

Novel bakuchiol derivatives inhibit migration and invasion of non-small cell lung cancers by suppressing epithelial-to-mesenchymal transition

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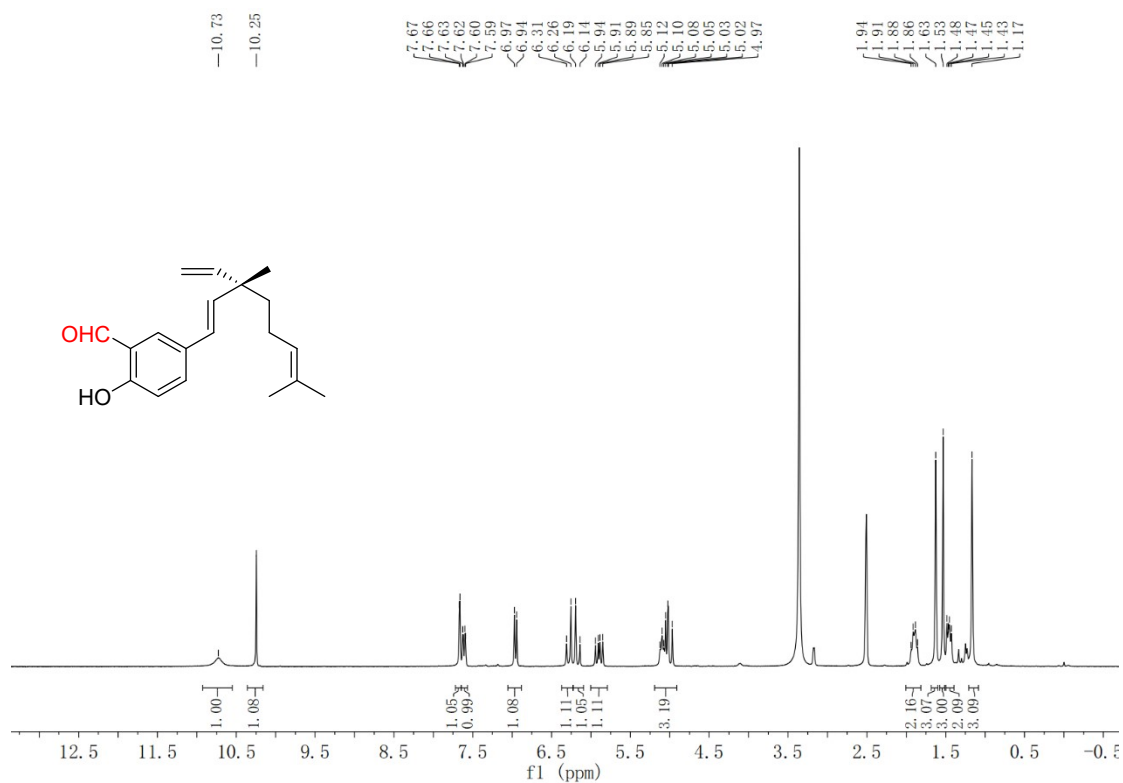


Figure S1 ¹H NMR spectrum of compound 1

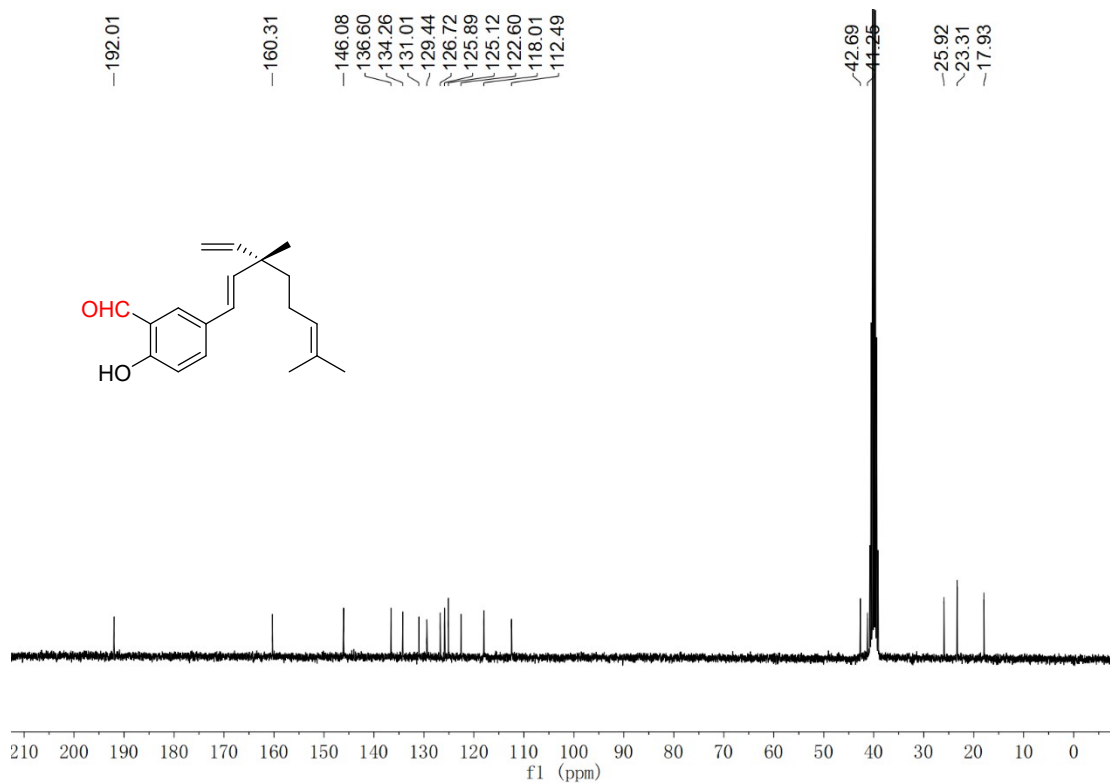


Figure S2 ¹³C NMR spectrum of compound 1

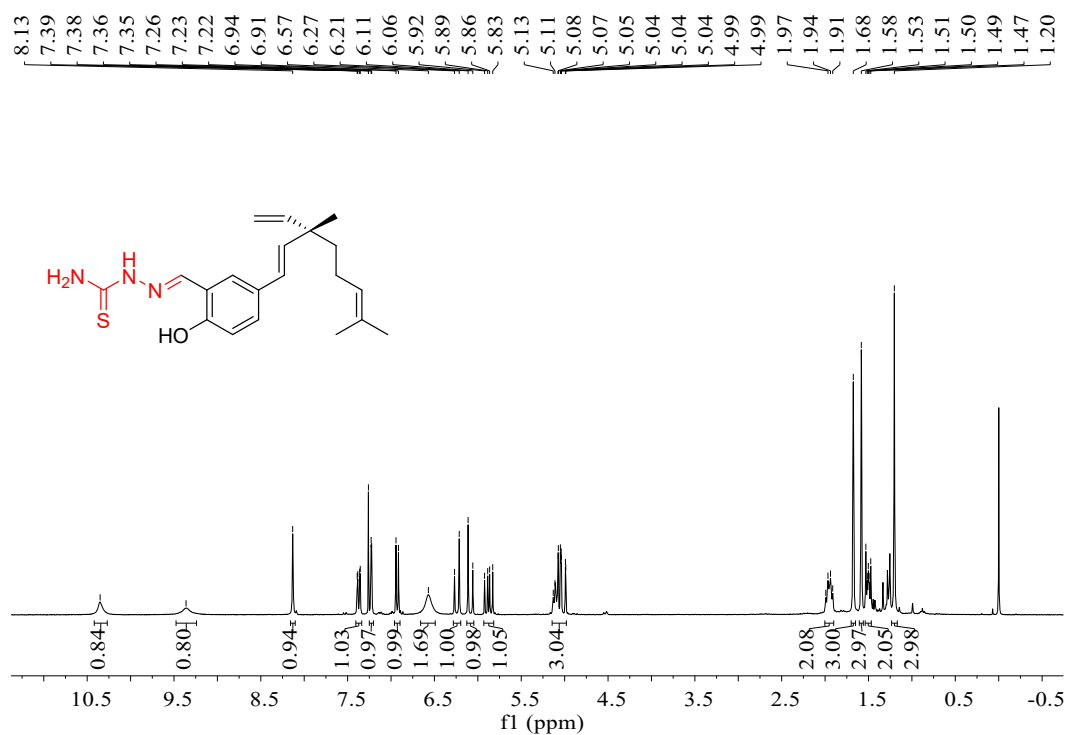


Figure S3 ¹H NMR spectrum of compound 2a

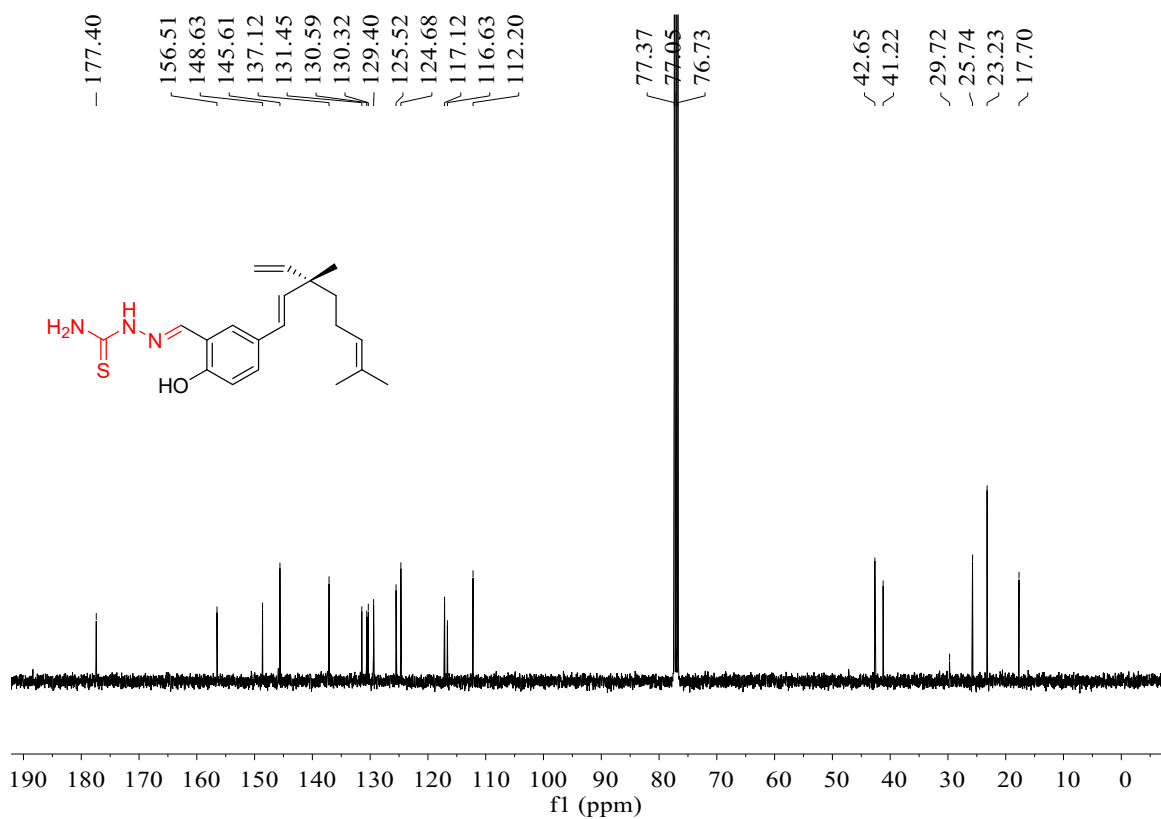


Figure S4 ¹³C NMR spectrum of compound 2a

136-WJA-4-A #18 RT: 0.10 AV: 1 NL: 2.05E8
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]

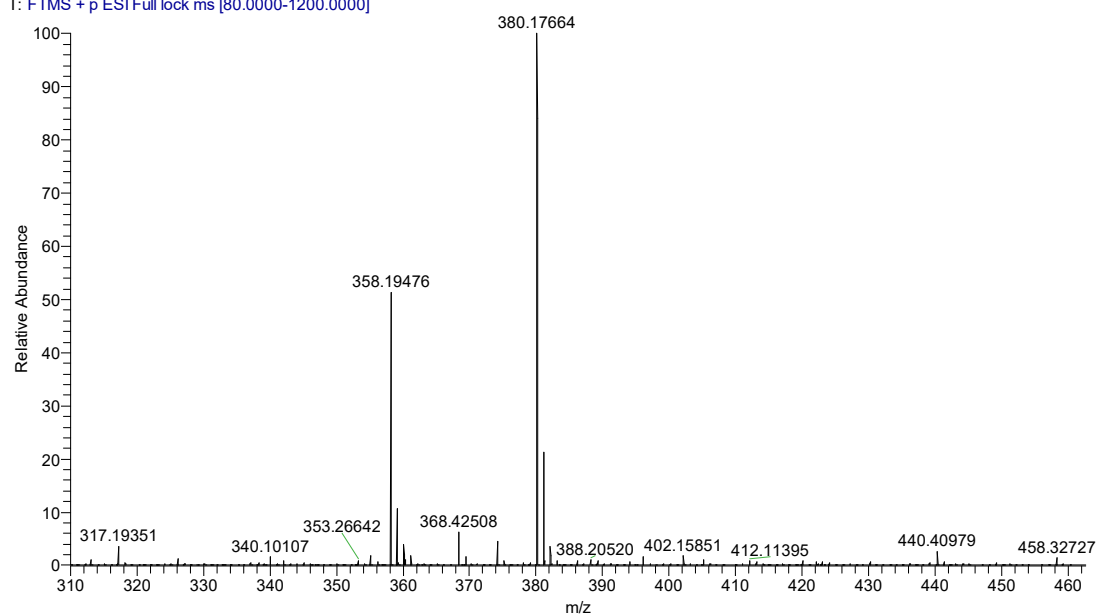


Figure S5 ESI-HRMS spectrum of compound 2a

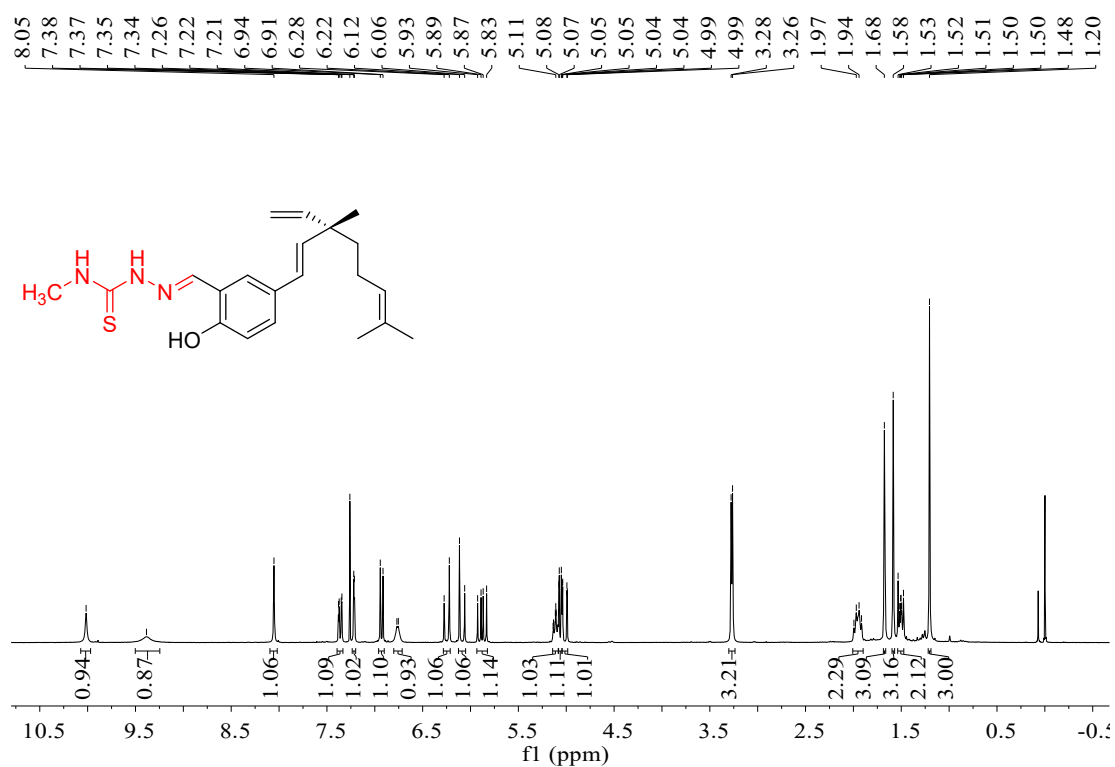


Figure S6 ¹H NMR spectrum of compound 2b

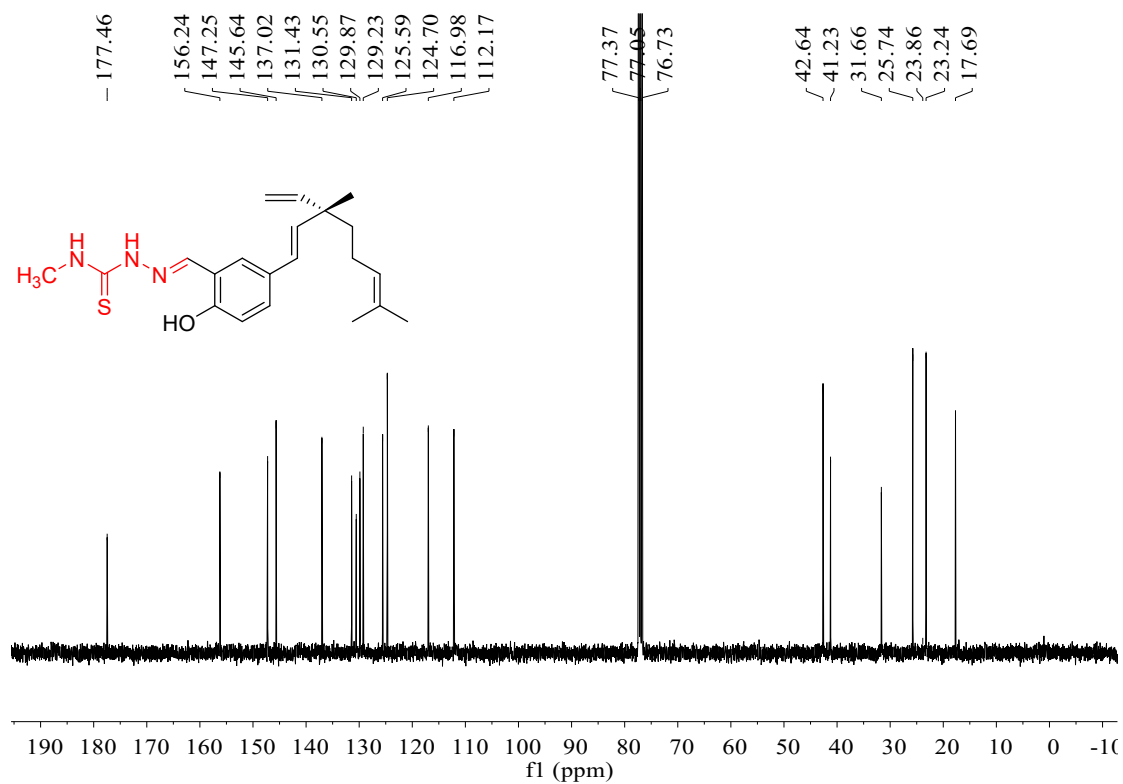


Figure S7 ¹³C NMR spectrum of compound 2b

136-XMF-2-13-11 #19 RT: 0.11 AV: 1 NL: 4.59E7
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]

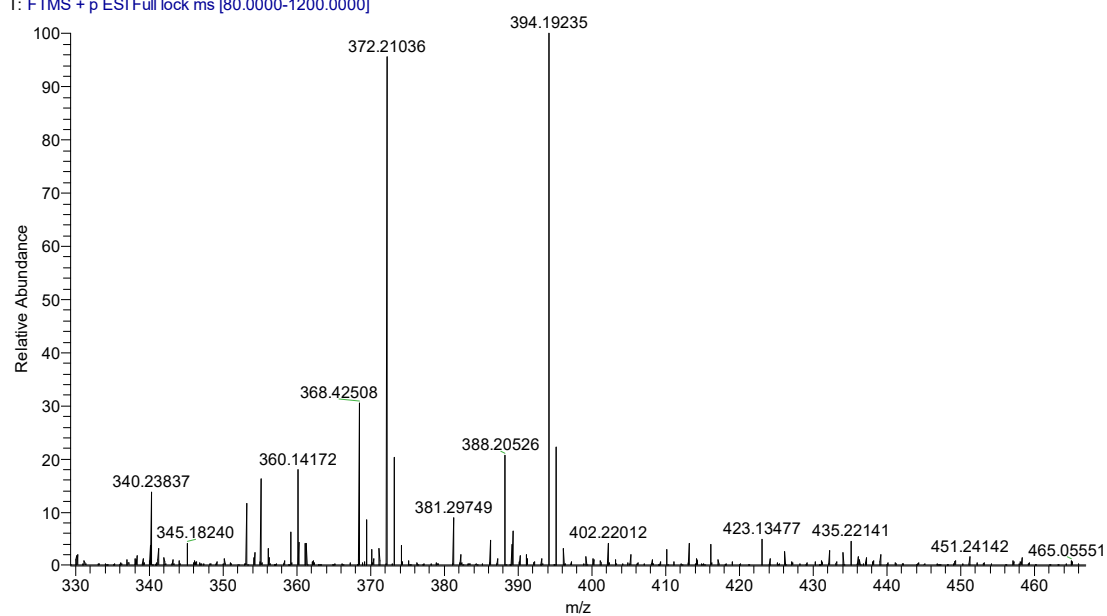


Figure S8 ESI-HRMS spectrum of compound 2b

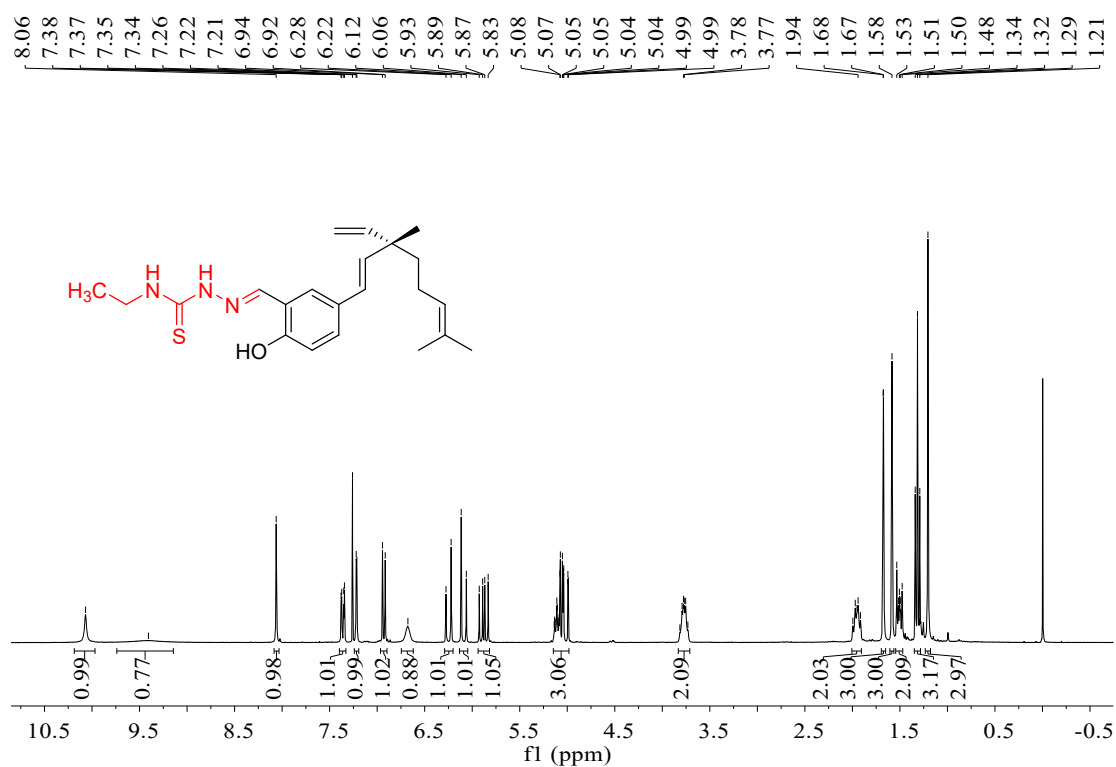


Figure S9 ¹H NMR spectrum of compound 2c

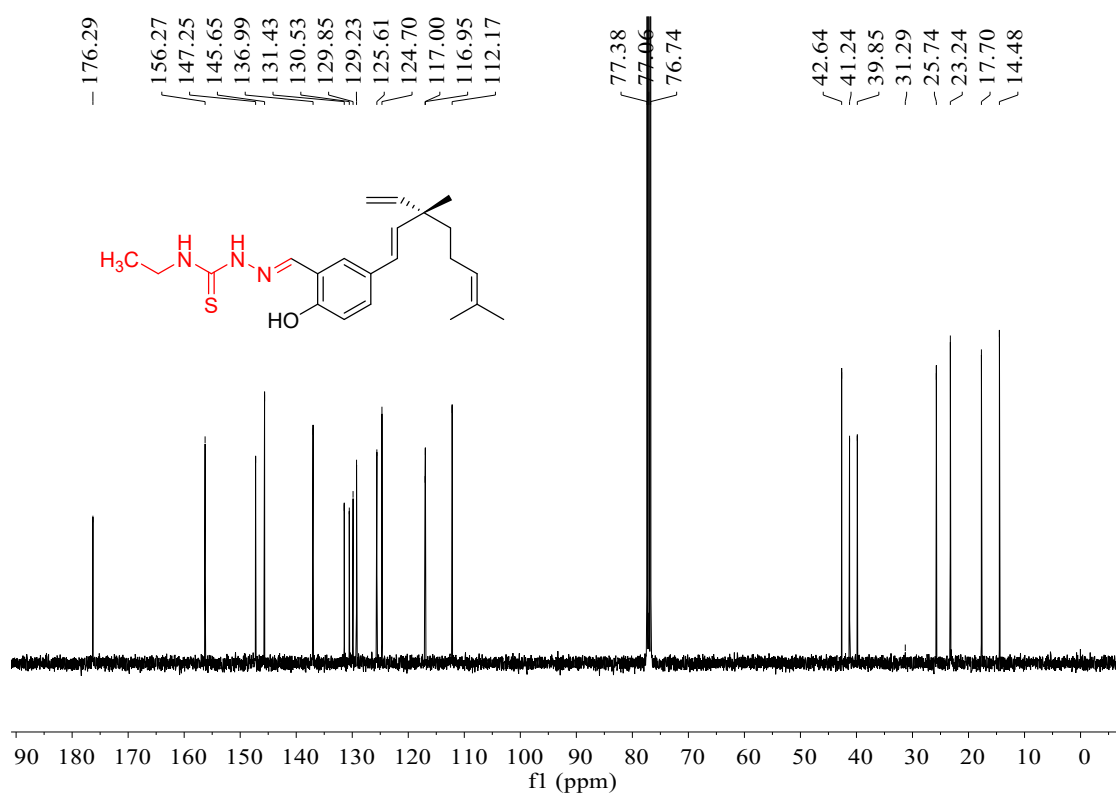


Figure S10 ¹³C NMR spectrum of compound 2c

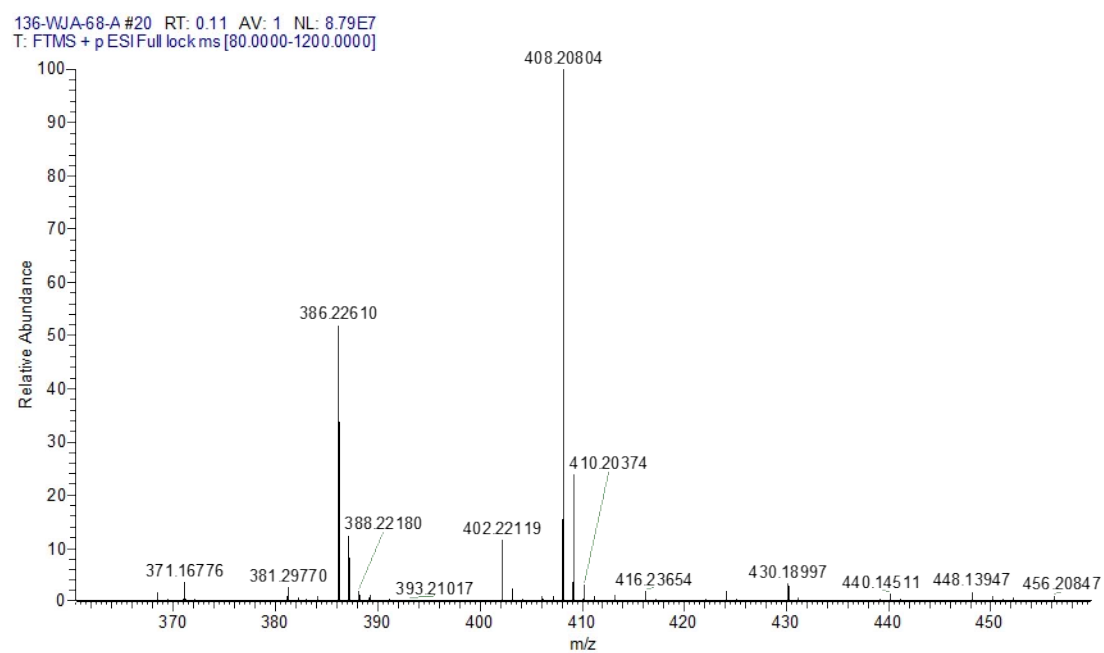


Figure S11 ESI-HRMS spectrum of compound 2c

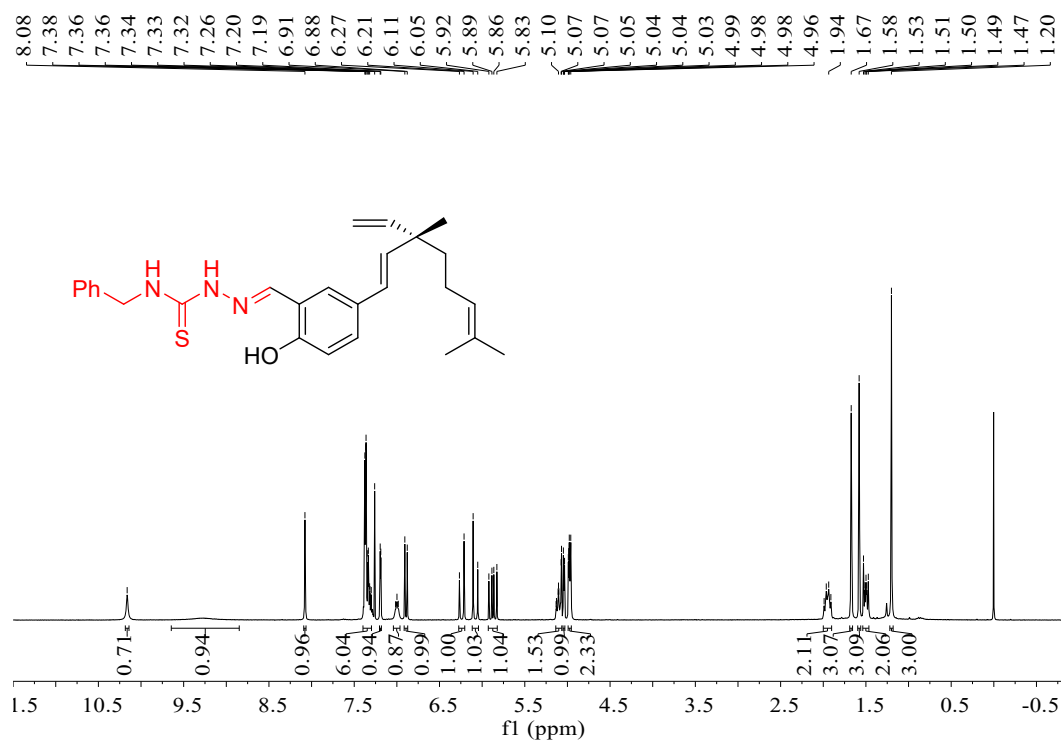


Figure S12 ¹H NMR spectrum of compound 2d

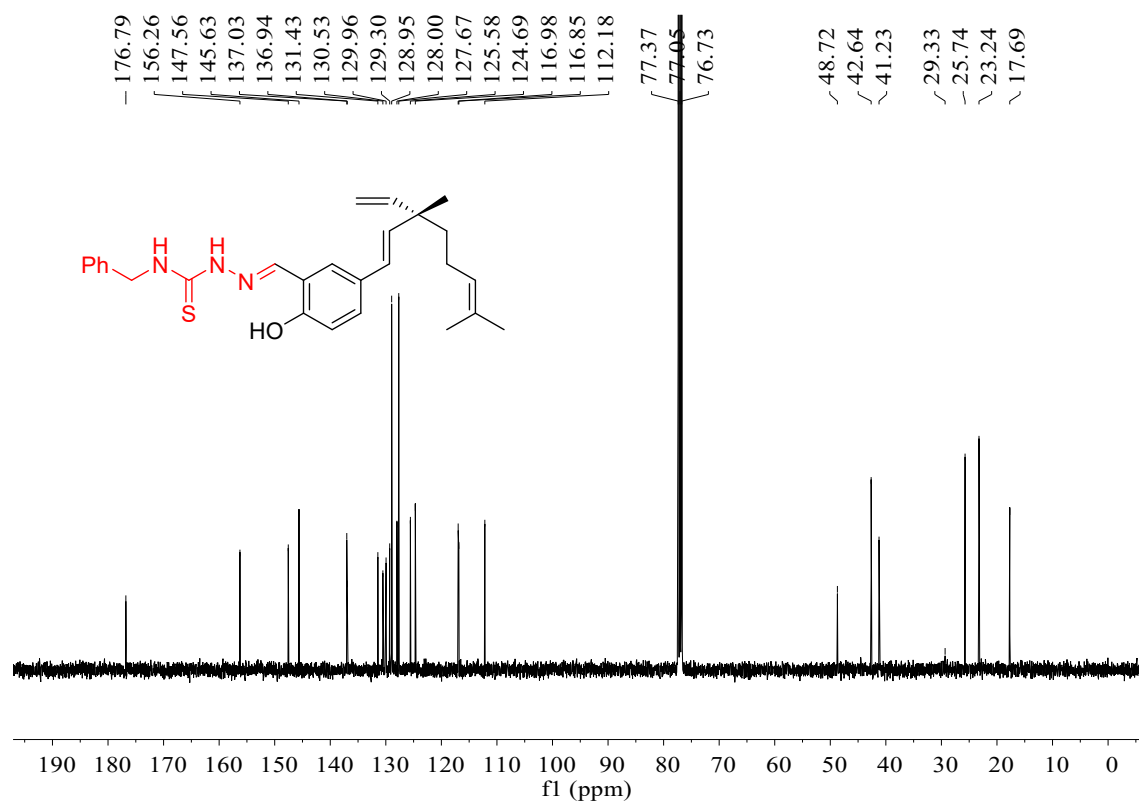


Figure S13 ¹³C NMR spectrum of compound 2d

136-WJA-66-A #17 RT: 0.09 AV: 1 NL: 1.21E7
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]

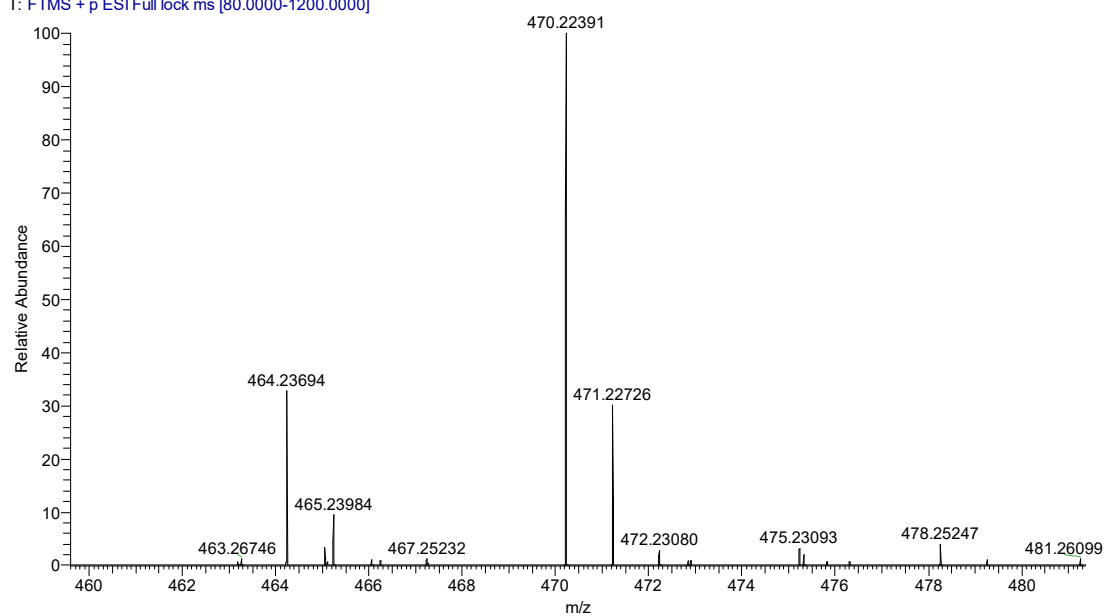


Figure S14 ESI-HRMS spectrum of compound 2d

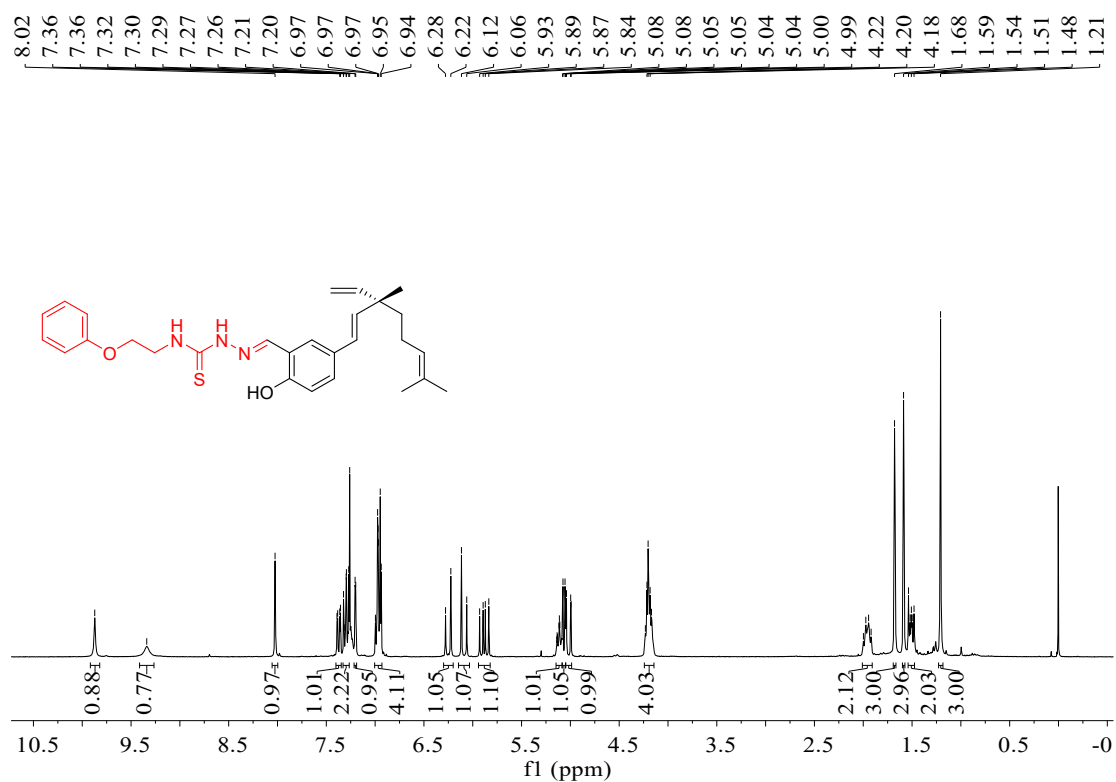


Figure S15 ¹H NMR spectrum of compound 2e

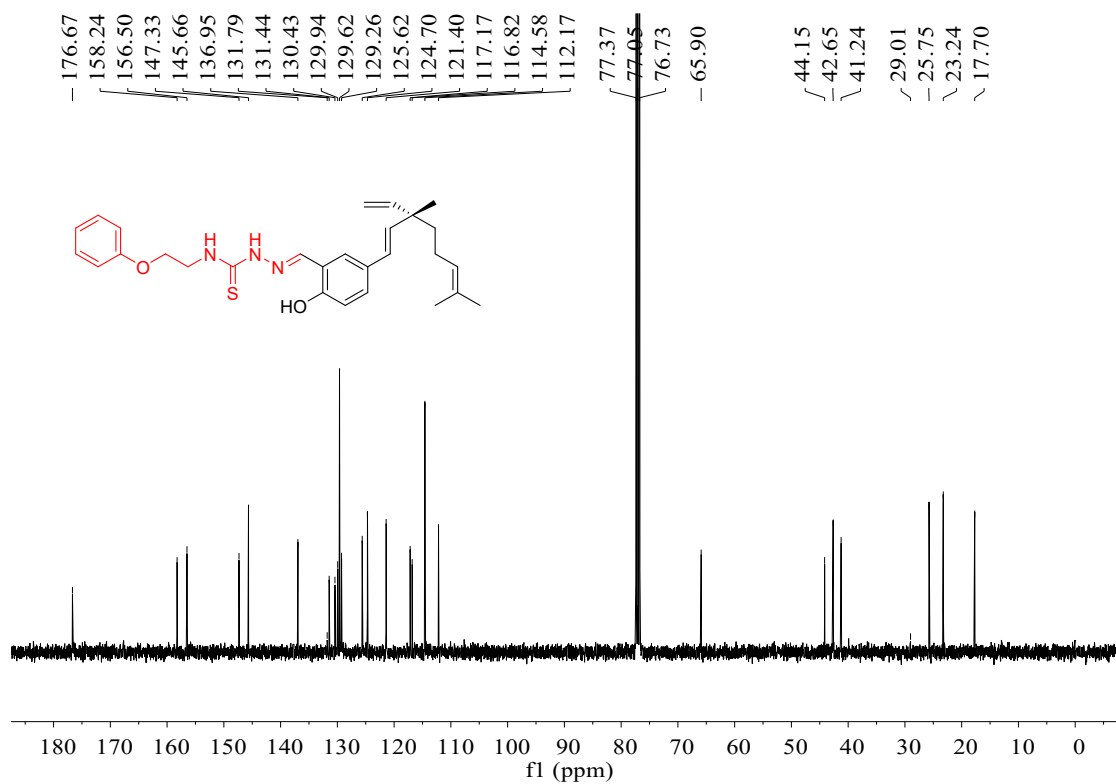


Figure S16 ¹³C NMR spectrum of compound 2e

136-WJA-73-A #19 RT: 0.11 AV: 1 NL: 3.16E7
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]

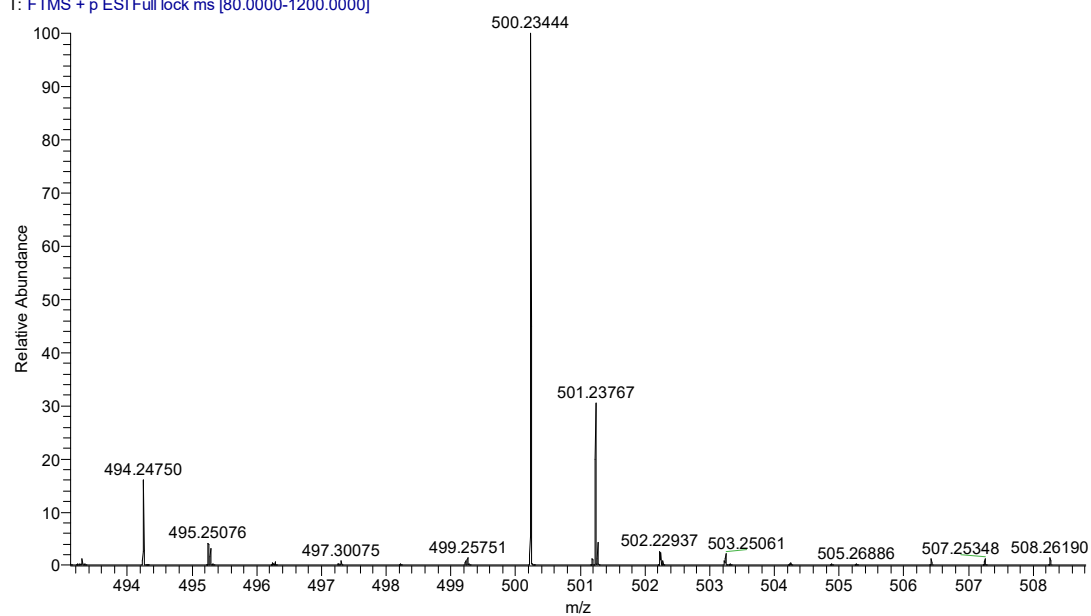


Figure S17 ESI-HRMS spectrum of compound 2e

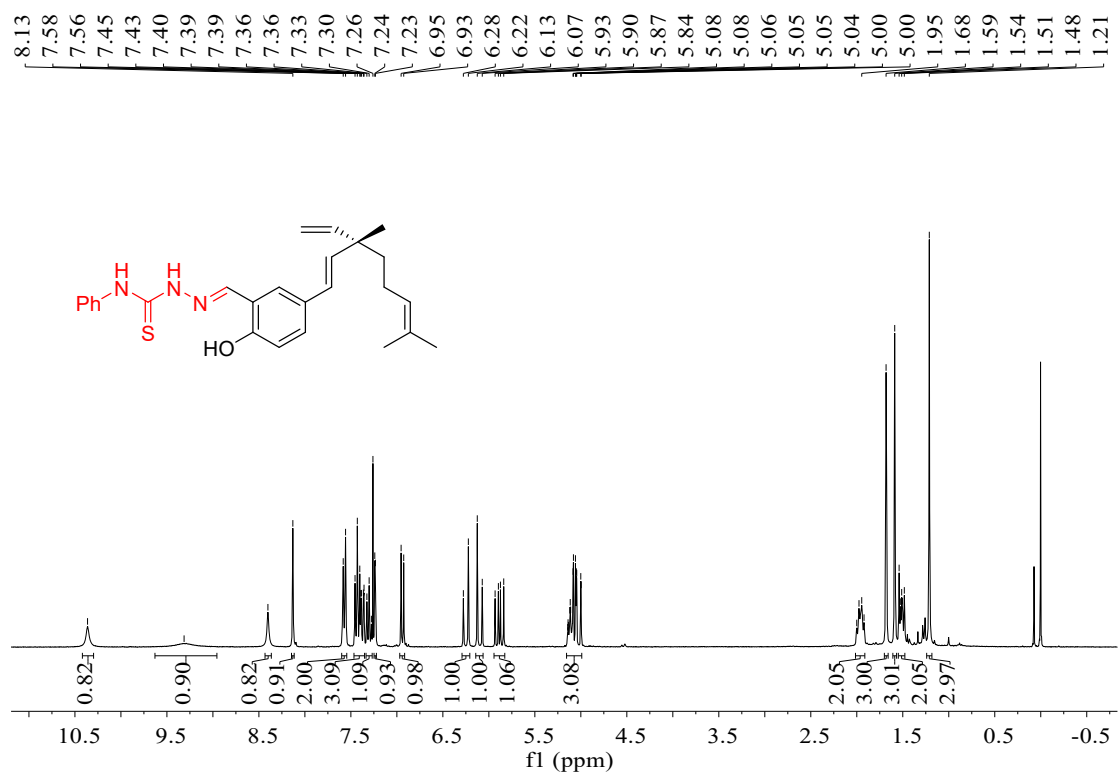


Figure S18 ¹H NMR spectrum of compound 2f

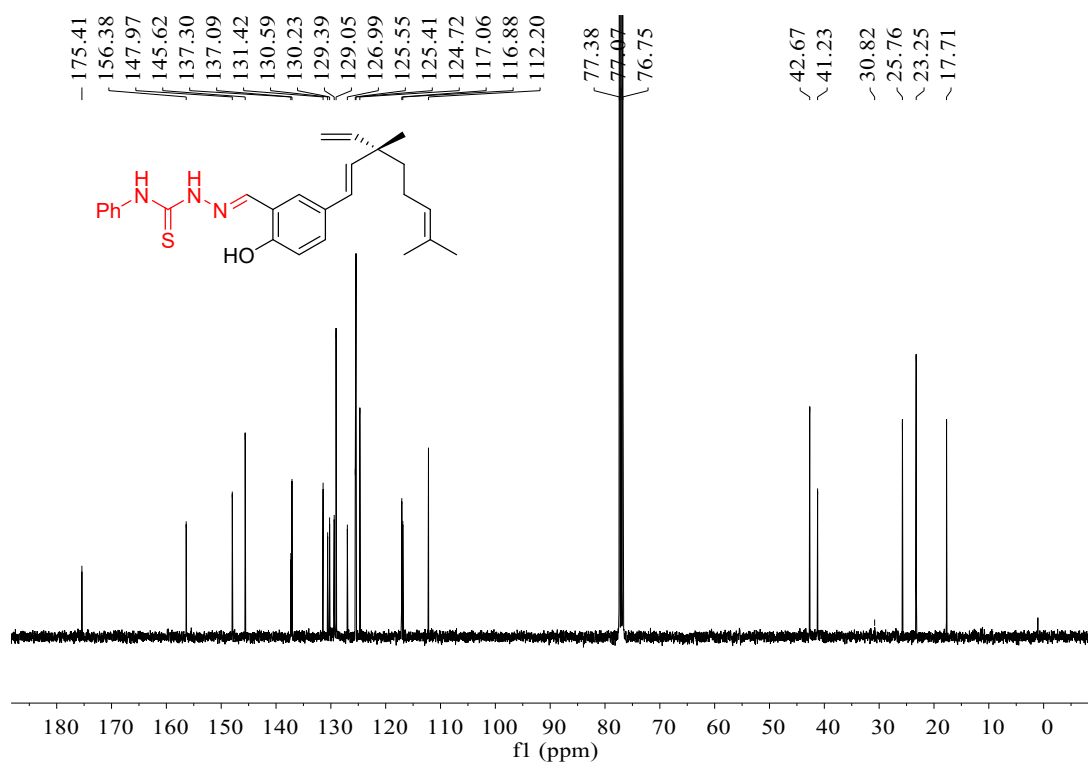


Figure S19 ¹³C NMR spectrum of compound 2f

136-WJA-67-A #14 RT: 0.08 AV: 1 NL: 1.66E8
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]

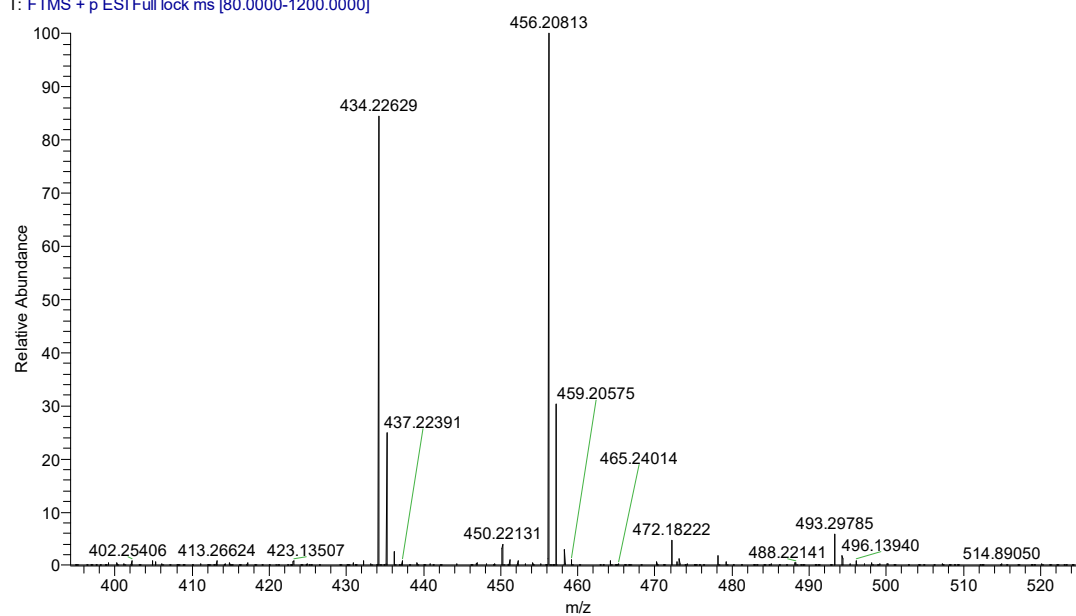


Figure S20 ESI-HRMS spectrum of compound 2f

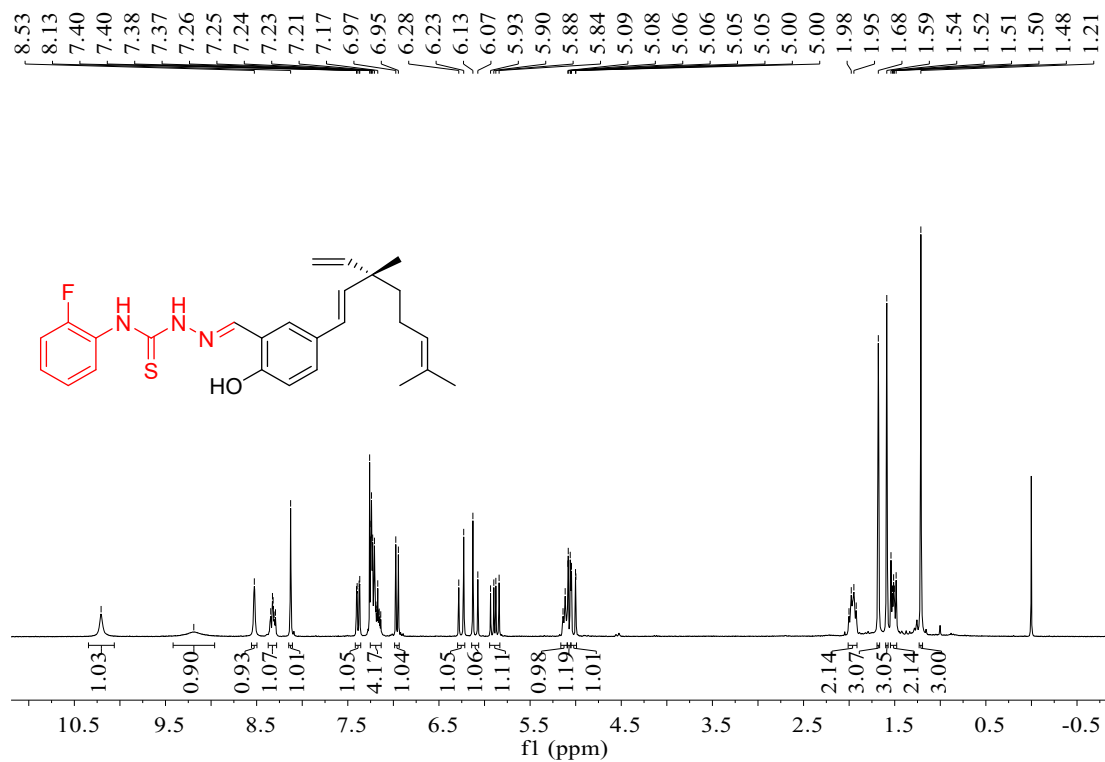


Figure S21 ¹H NMR spectrum of compound 2g

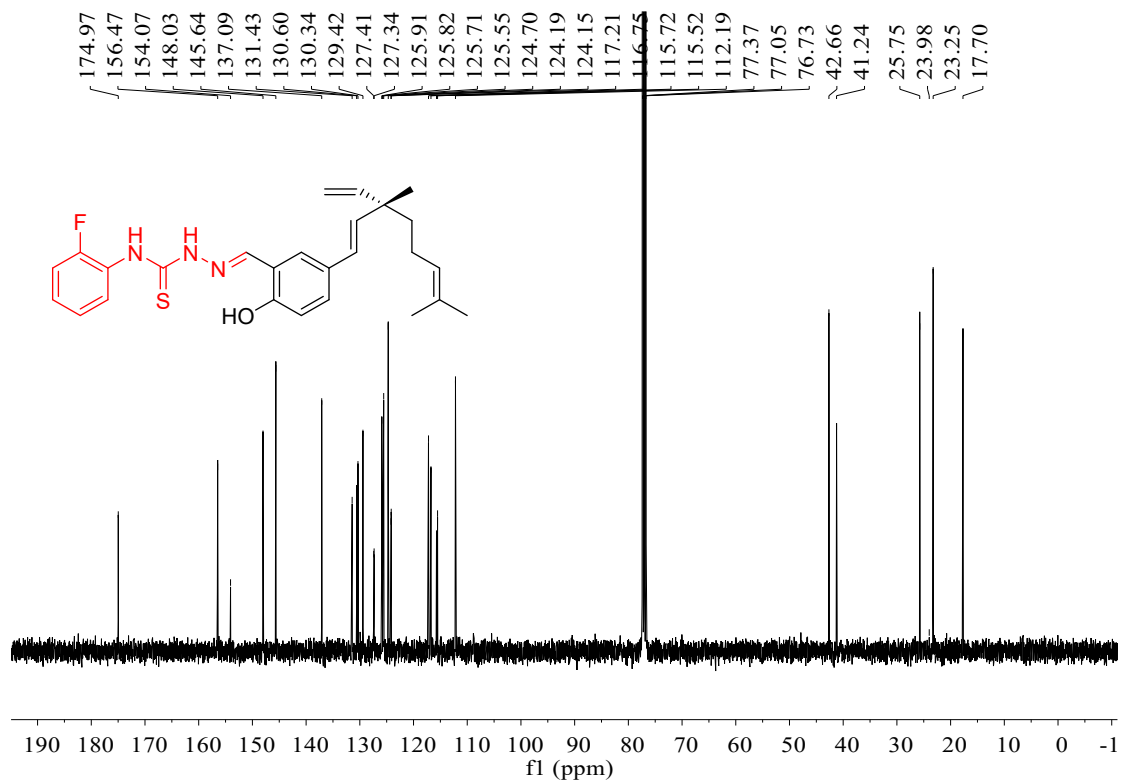


Figure S22 ¹³C NMR spectrum of compound 2g

136-XMF-2-13-5 #17 RT: 0.09 AV: 1 NL: 2.91E8
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]

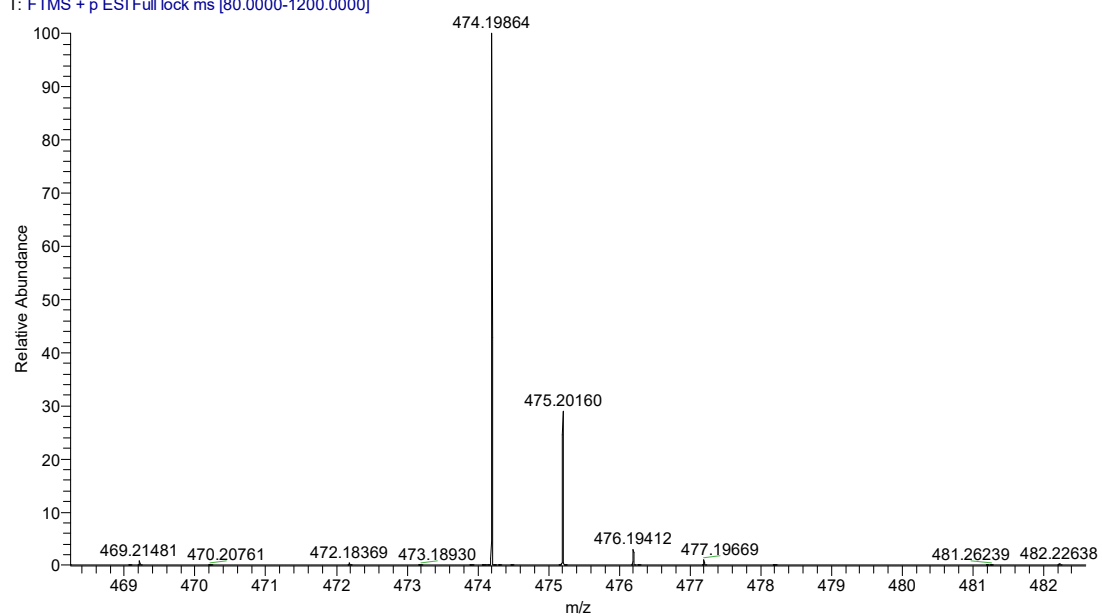


Figure S23 ESI-HRMS spectrum of compound 2g

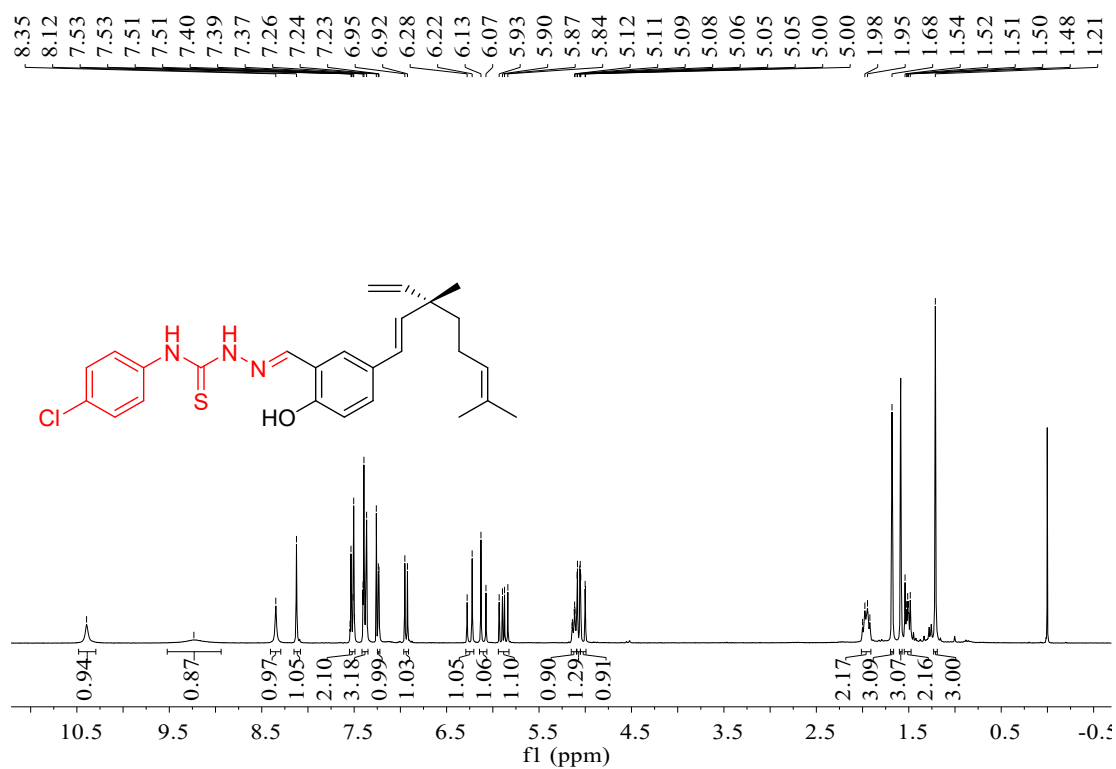


Figure S24 ¹H NMR spectrum of compound 2h

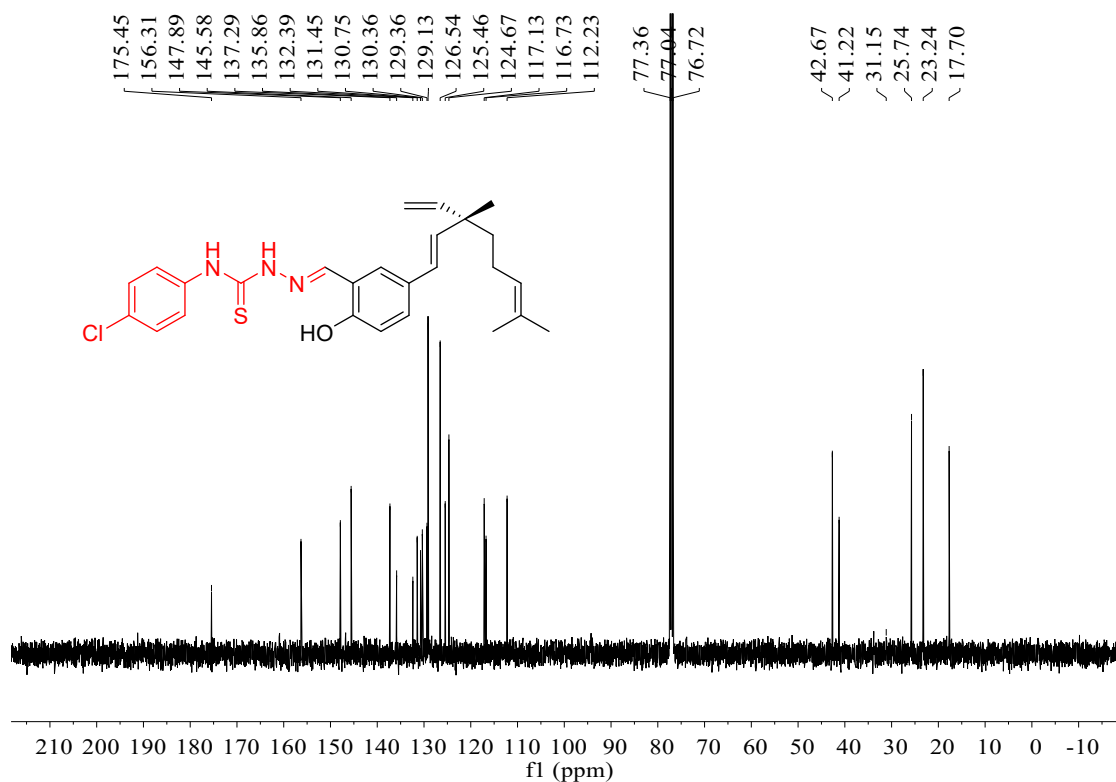


Figure S25 ¹³C NMR spectrum of compound 2h

136-XMF-2-13-2 #19 RT: 0.11 AV: 1 NL: 1.14E7
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]

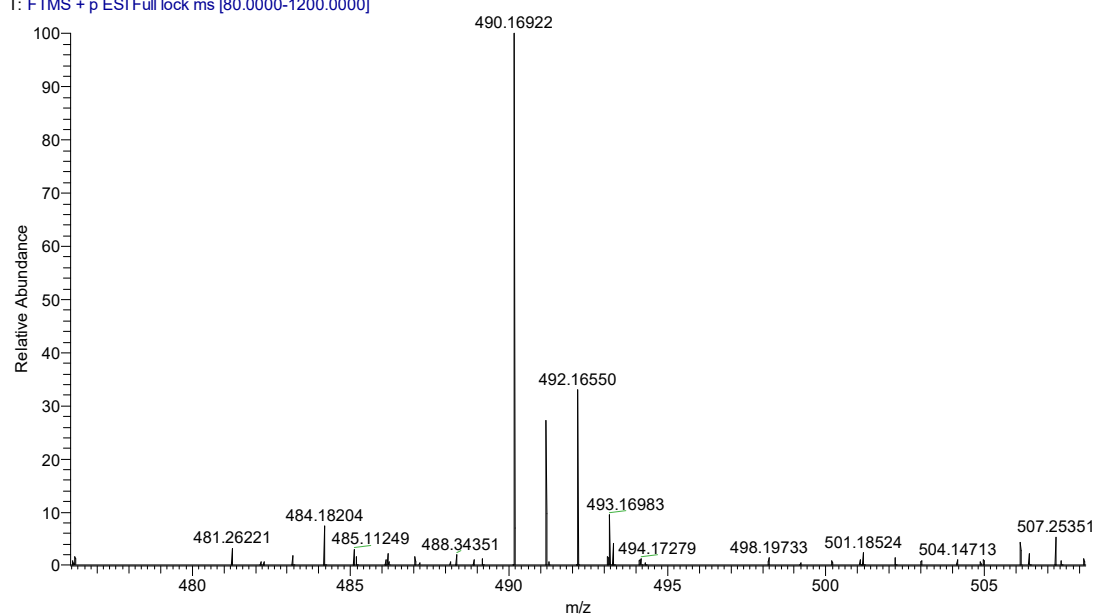


Figure S26 ESI-HRMS spectrum of compound 2h

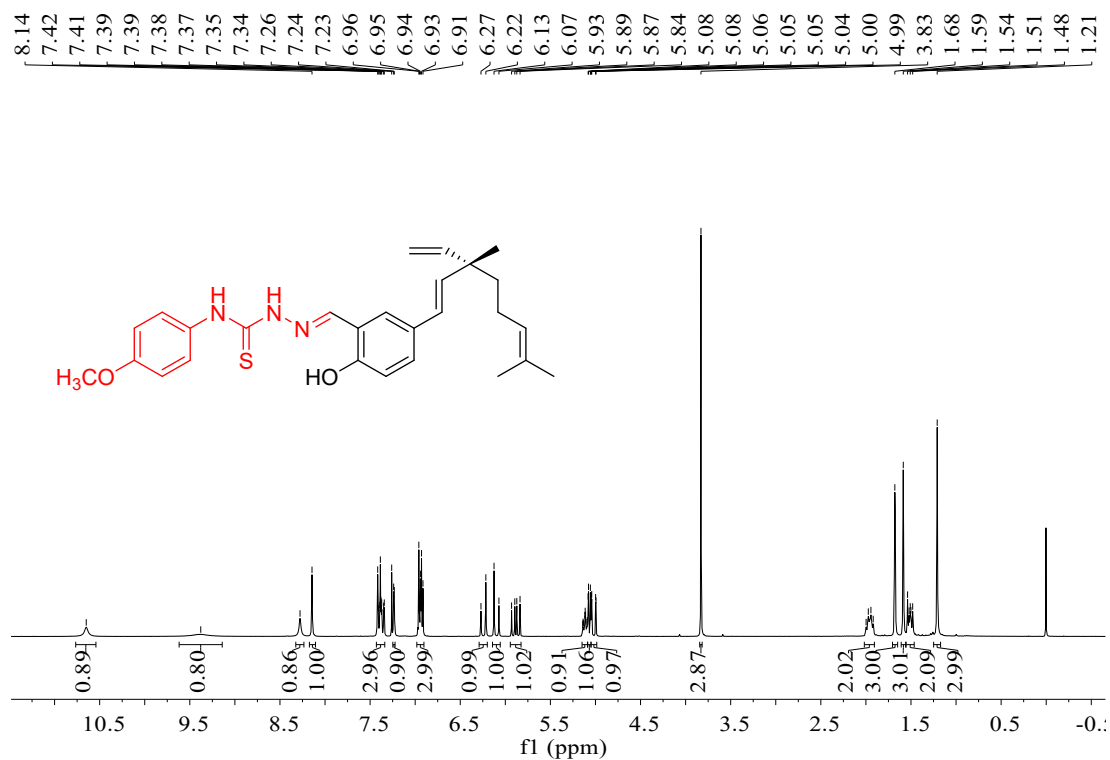


Figure S27 ¹H NMR spectrum of compound 2i

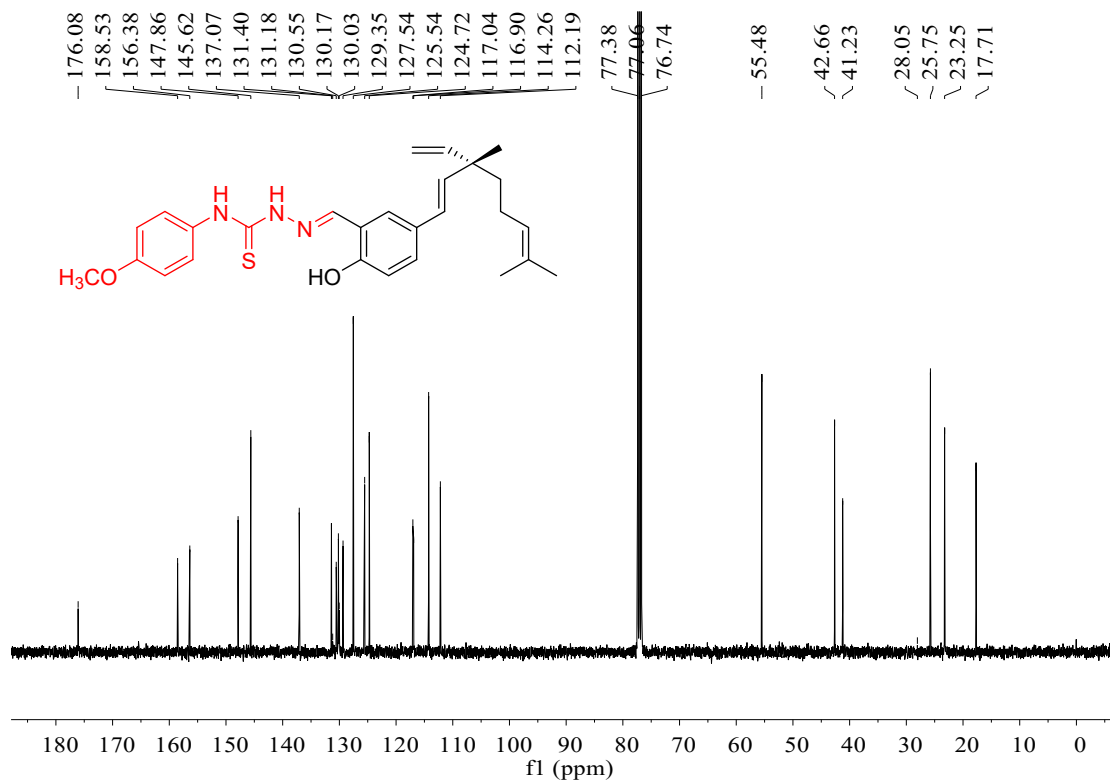


Figure S28 ¹³C NMR spectrum of compound 2i

136-WJA-81-A #20 RT: 0.11 AV: 1 NL: 1.37E7
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]

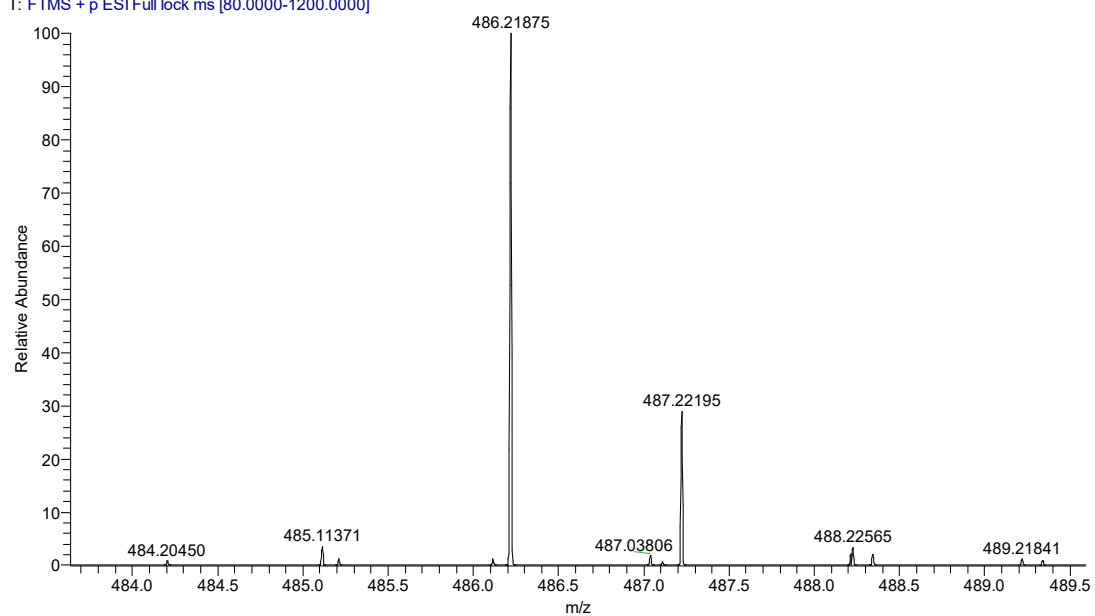


Figure S29 ESI-HRMS spectrum of compound 2i

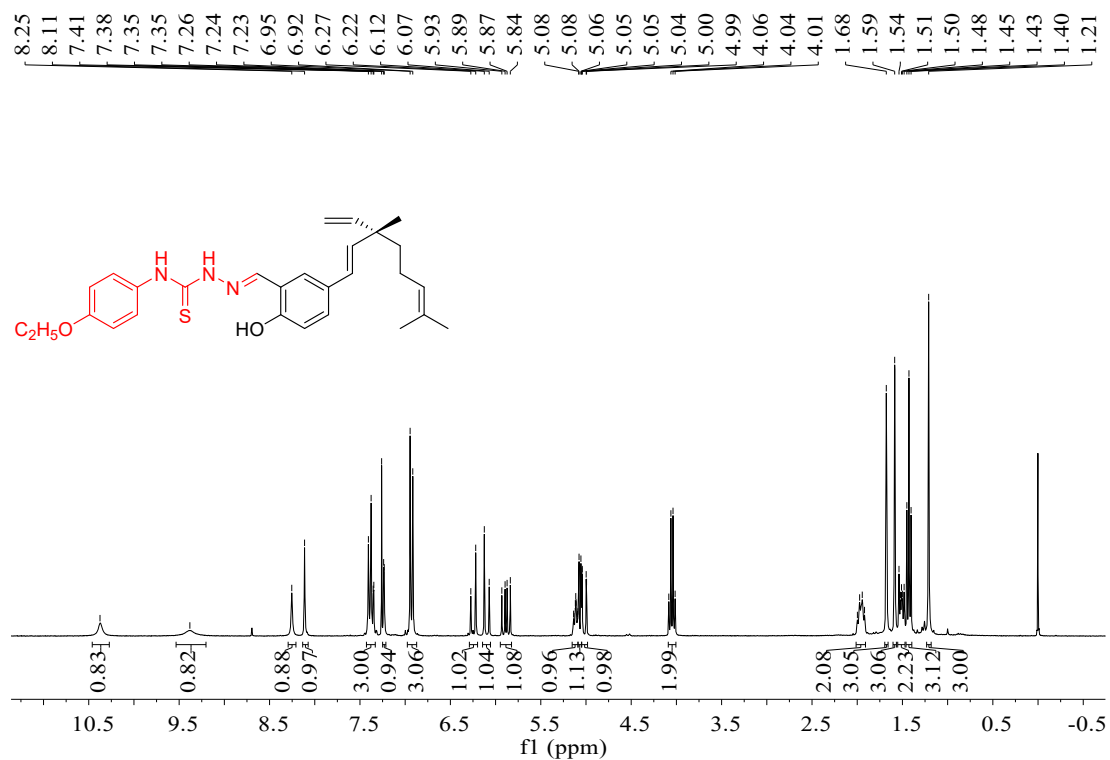


Figure S30 ¹H NMR spectrum of compound 2j

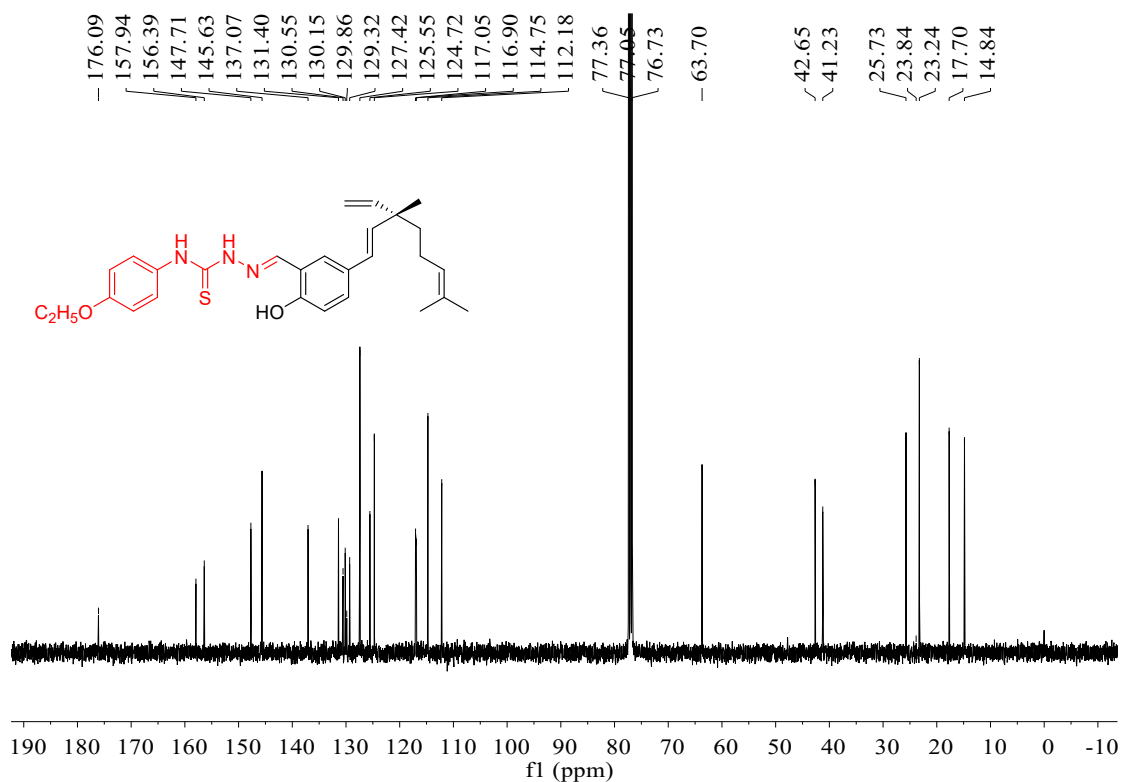


Figure S31 ¹³C NMR spectrum of compound 2j

136-XMF-2-13-17 #18 RT: 0.10 AV: 1 NL: 3.34E7
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]

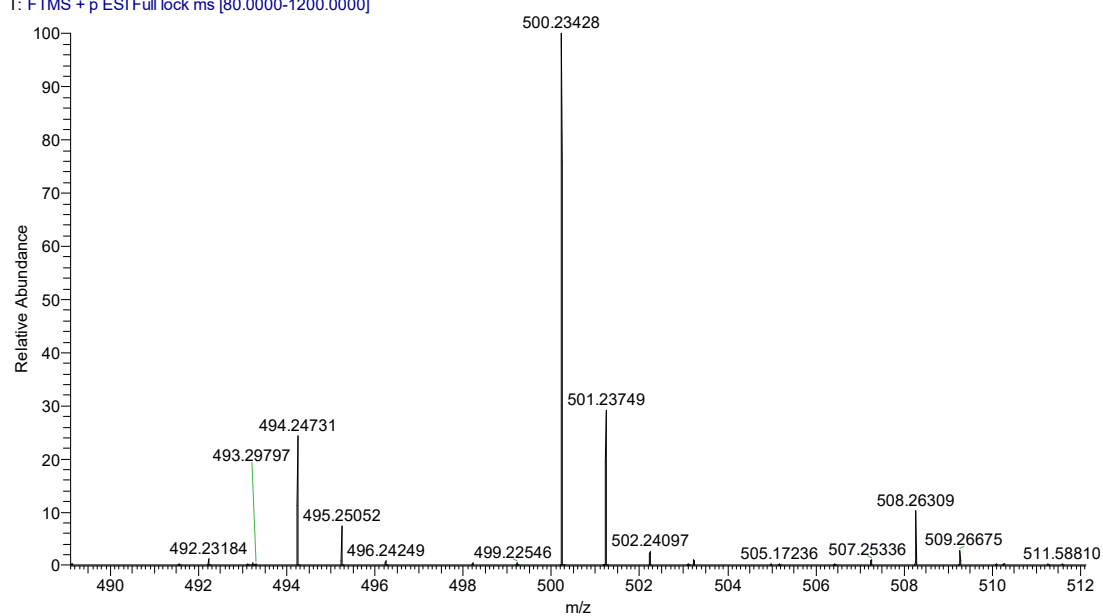


Figure S32 ESI-HRMS spectrum of compound 2j

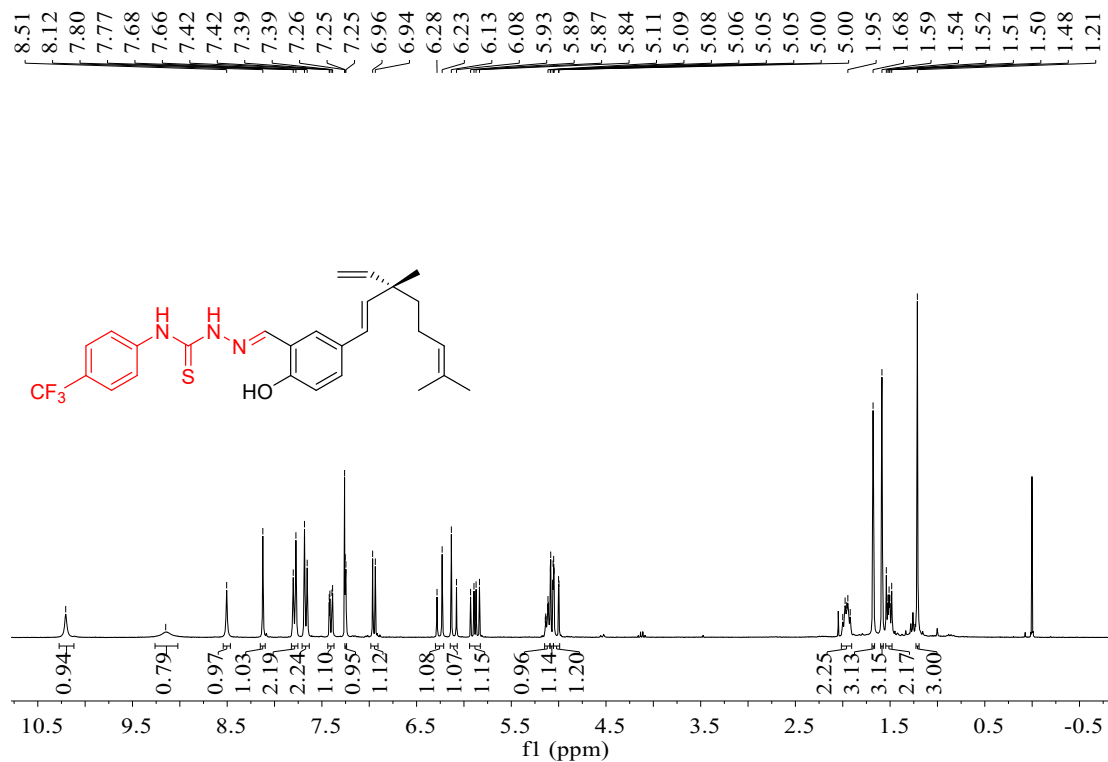


Figure S33 ¹H NMR spectrum of compound 2k

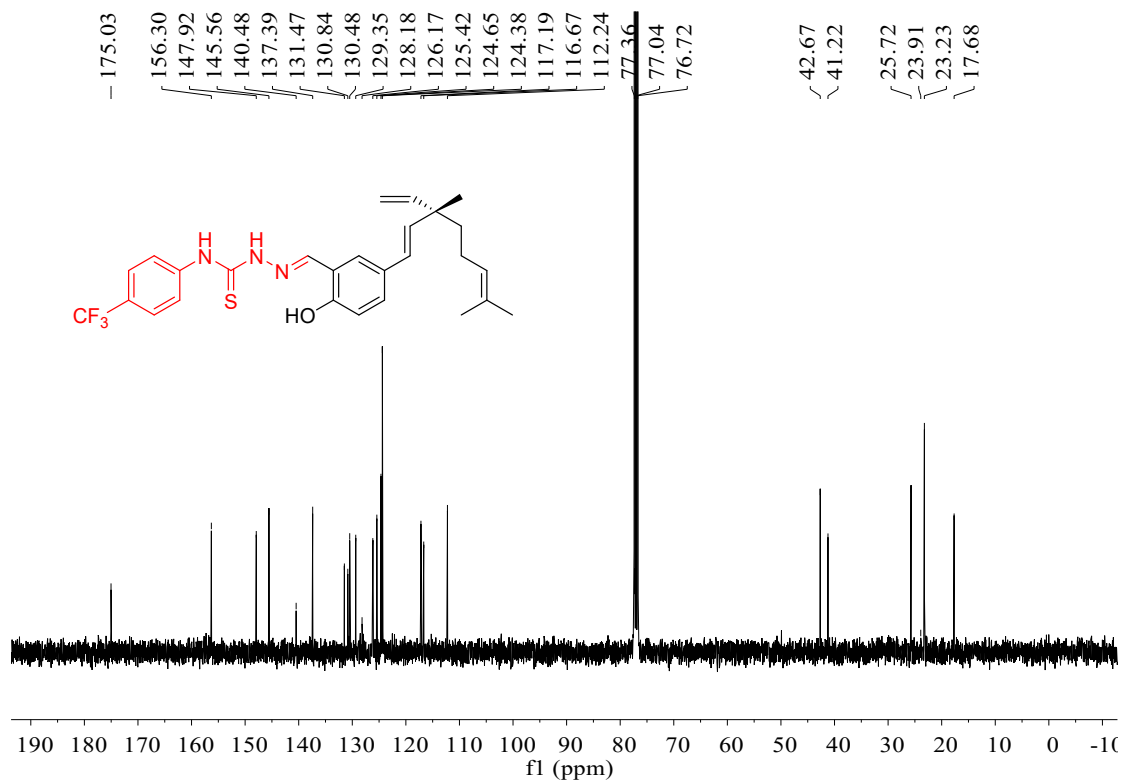


Figure S34 ¹³C NMR spectrum of compound 2k

136-XMF-2-13-6 #22 RT: 0.12 AV: 1 NL: 1.15E7
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]

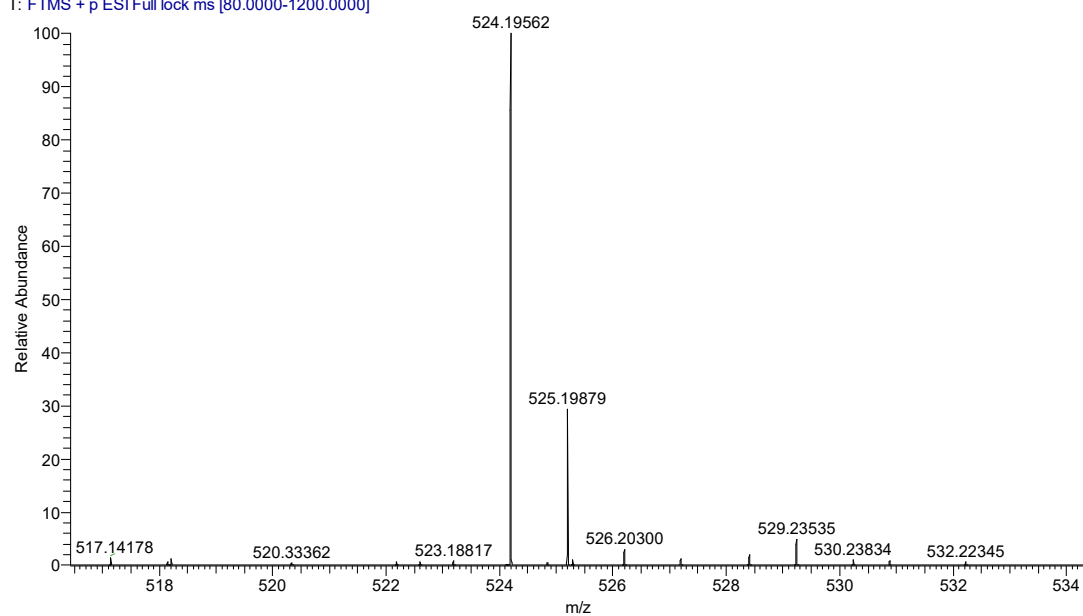


Figure S35 ESI-HRMS spectrum of compound 2k

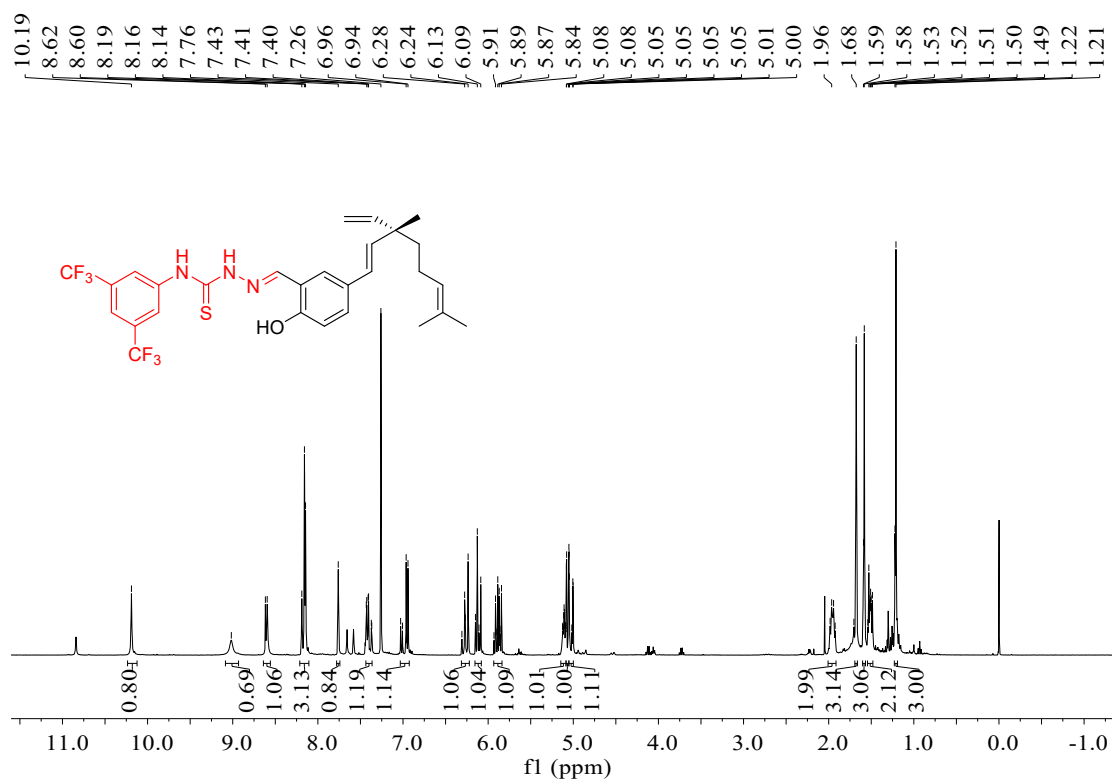


Figure S36 ¹H NMR spectrum of compound 2l

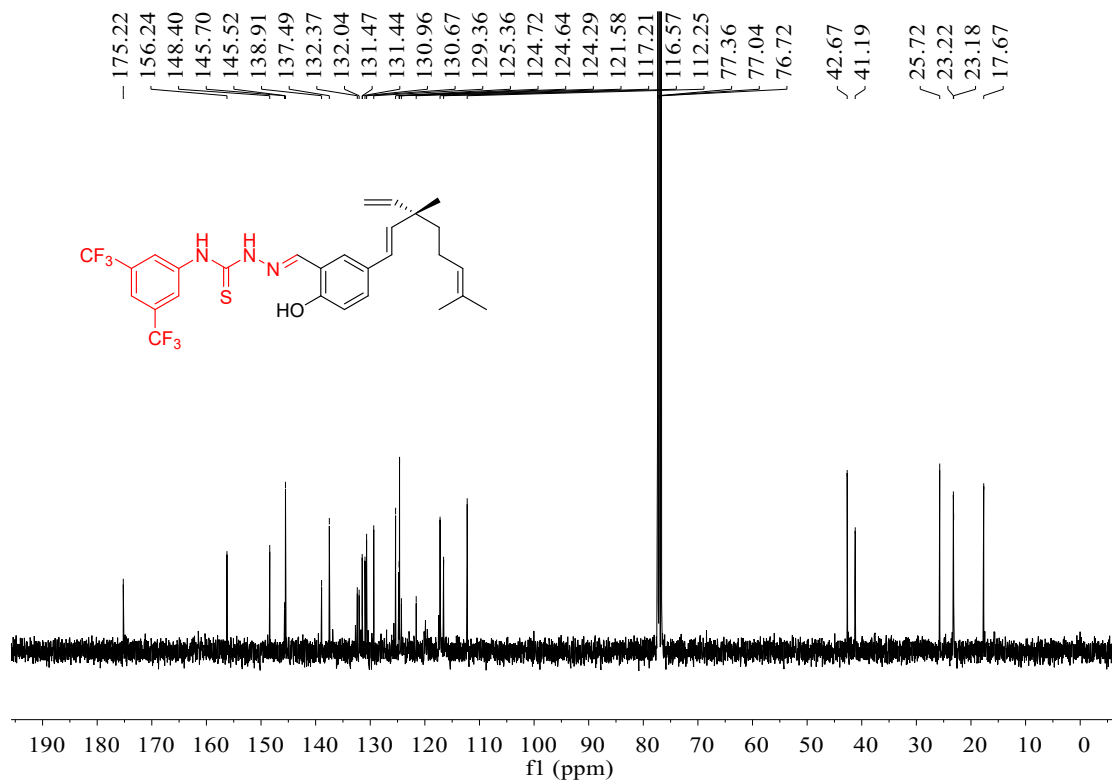


Figure S37 ¹³C NMR spectrum of compound 2l

136-XMF-2-13-16 #20 RT: 0.11 AV: 1 NL: 1.31E6
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]

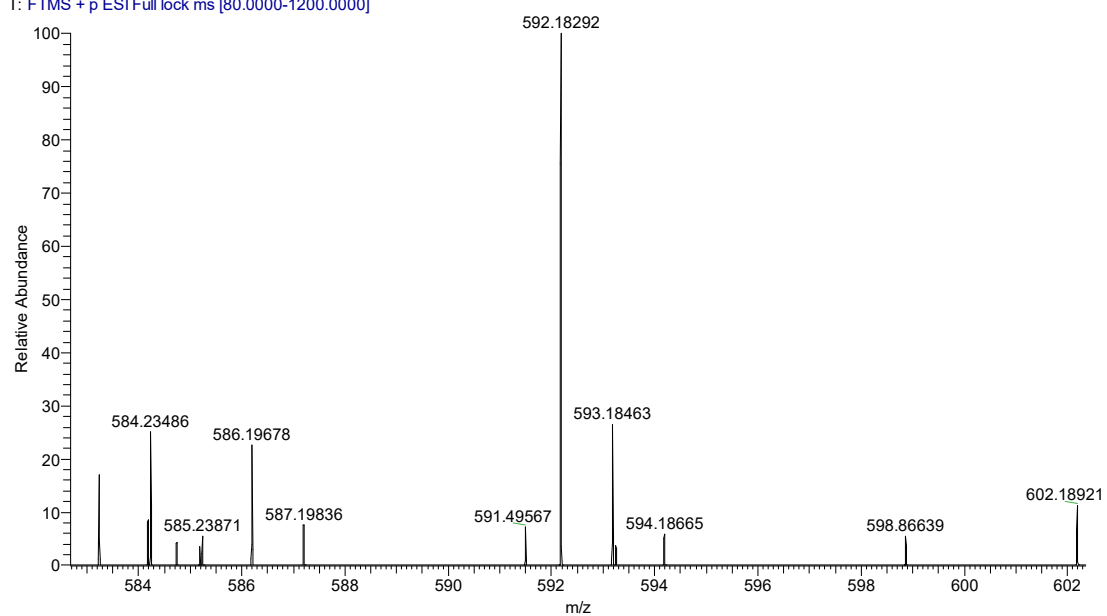


Figure S38 ESI-HRMS spectrum of compound 21

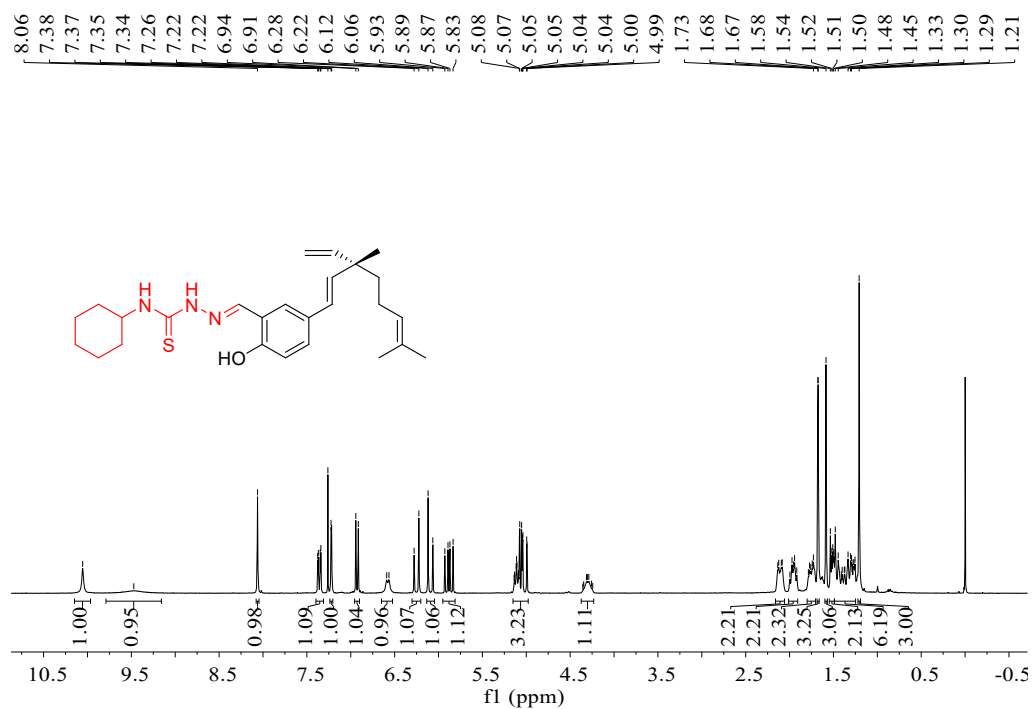


Figure S39 ¹H NMR spectrum of compound 2m

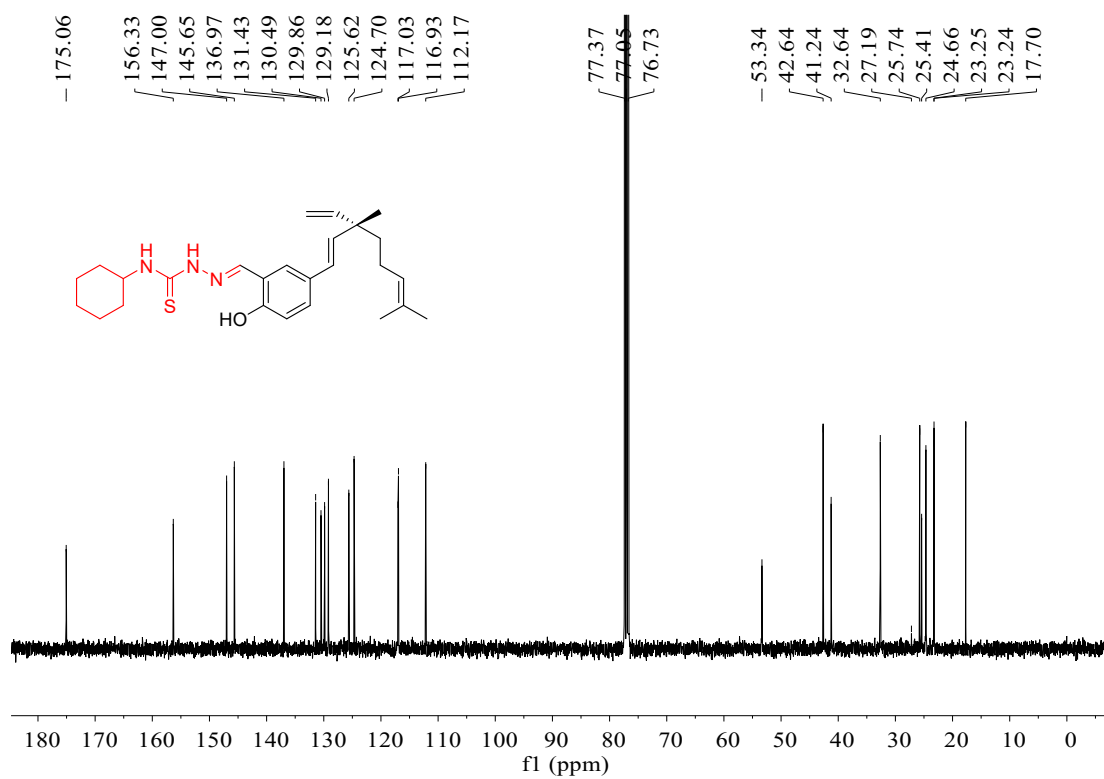


Figure S40 ¹³C NMR spectrum of compound 2m

136-WJA-69-A #12 RT: 0.07 AV: 1 NL: 7.83E7
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]

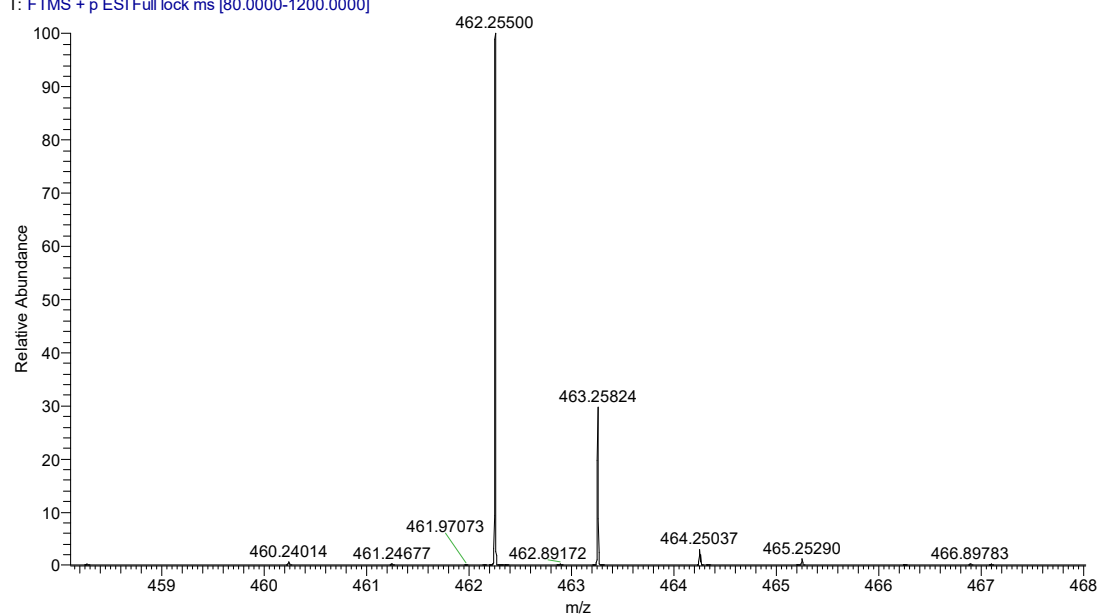


Figure S41 ESI-HRMS spectrum of compound 2m

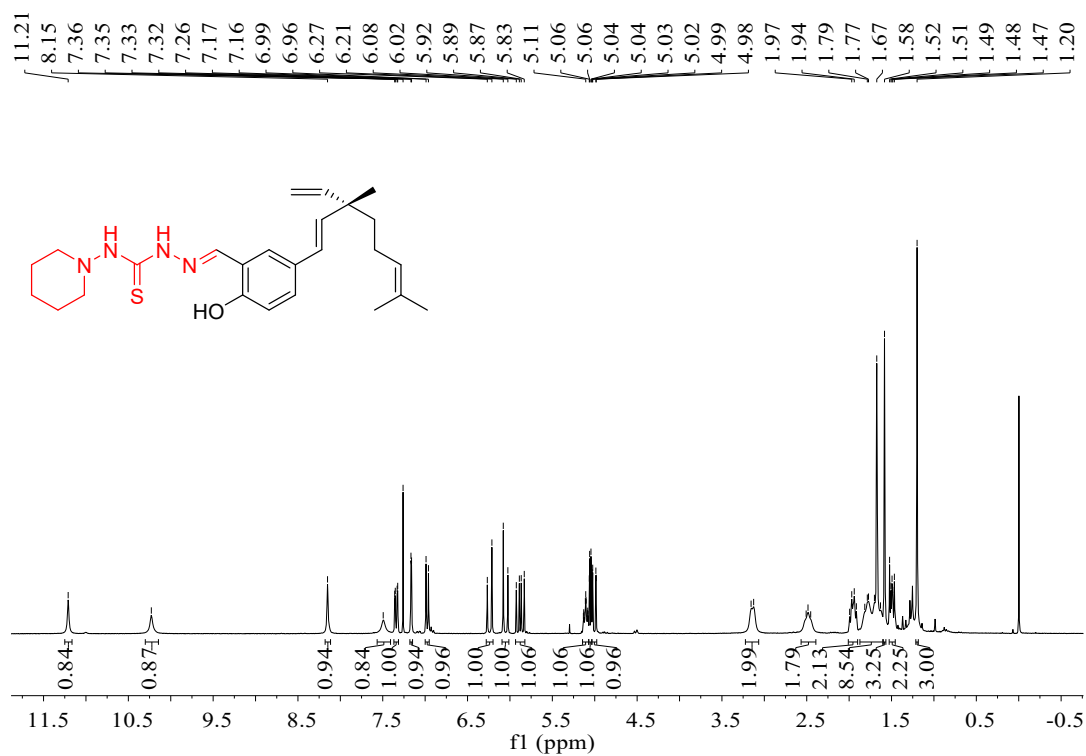


Figure S42 ¹H NMR spectrum of compound 2n

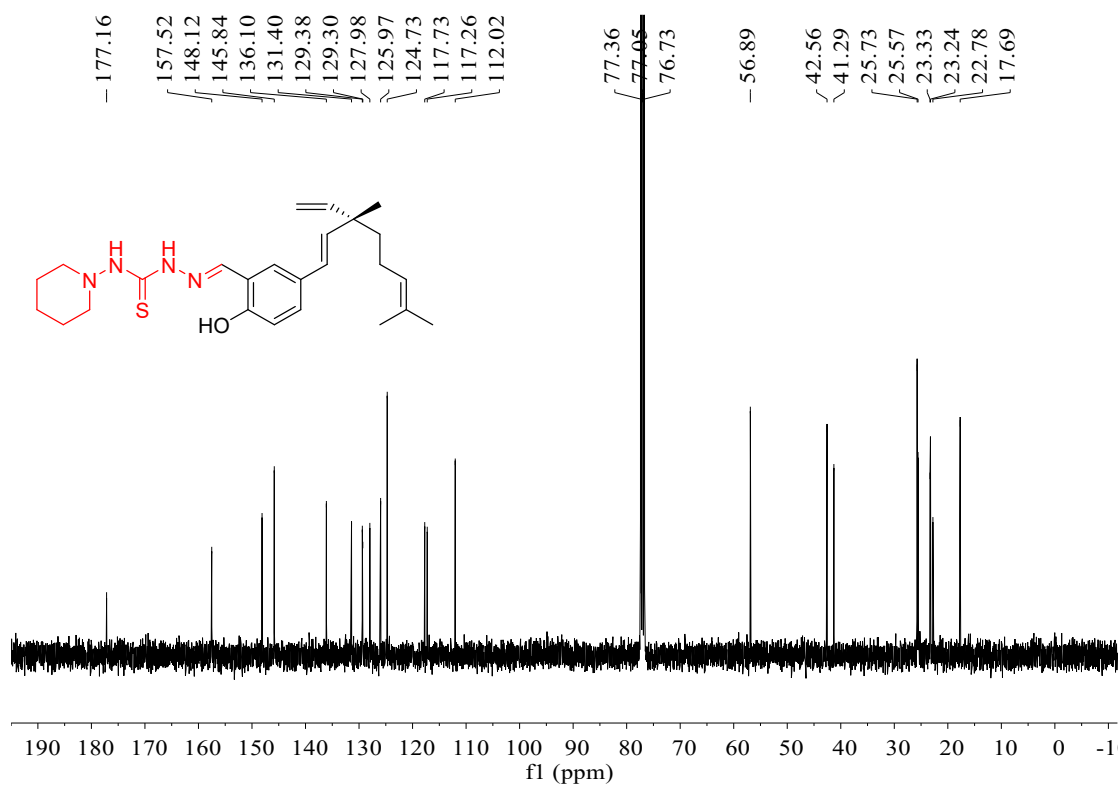


Figure S43 ¹³C NMR spectrum of compound 2n

136-XMF-2-13-3 #15 RT: 0.08 AV: 1 NL: 9.50E7
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]

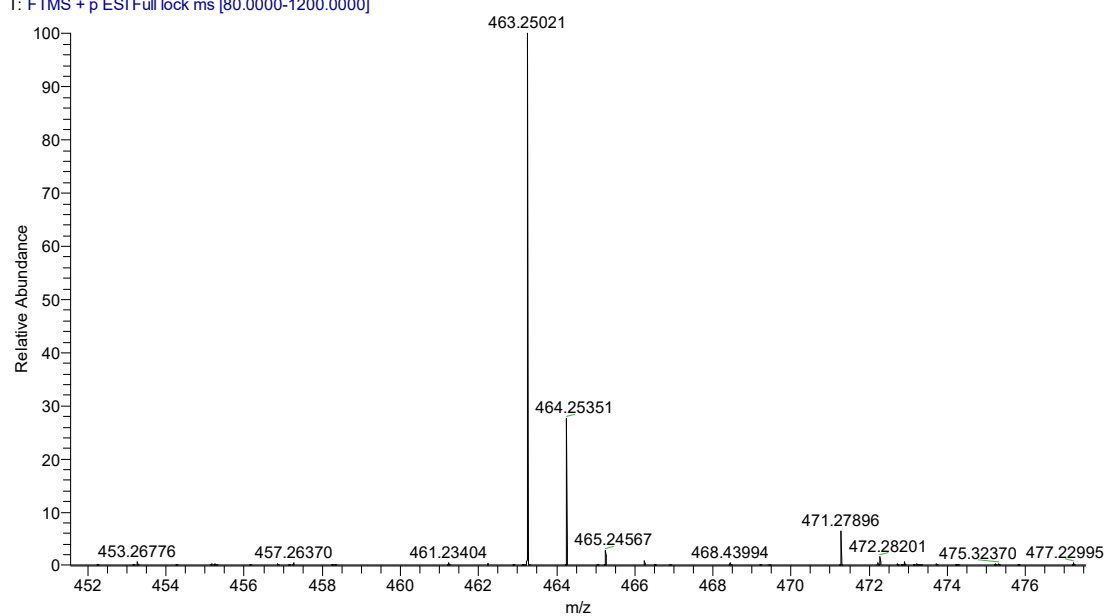


Figure S44 ESI-HRMS spectrum of compound 2n

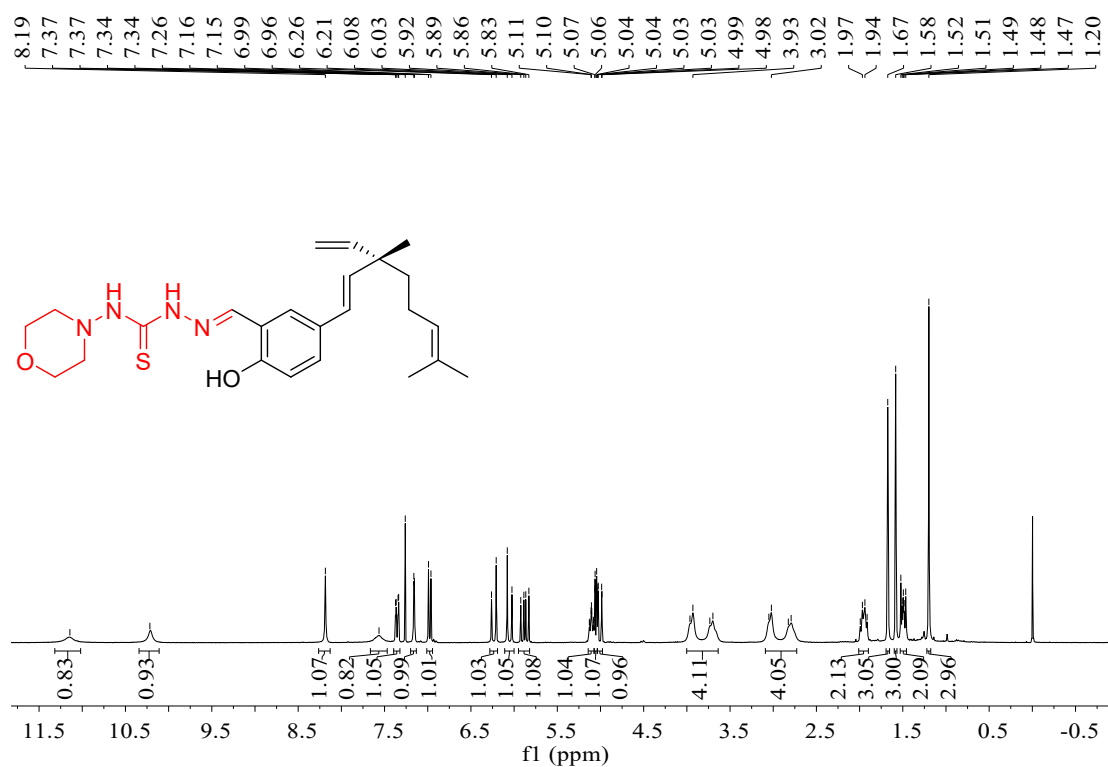


Figure S45 ¹H NMR spectrum of compound 2o

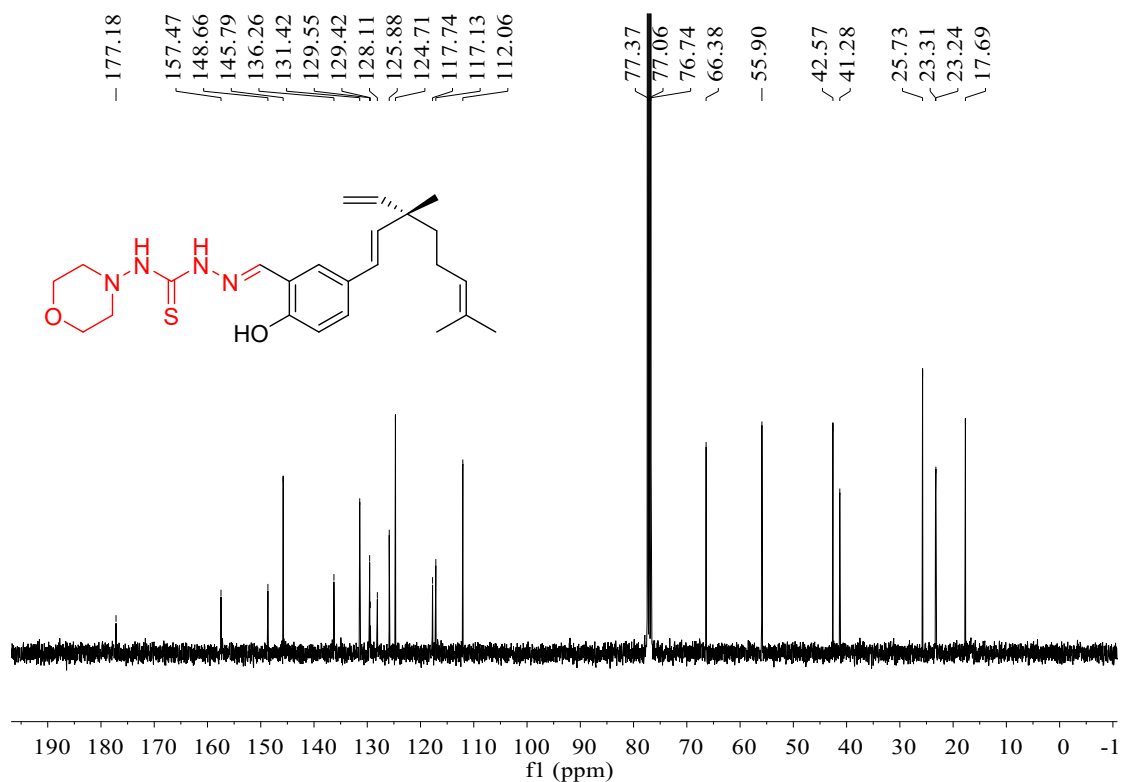


Figure S46 ¹³C NMR spectrum of compound 2o

136-XMF-2-13-4 #17 RT: 0.09 AV: 1 NL: 7.02E7
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]

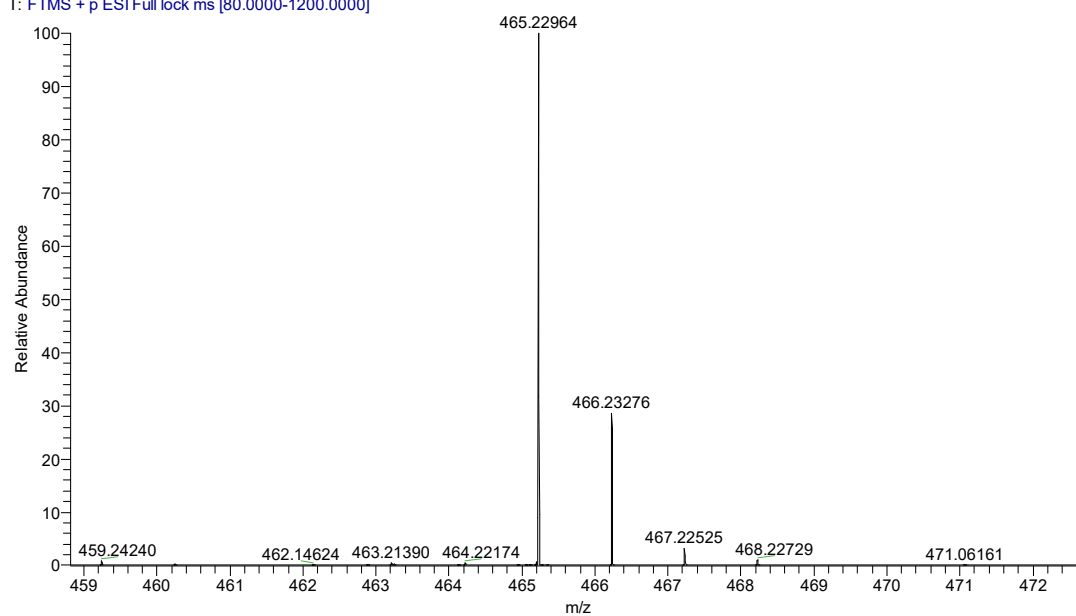


Figure S47 ESI-HRMS spectrum of compound 2o

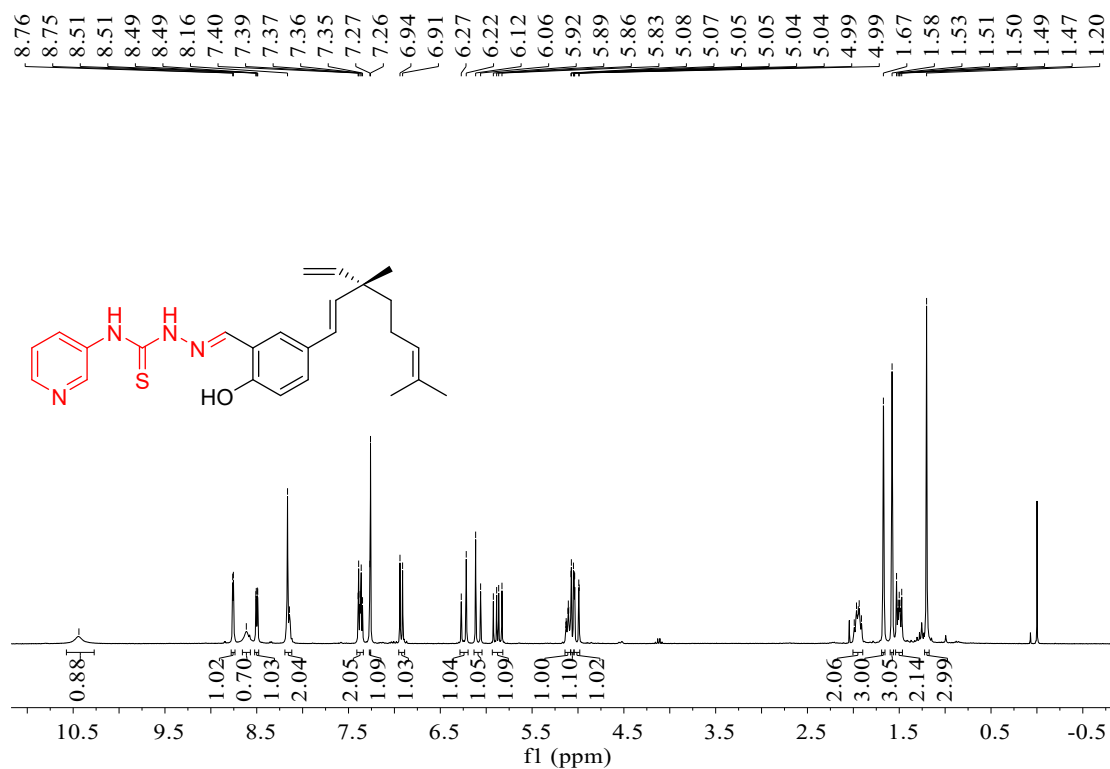


Figure S48 ¹H NMR spectrum of compound 2p

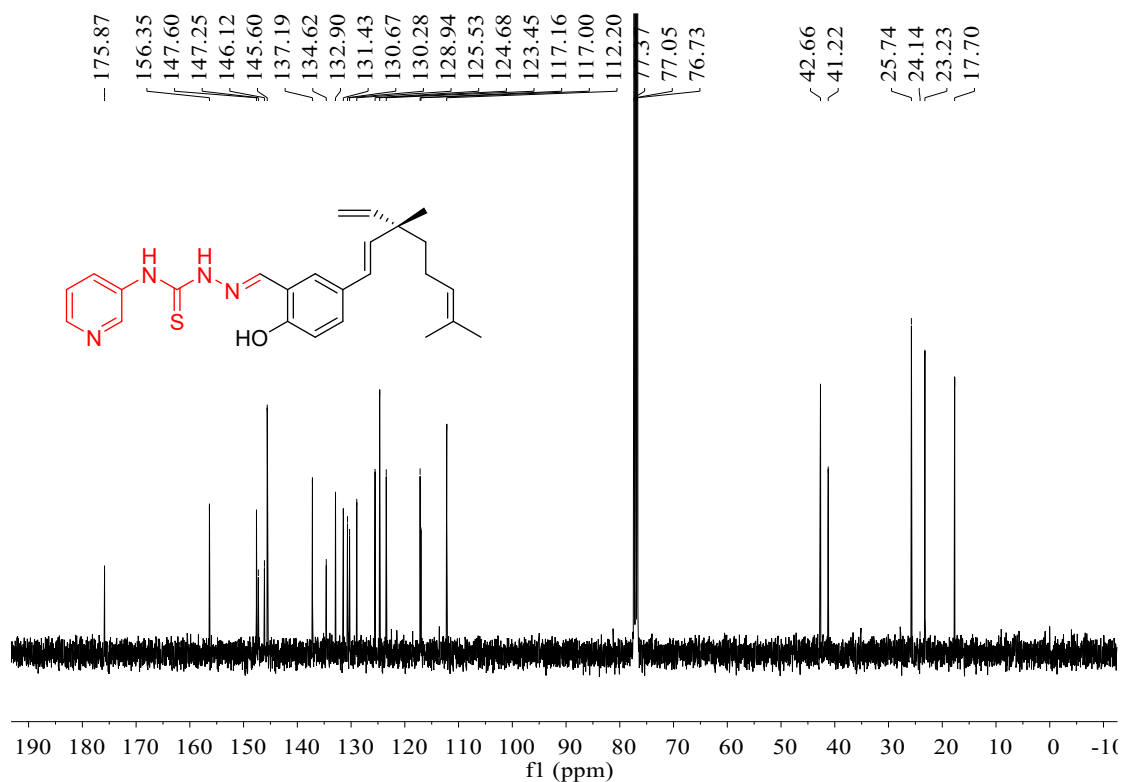


Figure S49 ¹³C NMR spectrum of compound 2p

136-XMF-2-13-7 #18 RT: 0.10 AV: 1 NL: 4.50E7
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]

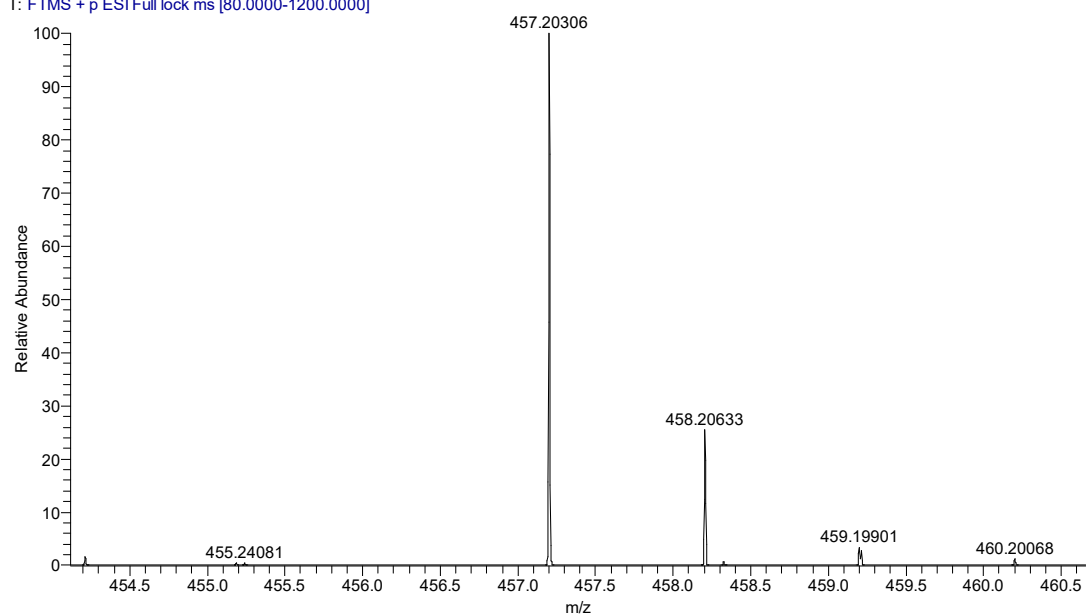


Figure S50 ESI-HRMS spectrum of compound 2p

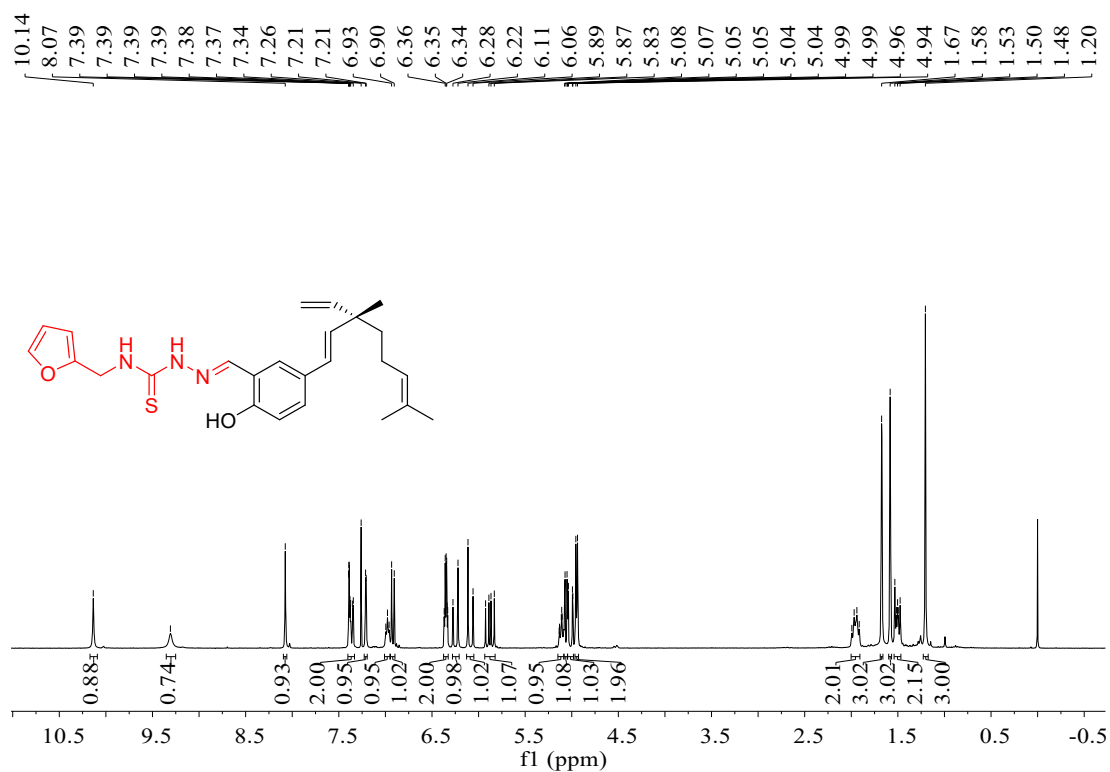


Figure S51 ¹H NMR spectrum of compound 2q

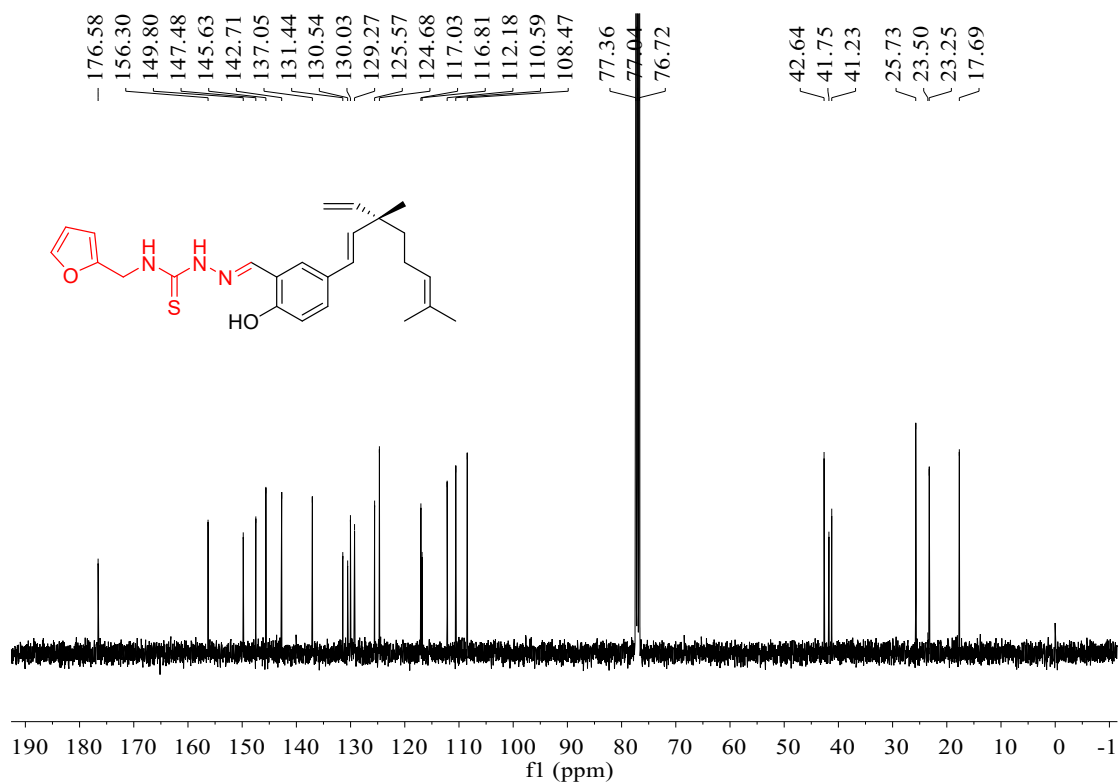


Figure S52 ¹³C NMR spectrum of compound 2q

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T: FTMS + p ESI Full lock ms [80.0000-1200.0000]

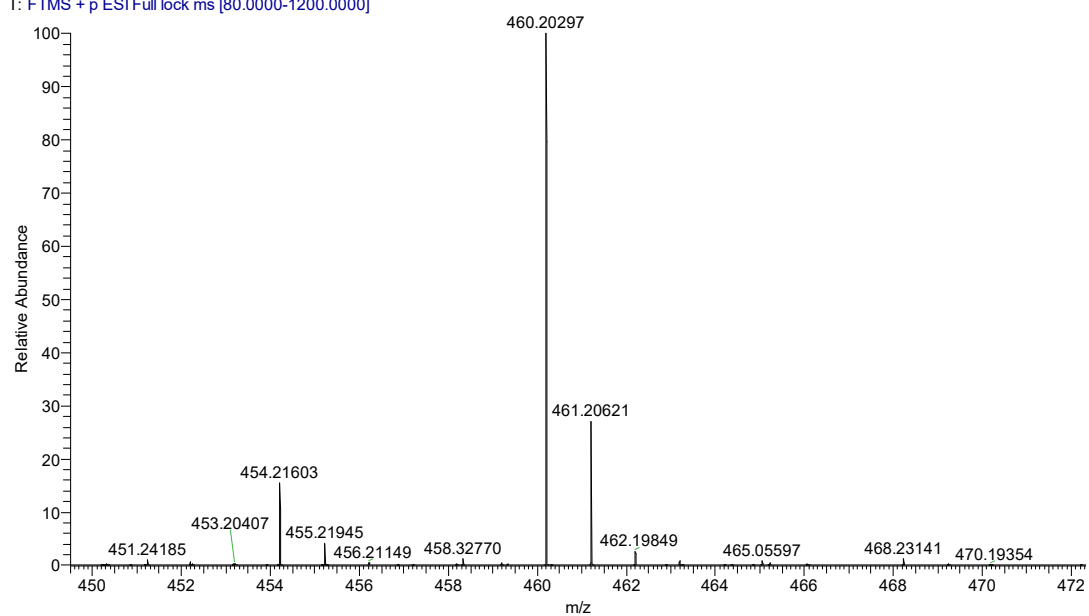


Figure S53 ESI-HRMS spectrum of compound 2q

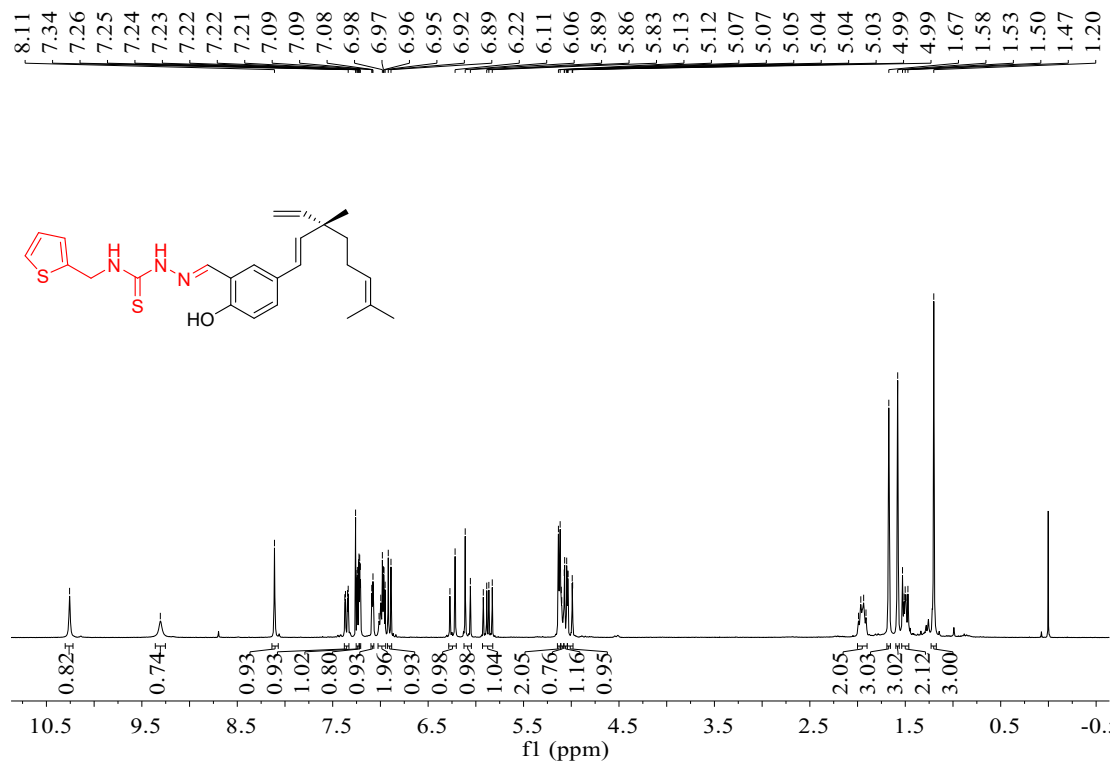


Figure S54 ¹H NMR spectrum of compound 2r

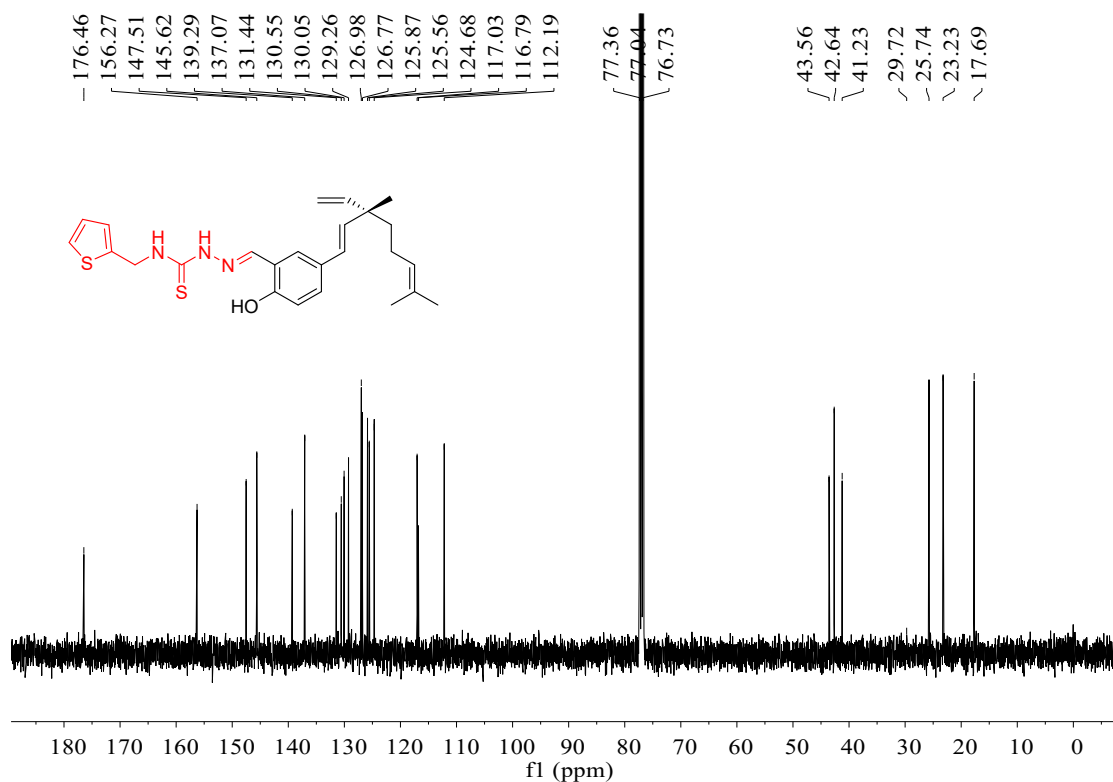


Figure S55 ¹³C NMR spectrum of compound 2r

136-WJA-72-A #17 RT: 0.09 AV: 1 NL: 1.10E7
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]

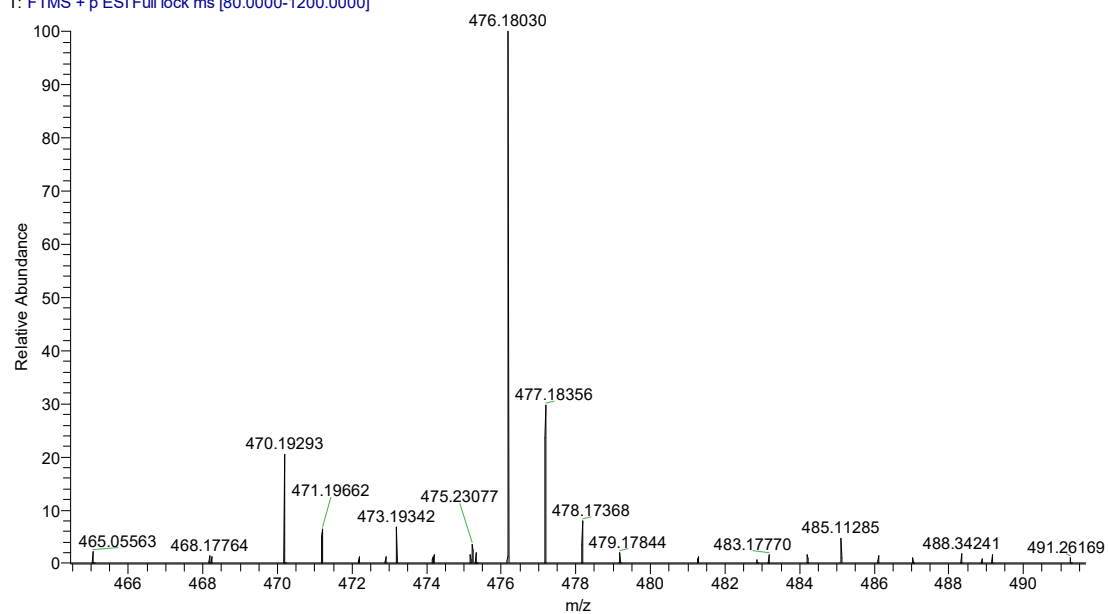


Figure S56 ESI-HRMS spectrum of compound 2r

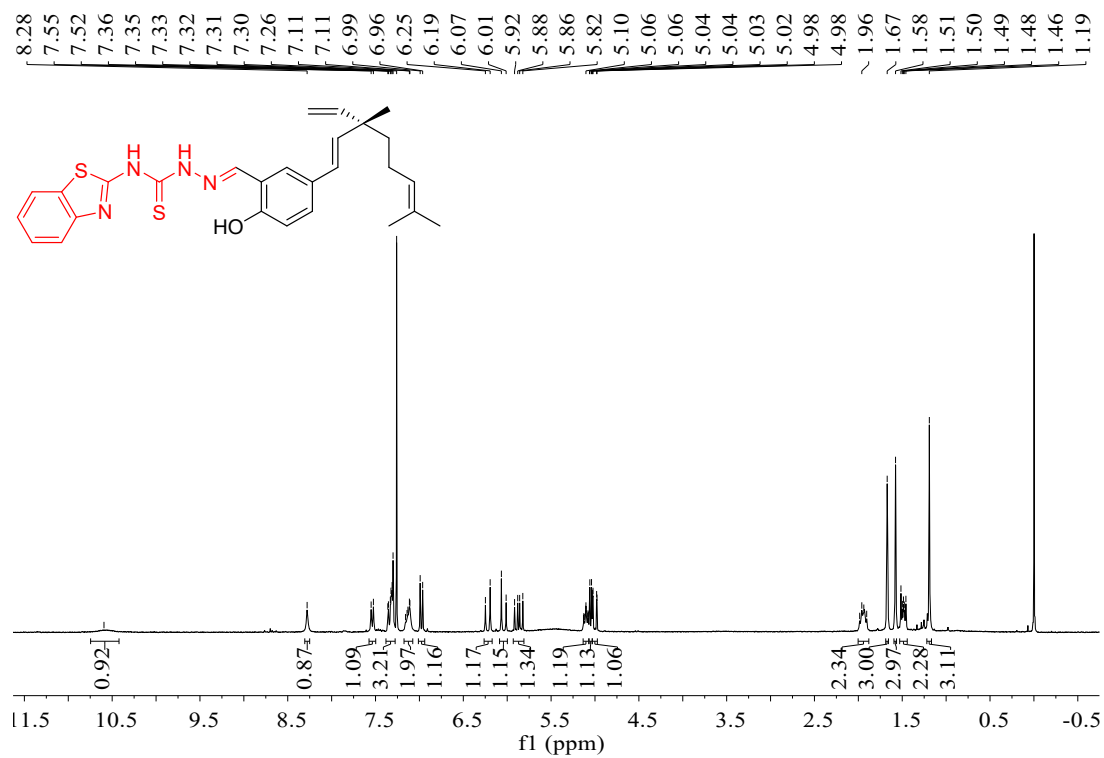


Figure S57 ¹H NMR spectrum of compound 2s

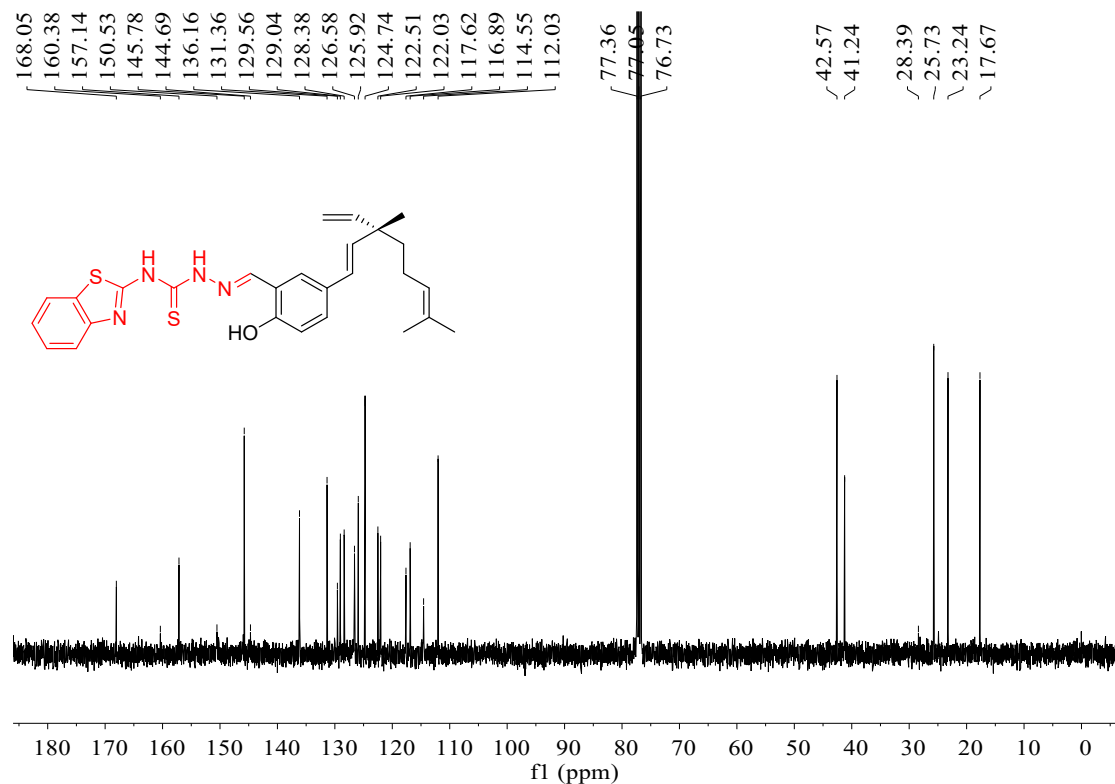


Figure S58 ¹³C NMR spectrum of compound 2s

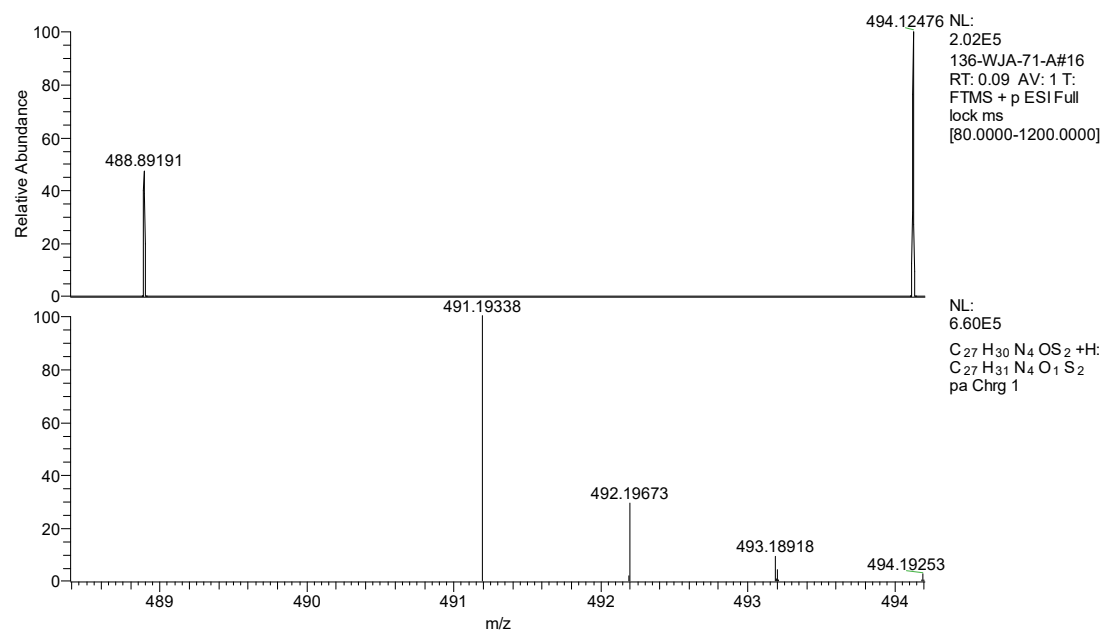


Figure S59 ESI-HRMS spectrum of compound 2s

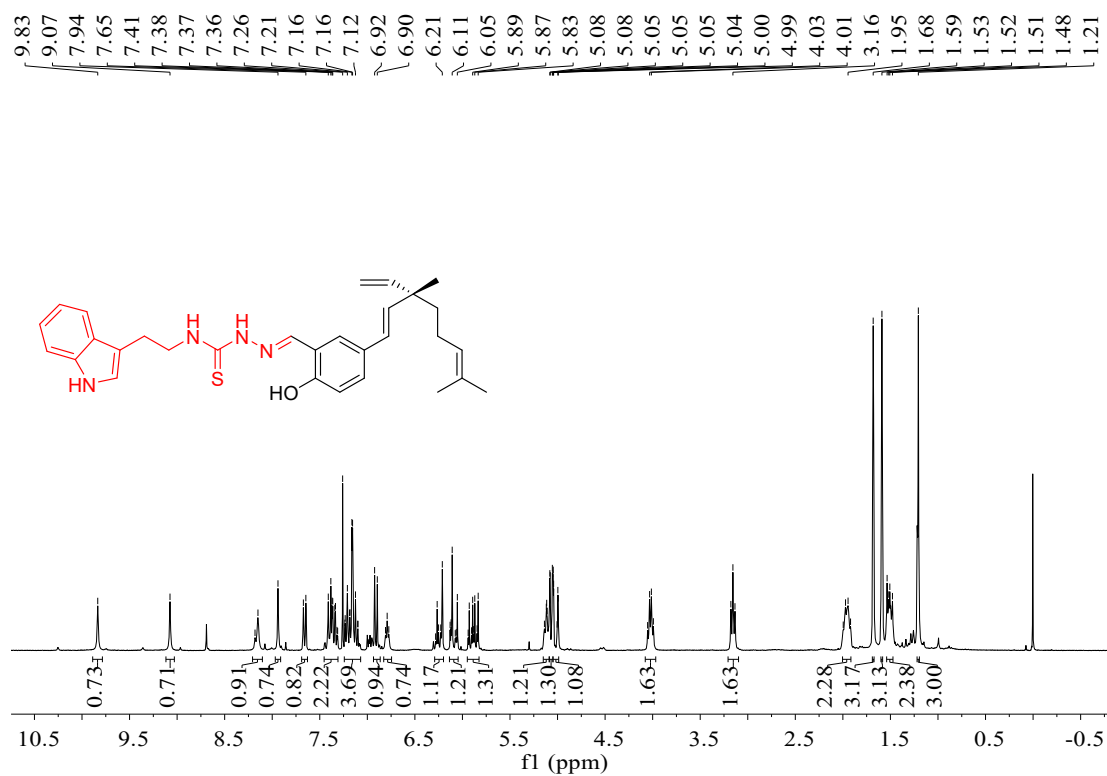


Figure S60 ¹H NMR spectrum of compound 2t

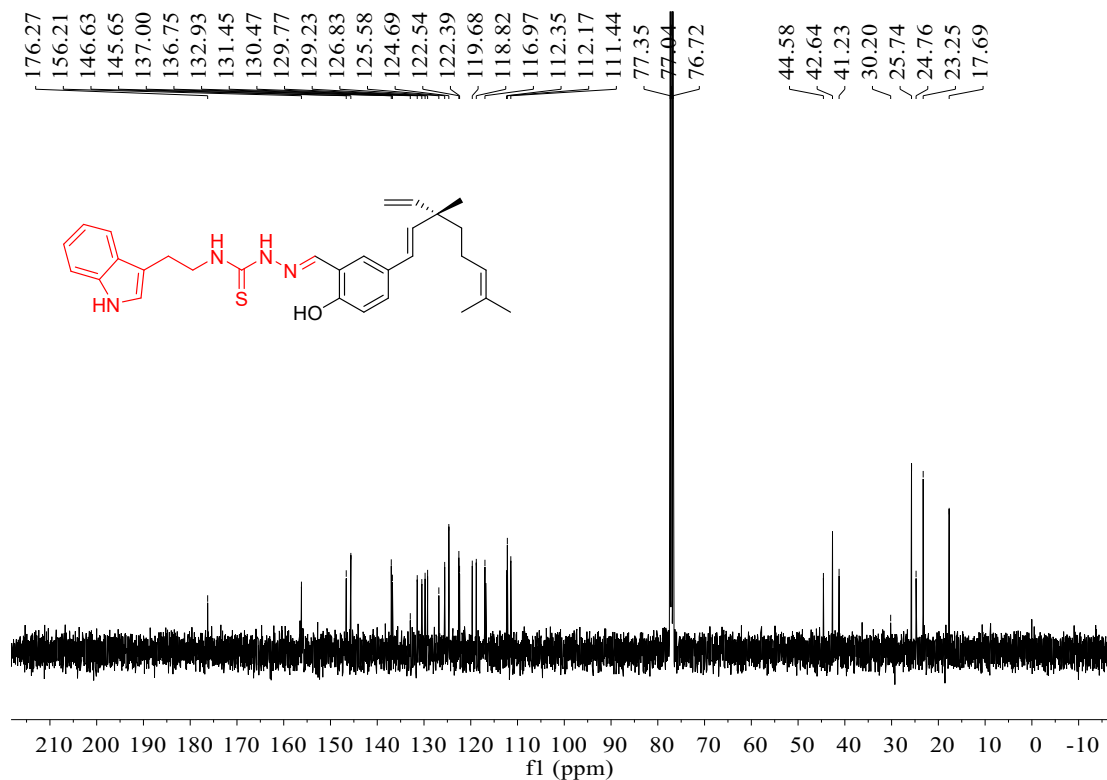


Figure S61 ¹³C NMR spectrum of compound 2t

136-XMF-2-13-15 #17 RT: 0.09 AV: 1 NL: 1.46E7
T: FTMS + p ESI Full lock ms [80.0000-1200.0000]

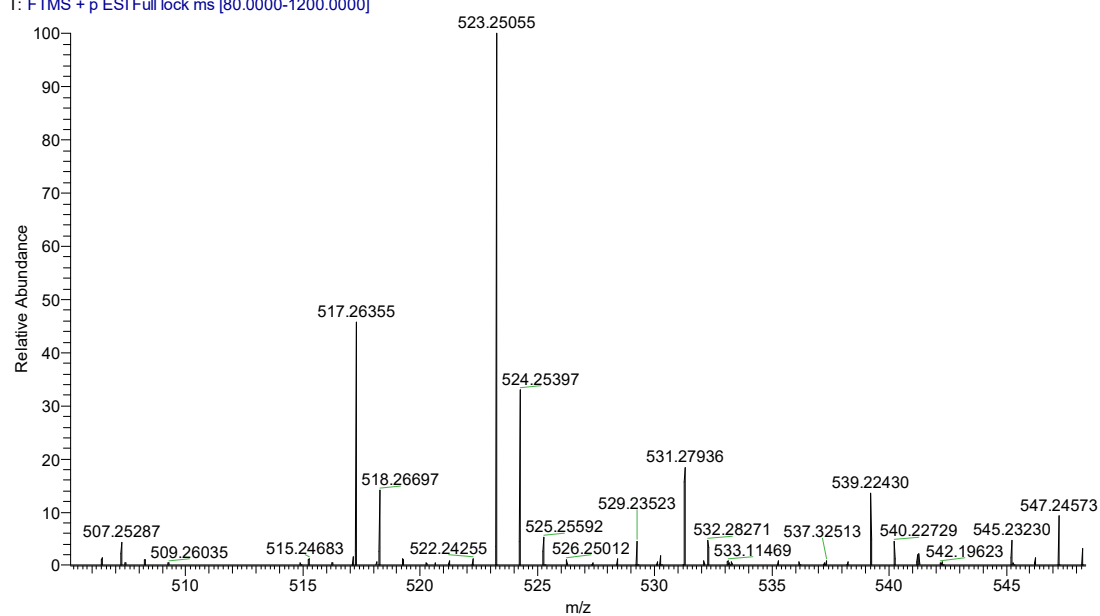
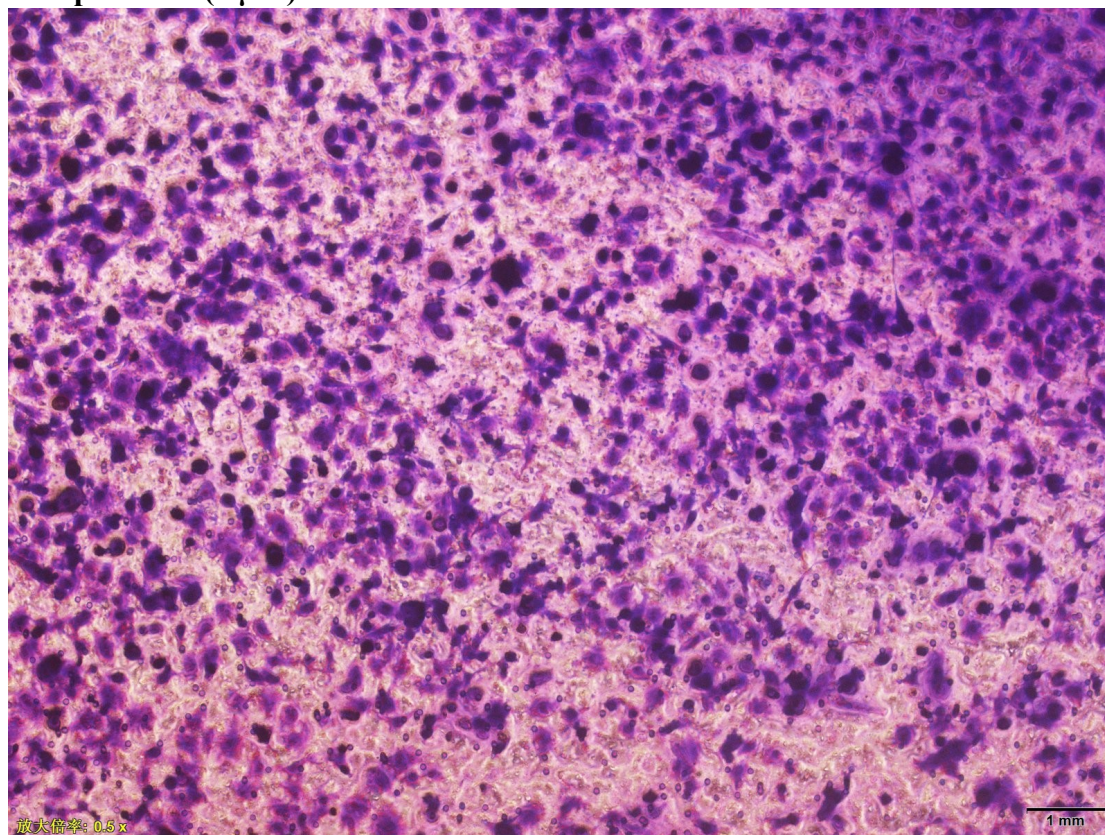


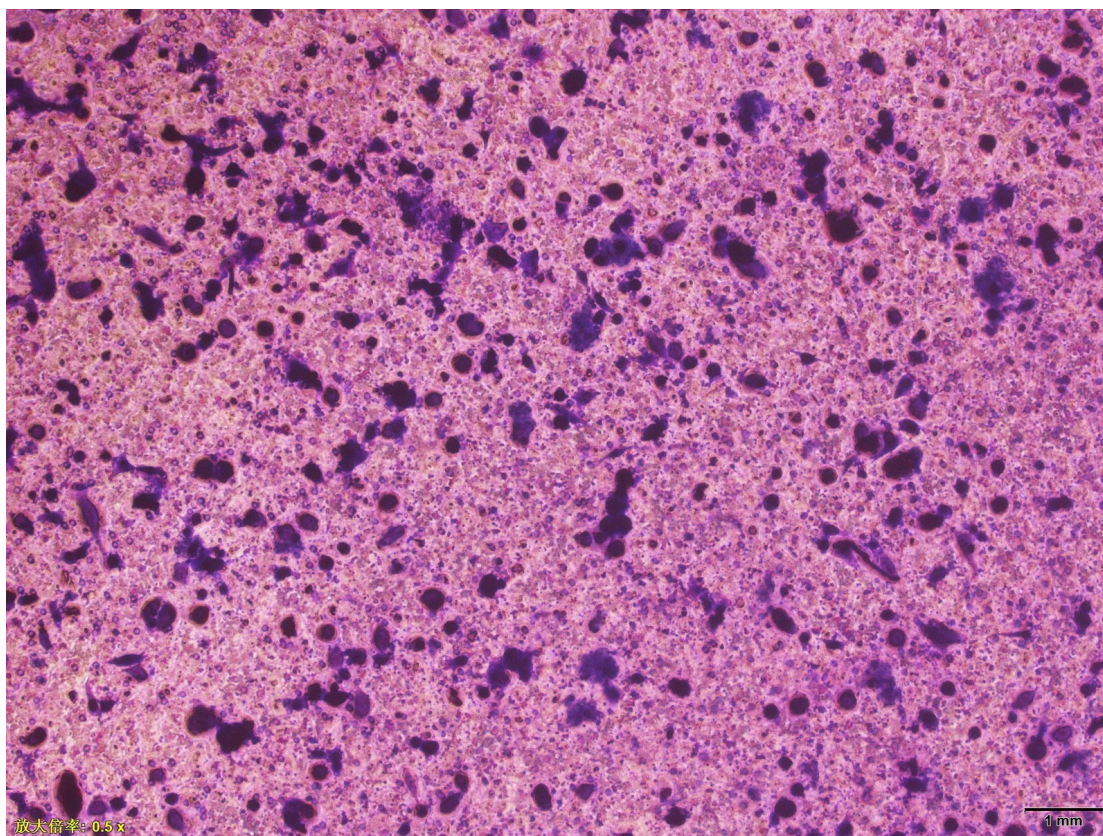
Figure S62 ESI-HRMS spectrum of compound 2t

Figure S63 Representative photomicrographs of migration. Cells treated with the compound 2f (0, 1, 2, 4 μ M) for 24 h.

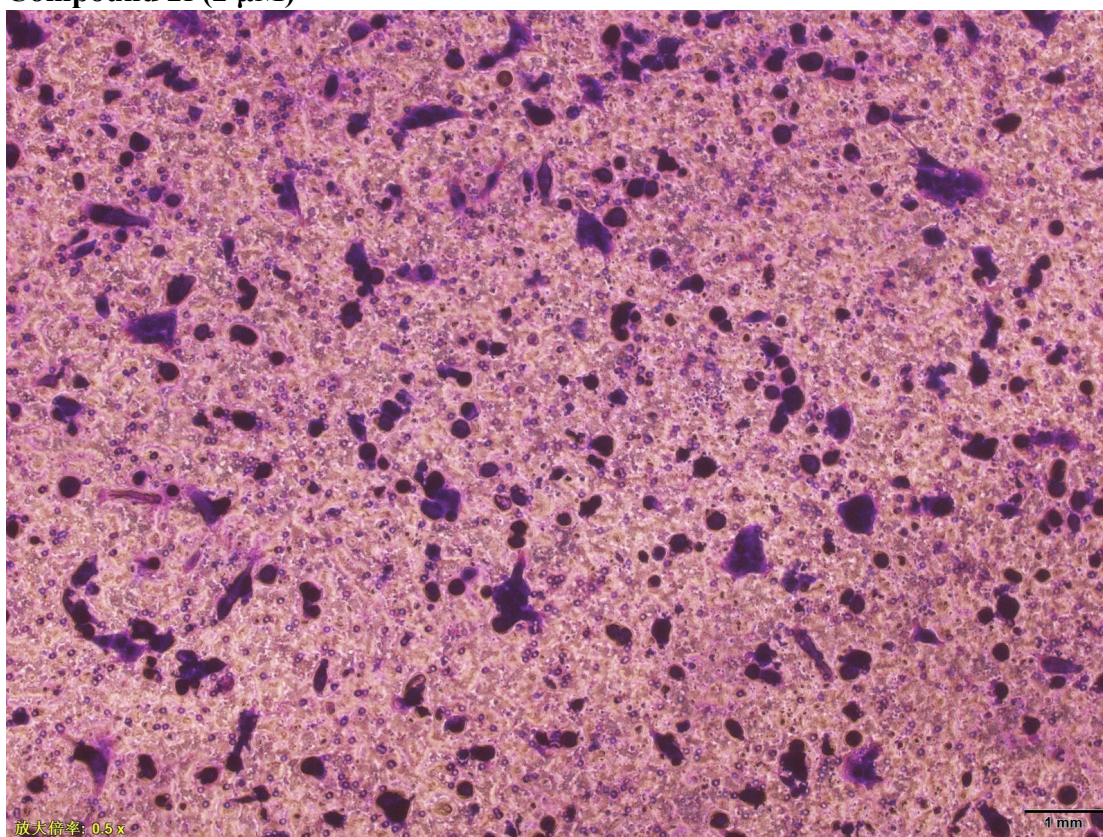
Compound 2f (0 μ M)



Compound 2f (1 μ M)



Compound 2f (2 μ M)



Compound 2f (4 μ M)

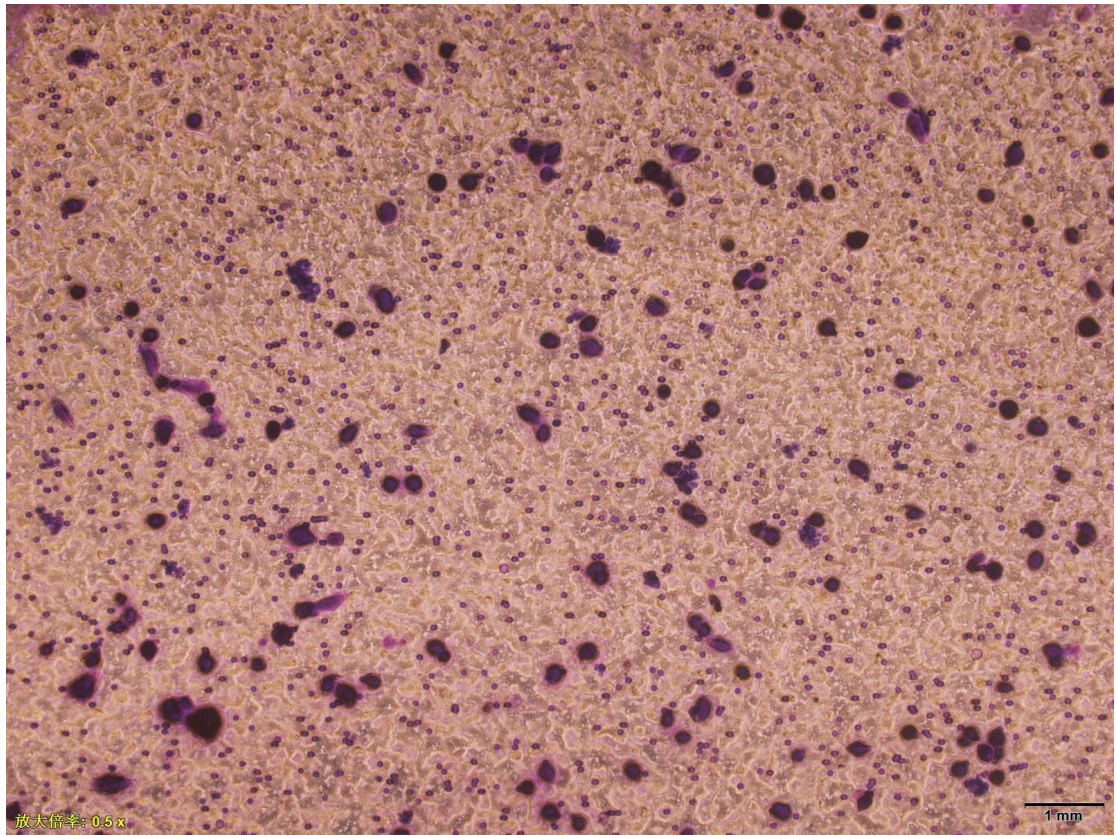
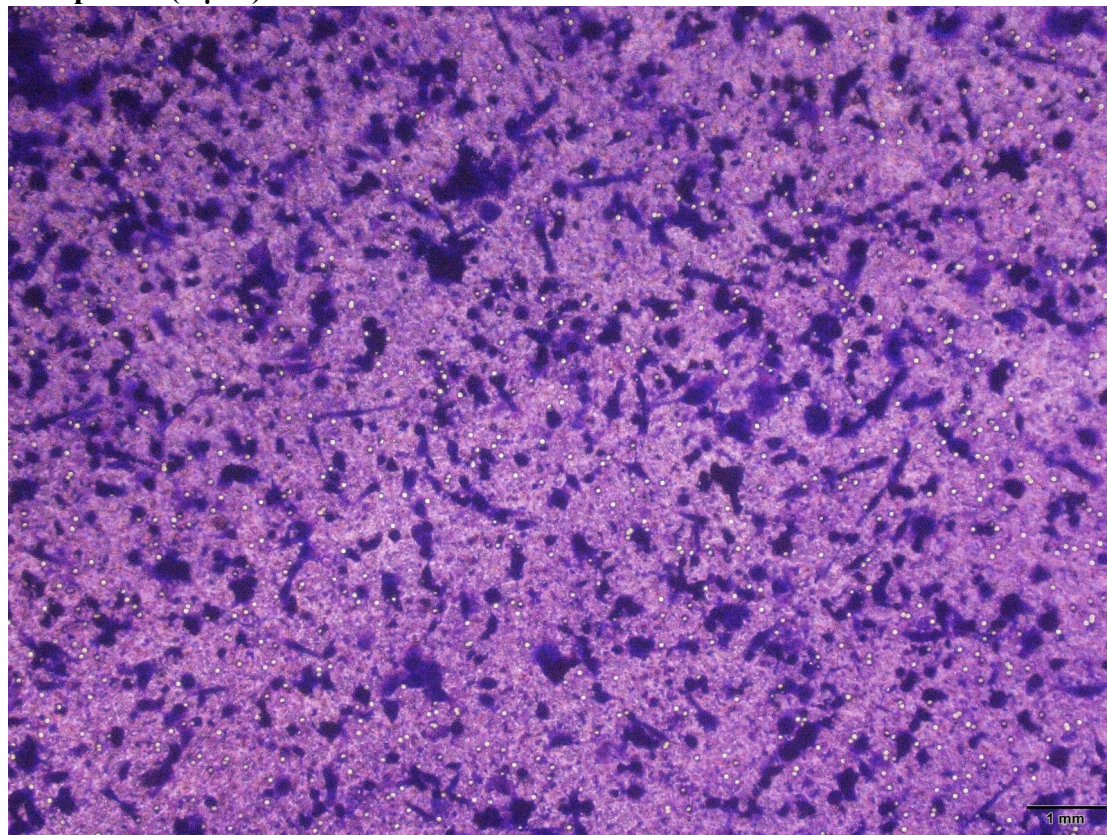
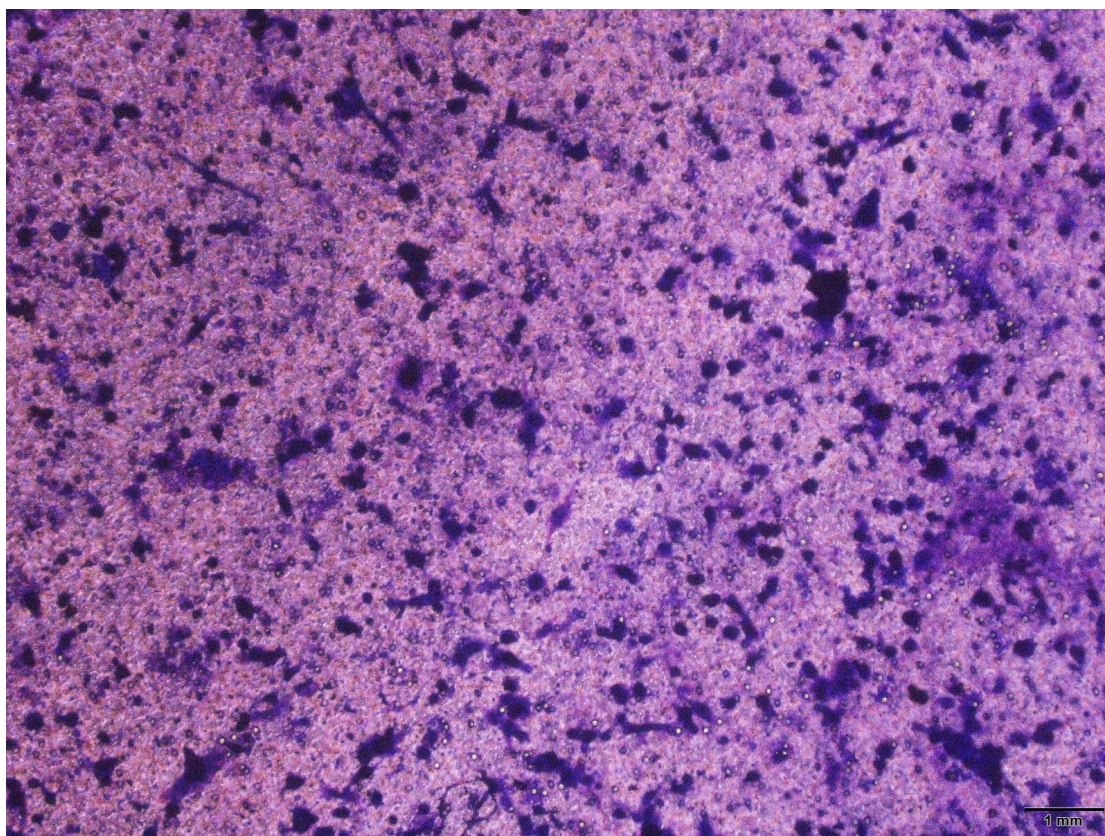


Figure S64 Representative photomicrographs of invasion. Cells treated with the compound 2f (0, 1, 2, 4 μ M) for 24 h.

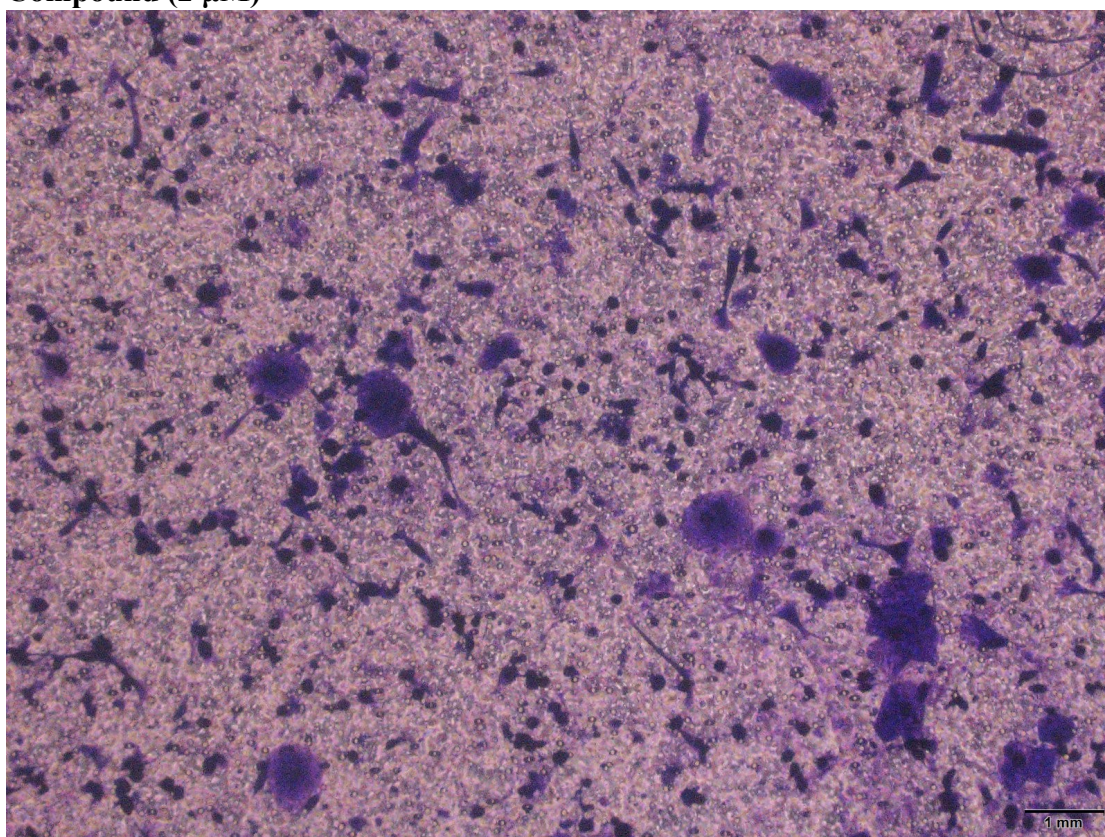
Compound (0 μ M)



Compound (1 μ M)



Compound (2 μ M)



Compound (4 μ M)

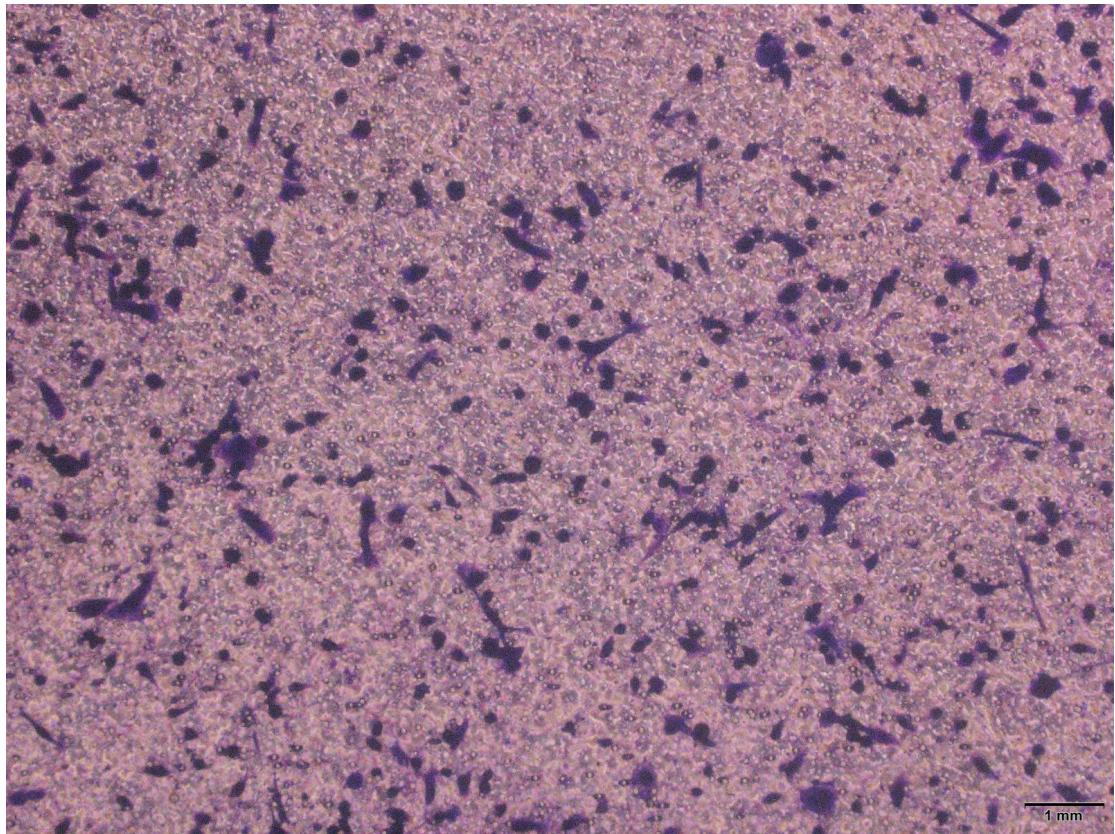
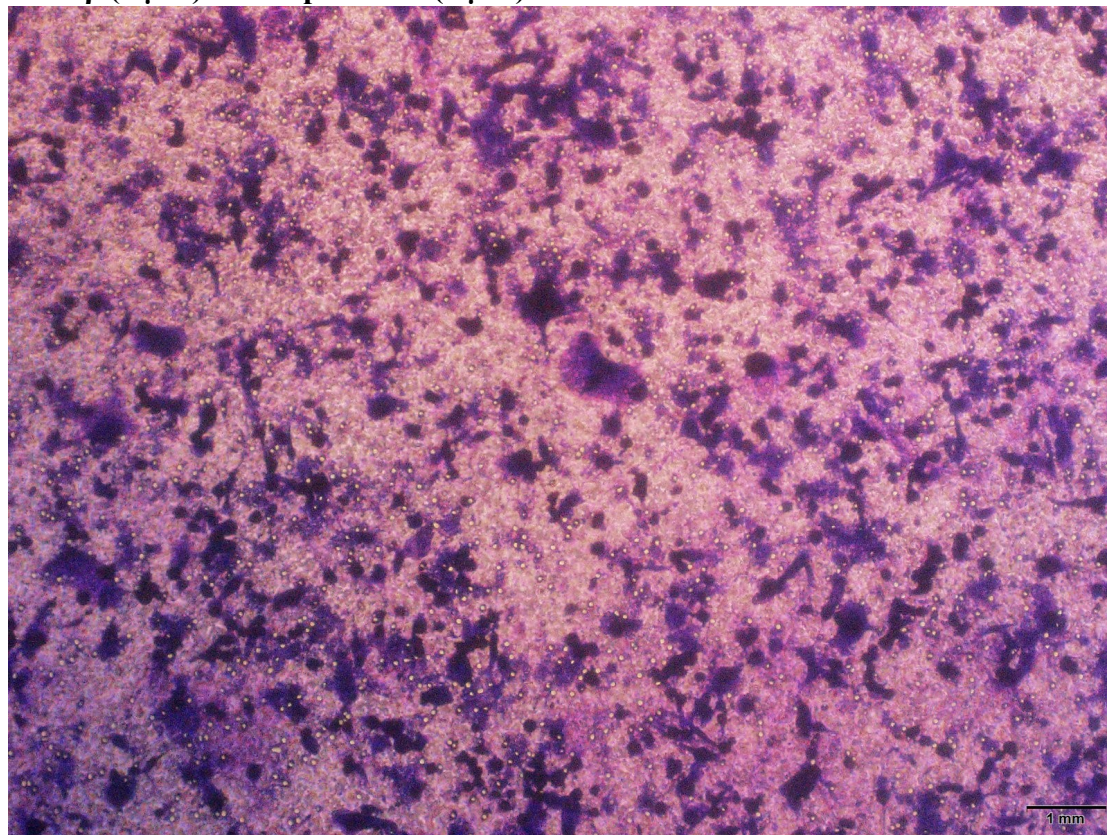
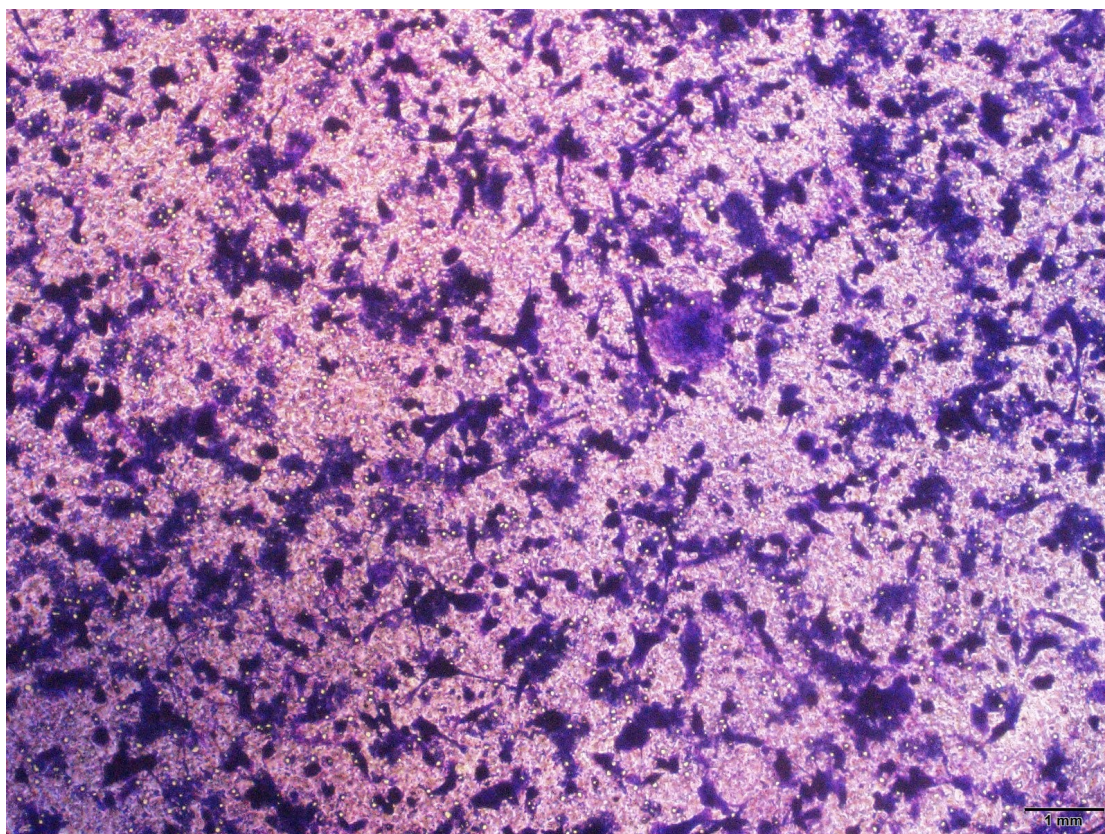


Figure S65 Representative photomicrographs of migration. Cells treated with the compound 2f (0, 2, 4 μ M), with or without 30 ng/mL TGF- β for 24 h.

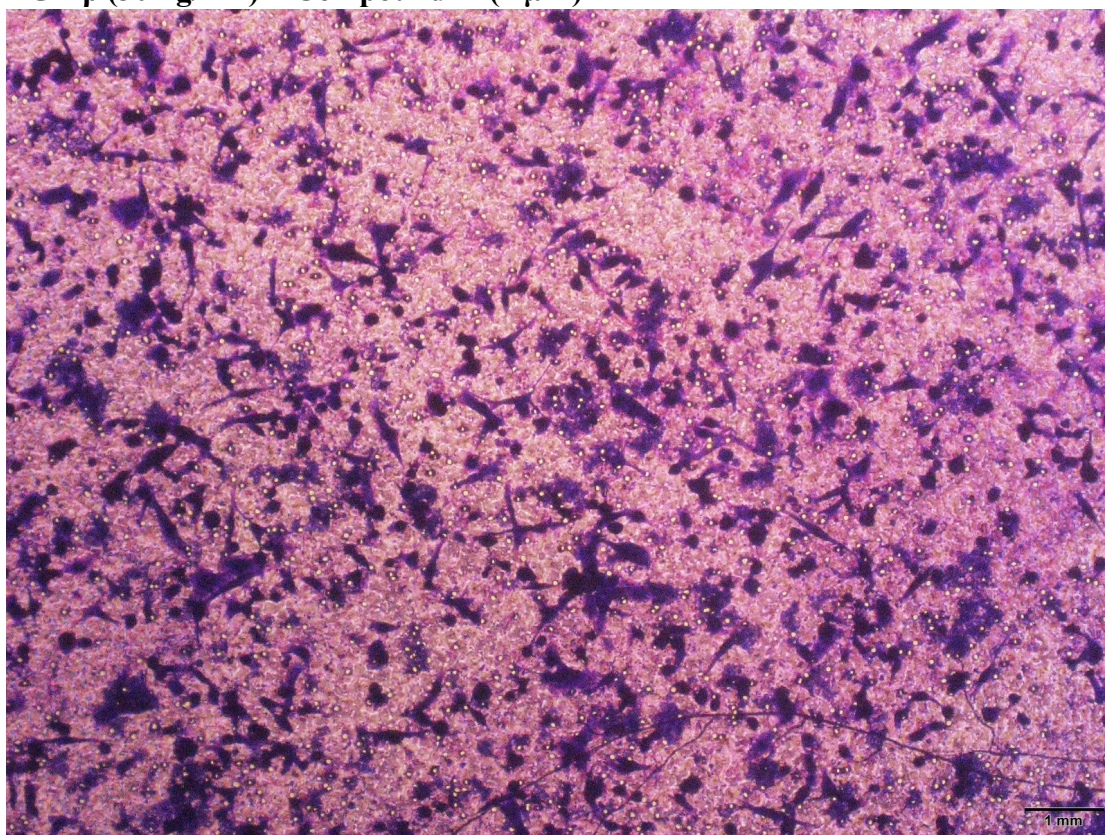
TGF- β (0 μ M) + Compound 2f (0 μ M)



TGF- β (30 ng/mL) + Compound 2f (0 μ M)



TGF- β (30 ng/mL) + Compound 2f (2 μ M)



TGF- β (30 ng/mL) + Compound 2f (4 μ M)

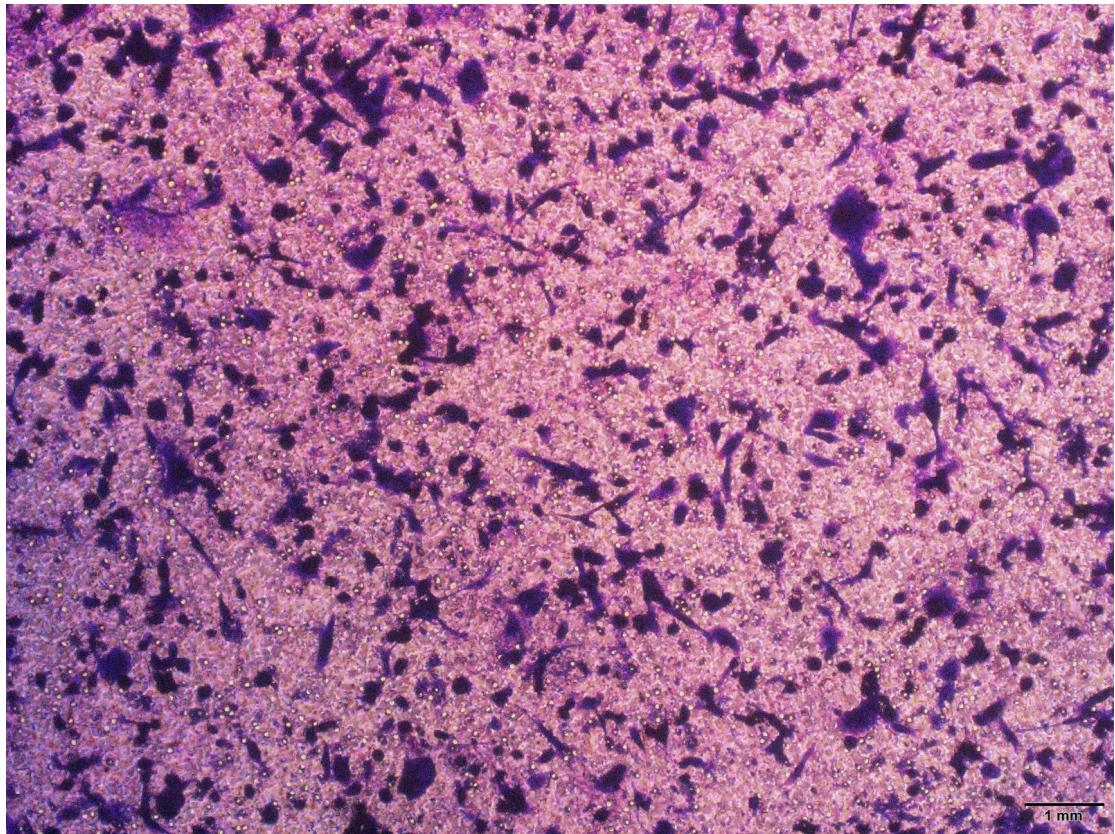
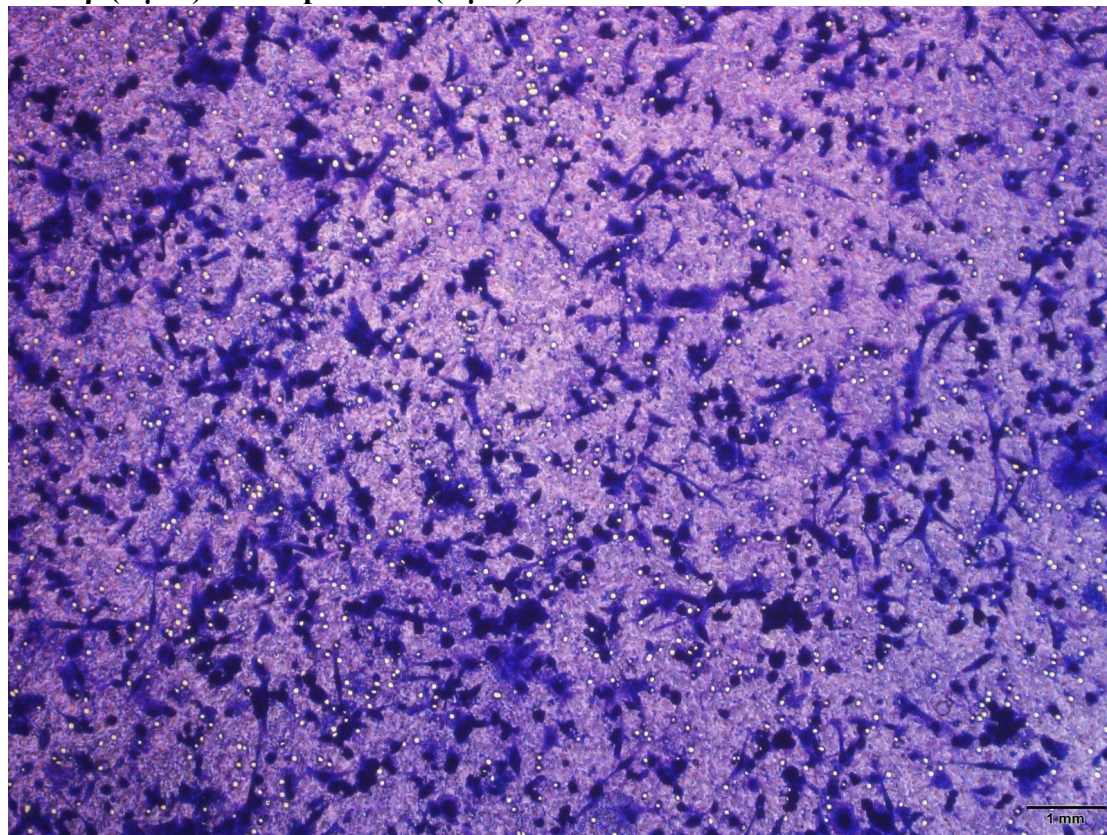
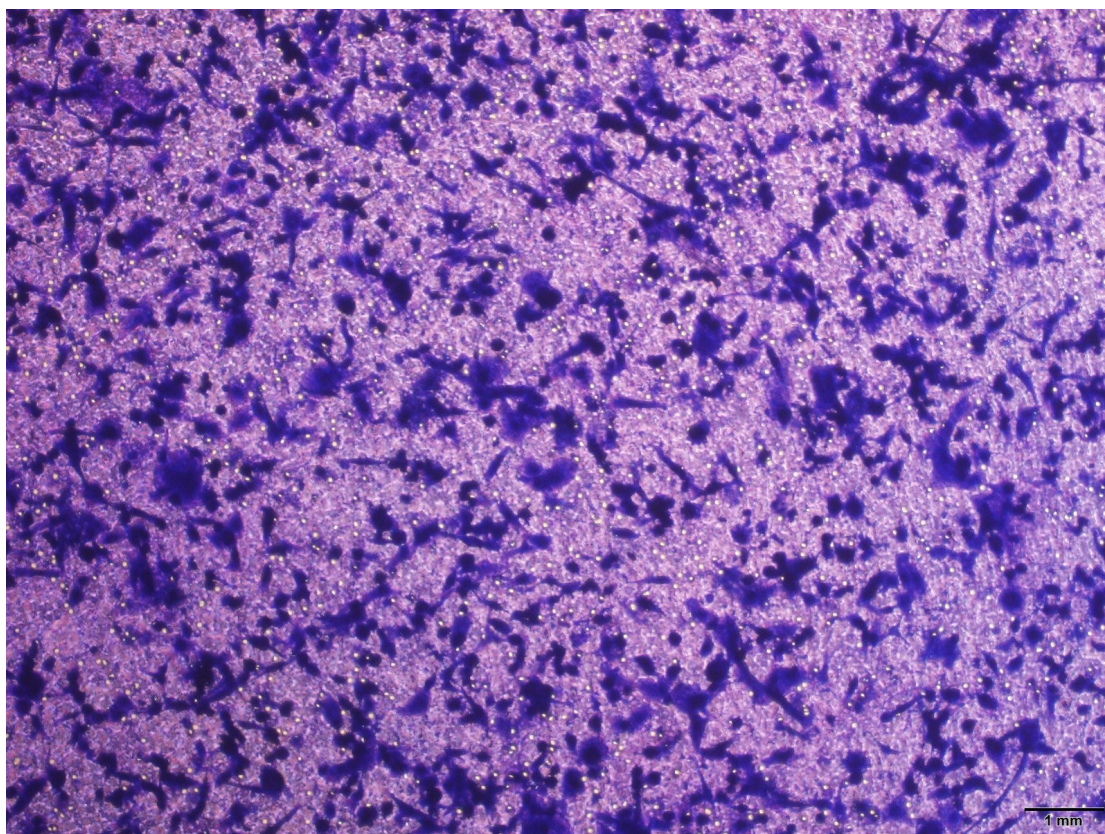


Figure S66 Representative photomicrographs of invasion. Cells treated with the compound 2f (0, 2, 4 μ M), with or without 30 ng/mL TGF- β for 24 h.

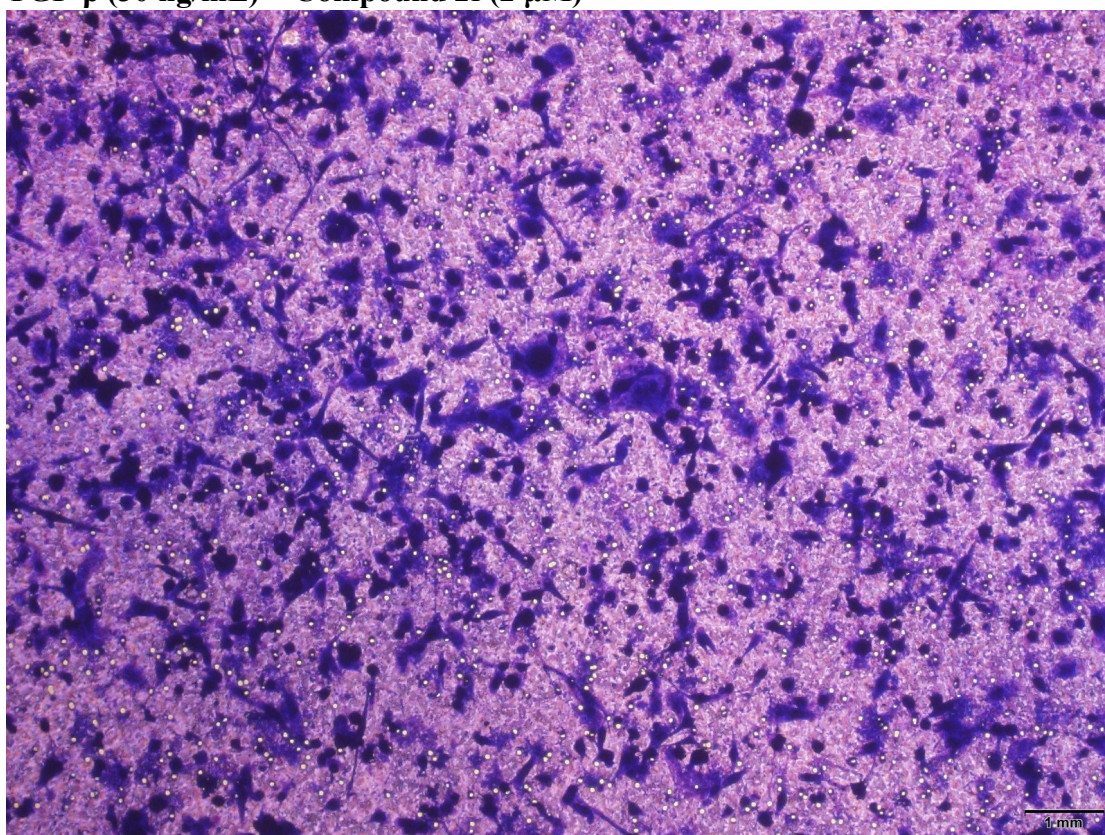
TGF- β (0 μ M) + Compound 2f (0 μ M)



TGF- β (30 ng/mL) + Compound 2f (0 μ M)



TGF- β (30 ng/mL) + Compound 2f (2 μ M)



TGF- β (30 ng/mL) + Compound 2f (4 μ M)

