

Supplemental Material

Novel Carbazolyl-thiazolyl-chromone and Carbazolyl-thiazolyl-pyrazole Hybrids: Synthesis, Cytotoxicity Evaluation and Molecular Docking Studies

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Copies of IR, NMR and MS Spectra for all the synthesized Compounds

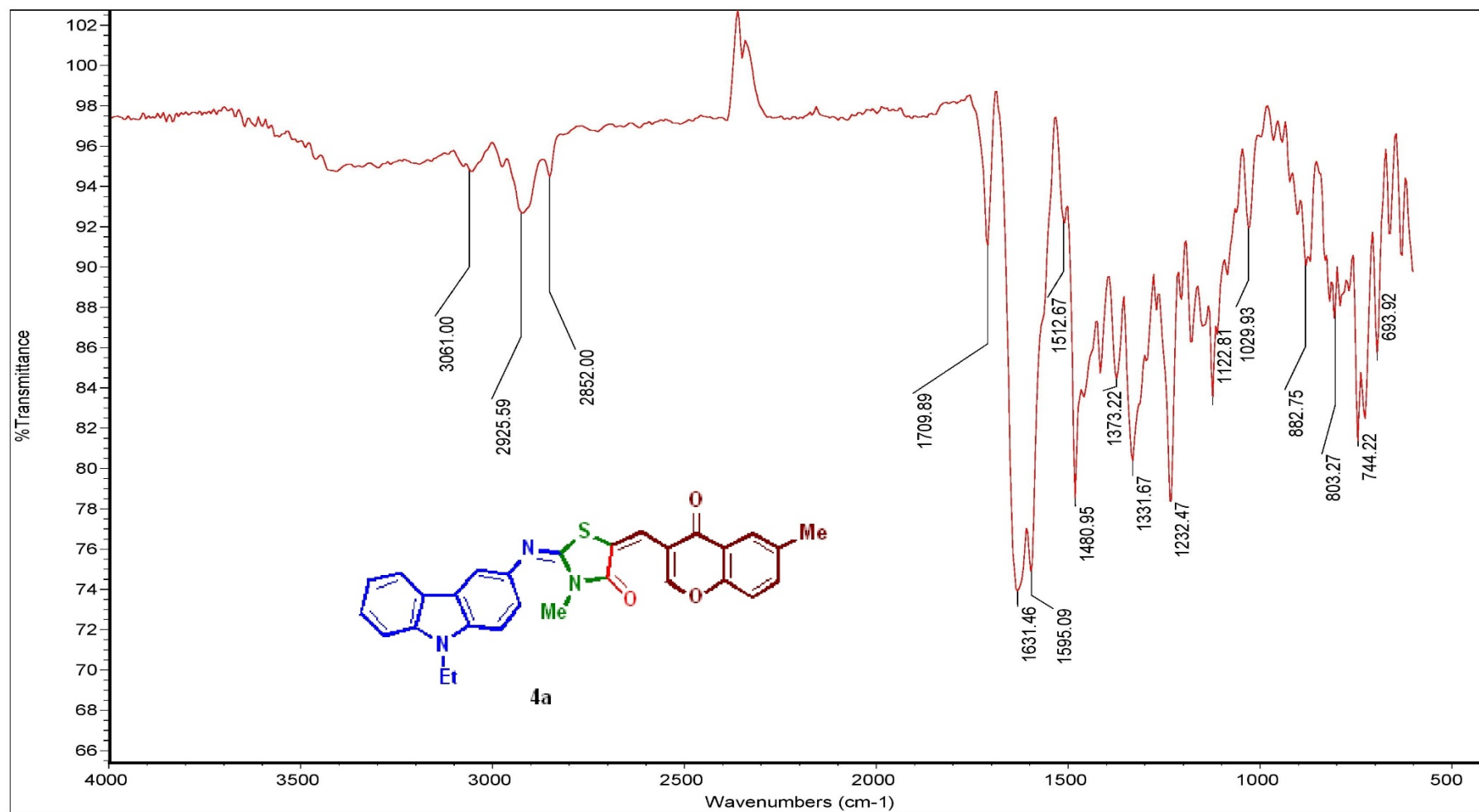


Figure S1: The IR spectrum of compound **4a**.

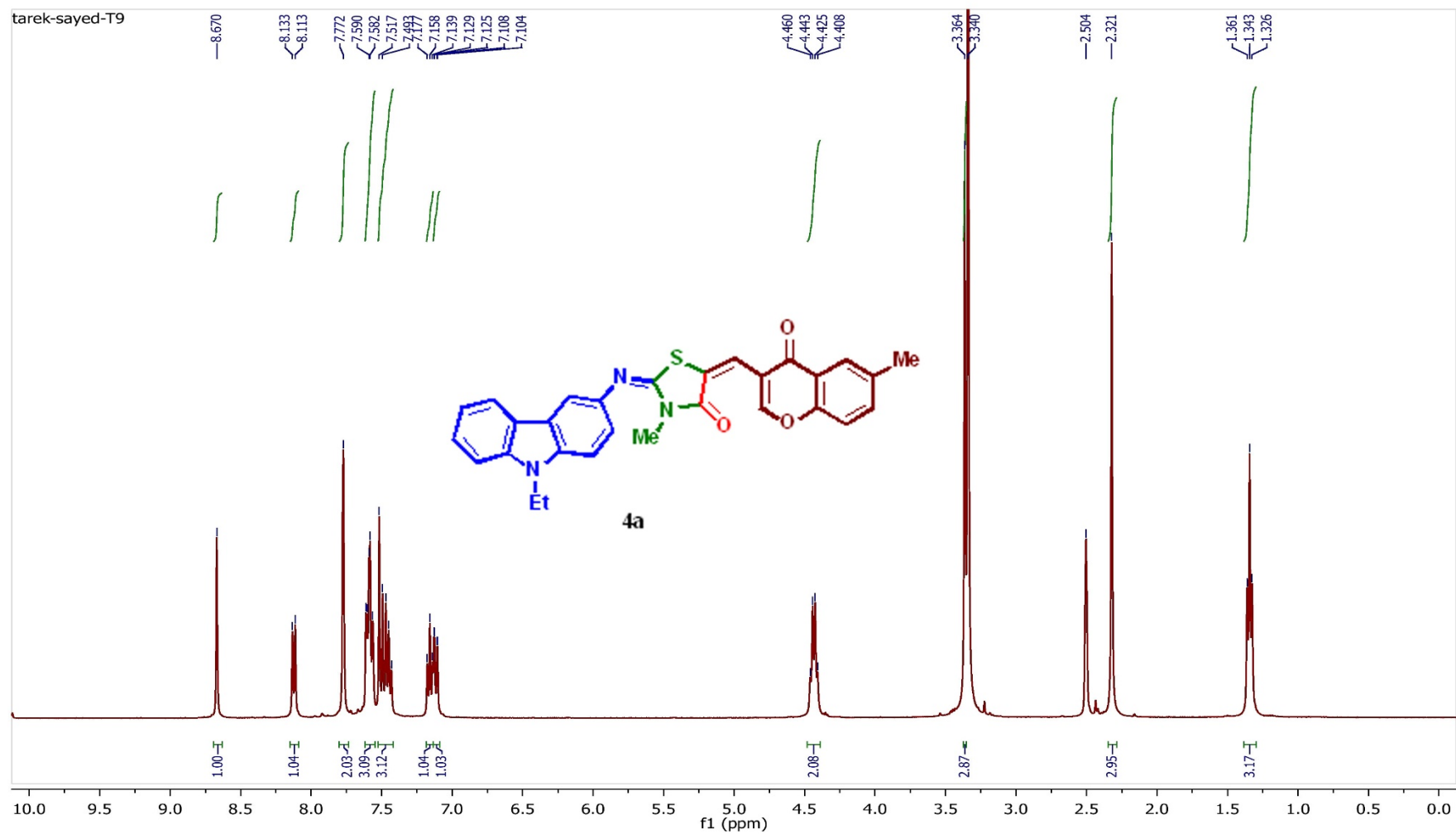


Figure S2: The ^1H -NMR spectrum of compound **4a**.

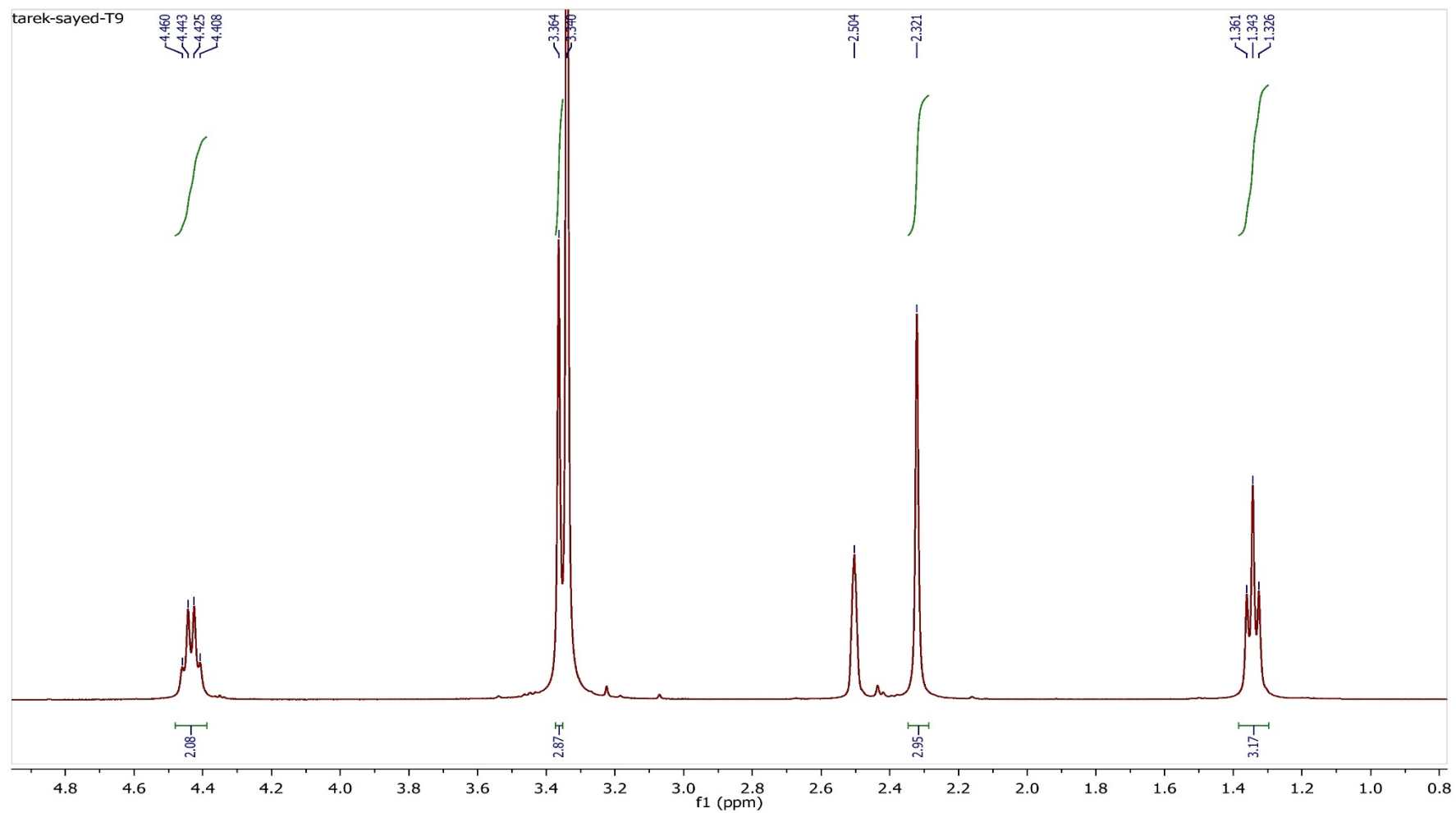


Figure S3: The enlargement of upfield region in ^1H -NMR spectrum of compound **4a**.

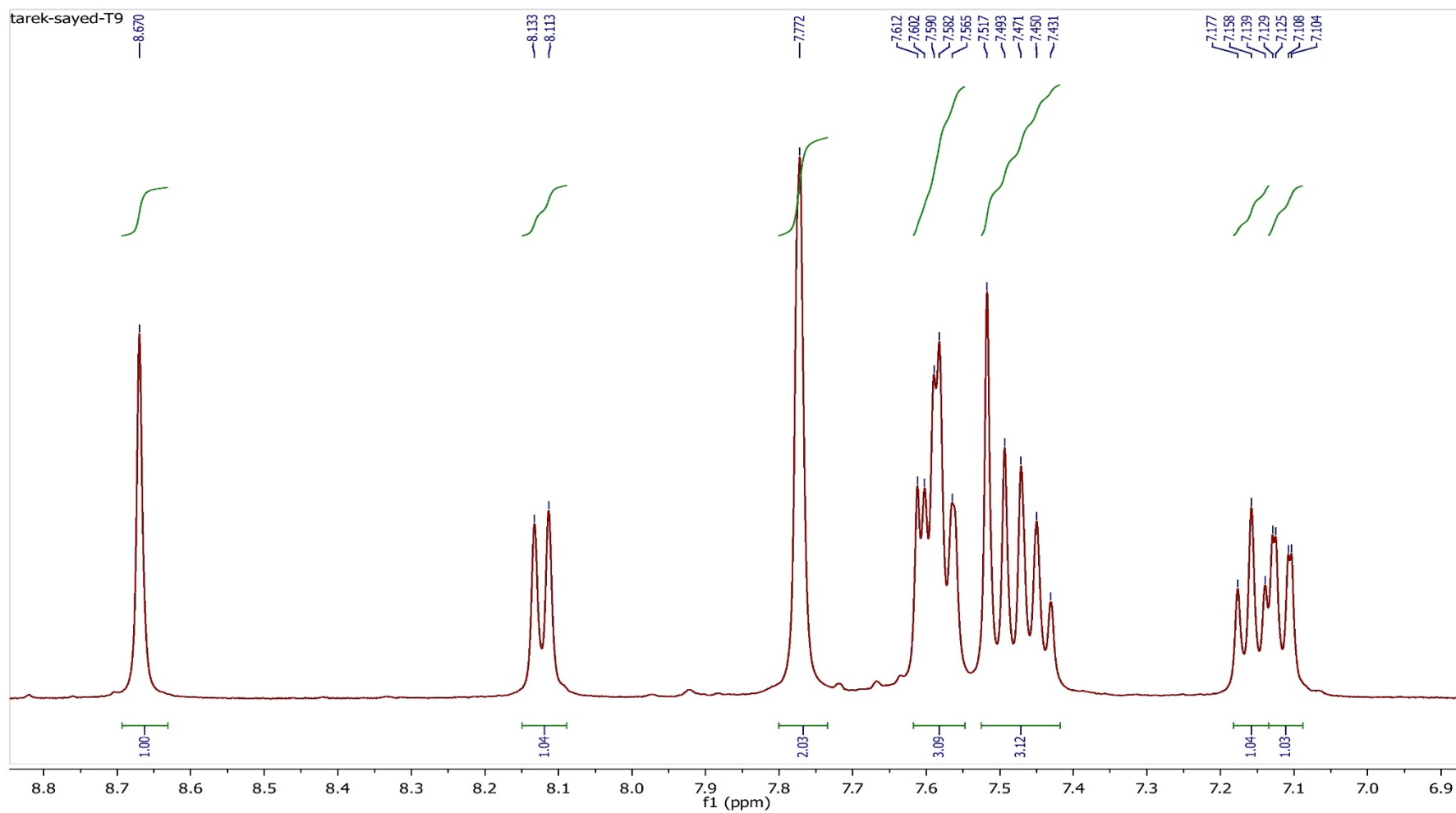


Figure S4: The enlargement of downfield region in ^1H -NMR spectrum of compound **4a**.

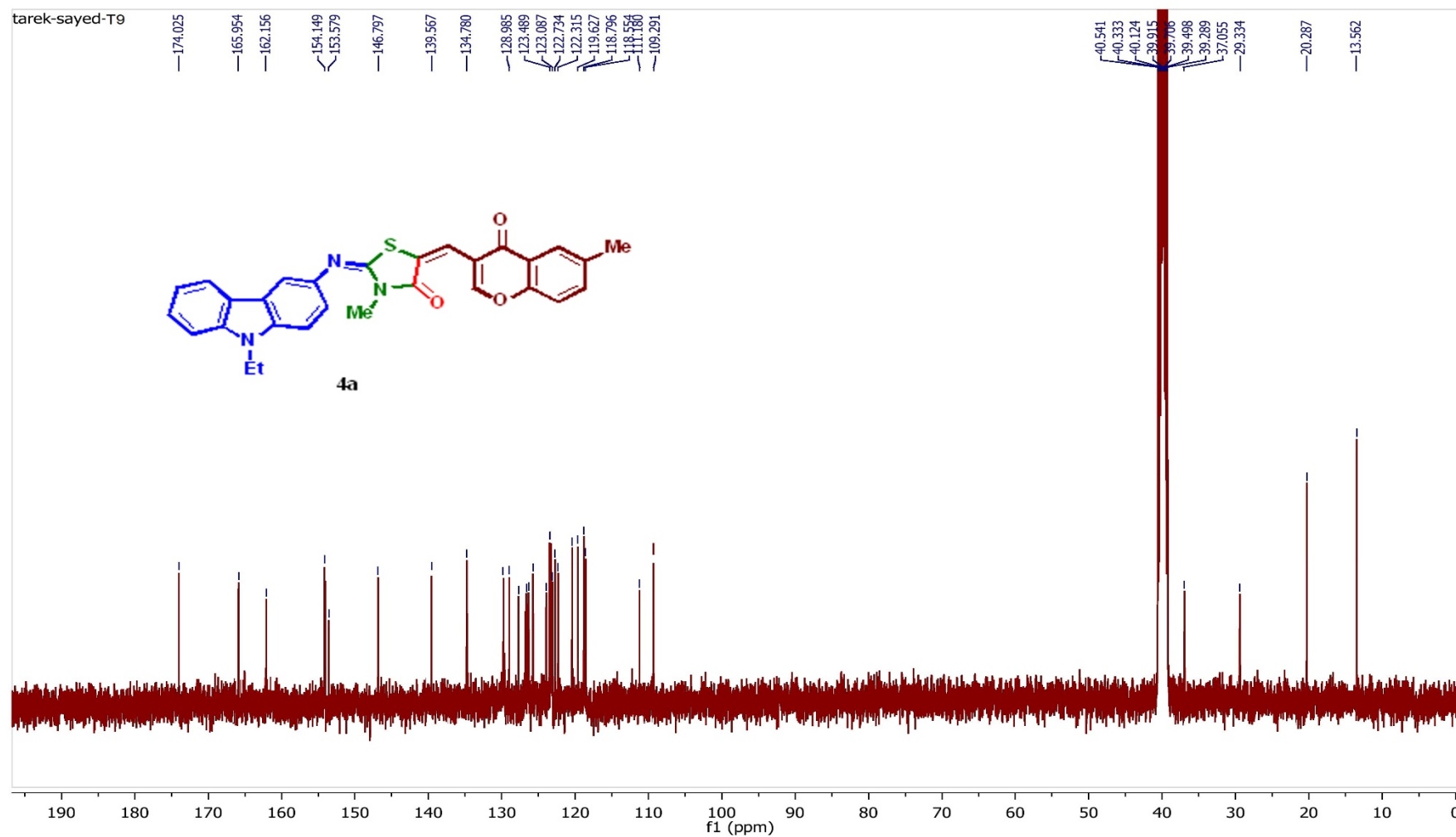


Figure S5: The ^{13}C -NMR spectrum of compound **4a**.

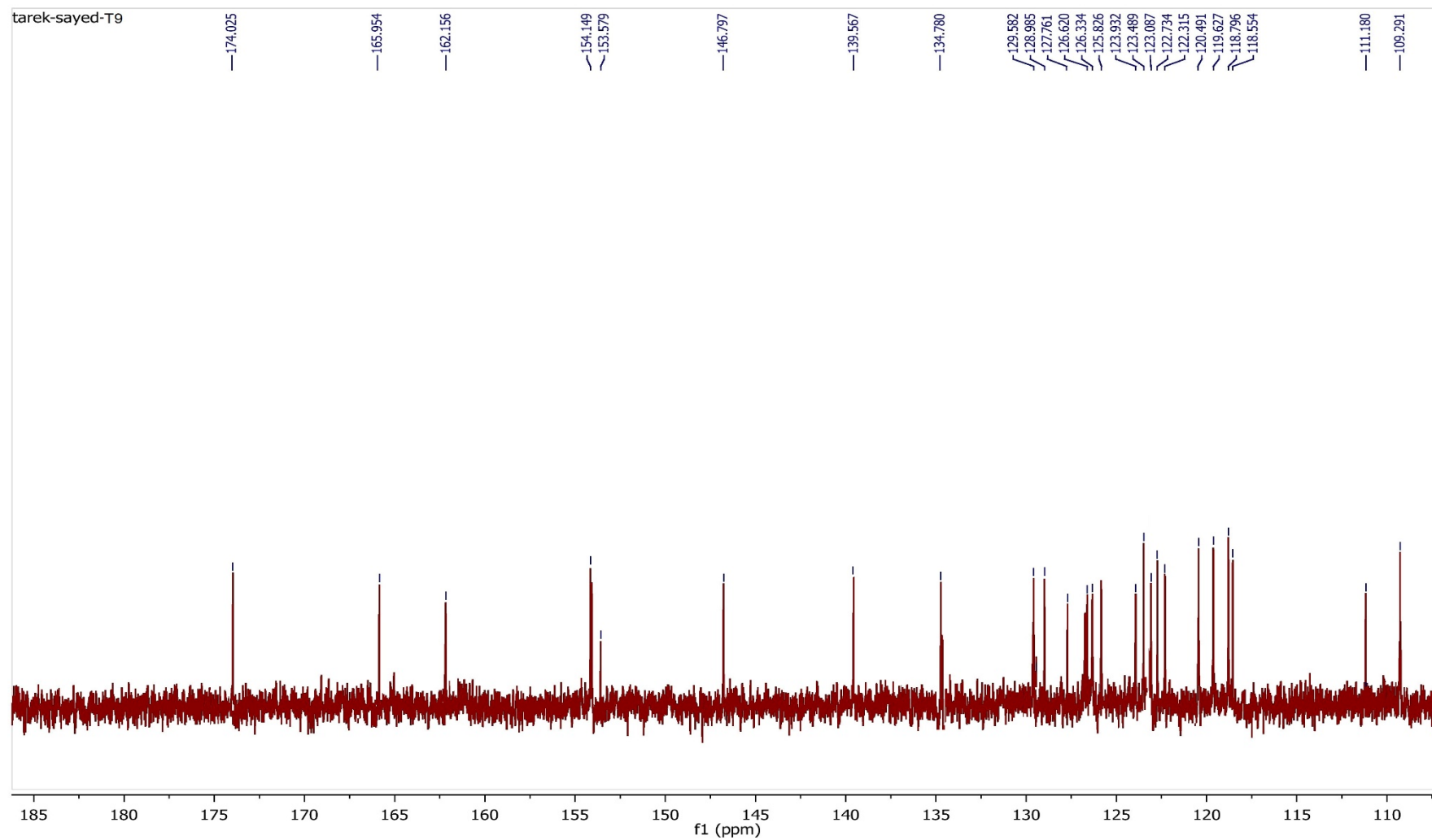


Figure S6: The enlargement of downfield region in ^{13}C -NMR spectrum of compound **4a**.

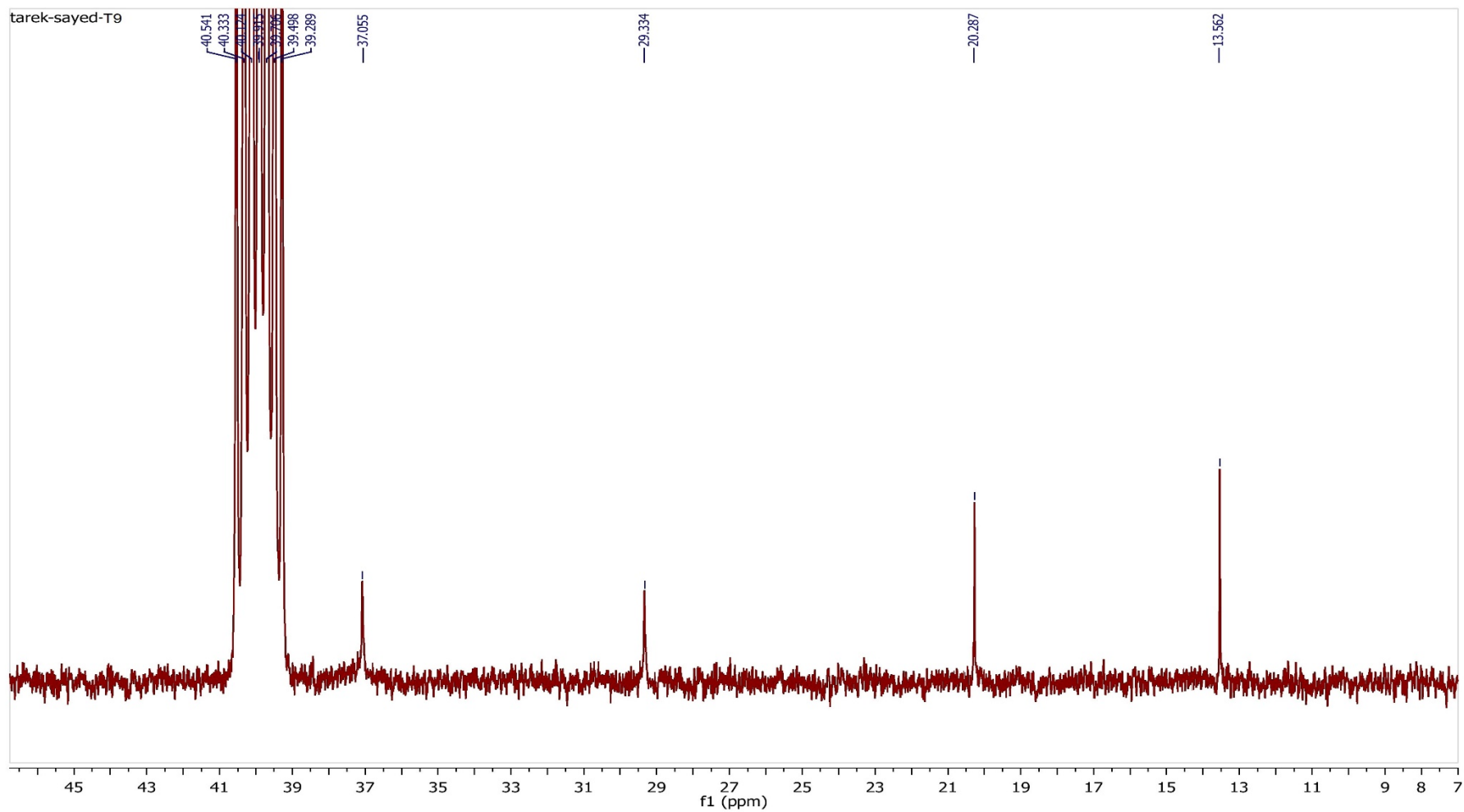


Figure S7: The enlargement of upfield region in ^{13}C -NMR spectrum of compound **4a**.

tarek-T9 #48-50 RT: 0.82-0.85 AV: 3 SB: 2 3.82, 3.53 NL: 1.58E2
T: (0,0) + c EI Full ms [40.00-1000.00]

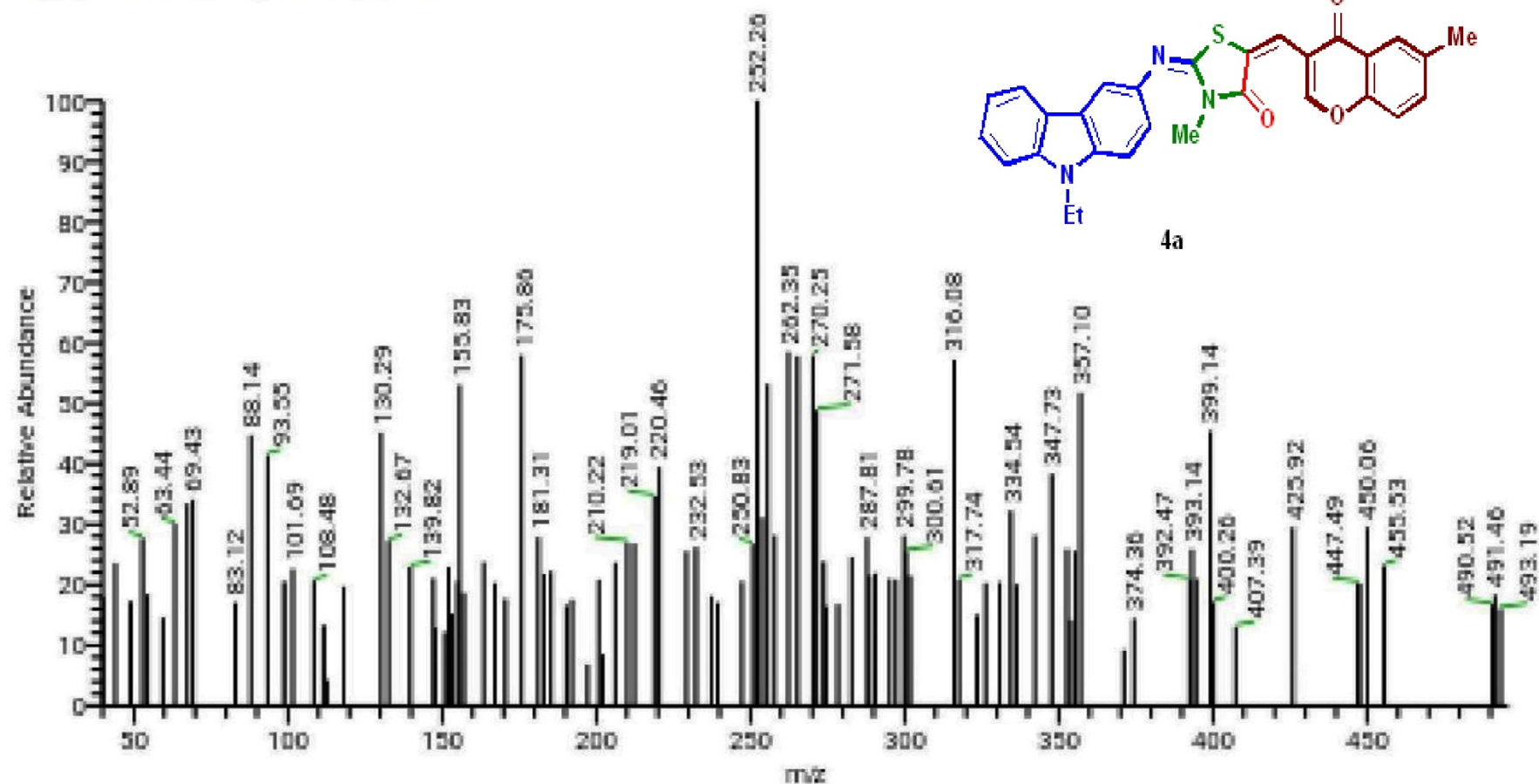


Figure S8: The mass spectrum of compound **4a**.

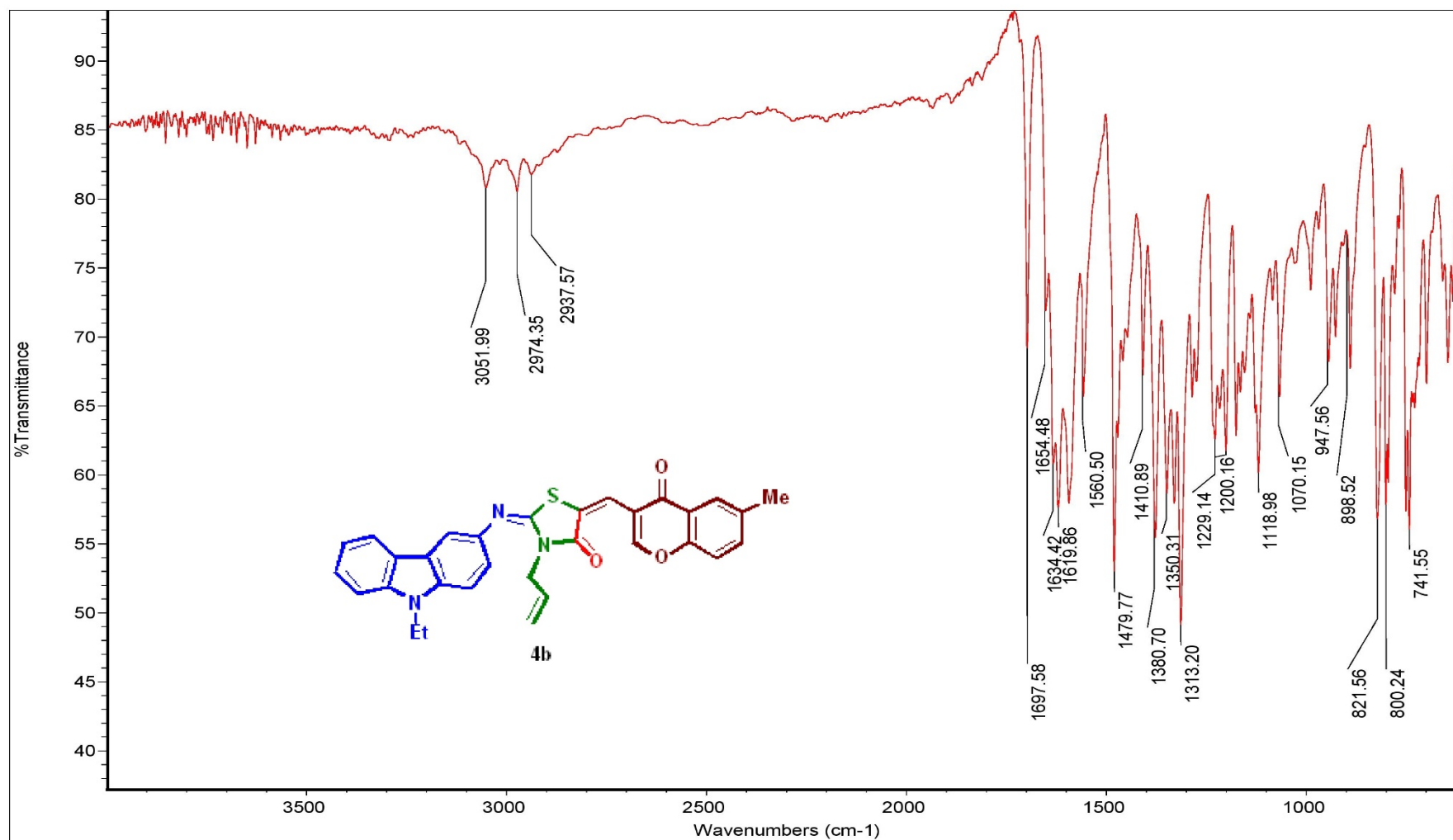


Figure S9: The IR spectrum of compound **4b**.

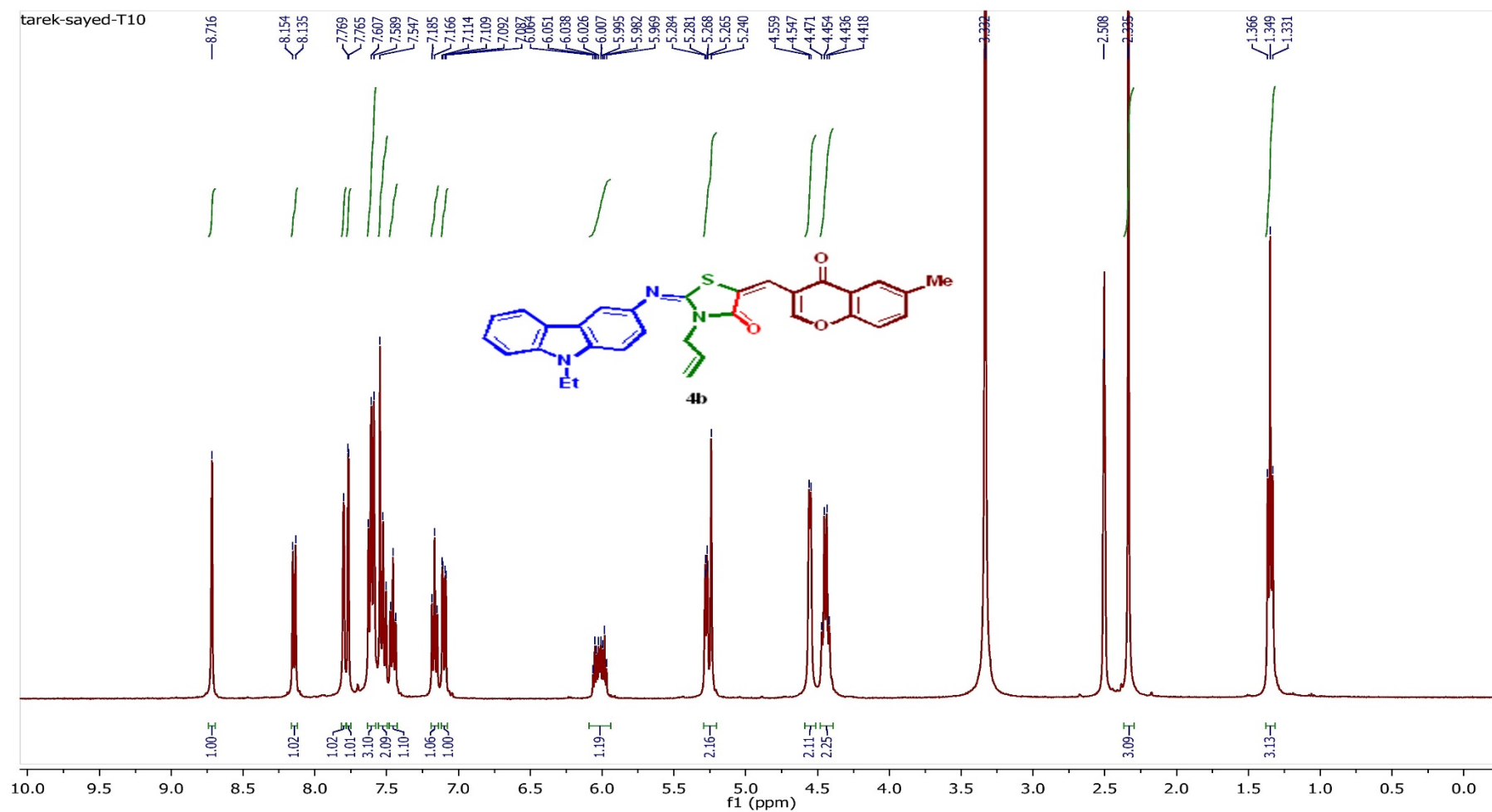


Figure S10: The ^1H -NMR spectrum of compound **4b**.

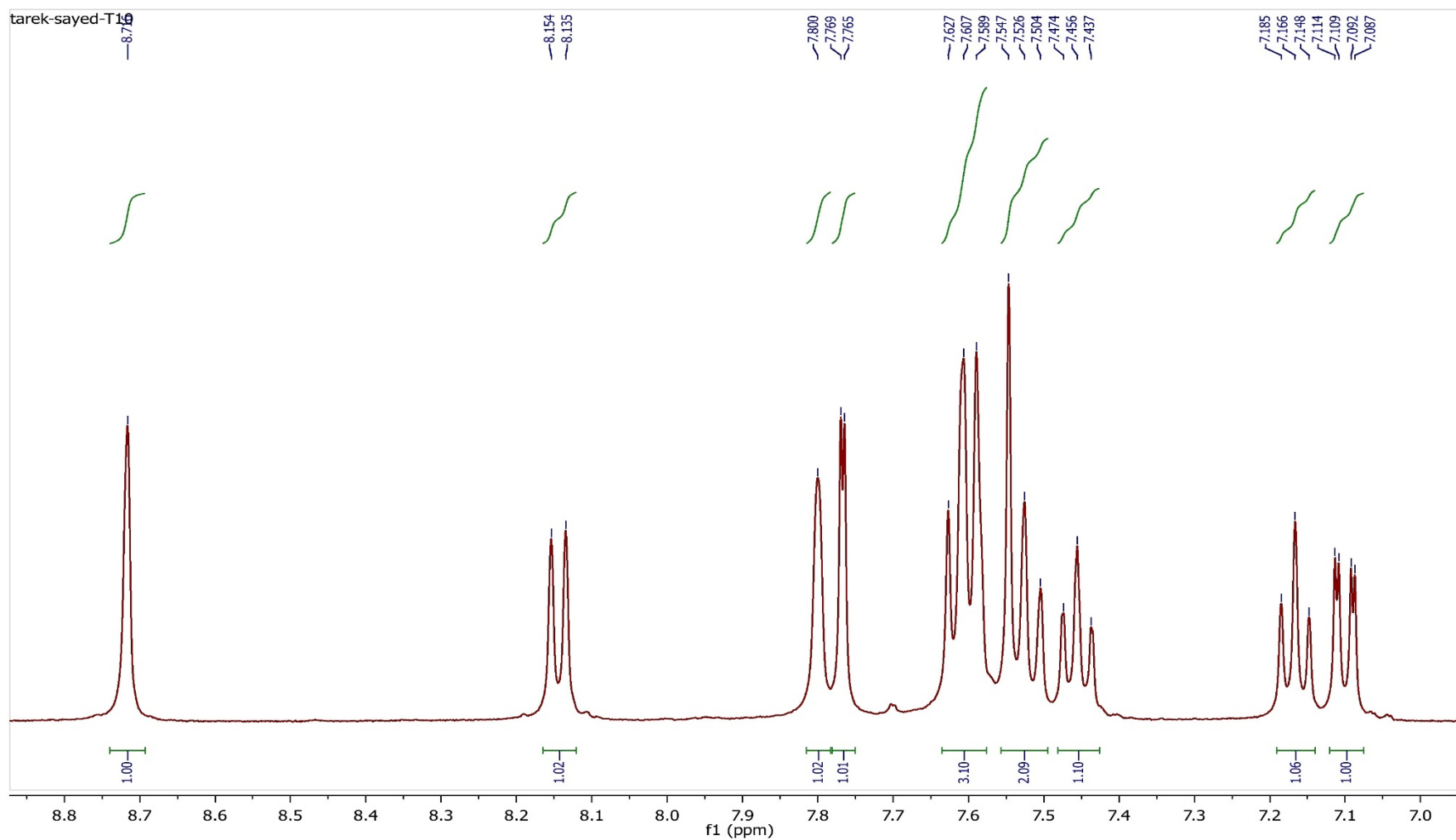


Figure S11: The enlargement of downfield region in ^1H -NMR spectrum of compound **4b**.

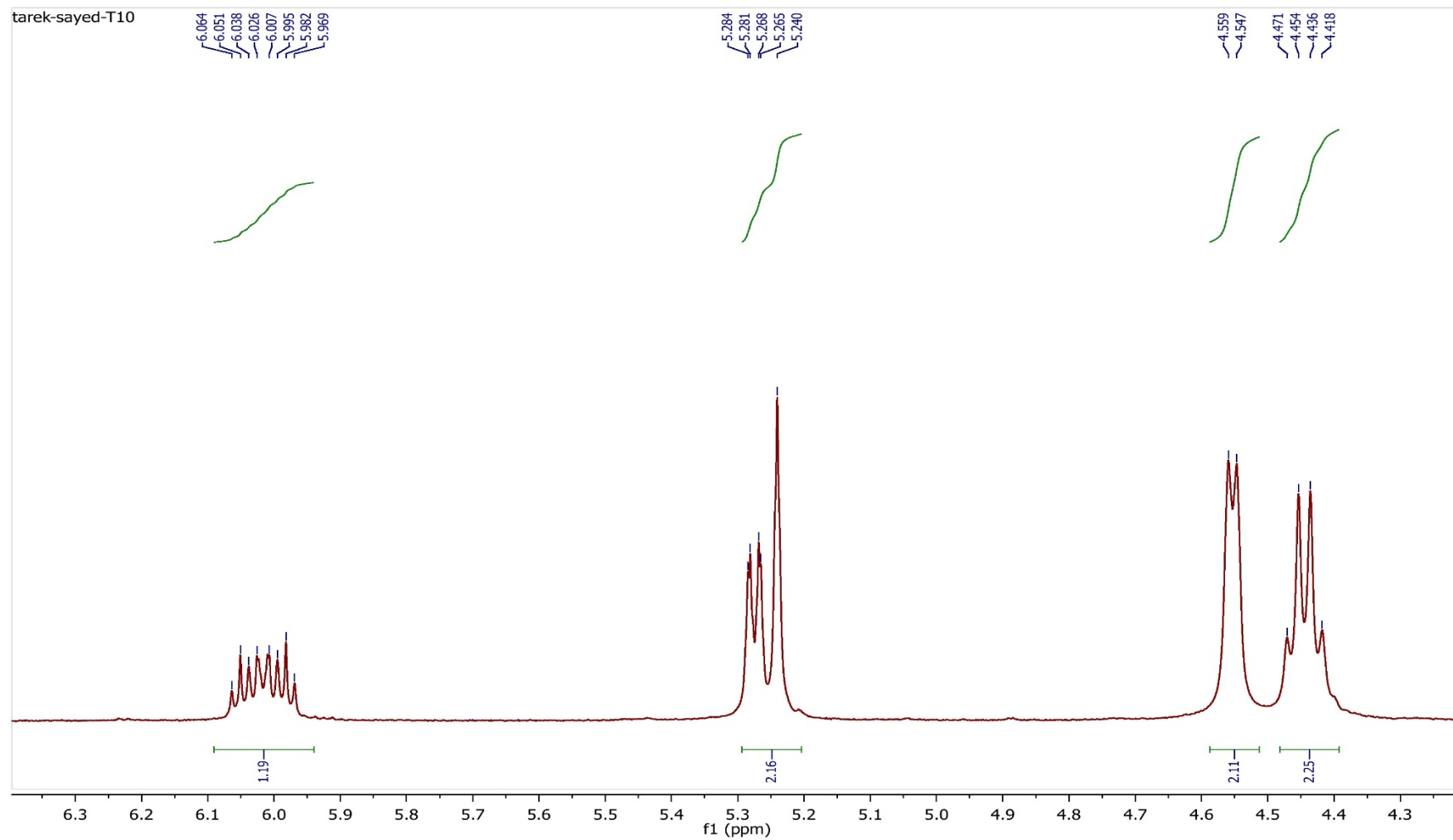


Figure S12: The enlargement of upfield region in ^1H -NMR spectrum of compound **4b**.

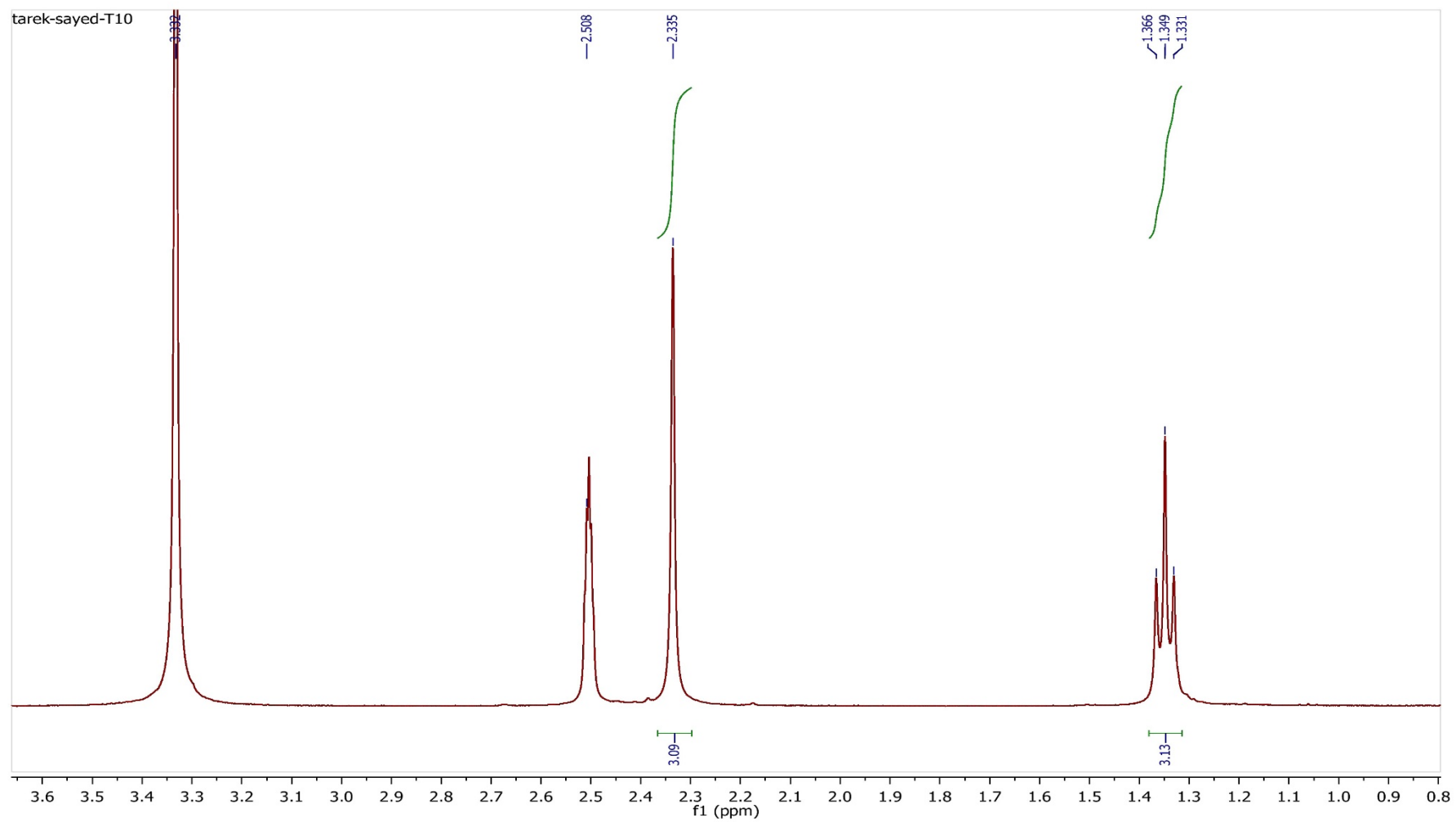


Figure S13: The enlargement of upfield region in ^1H -NMR spectrum of compound **4b**.

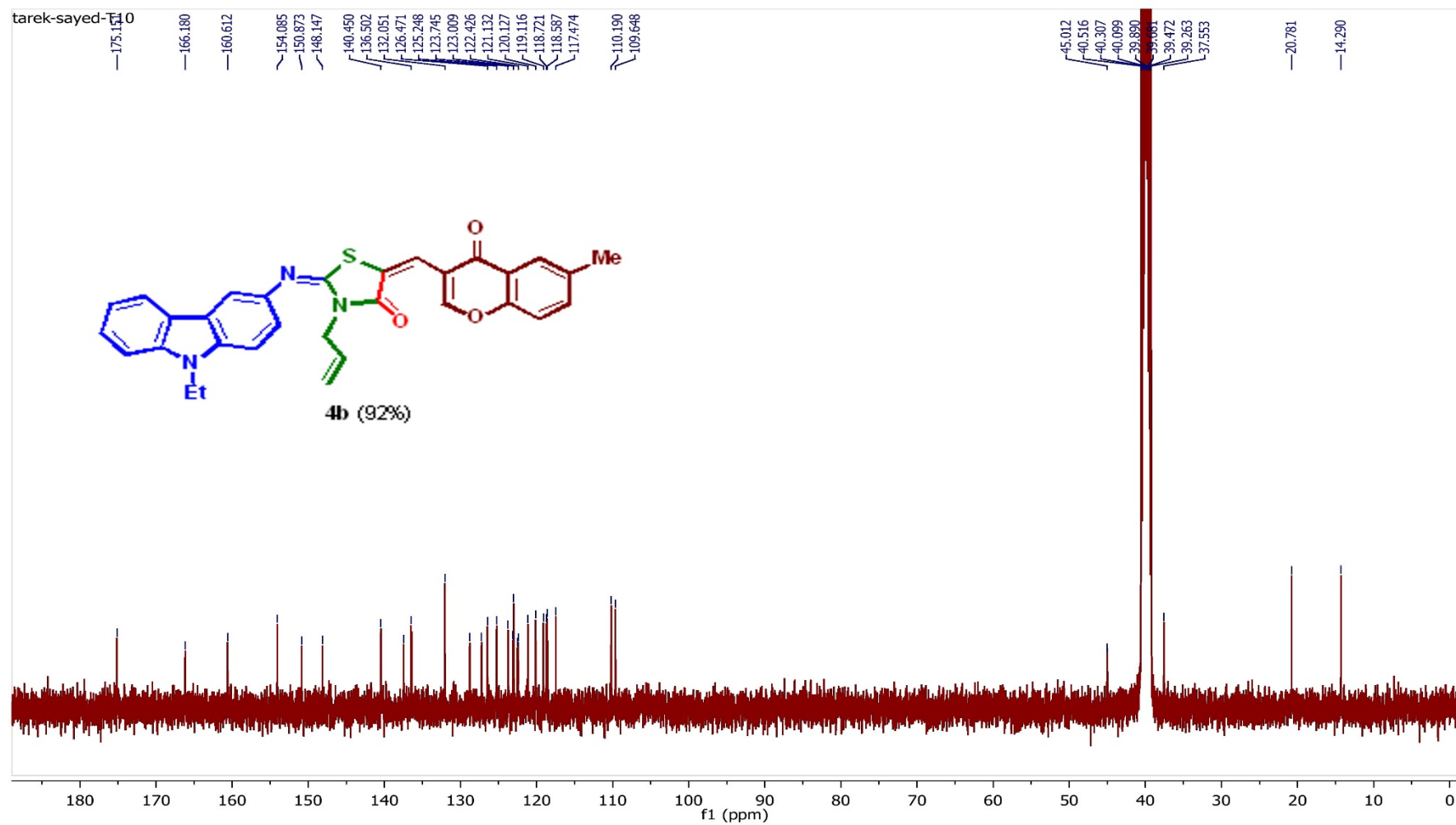


Figure S14: The ¹³C-NMR spectrum of compound **4b**.

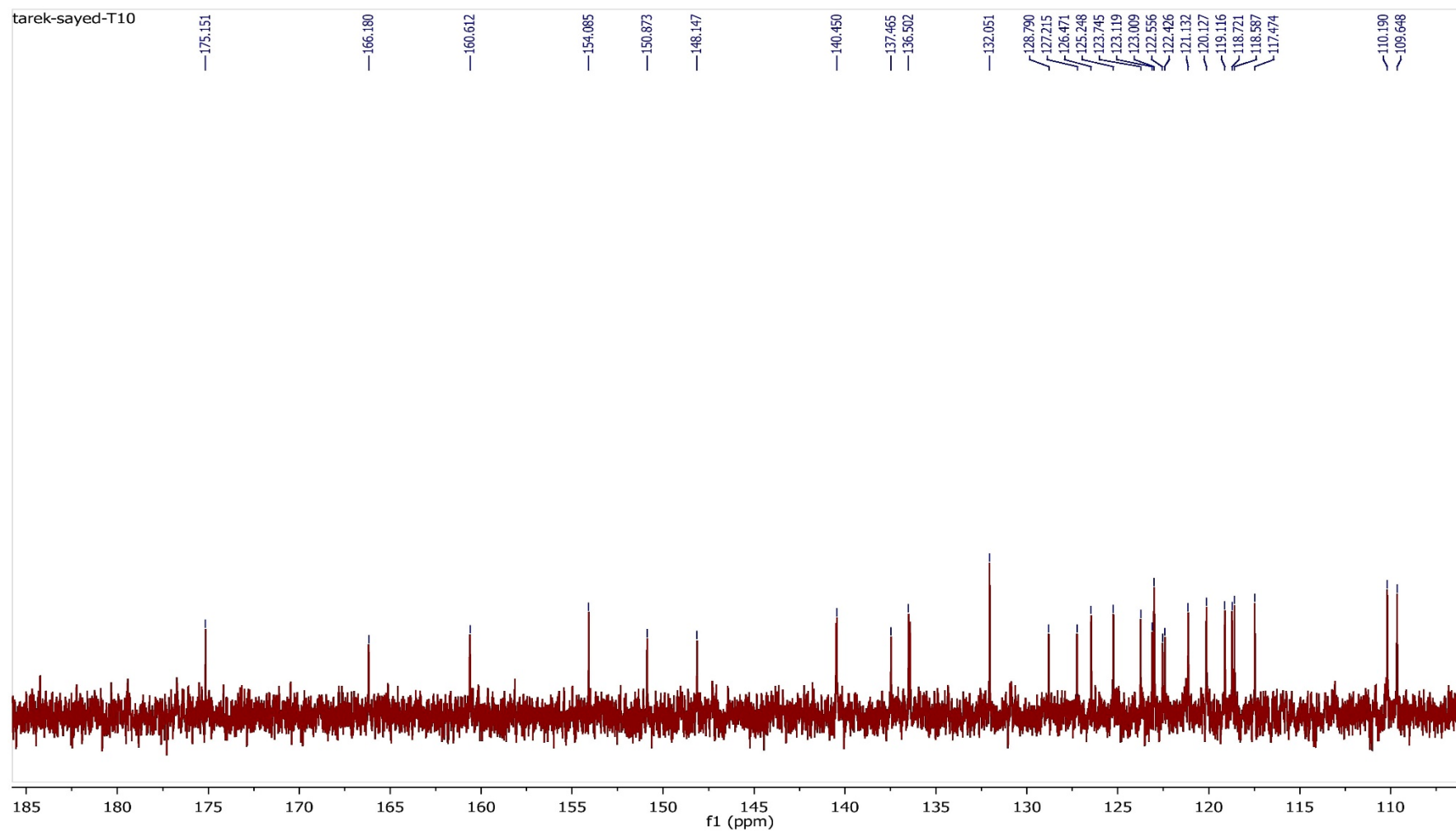


Figure S15: The enlargement of downfield region in ^{13}C -NMR spectrum of compound **4b**.

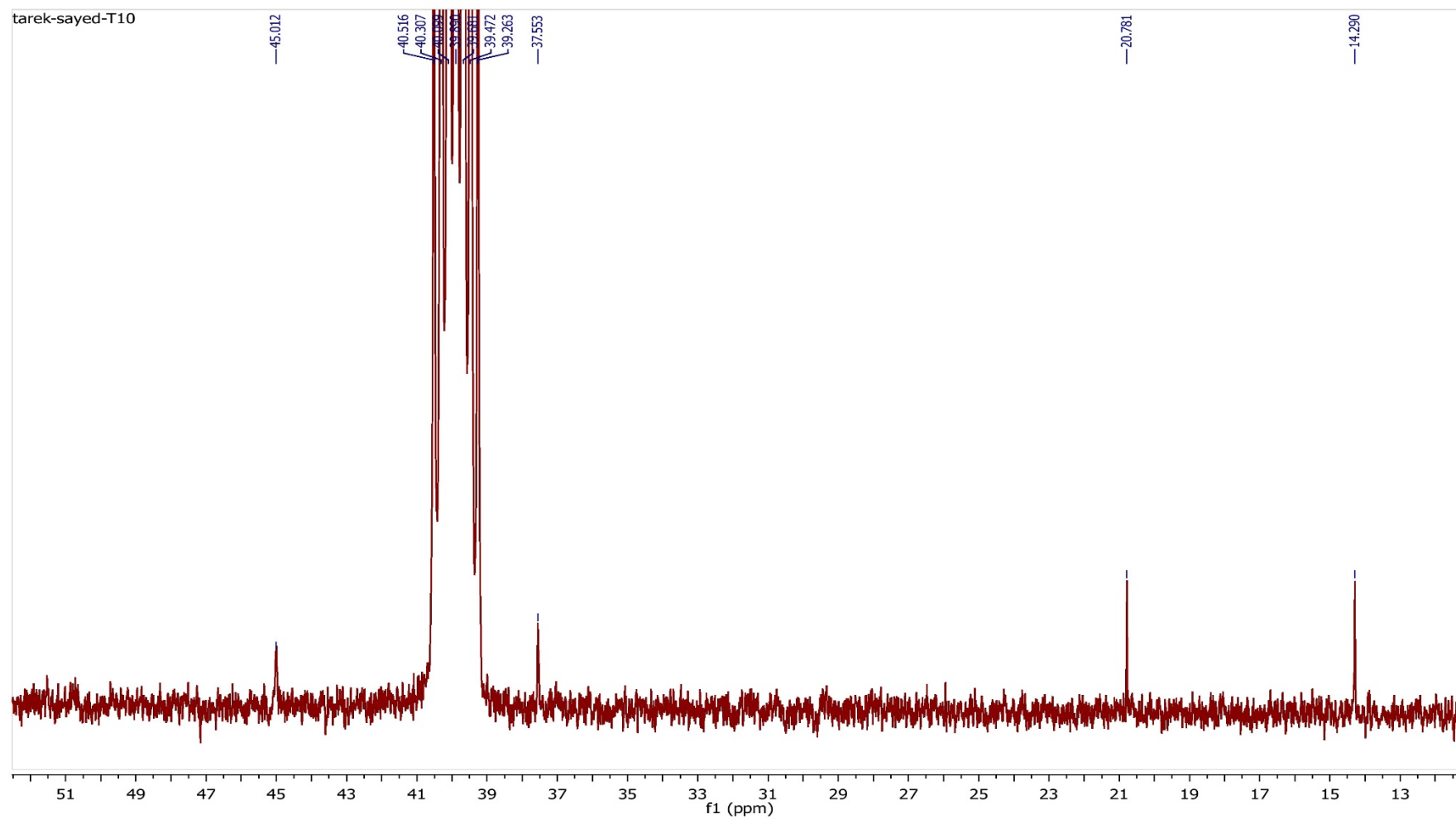


Figure S16: The enlargement of upfield region in ^{13}C -NMR spectrum of compound **4b**.

tarek-T10 #232-237 RT: 3.90-3.98 AV: 6 SB: 2 3.82, 3.53 NL: 1.51E2
T: (0,0) + e EI Full ms [40.00-1000.00]

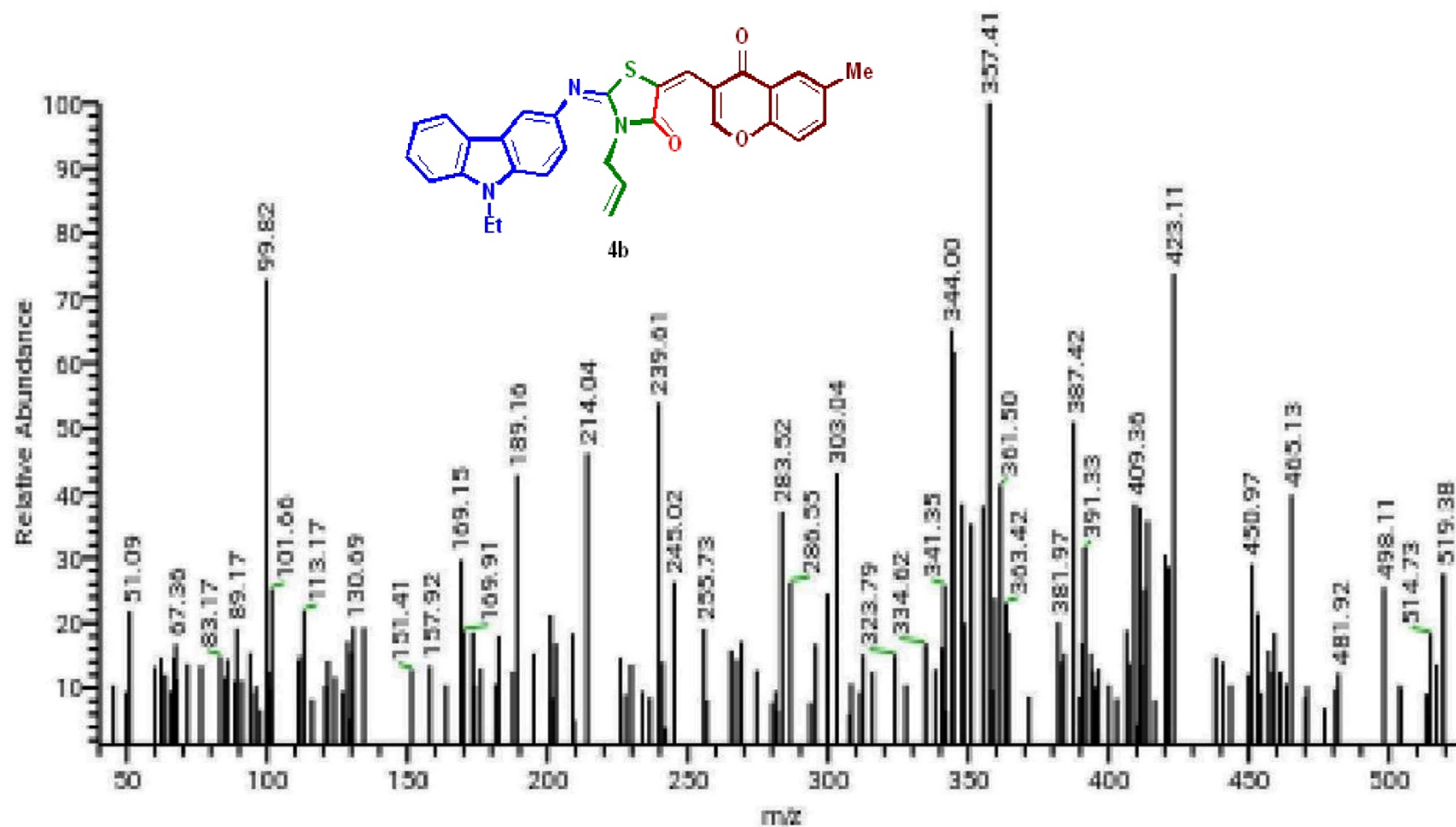


Figure S17: The mass spectrum of compound 4b.

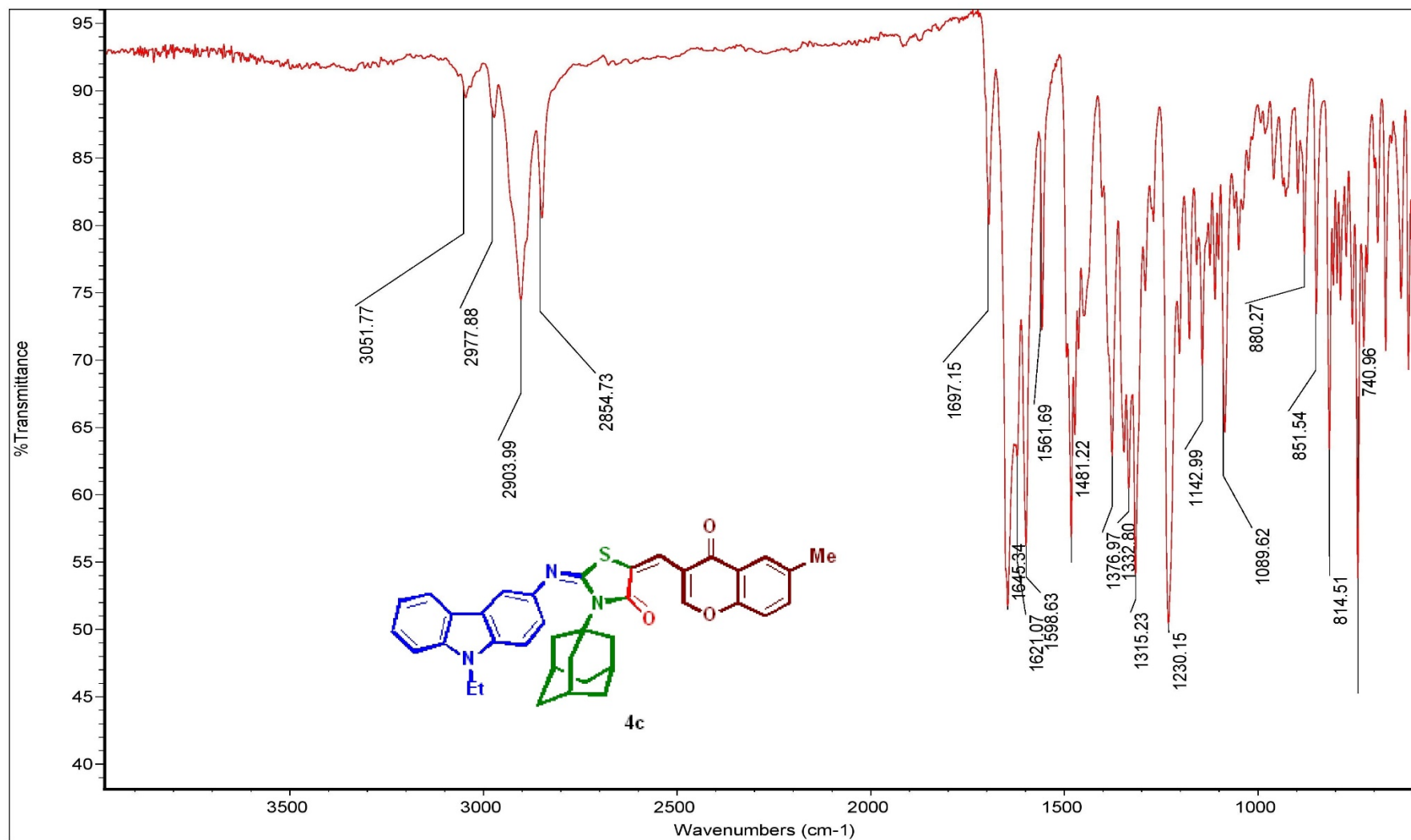


Figure S18: The IR spectrum of compound **4c**.

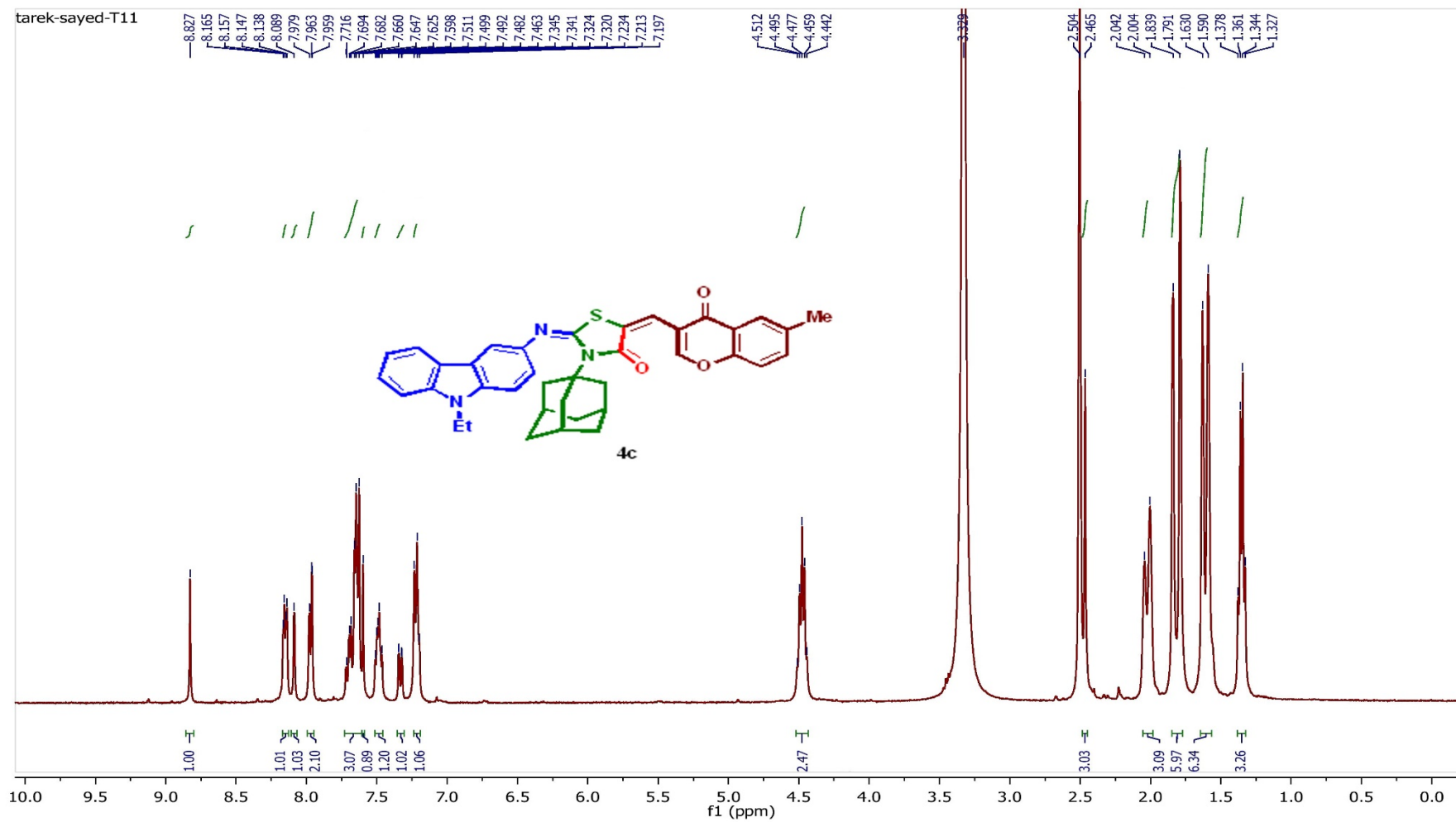


Figure S19: The ^1H -NMR spectrum of compound **4c**.

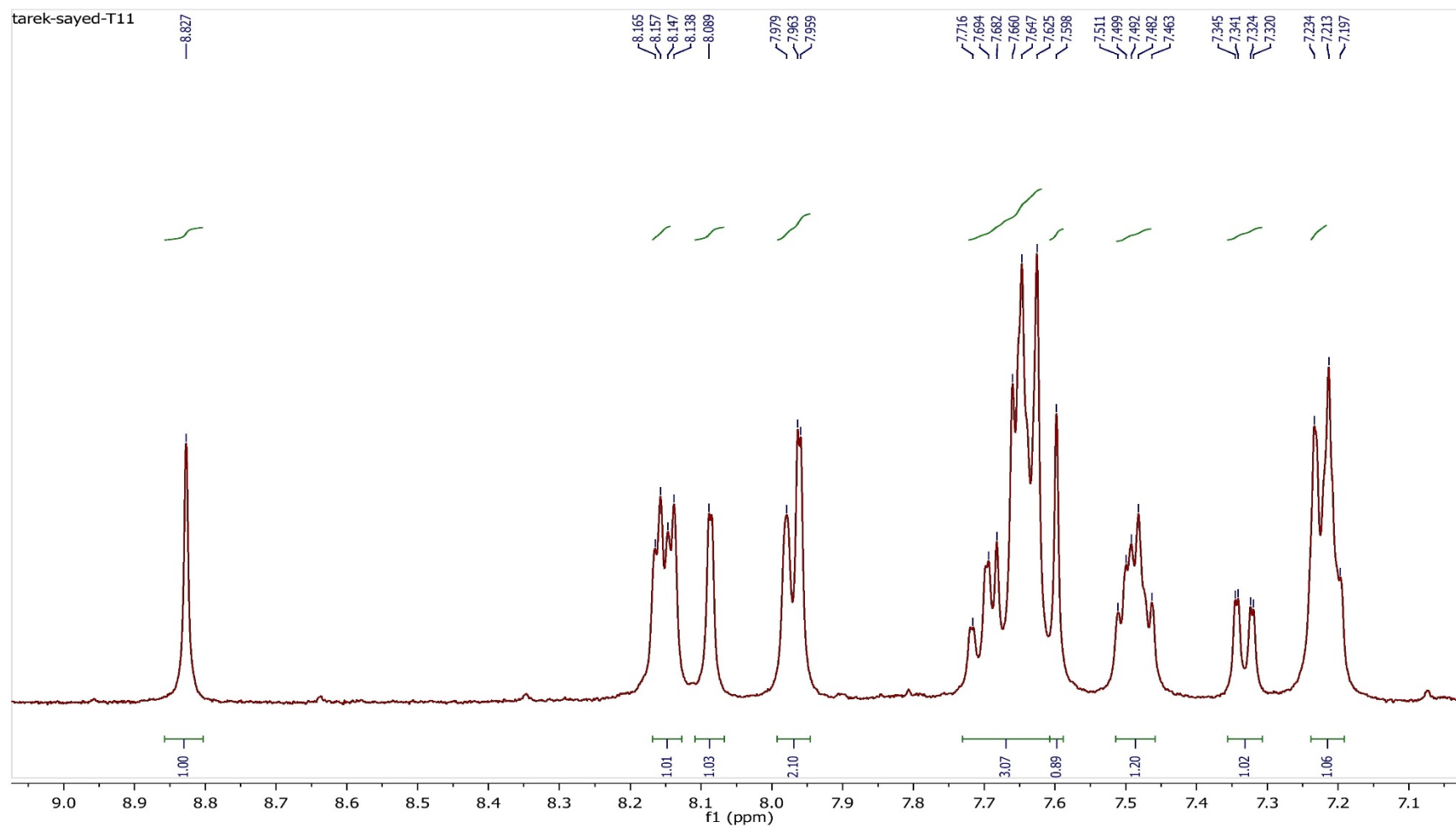


Figure S20: The enlargement of downfield region in ^1H -NMR spectrum of compound **4c**.

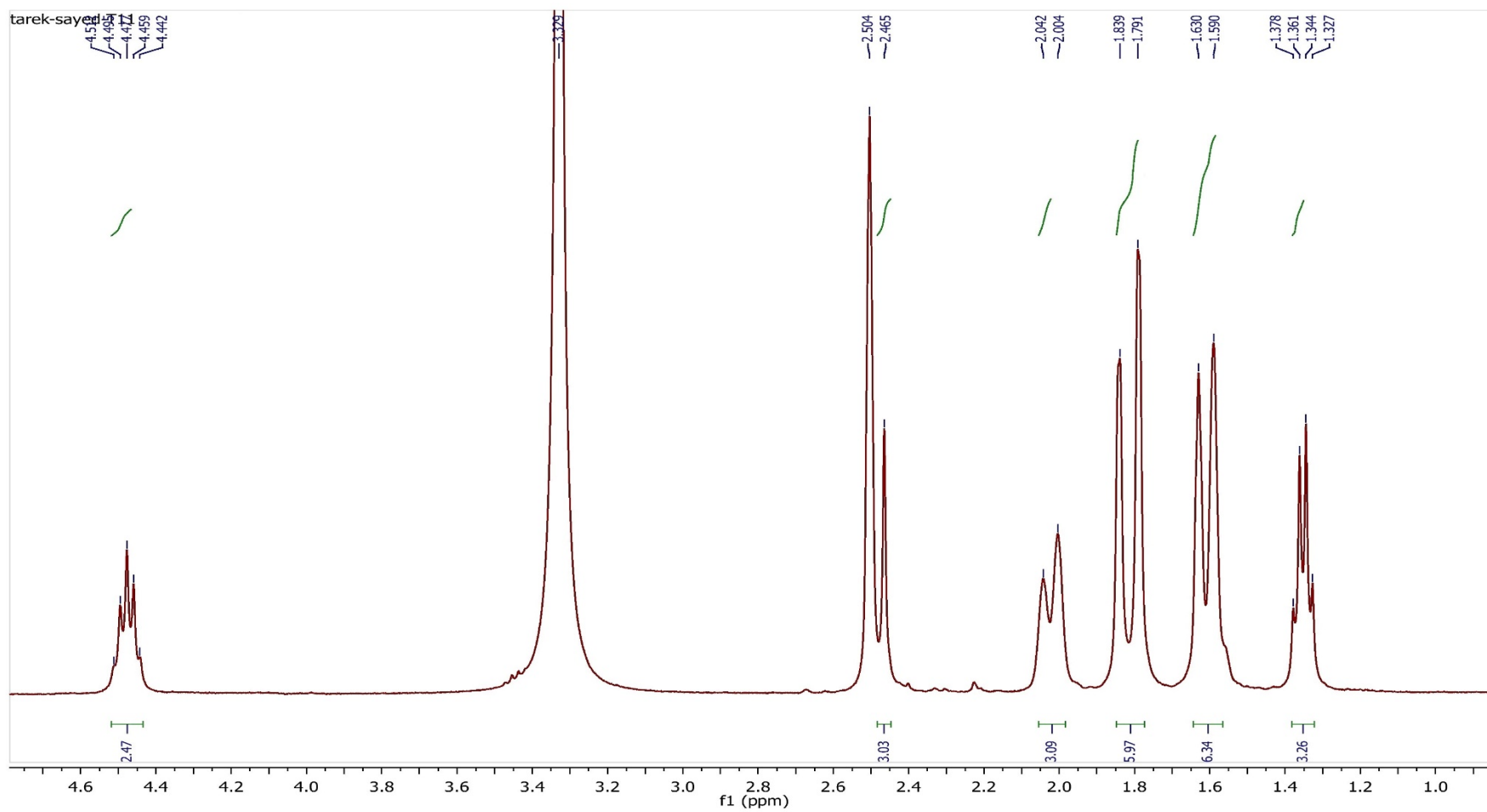


Figure S21: The enlargement of upfield region in ^1H -NMR spectrum of compound **4c**.

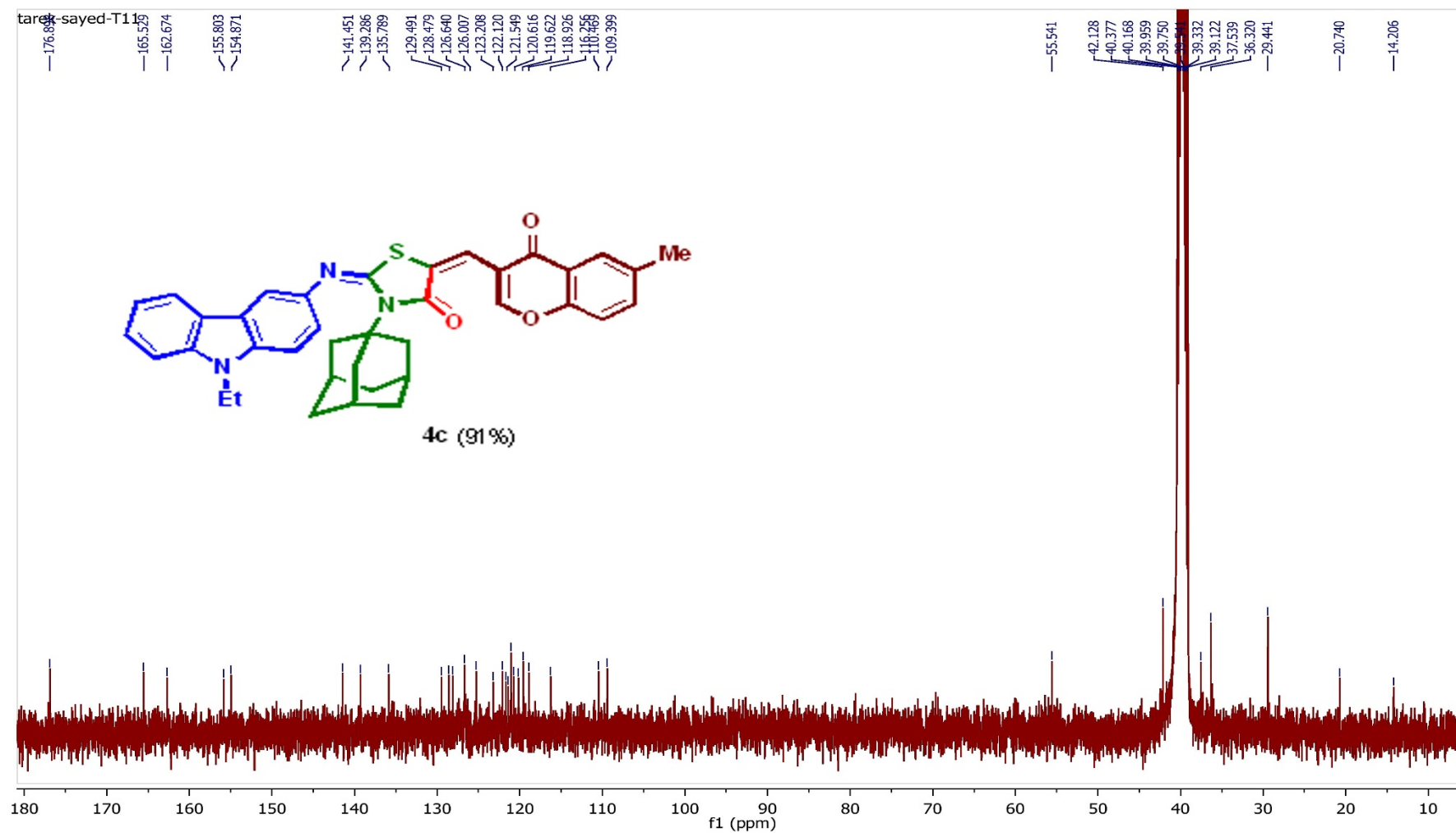


Figure S22: The ^{13}C -NMR spectrum of compound **4c**.

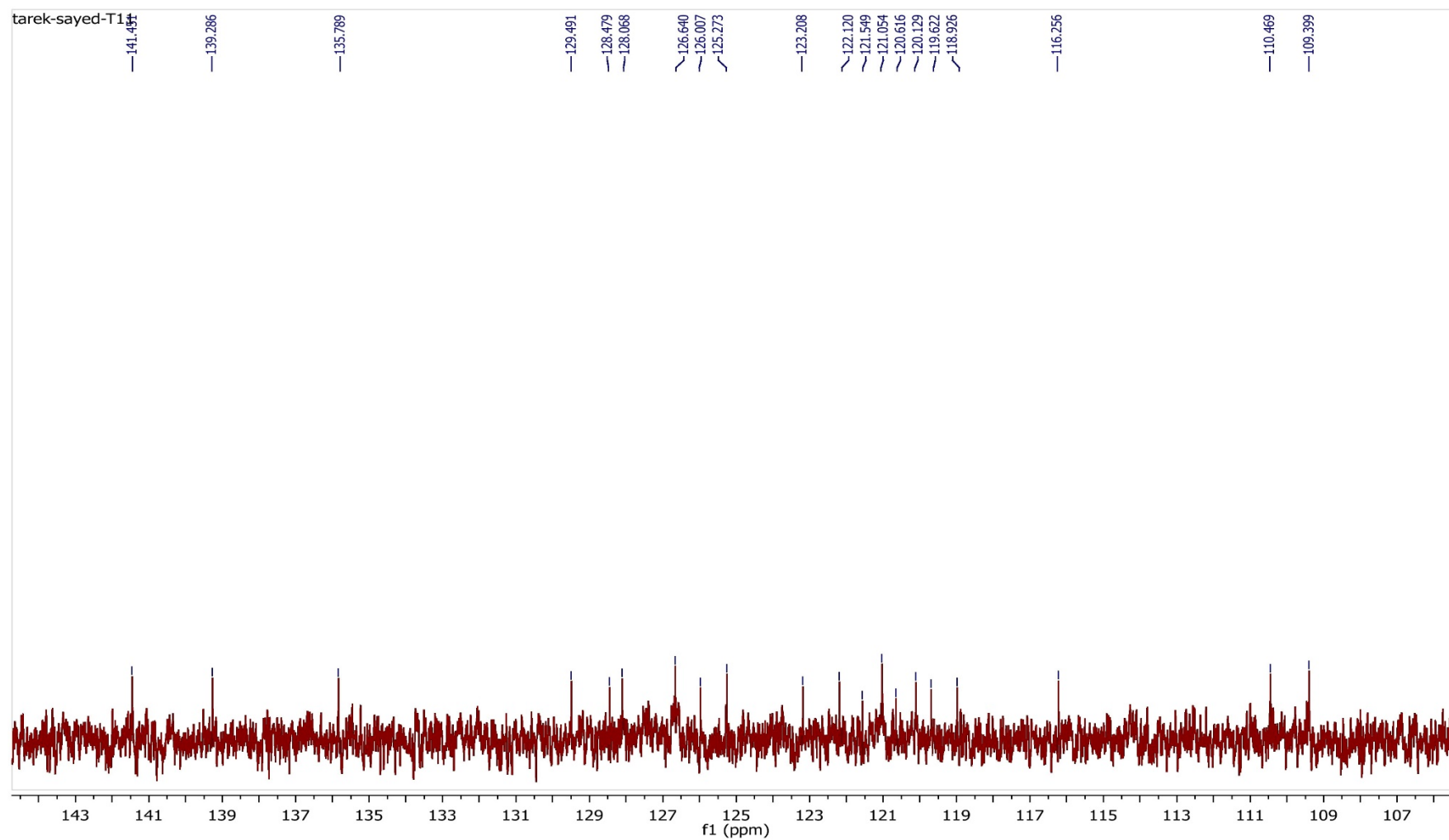


Figure S23: The enlargement of downfield region in ^{13}C -NMR spectrum of compound **4c**.

tarek-T11 #86-90 RT: 1.46-1.52 AV: 5 SB: 2 3.82, 3.53 NL: 3.01E2
T: (0,0) + e EI Full ms [40.00-1000.00]

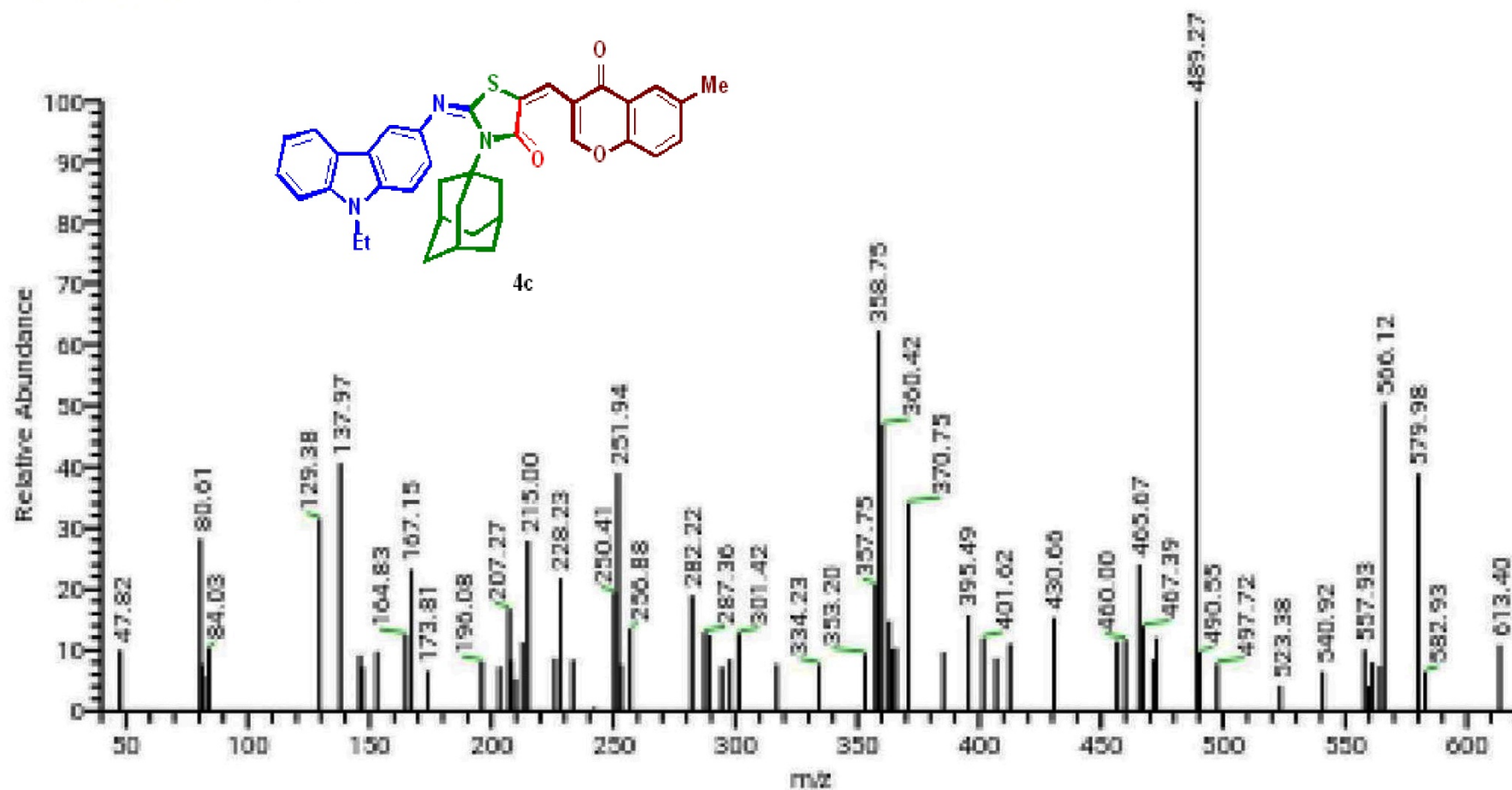


Figure S24: The mass spectrum of compound 4c.

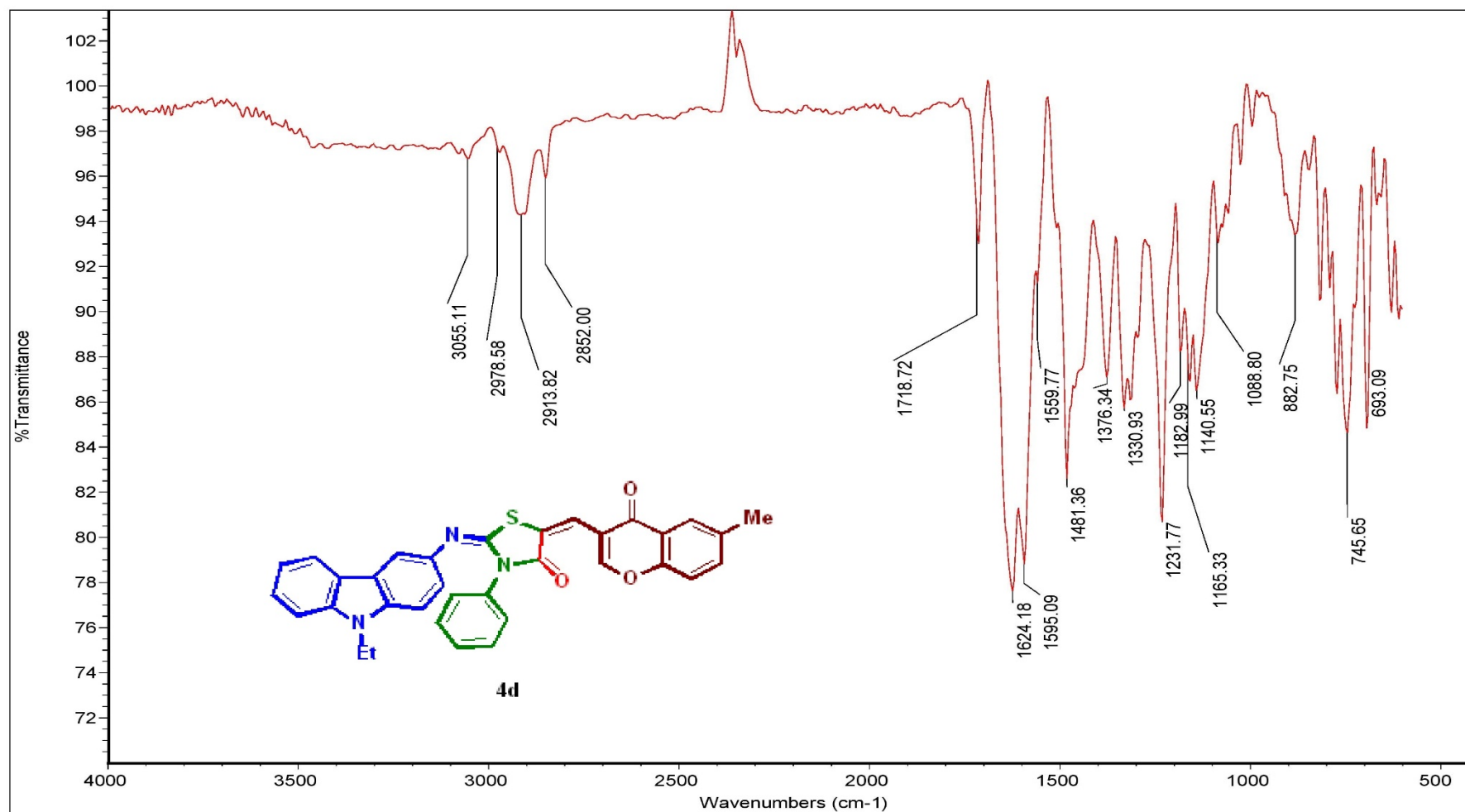


Figure S25: The IR spectrum of compound **4d**.

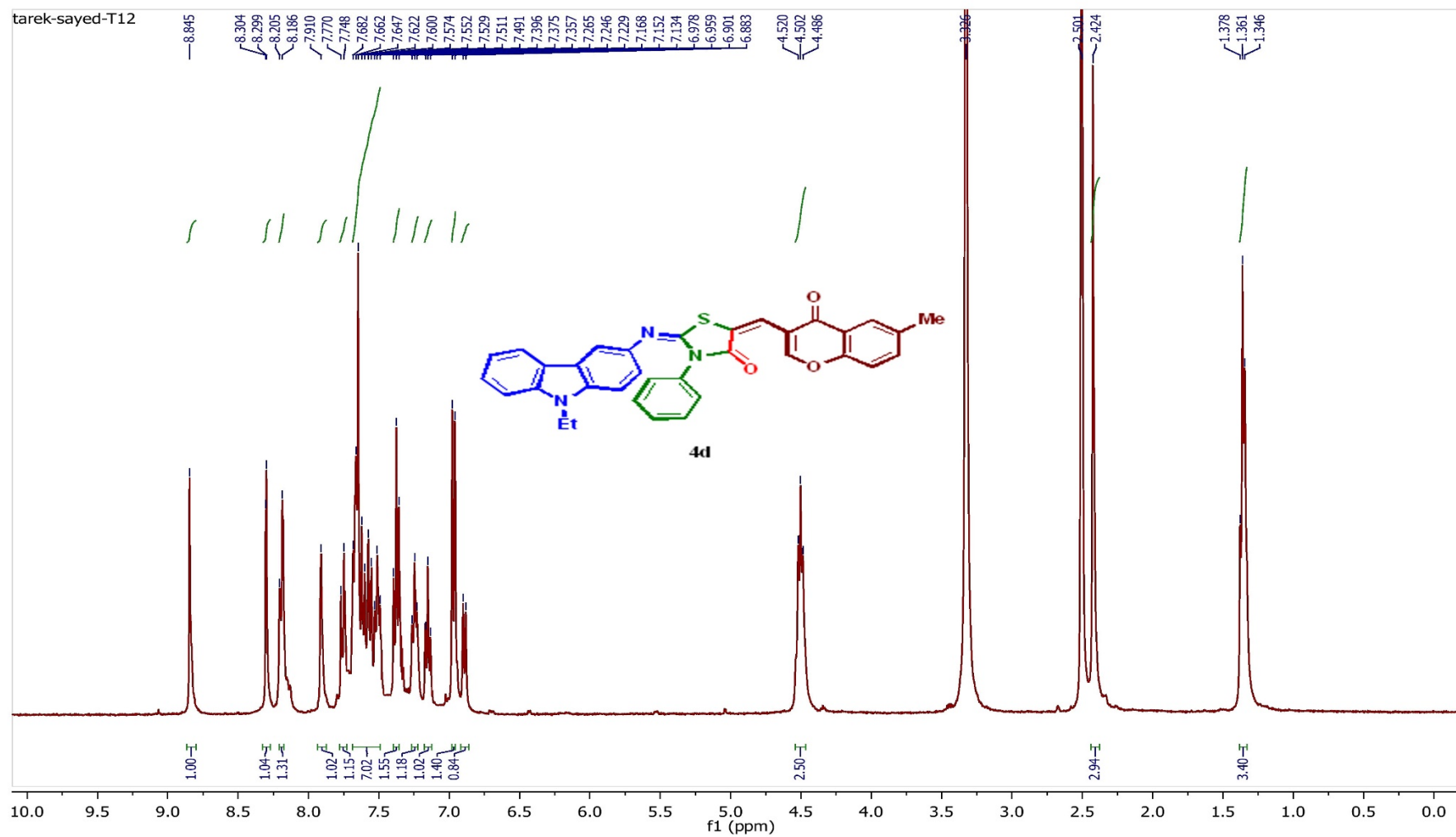


Figure S26: The ^1H -NMR spectrum of compound **4d**.

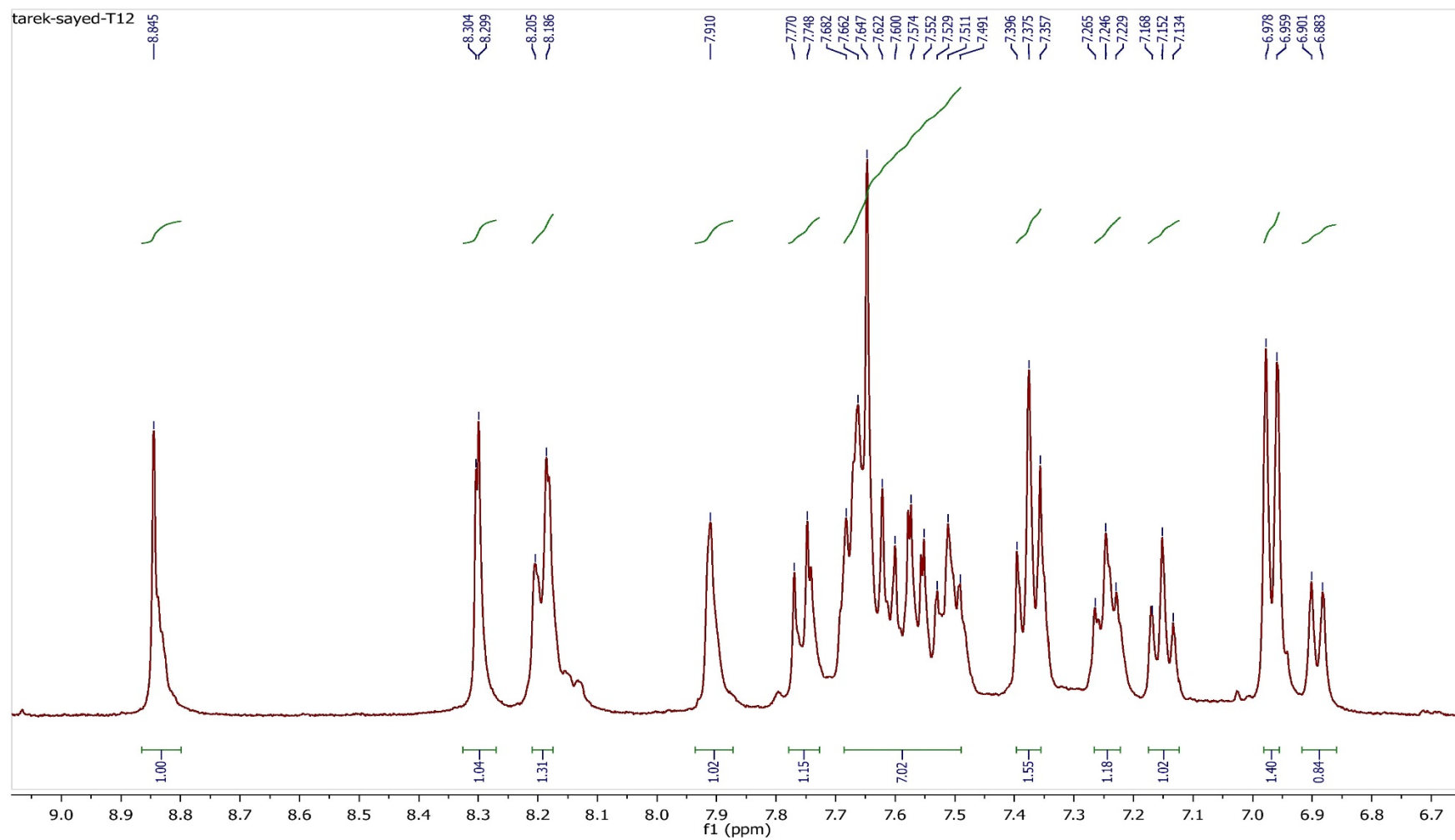


Figure S27: The enlargement of downfield region in ^1H -NMR spectrum of compound **4d**.

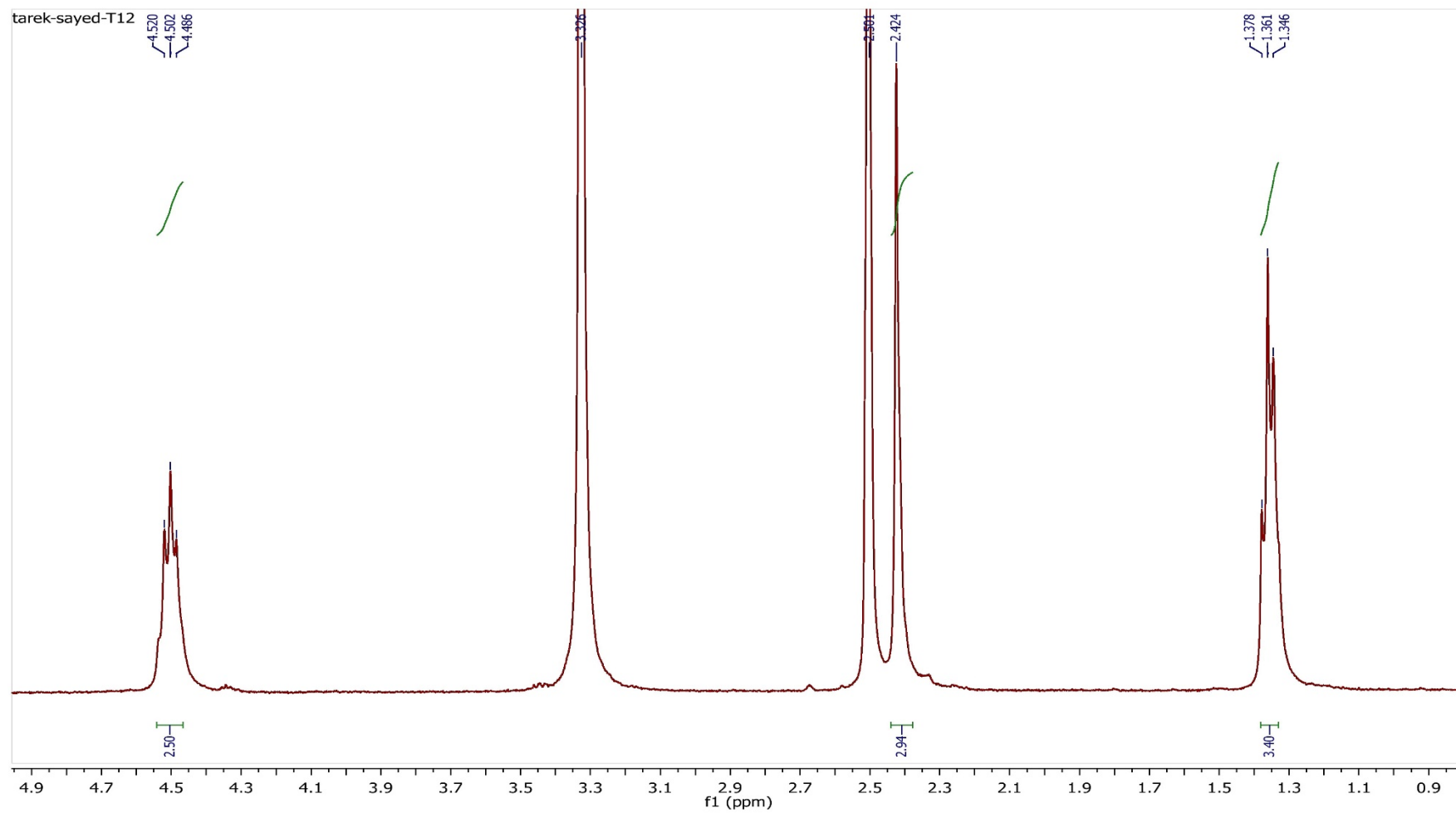


Figure S28: The enlargement of upfield region in ^1H -NMR spectrum of compound **4d**.

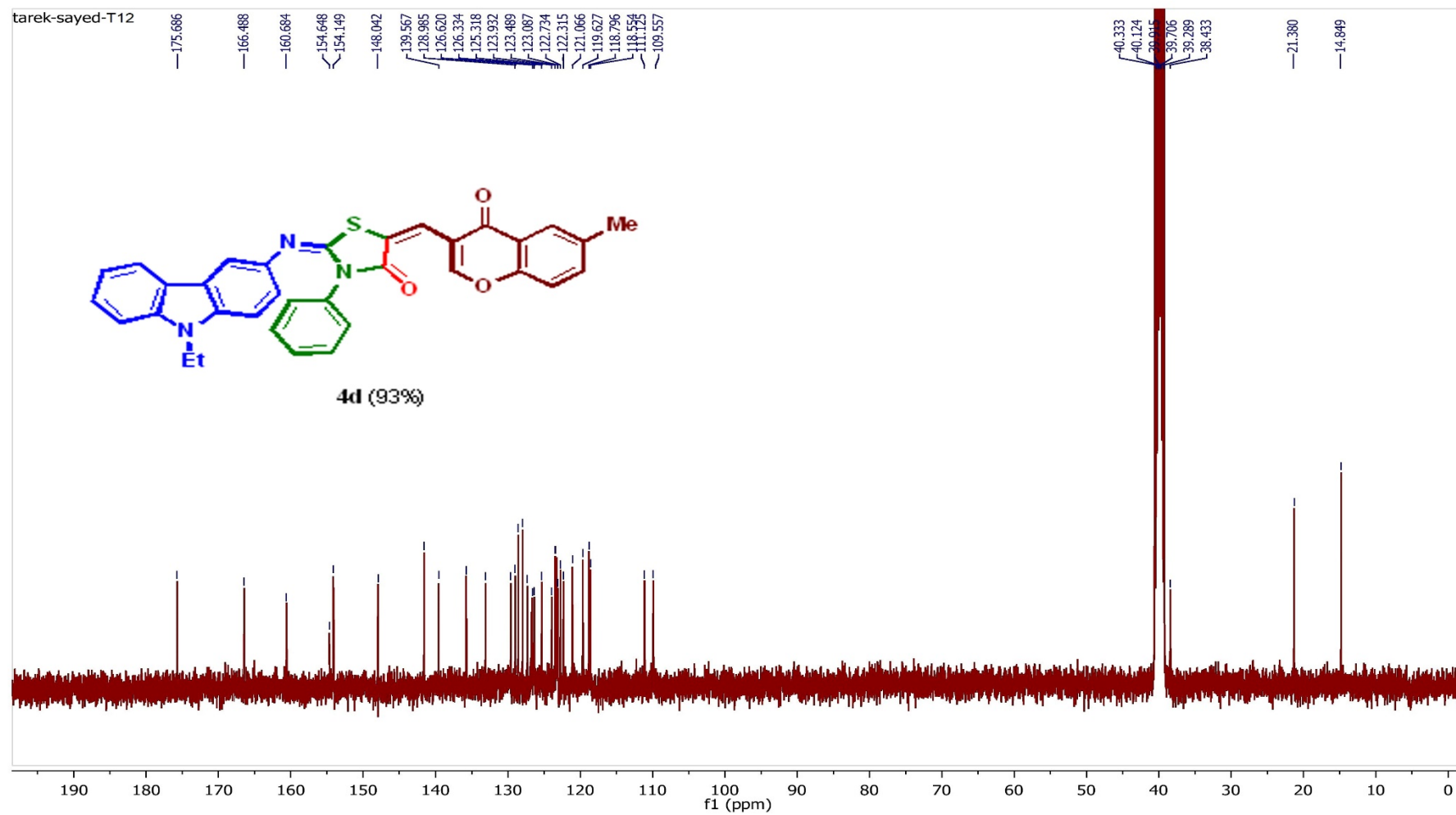


Figure S29: The ^{13}C -NMR spectrum of compound **4d**.

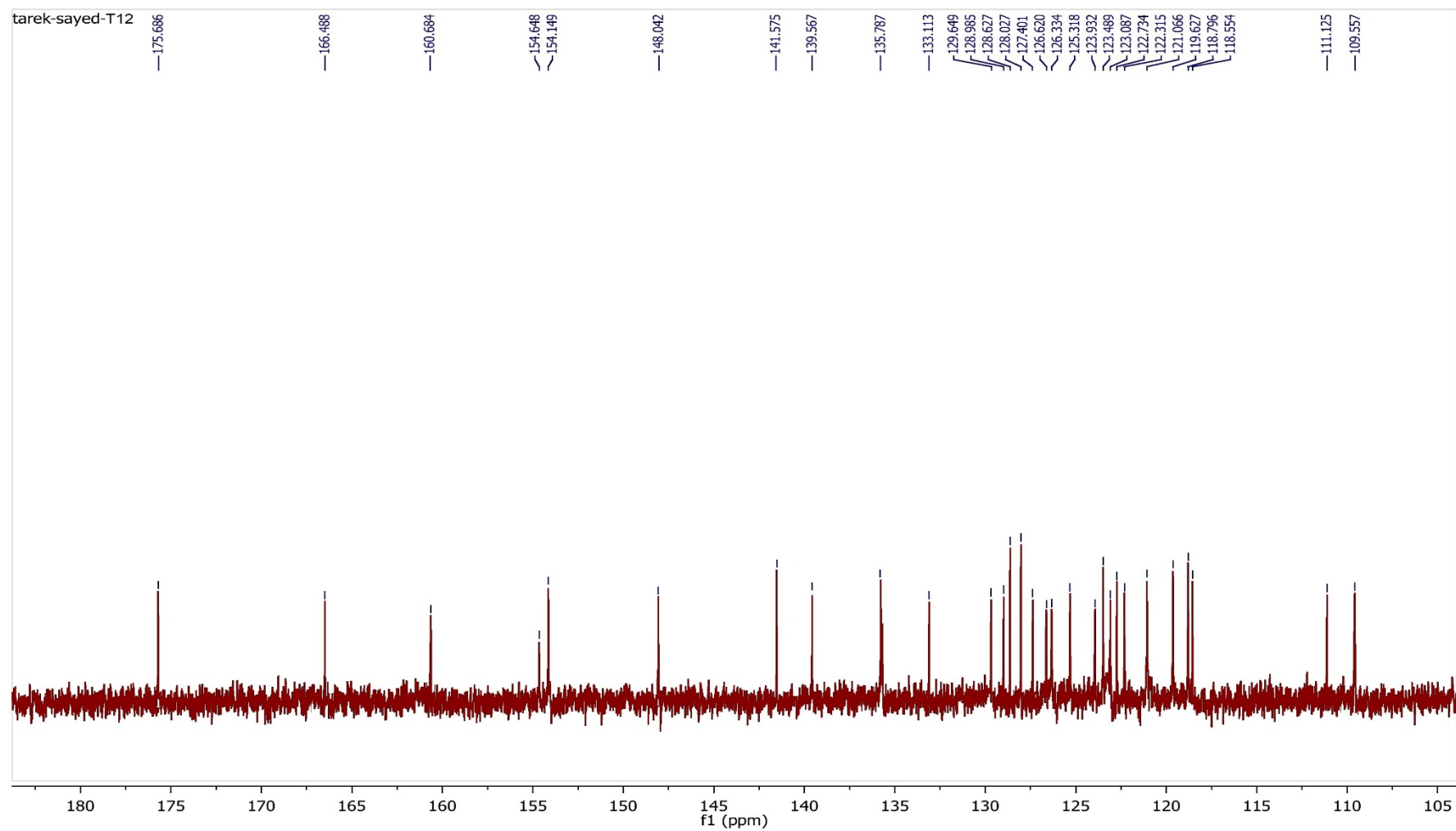


Figure S30: The enlargement of downfield region in ^{13}C -NMR spectrum of compound **4d**.

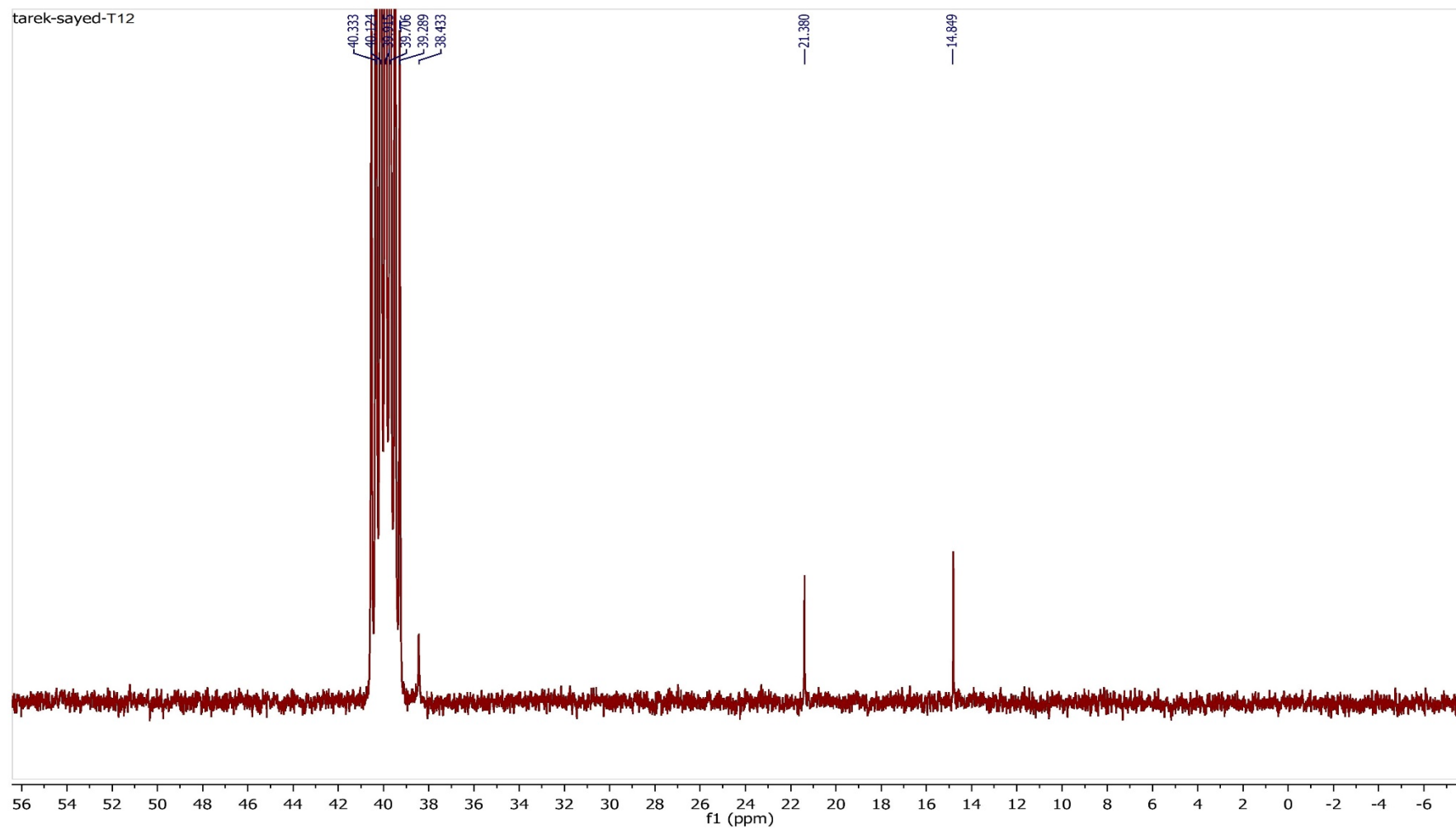


Figure S31: The enlargement of upfield region in ^{13}C -NMR spectrum of compound **4d**.

tarek-T12 #29 RT: 0.50 AV: 1 SB: 2 0.97, 1.05 NL: 0.02E2
T: {0,0} + e EI Full ms [40.00-1000.00]

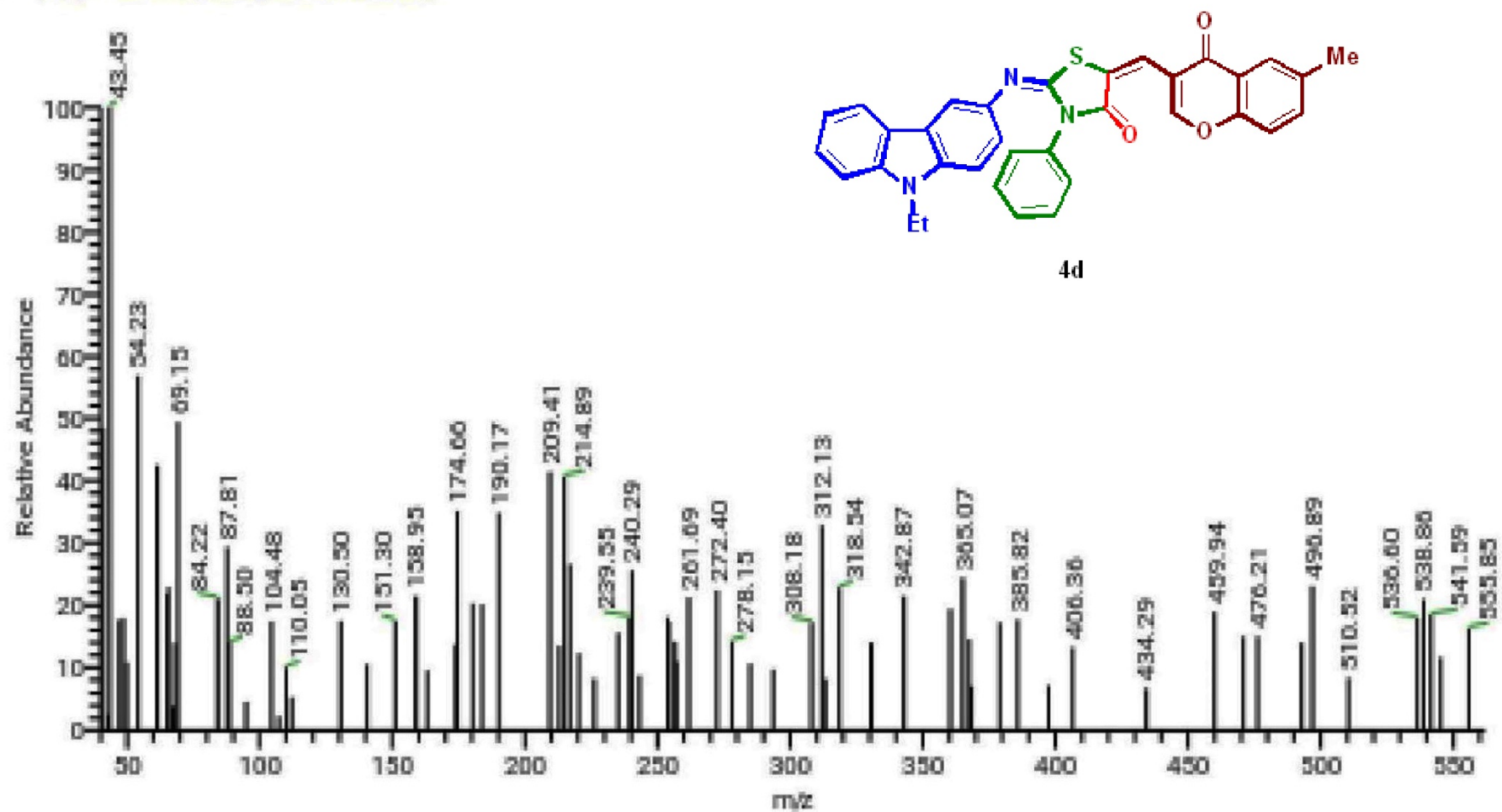


Figure S32: The mass spectrum of compound 4d.

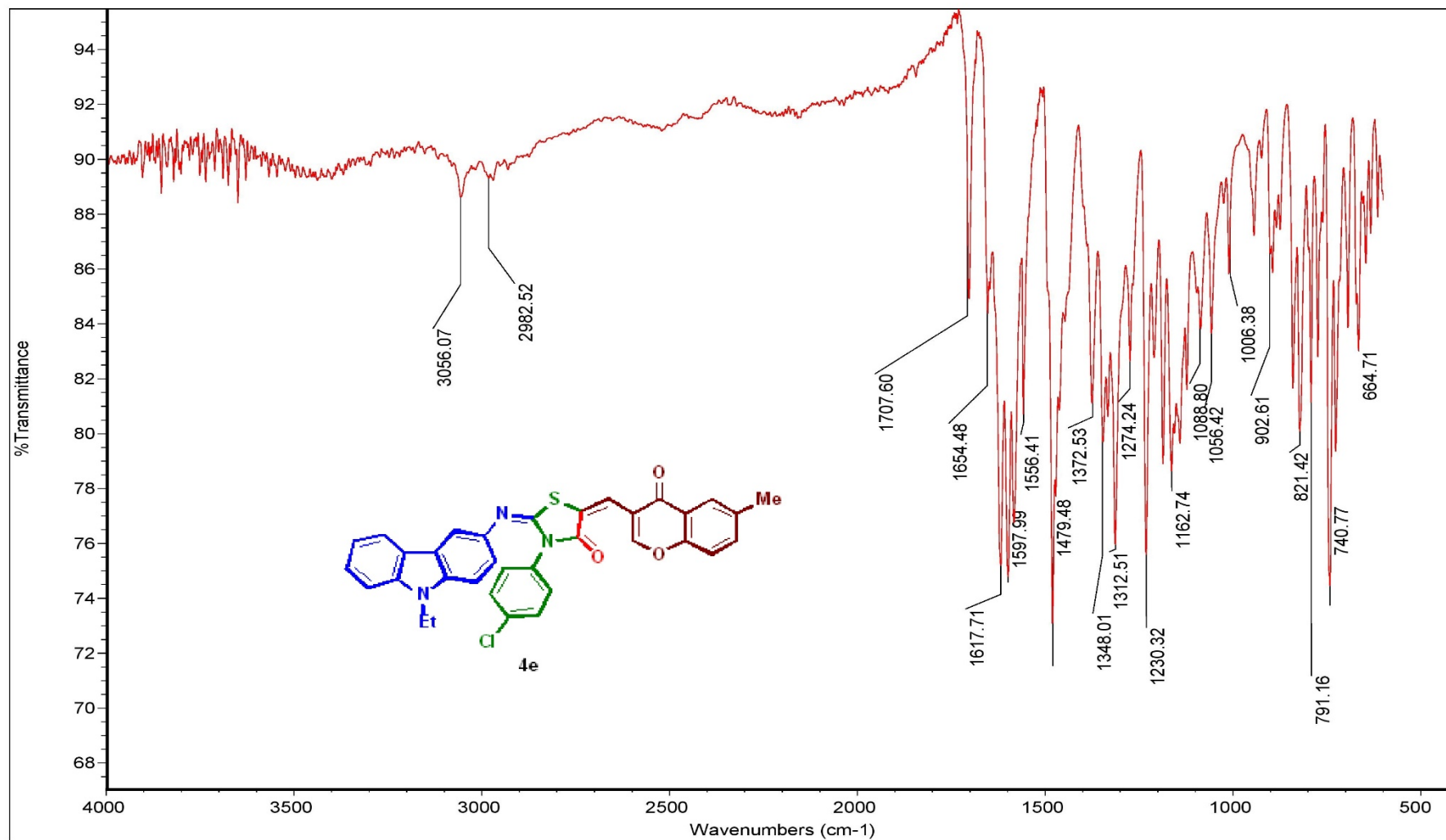


Figure S33: The IR spectrum of compound **4e**.

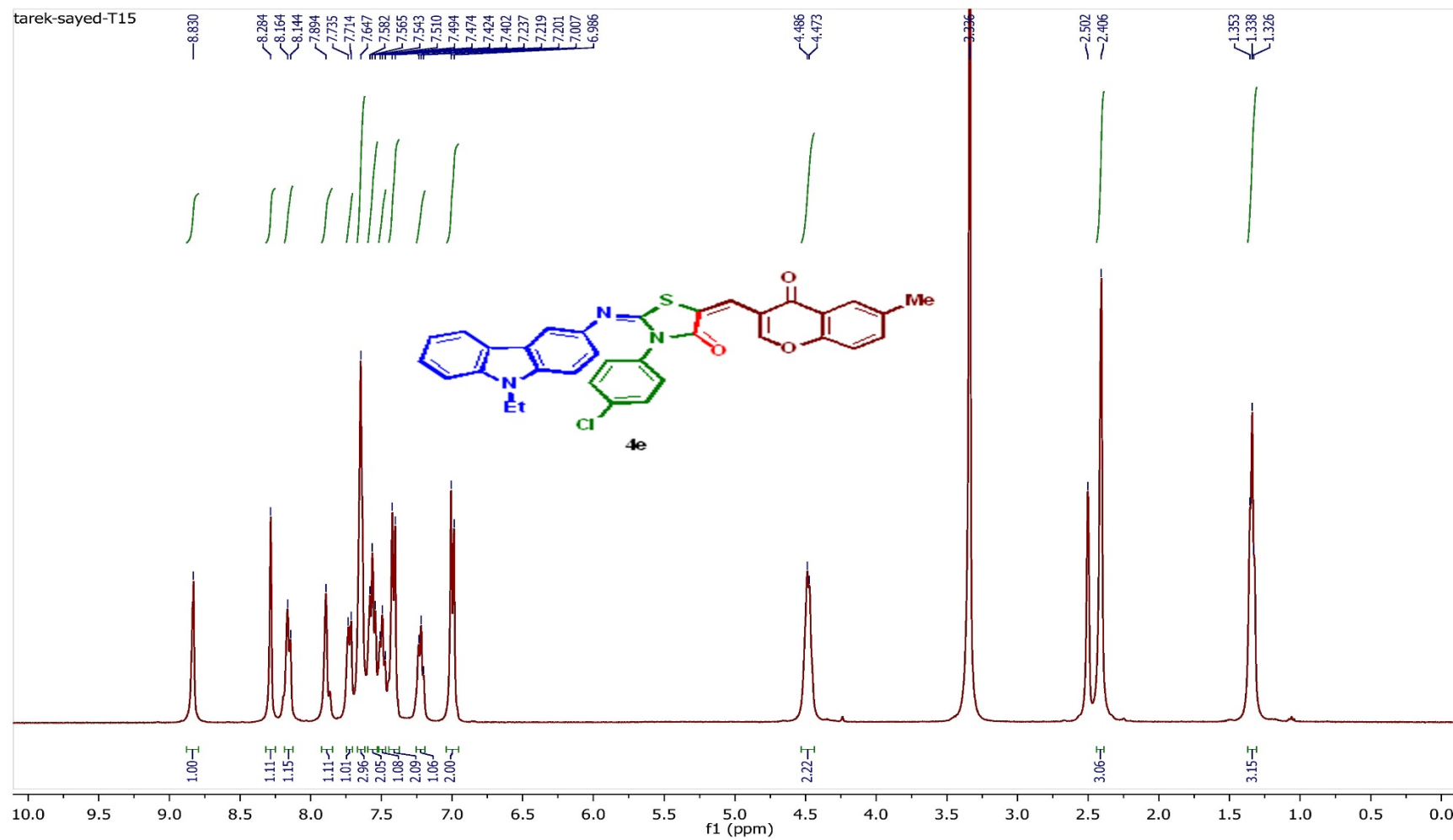


Figure S34: The ^1H -NMR spectrum of compound **4e**.

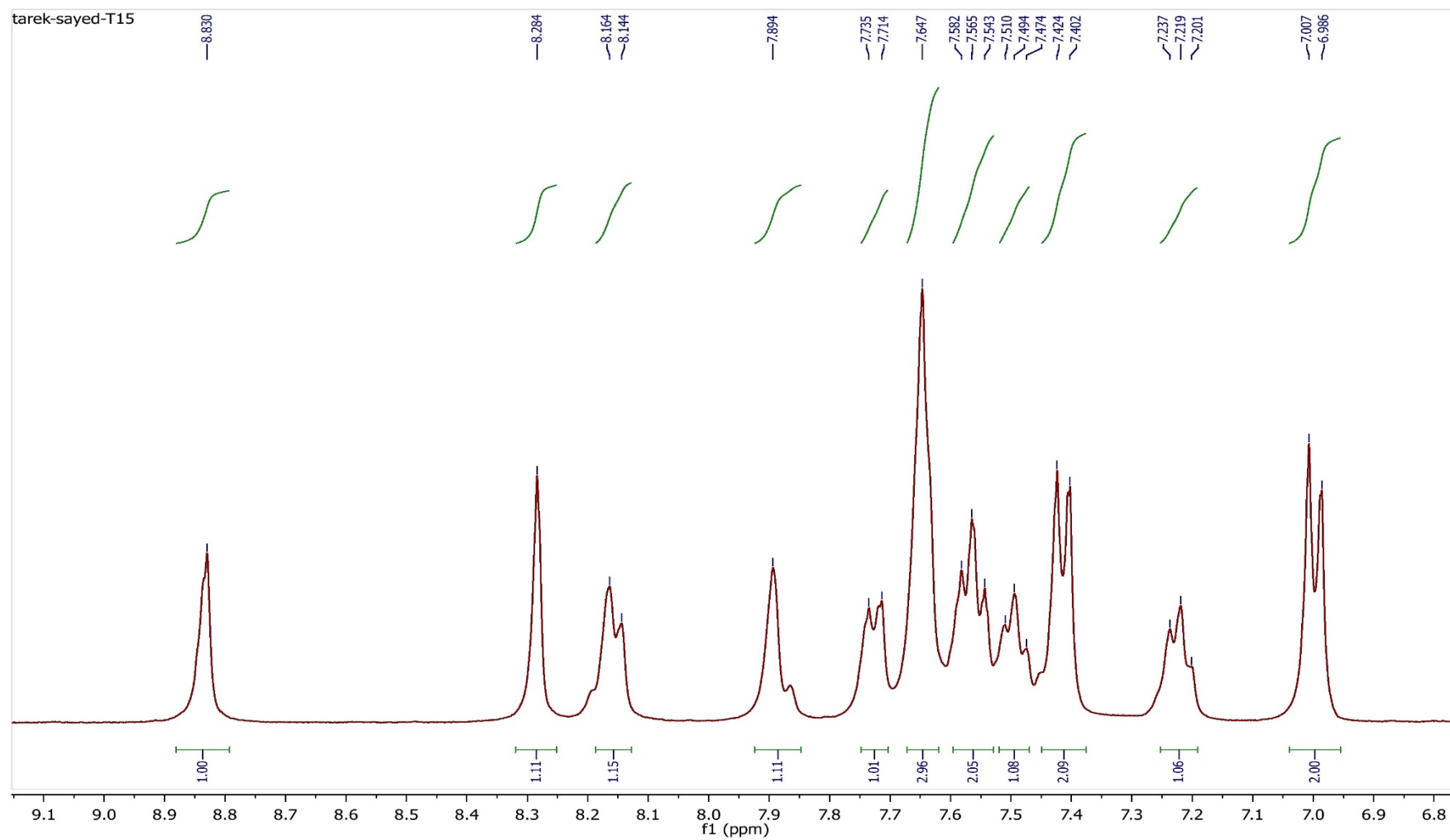


Figure S35: The enlargement of downfield region in ^1H -NMR spectrum of compound **4e**.

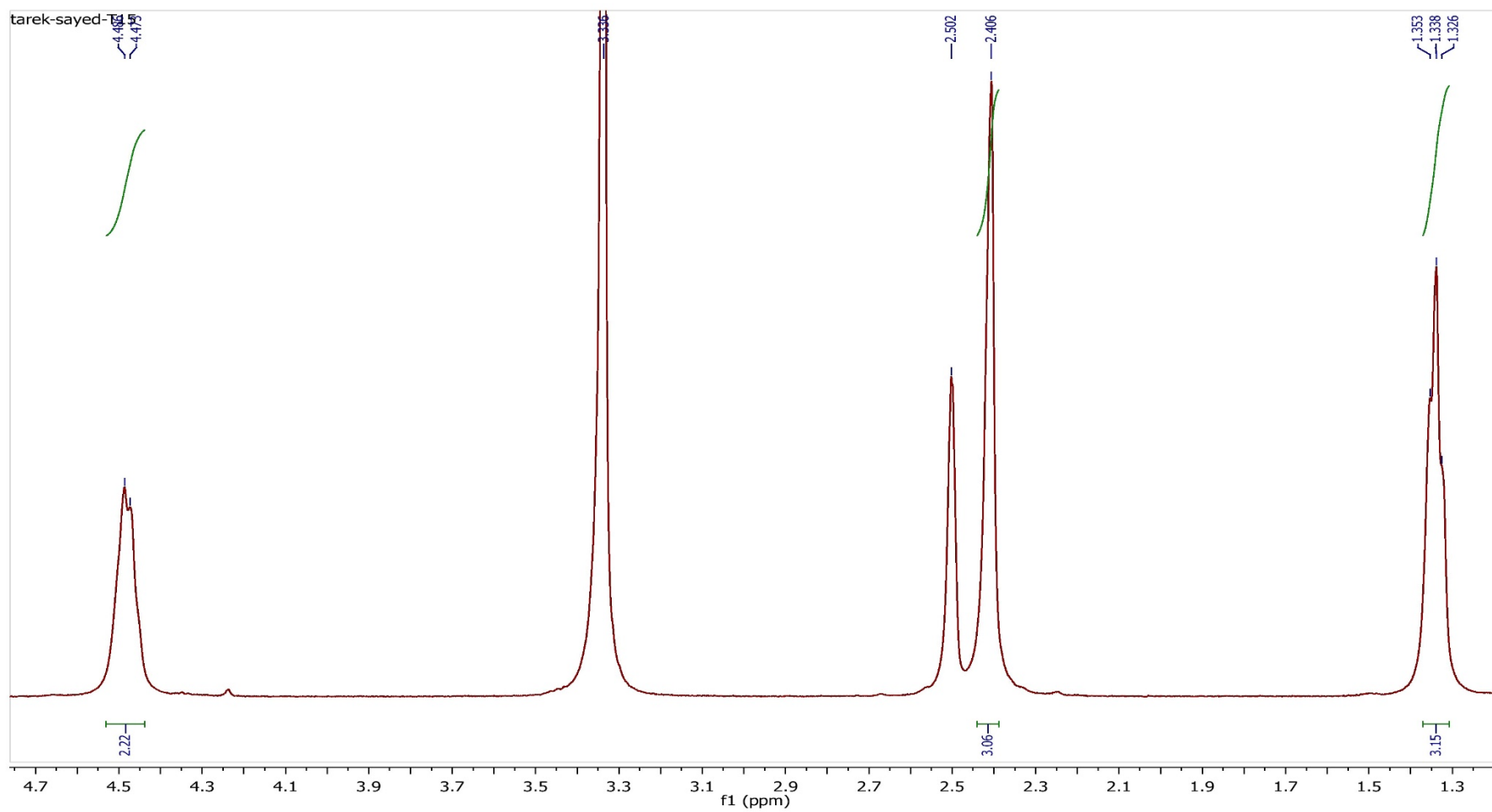


Figure S36: The enlargement of upfield region in ^1H -NMR spectrum of compound 4e.

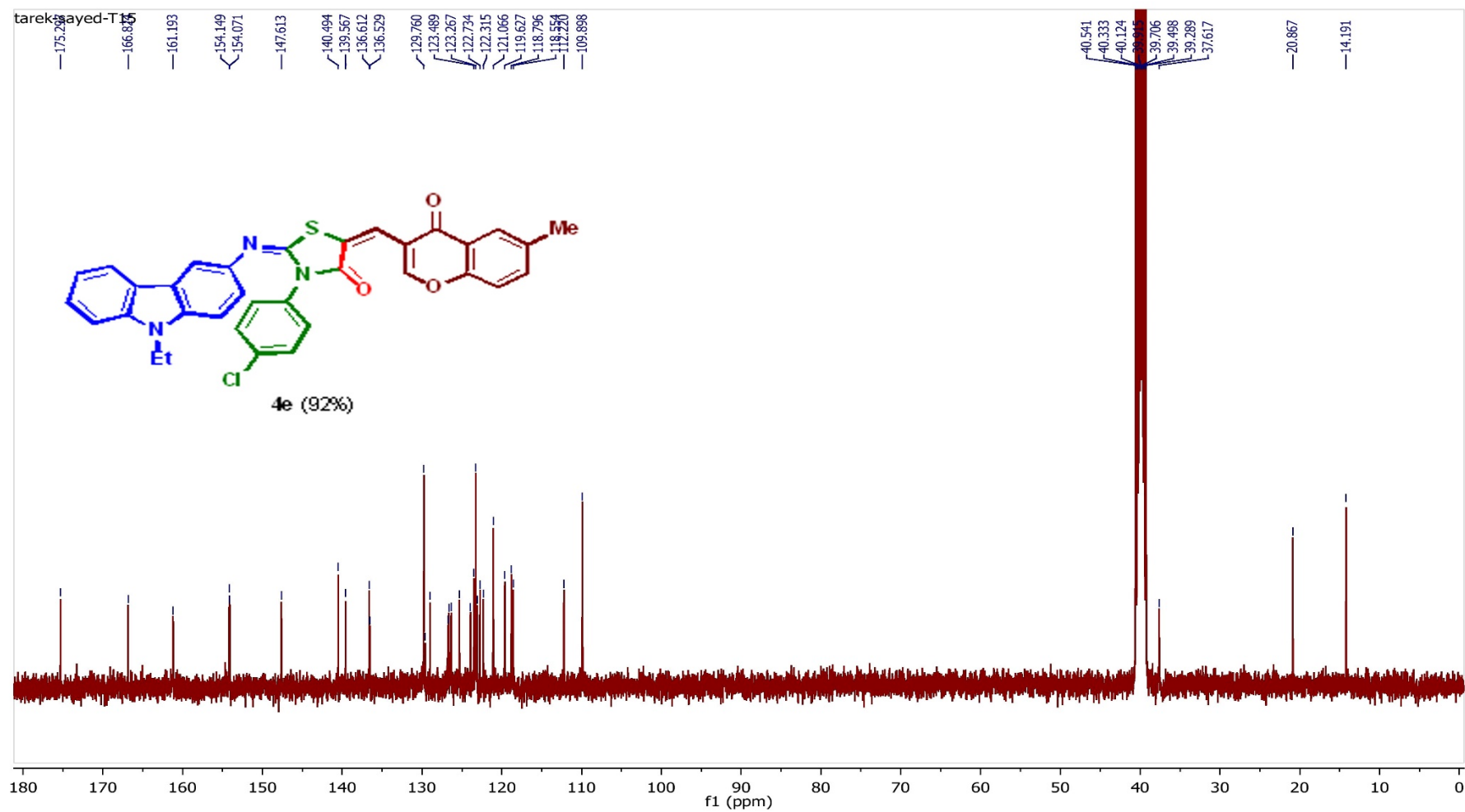


Figure S37: The ^{13}C -NMR spectrum of compound **4e**.

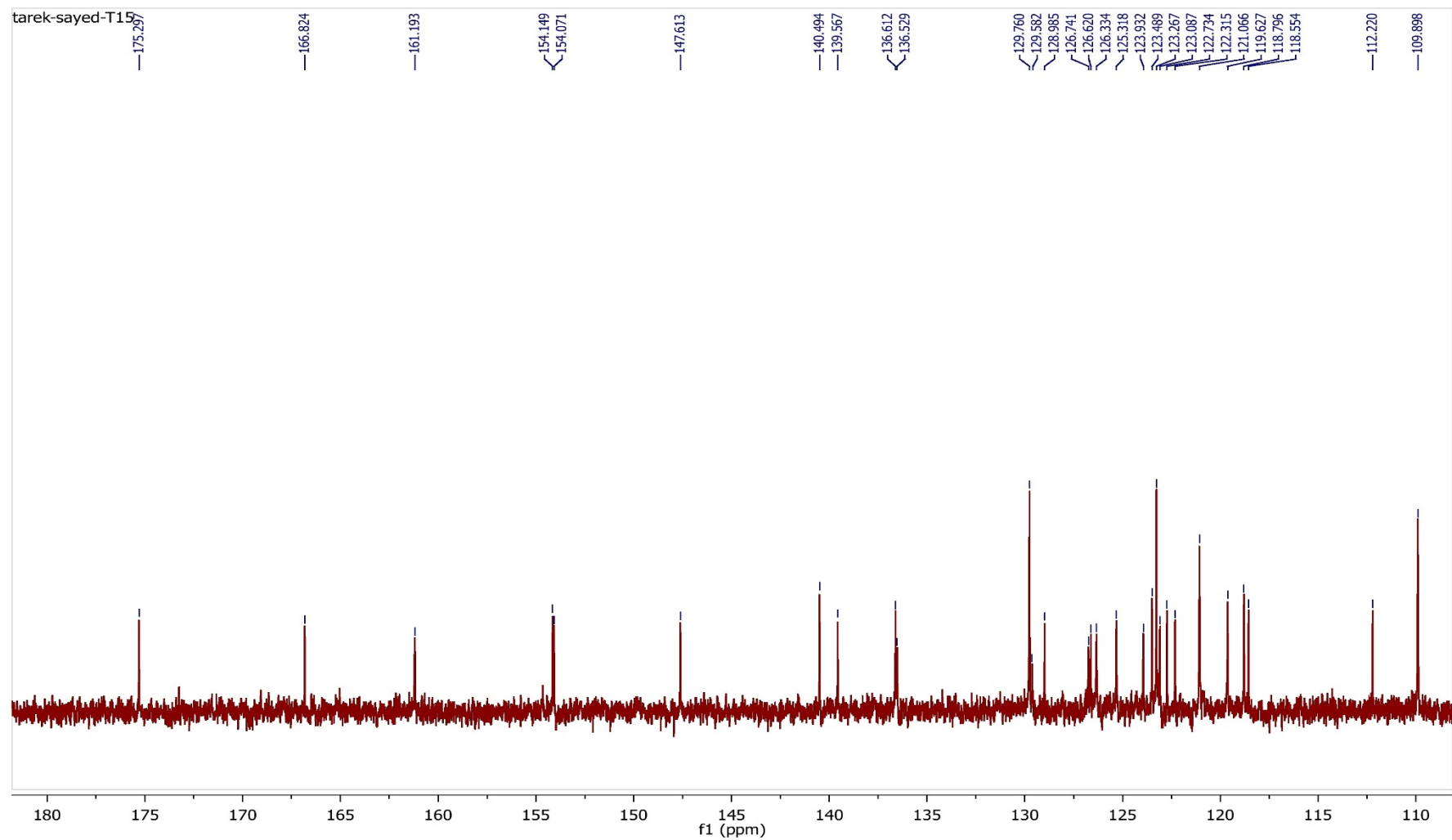


Figure S38: The enlargement of downfield region in ^{13}C -NMR spectrum of compound **4e**.

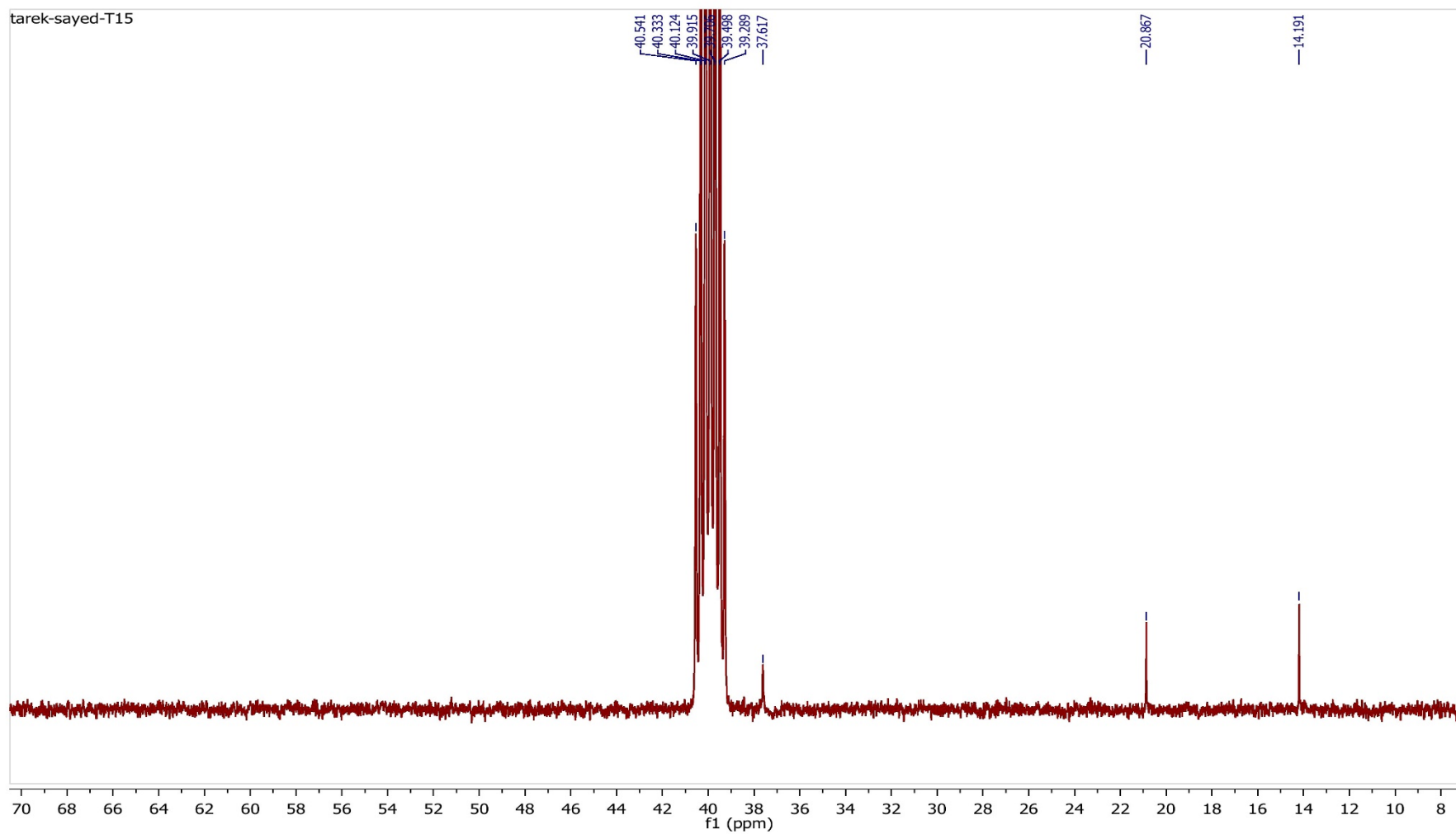


Figure S39: The enlargement of upfield region in ^{13}C -NMR spectrum of compound **4e**.

tarek-T15 #277 RT: 4.65 AV: 1 SB: 2 3.82, 3.53 NL: 4.34E2
T: (0,0) + e EI Full ms [40.00-1000.00]

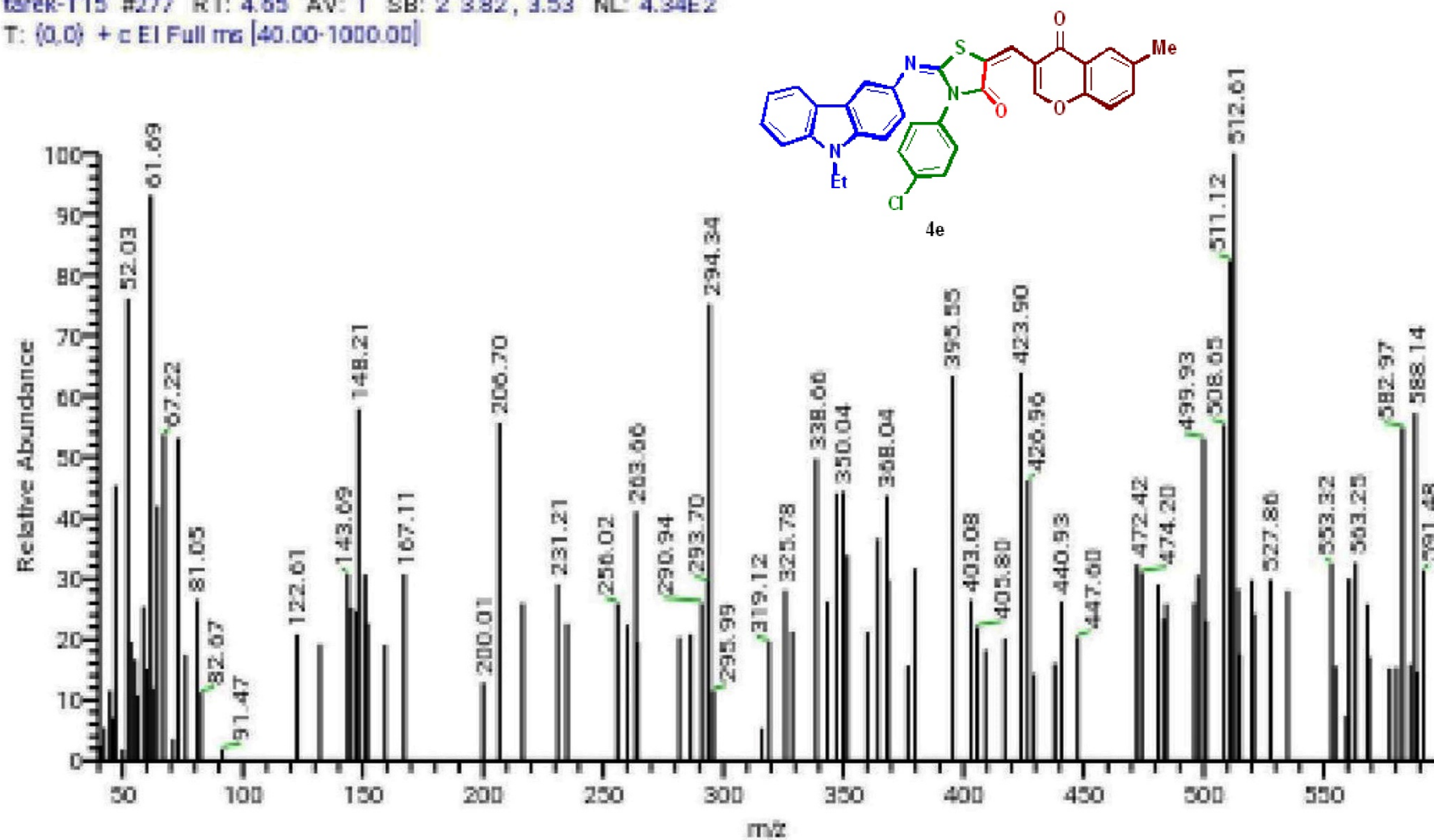


Figure S40: The mass spectrum of compound 4e.

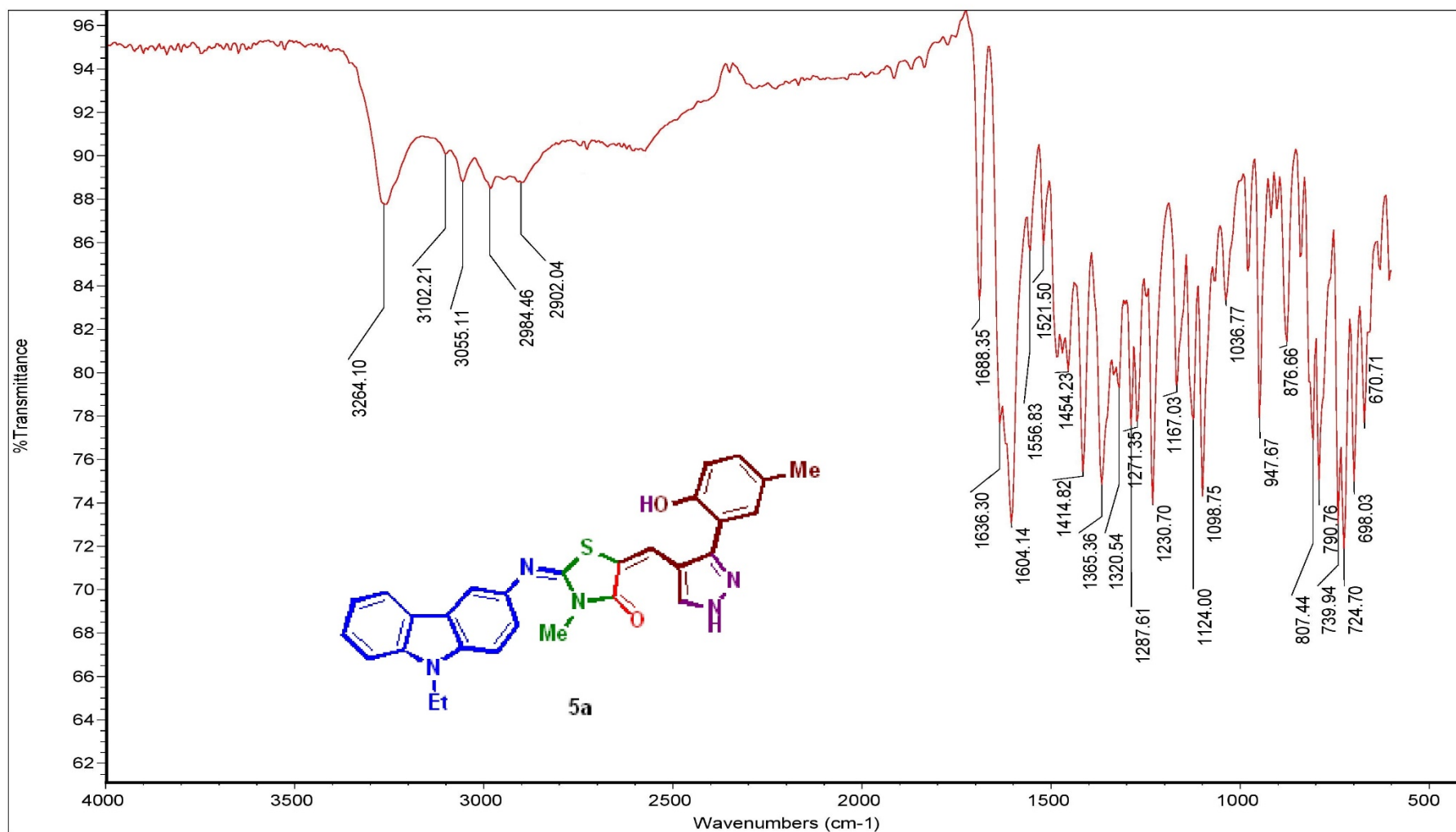


Figure S41: The IR spectrum of compound **5a**.

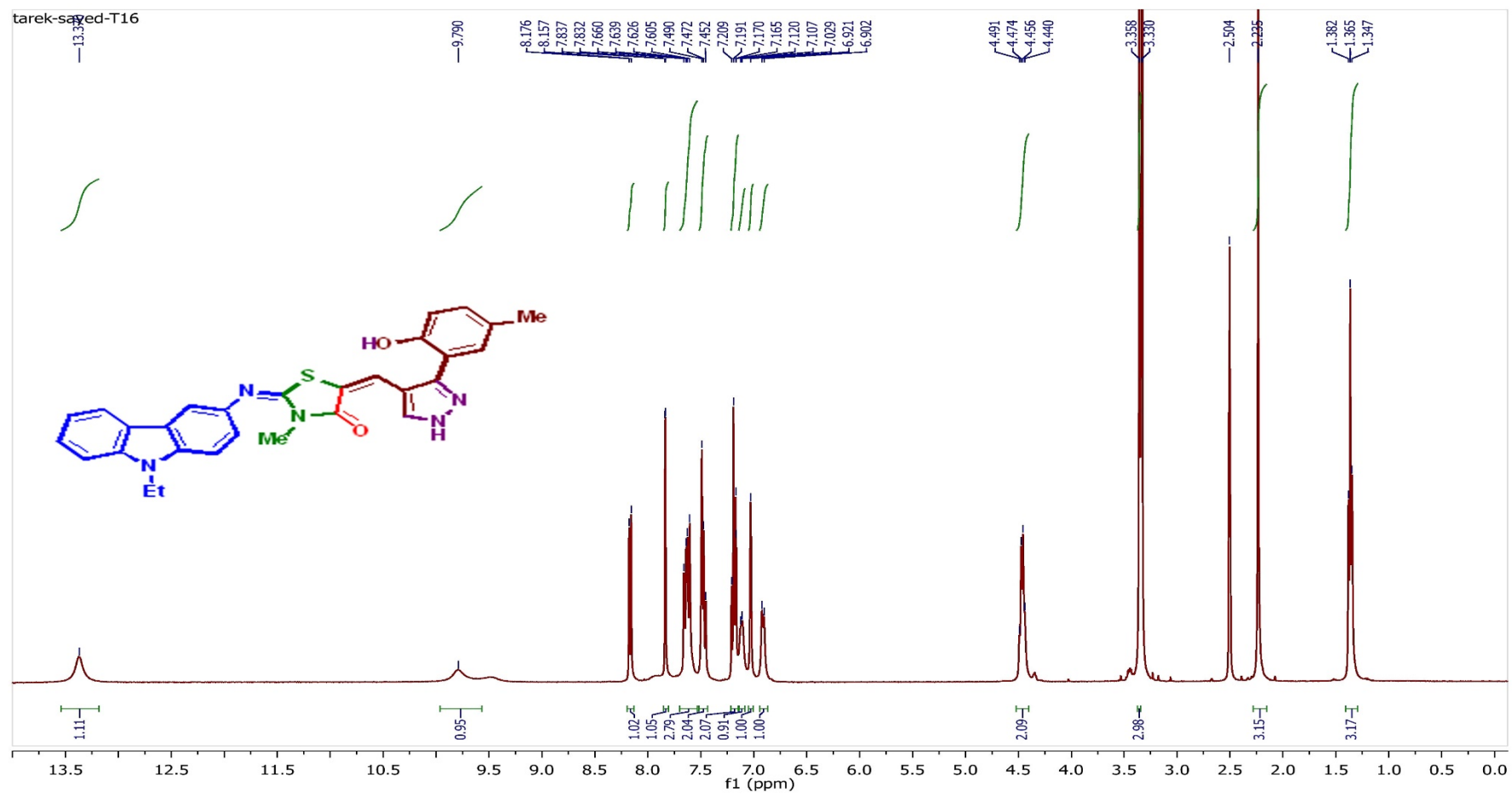


Figure S42: The ^1H -NMR spectrum of compound **5a**.

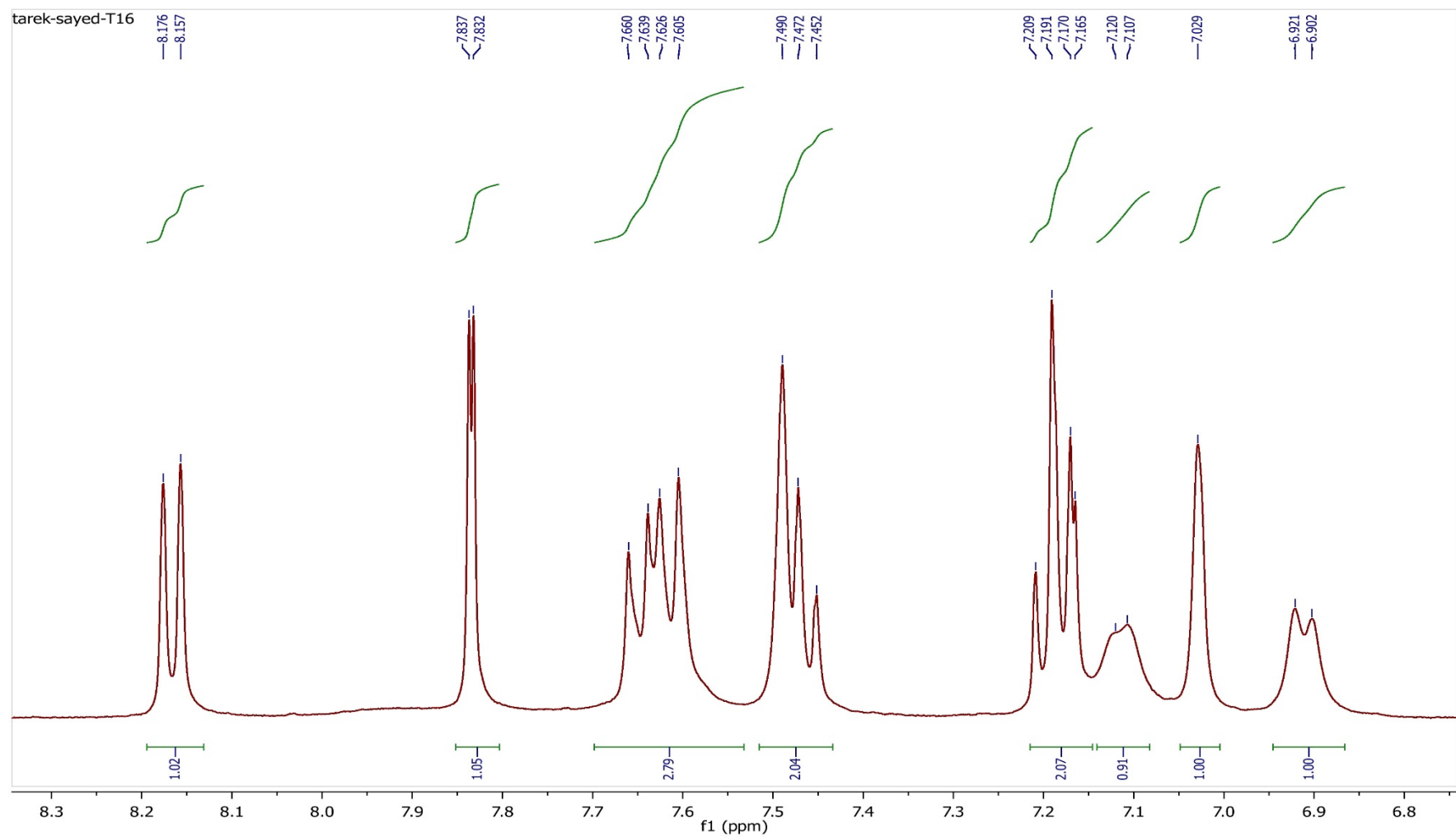


Figure S43: The enlargement of downfield region in ¹H-NMR spectrum of compound **5a**.

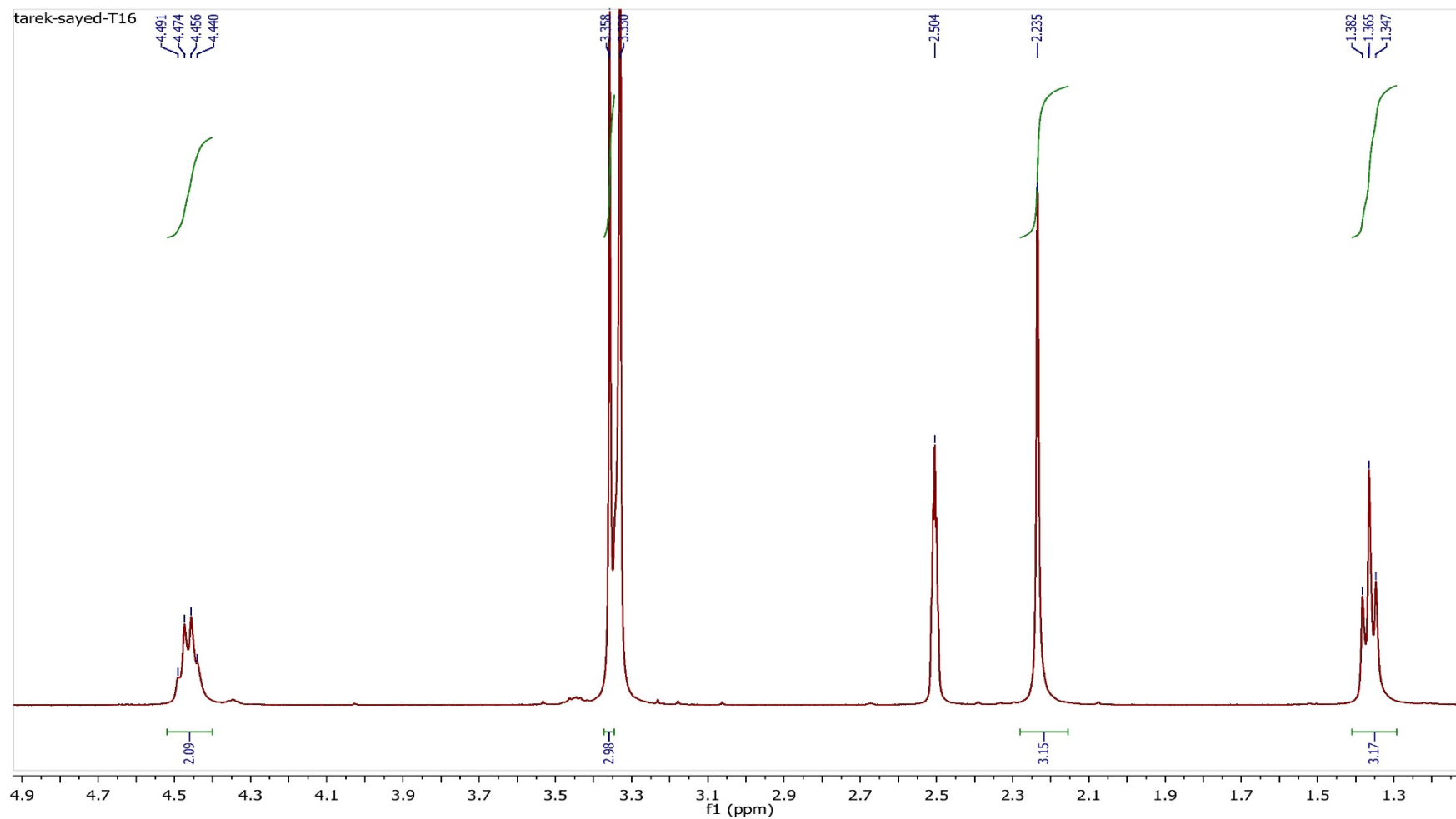


Figure S44: The enlargement of upfield region in ^1H -NMR spectrum of compound **5a**.

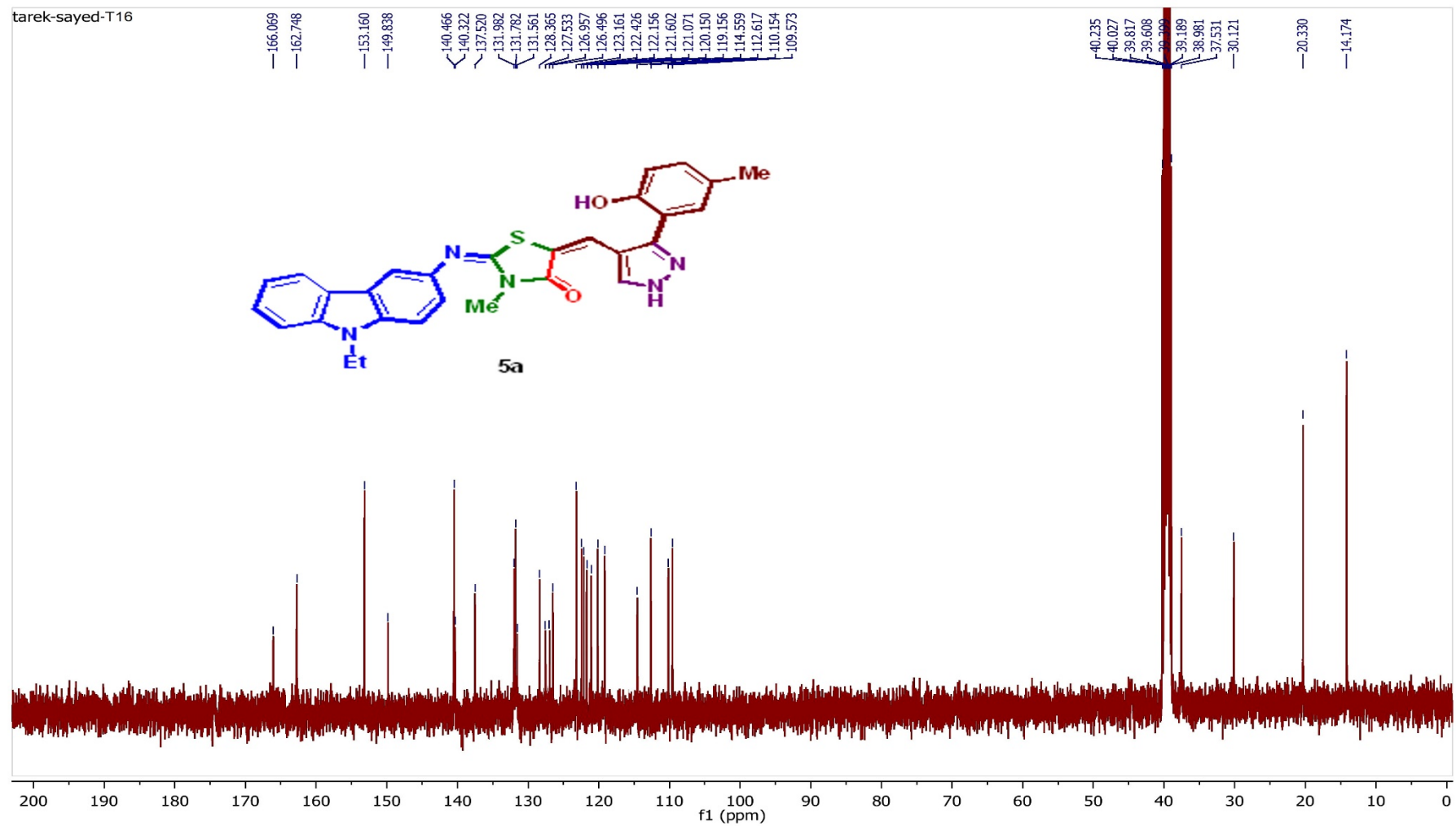


Figure S45: The ^{13}C -NMR spectrum of compound **5a**.

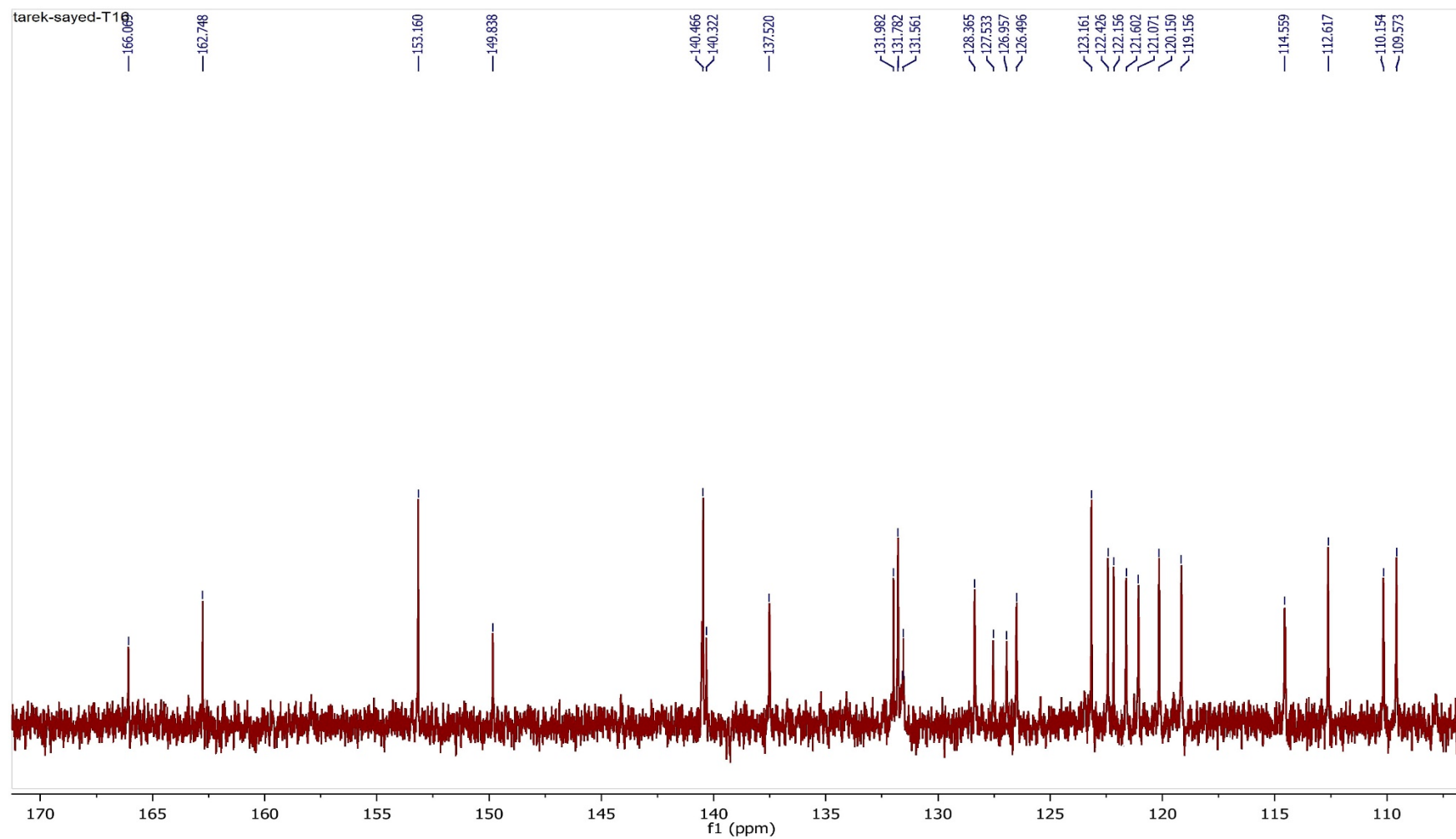


Figure S46: The enlargement of downfield region in ^{13}C -NMR spectrum of compound **5a**.

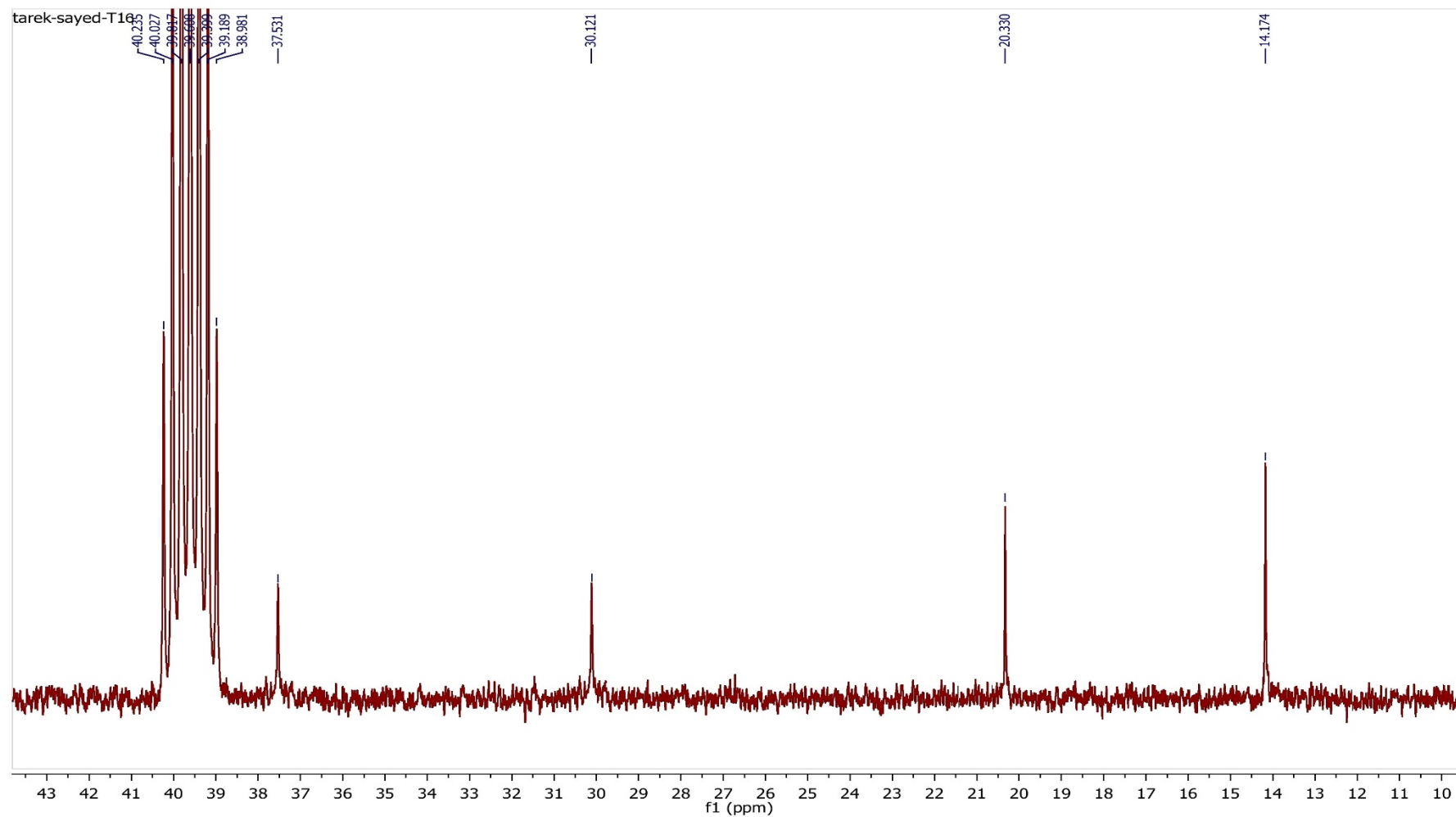


Figure S47: The enlargement of upfield region in ^{13}C -NMR spectrum of compound **5a**.

Chemical structure of compound **5a** is shown. It consists of a 2-ethyl-1H-indole-3-yl group connected to a 4-methyl-5-(2-hydroxy-4-methylphenyl)-1,3,4-thiazolidine-2-thione moiety.

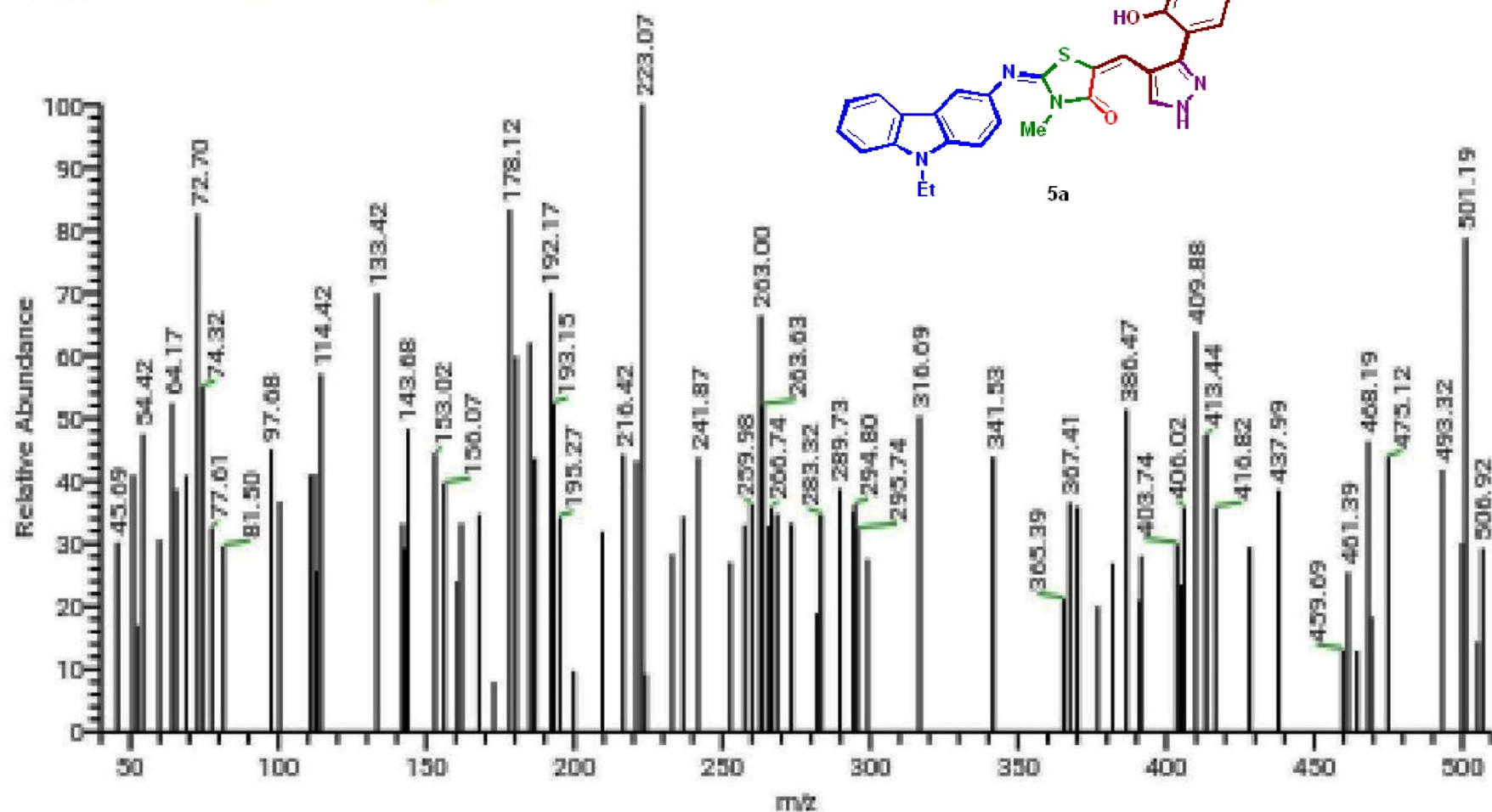


Figure S48: The mass spectrum of compound **5a**.

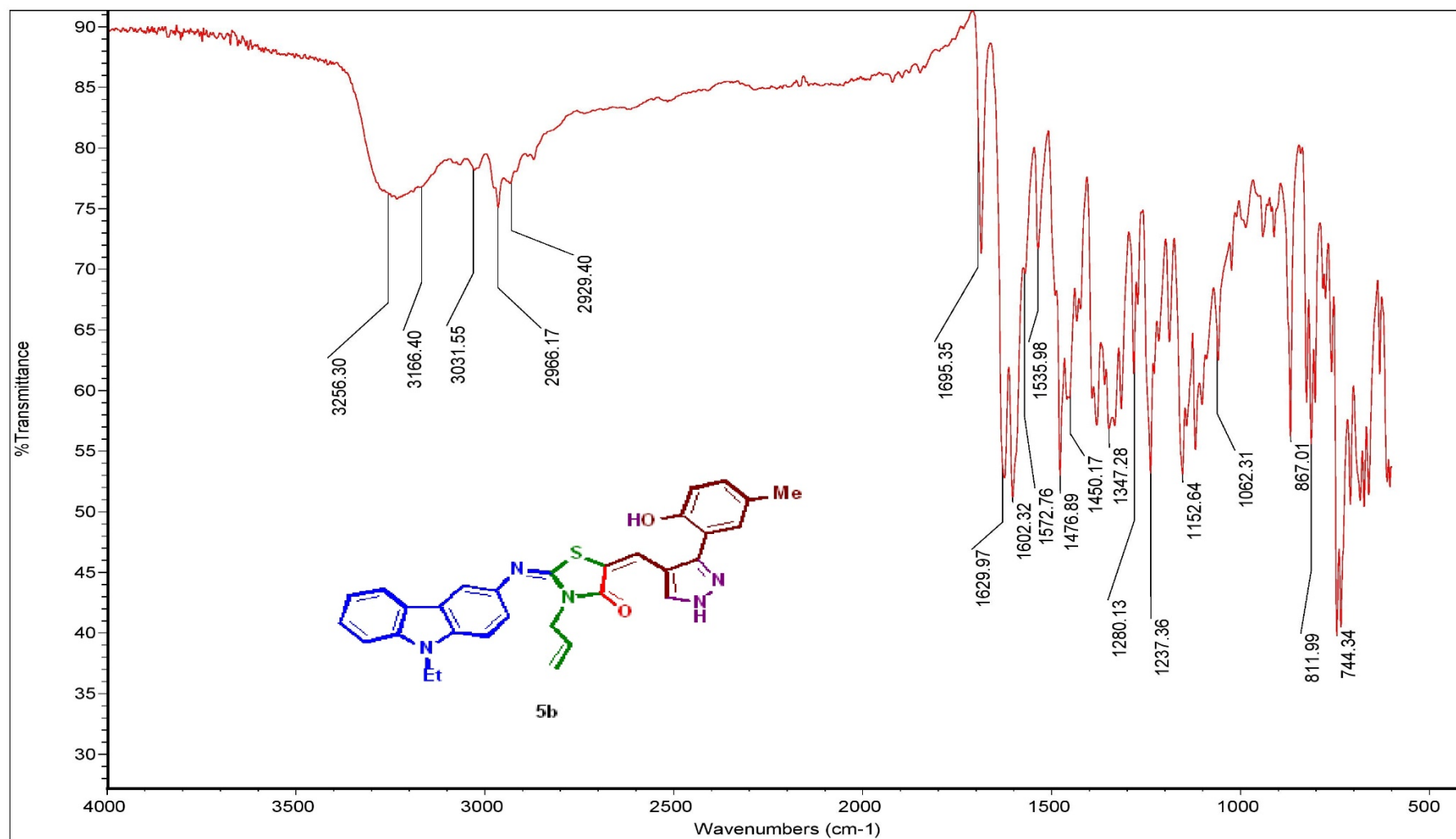


Figure S49: The IR spectrum of compound **5b**.

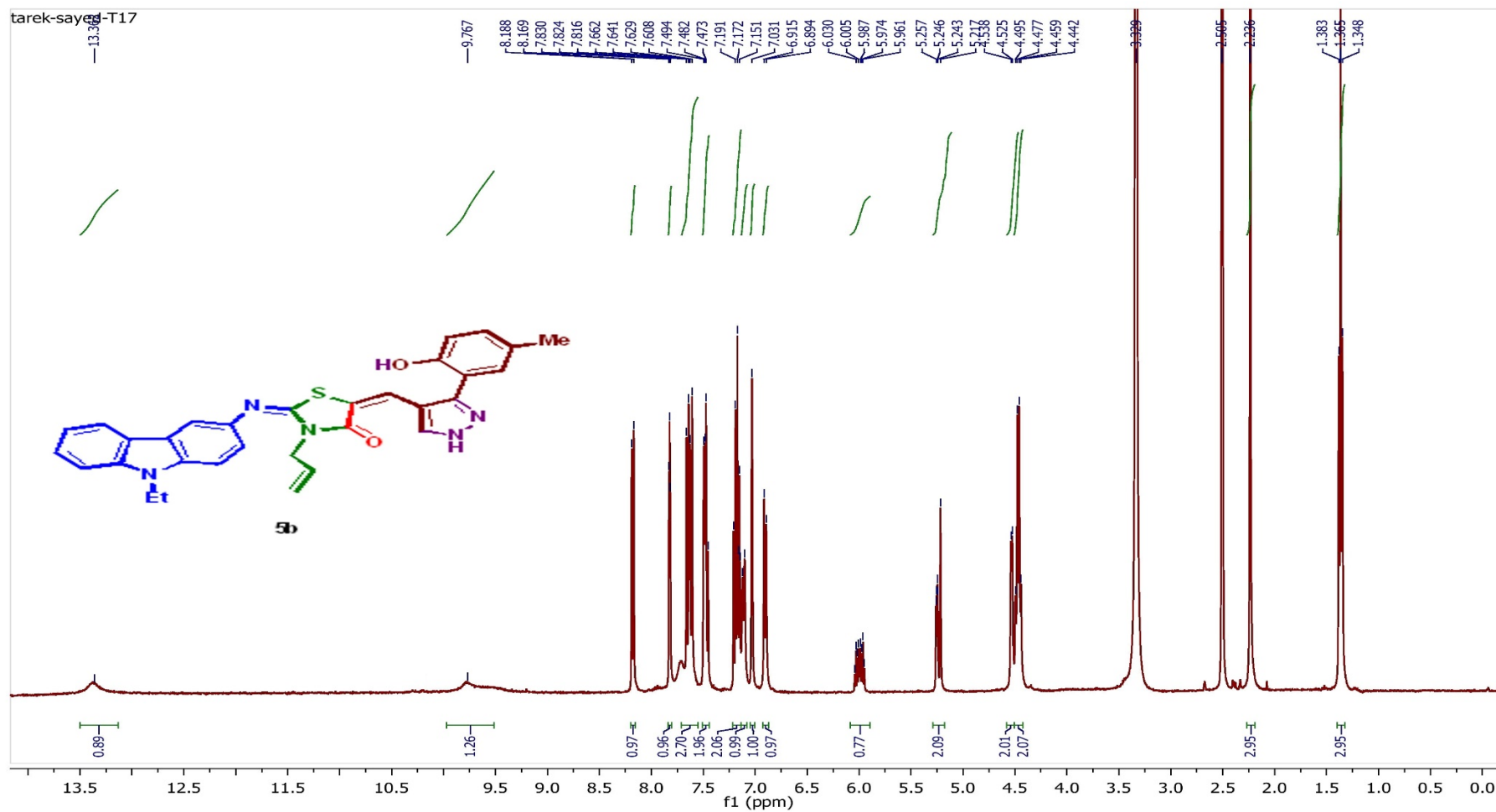


Figure S50: The ^1H -NMR spectrum of compound **5b**.

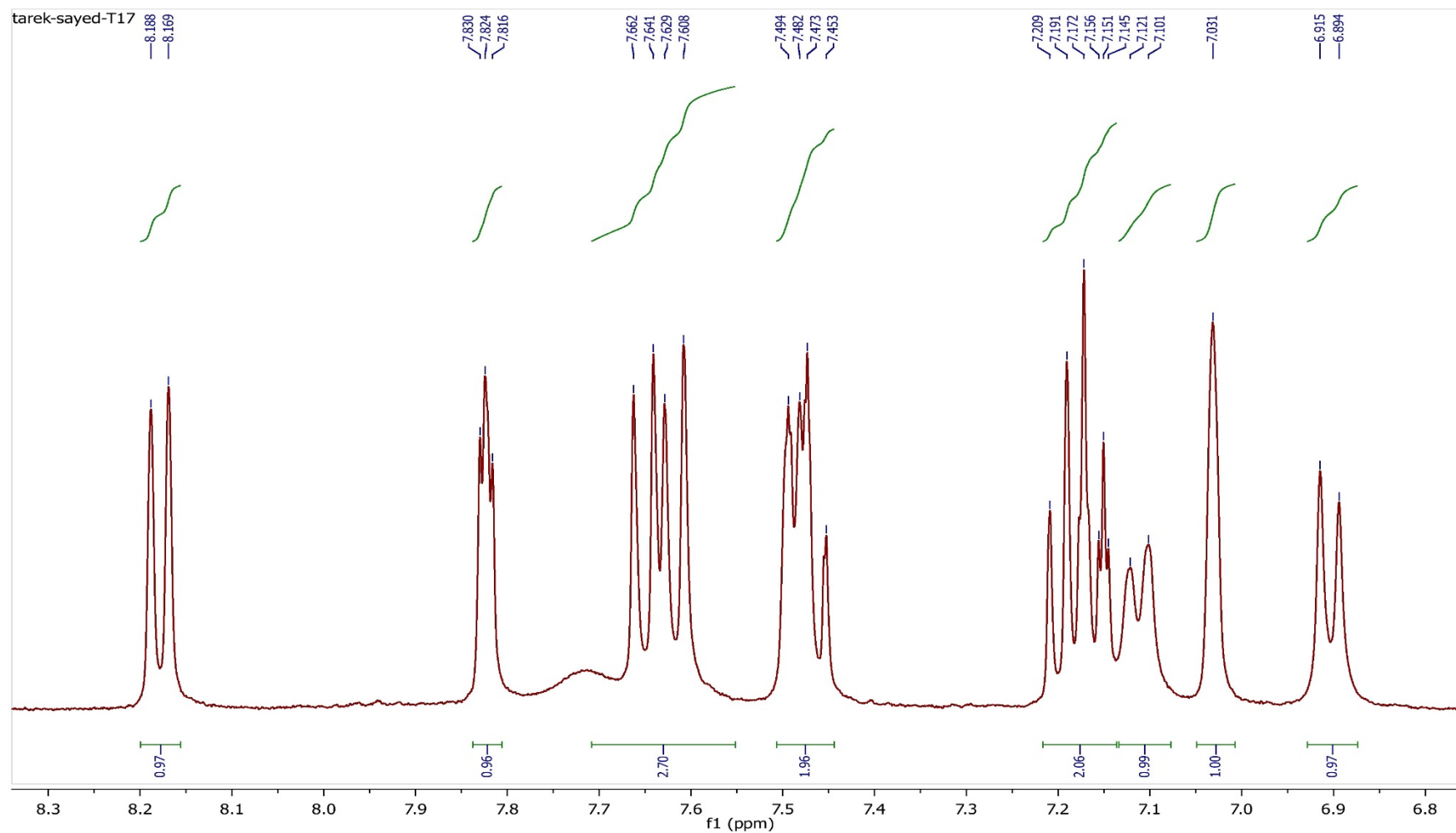


Figure S51: The enlargement of downfield region in ¹H-NMR spectrum of compound **5b**.

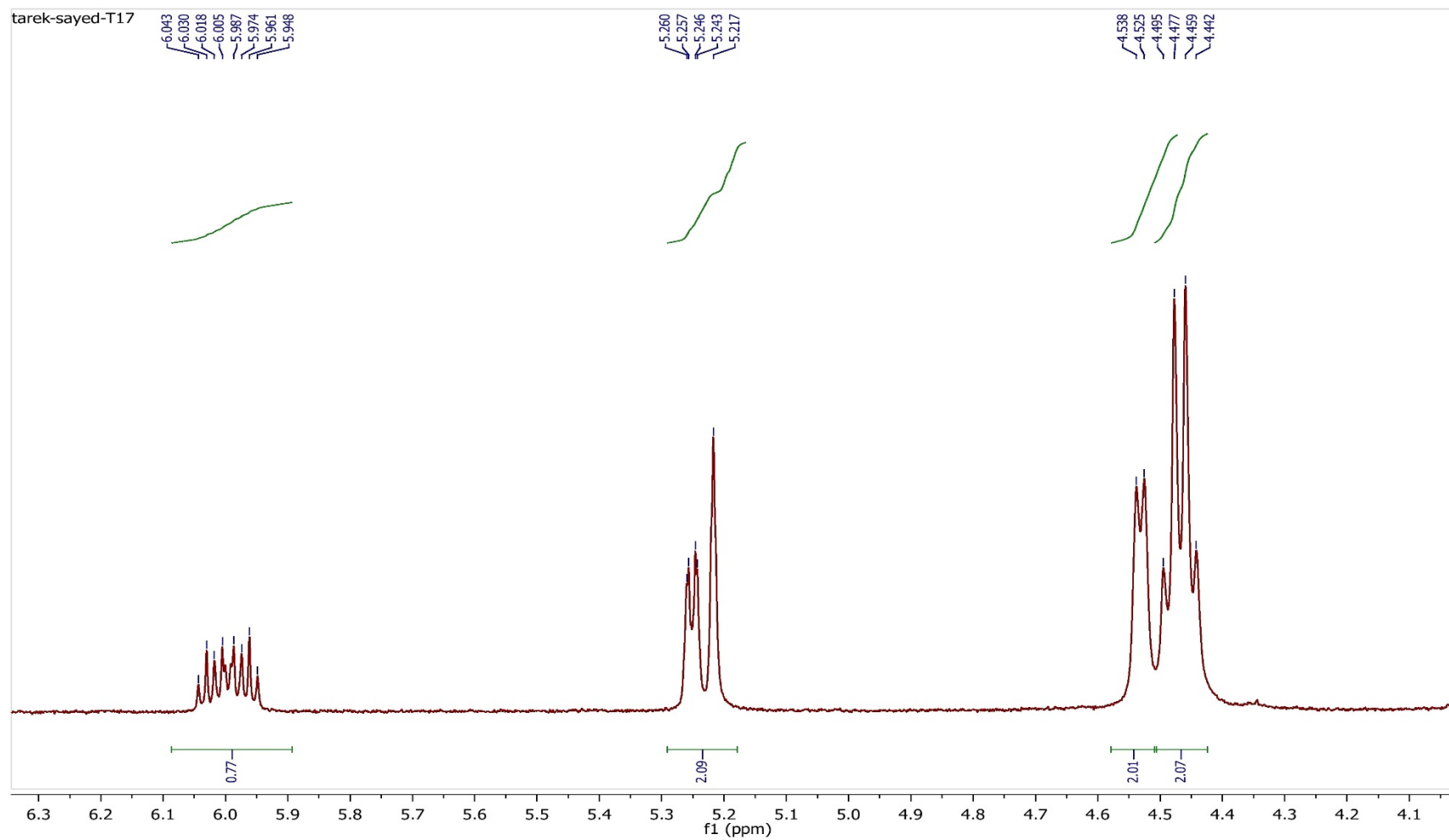


Figure S52: The enlargement of upfield region in ^1H -NMR spectrum of compound **5b**.

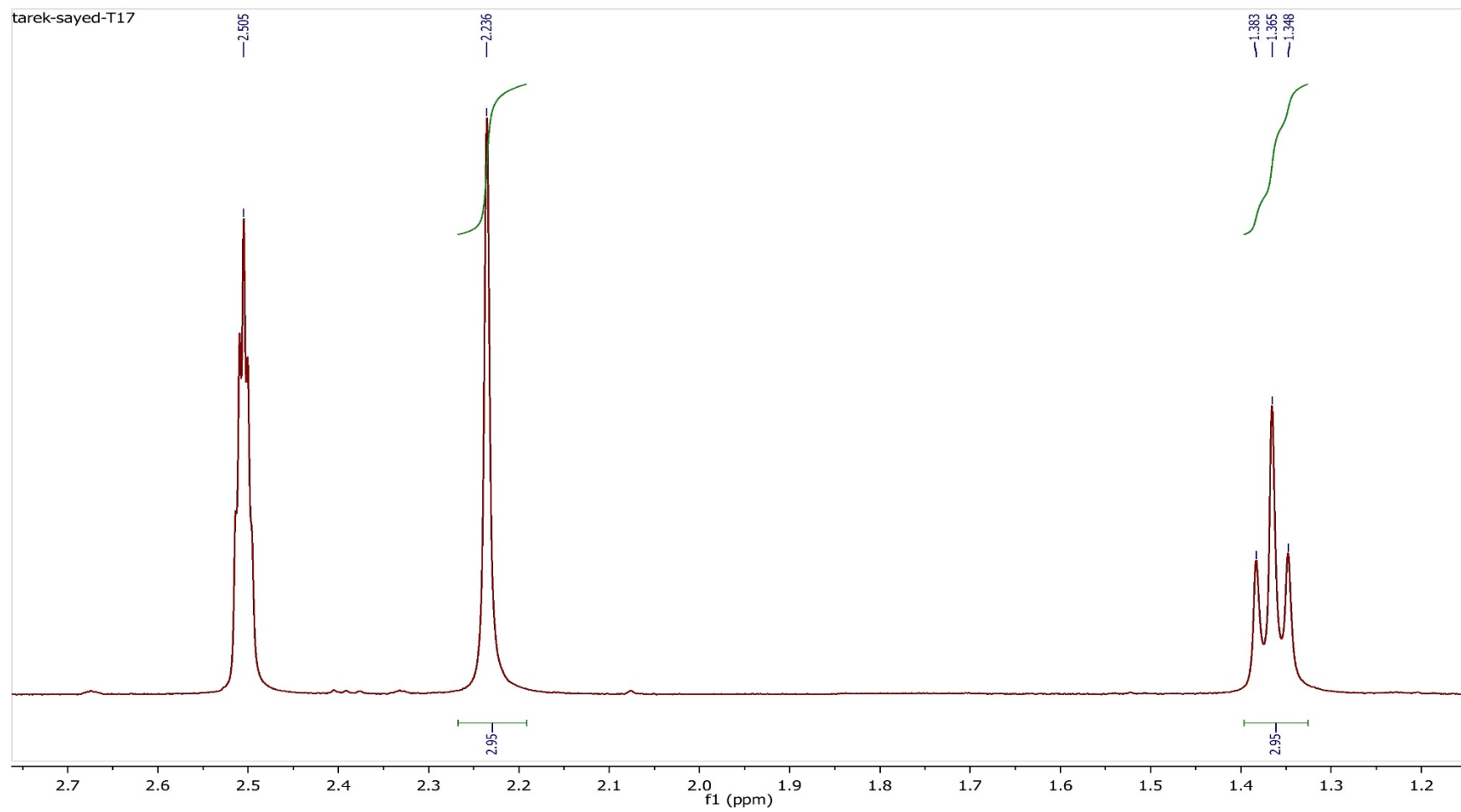


Figure S53: The enlargement of upfield region in ^1H -NMR spectrum of compound **5b**.

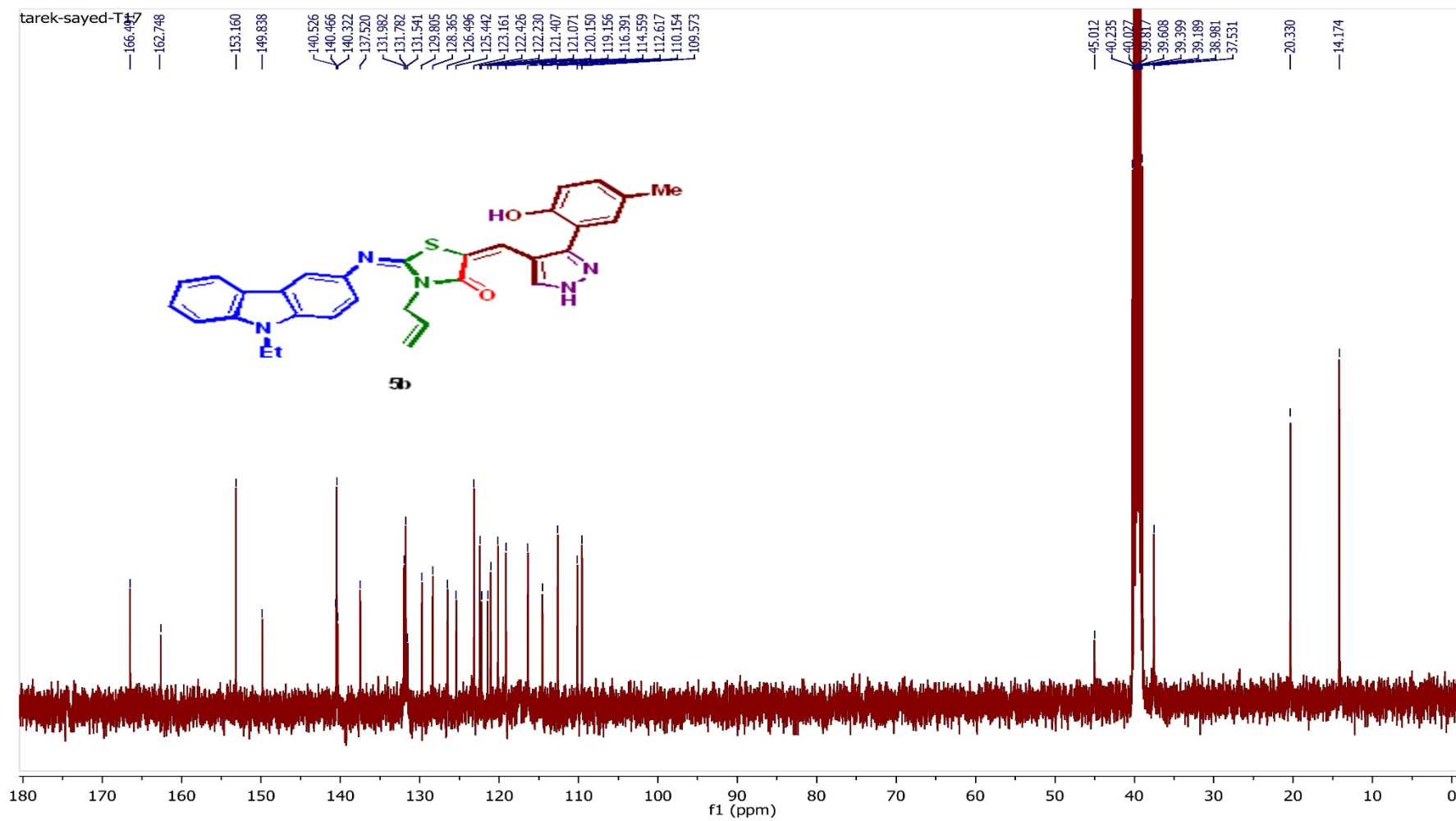


Figure S54: The ^{13}C -NMR spectrum of compound **5b**.

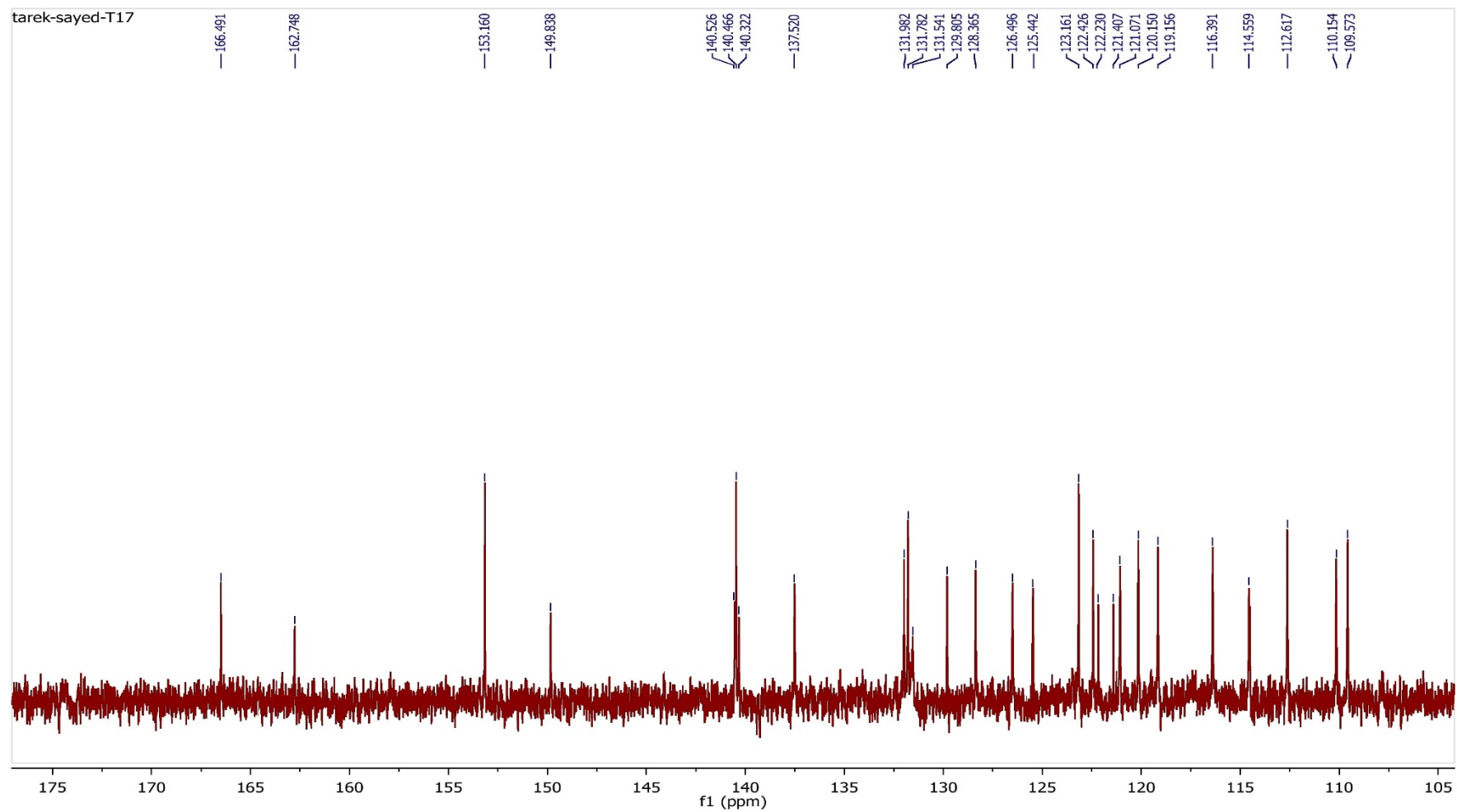


Figure S55: The enlargement of downfield region in ^{13}C -NMR spectrum of compound **5b**.

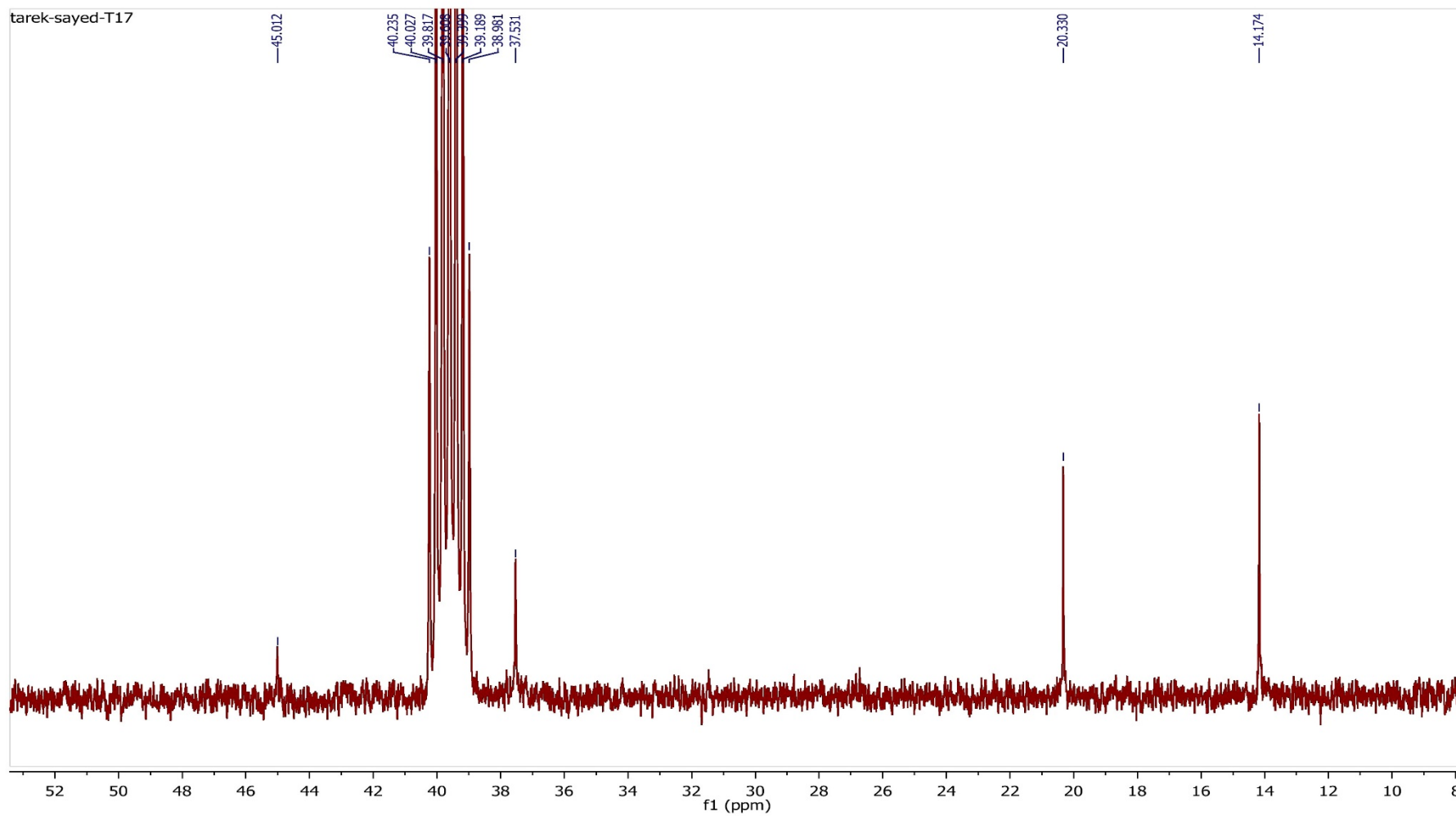


Figure S56: The enlargement of upfield region in ^{13}C -NMR spectrum of compound **5b**.

tarek-17 #48-50 RT: 0.82-0.85 AV: 3 SB: 2 3.82, 3.53 NL: 1.57E2
T: (0,0) +c EI Full ms [40.00-1000.00]

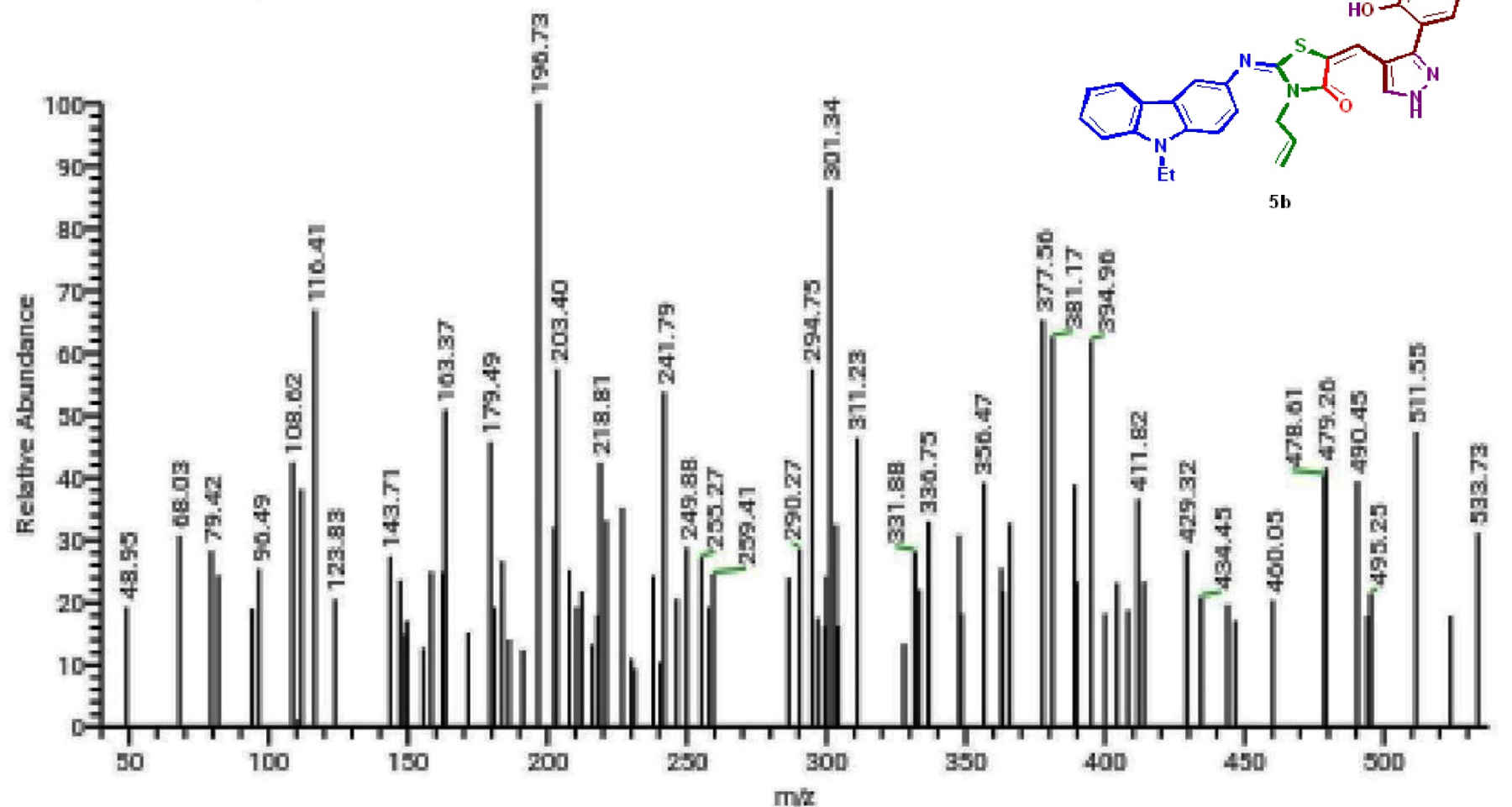


Figure S57: The mass spectrum of compound 5b.

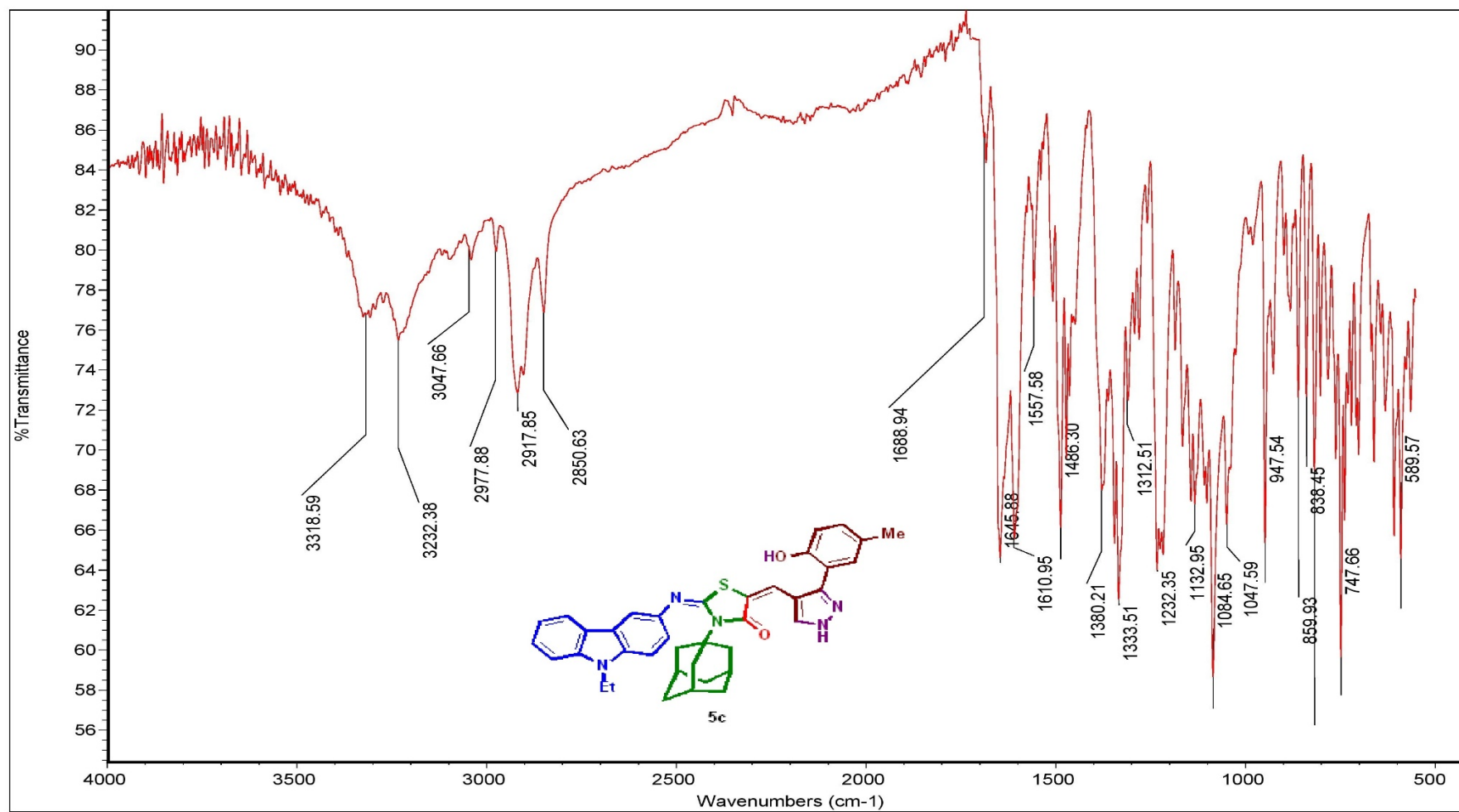


Figure S58: The IR spectrum of compound **5c**.

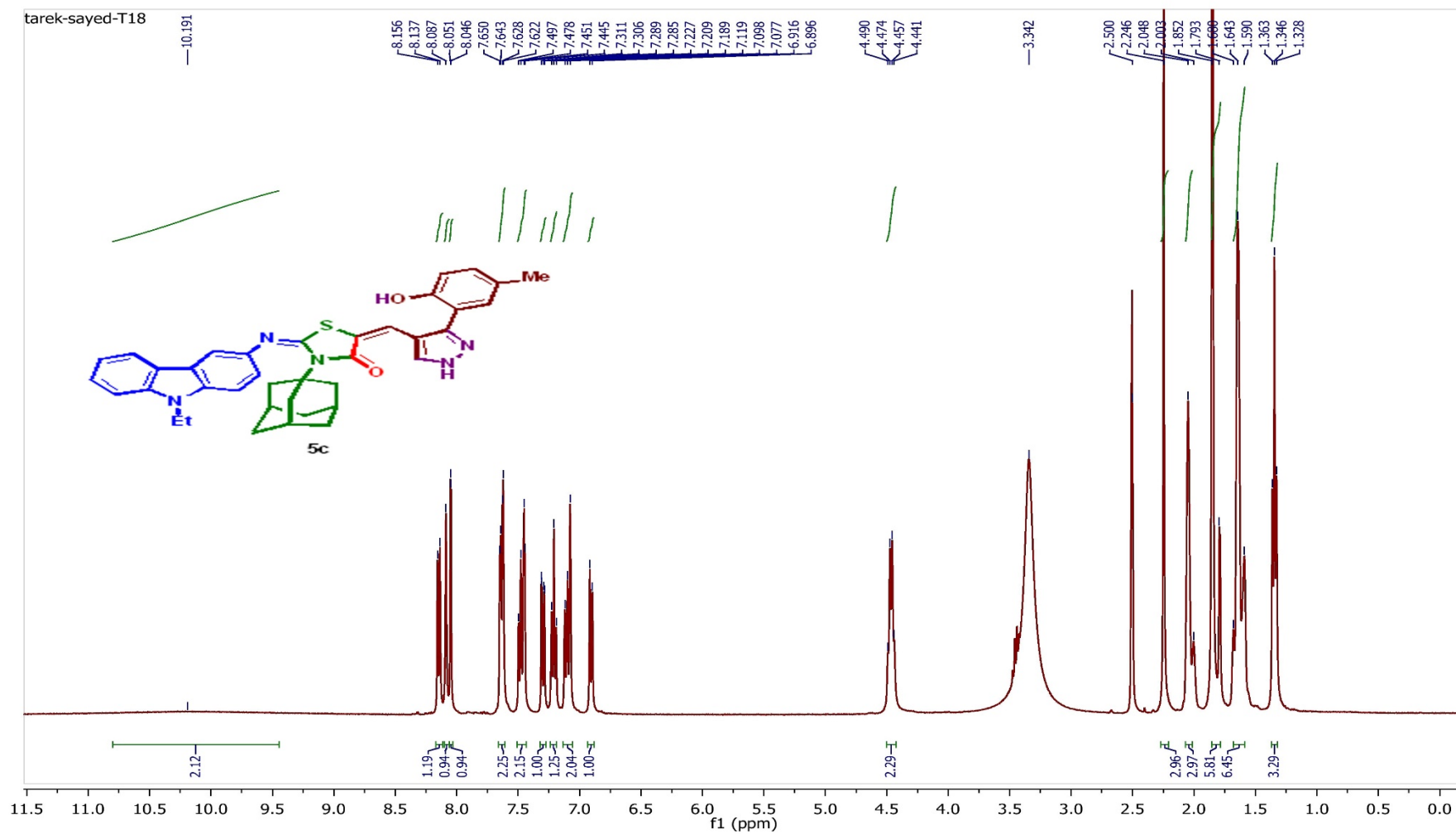


Figure S59: The ^1H -NMR spectrum of compound **5c**.

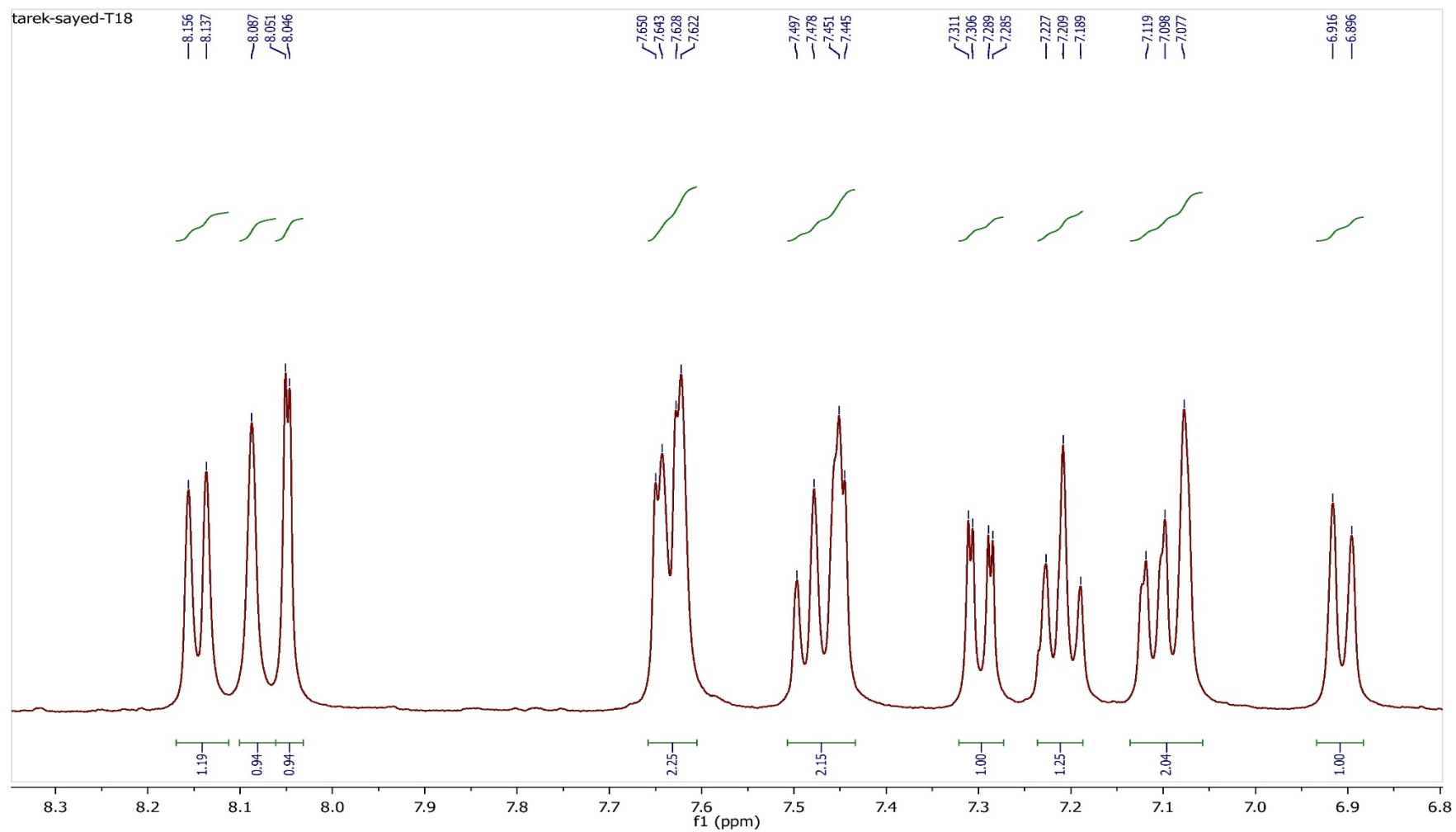


Figure S60: The enlargement of downfield region in ^1H -NMR spectrum of compound **5c**.

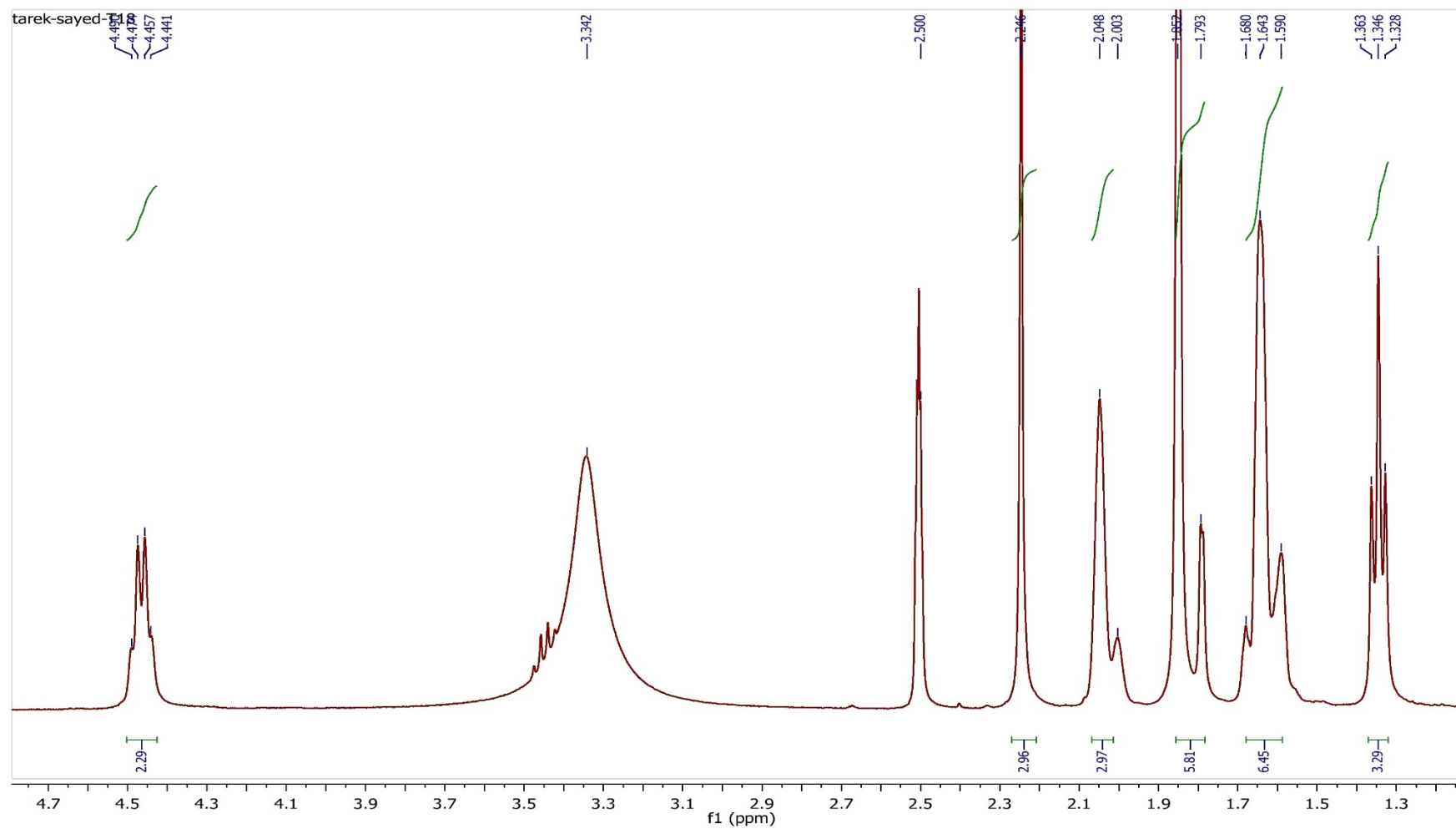


Figure S61: The enlargement of upfield region in ^1H -NMR spectrum of compound **5c**.

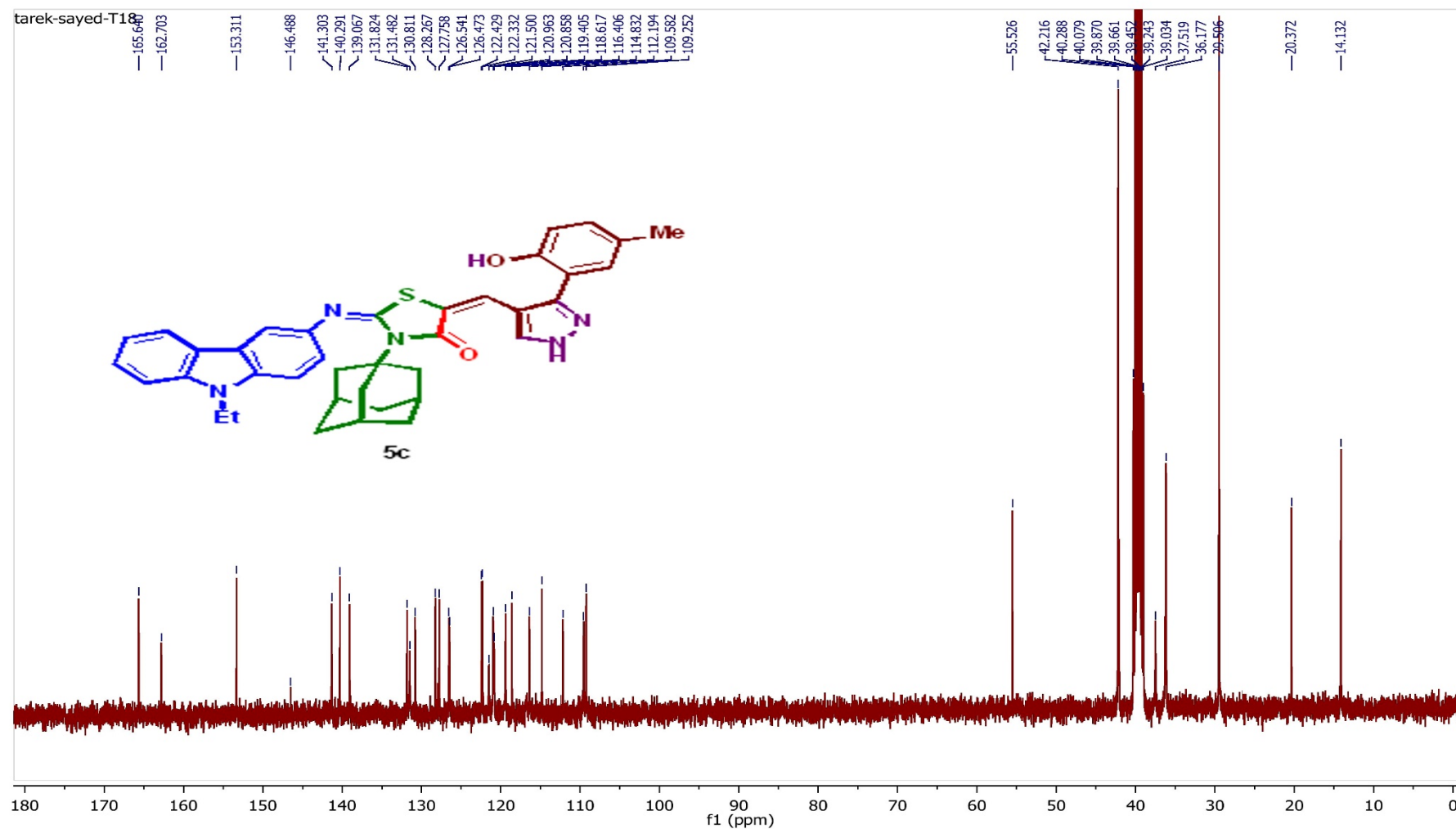


Figure S62: The ^{13}C -NMR spectrum of compound **5c**.

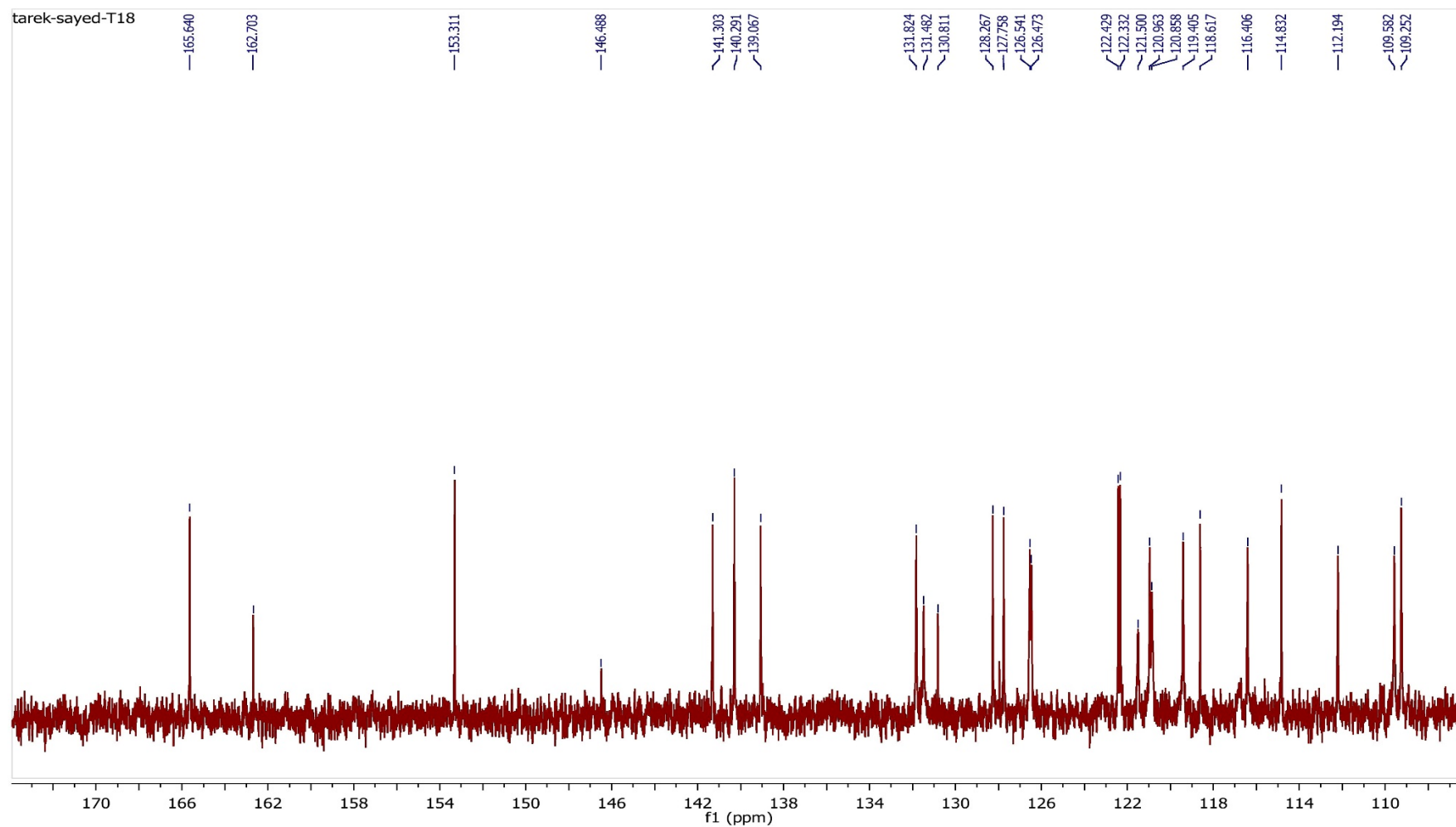


Figure S63: The enlargement of downfield region in ^{13}C -NMR spectrum of compound **5c**.

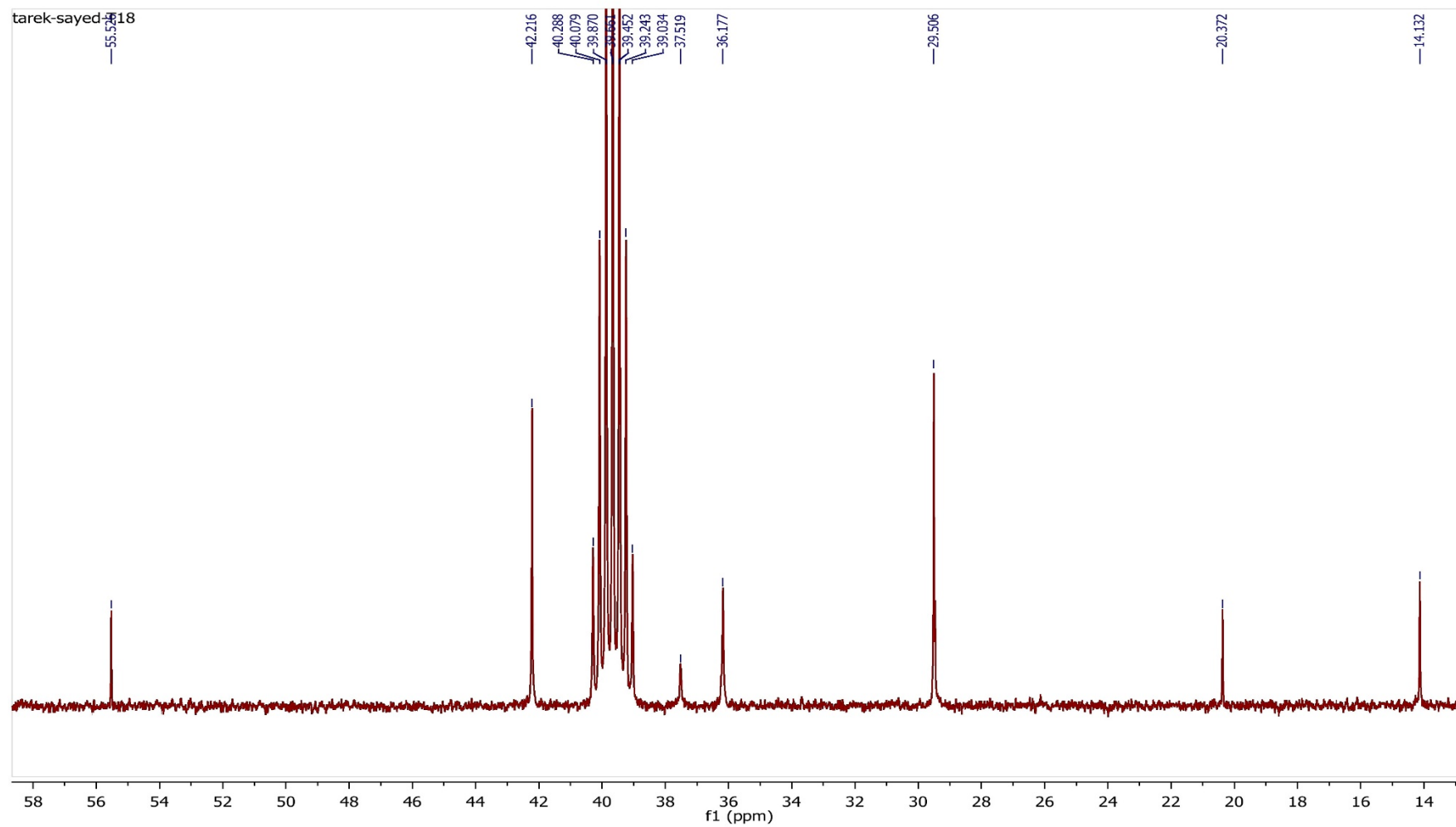


Figure S64: The enlargement of upfield region in ^{13}C -NMR spectrum of compound **5c**.

tarek-T18 #243 RT: 4.08 AV: 1 SB: 2 3.82, 3.53 NL: 2.07E3
T: (0,0) + e EI Full ms [40.00-1000.00]

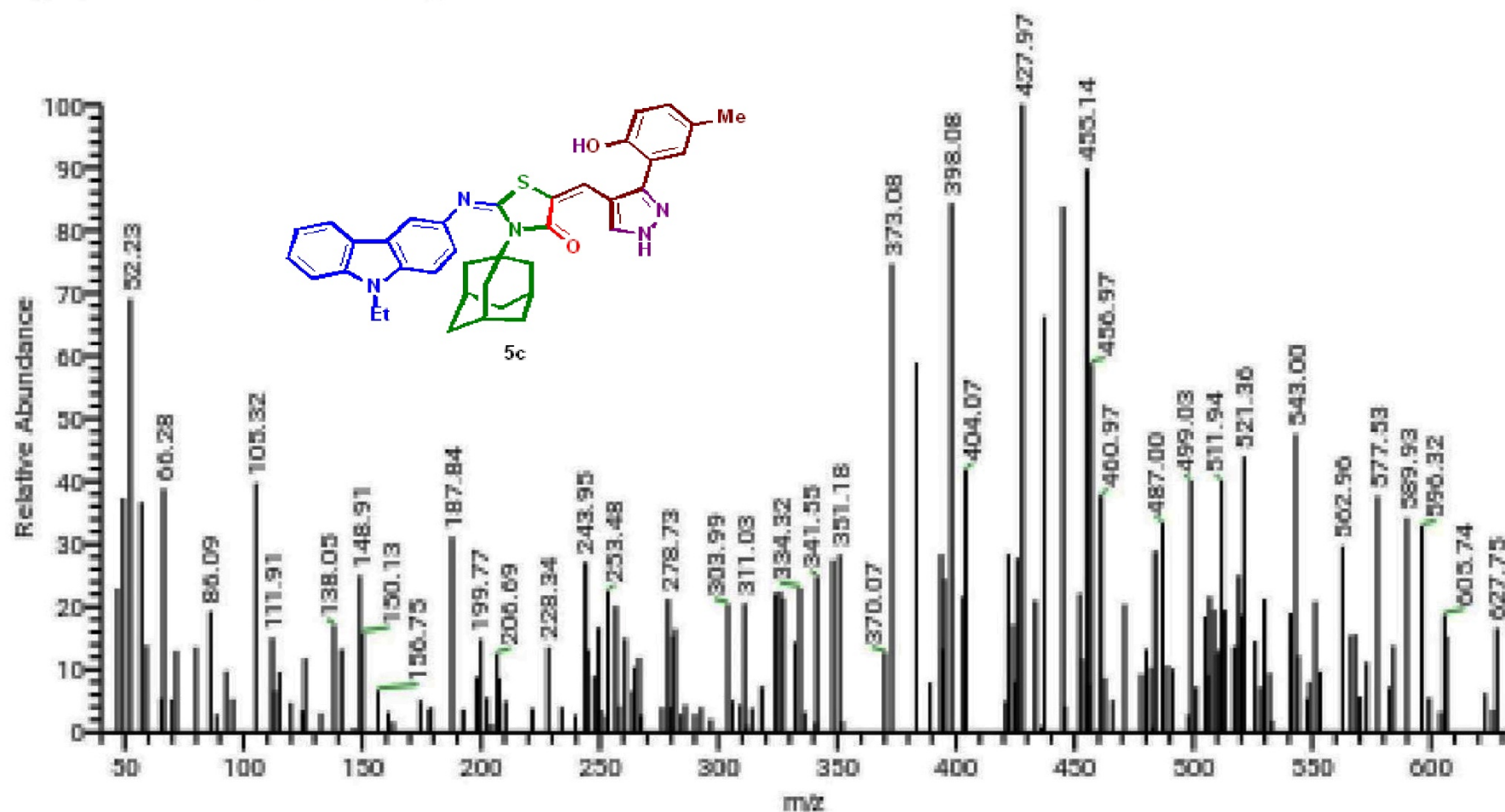


Figure S65: The mass spectrum of compound 5c.

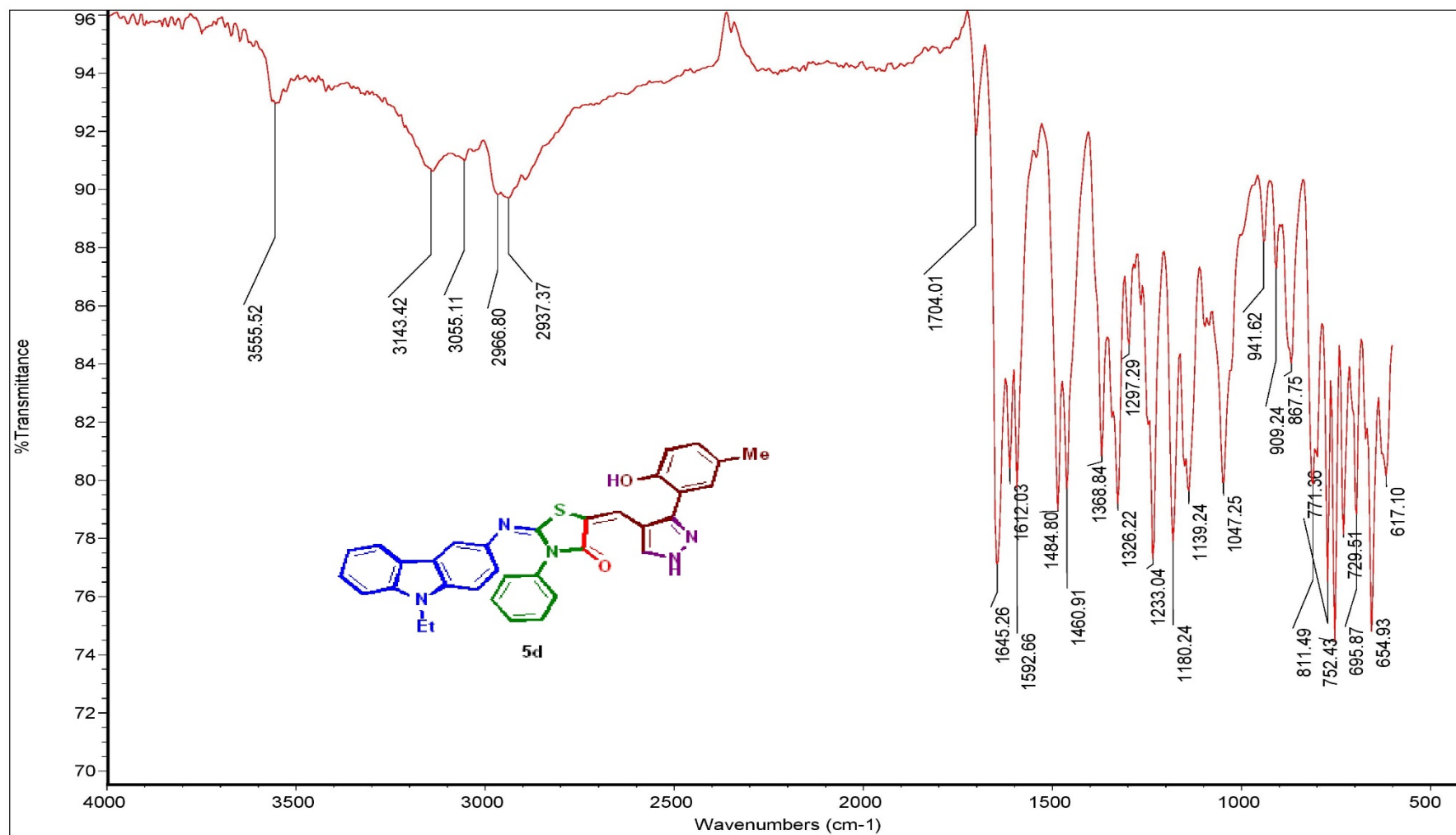


Figure S66: The IR spectrum of compound **5d**.

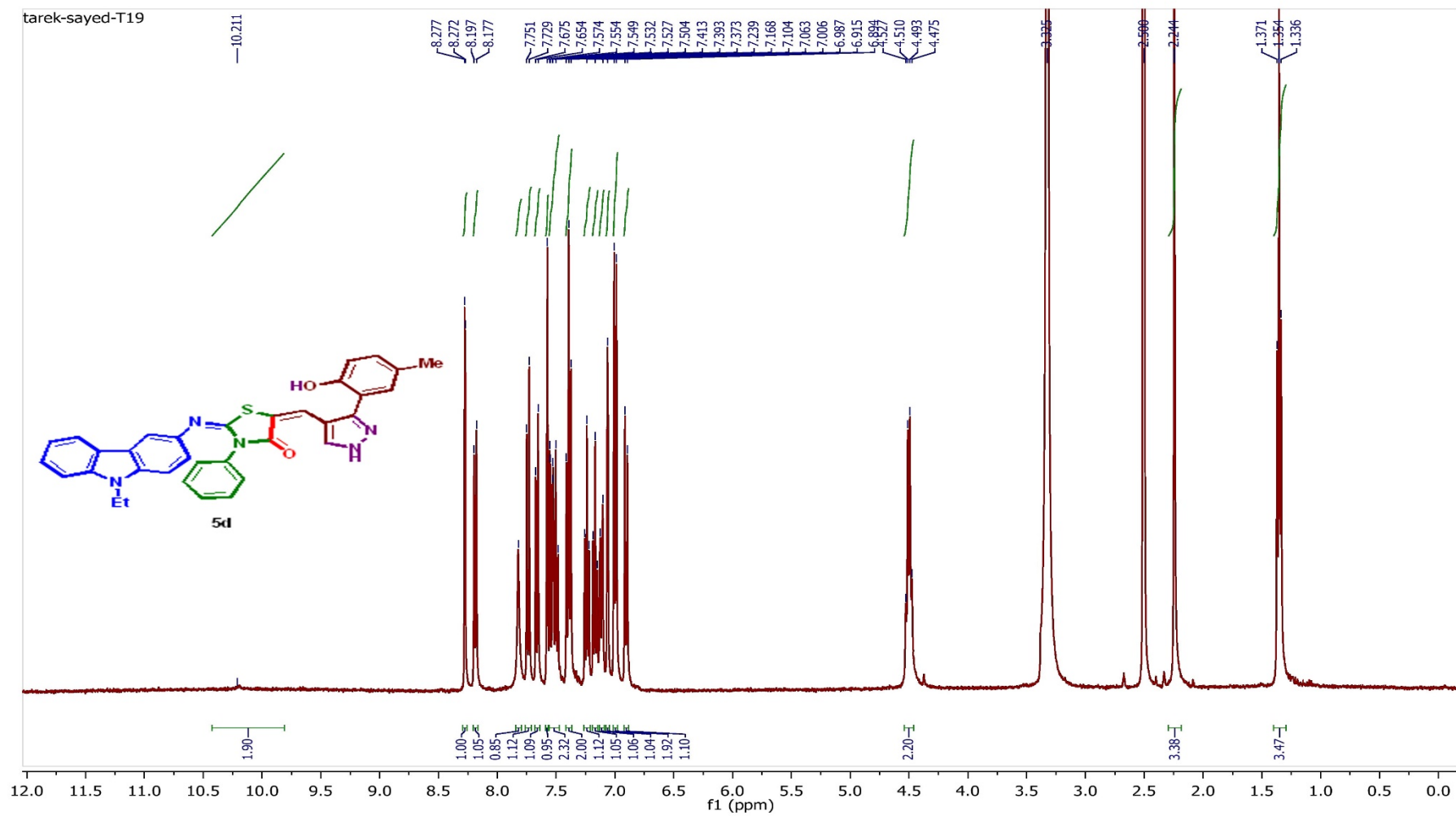


Figure S67: The ^1H -NMR spectrum of compound **5d**.

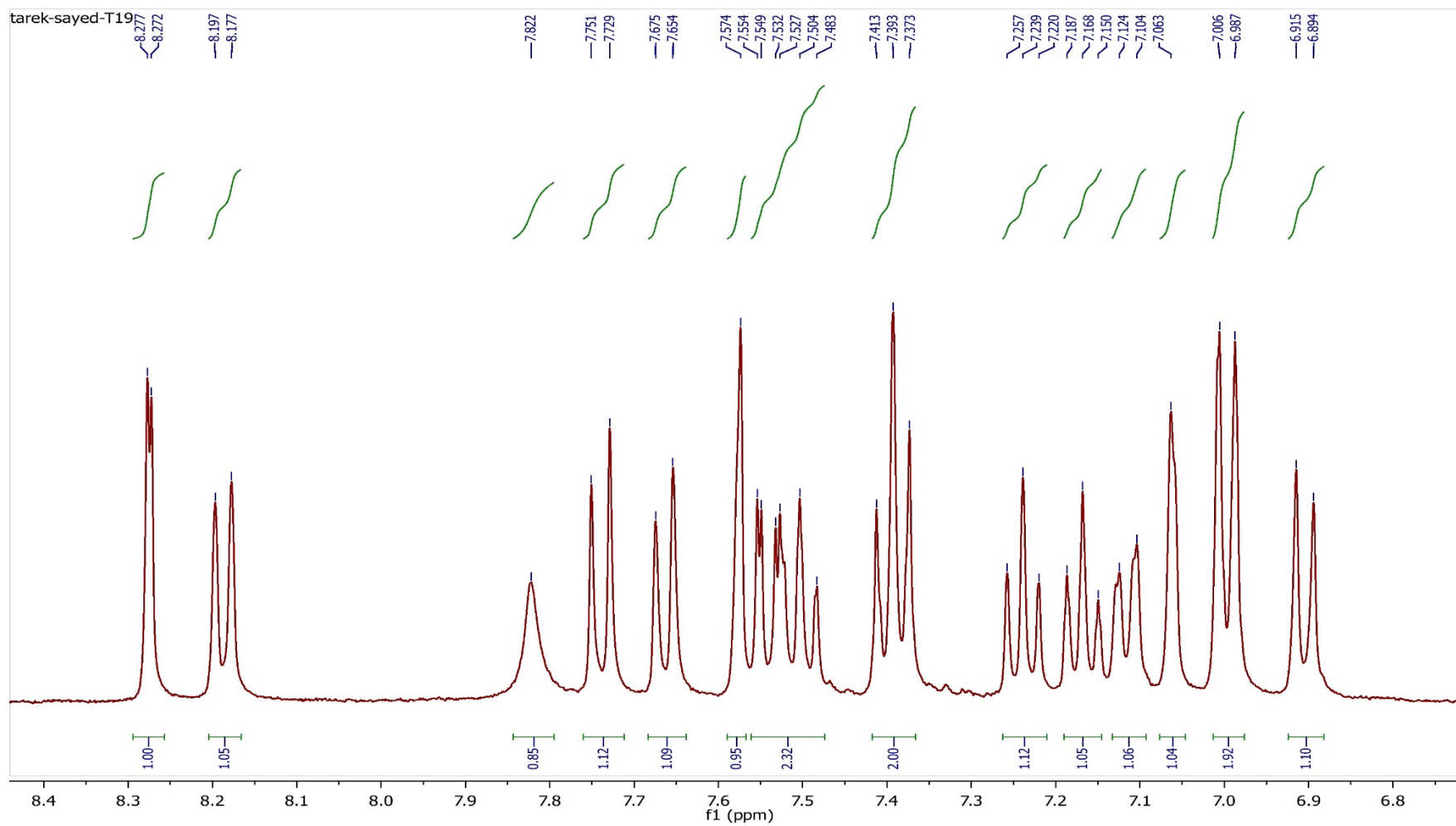


Figure S68: The enlargement of downfield region in ^1H -NMR spectrum of compound **5d**.

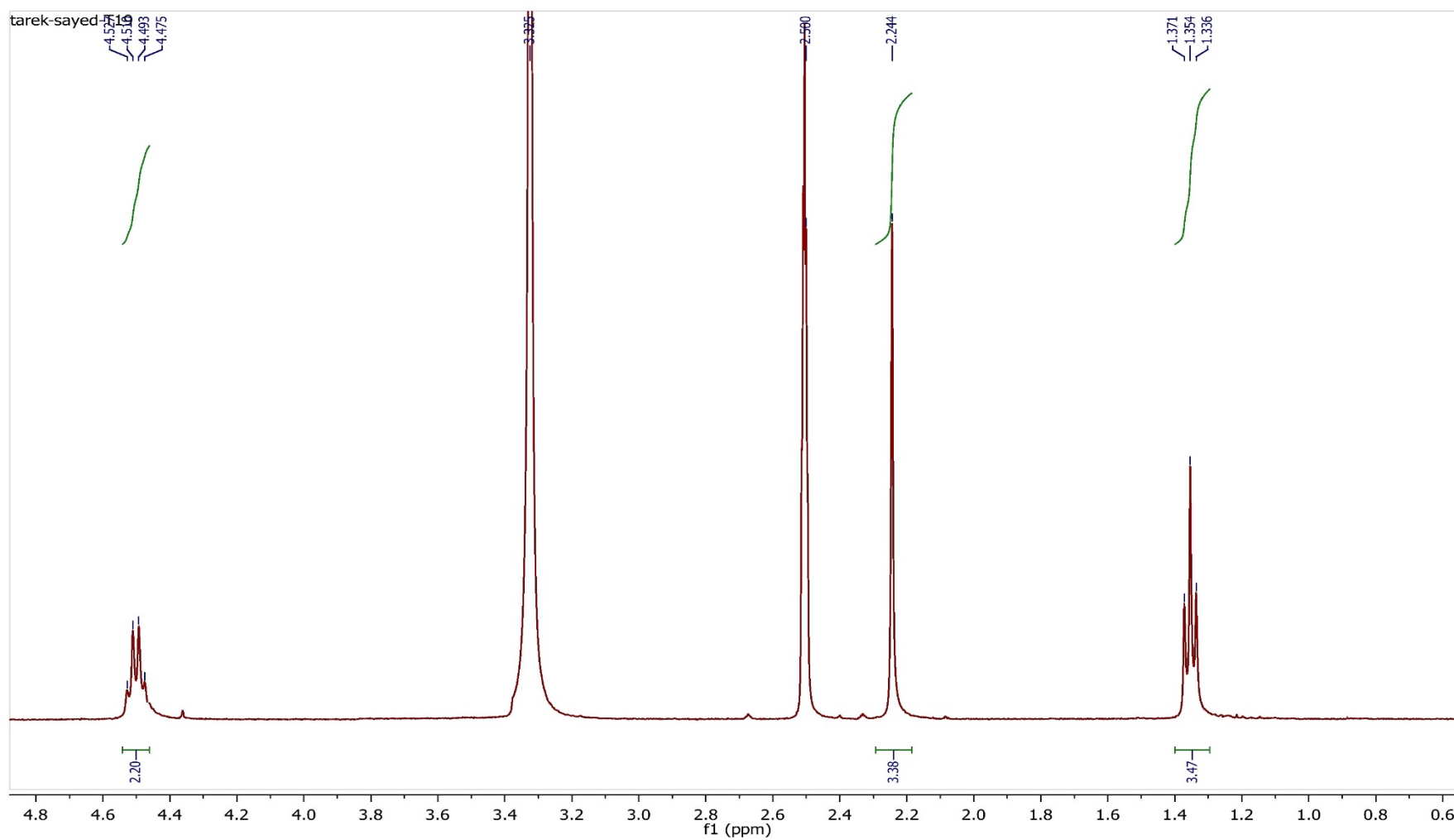


Figure S69: The enlargement of upfield region in ^1H -NMR spectrum of compound **5d**.

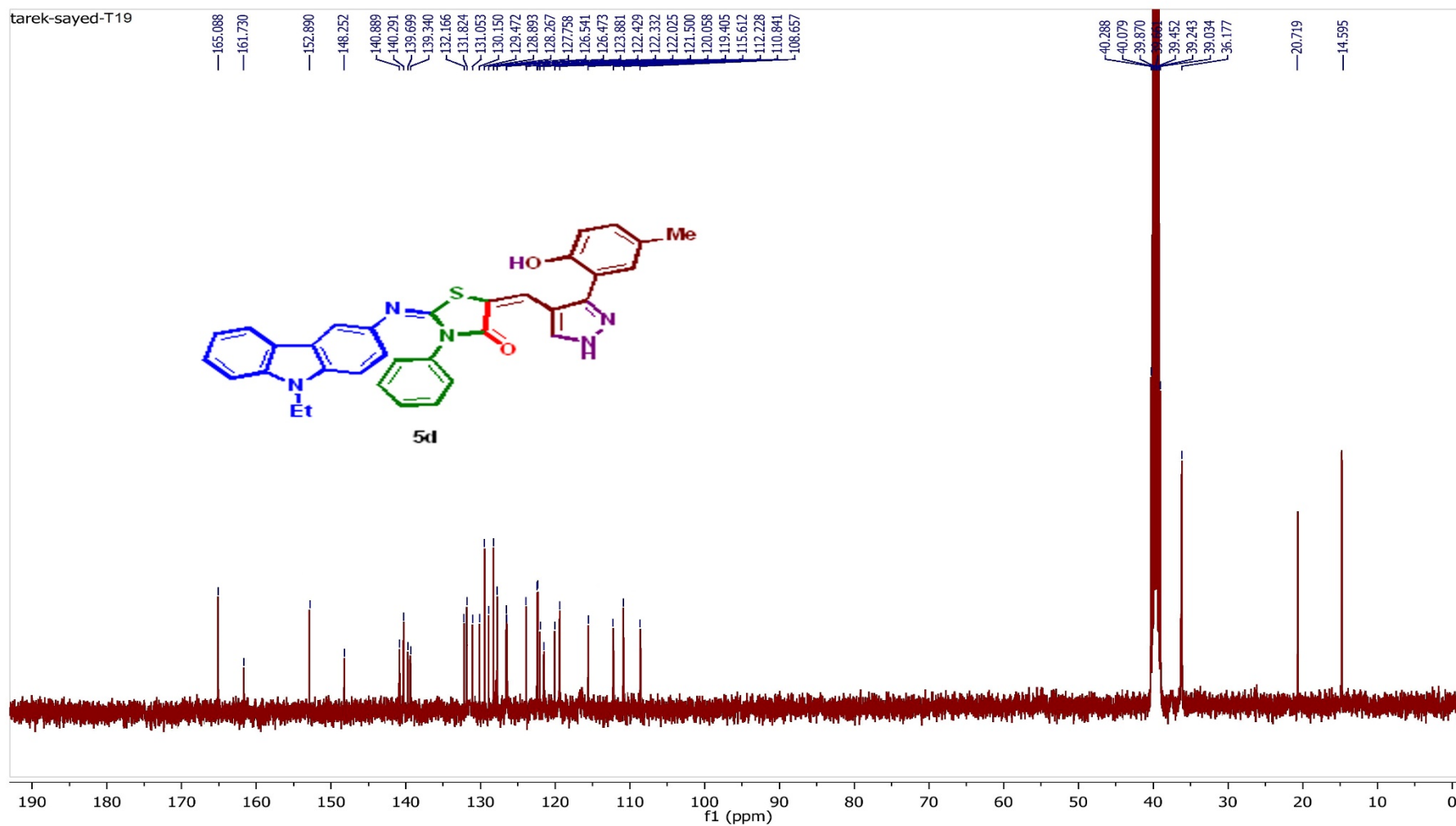


Figure S70: The ^{13}C -NMR spectrum of compound **5d**.

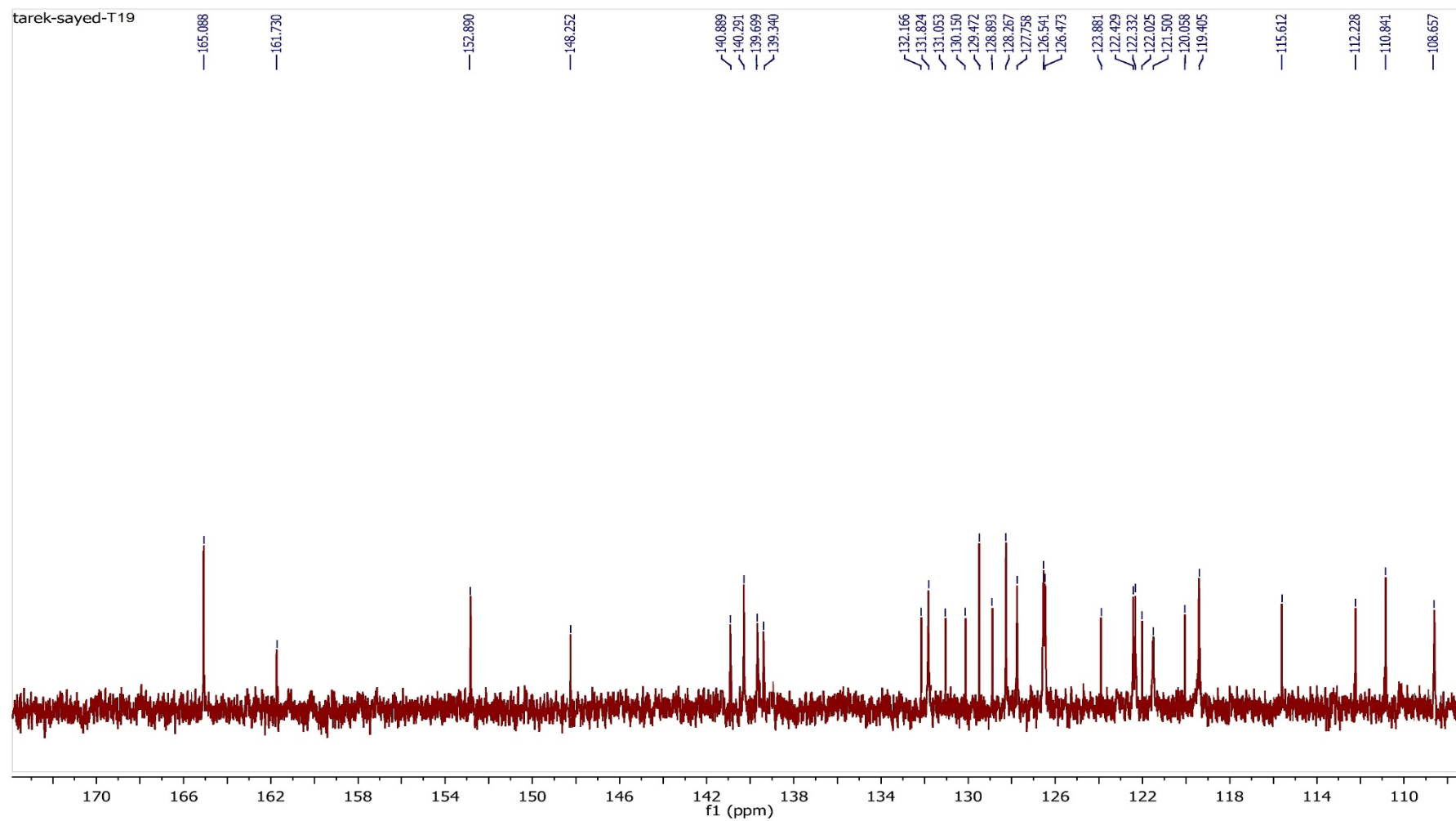


Figure S71: The enlargement of downfield region in ^{13}C -NMR spectrum of compound **5d**.

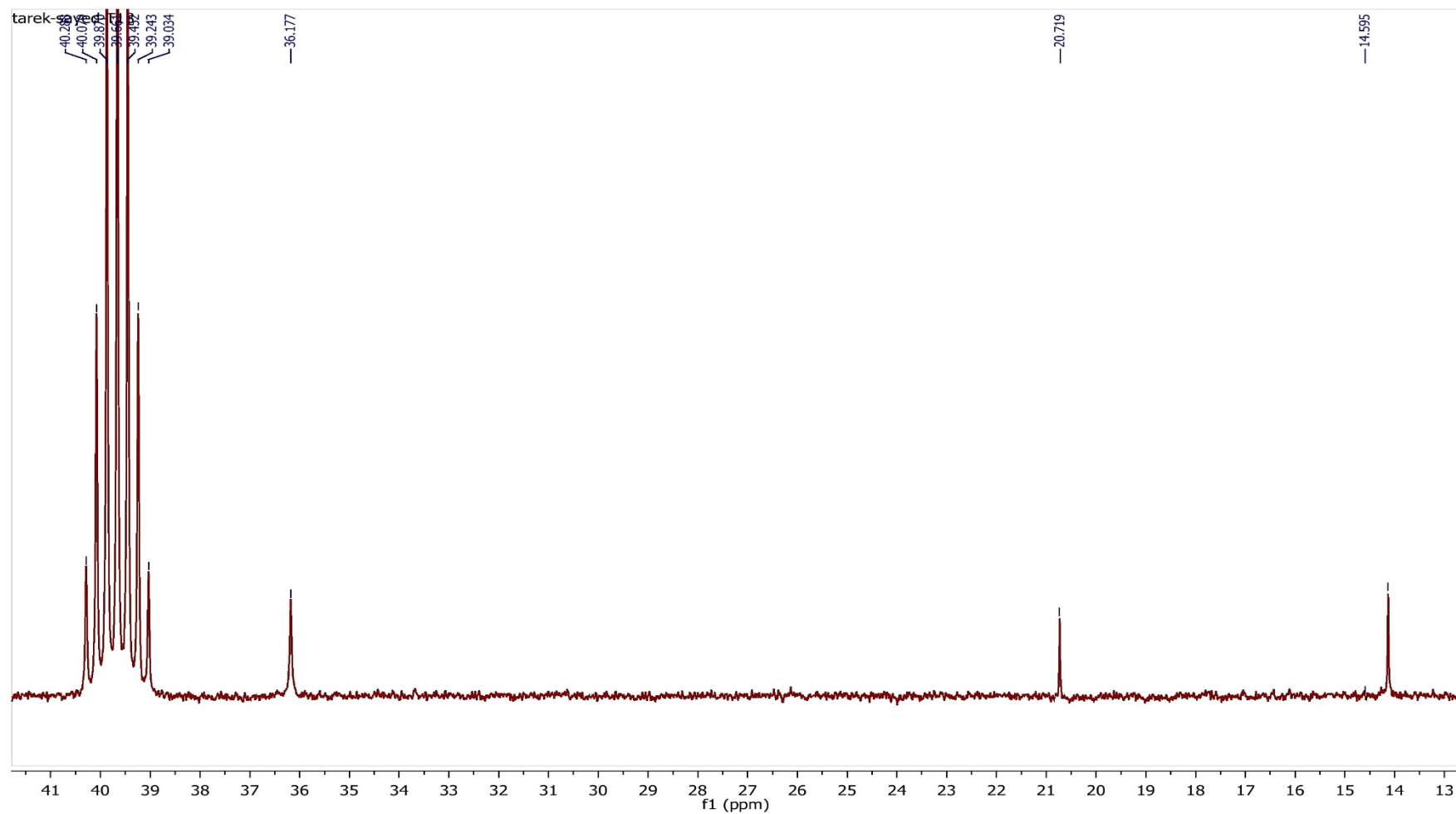


Figure S72: The enlargement of upfield region in ^{13}C -NMR spectrum of compound **5d**.

tarek-T19 #219 RT: 3.68 AV: 1 SB: 2 3.82, 3.53 NL: 3.43E2
T: (0,0) + e EI Full ms [40.00-1000.00]

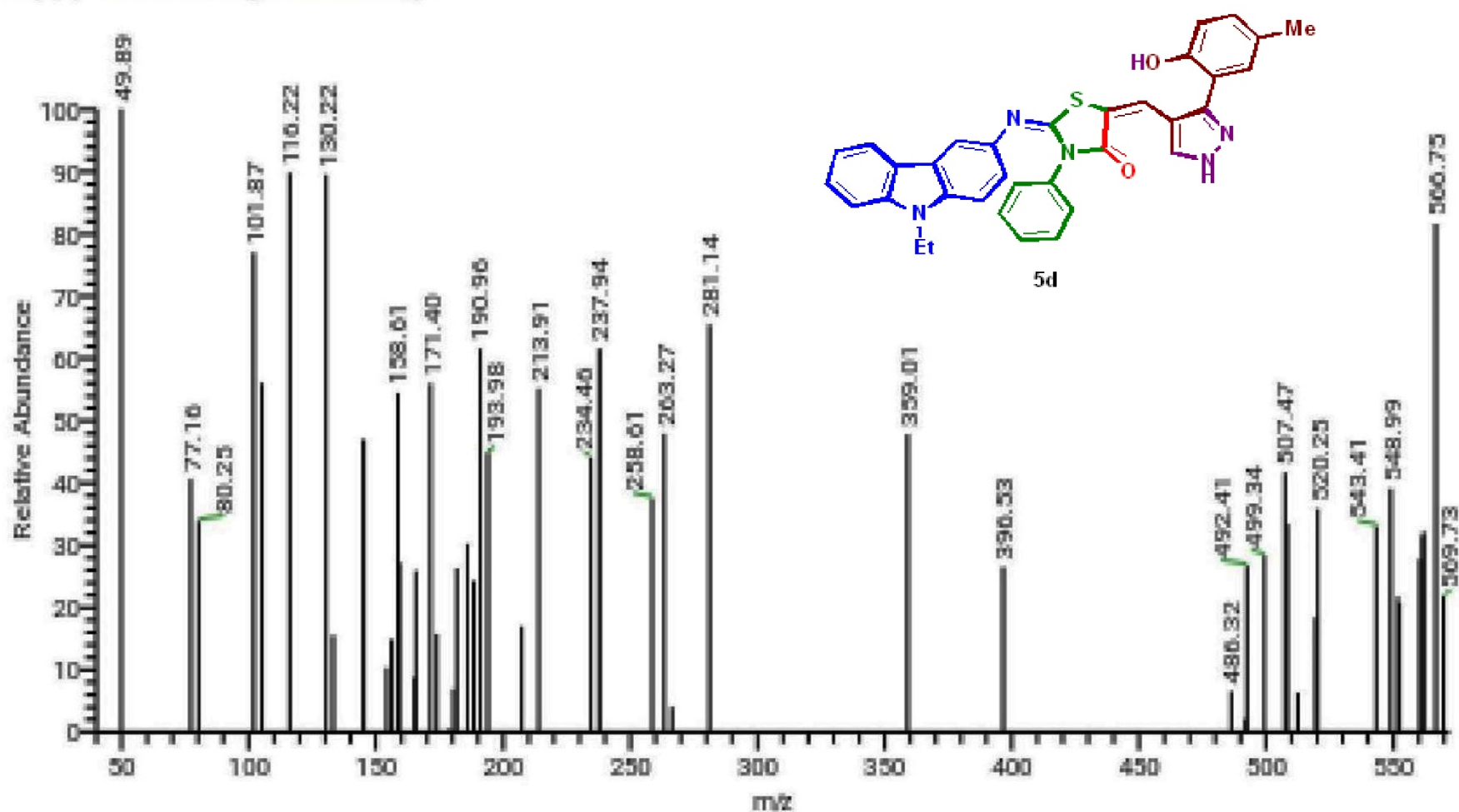


Figure S73: The mass spectrum of compound **5d**.

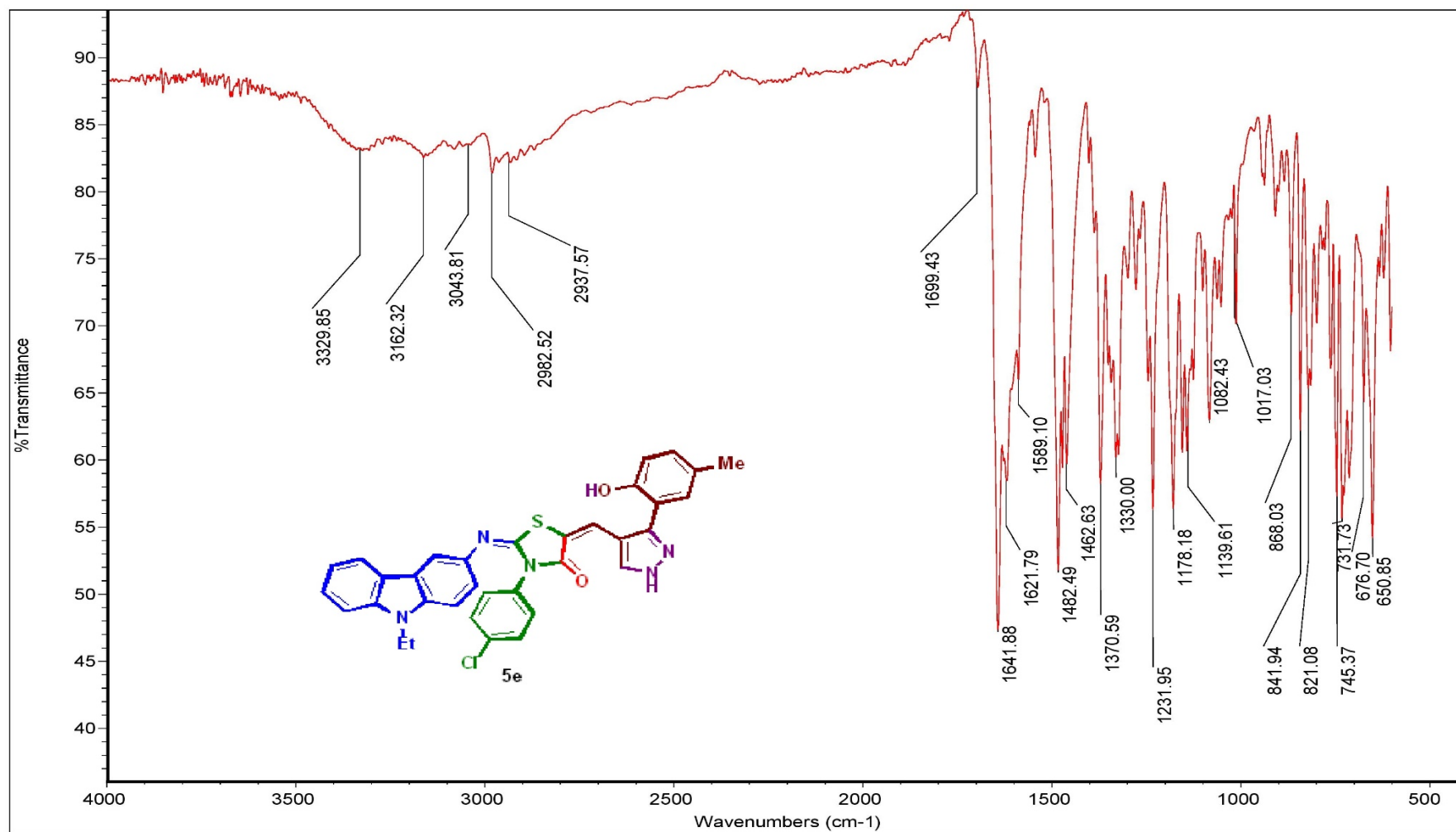


Figure S74: The IR spectrum of compound 5e.

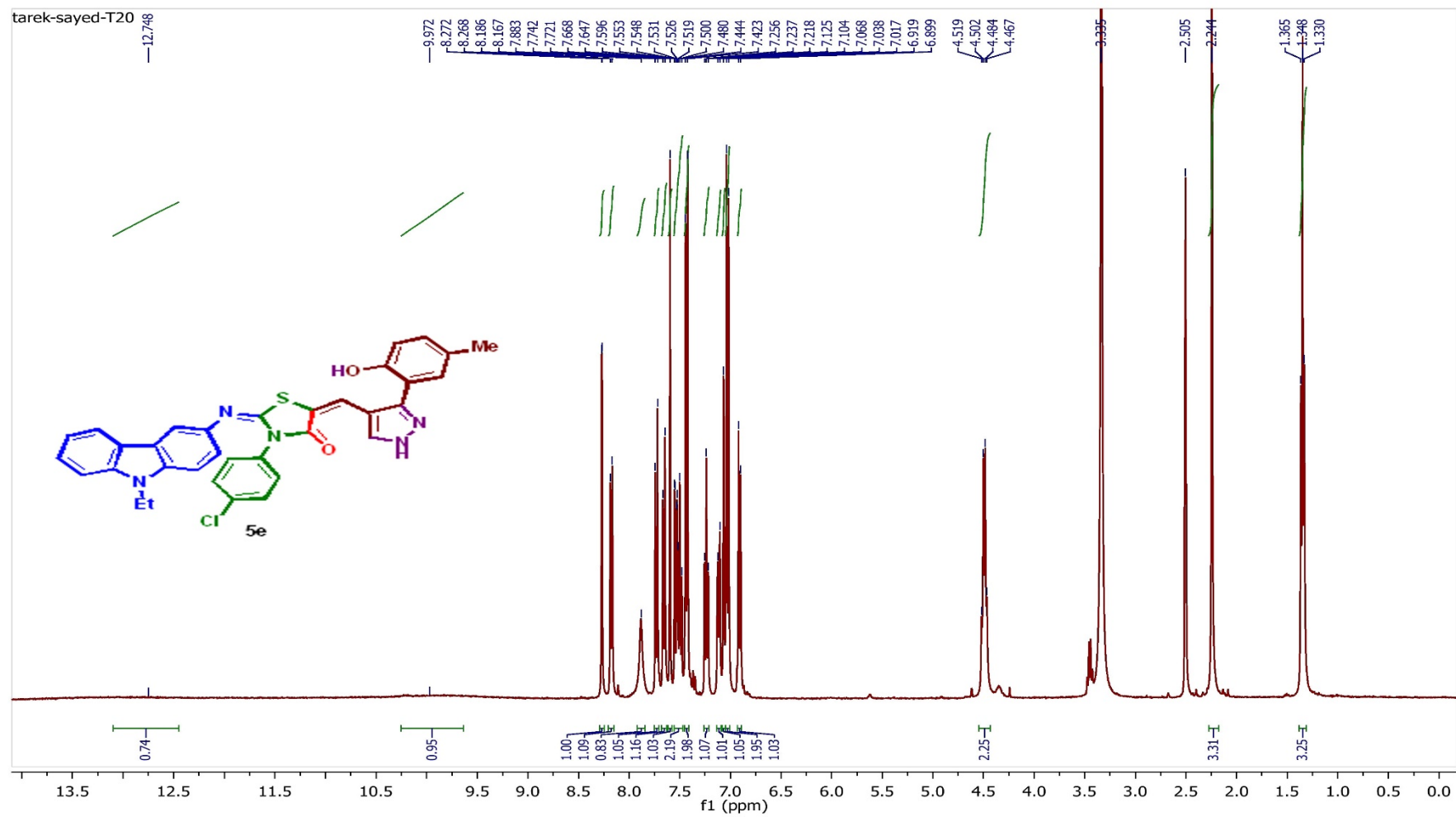


Figure S75: The ^1H -NMR spectrum of compound **5e**.

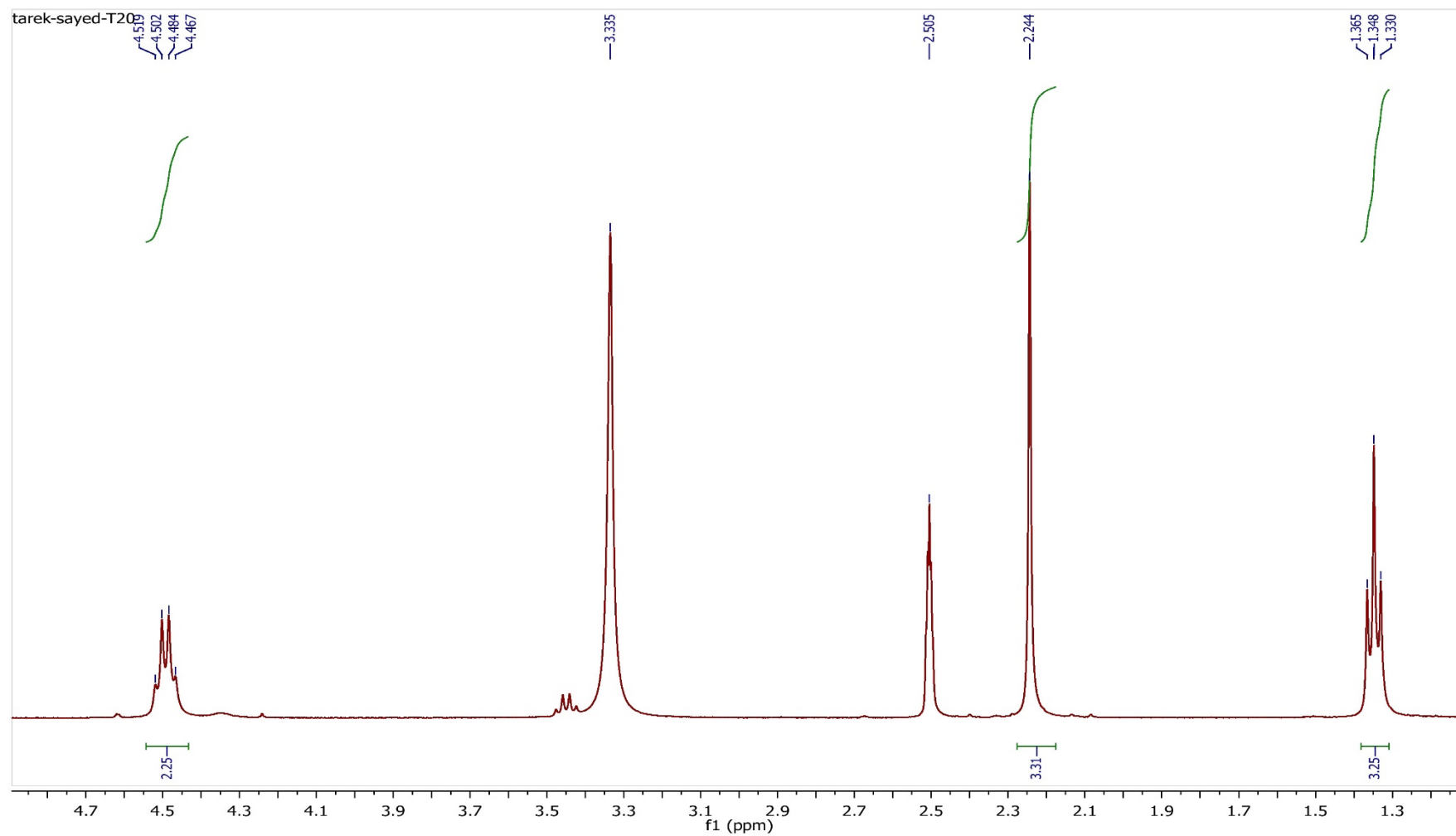


Figure S76: The enlargement of upfield region in ^1H -NMR spectrum of compound **5e**.

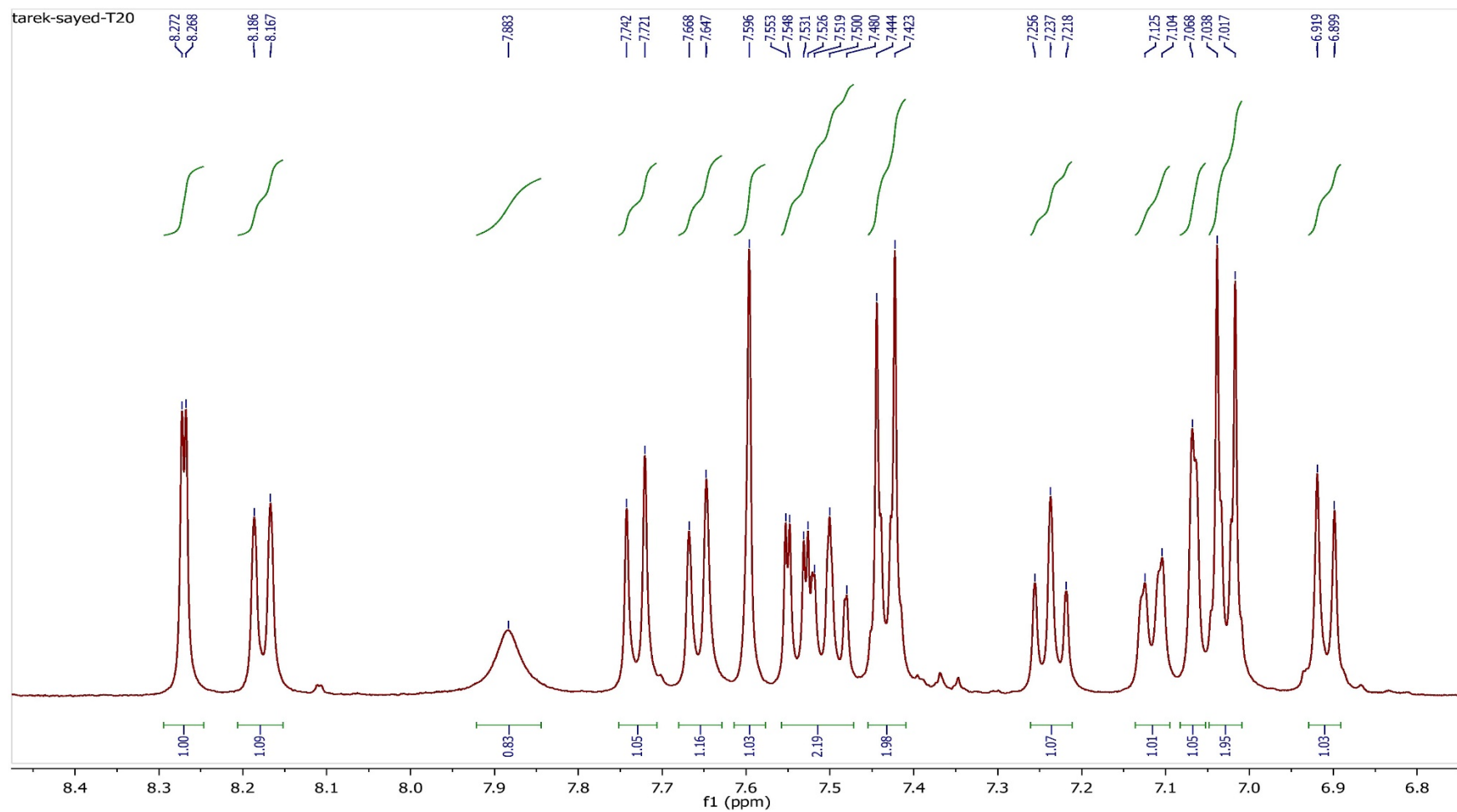


Figure S77: The enlargement of downfield region in ^1H -NMR spectrum of compound **5e**.

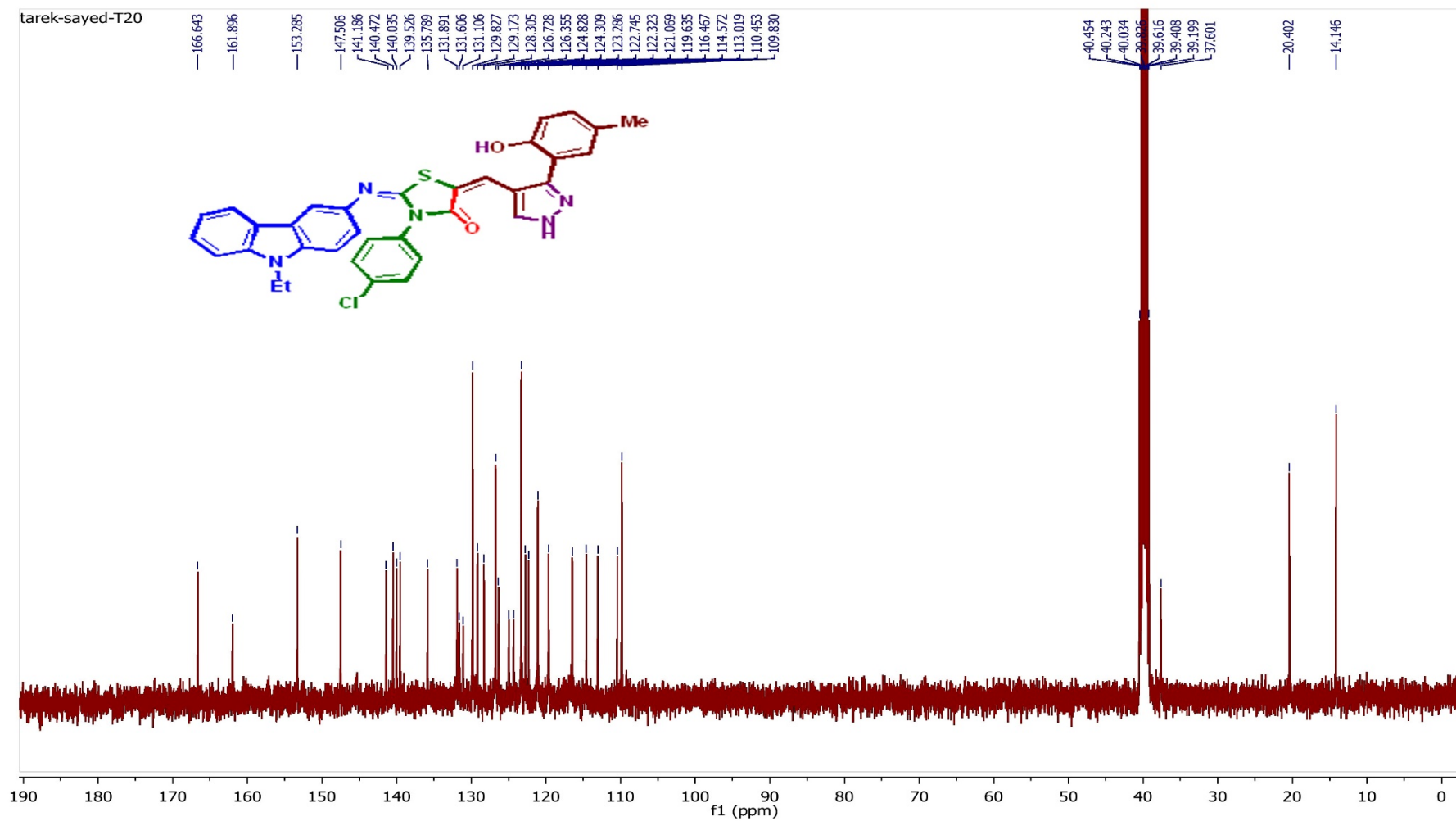


Figure S78: The ^{13}C -NMR spectrum of compound **5e**.

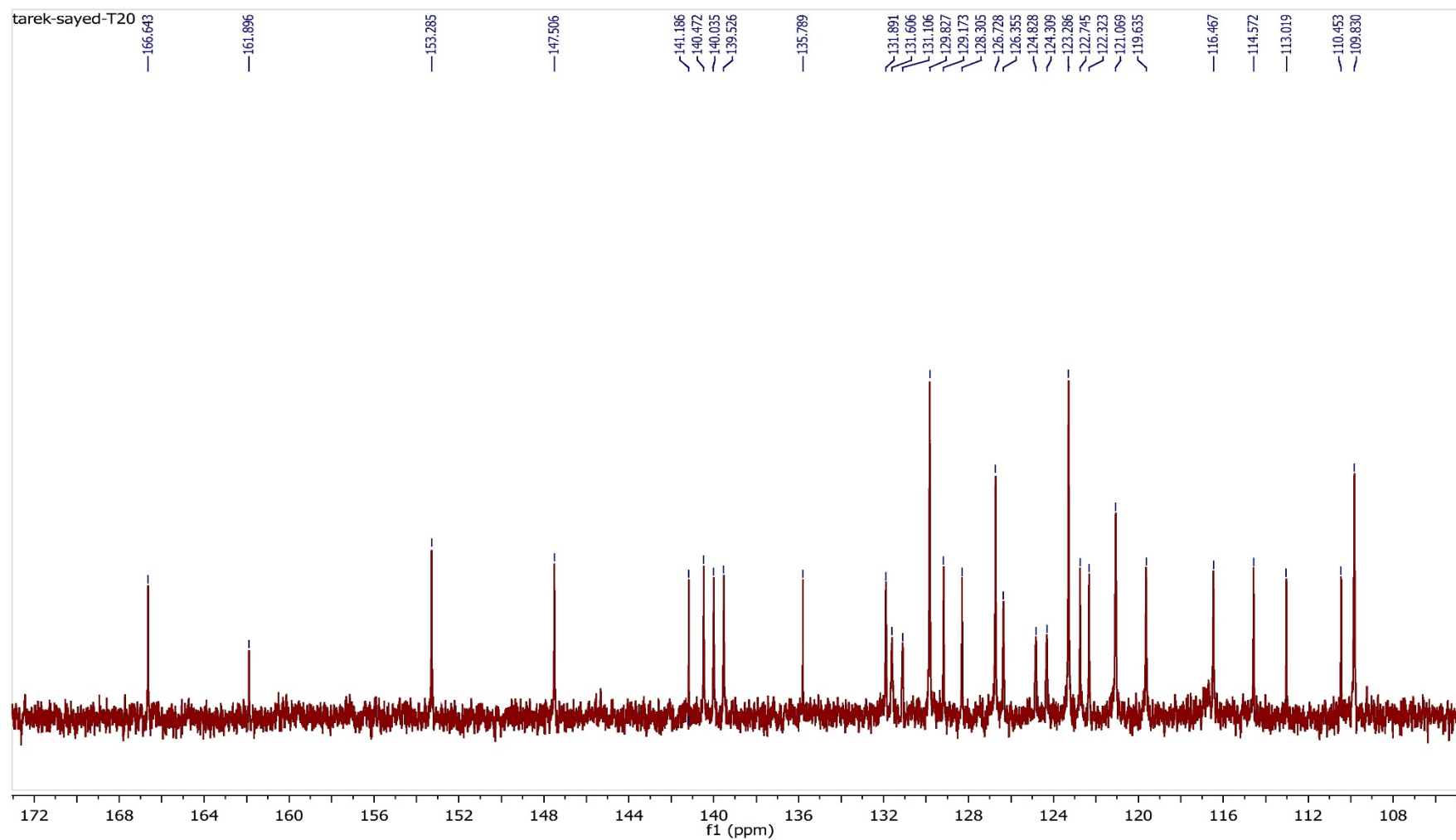


Figure S79: The enlargement of downfield region in ^{13}C -NMR spectrum of compound **5e**.

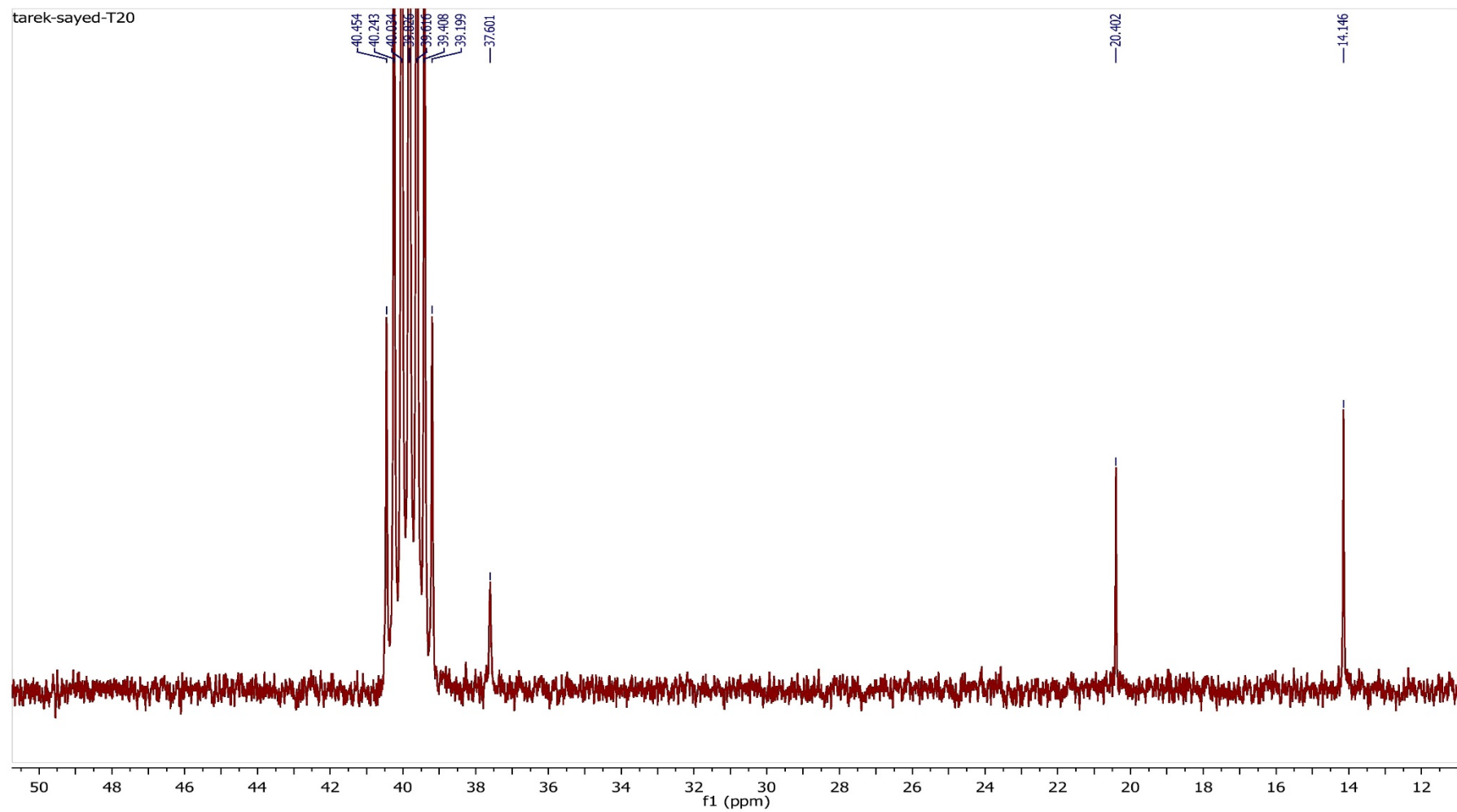


Figure S80: The enlargement of upfield region in ^{13}C -NMR spectrum of compound **5e**.

tarek-T20 #57-59 RT: 0.97-1.00 AV: 3 SB: 2 3.82, 3.53 NL: 1.77E2

T: (0,0) + e EI Full ms [40.00-1000.00]

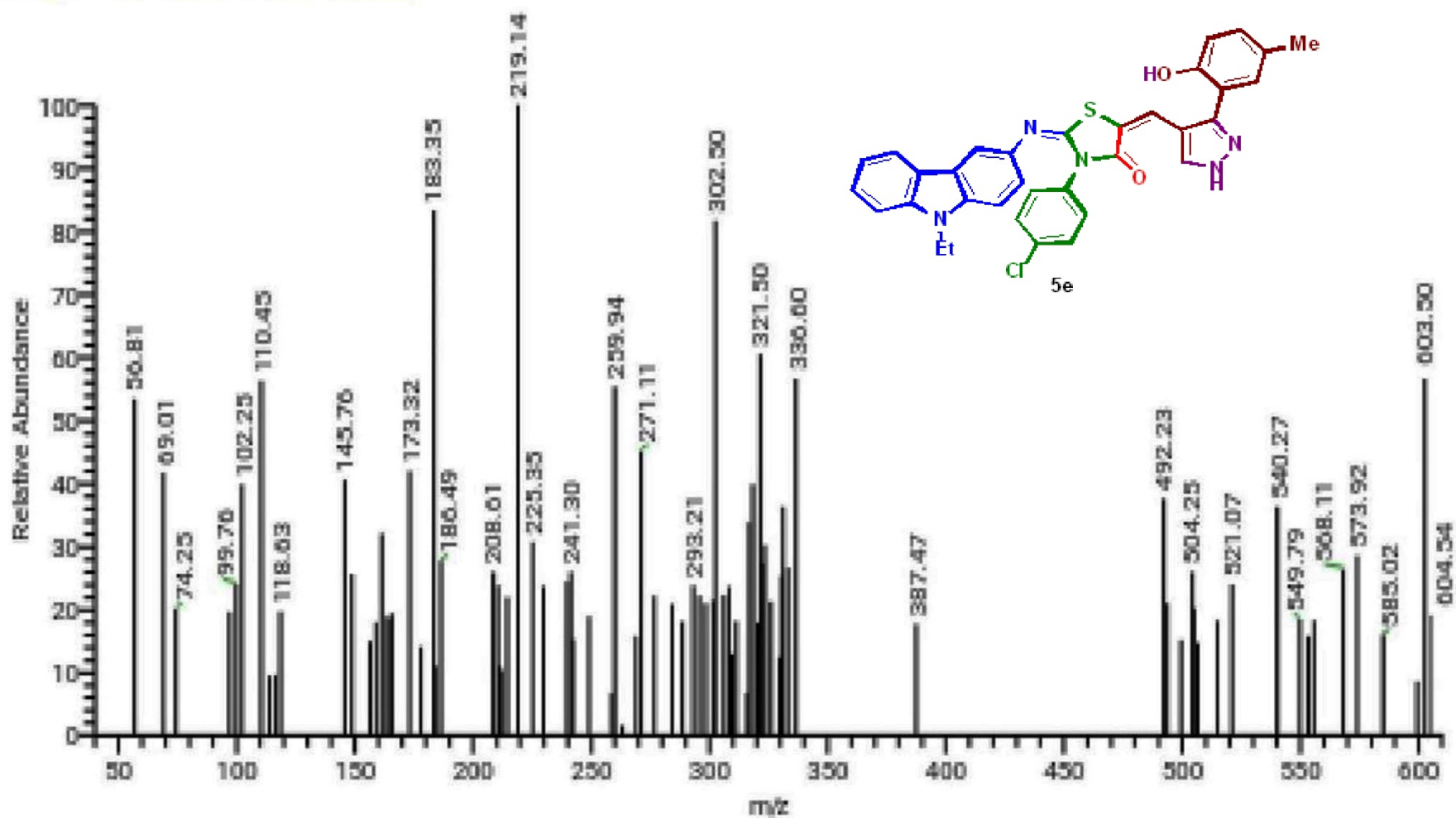


Figure S81: The mass spectrum of compound 5e.