

SUPPORTING INFORMATION FOR:

Potent combretastatin A-4 analogues containing quinoline: Design, Synthesis, antiproliferative, and anti-tubulin activity

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Figure S1; ^1H NMR for compound 19a

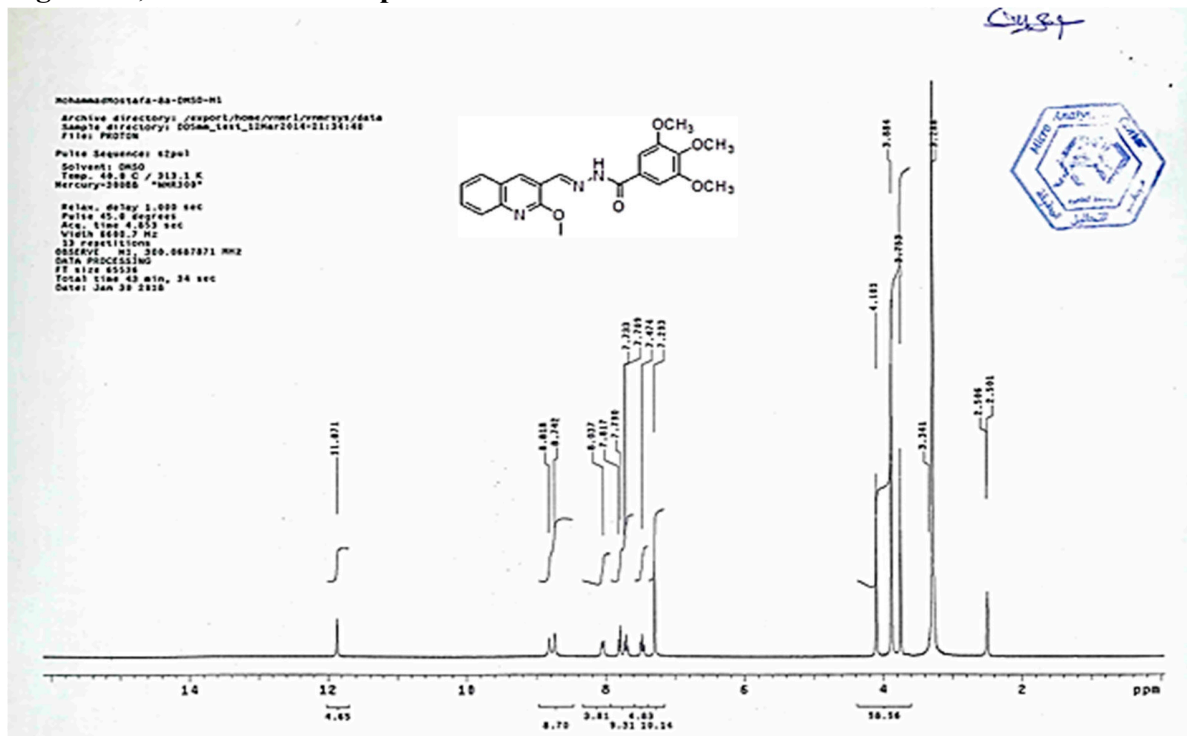


Figure S2; ^{13}C NMR for compound 19a

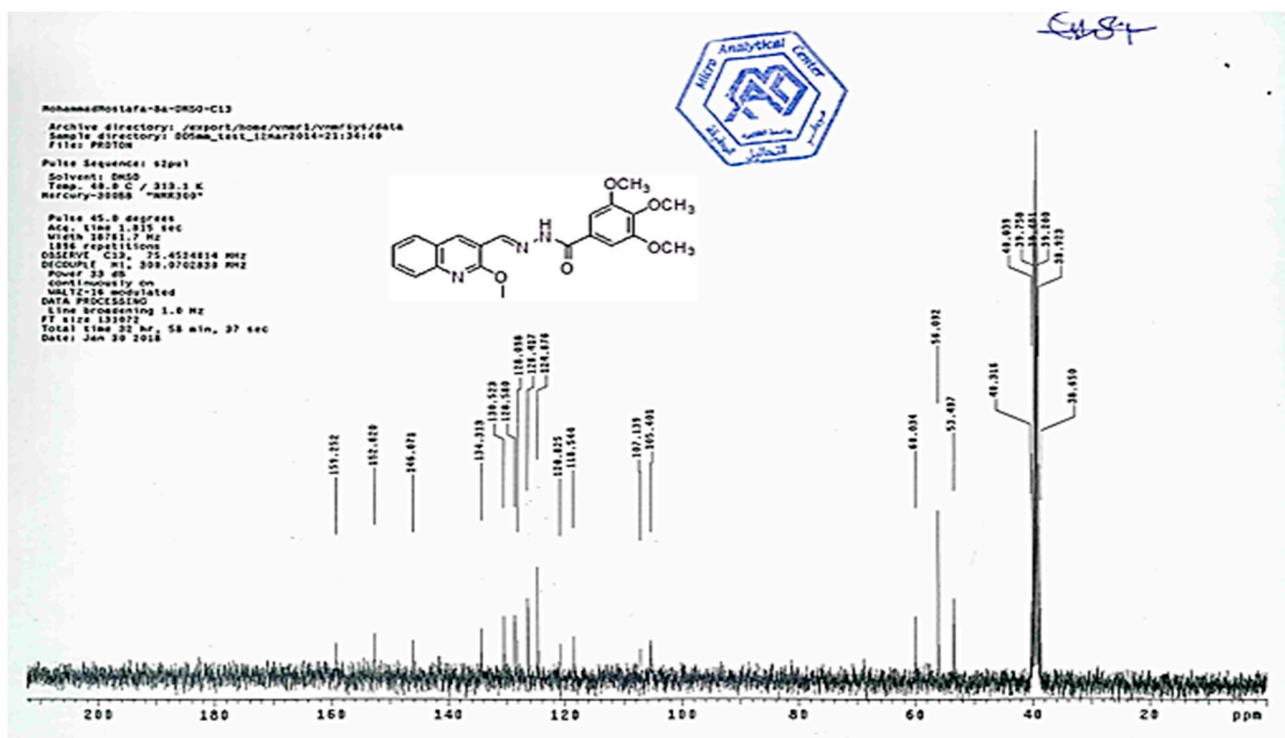


Figure S3; ^1H NMR for compound 19b

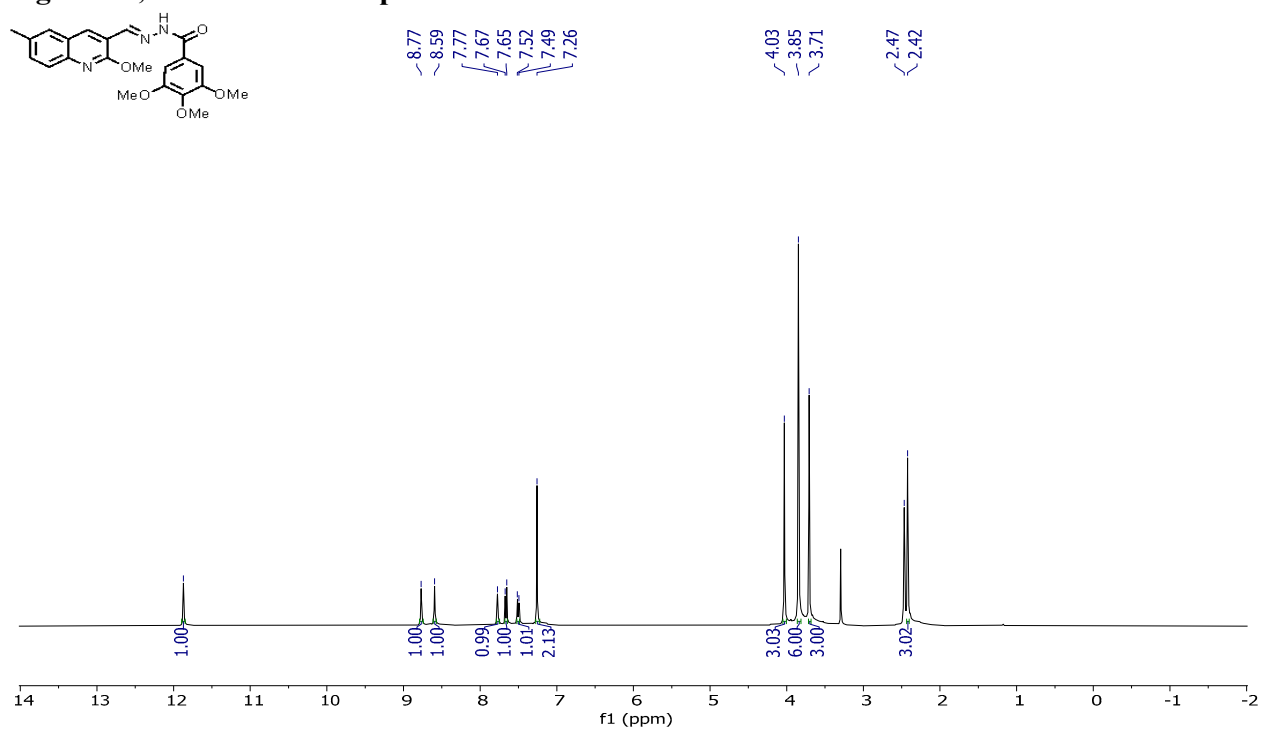


Figure S4; ^{13}C NMR for compound 19b

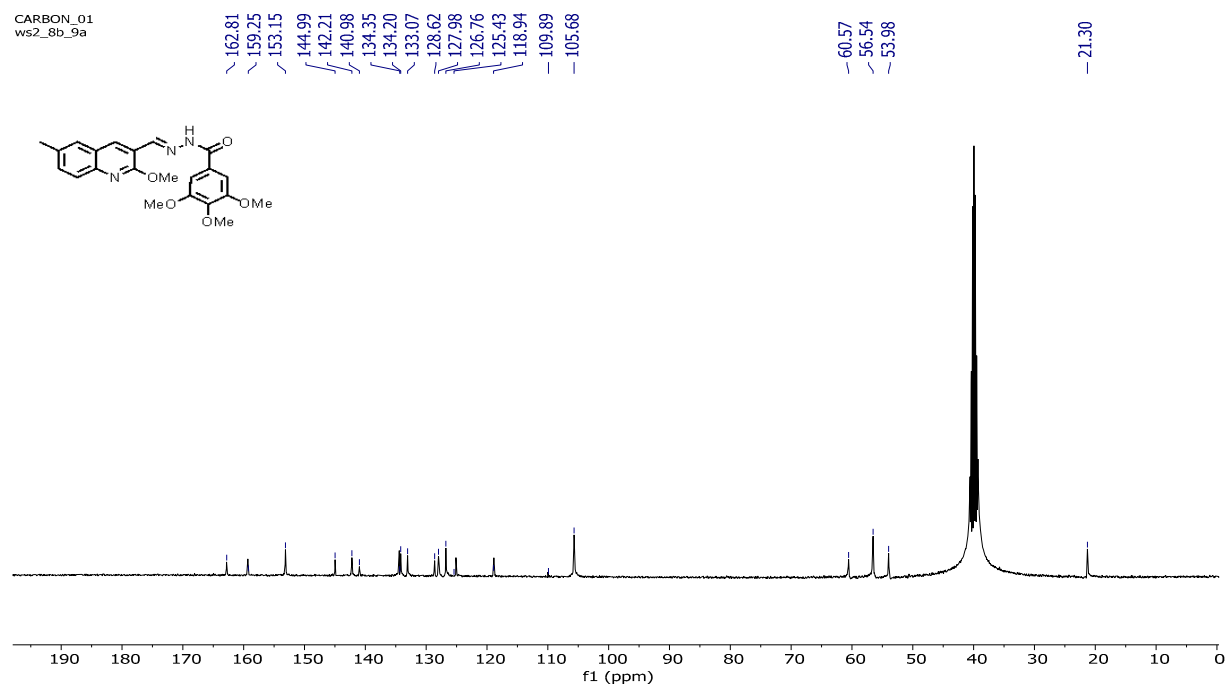


Figure S5; ^1H NMR for compound 19c

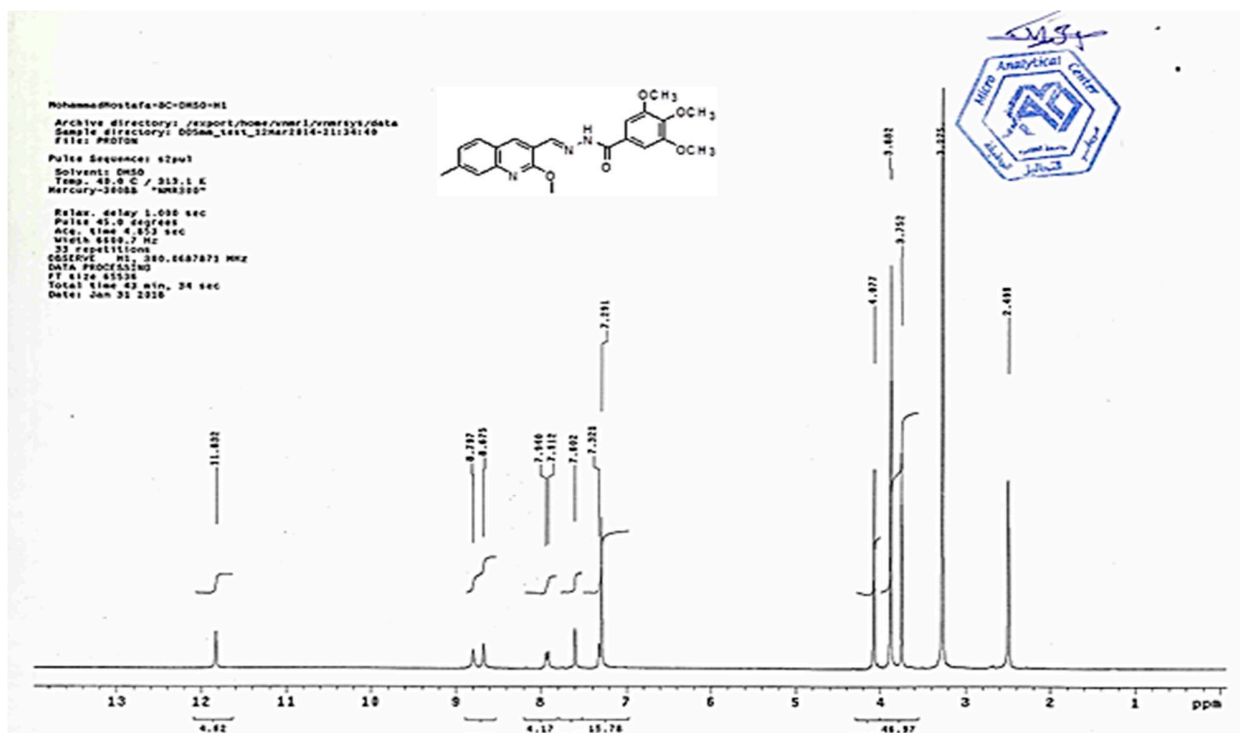


Figure S6; ^{13}C NMR for compound 19c

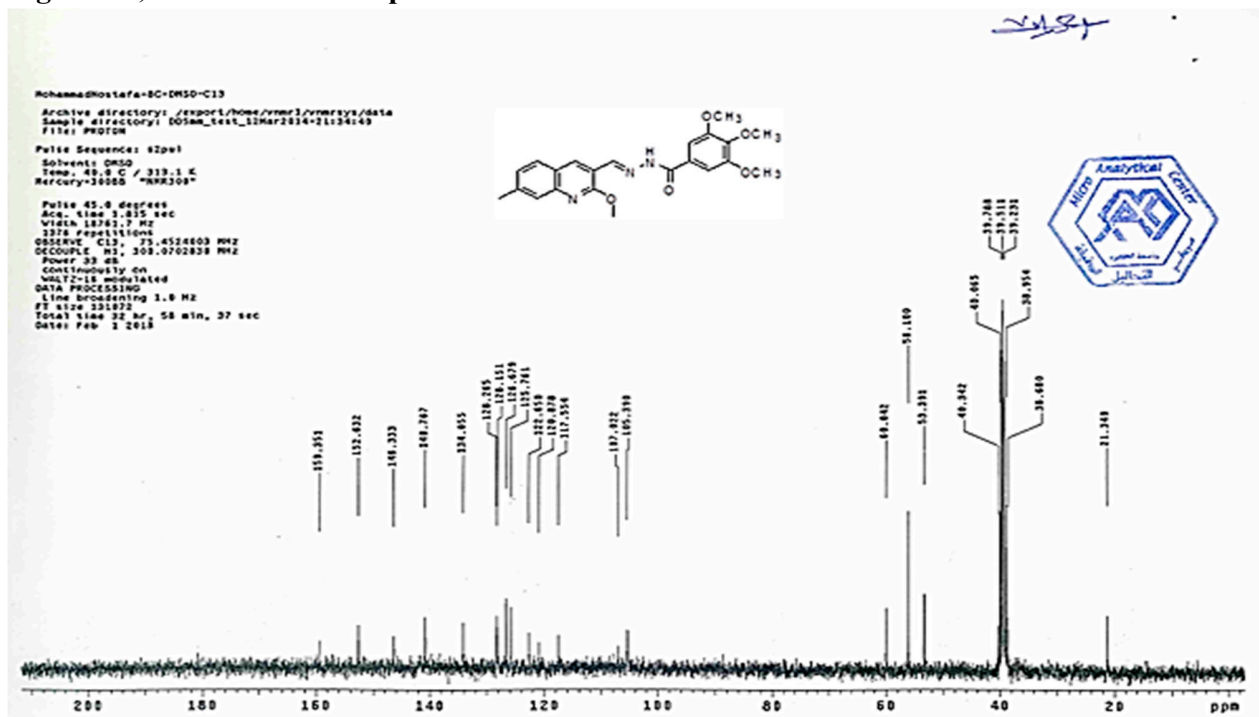


Figure S7; ¹H NMR for compound 19d

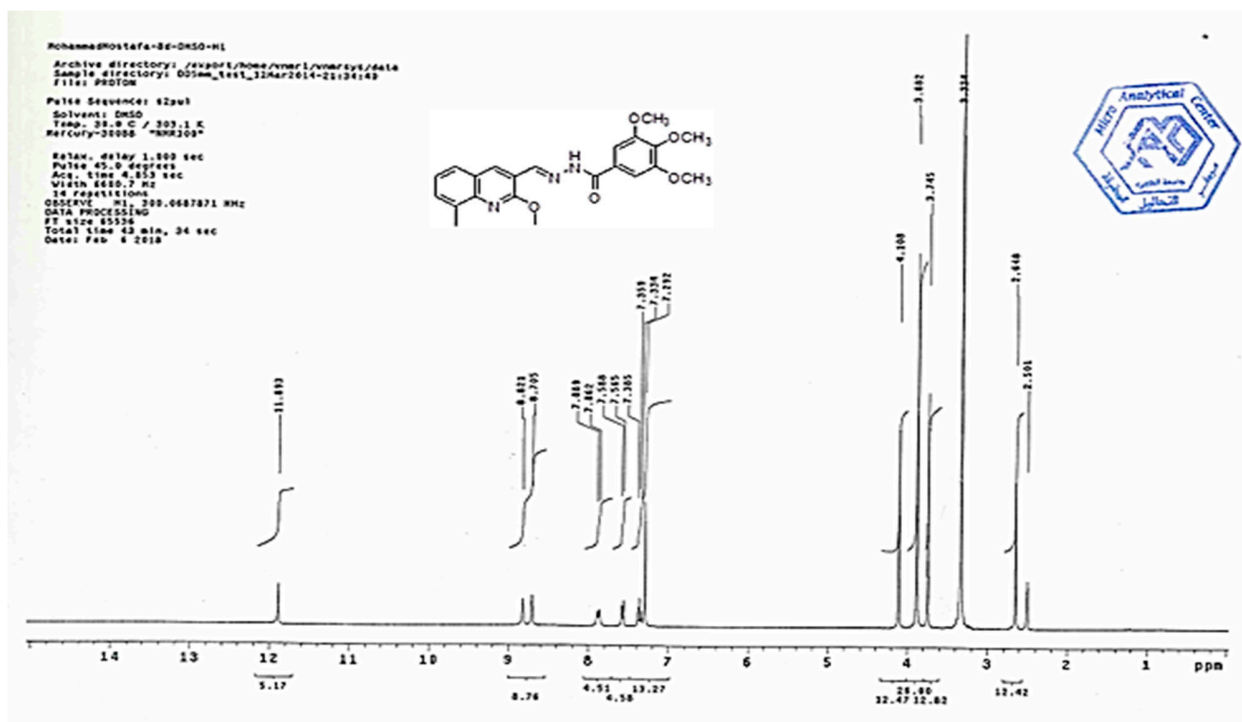


Figure S8; ¹³C NMR for compound 19d

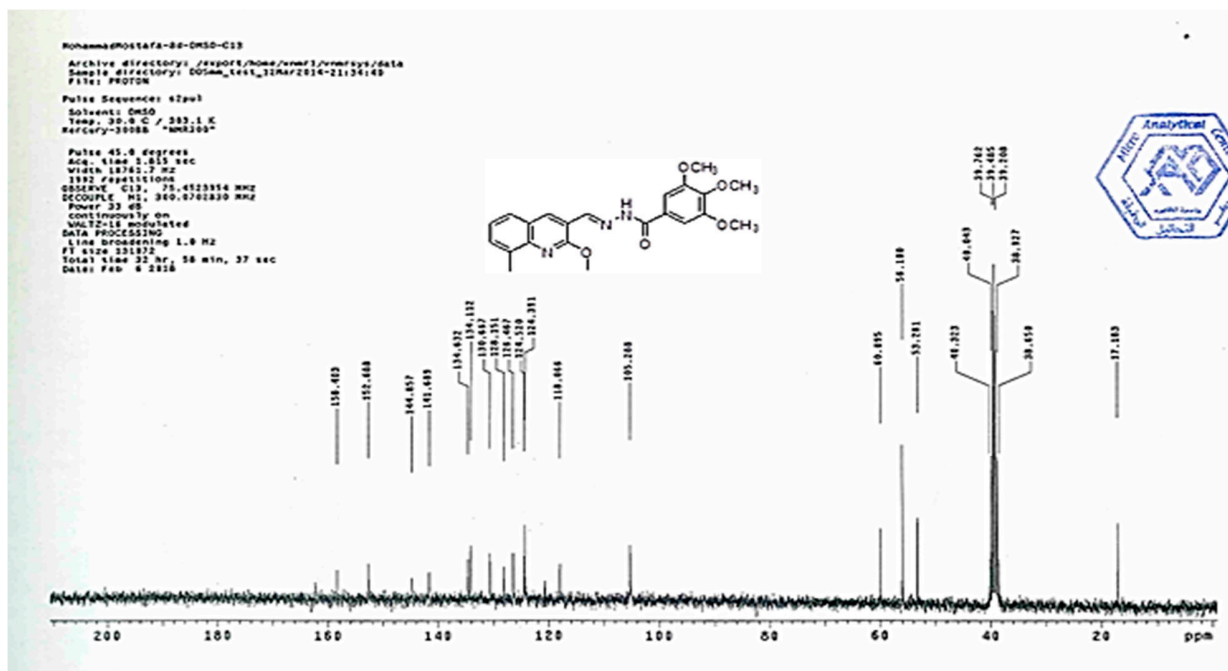


Figure S9; ^1H NMR for compound 19e

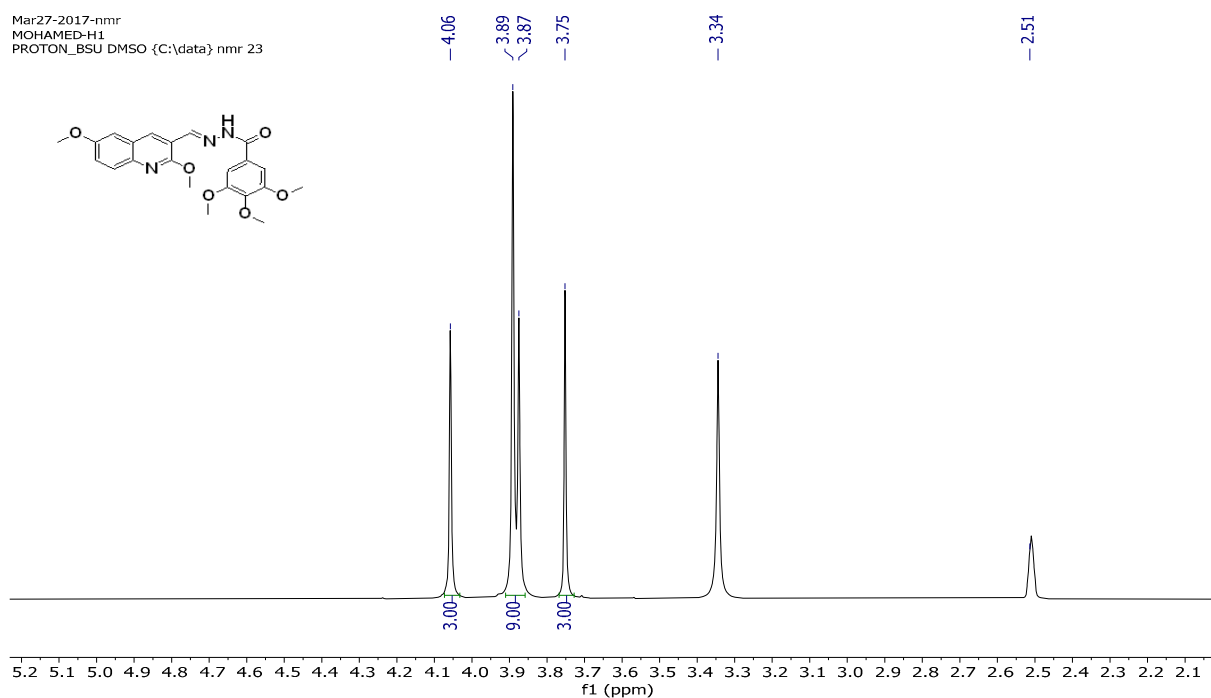
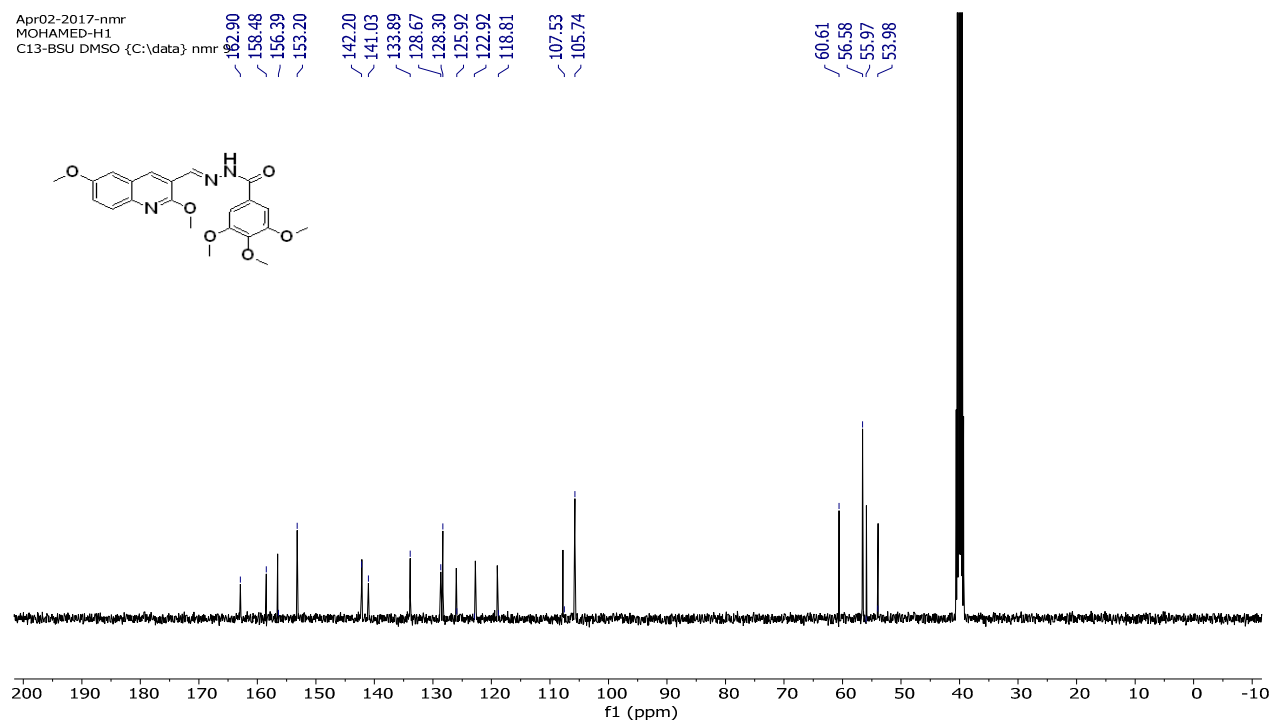


Figure S10; ^{13}C NMR for compound 19e



MOHAMMADHOSSAFA-SF-DMSO-H1

Archive directory: \export\hose\vwv\1\vwv\sys\data
Sample directory: OCSm_test_22Mar2016-22124149
File: PROTON

Pulse Sequence: zgpu1
Solvent: DMSO
Temp: 30.0 C / 269.1 K
Mercury-300SB "hmq3360"

Relax. delay 1.000 sec
Pulse: 45.0 degrees
Acq. time 4.855 sec
Width 6609.7 Hz
31 Repetitions
OBSERVE: HS, 300.9687871 MHz
DATA PROCESSING
FT size 85536
Total time 43 min, 34 sec
Date: Feb 8 2016

COc1cc(OC)c(C(=O)Nc2cc3cc(OC)cc(O)c3nc2C4=CC=CC=C4O)cc1OC

11.424
8.233
8.165
7.972
7.942
7.262
7.186
7.137
7.125
7.114
7.095
7.068
4.075
3.917
3.773
3.334
2.511

4.15
7.16
3.74
17.39
69.76
4.15

ppm

MohammedMostafa-87-DMSO-C13

Archive directory: /exp01/home/vnmr3/vnmrfsys/ATAA
Sample directory: D05mm_test_12Mar2014-21:34:49
File: F02108

Pulse Sequence: zgpg30
Solvent: DMSO
Temp: 30.0 C / 360.3 K
Acquire: 30588 "nmr330"

Pulse 45.0 degrees
Acc. time 1.815 sec
Width 12741.7 Hz
2458 Repetitions
Observed C13: 75.4522843 MHz
Decouple H1: 309.0702339 MHz
Power 33 dB
continuously on
VHFP+18 modulated
DATA PROCESSING
line broadening 3.0 Hz
F2 size 131972
Total time 20 hr, 58 min, 37 sec
Date: Feb 7 2018

COC1=CC(=C(C=C1)C(=N/C=N/C(=O)C2=CC(OC)=C(OC)C2)C3=CC(OC)=CC=C3)

40.454, 39.272, 39.160, 39.129, 38.842, 36.461, 46.395, 56.316, 56.111, 55.308, 55.239, 115.710, 116.740, 116.855, 117.515, 118.261, 118.419, 136.169, 142.400, 148.215, 155.496, 159.417, 161.515

ppm

Atomic Analytical Center
مركز التحليل الذري
جامعة القاهرة
Cairo University

Figure S13; ^1H NMR for compound 19g

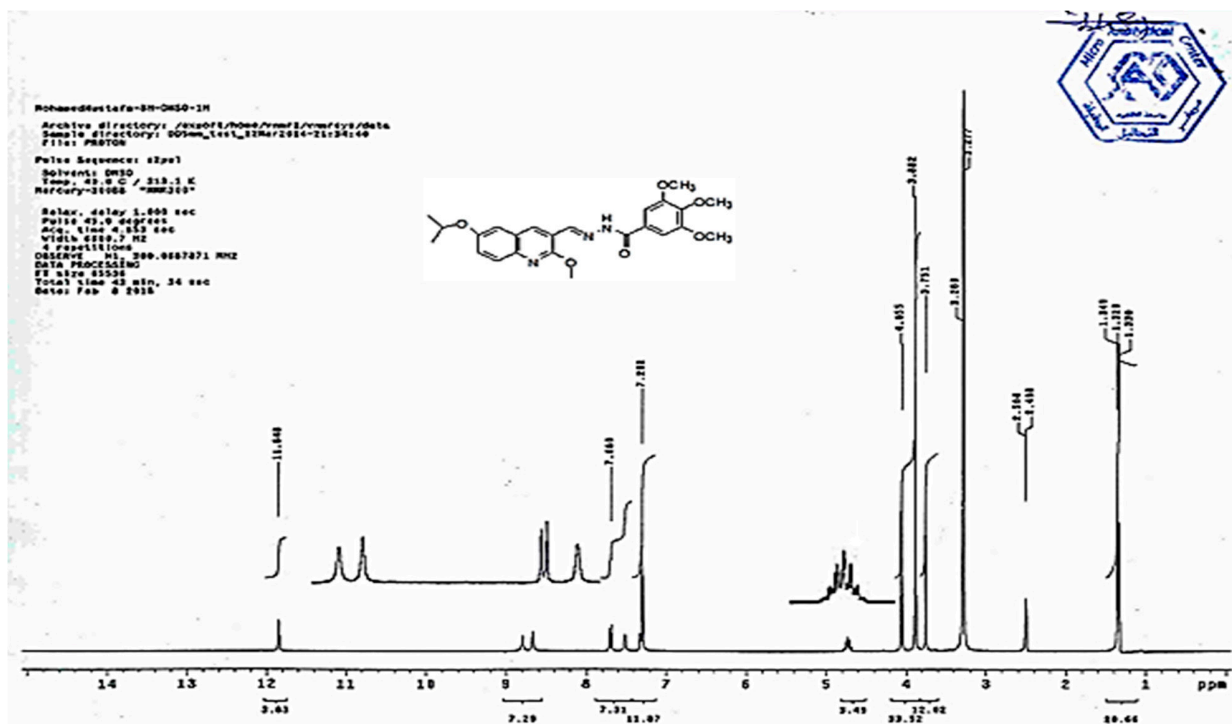


Figure S14; ^{13}C NMR for compound 19g

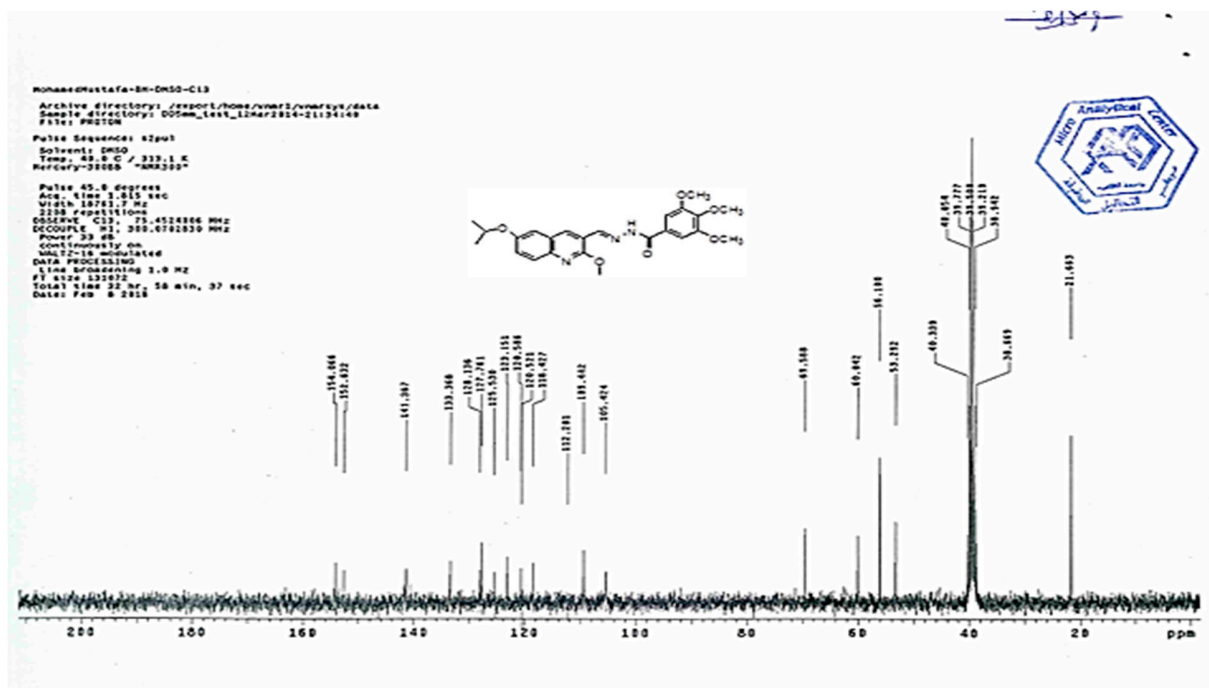


Figure S15; ^1H NMR for compound 19h

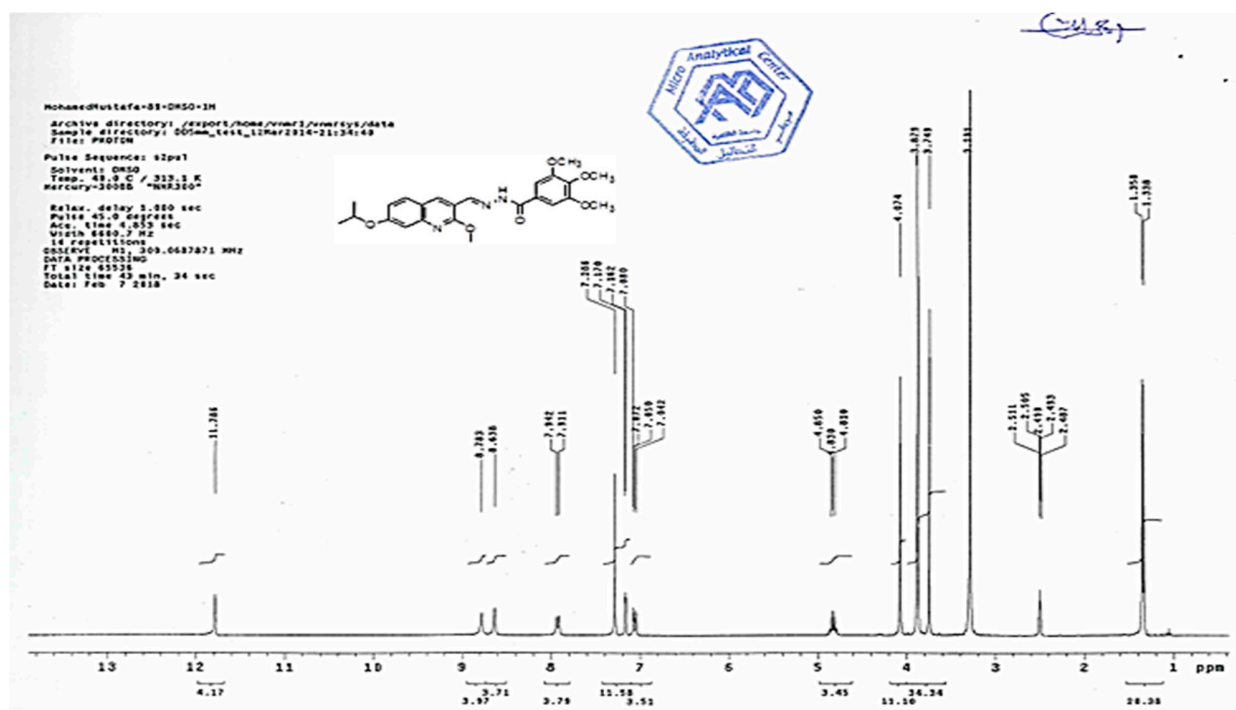


Figure S16; ^{13}C NMR for compound 19h

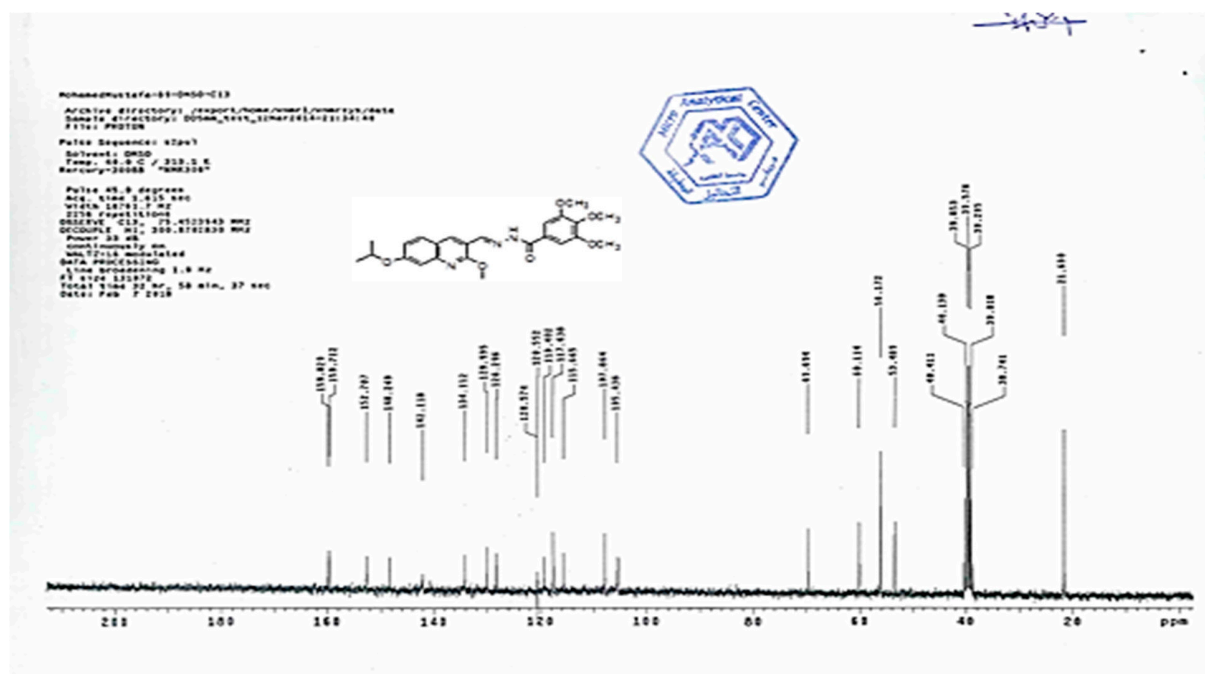


Figure S17; ^1H NMR for compound 19i

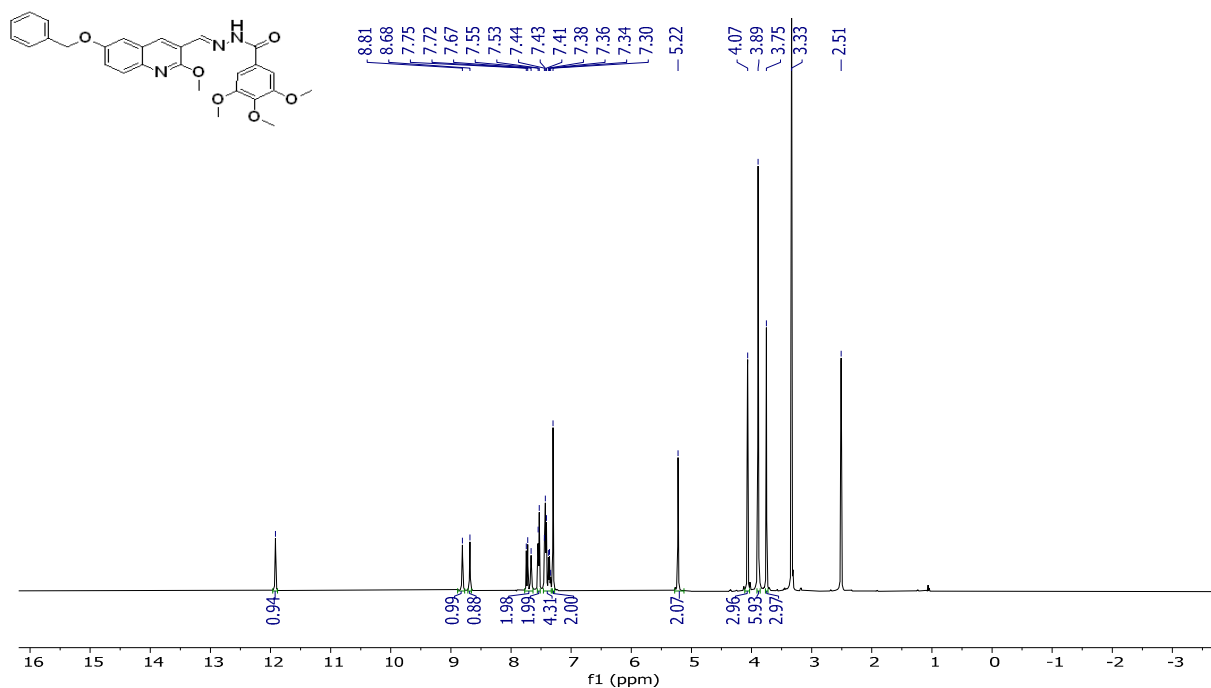


Figure S18; ^{13}C NMR for compound 19i

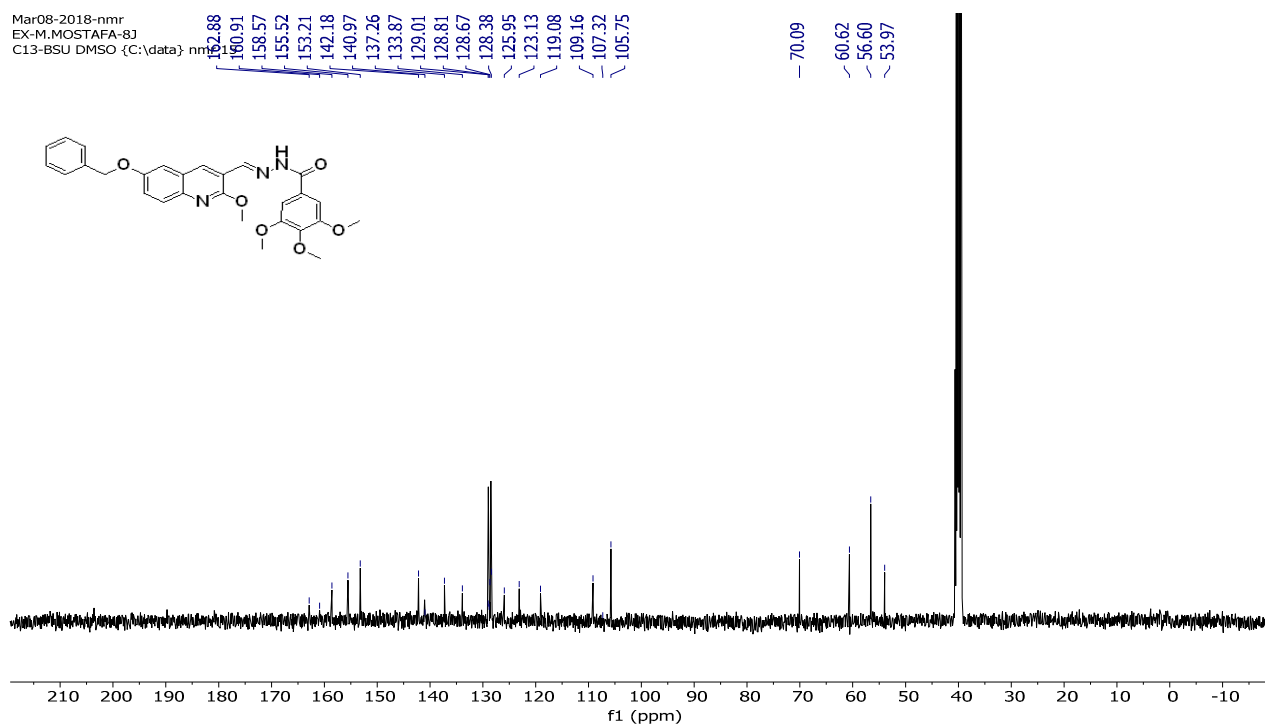


Figure S19; ^1H NMR for compound 19j

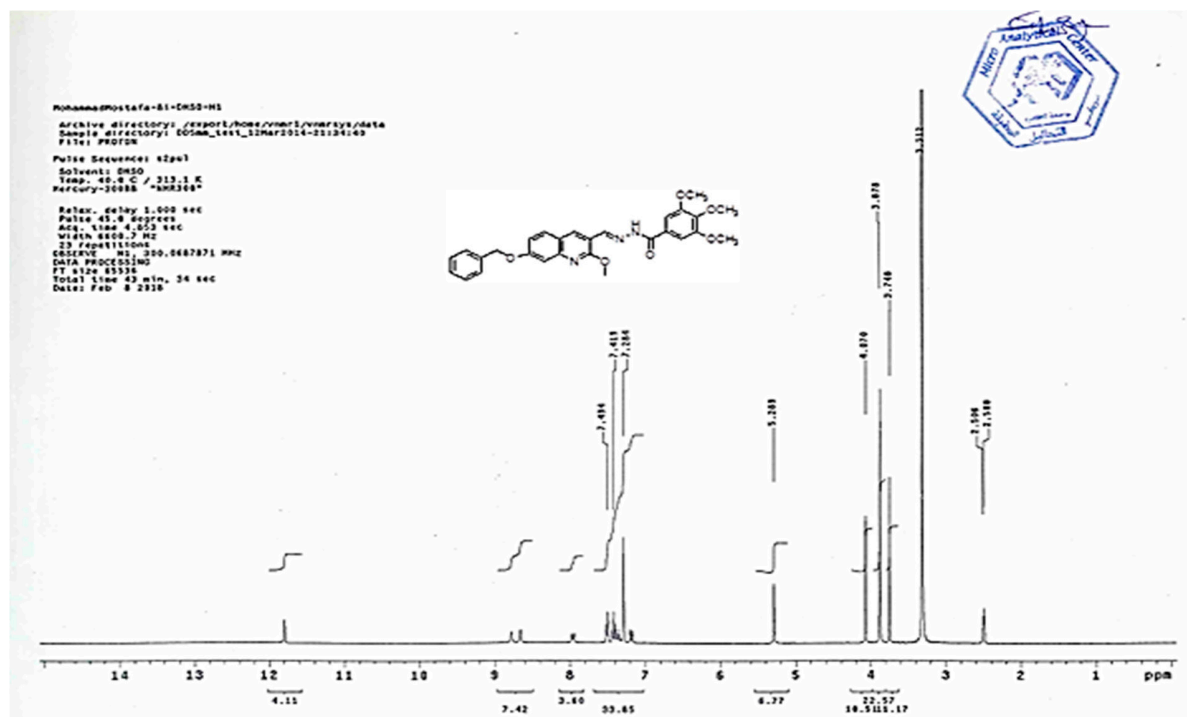


Figure S20; ^{13}C NMR for compound 19j

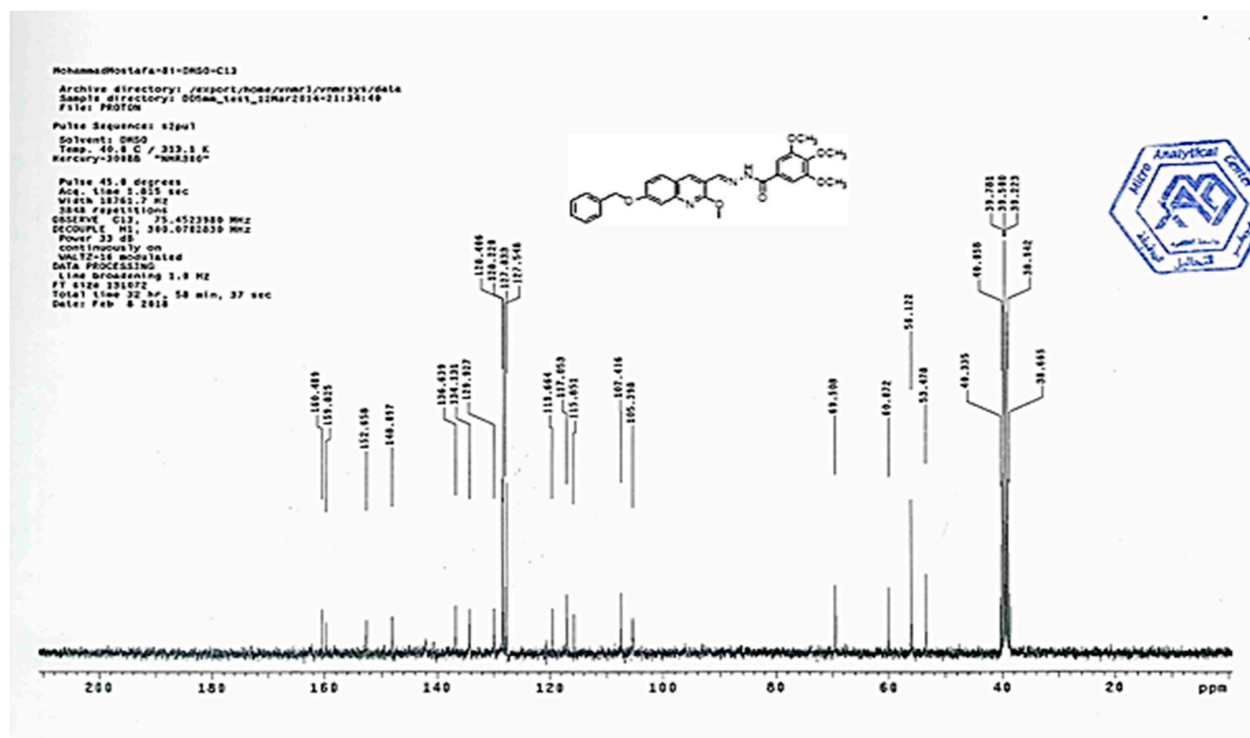


Figure S21; ^1H NMR for compound 20a

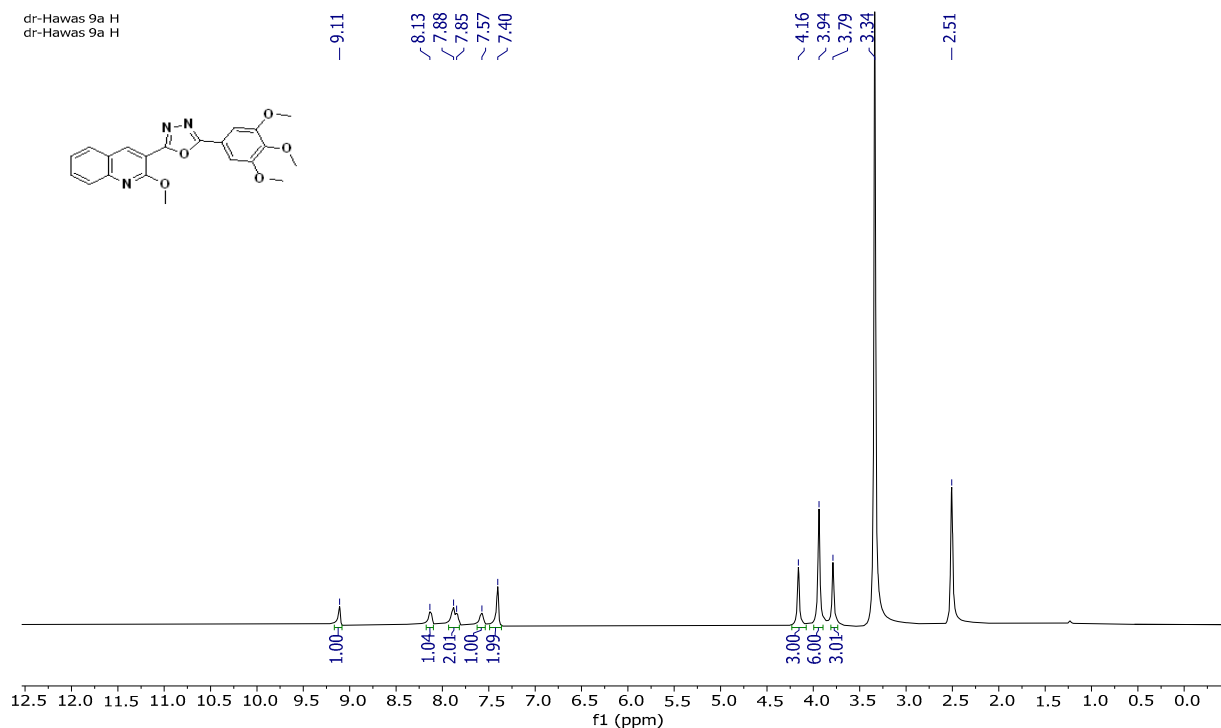


Figure S22; ^{13}C NMR for compound 20a

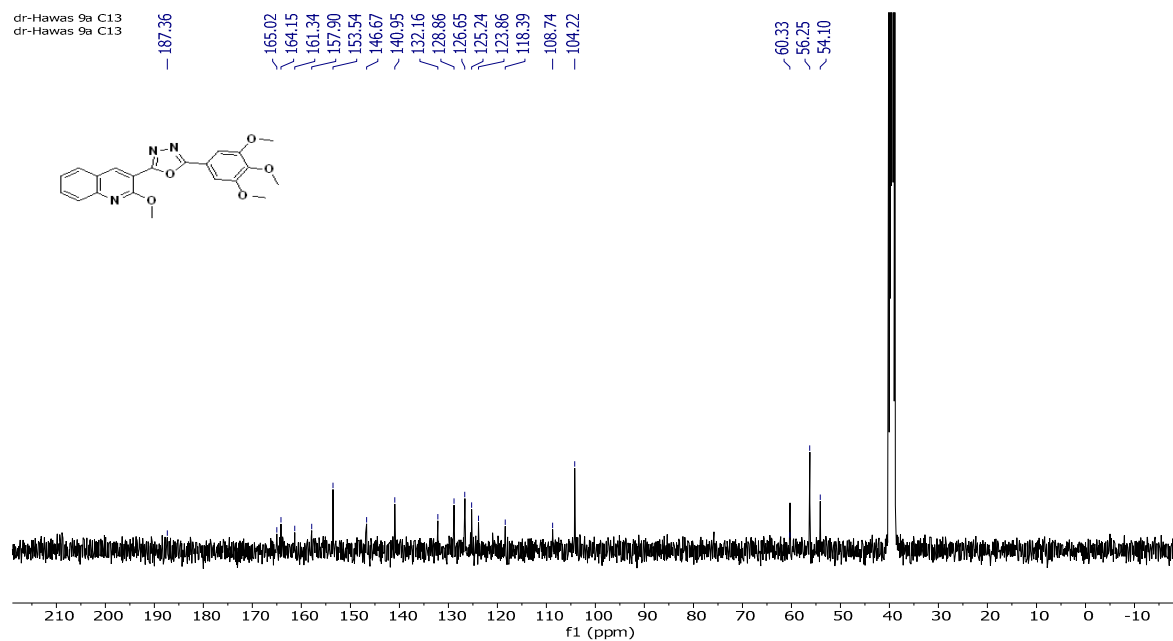


Figure S23; ^1H NMR for compound 20b

Jul02-2018-abeer
M MOSTAFA-9B
PROTON_BS0 DMSO {C:\data\} abeer 11

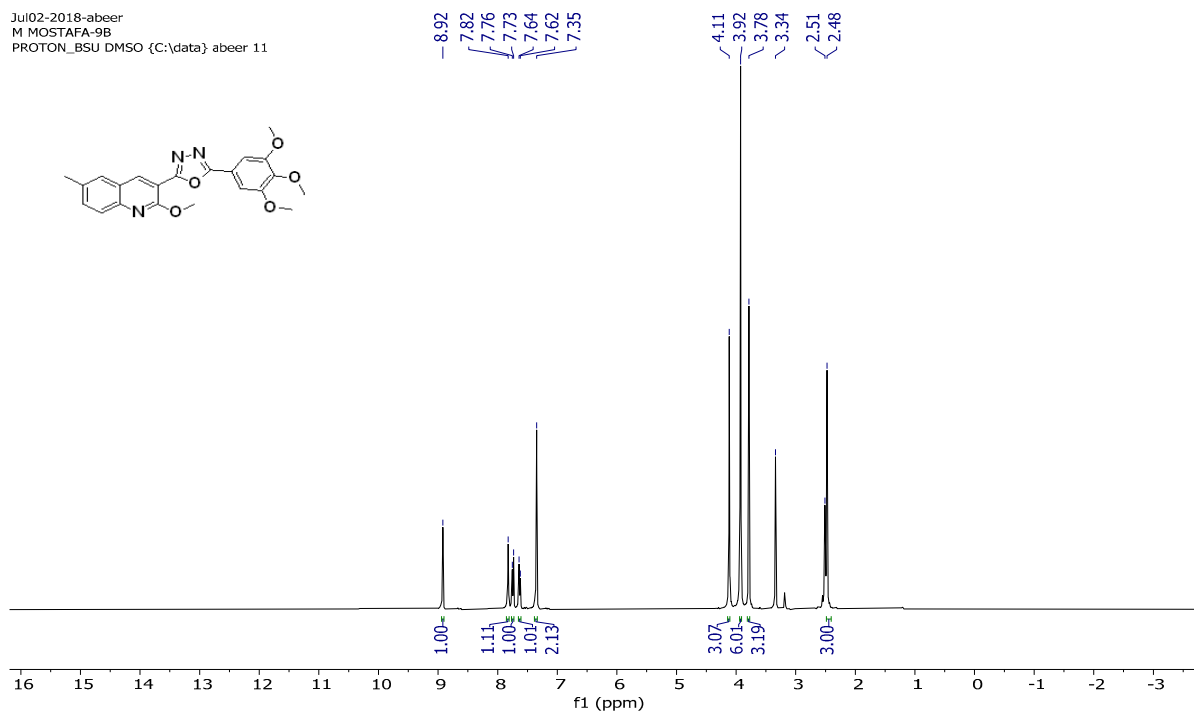


Figure S24; ^{13}C NMR for compound 20b

dr-Hawas 9b C13
dr-Hawas 9b C13

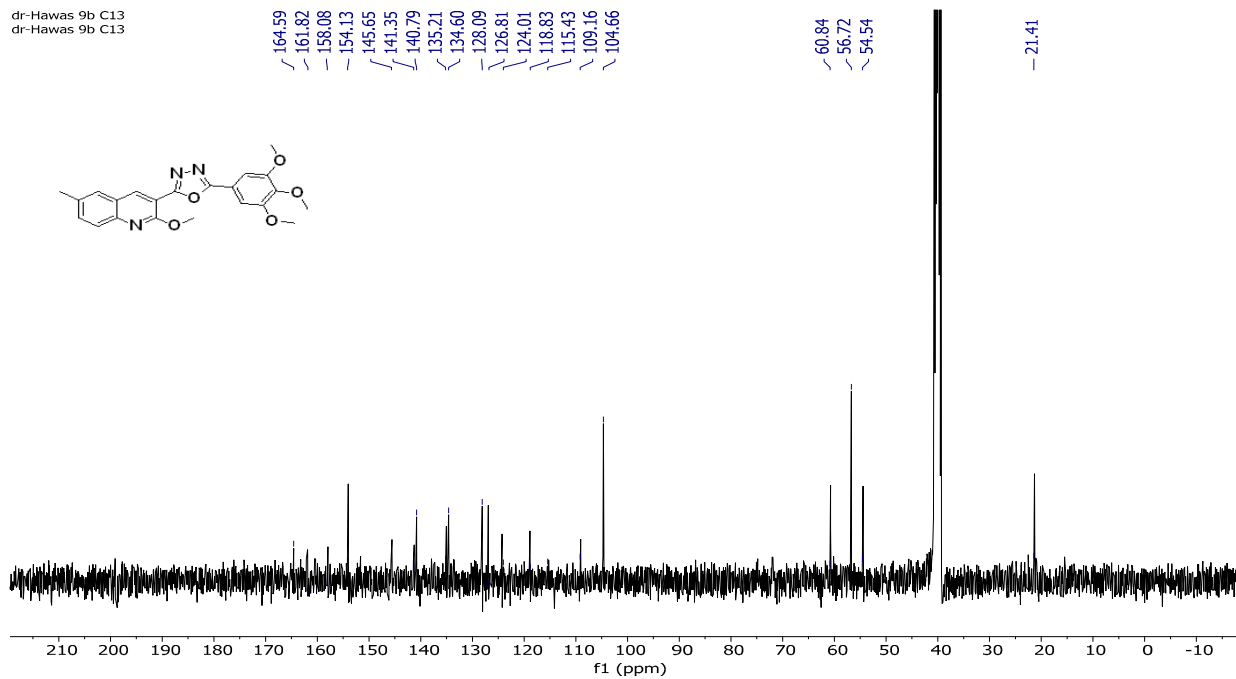


Figure S25; ^1H NMR for compound 20c

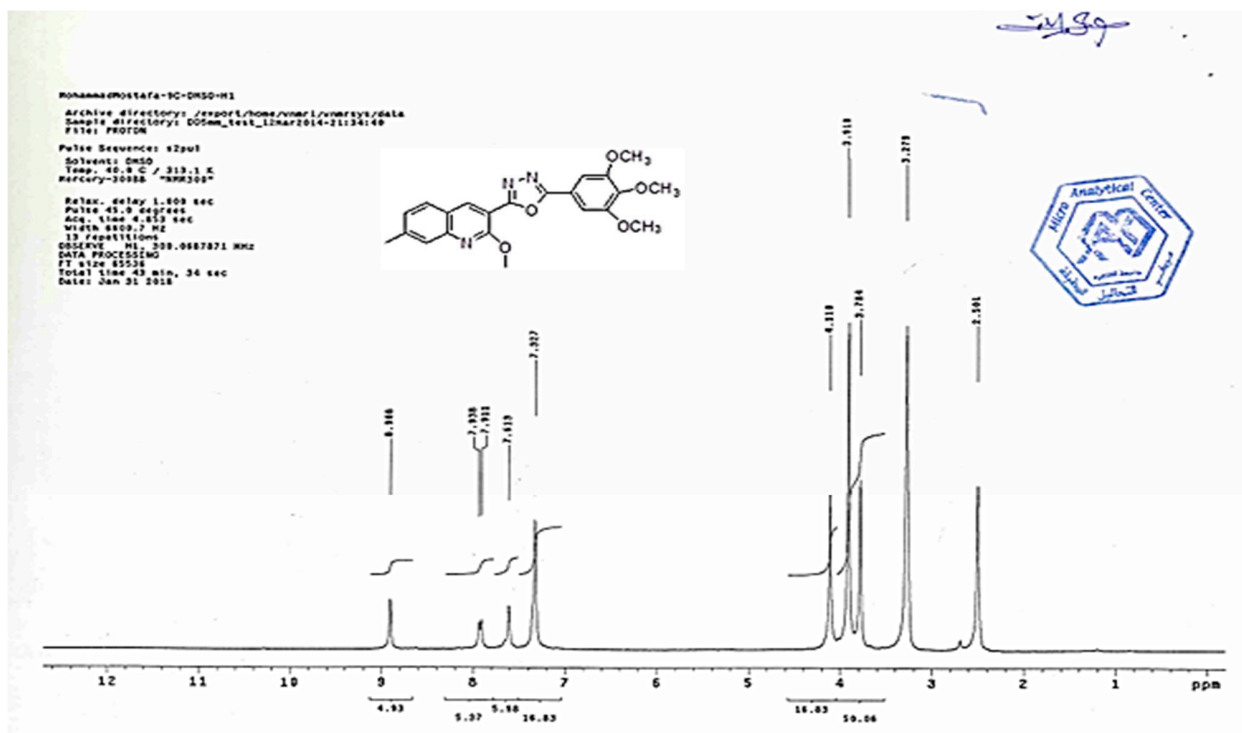


Figure S26; ^{13}C NMR for compound 20c

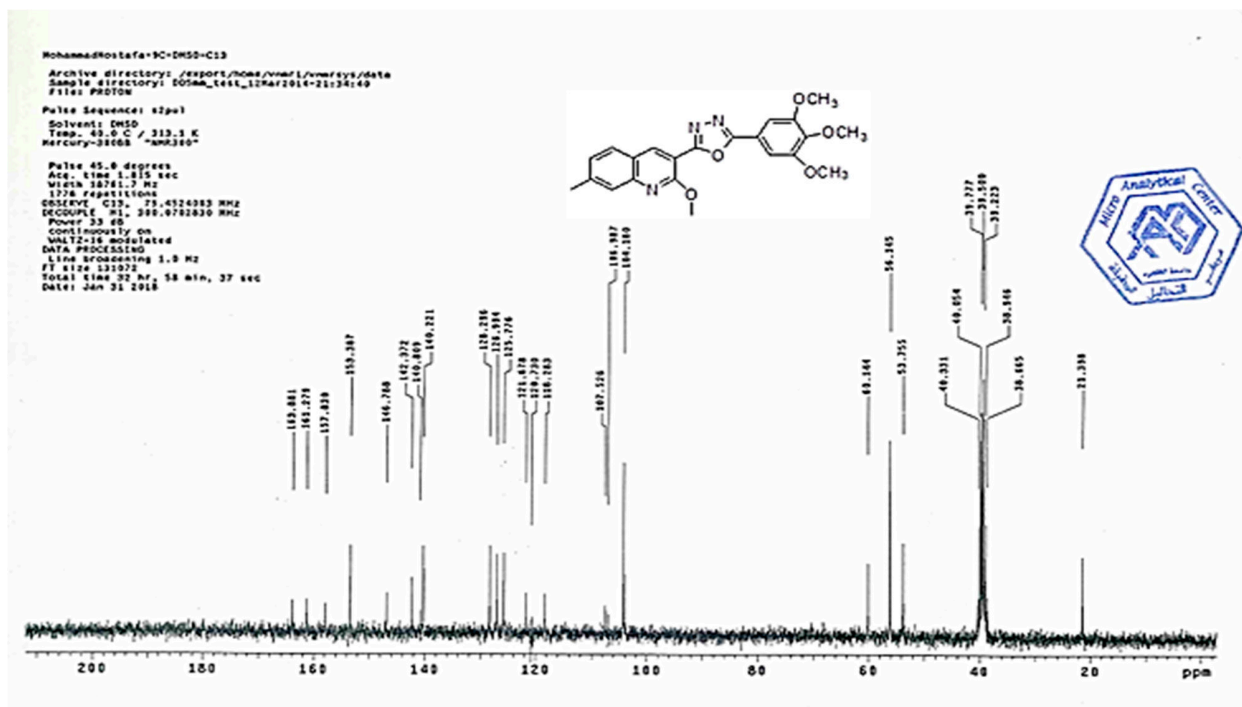


Figure S27; ^1H NMR for compound 20d

Jul02-2018-abeer
M MOSTAFA-9D
PROTON_BS DMSO {C:\data\} abeer 10

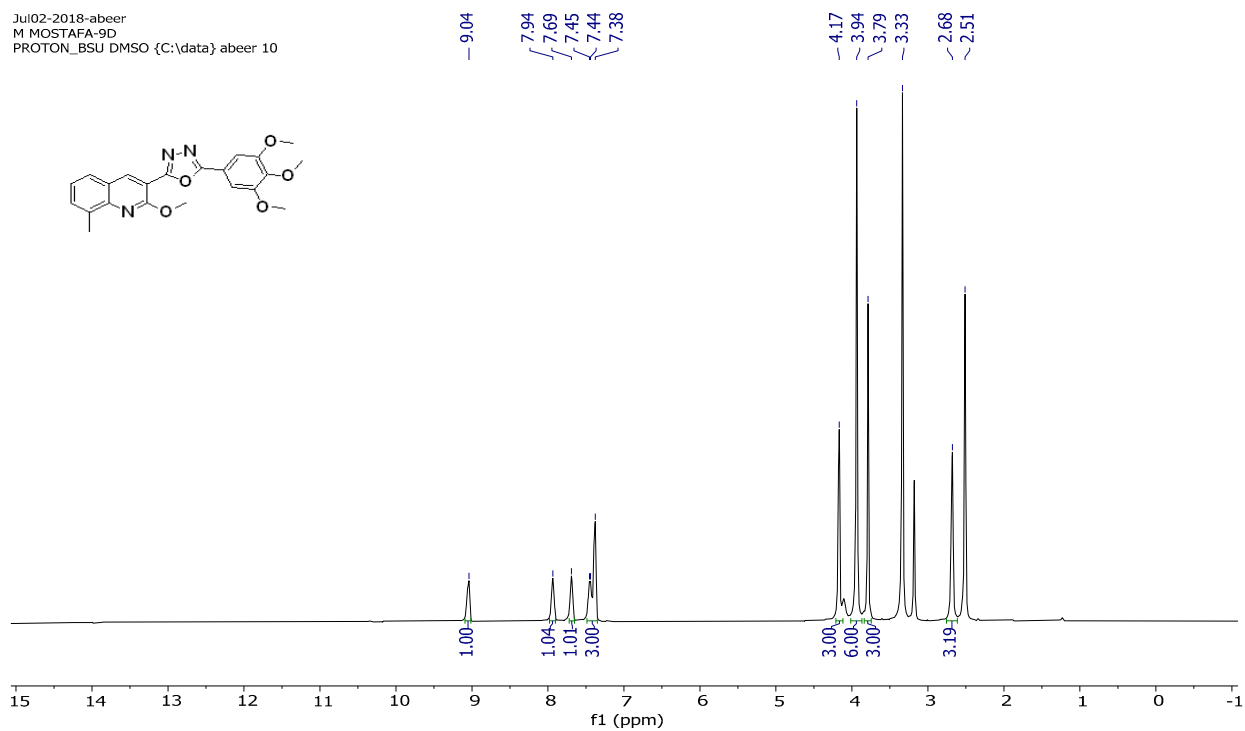


Figure S28; ^{13}C NMR for compound 20d

dr-Hawas 9d C13
dr-Hawas 9d C13

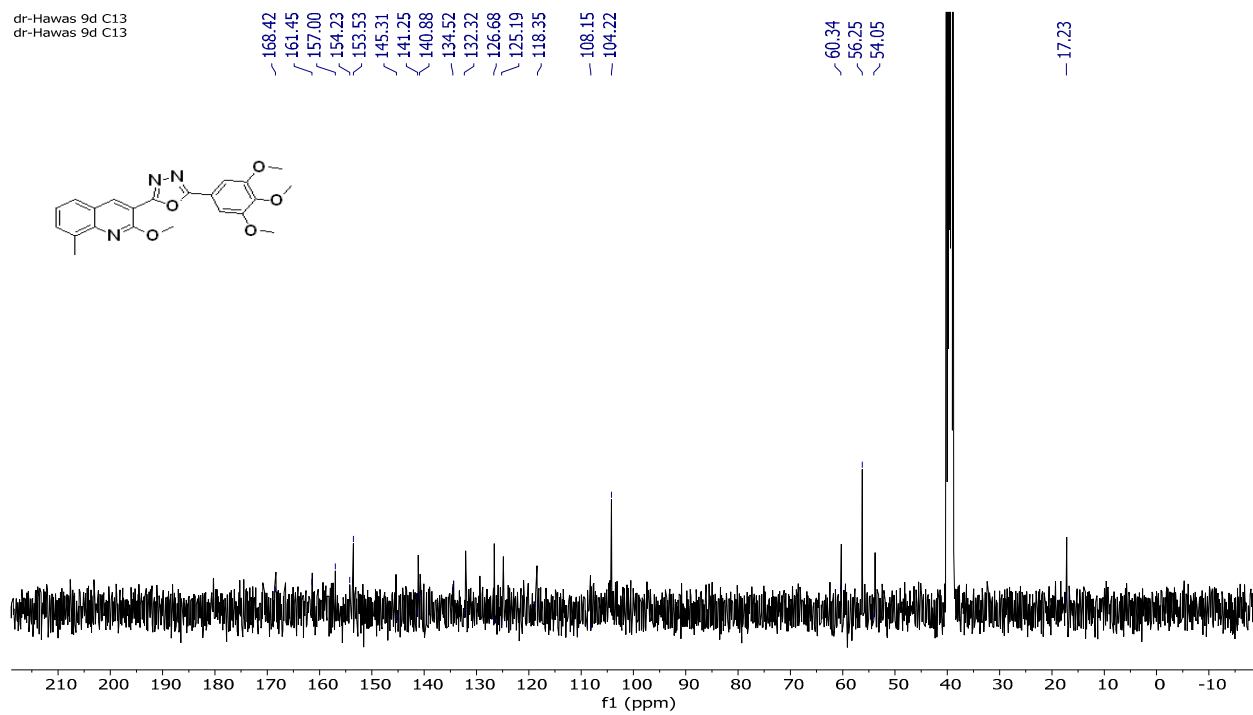


Figure S29; ^1H NMR for compound 20e

Mar27-2017-nmr
MOHAMED-D1
PROTON_BSUS DMSO {C:\data} nmr 24

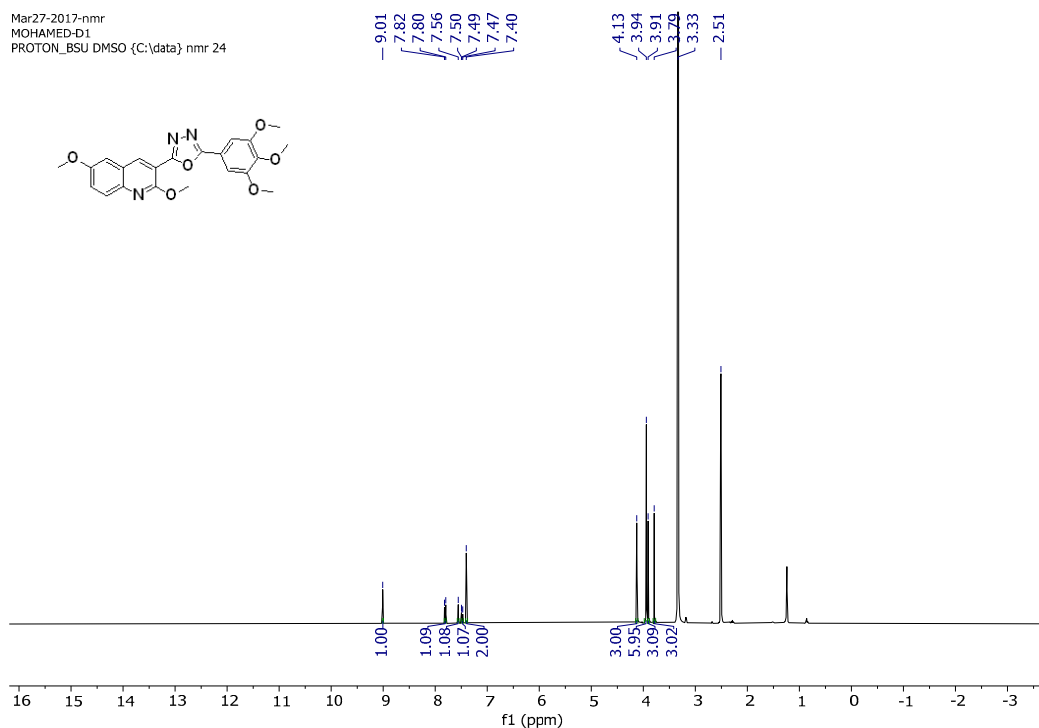


Figure S30; ^{13}C NMR for compound 20e

Apr05-2017-nmr
MOHAMED-D1
C13-BSUS DMSO {C:\data} nmr

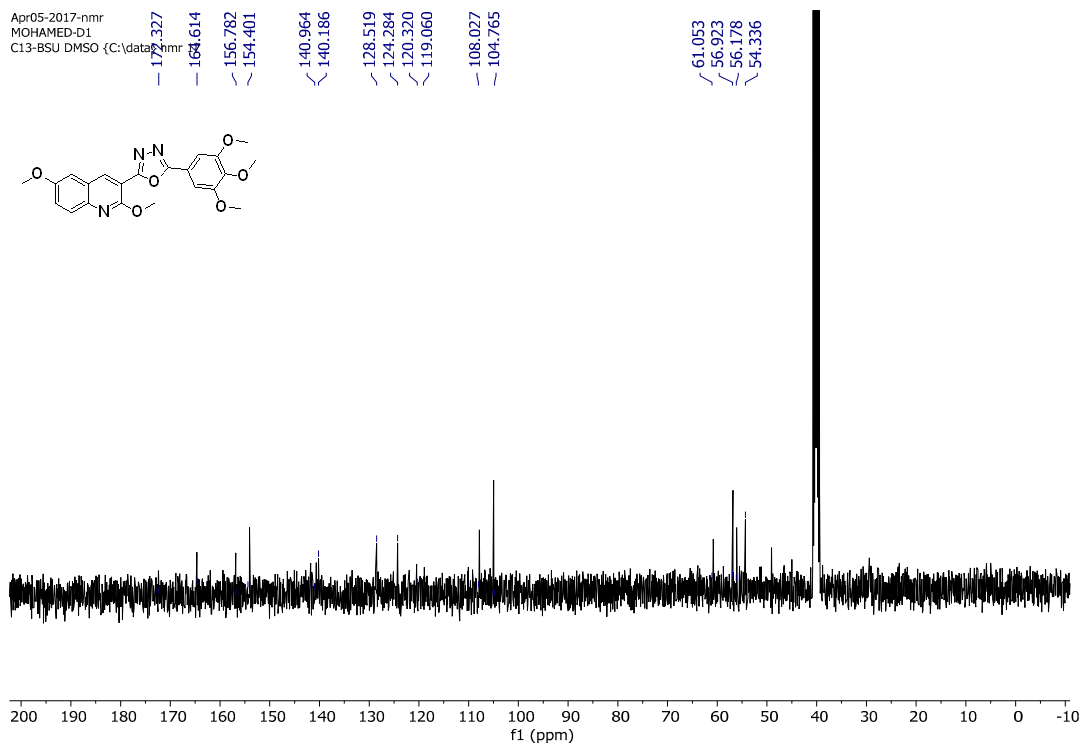


Figure S31; ^1H NMR for compound 20f

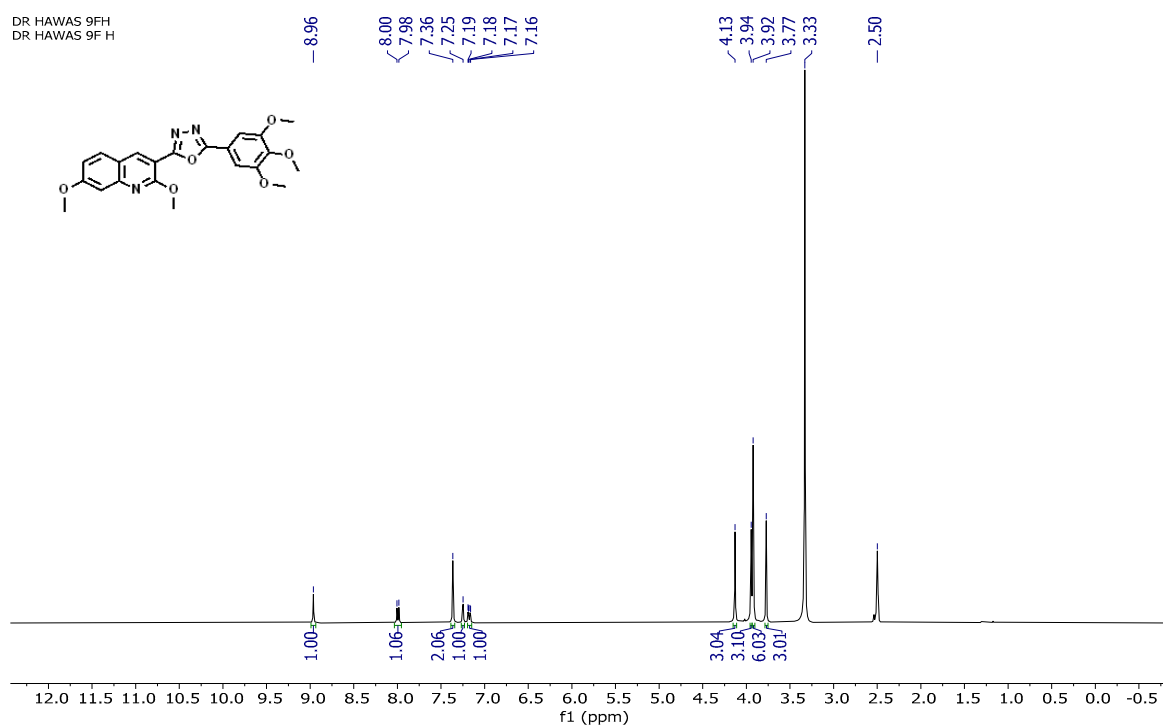


Figure S32; ^{13}C NMR for compound 20f

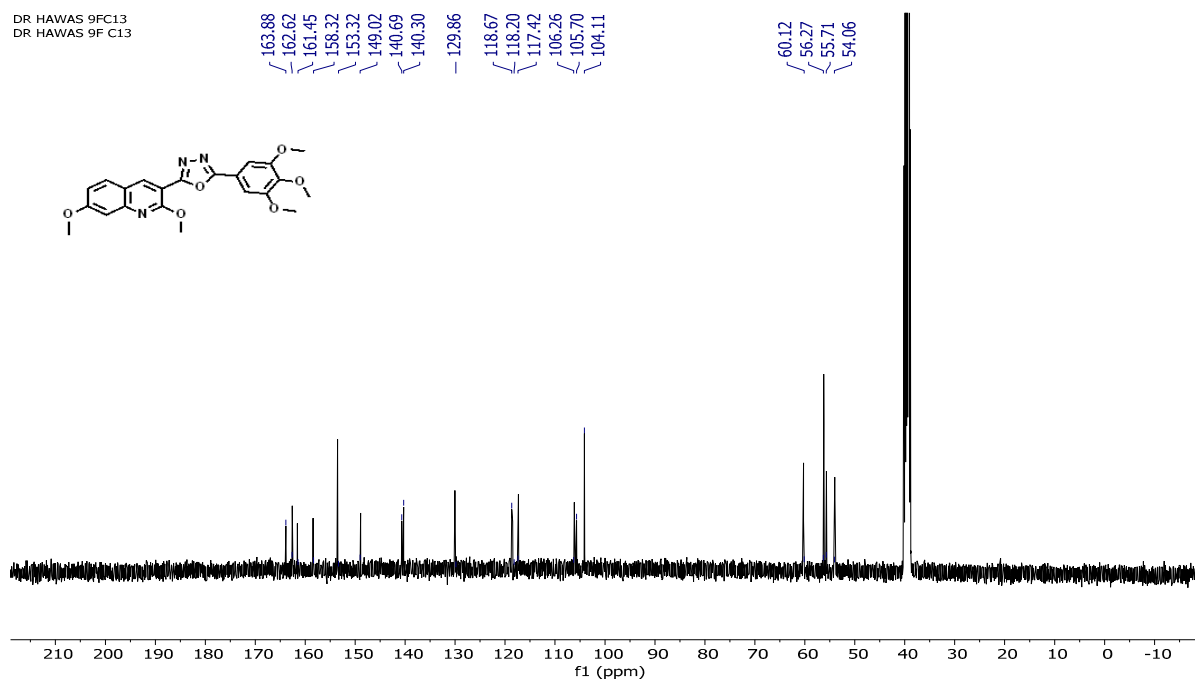


Figure S33; ^1H NMR for compound 20g

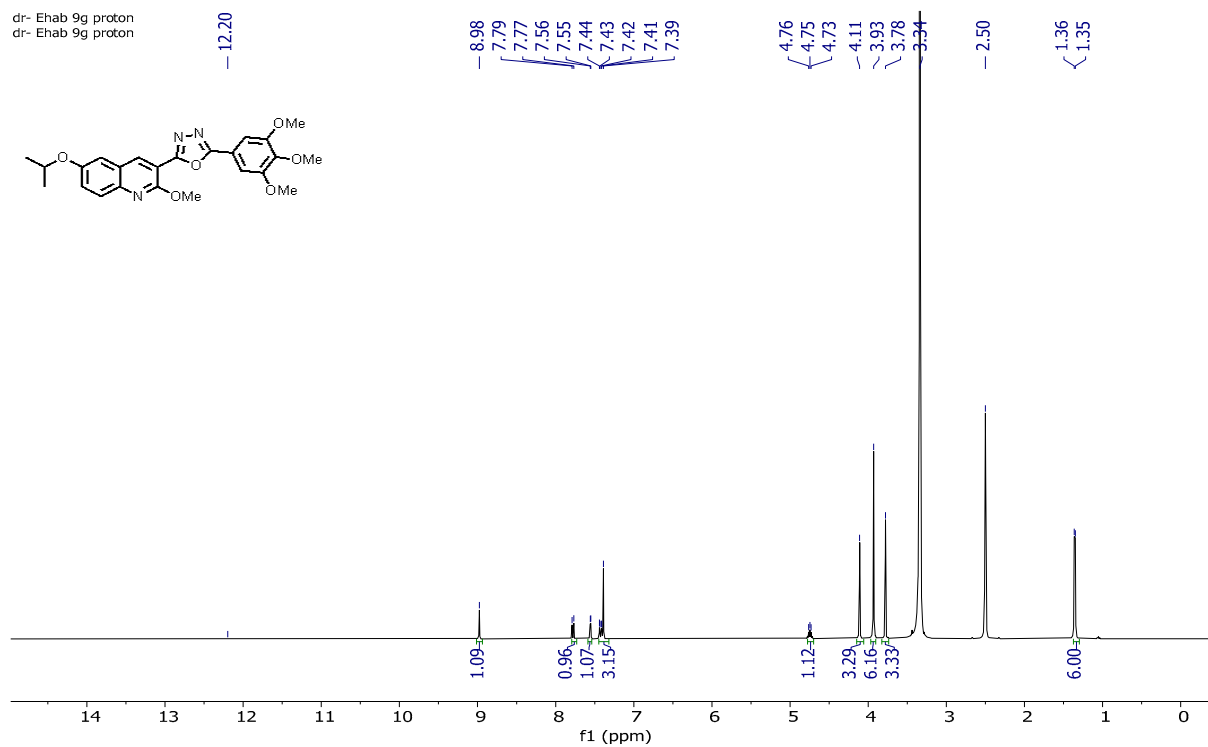


Figure S34; ^{13}C NMR for compound 20g

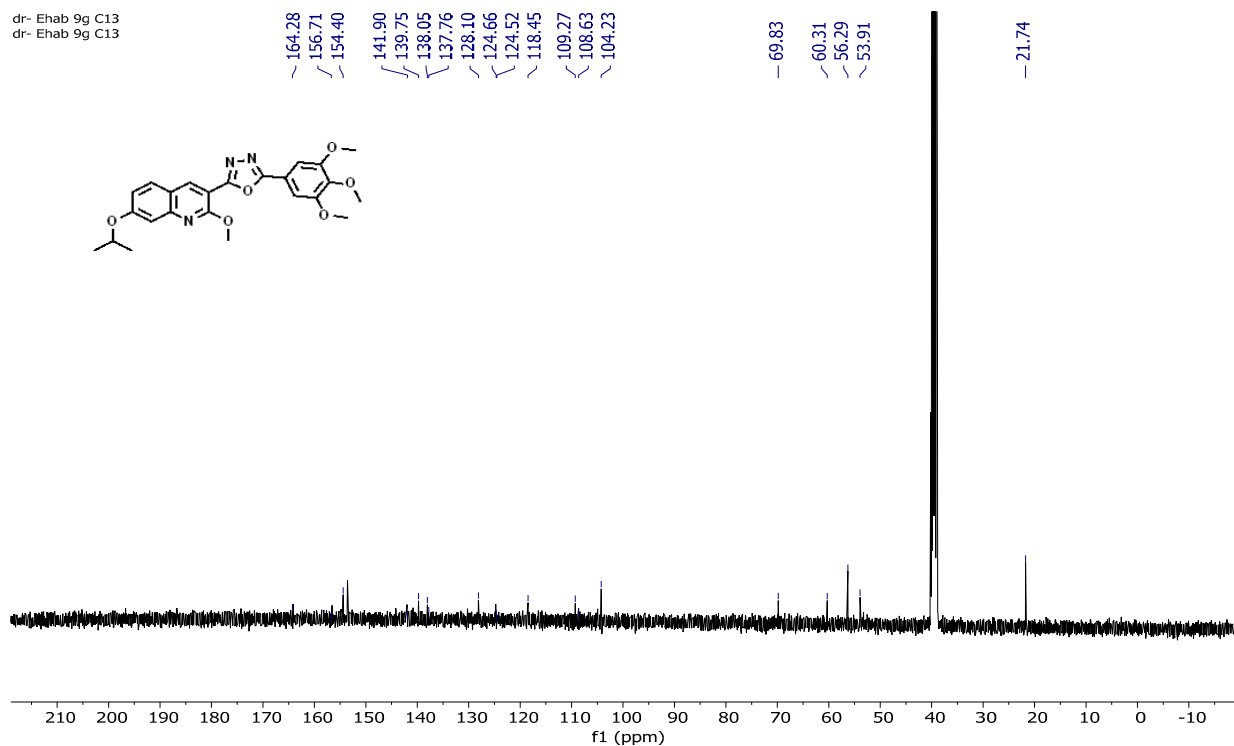


Figure S35; ^1H NMR f for compound 20h

Jul02-2018-abeer
M MOSTAFA-9G
PROTON_BS DMSO {C:\data} abeer 12

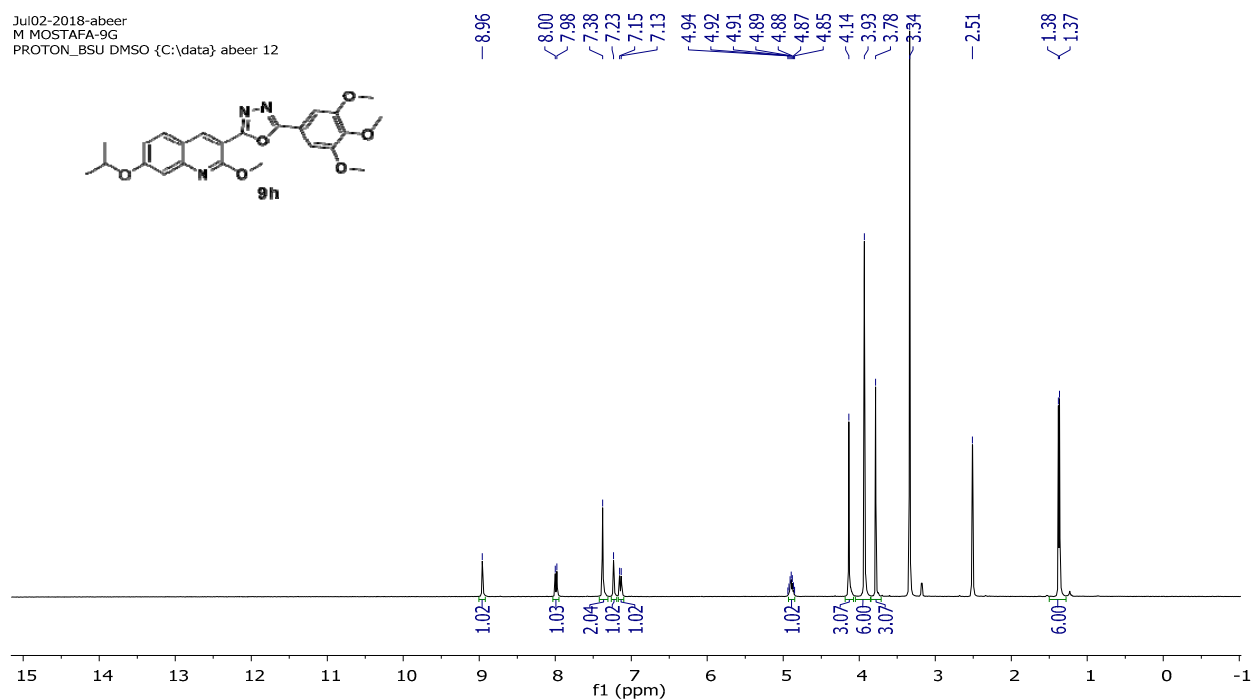


Figure S36; ^{13}C NMR for compound 20h

dr-Hwas 9h C13
dr-Hawas 9h C13

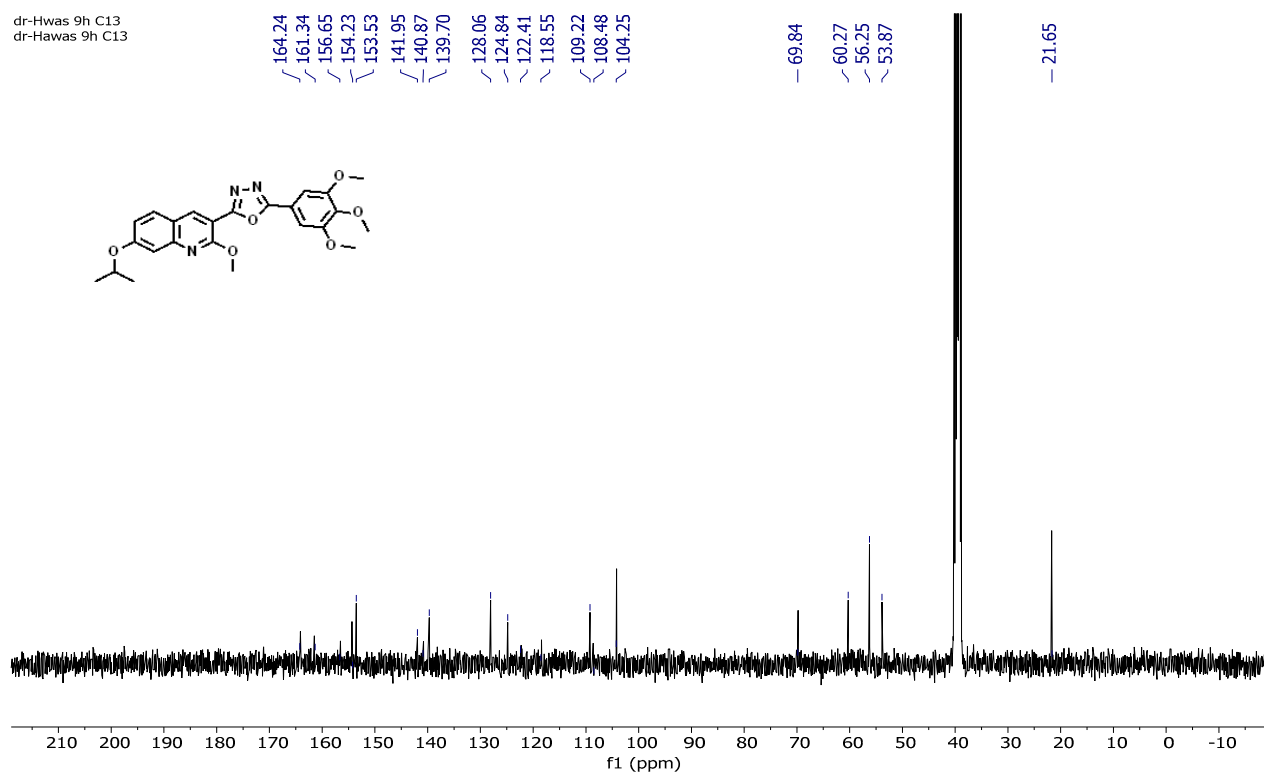


Figure S37; ^1H NMR for compound 20i

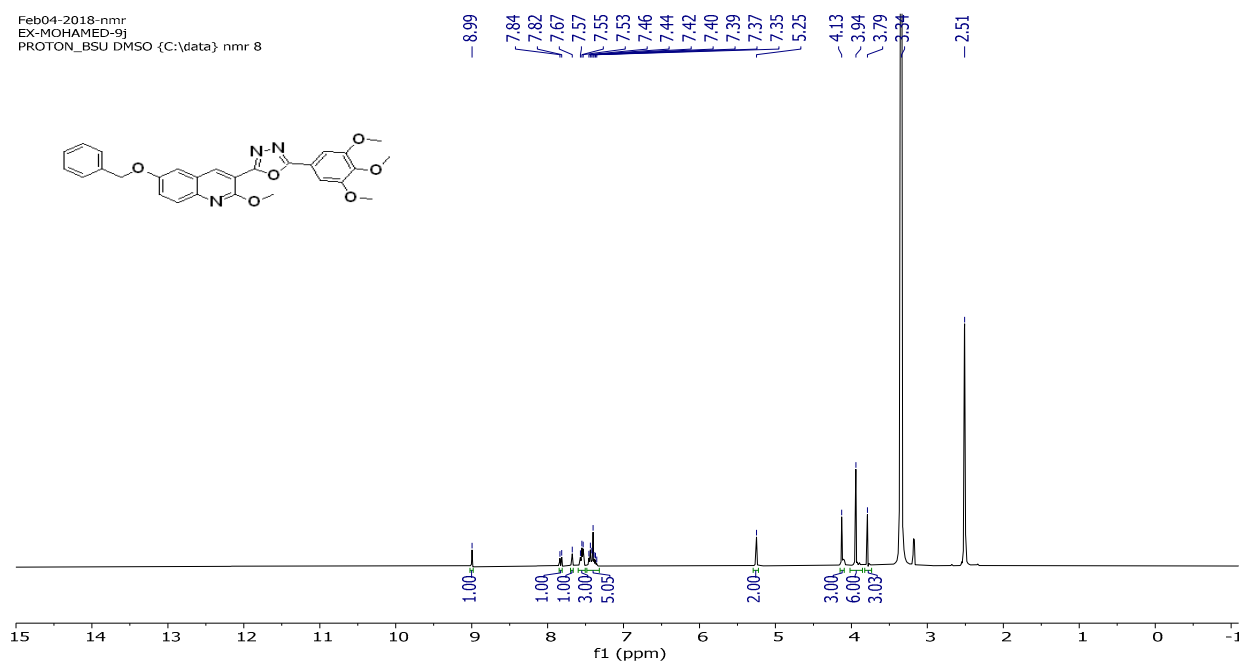


Figure S38; ^{13}C NMR for compound 20i

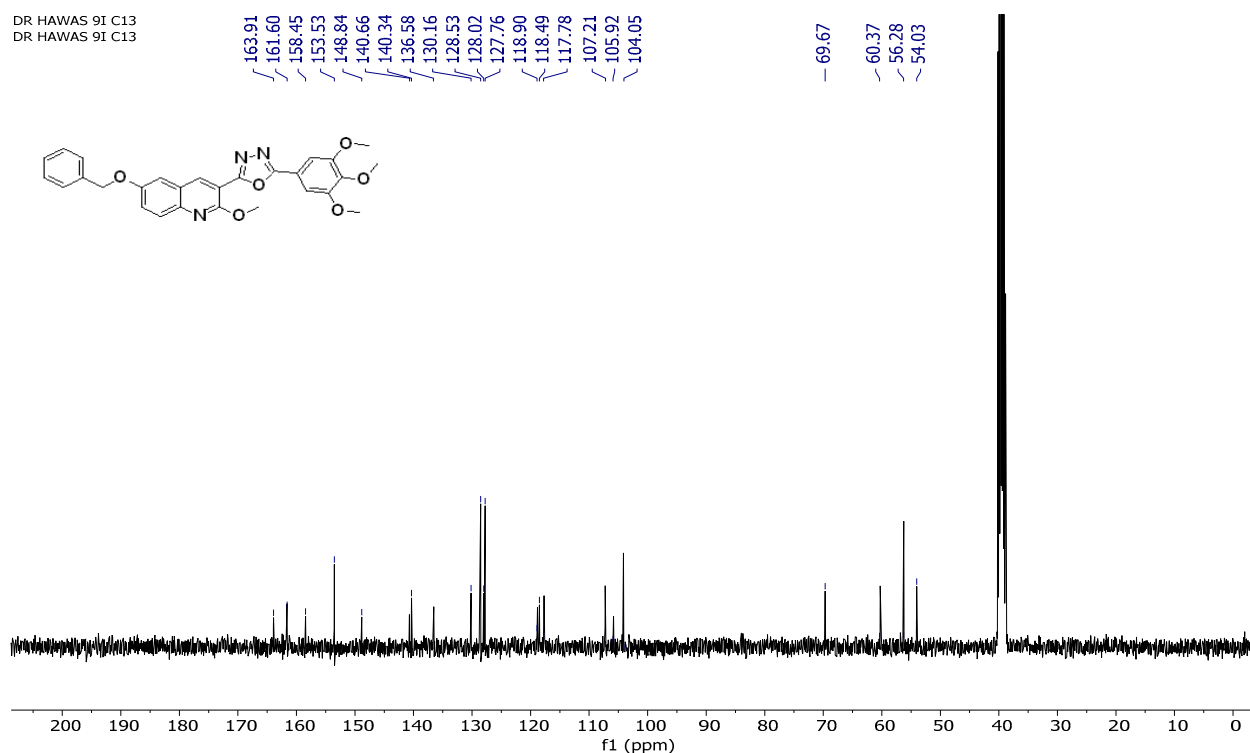


Figure S39; ^1H NMR for compound 20j

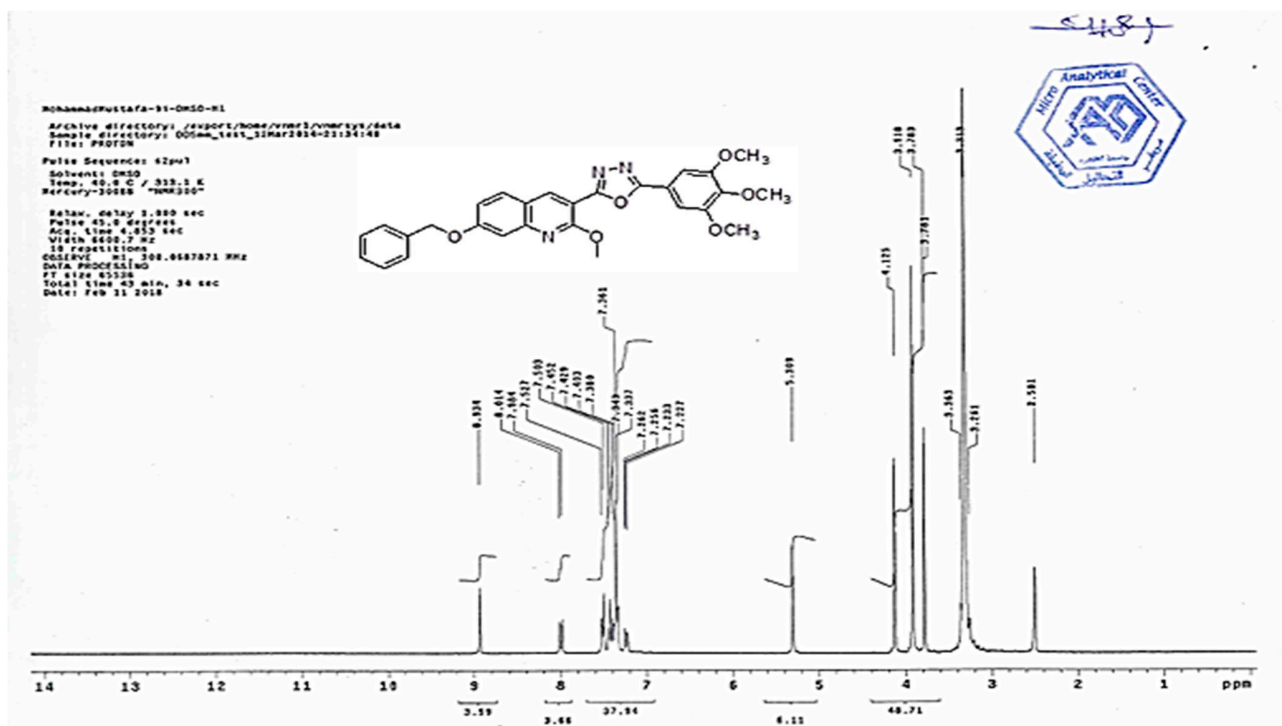
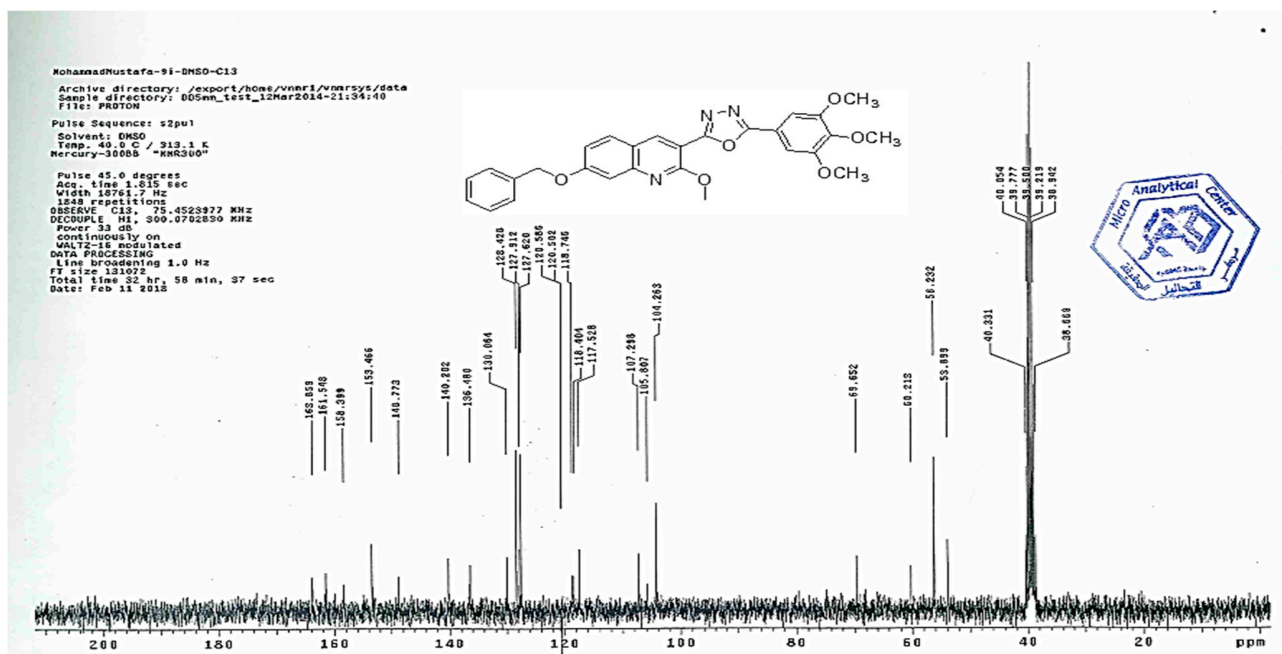


Figure S40; ^{13}C NMR for compound 20j



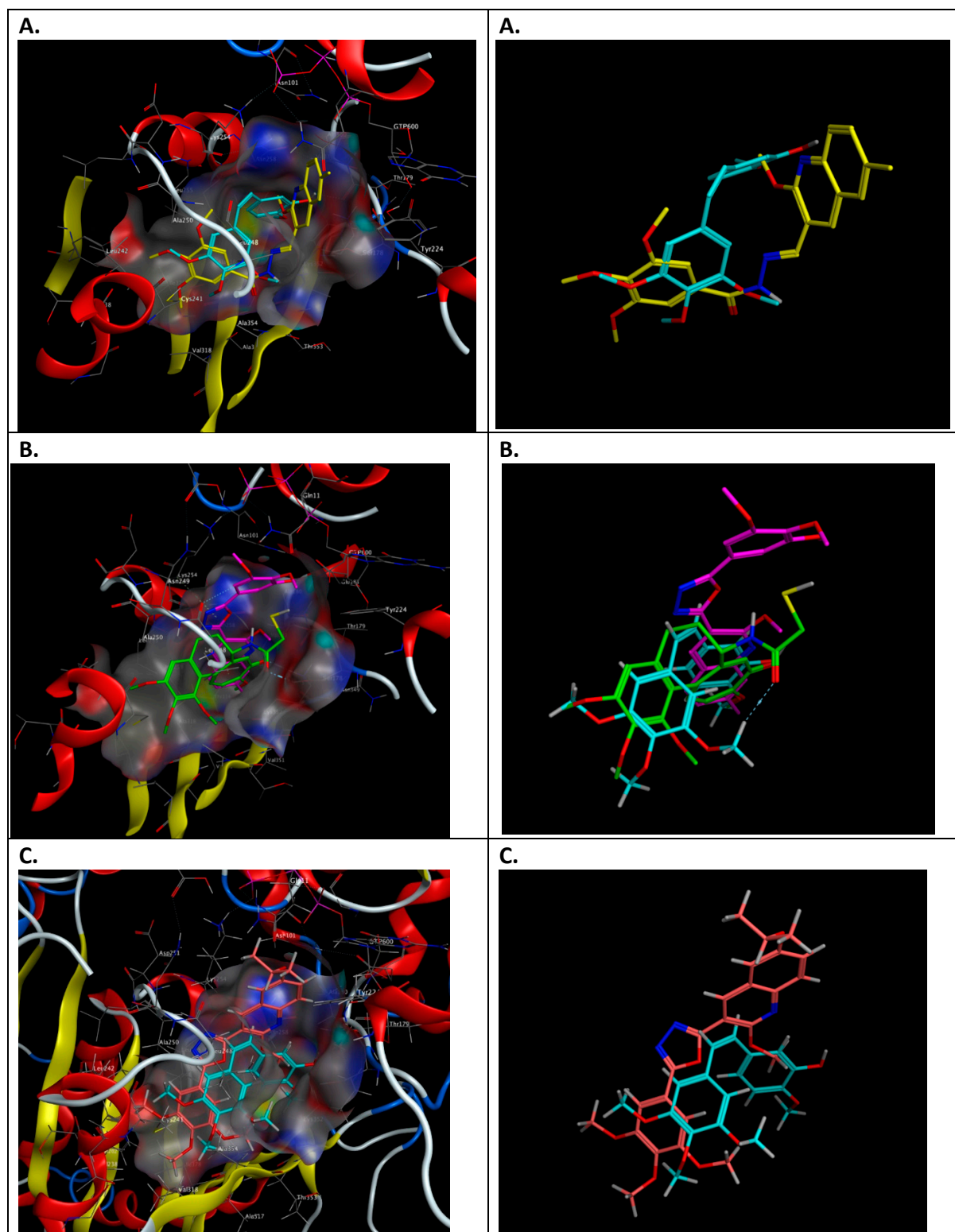


Figure S41. **A.** Quinoline **19b** (yellow) and CA-4 (cyan) docked at the colchicine-binding site of tubulin in co-crystal 1SAO. **B.** Quinoline **20c** (pink) and DAMA-colchicine (green) docked at the colchicine-binding site of tubulin in co-crystal 1SAO. **C.** Quinoline **9=20g** (red) and CA-4 (cyan) docked at the colchicine-binding site of tubulin in co-crystal 1SAO. Protein residues removed on right for clarity. (red = oxygen, grey = hydrogen).

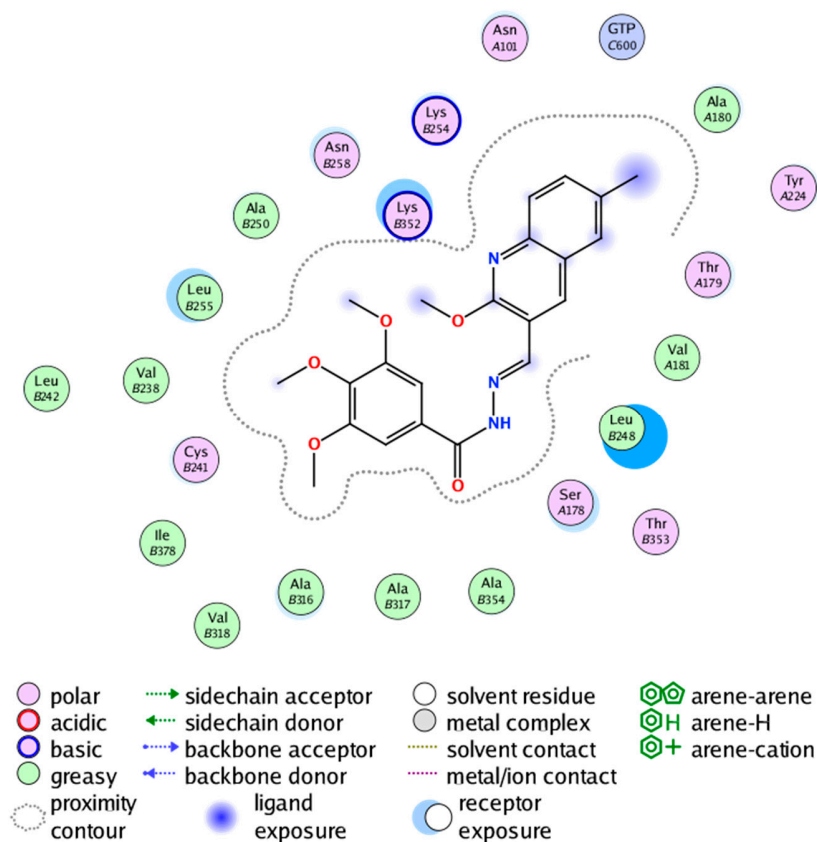


Figure S42. 2D Ligand Interaction Schematic for **19b** as generated by MOE

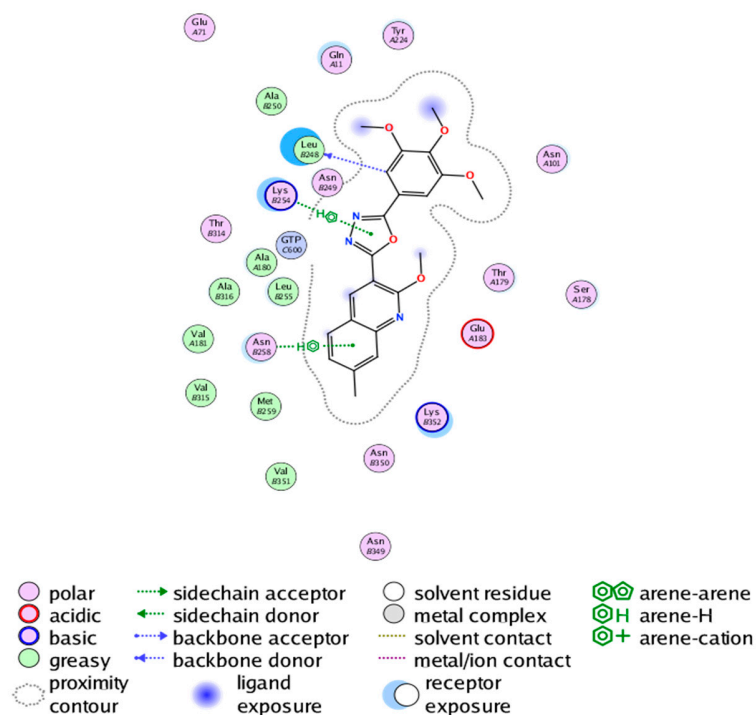


Figure S43. 2D Ligand Interaction Schematic for **20c** as generated by MOE

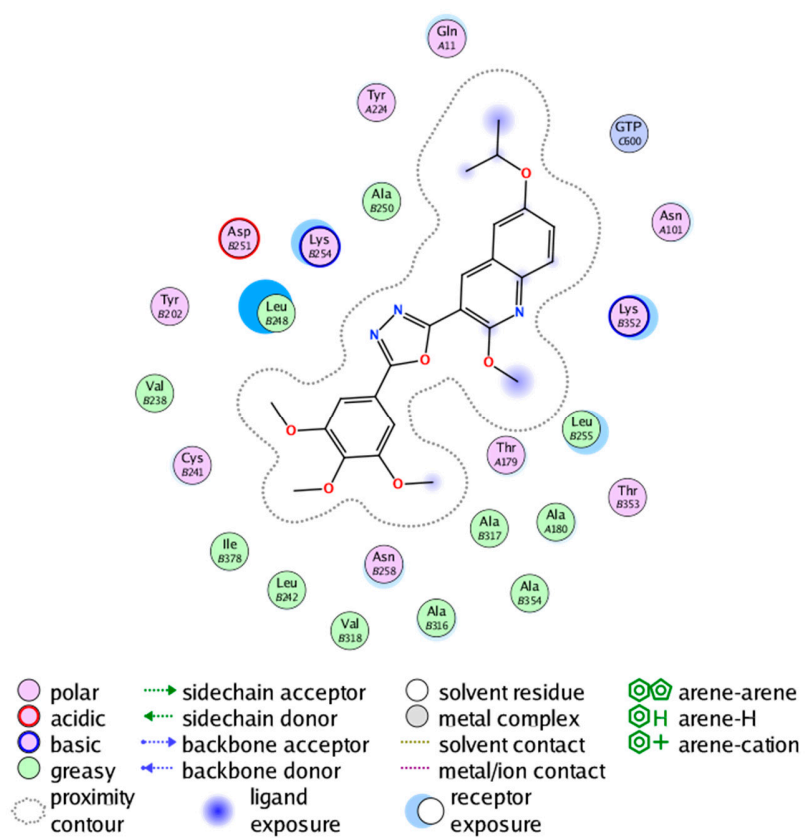


Figure S44. 2D Ligand Interaction Schematic for **20g** as generated by MOE