Electronic Supplementary Material (ESI) for Organic .

A Fluorescent Probe for Estimation of Adenosine Diphosphate and Monitoring of Glucose Metabolism

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Supporting Information

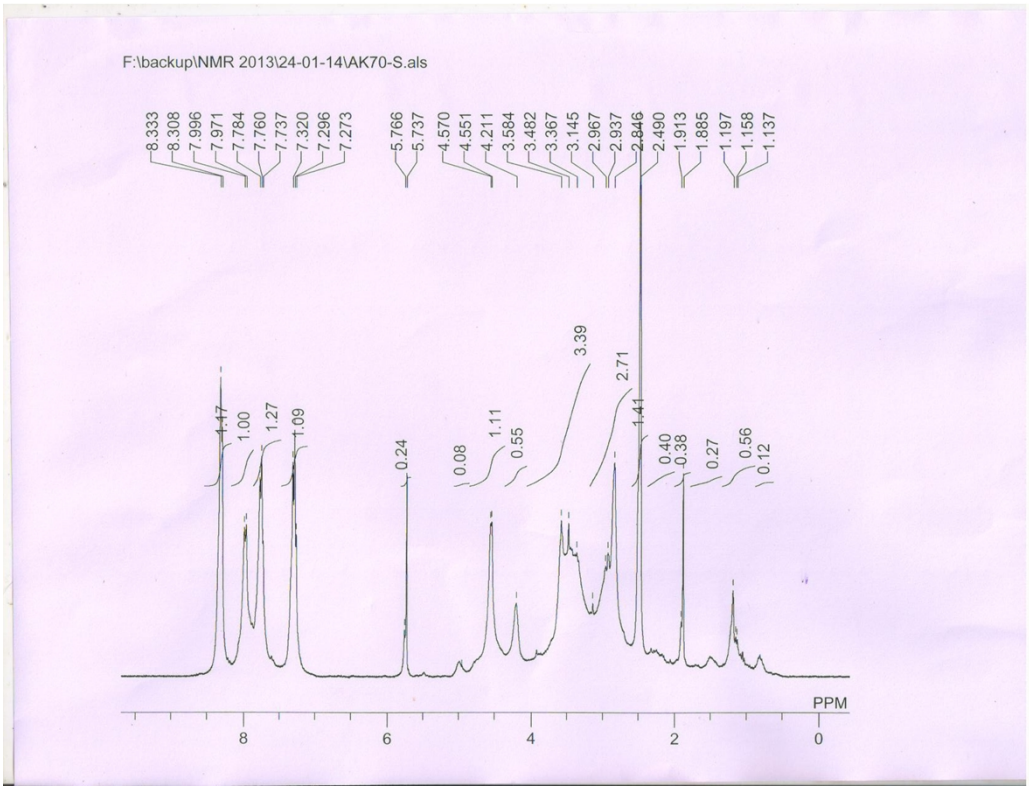


Figure S1a. [1]H NMR spectrum of compound **3** (DMSO δ 2.49).

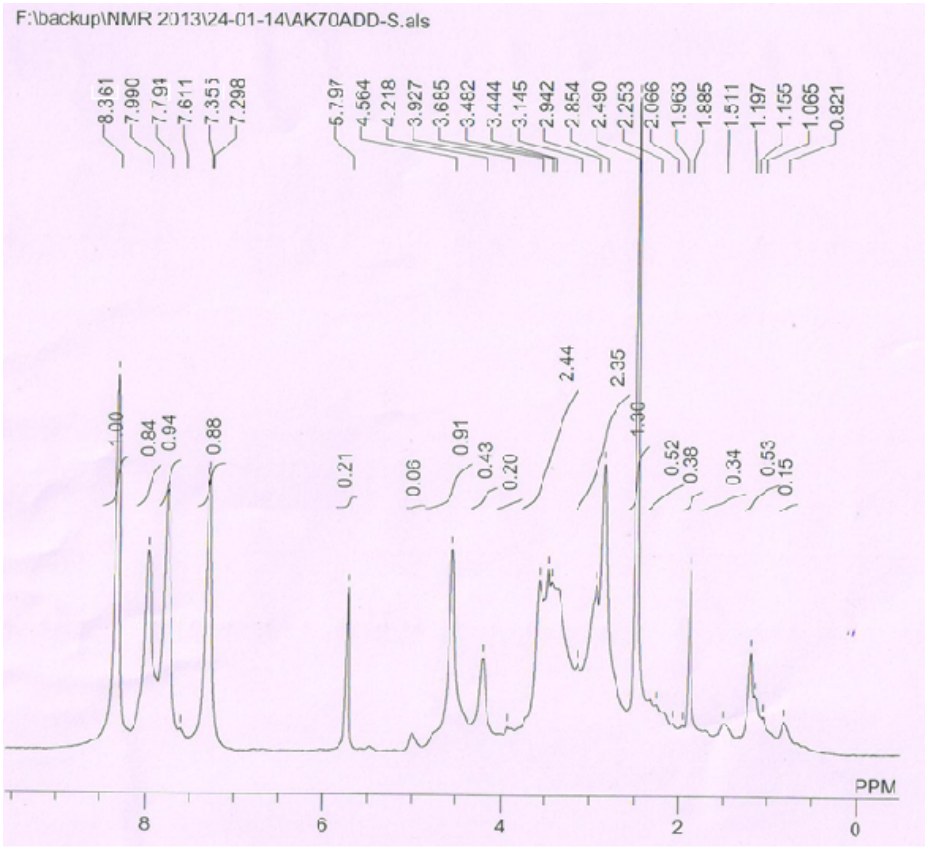


Figure S1b. [1]H NMR spectrum of compound **3**+ADP (DMSO δ 2.49).

Table S1. Physico-chemical parameters of compounds 2 and 3 and those reported earlier.[4m]

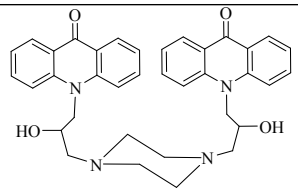
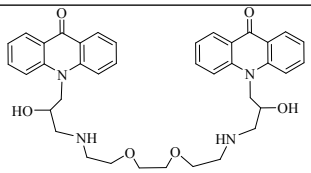
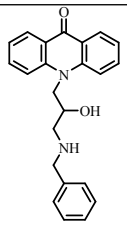
compound	logP	TPSA	ATP/ADP selectivity
	2.017	90.942	No selectivity
	0.745	126.988	ADP
	2.388	54.26	ATP
ATP	-2.56	279.15	
ADP	-1.55	232.61	

Table S2. Comparison of ADP/ATP quantification of different steps of glucose metabolism by fluorescence and mass spectral studies.

Step of Scheme 2	Description	ATP/ADP produced	Fluorescence studies	LC-MS QuantAnalysis
1	Phosphorylation of glucose	ADP	3.1 ng	3.0 ng
3	Phosphorylation of fructose-6-phosphate	ADP	3.1 ng	3.2 ng
6	Formation of 3-phosphoglycerate	ATP	55 ng	52 ng
8	Formation of pyruvate	ATP	55 ng	53 ng
	Mitochondria from pig liver	ADP	50 ng	48 ng

The amount of reagents in each reaction was as given in the text.

Benesi-Hildebrand plot of 3.ADP.

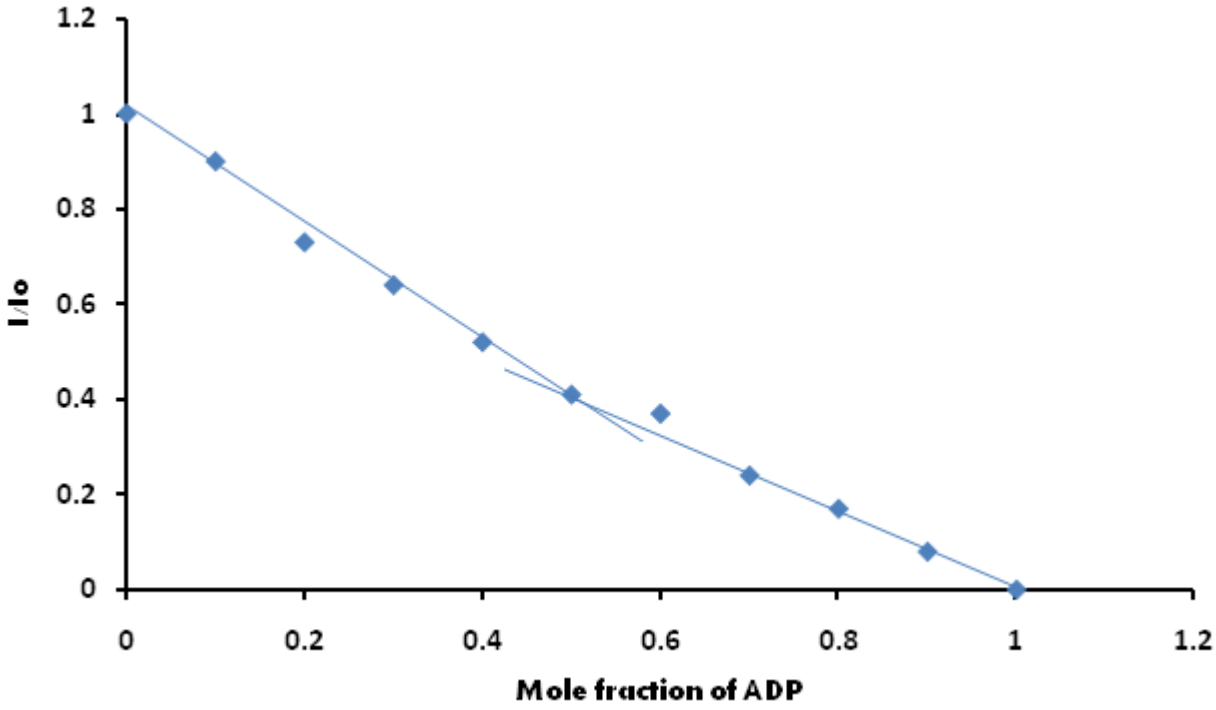


Figure S2. Benesi-Hildebrand plot of **3.ADP** indicating 1:1 stoichiometry.

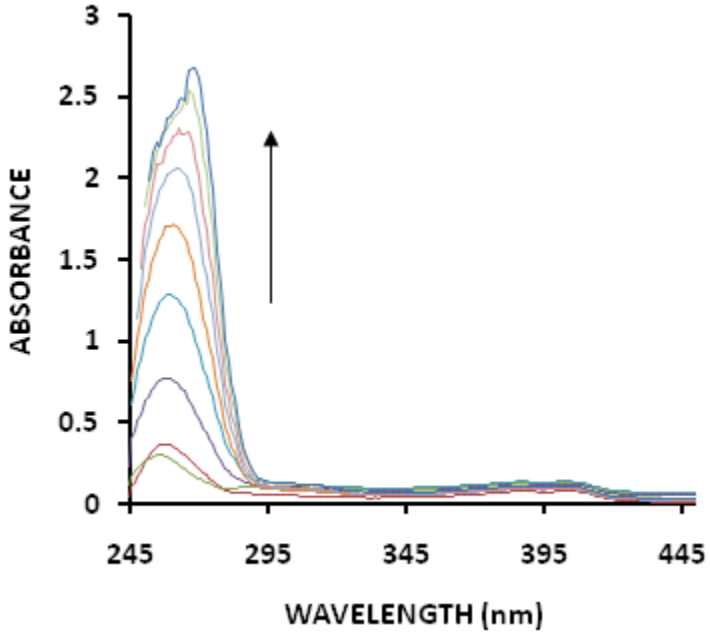


Figure S3. Absorbance spectrum of compound **3** (10^{-5} M) with 0-5 equiv of ADP in HEPES buffer.

Equation for calculation of binding constant

Binding constants of compound-anion complex were calculated using Benesi-Hildebrand Equation.

$1/(A_f - A_{obs}) = 1/(A_f - A_{fc}) + 1/ K(A_f - A_{fc})[L]$

Where A_f is absorbance of free host, A_{obs} is absorbance observed, A_{fc} is absorbance at saturation, K is the binding constant.

Binding constant of compound 3 with ADP

Compound.	Binding constant with ADP (M^{-1})
3	**2.14×10^5**

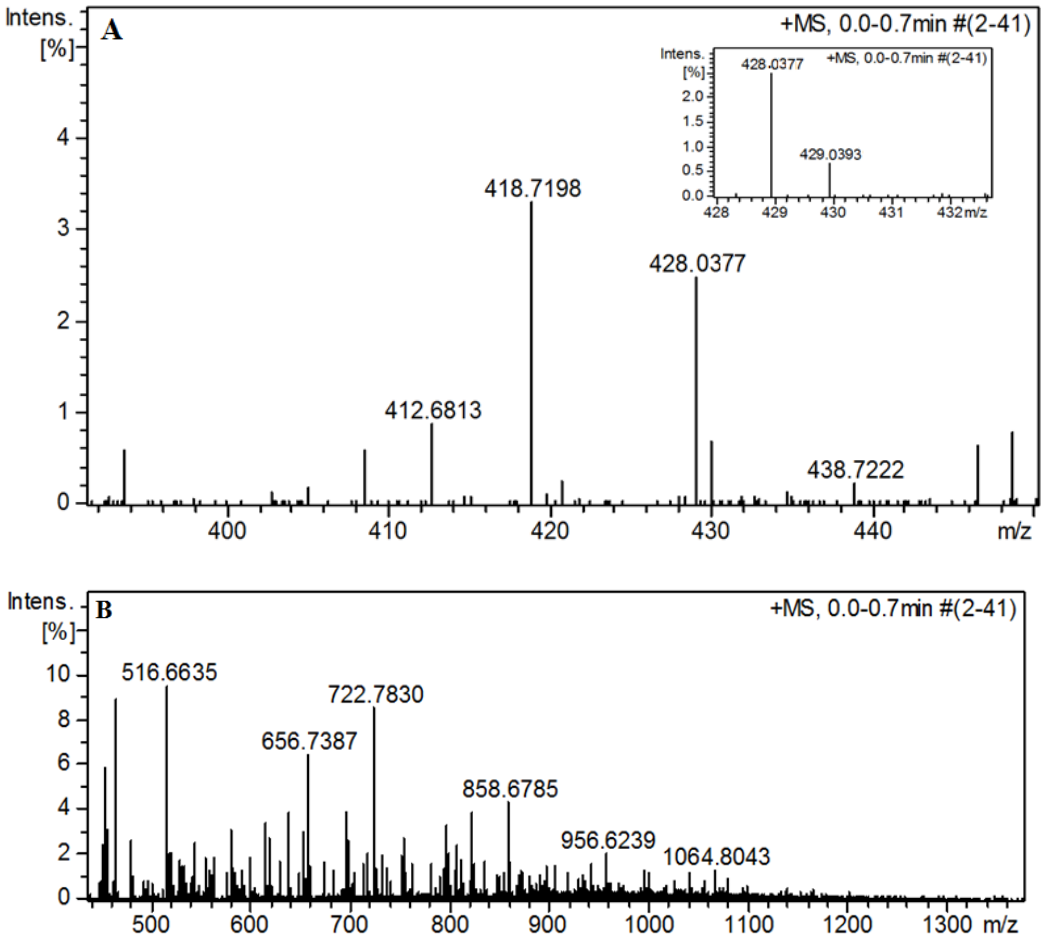


Figure S4. High resolution mass spectrum of mitochondrial solution. A) spectrum showing mass peak at *m/z* 428.0377 corresponding to mass of ADP. Inset: expansion showing isotopic pattern, B) mass spectrum in the higher region showing presence of other components in mitochondria.

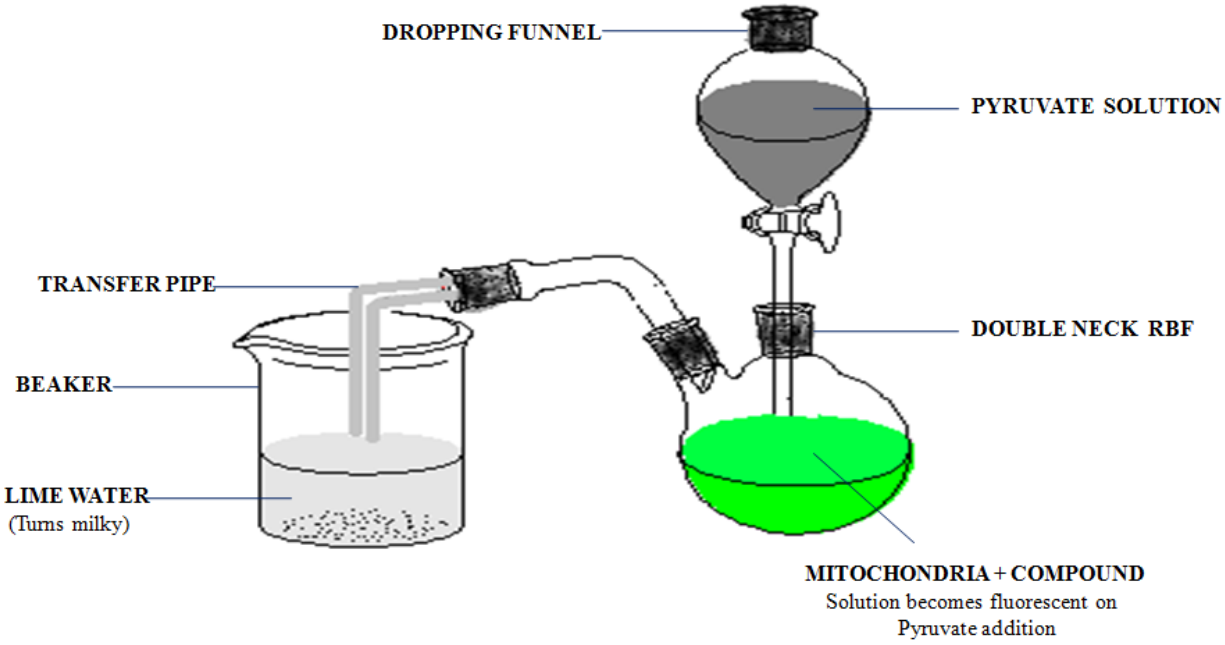


Figure S5. Apparatus set up for monitoring the breakdown of pyruvate in mitochondria.

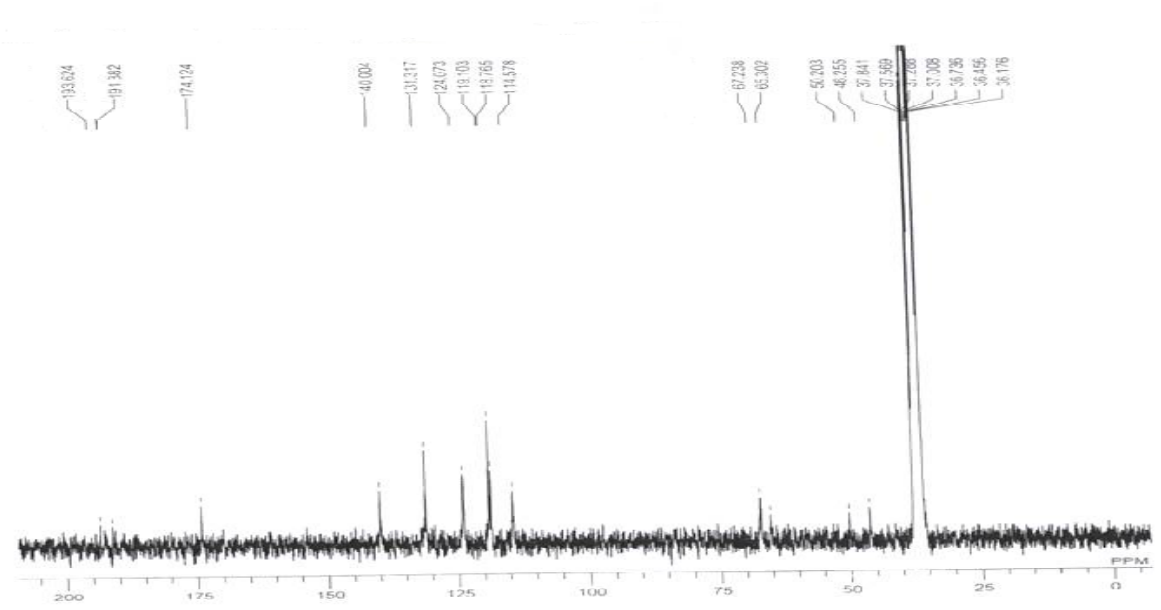


Figure S6. ^{13}C NMR spectrum of compound **3**.

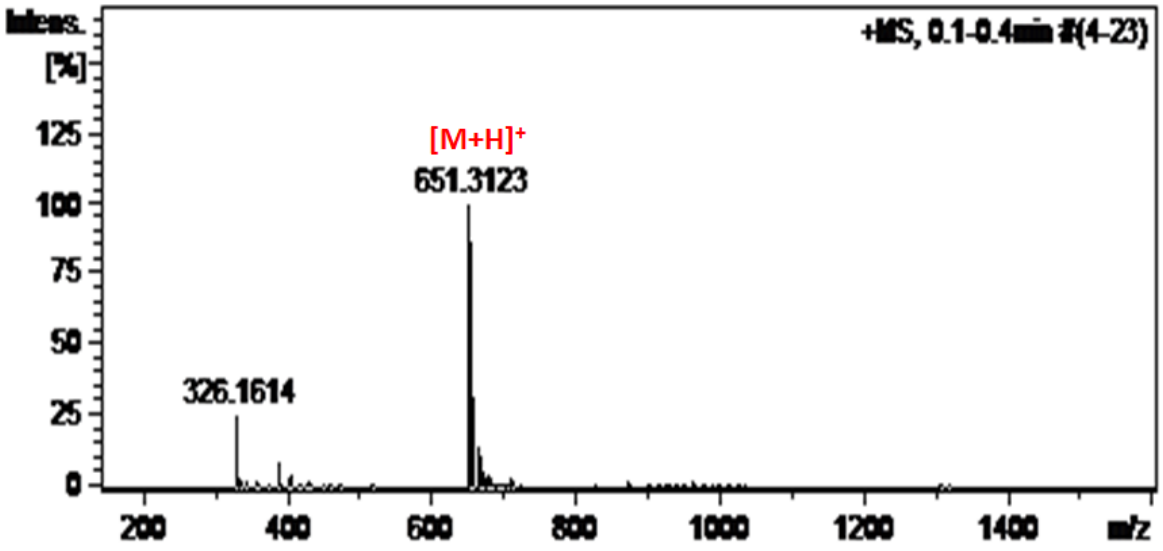


Figure S7. High Resolution Mass Spectrum of compound **3**.

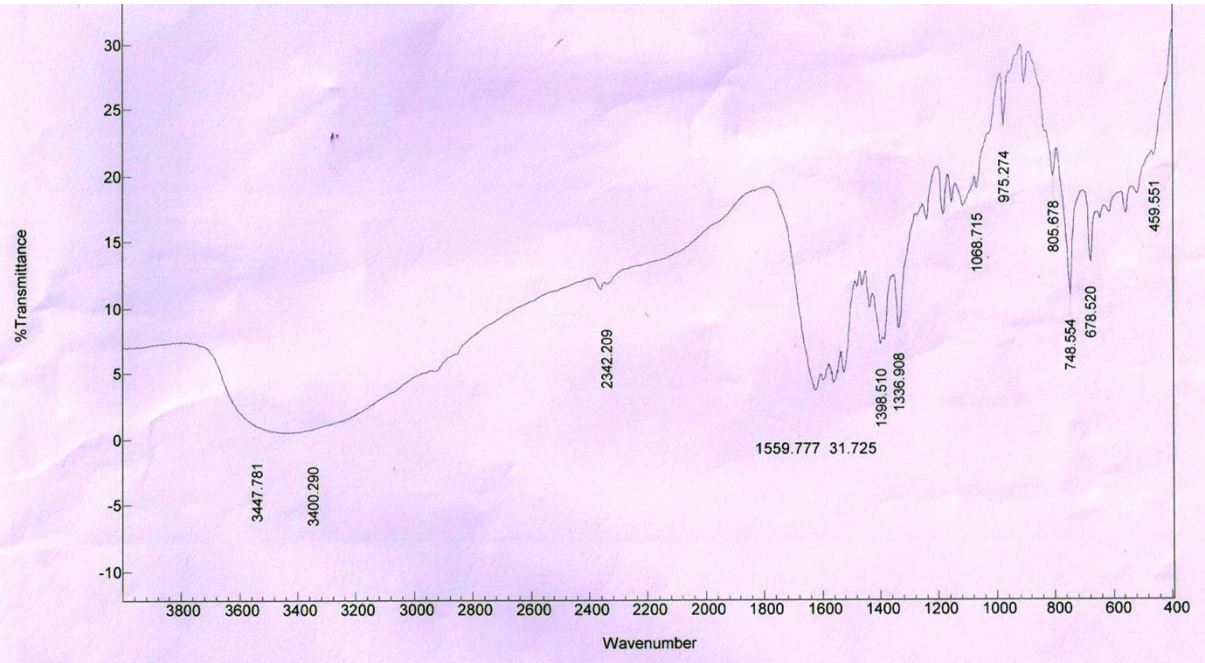


Figure S8. IR Spectrum of compound **3.**

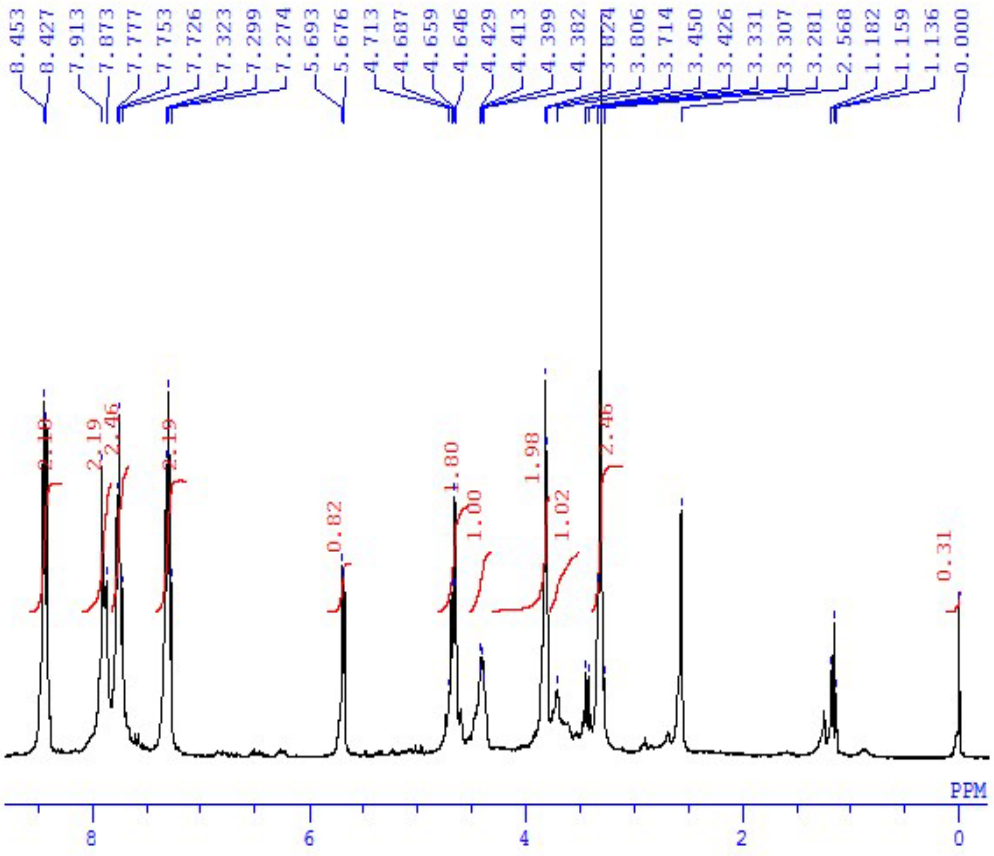


Figure S9. ^{1}H NMR spectrum of compound **2** ($CDCl_3$+DMSO-d_6). DMSO signal was suppressed.

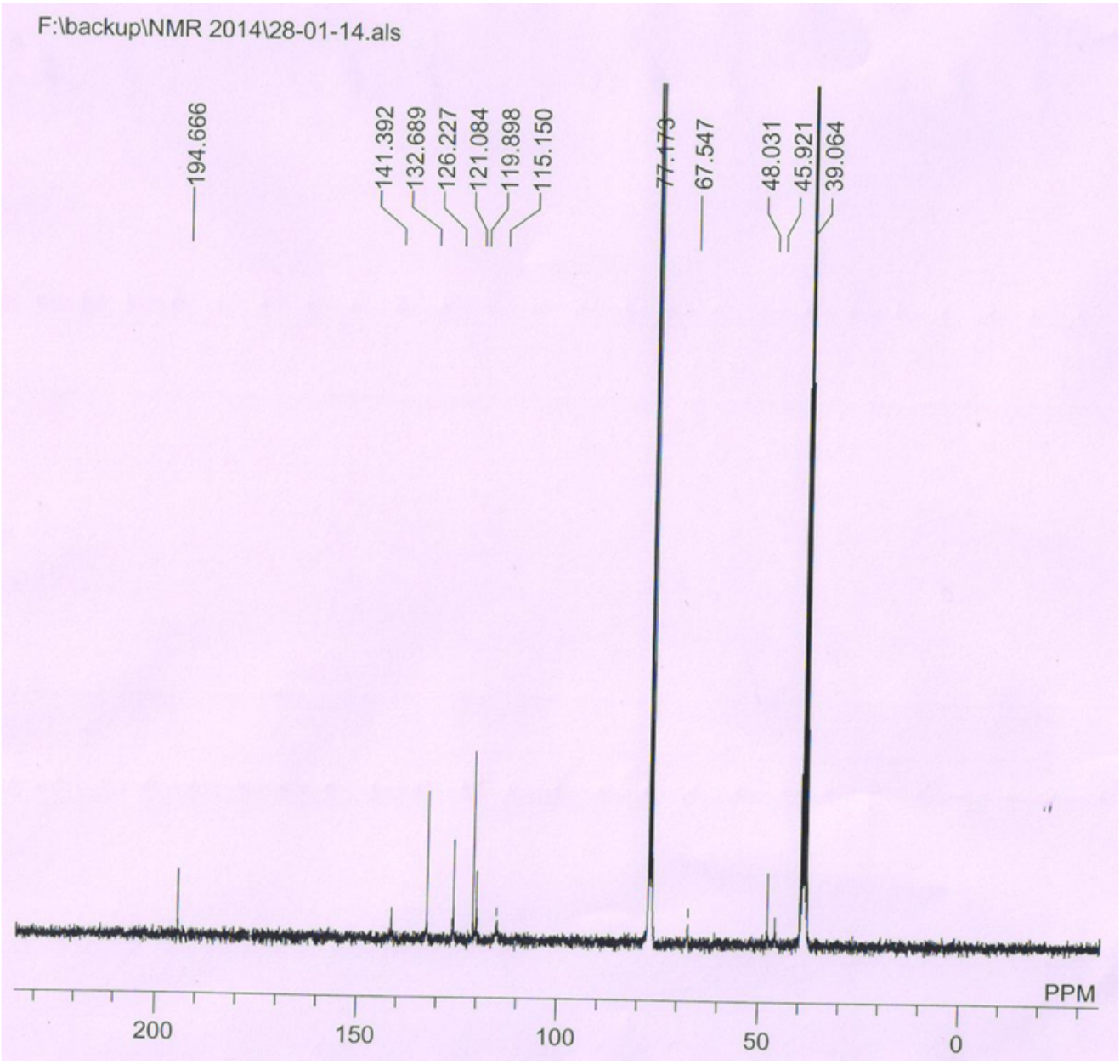


Figure S10. ^{13}C NMR spectrum of compound **2** ($CDCl_3$+DMSO-d_6).

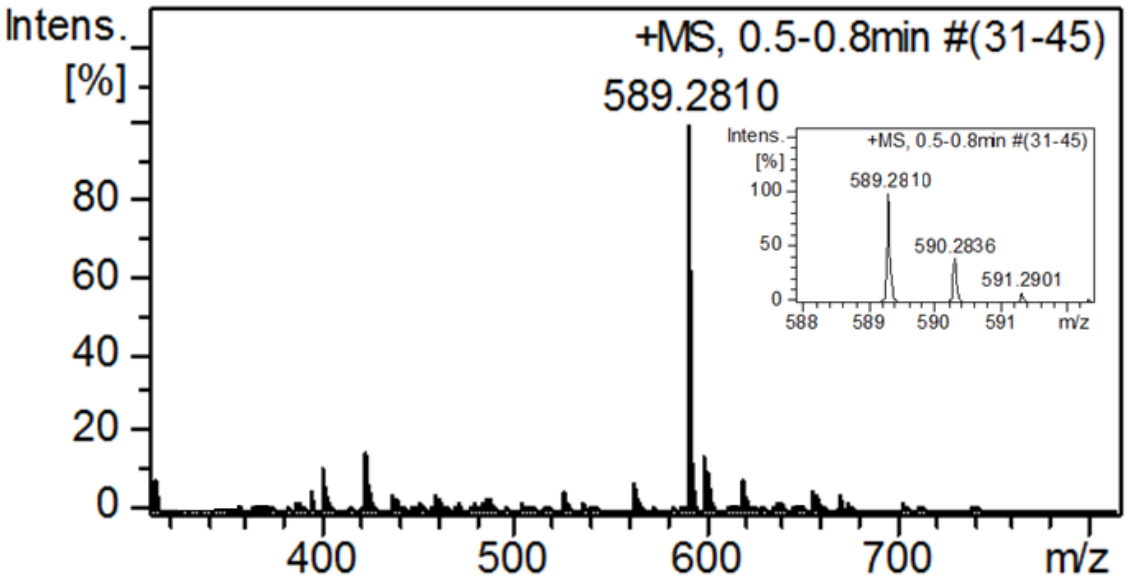


Figure S11. HRMS of compound **2**. Mass peak at *m/z* 589.2810 corresponds to mass of compound **2** (calcd *m/z* 589.2809, $[M+H]^+$).

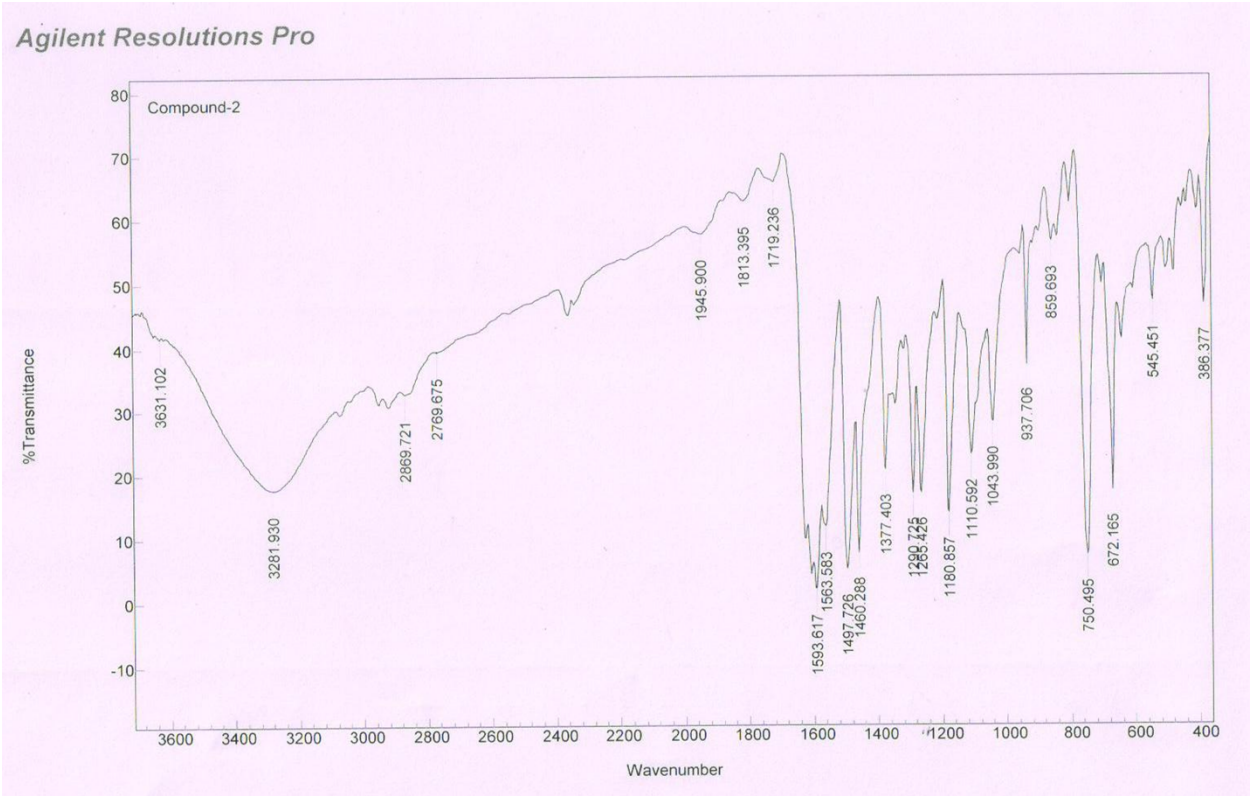


Figure S12. IR spectrum of compound **2**.