

Antiviral Activity of Pyrazole Derivatives bearing Hydroxyquinoline Scaffold against SARS-CoV-2, HCoV-229E, MERS-CoV, and IBV Propagation

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Supporting information:

Table S1. Physicochemical Properties / Lipophilicity / Drug-likeness properties of the prepared compounds.

Compds.	Molecular weight (g/mol)	Num. heavy atoms	Num. arom. heavy	Num. H-bond acceptor	Num. H-bond donors	Molar Refractivity	TPSA (Å ²)	Consensus Log P _{o/w}	Lipinski's Rule	Bioavailability Score	GI absorption	Log K _p (Skin permeation) (cm/s)
Hyd	422.48	32	23	4	2	124.13	90.01	3.36	Yes	0.55	High	-6.18
HQ	577.63	44	33	6	2	171.73	109.47	5.50	Yes	0.55	Low	-5.27
15A	559.62	43	33	5	1	173.52	83.61	5.83	No	0.17	Low	-4.67

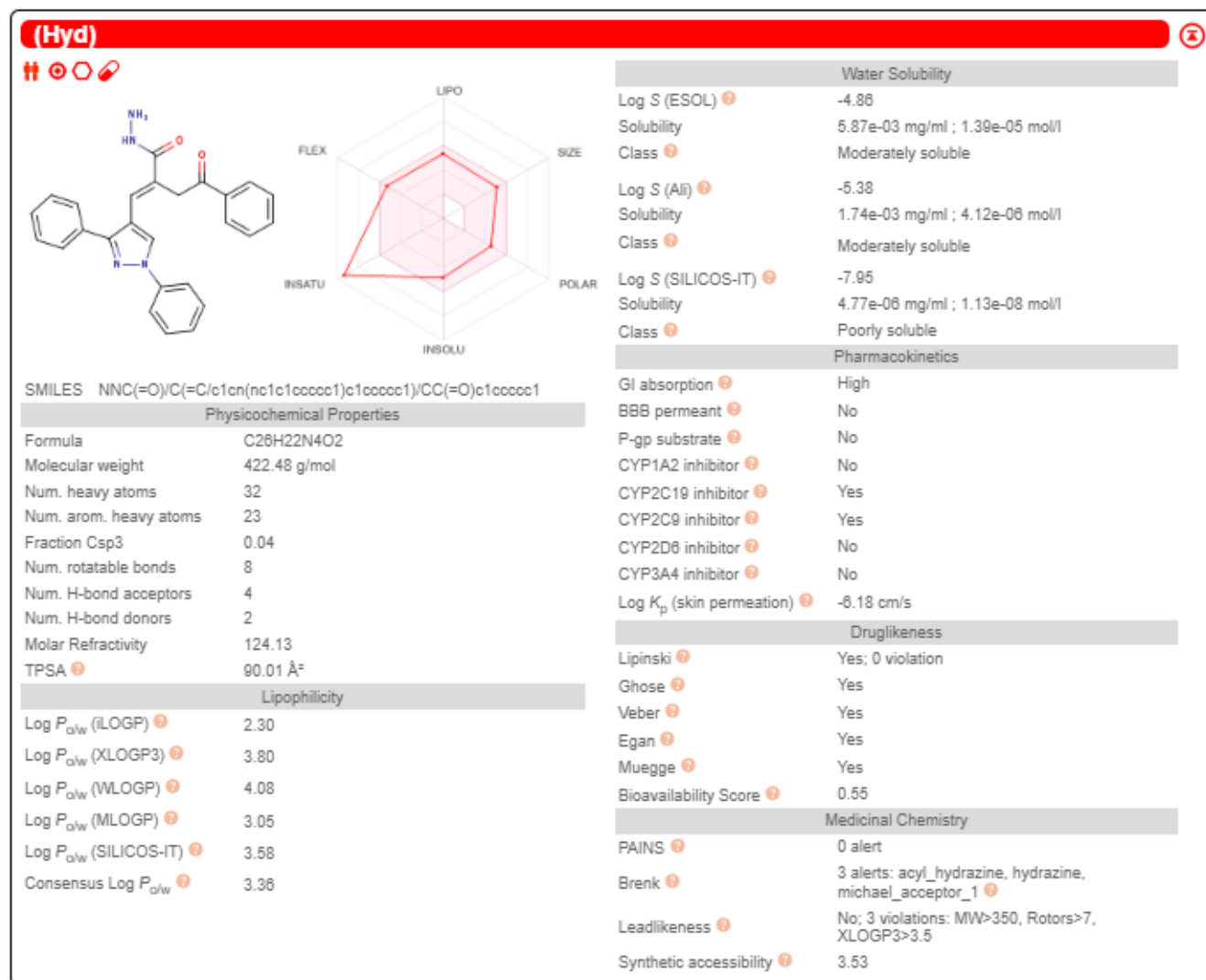


Fig. S1. ADME of compound **Hyd**.

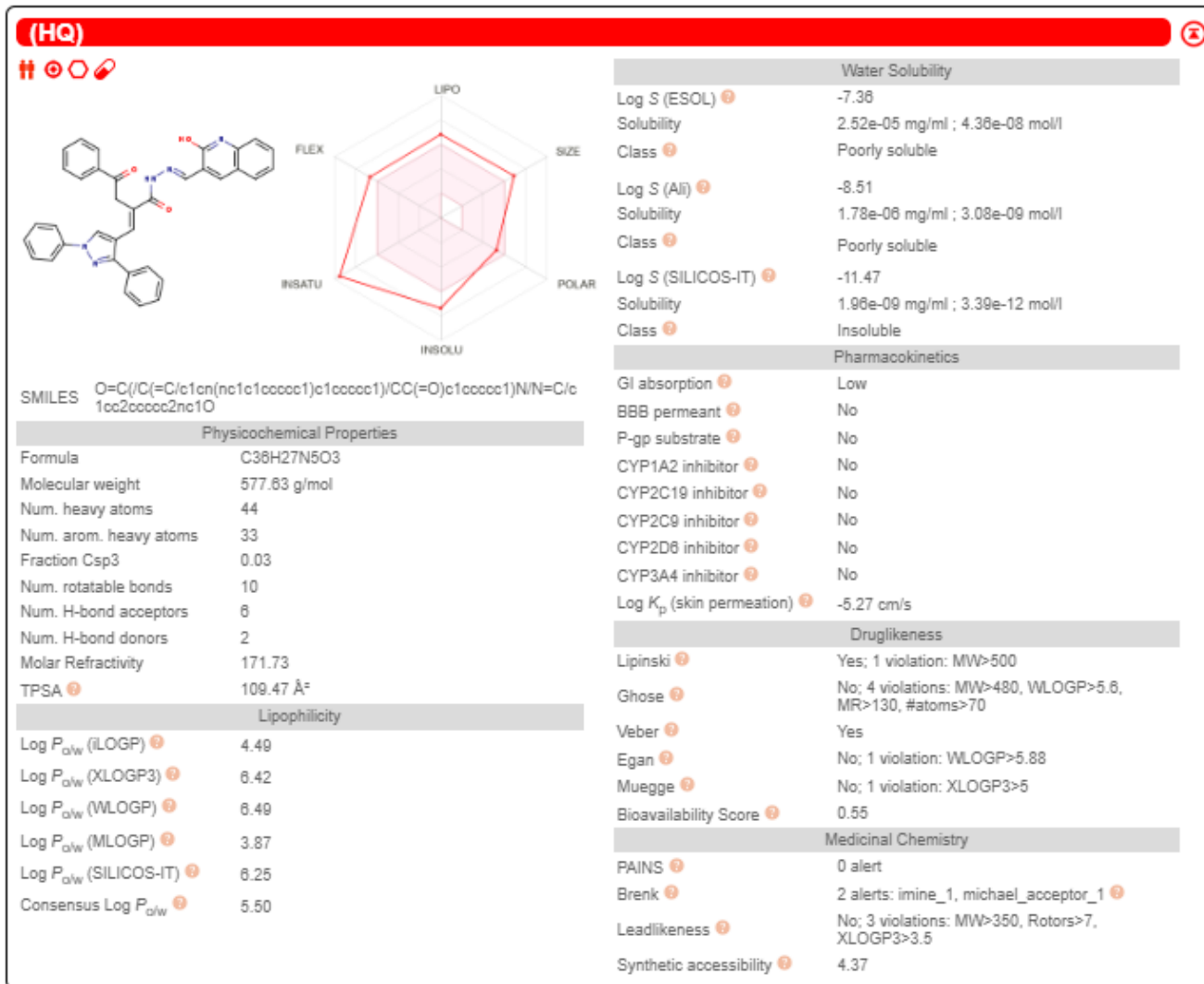


Fig. S2. ADME of compound HQ.

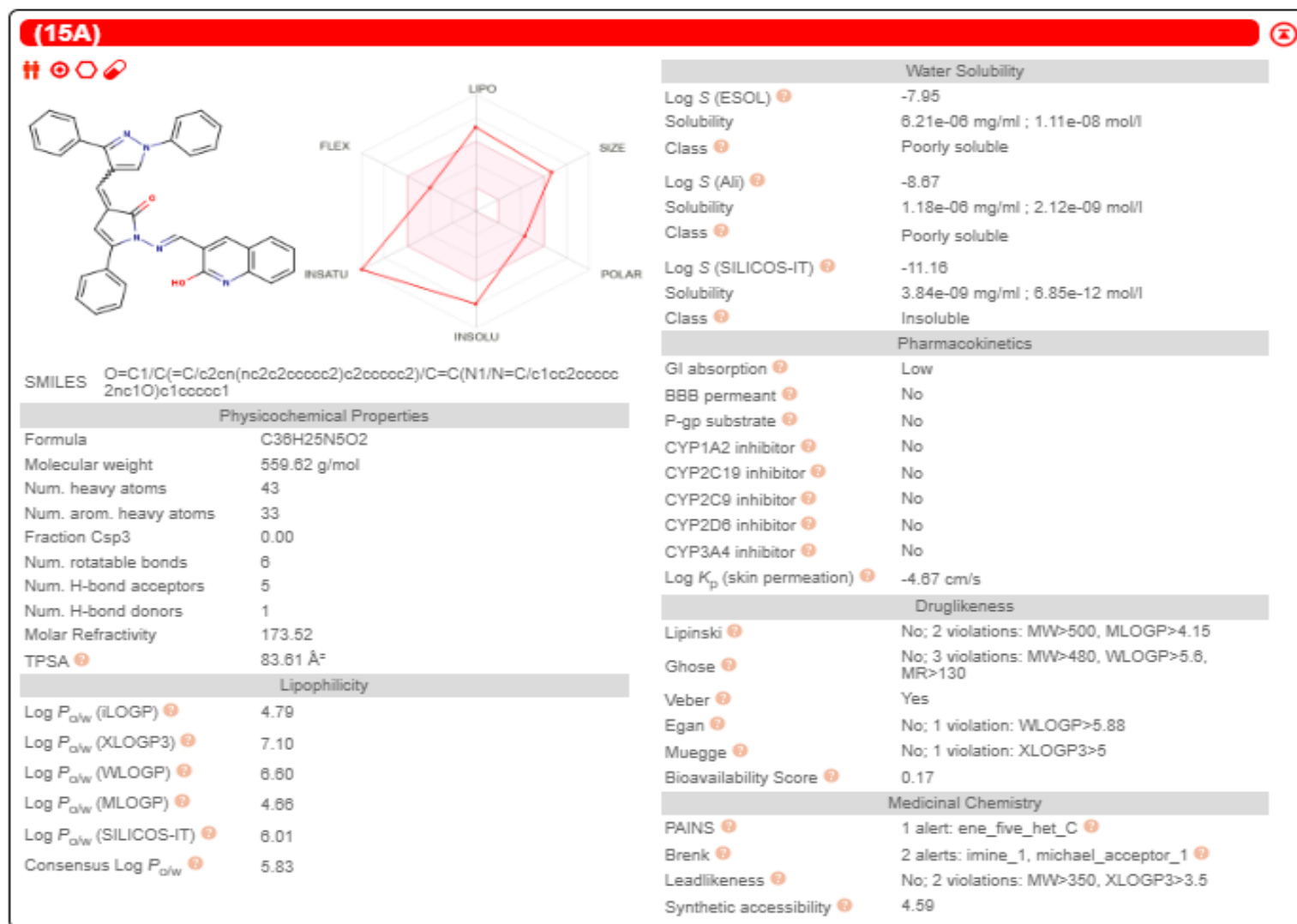


Fig. S3. ADME of compound 15A.

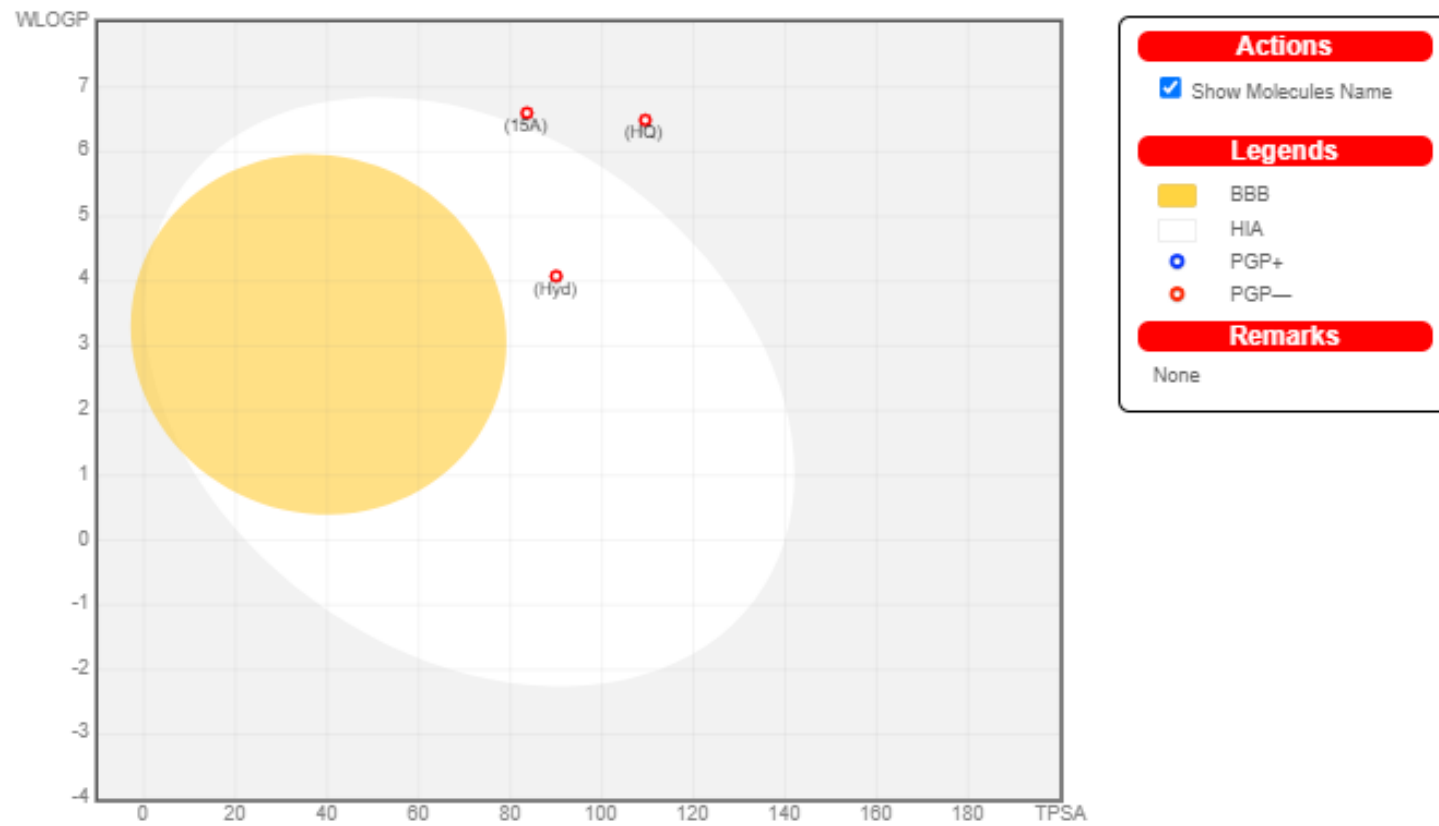
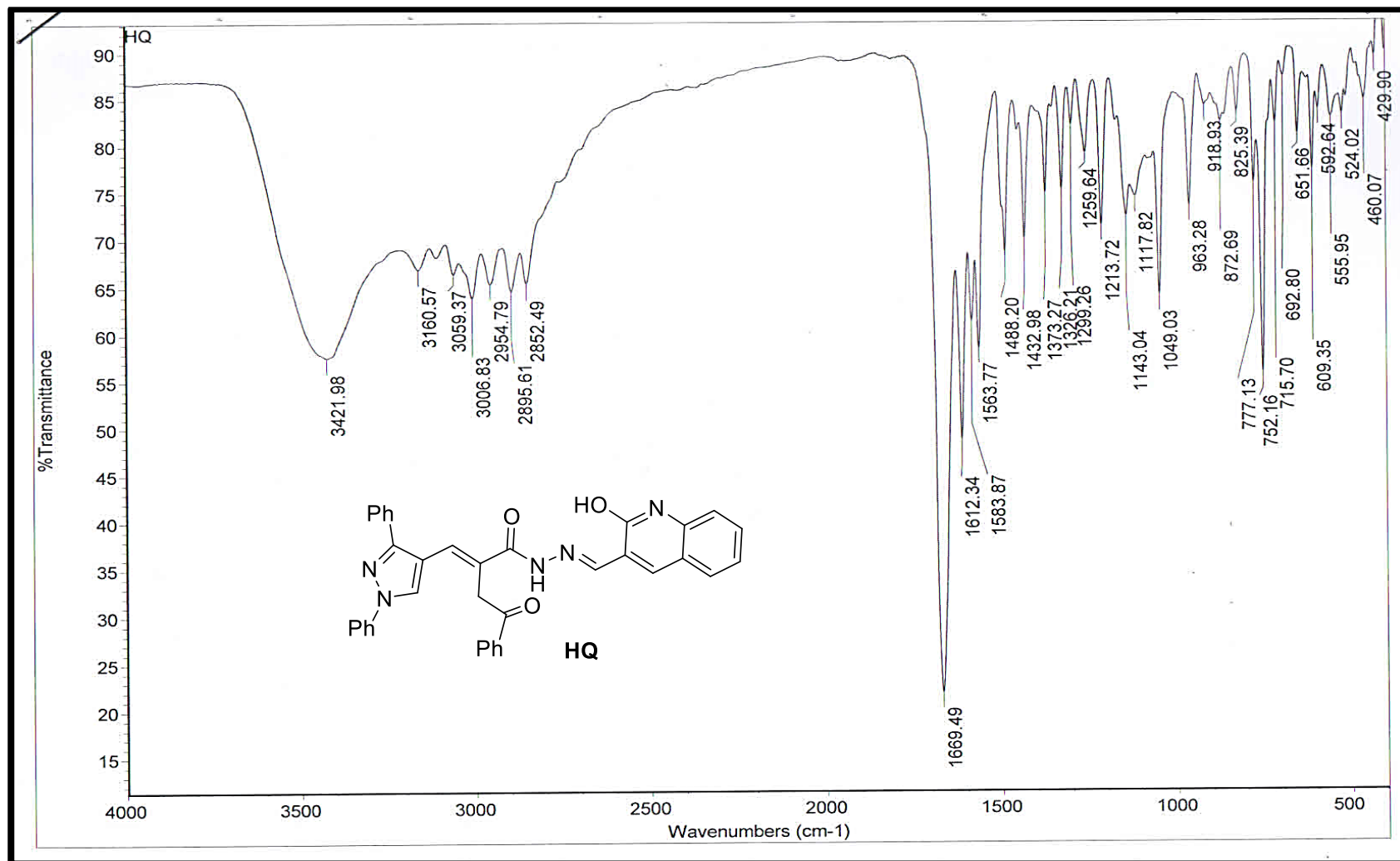


Fig. S4. BOILED-EGG of the synthesized compounds.

Spectral data:



FTIR spectrum of compound **HQ**



Dr_SayedKarm-HQ

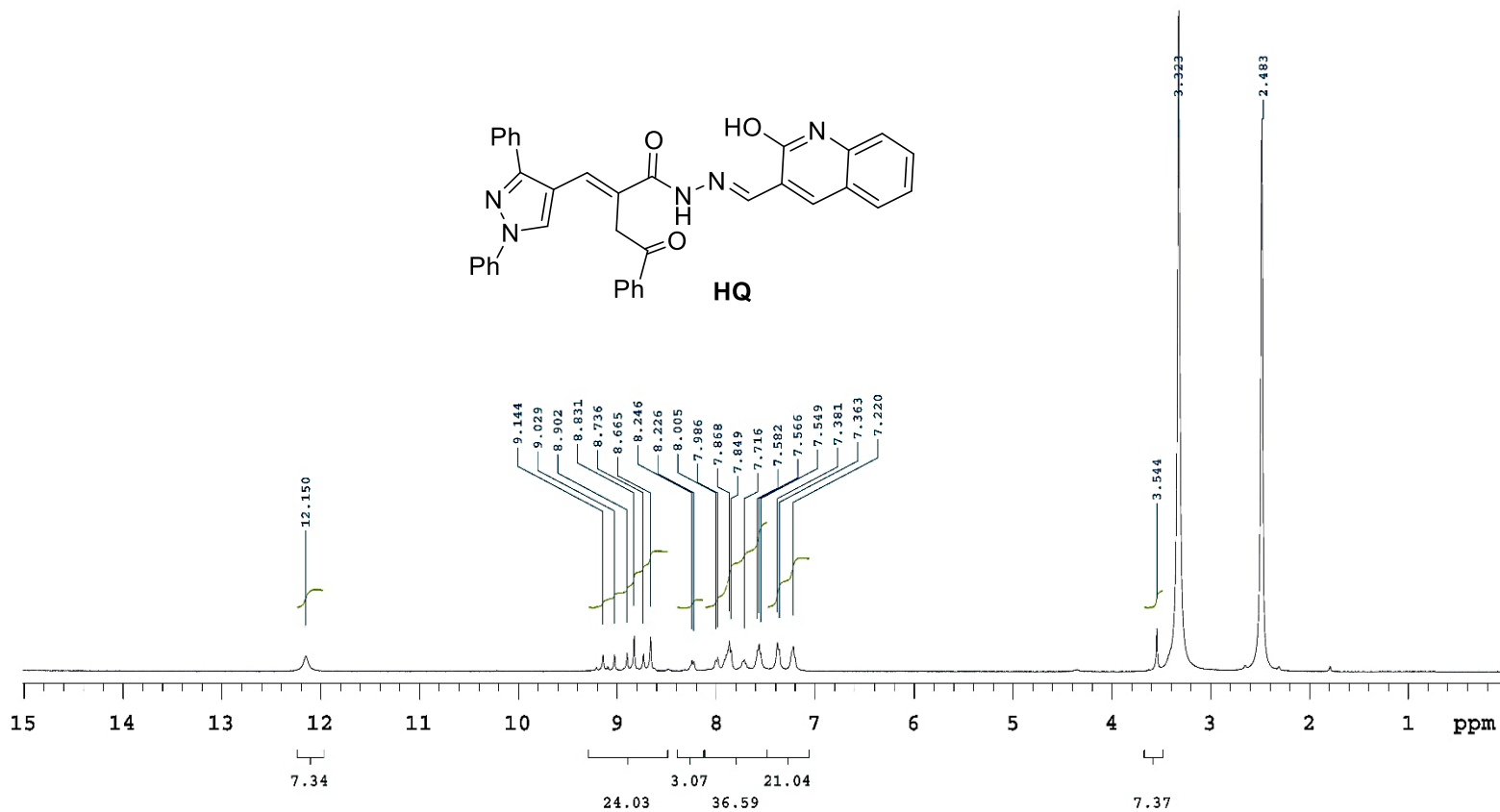
Dr_SayedKarm-HQ

Sample Name **Dr_SayedKarm-HQ**
Date collected **2018-01-30**

Pulse sequence **PROTON**
Solvent **DMSO**

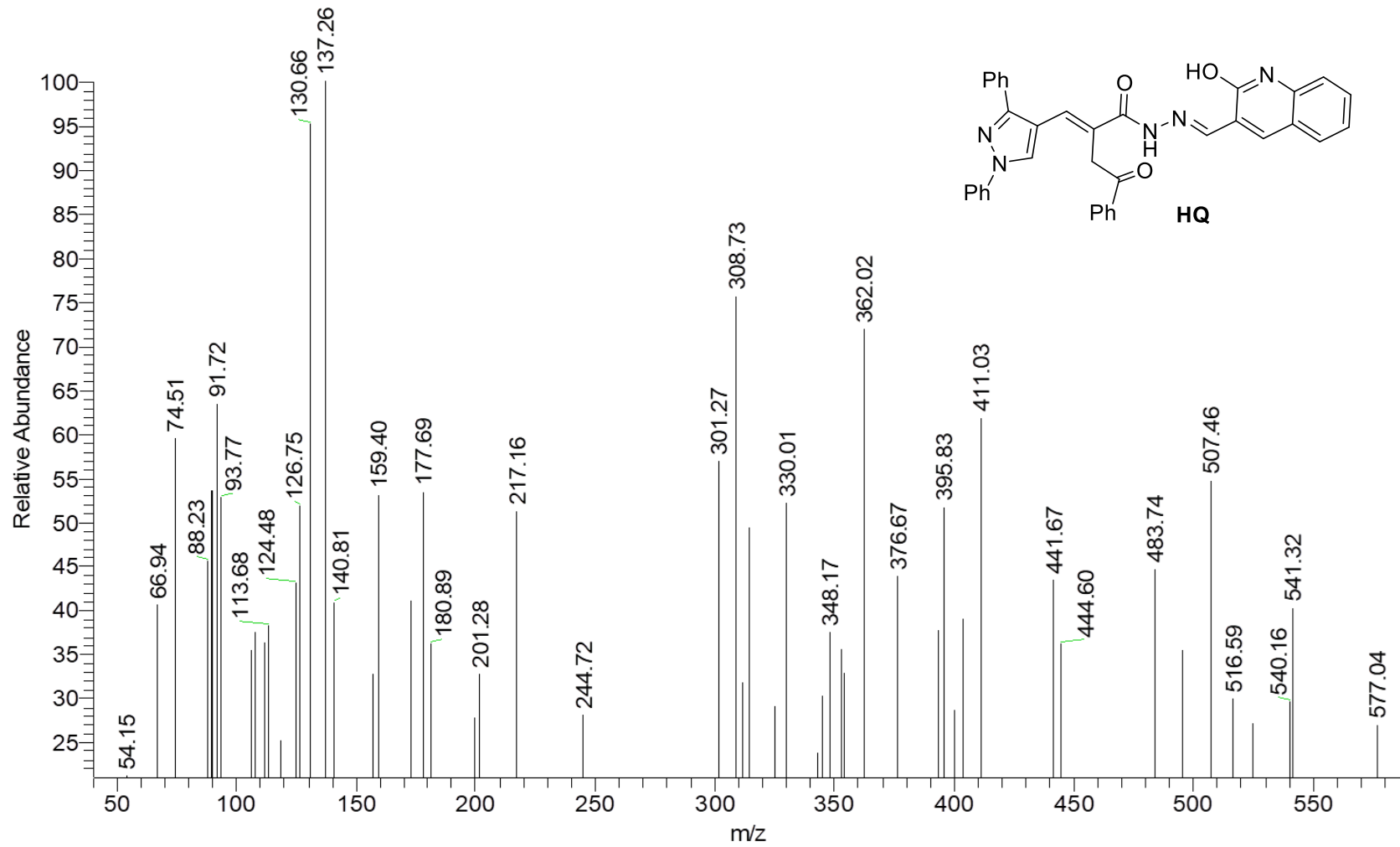
Temperature **25**
Spectrometer **nmr400-mercury400**

Study owner **vnmr1**
Operator **vnmr1**

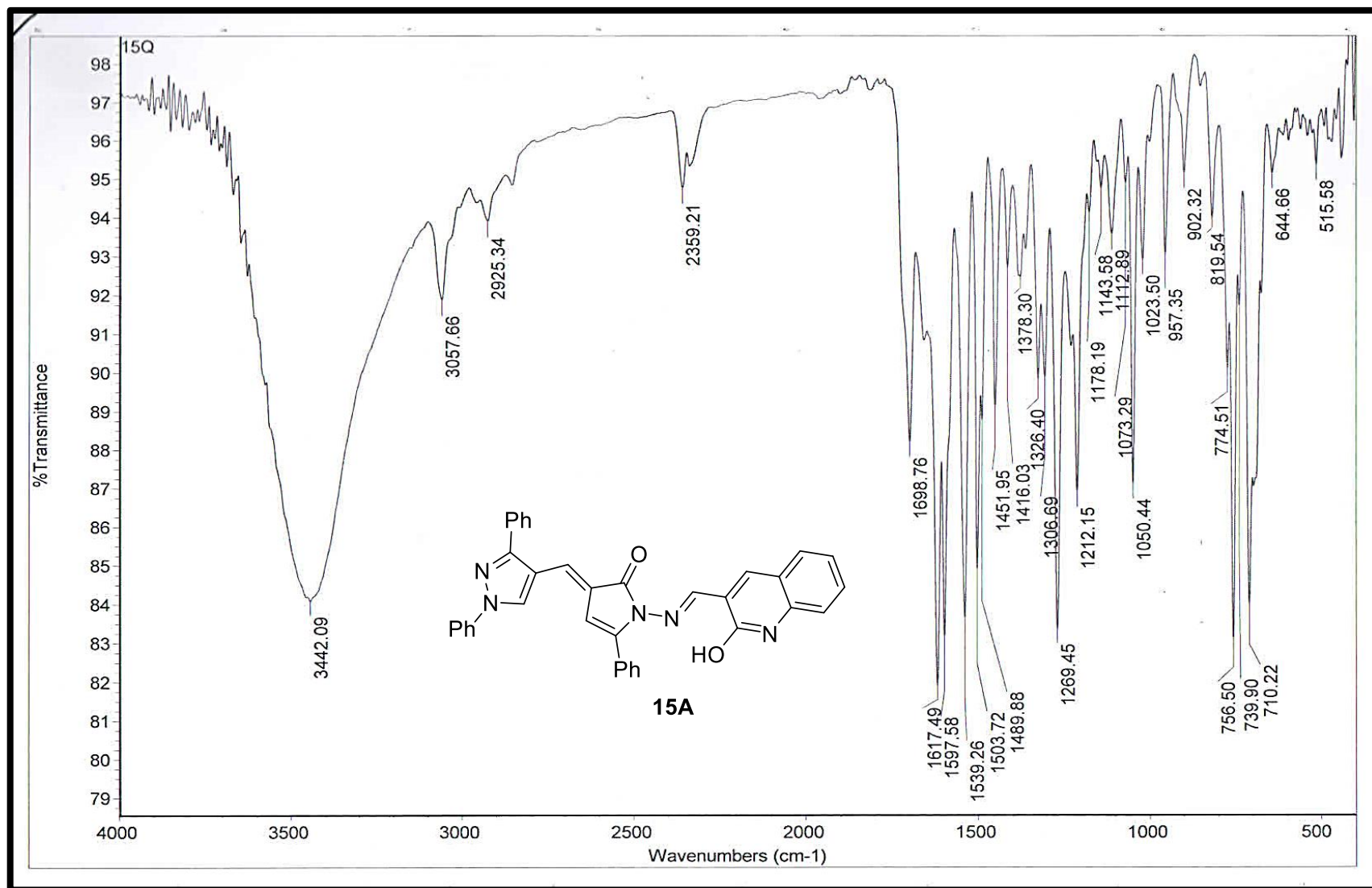


¹H NMR spectrum (DMSO-*d*₆) of compound **HQ**

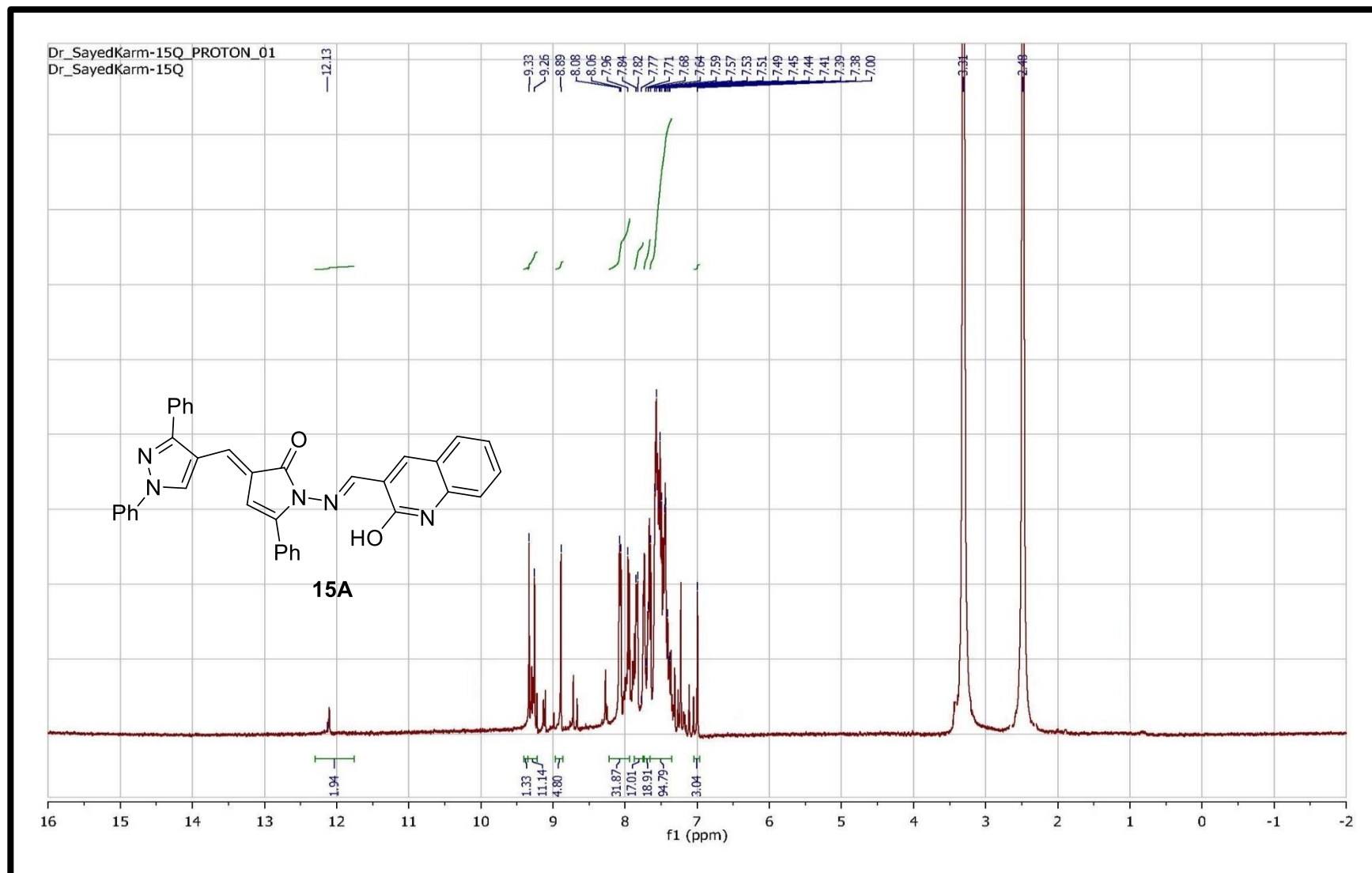
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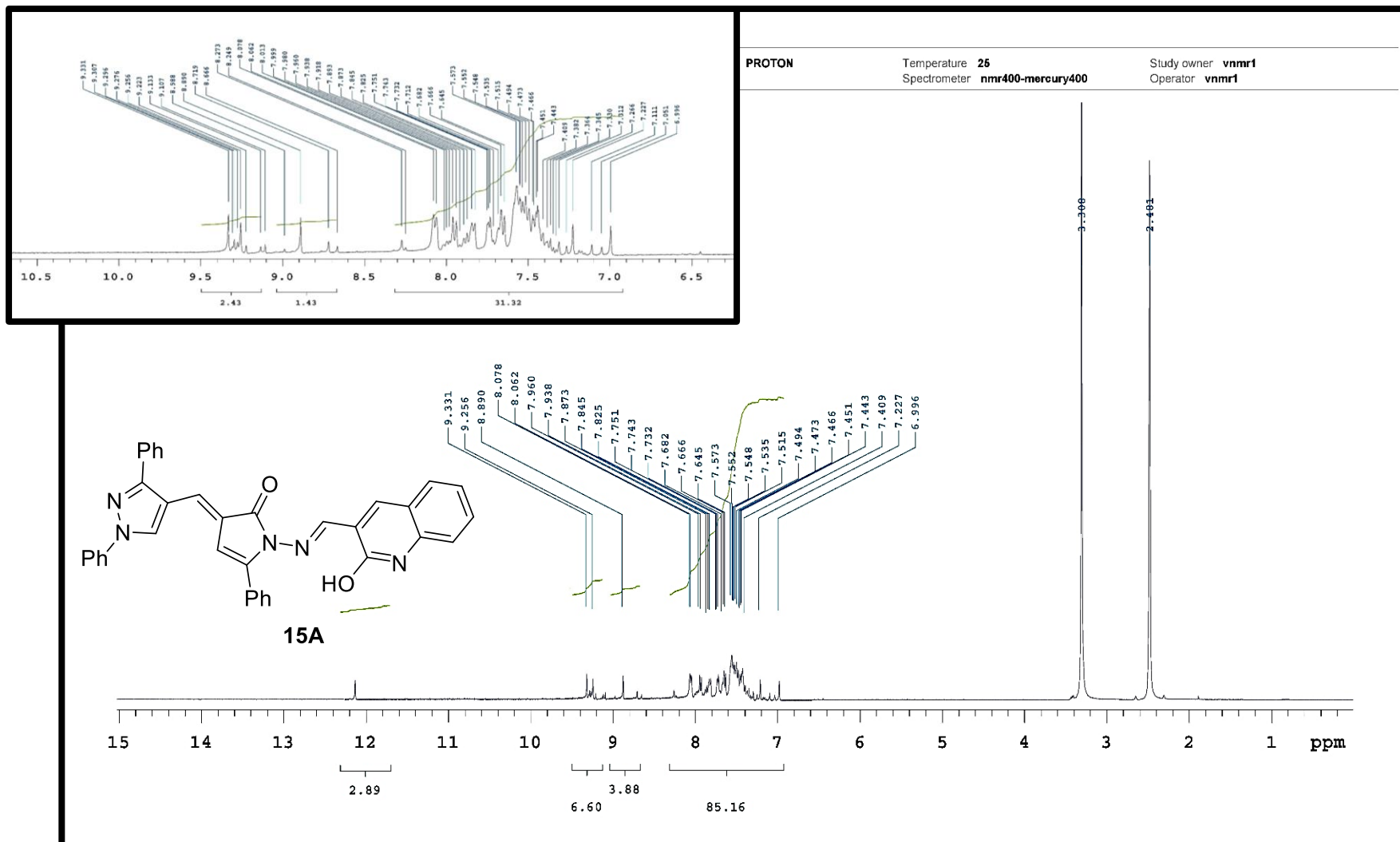
Mass spectrum of compound HQ



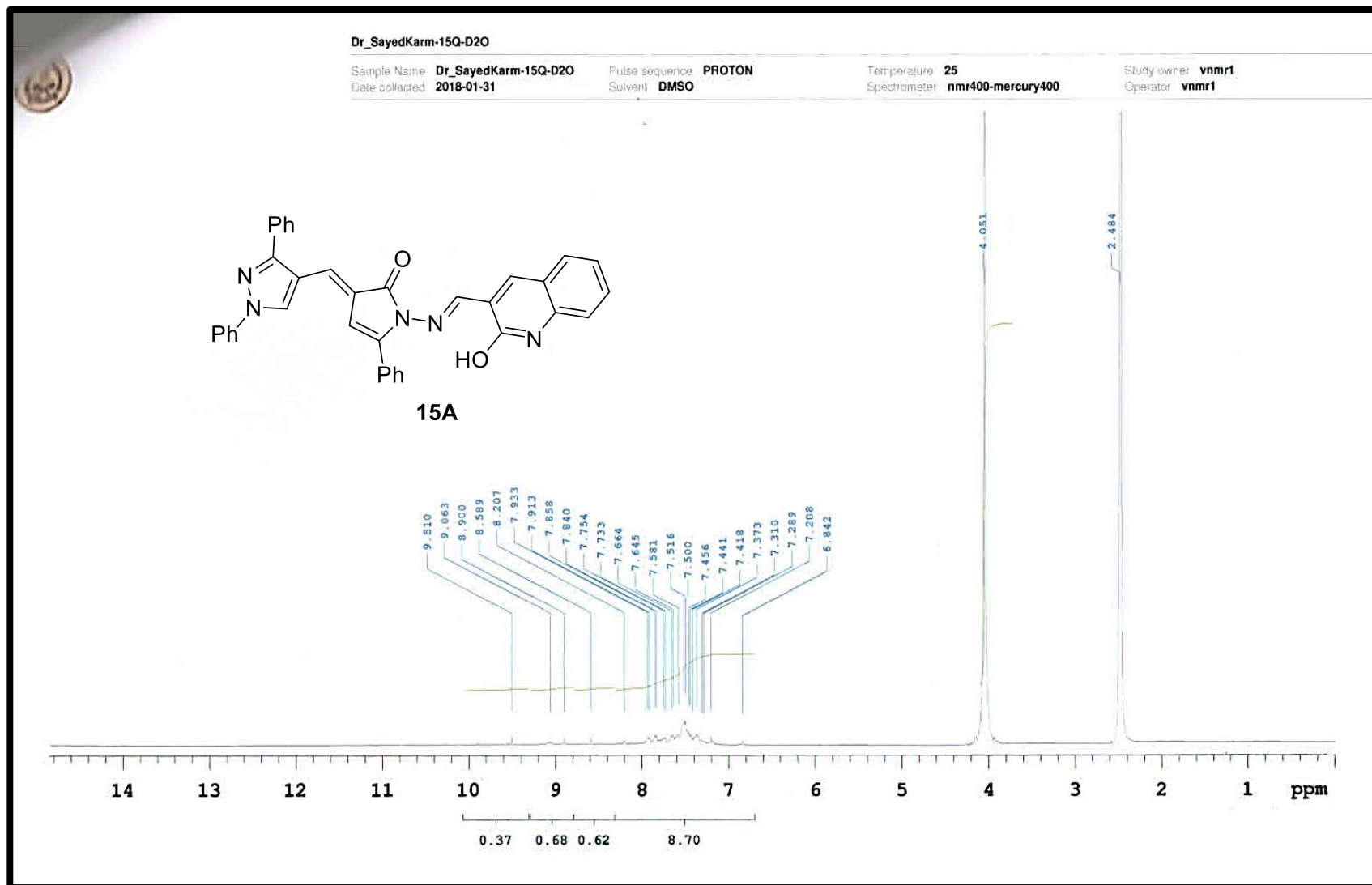
FTIR spectrum of compound 15A



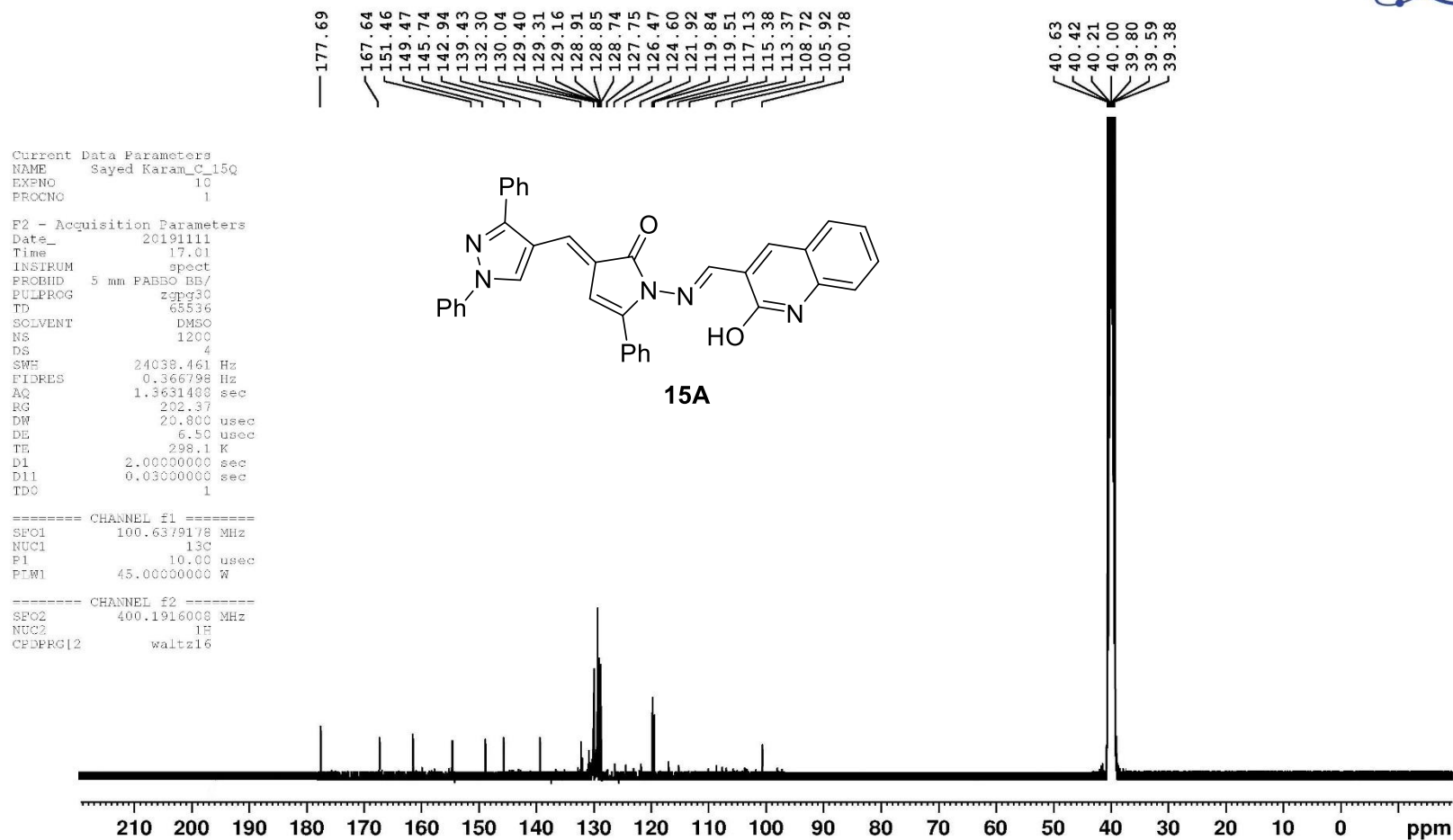
^1H NMR spectrum ($\text{DMSO-}d_6$) of compound **15A**



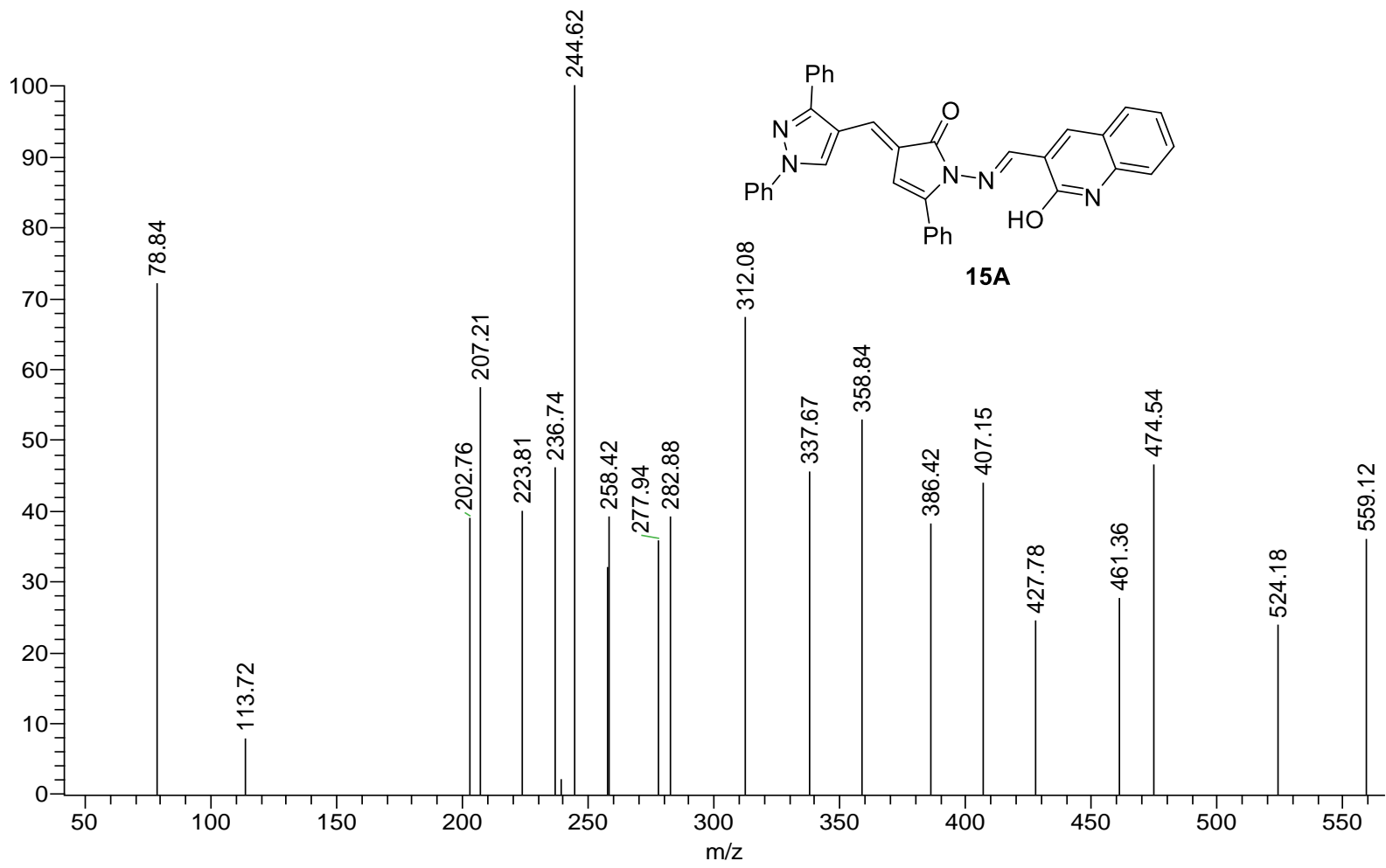
Cont. ^1H NMR spectrum ($\text{DMSO-}d_6$) of compound **15A**



¹H NMR spectrum (DMSO-*d*₆+D₂O) of compound 15A

¹³C NMR spectrum (DMSO-*d*₆) of compound **15A**

T: {0,0} + c EI Full ms [40.00-1000.00]



Mass spectrum of compound 15A