Supporting Information

Structure revision of the sponge-derived dibrominated bis-indole alkaloids, echinosulfone A and the echinosulfonic acids A to D

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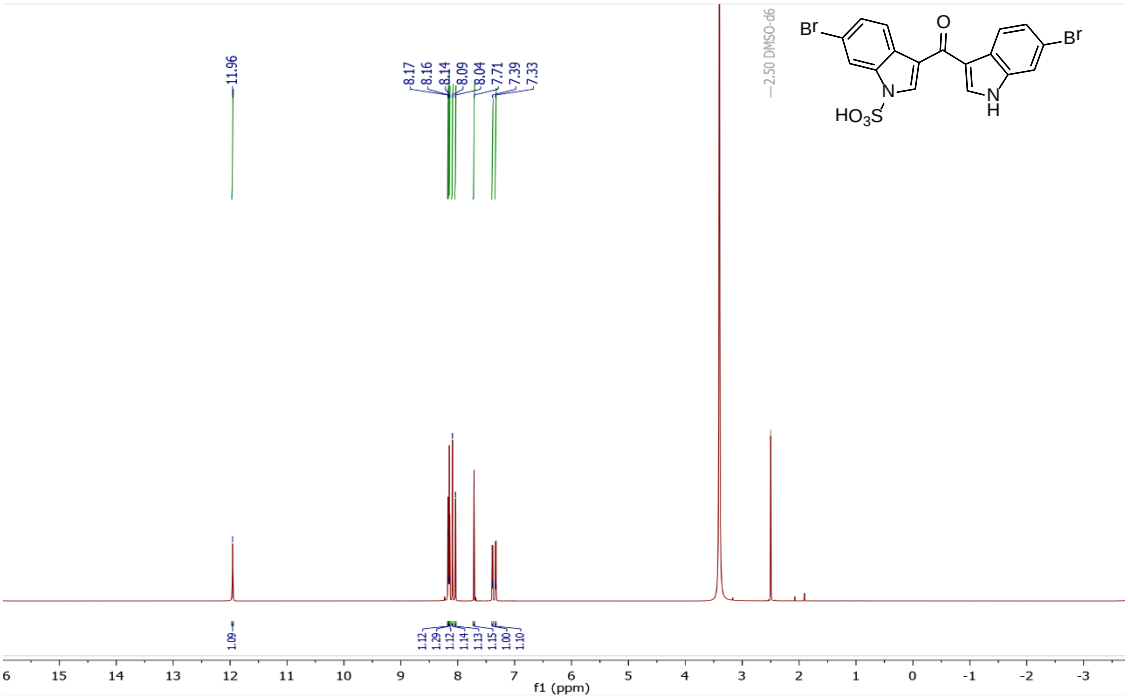
1.2 bis(6-bromo-1*H*-indol-3-yl)methanone (3) S9

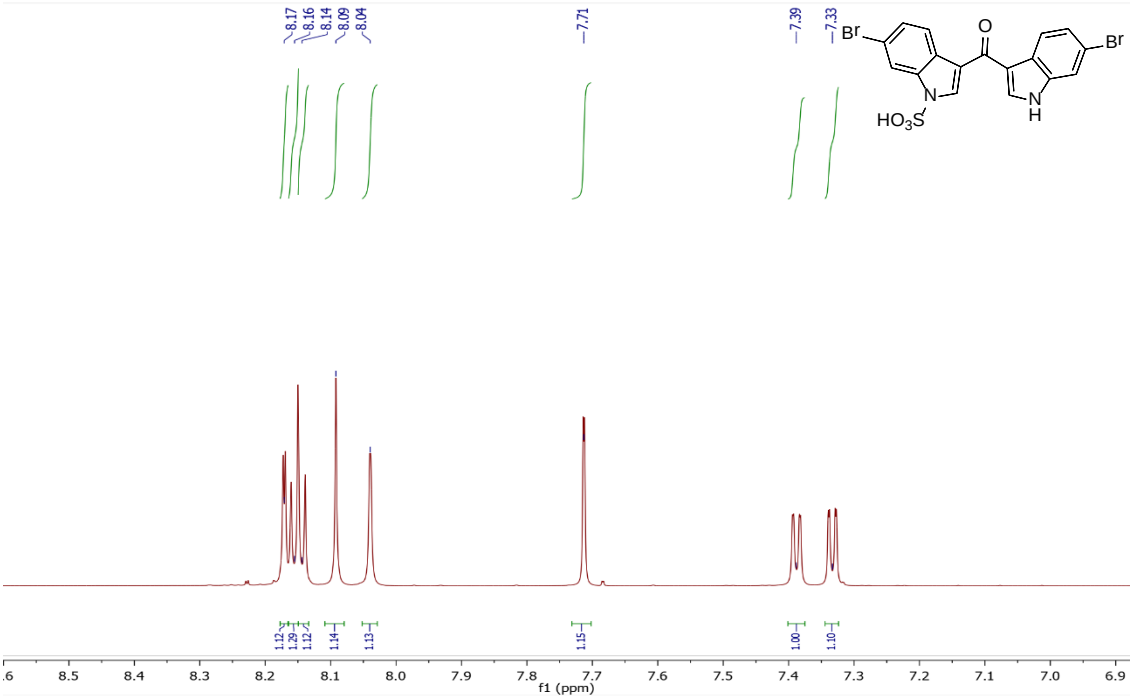
1. Spectra

1.1 6-bromo-3-(6-bromo-1*H*-indole-3-carbonyl)-1*H*-indole-1-sulfonate (2)

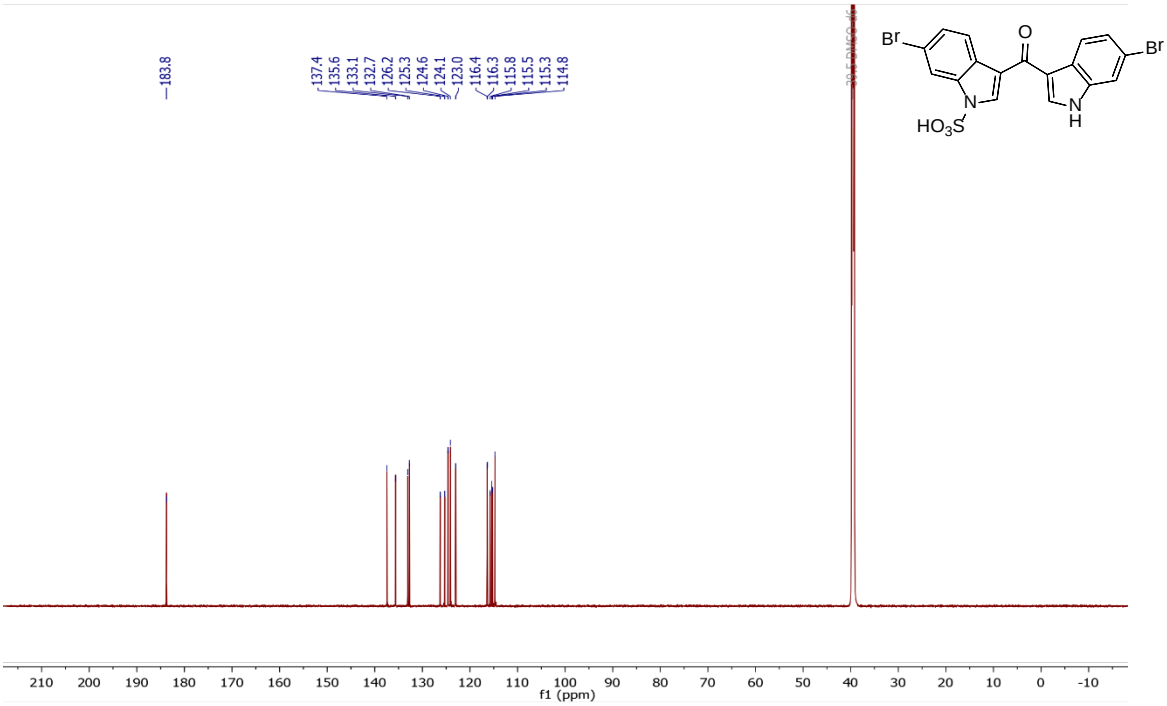
^{1}H NMR (800 MHz) spectrum of 2 in DMSO-d_6



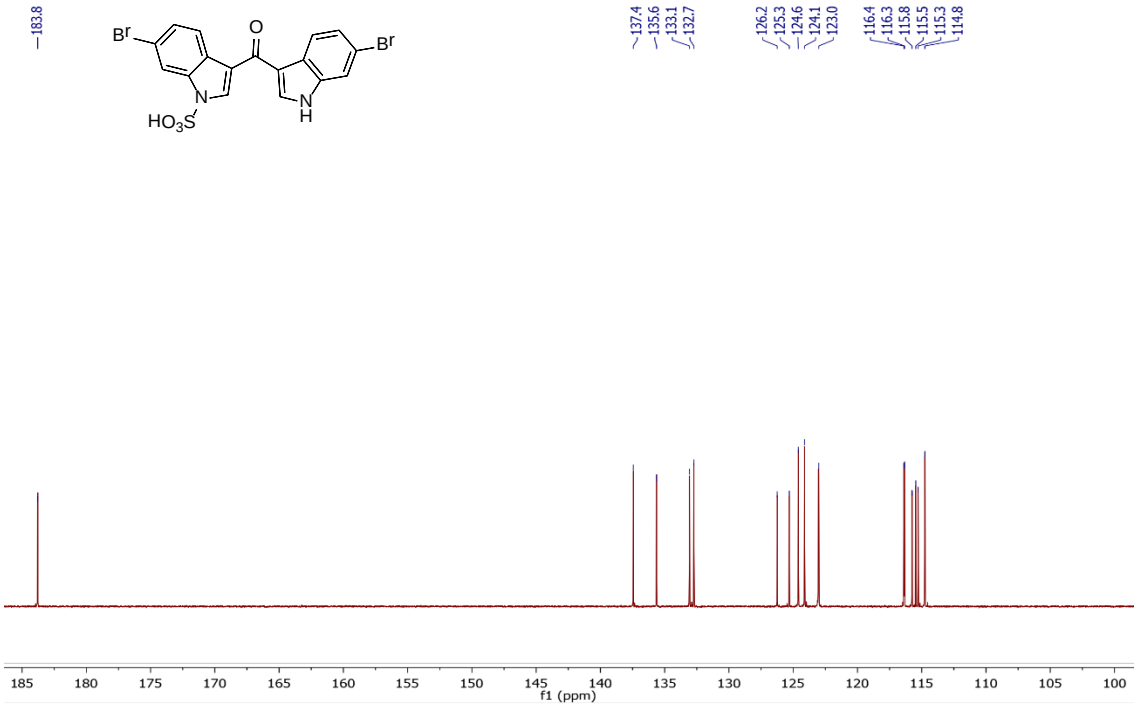
Expanded ^{1}H NMR (800 MHz) spectrum of 2 in DMSO-d_6



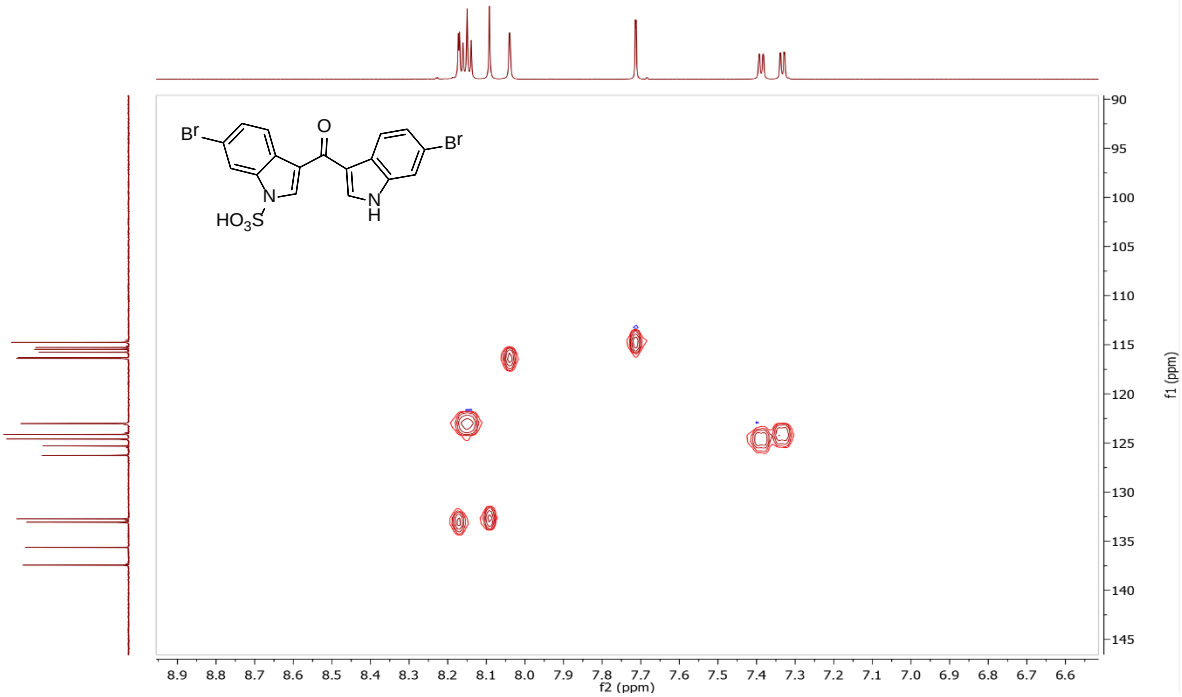
^{13}C NMR (200 MHz) spectrum of 2 in DMSO-*d*$_6$



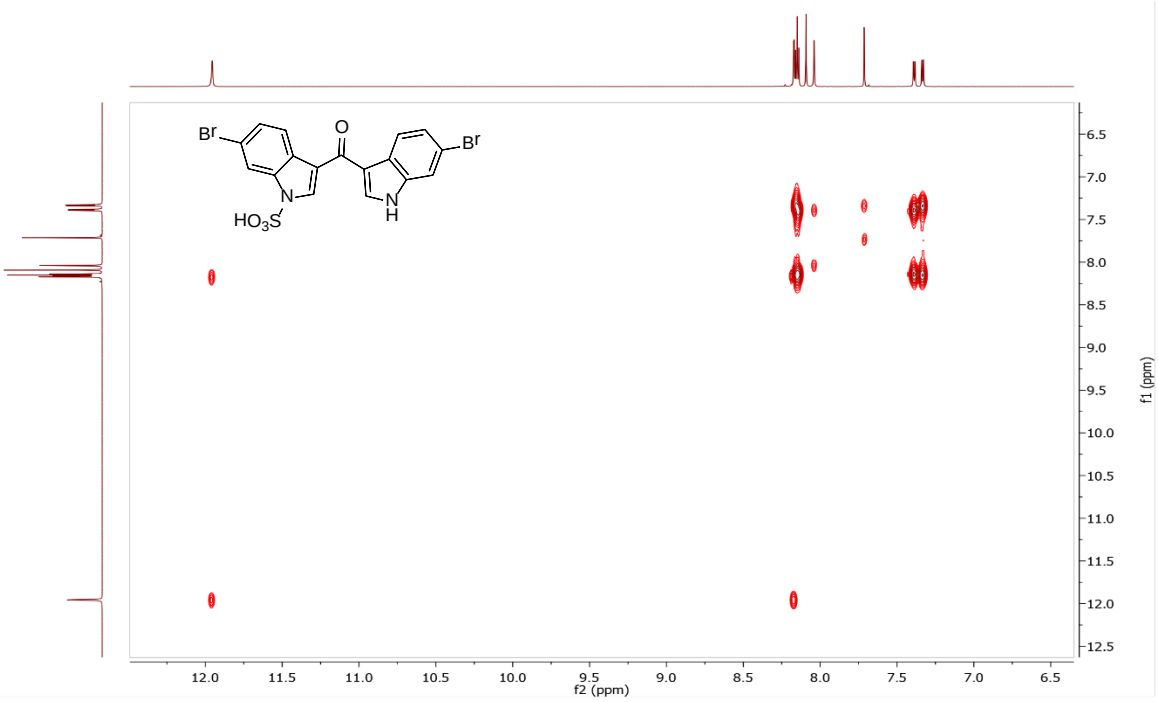
Expanded ^{13}C NMR (200 MHz) spectrum of 2 in DMSO-*d*$_6$



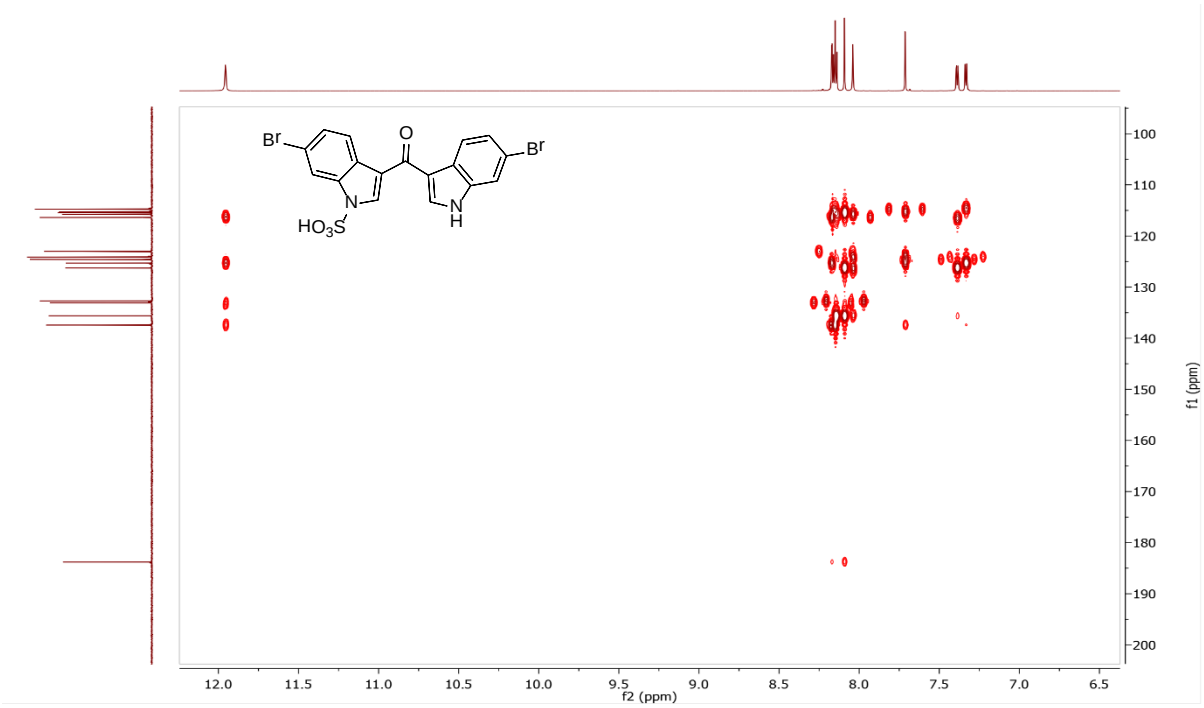
HSQC spectrum of 2 in DMSO-*d*$_6$



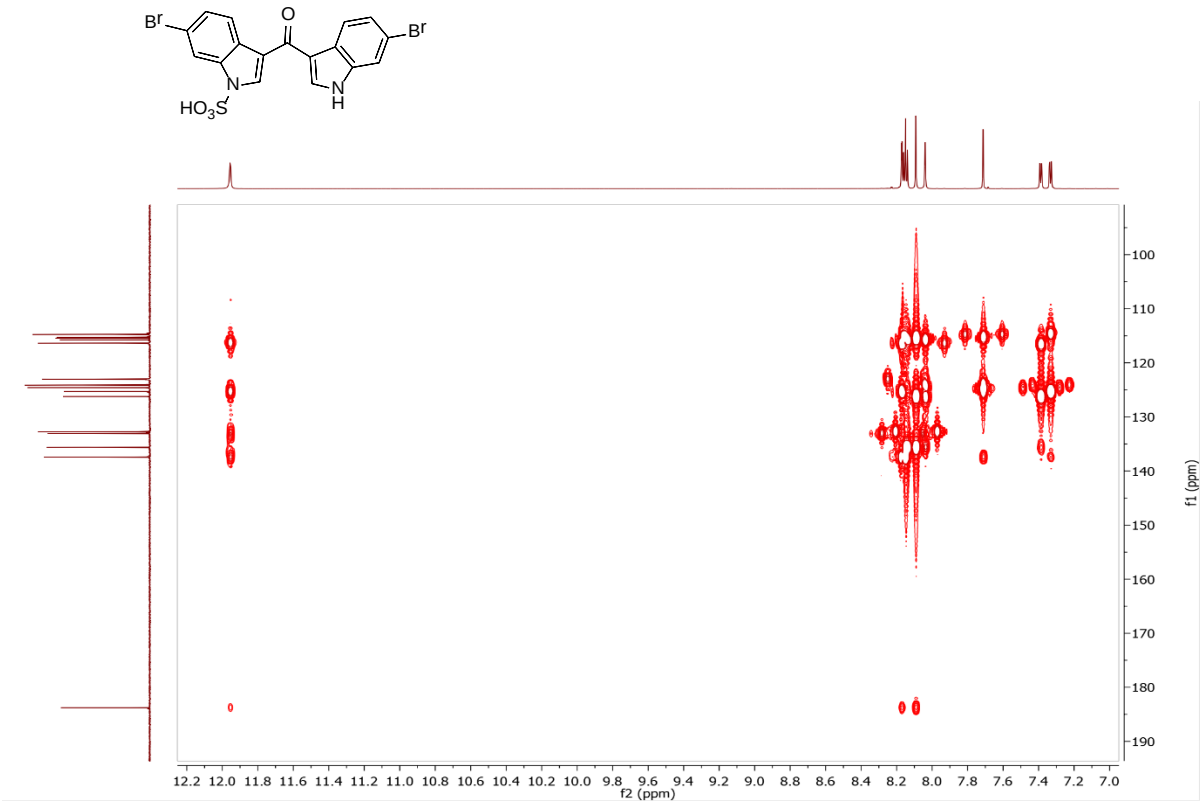
COSY spectrum of 2 in DMSO-*d*$_6$



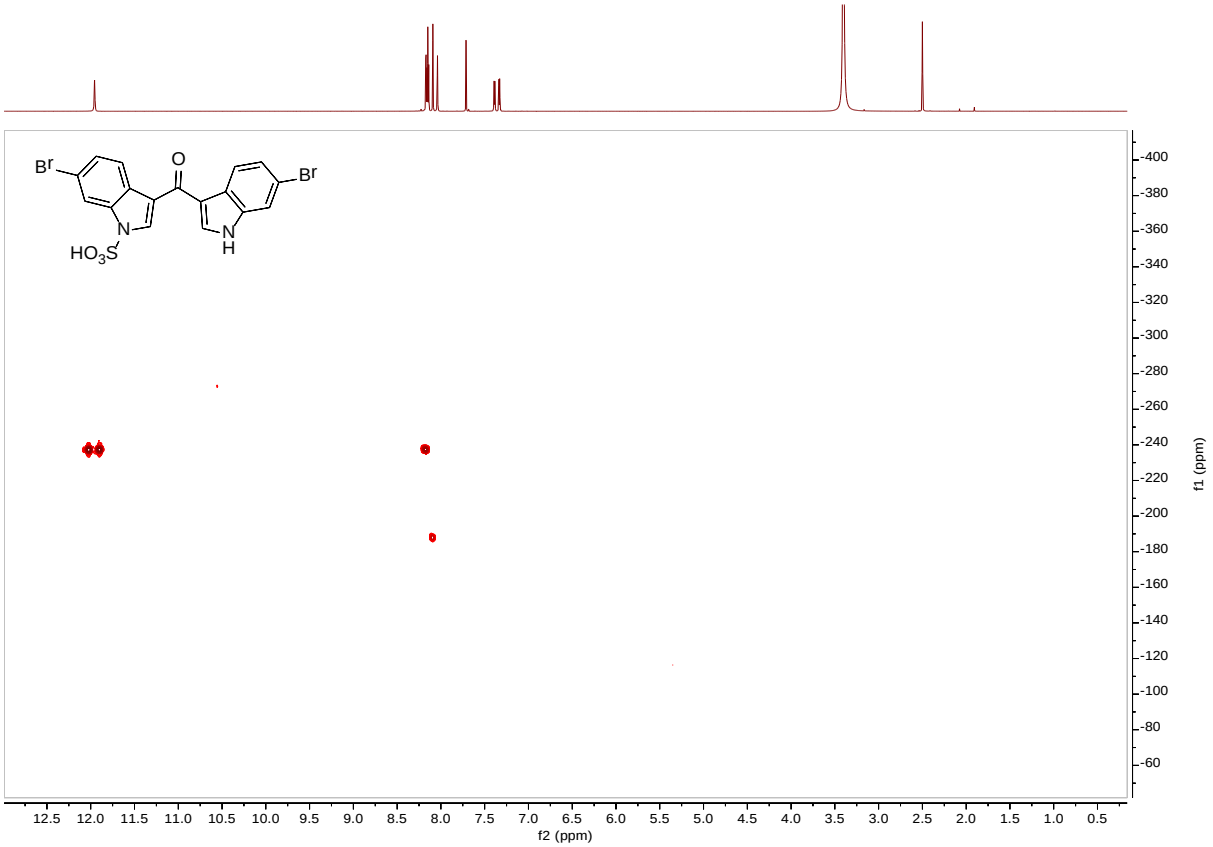
$^{1}H/^{13}C$ HMBC spectrum of 2 in DMSO-*d*$_6$



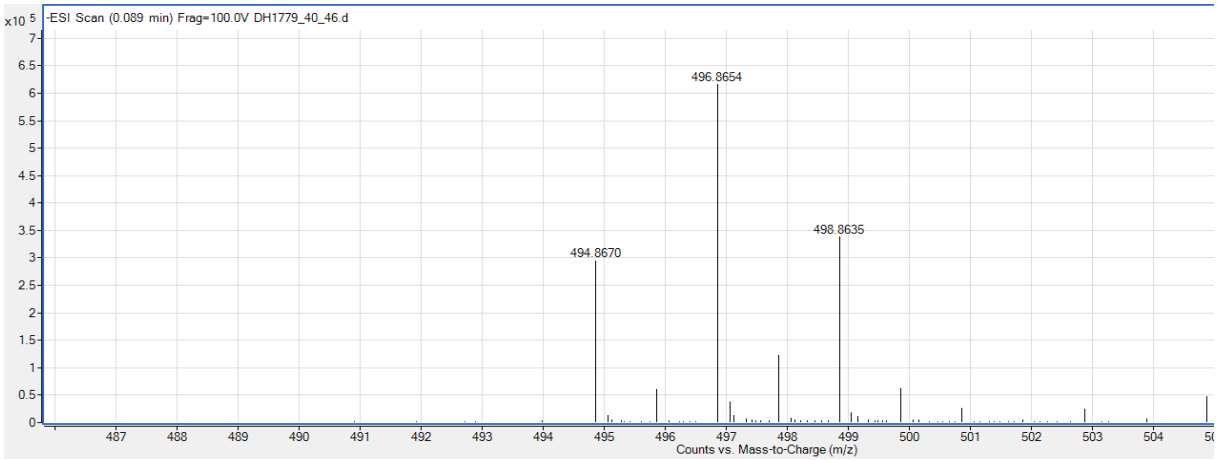
$^{1}H/^{13}C$ HMBC spectrum of 2 (increased intensity) in DMSO-*d*$_6$



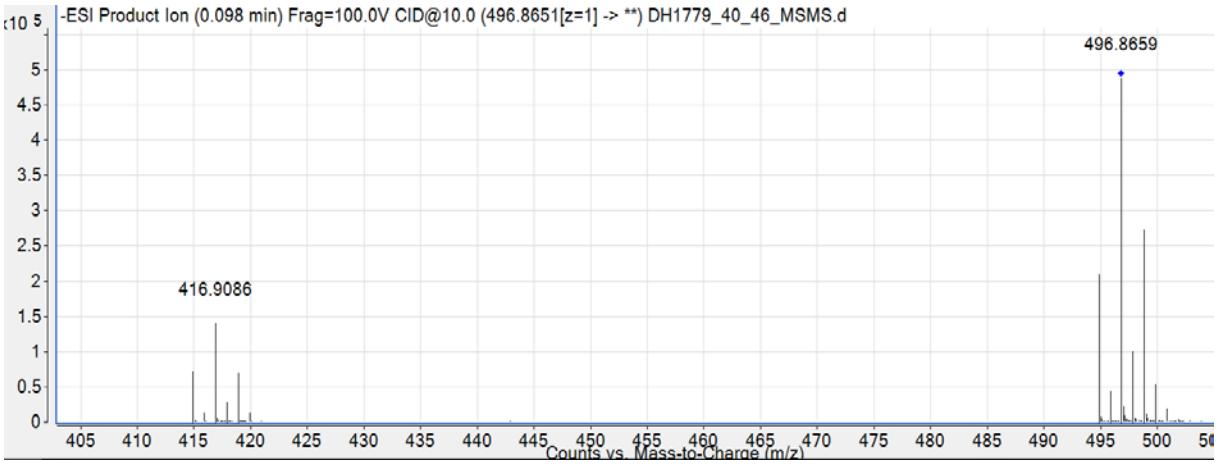
$^{1}H/^{15}N$ HMBC spectrum of 2 in DMSO-*d*$_6$ (externally referenced to CH_3NO_2 0 ppm)



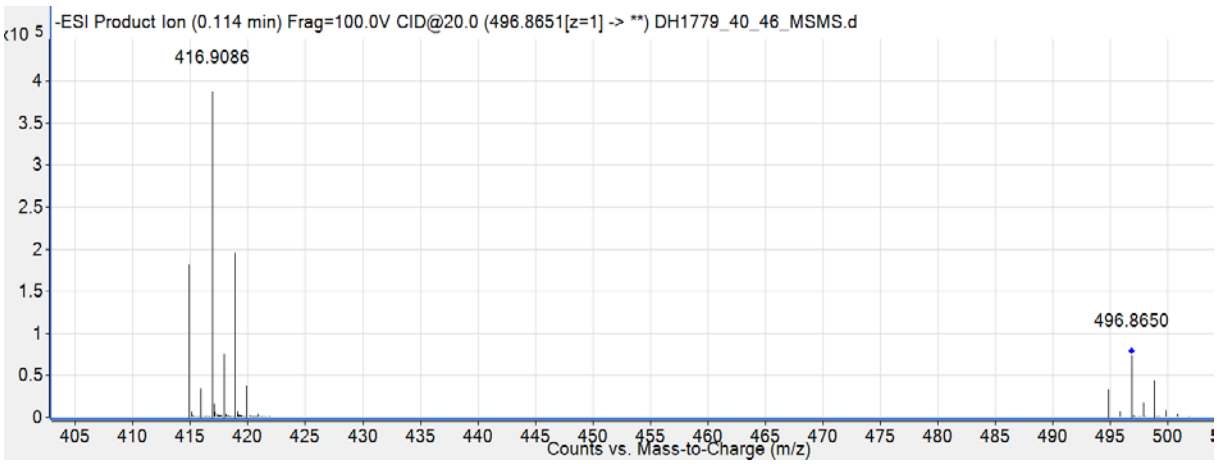
HRMS (ESI-QTOF) [M-H]$^-$ of 2



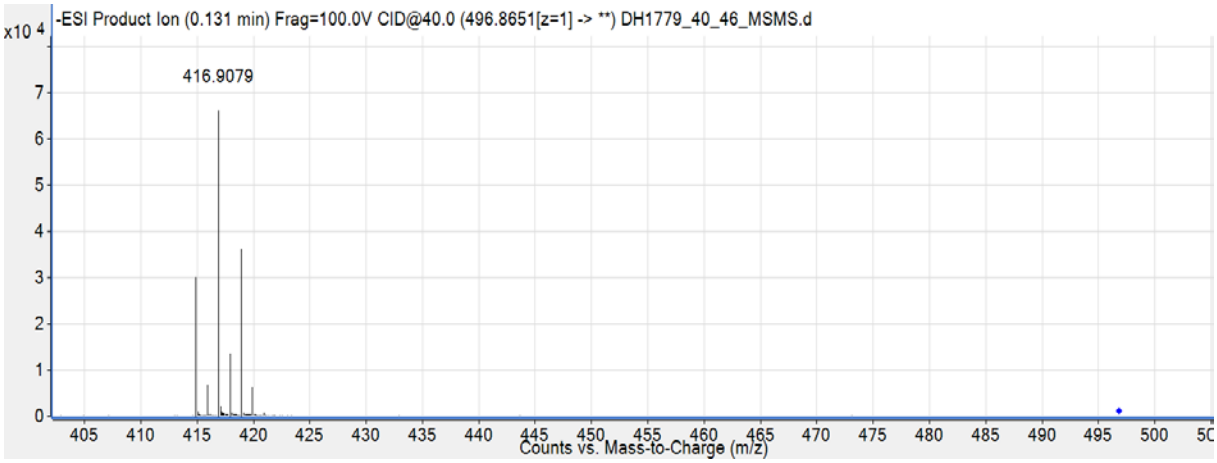
HRMS (ESI-QTOF) MS/MS (targeted 496.8650 *mz*) @ 10.0 eV of 2



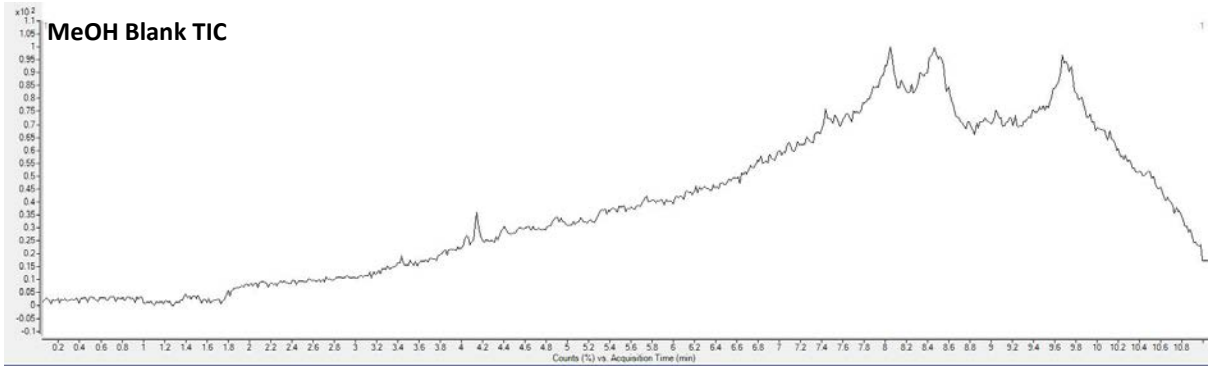
HRMS (ESI-QTOF) MS/MS (targeted 496.8650 *mz*) @ 20 eV of 2

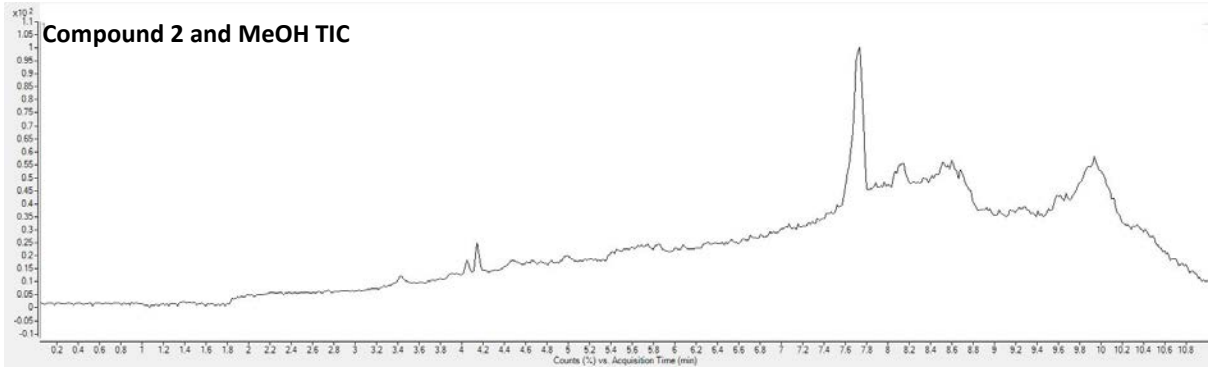


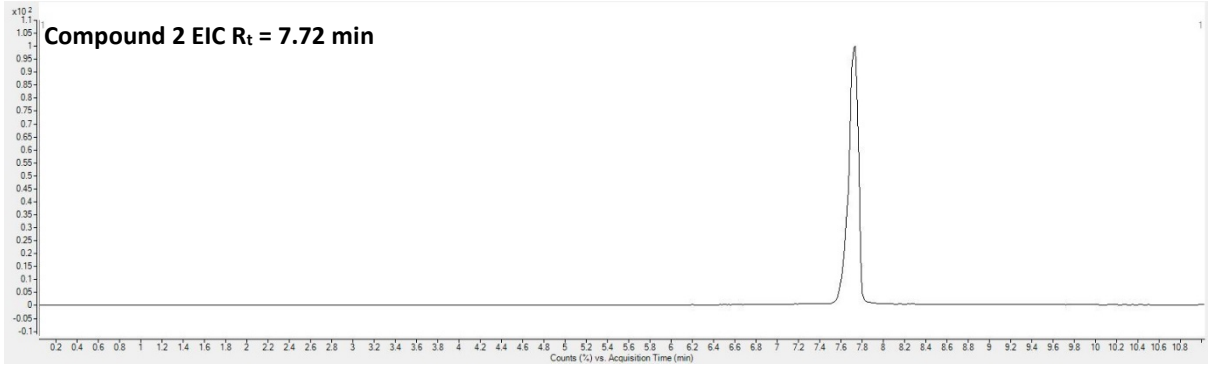
HRMS (ESI-QTOF) MS/MS (targeted 496.8650 *mz*) @ 40 eV of 2



LCMS trace for 2 in MeOH (100%H_2O to 100%ACN over 10 minutes)

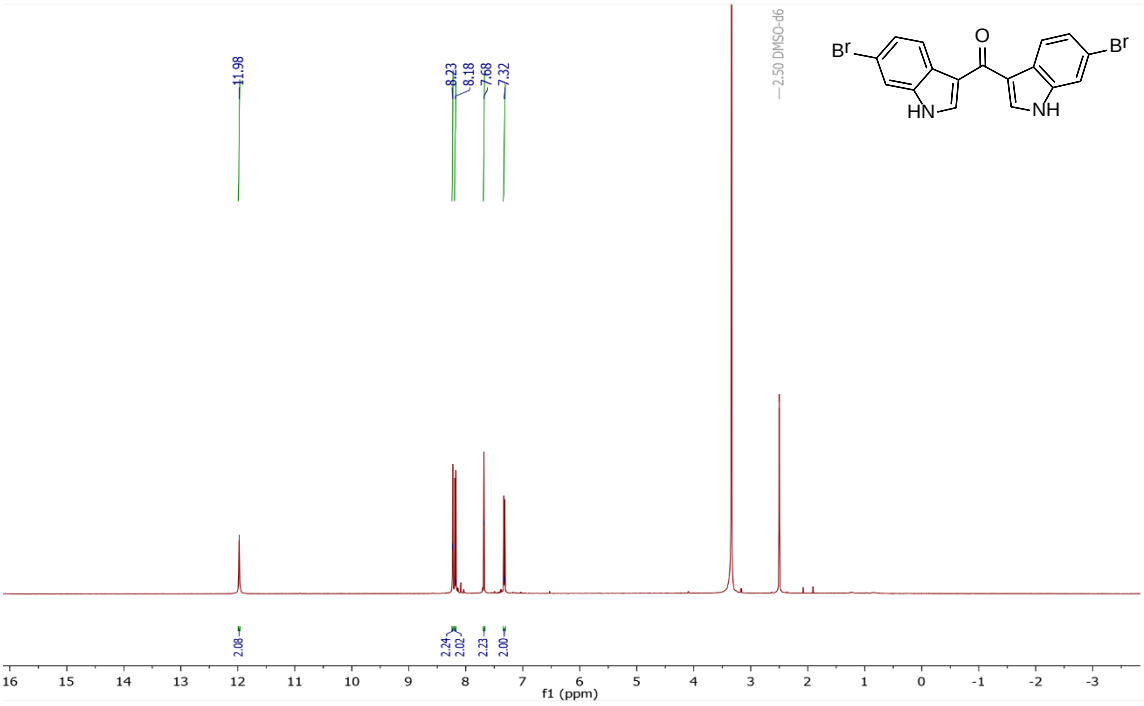




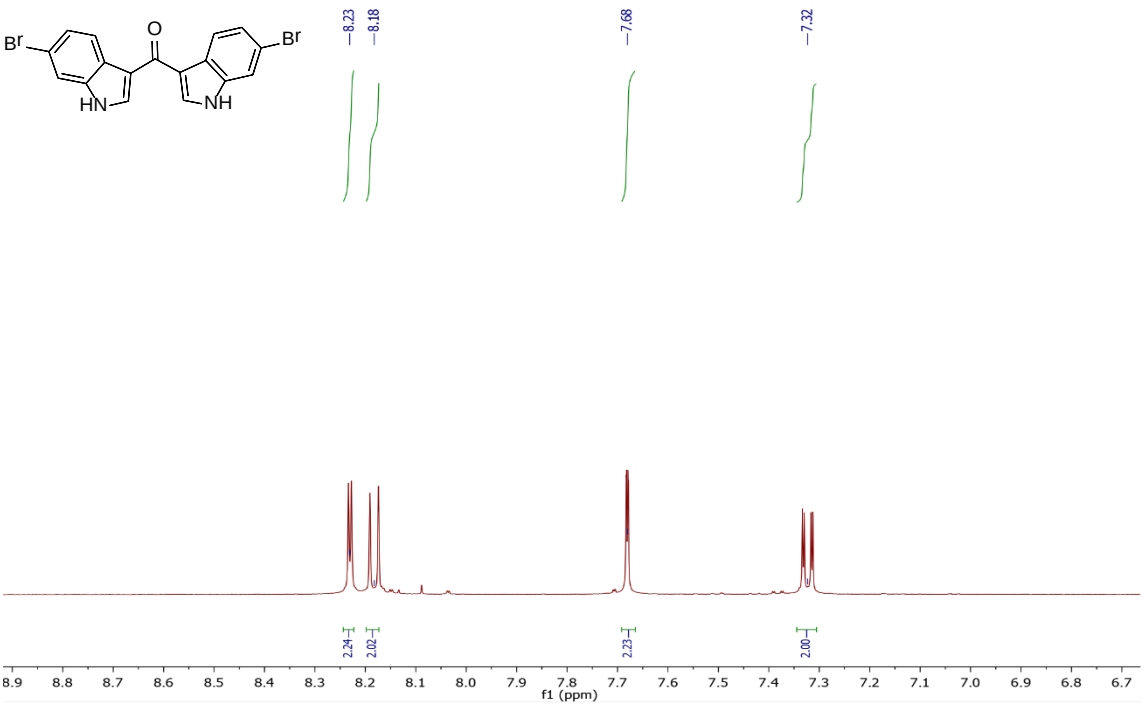


1.2 bis(6-bromo-1*H*-indol-3-yl)methanone (3)

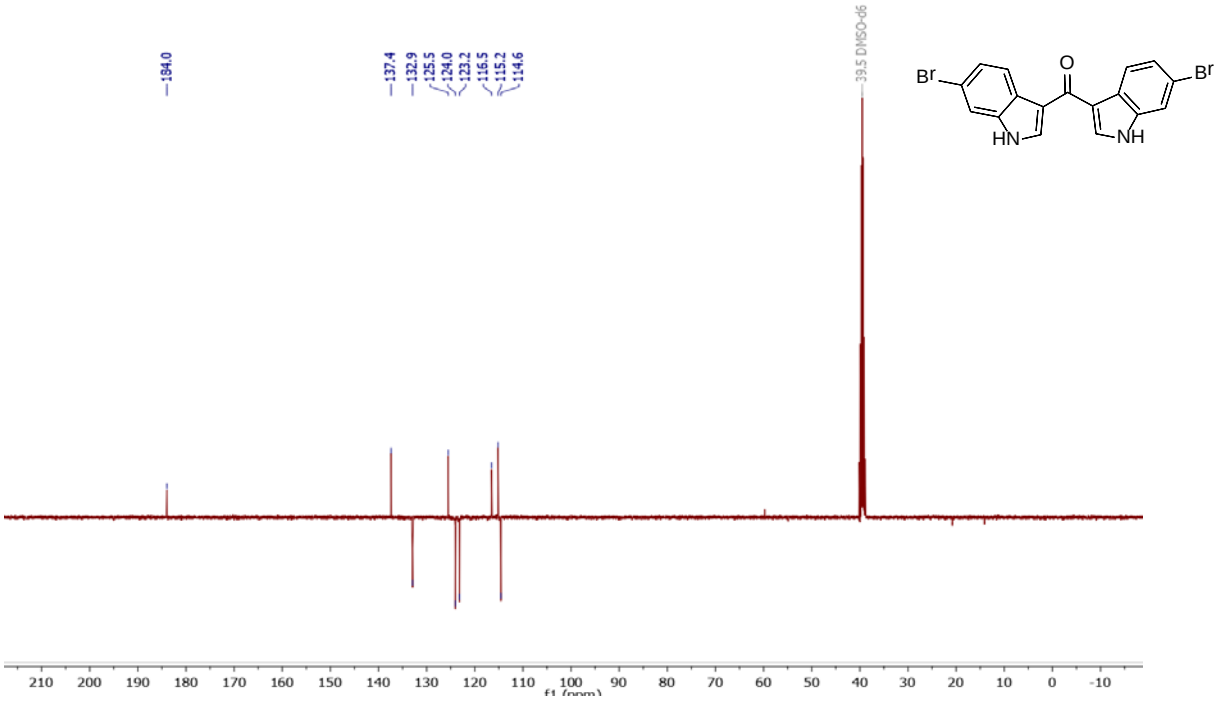
^{1}H NMR (400 MHz) spectrum of 3 in DMSO-*d*$_6$



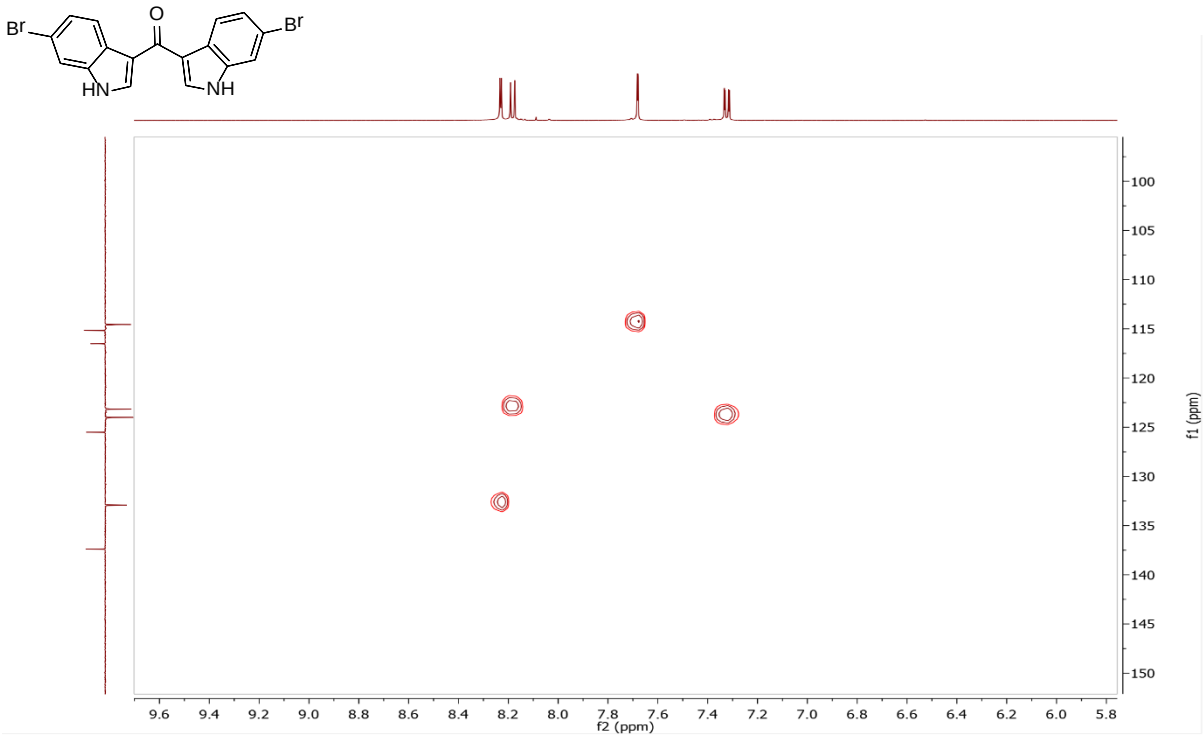
Expanded ^{1}H NMR (400 MHz) spectrum of 3 in DMSO-*d*$_6$



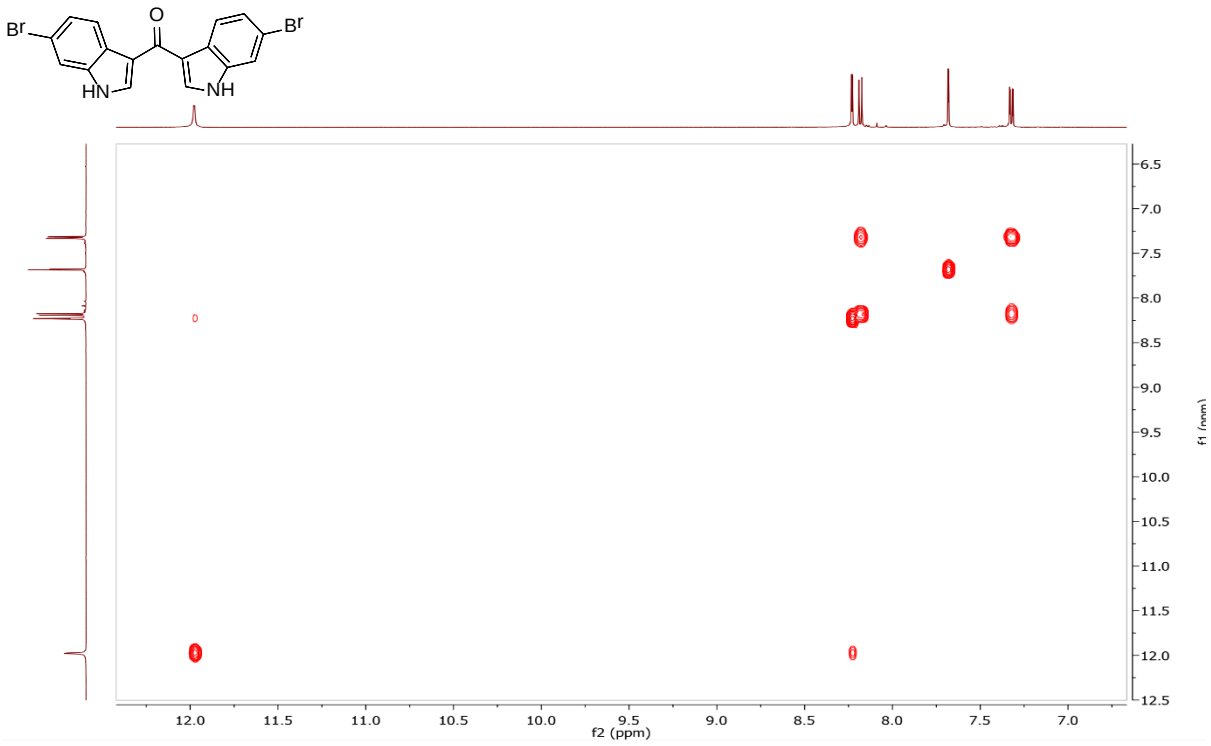
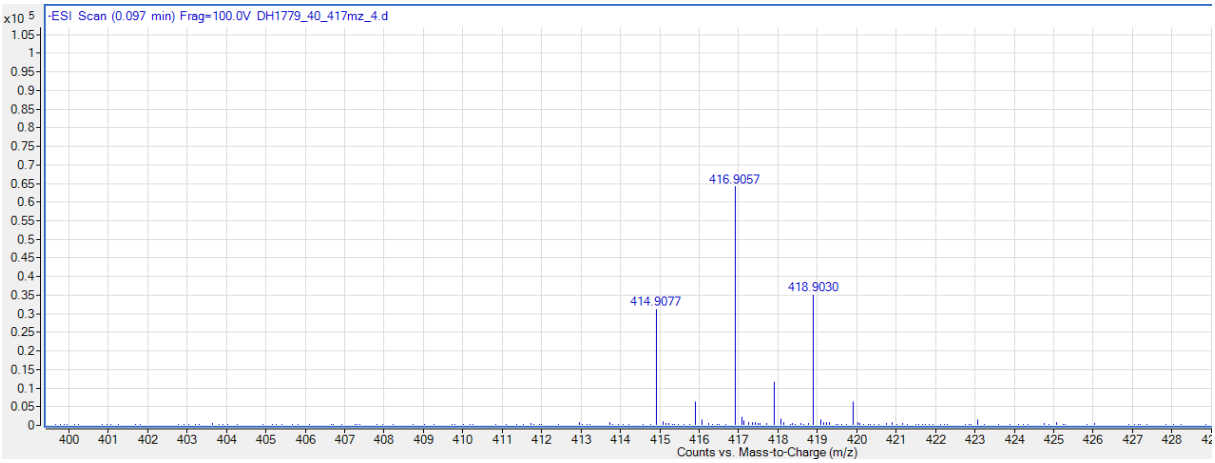
^{13}C DEPTQ (100 MHz) spectrum of 3 in DMSO-*d*$_6$



HSQC spectrum of 3 in DMSO-*d*$_6$



COSY spectrum of 3 in DMSO-d_6



HRSMS (ESI-QTOF) $[M-H]^-$ spectrum of 3