Electronic Supplementary Information

First report of trans-A2B-corrole derived from a lapachone derivative: Photophysical, TD-DFT and Photobiological assays

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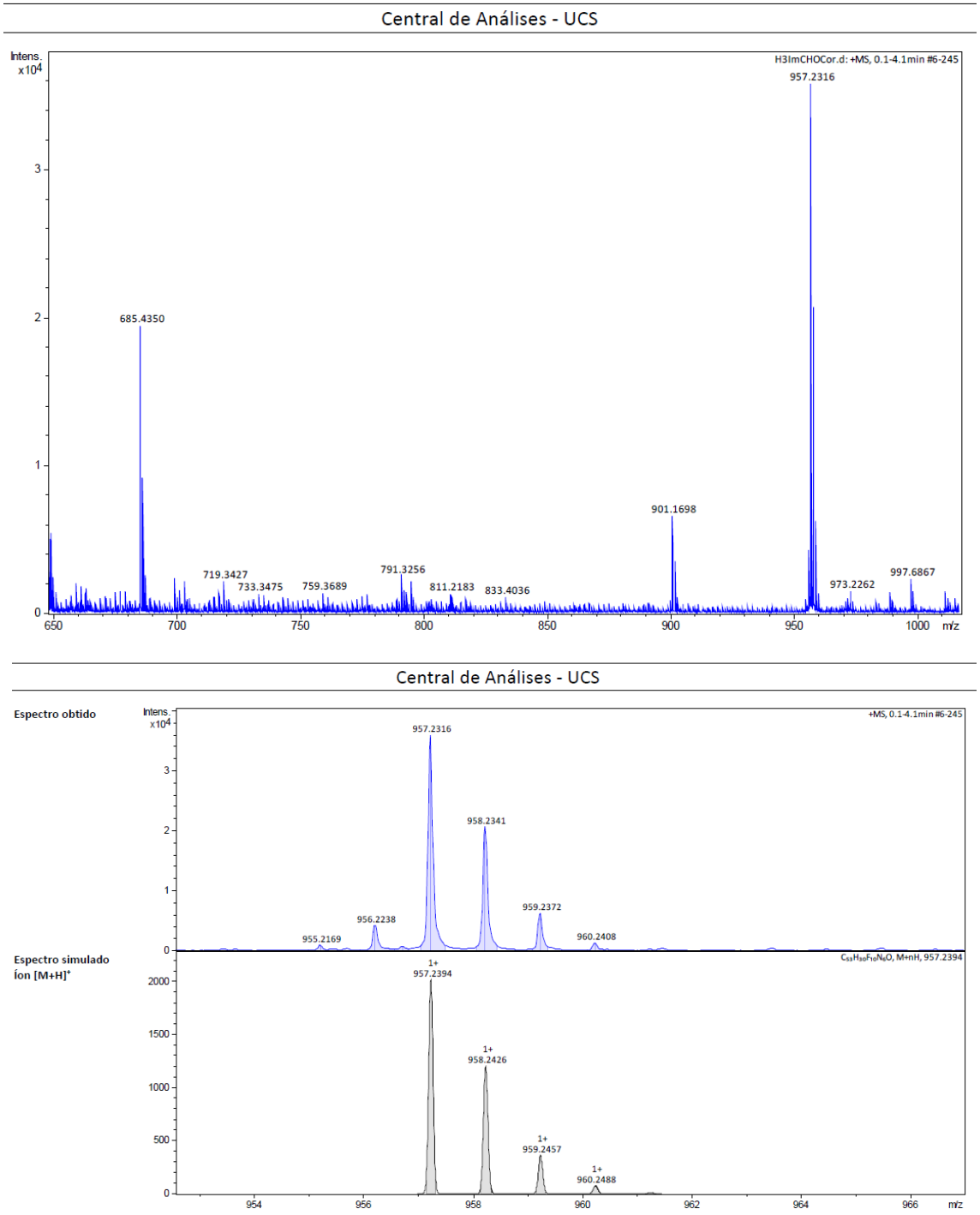


Figure S1. HRMS-ESI(+) spectrum of corrole **H_3LapCor**.

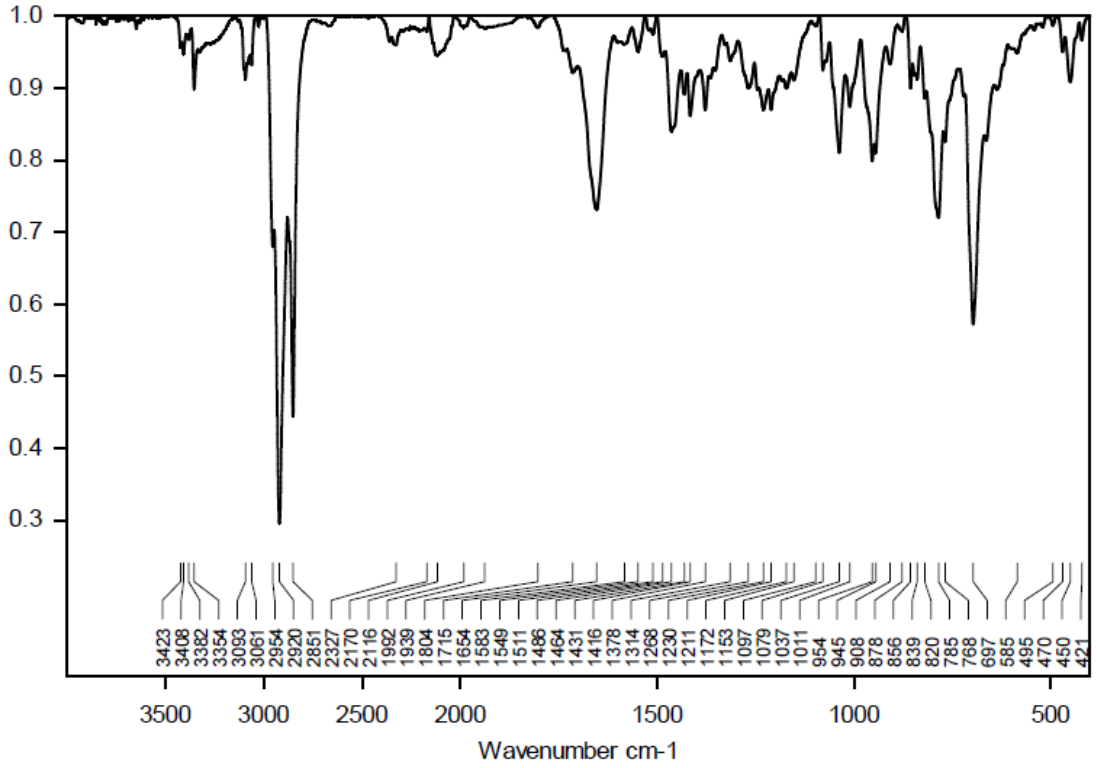
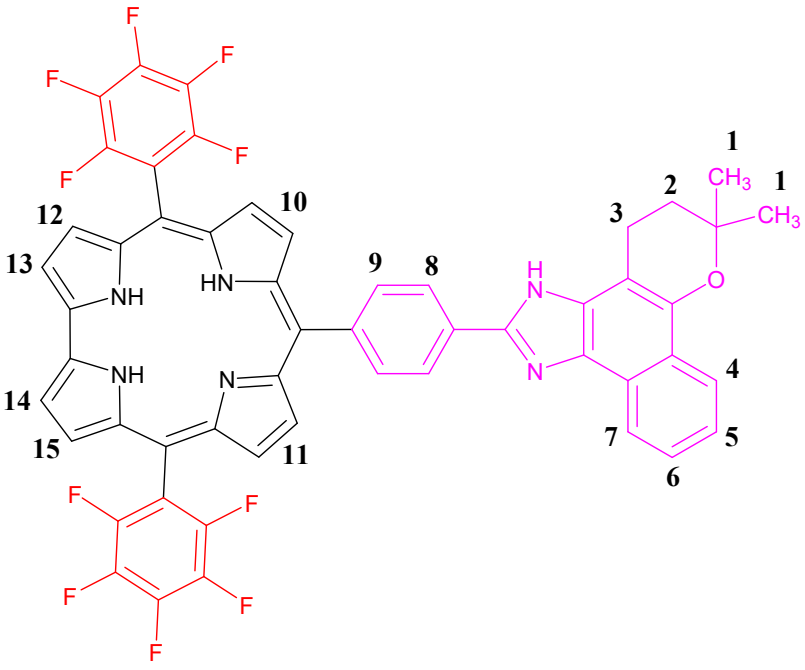
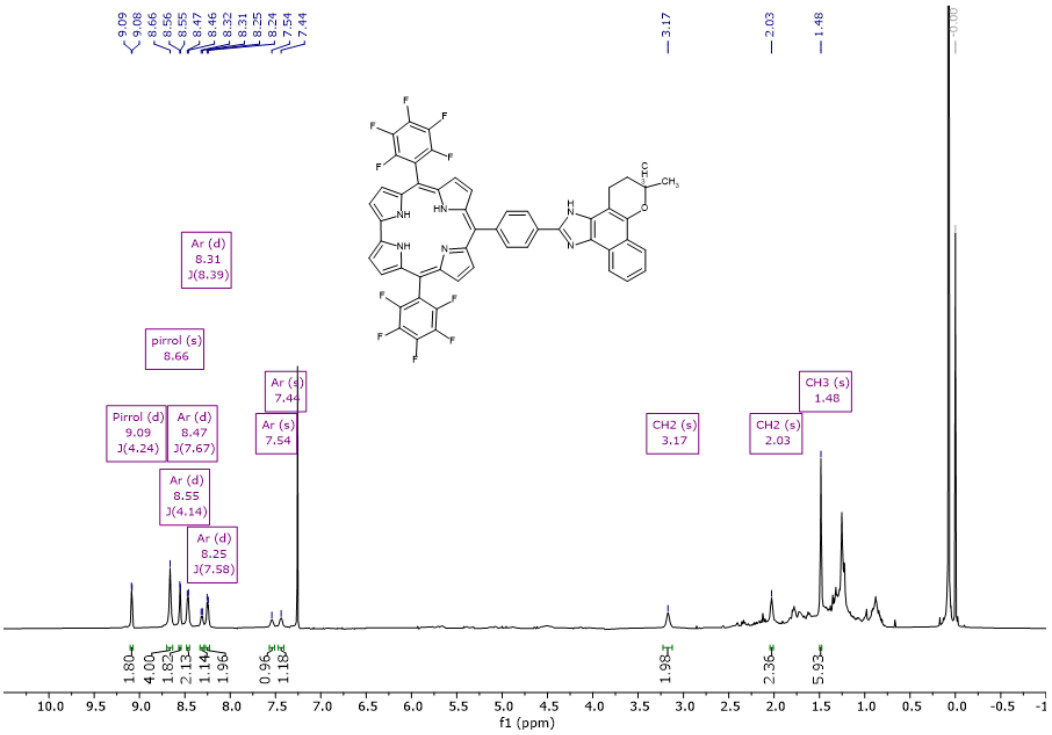


Figure S2. FTIR ATR spectrum of corrole **H_3LapCor**.

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J(8.39)
pirrol (s)
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Ar (s)
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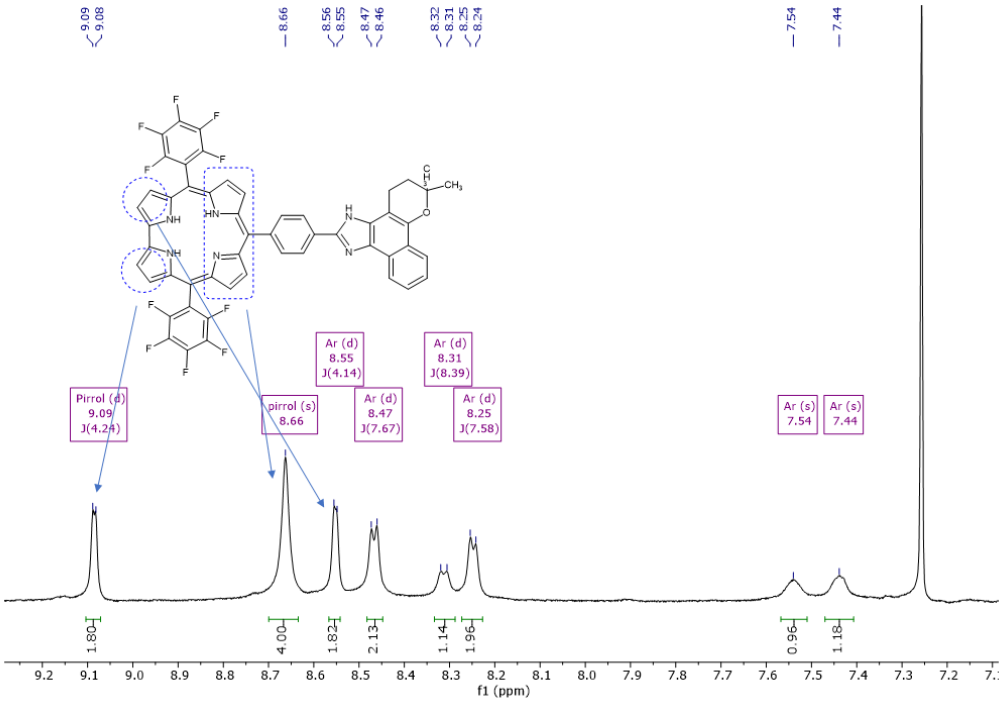
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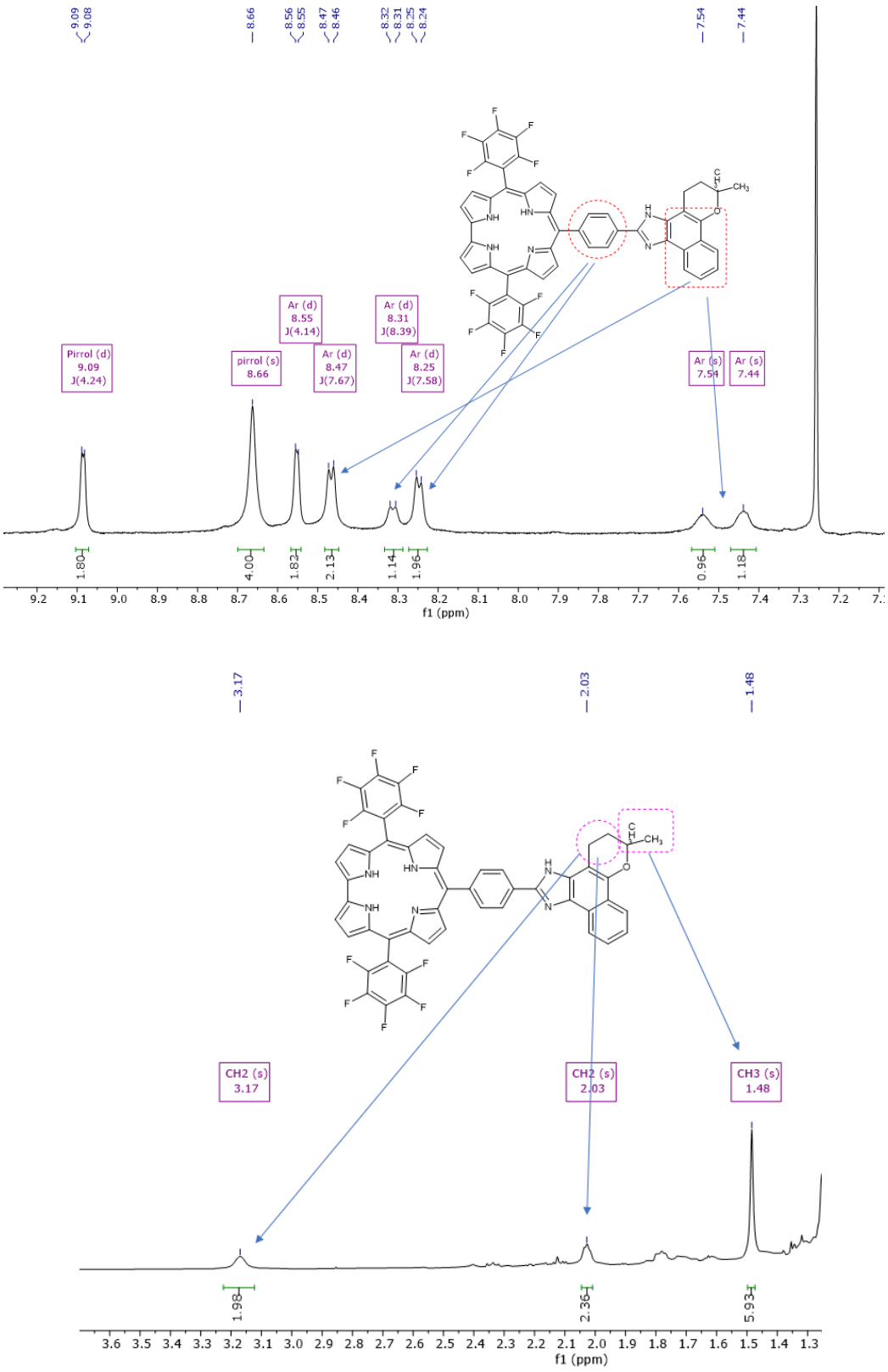
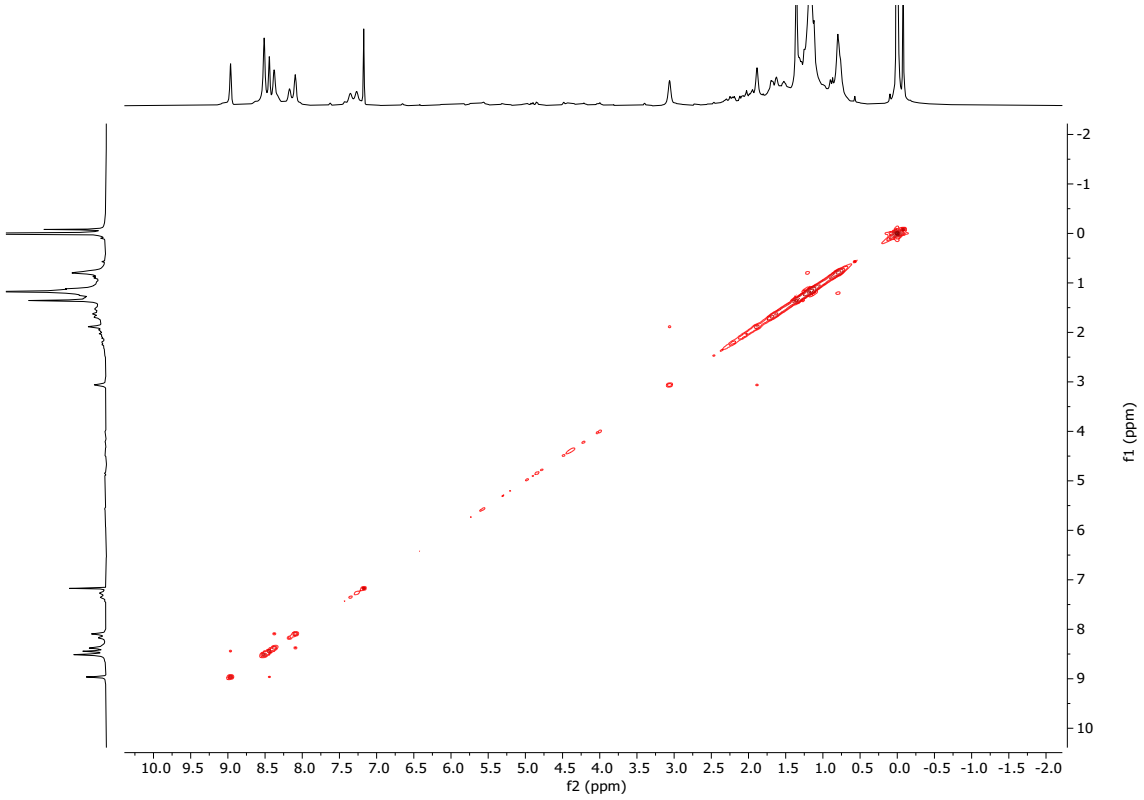


Figure S3. ^{1}H NMR spectrum (600 MHz) of corrole **H_3LapCor** in $CDCl_3$.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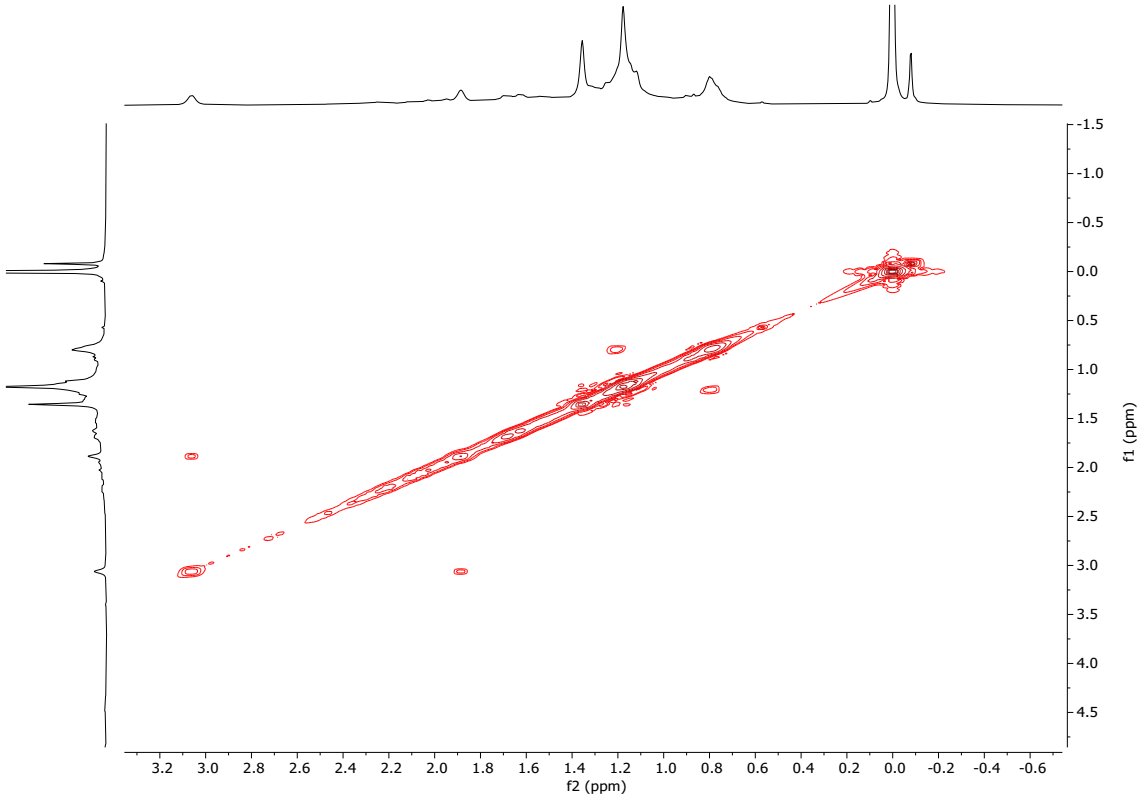
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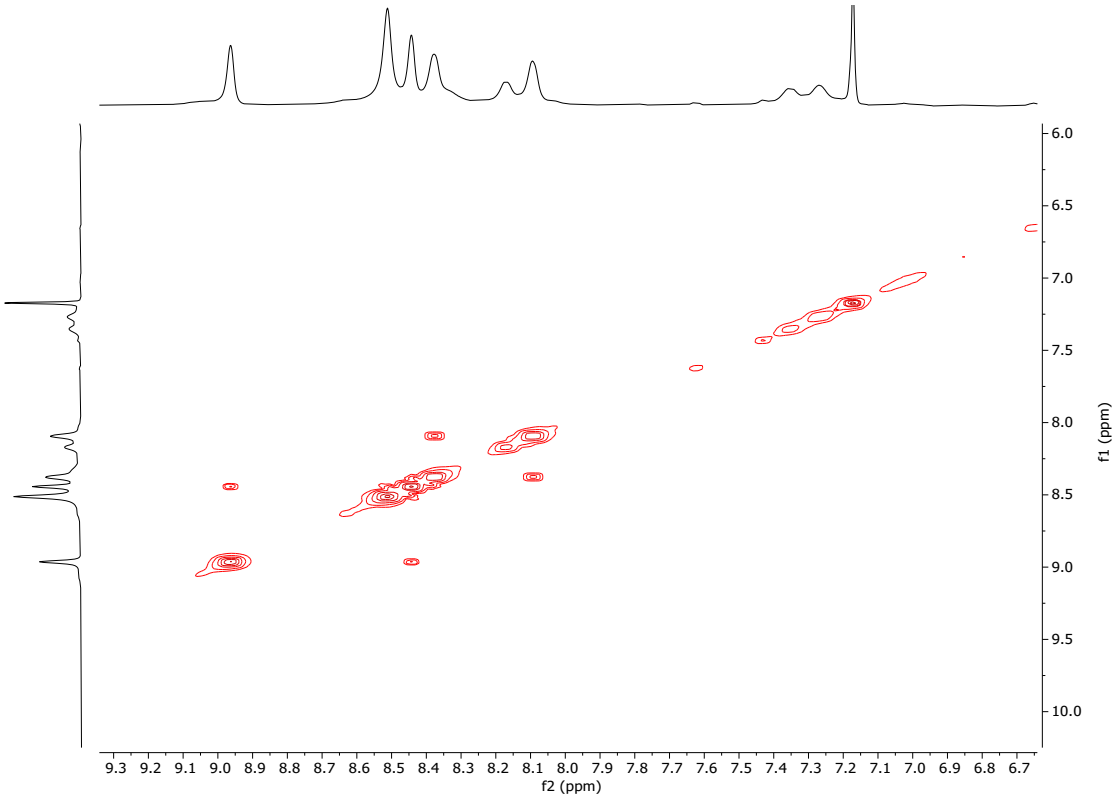

Figure S4. ^{1}H-^{1}H COSY 2D NMR spectrum of corrole **H_3LapCor** in $CDCl_3$.

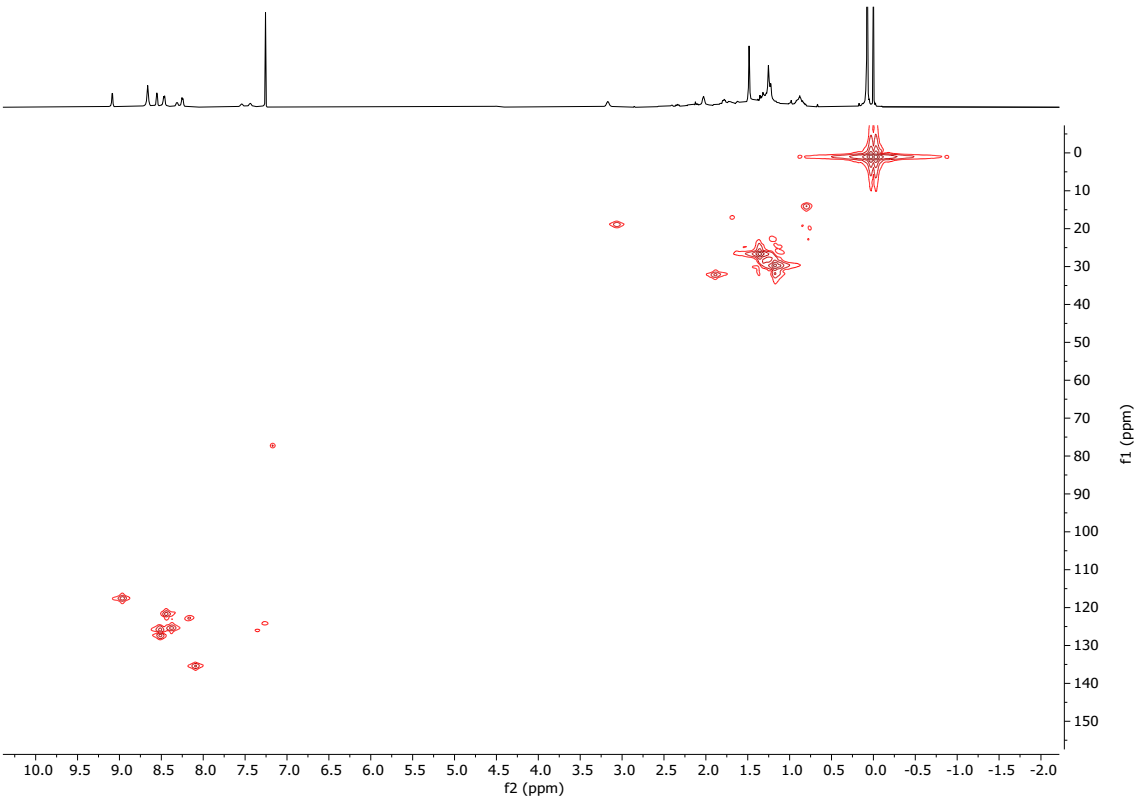

Figure S5. ^{1}H-^{13}C HMBC NMR spectrum of corrole **H_3LapCor** in $CDCl_3$.

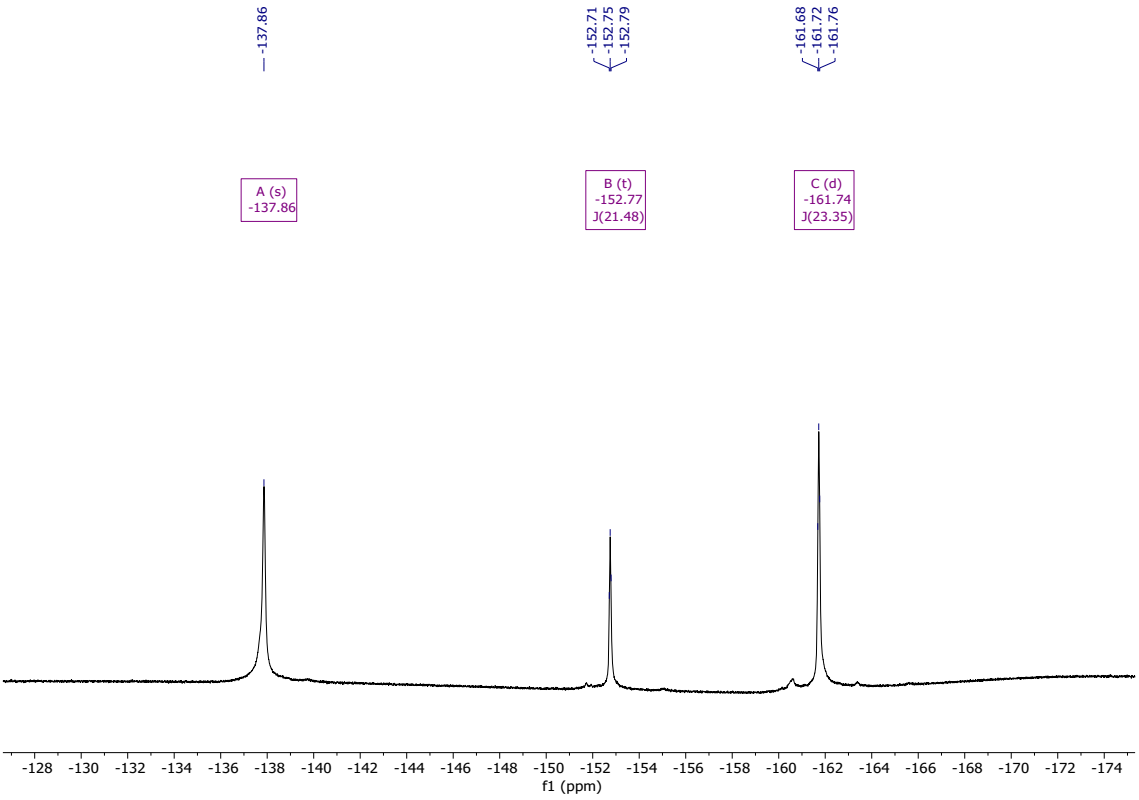

Figure S6. ^{19}F NMR spectrum (565 MHz) of corrole **H_3LapCor** in $CDCl_3$.

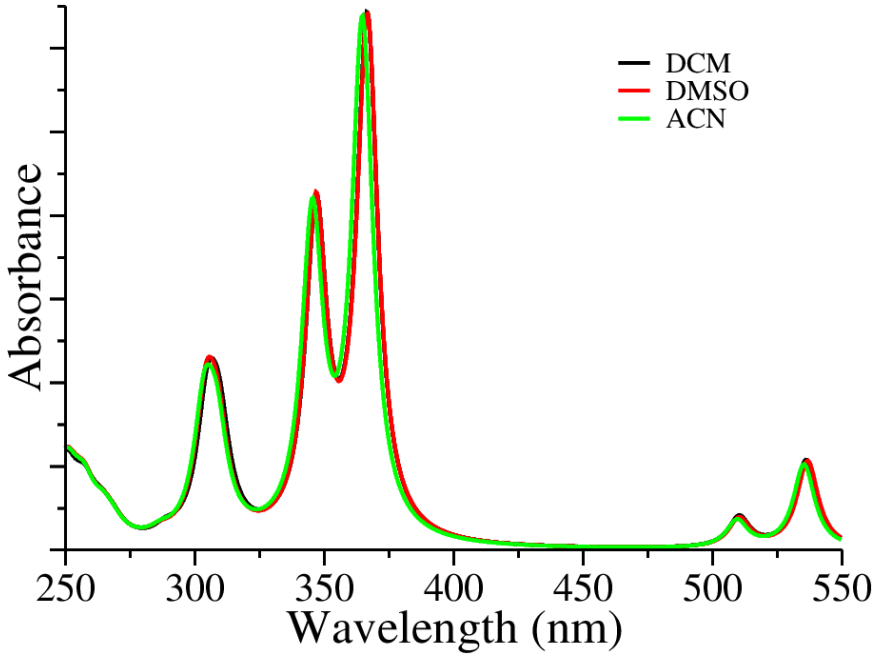

Figure S7. TD-DFT UV-Vis absorption spectra of corrole **H_3LapCor**.

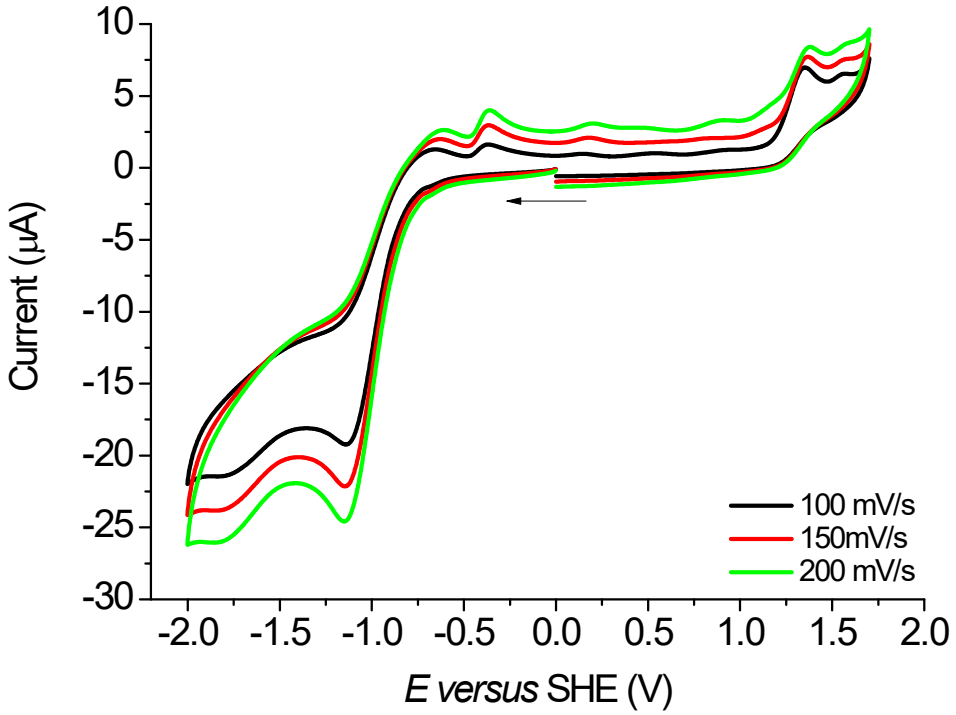

Figure S8. Cyclic voltametry of corrole **H_3LapCor** in dry DCM solution.

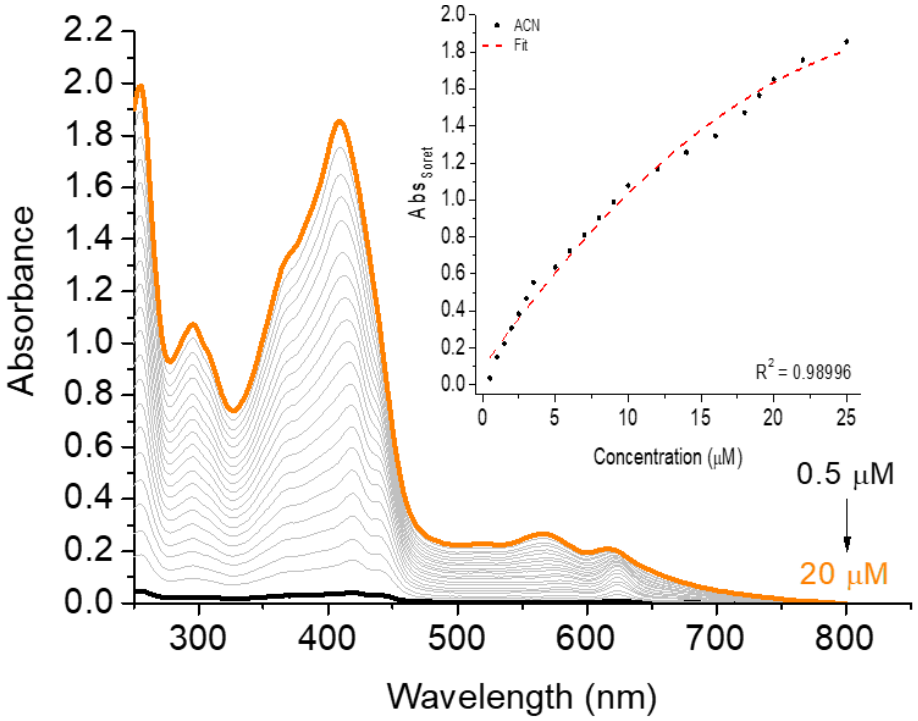

Figure S9. UV-Vis aggregation assays of corrole **H_3LapCor** in ACN solution, in the concentration variation from 0.5 to 20 μM. Inset: Abs_{Soret} versus concentration plot.

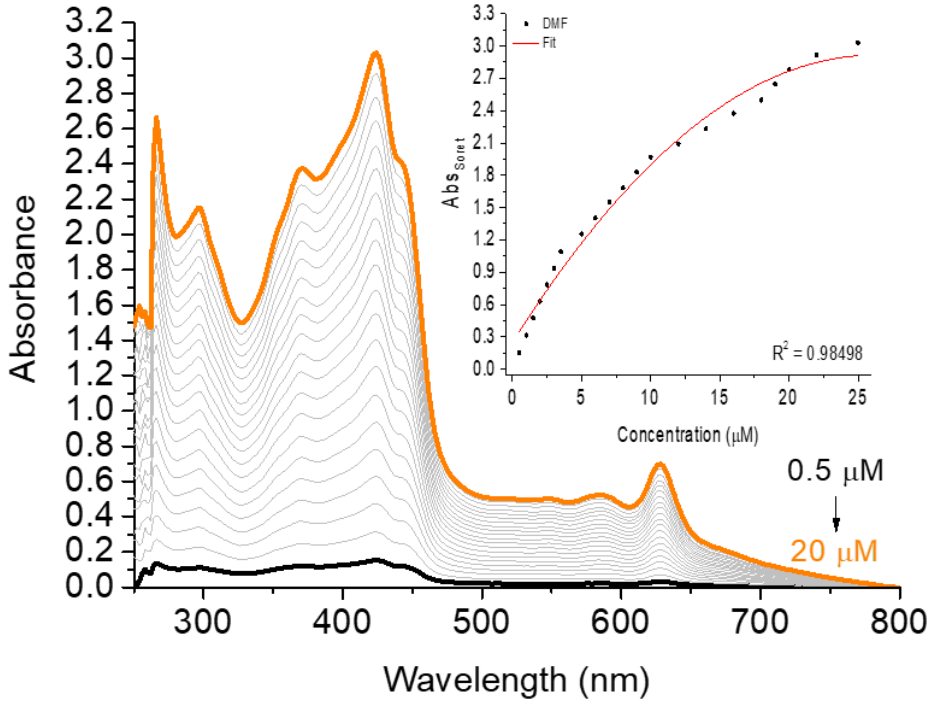

Figure S10. UV-Vis aggregation assays of corrole **H_3LapCor** in DMF solution, in the concentration variation from 0.5 to 20 μM. Inset: Abs_{Soret} versus concentration plot.

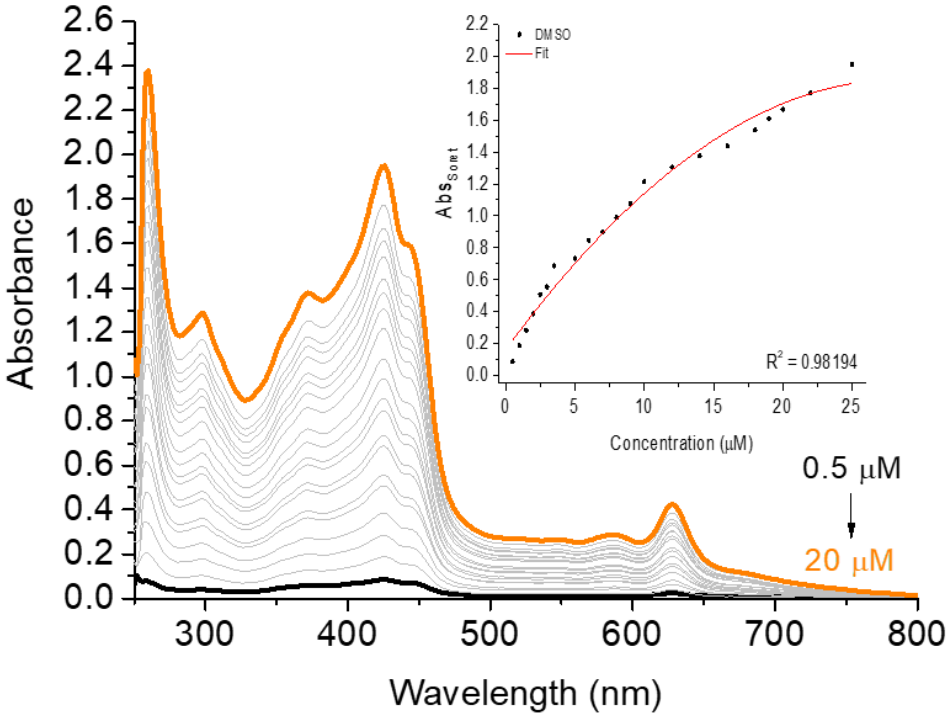

Figure S11. UV-Vis aggregation assays of corrole **H_3LapCor** in DMSO solution, in the concentration variation from 0.5 to 20 μM. Inset: Abs_{Soret} versus concentration plot.

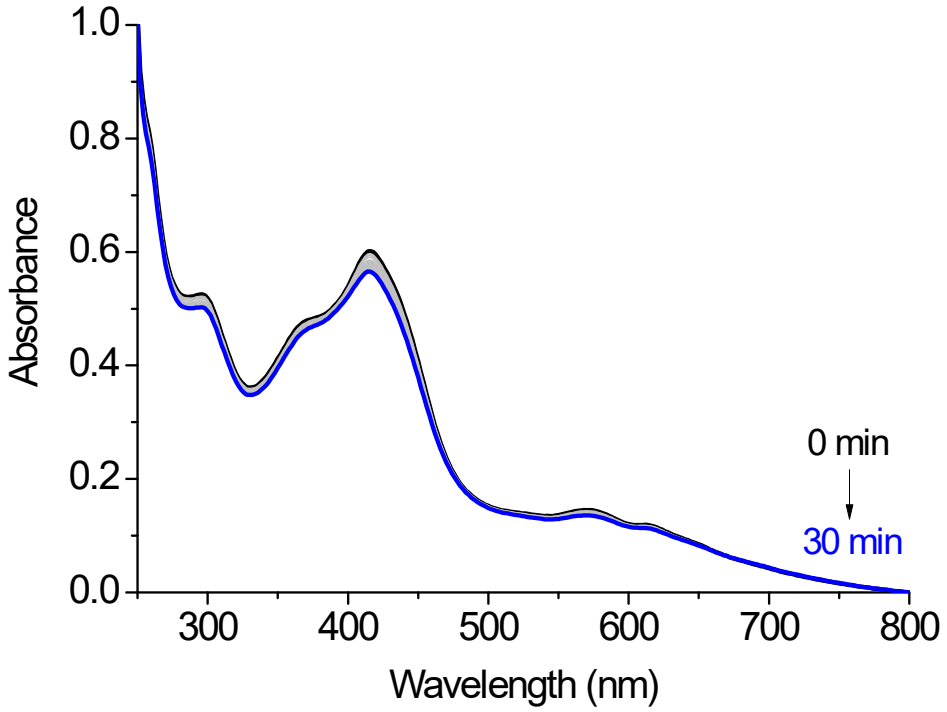

Figure S12. Photostability assays by UV-Vis analysis of corrole **H_3LapCor** in DMSO(5%)/Tris-HCl pH 7.4 buffer mixture solution, in white-light irradiation conditions, at period of 30 min.

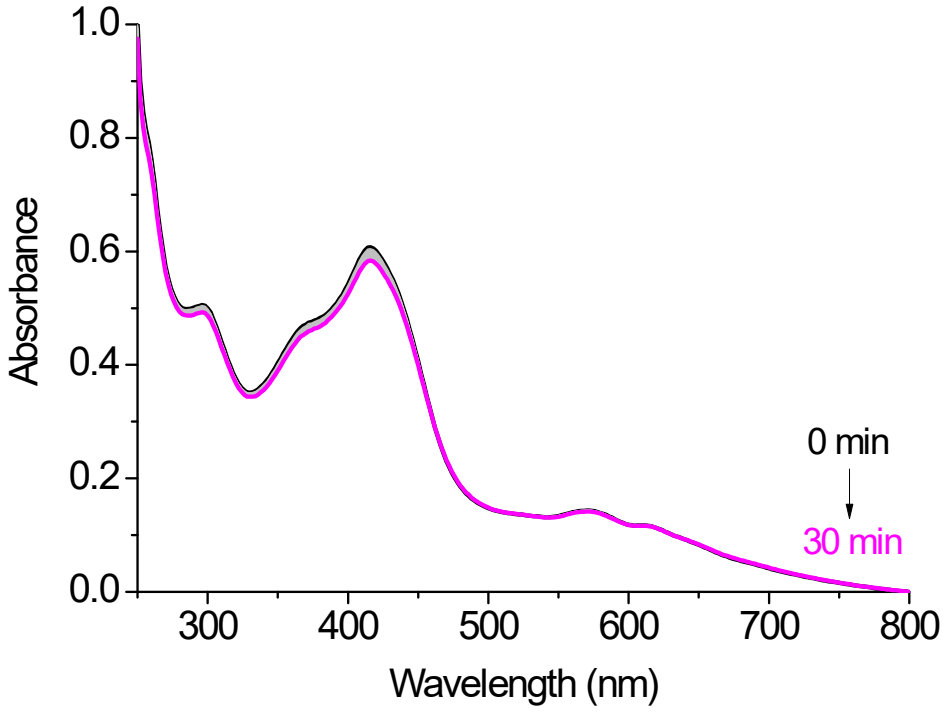

Figure S13. Photostability assays by UV-Vis analysis of corrole **H_3LapCor** in DMSO(5%)/Tris-HCl pH 7.4 buffer mixture solution, in red-light irradiation conditions, at period of 30 min.

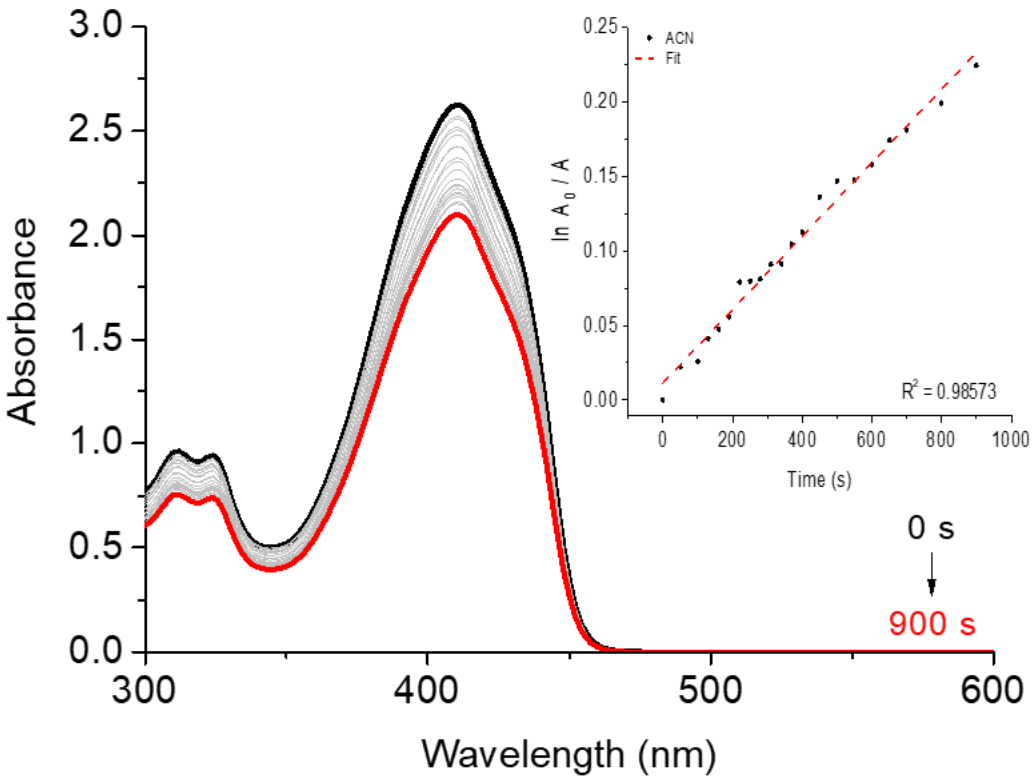

Figure S14. DPBF photo-oxidation experiment in ACN solution by irradiation with red-light LED source (660 nm; irradiance of 100 mW cm^{-2} and a total light dosage of 90 J cm^{-2}) in the presence of corrole **H_3LapCor**. The inset shows the first order kinetic profile.

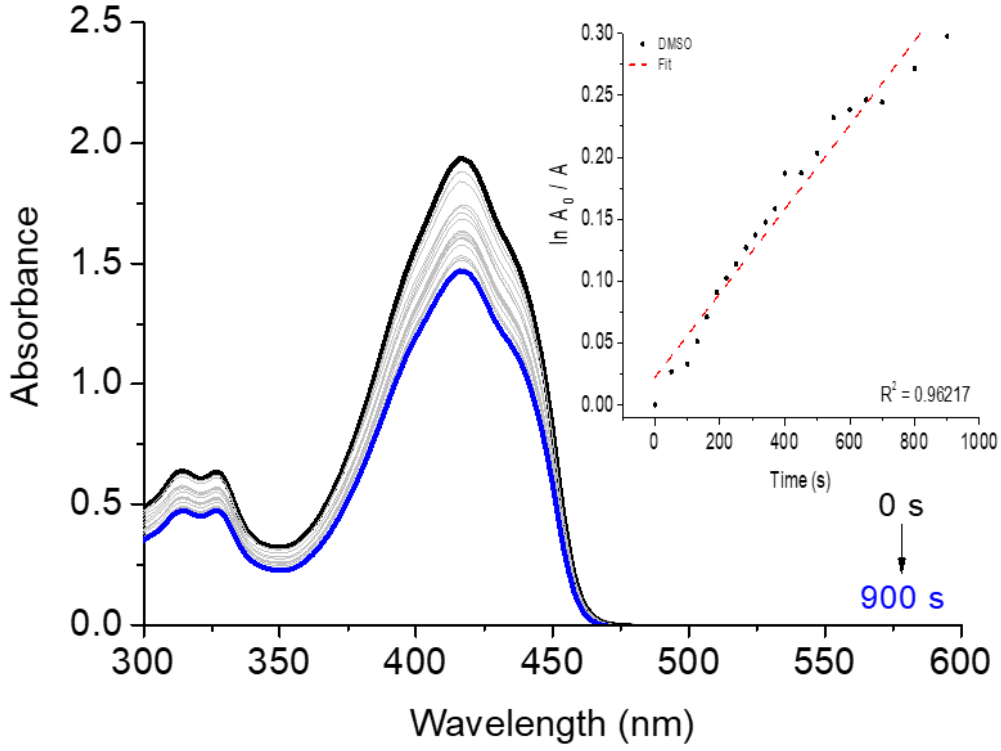

Figure S15. DPBF photo-oxidation experiment in DMSO solution by irradiation with red-light LED source (660 nm; irradiance of 100 mW cm^{-2} and a total light dosage of 90 J cm^{-2}) in the presence of corrole **H_3LapCor**. The inset shows the first order kinetic profile.

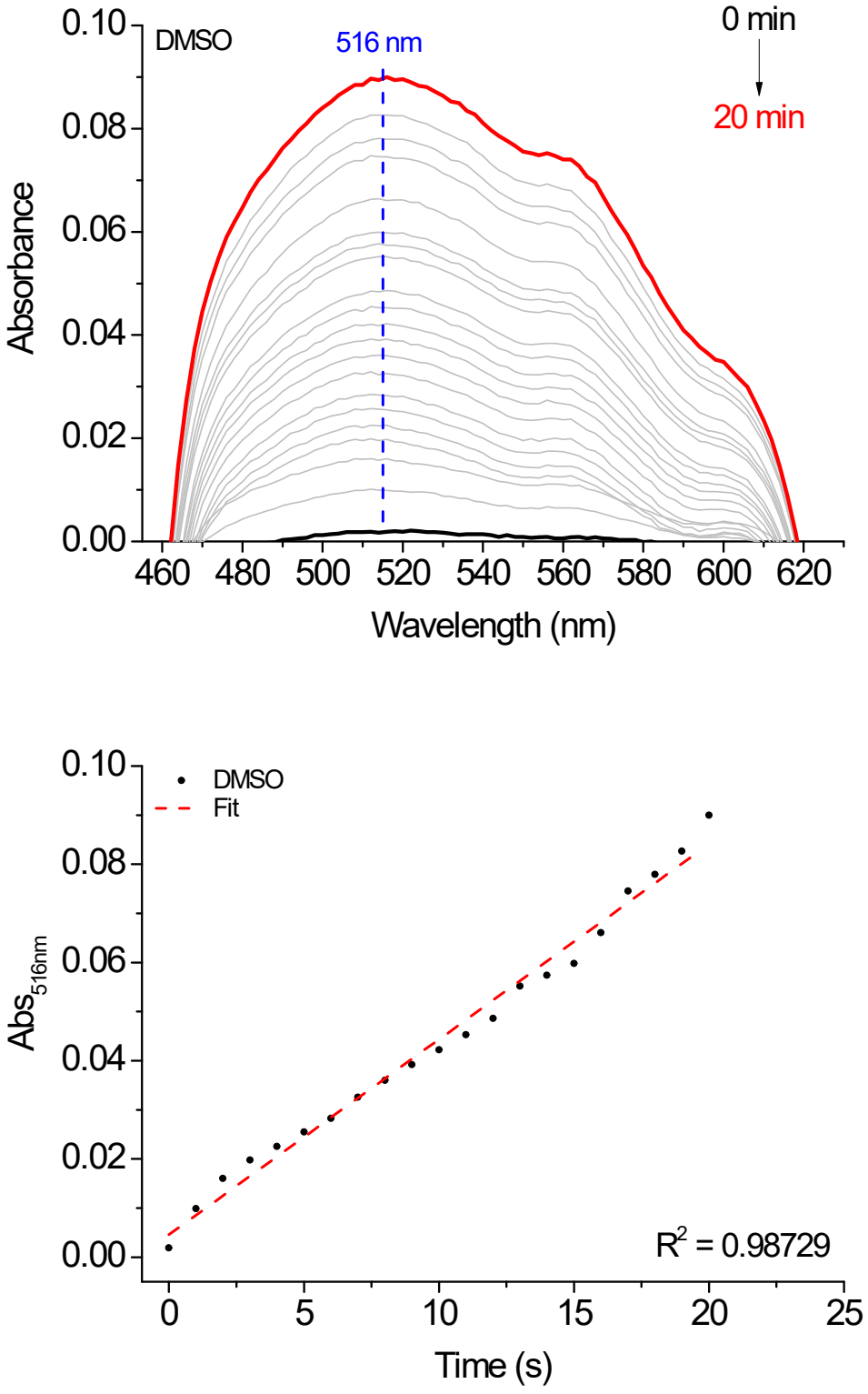

Figure S16. NBT reduction experiment in DMSO solution by irradiation with white-light LED source in the presence of corrole **H_3LapCor**.

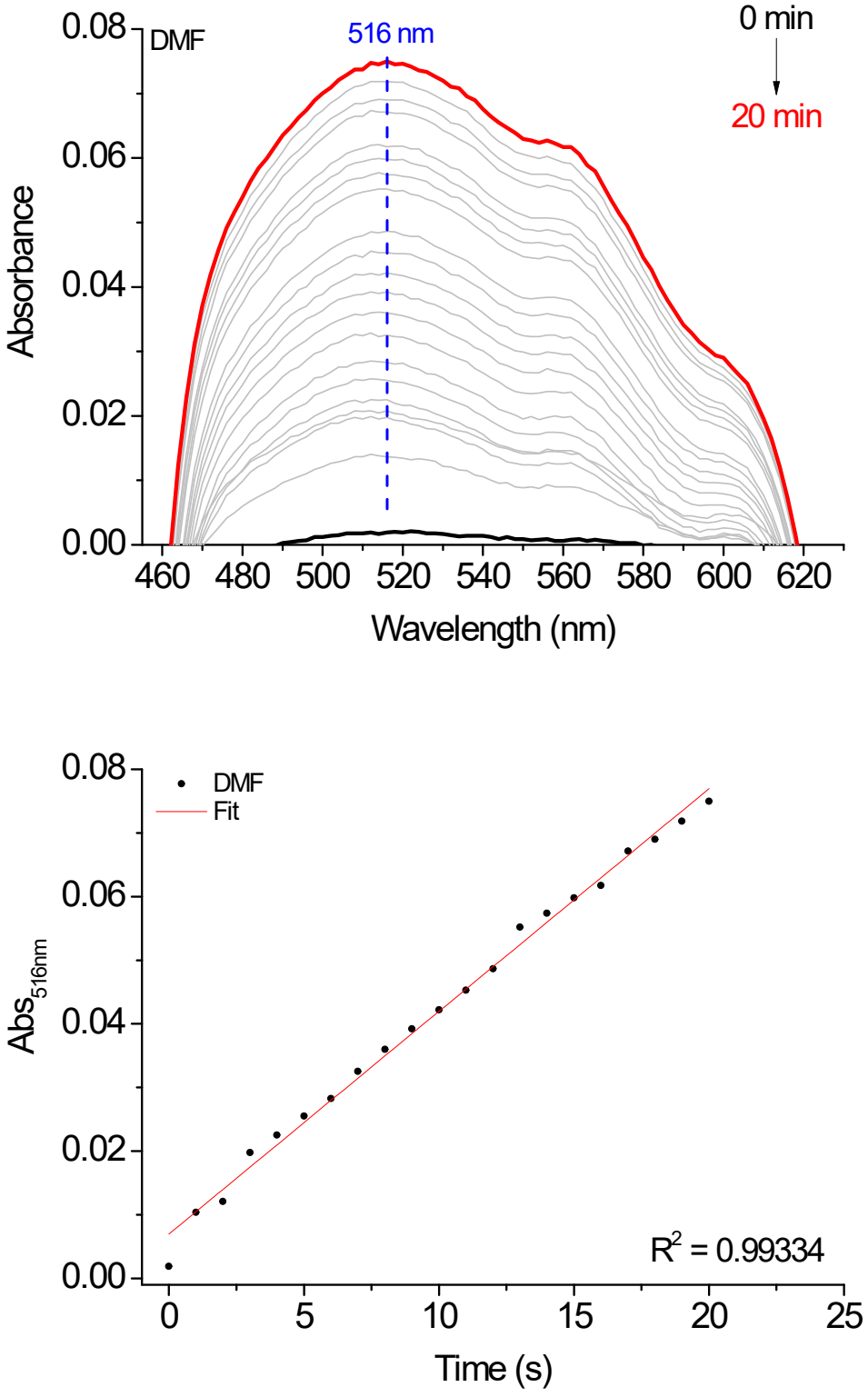

Figure S17. NBT reduction experiment in DMF solution by irradiation with white-light LED source in the presence of corrole **H_3LapCor**.

Table S1. Vertical transitions, Energy, oscillator strength (f), and Dipole Moment for the corrole-lapachone in three different solvent environments.

Environment	Transition	Energy eV(nm)	ƒ	Dipole Moment
DCM	$S_0 \rightarrow S_1$	2.3124 (536.17)	0.3321	7.1398
	$S_0 \rightarrow S_2$	2.4297 (510.29)	0.1145	
	$S_0 \rightarrow S_3$	3.3820 (366.60)	1.9428	
	$S_0 \rightarrow S_4$	3.5742 (346.89)	1.2044	
DMSO	$S_0 \rightarrow S_1$	2.3100 (536.74)	0.3287	7.7482
	$S_0 \rightarrow S_2$	2.4294 (510.34)	0.1085	
	$S_0 \rightarrow S_3$	3.3812 (366.68)	1.9382	
	$S_0 \rightarrow S_4$	3.5751 (346.79)	1.2154	
ACN	$S_0 \rightarrow S_1$	2.3160 (535.35)	0.3287	7.6981
	$S_0 \rightarrow S_2$	2.4335 (509.49)	0.1085	
	$S_0 \rightarrow S_3$	3.3994 (364.73)	1.9382	
	$S_0 \rightarrow S_4$	3.5897 (345.39)	1.2154	