

Supplementary Data

Antiproliferative Activity of New Neocryptolepine–Rhodanine– α -Aminophosphonate Conjugates: *In Vitro* and *In Silico* Evaluation

Hanem M. Awad ^{a*}, Abdullah A. S. Ahmed ^b, Yasmine S. Moemen ^c, Mohamed Aly Saad Aly ^d, Ahmed I. El-Tantawy ^e, Elshaymaa I. Elmongy ^f, and Ibrahim El Tantawy El Sayed ^{b*}

^a Department of Tanning Materials and Leather Technology, National Research Centre, Dokki, Giza 12611, Egypt

^b Chemistry Department, Faculty of Science, Menoufia University, Shebin El-Kom 32511, Egypt

^c Clinical Pathology Department, National Liver Institute, Menoufia University, Shebin El-Kom 32511, Egypt

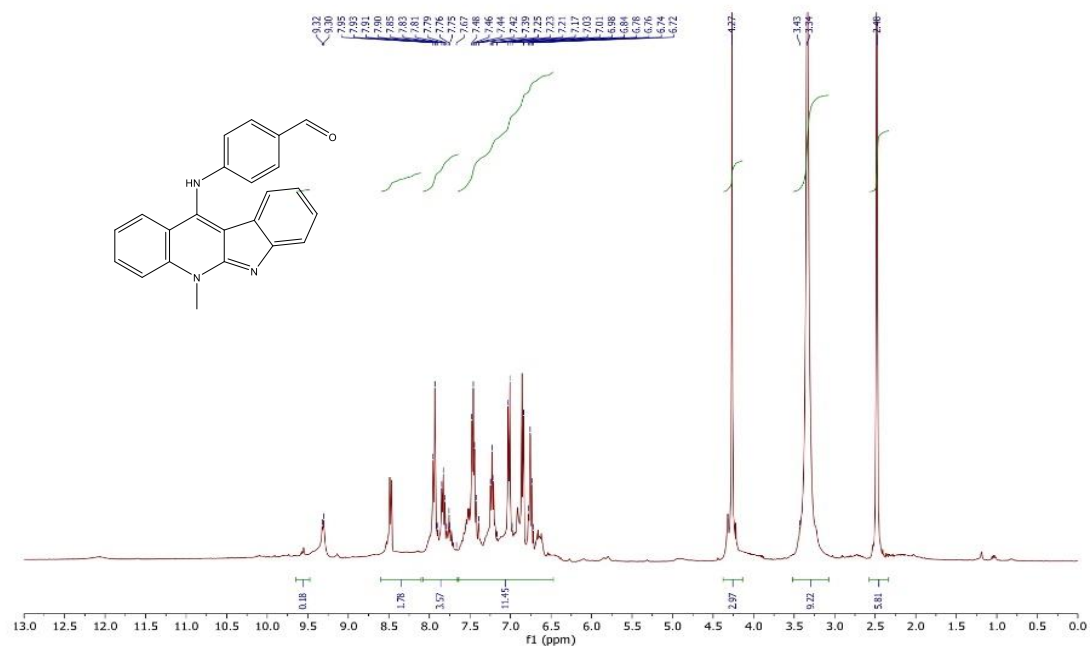
^d Department of Electrical and Computer Engineering at Georgia Tech Shenzhen Institute (GTSI), Tianjin University. Shenzhen, Guangdong, 518055, China.

^e Research Institute for Interdisciplinary Science, Okayama University, Tsushima-naka, Kita-ku, Okayama 700-8530, Japan

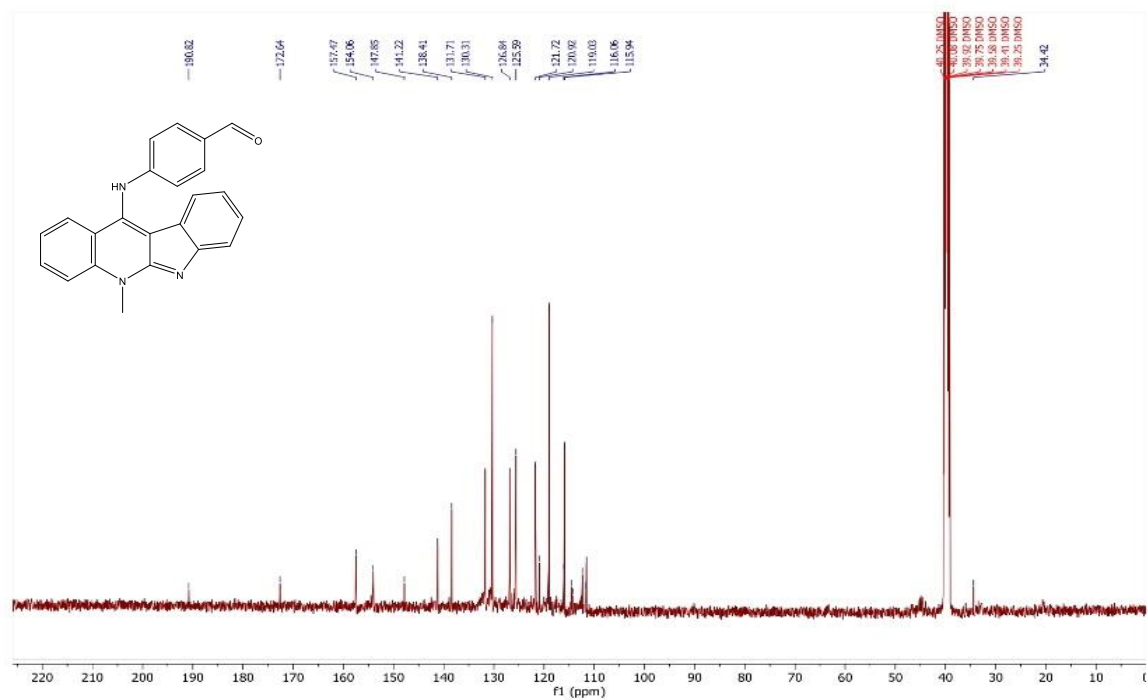
^f Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Capital University (formerly Helwan), Ain Helwan,

Corresponding authors:

Ibrahim El Tantawy El Sayed, ibrahimtantawy@science.menofia.edu.eg

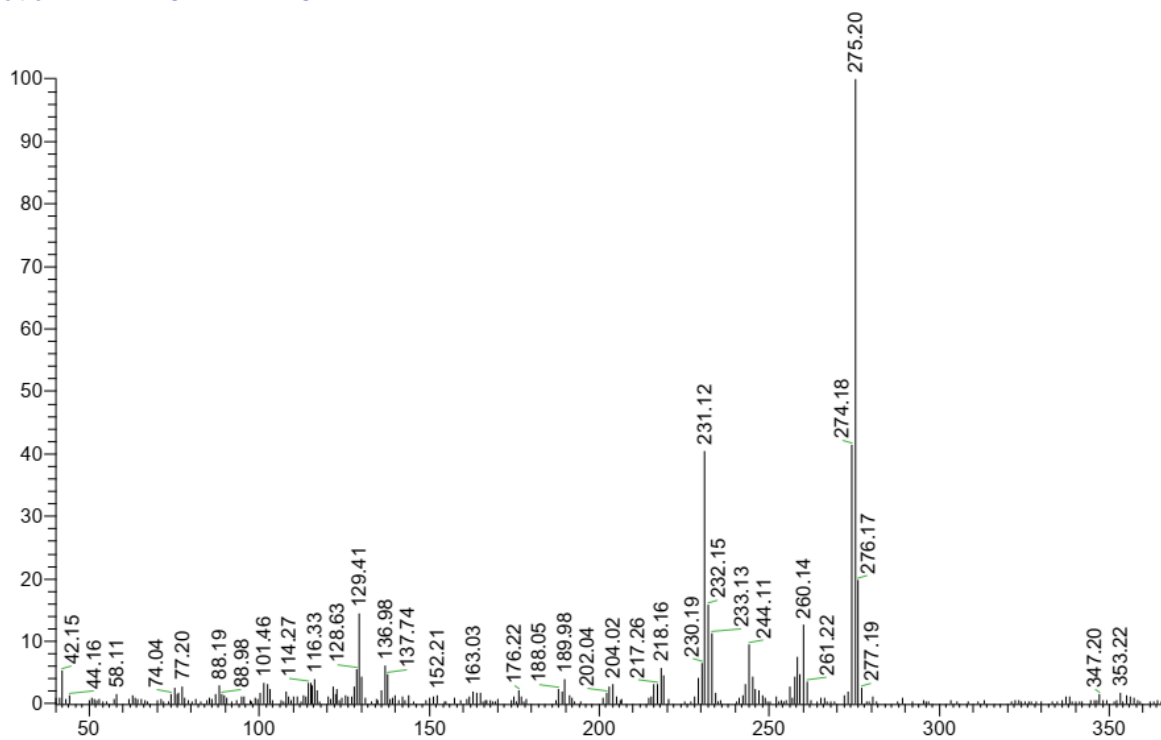


¹H NMR of 3b in DMSO.

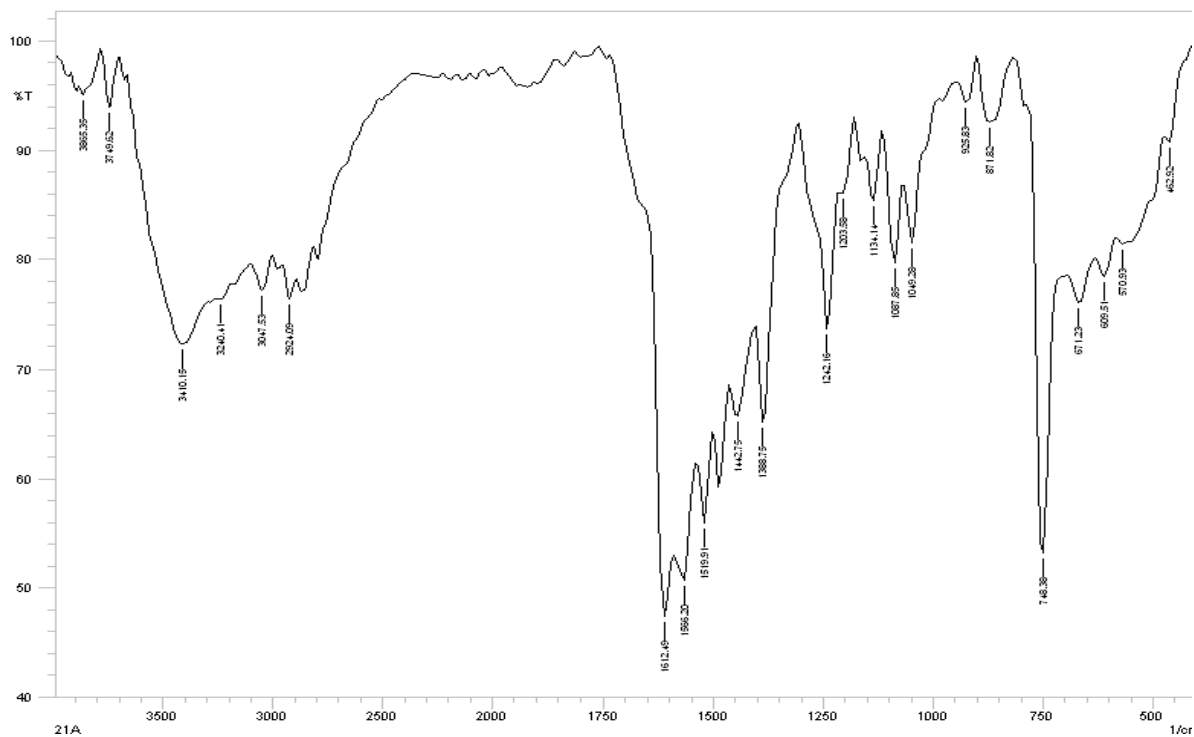


¹³C NMR of 3b in DMSO.

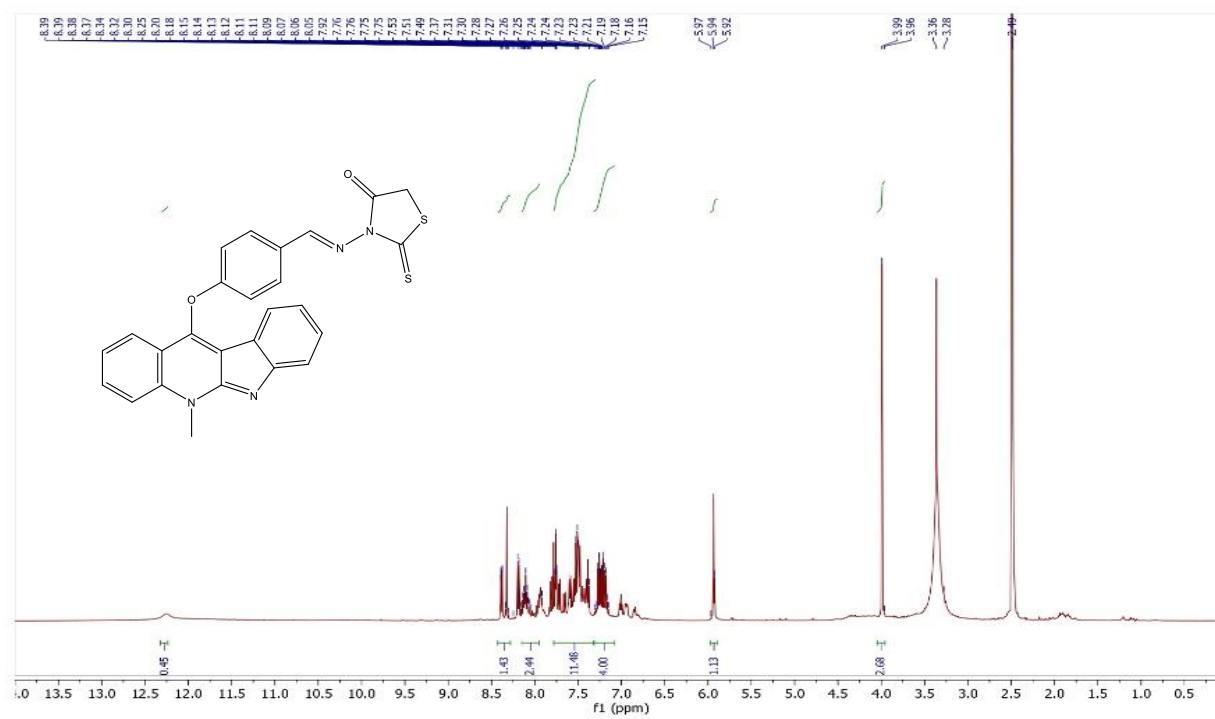
abdallah-ahmed-mohamed-21a #125 RT: 2.11 AV: 1 SB: 2 4.55 , 4.57 NL: 1.97E5
T: {0,0} + c EI Full ms [40.00-1000.00]



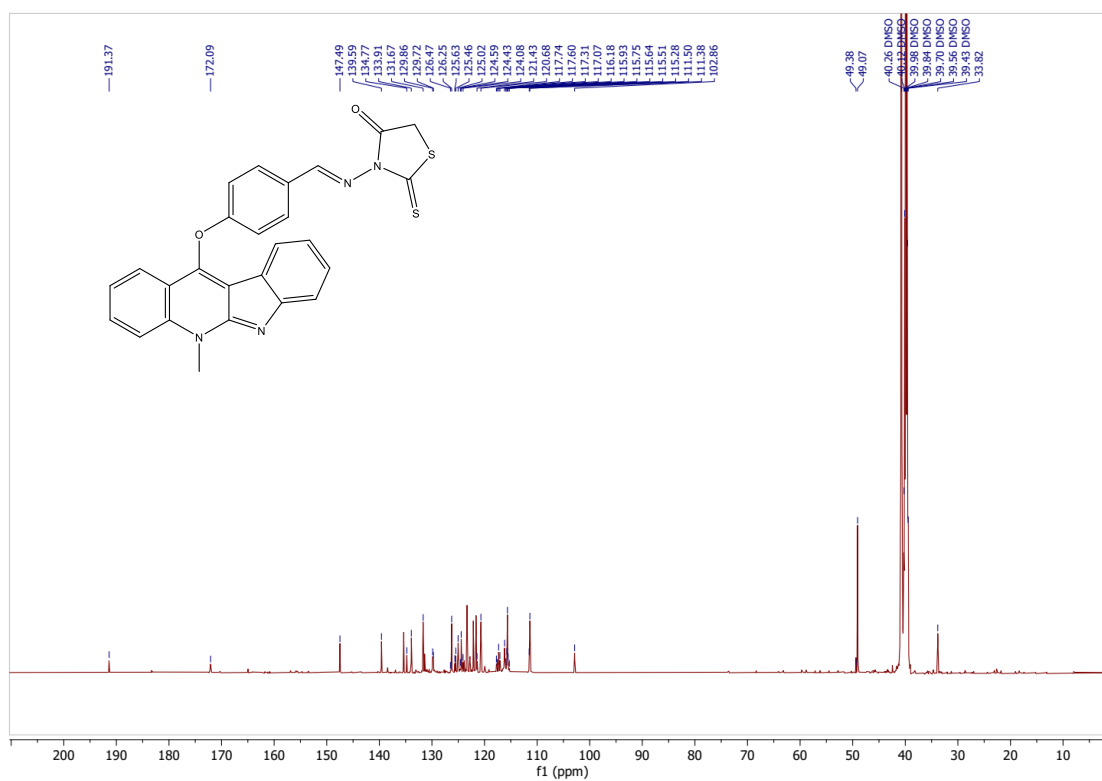
EI-MS of 3b.



FT IR of compound 3b.

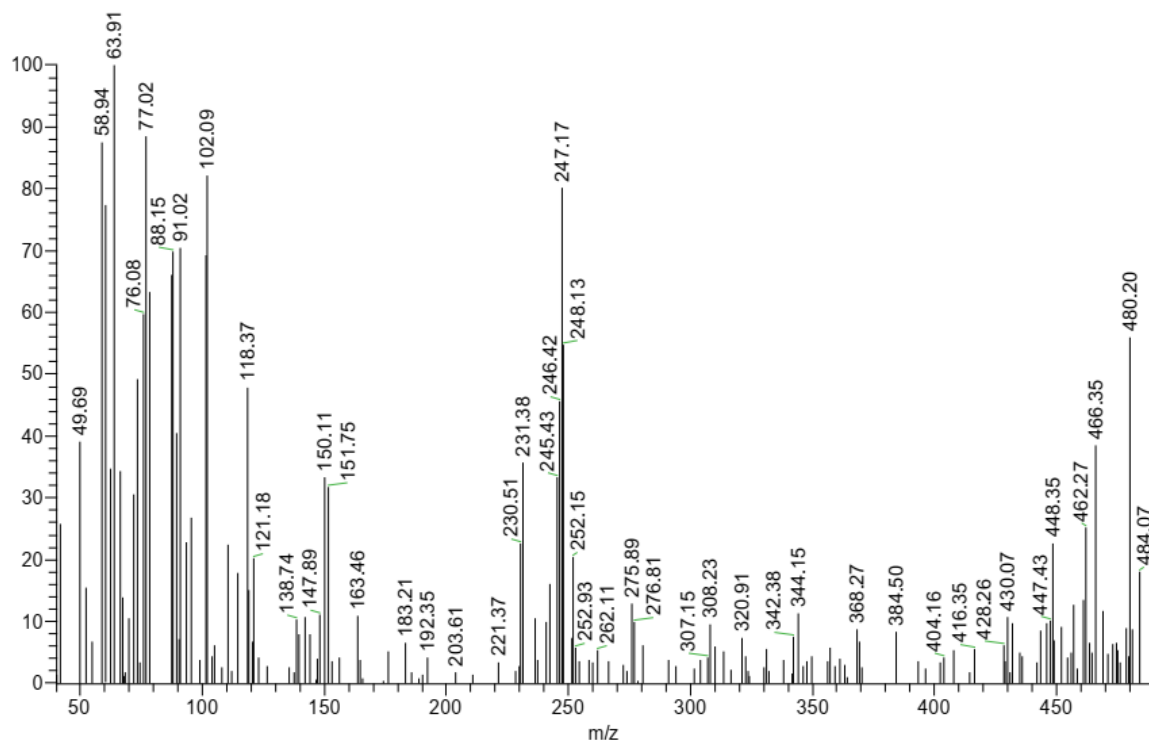


¹H NMR of 5a in DMSO.

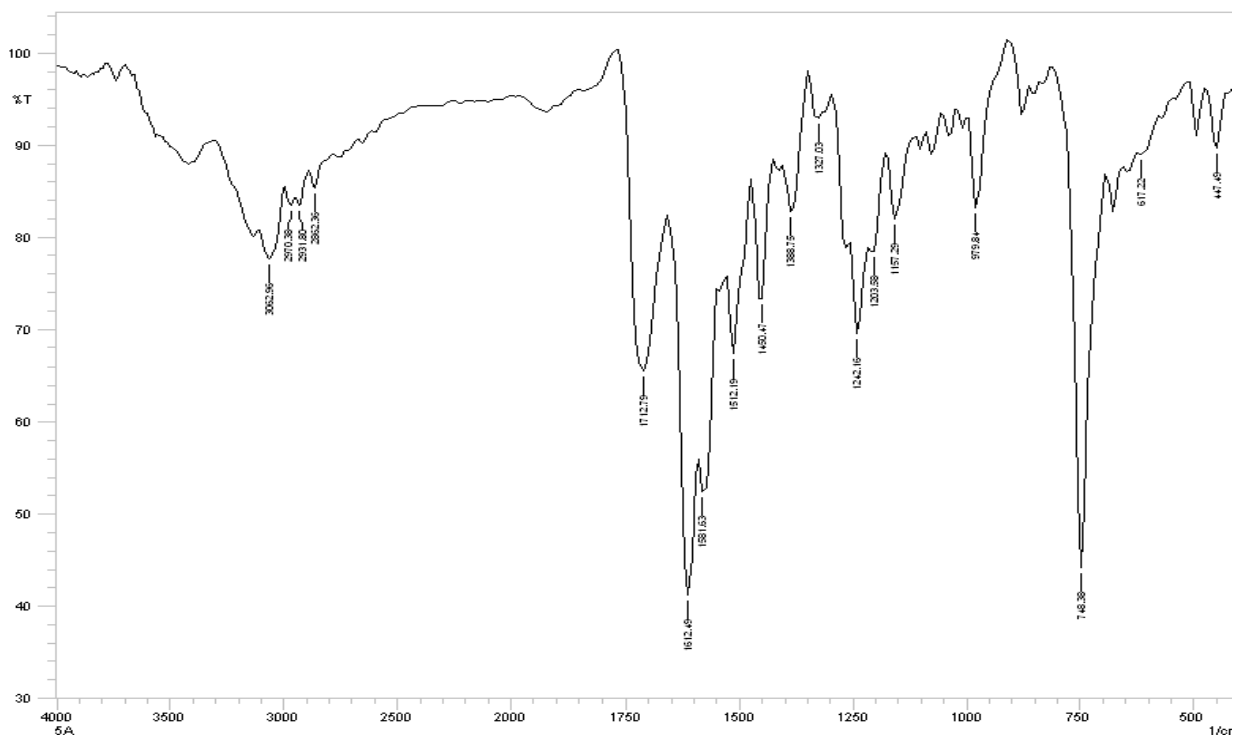


¹³C NMR of 5a in DMSO.

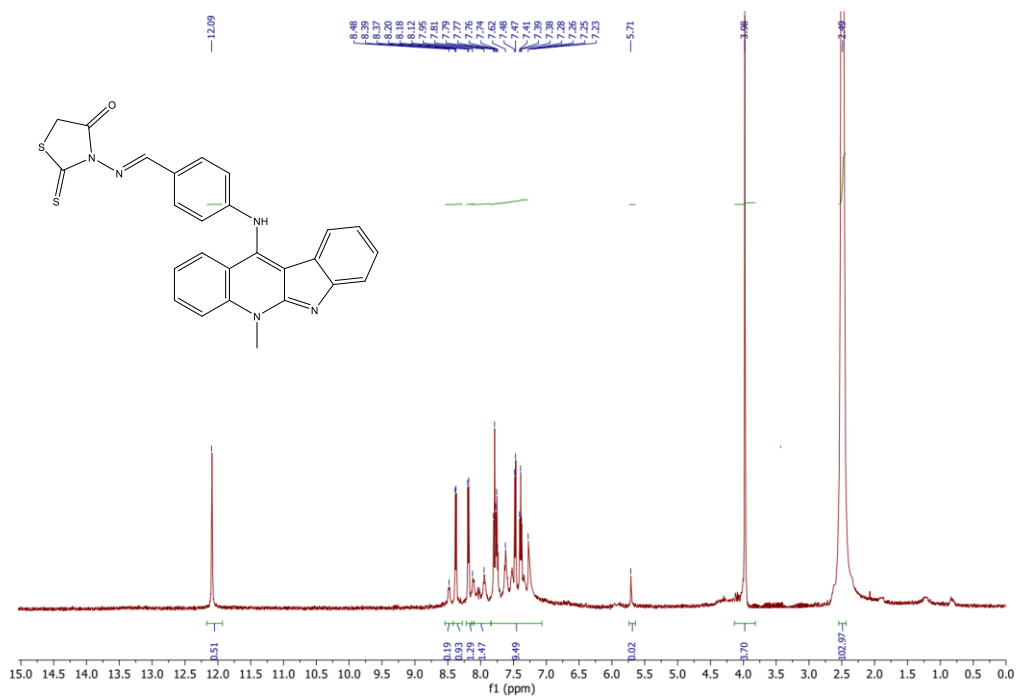
abdallah-ahmed-mohamed-3a #217 RT: 3.65 AV: 1 SB: 2 4.55, 4.59 NL: 2.98E3
T: {0,0} + c EI Full ms [40.00-1000.00]



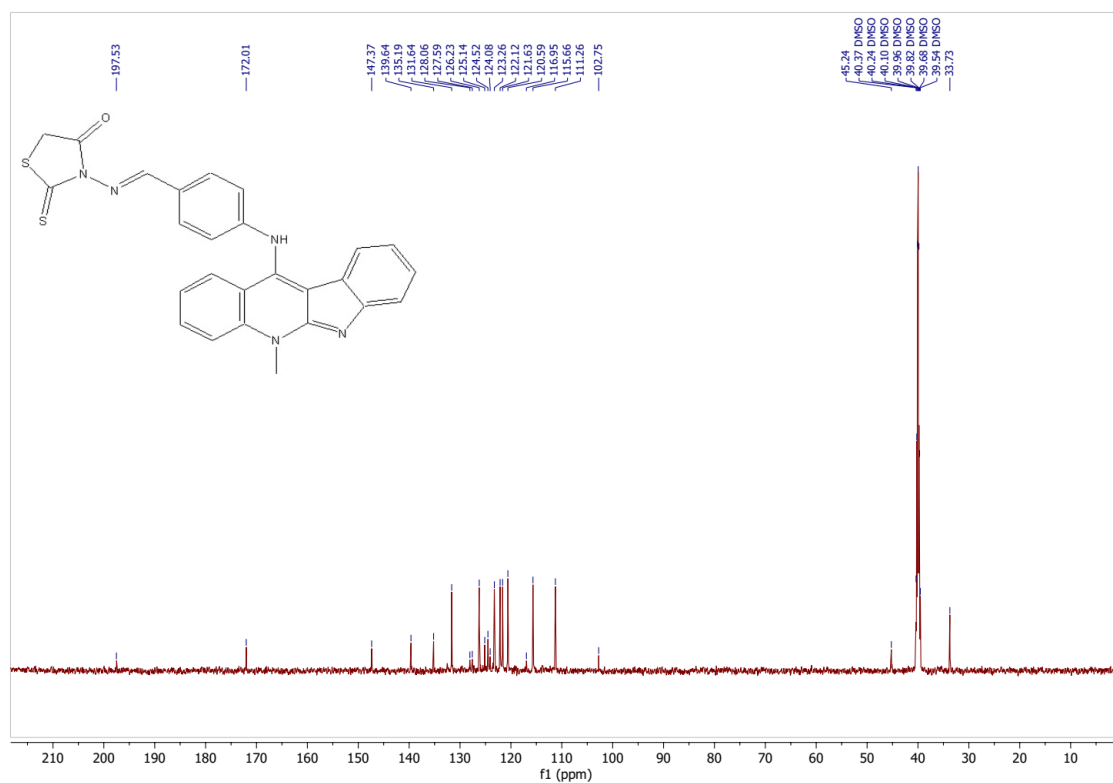
EI-MS of 5a.



FT IR of compound 5a.

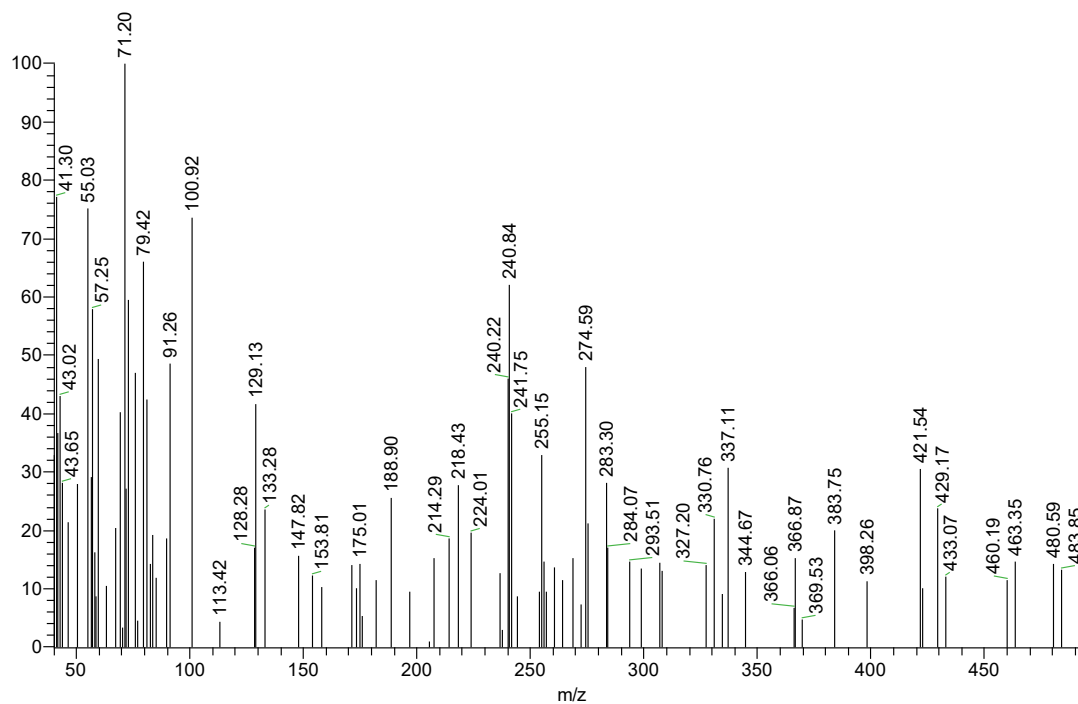


¹H-NMR of 5b in DMSO.

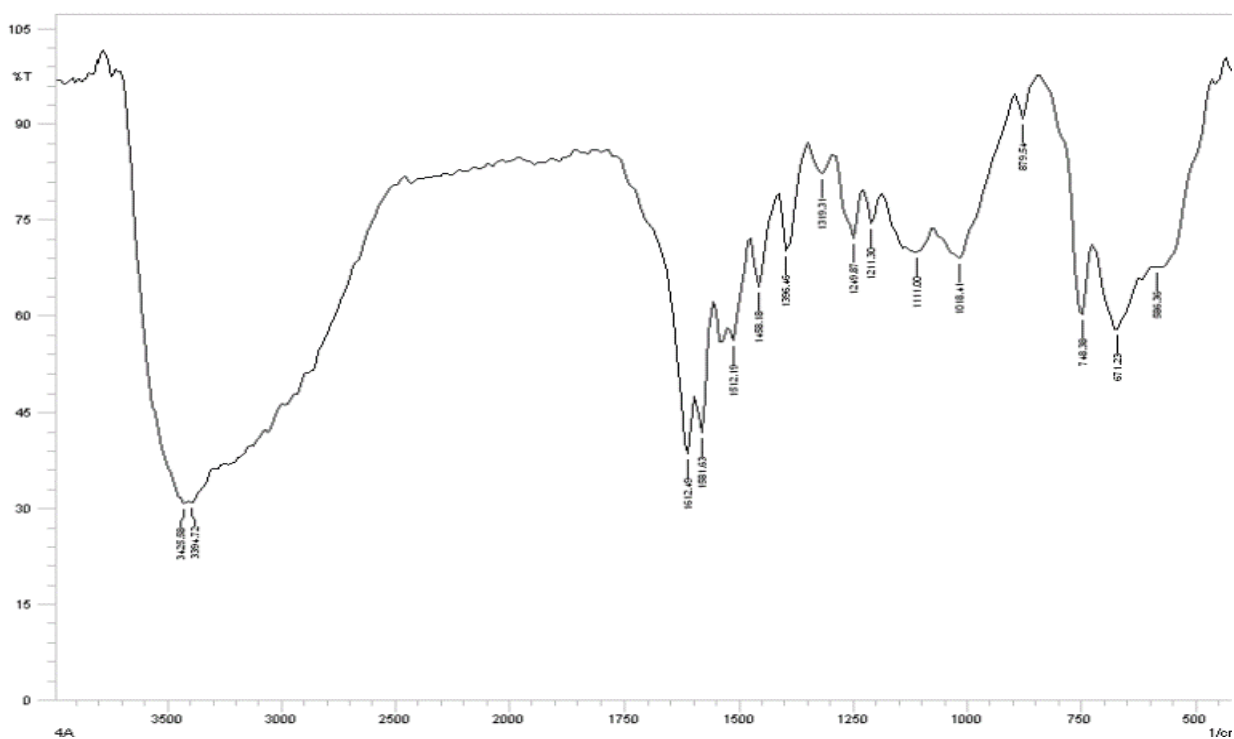


¹³C-NMR of 5b in DMSO.

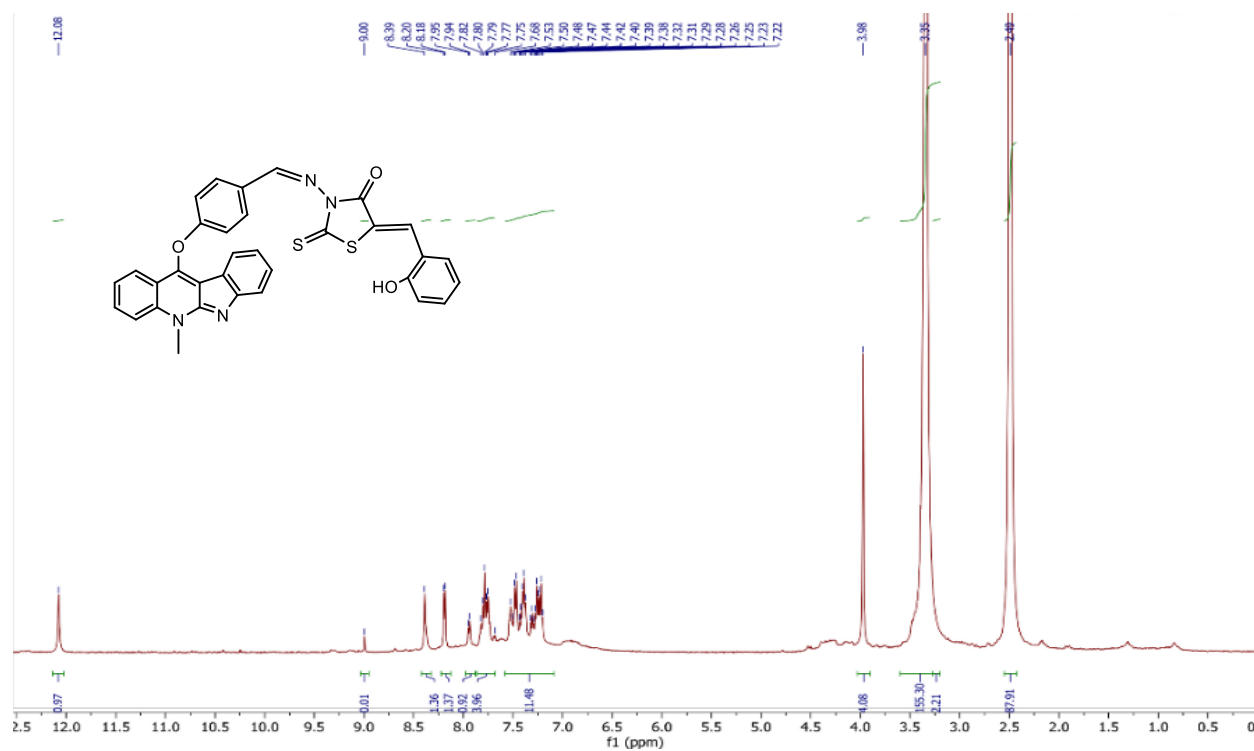
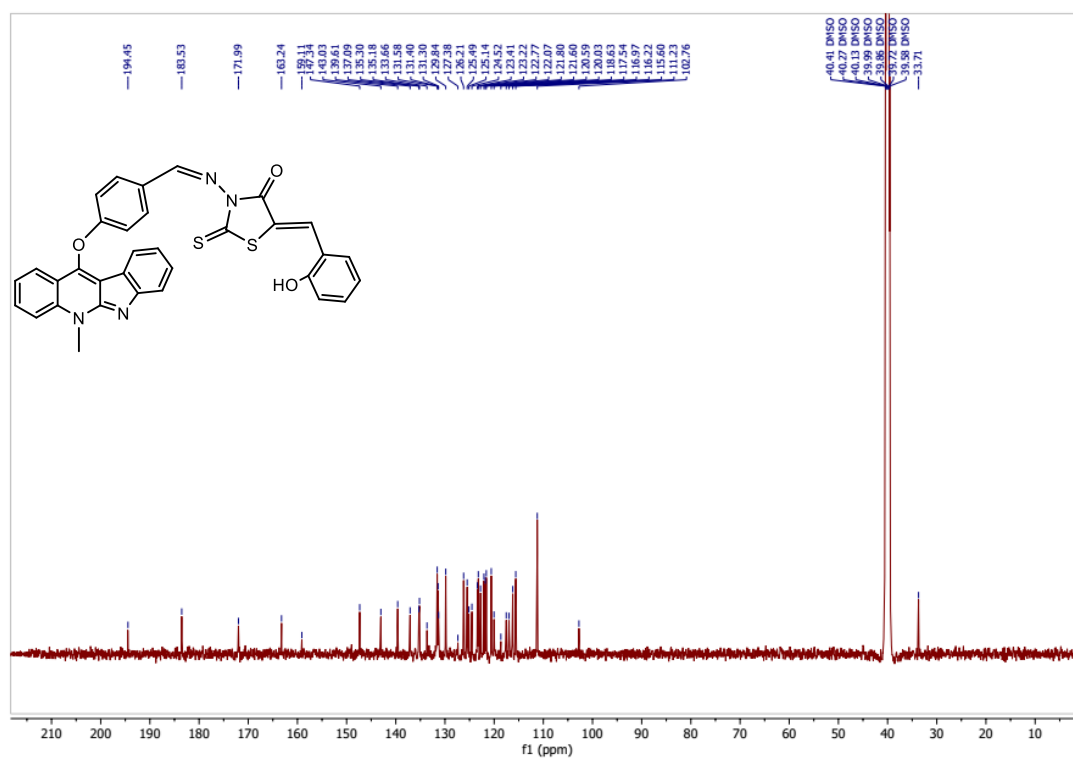
abdallah-ahmed-mohamed-4a #153 RT: 2.58 AV: 1 SB: 2 4.55 , 4.59 NL: 7.98E2
T: {0,0} + c EI Full ms [40.00-1000.00]



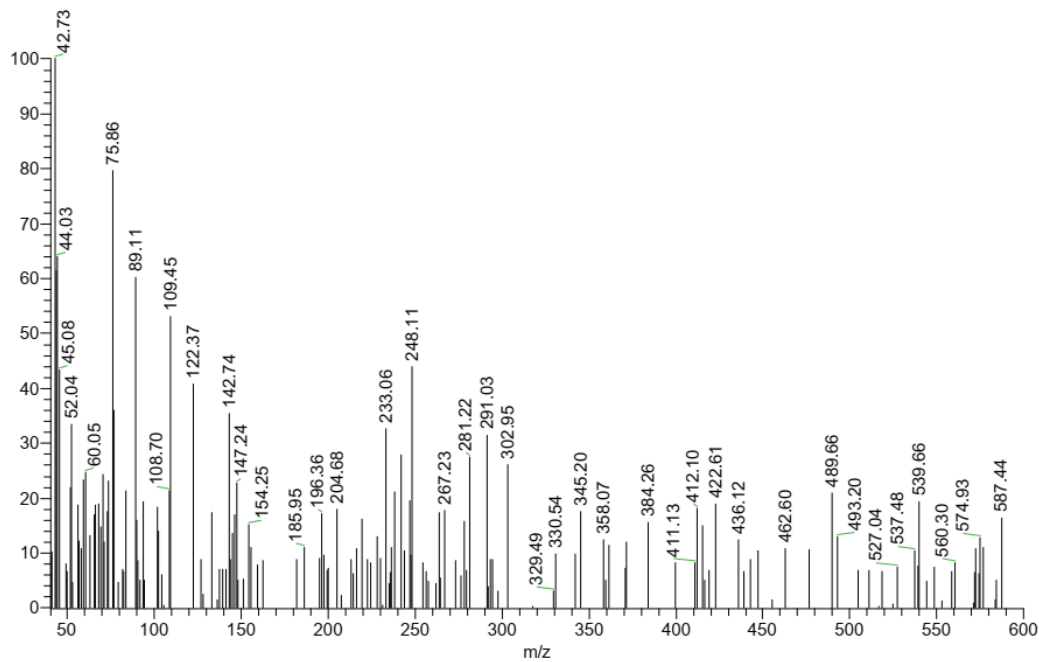
EI-MS of 5b.



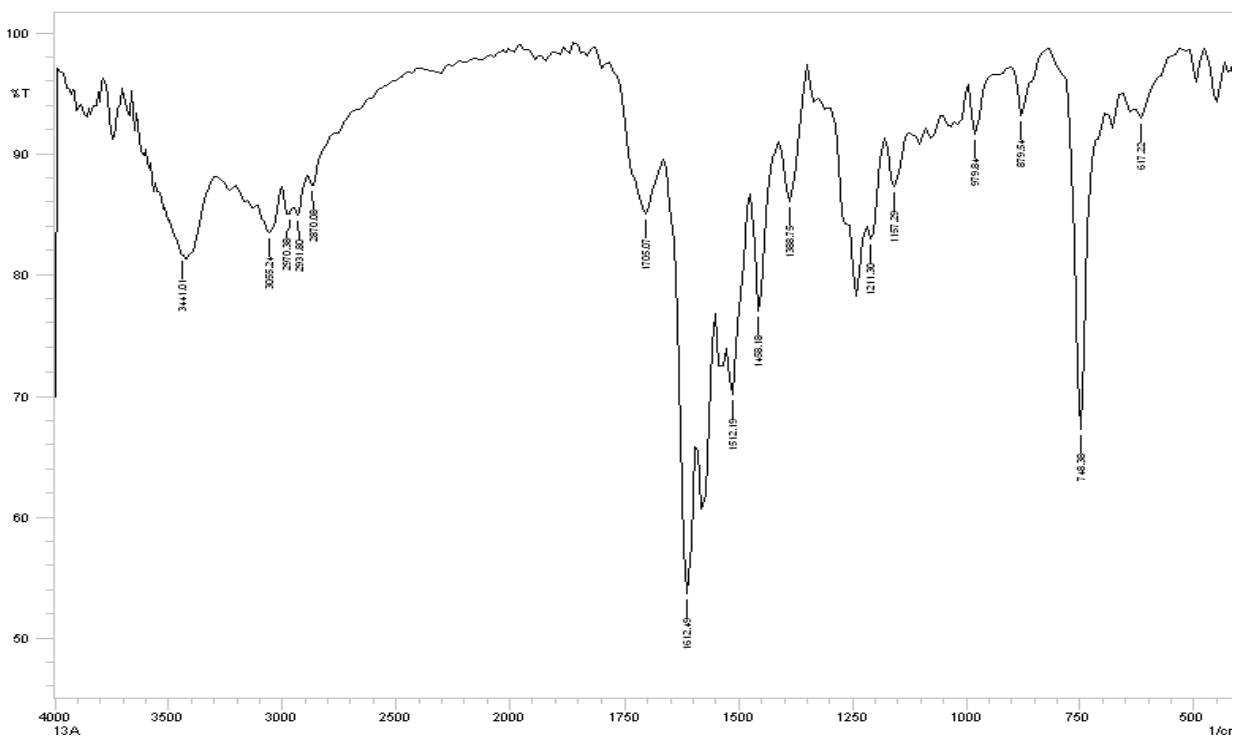
FT IR of compound 5b.

¹H NMR of 7a in DMSO¹³C NMR of 7a in DMSO

abdallah-ahmed-mohamed-13a #222 RT: 3.73 AV: 1 SB: 2 4.50, 4.50 NL: 1.12E3
T: {0,0} + c EIFull ms [40.00-1000.00]



EI-MS of 7a



FT IR of compound 7a.

Chemical Structure of 10: CN1c2ccccc2c3nc4ccccc4n3C(=O)N1Cc1ccc(cc1)/C=N/C(=O)N2C(=O)S(=O)C2=Cc3ccccc3O

¹H NMR (CDCl₃):

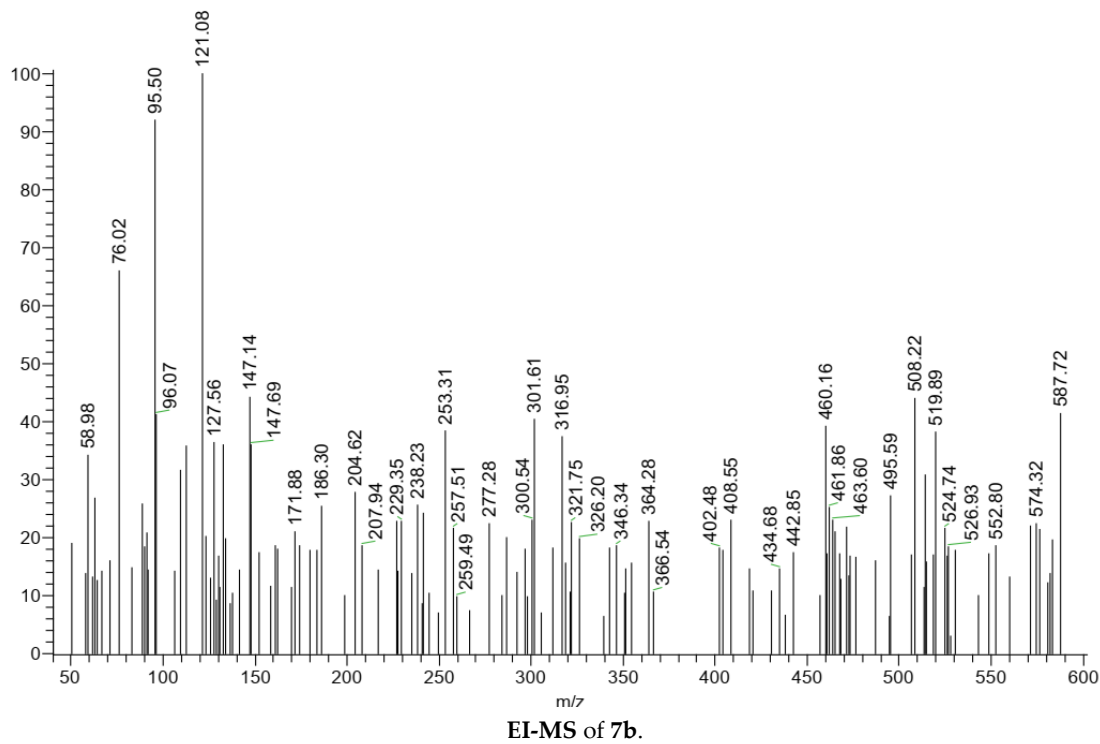
- 7.45 (d, 2H, ArH)
- 7.35 (d, 2H, ArH)
- 7.25 (d, 2H, ArH)
- 7.15 (d, 2H, ArH)
- 6.40 (s, 1H, ArH)
- 3.80 (s, 3H, OCH₃)
- 3.40 (s, 1H, OH)

¹³C NMR (DMSO-d₆):

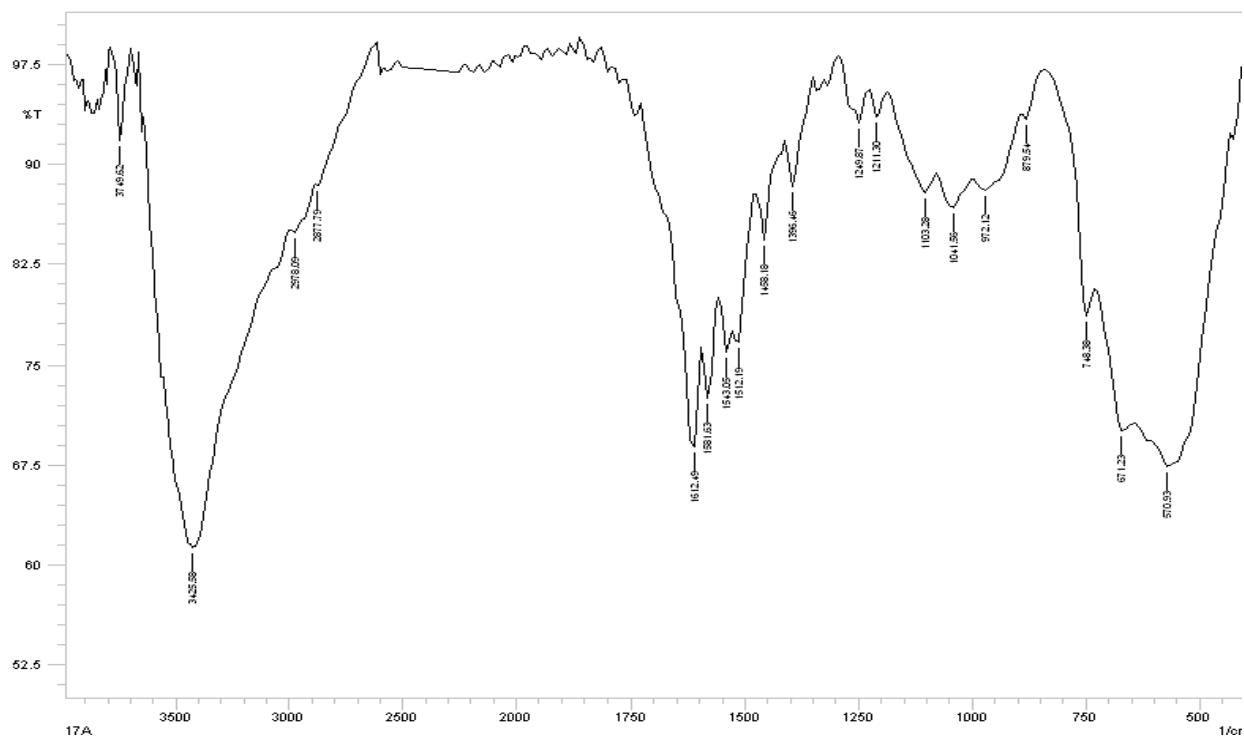
- 195.19, 172.04 (C=O)
- 147.40, 139.66, 135.21, 135.16, 130.74, 129.83, 126.26, 125.16, 124.94, 123.97, 122.29, 122.16, 121.67, 120.63, 120.36, 118.27, 115.70, 111.28, 102.77 (Aromatic)
- 40.38, 40.24, 40.11, 39.97, 39.83, 39.69, 39.51, 33.75 (Aliphatic)

¹³C NMR of **7b** in DMSO.

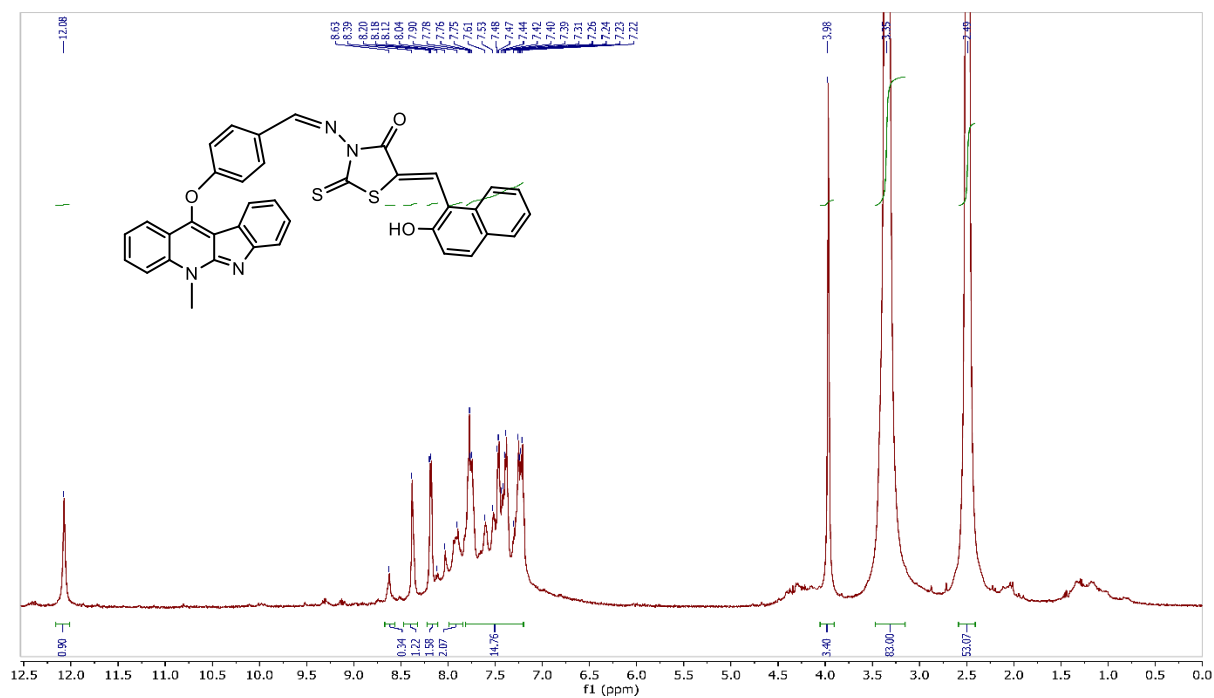
abdallah-ahmed-mohamed-17a #271 RT: 4.55 AV: 1 SB: 2 4.55, 4.57 NL: 2.77E2
T: {0,0} + c EI Full ms [40.00-1000.00]



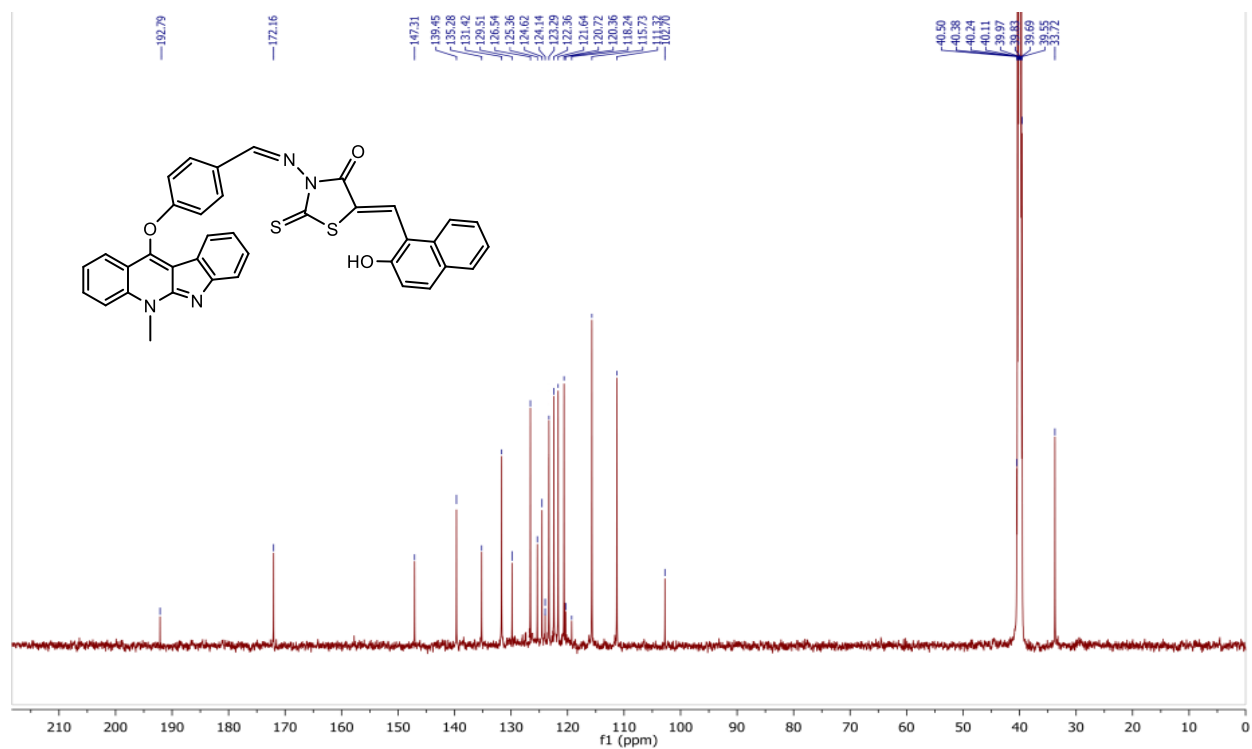
EI-MS of 7b.



FT IR of compound 7b.

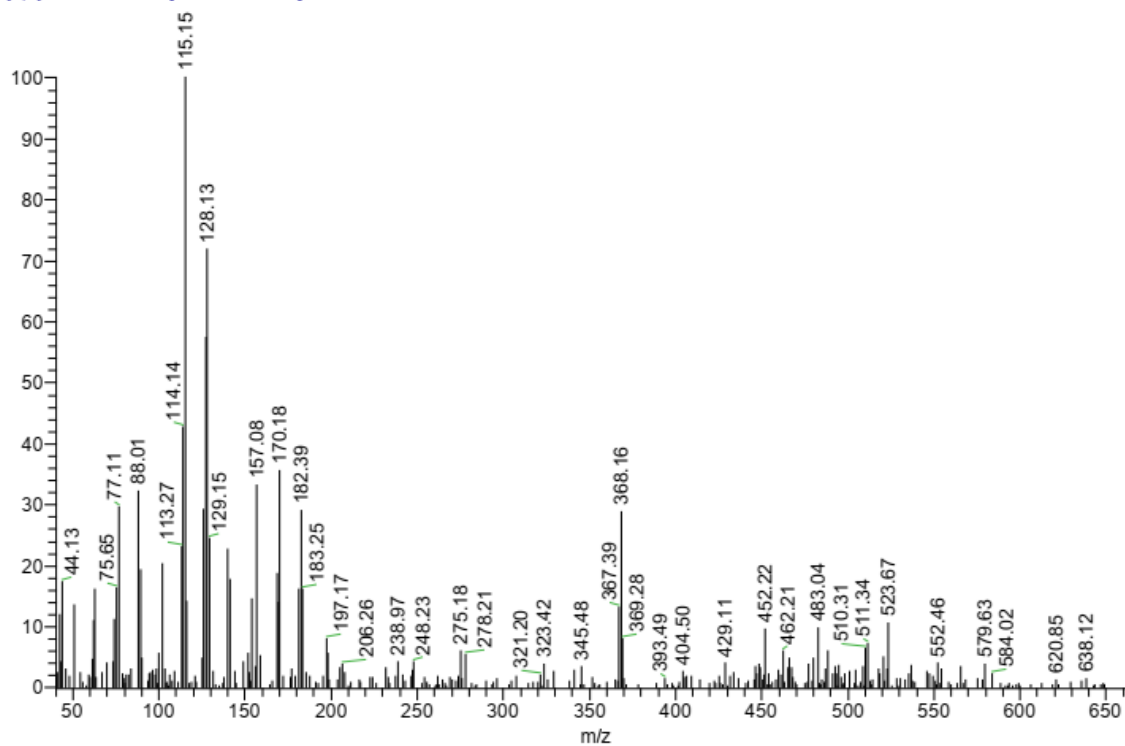


¹H NMR of 7c in DMSO

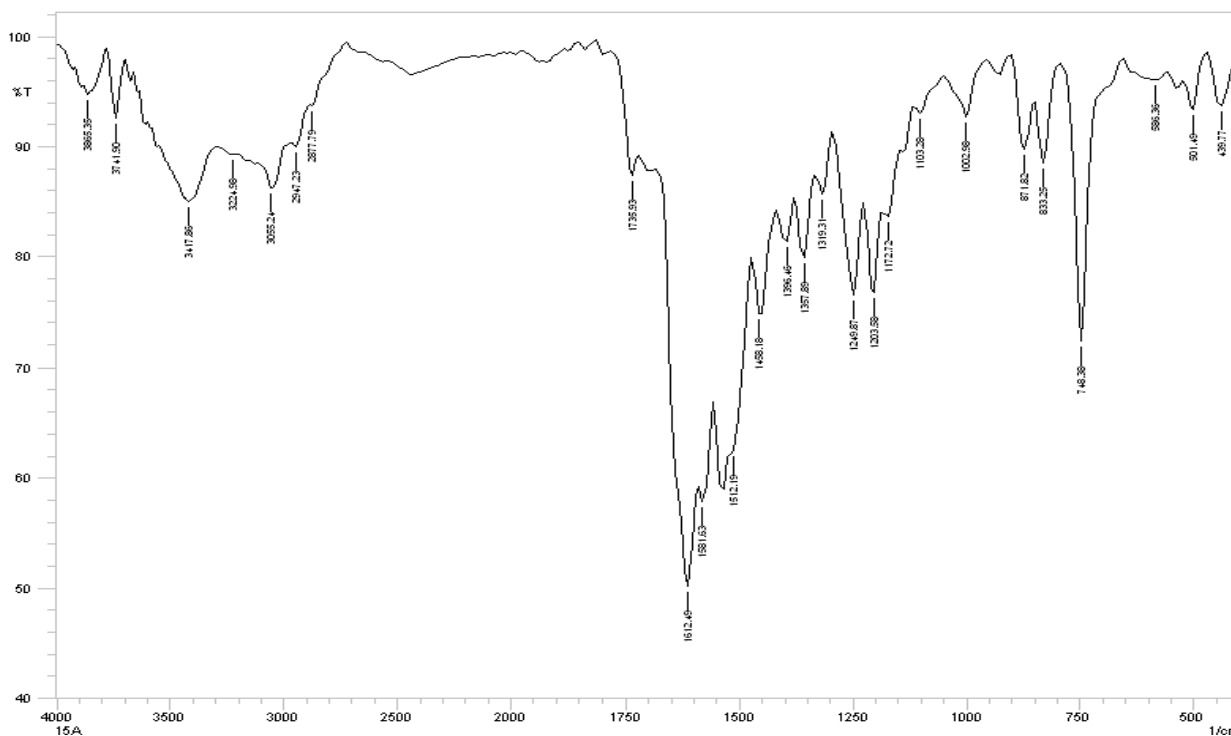


¹³C NMR of 7c in DMSO

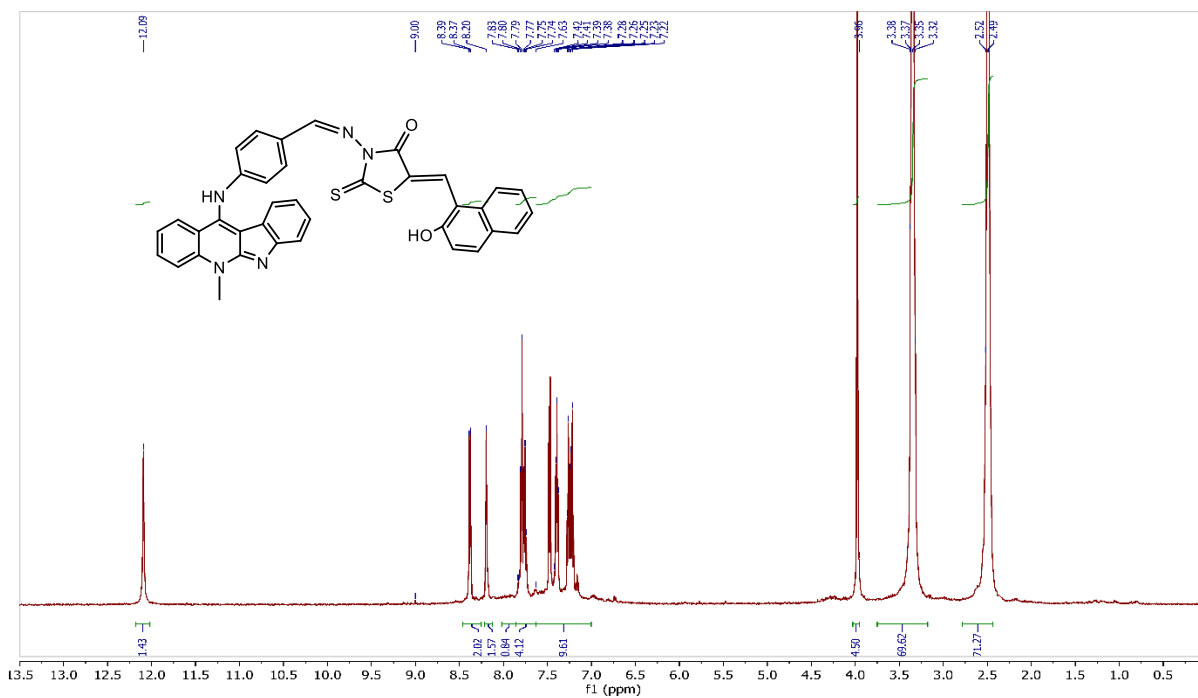
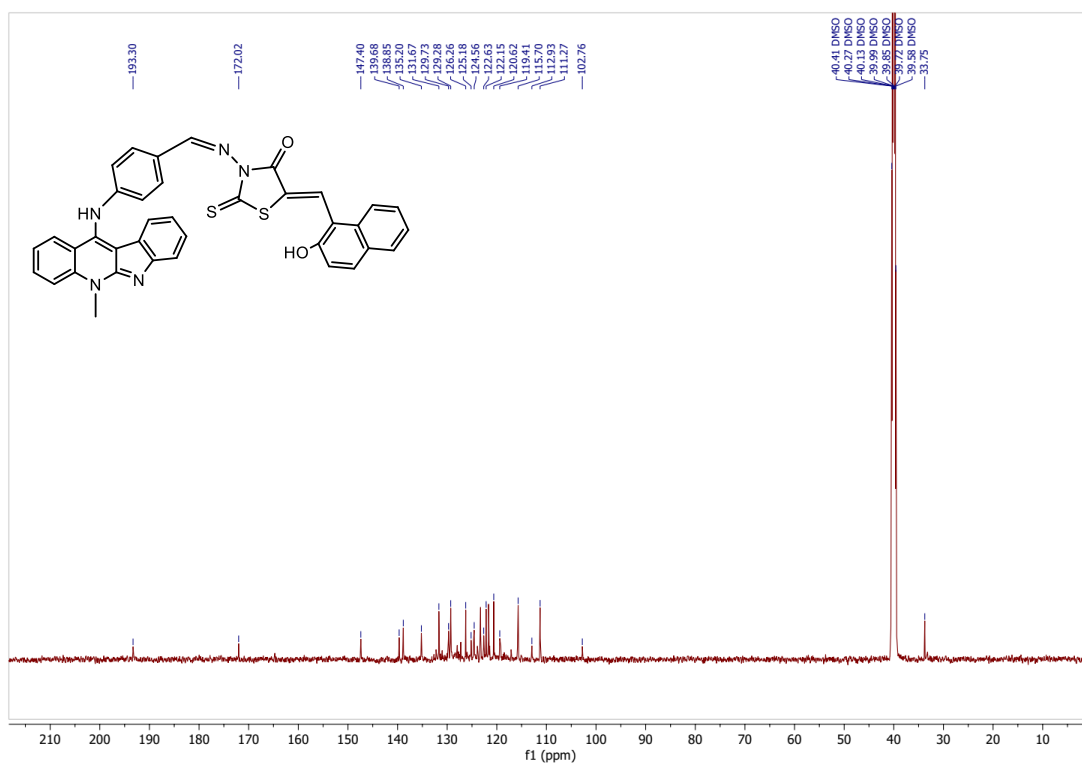
abdallah-ahmed-mohamed-15a #167 RT: 2.81 AV: 1 SB: 2 4.44, 4.44 NL: 1.77E4
T: {0,0} + c EI Full ms [40.00-1000.00]



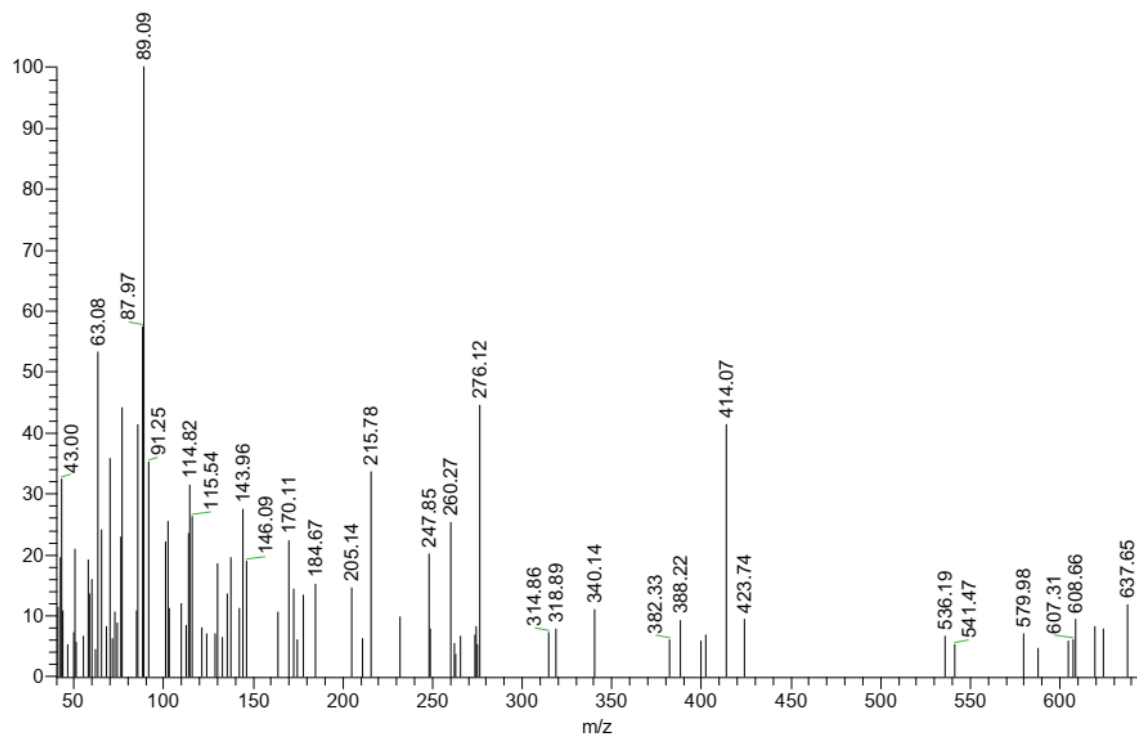
EI-MS of 7c



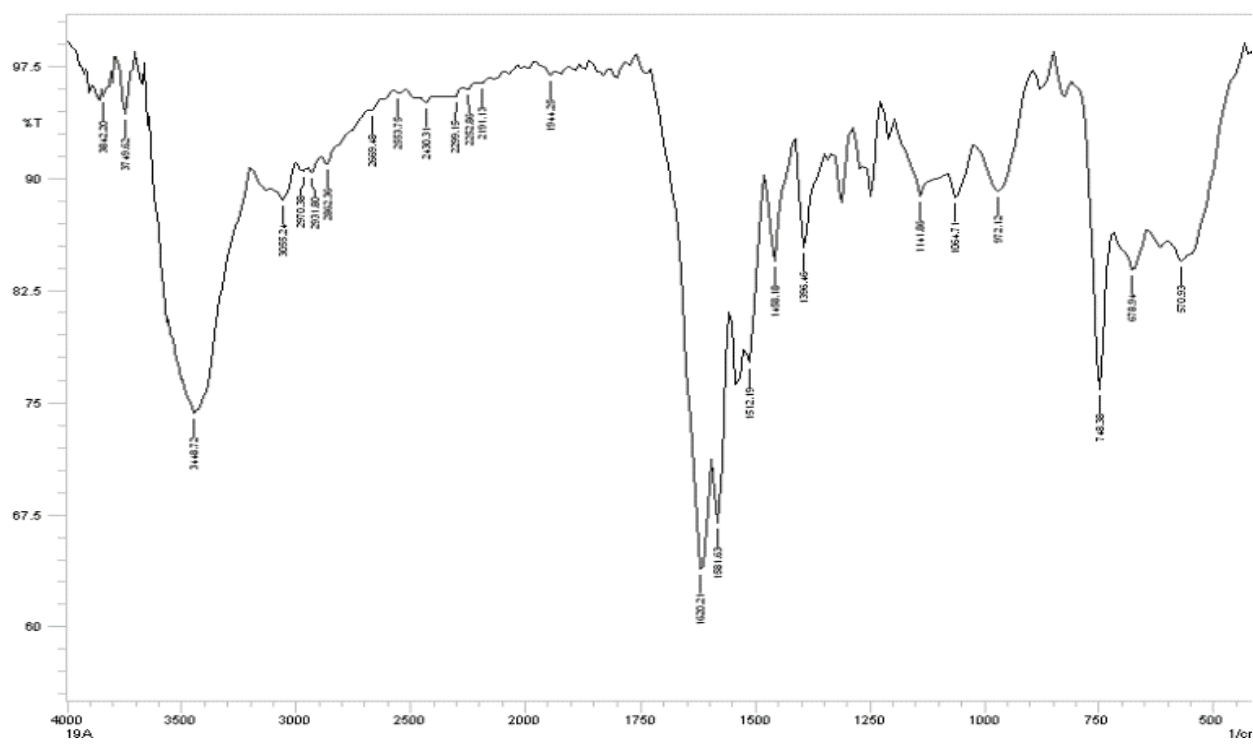
FT IR of compound 7c

¹H NMR of 7d in DMSO¹³C NMR of 7d in DMSO

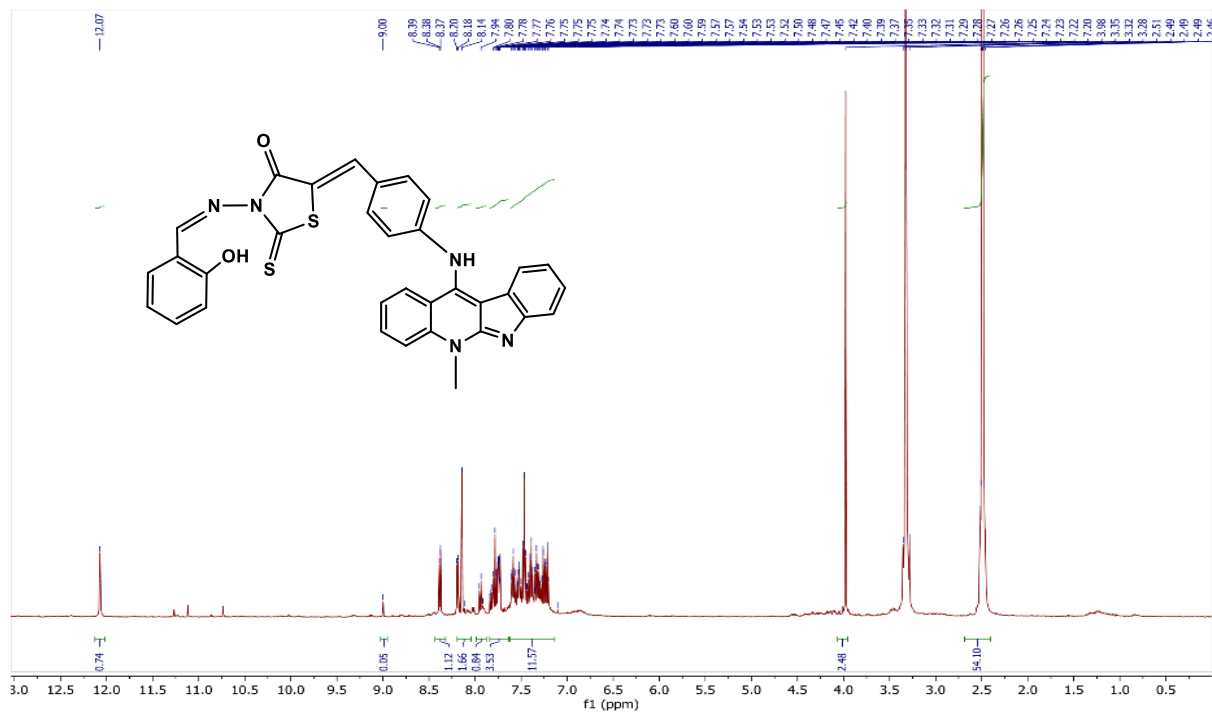
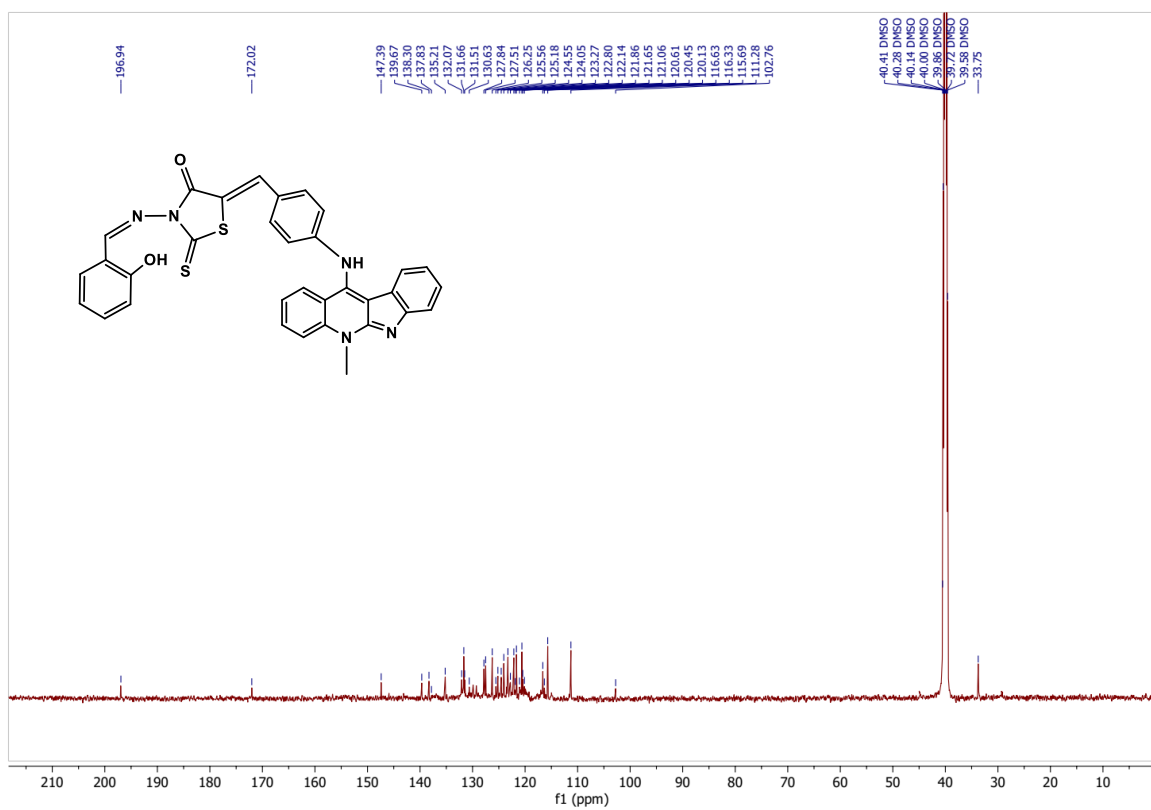
abdallah-ahmed-mohamed-19a #116 RT: 1.96 AV: 1 SB: 2 4.42, 4.42 NL: 1.65E3
T: {0,0} + c EI Full ms [40.00-1000.00]



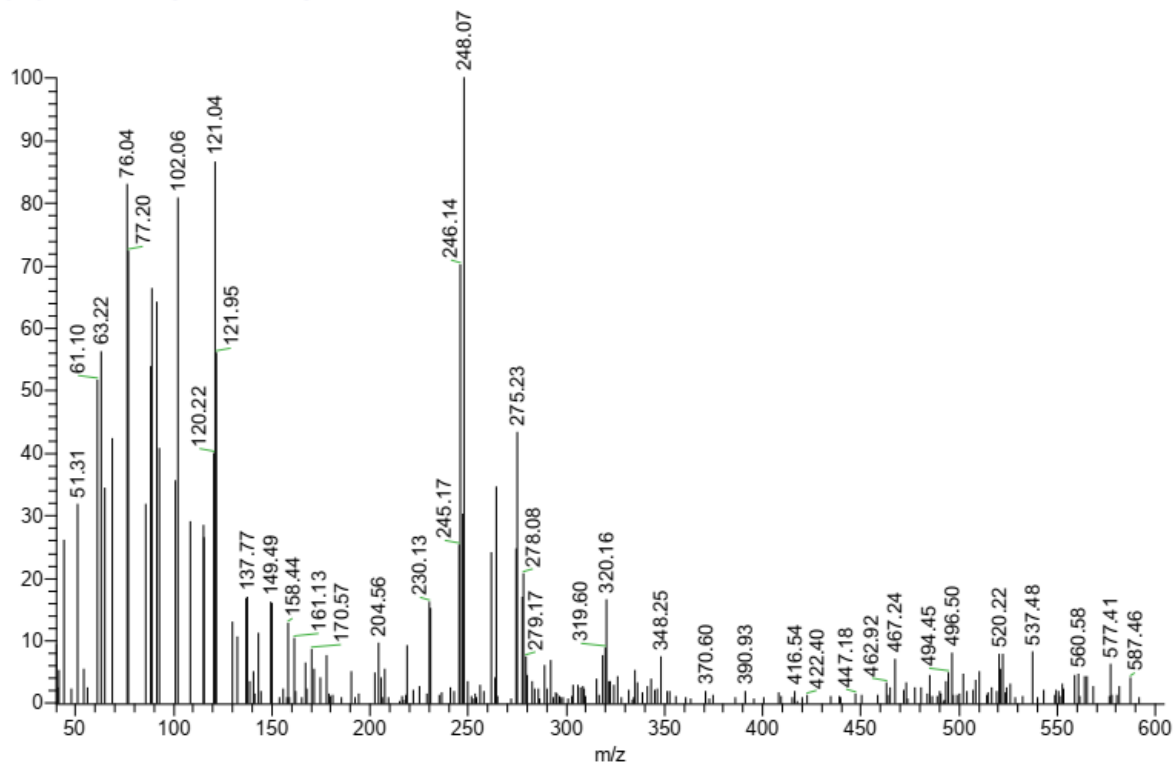
EI-MS of 7d



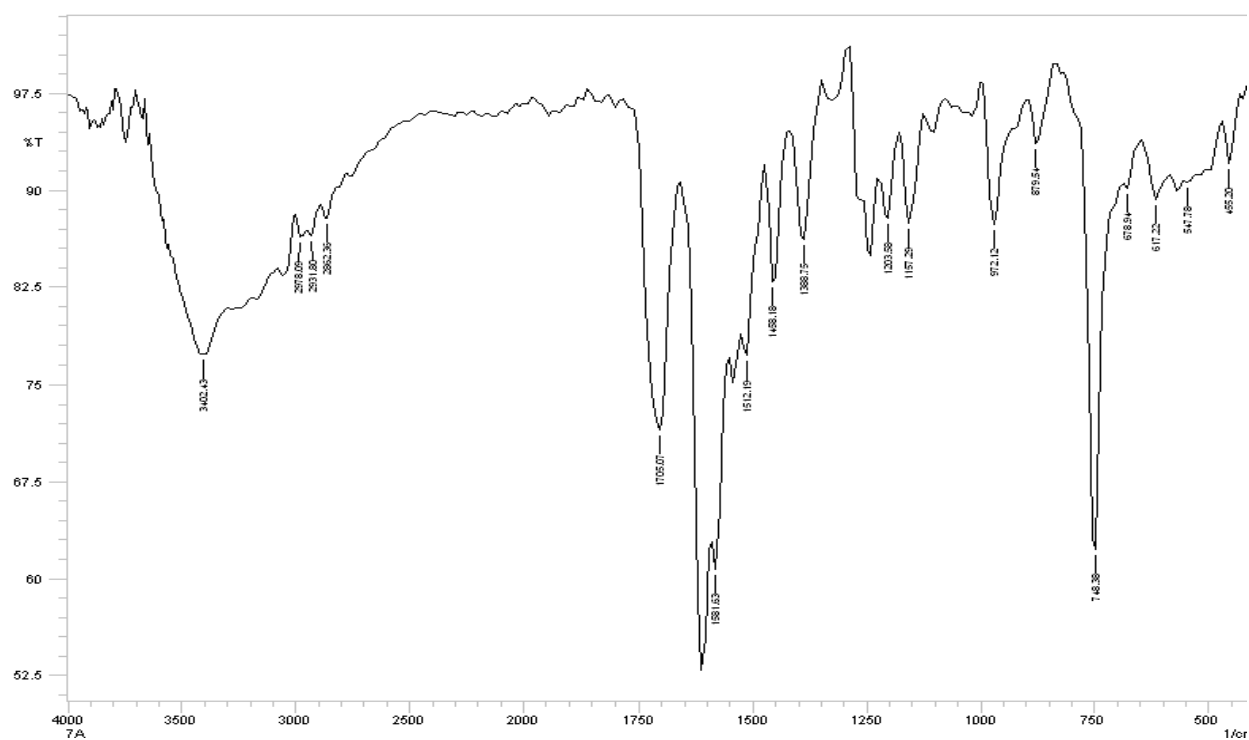
FT IR of compound 7d

¹H NMR of **9b** in DMSO¹³C NMR of **9b** in DMSO

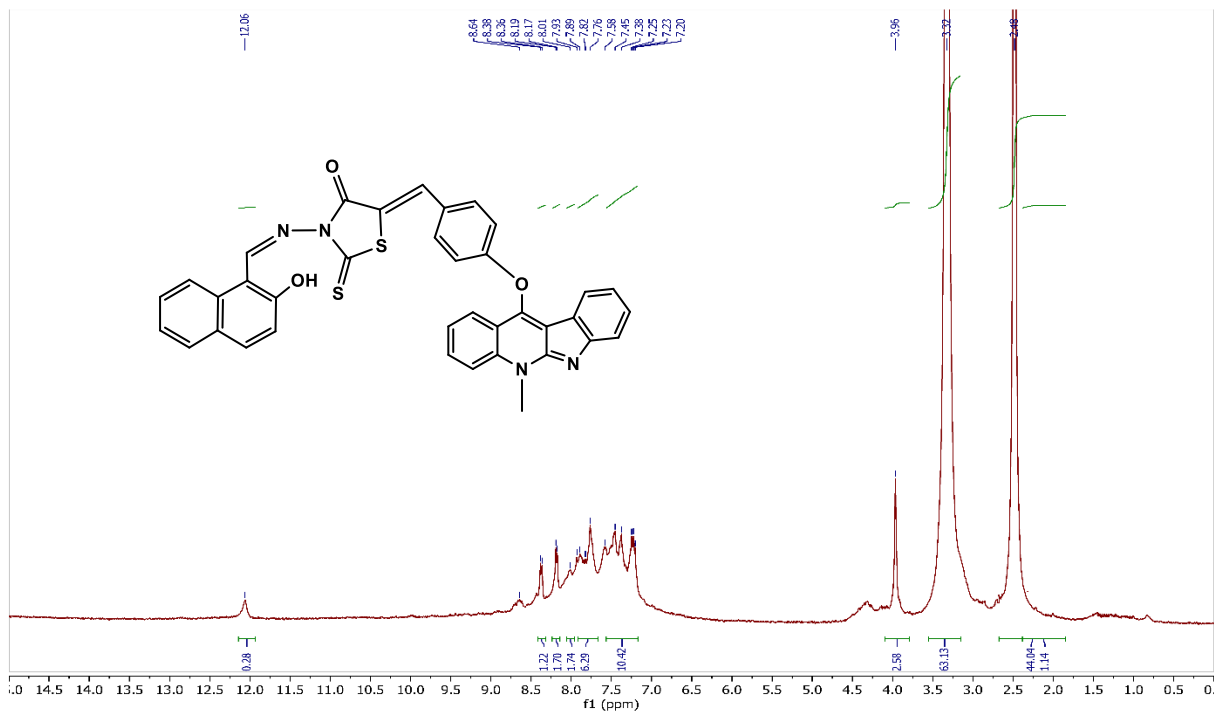
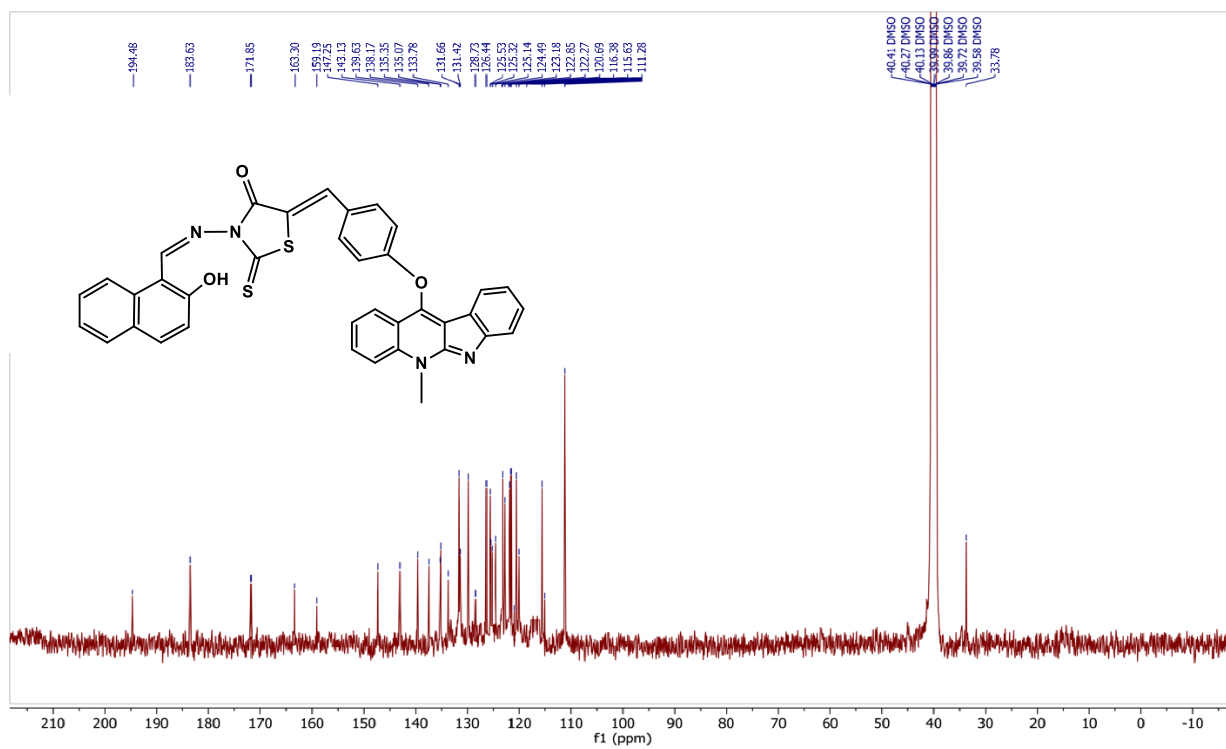
abdallah-ahmed-mohamed-7a #189 RT: 3.18 AV: 1 SB: 2 4.42, 4.42 NL: 9.91E3
T: {0,0} + c EI Full ms [40.00-1000.00]



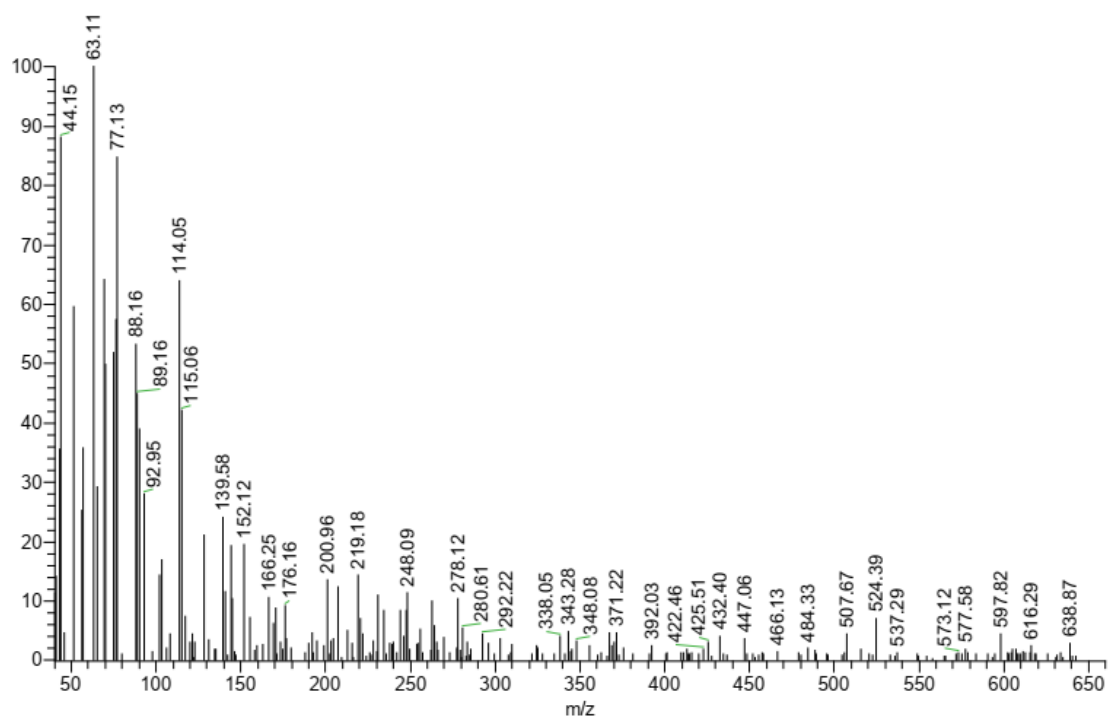
EI-MS of 9b



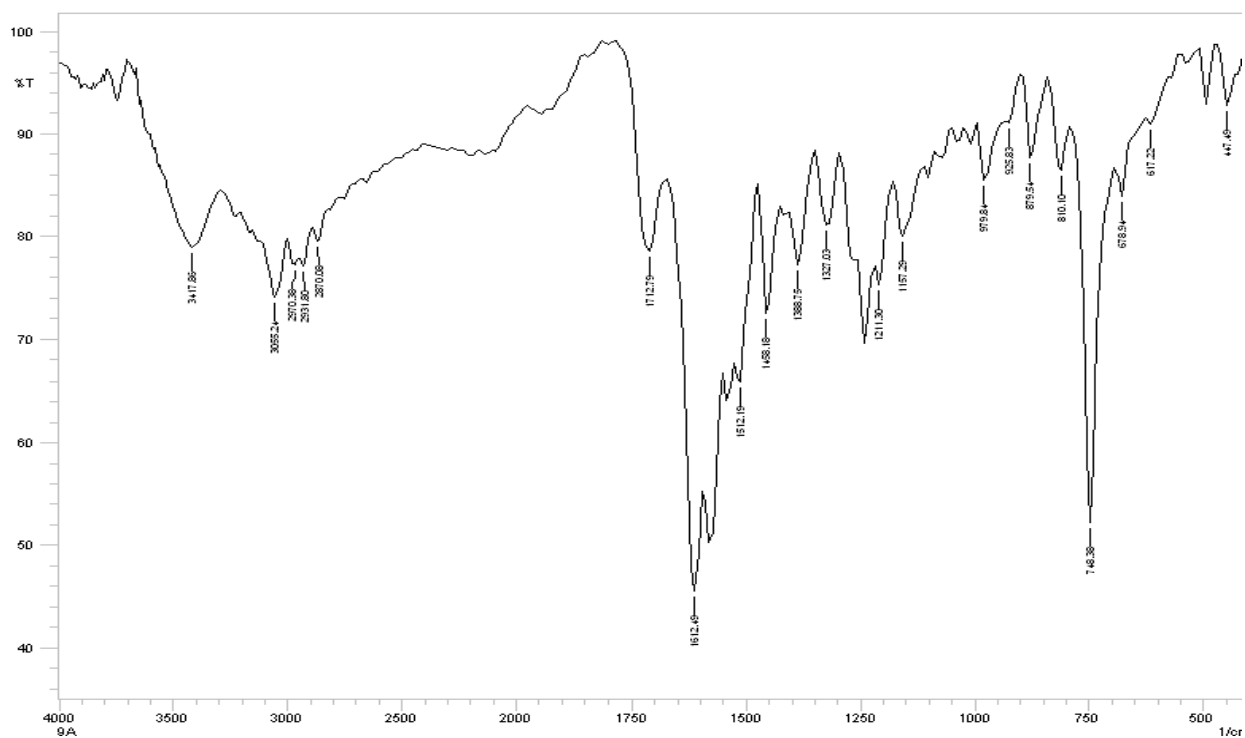
FT IR of compound 9b

¹H NMR of 9c in DMSO¹³C NMR of 9c in DMSO

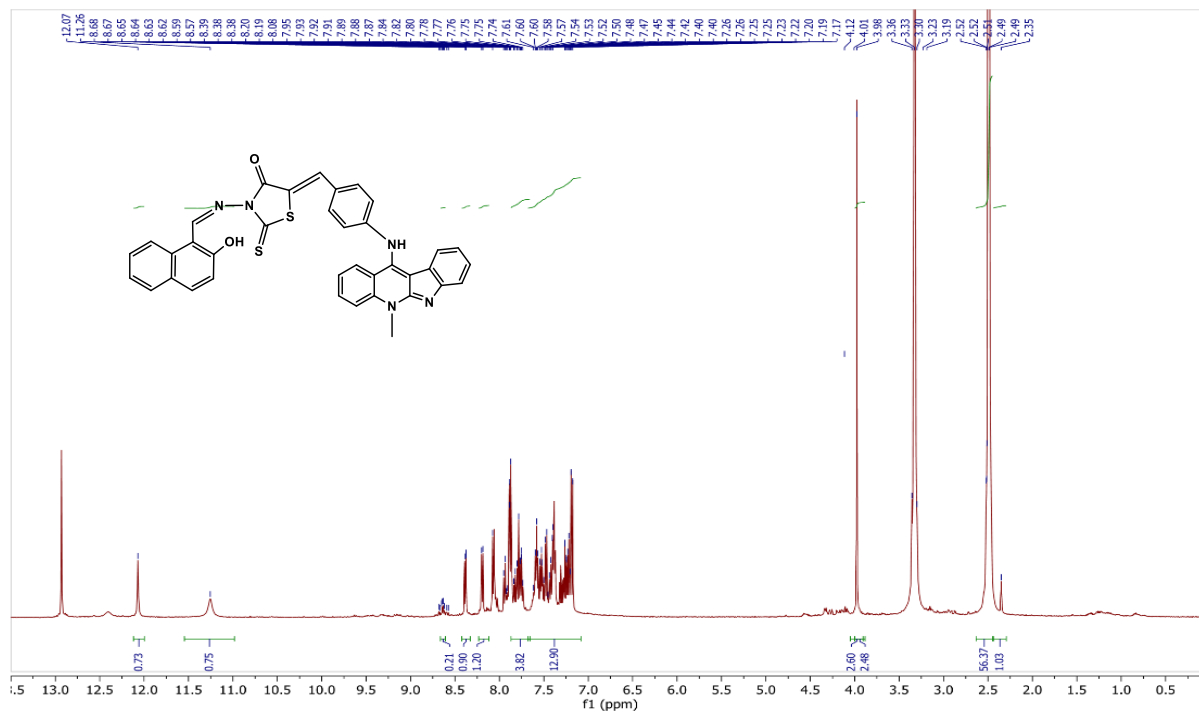
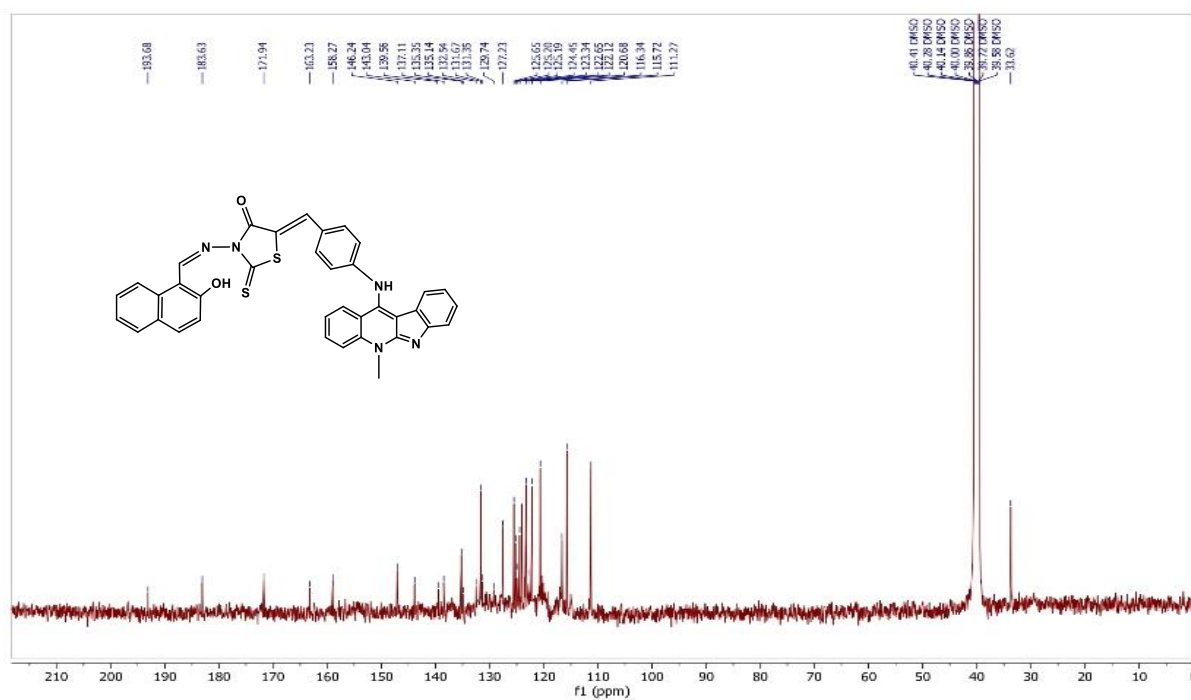
abdallah-ahmed-mohamed-9a #230 RT: 3.87 AV: 1 SB: 2 4.49, 4.49 NL: 1.03E4
T: {0,0} + c EI Full ms [40.00-1000.00]



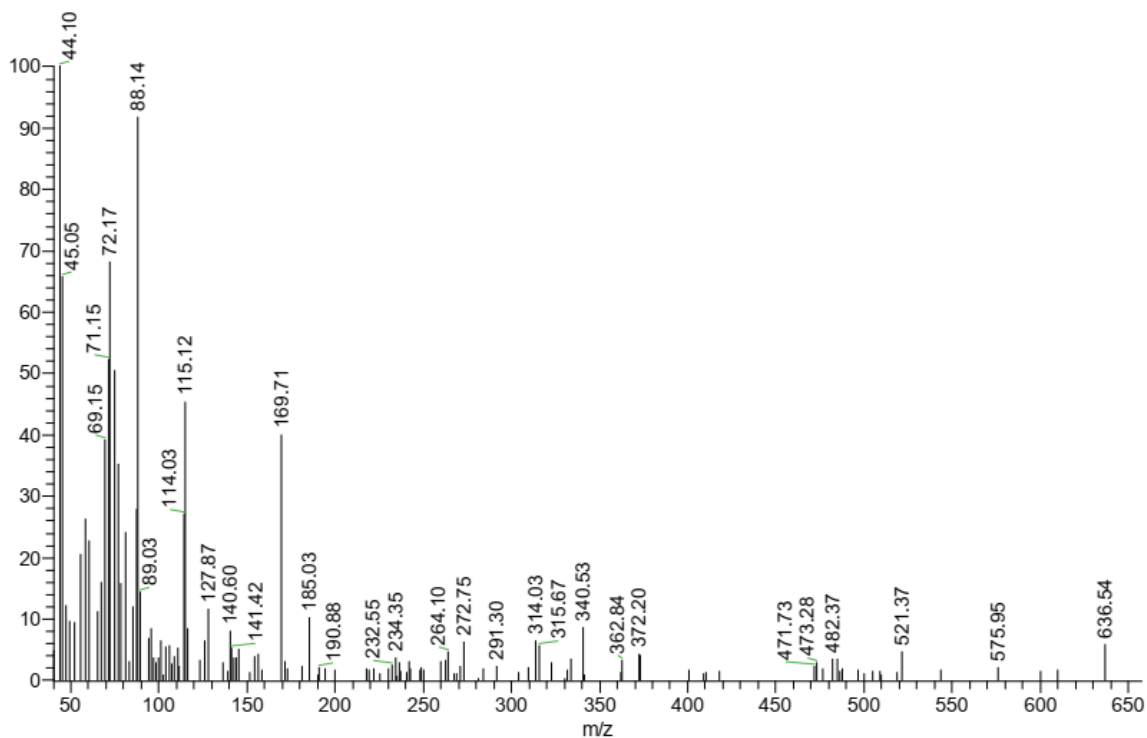
EI-MS of 9c



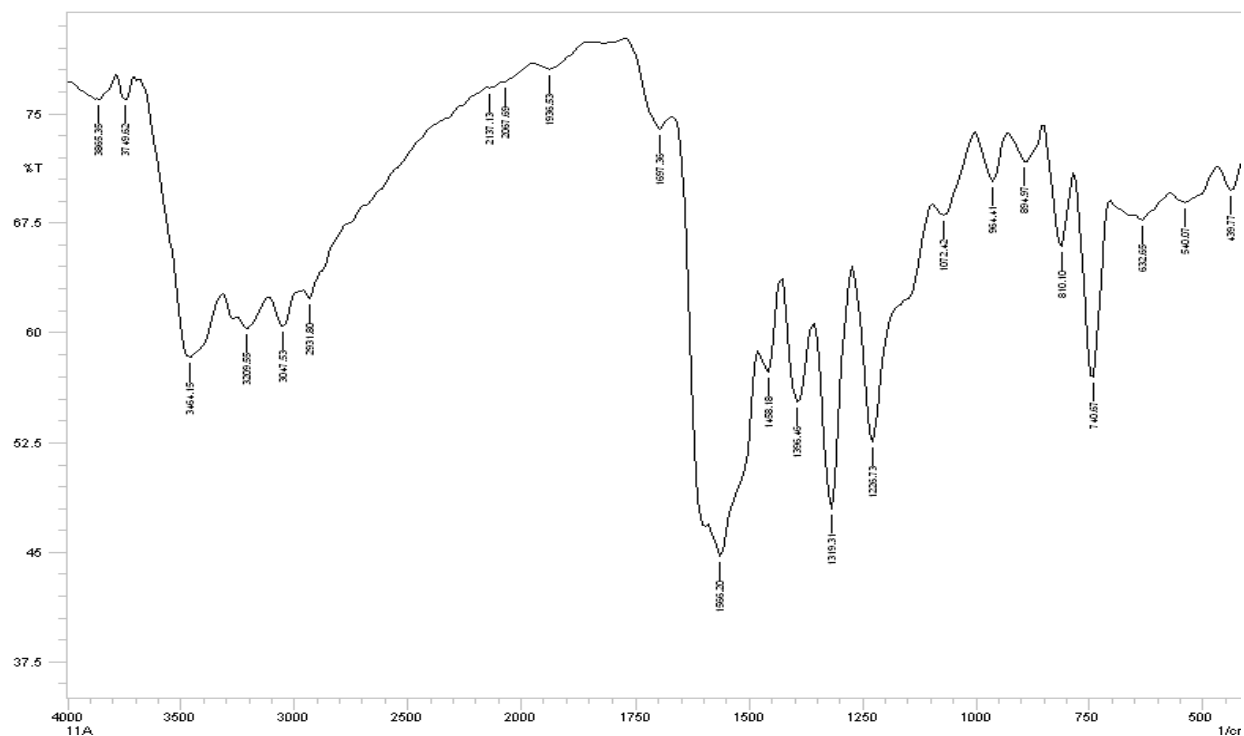
FT IR of compound 9c

¹H NMR of 9d in DMSO

abdallah-ahmed-mohamed-11a #154 RT: 2.59 AV: 1 SB: 2 4.49, 4.49 NL: 6.14E3
T: {0,0} + c EI Full ms [40.00-1000.00]



EL-MS of 9d

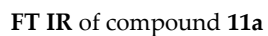


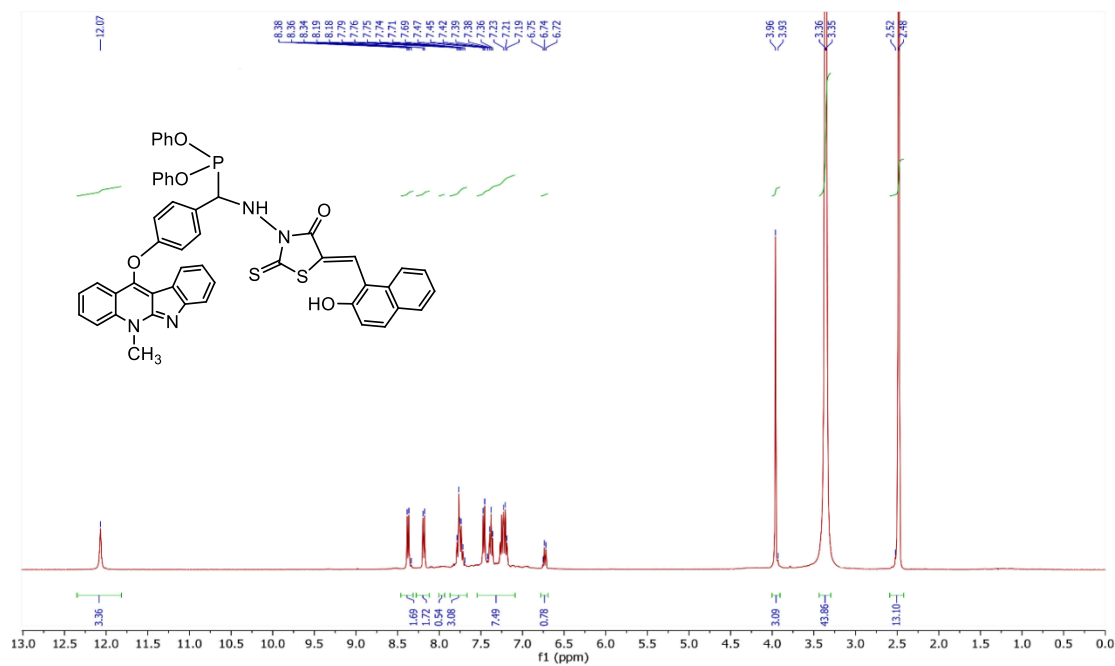
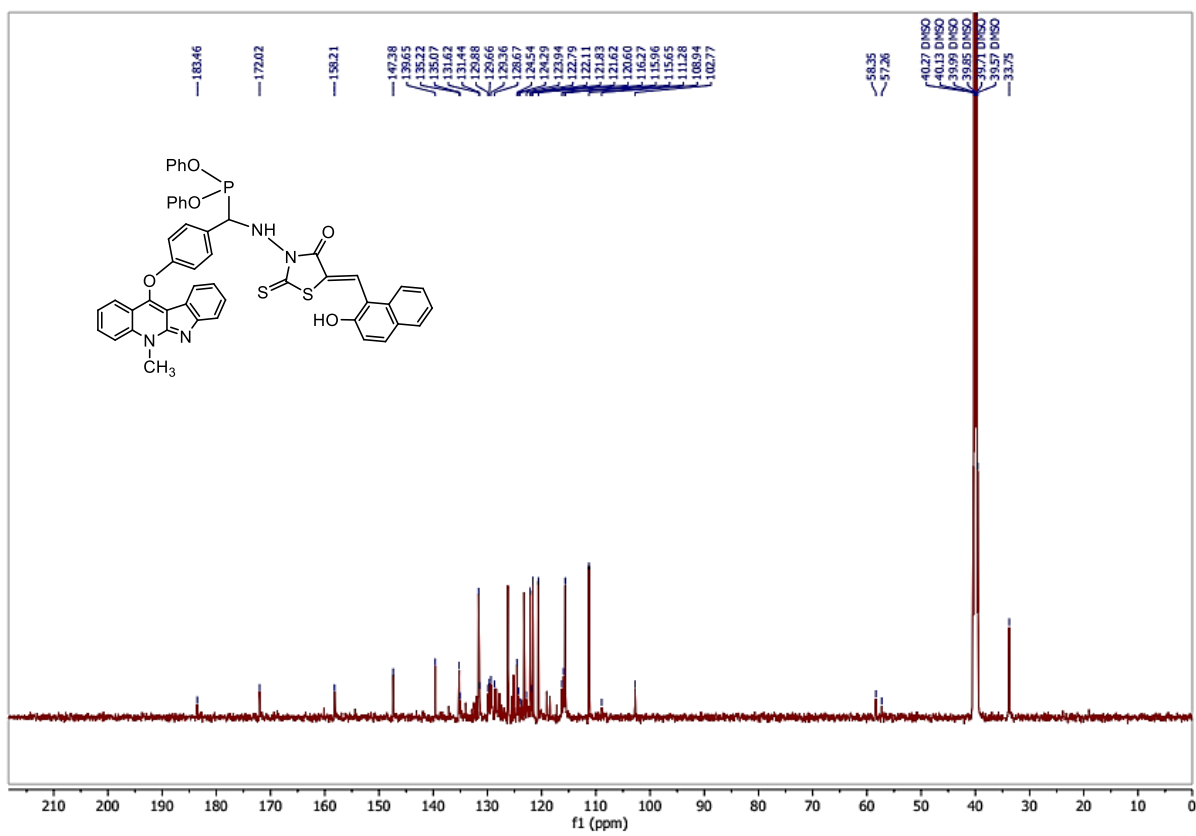
FT IR of compound 9d

Chemical structure of compound 10 is shown. The structure is a complex molecule featuring a 4-methyl-1H-indole-3-carboxamide derivative linked via a phosphonate group to a 4-((4-((4-hydroxyphenyl)vinyl)thio)thio)phenyl group.

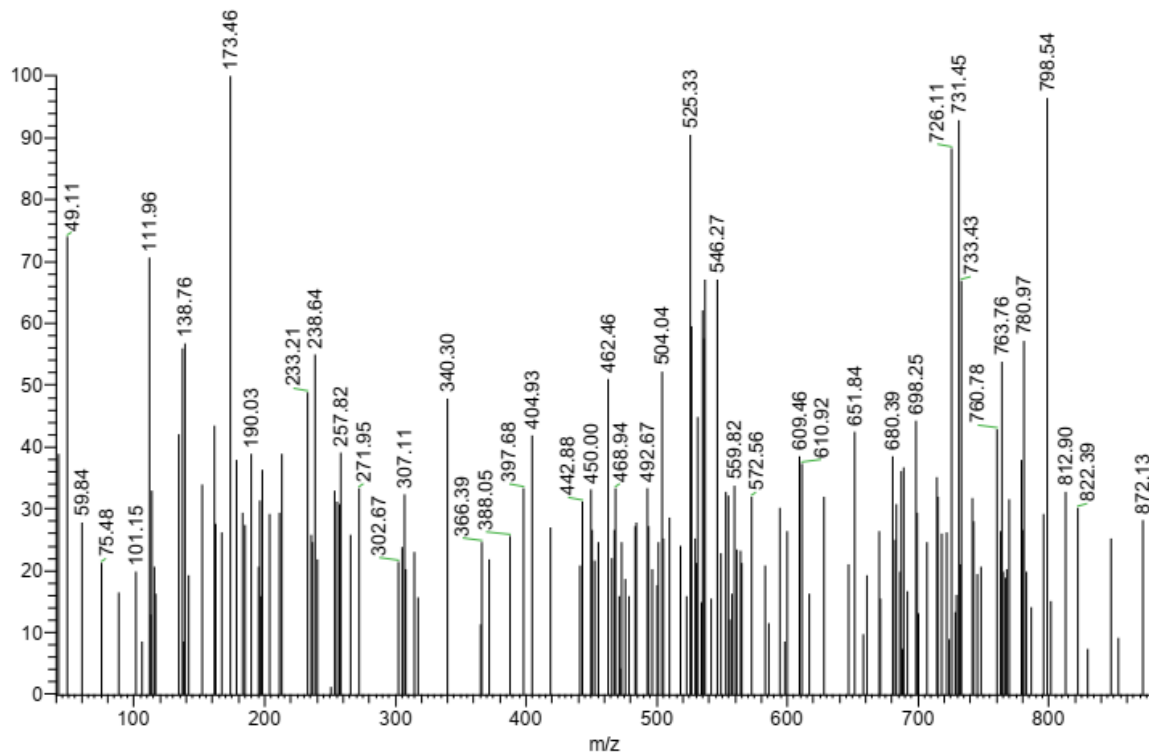
¹³C NMR spectrum (f1 (ppm)) of compound 10. The spectrum shows peaks corresponding to the chemical structure, with labeled chemical shifts (ppm): 193.41, 172.03, 158.26, 147.61, 139.54, 135.22, 132.56, 132.55, 132.54, 132.53, 132.52, 132.51, 132.50, 132.49, 132.48, 132.47, 132.46, 132.45, 132.44, 132.43, 132.42, 132.41, 132.40, 132.39, 132.38, 132.37, 132.36, 132.35, 132.34, 132.33, 132.32, 132.31, 132.30, 132.29, 132.28, 132.27, 132.26, 132.25, 132.24, 132.23, 132.22, 132.21, 132.20, 132.19, 132.18, 132.17, 132.16, 132.15, 132.14, 132.13, 132.12, 132.11, 132.10, 132.09, 132.08, 132.07, 132.06, 132.05, 132.04, 132.03, 132.02, 132.01, 132.00, 131.99, 131.98, 131.97, 131.96, 131.95, 131.94, 131.93, 131.92, 131.91, 131.90, 131.89, 131.88, 131.87, 131.86, 131.85, 131.84, 131.83, 131.82, 131.81, 131.80, 131.79, 131.78, 131.77, 131.76, 131.75, 131.74, 131.73, 131.72, 131.71, 131.70, 131.69, 131.68, 131.67, 131.66, 131.65, 131.64, 131.63, 131.62, 131.61, 131.60, 131.59, 131.58, 131.57, 131.56, 131.55, 131.54, 131.53, 131.52, 131.51, 131.50, 131.49, 131.48, 131.47, 131.46, 131.45, 131.44, 131.43, 131.42, 131.41, 131.40, 131.39, 131.38, 131.37, 131.36, 131.35, 131.34, 131.33, 131.32, 131.31, 131.30, 131.29, 131.28, 131.27, 131.26, 131.25, 131.24, 131.23, 131.22, 131.21, 131.20, 131.19, 131.18, 131.17, 131.16, 131.15, 131.14, 131.13, 131.12, 131.11, 131.10, 131.09, 131.08, 131.07, 131.06, 131.05, 131.04, 131.03, 131.02, 131.01, 131.00, 130.99, 130.98, 130.97, 130.96, 130.95, 130.94, 130.93, 130.92, 130.91, 130.90, 130.89, 130.88, 130.87, 130.86, 130.85, 130.84, 130.83, 130.82, 130.81, 130.80, 130.79, 130.78, 130.77, 130.76, 130.75, 130.74, 130.73, 130.72, 130.71, 130.70, 130.69, 130.68, 130.67, 130.66, 130.65, 130.64, 130.63, 130.62, 130.61, 130.60, 130.59, 130.58, 130.57, 130.56, 130.55, 130.54, 130.53, 130.52, 130.51, 130.50, 130.49, 130.48, 130.47, 130.46, 130.45, 130.44, 130.43, 130.42, 130.41, 130.40, 130.39, 130.38, 130.37, 130.36, 130.35, 130.34, 130.33, 130.32, 130.31, 130.30, 130.29, 130.28, 130.27, 130.26, 130.25, 130.24, 130.23, 130.22, 130.21, 130.20, 130.19, 130.18, 130.17, 130.16, 130.15, 130.14, 130.13, 130.12, 130.11, 130.10, 130.09, 130.08, 130.07, 130.06, 130.05, 130.04, 130.03, 130.02, 130.01, 130.00, 129.99, 129.98, 129.97, 129.96, 129.95, 129.94, 129.93, 129.92, 129.91, 129.90, 129.89, 129.88, 129.87, 129.86, 129.85, 129.84, 129.83, 129.82, 129.81, 129.80, 129.79, 129.78, 129.77, 129.76, 129.75, 129.74, 129.73, 129.72, 129.71, 129.70, 129.69, 129.68, 129.67, 129.66, 129.65, 129.64, 129.63, 129.62, 129.61, 129.60, 129.59, 129.58, 129.57, 129.56, 129.55, 129.54, 129.53, 129.52, 129.51, 129.50, 129.49, 129.48, 129.47, 129.46, 129.45, 129.44, 129.43, 129.42, 129.41, 129.40, 129.39, 129.38, 129.37, 129.36, 129.35, 129.34, 129.33, 129.32, 129.31, 129.30, 129.29, 129.28, 129.27, 129.26, 129.25, 129.24, 129.23, 129.22, 129.21, 129.20, 129.19, 129.18, 129.17, 129.16, 129.15, 129.14, 129.13, 129.12, 129.11, 129.10, 129.09, 129.08, 129.07, 129.06, 129.05, 129.04, 129.03, 129.02, 129.01, 129.00, 128.99, 128.98, 128.97, 128.96, 128.95, 128.94, 128.93, 128.92, 128.91, 128.90, 128.89, 128.88, 128.87, 128.86, 128.85, 128.84, 128.83, 128.82, 128.81, 128.80, 128.79, 128.78, 128.77, 128.76, 128.75, 128.74, 128.73, 128.72, 128.71, 128.70, 128.69, 128.68, 128.67, 128.66, 128.65, 128.64, 128.63, 128.62, 128.61, 128.60, 128.59, 128.58, 128.57, 128.56, 128.55, 128.54, 128.53, 128.52, 128.51, 128.50, 128.49, 128.48, 128.47, 128.46, 128.45, 128.44, 128.43, 128.42, 128.41, 128.40, 128.39, 128.38, 128.37, 128.36, 128.35, 128.34, 128.33, 128.32, 128.31, 128.30, 128.29, 128.28, 128.27, 128.26, 128.25, 128.24, 128.23, 128.22, 128.21, 128.20, 128.19, 128.18, 128.17, 128.16, 128.15, 128.14, 128.13, 128.12, 128.11, 128.10, 128.09, 128.08, 128.07, 128.06, 128.05, 128.04, 128.03, 128.02, 128.01, 128.00, 127.99, 127.98, 127.97, 127.96, 127.95, 127.94, 127.93, 127.92, 127.91, 127.90, 127.89,

 ^{13}C NMR of **11a** in DMSO

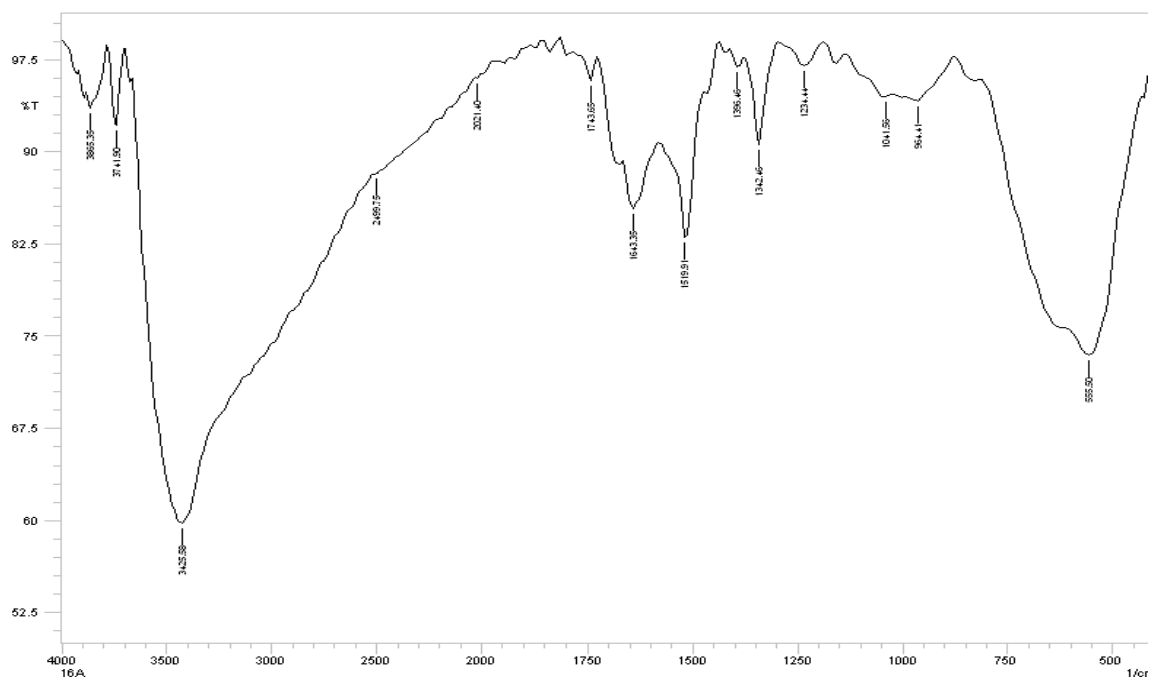


¹H NMR of 11c in DMSO¹³C NMR of 11c in DMSO

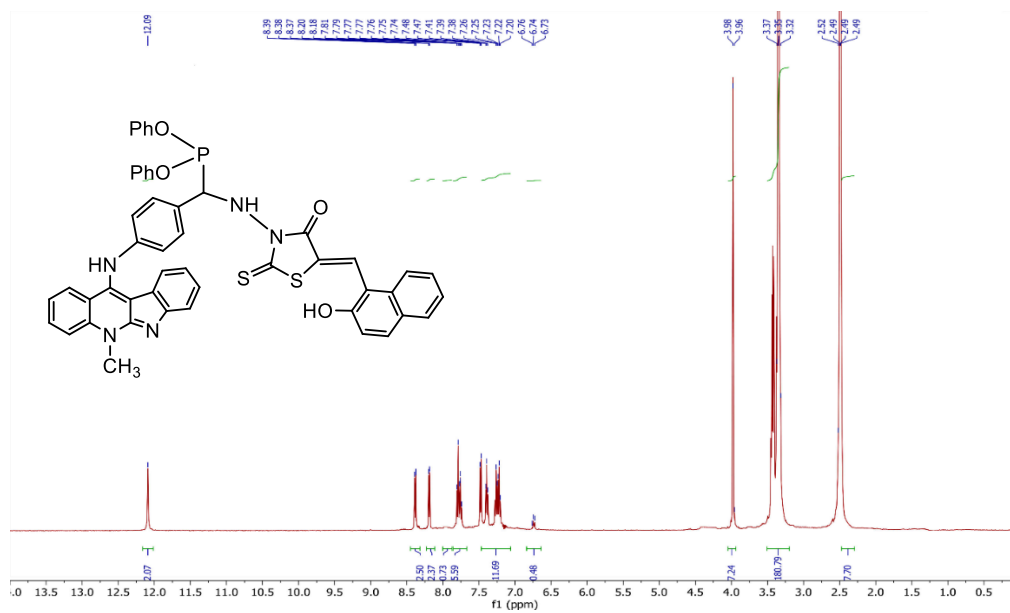
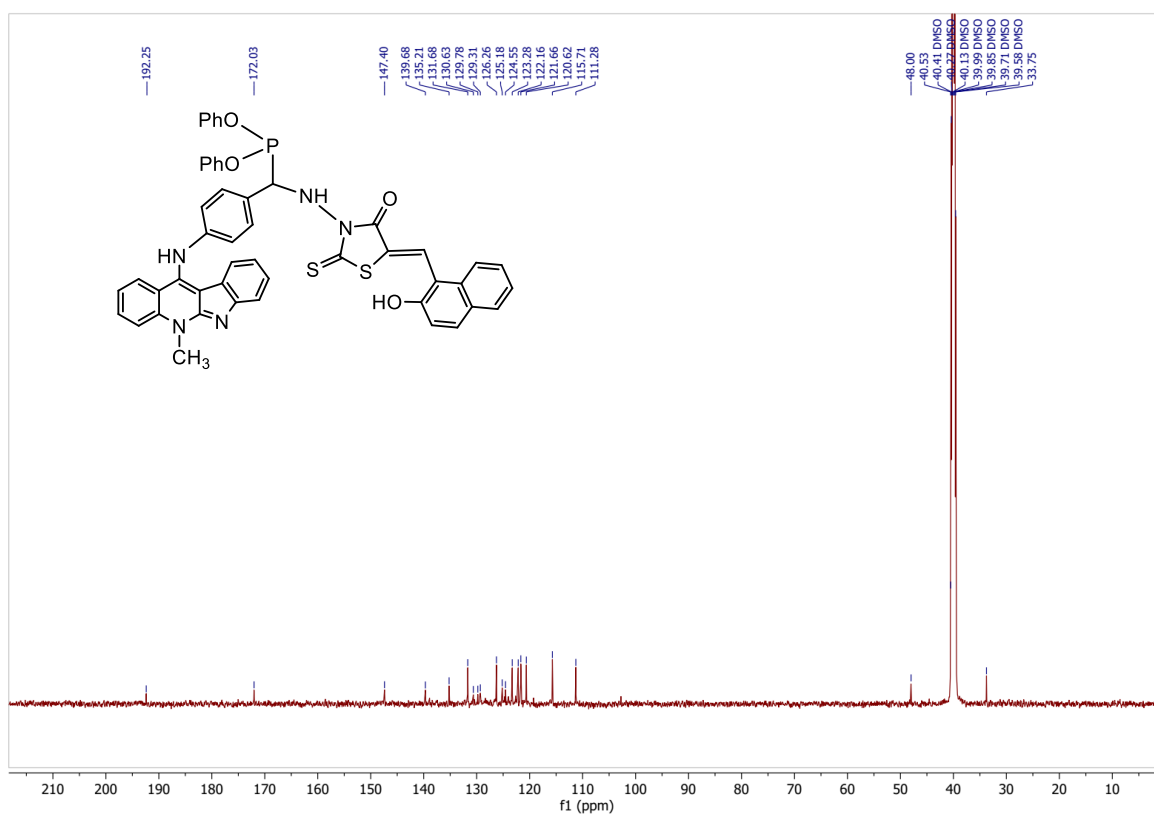
abdallah-ahmed-mohamed-16a #58 RT: 0.99 AV: 1 SB: 2 4.55, 4.55 NL: 3.94E2
T: {0,0} + c EI Full ms [40.00-1000.00]



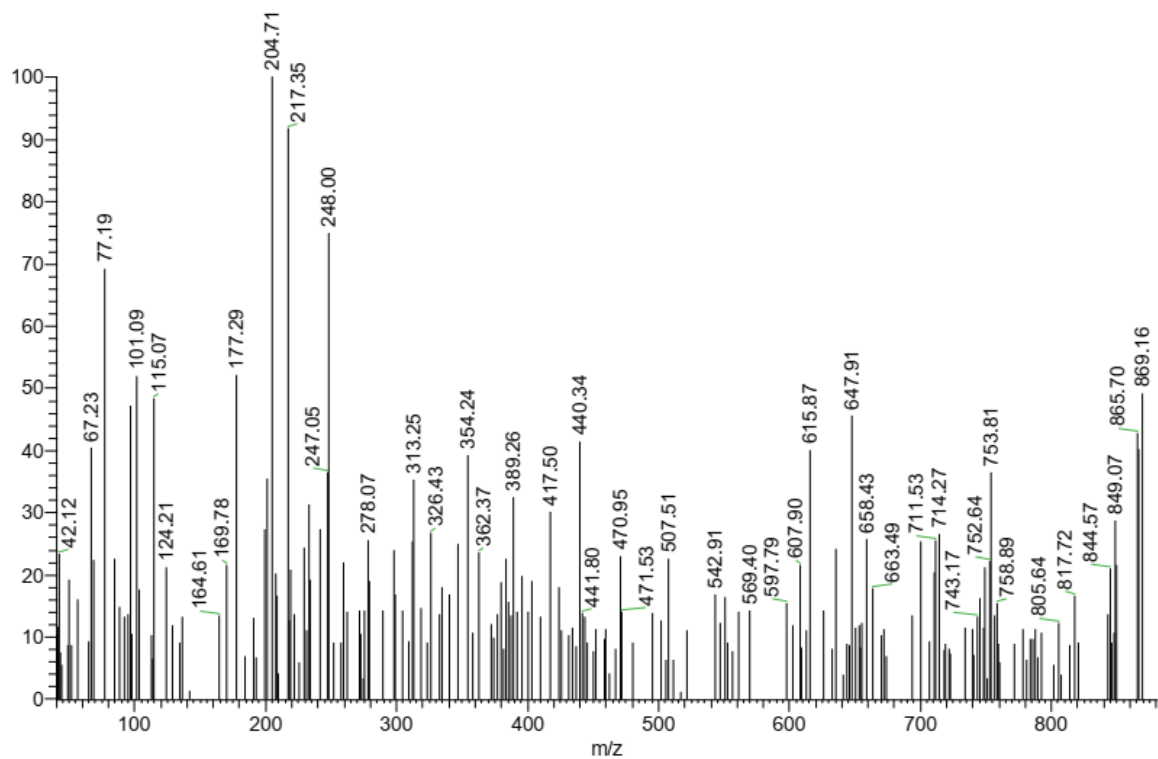
EI-MS of 11c



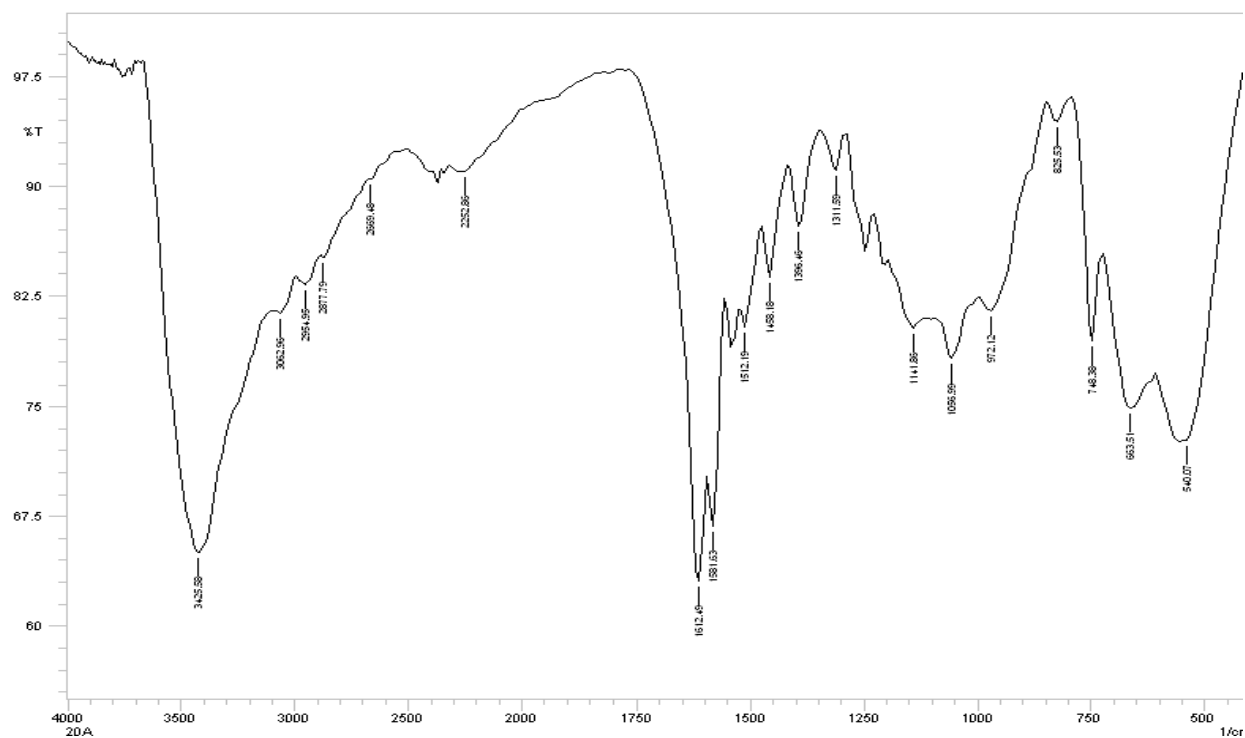
FT IR of compound 11c

¹H NMR of 11d in DMSO ^{13}C NMR of **11d** in DMSO

abdallah-ahmed-mohamed-20a #162 RT: 2.73 AV: 1 SB: 2 4.54, 4.54 NL: 9.08E2
T: {0,0} + c EI Full ms [40.00-1000.00]



EL-MS of 11d



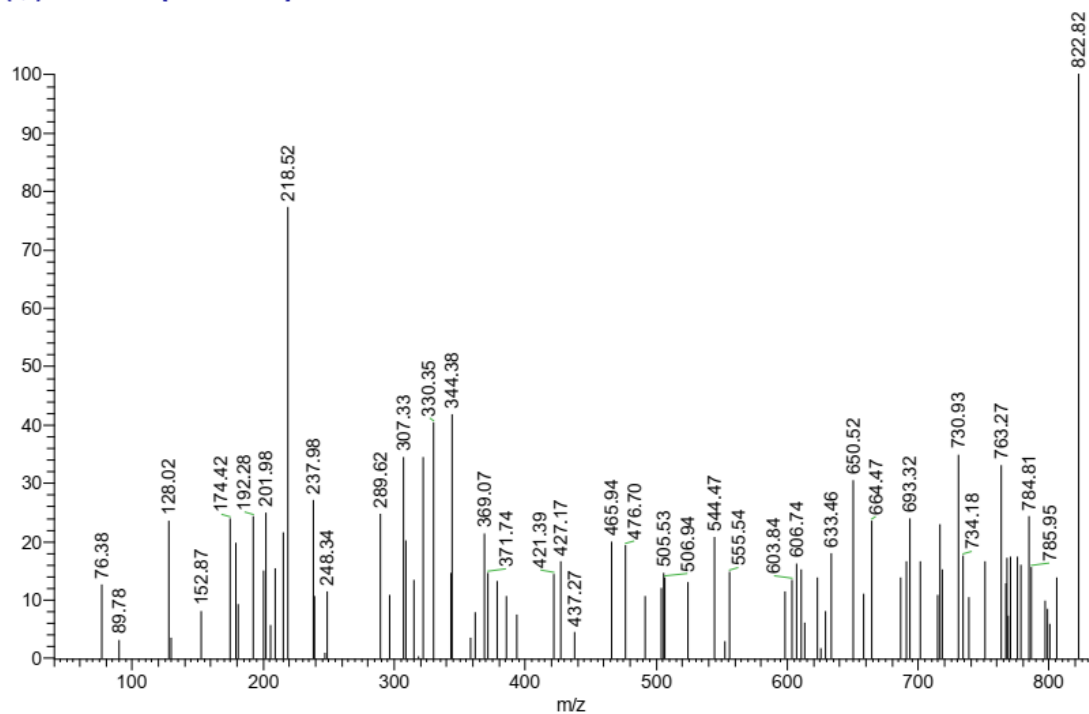
FT IR of compound 11d

Chemical structure of compound 10 is shown above the spectrum. The spectrum displays the following peak values (ppm):

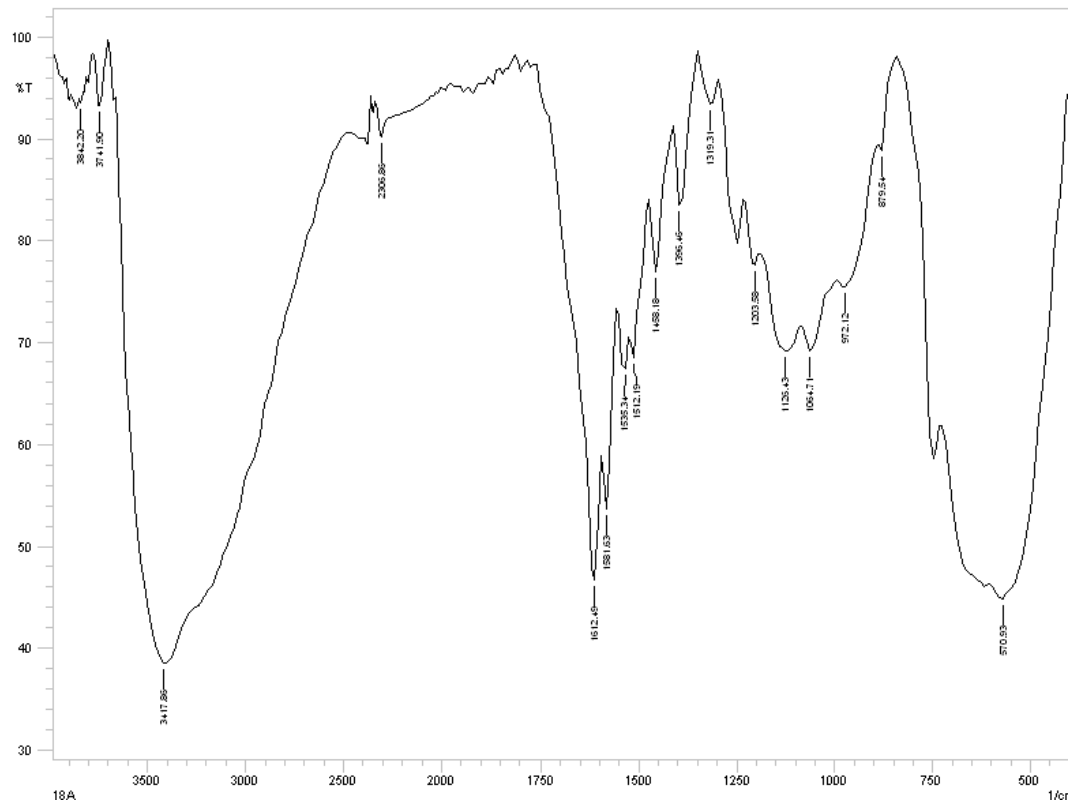
Peak Value (ppm)
183.49
172.01
147.33
143.02
139.60
138.39
135.29
135.18
131.57
131.39
128.83
128.20
125.49
125.33
124.52
123.40
123.22
122.77
122.07
121.80
121.60
120.38
119.44
117.54
116.21
115.60
111.25
102.75
58.80
58.15
40.29
40.16
39.88
39.75
34.67
33.72

 ^{13}C -NMR of **12a** in DMSO

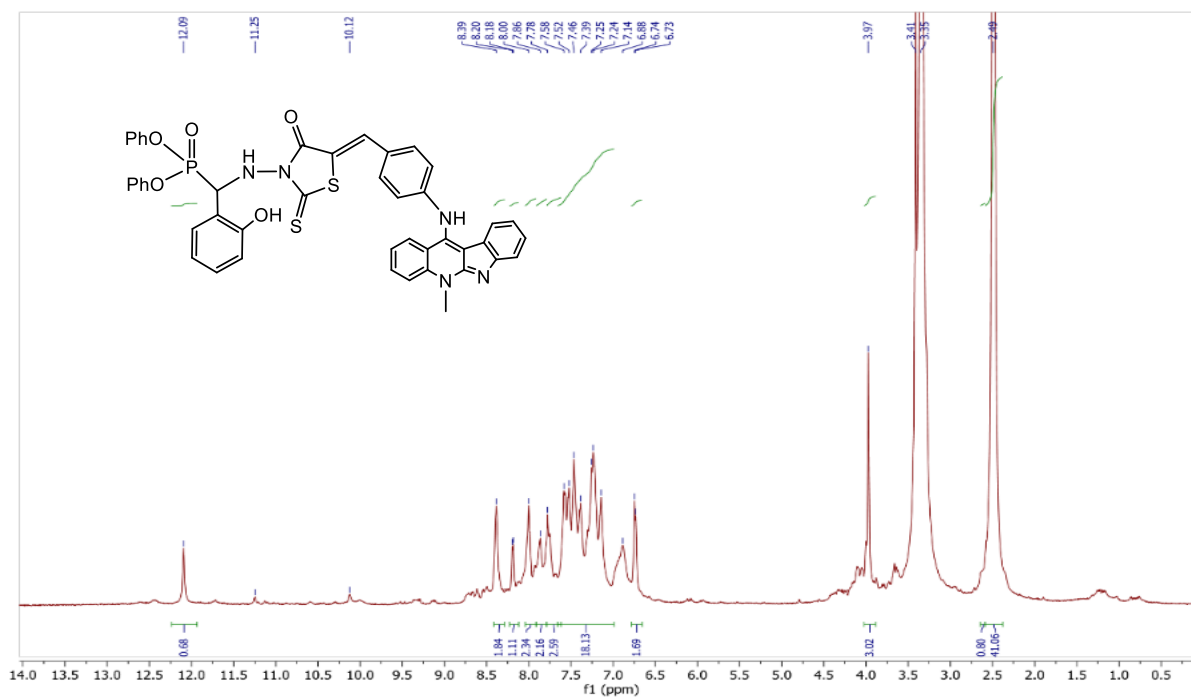
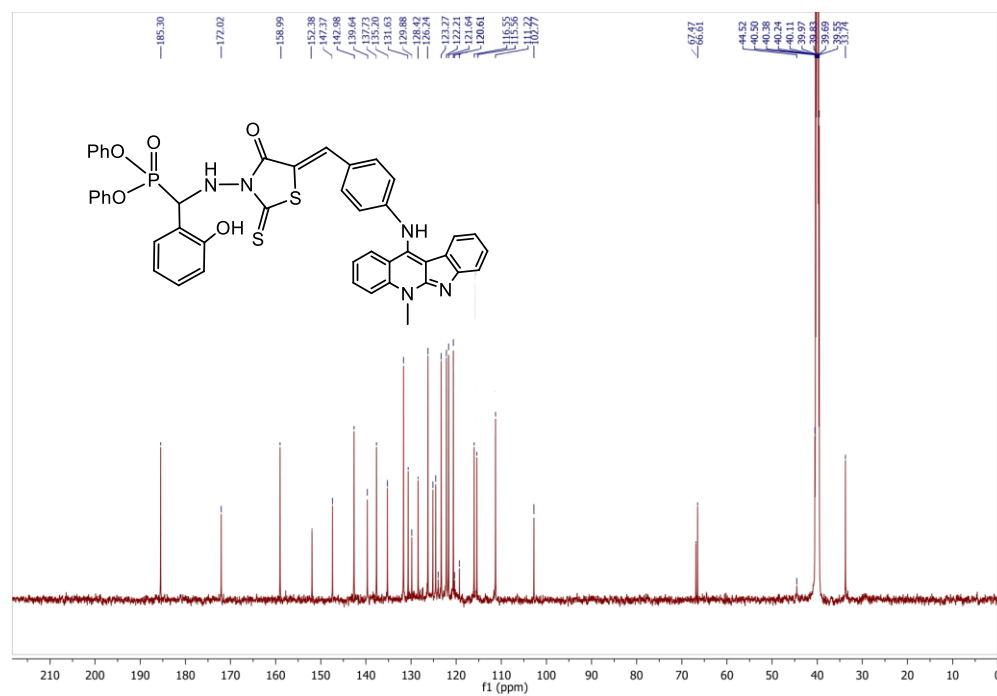
abdallah-ahmed-mohamed-6a #182 RT: 3.06 AV: 1 SB: 2 4.55, 4.59 NL: 6.75E2
T: {0,0} + c EI Full ms [40.00-1000.00]



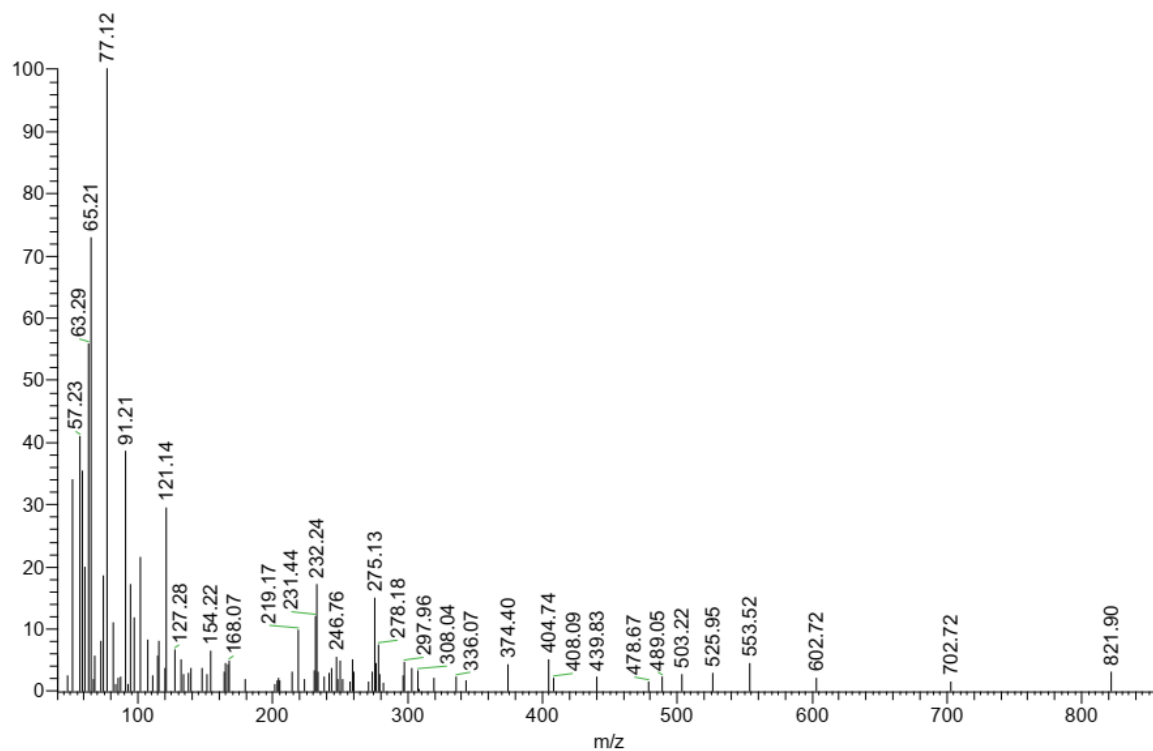
EI-MS of 12a



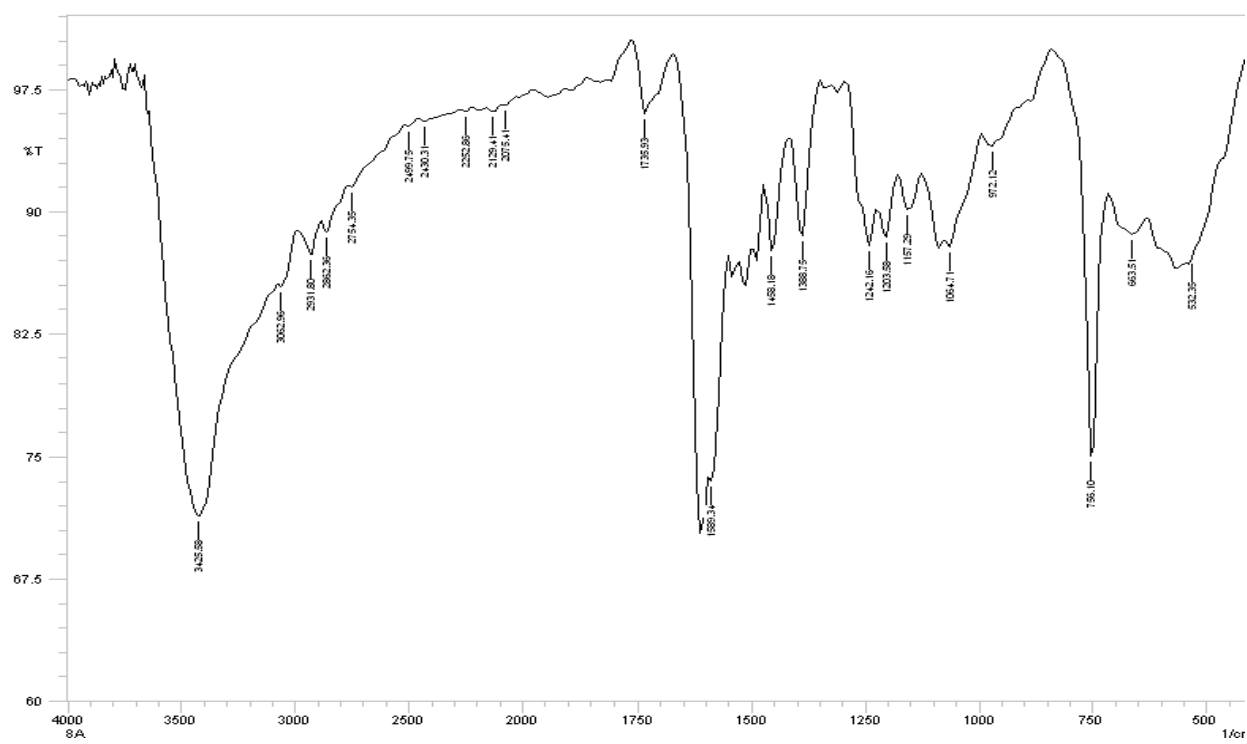
FT IR of compound 12a

¹H NMR of 12b in DMSO¹³C NMR of 12b in DMSO

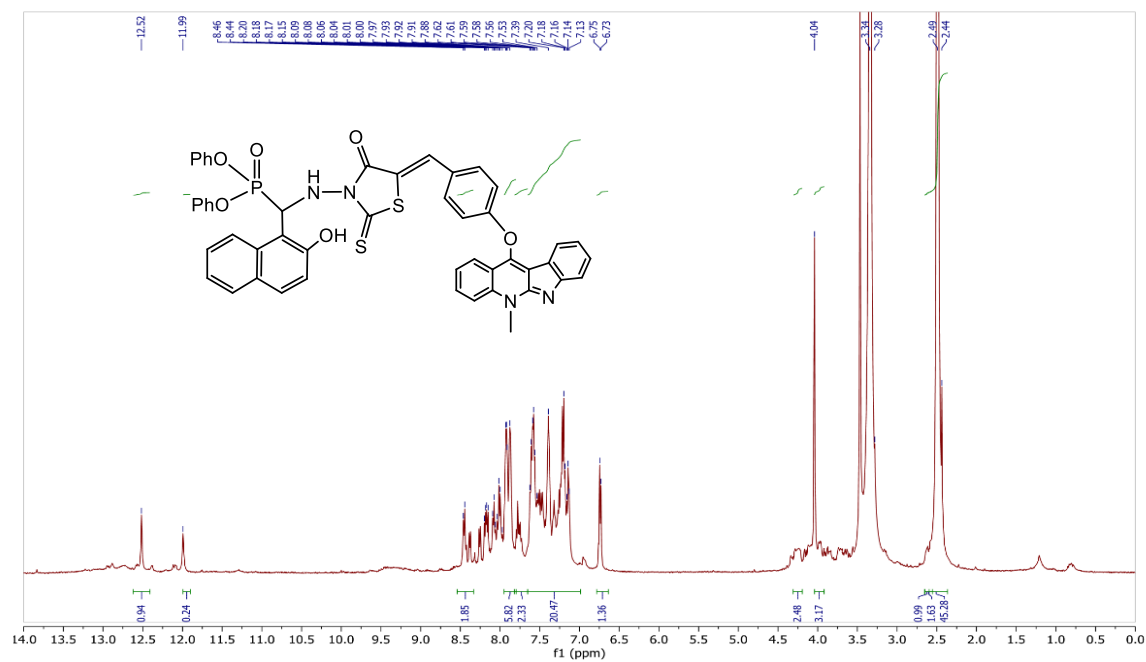
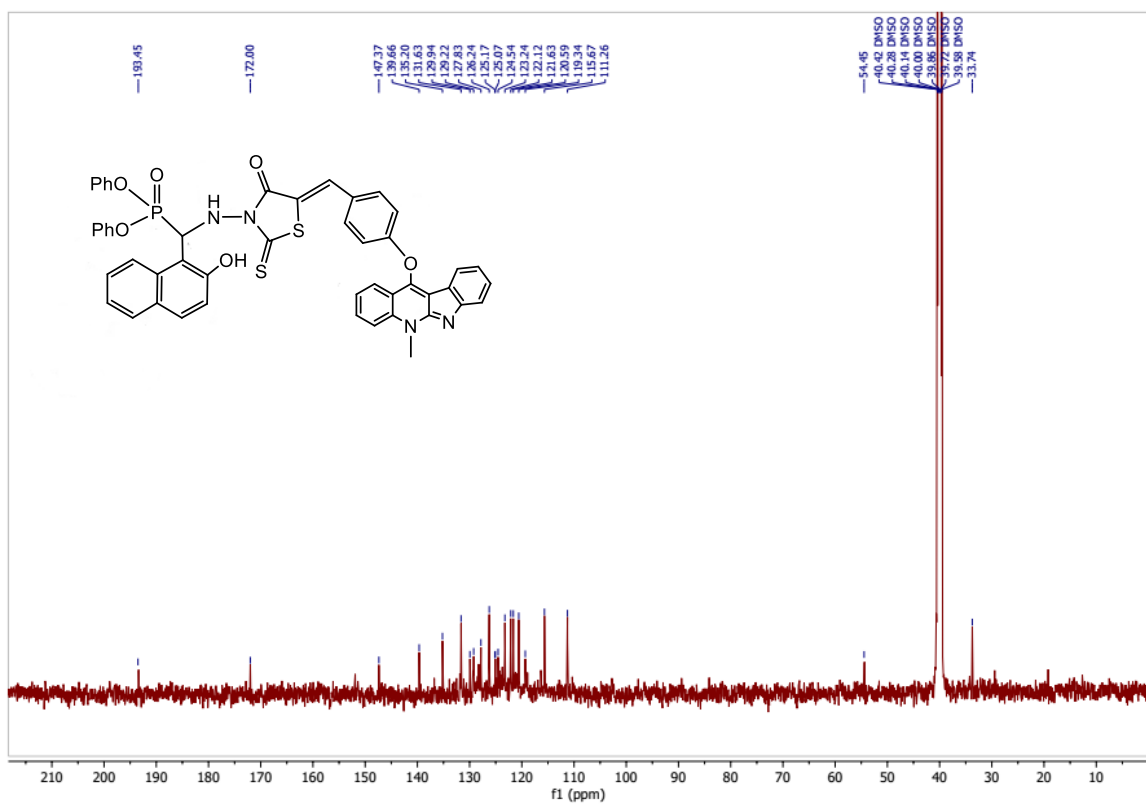
abdallah-ahmed-mohamed-8a #143 RT: 2.41 AV: 1 SB: 2 4.43, 4.43 NL: 6.01E3
T: {0,0} + c EI Full ms [40.00-1000.00]



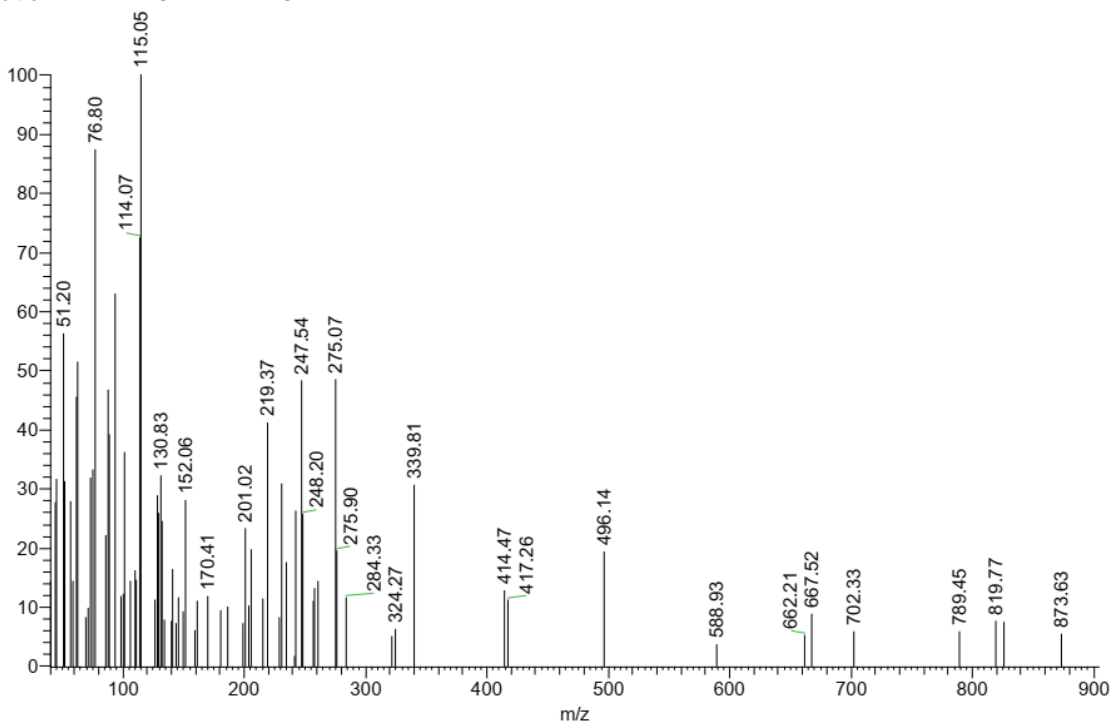
EI-MS of 12b



FT IR of compound 12b

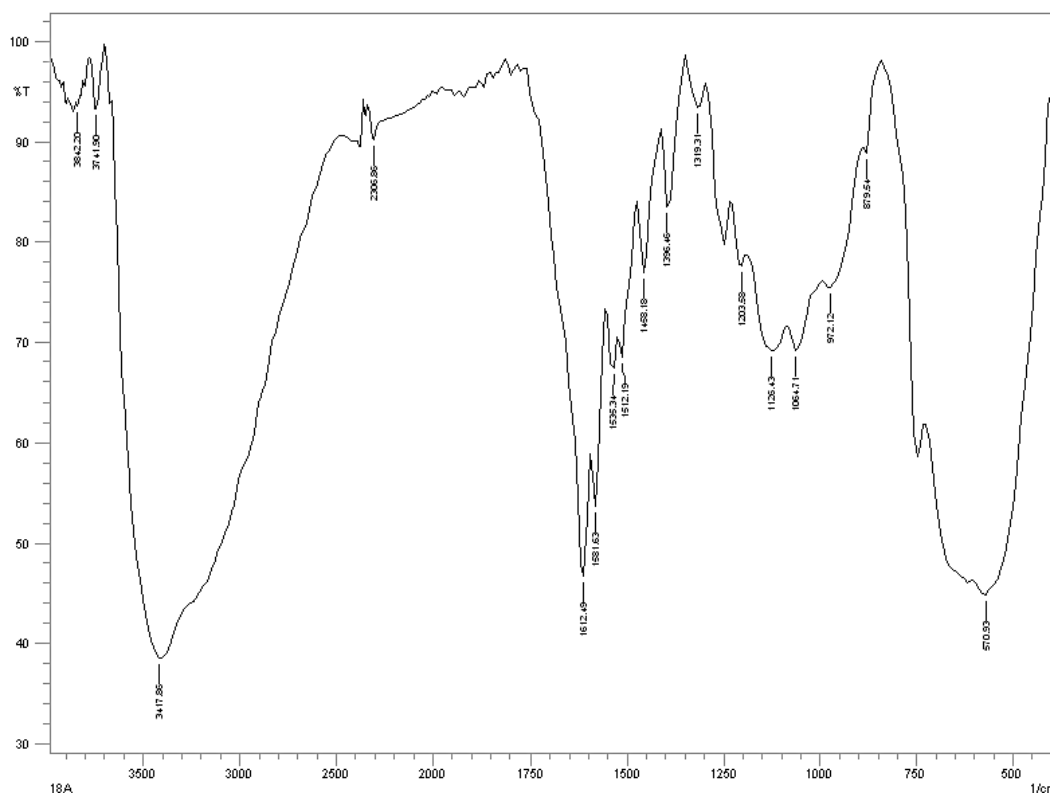
¹H NMR of 12c in DMSO¹³C NMR of 12c in DMSO

adallah-ahmed-mohamed-10a #170 RT: 2.86 AV: 1 SB: 2 4.42, 4.42 NL: 2.01E3
{0,0} + c EI Full ms [40.00-1000.00]

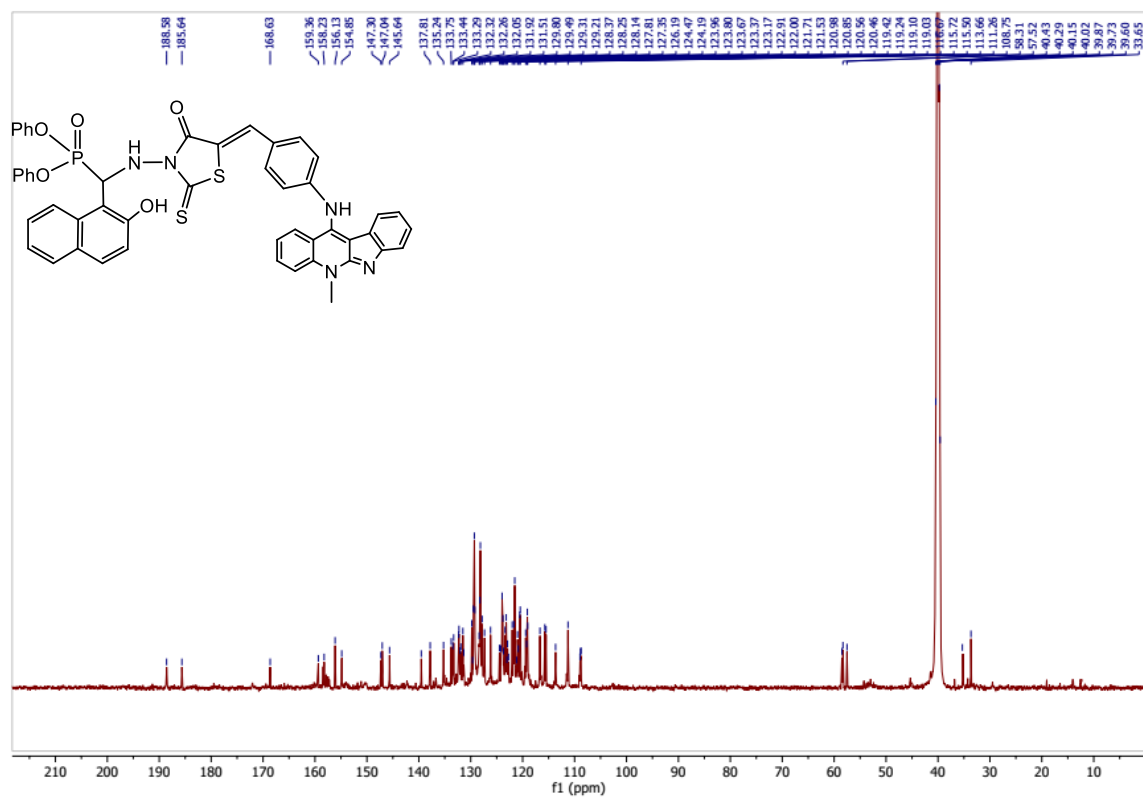


EI-MS

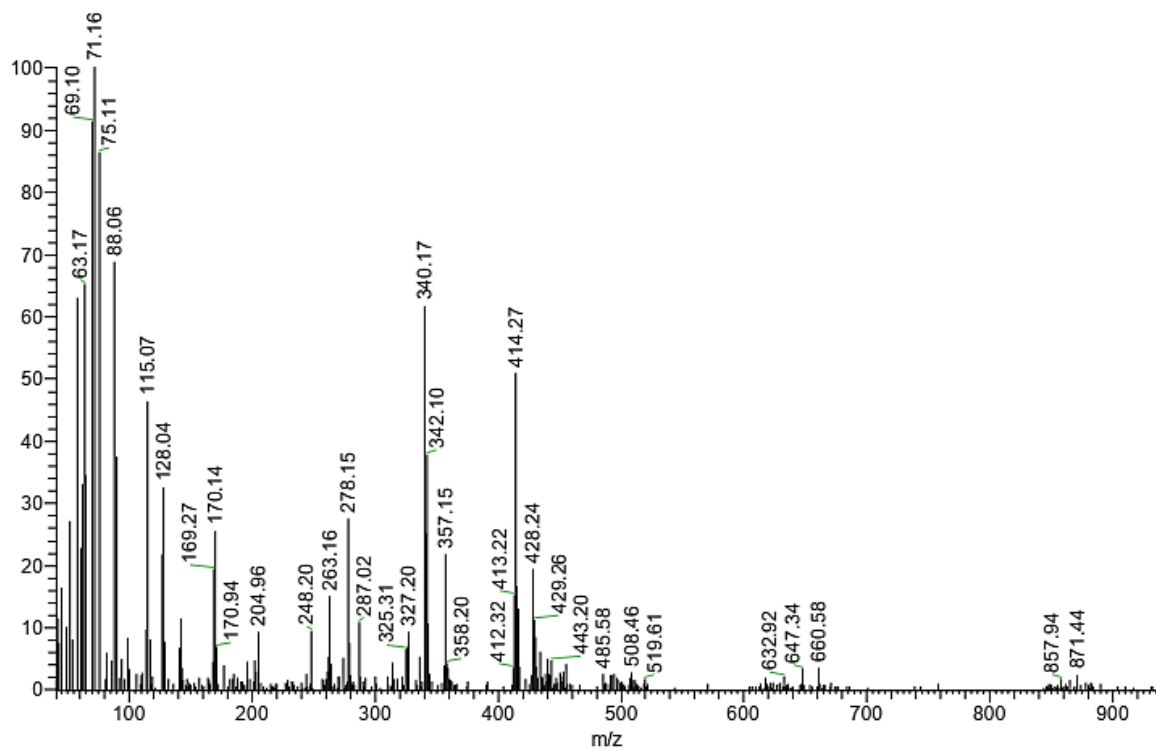
of 12c



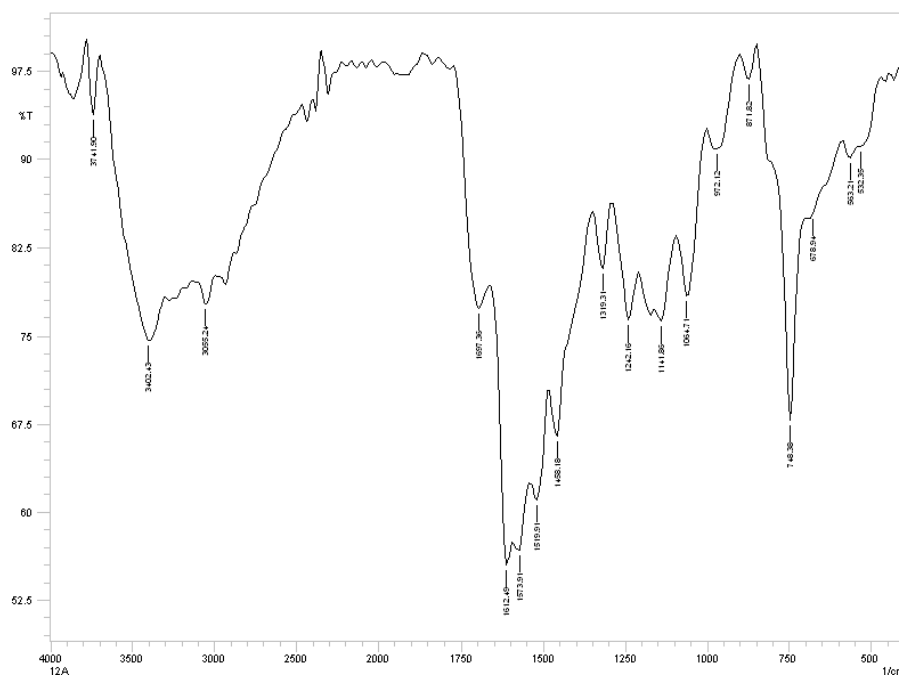
FT IR of compound 12c



abdallah-ahmed-mohamed-12a #114 RT: 1.92 AV: 1 SB: 2 4.47, 4.47 NL: 2.88E4
T: {0,0} + c EI Full ms [40.00-1000.00]



EI-MS of 12d



FT IR of compound 12d