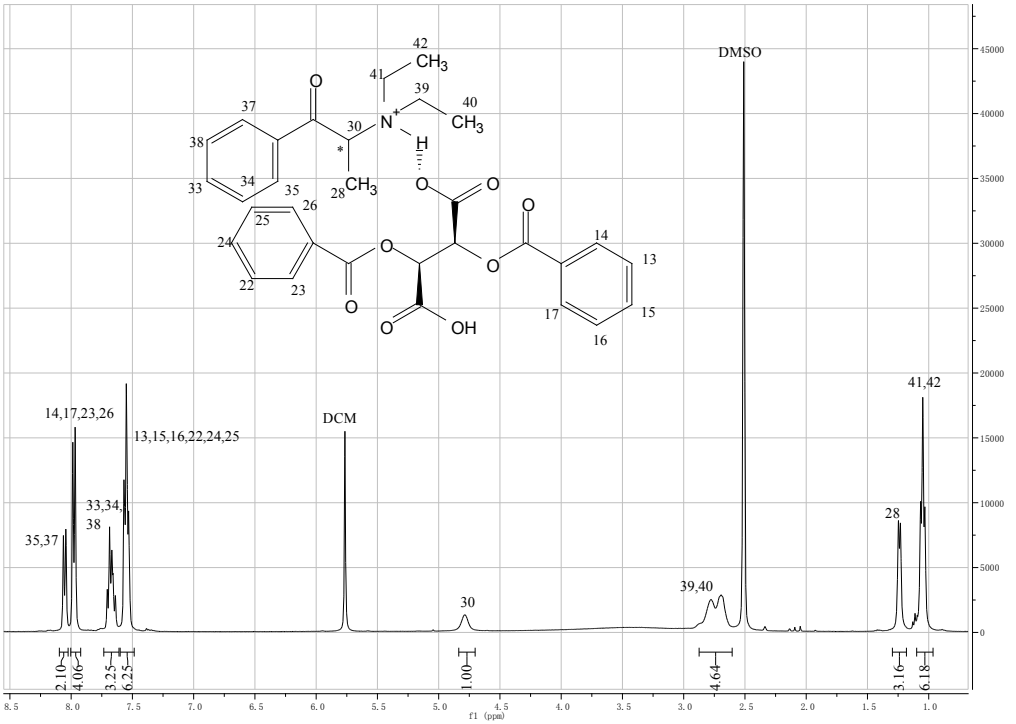


Figure S8 ^{1}H NMR spectrum of (±)-*N,N*-diethylcathinone *D*-DBT salt (**2**-*D*-DBT) (DMSO-D_6, 20 ºC).

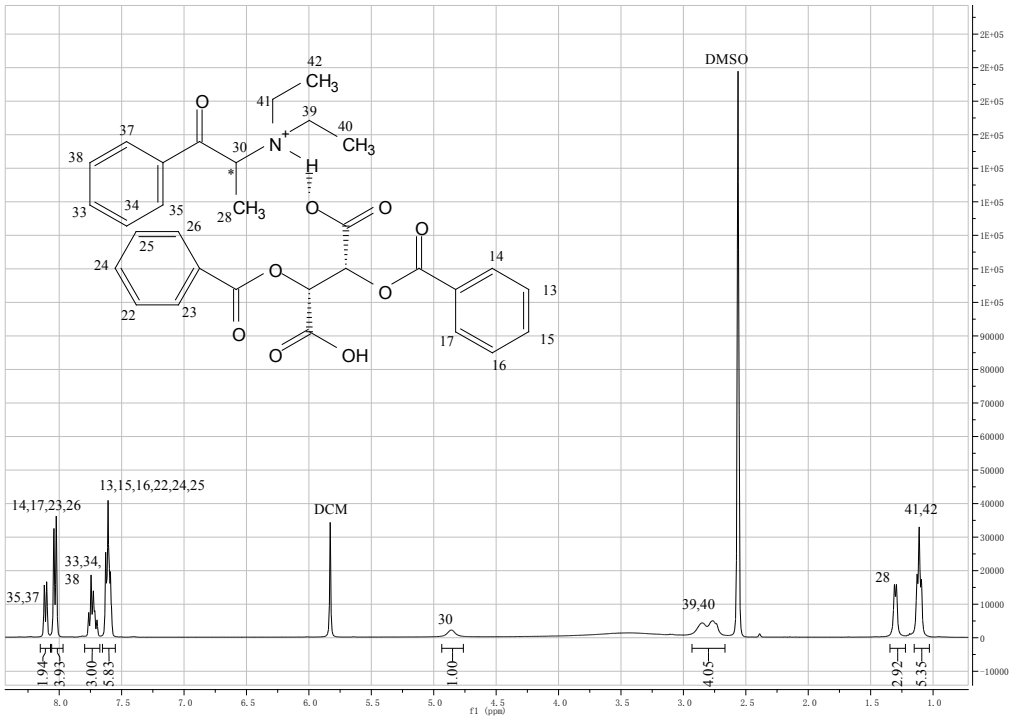


Figure S9 ^{1}H NMR spectrum of (±)-*N,N*-diethylcathinone *L*-DBT salt (**2**-*L*-DBT) (DMSO-D_6, 20 ºC).

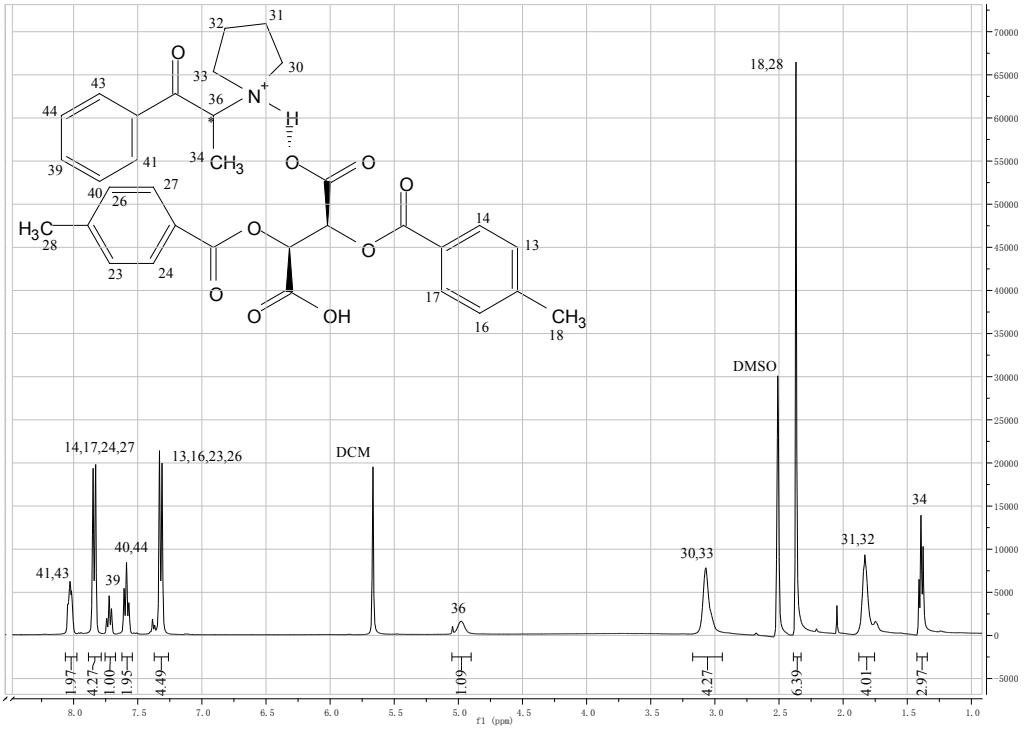


Figure S10 ^{1}H NMR spectrum of (±)-2-(1-pyrrolidinyl)-propiophenone *D*-DTT salt (**3**-*D*-DTT) (DMSO-D_6, 20 ºC).

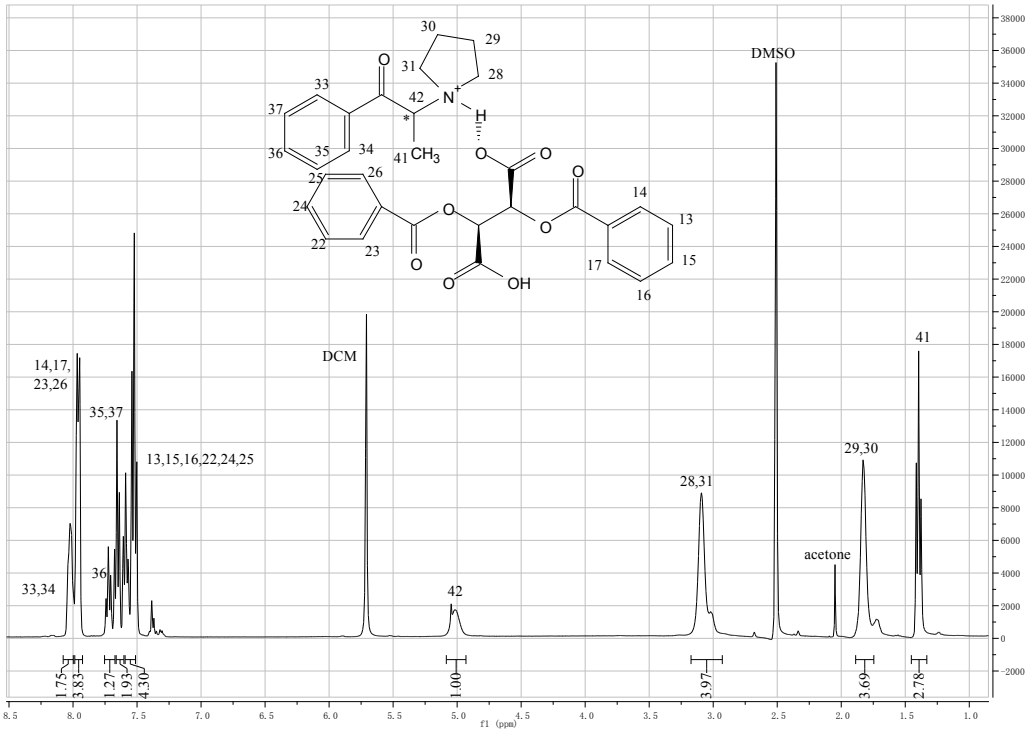


Figure S11 ^{1}H NMR spectrum of (±)-2-(1-pyrrolidinyl)-propiophenone *D*-DBT salt (**3**-*D*-DBT) (DMSO-D_6, 20 ºC).

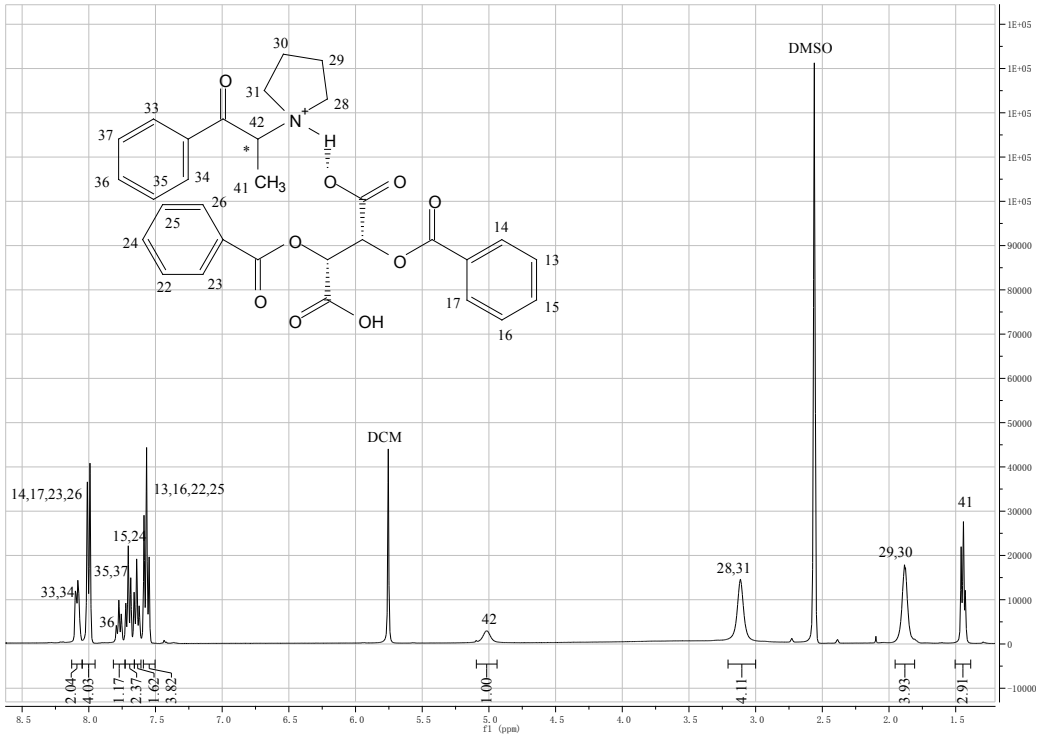


Figure S12 ^{1}H NMR spectrum of (±)-2-(1-pyrrolidinyl)-propiophenone *L*-DBT salt (**3**-*L*-DBT) (DMSO-$D_{6,}$ 20 ºC).

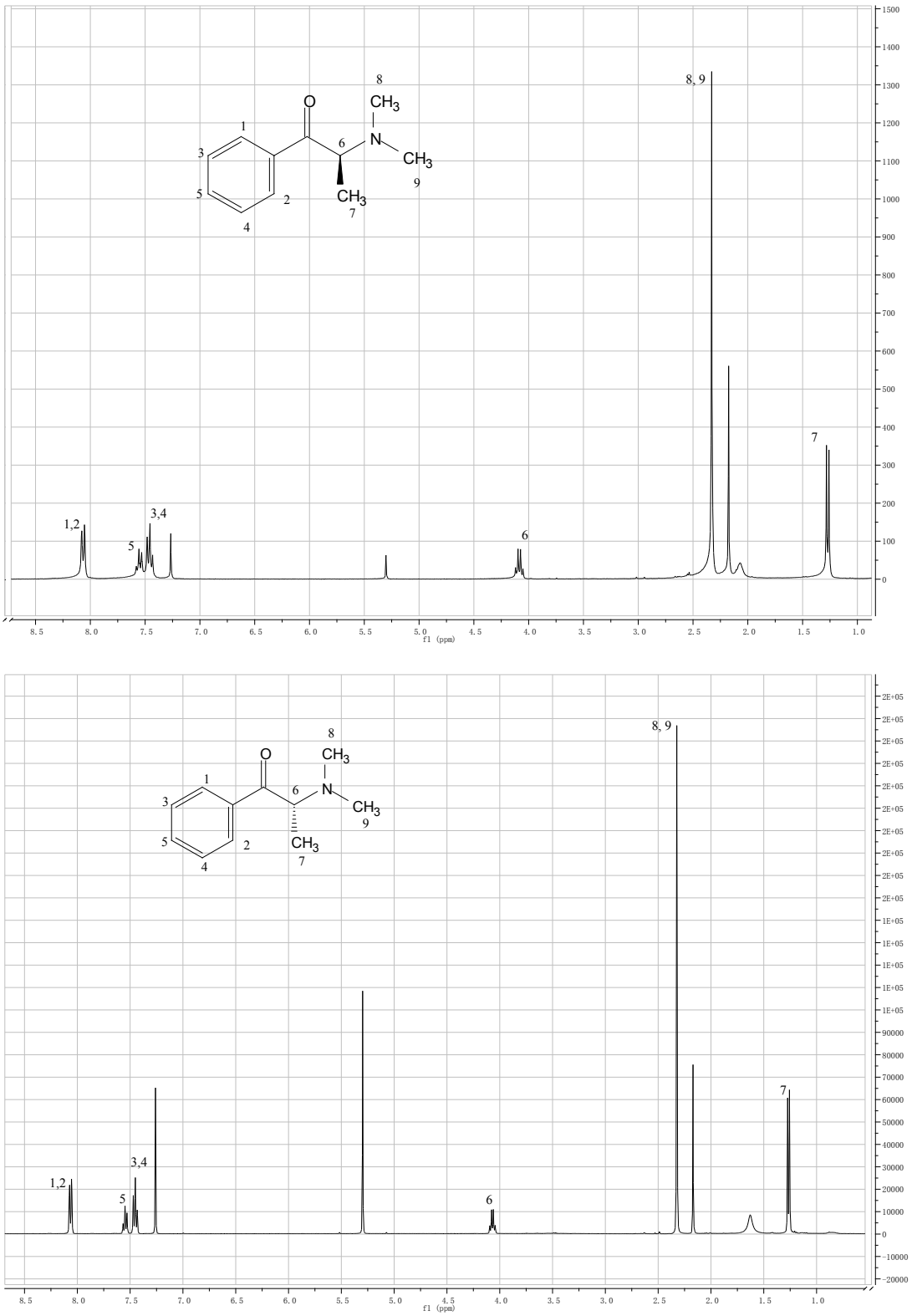


Figure S13 ^{1}H NMR spectra of compound (a) *S*-*N,N*-dimethylcathinone (*S*-**1**) and (b) *R*-*N,N*-dimethylcathinone (*R*-**1**) ($CDCl_3$, 20 ^{o}C).

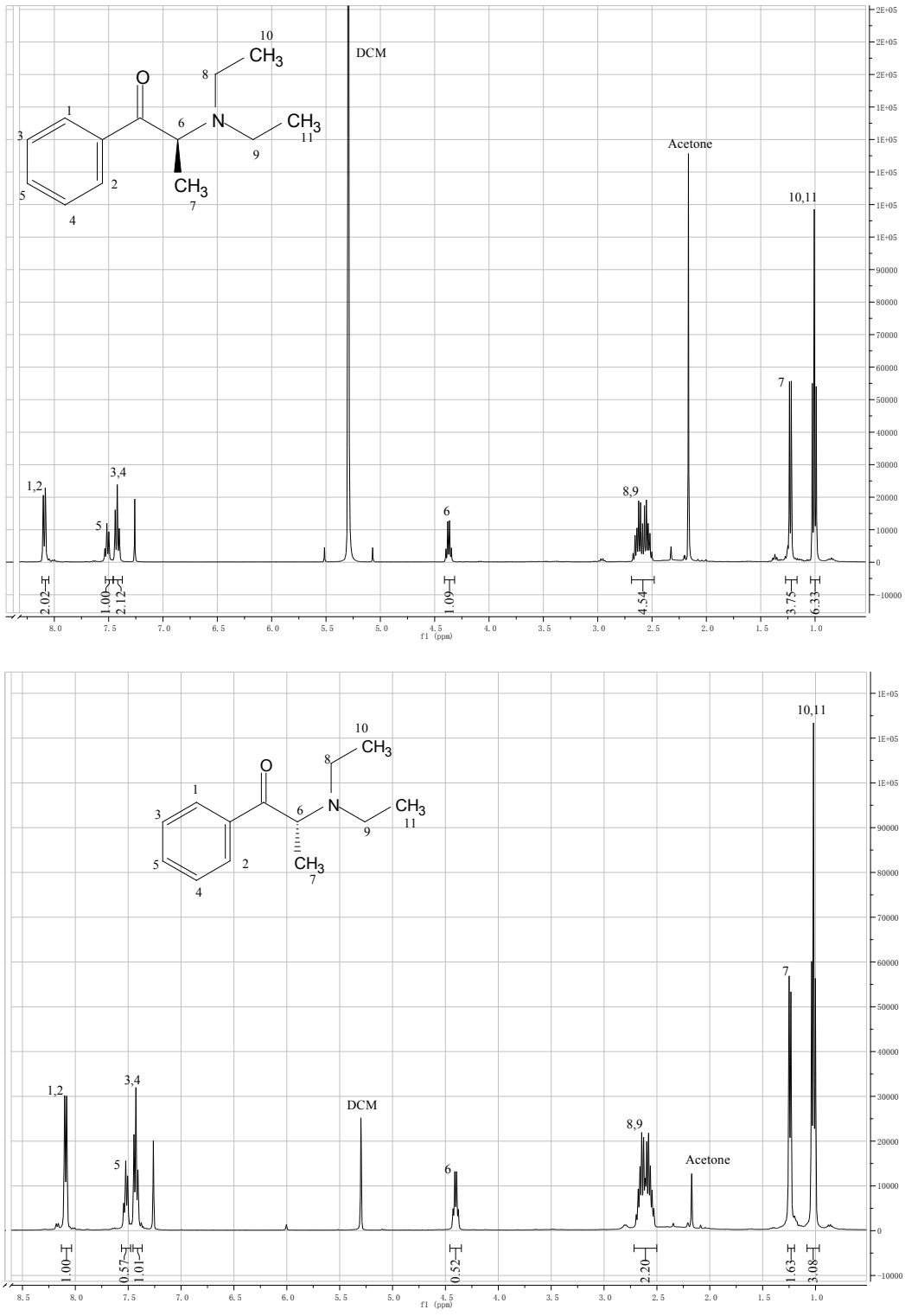


Figure S14 ^{1}H NMR spectra of compound (a) *S*-*N,N*-diethylcathinone (*S*-**2**) and (b) *R*-*N,N*-diethylcathinone (*R*-**2**) ($CDCl_3$, 20 ^{o}C).

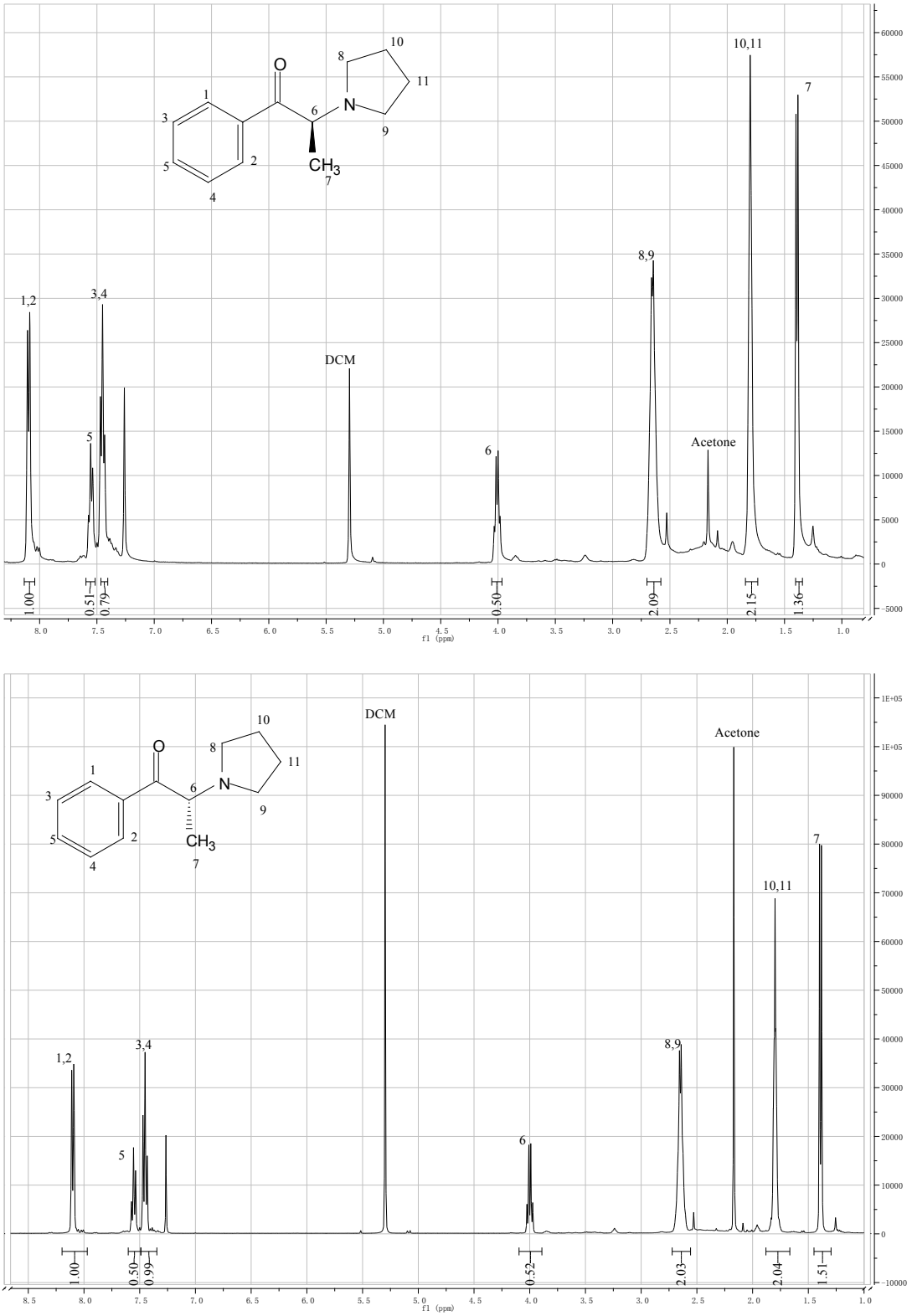
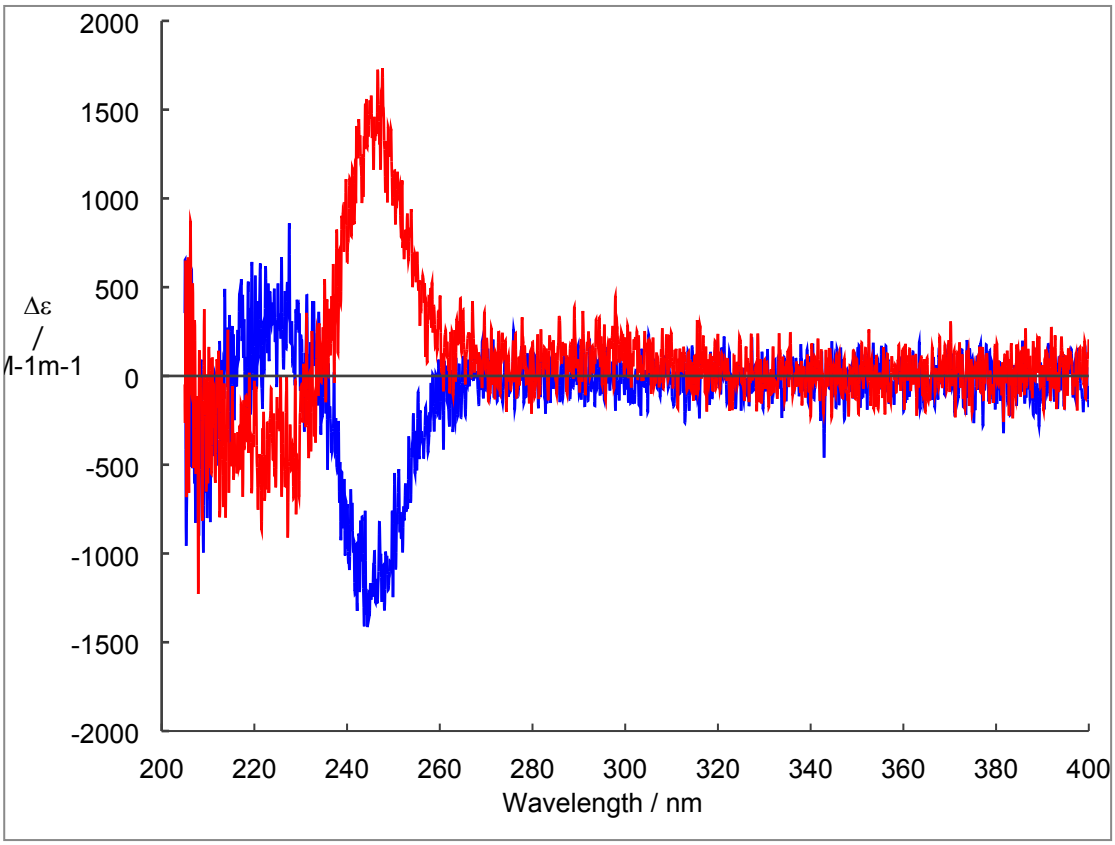


Figure S15 ^{1}H NMR spectra of compound (a) *S*-2-(1-pyrrolidinyl)-propiophenone (*S*-**3**) and (b) *R*-2-(1-pyrrolidinyl)-propiophenone (*R*-**3**) ($CDCl_3$, 20 ^{o}C).

(a)



(b)

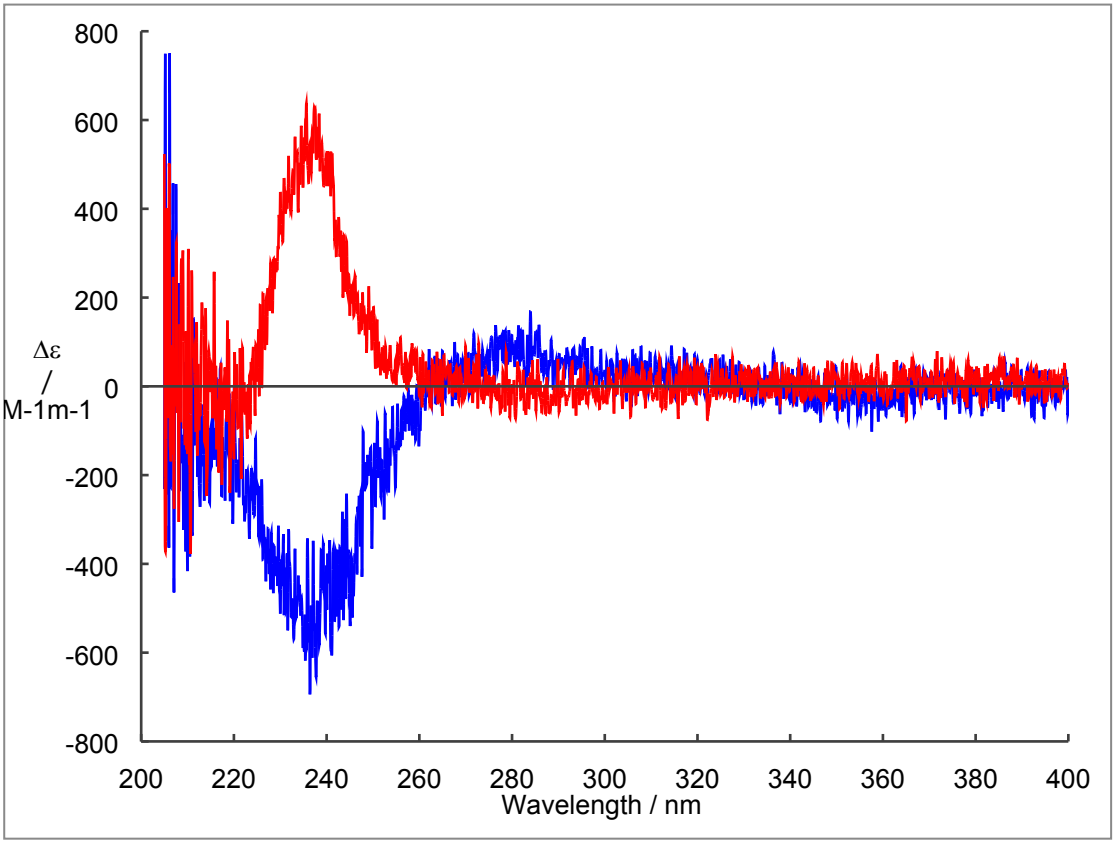


Figure S16 Circular Dichroism spectra of (a) *S*-**2** (red) and ***R*-1** (blue) and (b) *S*-**3** (red) and *R*-**3** (blue) (approx. 4 x 10^{-5} mol dm^{-3} in methanol 293 K).

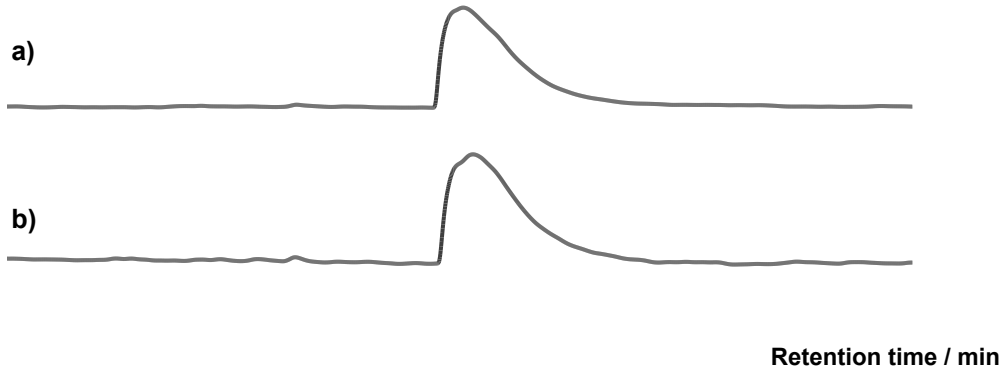


Figure S17 HPLC traces of (a) *S*-**1** and (b) *R*-**1** CHIRACEL® OJ-H HPLC column, 2% 2-propanol in *n*-hexane, 298K)

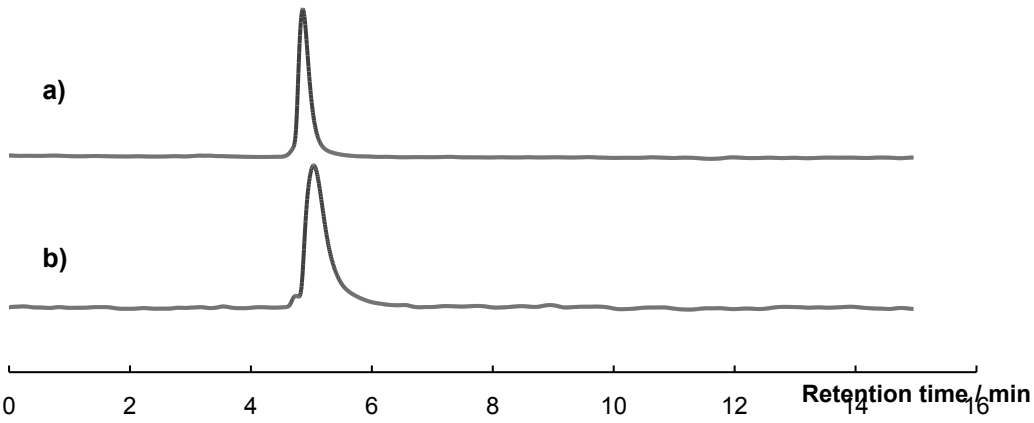


Figure S18 HPLC traces of (a) *S*-**2** and (b) *R*-**2** CHIRACEL® OJ-H HPLC column, 3% 2-propanol in *n*-hexane, 298K)

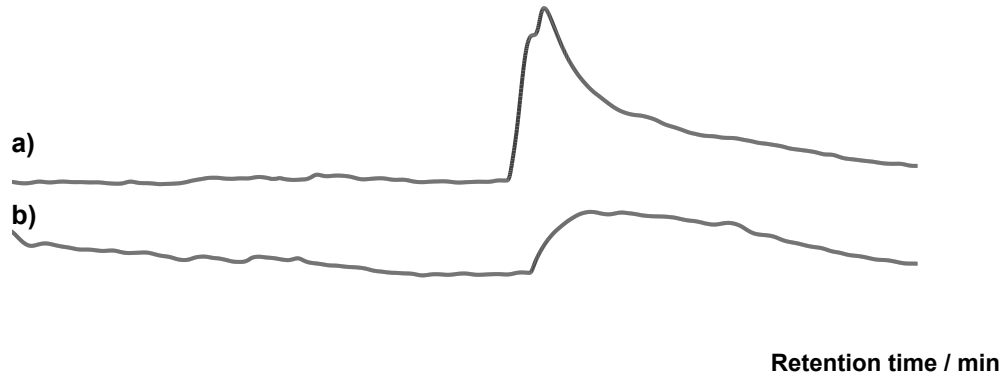


Figure S19 HPLC traces of (a) *S*-**3** and (b) *R*-**3** CHIRACEL® OJ-H HPLC column, 2% 2-propanol in *n*-hexane, 298K)