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Supporting Information

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Supporting Information

Modular Synthesis of New Pyrroloquinoline Quinone Derivatives

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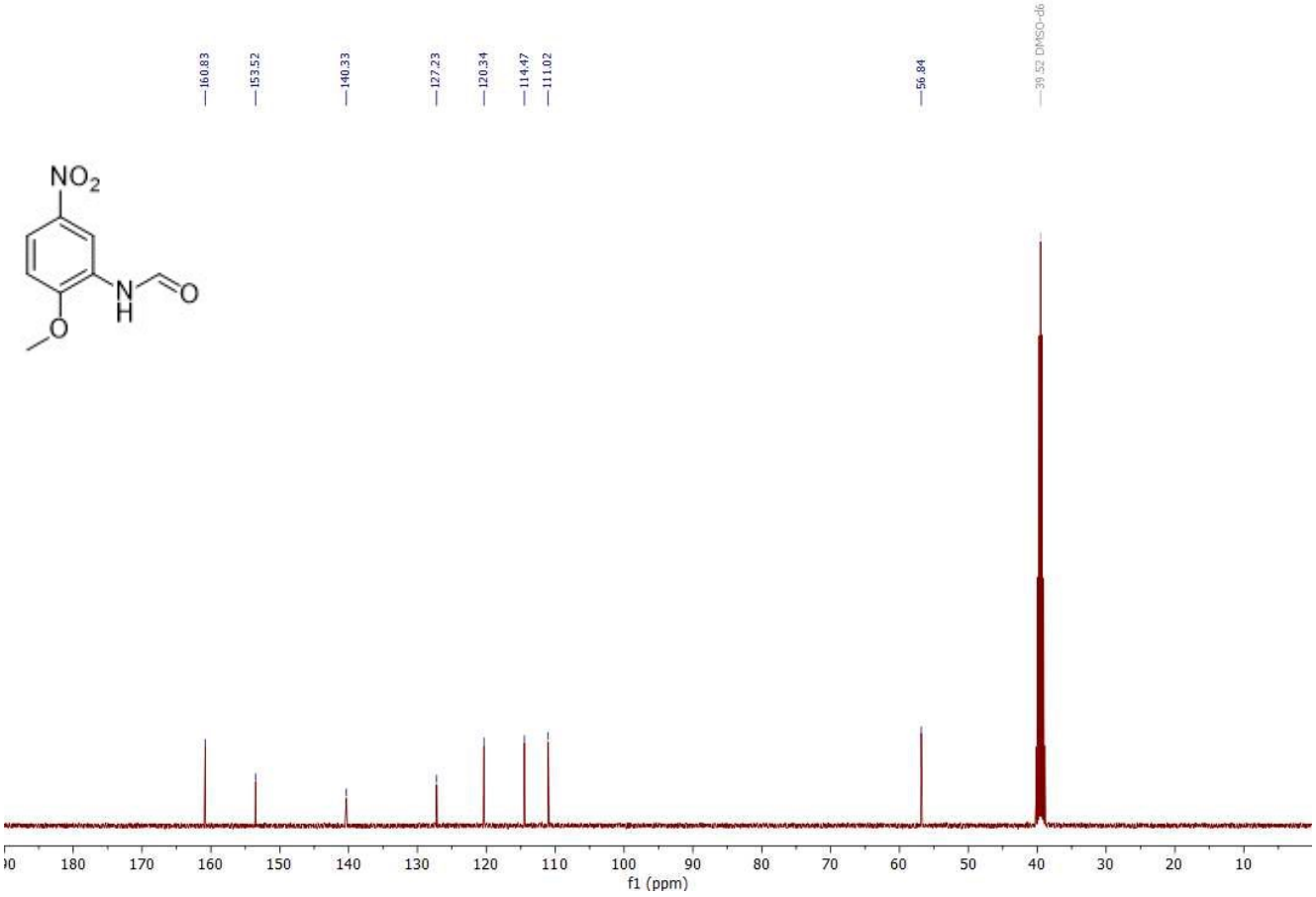
Copies of ^{1}H und ^{13}C NMR spectra

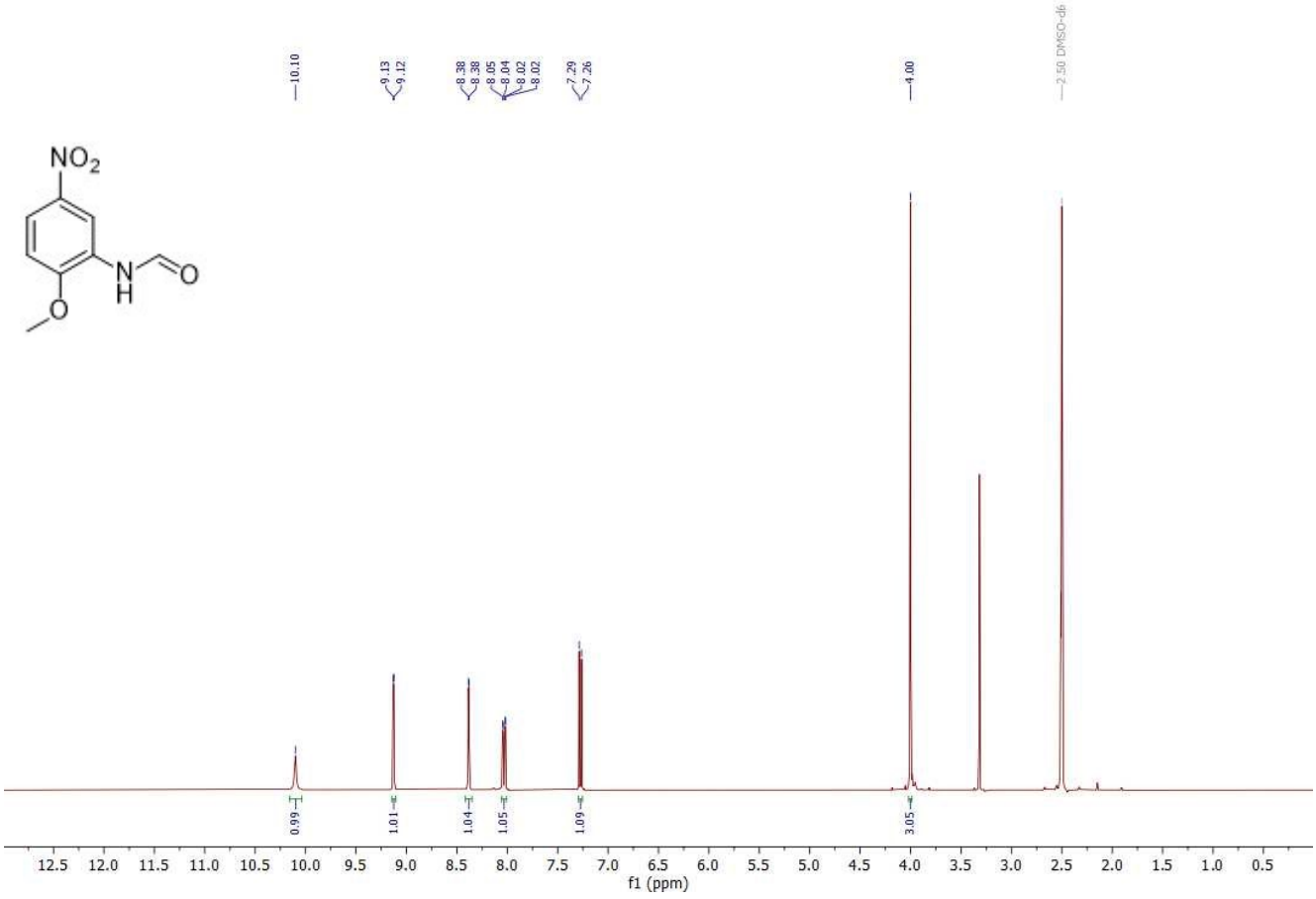
Crystal Structure

Primary Data (NMR, IR, MS and more detailed reaction procedures) are accessible at the Chemotion Online Repository. https://dx.doi.org/10.14272/collection/RAJ_2022-08-25

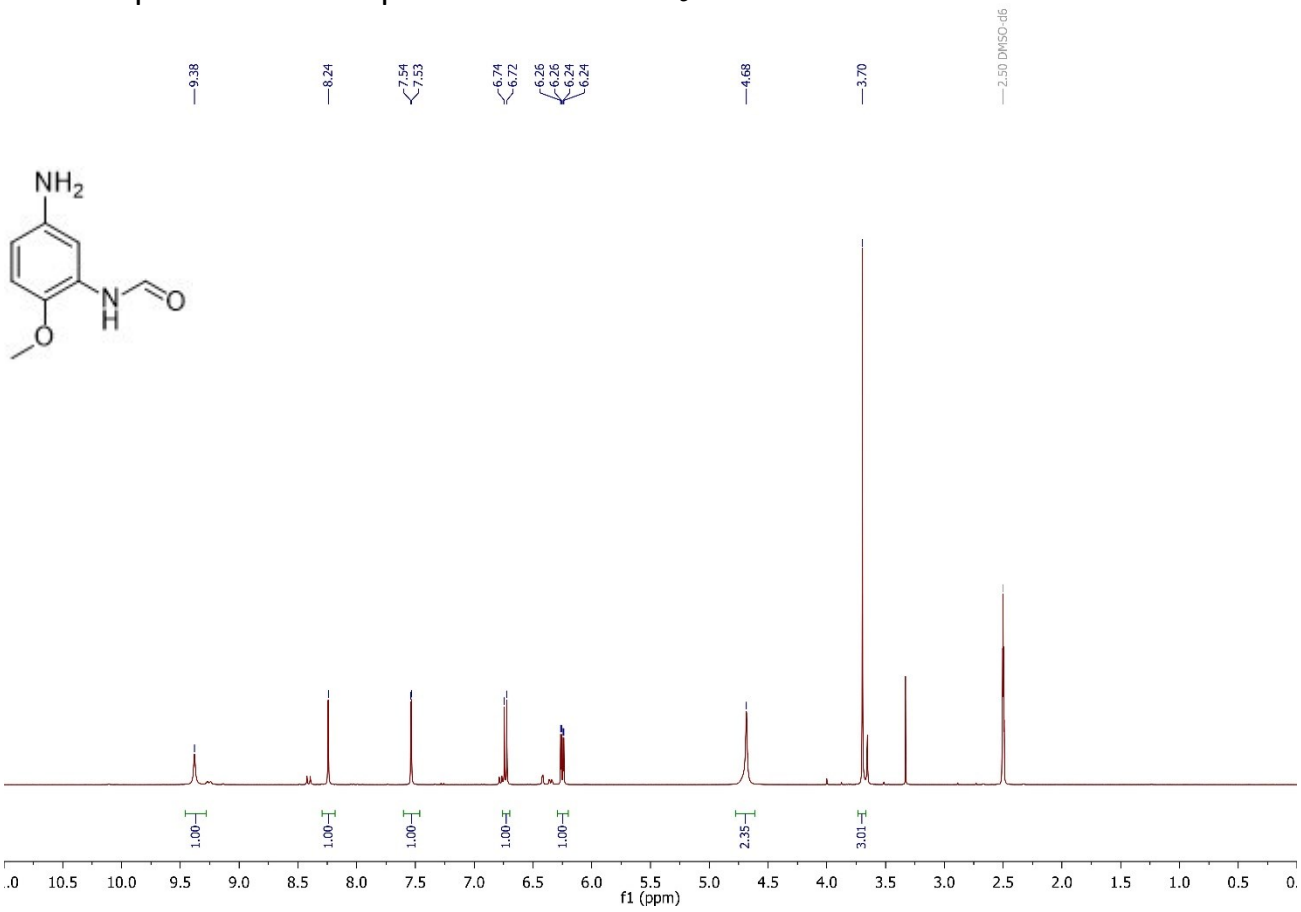
^{1}H NMR Spectrum of Compound **2** in DMSO-d_6



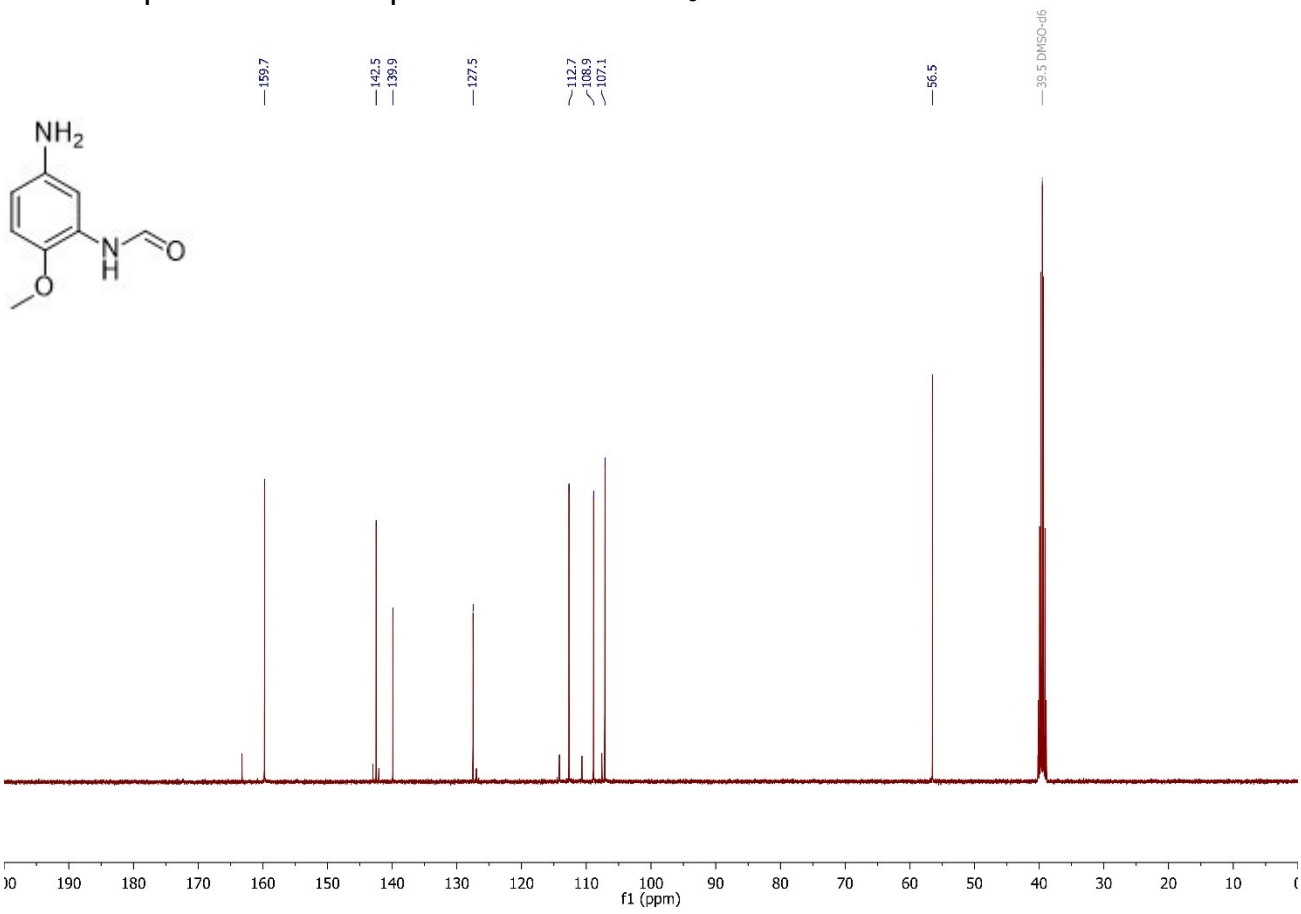
^{13}C NMR Spectrum of Compound **2** in DMSO-d_6



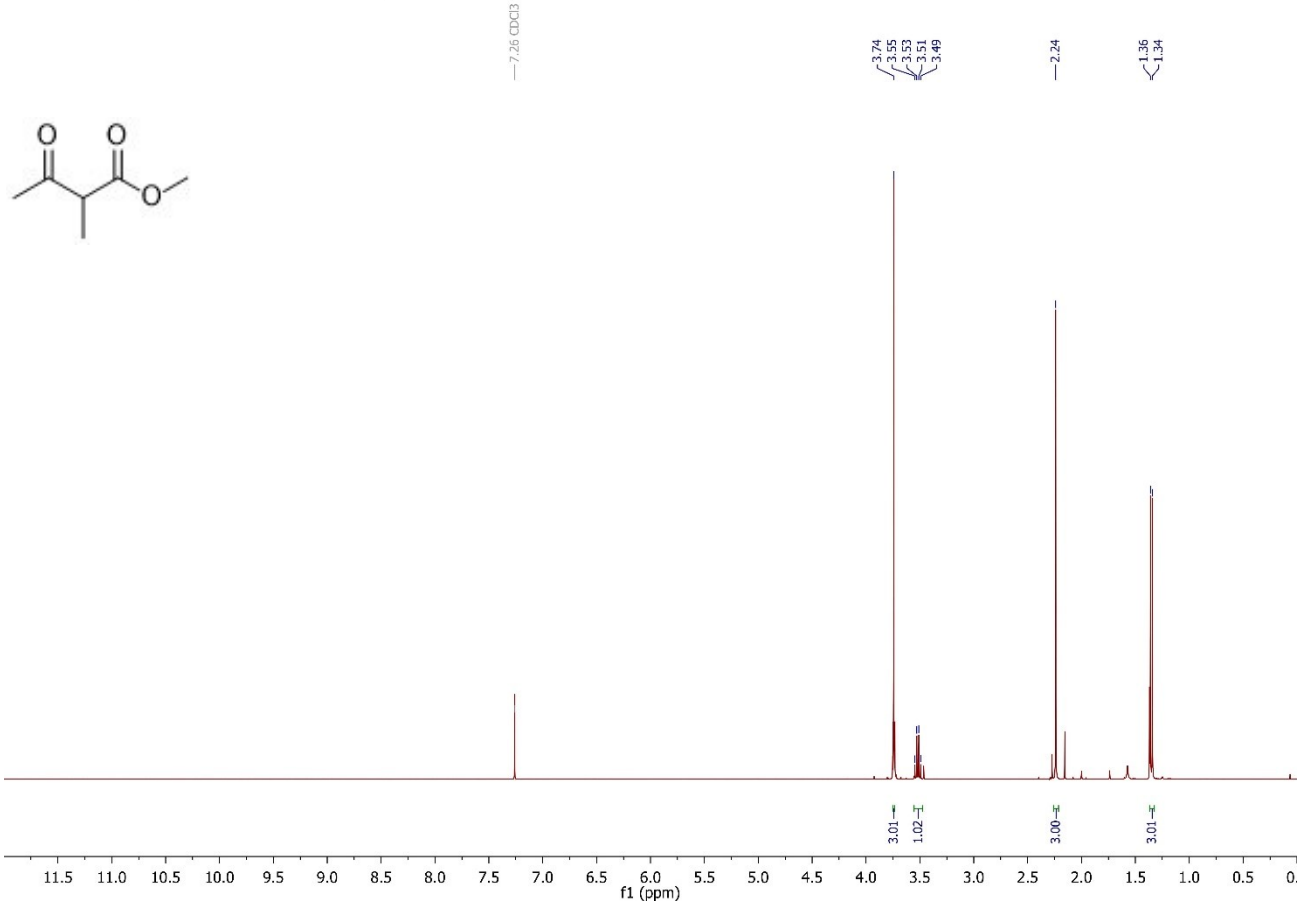
^{1}H NMR Spectrum of Compound **3** in DMSO-d_6



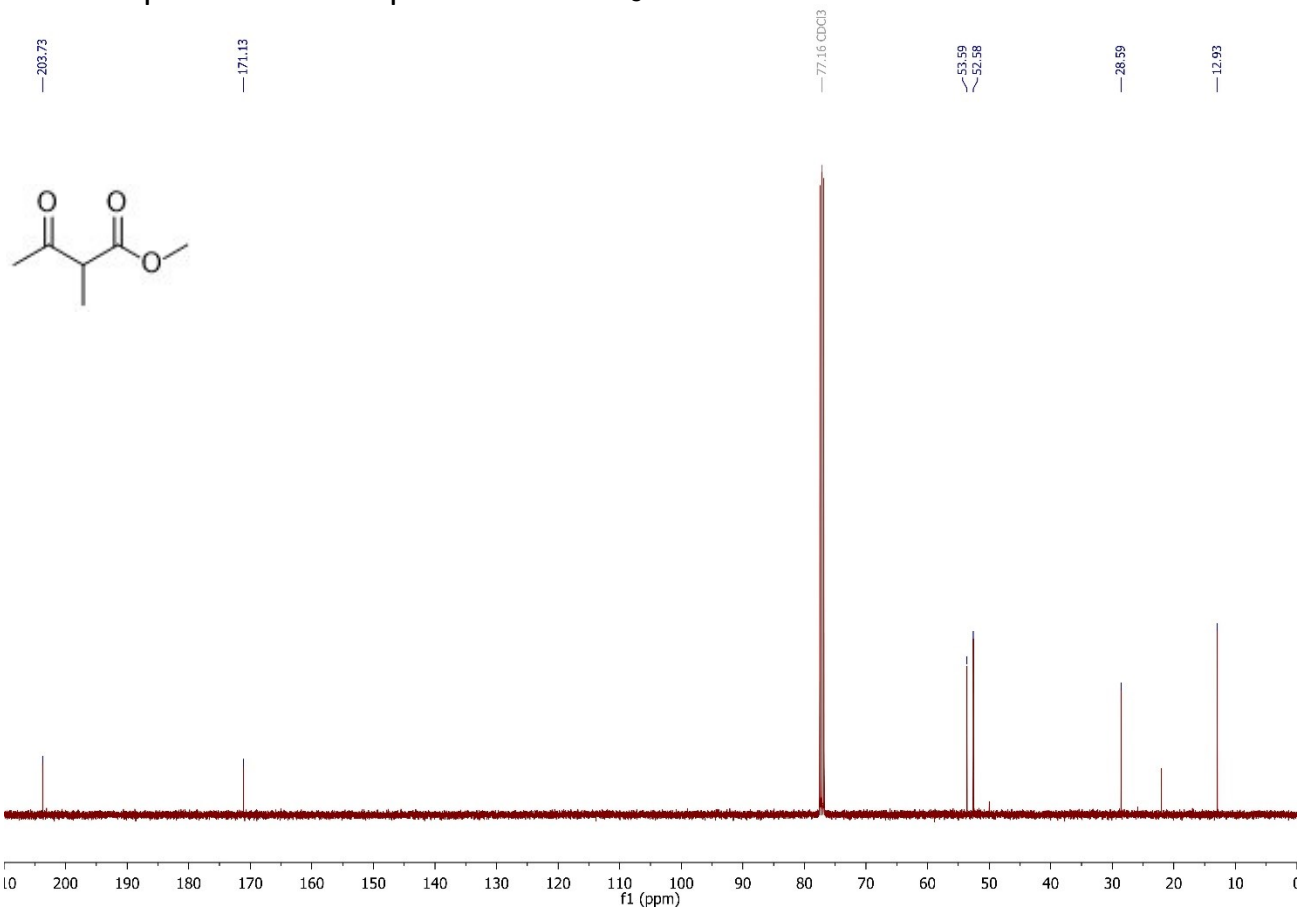
^{13}C NMR Spectrum of Compound **3** in DMSO-d_6



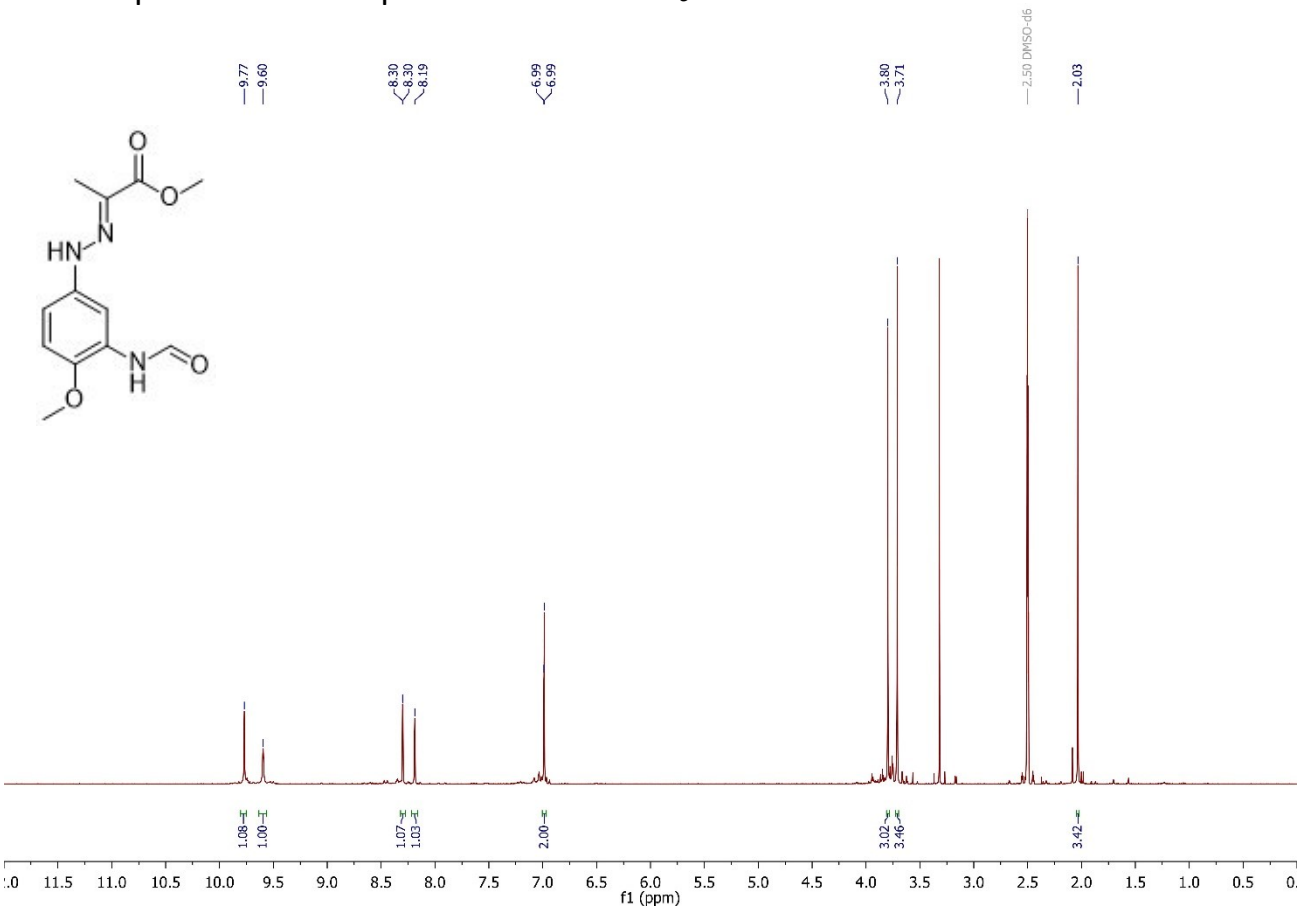
^{1}H NMR Spectrum of Compound **4** in $CDCl_3$



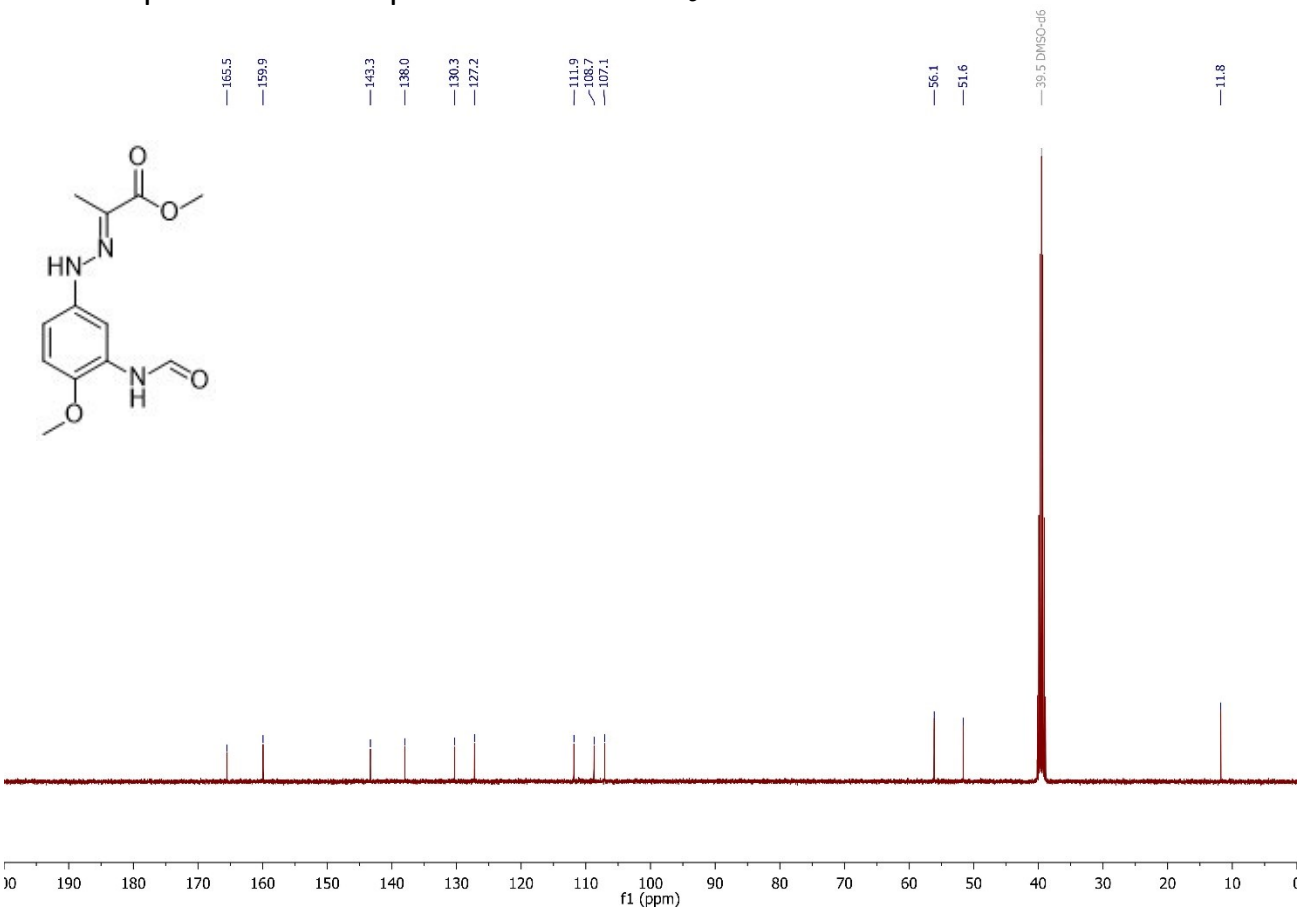
^{13}C NMR Spectrum of Compound **4** in $CDCl_3$



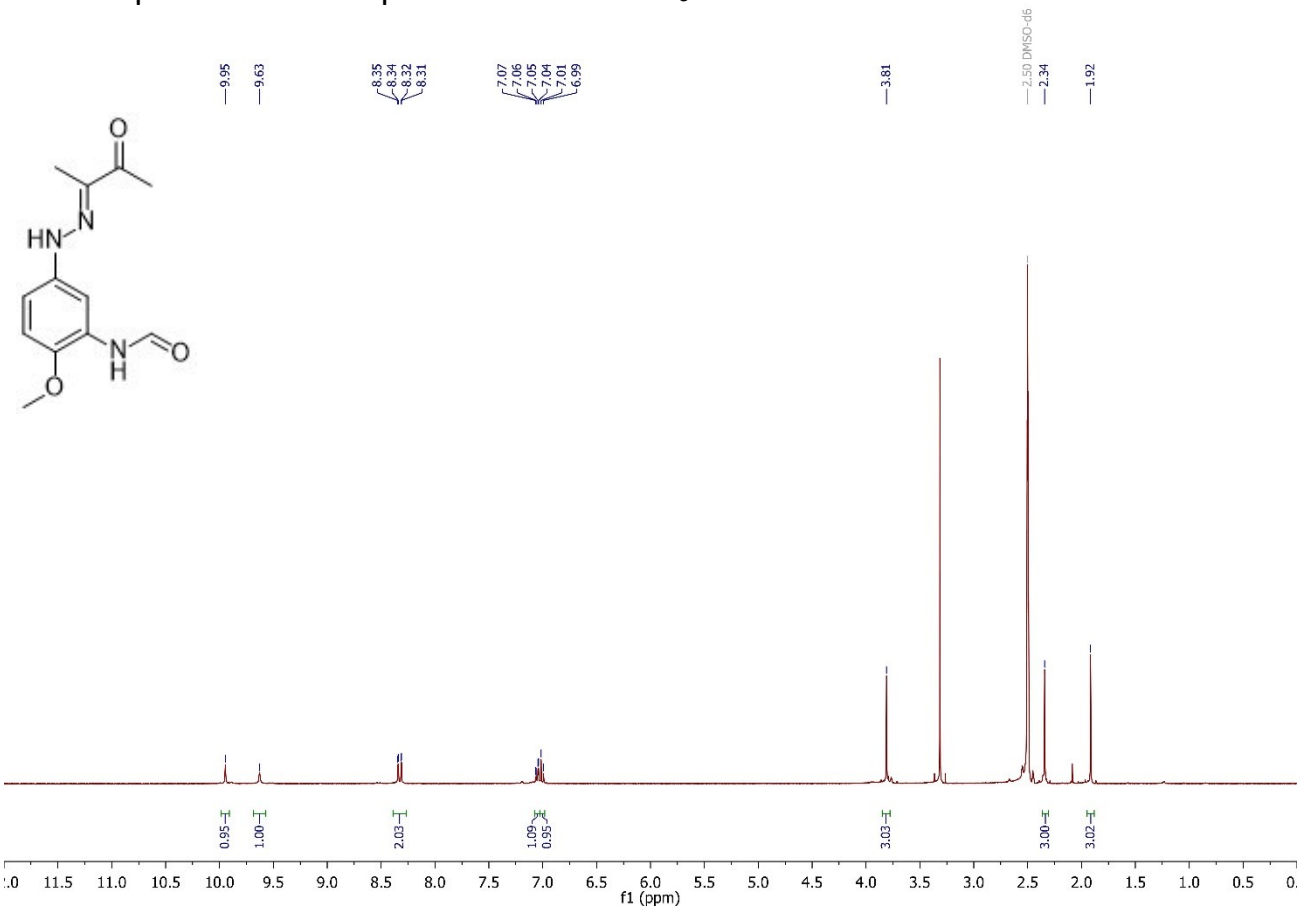
^{1}H NMR Spectrum of Compound **5** in DMSO-d_6



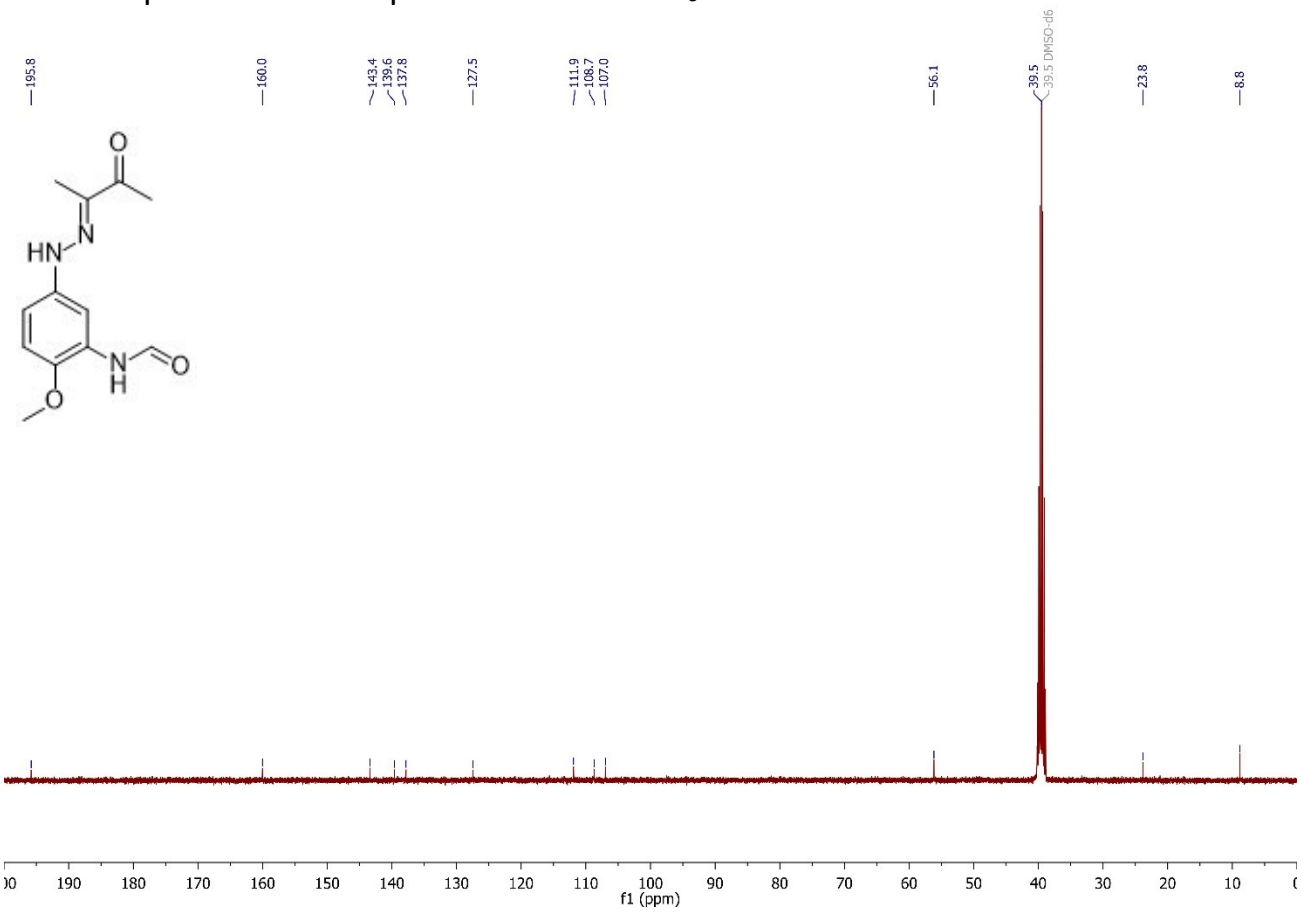
^{13}C NMR Spectrum of Compound **5** in DMSO-d_6



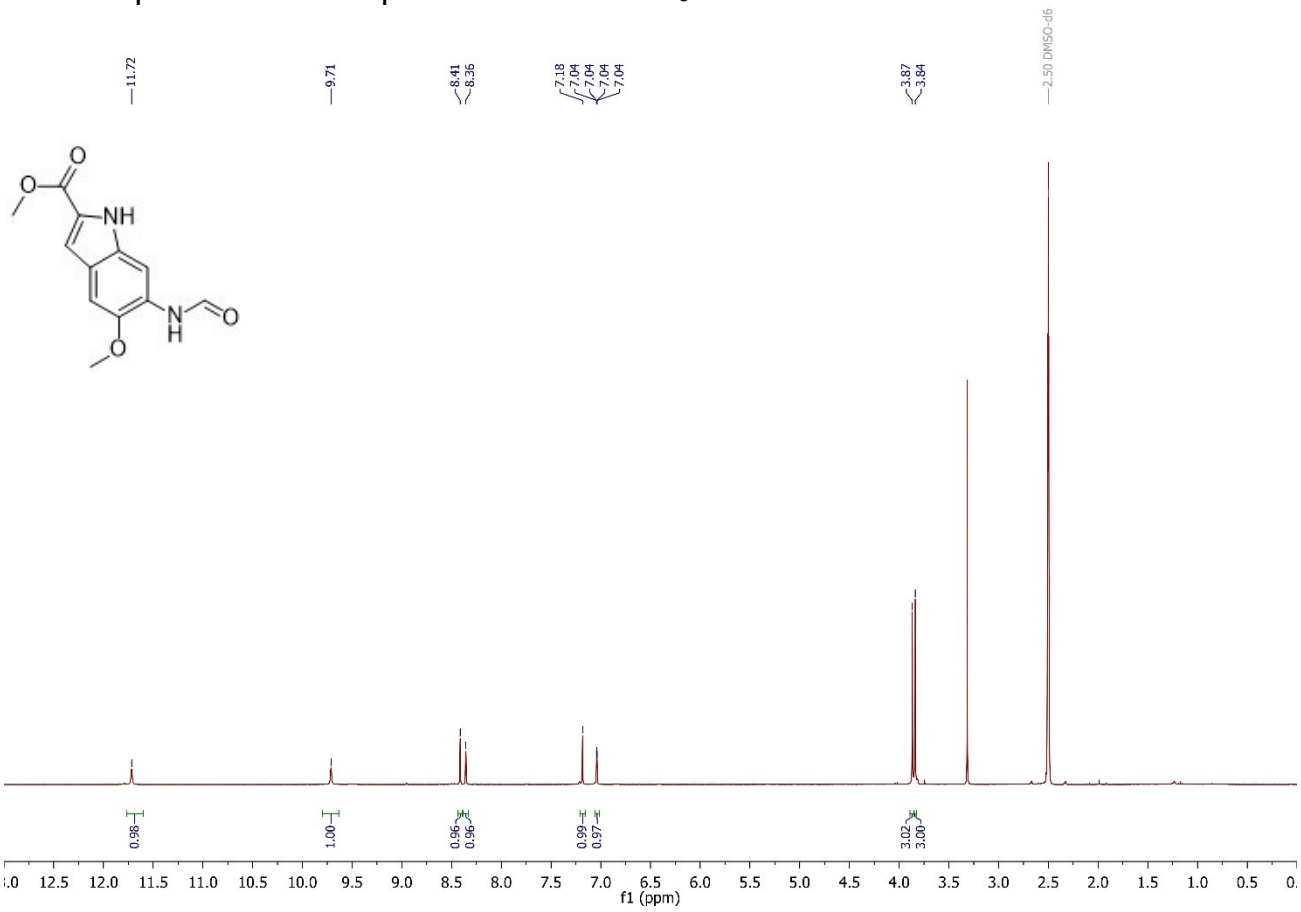
^{1}H NMR Spectrum of Compound **6** in DMSO-d_6



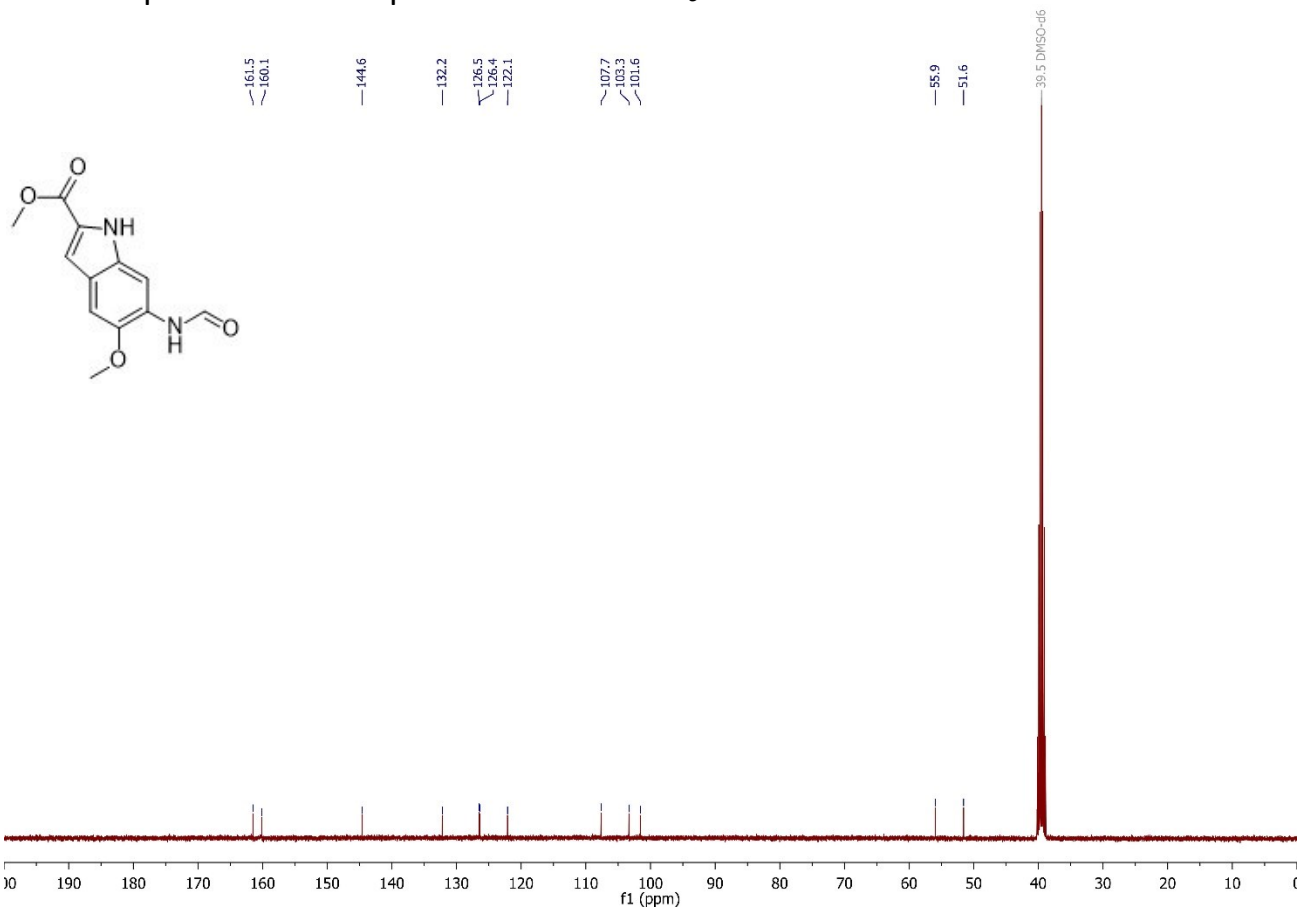
^{13}C NMR Spectrum of Compound **6** in DMSO-d_6



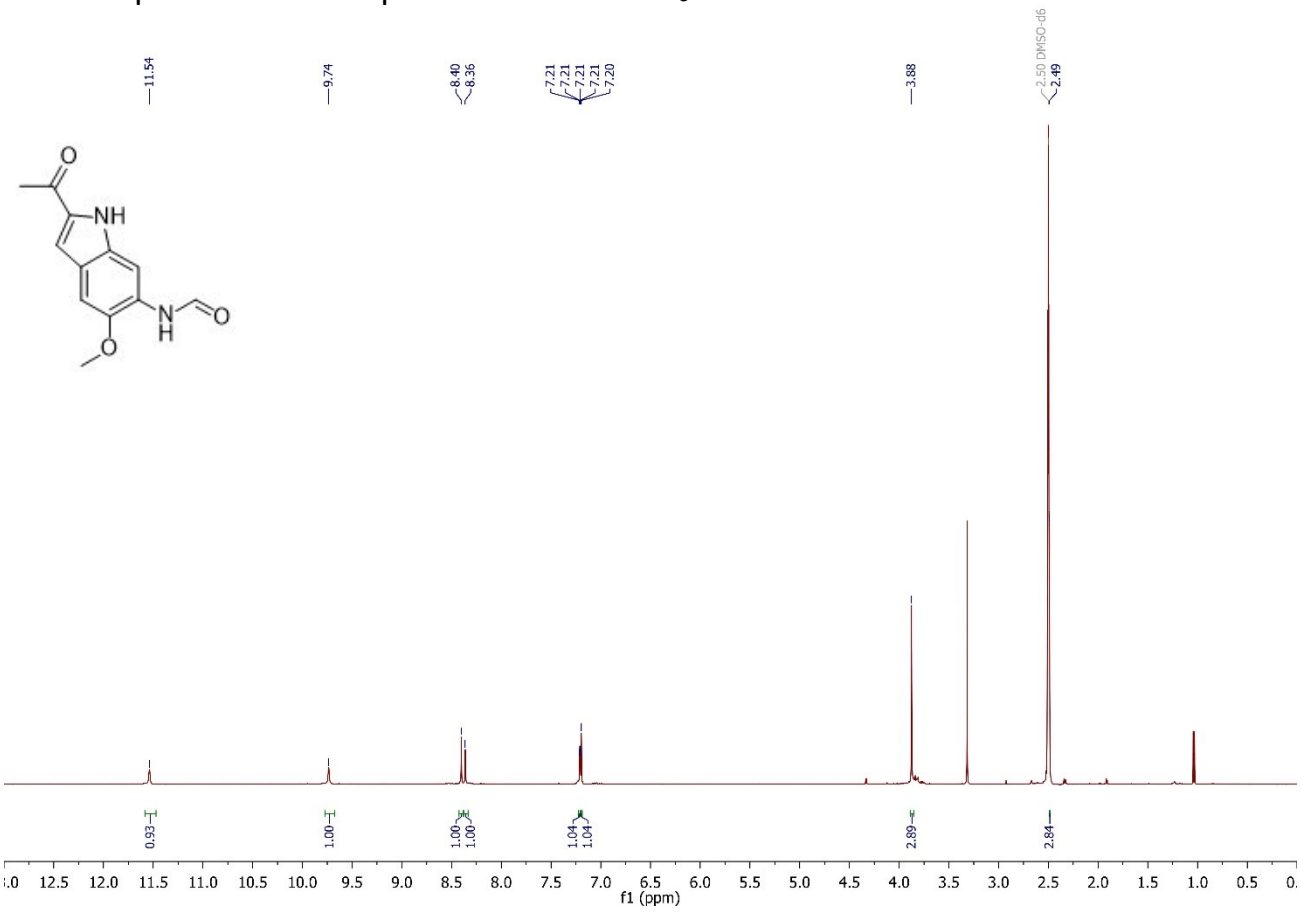
^{1}H NMR Spectrum of Compound **7** in DMSO-d_6



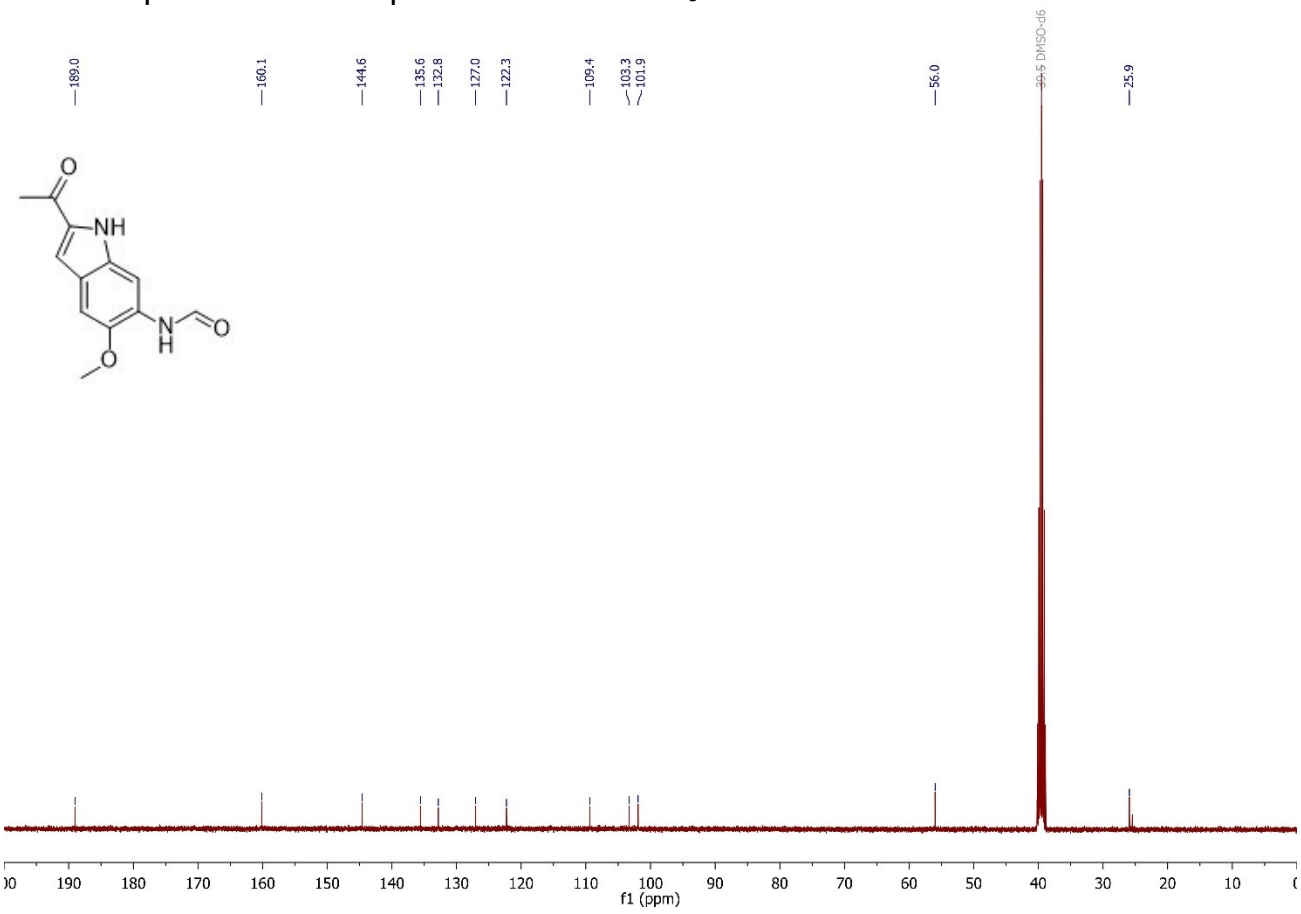
^{13}C NMR Spectrum of Compound **7** in DMSO-d_6



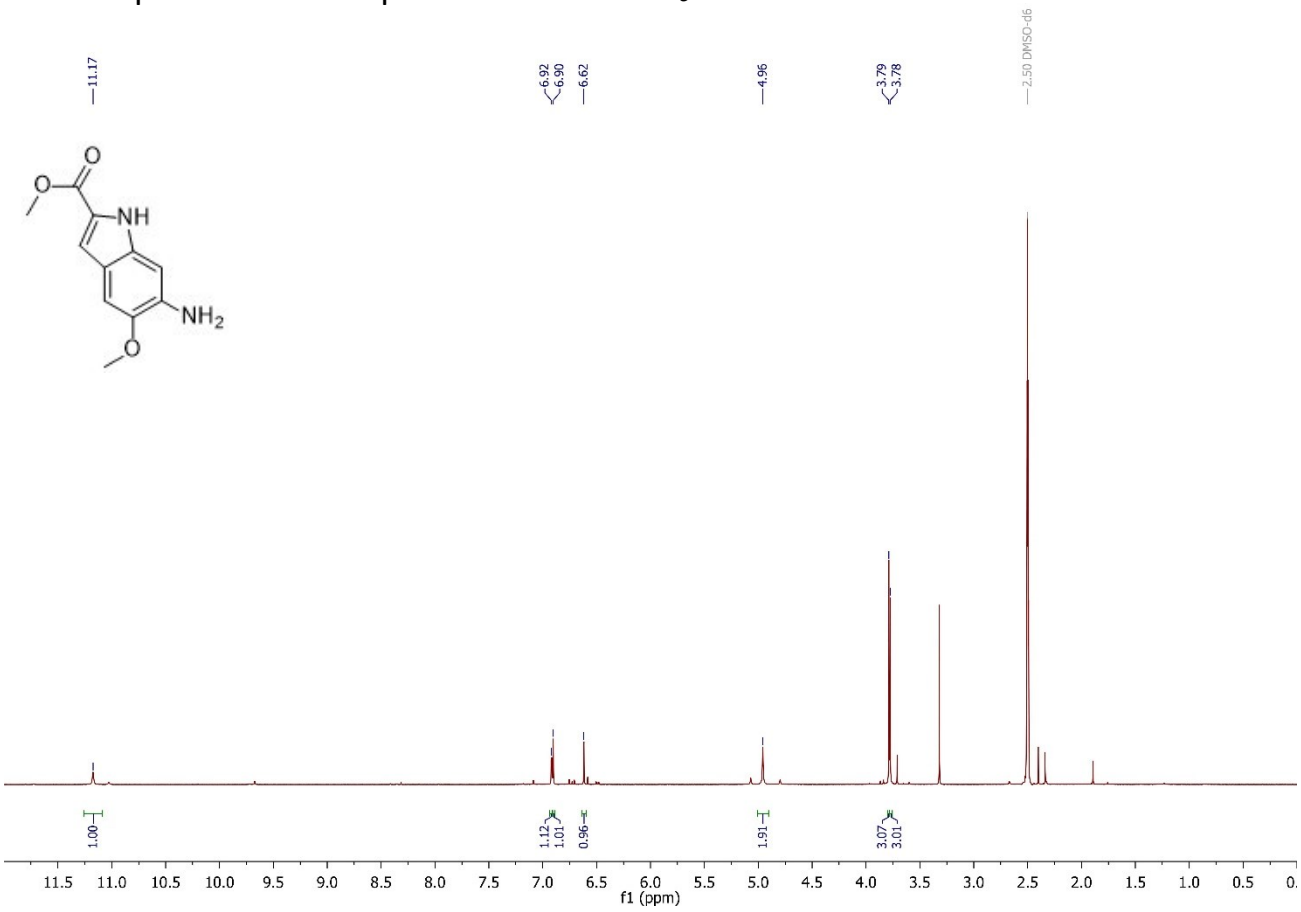
^{1}H NMR Spectrum of Compound **8** in DMSO-d_6



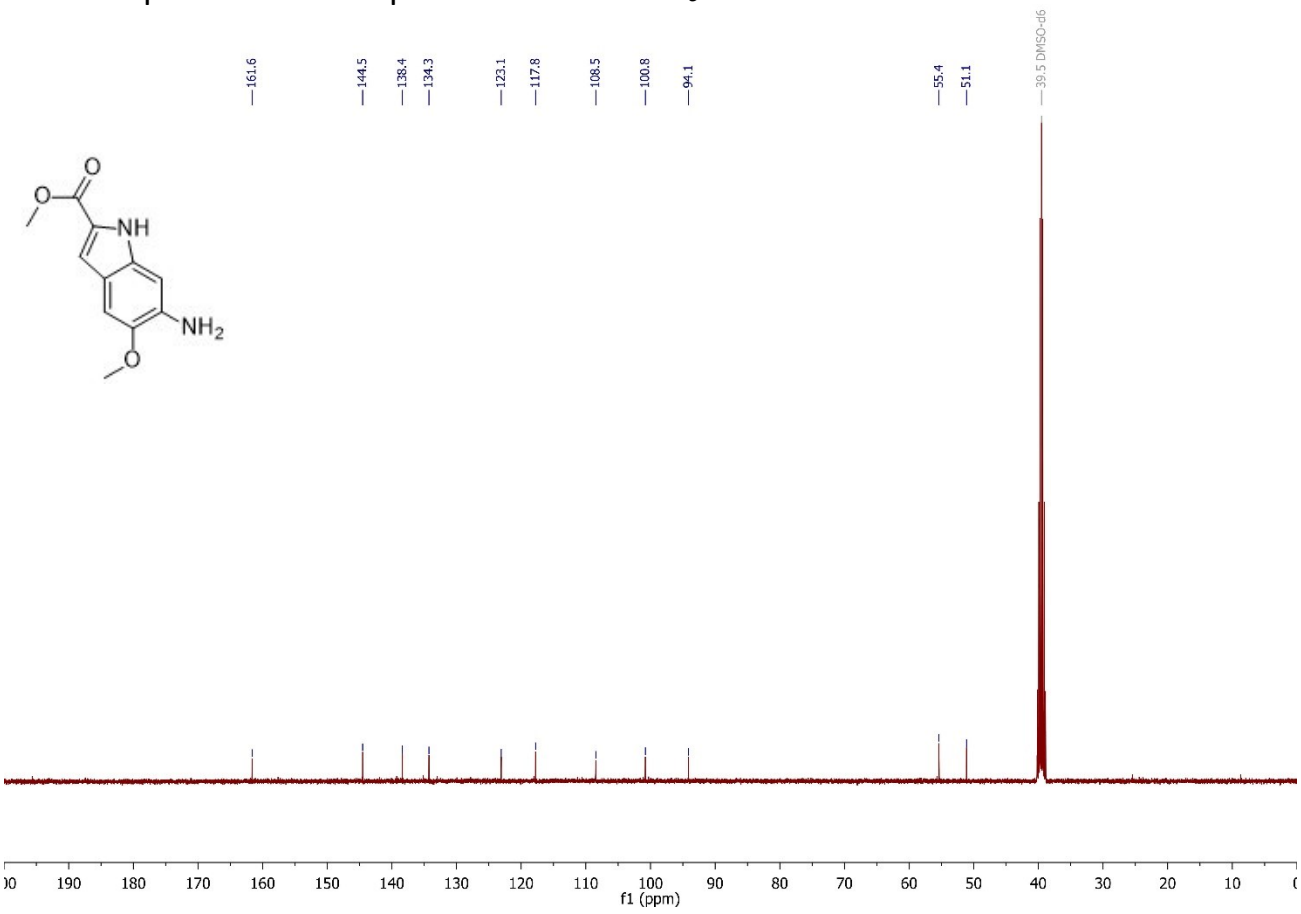
^{13}C NMR Spectrum of Compound **8** in DMSO-d_6



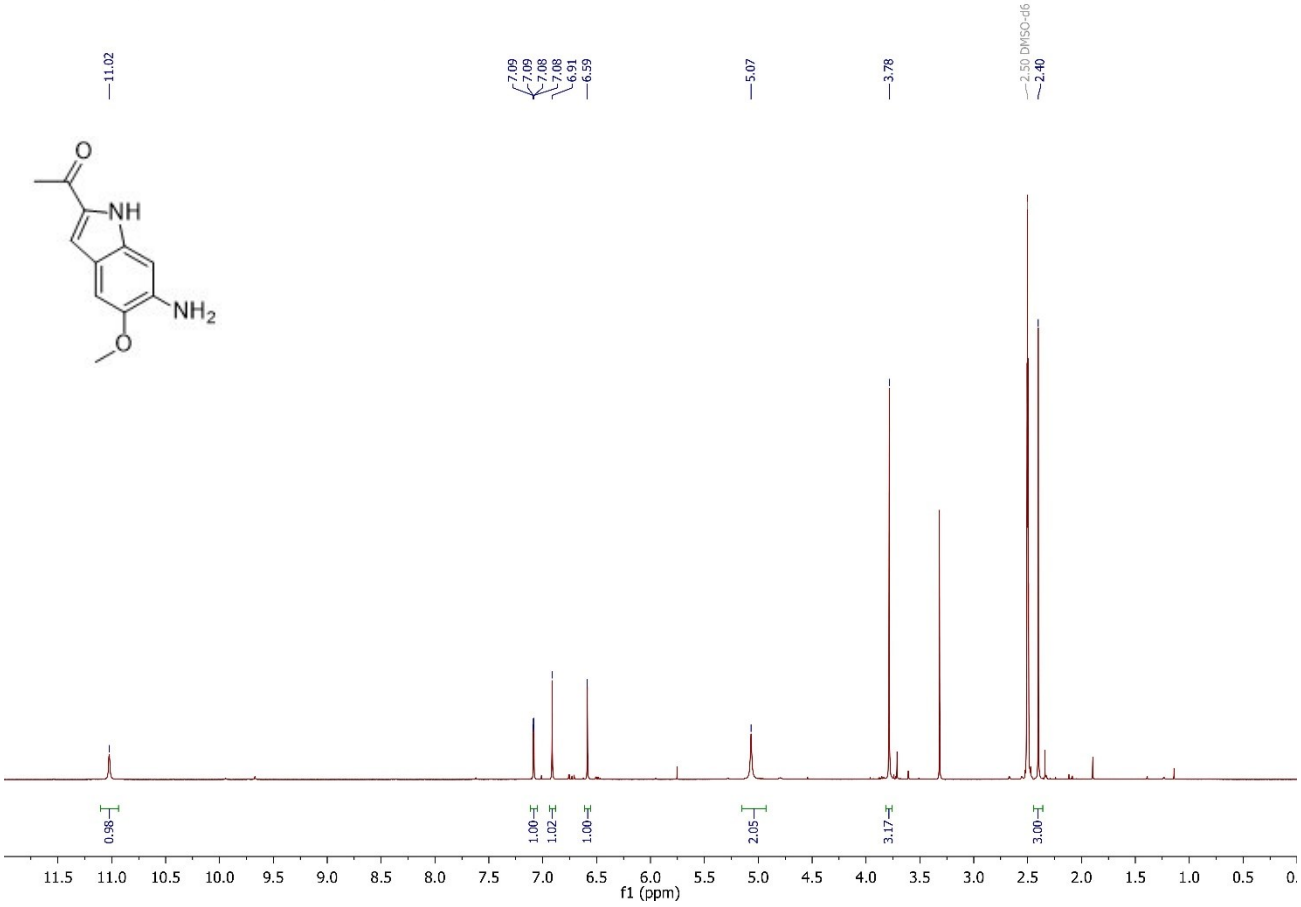
^{1}H NMR Spectrum of Compound **9** in DMSO-d_6



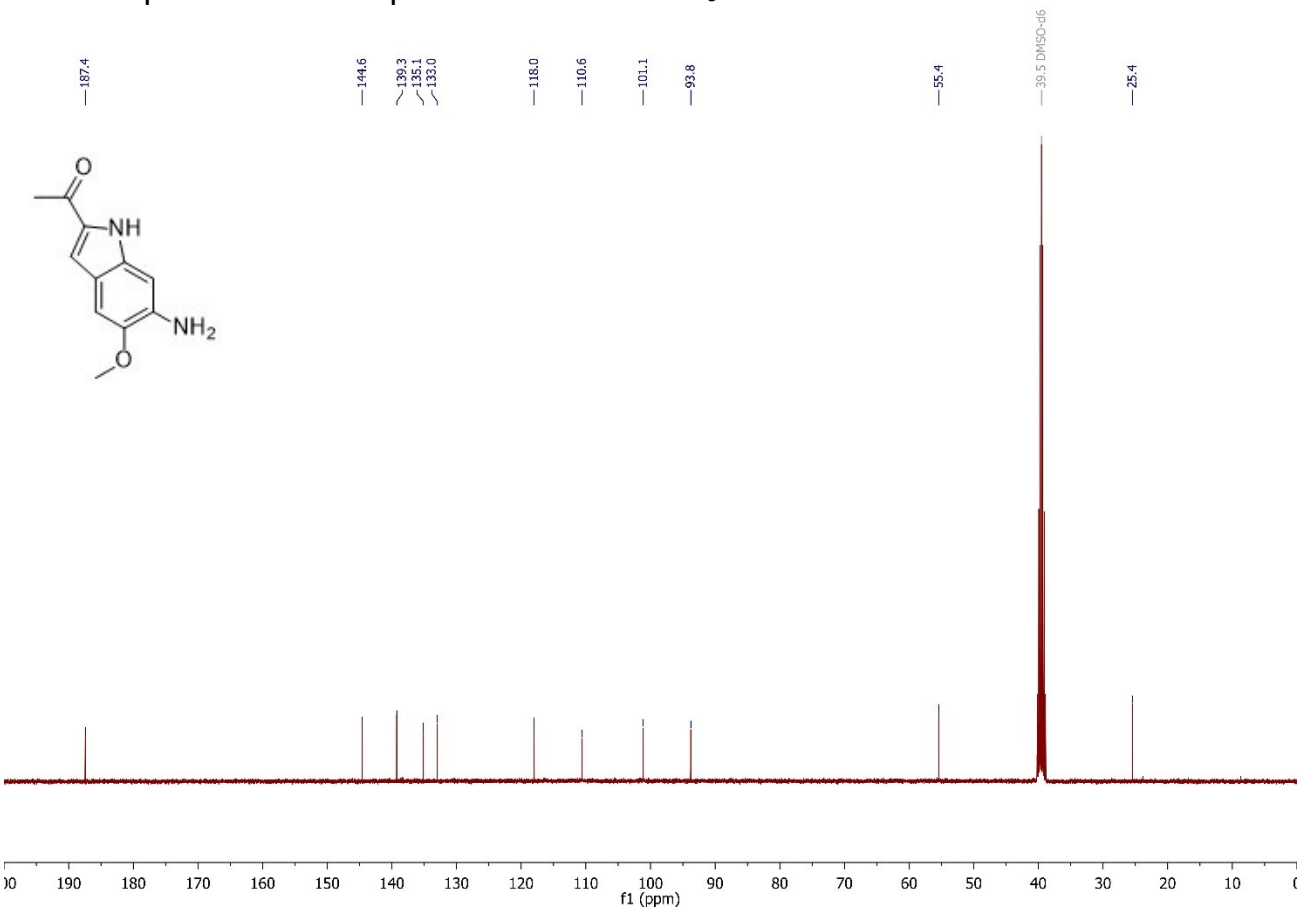
^{13}C NMR Spectrum of Compound **9** in DMSO-d_6



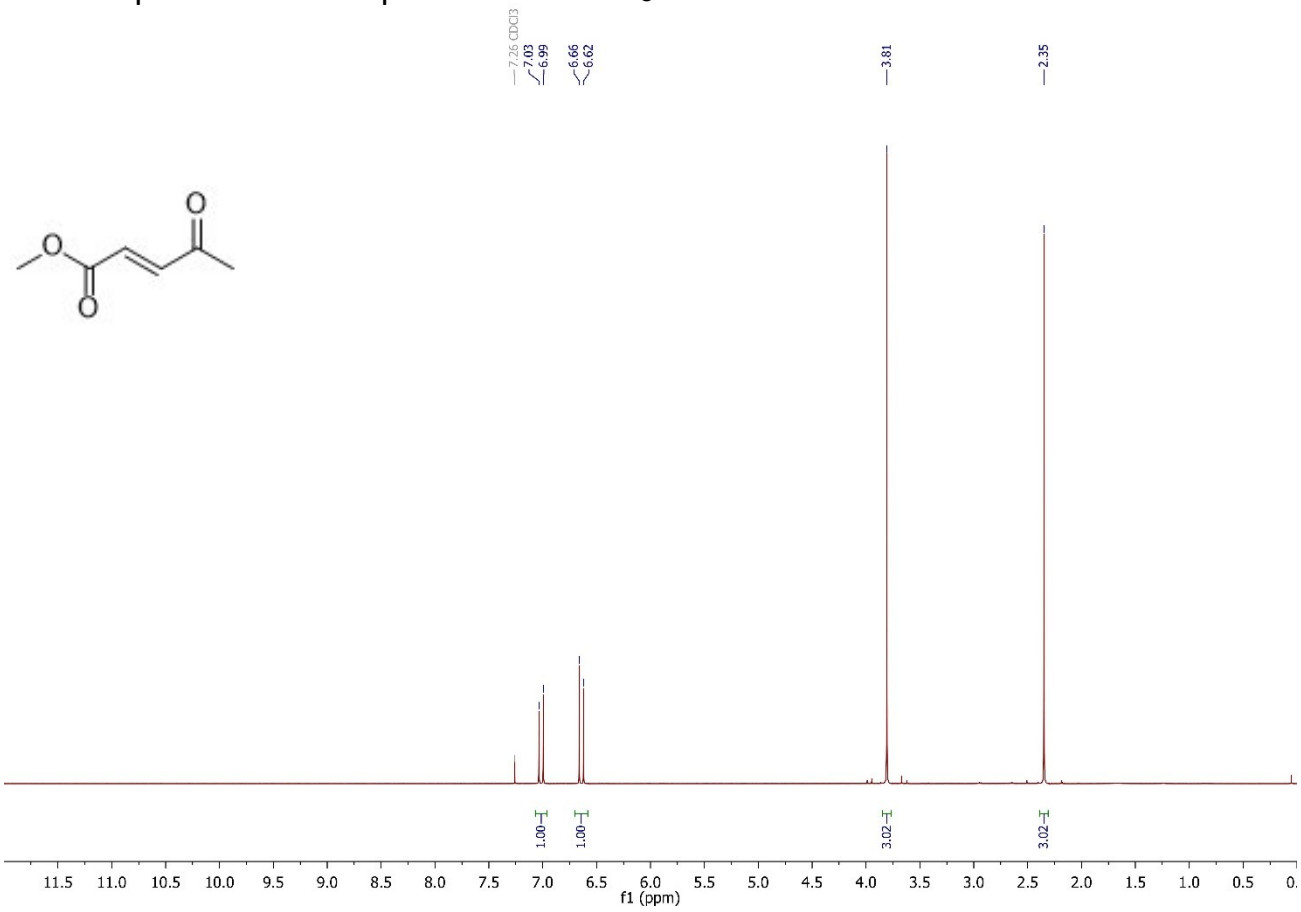
^{1}H NMR Spectrum of Compound **10** in DMSO-d_6



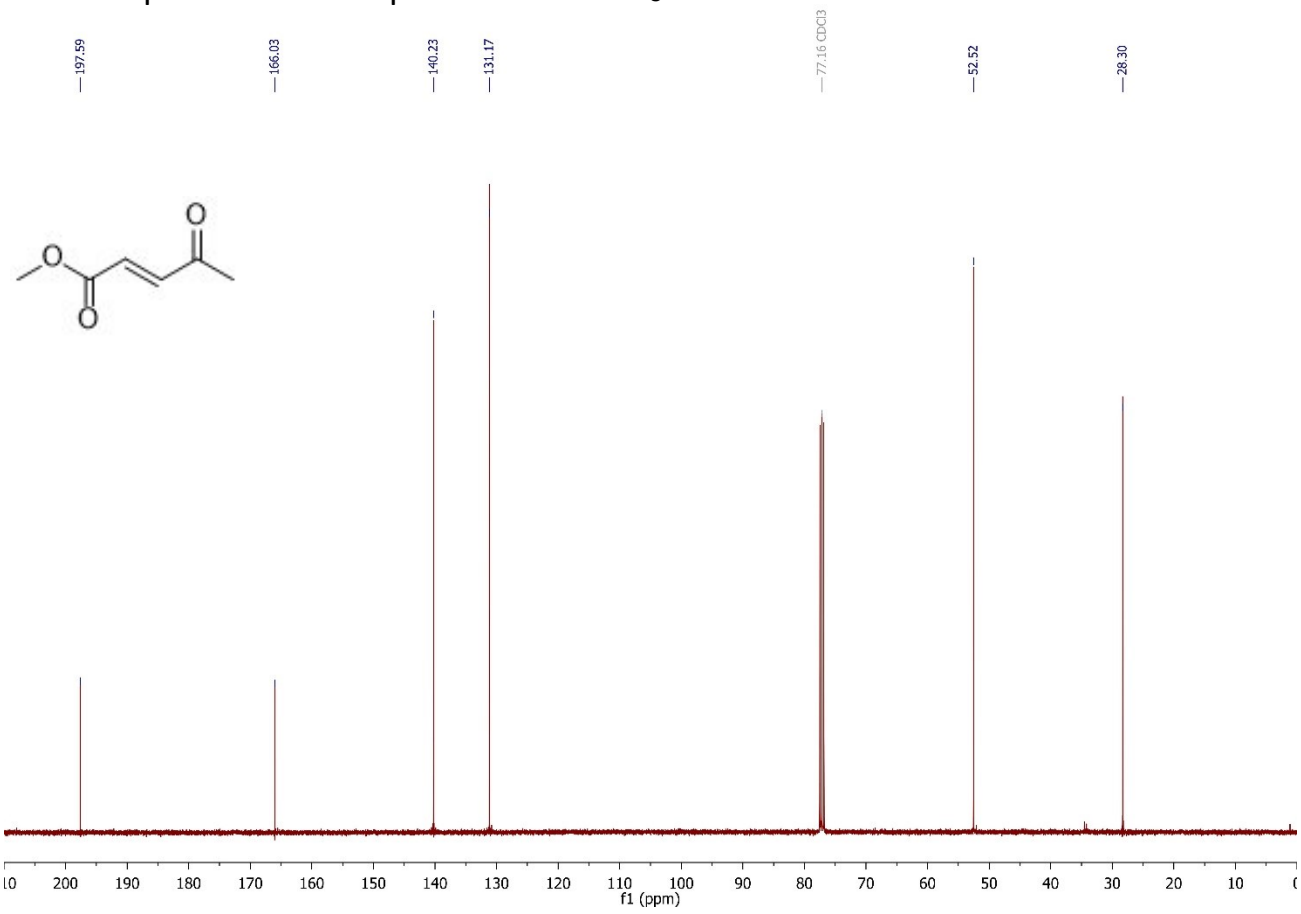
^{13}C NMR Spectrum of Compound **10** in DMSO-d_6



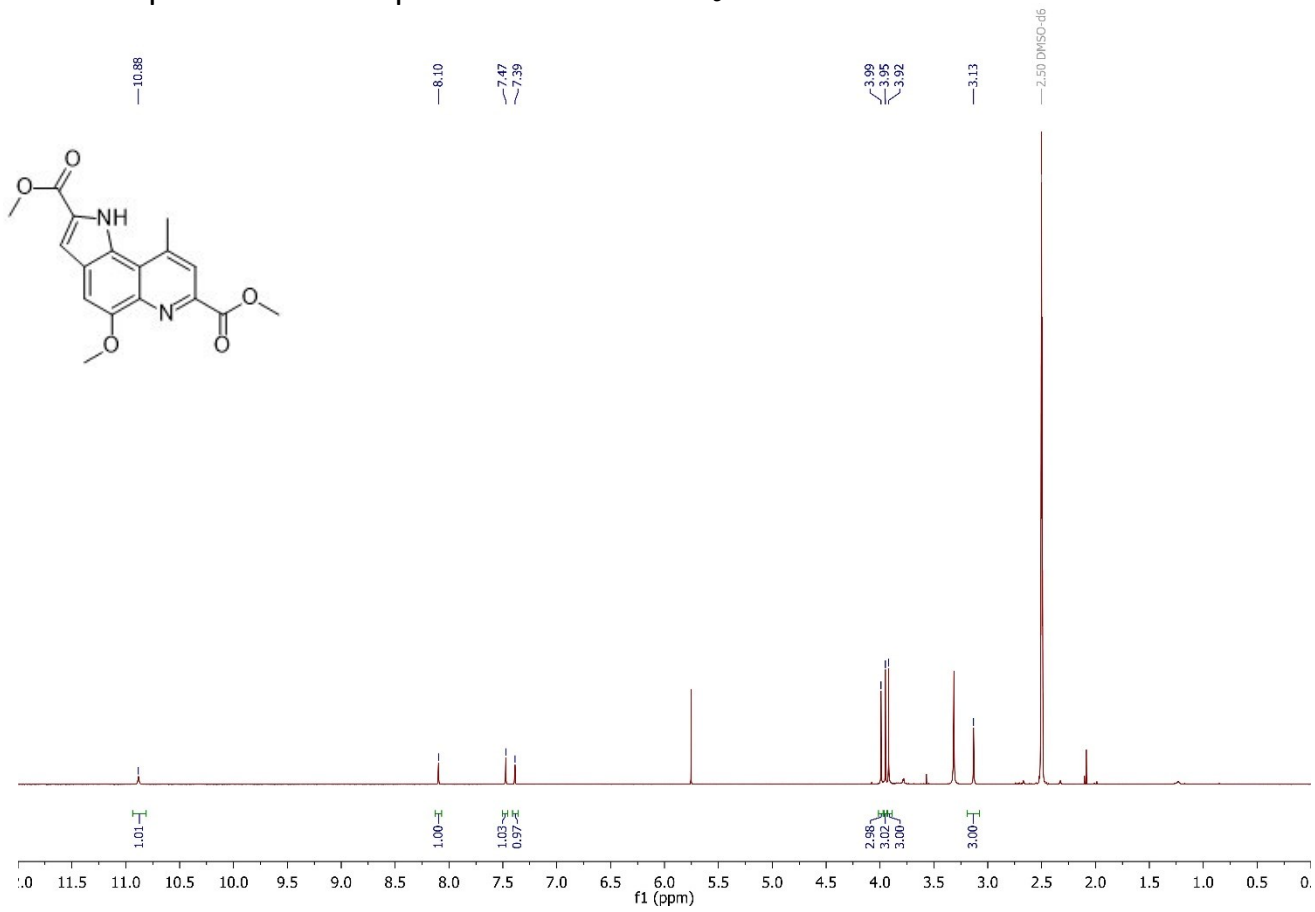
^{1}H NMR Spectrum of Compound **12** in $CDCl_3$



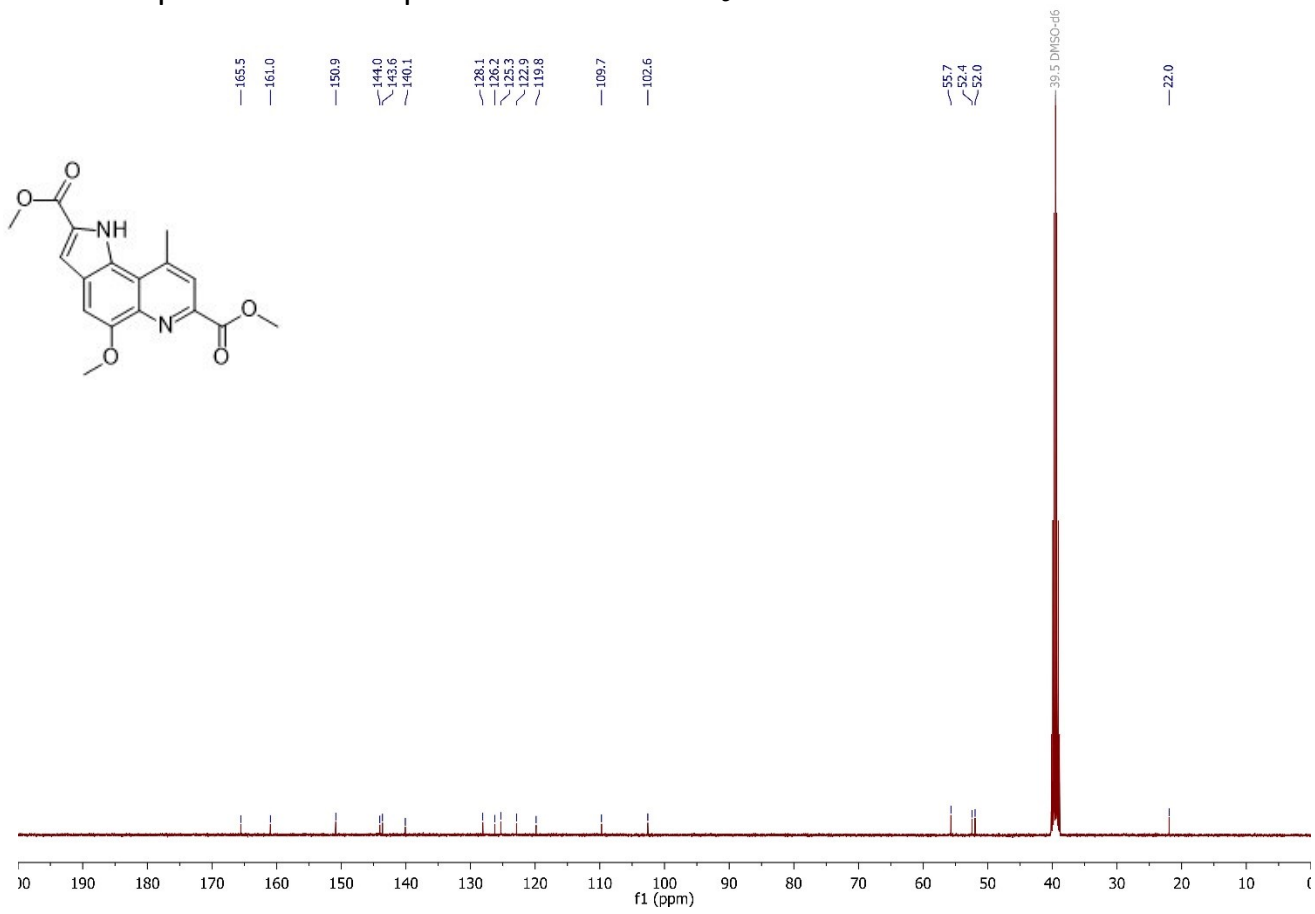
^{13}C NMR Spectrum of Compound **12** in $CDCl_3$



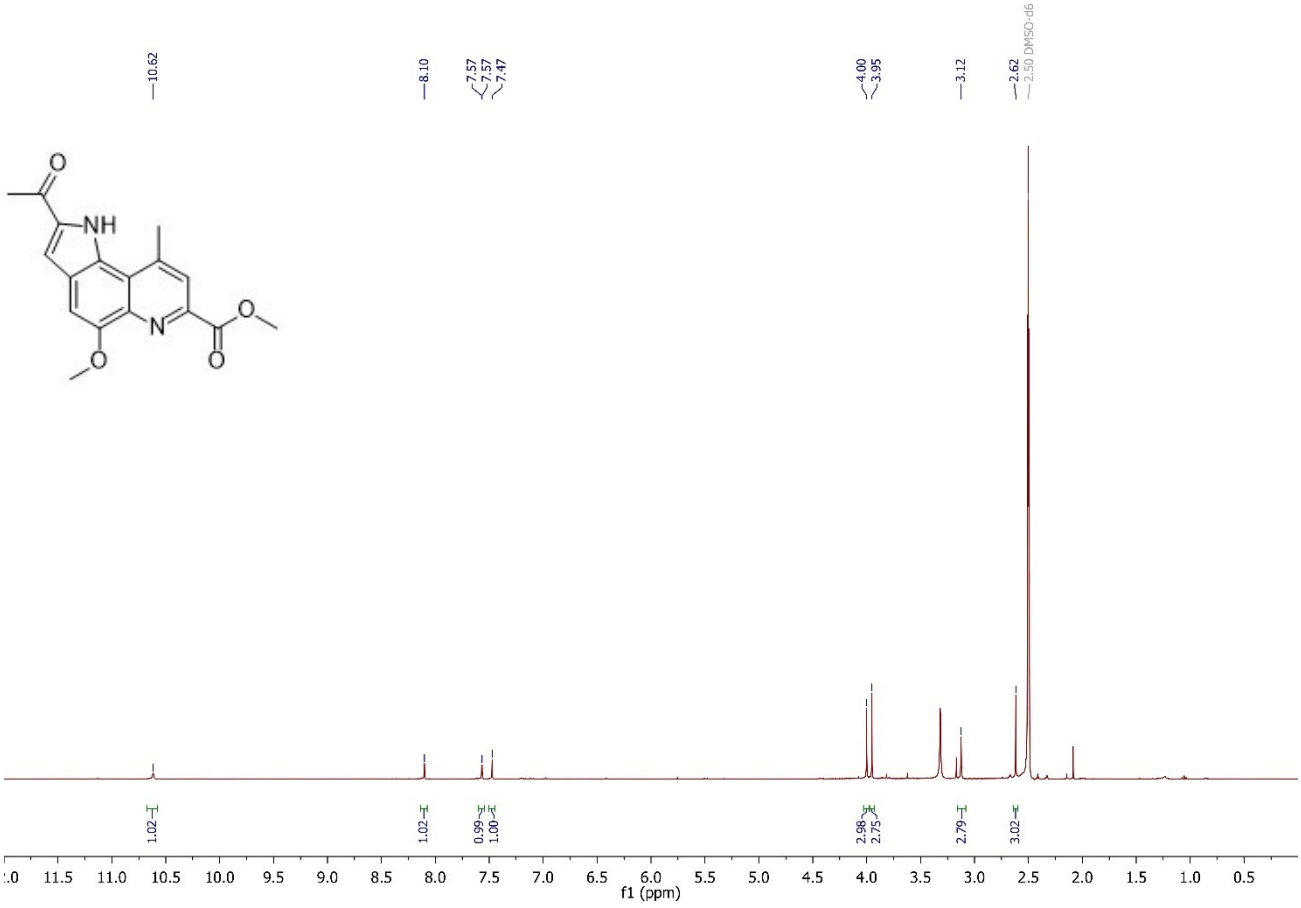
^{1}H NMR Spectrum of Compound **13** in DMSO-d_6



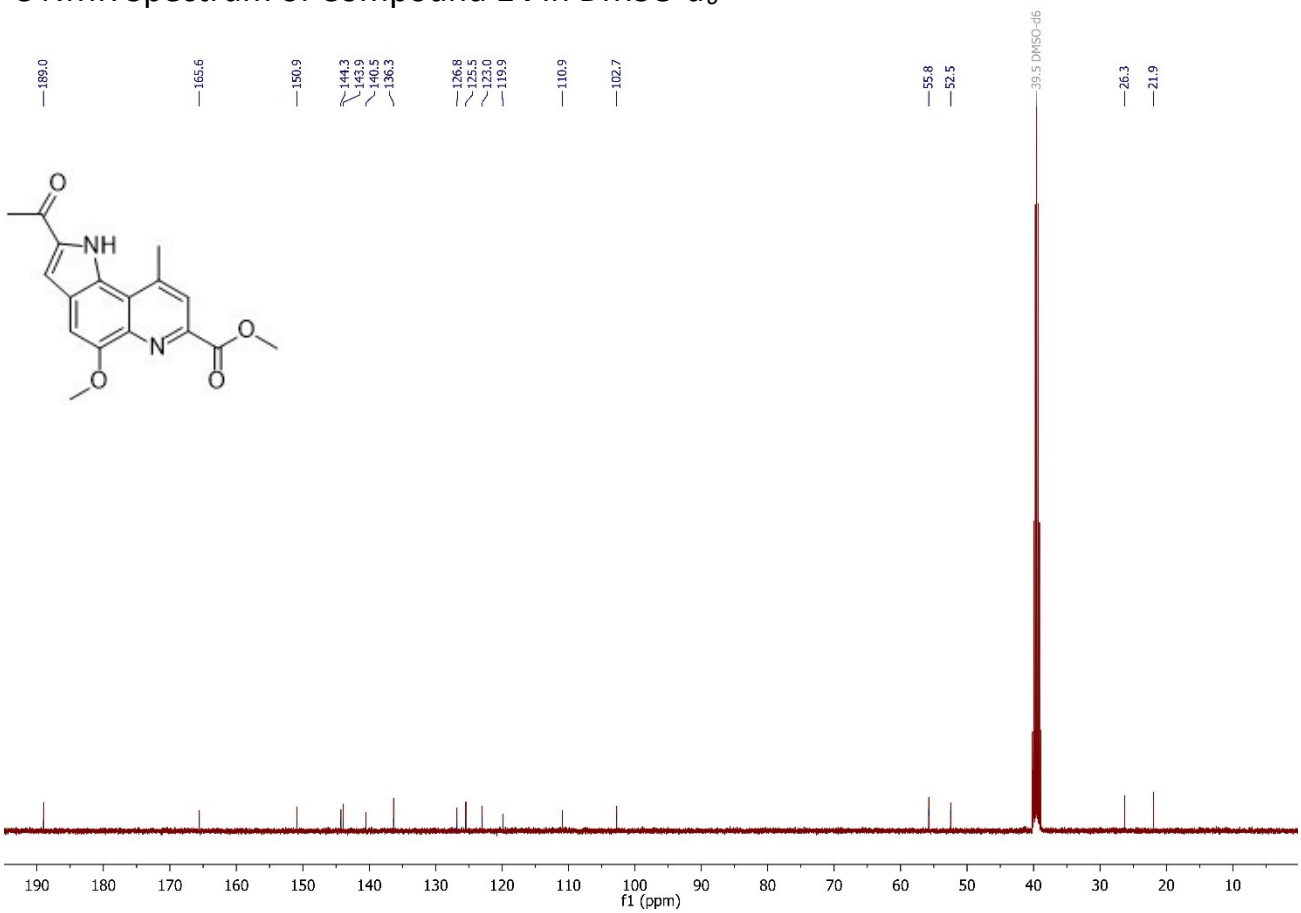
^{13}C NMR Spectrum of Compound **13** in DMSO-d_6



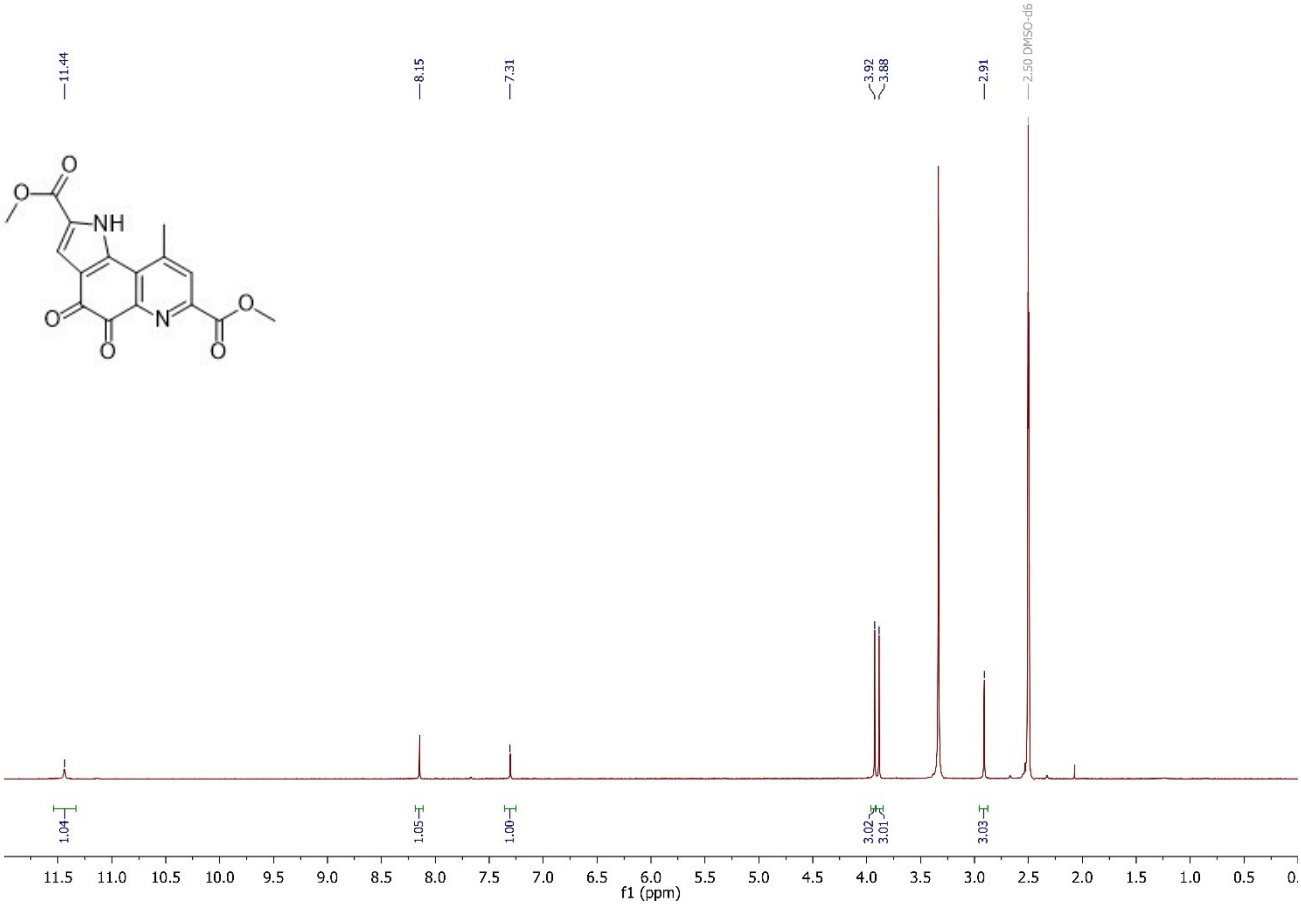
^{1}H NMR Spectrum of Compound **14** in DMSO-d_6



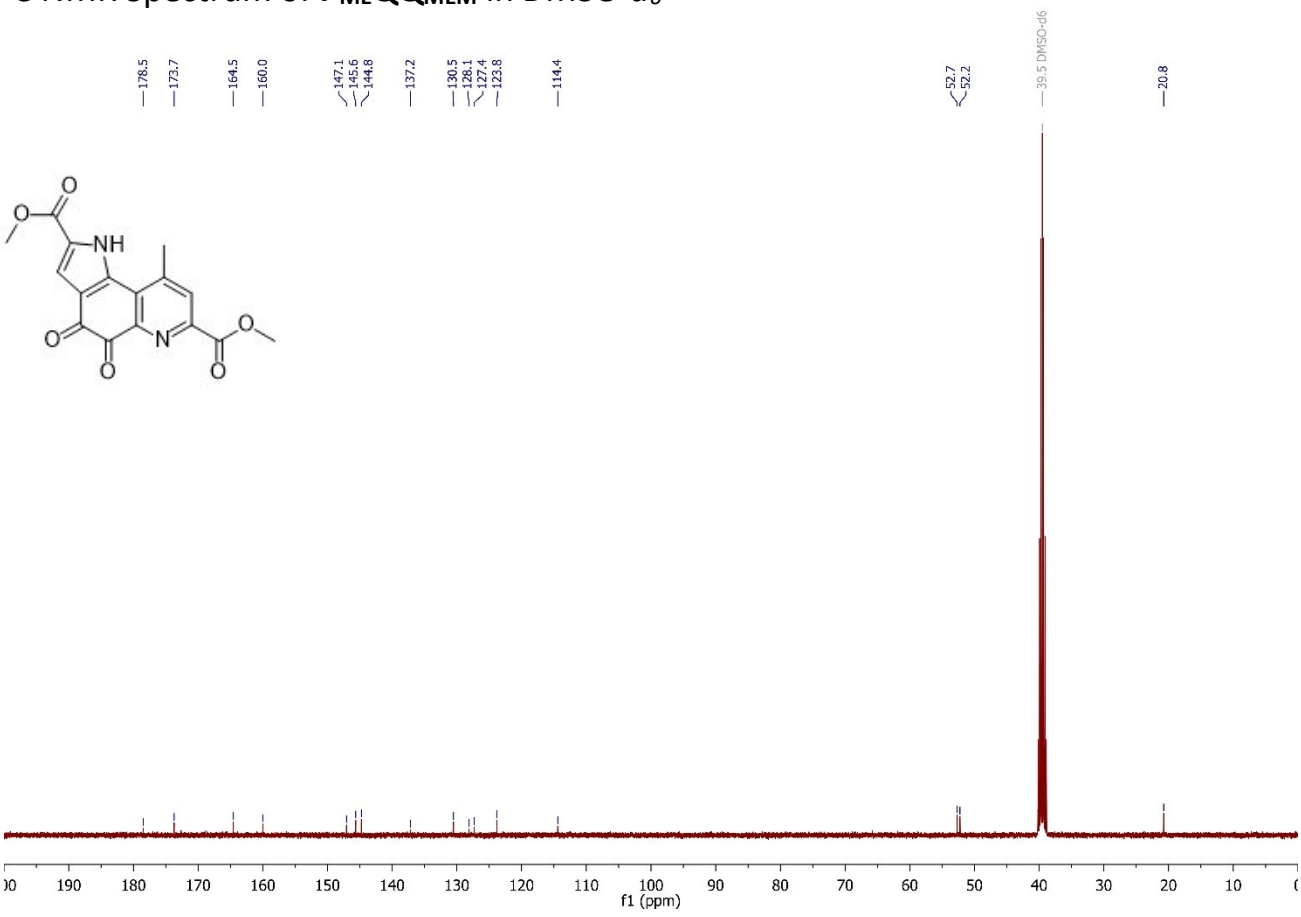
^{13}C NMR Spectrum of Compound **14** in DMSO-d_6



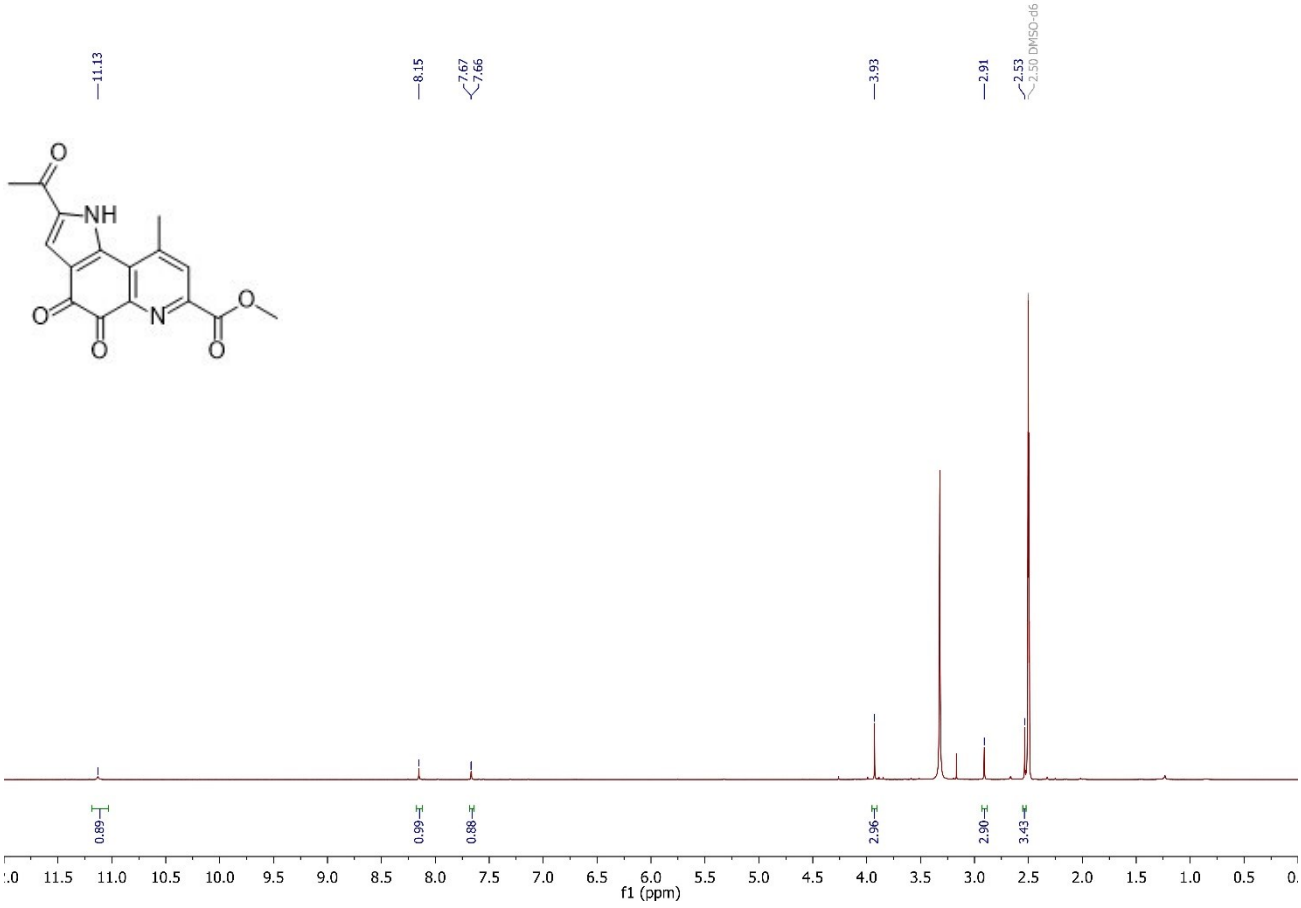
^{1}H NMR Spectrum of **$P_{ME}QQ_{MEM}$** in DMSO-*d_6*



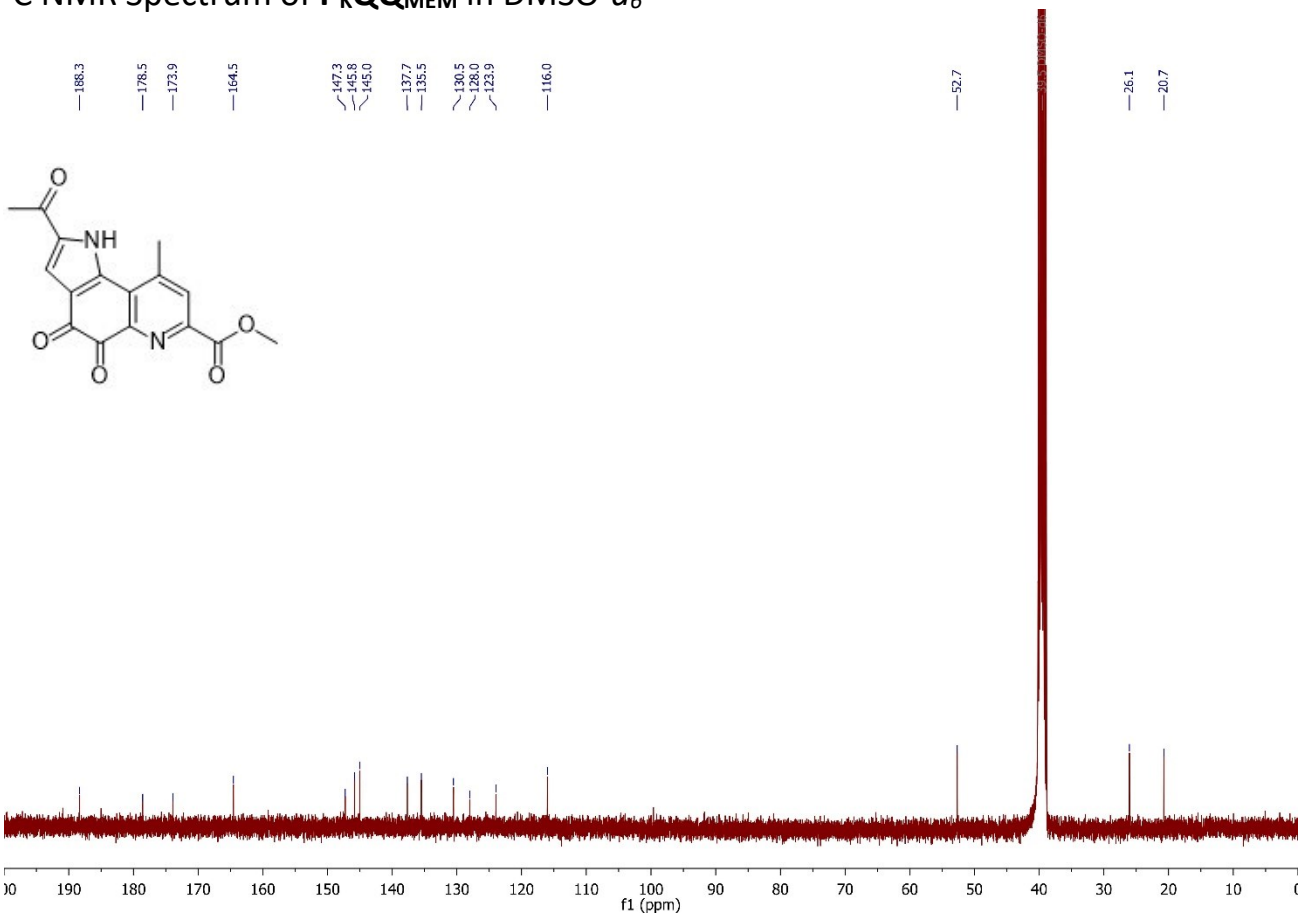
^{13}C NMR Spectrum of **$P_{ME}QQ_{MEM}$** in DMSO-*d_6*



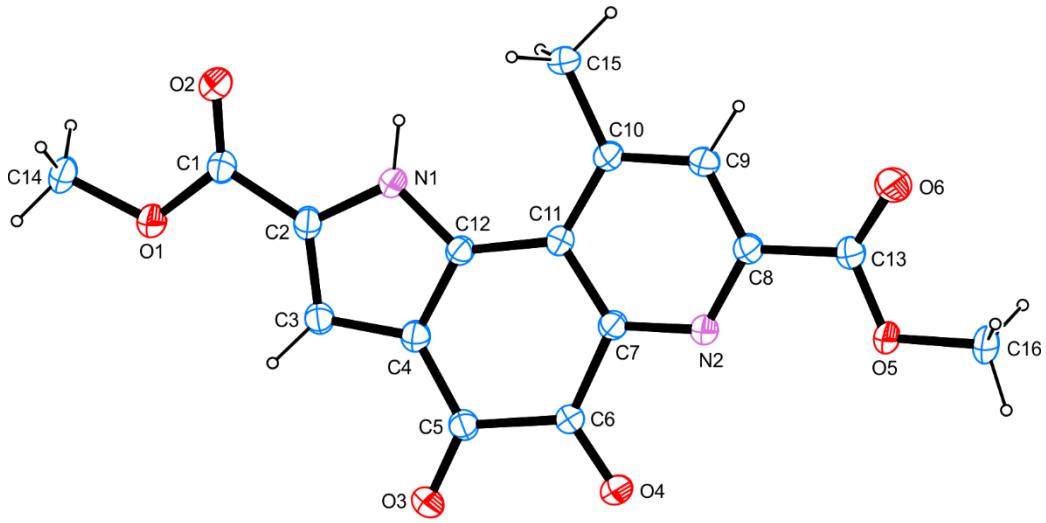
^{1}H NMR Spectrum of **P_KQQ_{MEM}** in DMSO-*d_6*



^{13}C NMR Spectrum of **P_KQQ_{MEM}** in DMSO-*d_6*



Crystallographic Data of **$P_{ME}QQ_{MEM}$**



$P_{ME}QQ_{MEM}$	
net formula	$C_{16}H_{12}N_2O_6$
M_r/g mol^{-1}	328.28
crystal size/mm	0.060 × 0.050 × 0.030
T/K	102.(2)
radiation	MoKα
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'C 1 2/c 1'
a/Å	8.5929(5)
b/Å	21.5998(13)
c/Å	15.3761(10)
α/°	90
β/°	105.320(2)
γ/°	90
V/Å^3	2752.5(3)
Z	8
calc. density/g cm^{-3}	1.584
μ/mm^{-1}	0.124
absorption correction	Multi-Scan
transmission factor range	0.93–1.00
refls. measured	26705
R_{int}	0.0483

mean σ(I)/I	0.0266
θ range	2.632–27.485
observed refls.	2584
x, y (weighting scheme)	0.0419, 4.3094
hydrogen refinement	H(C) constr, H(N) refall
refls in refinement	3158
parameters	224
restraints	0
$R(F_{obs})$	0.0415
$R_w(F^2)$	0.1101
S	1.043
shift/error$_{max}$	0.001
max electron density/e Å^{-3}	0.380
min electron density/e Å^{-3}	−0.441

Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre, CCDC, 12 Union Road, Cambridge CB21EZ, UK. Copies of the data can be obtained free of charge on quoting the depository numbers CCDC-2193479 (https://www.ccdc.cam.ac.uk/structures/).