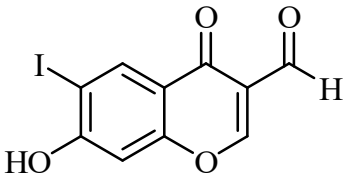
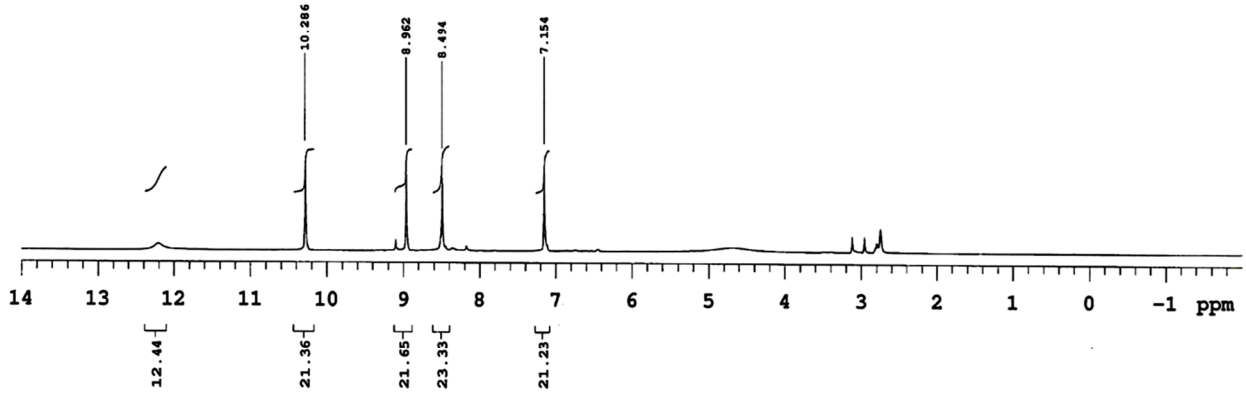
Supplementary Materials

Figure S1: Copies of ^{1}H-NMR and ^{13}C-NMR spectra for compounds 1, 2a–i and 3a–i.





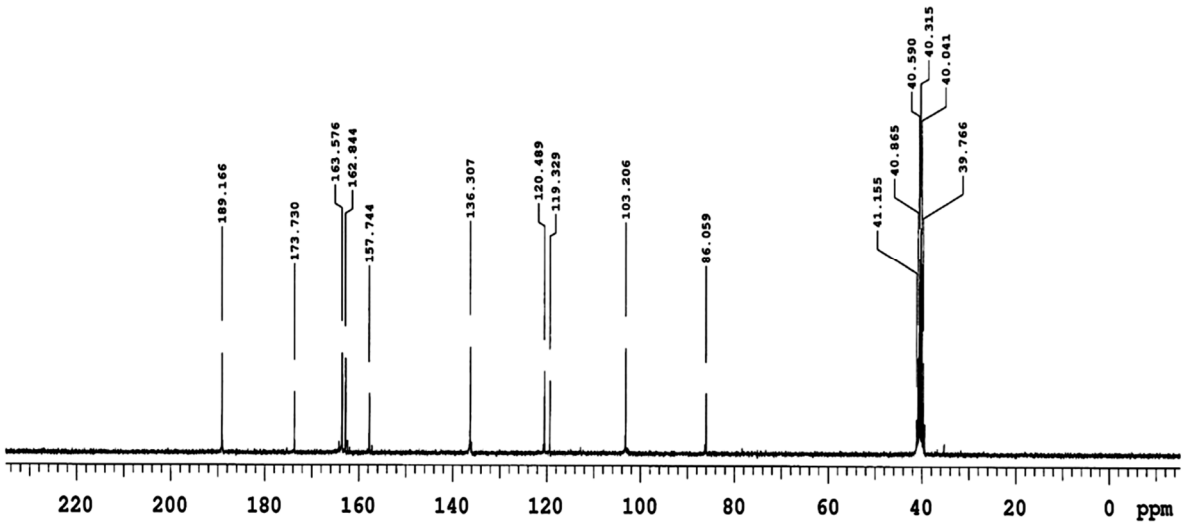


Figure S1.1: ^{1}H- and ^{13}C-NMR spectra of **1** in DMSO-d_6 at 300 and 75 MHz, respectively.

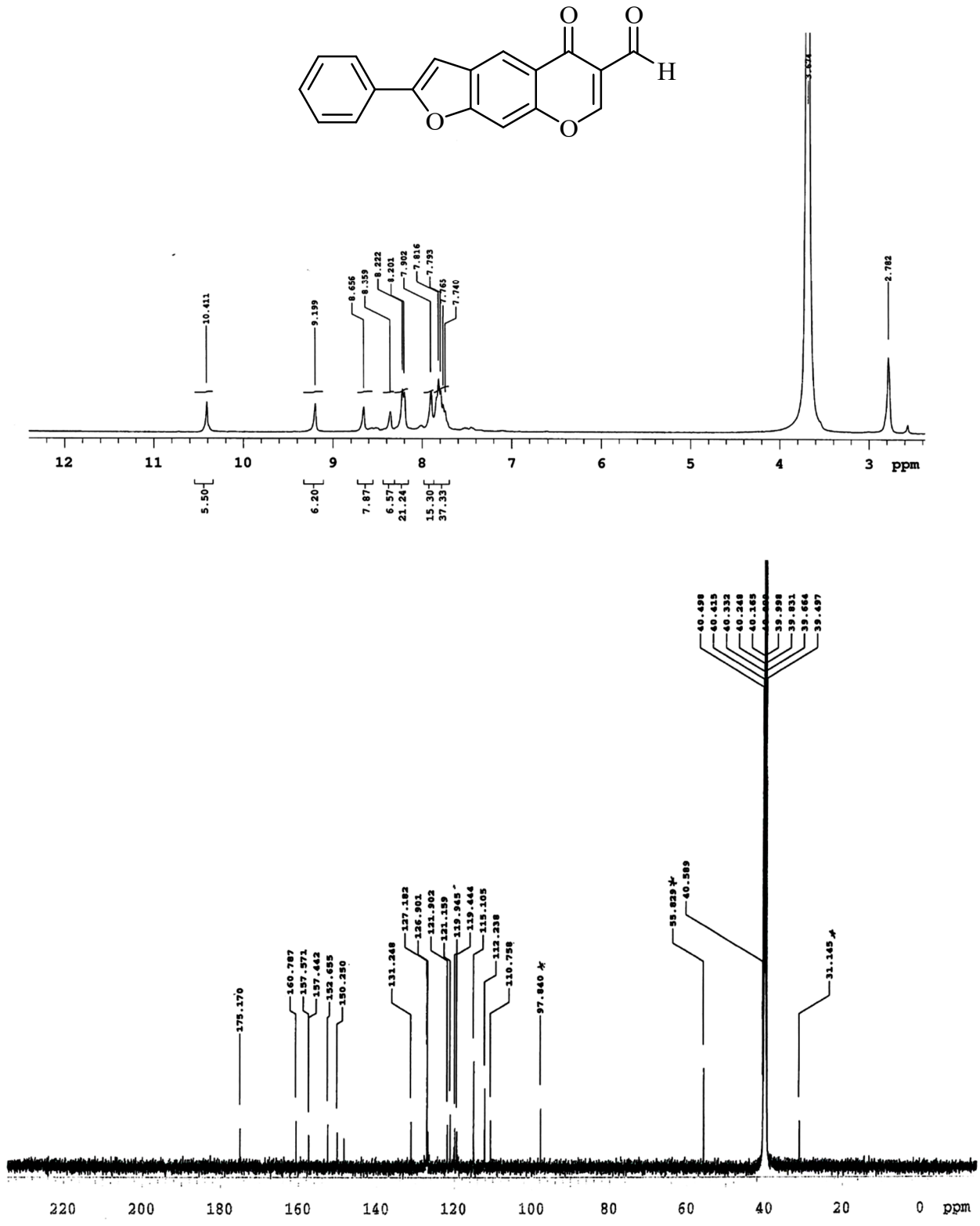


Figure S1.3: [1]H- and [13]C-NMR spectra of **2a** in DMSO-d_6 at 300 and 75 MHz, respectively.

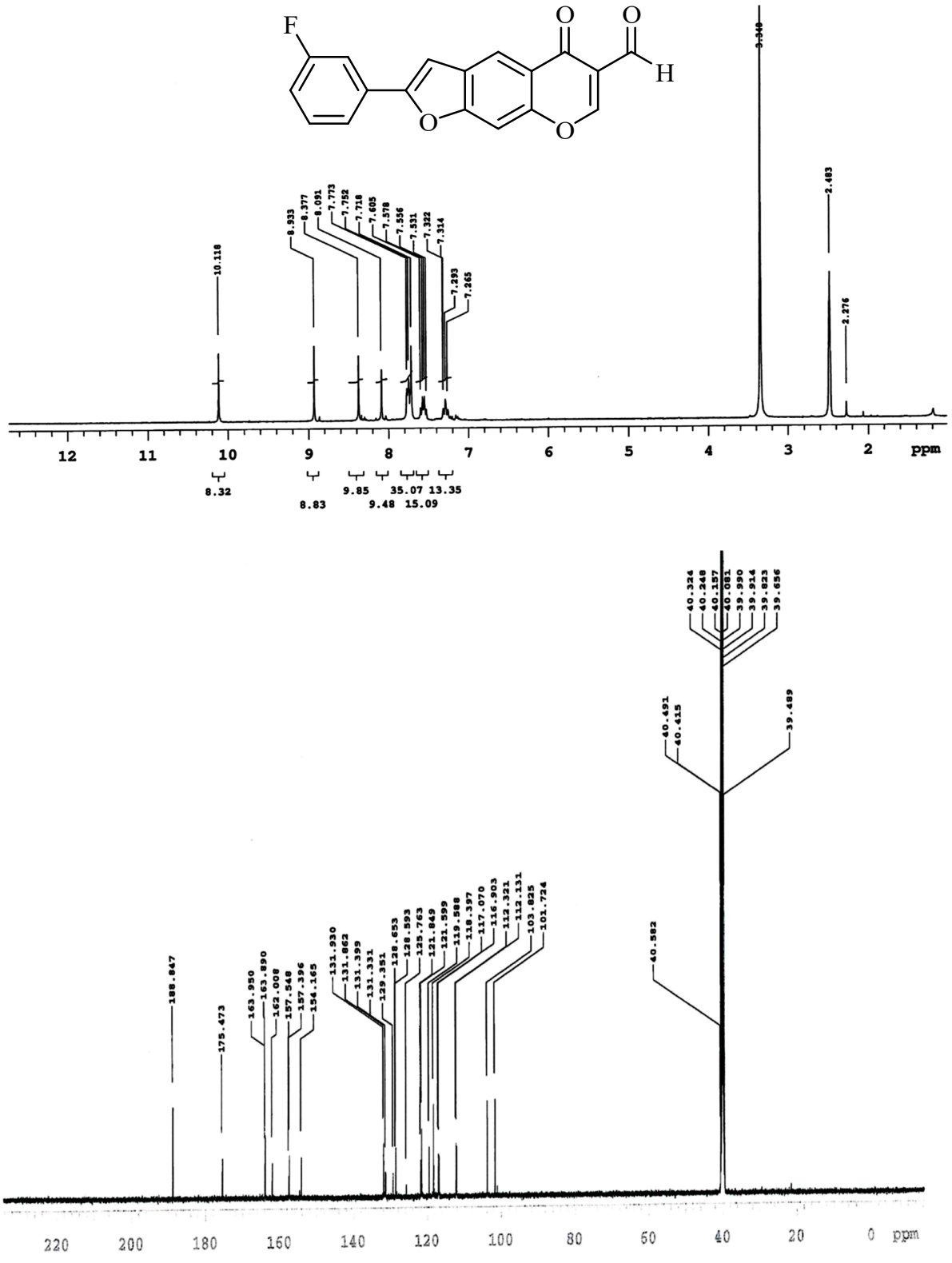


Figure S1.4: [1]H- and [13]C-NMR spectra of **2b** in DMSO-d_6 at 300 and 75 MHz, respectively.

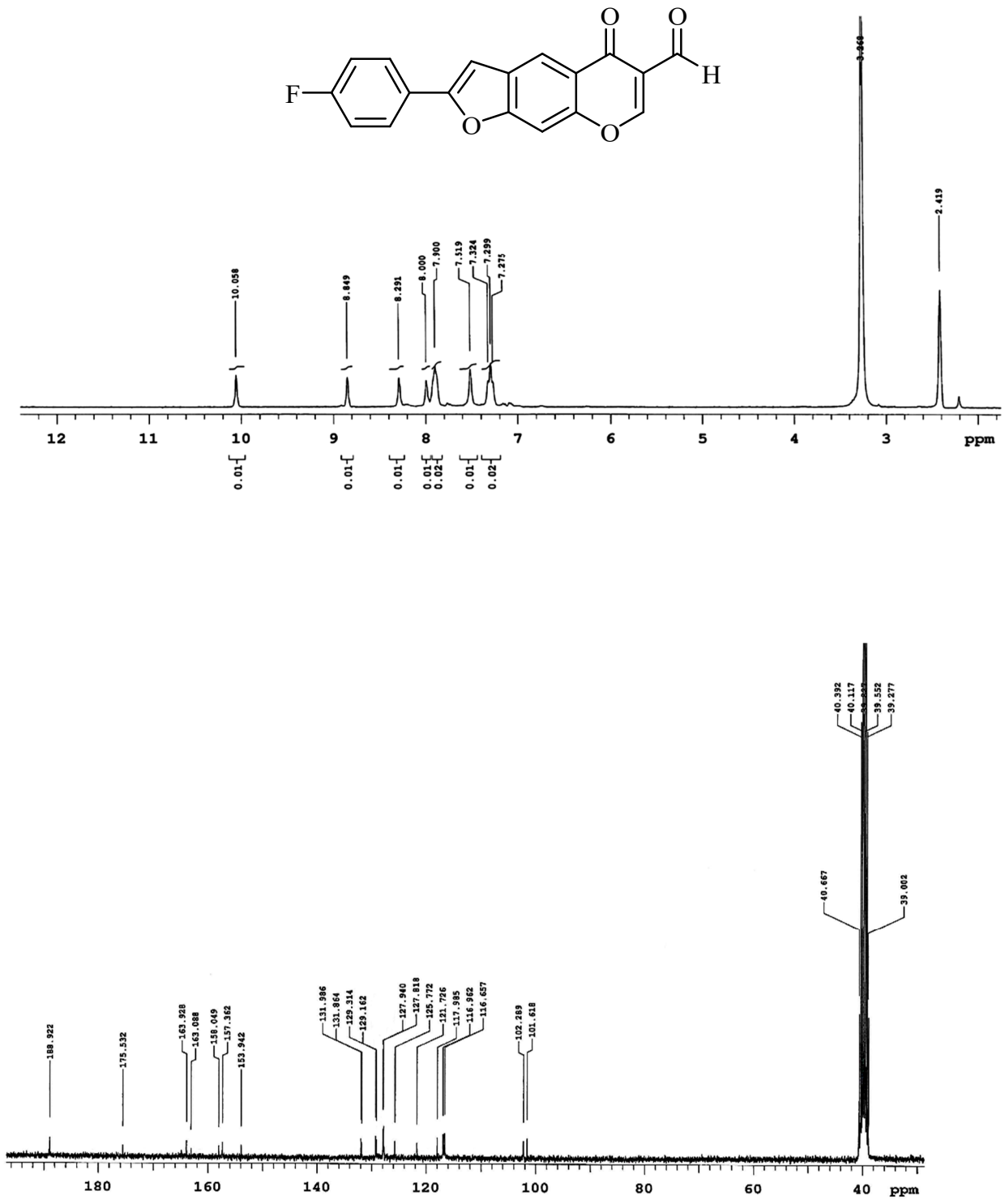


Figure S1.5: [1]H- and [13]C-NMR spectra of **2c** in DMSO-d_6 at 300 and 75 MHz, respectively.

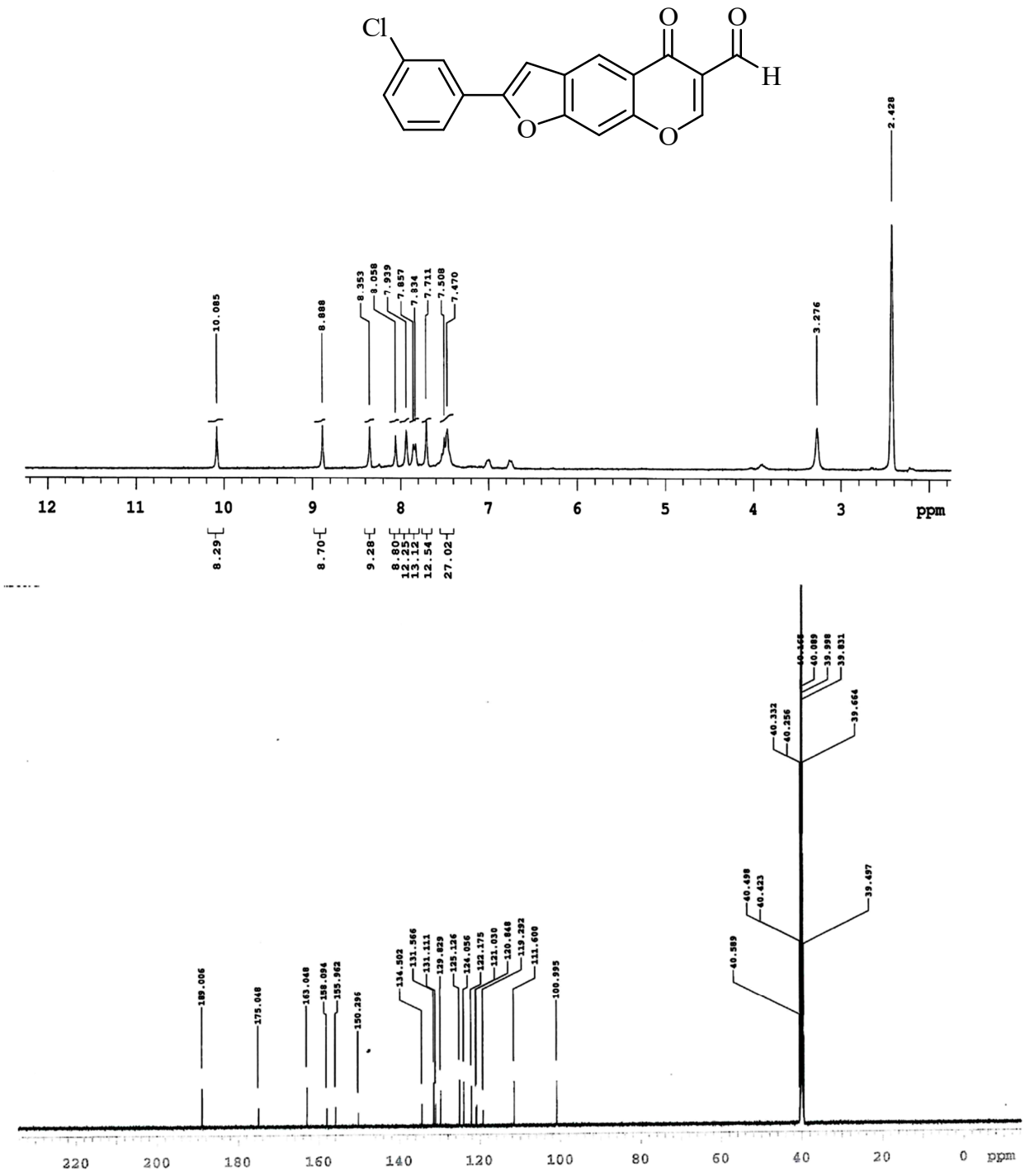


Figure S1.6: [1]H- and [13]C-NMR spectra of **2d** in DMSO-d_6 at 300 and 75 MHz, respectively.

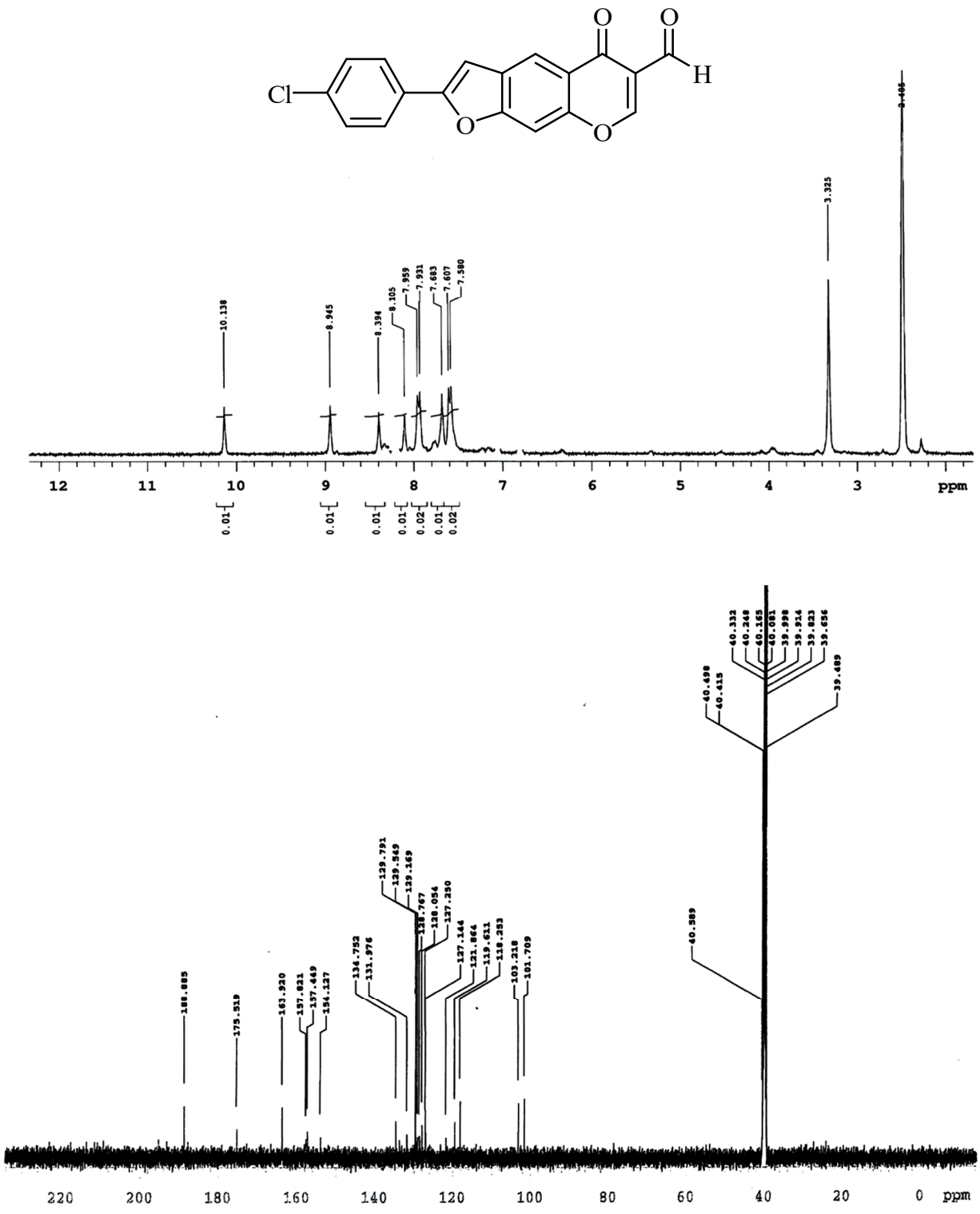


Figure S1.7: [1]H- and [13]C-NMR spectra of **2e** in DMSO-d_6 at 300 and 75 MHz, respectively.

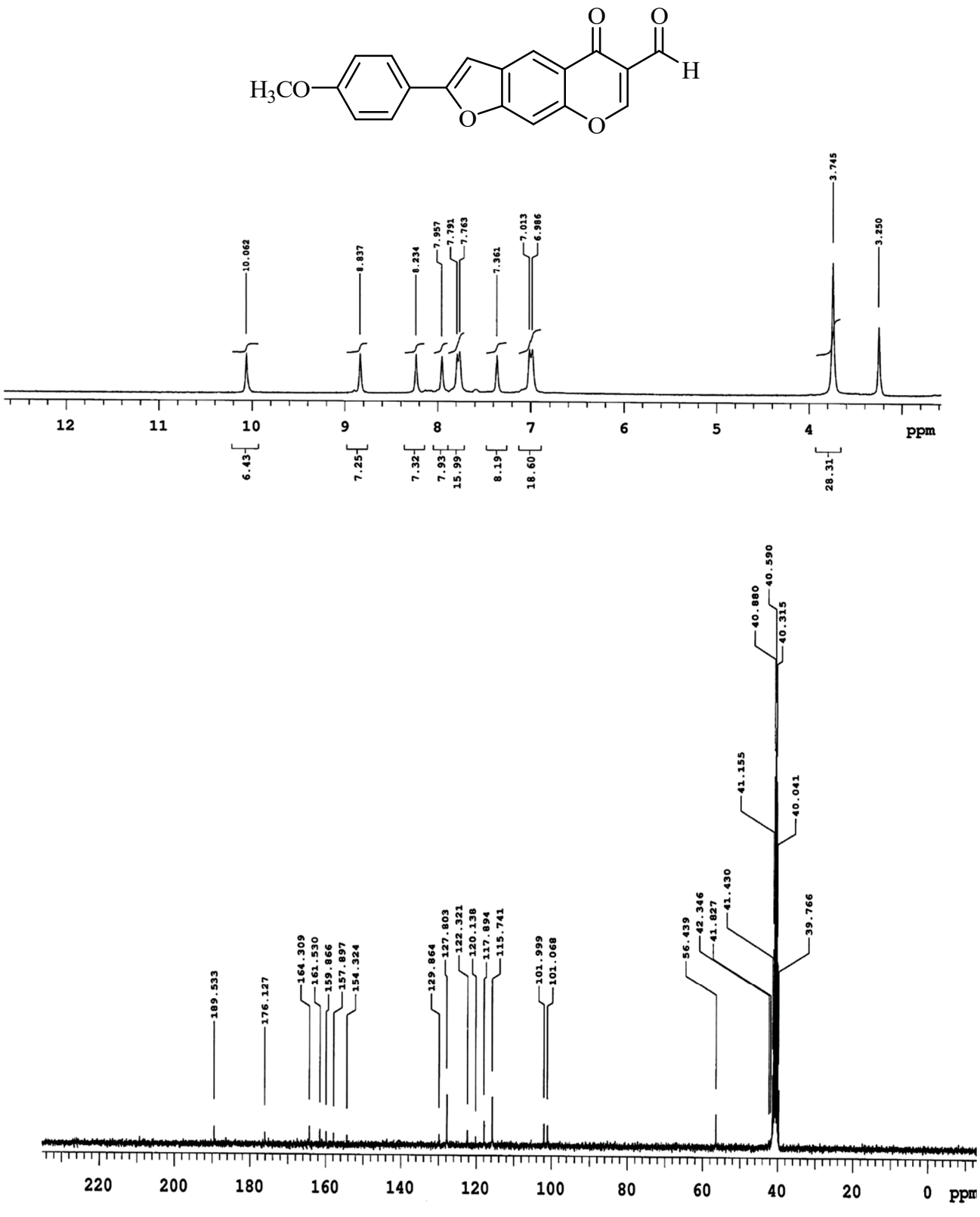


Figure S1.8: [1]H- and [13]C-NMR spectra of **2f** in DMSO-d_6 at 300 and 75 MHz, respectively.

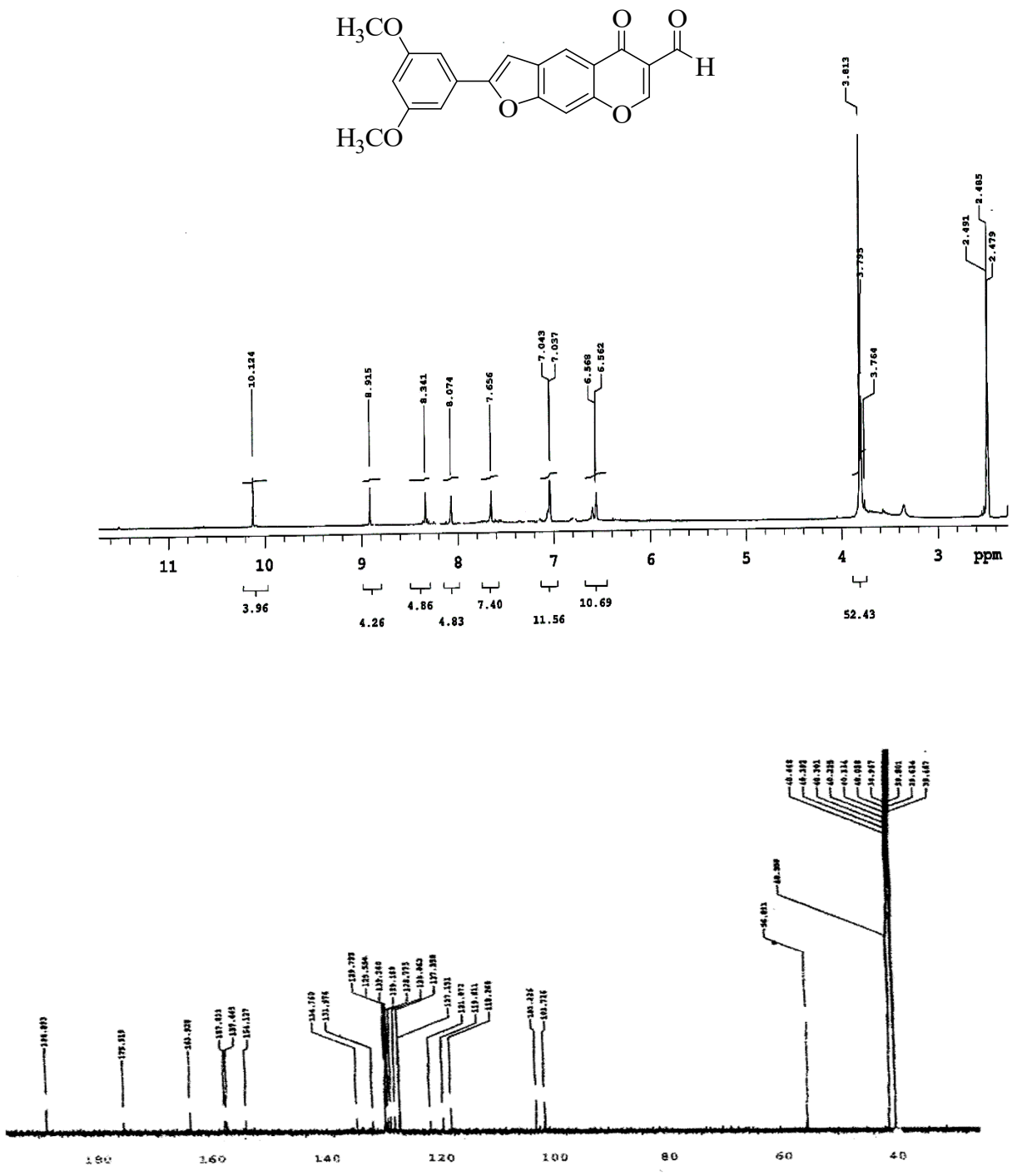


Figure S1.9: [1]H- and [13]C-NMR spectra of **2g** in DMSO-d_6 at 300 and 75 MHz, respectively

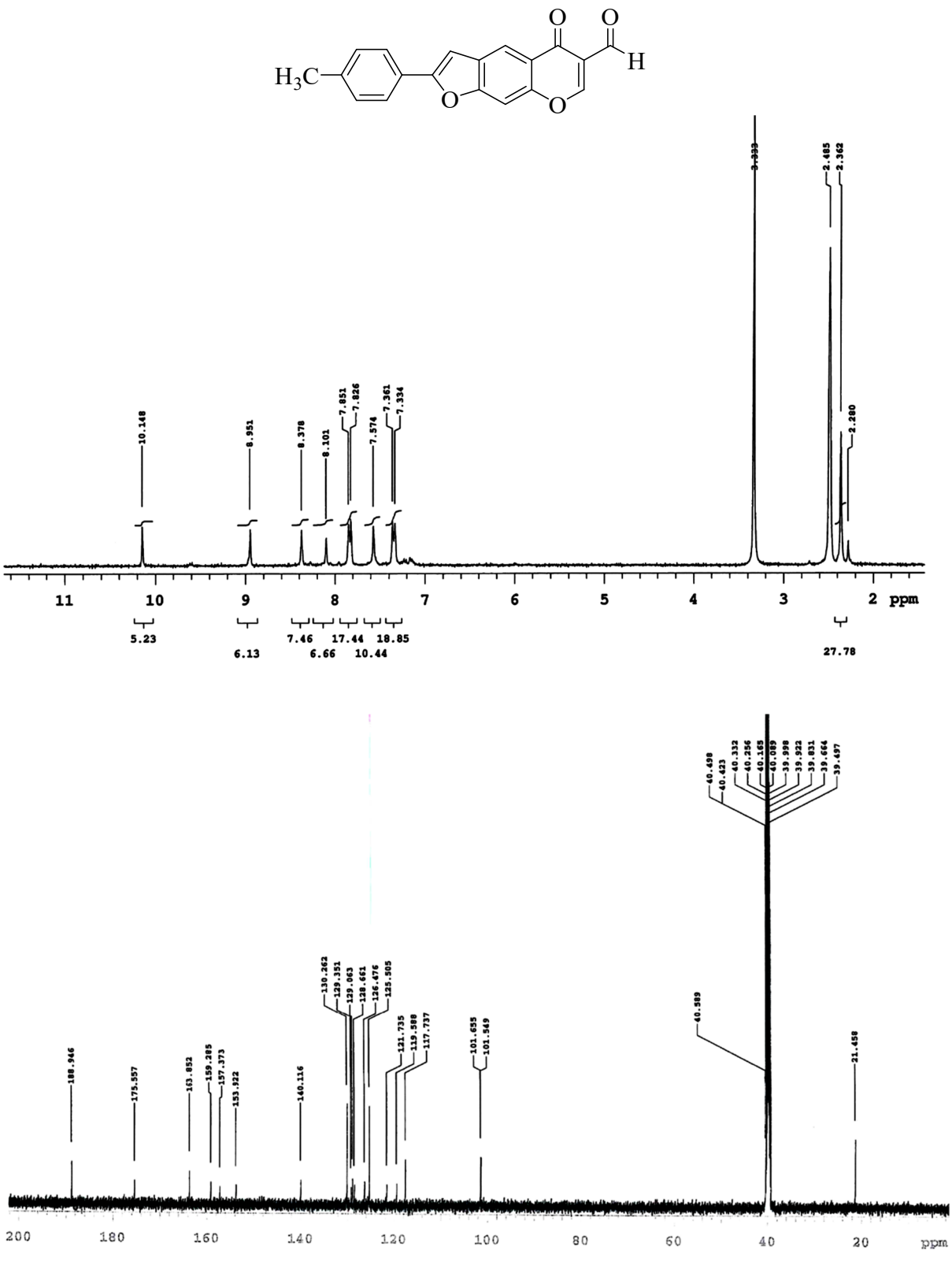


Figure S1.10: [1]H- and [13]C-NMR spectra of **2h** in DMSO-d_6 at 300 and 75 MHz, respectively.

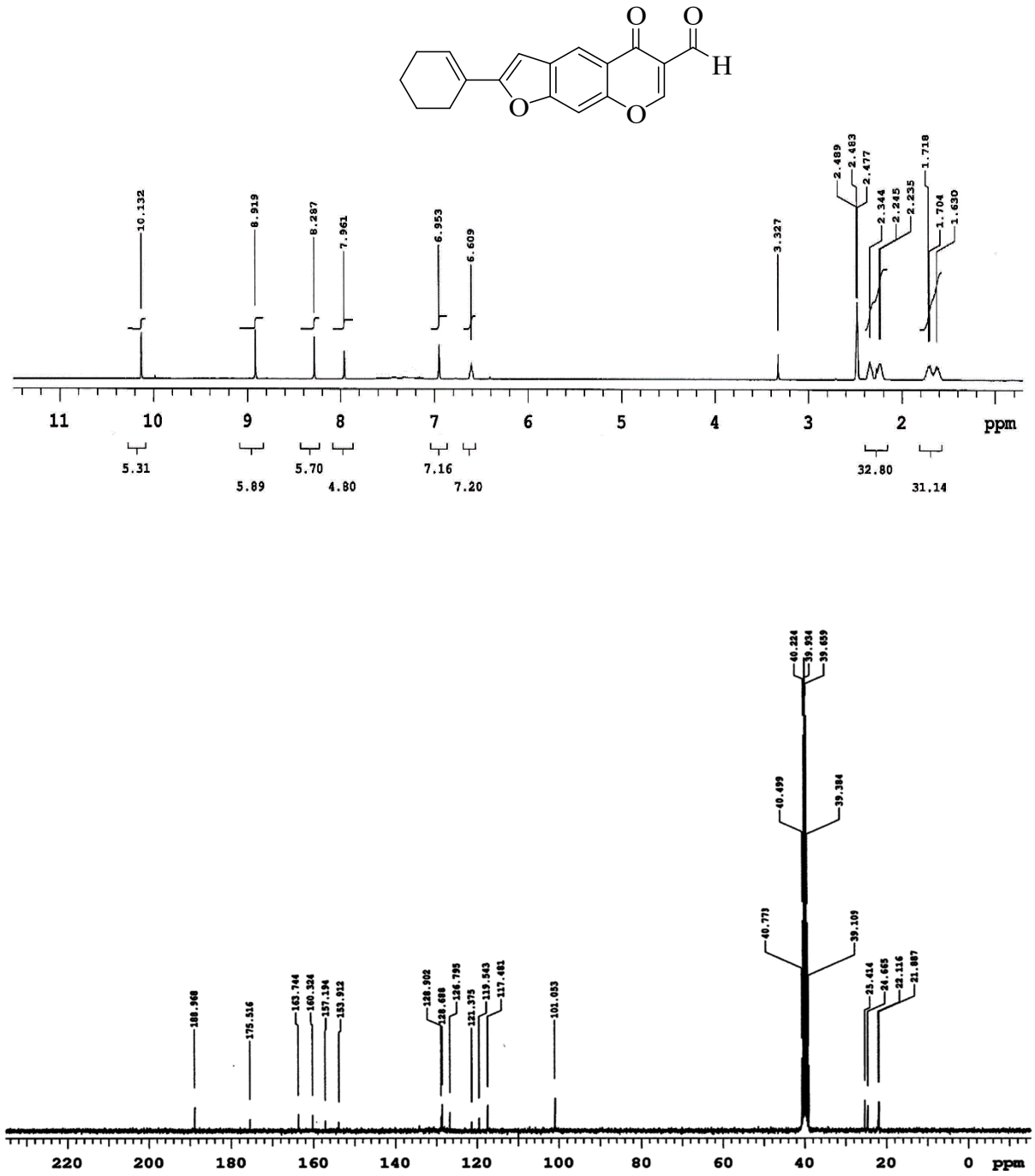


Figure S1.11: [1]H- and [13]C-NMR spectra of **2i** in DMSO-d_6 at 300 and 75 MHz, respectively.

Figure S1.12: ^{1}H- and ^{13}C-NMR spectra of **3a** in DMSO-d_6 at 300 and 75 MHz, respectively.

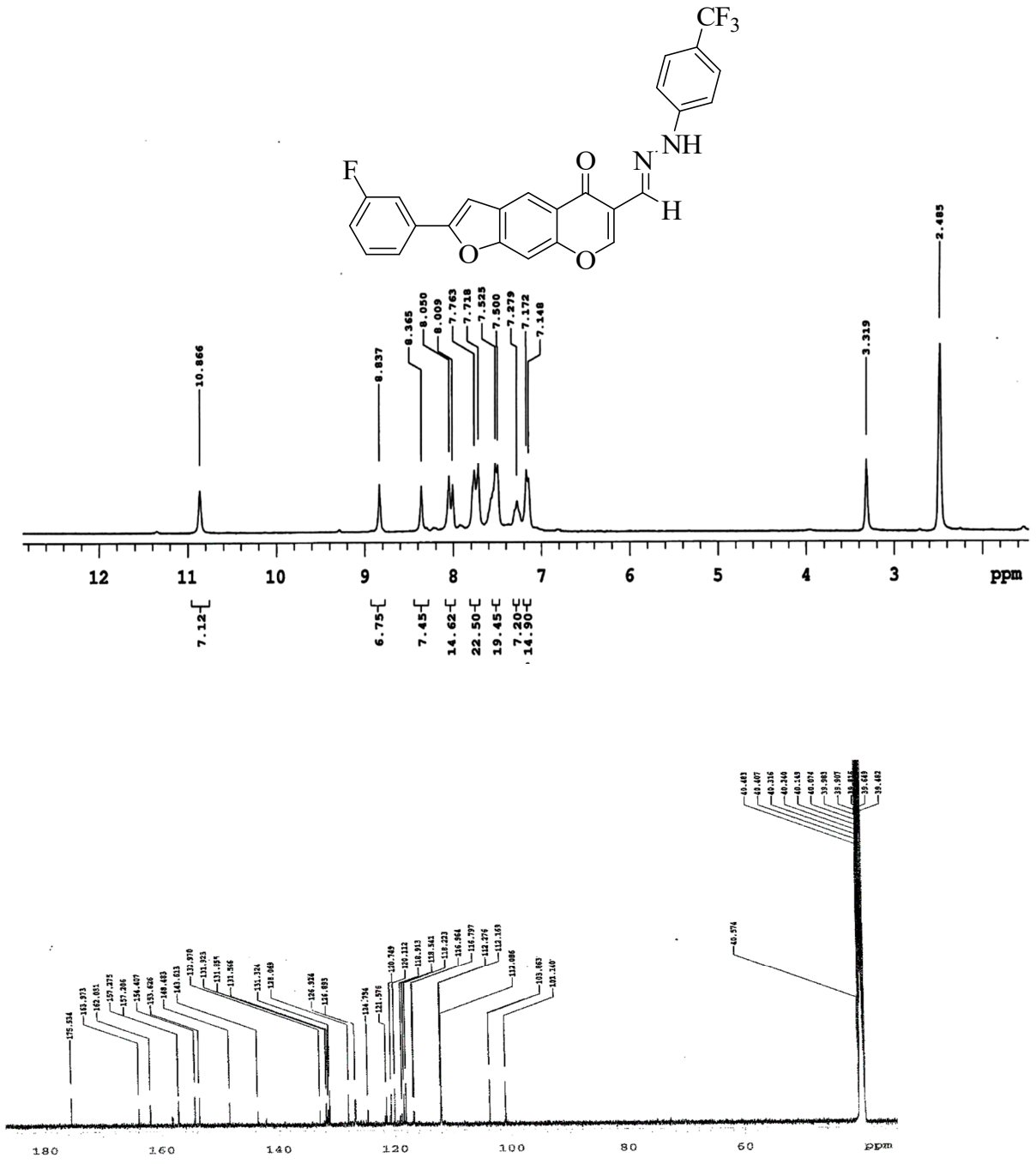


Figure S1.13: [1]H- and [13]C-NMR spectra of **3b** in DMSO-d_6 at 300 and 75 MHz, respectively.

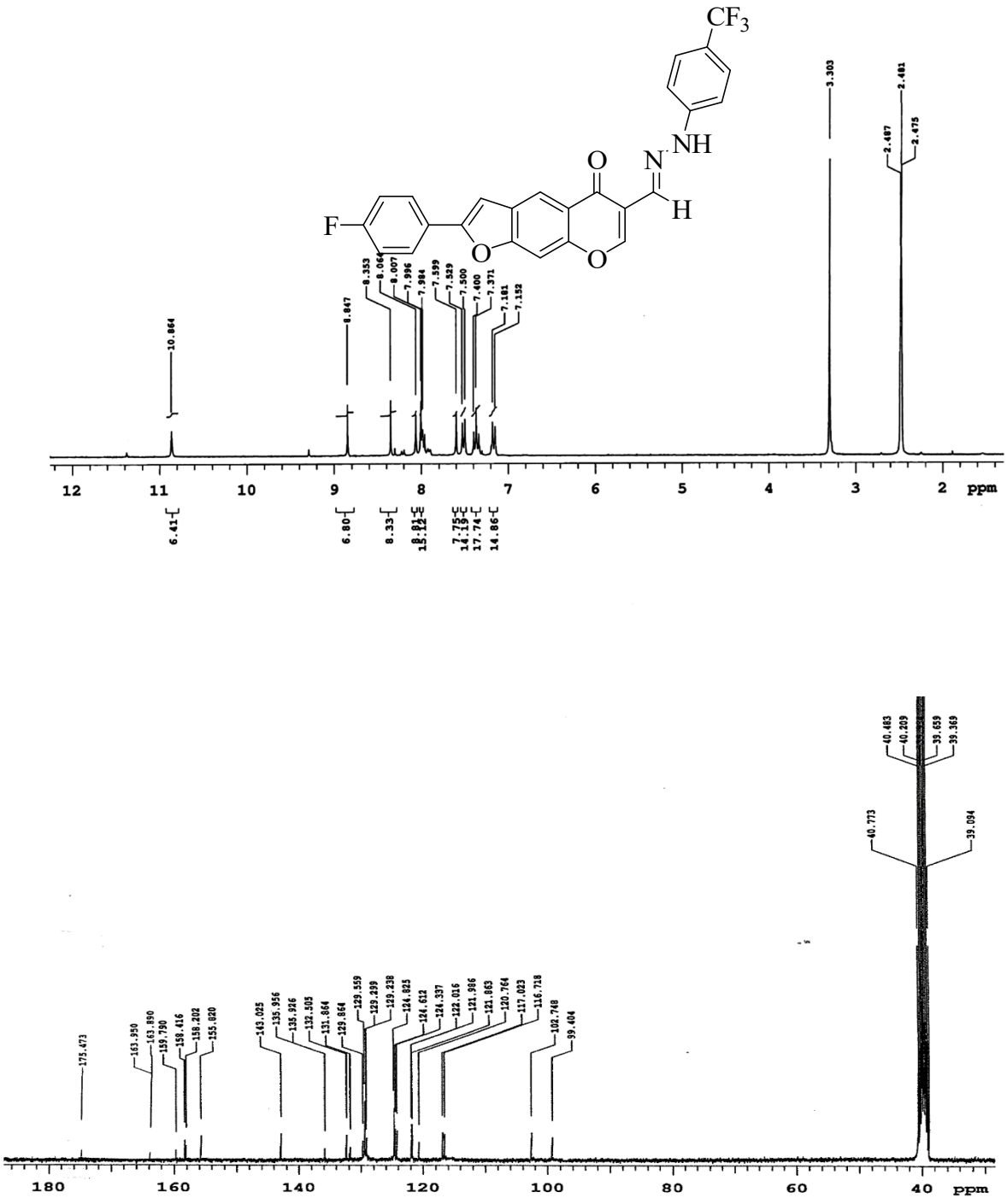


Figure S1.14: [1]H- and [13]C-NMR spectra of **3c** in DMSO-d_6 at 300 and 75 MHz, respectively.

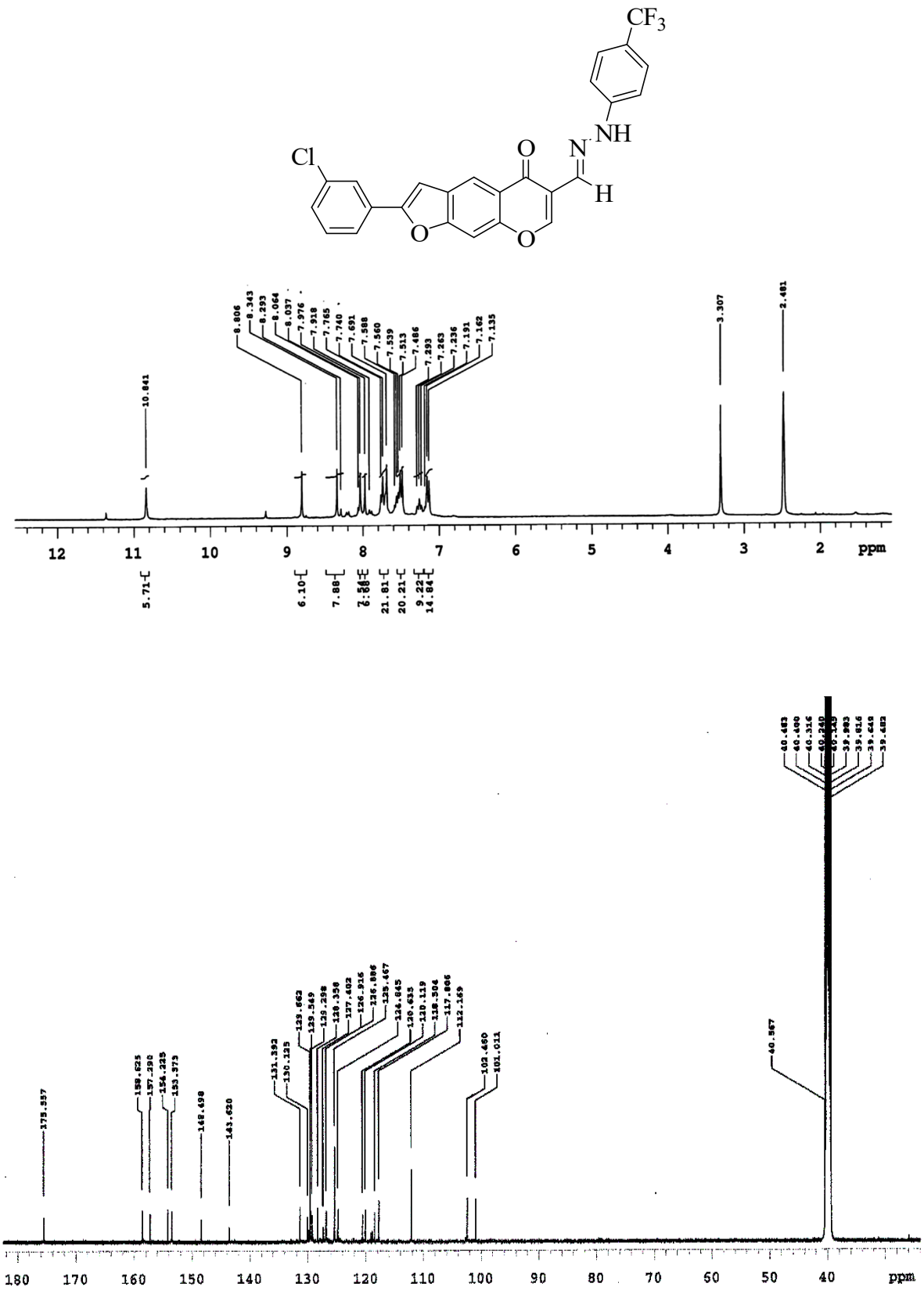


Figure S1.15: [1]H- and [13]C-NMR spectra of **3d** in DMSO-d_6 at 300 and 75 MHz, respectively.

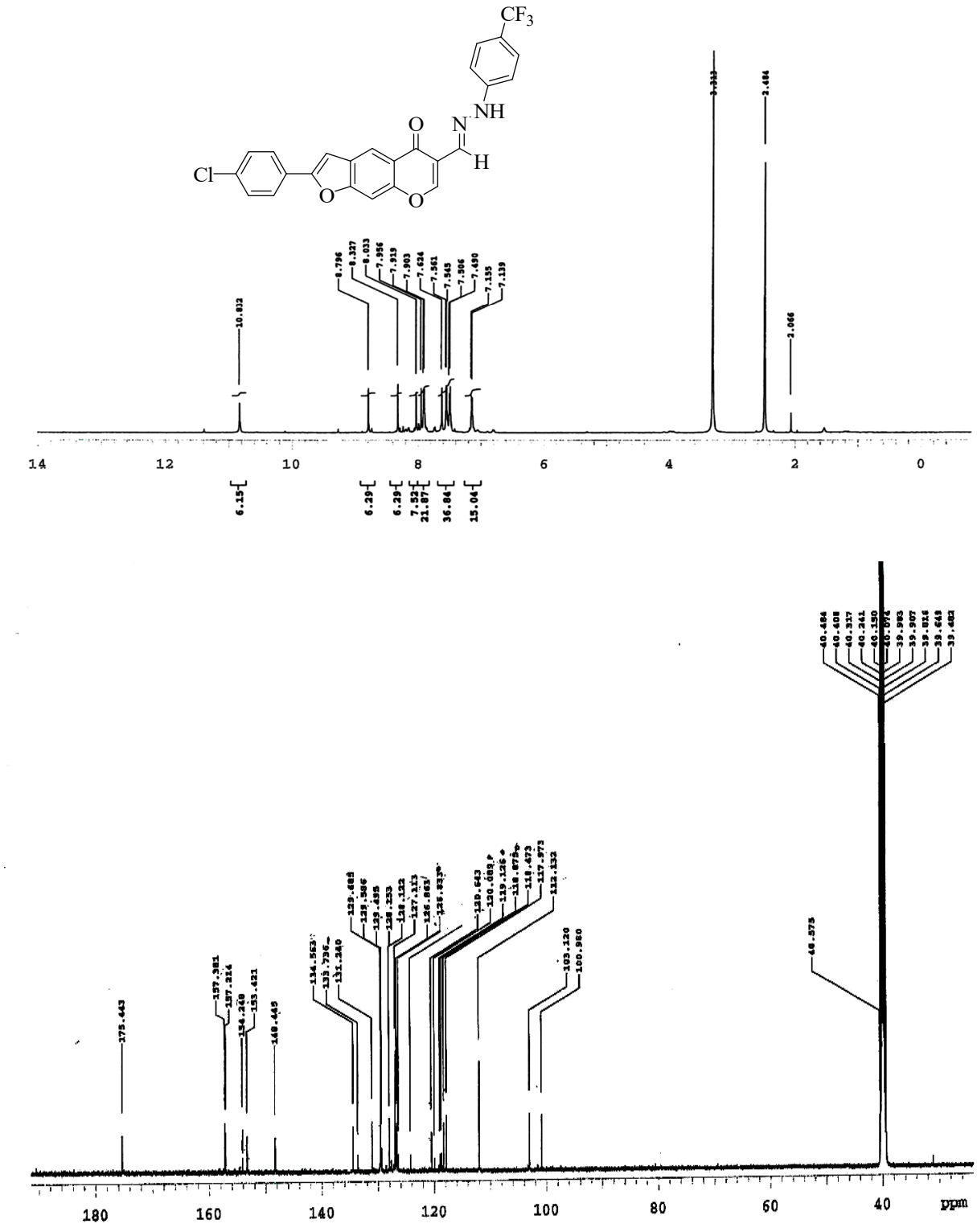


Figure S1.16: [1]H- and [13]C-NMR spectra of **3e** in DMSO-d_6 at 300 and 75 MHz, respectively.

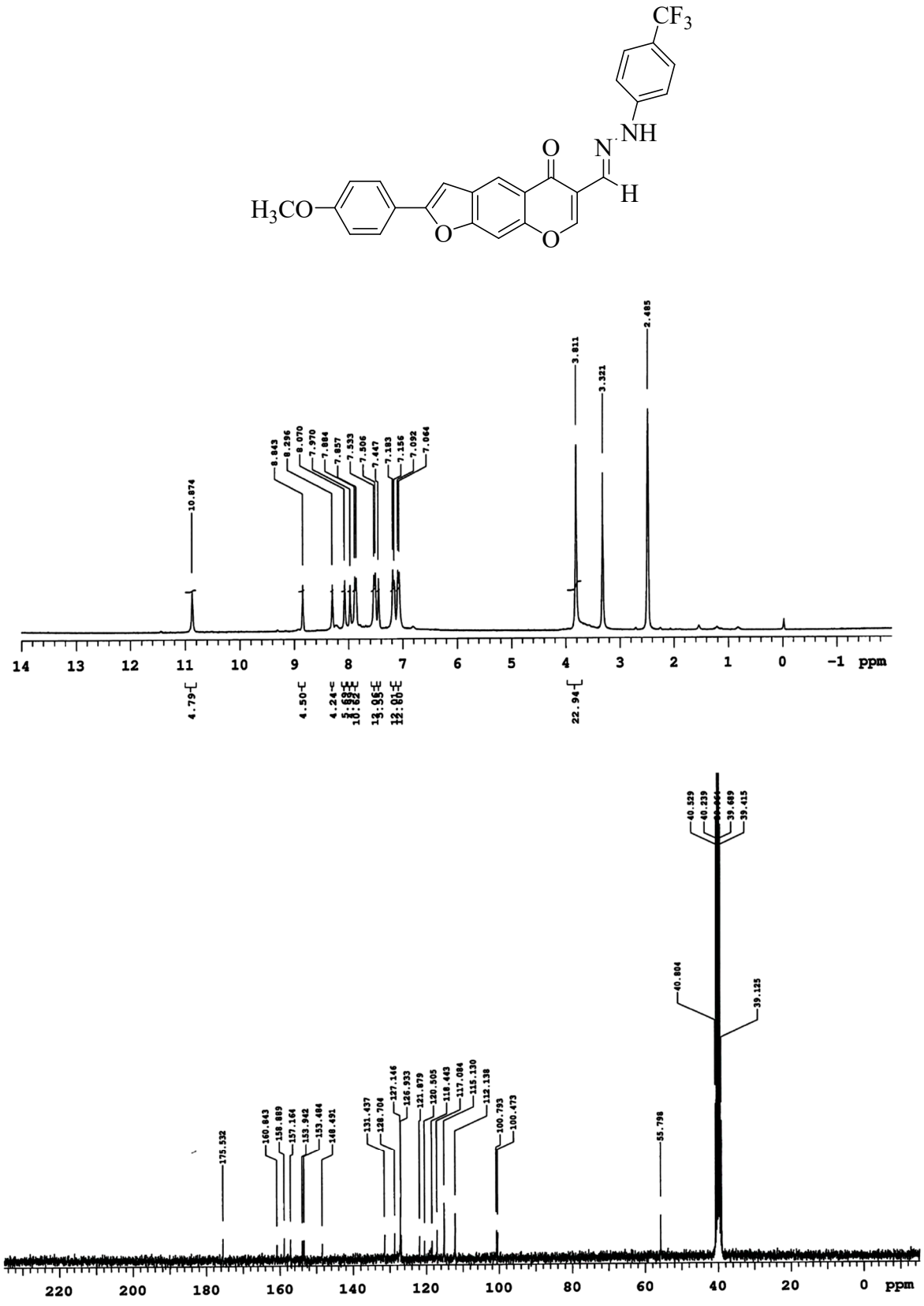


Figure S1.17: [1]H- and [13]C-NMR spectra of **3f** in DMSO-d_6 at 300 and 75 MHz, respectively.

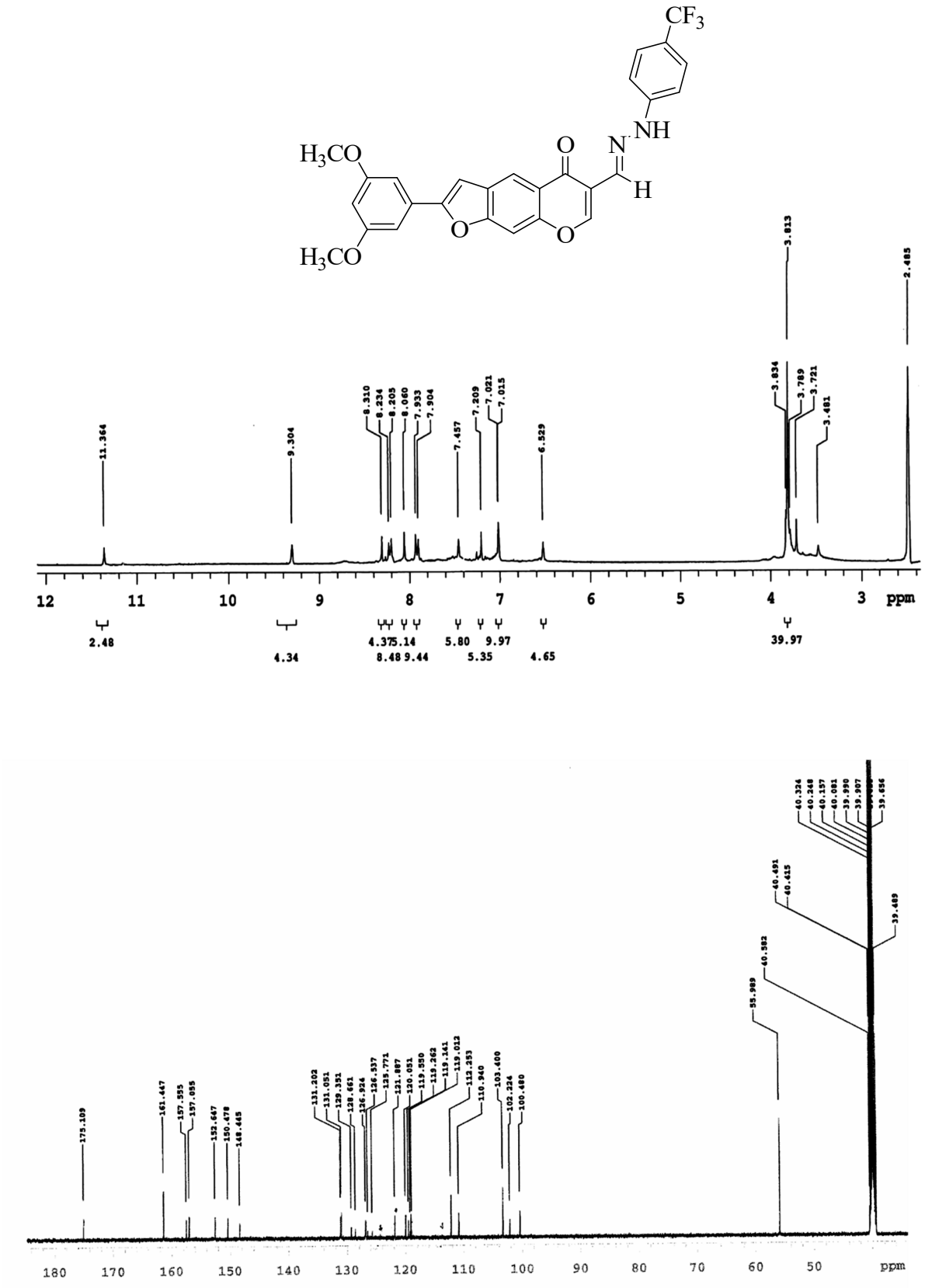


Figure S1.18: [1]H- and [13]C-NMR spectra of **3g** in DMSO-d_6 at 300 and 75 MHz, respectively.

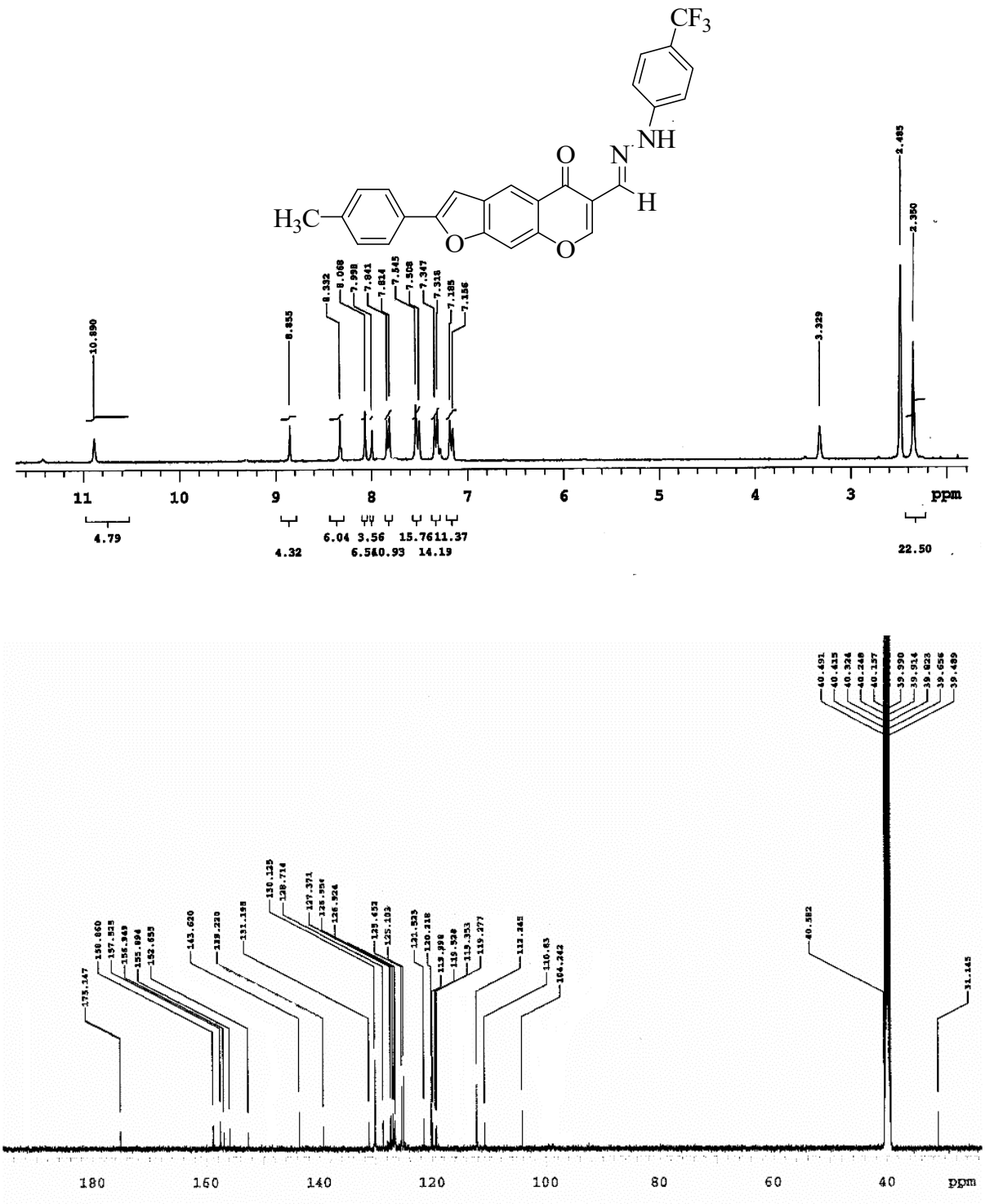


Figure S1.19: [1]H- and [13]C-NMR spectra of **3h** in DMSO-d_6 at 300 and 75 MHz, respectively.

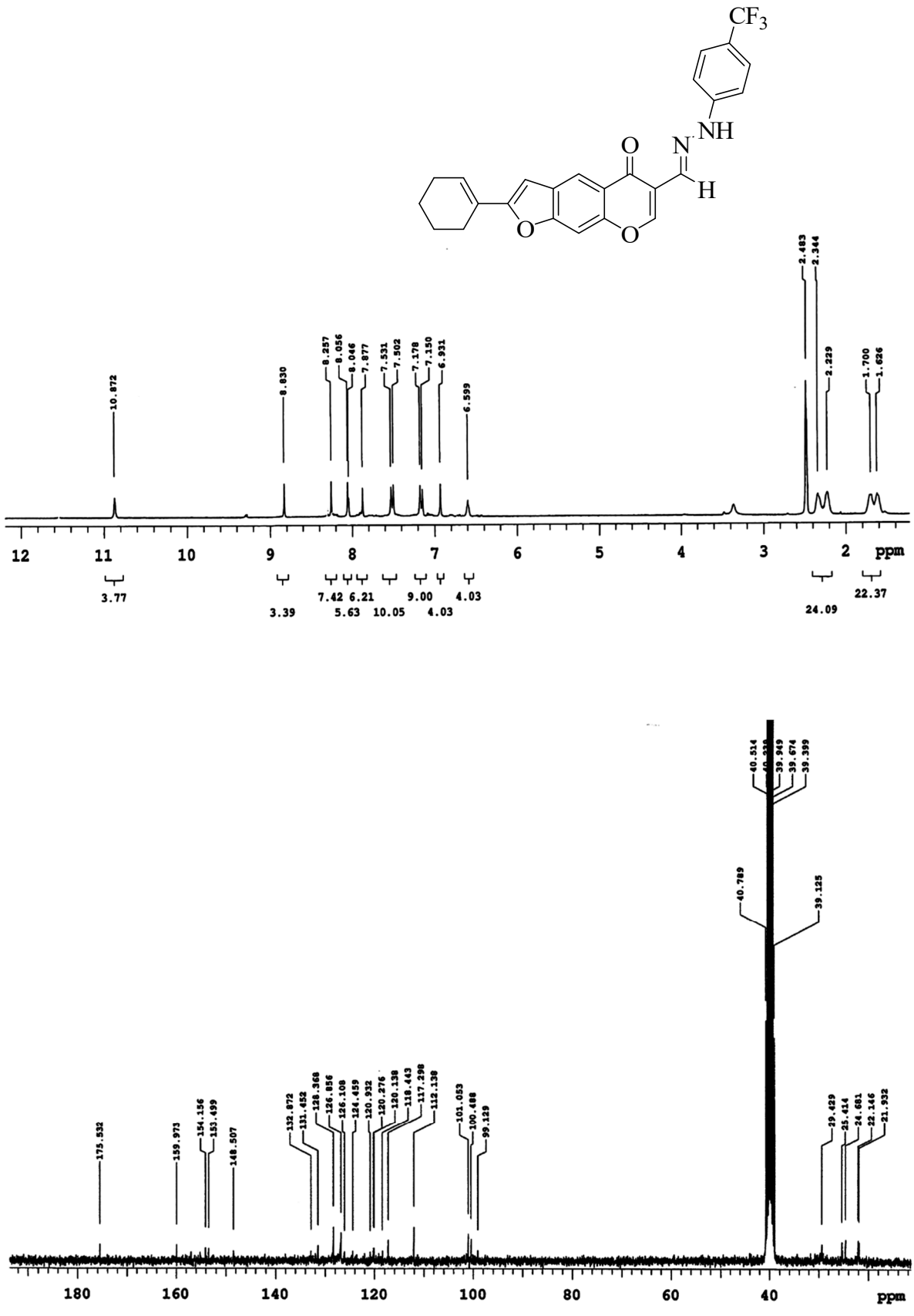
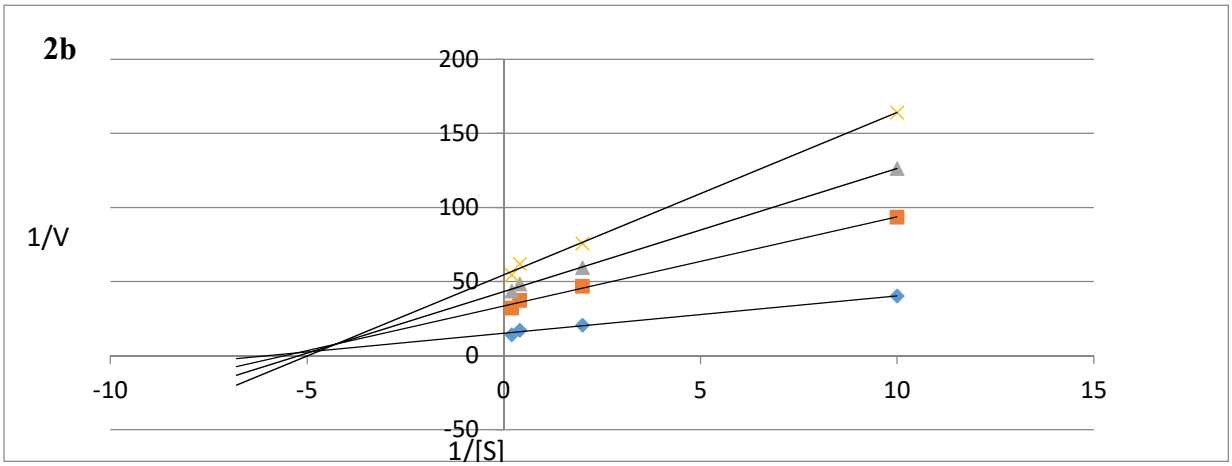
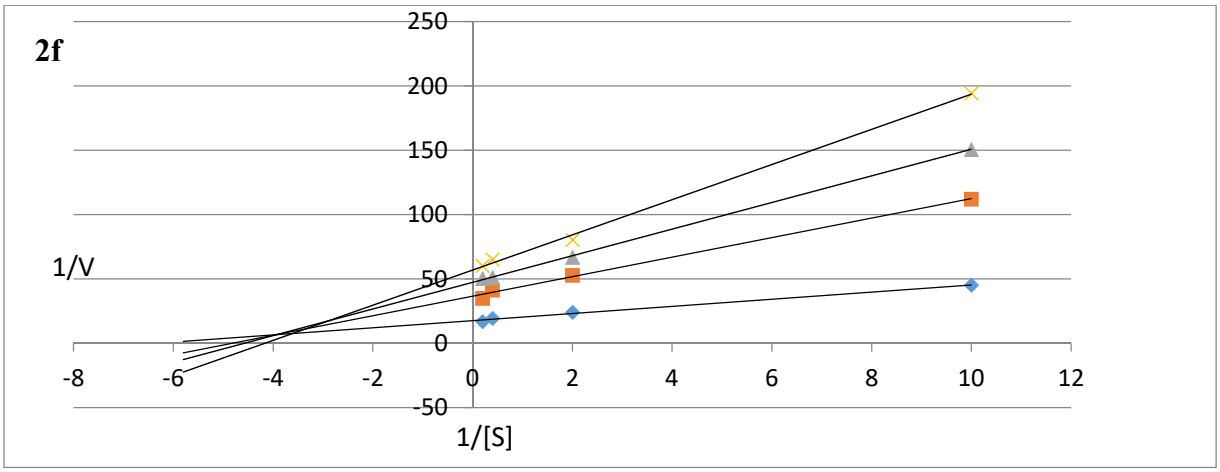
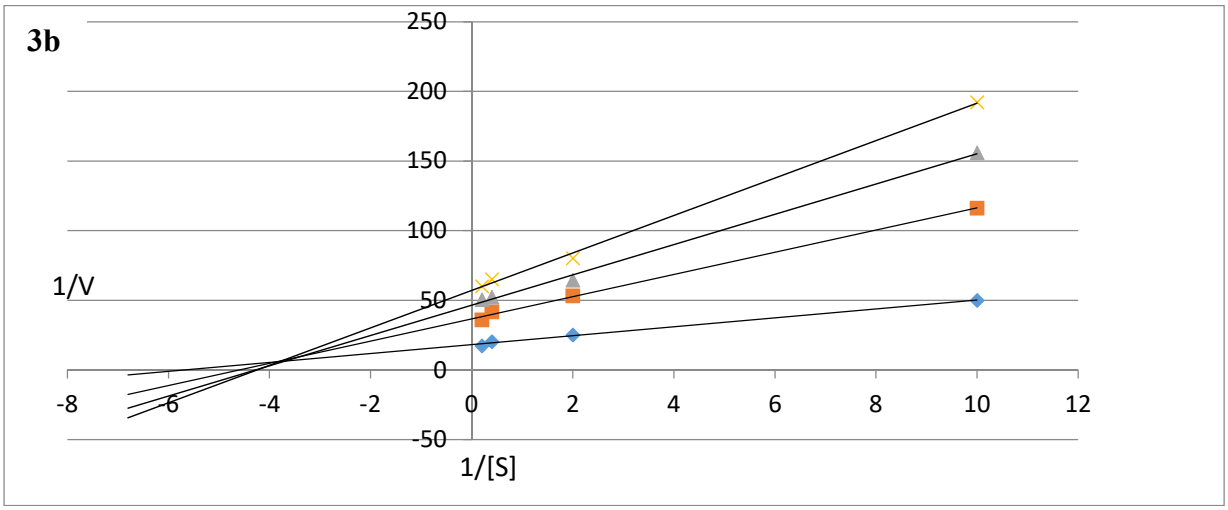


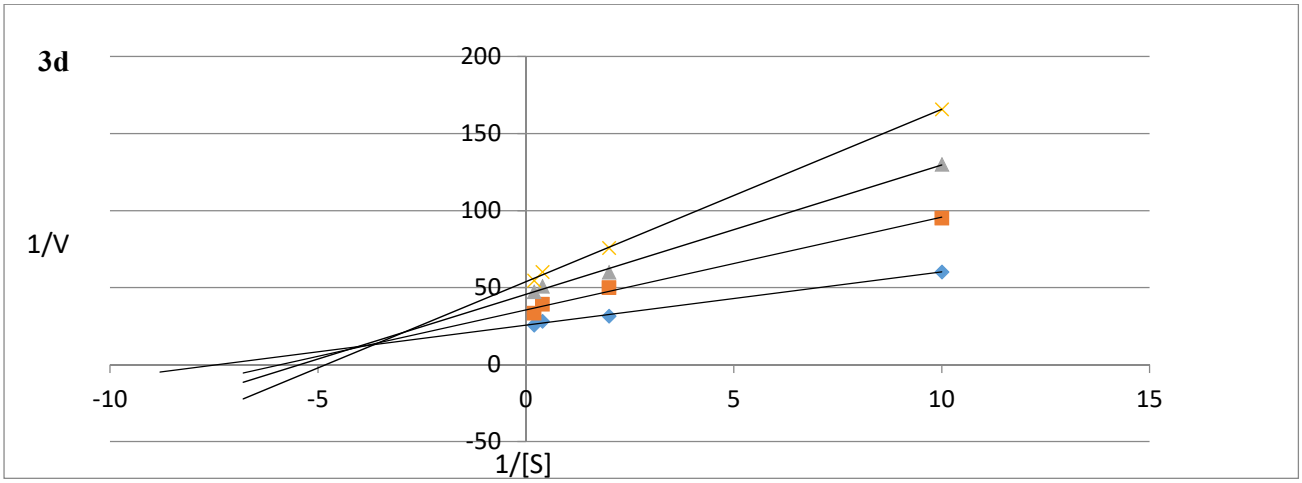
Figure S1.20: [1]H- and [13]C-NMR spectra of **3i** in DMSO-d_6 at 300 and 75 MHz, respectively.

Figure S2.1: Lineweaver-Burk and Dixon plots of 2b, 2f, 3b, 3d and 3f against ACh.









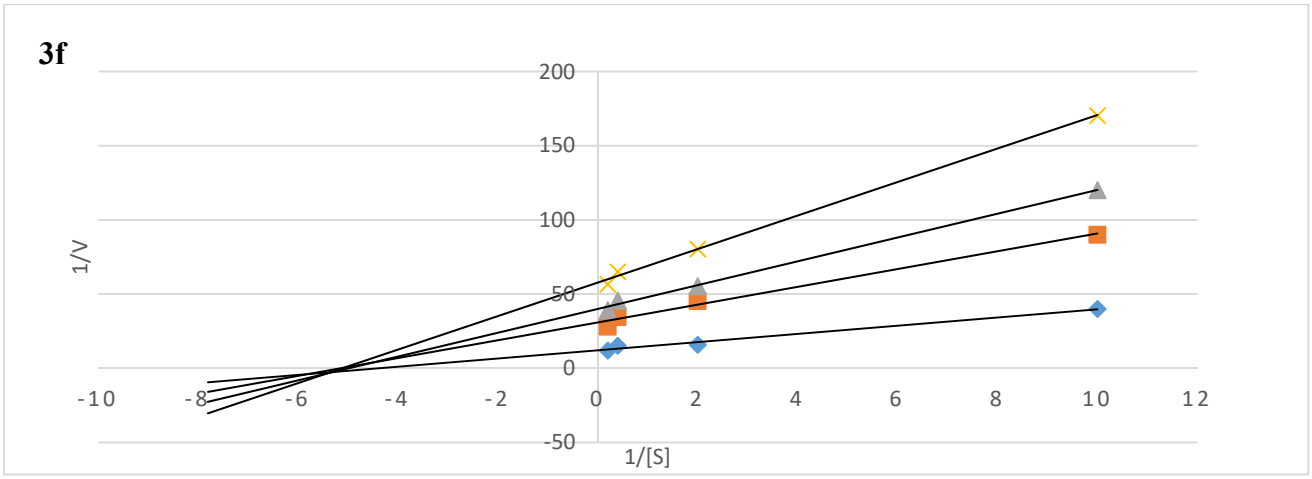
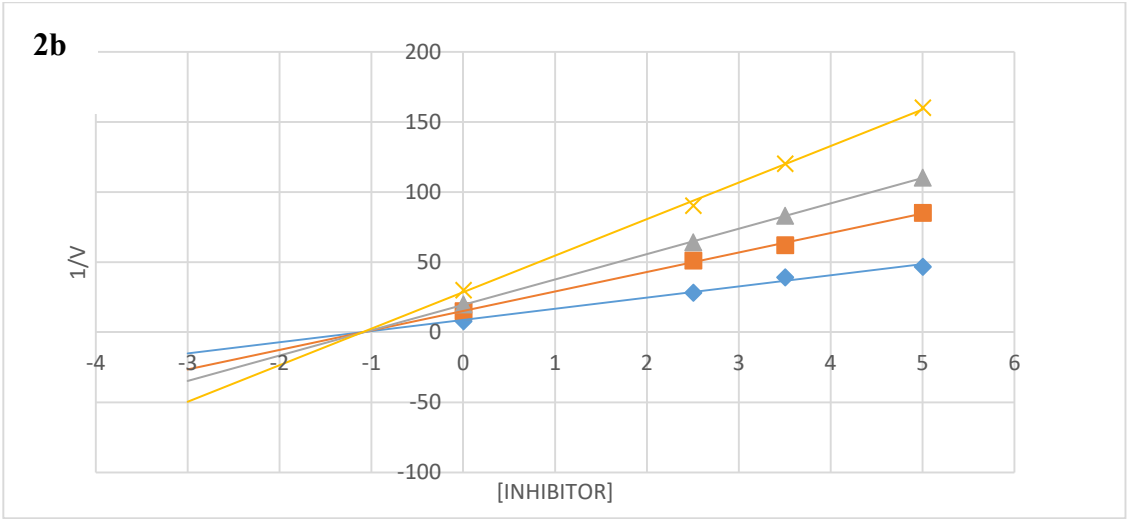


Figure S2.1.1: Lineweaver–Burk plots for inhibition of AChE by **2b**, **2f**, **3b**, **3d**, **3f**. Blue symbols and fitted straight lines represent enzyme activity in the absence of inhibitor, while orange (2.5 μM), grey (3.5 μM) and yellow (5 μM) represent various concentrations of inhibitor.

2b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100
50
0
-50
-100
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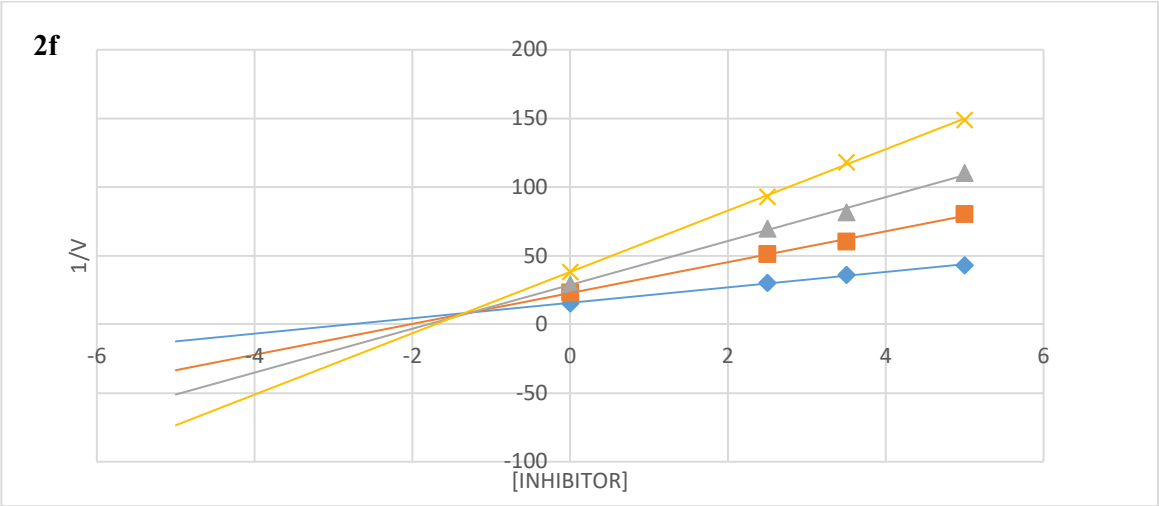
-4
-3
-2
-1
0
1
2
3
4
5
6
[INHIBITOR]

2f


200
150
100
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0
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1/V
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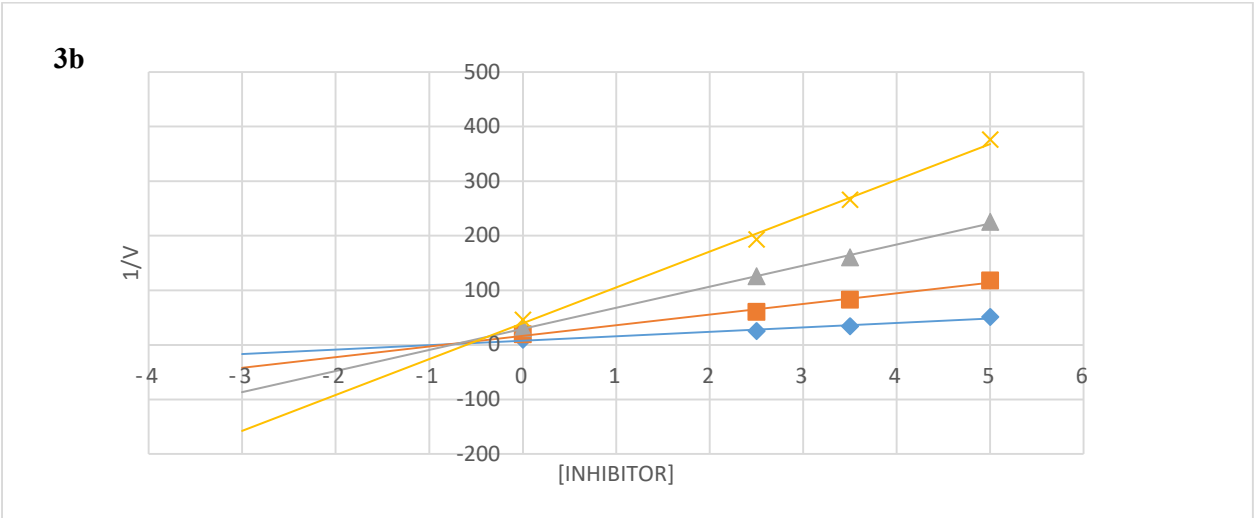
0
2
4
6
[INHIBITOR]

3b


500
400
300
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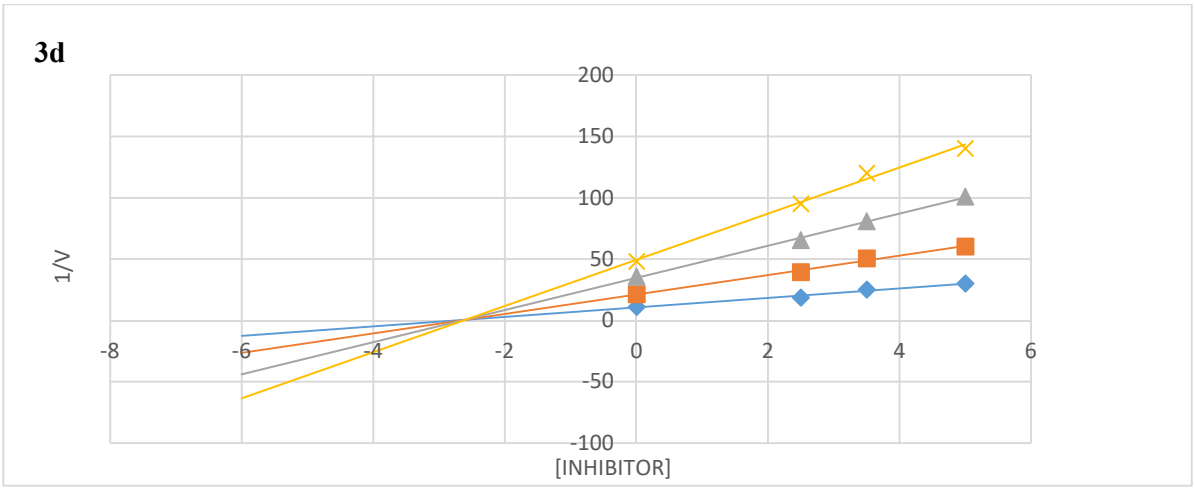
6
[INHIBITOR]



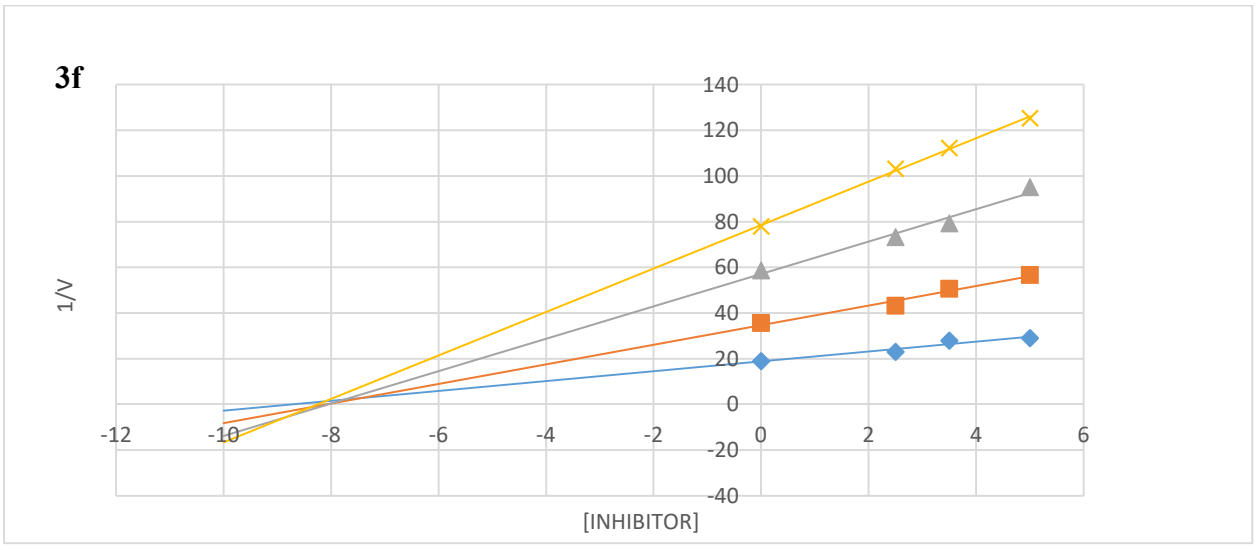
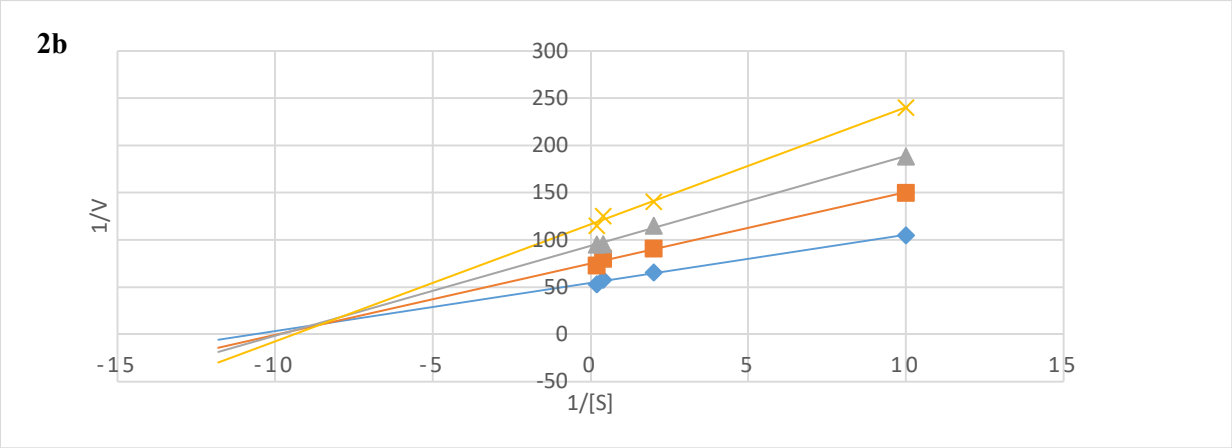
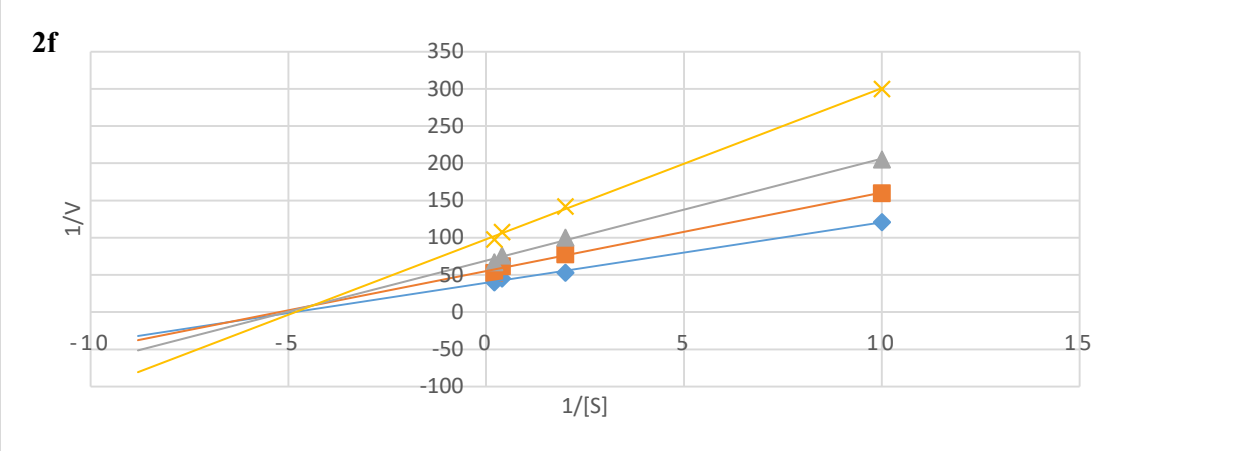
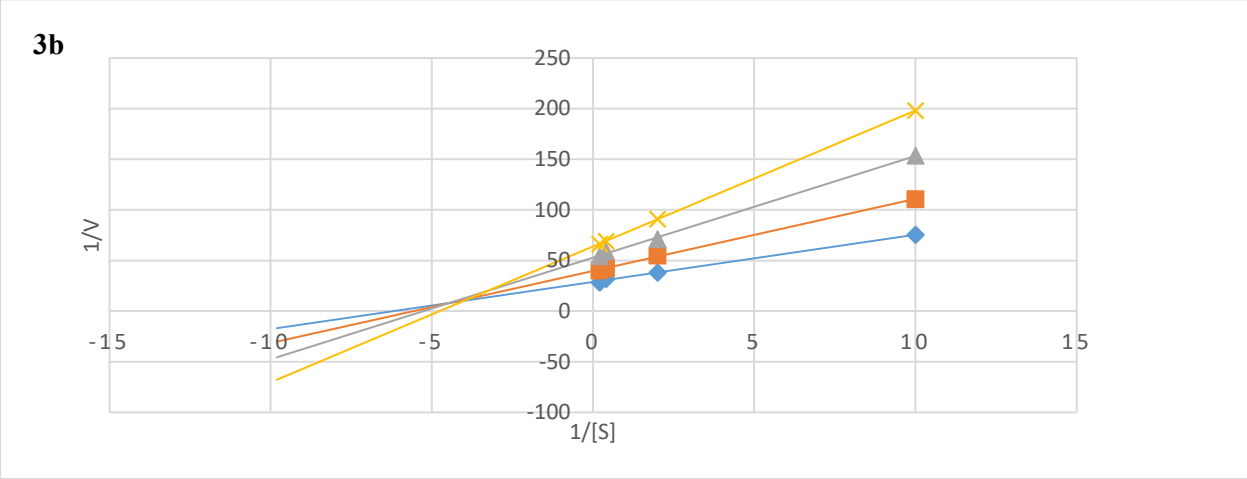


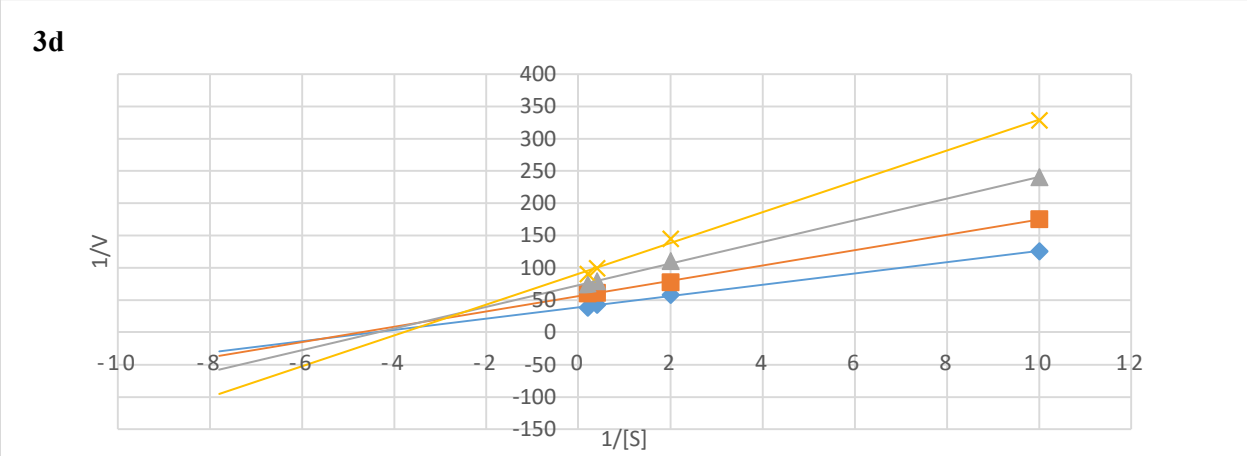
Figure S2.1.2: Dixon plots for inhibition of AChE by **2b**, **2f**, **3b**, **3d**, **3f**. Blue symbols and fitted straight lines represent enzyme activity with 5 mM substrate, while orange (2.5 mM), grey (0.5 mM) and yellow (0.1 mM) represent various concentrations of substrate.

Figure S2.2: Lineweaver-Burk and Dixon plots of 2b, 2f, 3b, 3d and 3f against BChE.









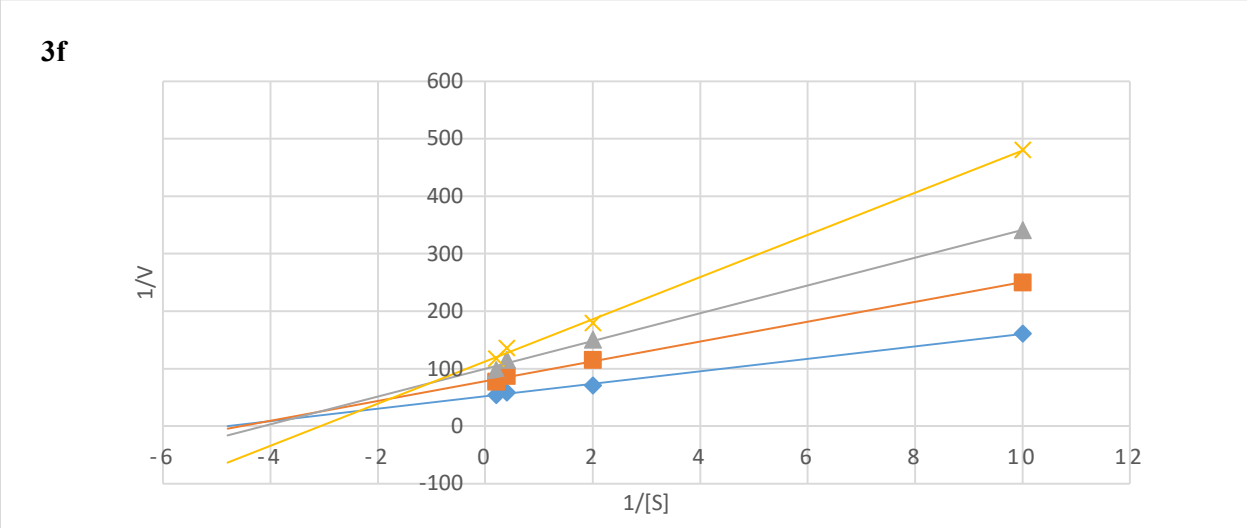
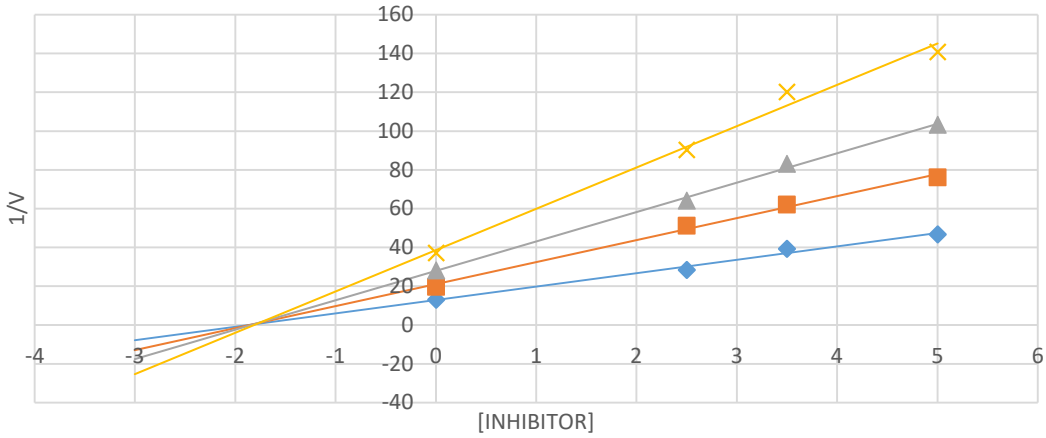


Figure S2.2.1: Lineweaver–Burk plots for inhibition of BChE by **2b**, **2f**, **3b**, **3d**, **3f**. Blue symbols and fitted straight lines represent enzyme activity in the absence of inhibitor, while orange (2.5 μM), grey (3.5 μM) and yellow (5 μM) represent various concentrations of inhibitor.

2b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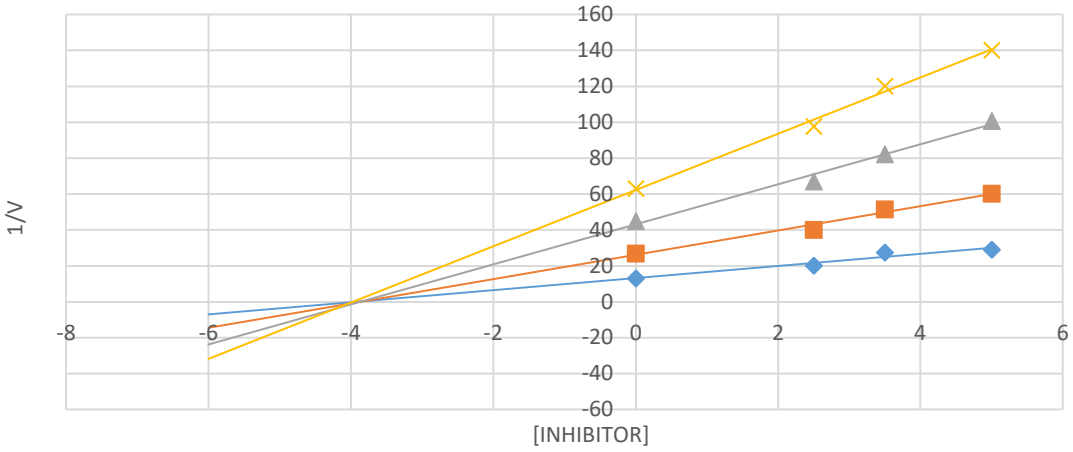
[INHIBITOR]

2f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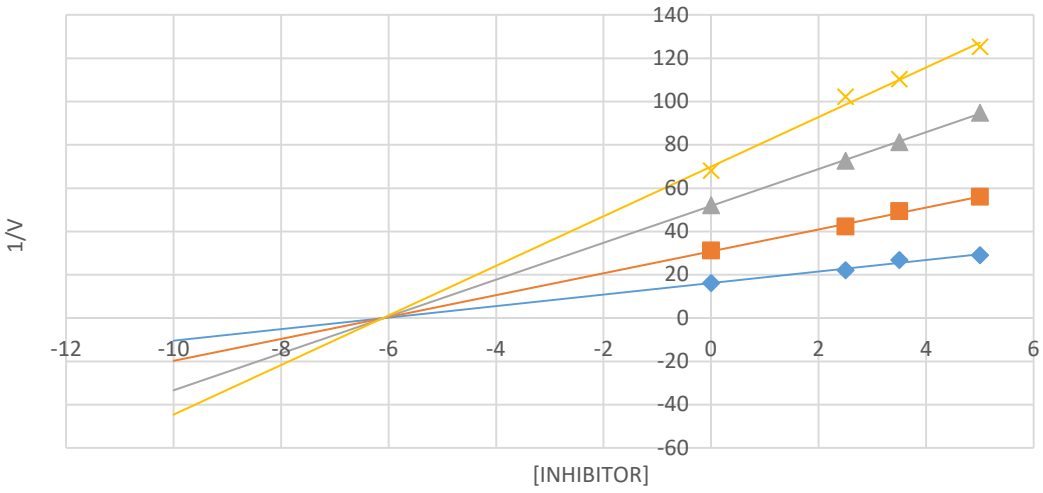
3b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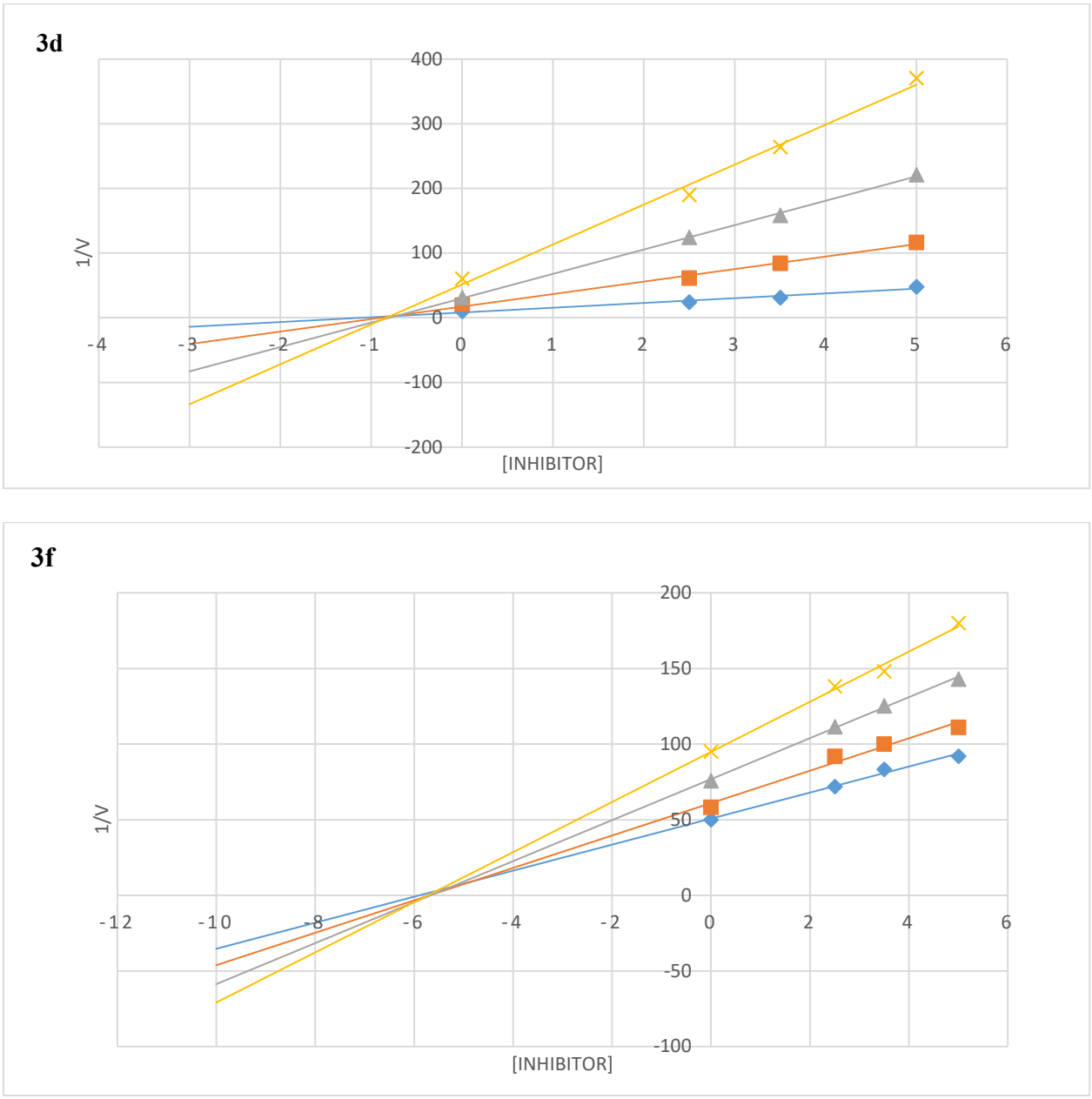

Figure S2.2.2: Dixon plots for inhibition of BChE by **2b**, **2f**, **3b**, **3d**, **3f**. Blue symbols and fitted straight lines represent enzyme activity with 5 mM substrate, while orange (2.5 mM), grey (0.5 mM) and yellow (0.1 mM) represent various concentrations of substrate.

Figure S2.3: Lineweaver-Burk and Dixon plots of 2f against BACE-1.

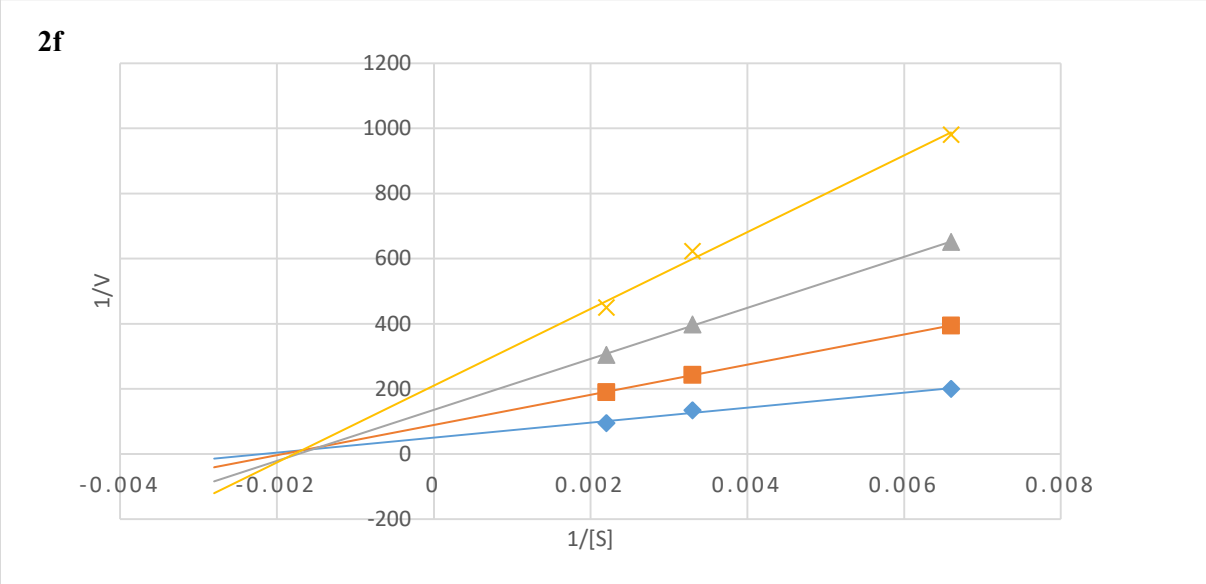

Figure S2.3.1: Lineweaver–Burk plots for inhibition of BACE-1 by **2f**. Blue symbols and fitted straight lines represent enzyme activity in the absence of inhibitor, while orange (2.5 μM), grey (3.5 μM) and yellow (5 μM) represent various concentrations of inhibitor.

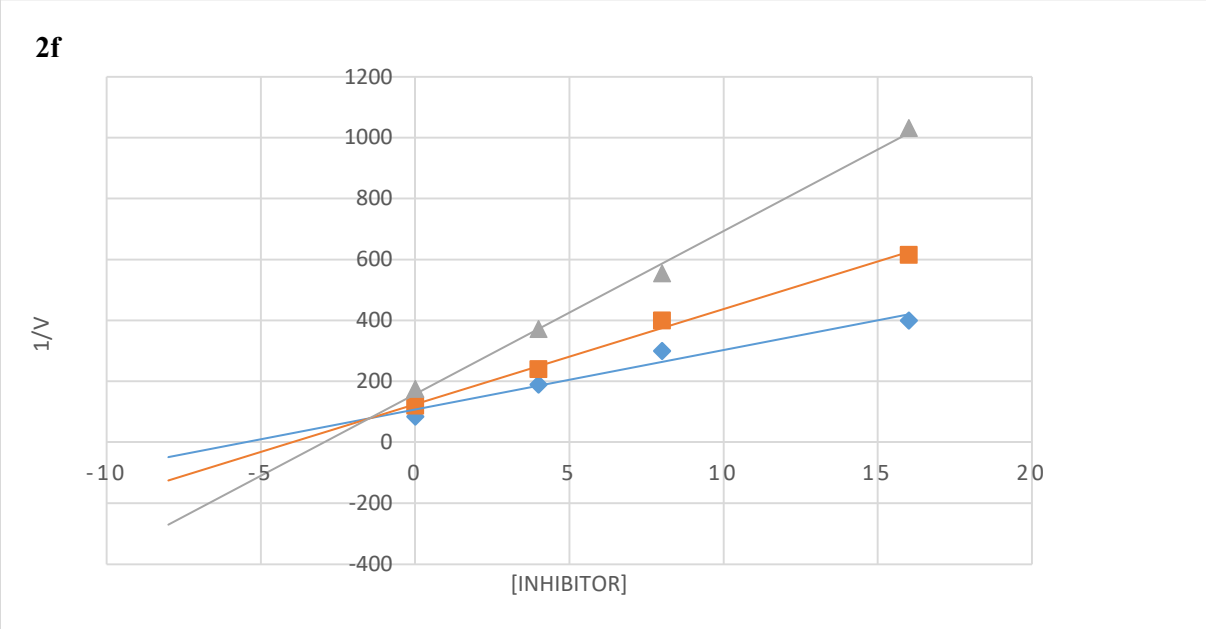

Figure S2.3.2: Dixon plots for inhibition of BACE-1 by **2f**. Blue symbols and fitted straight lines represent enzyme activity in the presence of 450 nM substrate and orange and grey, 300 nM and 150 nM substrate, respectively.

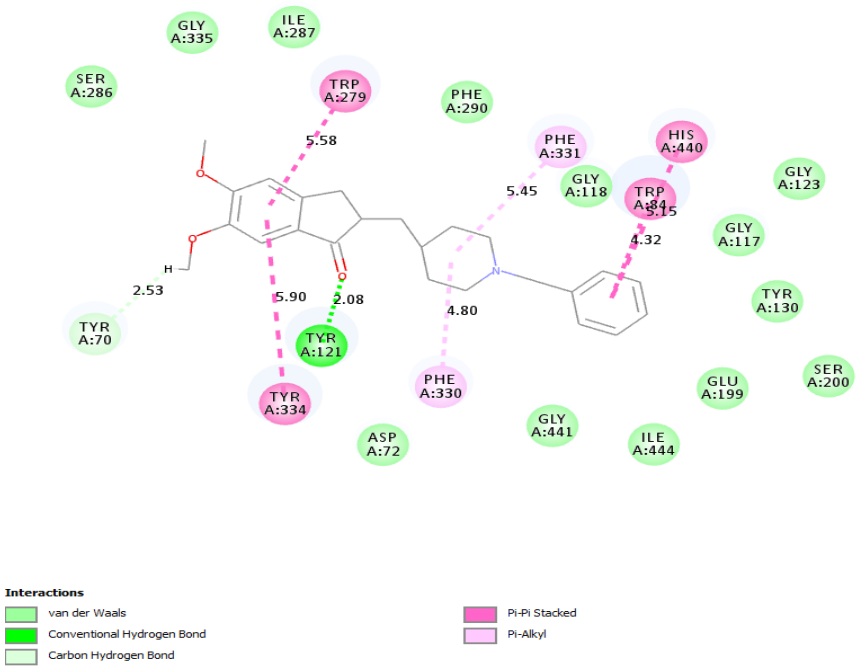

Figure S3: Docking pose of donepezil showing interaction with AChE protein residues.

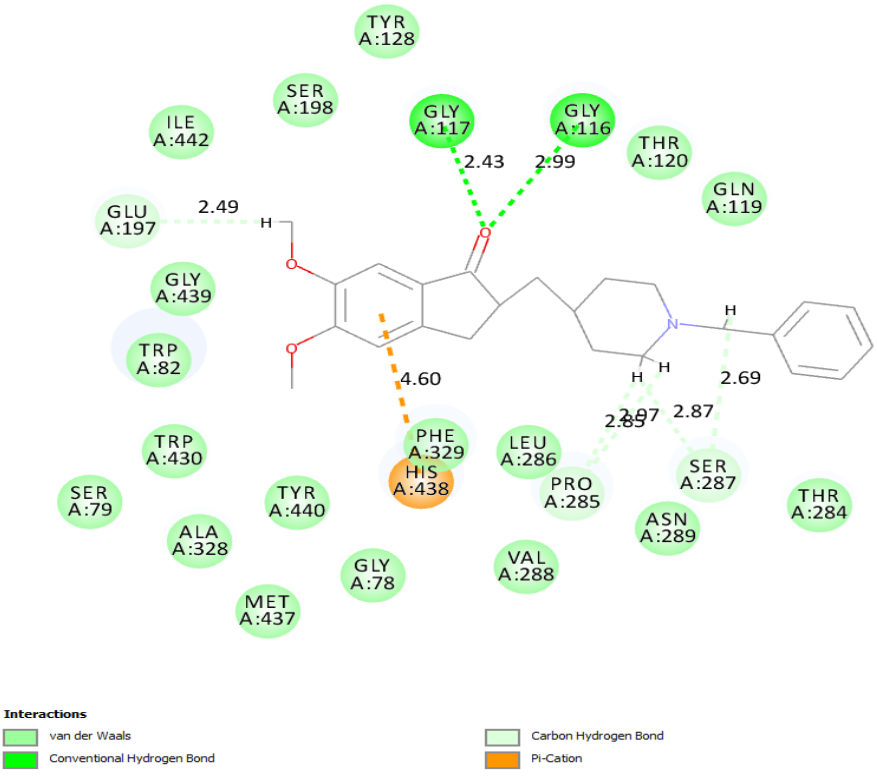

Figure S4: Docking pose of donepezil showing interaction with BChE protein residues.

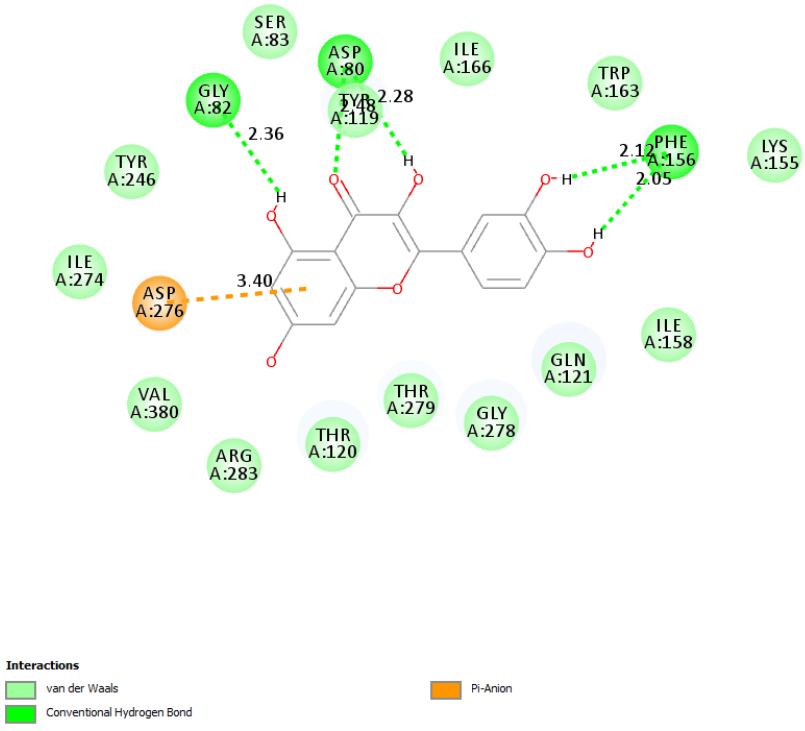

Figure S5: **Docking pose of quercetin showing interaction with BACE-1 protein residues.**

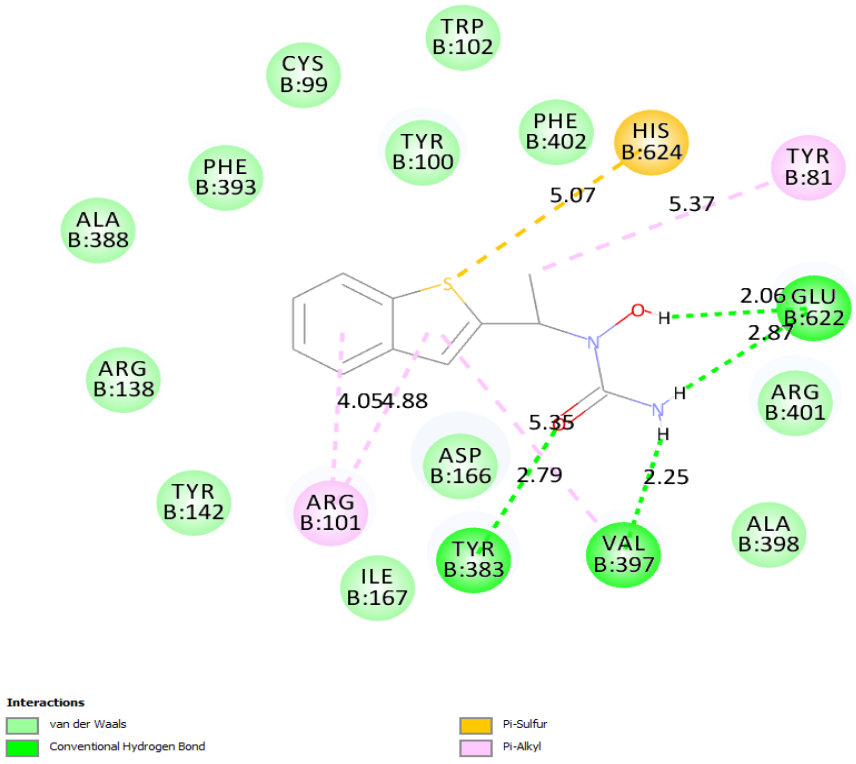

Figure S6: **Docking pose of zileuton showing interaction with LOX-5 protein residues.**

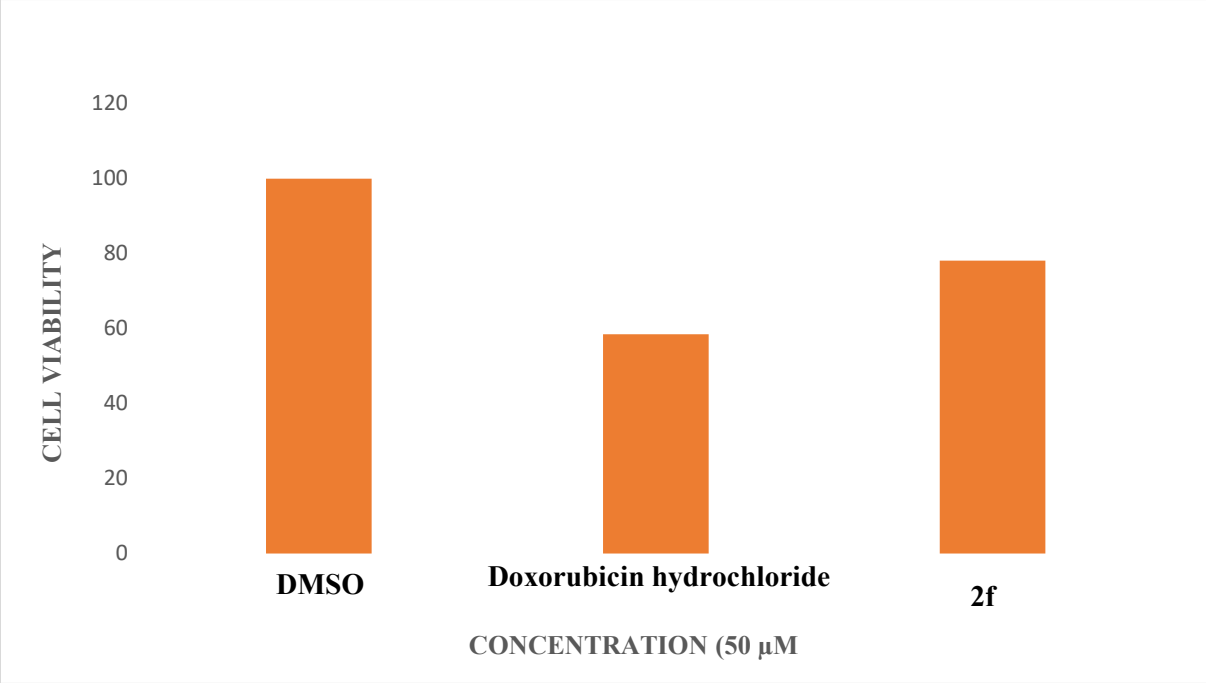

Figure S7: Evaluation of toxicity of **2f** in Hek293-T.