

Supplementary Information

Characterization of the 2-hydroxy-5-methylacetophenone and some aromatic aldehydes condensation products by NMR and computational methods

I G Mamedov*^a & E I Mamedov^b

^a Baku State University, Faculty of Chemistry, Z. Khalilov St. 23, Az-1148

^b Azerbaijan Medicinal University, A. Bakikhanov St. 23, Az-1022

E-mail: bsu.nmrlab@gmail.com

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A two-component Claisen-Schmidt condensation between the 2-hydroxy-5-methylacetophenone and some aromatic aldehydes has been carried out for the synthesis of chalcone derivatives at ambient temperature. The products were obtained with good yields and as a mixture of two compounds or a single product. Piperidine was used as a catalyst for the in-situ generation of carbanion from ketone. The possibility of the formation of different products was investigated on the based PM7 optimization, HMO theory and NMR methods.

General procedure for preparation of spiropyrrolidinones

A mixture of 0.2 mmol (0.03 g) 2-hydroxy-5-methylacetophenone **1**, 0.2 mmol (0.02 g) benzaldehyde **2** [or 0.2 mmol (0.02 g) 3-pyridinecarboxaldehyde **3**; 0.2 mmol (0.03 g) 4-nitrobenzaldehyde **4**] in 15 ml 96% ethanol, at presence of catalytic amount piperidine were stirred at 25°C for 3 h. The solid formed in the reaction mixture was filtered and to obtain the pure products (chromemenone) recrystallized from EtOH. After evaporation of solvent obtained solid (chalcones) recrystallized from methanol.

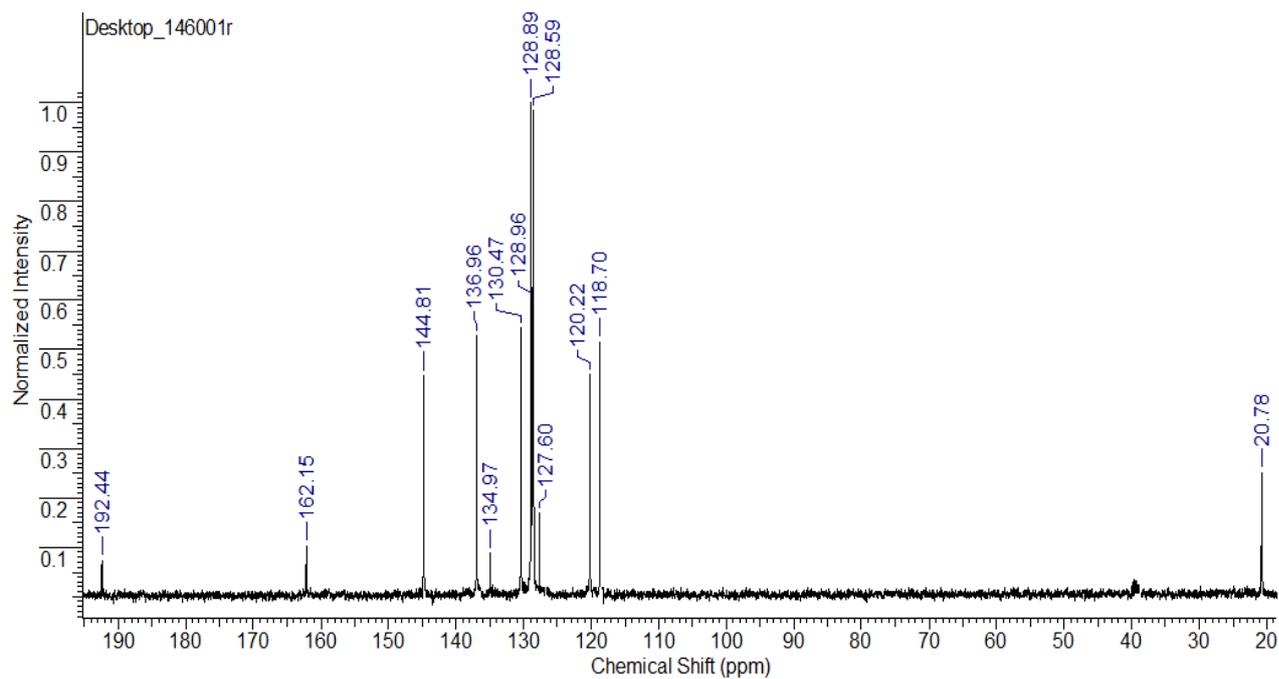
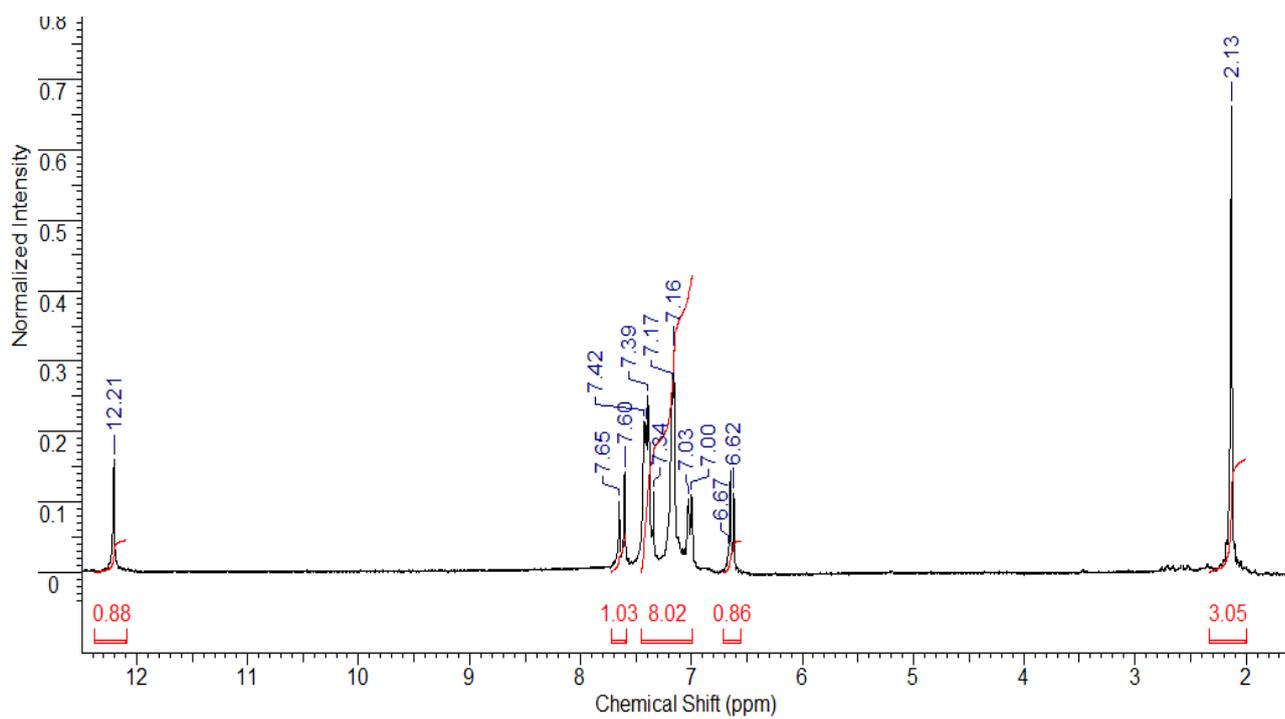


Figure S1- ^1H and ^{13}C NMR contour plot of **5** in $\text{DMSO-}d_6$

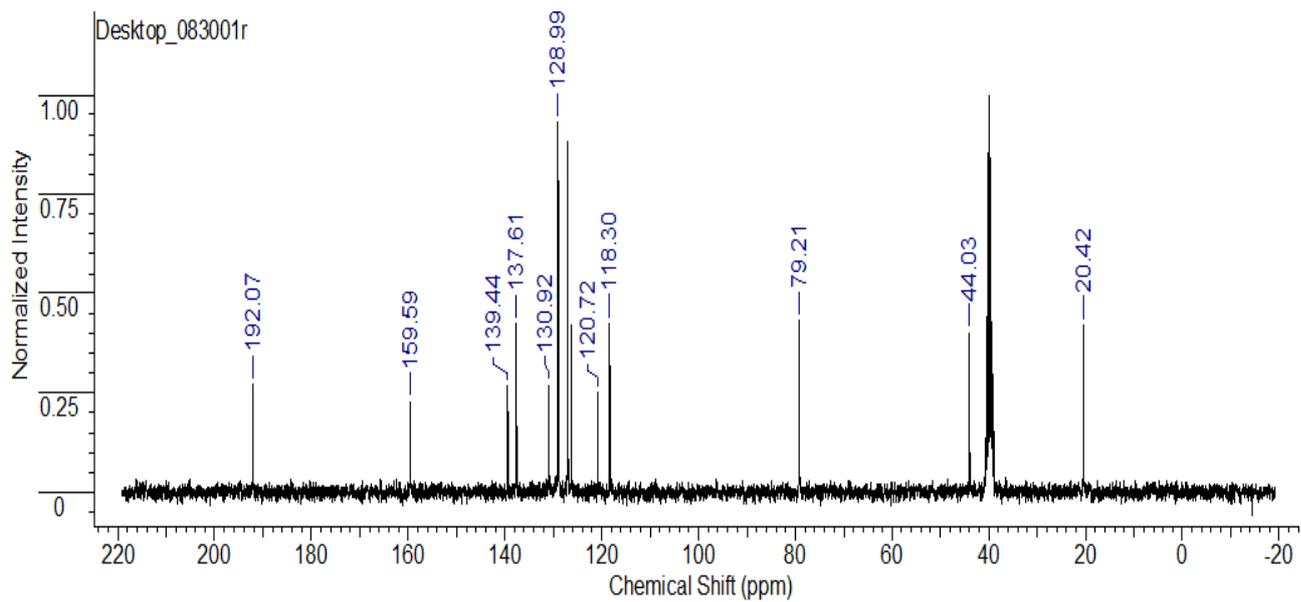
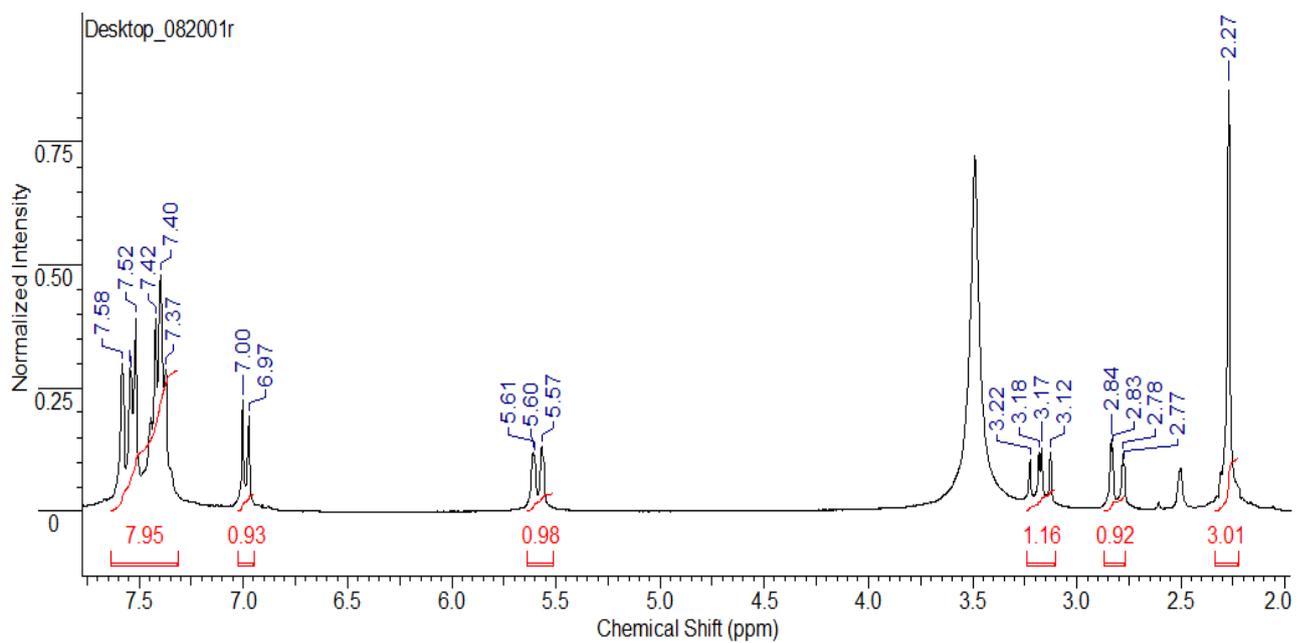


Figure S2- ^1H and ^{13}C NMR contour plot of **6** in $\text{DMSO-}d_6$

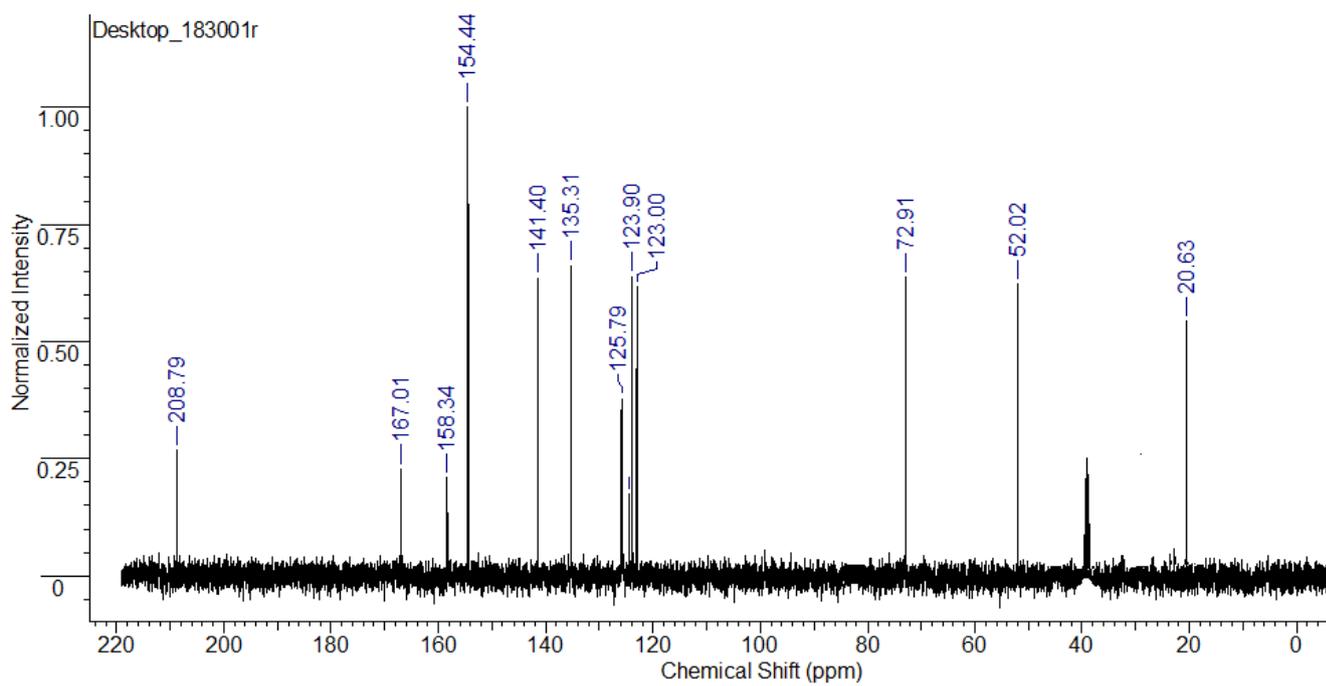
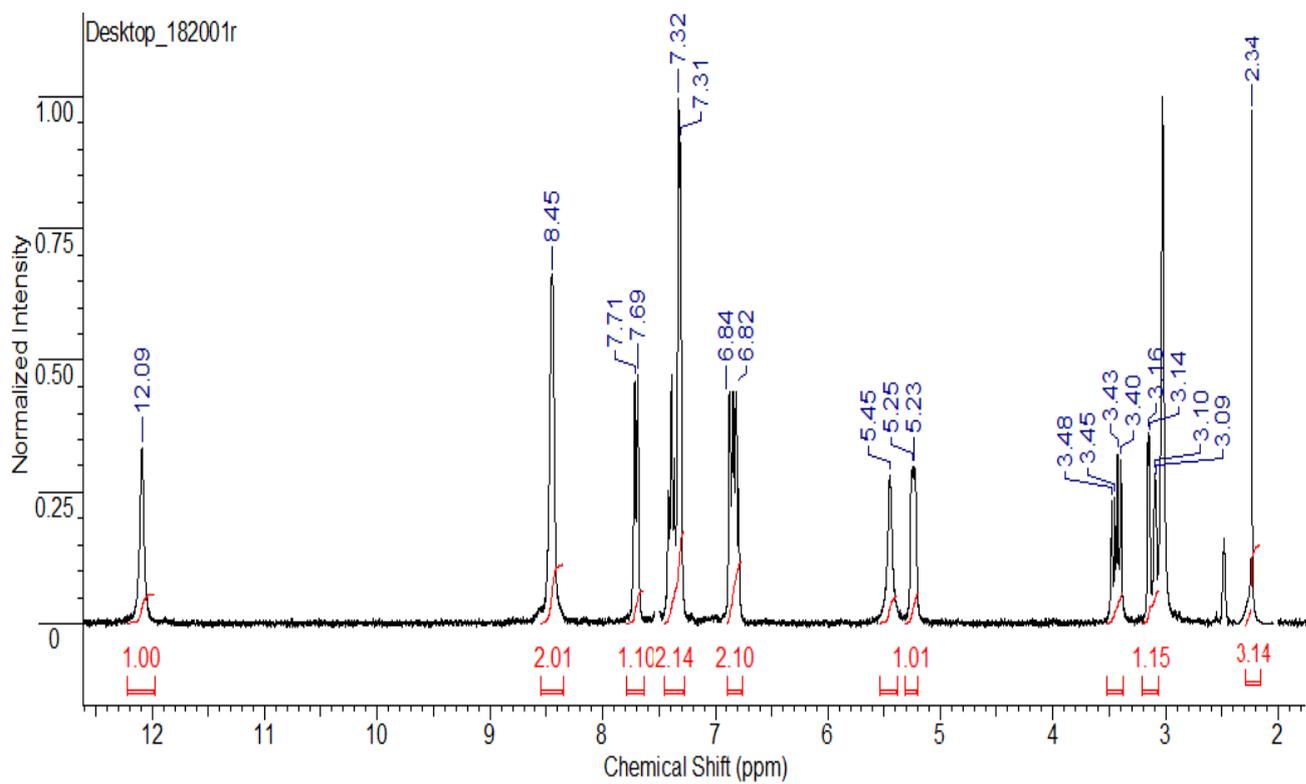


Figure S3- ^1H and ^{13}C NMR contour plot of **10** in $\text{DMSO-}d_6$

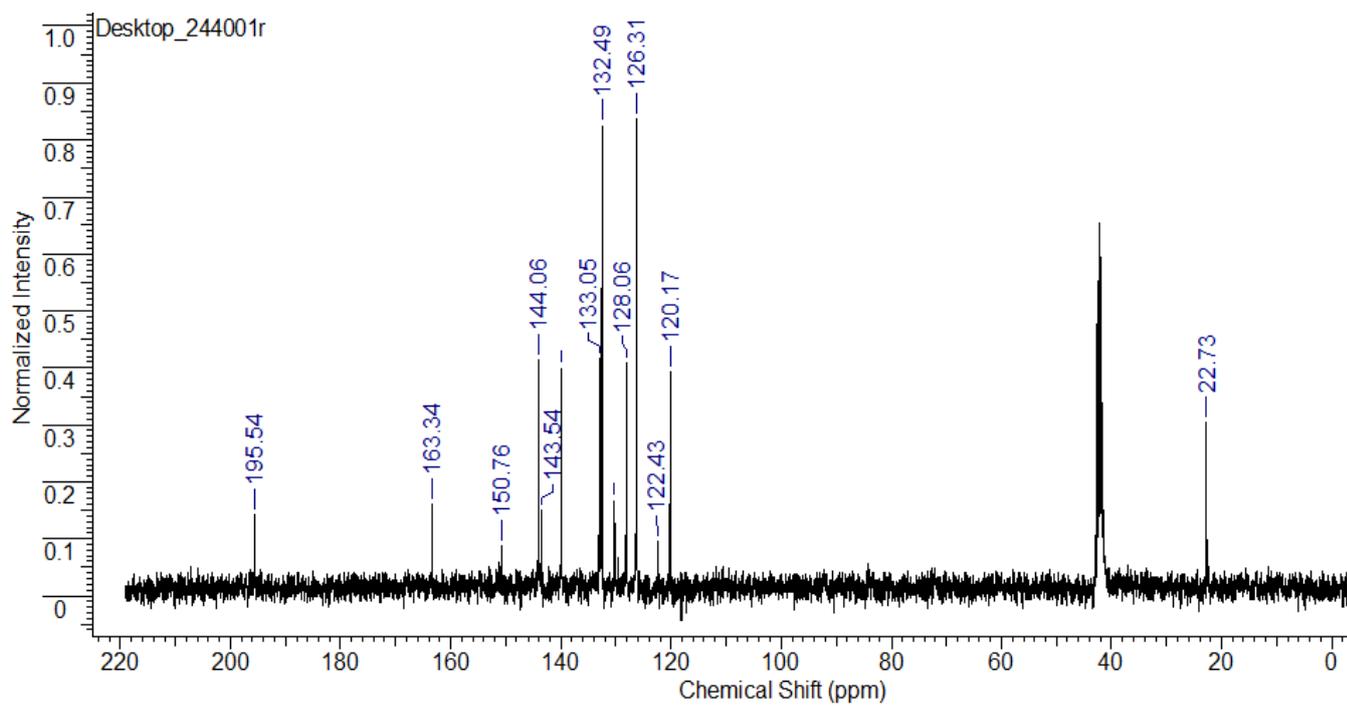
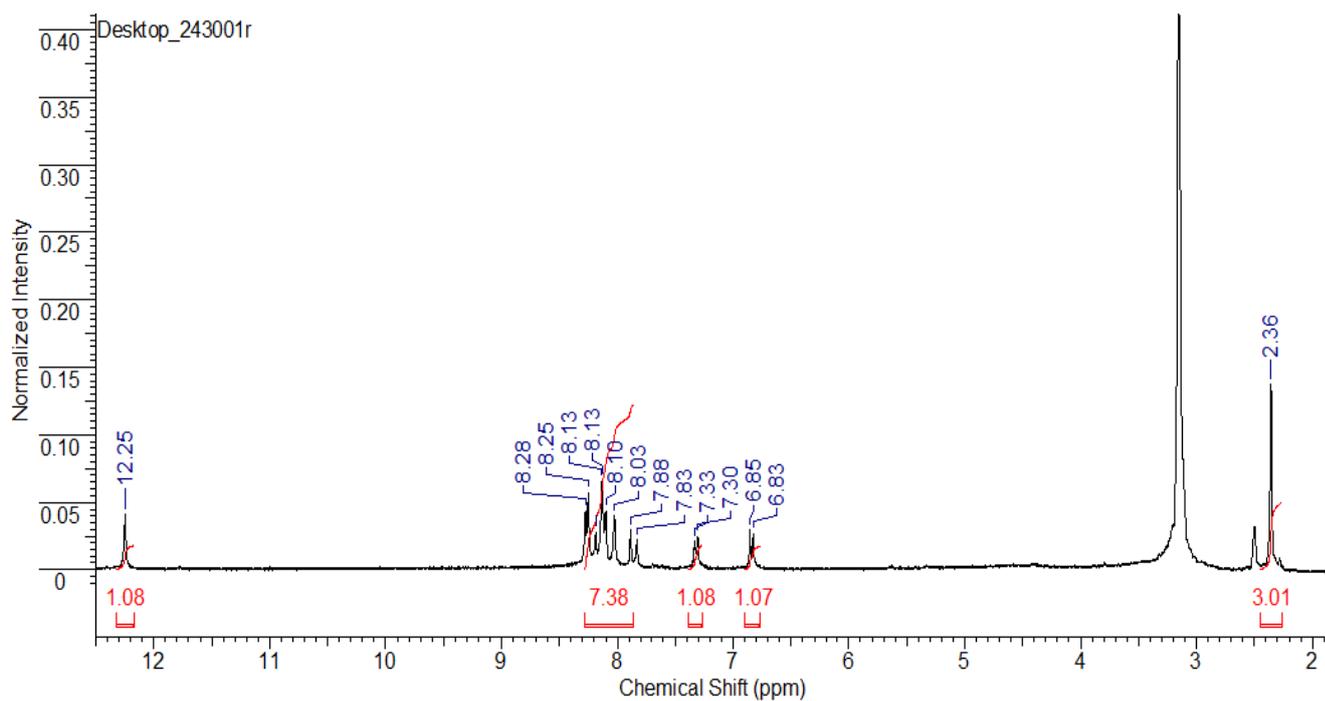


Figure S4- ^1H and ^{13}C NMR contour plot of **11** in $\text{DMSO-}d_6$

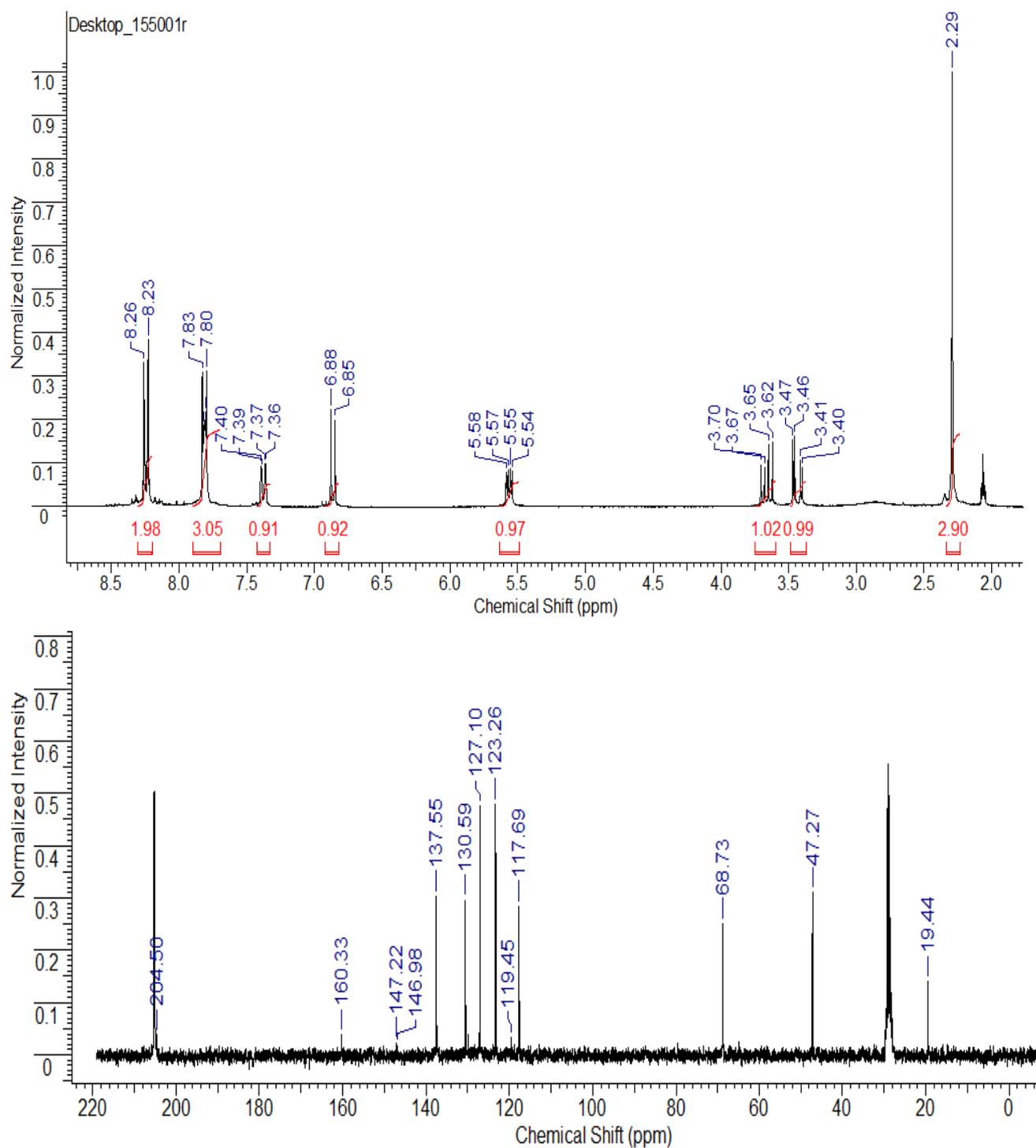


Figure S5- ^1H and ^{13}C NMR contour plot of **12** in acetone- d_6

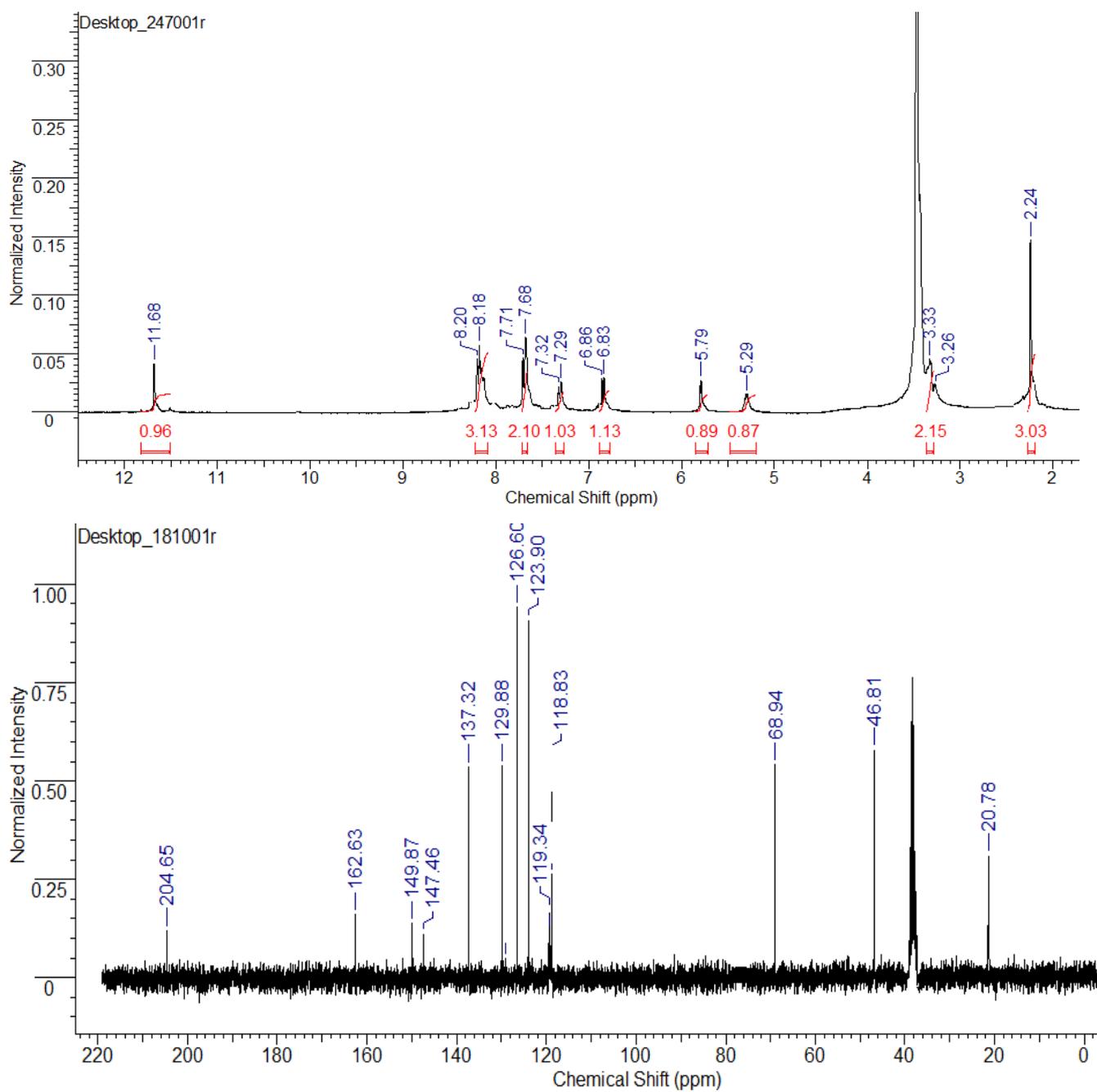
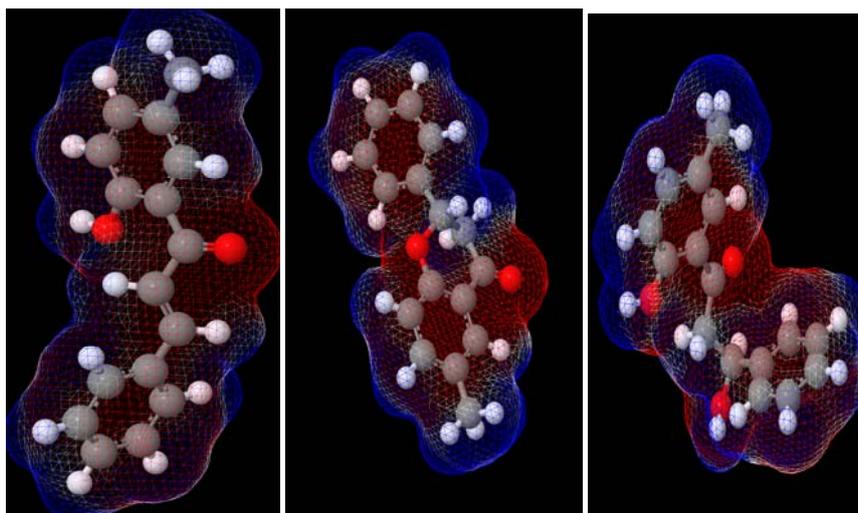


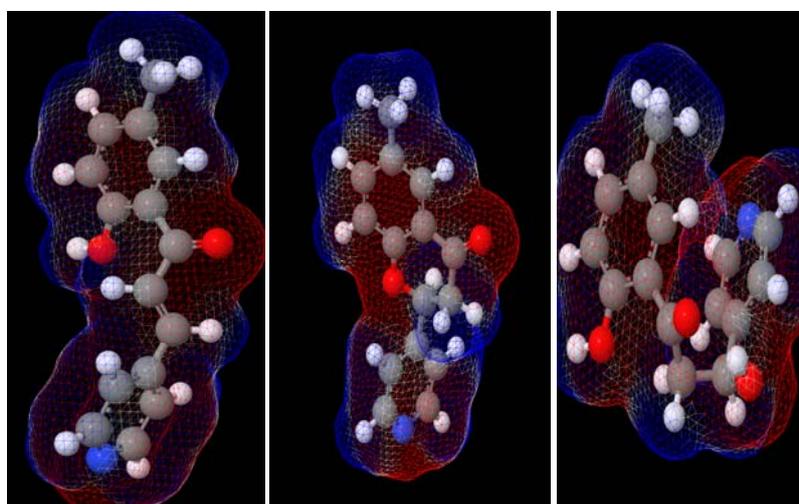
Figure S6- ¹H and ¹³C NMR contour plot of **13** in DMSO-*d*₆



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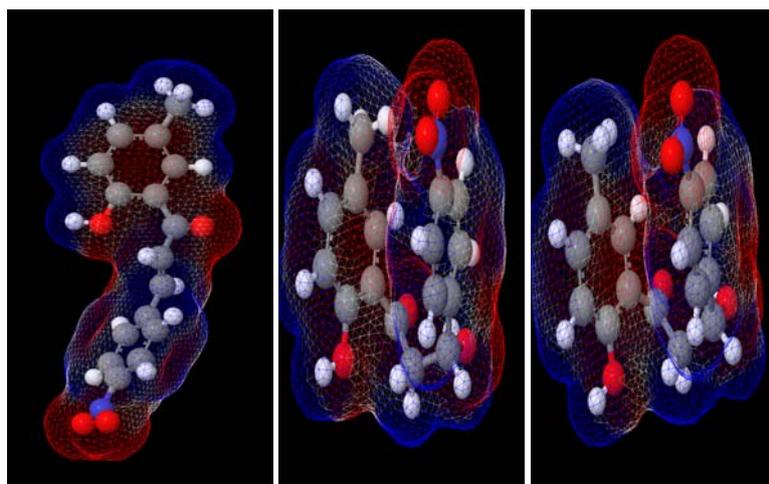
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Figure S7- Electrostatic potentials for all isomers