SUPPORTING INFORMATION

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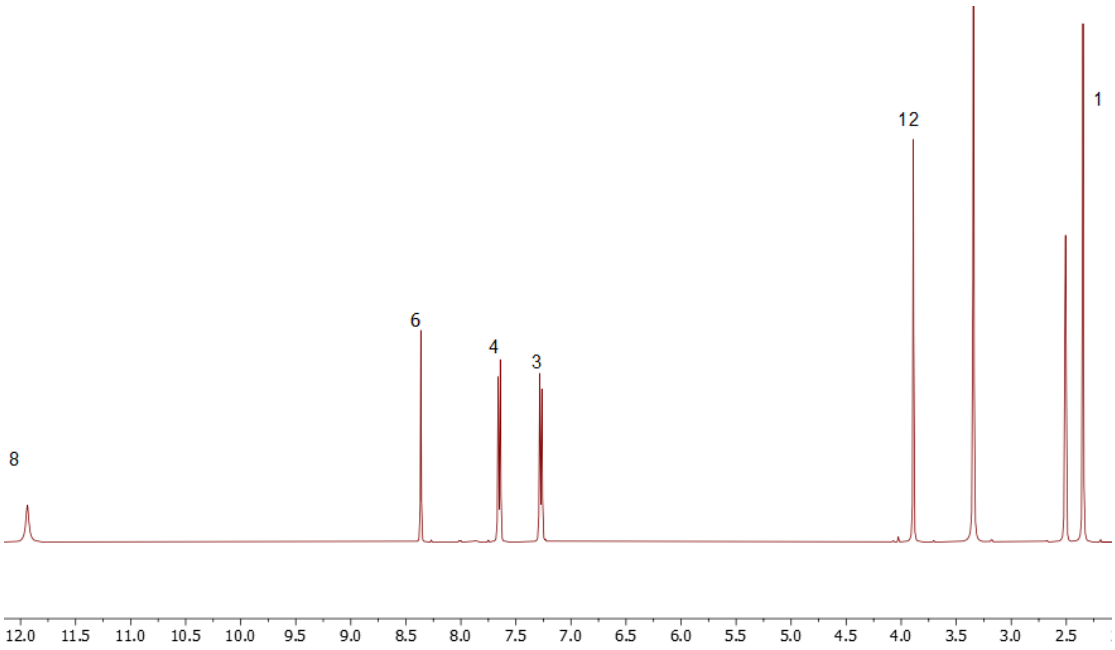

Figure S1. [1]H-NMR spectra. The spectra were recorded in DMSO-d6 on a Bruker AC 400MHz spectrometer at 25ºC.

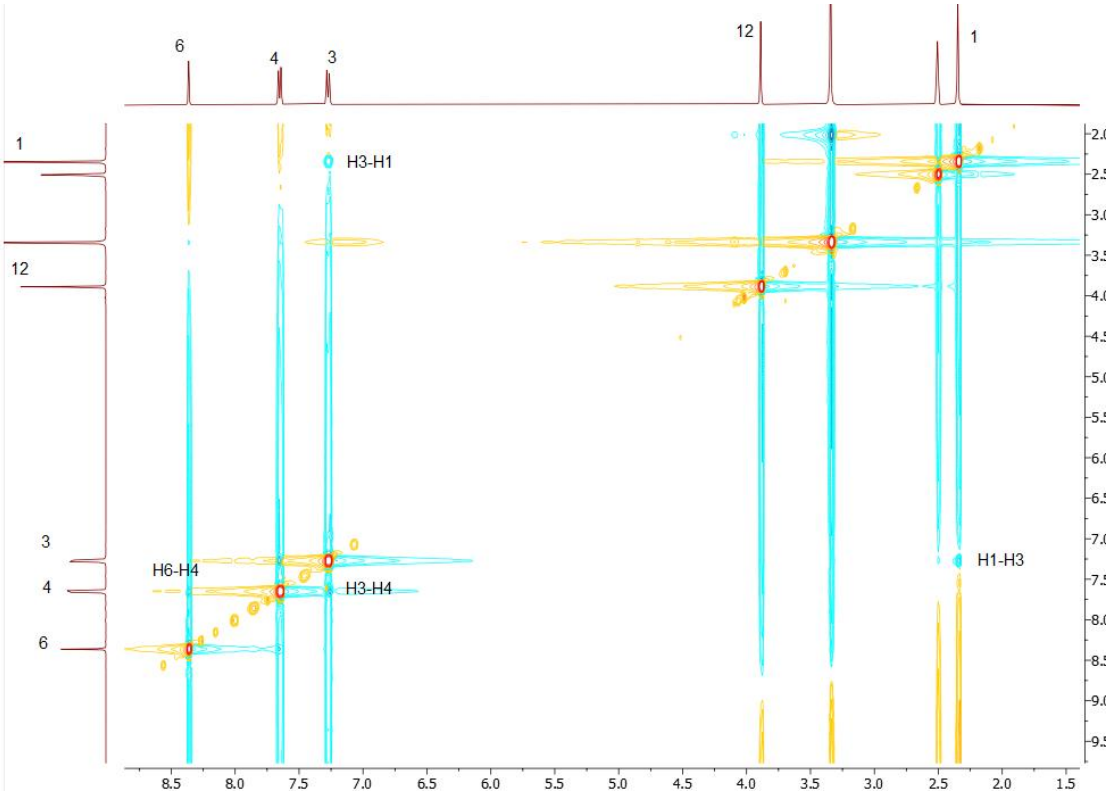

Figure S2. 2D-NOESY-NMR spectra. The spectra were recorded in DMSO-d6 on a Bruker AC 400MHz spectrometer at 25ºC.

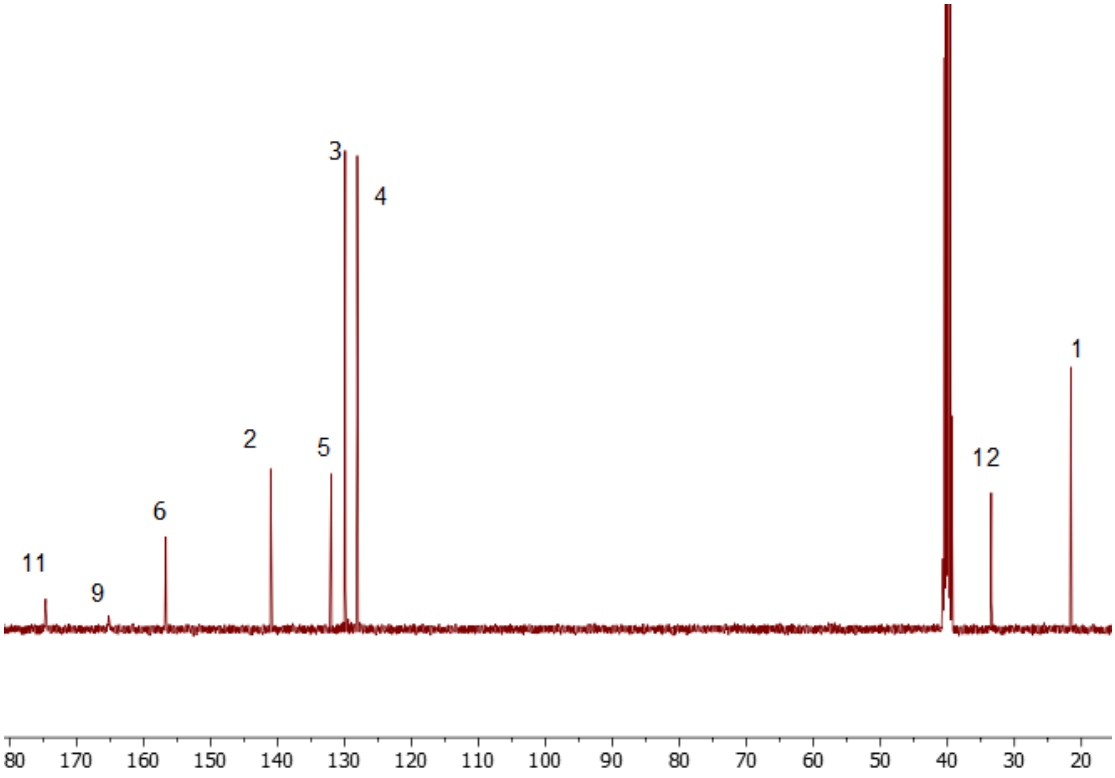

Figure S3. ^{13}C-NMR spectra. The spectra were recorded in DMSO-d6 on a Bruker AC 400MHz spectrometer at 25ºC.

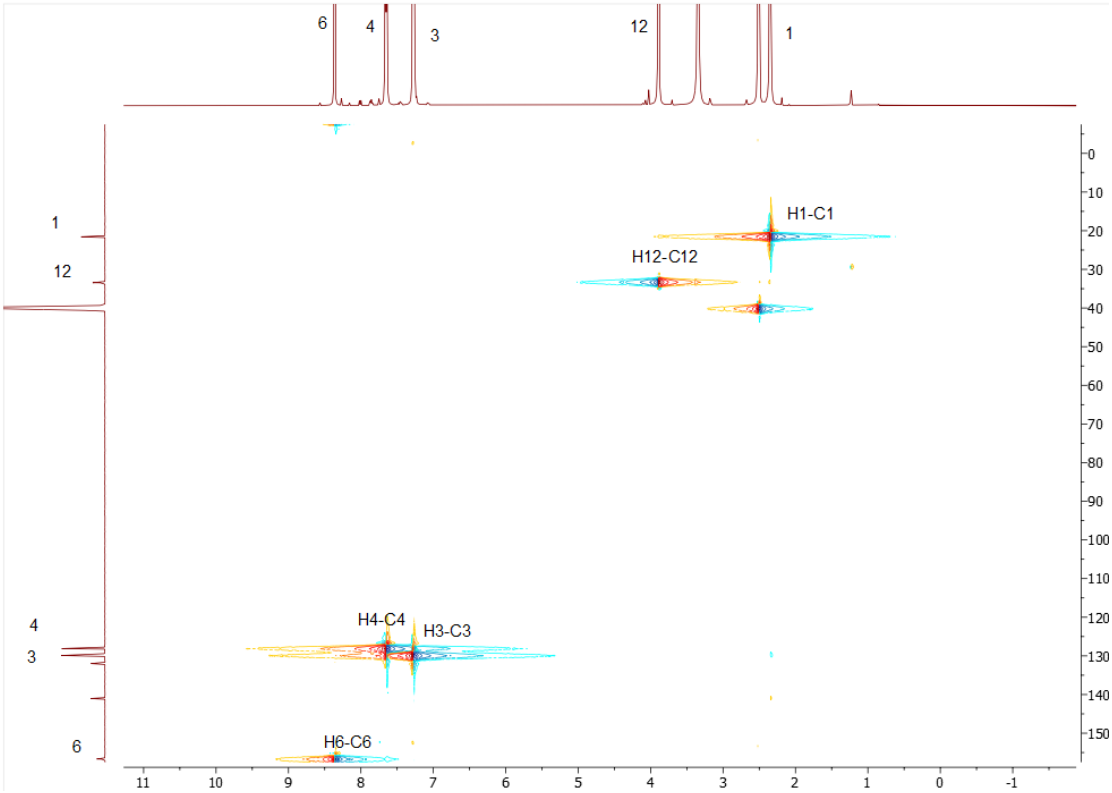

Figure S4. 2D-HSQC-NMR spectra. The spectra were recorded in DMSO-d6 on a Bruker AC 400MHz spectrometer at 25ºC.

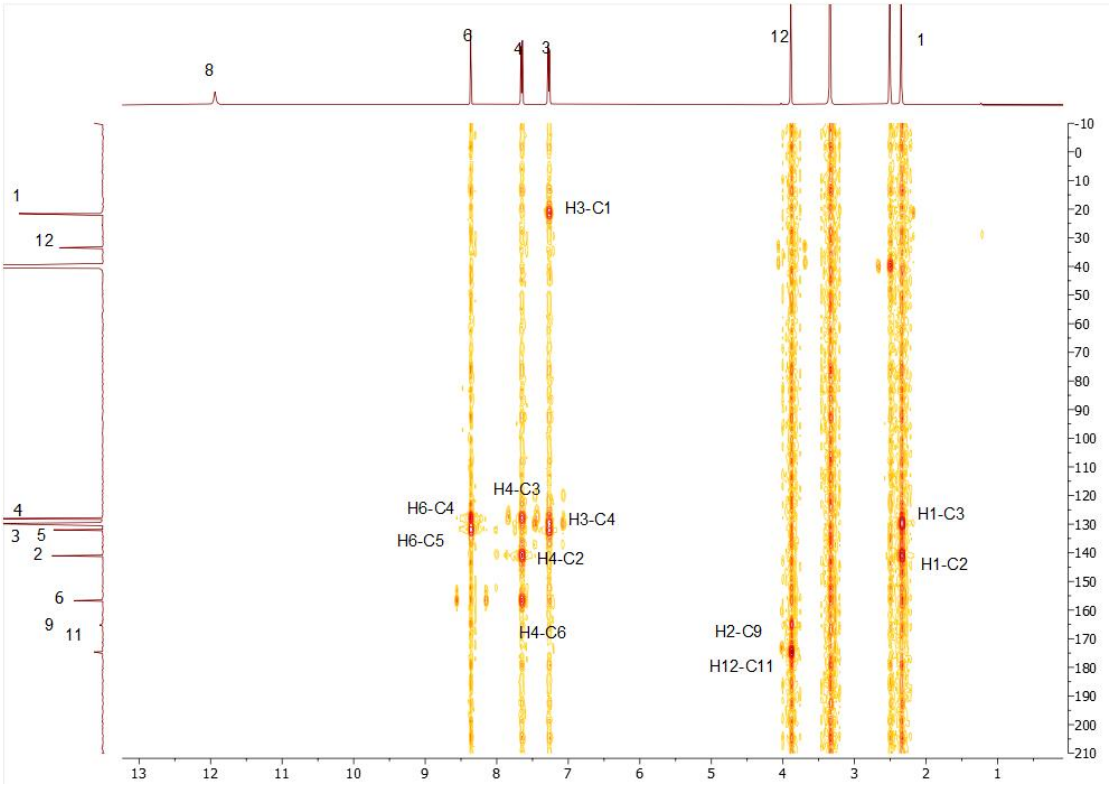

Figure S5. 2D-HMBC-NMR spectra. The spectra were recorded in DMSO-d6 on a Bruker AC 400MHz spectrometer at 25ºC.

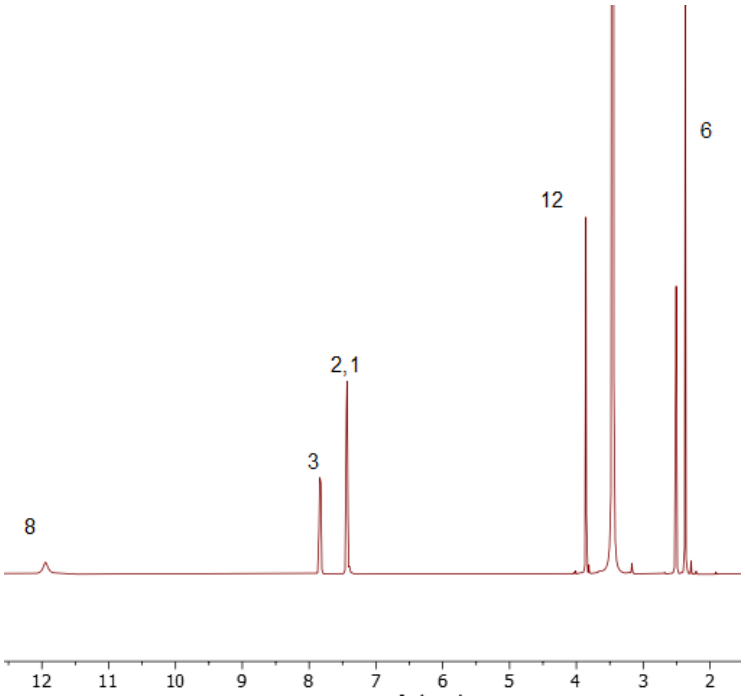

Figure S6. [1]H-NMR spectra. The spectra were recorded in DMSO-d6 on a Bruker AC 400MHz spectrometer at 25ºC.

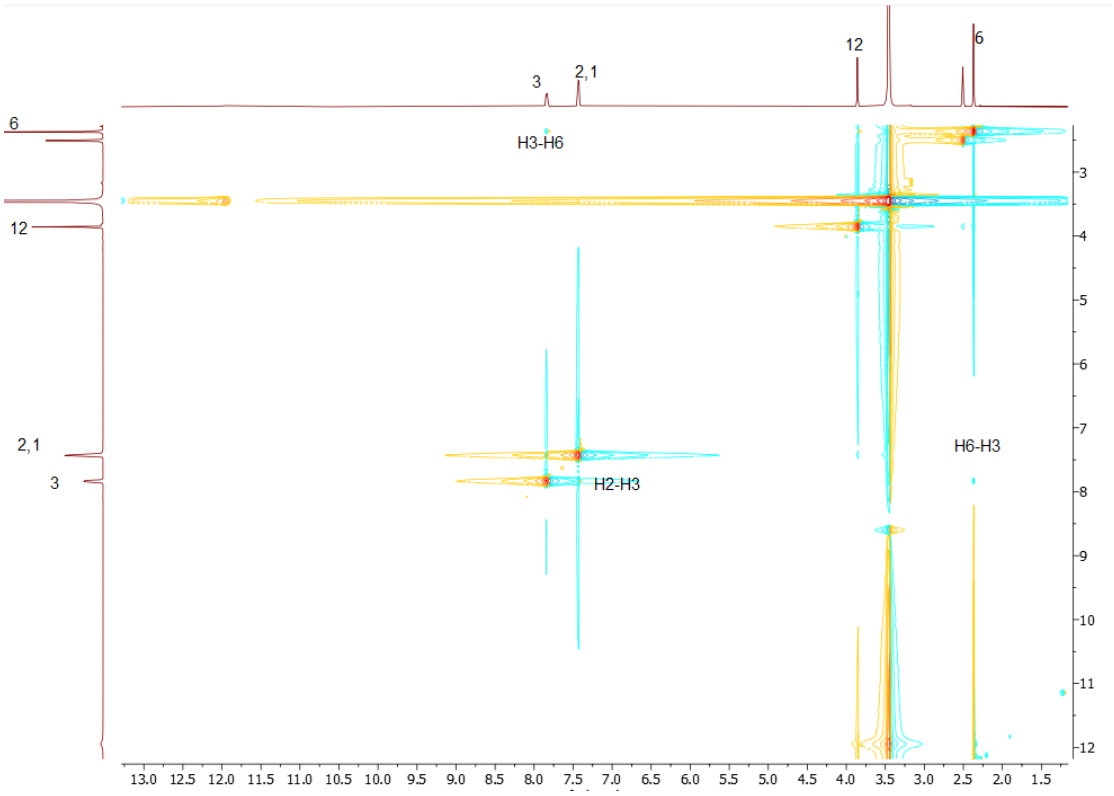

Figure S7. 2D-NOESY-NMR spectra. The spectra were recorded in DMSO-d6 on a Bruker AC 400MHz spectrometer at 25ºC.

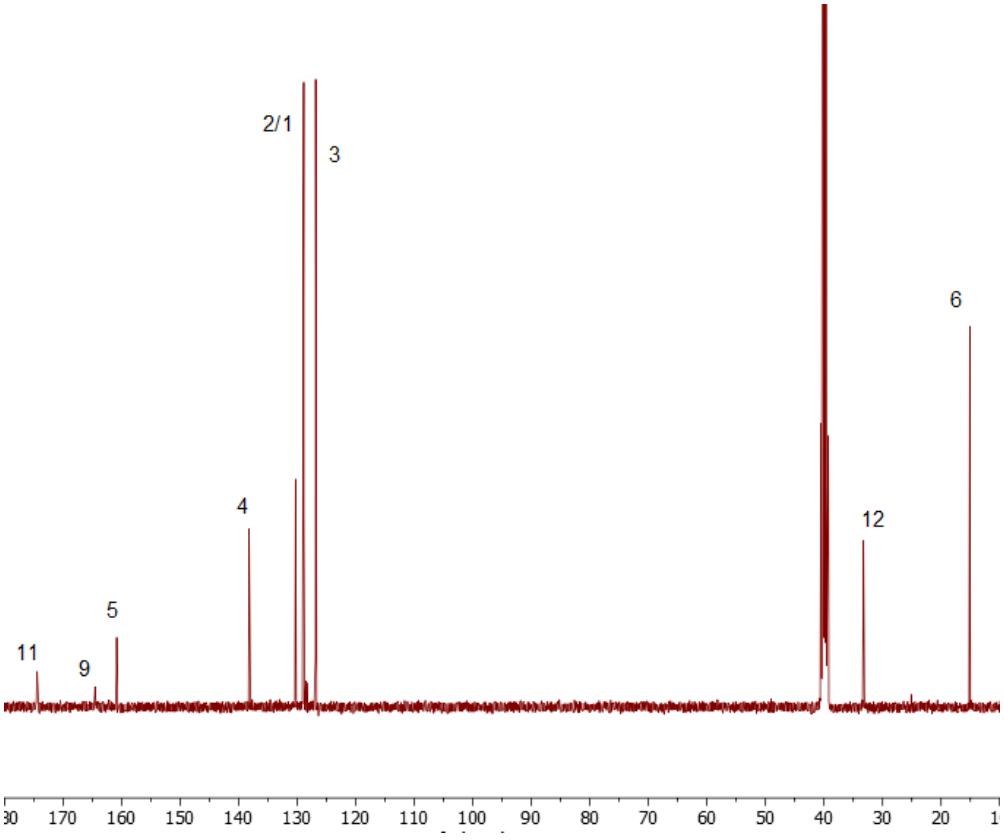

Figure S8. ^{13}C-NMR spectra. The spectra were recorded in DMSO-d6 on a Bruker AC 400MHz spectrometer at 25ºC.

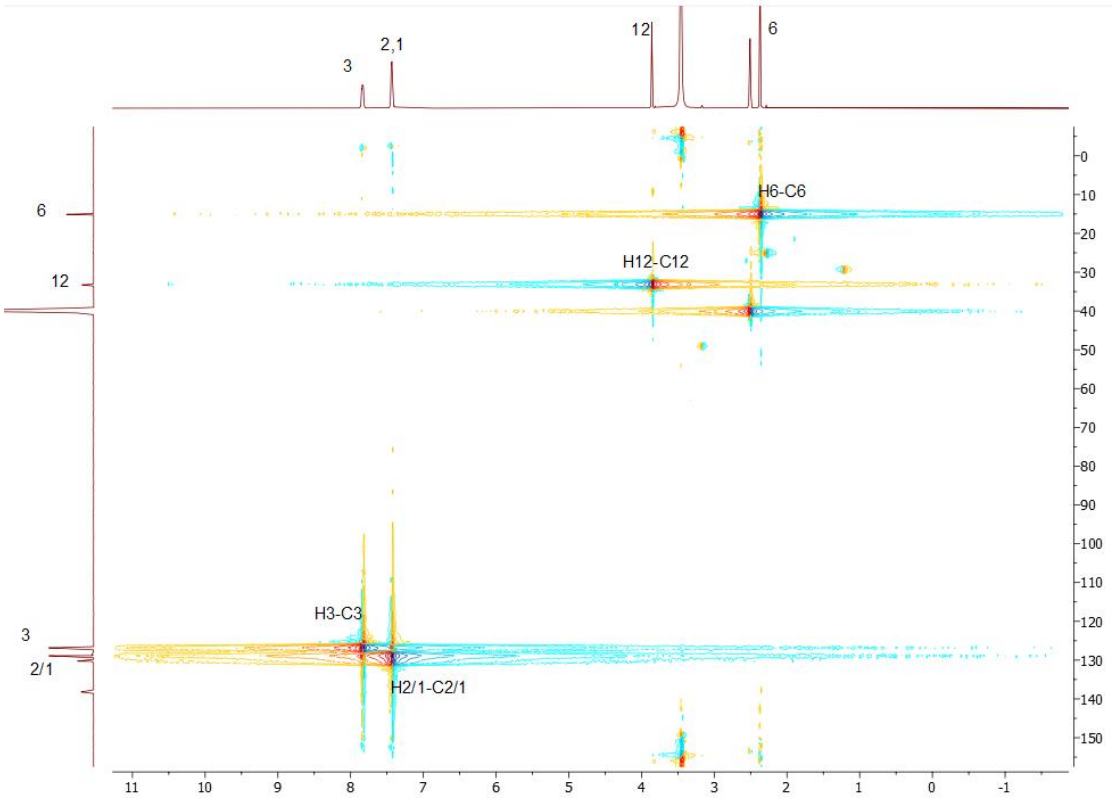

Figure S9. 2D-HSQC-NMR spectra. The spectra were recorded in DMSO-d6 on a Bruker AC 400MHz spectrometer at 25ºC.

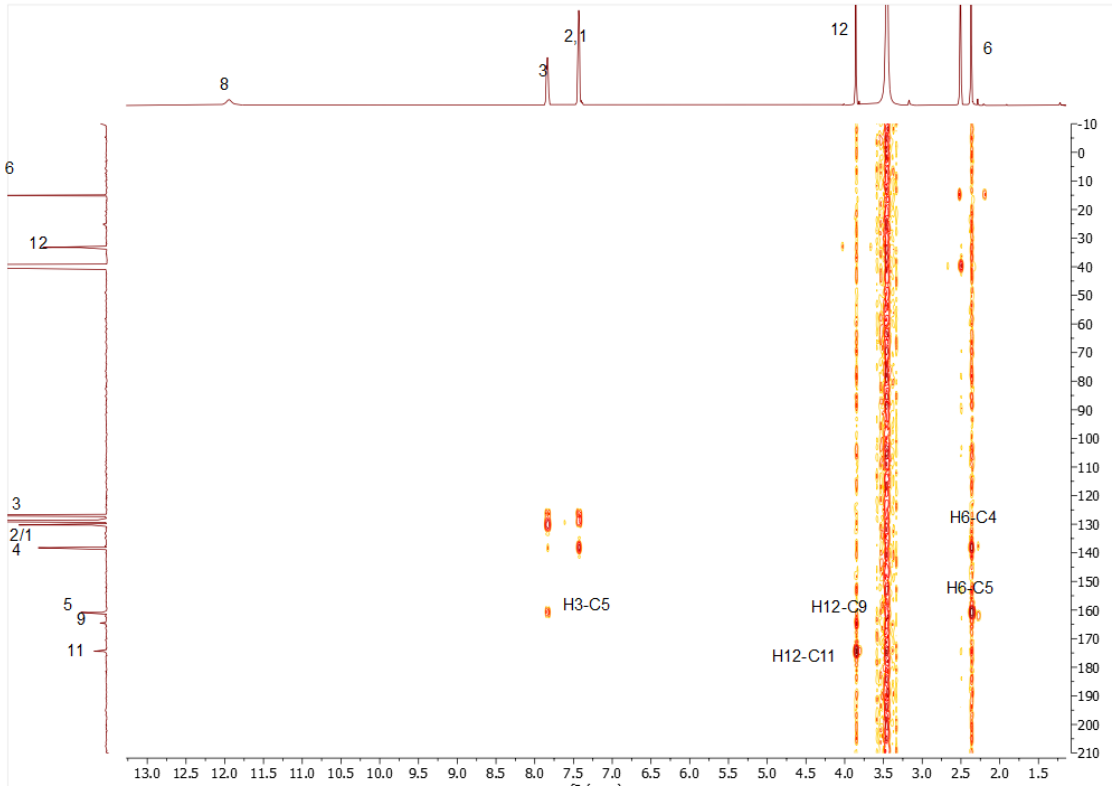

Figure S10. 2D-HMBC-NMR spectra. The spectra were recorded in DMSO-d6 on a Bruker AC 400MHz spectrometer at 25ºC.

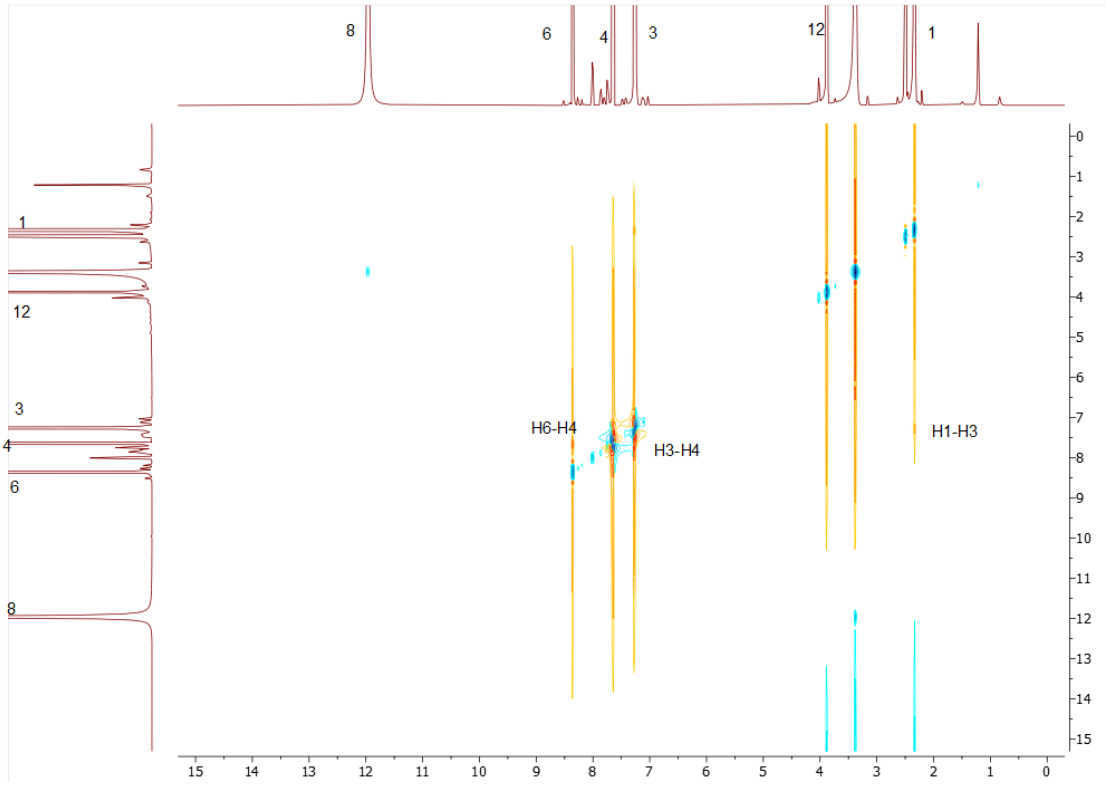

Figure S11. 2D-ROESY-NMR spectra. The spectra were recorded in DMSO-d6 on a Bruker AC 500MHz spectrometer at 25ºC using P15=150.000 us.

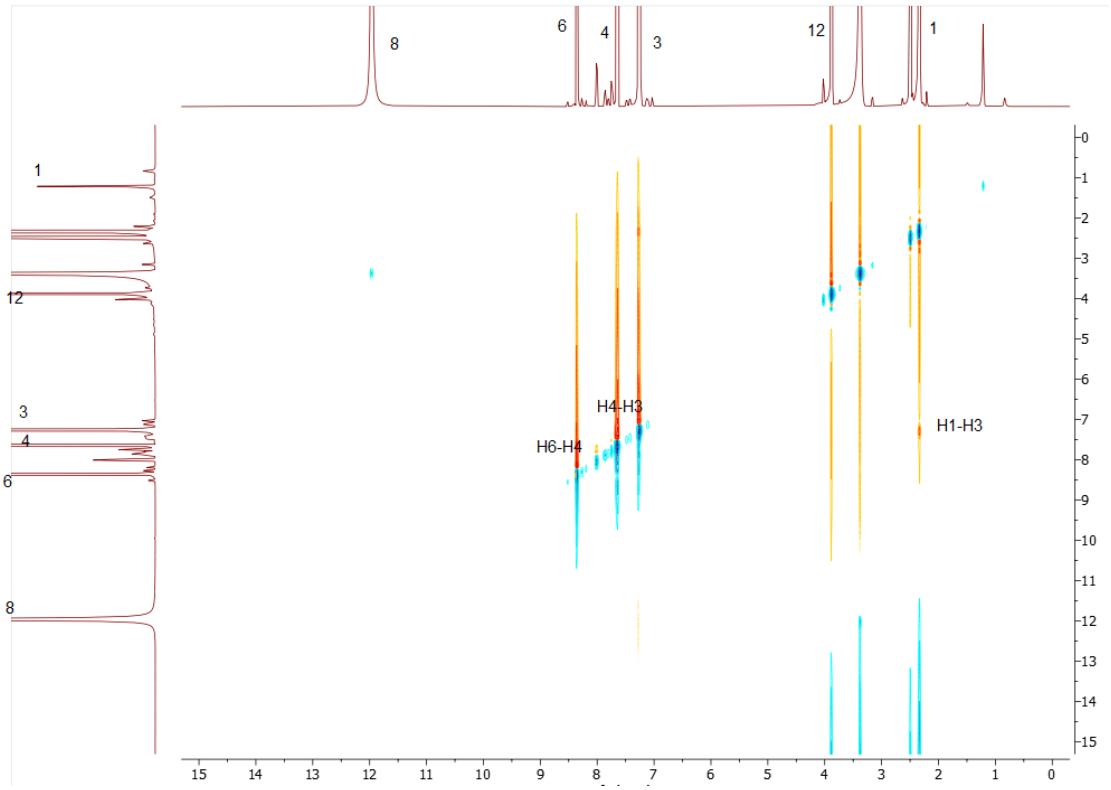

Figure S12. 2D-ROESY-NMR spectra. The spectra were recorded in DMSO-d6 on a Bruker AC 500MHz spectrometer at 25ºC using P15=300.000 us.

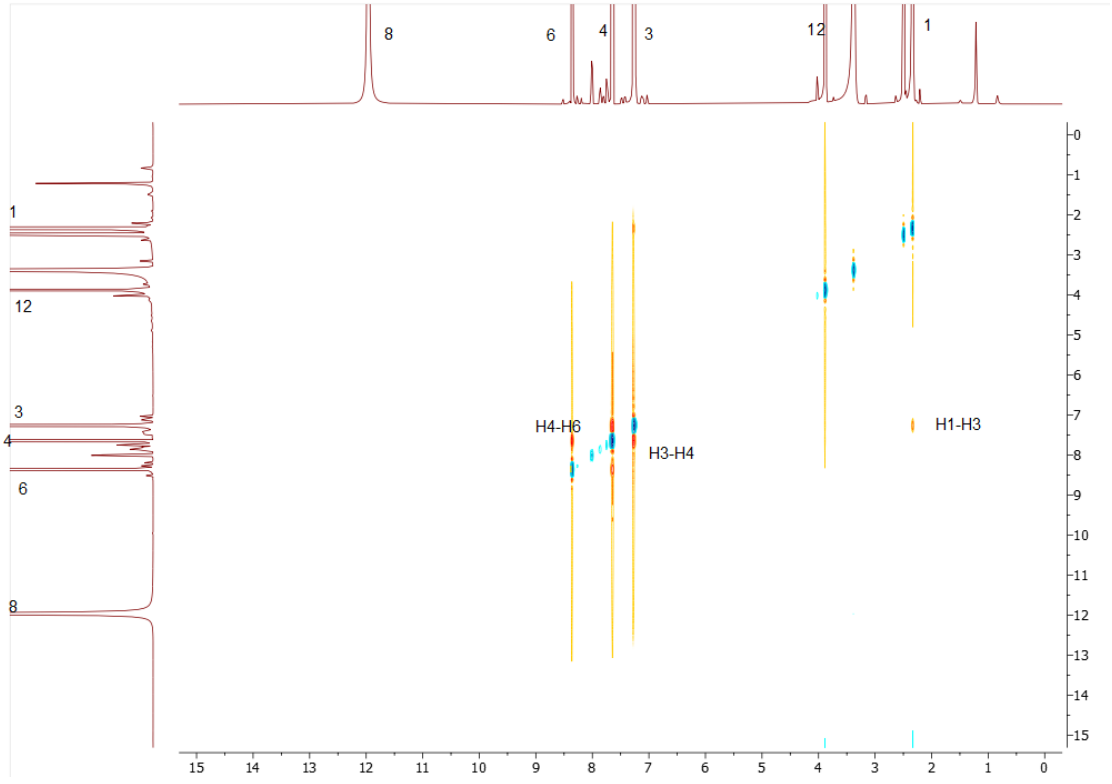

Figure S13. 2D-ROESY-NMR spectra. The spectra were recorded in DMSO-d6 on a Bruker AC 500MHz spectrometer at 25ºC using P15=500.000 us.

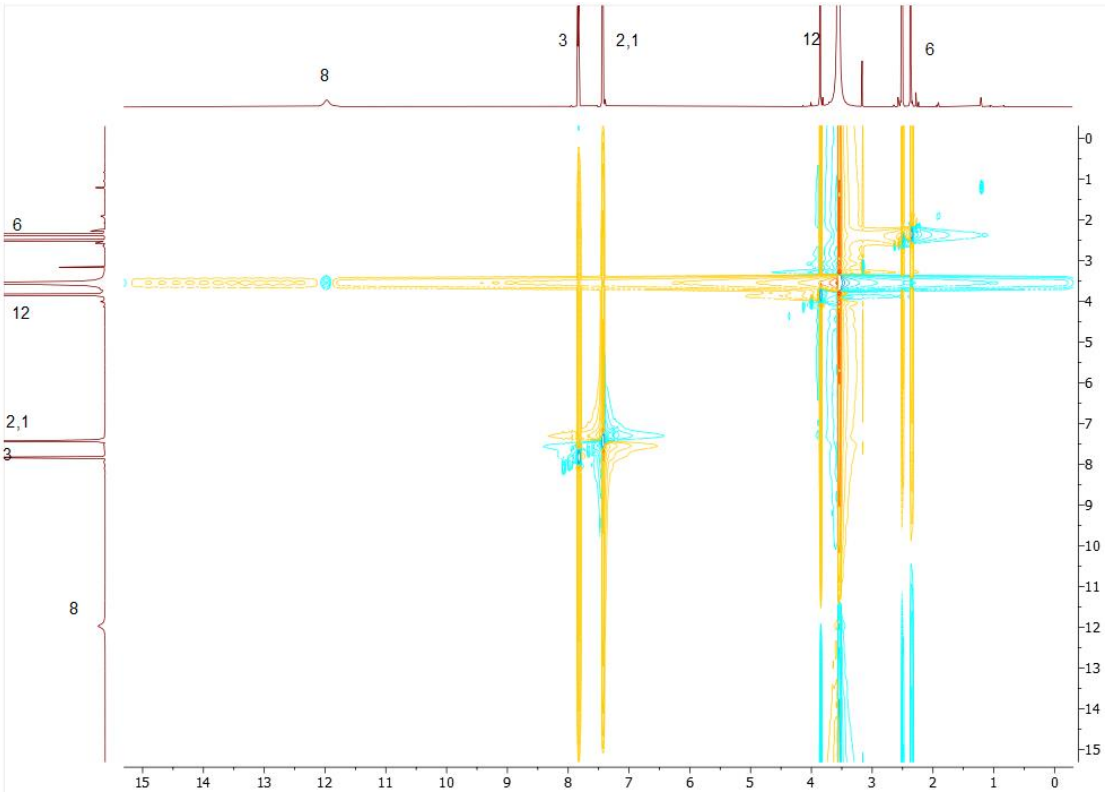

Figure S14. 2D-ROESY-NMR spectra. The spectra were recorded in DMSO-d6 on a Bruker AC 500MHz spectrometer at 25ºC using P15=150.000 us.

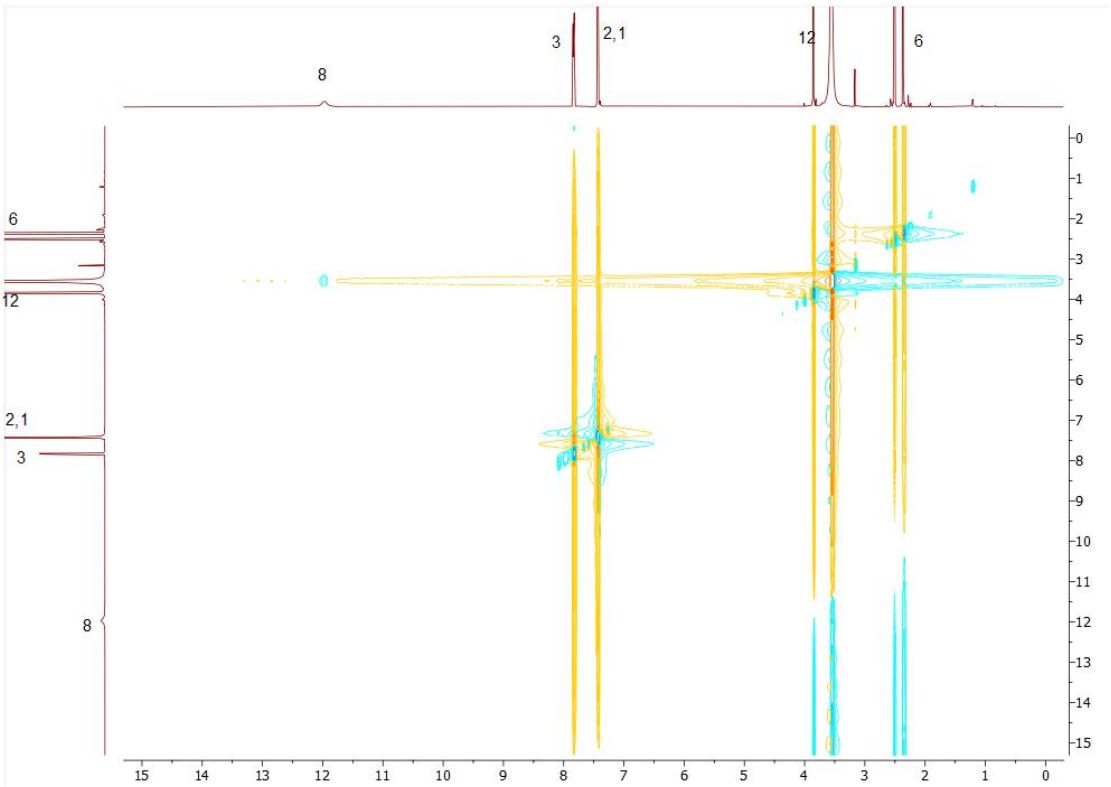

Figure S15. 2D-ROESY-NMR spectra. The spectra were recorded in DMSO-d6 on a Bruker AC 500MHz spectrometer at 25ºC using P15=300.000 us.

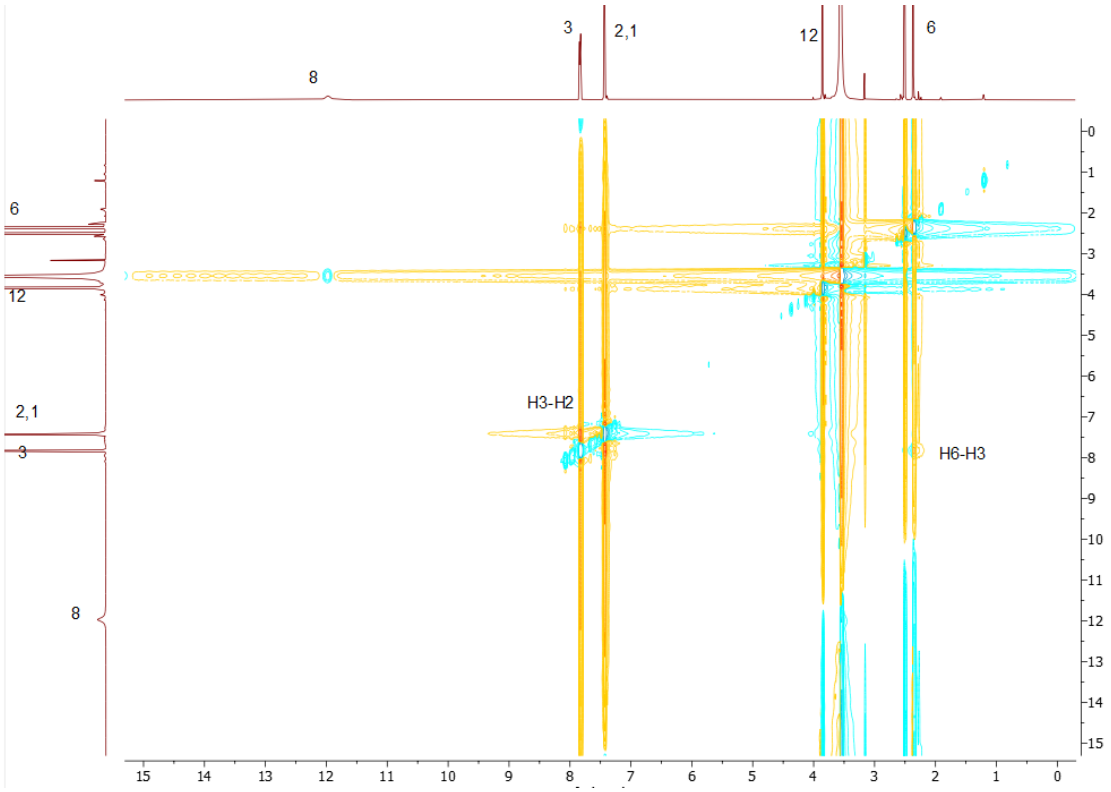

Figure S16. 2D-ROESY-NMR spectra. The spectra were recorded in DMSO-d6 on a Bruker AC 500MHz spectrometer at 25ºC using P15=500.000 us.

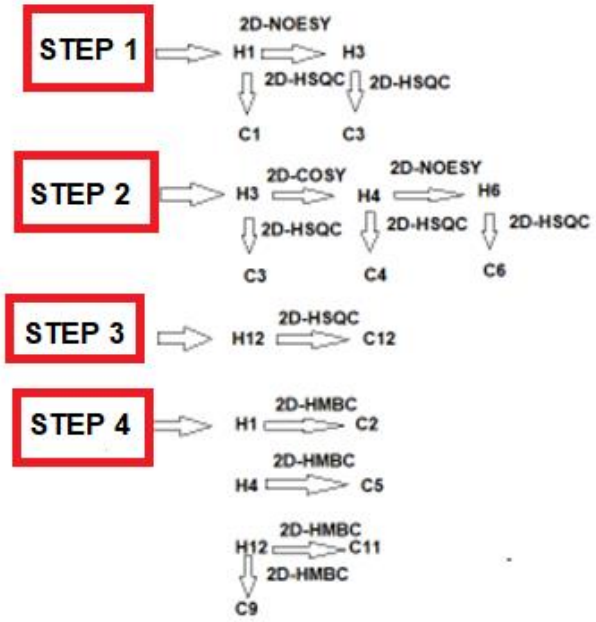

Figure S17. Overall diagram showing the identification strategy of the **DKI21** compound in DMSO.

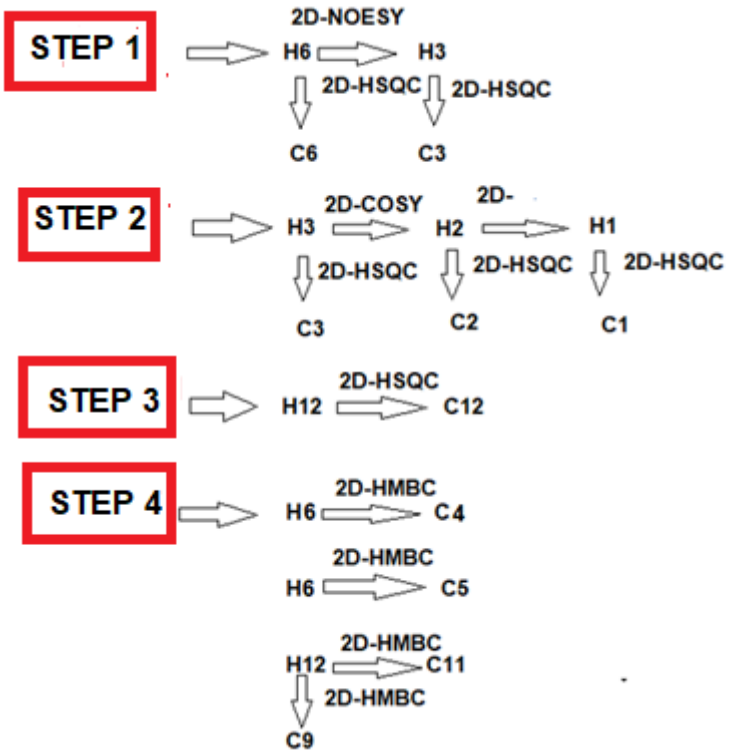

Figure S18. Overall diagram showing the identification strategy of the **DKI24** compound in DMSO.

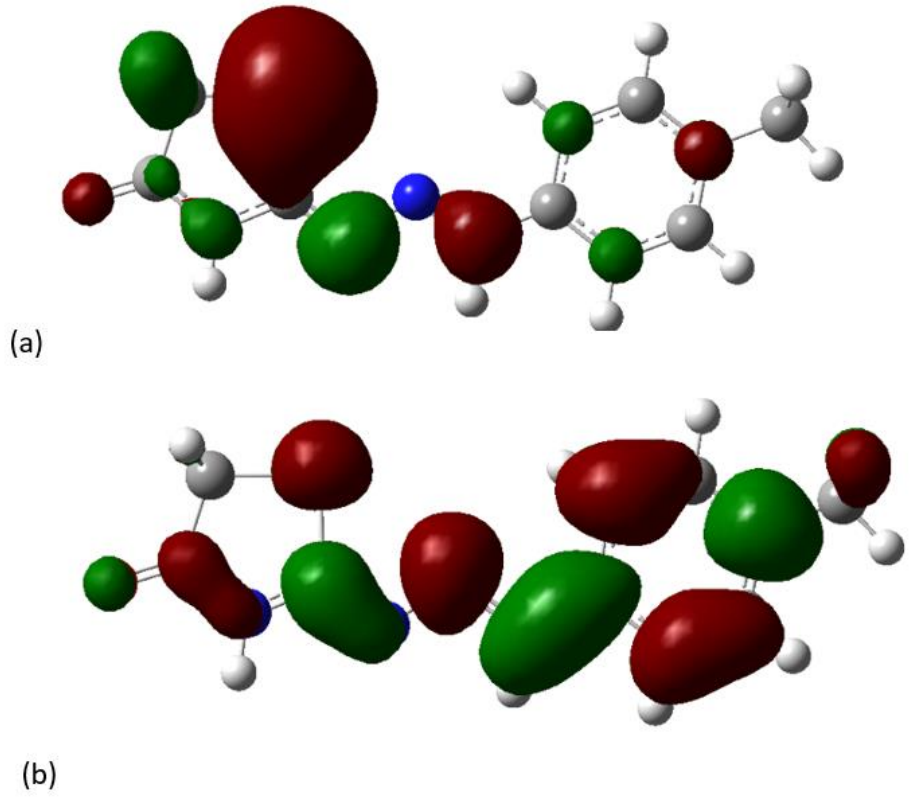

Figure S19. Orbitals in HOMO (top) and LUMO (bottom) in **DKI21** exo conformation.

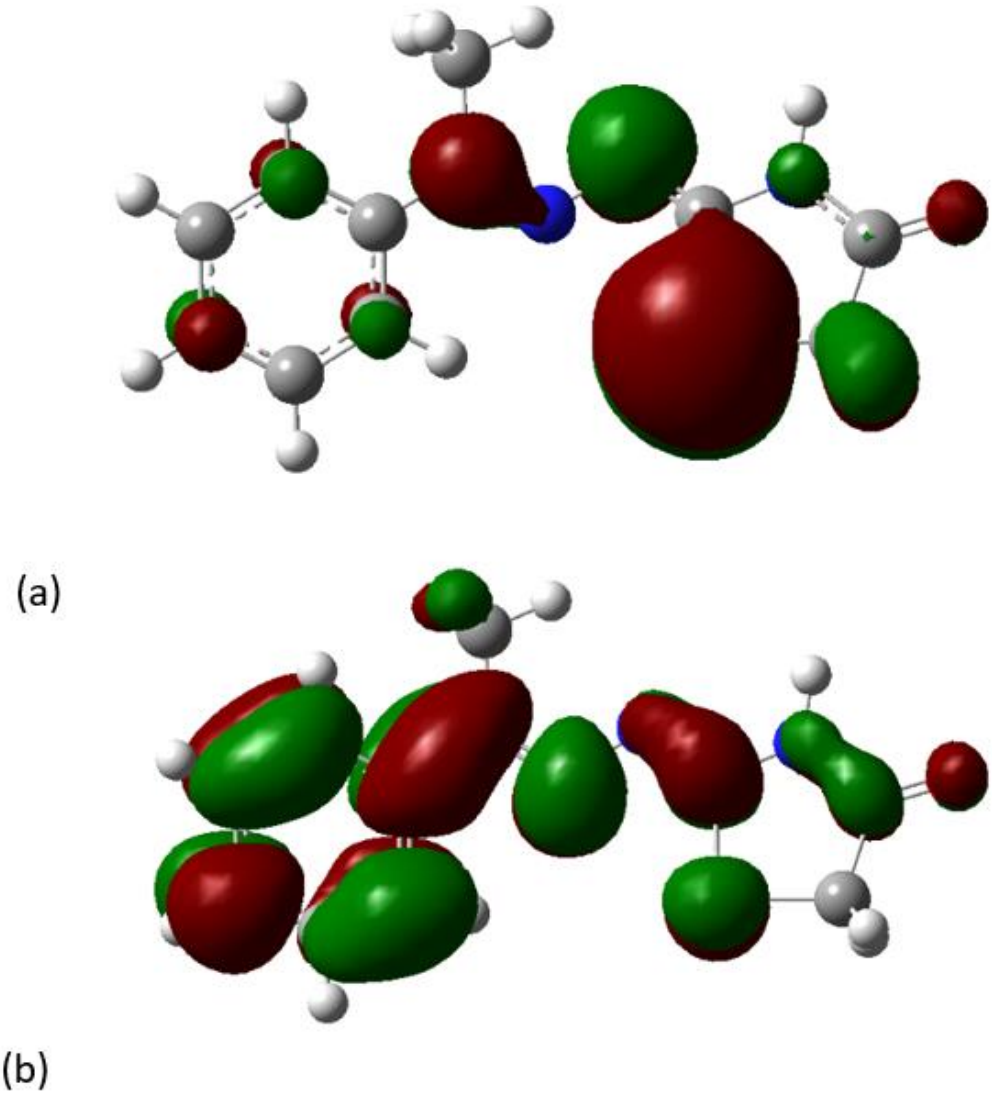

Figure S20. Orbitals in HOMO (top) and LUMO (bottom) in **DKI24** exo conformation

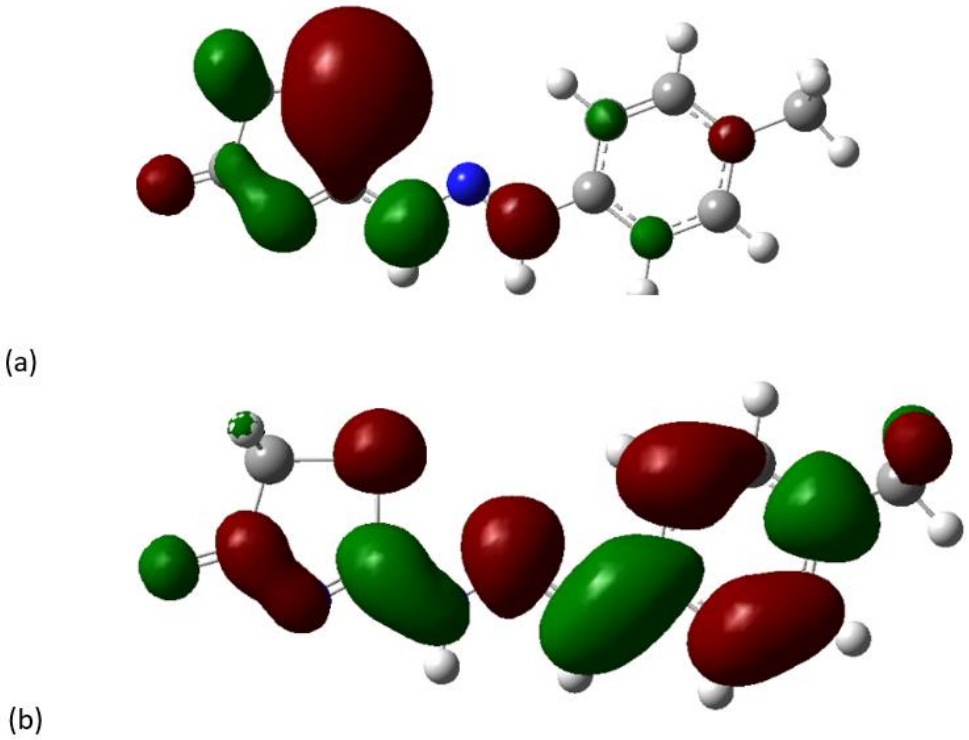

Figure S21. Orbitals in HOMO (top) and LUMO (bottom) in **DKI21** endo conformation.

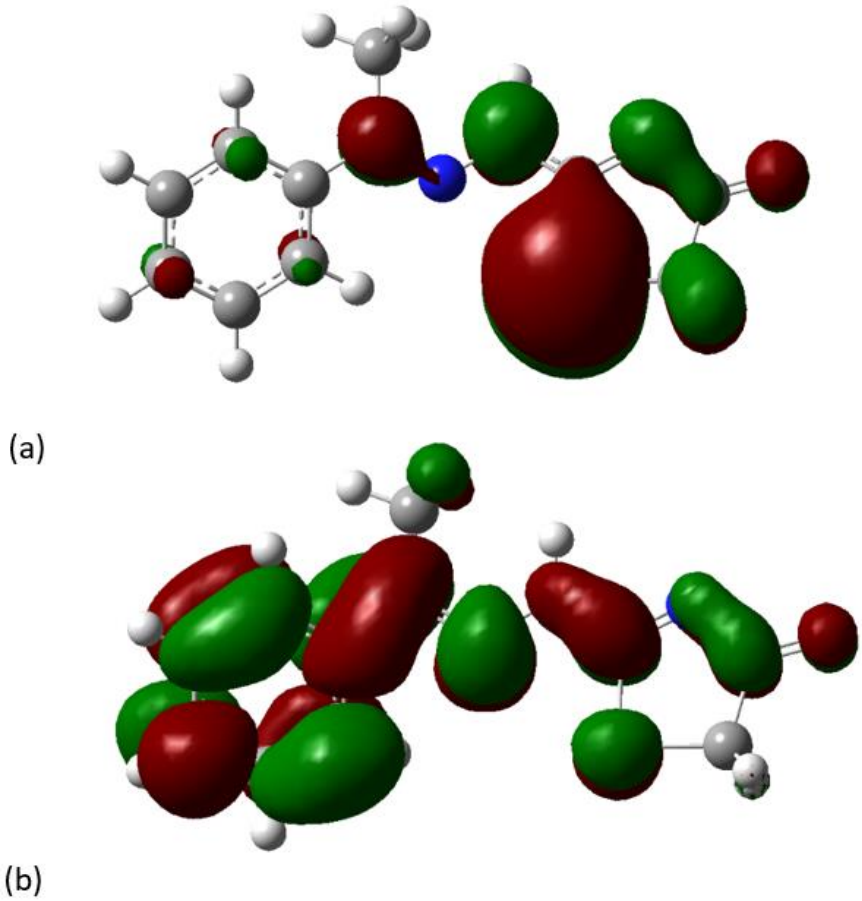

Figure S22. Orbitals in HOMO (top) and LUMO (bottom) in **DKI24** endo conformation.

Table S1. HOMO- LUMO gap, hardness, and softness of lowest in energy endo and exo conformers .

	DKI21 endo	DKI21 exo	DKI24 endo	DKI24 exo
H-L	4.302	4.237	4.549	4.364
η	2.151	2.118	2.275	2.182
μ	-4.331	-4.160	-4.349	-4.144
S	0.465	0.472	0.440	0.458