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SUPPLEMENTARY MATERIALS

Cyclization of Arylhydrazones of Cross-Conjugated Enynones: Synthesis of Luminescent 1,5-Diaryl-3-styryl-1*H*-pyrazoles

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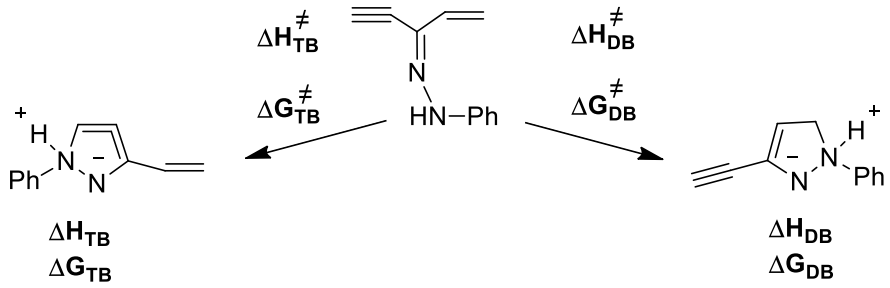
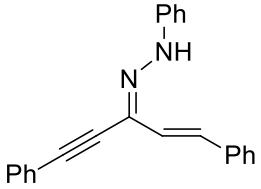


Method	$\Delta H_{TB}^{\neq}$	$\Delta G_{TB}^{\neq}$	ΔH_{TB}	ΔG_{TB}	$\Delta H_{DB}^{\neq}$	$\Delta G_{DB}^{\neq}$	ΔH_{DB}	ΔG_{DB}
SMD(DMF)–M06-2X/MG3S	**24.67**	**25.74**	**15.39**	**16.84**	**34.56**	**35.66**	**18.84**	**20.26**
SMD(DMF)–M06-2X/6-311+G(2df,2pd)//SMD(DMF)–M06-2X/6-31+G(d,p)	24.69	25.78	15.48	16.89	34.48	35.91	18.96	20.66
SMD(DMF)–M06-2X/6-31+G(d,p)	22.42	23.51	12.55	13.95	32.93	34.38	17.91	19.61
SMD(DMF)–M06-2X/6-311+G(2df,2pd)//SMD(DMF)–B3LYP/6-31+G(d,p)	24.48	26.06	15.25	16.40	34.33	35.88	18.73	20.29
SMD(DMF)–B3LYP/6-31+G(d,p)	18.98	20.56	13.38	14.53	32.91	34.46	22.47	24.04
SMD(DMF)–M06-2X/6-311+G(2df,2pd)//SMD(DMF)–B3LYP/6-31G(d)	**24.32**	**25.90**	**15.20**	**16.61**	**34.30**	**35.88**	**18.78**	**20.08**
SMD(DMF)–B3LYP/6-31G(d)	20.45	22.03	16.67	18.08	34.54	36.13	24.85	26.14

Geometries of molecules and transition states

SMD(DMFA)-M062X/6-311+G(2df,2pd)//SMD(DMFA)- B3LYP/6-31G(d)



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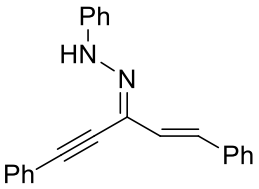

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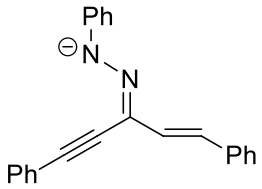

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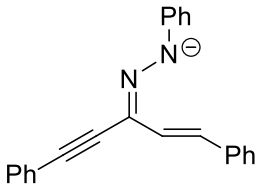

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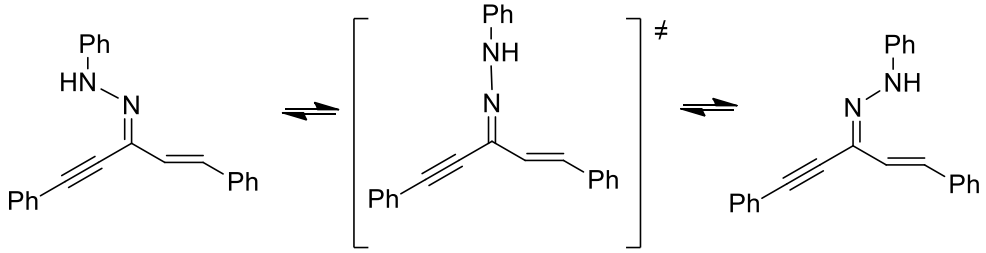

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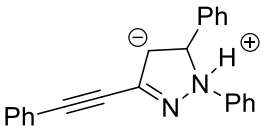

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H,0,0.8277116481,-1.6680796659,-1.5718677065
C,0,3.604220105,0.4916132891,0.0778220616
H,0,2.0154647233,1.2830487956,1.3138910196
C,0,1.8124696436,-4.6809379717,2.0191391787
H,0,2.9929123134,-3.5933392701,3.462789973
H,0,0.4534092313,-5.5005087933,0.5568556832
C,0,-7.9398628608,-2.0457022016,-2.0559459443
H,0,-6.642791982,-2.2464617277,-0.344914452
C,0,-6.9838092753,-0.9462084691,-3.9877107054
H,0,-4.9409250253,-0.2862686233,-3.7847986696
C,0,3.9341334503,-0.3932080988,-0.9514687371
H,0,3.1917926616,-1.8598153047,-2.3500231668
H,0,4.3708155199,1.1088995479,0.5372312309
H,0,2.3859585377,-5.5988074538,2.119617385
C,0,-8.0655434951,-1.5791502347,-3.3679432195
H,0,-8.7777234692,-2.5383557879,-1.5699554595
H,0,-7.0767922471,-0.5820290368,-5.007310207
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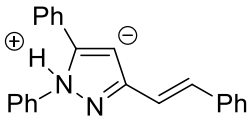
H,0,-9.0014825518,-1.7081570934,-3.9046695199



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C,0,0.2662867511,-1.2119089482,0.0808068324
C,0,0.5008178157,-1.0647273536,1.4470838267
N,0,1.3239089096,-0.8236227758,-0.8719349513
C,0,-0.5082471523,-1.4197843522,2.3409344069
H,0,1.4525872698,-0.6838374506,1.8031651149
C,0,-0.9425806263,-1.6964770016,-0.4095687119
N,0,1.5008453247,0.6279500459,-0.8691266346
H,0,1.0008912092,-1.0636123127,-1.8189728313
C,0,-1.7296670412,-1.9125001565,1.8692249694
H,0,-0.3389480425,-1.3111642213,3.4082464377
C,0,-1.9453095137,-2.0502053562,0.4972698851
H,0,-1.1006018515,-1.795381187,-1.4802750585
C,0,2.7899863427,0.8028940137,-0.6558696449
H,0,-2.510682914,-2.1884818938,2.5719558236
H,0,-2.8921891767,-2.4307469273,0.1257496528
C,0,3.2654344074,2.1783892583,-0.5992024639
C,0,3.6403831451,-0.3978489859,-0.5062604374
C,0,4.5715216446,2.4794757563,-0.4302694758
H,0,2.5091517585,2.9524272953,-0.7077731024
C,0,2.7548135402,-1.4013375168,-0.6417772686
H,0,5.2628565723,1.6437945047,-0.3376302074
C,0,2.9051660615,-2.8606695707,-0.6334902476
C,0,1.9901994316,-3.7478521065,-1.2323734276
C,0,4.0500202237,-3.4054975372,-0.0148467221
C,0,2.211772787,-5.126164008,-1.2062364194
H,0,1.107935536,-3.3749730452,-1.7433467345
C,0,4.2687384682,-4.779630819,0.0052160964
H,0,4.7607076717,-2.729127397,0.4497660544
C,0,3.3478597652,-5.6501315589,-0.5878540594
H,0,1.4923602318,-5.7898846019,-1.6787700826
H,0,5.1572855321,-5.174037705,0.4916045352
H,0,3.5163021552,-6.7234763374,-0.5688053207
C,0,5.1757266294,3.8101510166,-0.3615340446
C,0,4.4328787411,5.0062125418,-0.4444794411
C,0,6.5729128937,3.9023640274,-0.2072223511
C,0,5.0691298561,6.2422544898,-0.3764650397
H,0,3.3538517354,4.9692302183,-0.5622093788
C,0,7.2090979692,5.141147516,-0.139831495
H,0,7.1576722283,2.9879618078,-0.1414872832
C,0,6.4589472635,6.3161642984,-0.2244523825
H,0,4.4812032327,7.1540144509,-0.4418123697
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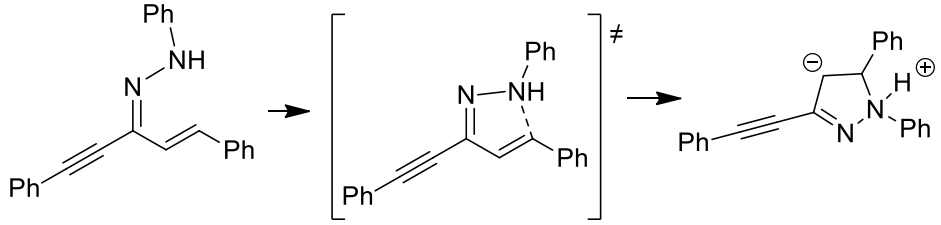
H,0,6.9507911633,7.2838324806,-0.1725972331

Transition state for the reaction



Charge = 0 Multiplicity = 1

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C,0,-1.9041878137,0.9016728257,-0.3118051791
N,0,-0.7105299334,-1.1579137163,-0.2544692533
C,0,-0.5746118192,1.5002728662,-0.2106327682
H,0,-2.7917639305,1.4304144444,0.017556243
C,0,-3.0807164631,-1.2694767964,-0.4182202207
N,0,0.3090813262,-0.1653918748,-0.2841486197
C,0,-0.2355951656,2.3885247542,0.9273141505
H,0,-0.0863712172,1.8366642432,-1.1261424615
C,0,-4.1011930513,-1.92939851,-0.4708839238
C,0,1.4058913739,-0.3967882072,0.6242579386
H,0,0.6739047308,-0.0570080501,-1.2317722888
C,0,-0.8494745335,2.2343454478,2.1831673748
C,0,0.7434092972,3.385965116,0.7694824667
C,0,-5.3045350325,-2.694943389,-0.5288630194
C,0,1.1650784667,-0.9628780911,1.8774689361
C,0,2.6904218289,0.0079782602,0.2514320565
C,0,-0.5086547171,3.0711989268,3.245011561
H,0,-1.5957571959,1.4565742566,2.3182589353
C,0,1.0842337423,4.2227782665,1.8312591577
H,0,1.2270085036,3.5076608348,-0.1971086361
C,0,-5.2571580108,-4.1043940709,-0.5310553975
C,0,-6.5579405766,-2.0508762074,-0.5857680946
C,0,2.2328289674,-1.14055632,2.7585878434
H,0,0.1597270636,-1.2725410619,2.1397997007
C,0,3.7489518352,-0.1686304311,1.1428877146
H,0,2.8578281253,0.4468070918,-0.7293844599
C,0,0.4574731287,4.0672001611,3.0715515748
H,0,-0.992773473,2.9453420127,4.2099047899
H,0,1.8354874162,4.9958364885,1.6930812334
C,0,-6.4354973921,-4.8452839027,-0.5889764866
H,0,-4.2947024434,-4.6054647874,-0.4875607556
C,0,-7.7300505729,-2.8015506838,-0.6425381813
H,0,-6.6001114768,-0.9656813872,-0.5840350499
C,0,3.523202801,-0.7437819274,2.3967116289
H,0,2.0538251197,-1.5890990558,3.731896677
H,0,4.7501353159,0.1382247935,0.853628409
H,0,0.7235283369,4.7173099289,3.9009446391
C,0,-7.6738262045,-4.1985610804,-0.6446160337
H,0,-6.3872850467,-5.9308916605,-0.5909114533
H,0,-8.6902592448,-2.2946639452,-0.6855594447
H,0,4.3498154746,-0.8831006216,3.087843216
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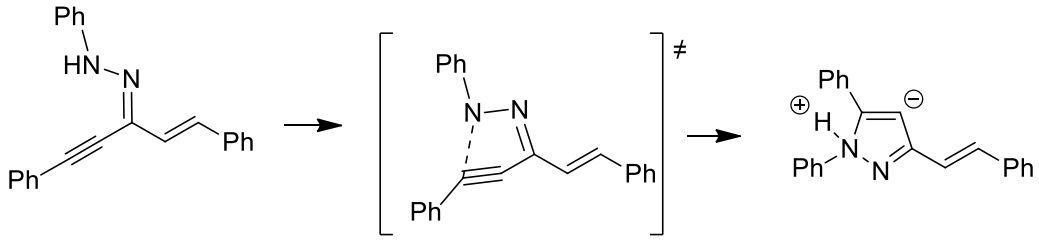
Transition state for the reaction



Charge = 0 Multiplicity = 1

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C,0,3.3688494476,2.1932850655,-0.4202524708
N,0,1.4868458073,0.7744697895,-0.6018889396
C,0,4.6997254534,2.4220581567,-0.4548571005
H,0,2.6534112842,2.9951139751,-0.2553683658
C,0,3.5974639888,-0.349622984,-0.8137283042
N,0,1.1045868535,-0.5839538685,-0.8184482652
C,0,5.3859380643,3.7029447421,-0.2846233909
H,0,5.3469005849,1.5651749459,-0.6340708651
C,0,2.8185382914,-1.3775109116,-0.9545977402
C,0,0.1772358863,-1.0942919187,0.1626249089
H,0,0.6893403204,-0.6433136462,-1.7536347939
C,0,6.7917979623,3.7248564464,-0.3712855332
C,0,4.7128637862,4.9187115124,-0.0434629706
C,0,2.7854527049,-2.8137552126,-1.1420391123
C,0,0.4605036428,-0.9436459708,1.5240514572
C,0,-0.964699985,-1.7818229722,-0.2568772851
C,0,7.5031157823,4.9148640926,-0.2238965413
H,0,7.3233807558,2.7946376474,-0.5570834775
C,0,5.4242394238,6.1059510804,0.103449806
H,0,3.6293520538,4.9354449244,0.0287339444
C,0,1.7816777188,-3.4660568302,-1.8826809561
C,0,3.8223014592,-3.5880495505,-0.5788195263
C,0,-0.4137000918,-1.4834328877,2.4662932939
H,0,1.3509242759,-0.4088253429,1.8379332972
C,0,-1.8295062063,-2.3236944754,0.6962352783
H,0,-1.1784064135,-1.8833365375,-1.3177903468
C,0,6.8214096176,6.1103811725,0.0138501319
H,0,8.5874902397,4.9088262114,-0.2954454322
H,0,4.8894358926,7.0338437539,0.2884908975
C,0,1.8121842388,-4.8504626688,-2.0479350548
H,0,0.9864226229,-2.8901053077,-2.3446674795
C,0,3.8497793707,-4.9691807114,-0.7545488867
H,0,4.5985764167,-3.0921322226,-0.0041010852
C,0,-1.558467142,-2.1757432784,2.0579773199
H,0,-0.196977182,-1.3643731052,3.5242735327
H,0,-2.7192153522,-2.8544794191,0.3691321766
H,0,7.3719183566,7.0403215791,0.1284233706
C,0,2.843275705,-5.6072156383,-1.4862557357
H,0,1.0303173155,-5.3373047307,-2.6246059766
H,0,4.6559700579,-5.5496305534,-0.3137237457
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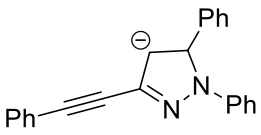

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N,0,0.0582733521,-1.0051083699,0.3103231418
C,0,1.5316829143,0.4530654582,-0.9898977661
H,0,-0.3031186765,1.6011210629,-1.7813982267
C,0,-2.0755855963,-0.0783128784,-0.2408655991
N,0,1.4006770416,-0.7105860989,-0.0774908677
C,0,2.3202871443,1.631732945,-0.3923525184
H,0,2.0789216783,0.1501386344,-1.9058186827
C,0,-3.2874136178,-0.0617837279,-0.115842262
C,0,2.4046231225,-1.5953844197,0.1982173203
C,0,2.1563868213,2.0111987708,0.9477868984
C,0,3.1697541514,2.3931848441,-1.2048028153
C,0,-4.7064261726,-0.0423672565,0.0341257789
C,0,2.1532574601,-2.7727593941,0.9569052876
C,0,3.7350556274,-1.3774895546,-0.2536957079
C,0,2.8290632993,3.120521562,1.4622419132
H,0,1.5021676874,1.4273607983,1.590832326
C,0,3.8366781796,3.5126558253,-0.6973123374
H,0,3.312216688,2.1036166488,-2.2448913837
C,0,-5.3473505866,-0.9467709194,0.9074188723
C,0,-5.4938311945,0.880990334,-0.6860100002
C,0,3.179443856,-3.66775506,1.2391339526
H,0,1.1441285287,-2.9627059886,1.3020347495
C,0,4.7435603277,-2.292546034,0.0400985393
H,0,3.9744063267,-0.490653284,-0.8297377353
C,0,3.6696677768,3.8791980516,0.6398207282
H,0,2.6977418329,3.3957043583,2.5062400364
H,0,4.4907564751,4.0925857022,-1.3444300052
C,0,-6.7327280399,-0.924009079,1.0528273603
H,0,-4.7492614907,-1.6610193172,1.4658032234
C,0,-6.8787125228,0.8951237586,-0.5336453749
H,0,-5.009436344,1.581242784,-1.3603308599
C,0,4.4884704395,-3.4463729961,0.7899347613
H,0,2.9509046938,-4.5592172233,1.8207894785
H,0,5.7497841482,-2.0942402561,-0.3246014206
H,0,4.1908212303,4.7452196777,1.0400471099
C,0,-7.5038877245,-0.0049913214,0.3347125253
H,0,-7.2122841954,-1.626614448,1.7292970566
H,0,-7.4722017806,1.6119650565,-1.0950483032
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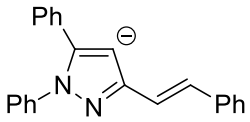

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N,0,0.0494281152,1.2182383835,-0.074718386
C,0,3.2695509398,-0.5264135816,-0.0464555135
H,0,2.5607424726,1.4609527939,-0.2433929711
C,0,0.2085394562,-1.124364223,0.1835857118
N,0,-1.1934096721,0.6964574497,0.0600988101
C,0,4.7158965984,-0.3133400166,-0.1419941669
H,0,2.9574731267,-1.5622203266,0.0855872022
C,0,-1.119234291,-0.7042567275,0.212705958
C,0,-2.2781821117,1.6044008472,0.1854425453
C,0,5.5741669306,-1.4307337935,-0.0760220005
C,0,5.311428234,0.9574983266,-0.2978321088
C,0,-2.3238741799,-1.560387307,0.2505652689
C,0,-2.3674140056,2.6953668746,-0.6920675261
C,0,-3.2410847722,1.4430113129,1.191618782
C,0,6.9591451561,-1.2904412371,-0.1631291519
H,0,5.1399918505,-2.420829053,0.0449459169
C,0,6.6943284814,1.0969949581,-0.3850557744
H,0,4.6864065778,1.8445650255,-0.3502782776
C,0,-3.4654119175,-1.3212393215,-0.5403261086
C,0,-2.316181455,-2.7177763039,1.0537852561
C,0,-3.4119534598,3.610275942,-0.5637097388
H,0,-1.6148843623,2.8166730287,-1.4642649226
C,0,-4.2906182162,2.3564205925,1.3025755424
H,0,-3.1590825634,0.6169052449,1.8896425472
C,0,7.5292680562,-0.0246633724,-0.3188735403
H,0,7.5936740766,-2.1718133816,-0.1093416134
H,0,7.1253094283,2.088098306,-0.504980912
C,0,-4.5548151215,-2.1939407948,-0.5155972441
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H,0,-1.4375461168,-2.9239653883,1.6582634849
C,0,-4.3820109973,3.4430392468,0.4291242569
H,0,-3.4708338927,4.4531589643,-1.2474858849
H,0,-5.0311711269,2.223259065,2.0869380412
H,0,8.607920275,0.0890970364,-0.3871052161
C,0,-4.5326035156,-3.3325839396,0.2939558495
H,0,-5.420477182,-1.9869305325,-1.140448469
H,0,-3.3686699482,-4.4756970467,1.7081909354
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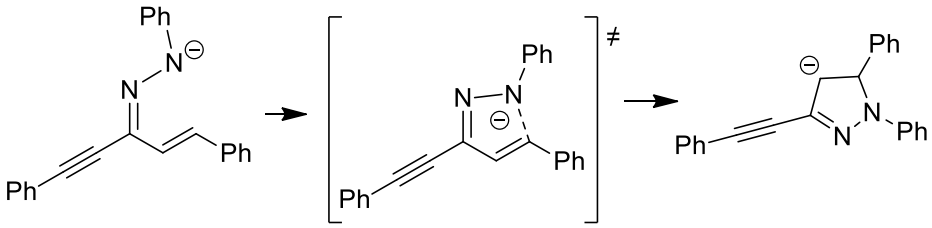
Transition state for the reaction



Charge = -1 Multiplicity = 1

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C,0,2.1356389845,0.0351453048,-0.4701140345
N,0,-1.2341081647,1.0094749824,-0.9241269443
C,0,-2.3807905863,-1.7282273988,-0.5012773548
H,0,-1.8217730665,-0.6612799433,-2.2520305729
C,0,3.3331296175,-0.0023003055,-0.2414370058
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C,0,-3.6577952901,-2.0088723878,-1.0262488691
C,0,4.7322261856,-0.0428889372,0.0306025974
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C,0,-4.5817285421,-2.7712840454,-0.3114971214
H,0,-3.9158070818,-1.6335426065,-2.0147483426
C,0,5.4223786408,1.1213833144,0.4324132522
C,0,5.4546607403,-1.2492972728,-0.0958795934
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H,0,-2.7331314083,-3.3624643578,2.4842821217
H,0,-5.5574987752,-2.9834456606,-0.7422682904
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H,0,4.8763132283,2.0549318797,0.5326768999
C,0,6.8213078058,-1.2846256134,0.1721103634
H,0,4.9334118507,-2.1511777154,-0.4037801761
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H,0,-2.6056899959,4.1573532275,2.1738653628
H,0,-5.5749876354,2.2734973629,-0.3068052263
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C,0,7.4948654272,-0.1255345399,0.5697641187
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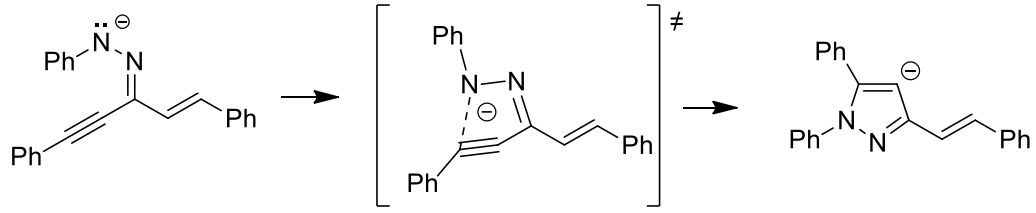
H,0,7.3629349067,-2.2214647682,0.0703076141
H,0,-4.9893167467,3.9142291618,1.4820795387
H,0,8.5608201769,-0.1573530584,0.7783217439

Transition state for the reaction



Charge = -1 Multiplicity = 1

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H,0,2.9008953931,-1.587420105,-0.398869518
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H,0,-5.3915658624,-2.3837193801,1.2281309419
H,0,-4.8307078615,4.6073932916,1.4301603014
H,0,-5.6069850211,-4.0925089824,-0.5707756201

X-ray analysis of compound **4a** was performed on a Bruker Quest diffractometer (Bruker AXS, Inc., Madison, WI, USA) equipped with a Mo anode and multilayer optics (λ = 0.71073 Å). At 100.0(2) K single crystal of $C_{23}H_{18}N_2$ (Fw = 323.3) is monoclinic, space group C2/c: a = 42.8149(15), b = 5.8284(2), c = 30.8813(9) Å, β = 118.624(2)°, V = 6764.4(4) $Å^3$, Z = 16, F(000) = 2736, dcalc = 1.270 g cm^{-3}, μ = 0.075 mm^{-1}. Crystal structures were solved applying SHELXT[3] program and refined with SHELXL[4] using OLEX2 software[5]. The structures were refined by full-matrix least-squares procedure against F^2(hkl). Non-hydrogen atoms were refined anisotropically. There were H(C) positions calculated; the H(N) and H(O) atoms were located on difference Fourier maps and refined using the riding model. Convergence factors were equal to R_1 = 0.088 (for 5364 observed reflections), wR_2 = 0.188, GOF = 1.013 (for 10386 independent reflections, R_{int} = 0.142).

CCDC 2175716 contains the supplementary crystallographic data for this paper. This data can be obtained free of charge via http://www.ccdc.cam.ac.uk/structures/.

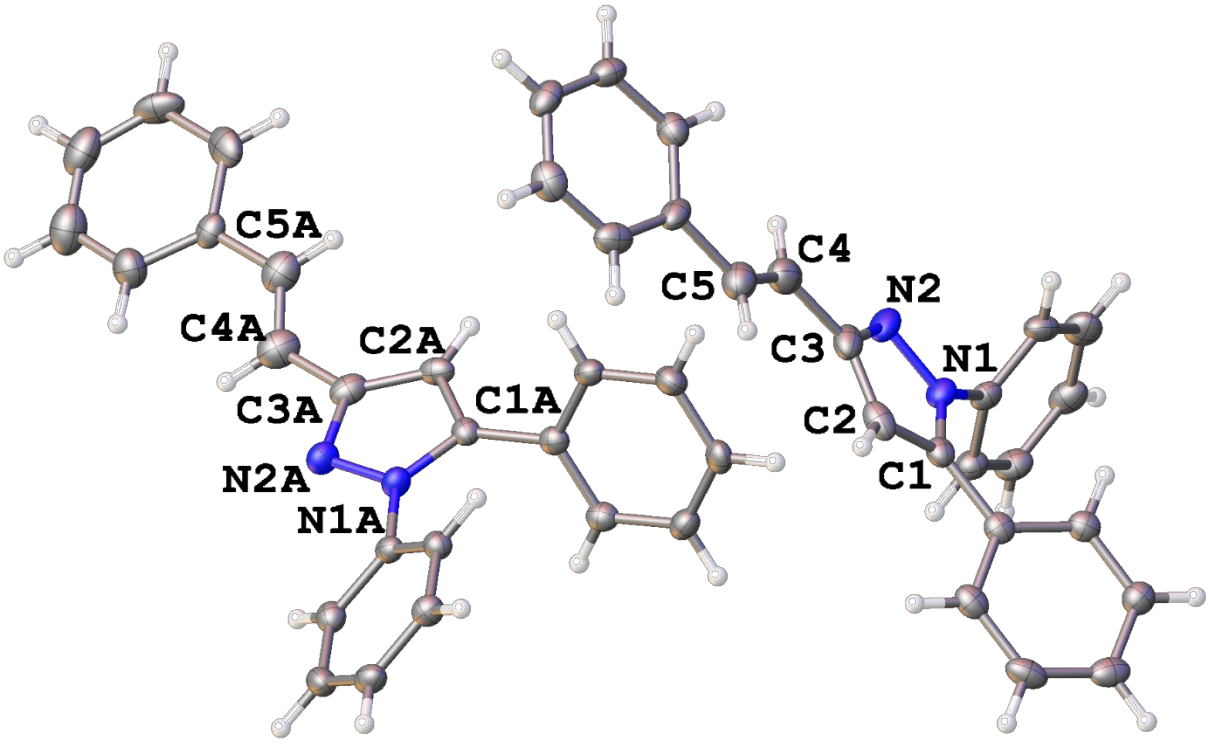


Figure 1. Asymmetric unit of **4a** in representation of atoms with thermal ellipsoids.

Table 1 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **4a**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N1	7527.4(6)	7185(4)	6242.7(8)	23.8(5)
N2	7266.6(6)	8799(4)	6120.0(9)	29.3(6)
C1	7562.7(7)	5780(5)	6618.2(10)	22.2(6)
C2	7307.8(8)	6520(5)	6740.5(11)	29.4(7)
C3	7136.2(7)	8383(5)	6427.3(11)	30.5(7)
C4	6850.5(8)	9968(6)	6388.0(11)	33.9(7)
C5	6678.9(8)	9836(6)	6633.6(12)	35.3(7)
C6	6390.3(7)	11427(5)	6569.3(11)	27.6(6)
C7	6159.9(8)	10715(5)	6741.2(10)	30.3(7)
C8	5874.5(8)	12054(6)	6674.4(11)	33.1(7)
C9	5815.6(8)	14134(5)	6439.9(11)	30.3(7)
C10	6044.7(8)	14888(5)	6273.5(11)	28.6(6)
C11	6331.6(8)	13546(5)	6336.2(11)	28.5(6)
C12	7841.1(7)	4015(5)	6850.3(10)	22.2(6)
C13	7772.7(8)	2090(5)	7056.7(10)	26.1(6)
C14	8031.8(8)	428(5)	7287.6(10)	30.3(7)
C15	8363.3(8)	652(5)	7314.7(10)	29.7(7)
C16	8436.0(8)	2580(5)	7116.0(10)	27.4(6)
C17	8178.3(7)	4258(5)	6887.6(10)	23.7(6)
C18	7698.9(7)	7088(5)	5944.2(10)	22.8(6)
C19	7885.3(7)	8986(5)	5922.6(10)	27.3(6)
C20	8041.7(8)	8936(6)	5620.7(11)	33.5(7)
C21	8010.4(8)	7004(5)	5344.5(11)	32.3(7)
C22	7827.5(8)	5108(5)	5371.3(11)	29.1(7)
C23	7669.8(7)	5134(5)	5672.6(10)	25.1(6)
N1A	5348.2(6)	2779(4)	4144.7(8)	22.3(5)
N2A	5033.5(6)	3077(4)	3721.4(8)	26.4(5)
C1A	5601.1(7)	4275(5)	4169.5(10)	20.2(5)
C2A	5445.5(7)	5630(5)	3755.6(10)	23.8(6)
C3A	5096.1(8)	4836(5)	3486.6(10)	27.0(6)
C4A	4785.0(9)	5567(6)	3024.5(12)	38.4(8)
C5A	4751.7(9)	7499(6)	2801.8(12)	37.1(8)
C6A	4438.5(7)	8246(5)	2343.9(10)	25.0(6)
C7A	4452.5(8)	10395(6)	2138.2(13)	37.7(8)
C8A	4156.2(10)	11099(6)	1682.9(13)	40.6(8)
C9A	3867.4(9)	9699(7)	1459.6(13)	43.6(9)
C10A	3855.0(9)	7690(7)	1662.3(13)	46.3(9)

Table 1 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **4a**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C11A	4130.3(8)	6979(6)	2088.9(12)	35.3(7)
C12A	5967.6(7)	4399(5)	4576.9(10)	21.3(6)
C13A	6081.5(7)	6384(5)	4860.9(10)	22.9(6)
C14A	6421.5(7)	6504(5)	5256.4(11)	27.1(6)
C15A	6652.3(7)	4660(5)	5370.5(10)	25.0(6)
C16A	6541.4(7)	2691(5)	5084.6(10)	24.6(6)
C17A	6200.4(7)	2553(5)	4690.1(10)	23.5(6)
C18A	5363.9(7)	1132(5)	4500.4(10)	20.3(5)
C19A	5566.9(7)	1556(5)	5003.8(10)	21.5(6)
C20A	5569.3(7)	-53(5)	5335.7(10)	24.4(6)
C21A	5369.9(7)	-2043(5)	5171.3(11)	26.9(6)
C22A	5163.1(7)	-2425(5)	4668.6(11)	27.0(6)
C23A	5161.0(7)	-839(5)	4333.7(10)	24.2(6)

Table 2 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **4a**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	23.2(12)	23.3(12)	25.7(13)	-3.7(10)	12.5(10)	3.7(9)
N2	24.4(12)	29.2(14)	32.3(14)	-7.7(11)	11.8(11)	5.6(10)
C1	22.4(13)	22.0(14)	23.3(14)	-6.5(11)	11.8(11)	-3.5(10)
C2	31.1(16)	35.7(18)	29.3(16)	-15.1(13)	20.8(13)	-12.4(13)
C3	22.8(14)	30.6(17)	36.0(17)	-13.1(13)	12.3(13)	-2.8(12)
C4	31.6(17)	33.3(18)	30.5(17)	-1.7(13)	9.9(14)	-2.8(13)
C5	30.9(16)	36.2(18)	37.9(18)	-7.7(14)	15.6(15)	0.0(13)
C6	22.8(14)	25.6(15)	28.6(15)	-8.2(12)	7.7(12)	4.9(11)
C7	38.4(17)	26.5(16)	20.8(15)	-0.2(12)	10.1(13)	0.5(13)
C8	35.8(17)	41.9(19)	28.3(16)	-5.5(14)	20.8(14)	-5.2(14)
C9	26.4(15)	34.4(17)	27.6(16)	-6.4(13)	10.9(13)	8.0(12)
C10	32.8(16)	23.0(15)	27.3(15)	0.3(12)	12.2(13)	5.9(12)
C11	27.9(15)	30.2(17)	31.1(16)	-6.2(13)	17.1(13)	-3.6(12)
C12	25.0(14)	24.8(15)	17.6(13)	-4.1(11)	10.8(11)	-2.3(11)
C13	31.0(15)	28.3(16)	21.0(14)	-5.5(12)	13.9(12)	-7.3(12)
C14	46.7(19)	22.3(15)	23.7(15)	-1.8(12)	18.3(14)	-7.8(13)
C15	41.2(18)	22.8(15)	20.2(14)	-3.1(11)	10.8(13)	3.7(13)
C16	27.6(15)	28.9(16)	24.6(15)	-1.2(12)	11.6(12)	1.1(12)
C17	27.9(14)	24.3(15)	19.9(14)	-1.4(11)	12.1(12)	-1.2(11)

Table 2 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **4a**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C18	24.6(14)	22.7(14)	19.6(13)	2.2(11)	9.3(11)	5.4(11)
C19	32.0(16)	18.7(14)	26.8(15)	1.2(11)	10.5(13)	2.0(11)
C20	38.0(17)	31.5(18)	33.2(17)	12.1(14)	18.9(14)	2.8(13)
C21	37.1(17)	33.3(18)	32.1(17)	10.1(13)	21.1(14)	9.6(13)
C22	36.8(17)	27.0(16)	27.0(15)	-1.1(12)	17.9(13)	6.8(12)
C23	27.1(14)	22.8(15)	24.3(14)	-0.8(11)	11.5(12)	2.1(11)
N1A	21.3(11)	24.9(13)	20.5(12)	3.0(9)	9.7(9)	1.9(9)
N2A	25.9(12)	28.4(14)	22.4(12)	1.5(10)	9.8(10)	2.8(10)
C1A	20.9(13)	20.0(13)	22.1(13)	-3.7(10)	12.3(11)	-0.1(10)
C2A	32.2(15)	20.1(14)	28.3(15)	3.6(11)	21.9(13)	2.7(11)
C3A	34.1(16)	27.7(16)	22.5(14)	0.5(12)	16.3(13)	7.9(12)
C4A	46(2)	41(2)	33.0(18)	2.0(15)	23.1(16)	6.8(15)
C5A	37.3(17)	47(2)	31.6(17)	2.2(15)	20.2(14)	5.9(15)
C6A	21.8(13)	33.5(16)	23.4(14)	2.3(12)	13.7(11)	4.5(11)
C7A	32.7(17)	41.0(19)	53(2)	-7.9(16)	31.3(16)	-5.6(14)
C8A	64(2)	30.6(19)	45(2)	17.1(15)	41.3(18)	14.7(16)
C9A	32.8(18)	64(3)	36.2(19)	4.5(18)	18.2(15)	13.6(17)
C10A	35.2(19)	68(3)	35.3(19)	1.0(18)	16.9(16)	1.3(17)
C11A	31.3(16)	40.4(19)	36.1(18)	-0.6(14)	17.7(14)	-4.0(13)
C12A	23.7(13)	21.5(14)	22.7(14)	1.5(11)	14.4(11)	-0.2(10)
C13A	24.1(14)	19.3(14)	28.5(15)	2.9(11)	15.1(12)	2.3(10)
C14A	27.8(15)	21.7(15)	33.0(16)	-2.5(12)	15.6(13)	-3.4(11)
C15A	19.8(13)	29.3(16)	27.6(15)	2.6(12)	12.5(12)	-3.5(11)
C16A	22.6(14)	26.3(15)	26.6(15)	5.2(12)	13.1(12)	4.2(11)
C17A	28.0(14)	21.9(14)	24.6(14)	-0.9(11)	15.9(12)	0.4(11)
C18A	20.1(13)	19.5(14)	25.1(14)	2.7(11)	13.8(11)	2.1(10)
C19A	21.7(13)	20.8(14)	22.7(14)	-1.3(11)	11.2(11)	-0.5(10)
C20A	26.2(14)	26.2(15)	23.4(14)	2.2(11)	14.0(12)	2.0(11)
C21A	27.5(15)	24.4(15)	33.1(16)	7.2(12)	17.9(13)	3.4(11)
C22A	23.5(14)	22.1(15)	36.3(17)	-1.1(12)	15.0(13)	-2.0(11)
C23A	22.6(14)	25.4(15)	26.2(15)	-3.5(12)	13.1(12)	0.6(11)

Table 3 Bond Lengths for **4a**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	N2	1.367(3)	N1A	N2A	1.366(3)
N1	C1	1.368(4)	N1A	C1A	1.364(3)
N1	C18	1.429(3)	N1A	C18A	1.436(3)
N2	C3	1.333(4)	N2A	C3A	1.354(4)
C1	C2	1.384(4)	C1A	C2A	1.373(4)
C1	C12	1.474(4)	C1A	C12A	1.469(4)
C2	C3	1.405(4)	C2A	C3A	1.397(4)
C3	C4	1.491(4)	C3A	C4A	1.473(4)
C4	C5	1.286(4)	C4A	C5A	1.291(5)
C5	C6	1.480(4)	C5A	C6A	1.473(4)
C6	C7	1.389(4)	C6A	C7A	1.418(4)
C6	C11	1.390(4)	C6A	C11A	1.382(4)
C7	C8	1.379(4)	C7A	C8A	1.430(5)
C8	C9	1.372(4)	C8A	C9A	1.361(5)
C9	C10	1.379(4)	C9A	C10A	1.341(5)
C10	C11	1.389(4)	C10A	C11A	1.345(4)
C12	C13	1.389(4)	C12A	C13A	1.391(4)
C12	C17	1.399(4)	C12A	C17A	1.393(4)
C13	C14	1.386(4)	C13A	C14A	1.383(4)
C14	C15	1.387(4)	C14A	C15A	1.386(4)
C15	C16	1.386(4)	C15A	C16A	1.386(4)
C16	C17	1.387(4)	C16A	C17A	1.385(4)
C18	C19	1.384(4)	C18A	C19A	1.392(4)
C18	C23	1.384(4)	C18A	C23A	1.382(4)
C19	C20	1.385(4)	C19A	C20A	1.385(4)
C20	C21	1.380(4)	C20A	C21A	1.384(4)
C21	C22	1.379(4)	C21A	C22A	1.388(4)
C22	C23	1.387(4)	C22A	C23A	1.384(4)

Table 4 Bond Angles for **4a**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	N1	C1	113.0(2)	N2A	N1A	C18A	118.7(2)
N2	N1	C18	116.9(2)	C1A	N1A	N2A	111.4(2)
C1	N1	C18	129.9(2)	C1A	N1A	C18A	129.8(2)
C3	N2	N1	104.0(2)	C3A	N2A	N1A	104.5(2)
N1	C1	C2	105.3(2)	N1A	C1A	C2A	107.3(2)
N1	C1	C12	124.4(2)	N1A	C1A	C12A	125.0(2)
C2	C1	C12	130.1(3)	C2A	C1A	C12A	127.7(3)
C1	C2	C3	105.9(3)	C1A	C2A	C3A	105.5(2)
N2	C3	C2	111.8(3)	N2A	C3A	C2A	111.3(2)
N2	C3	C4	115.9(3)	N2A	C3A	C4A	114.8(3)
C2	C3	C4	132.3(3)	C2A	C3A	C4A	133.9(3)
C5	C4	C3	126.4(3)	C5A	C4A	C3A	125.9(3)
C4	C5	C6	124.0(3)	C4A	C5A	C6A	125.9(3)
C7	C6	C5	117.5(3)	C7A	C6A	C5A	118.4(3)
C7	C6	C11	118.5(3)	C11A	C6A	C5A	124.8(3)
C11	C6	C5	123.9(3)	C11A	C6A	C7A	116.8(3)
C8	C7	C6	121.0(3)	C6A	C7A	C8A	119.1(3)
C9	C8	C7	120.3(3)	C9A	C8A	C7A	119.2(3)
C8	C9	C10	119.6(3)	C10A	C9A	C8A	121.1(3)
C9	C10	C11	120.5(3)	C9A	C10A	C11A	121.0(4)
C10	C11	C6	120.1(3)	C10A	C11A	C6A	122.9(3)
C13	C12	C1	119.2(3)	C13A	C12A	C1A	119.3(2)
C13	C12	C17	118.7(3)	C13A	C12A	C17A	119.4(3)
C17	C12	C1	122.1(3)	C17A	C12A	C1A	121.3(3)
C14	C13	C12	120.5(3)	C14A	C13A	C12A	120.1(3)
C13	C14	C15	120.6(3)	C13A	C14A	C15A	120.4(3)
C16	C15	C14	119.3(3)	C16A	C15A	C14A	119.7(3)
C15	C16	C17	120.3(3)	C17A	C16A	C15A	120.3(3)
C16	C17	C12	120.6(3)	C16A	C17A	C12A	120.1(3)
C19	C18	N1	119.1(3)	C19A	C18A	N1A	120.7(2)
C23	C18	N1	119.9(3)	C23A	C18A	N1A	118.7(2)
C23	C18	C19	121.0(3)	C23A	C18A	C19A	120.5(3)
C18	C19	C20	119.4(3)	C20A	C19A	C18A	119.0(3)
C21	C20	C19	119.9(3)	C21A	C20A	C19A	120.7(3)
C22	C21	C20	120.4(3)	C20A	C21A	C22A	119.7(3)
C21	C22	C23	120.3(3)	C23A	C22A	C21A	120.0(3)
C18	C23	C22	118.9(3)	C18A	C23A	C22A	119.9(3)

Table 5 Torsion Angles for **4a**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N1	N2	C3	C2	-0.5(3)	N1A	N2A	C3A	C2A	0.3(3)
N1	N2	C3	C4	177.9(2)	N1A	N2A	C3A	C4A	-177.0(2)
N1	C1	C2	C3	-0.8(3)	N1A	C1A	C2A	C3A	-1.1(3)
N1	C1	C12	C13	-151.9(3)	N1A	C1A	C12A	C13A	-116.3(3)
N1	C1	C12	C17	30.8(4)	N1A	C1A	C12A	C17A	62.4(4)
N1	C18	C19	C20	-177.7(3)	N1A	C18A	C19A	C20A	178.6(2)
N1	C18	C23	C22	177.7(2)	N1A	C18A	C23A	C22A	-178.2(2)
N2	N1	C1	C2	0.6(3)	N2A	N1A	C1A	C2A	1.3(3)
N2	N1	C1	C12	-174.9(2)	N2A	N1A	C1A	C12A	180.0(2)
N2	N1	C18	C19	61.7(3)	N2A	N1A	C18A	C19A	-143.0(3)
N2	N1	C18	C23	-116.8(3)	N2A	N1A	C18A	C23A	34.2(3)
N2	C3	C4	C5	177.3(3)	N2A	C3A	C4A	C5A	162.1(3)
C1	N1	N2	C3	0.0(3)	C1A	N1A	N2A	C3A	-1.0(3)
C1	N1	C18	C19	-124.1(3)	C1A	N1A	C18A	C19A	32.5(4)
C1	N1	C18	C23	57.5(4)	C1A	N1A	C18A	C23A	-150.3(3)
C1	C2	C3	N2	0.9(3)	C1A	C2A	C3A	N2A	0.4(3)
C1	C2	C3	C4	-177.2(3)	C1A	C2A	C3A	C4A	177.1(3)
C1	C12	C13	C14	-178.5(2)	C1A	C12A	C13A	C14A	177.8(3)
C1	C12	C17	C16	178.9(3)	C1A	C12A	C17A	C16A	-178.2(2)
C2	C1	C12	C13	33.8(4)	C2A	C1A	C12A	C13A	62.1(4)
C2	C1	C12	C17	-143.5(3)	C2A	C1A	C12A	C17A	-119.2(3)
C2	C3	C4	C5	-4.7(5)	C2A	C3A	C4A	C5A	-14.5(6)
C3	C4	C5	C6	-178.3(3)	C3A	C4A	C5A	C6A	-179.0(3)
C4	C5	C6	C7	161.1(3)	C4A	C5A	C6A	C7A	-177.5(3)
C4	C5	C6	C11	-17.0(5)	C4A	C5A	C6A	C11A	1.0(5)
C5	C6	C7	C8	-177.0(3)	C5A	C6A	C7A	C8A	177.4(3)
C5	C6	C11	C10	177.3(3)	C5A	C6A	C11A	C10A	-177.6(3)
C6	C7	C8	C9	-0.7(5)	C6A	C7A	C8A	C9A	0.4(5)
C7	C6	C11	C10	-0.9(4)	C7A	C6A	C11A	C10A	0.9(5)
C7	C8	C9	C10	-0.4(5)	C7A	C8A	C9A	C10A	0.8(5)
C8	C9	C10	C11	0.8(4)	C8A	C9A	C10A	C11A	-1.1(6)
C9	C10	C11	C6	-0.2(4)	C9A	C10A	C11A	C6A	0.2(5)
C11	C6	C7	C8	1.3(4)	C11A	C6A	C7A	C8A	-1.2(4)
C12	C1	C2	C3	174.3(3)	C12A	C1A	C2A	C3A	-179.6(3)
C12	C13	C14	C15	-0.3(4)	C12A	C13A	C14A	C15A	0.6(4)
C13	C12	C17	C16	1.5(4)	C13A	C12A	C17A	C16A	0.5(4)
C13	C14	C15	C16	1.2(4)	C13A	C14A	C15A	C16A	0.3(4)

Table 5 Torsion Angles for **4a**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C14	C15	C16	C17	-0.7(4)	C14A	C15A	C16A	C17A	-0.7(4)
C15	C16	C17	C12	-0.7(4)	C15A	C16A	C17A	C12A	0.4(4)
C17	C12	C13	C14	-1.0(4)	C17A	C12A	C13A	C14A	-1.0(4)
C18	N1	N2	C3	175.1(2)	C18A	N1A	N2A	C3A	175.2(2)
C18	N1	C1	C2	-173.9(3)	C18A	N1A	C1A	C2A	-174.4(3)
C18	N1	C1	C12	10.6(4)	C18A	N1A	C1A	C12A	4.2(4)
C18	C19	C20	C21	0.1(4)	C18A	C19A	C20A	C21A	-0.8(4)
C19	C18	C23	C22	-0.8(4)	C19A	C18A	C23A	C22A	-1.0(4)
C19	C20	C21	C22	-0.7(5)	C19A	C20A	C21A	C22A	-0.5(4)
C20	C21	C22	C23	0.7(5)	C20A	C21A	C22A	C23A	1.0(4)
C21	C22	C23	C18	0.1(4)	C21A	C22A	C23A	C18A	-0.3(4)
C23	C18	C19	C20	0.7(4)	C23A	C18A	C19A	C20A	1.5(4)

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **4a**.

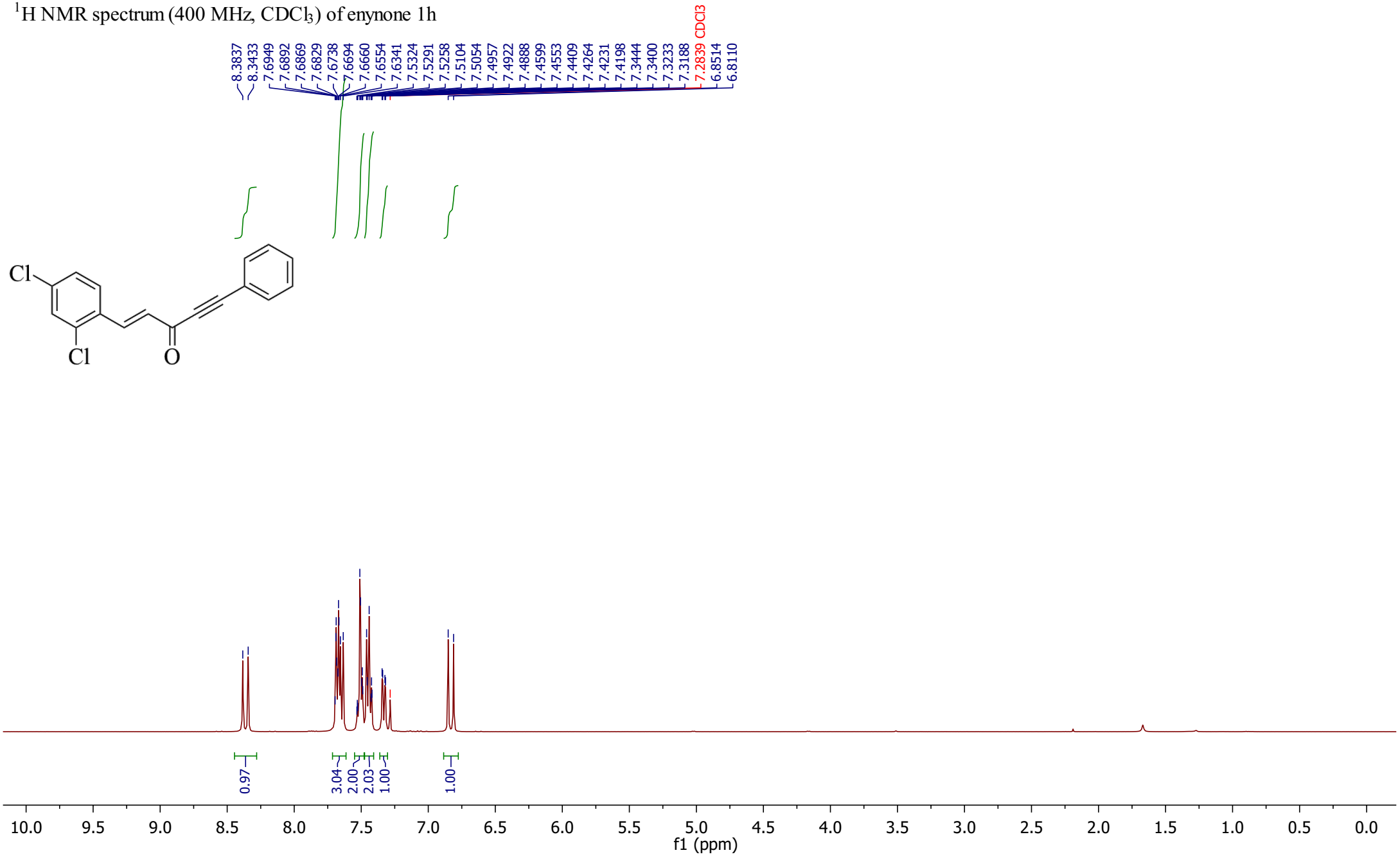
Atom	*x*	*y*	*z*	U(eq)
H2	7258.9	5896.88	6985.95	35
H4	6789.04	11194.88	6159.07	41
H5	6741.3	8645.08	6870.82	42
H7	6199.38	9285.76	6907.18	36
H8	5718.13	11533.48	6791.34	40
H9	5618.07	15049.4	6392.37	36
H10	6006.11	16336.84	6114.83	34
H11	6487.74	14076.38	6219.76	34
H13	7546.43	1911.83	7039.33	31
H14	7982	-877.03	7428.58	36
H15	8538.67	-505.84	7468.11	36
H16	8663.26	2754.06	7136.12	33
H17	8231.28	5582.19	6755.53	28
H19	7905.71	10312.39	6113.36	33
H20	8170.4	10229.72	5603.71	40
H21	8115.48	6978.82	5134.58	39
H22	7809.53	3779.43	5182.59	35
H23	7543.86	3830.91	5692.26	30
H2A	5552.9	6849.46	3670.1	29
H4A	4591.55	4522.89	2877	46
H5A	4946.82	8532.8	2946.36	44

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **4a**.

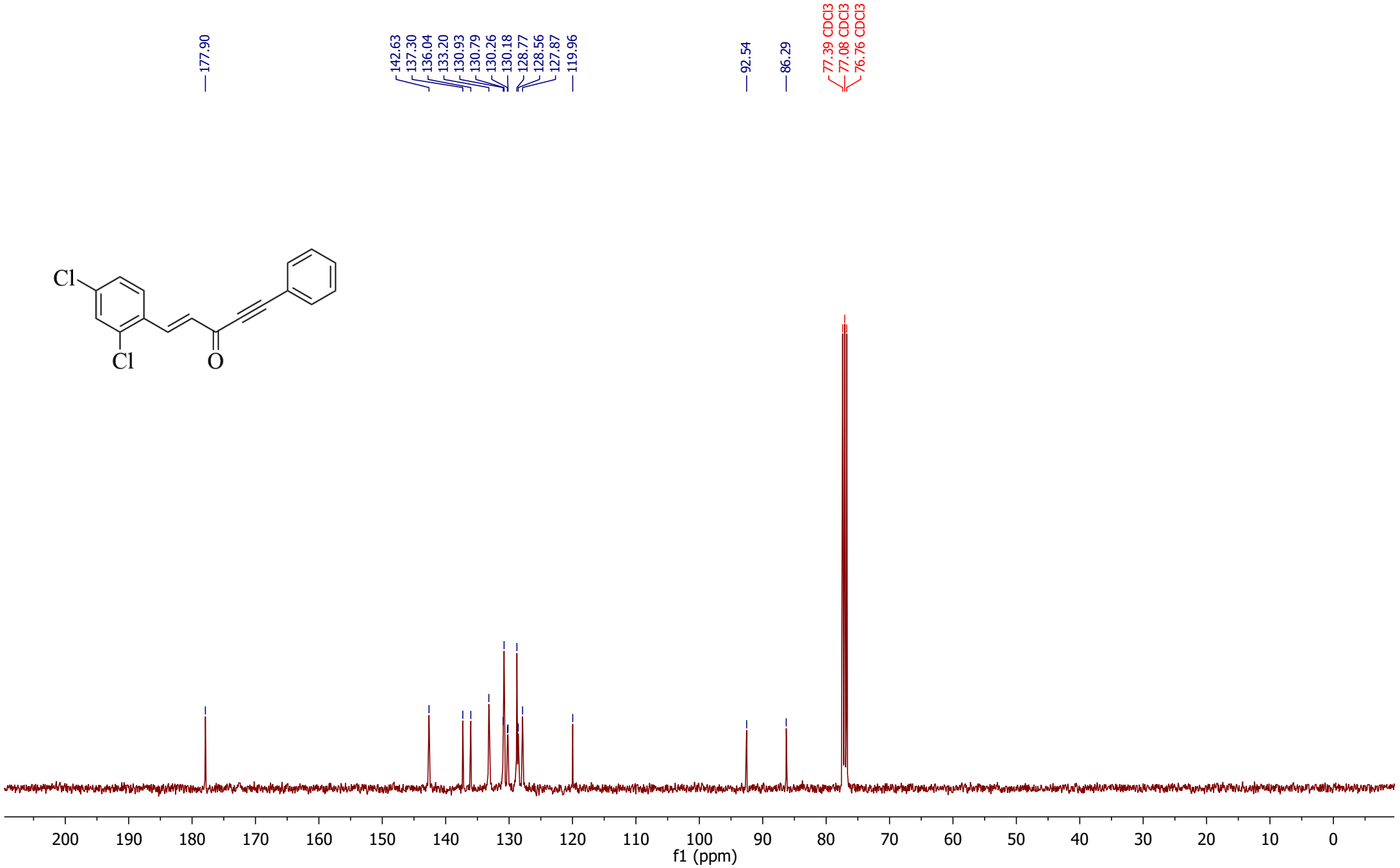
Atom	***x***	***y***	***z***	**U(eq)**
H7A	4655.88	11352.02	2300.51	45
H8A	4160.88	12527.81	1538.02	49
H9A	3671.45	10153.17	1155.1	52
H10A	3648.83	6755.45	1502.26	56
H11A	4112.15	5543.23	2220.81	42
H13A	5925.5	7658.84	4782.87	27
H14A	6497.29	7857.94	5451.05	32
H15A	6885.29	4745.82	5643.43	30
H16A	6699.89	1431.8	5159.54	29
H17A	6125.23	1195.87	4496.34	28
H19A	5701.79	2927.83	5118.04	26
H20A	5709.34	212.71	5679.87	29
H21A	5374.69	-3141.9	5401.55	32
H22A	5022.86	-3776.71	4554.4	32
H23A	5020.2	-1104.49	3989.68	29

Spectroscopic Data

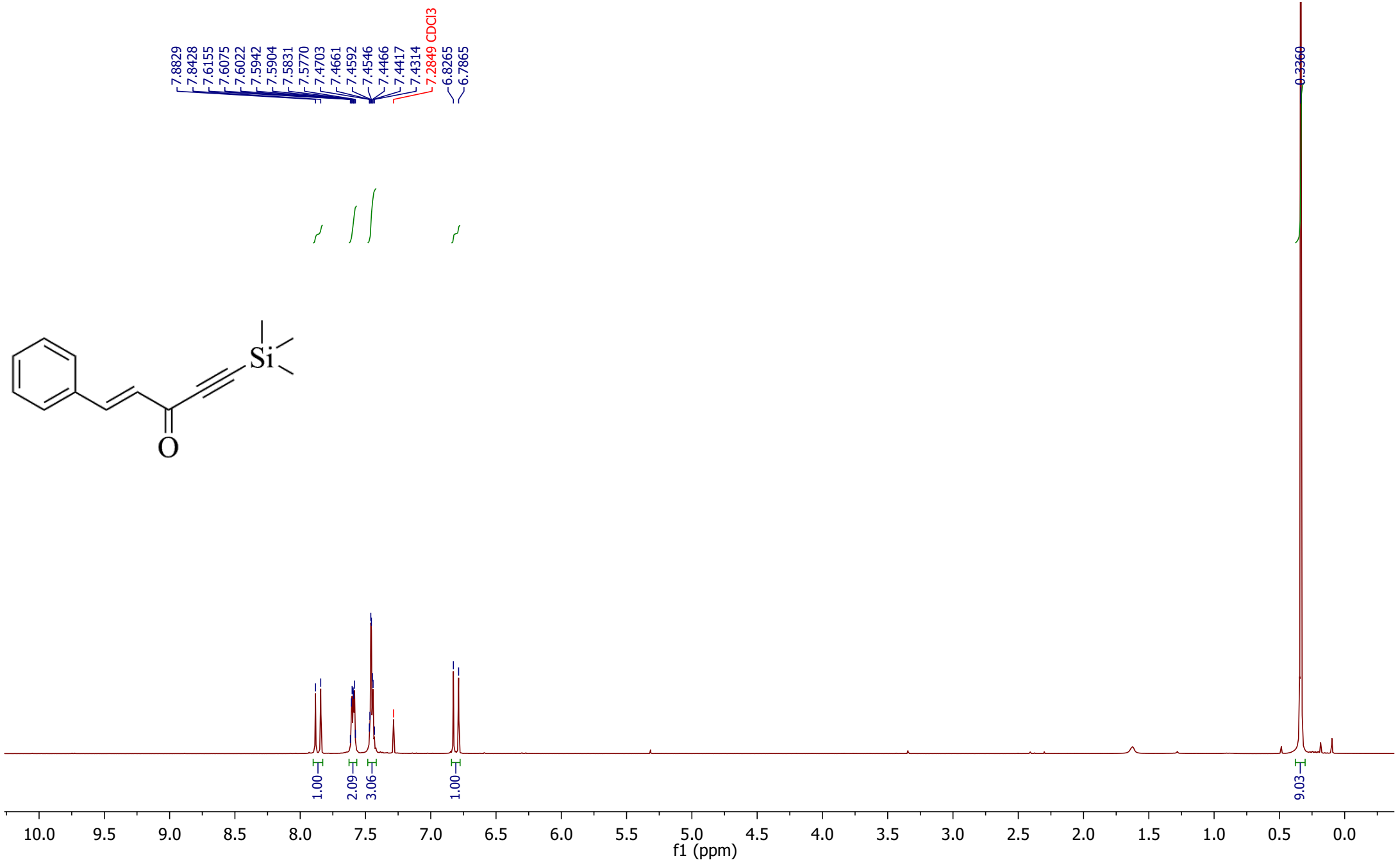
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of enynone 1h



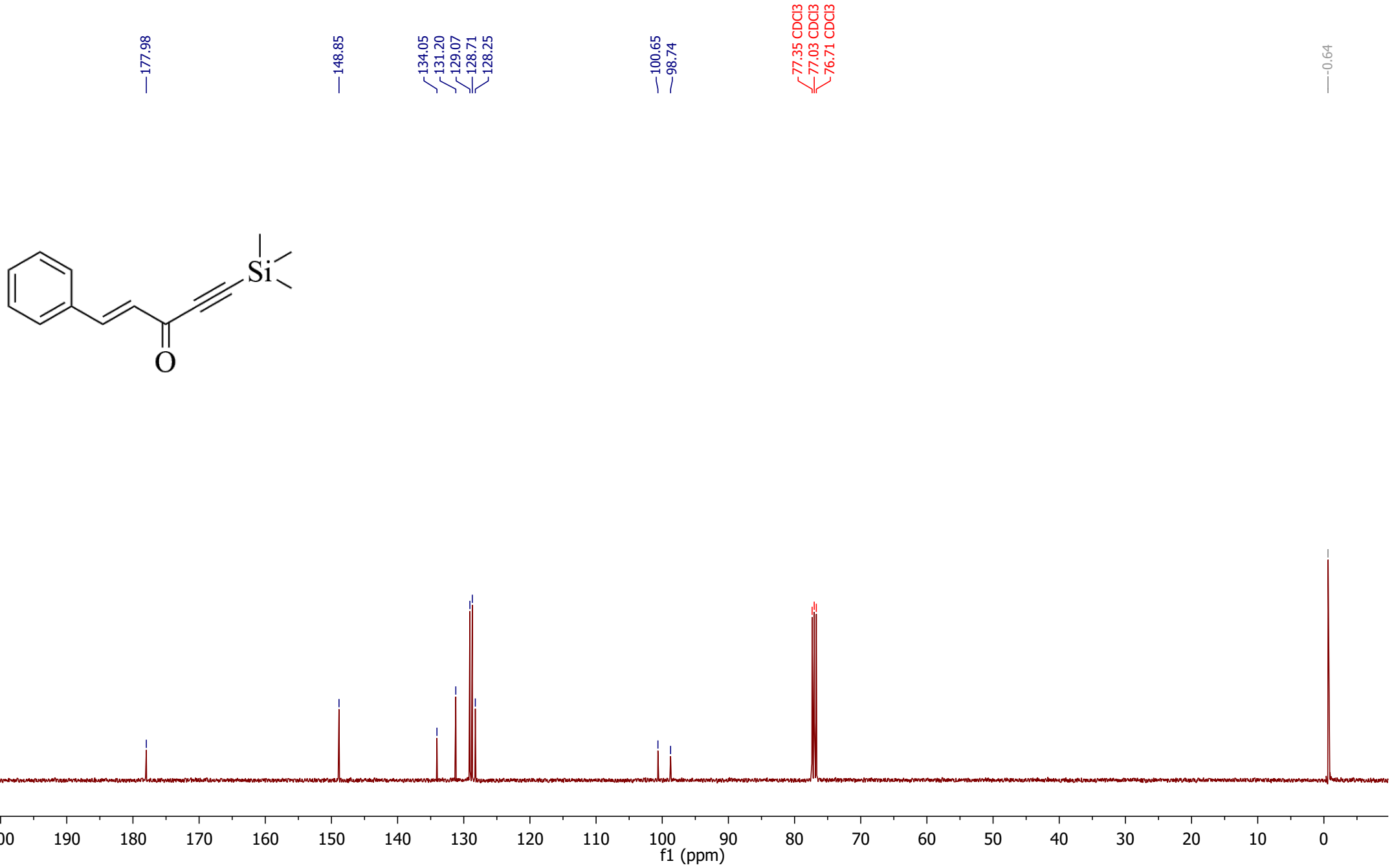
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of enynone 1h



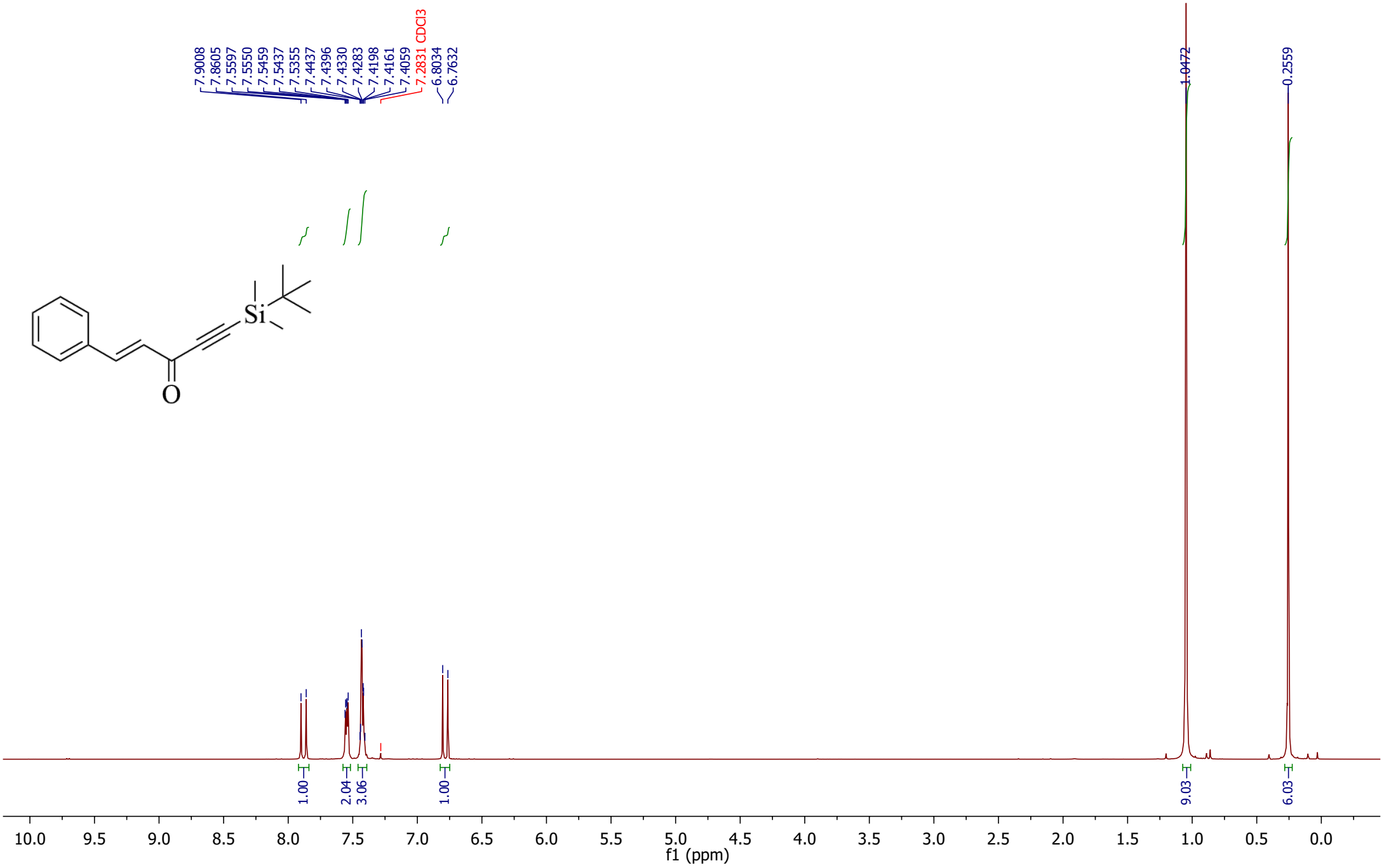
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of enynone 1p



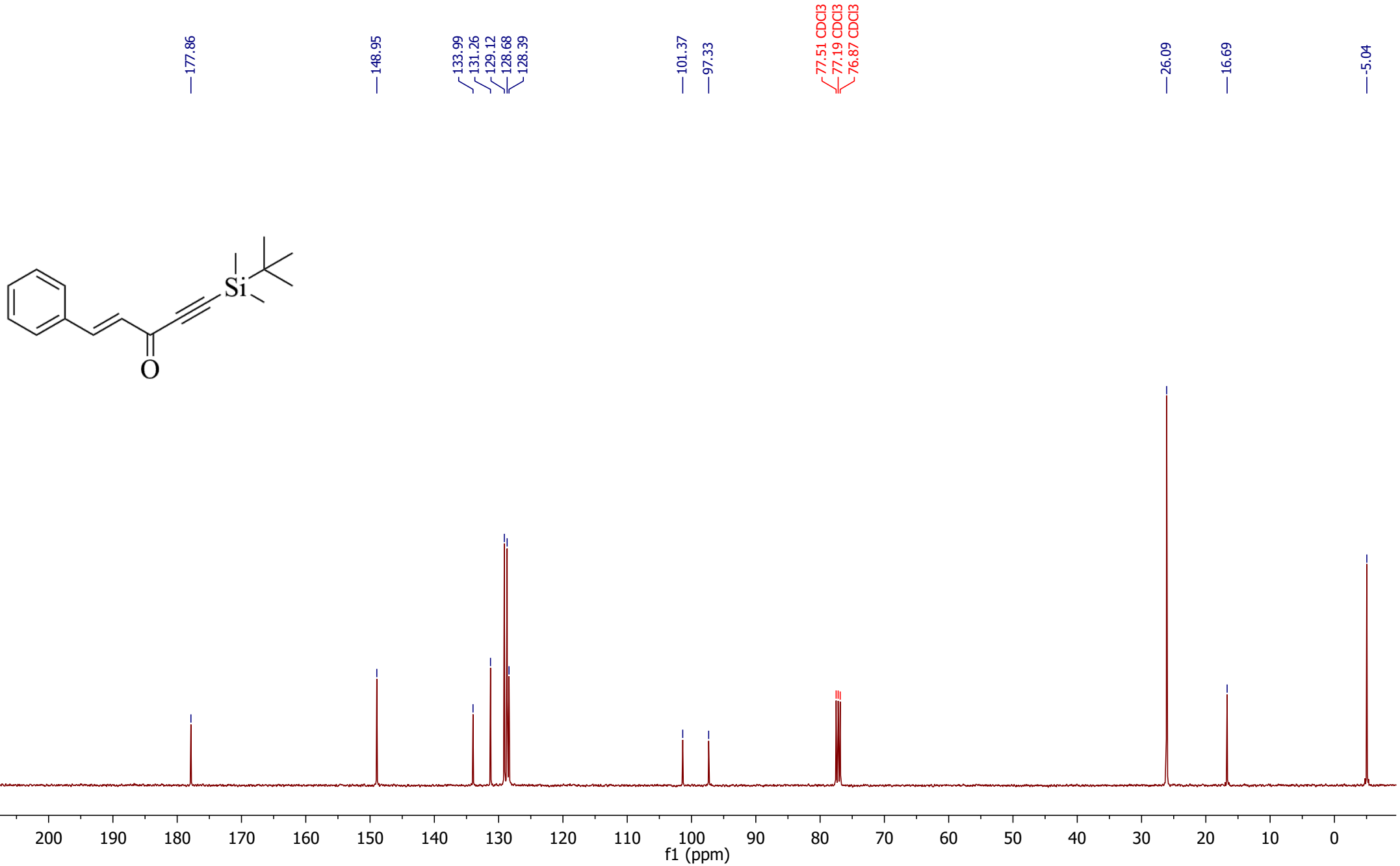
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of enynone 1p



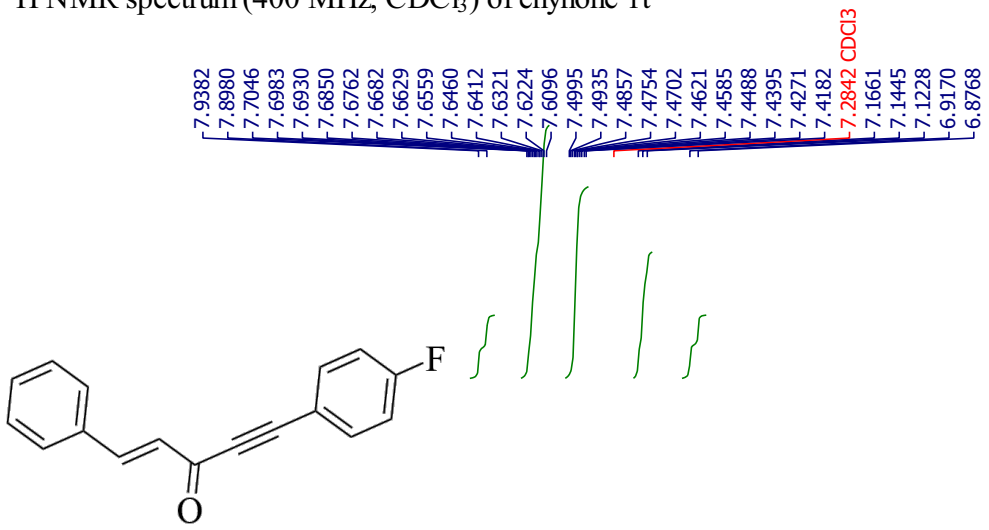
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of enynone 1q

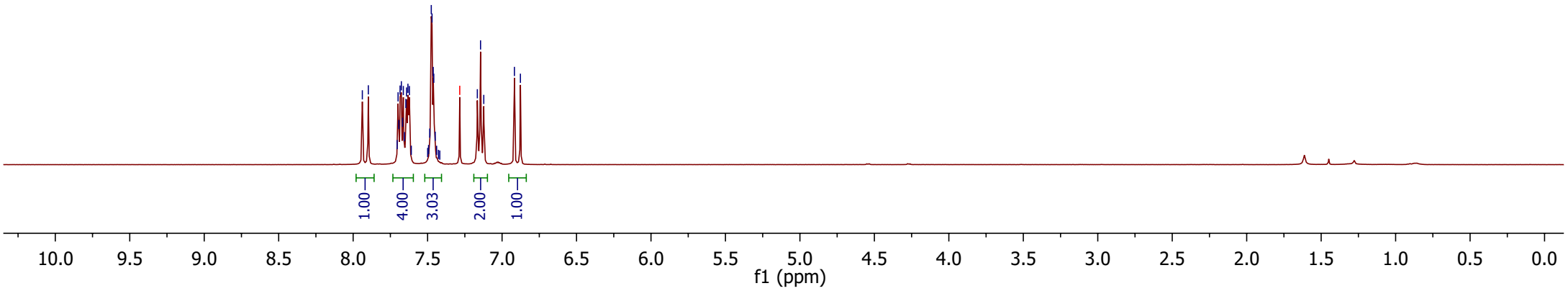


$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of enynone 1q

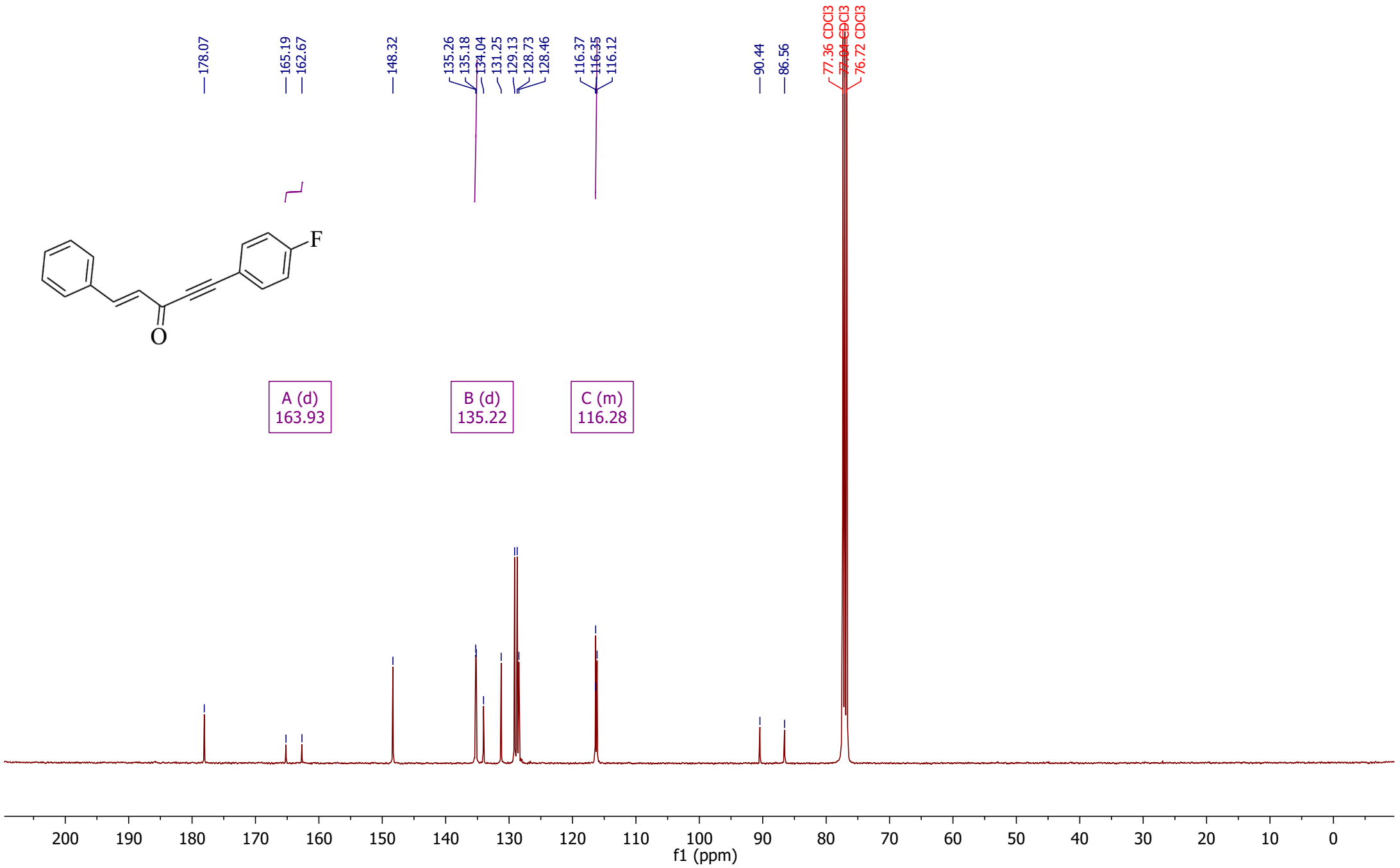


^{1}H NMR spectrum (400 MHz, $CDCl_3$) of enynone 1t

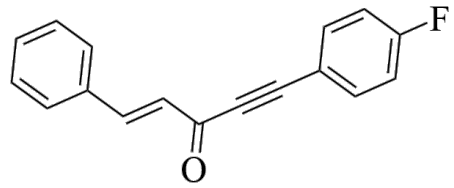




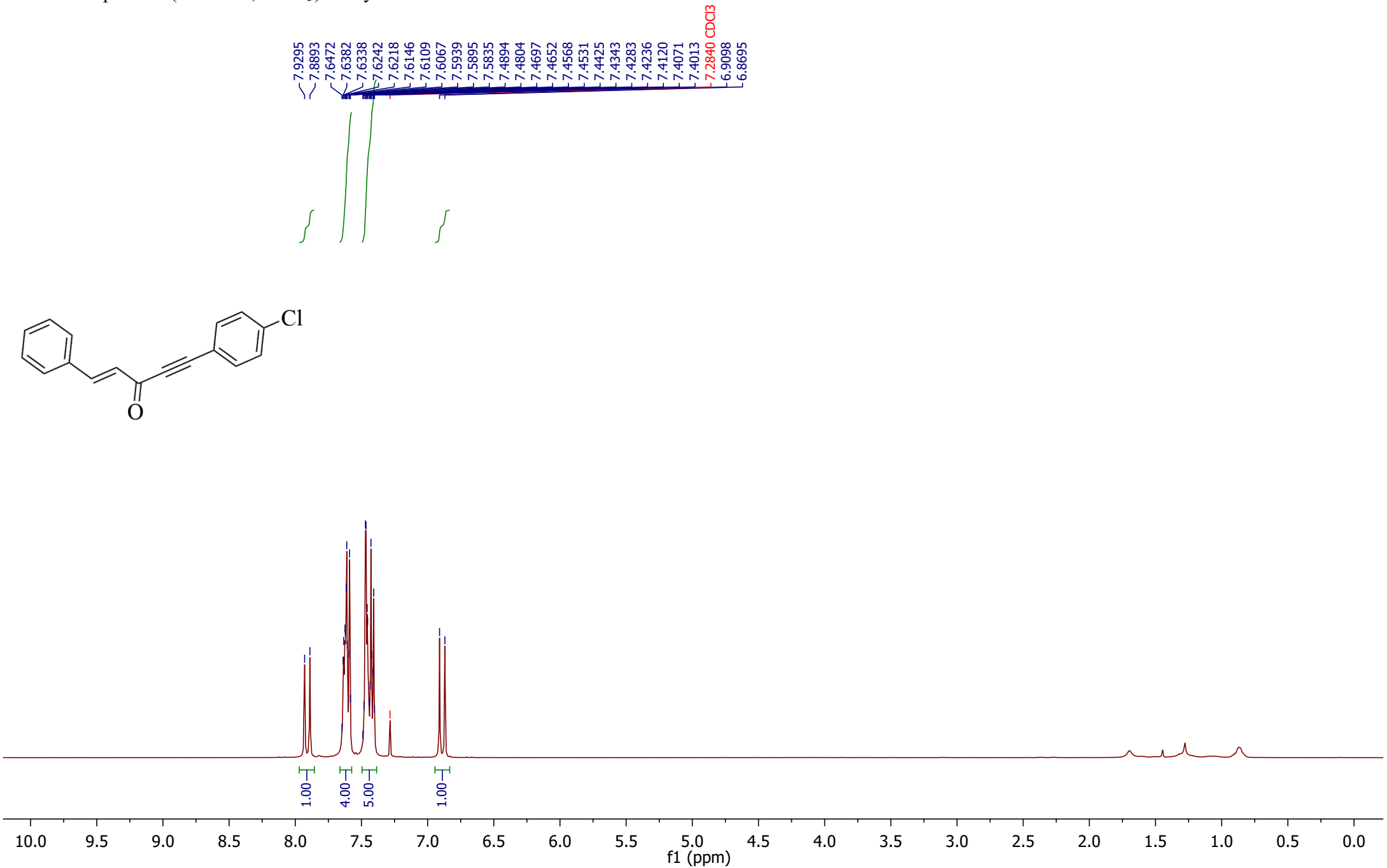
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of enynone 1t



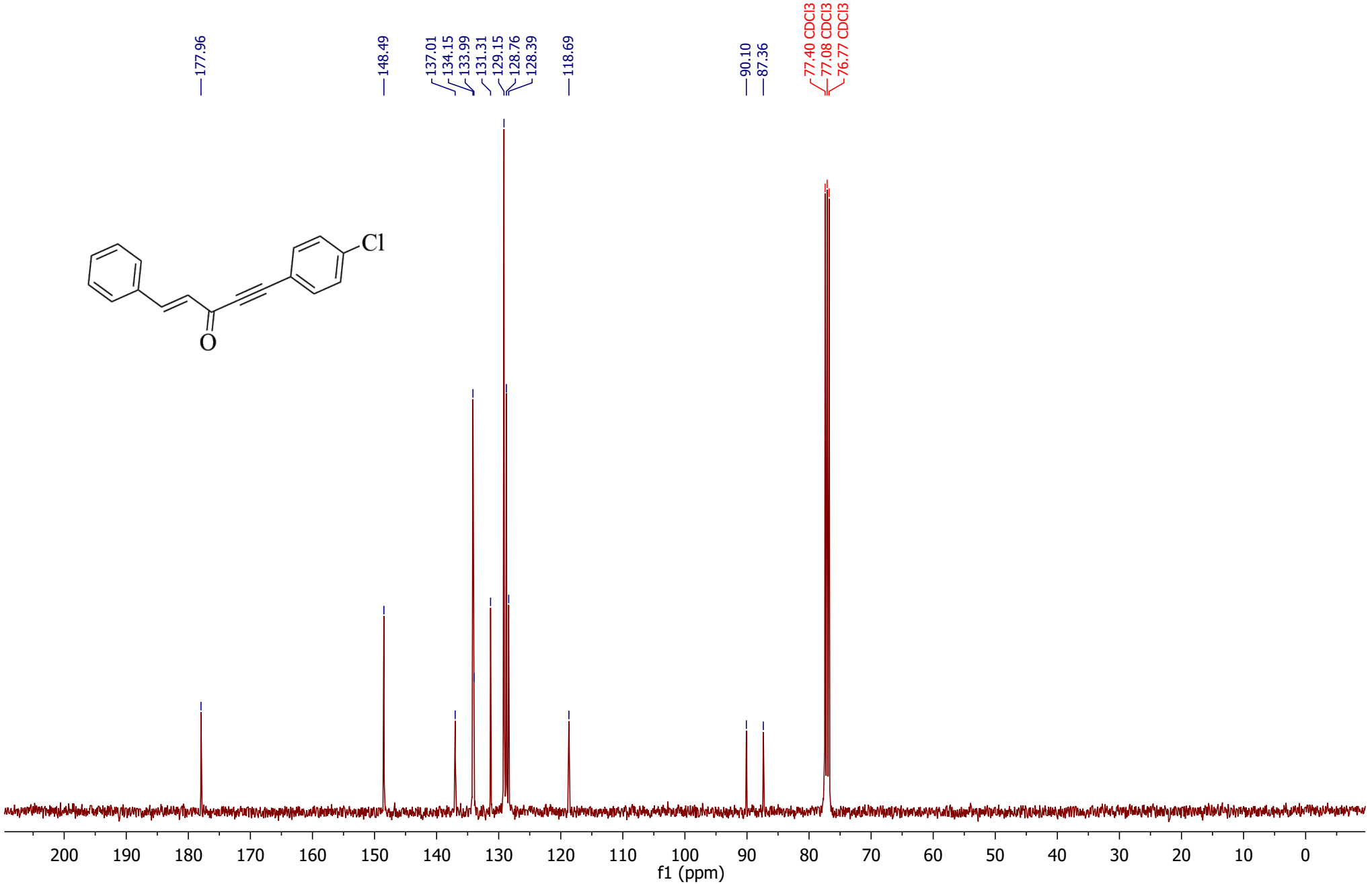
^{19}F NMR spectrum (376 MHz, $CDCl_3$) of enynone 1t



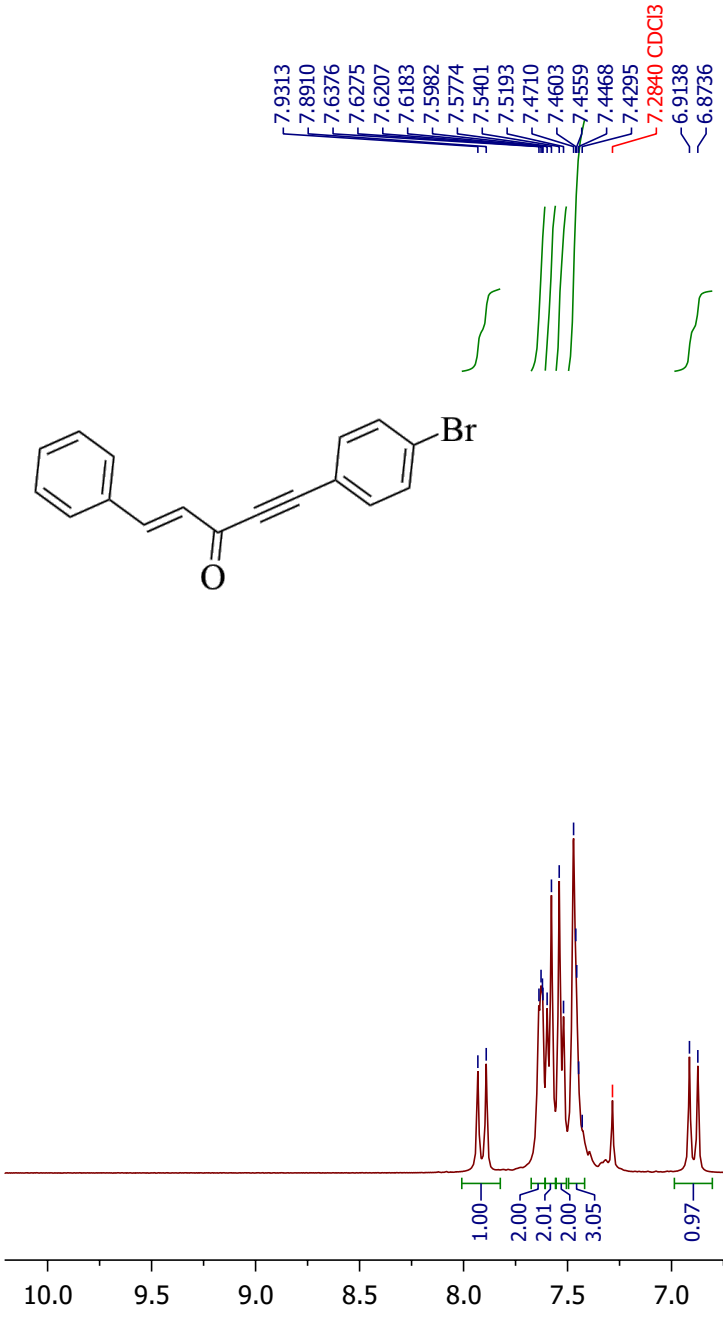
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of enynone 1u



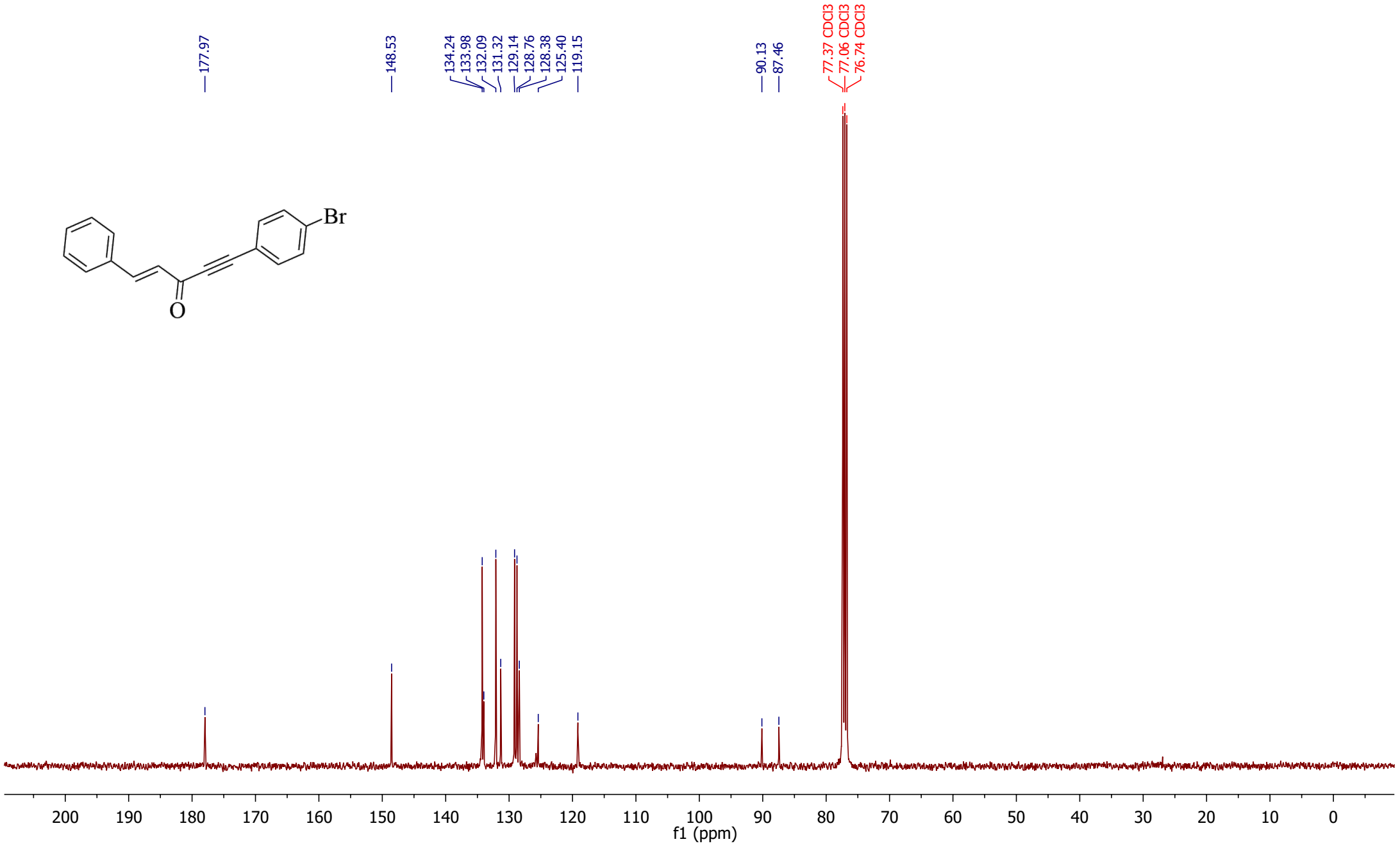
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of enynone 1u



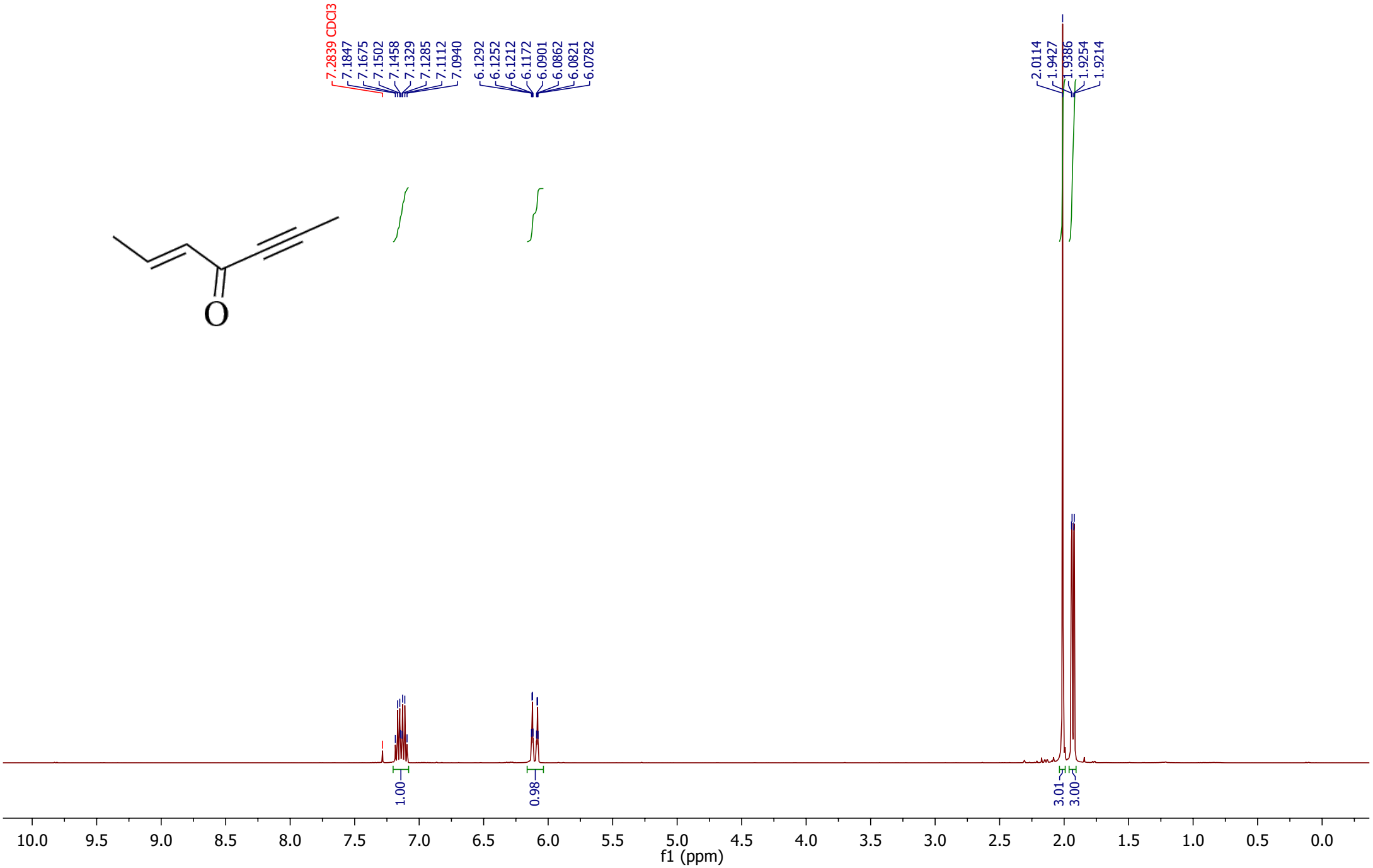
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of enynone 1v



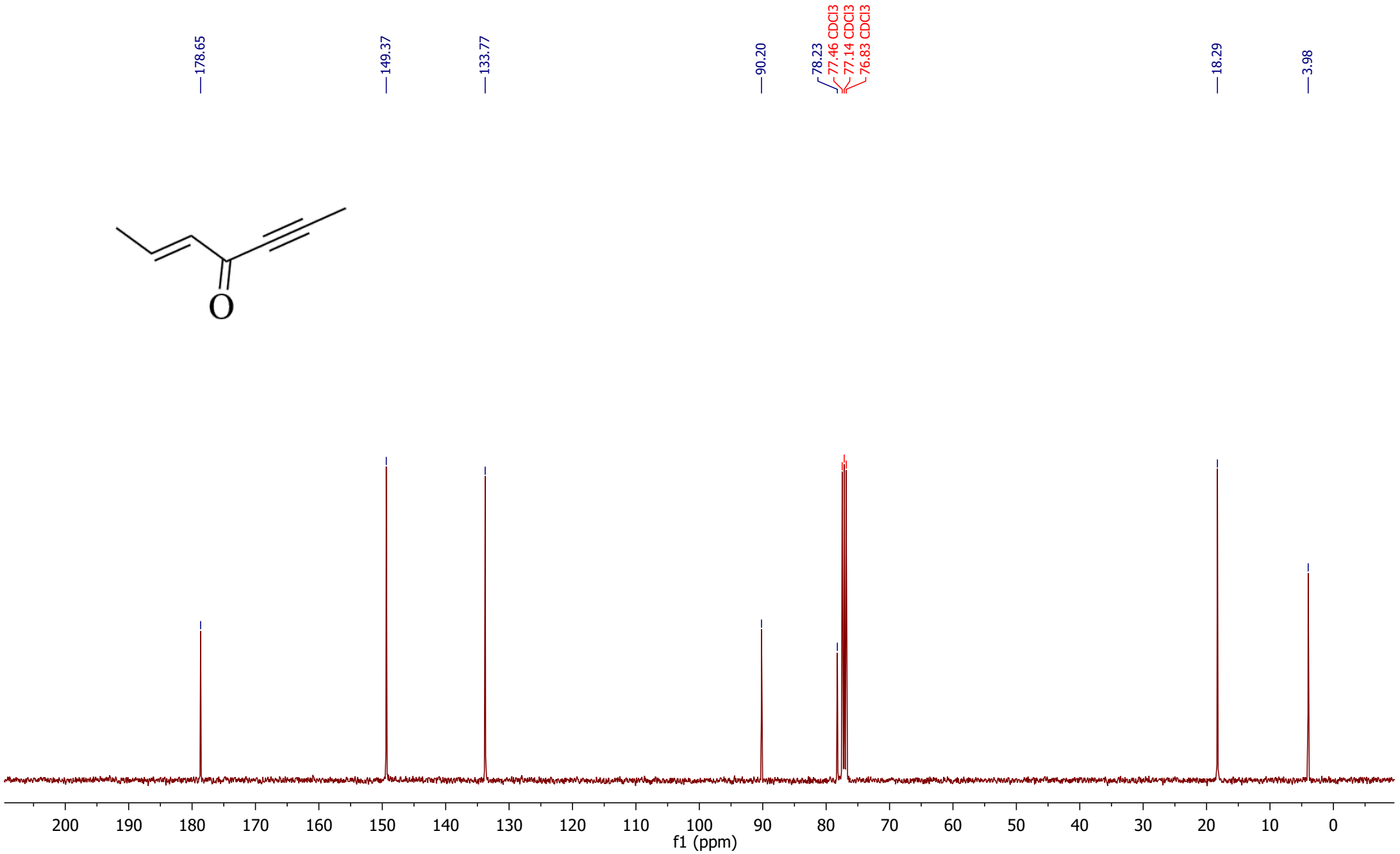
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of enynone 1v



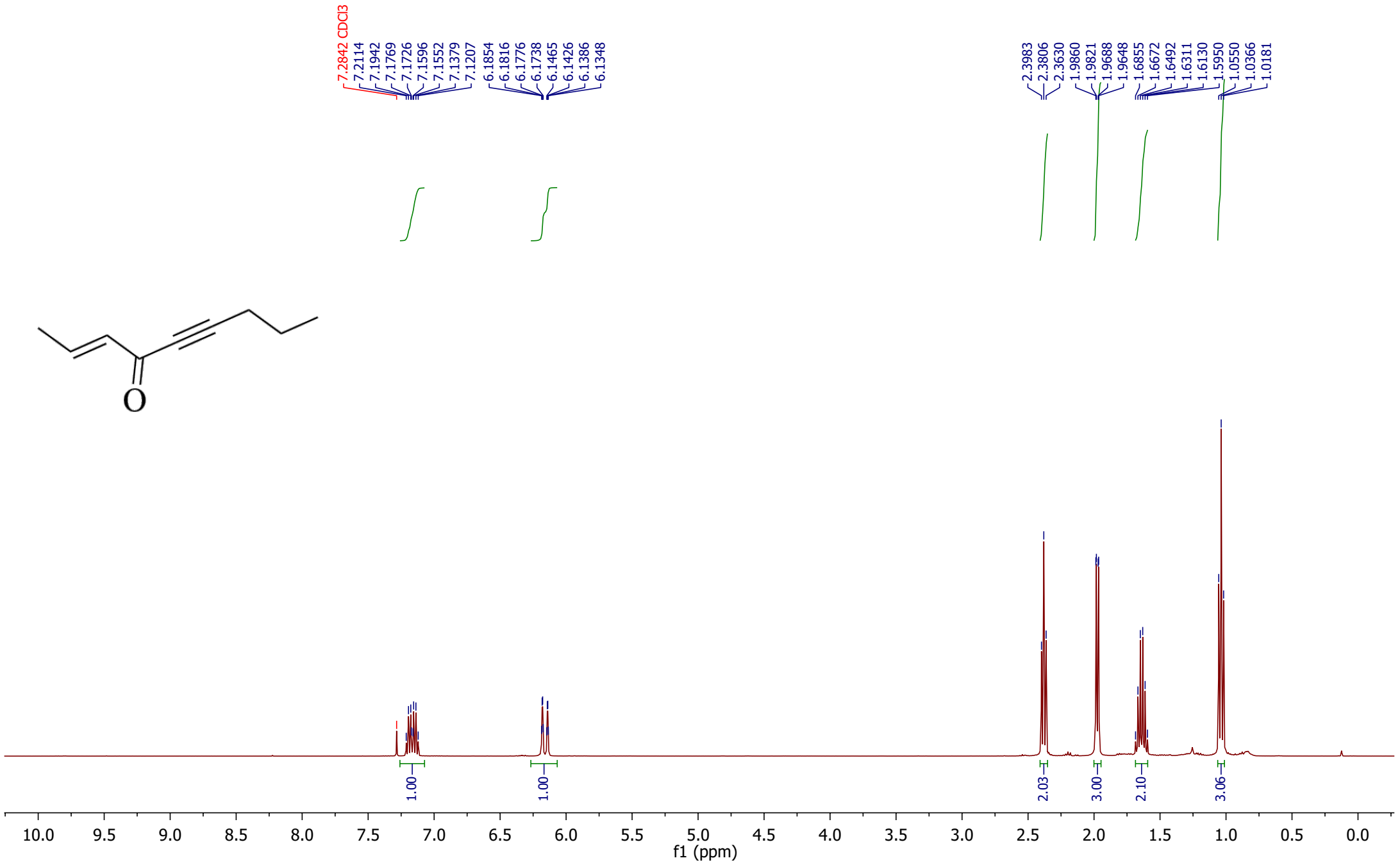
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of enynone 1w



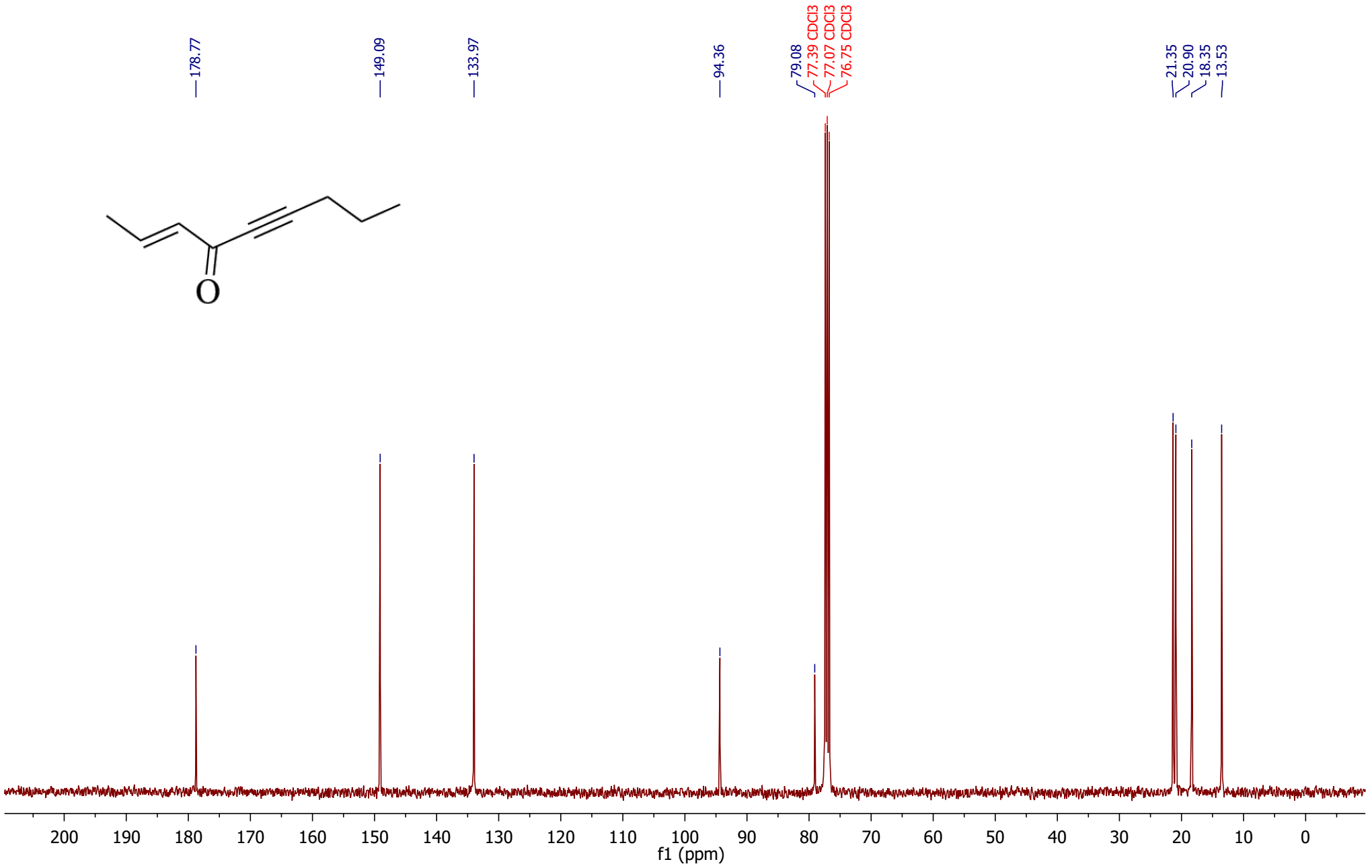
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of enynone 1w



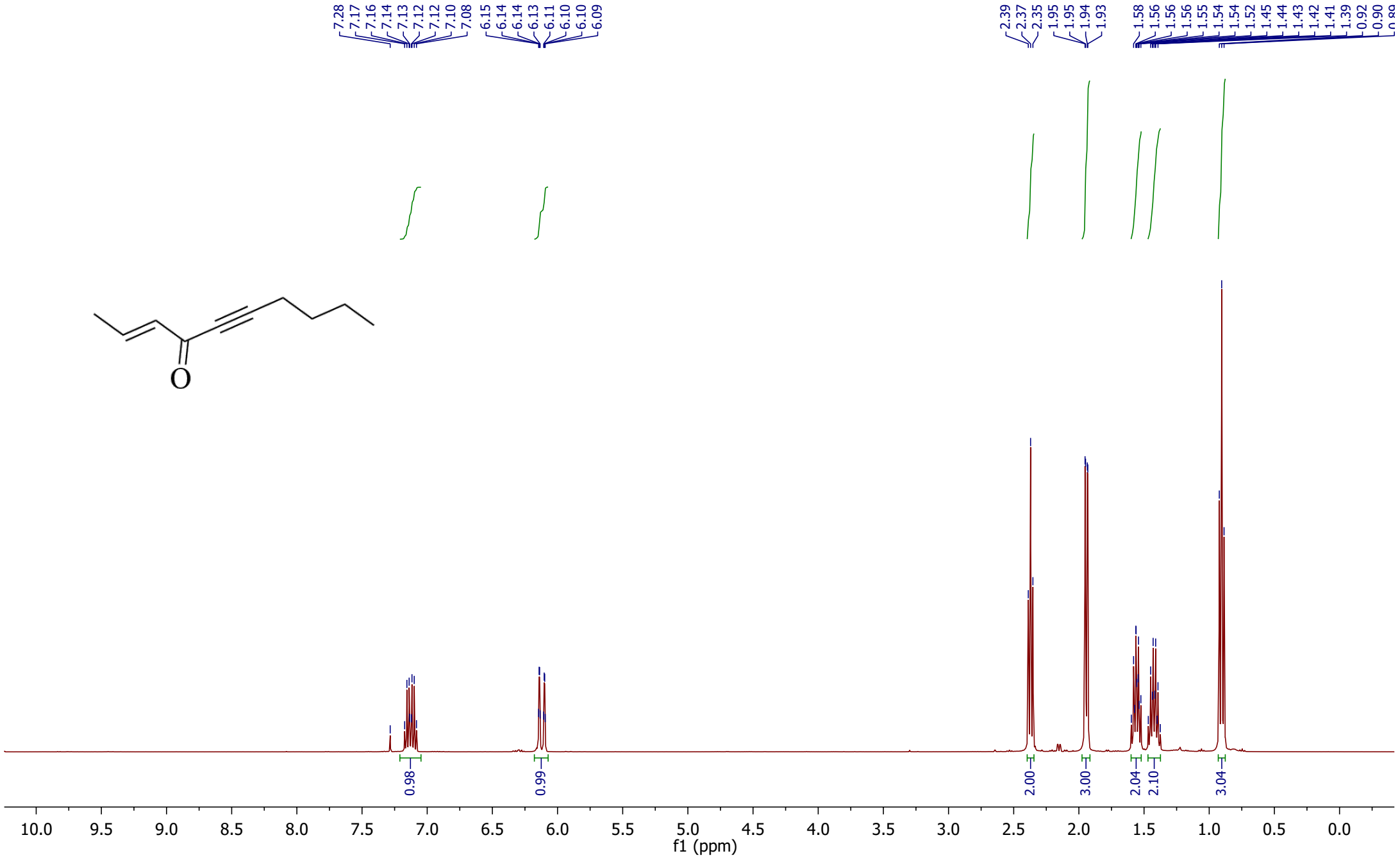
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of enynone 1x



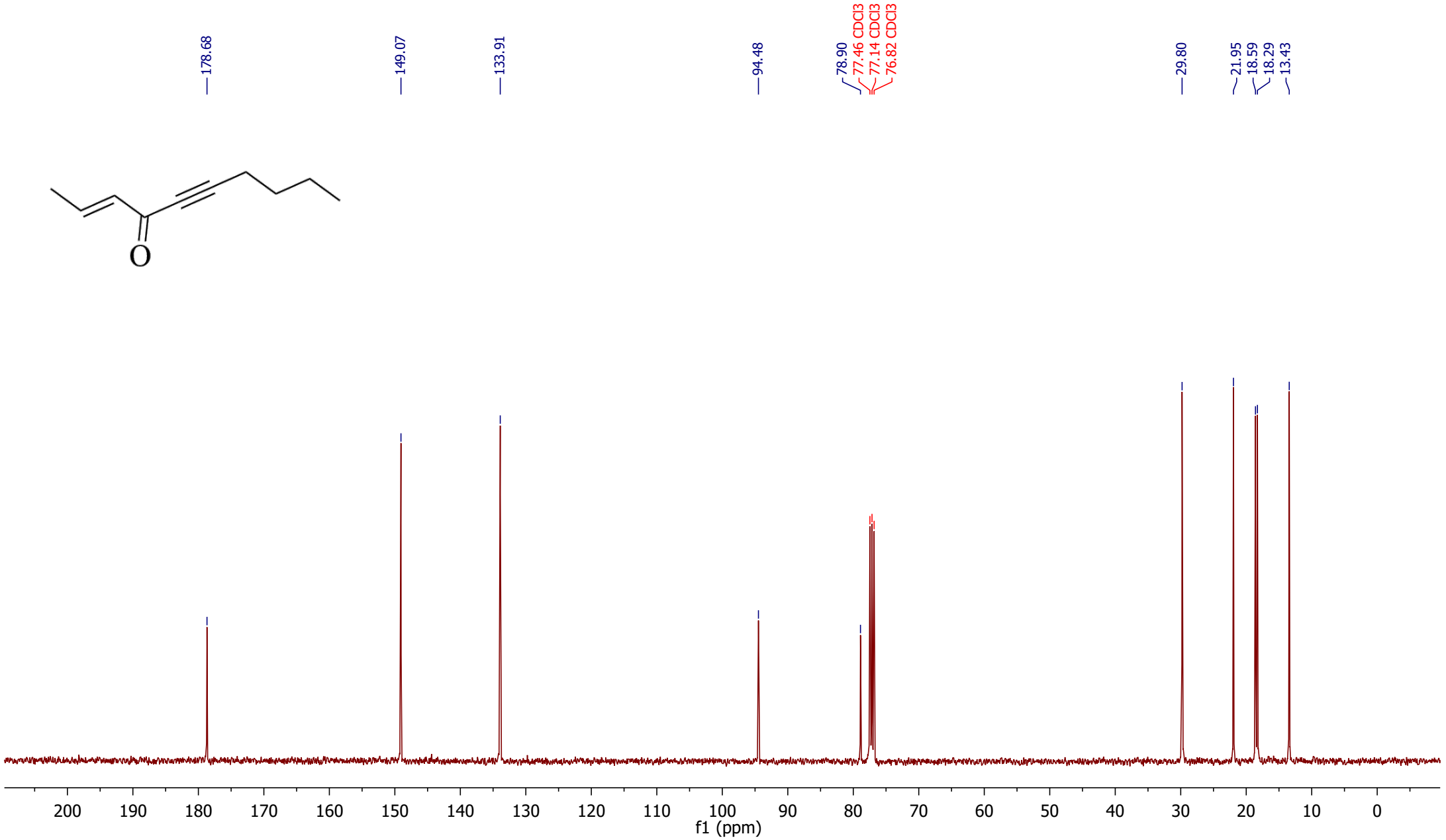
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of enynone 1x



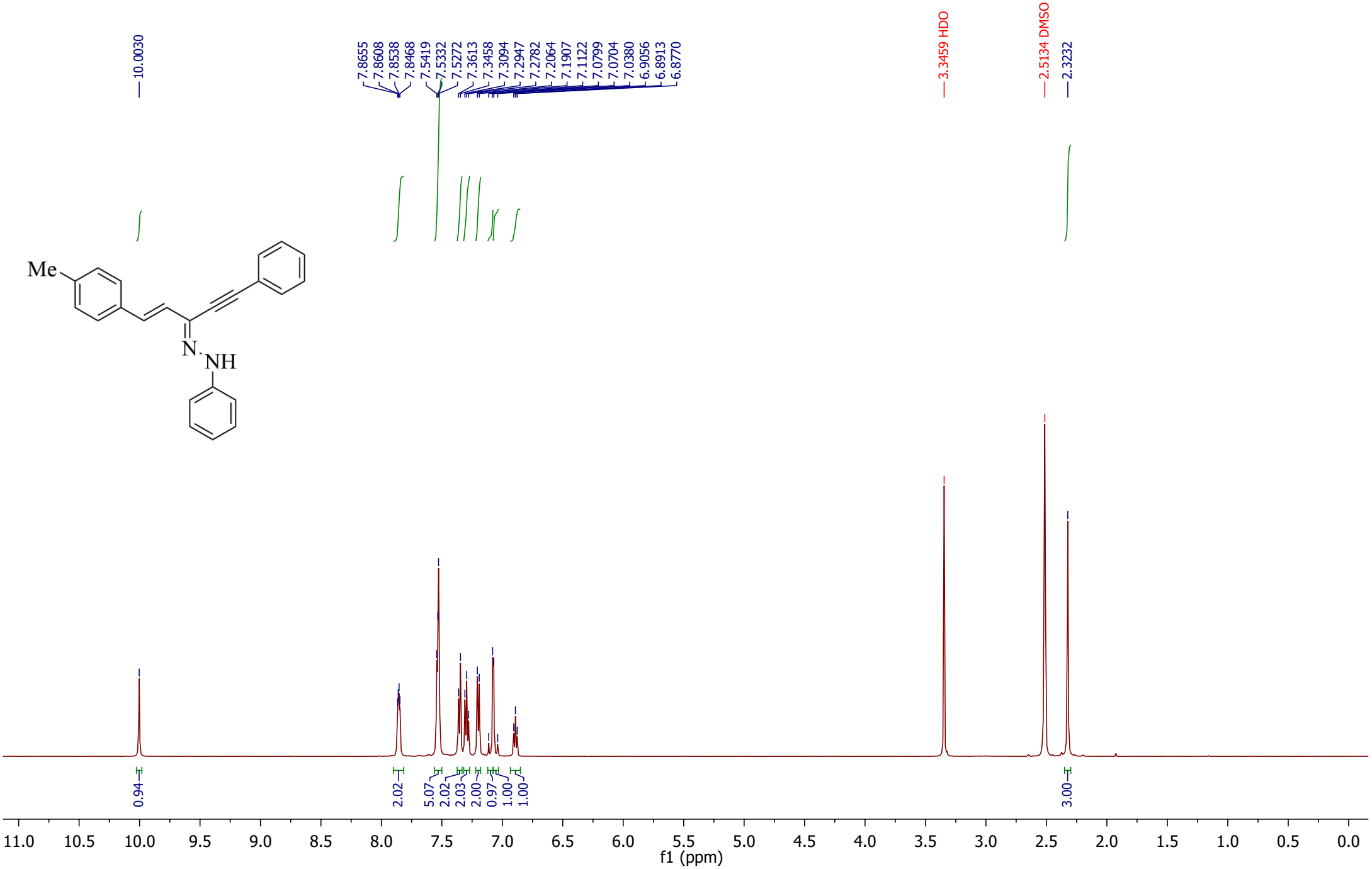
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of enynone 1y



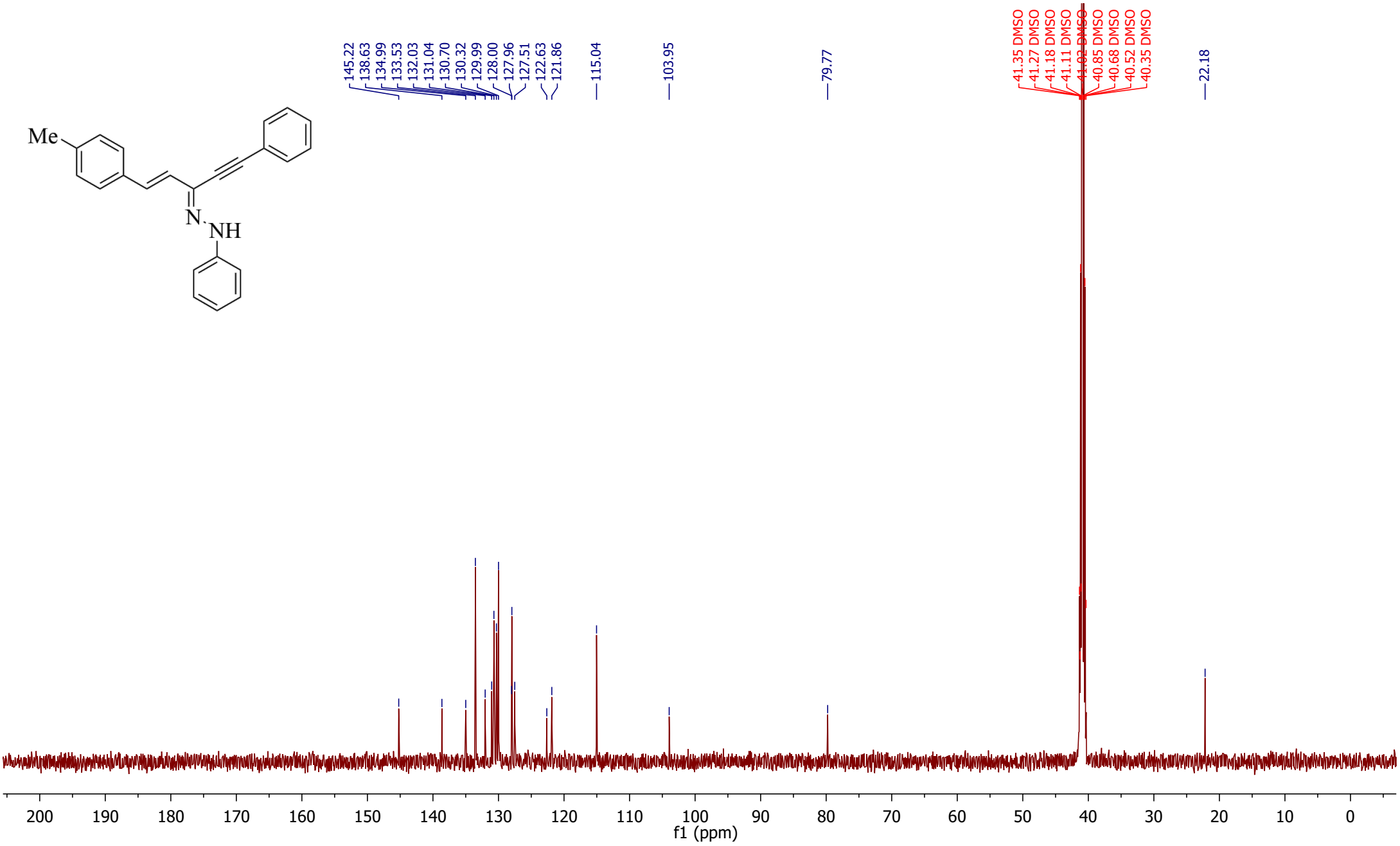
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of enynone 1y



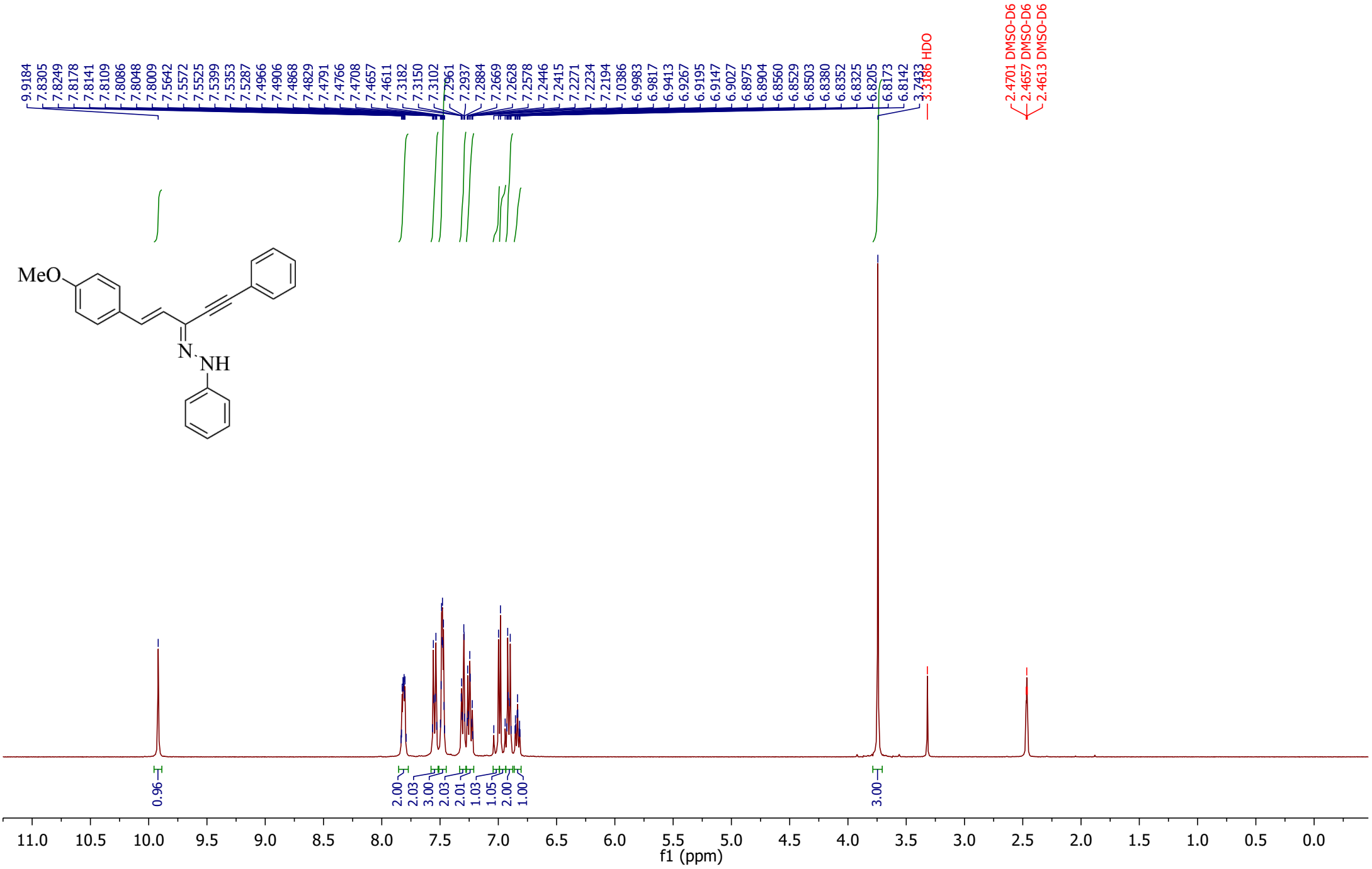
^{1}H NMR spectrum (500 MHz, DMSO-d_6) of phenylhydrazone 5b



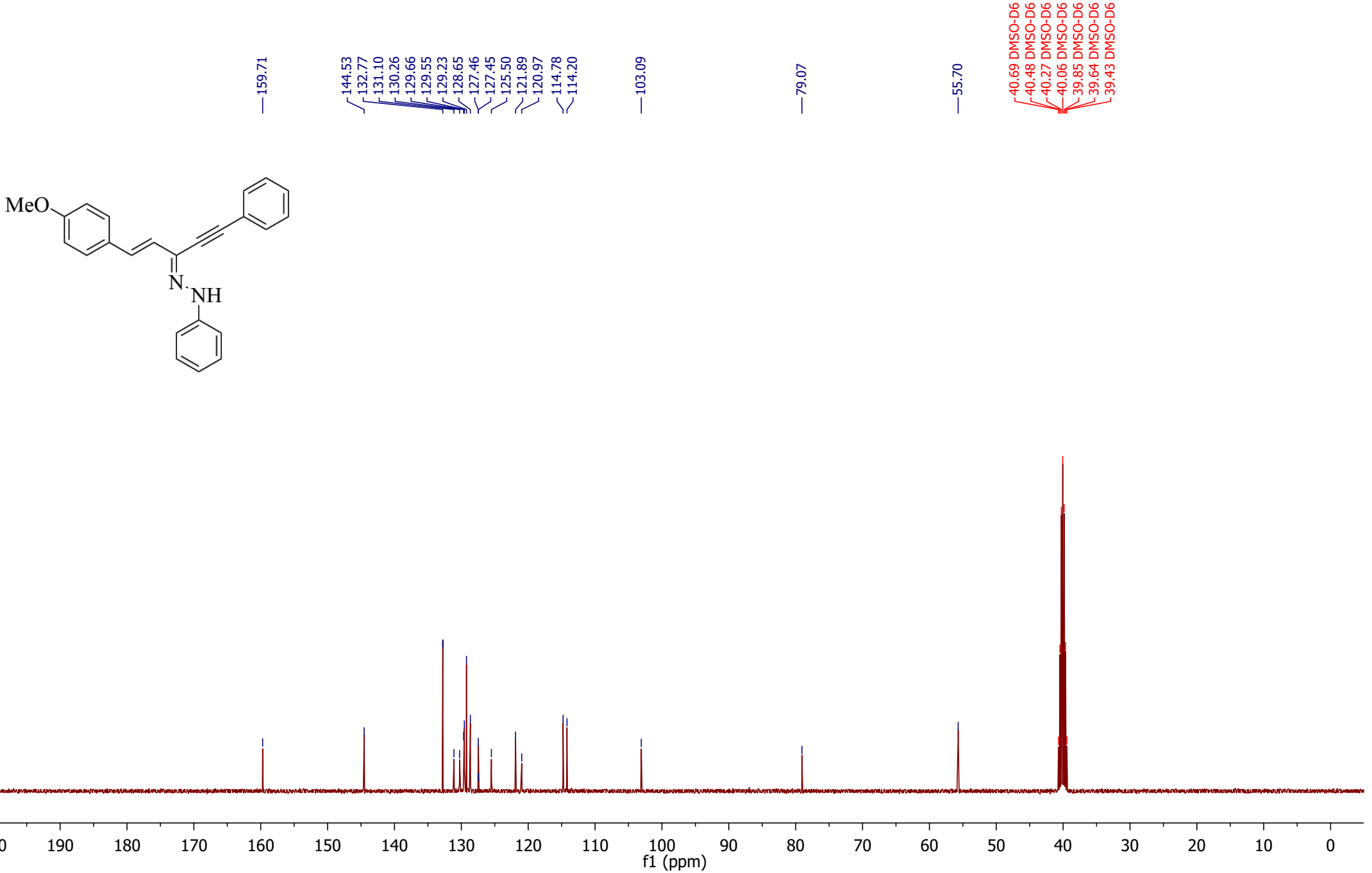
$^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, DMSO-d_6) of phenylhydrazone 5b



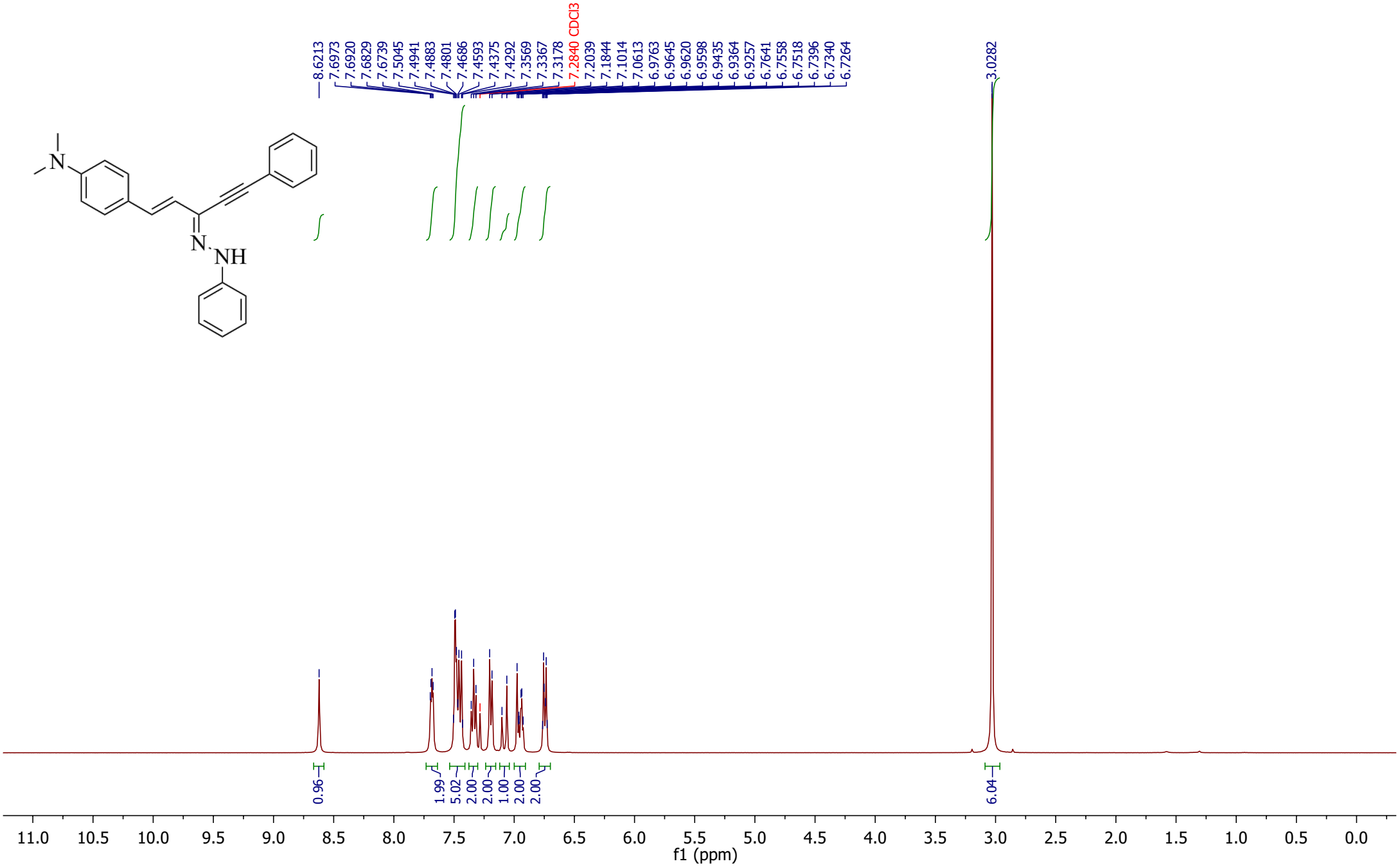
^{1}H NMR spectrum (400 MHz, DMSO-d_6) of phenylhydrazone 5c



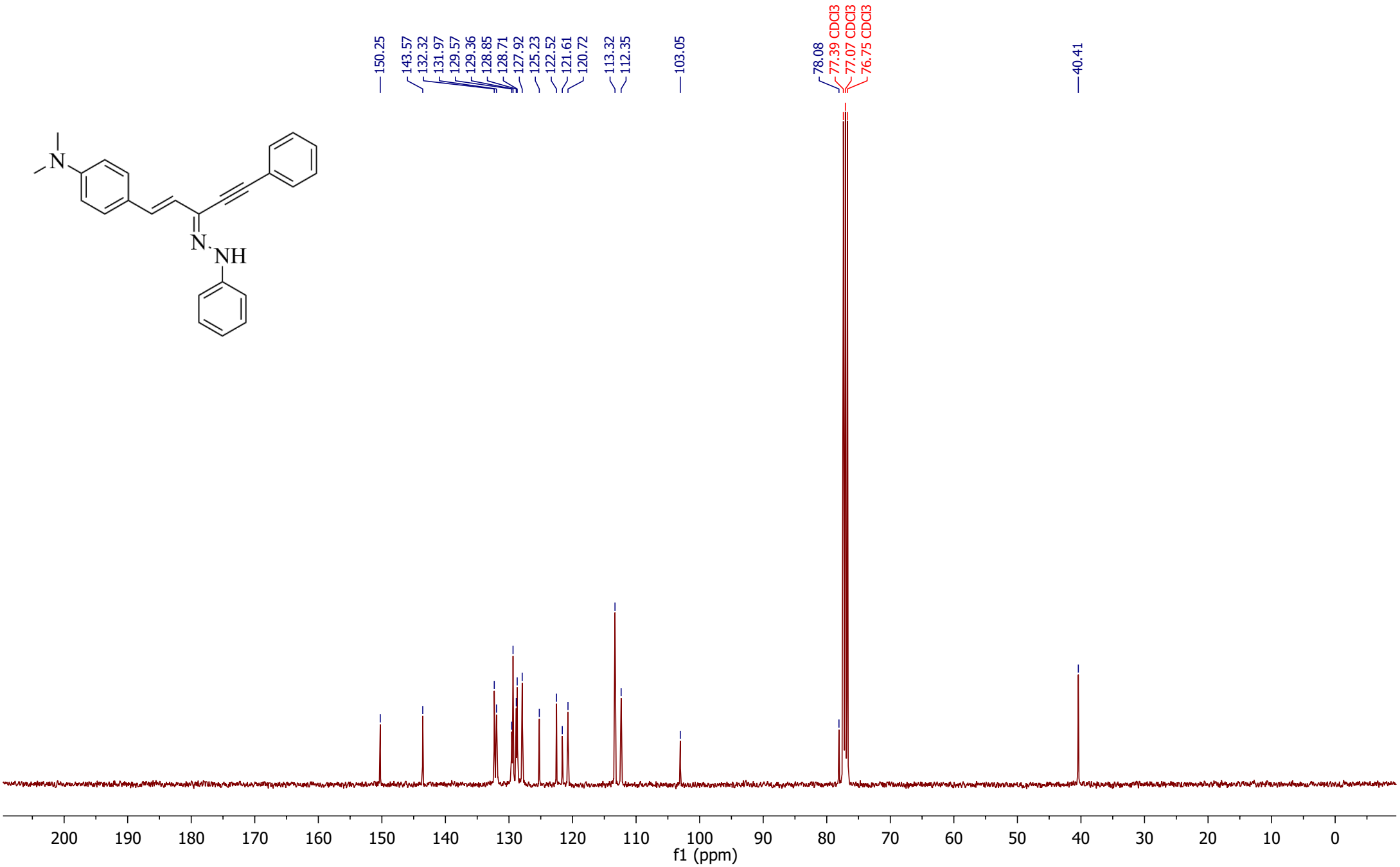
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, DMSO-d_6) of phenylhydrazone 5c



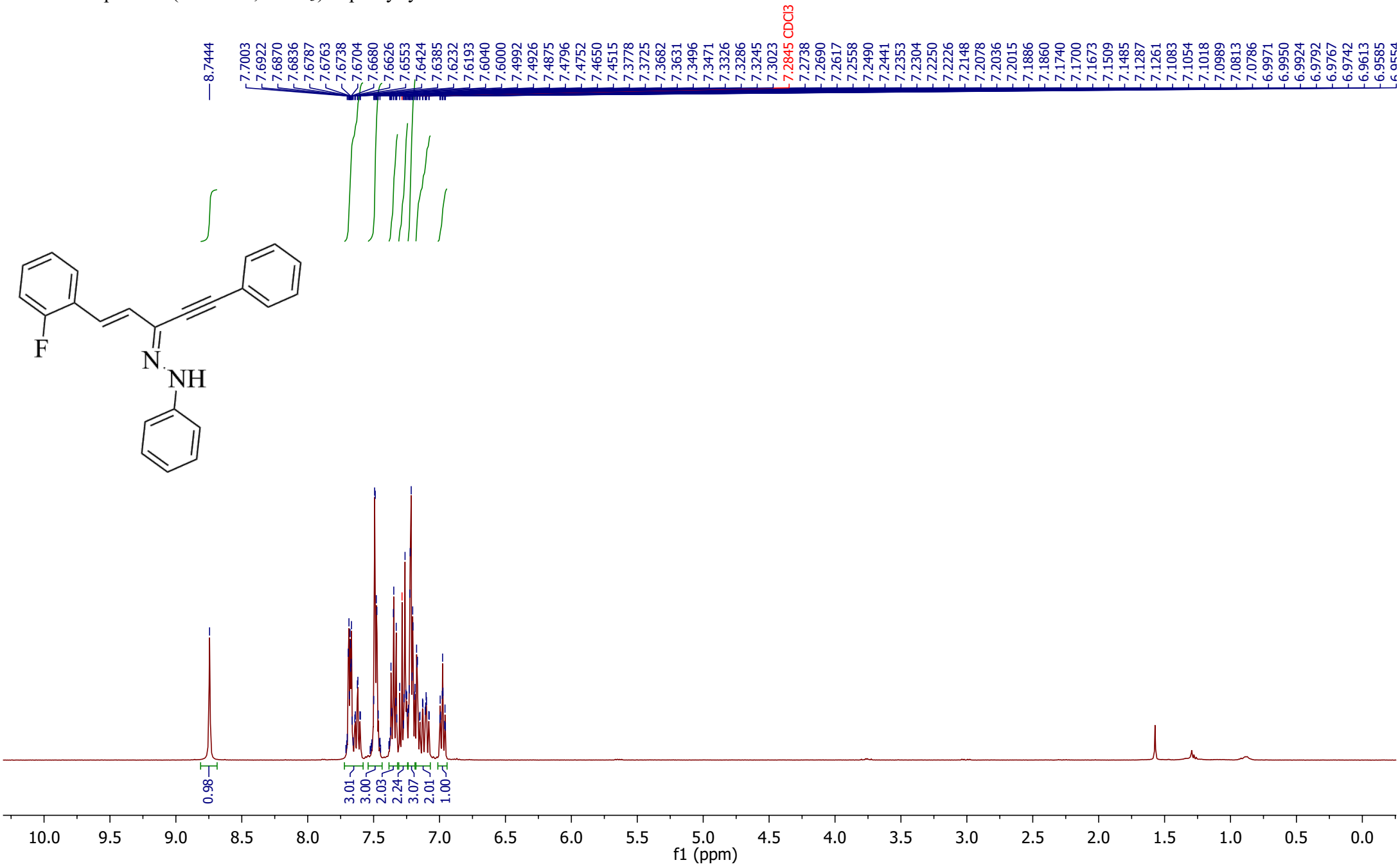
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of phenylhydrazone 5d



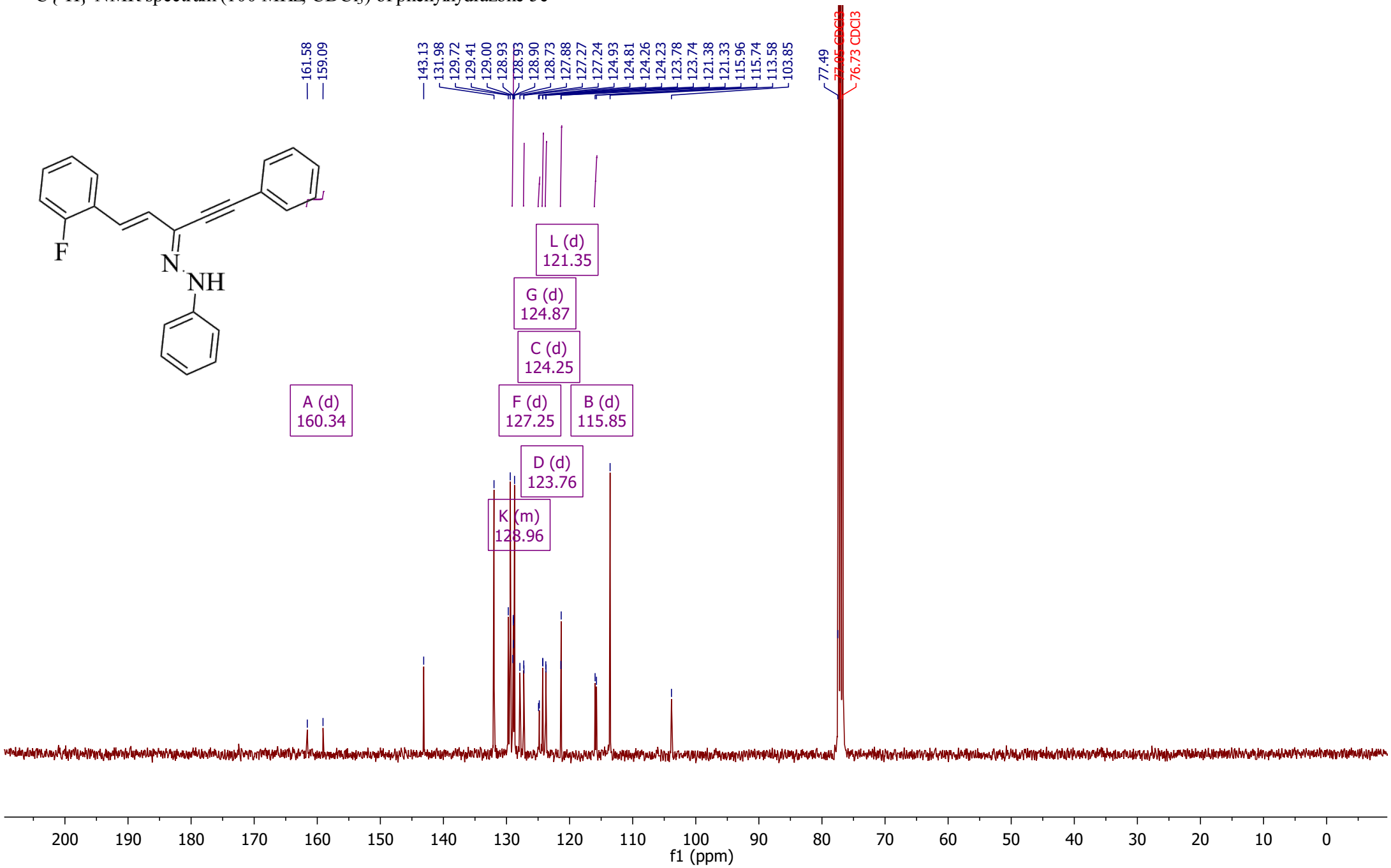
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of phenylhydrazone 5d



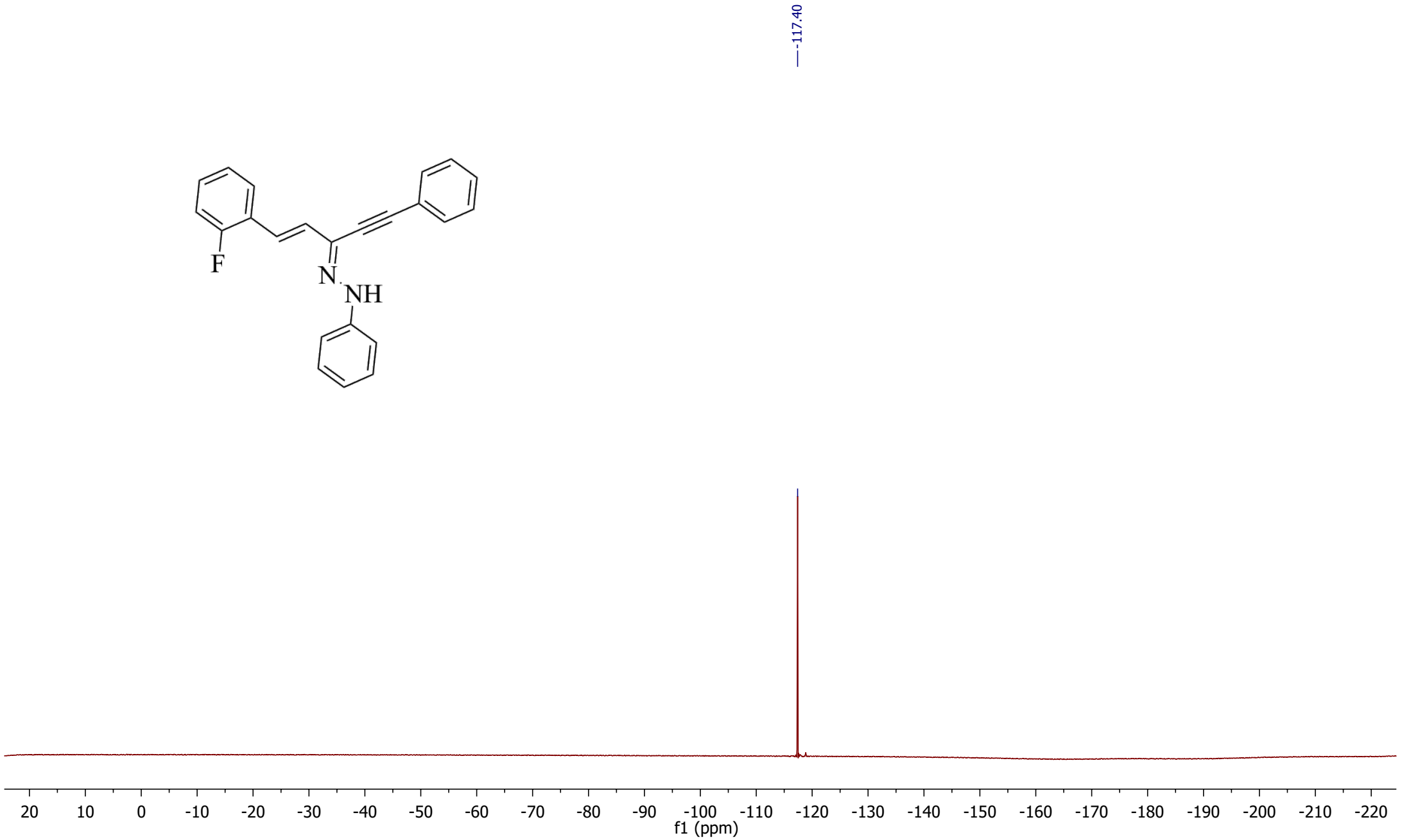
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of phenylhydrazone 5e



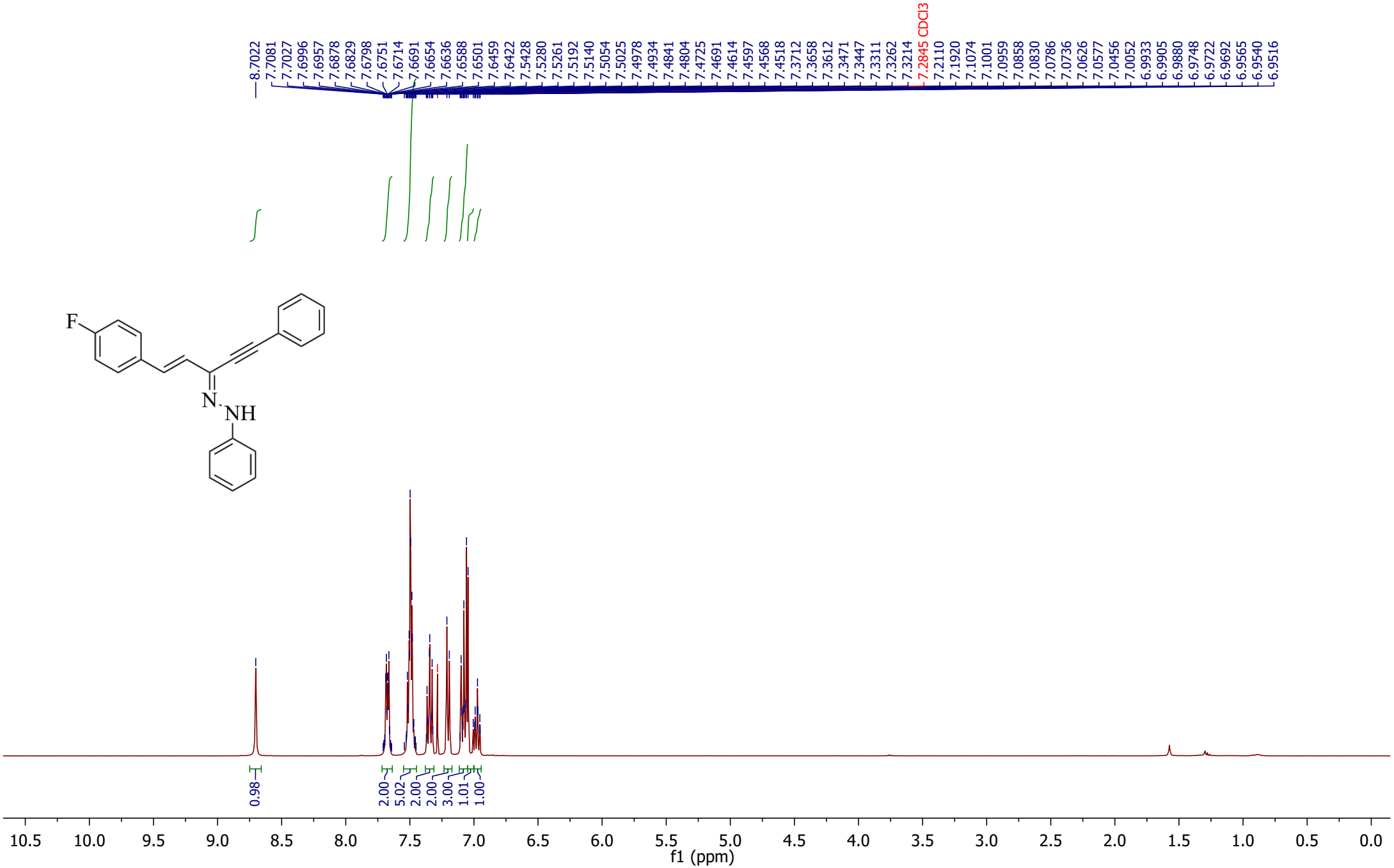
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of phenylhydrazone 5e



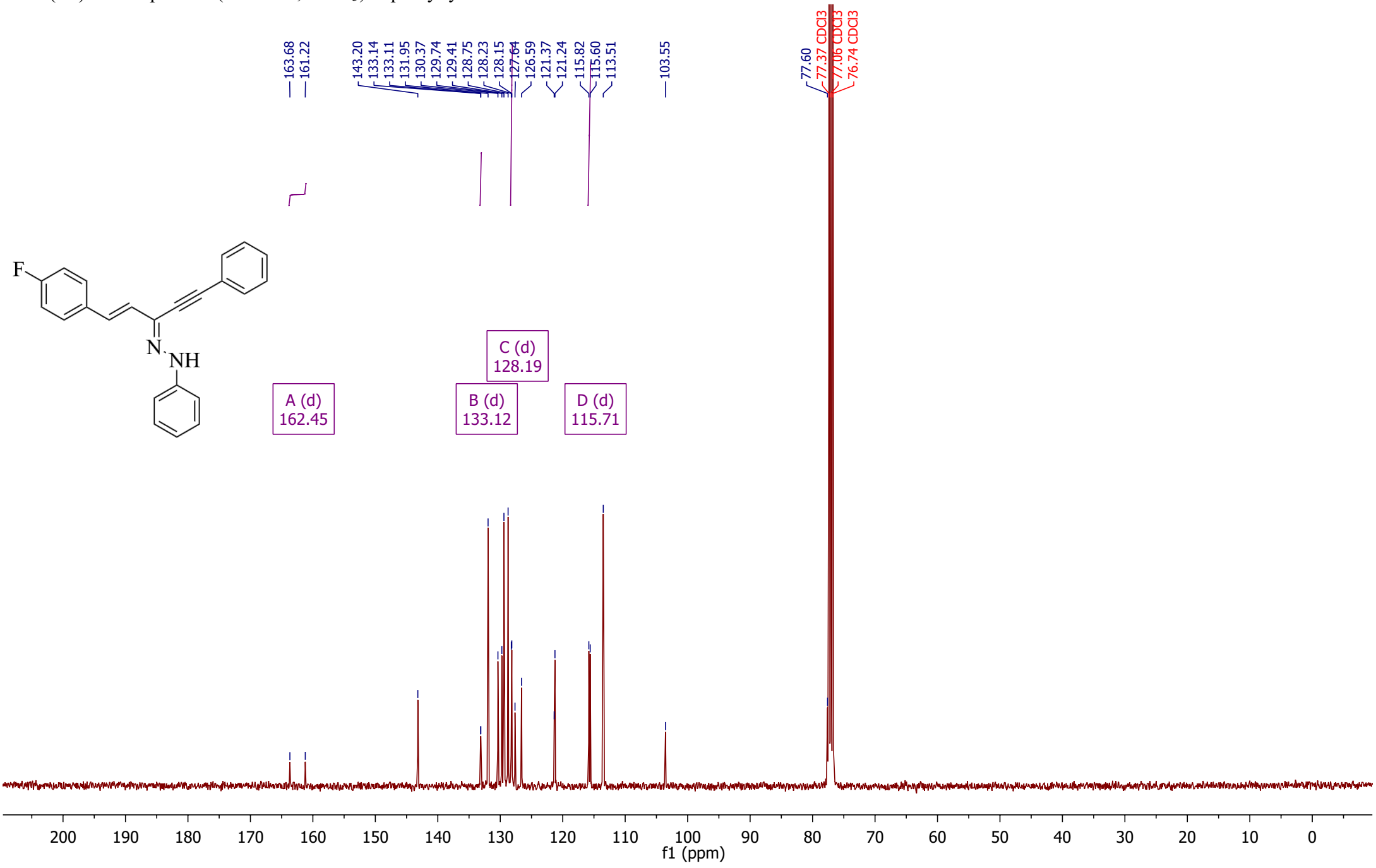
^{19}F NMR spectrum (100 MHz, $CDCl_3$) of phenylhydrazone 5e



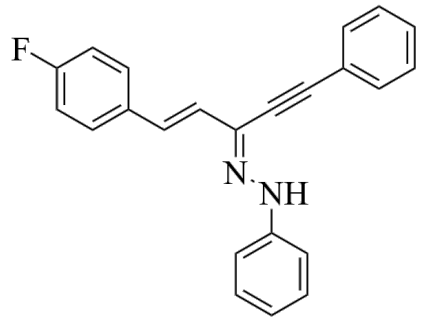
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of phenylhydrazone 5f



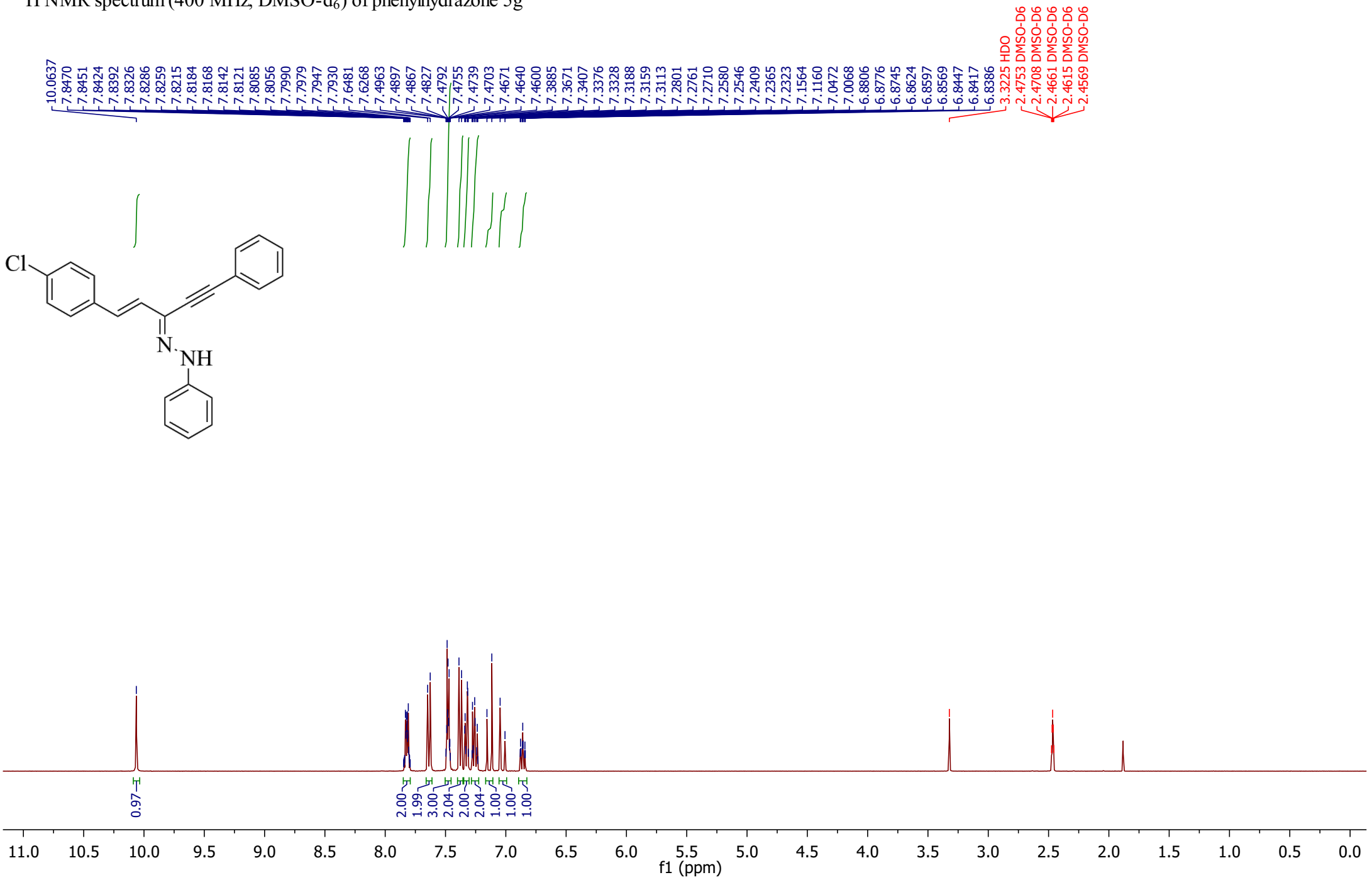
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of phenylhydrazone 5f



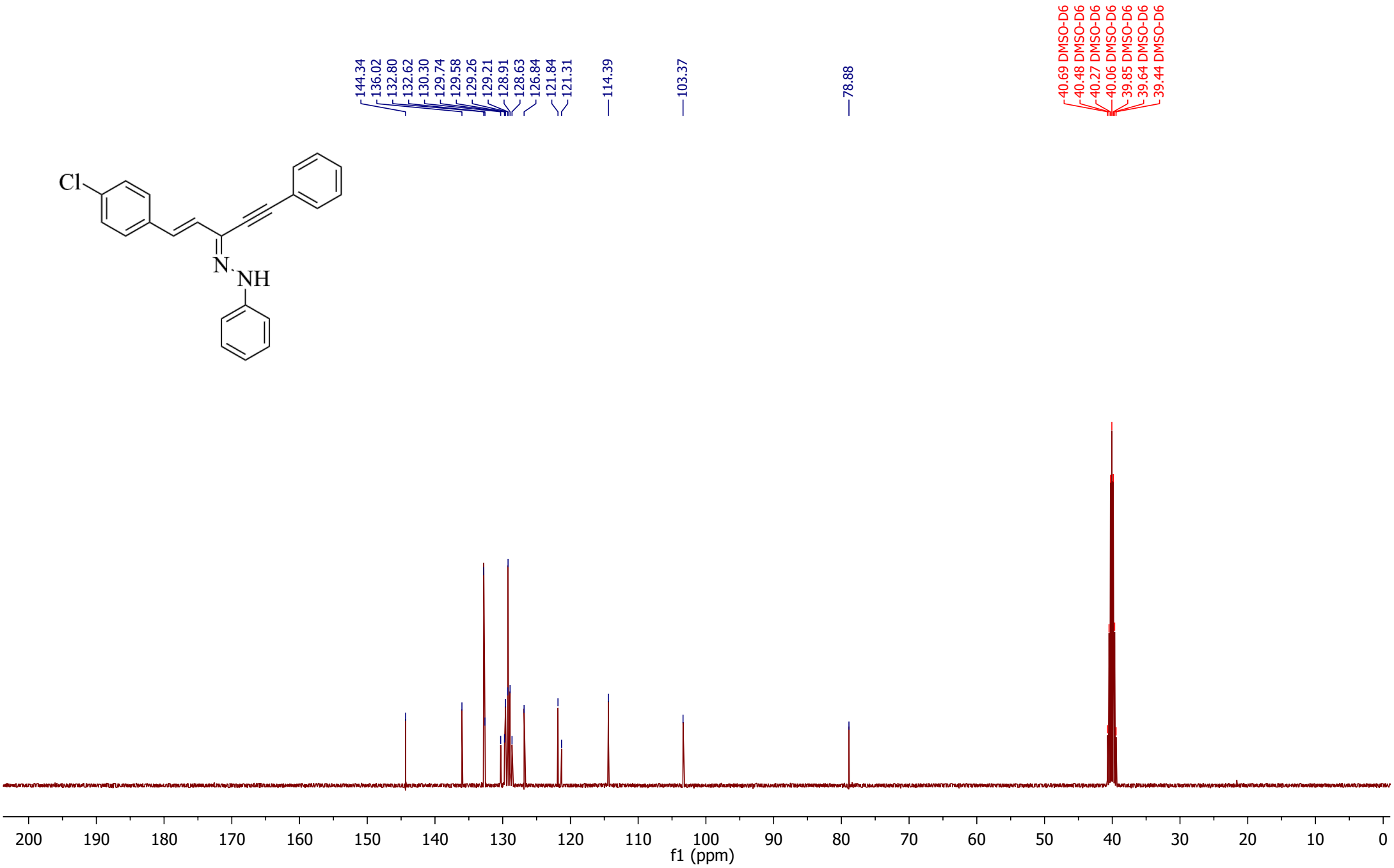
^{19}F NMR spectrum (376 MHz, $CDCl_3$) of phenylhydrazone 5f



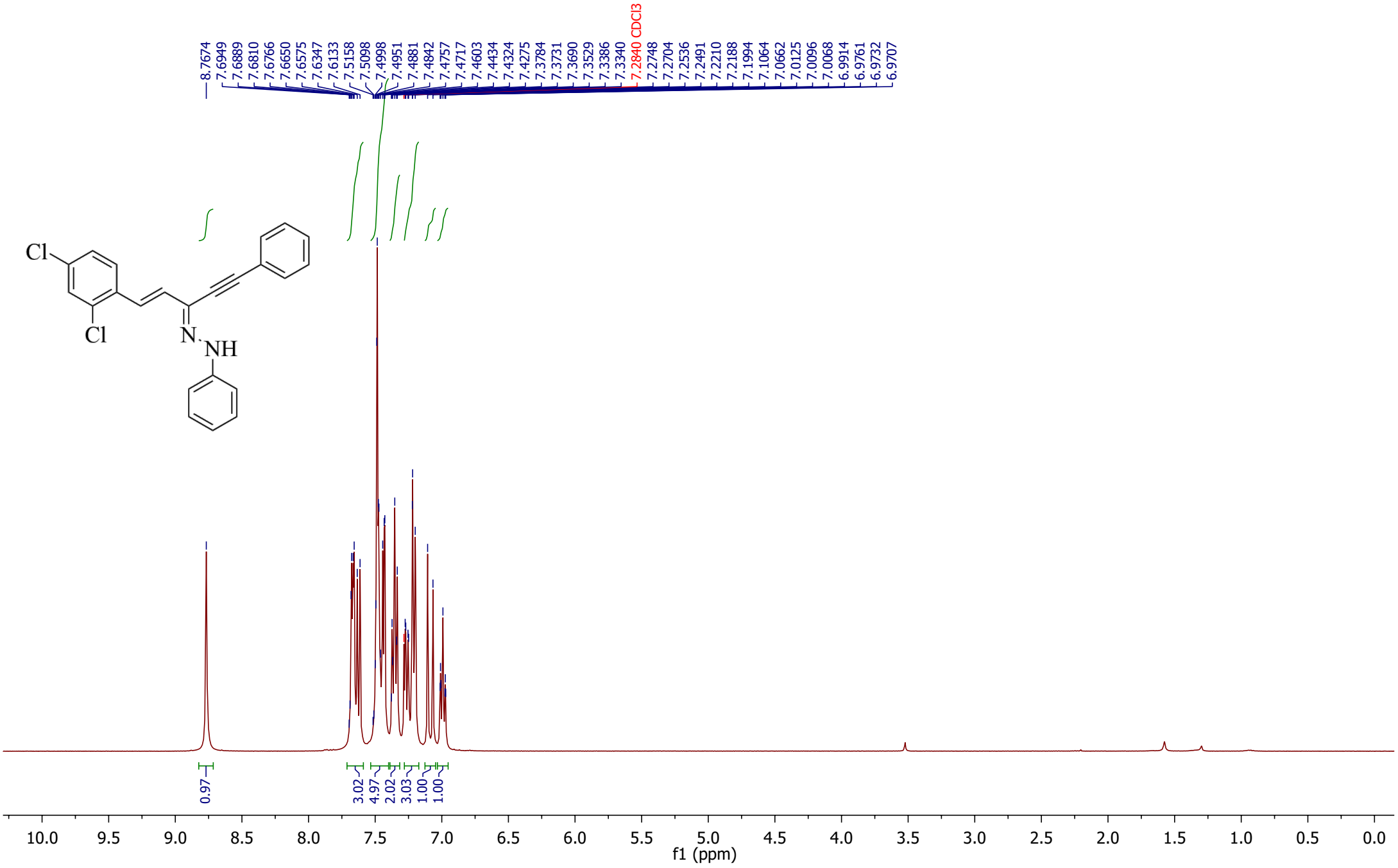
^{1}H NMR spectrum (400 MHz, DMSO-d_6) of phenylhydrazone 5g



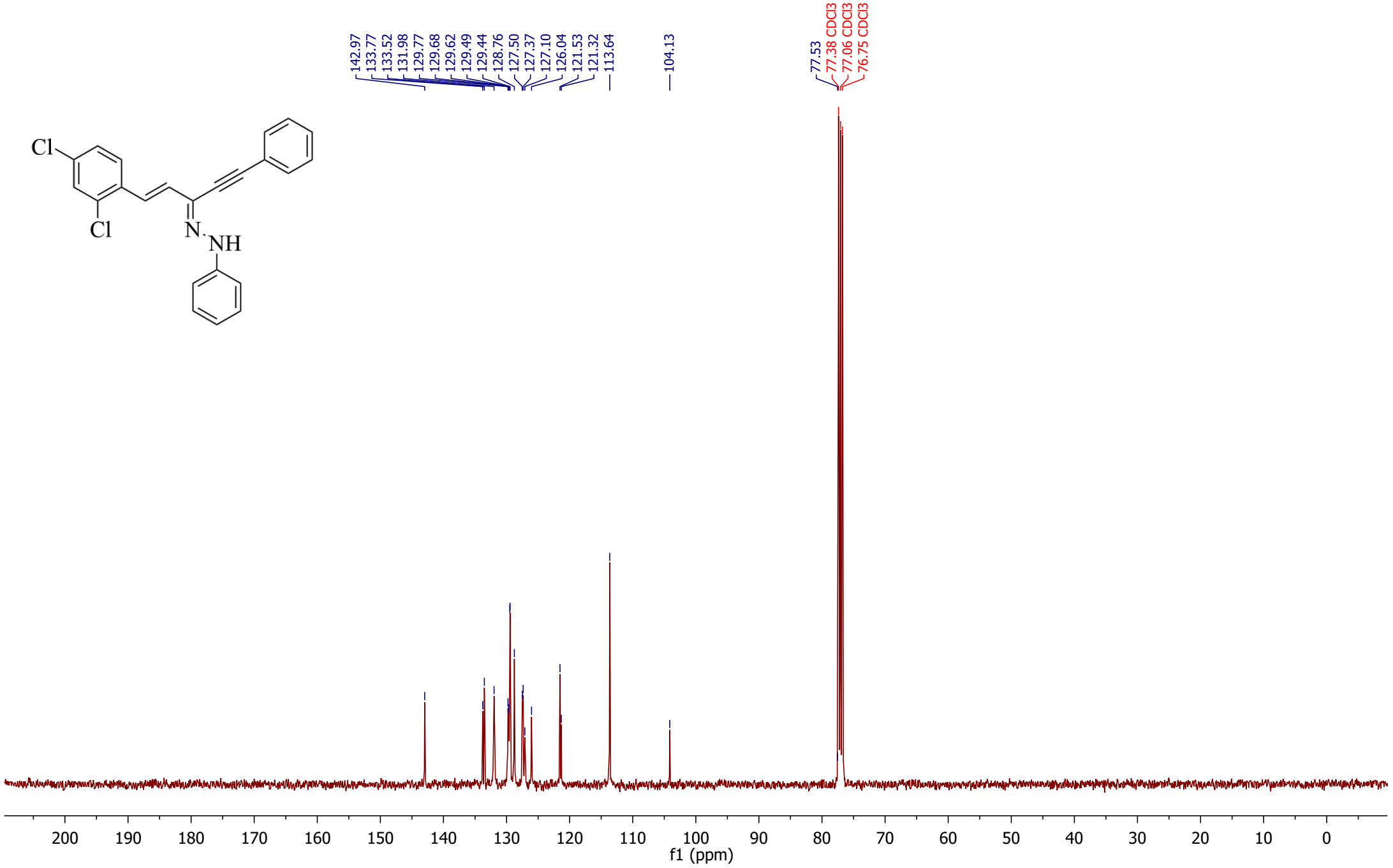
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, DMSO-d_6) of phenylhydrazone 5g



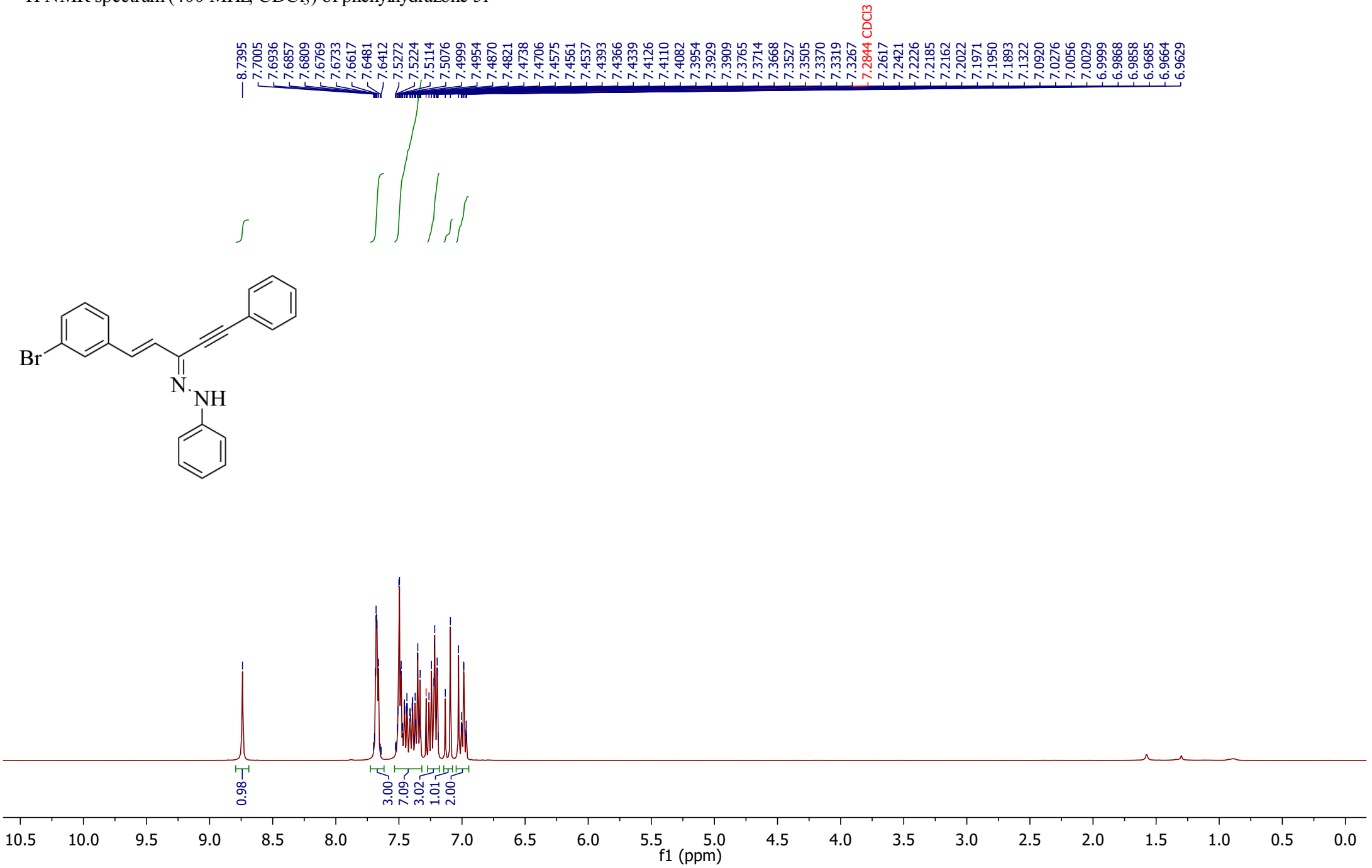
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of phenylhydrazone 5h



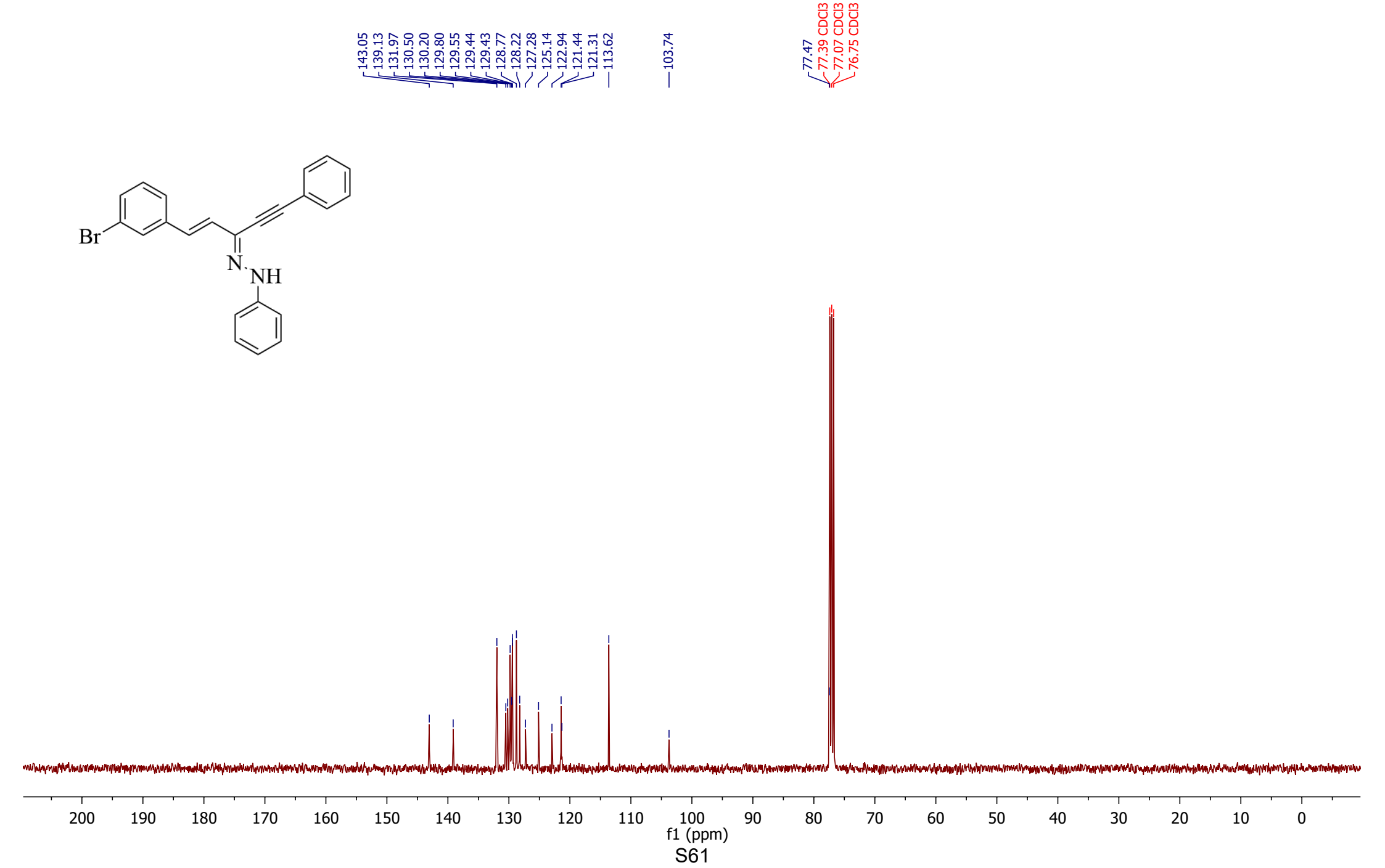
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of phenylhydrazone 5h



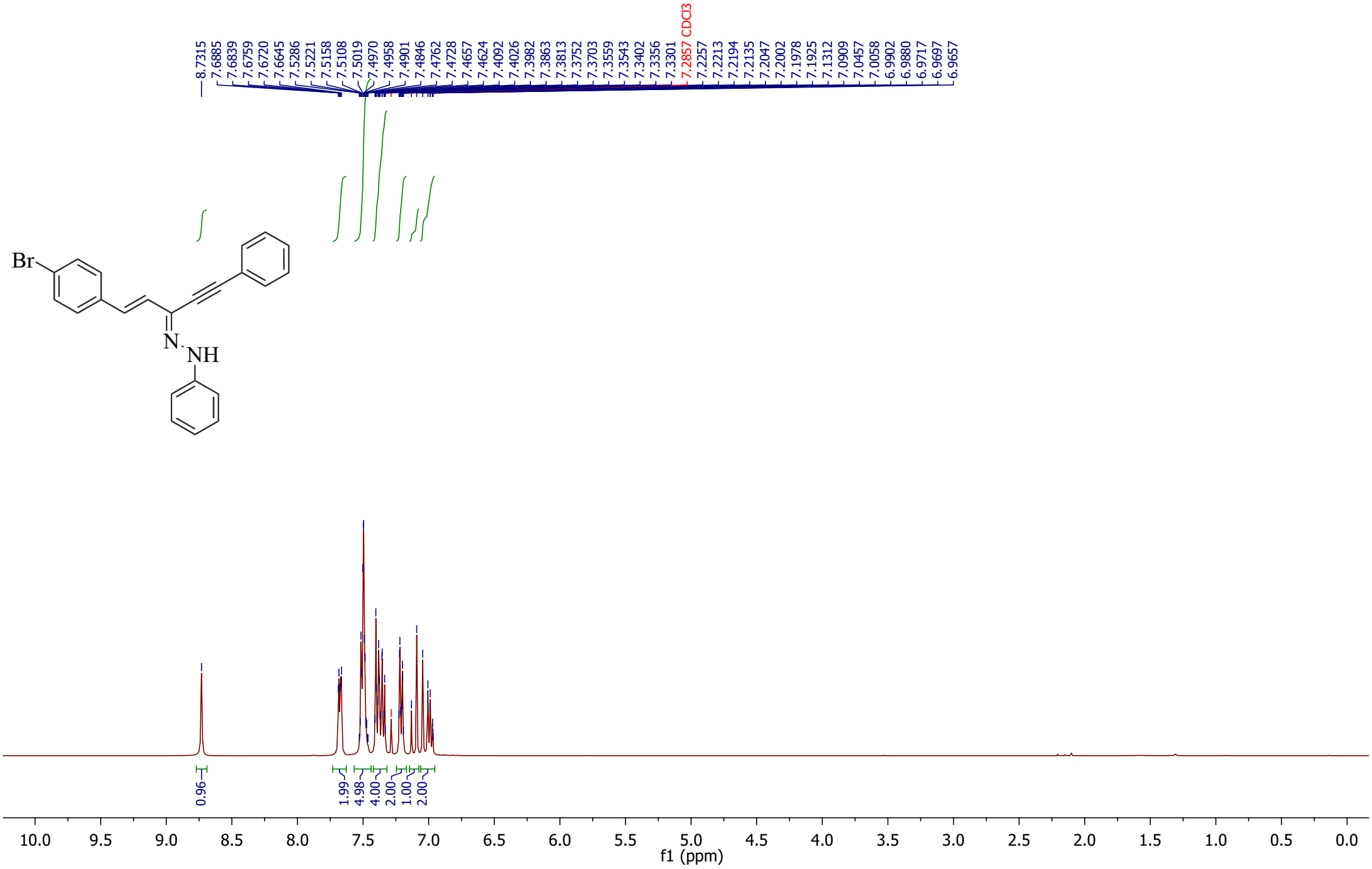
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of phenylhydrazone 5i



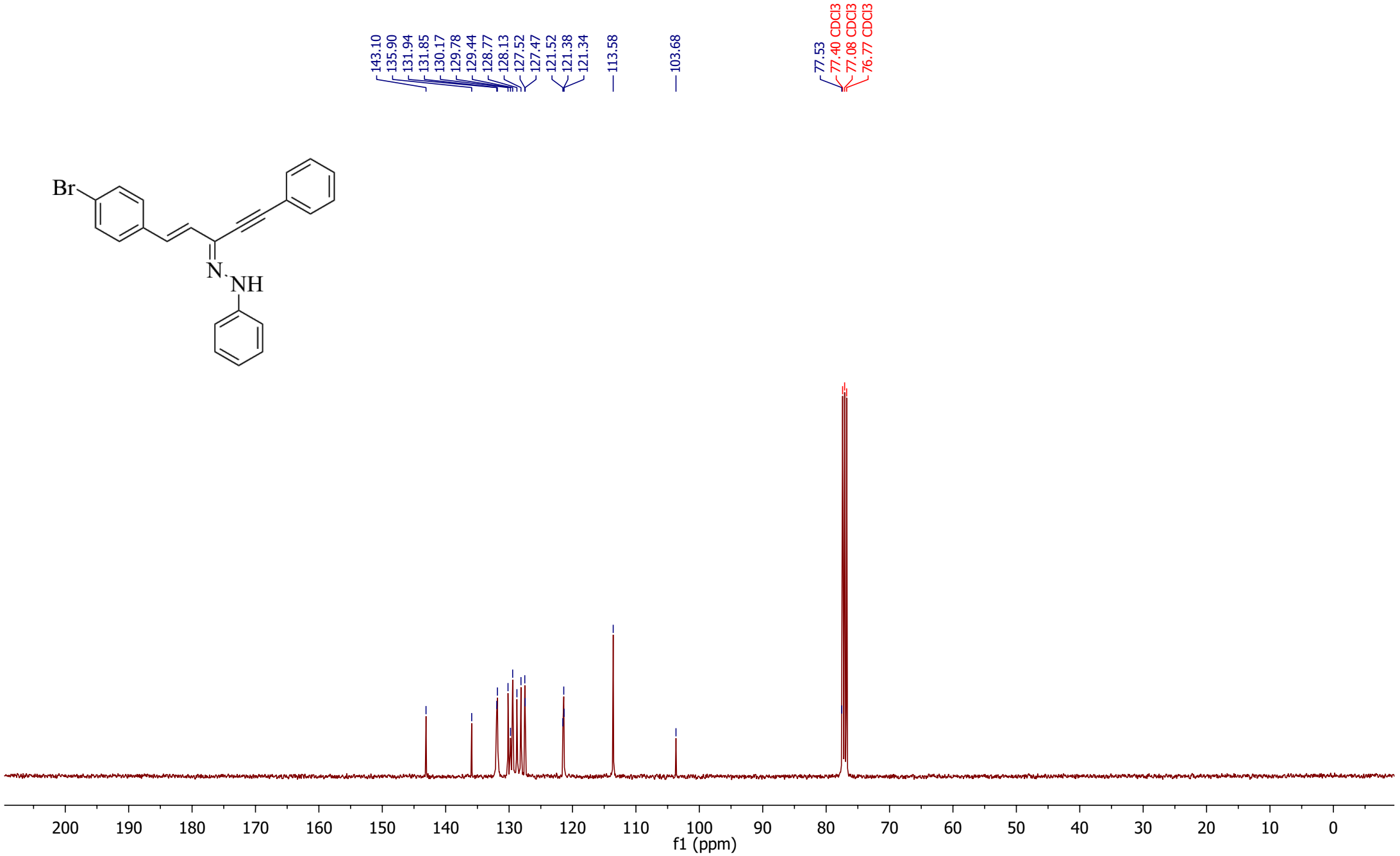
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of phenylhydrazone 5i



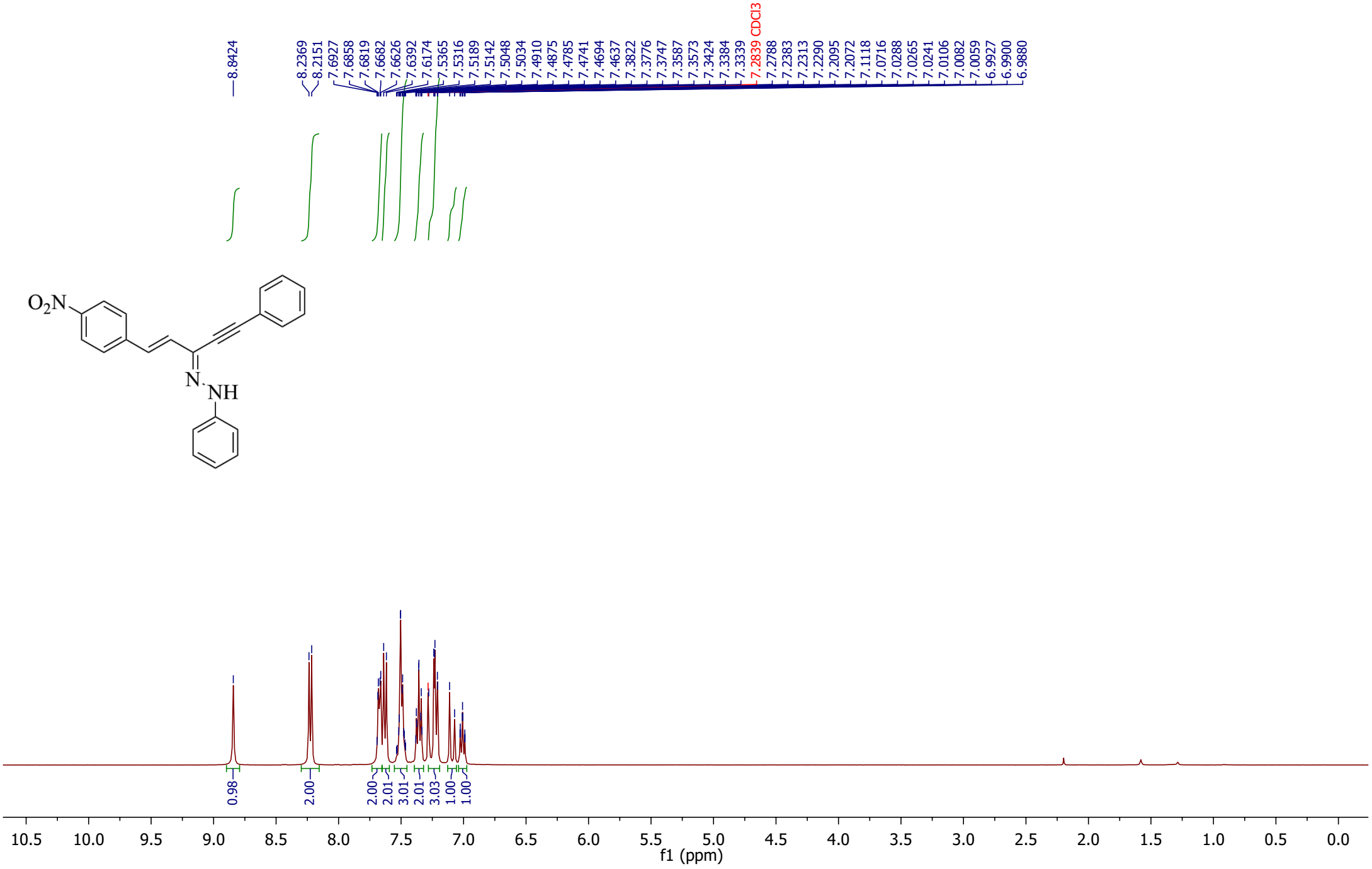
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of phenylhydrazone 5j



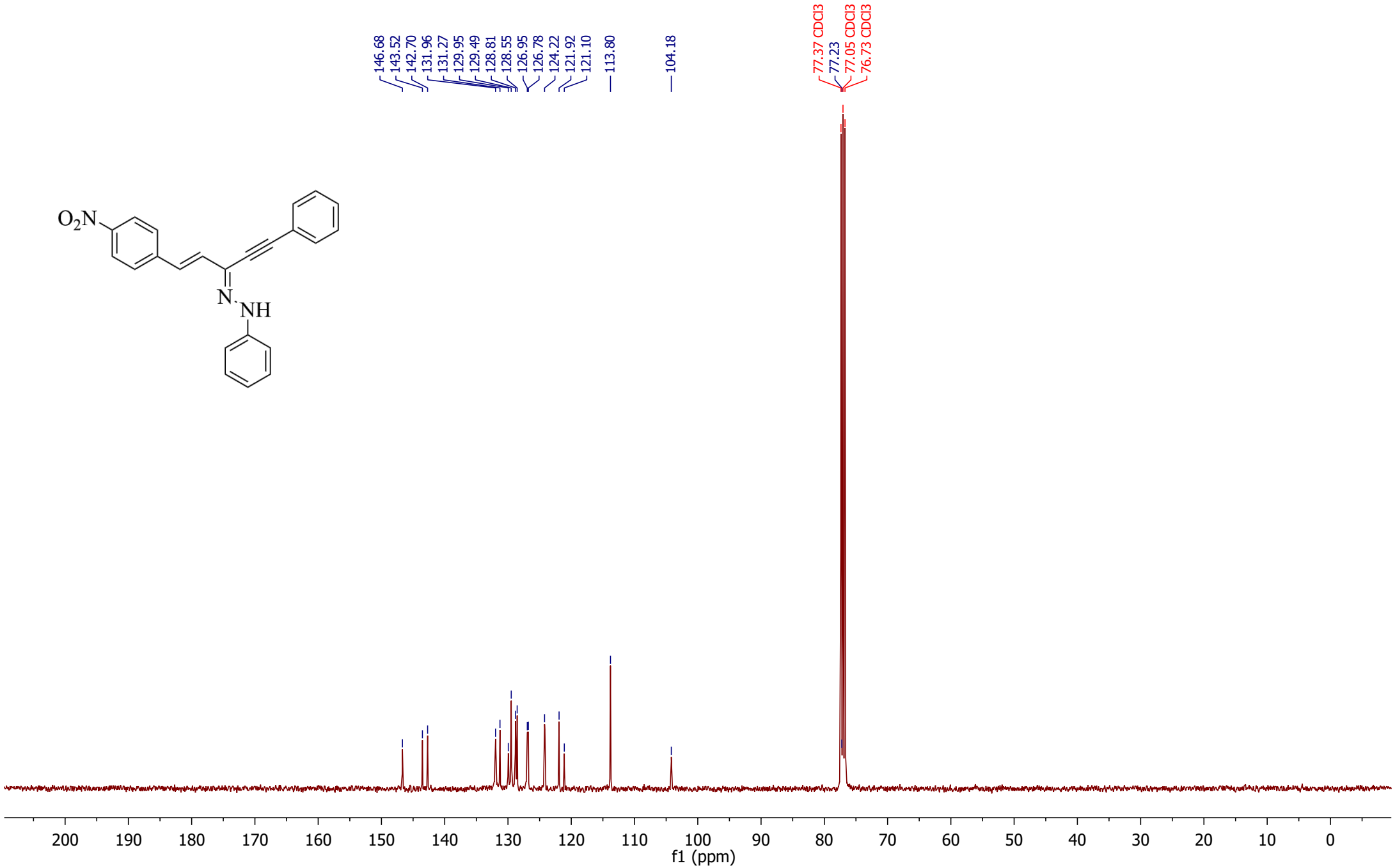
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of phenylhydrazone 5j



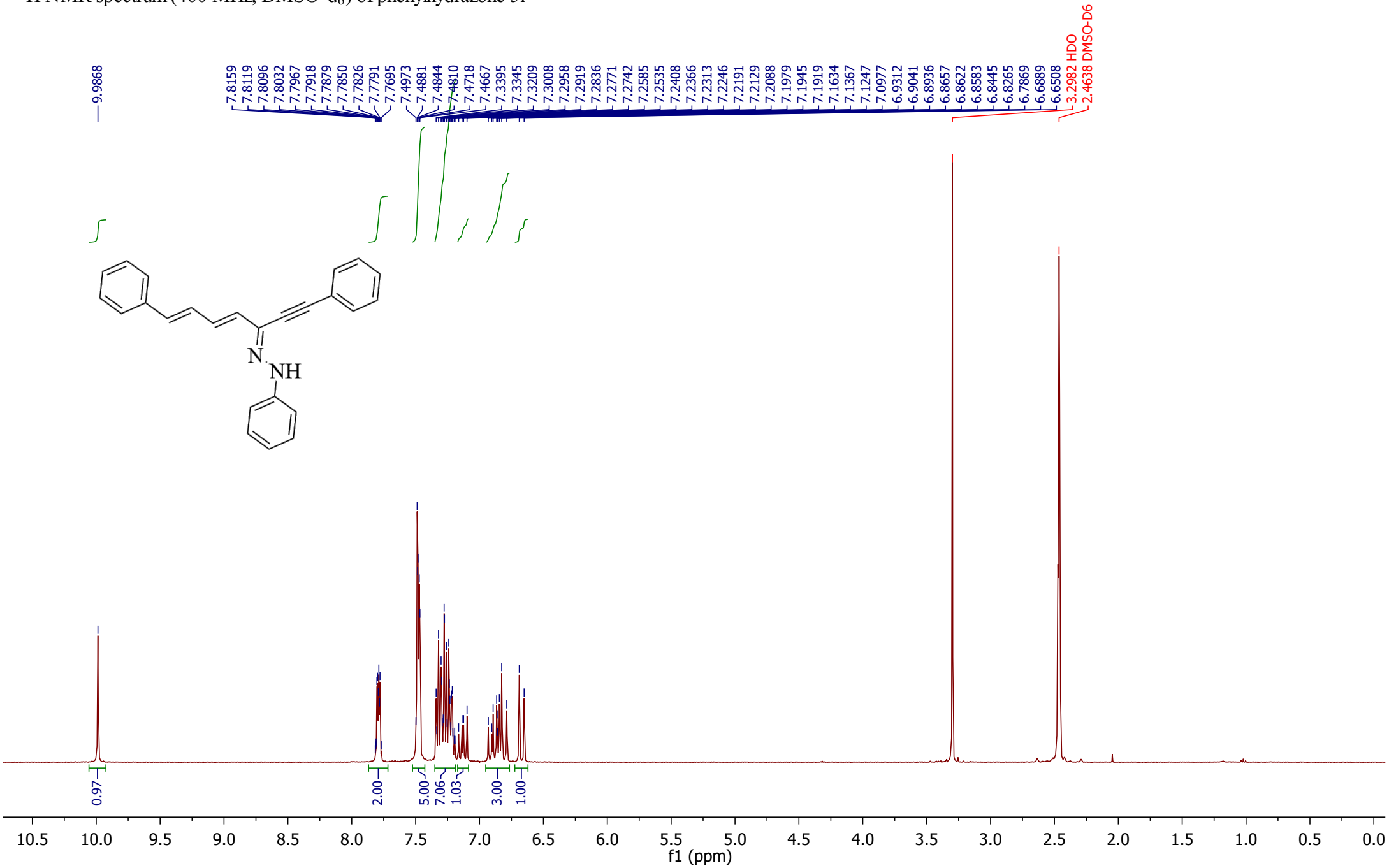
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of phenylhydrazone 5k



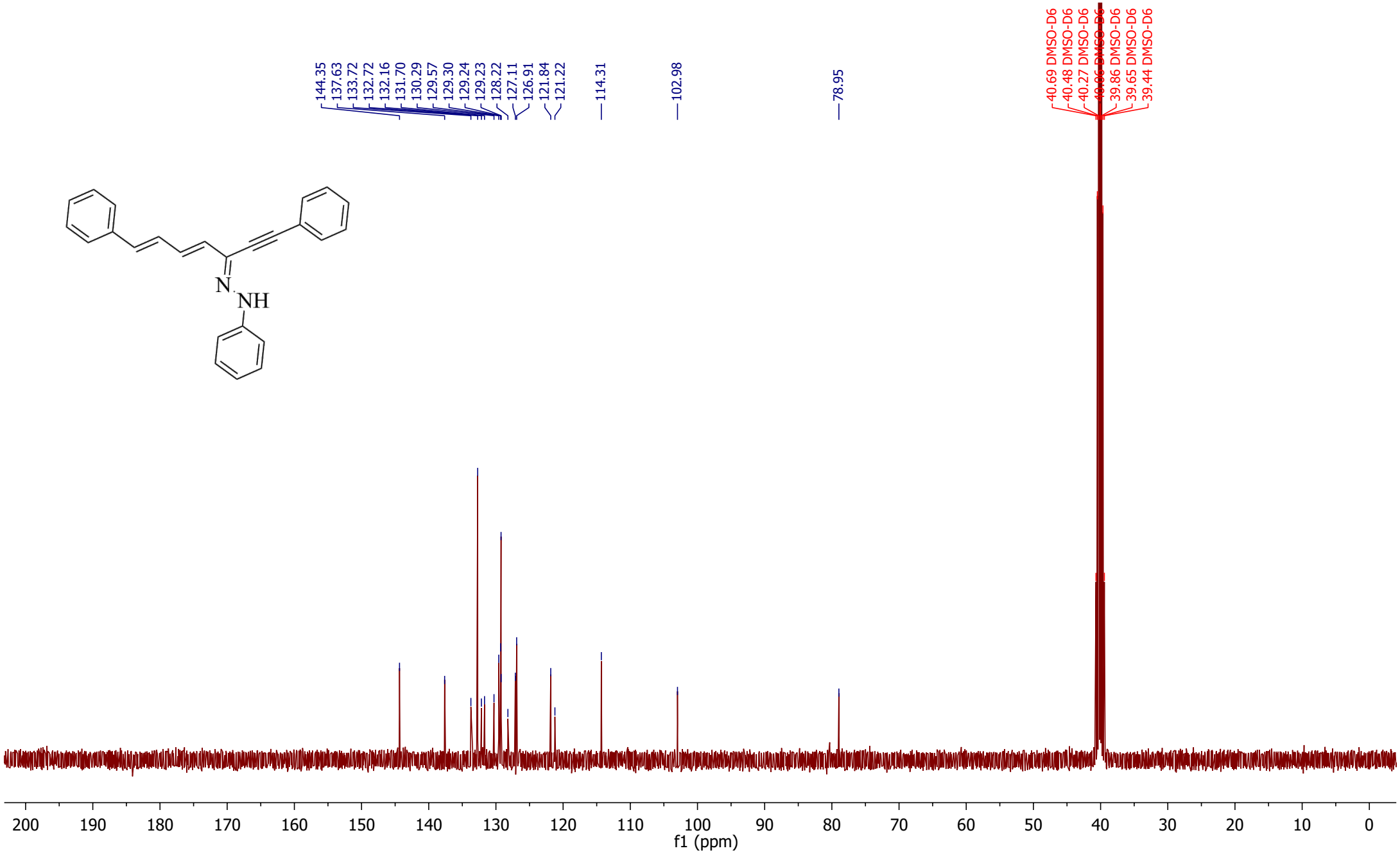
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of phenylhydrazone 5k



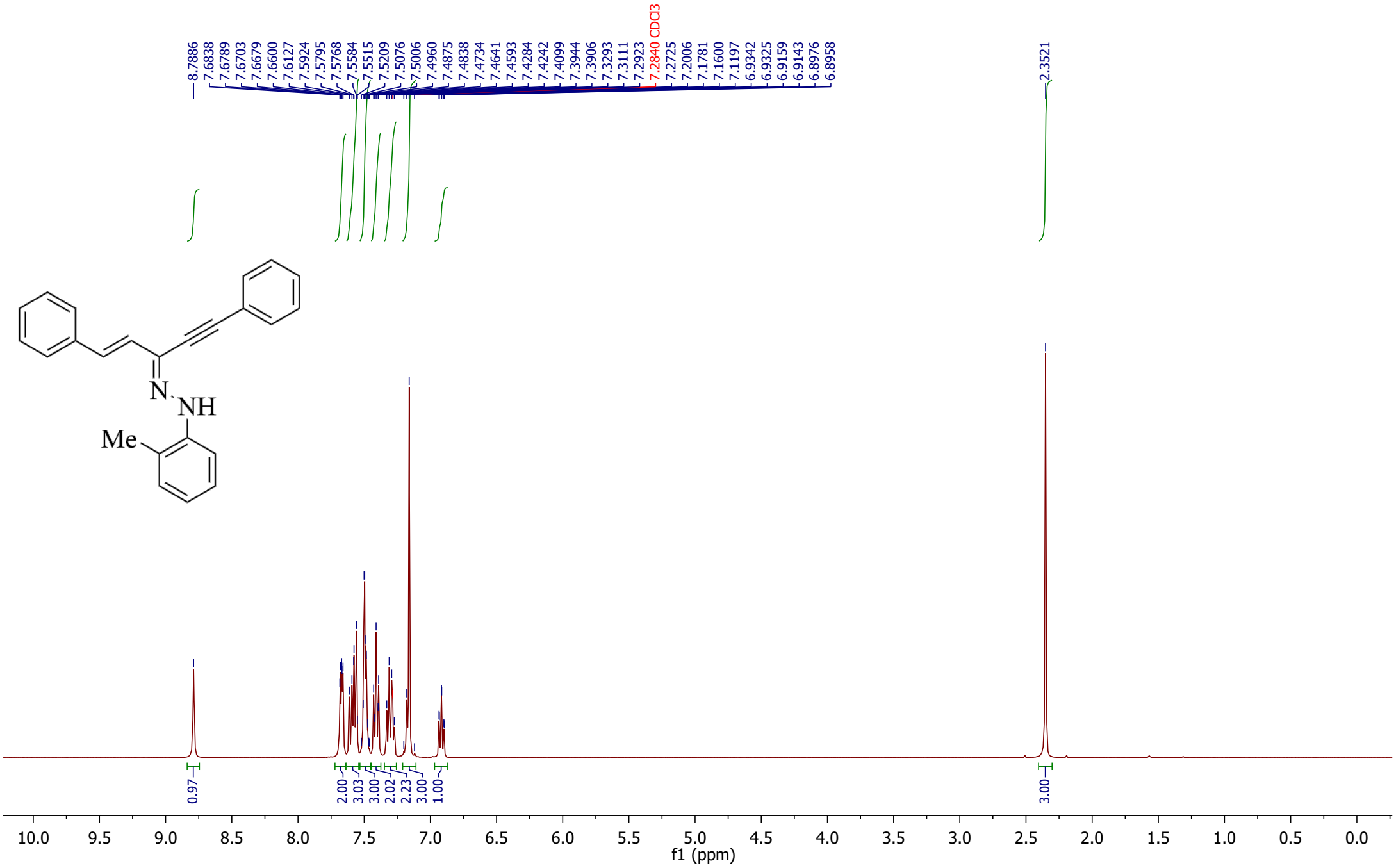
^{1}H NMR spectrum (400 MHz, DMSO-d_6) of phenylhydrazone 5l



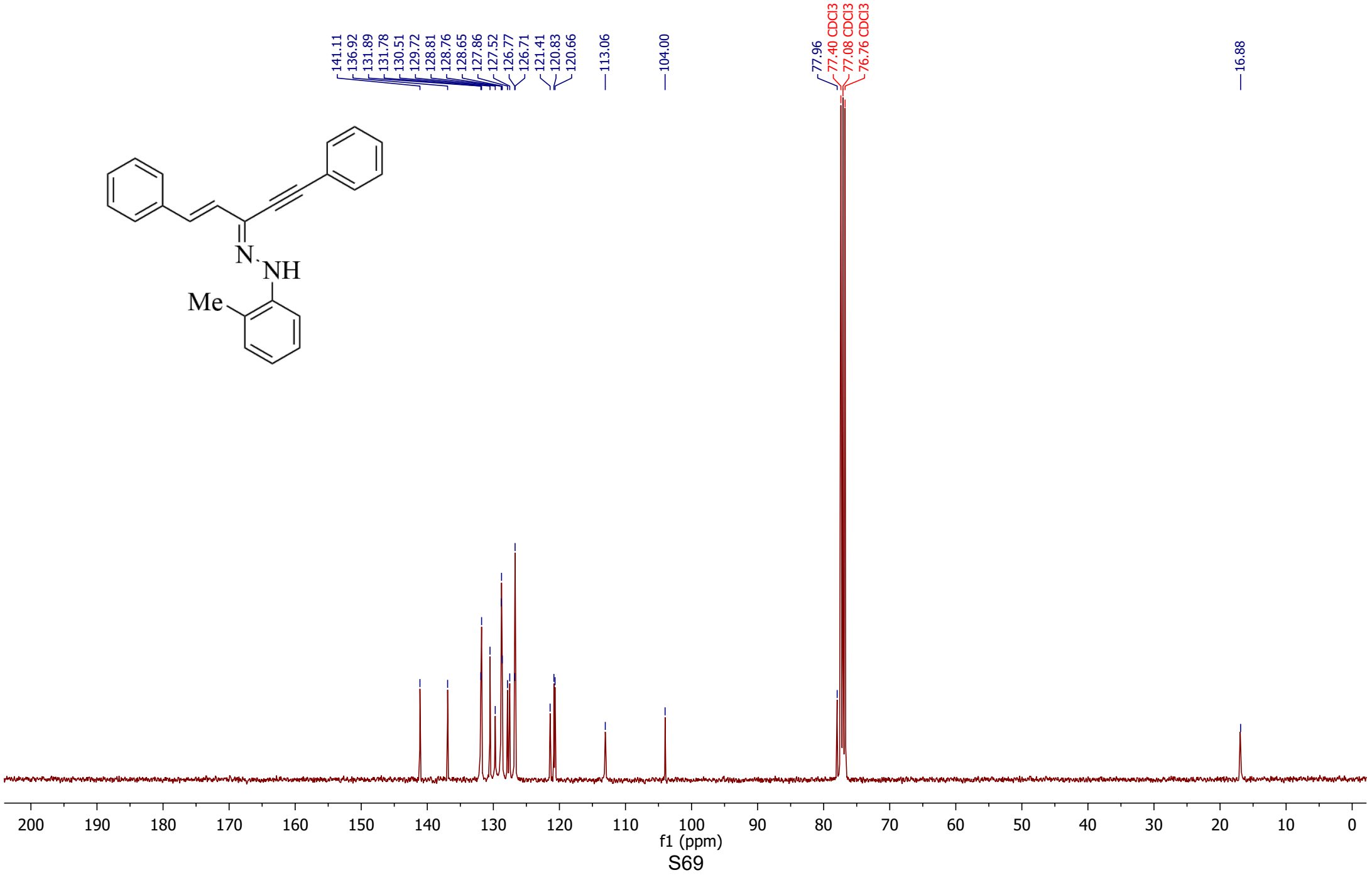
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, DMSO-d_6) of phenylhydrazone 5l



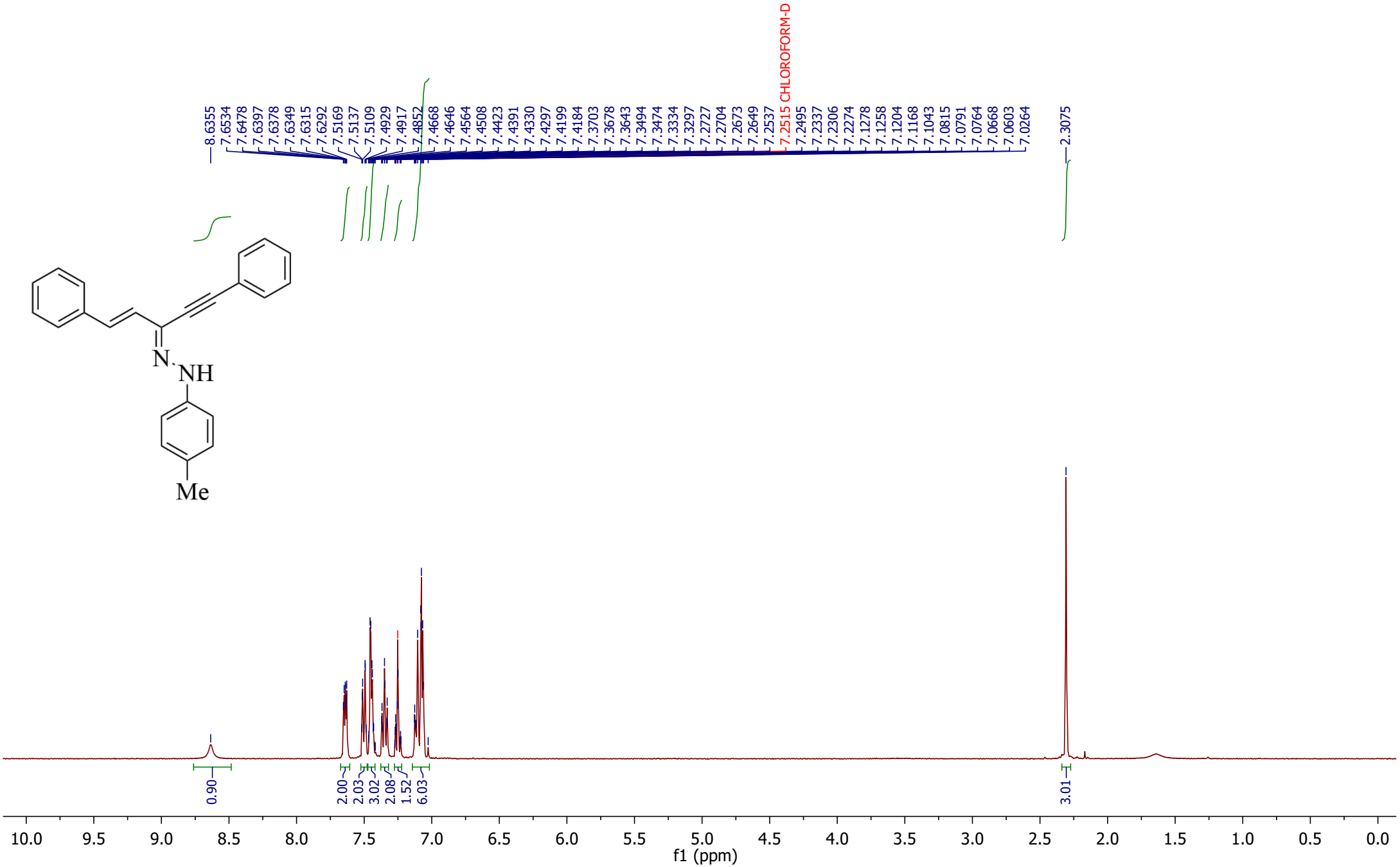
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 2-methylphenylhydrazone 5p



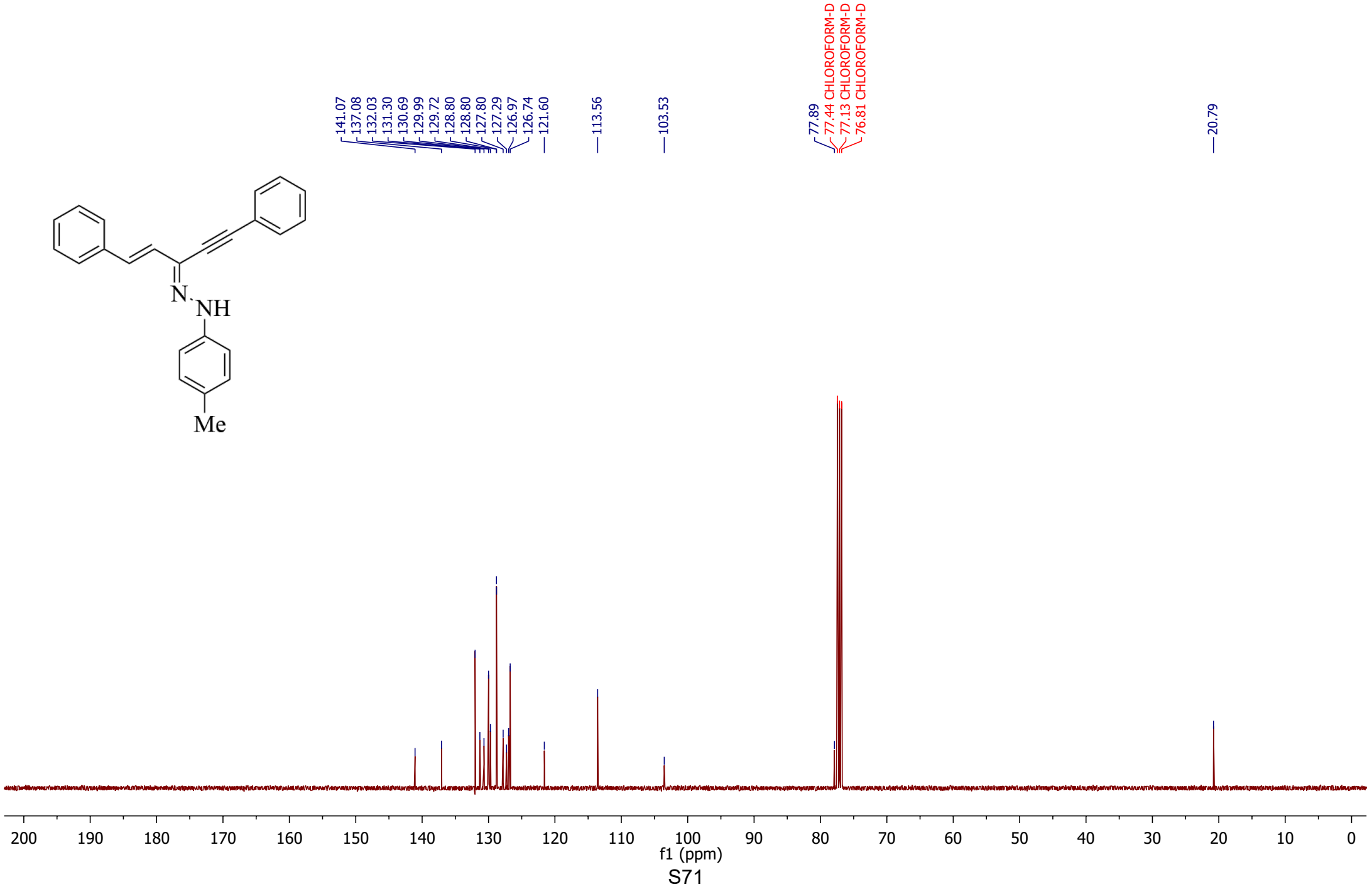
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 2-methylphenylhydrazone 5p



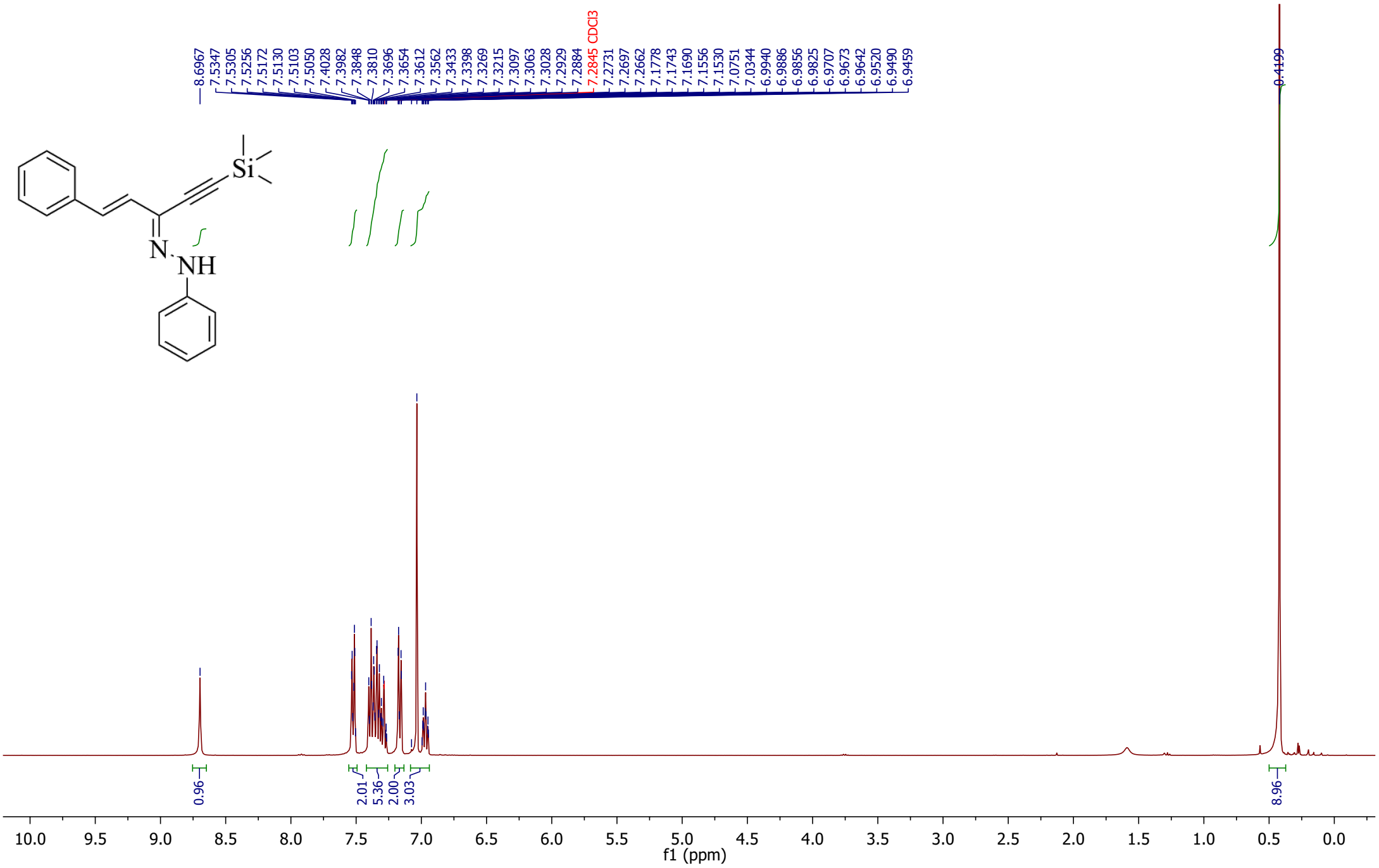
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4-methylphenylhydrazone 5q



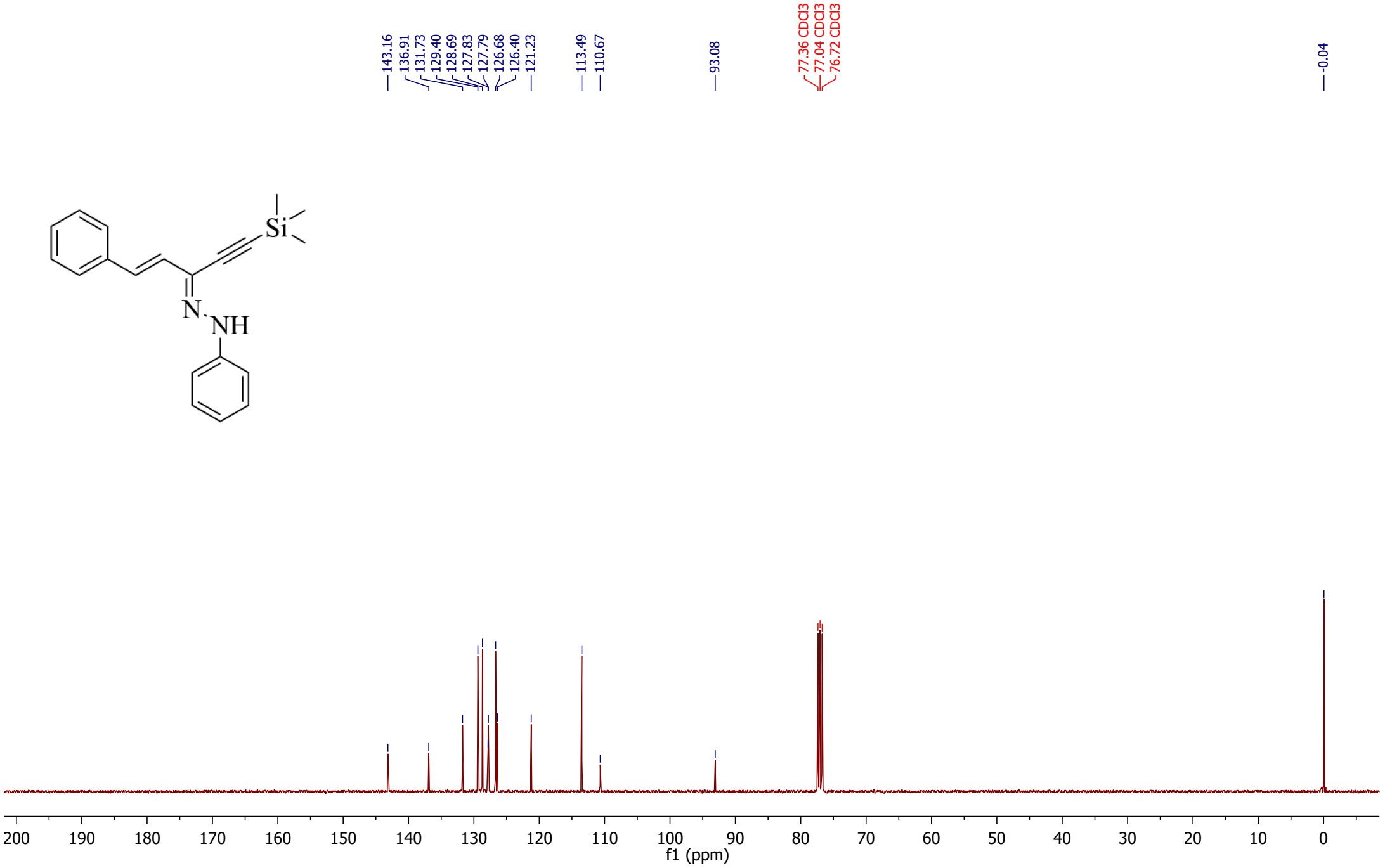
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 4-methylphenylhydrazone 5q



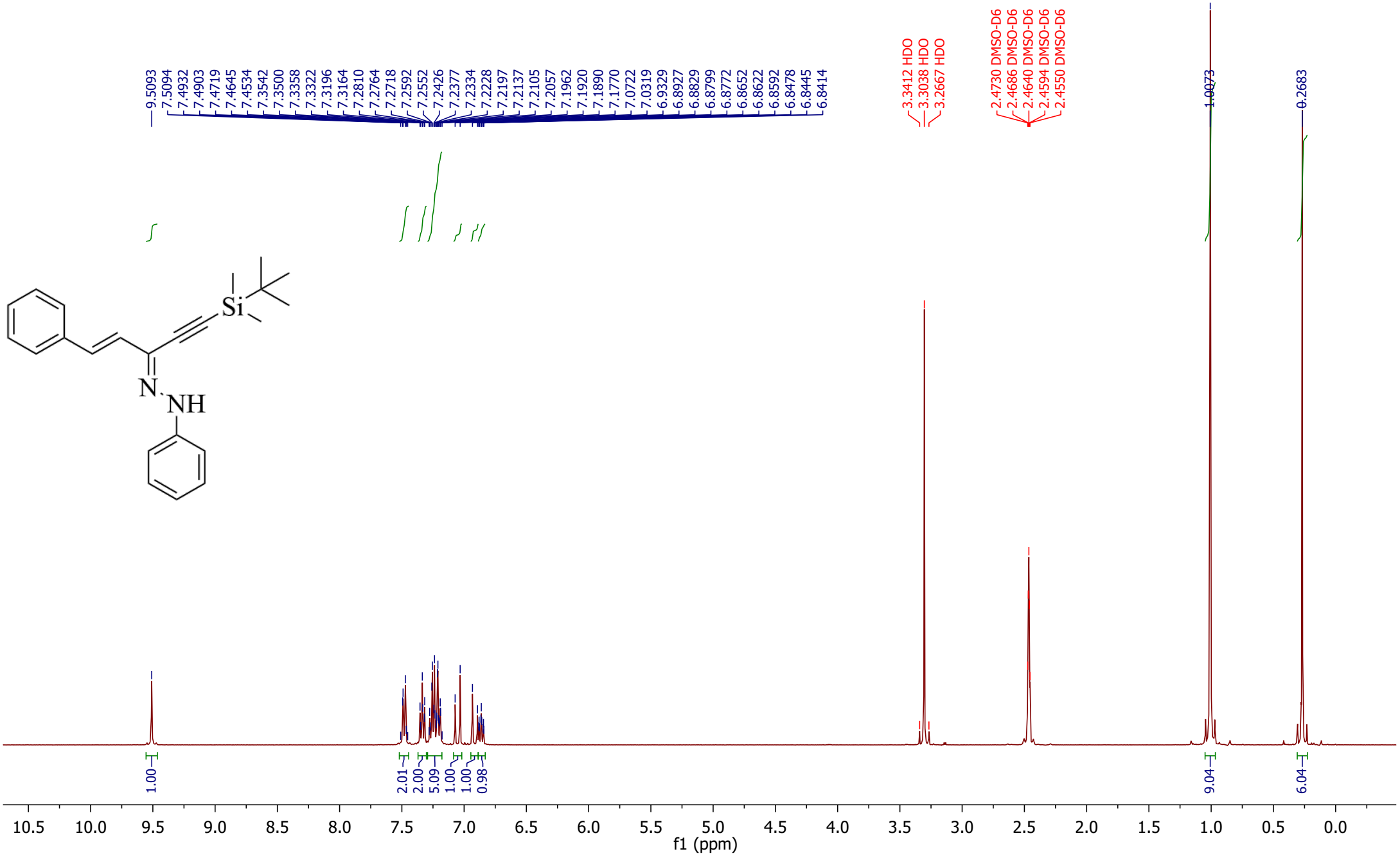
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of phenylhydrazone 5s



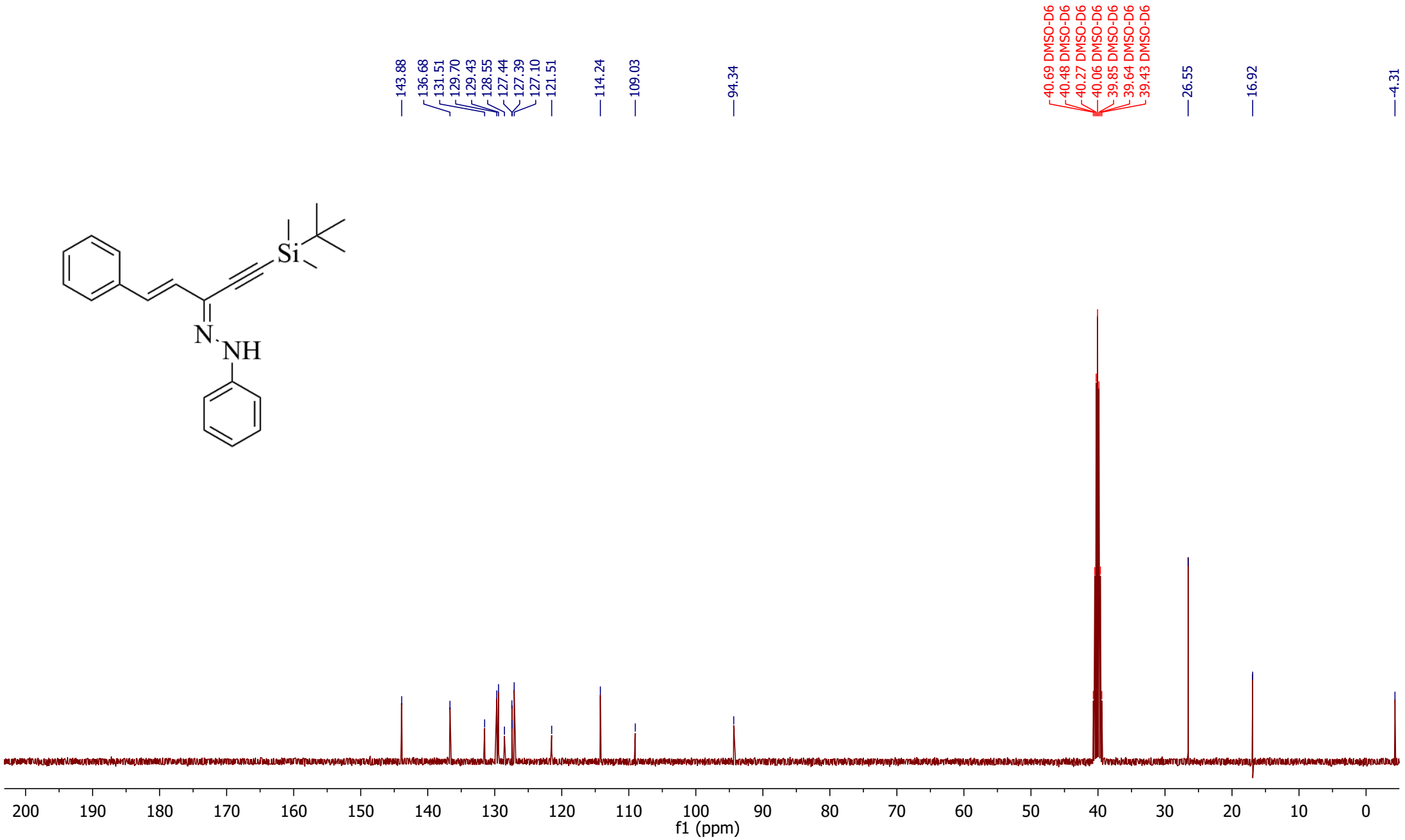
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of phenylhydrazone 5s



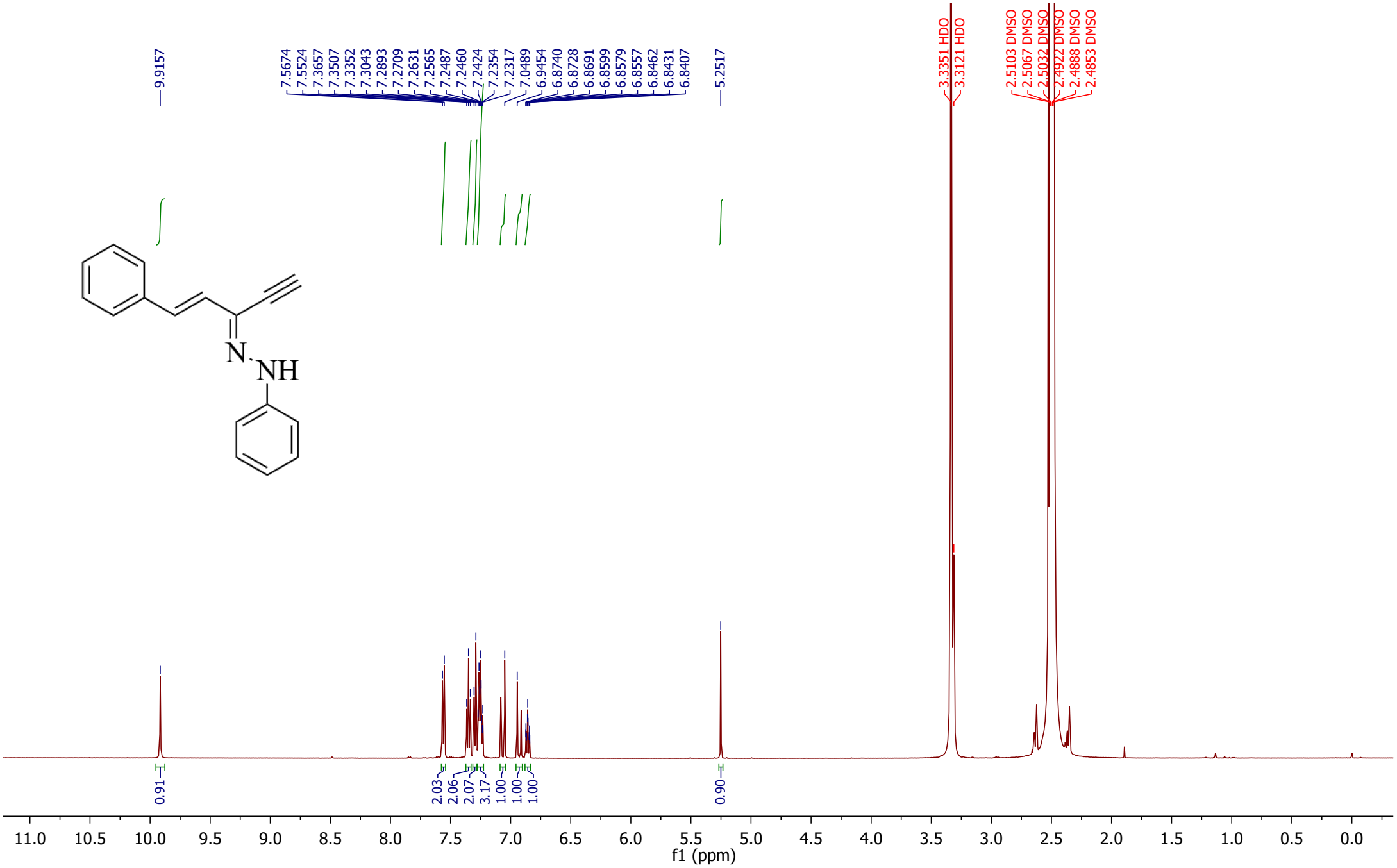
^{1}H NMR spectrum (400 MHz, DMSO-d_6) of phenylhydrazone 5t



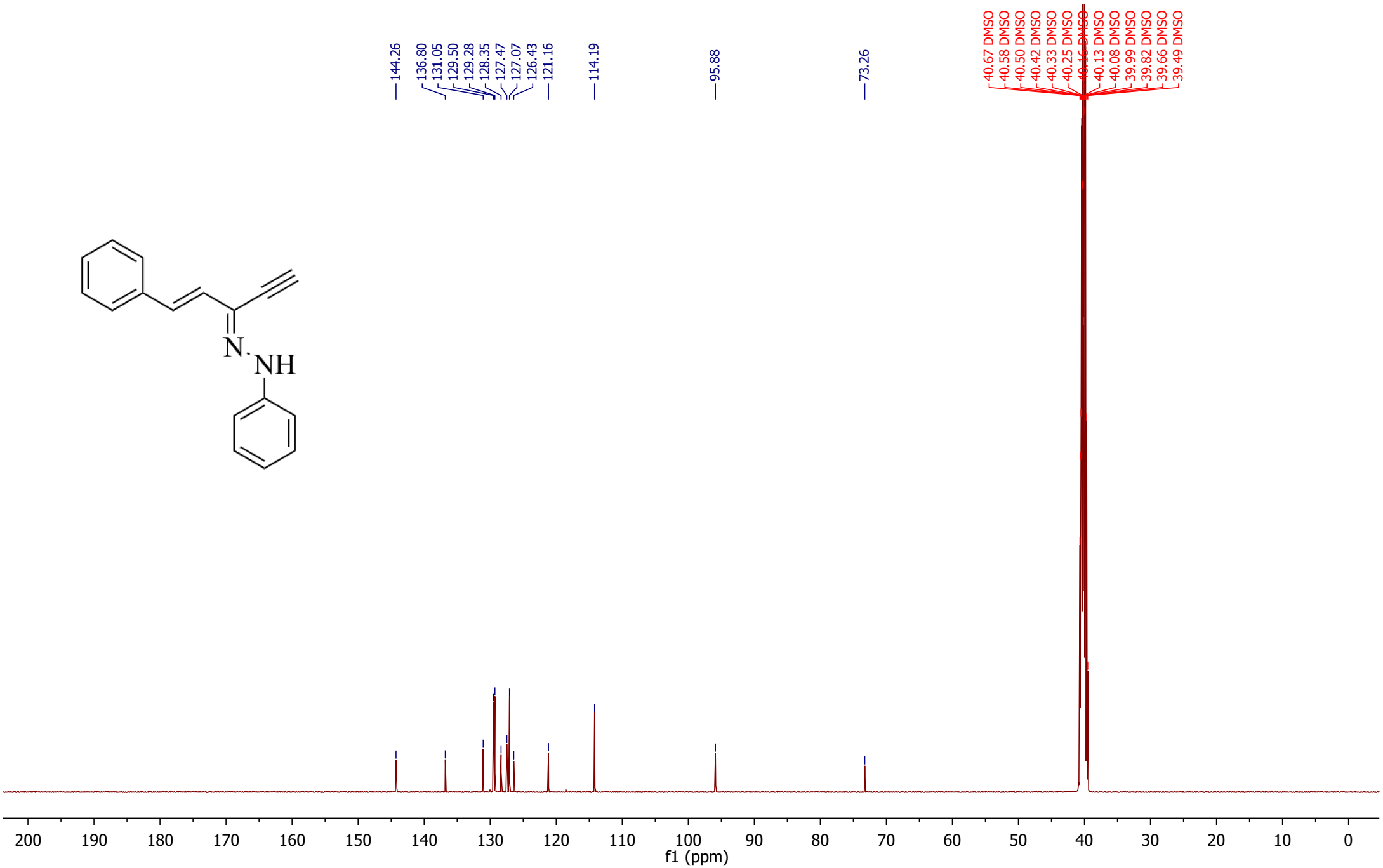
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, DMSO-d_6) of phenylhydrazone 5t



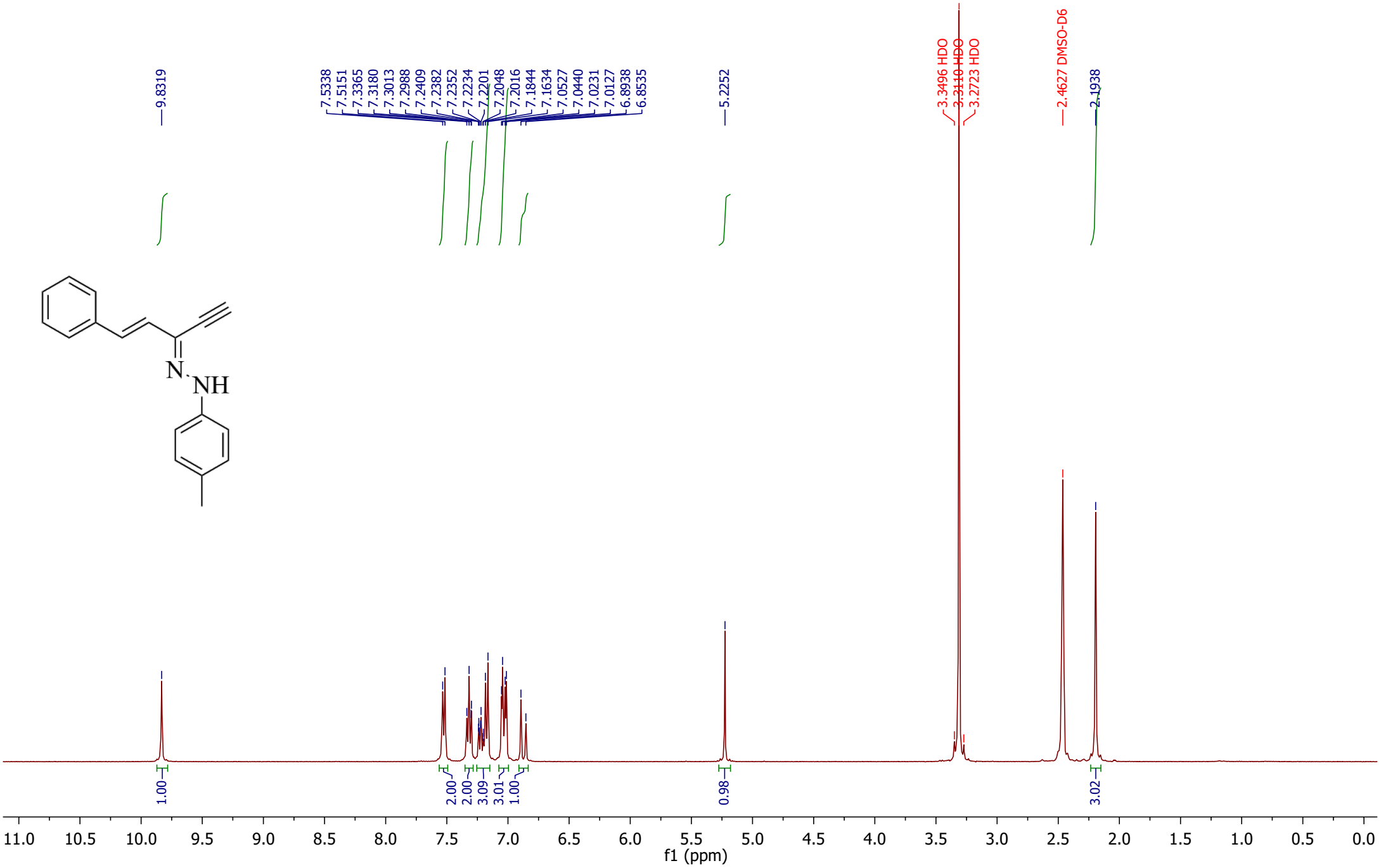
^{1}H NMR spectrum (500 MHz, DMSO-d_6) of phenylhydrazone 5u



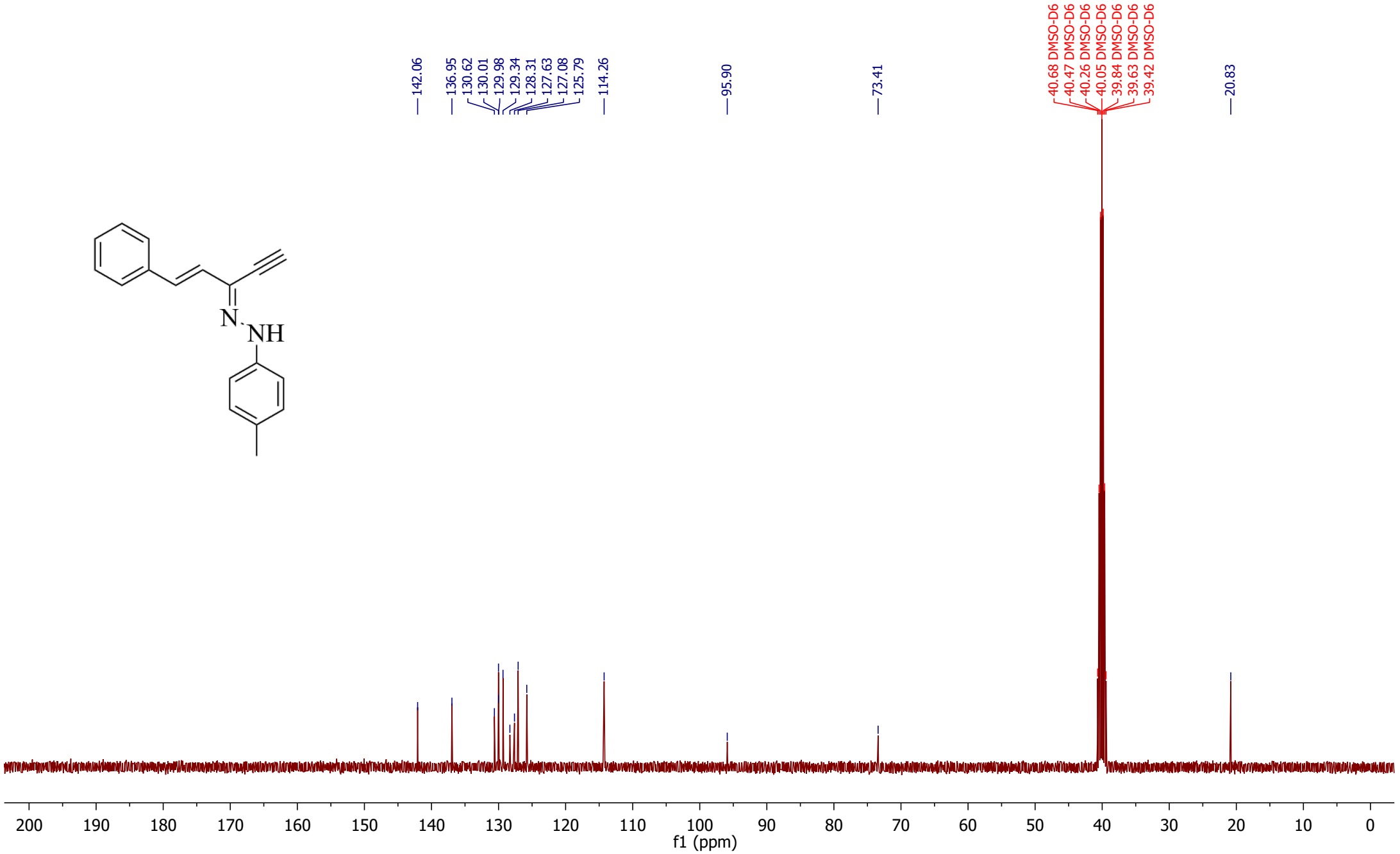
$^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, DMSO-d_6) of phenylhydrazone 5u



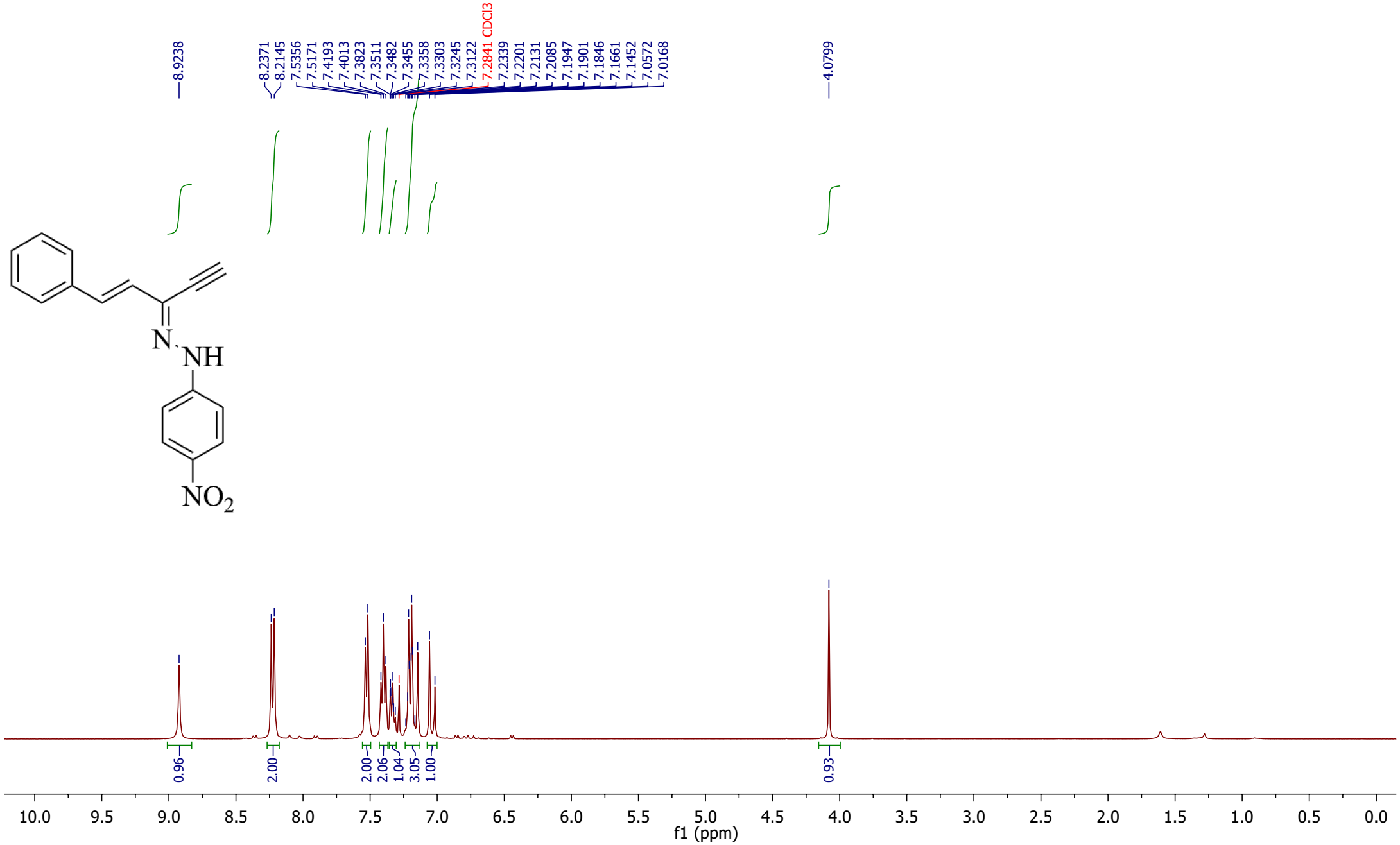
^{1}H NMR spectrum (400 MHz, DMSO-d_6) of 4-methylphenylhydrazone 5v



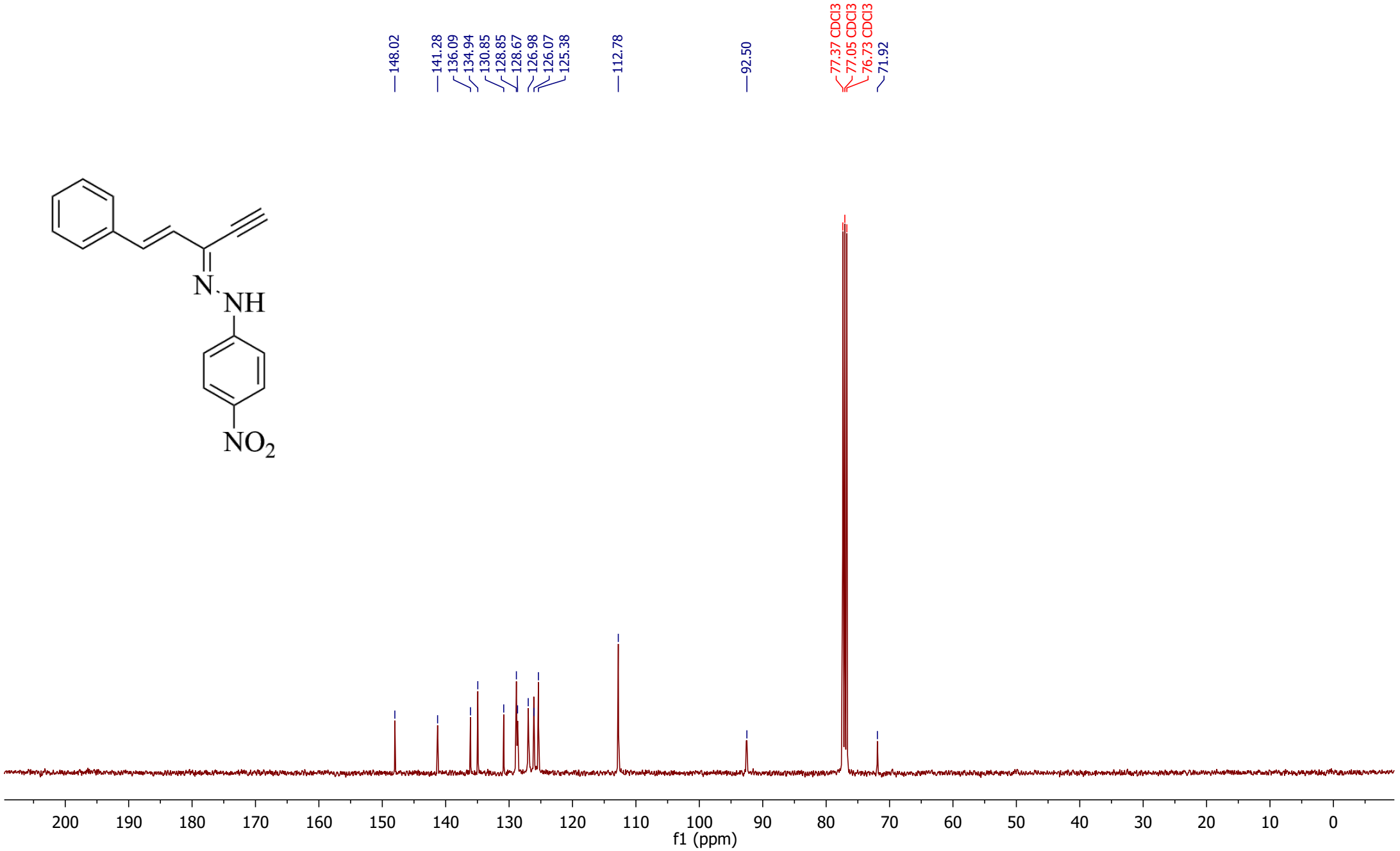
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, DMSO-d_6) of 4-methylphenylhydrazone 5v



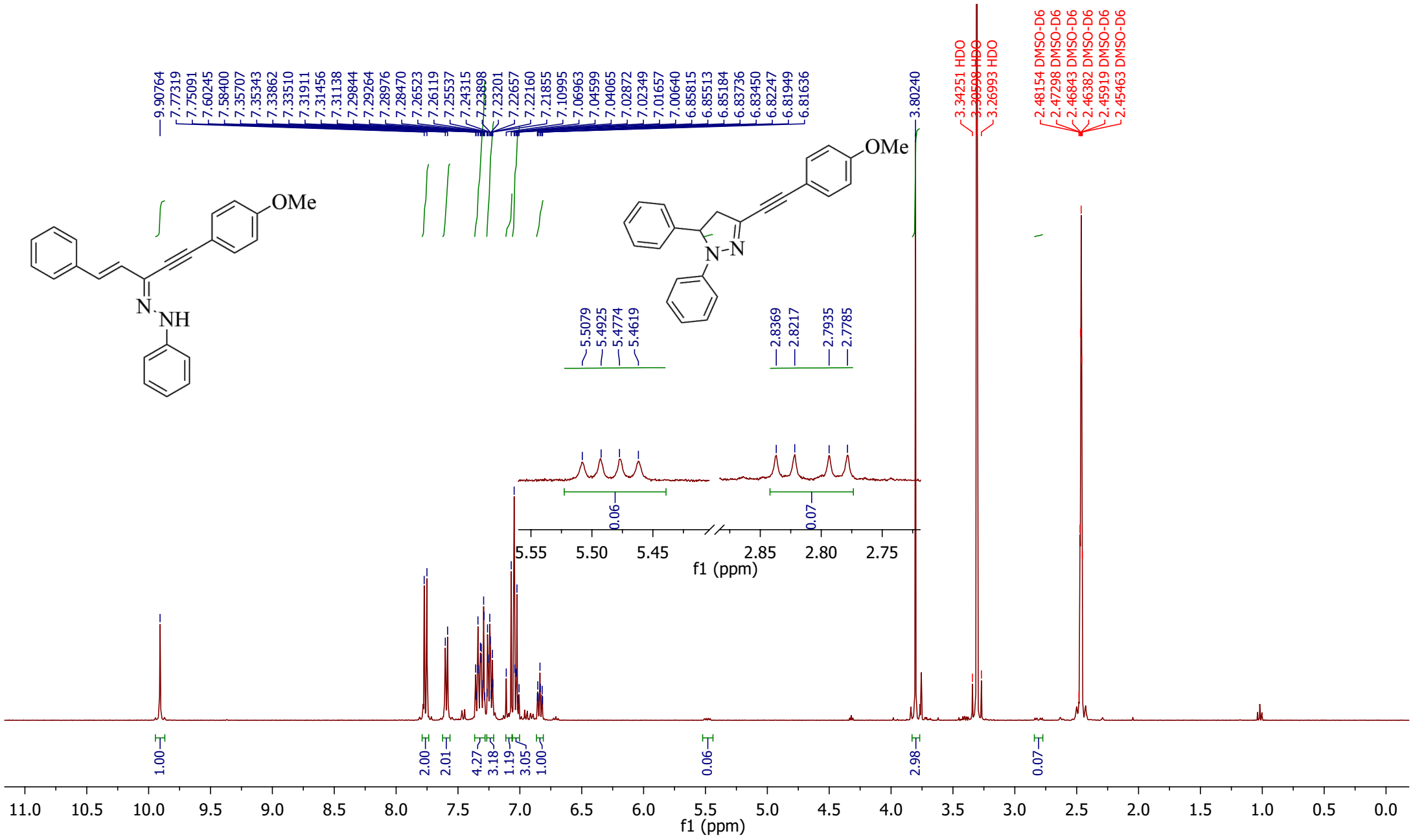
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4-nitrophenylhydrazone 5w



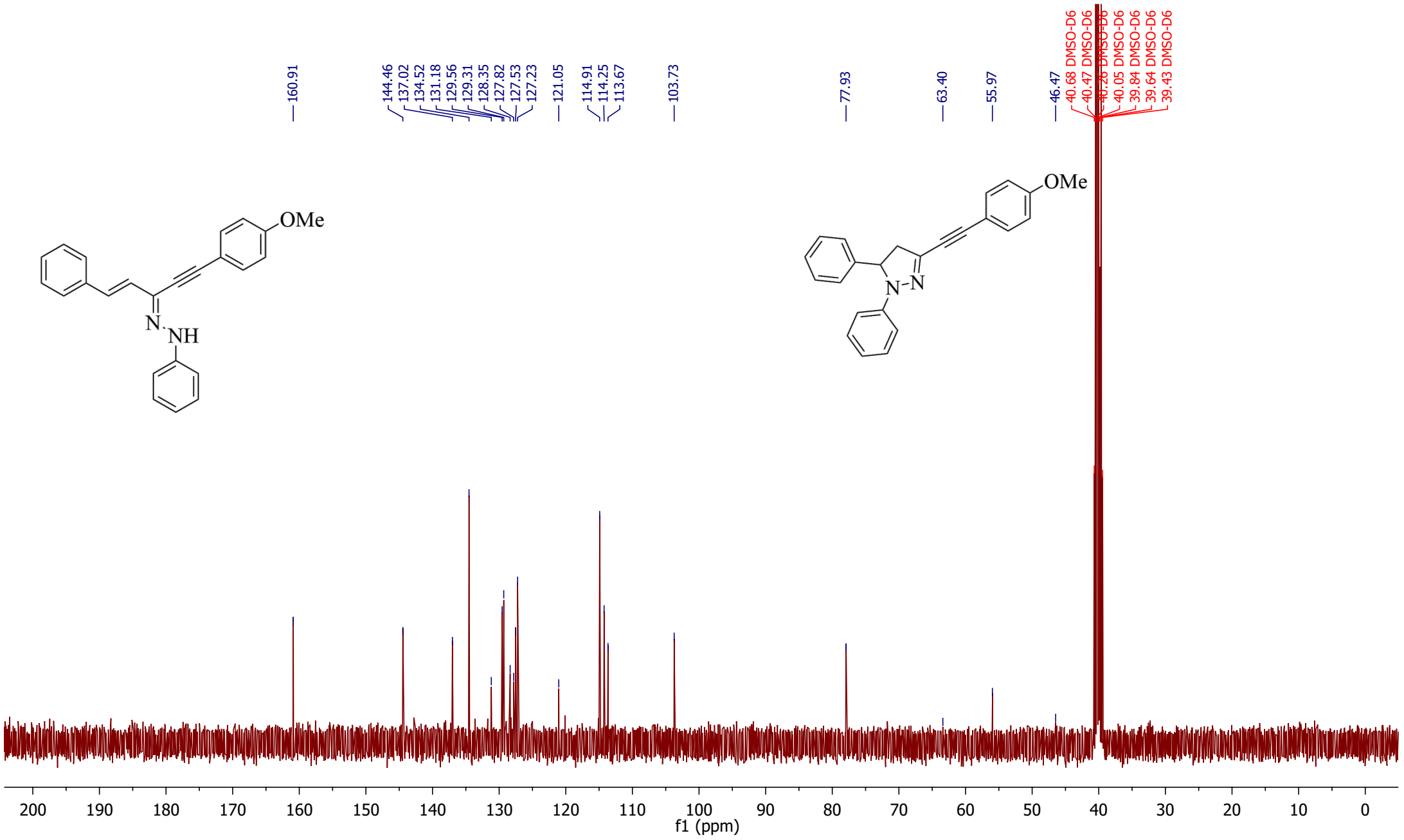
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 4-nitrophenylhydrazone 5w



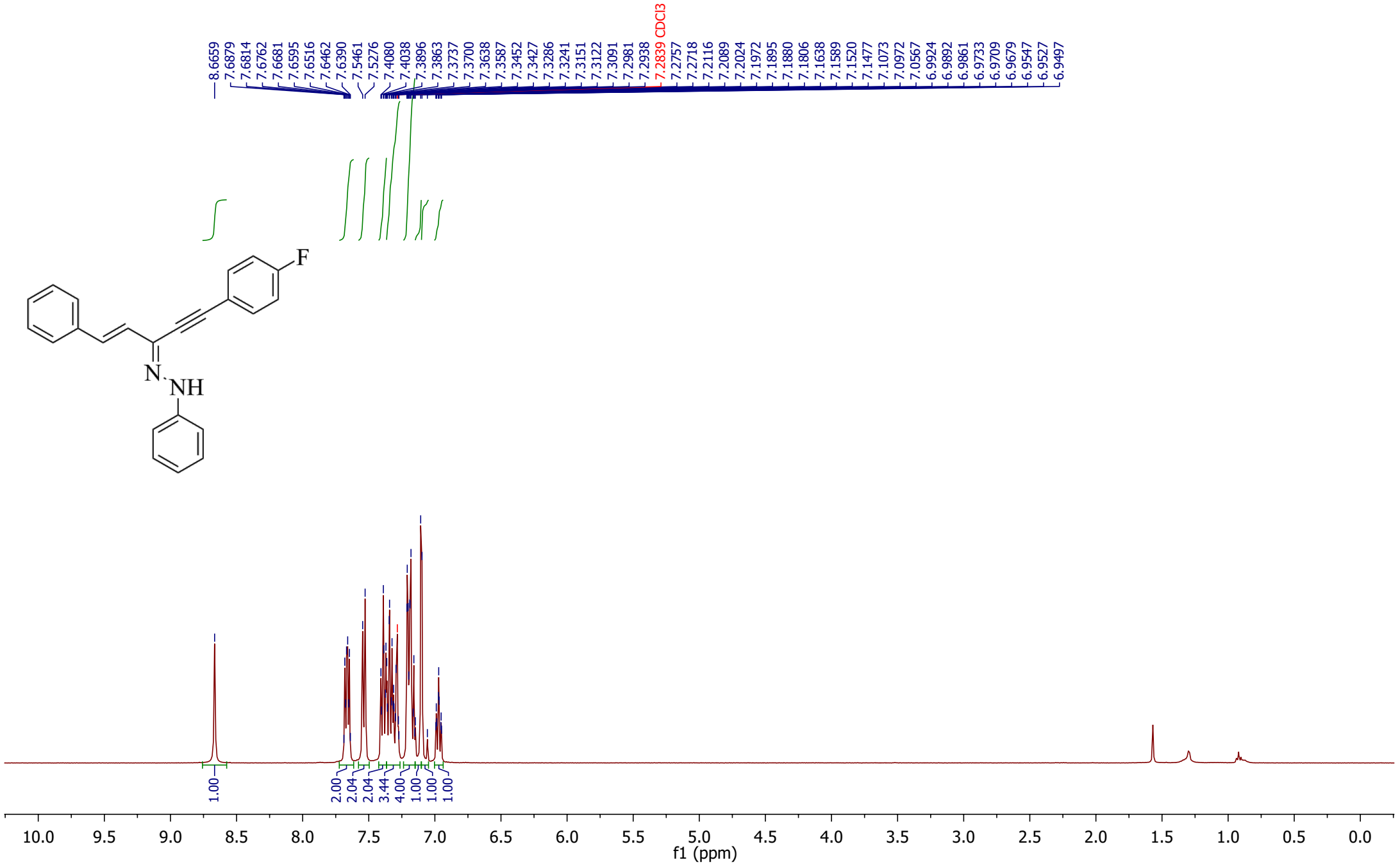
^{1}H NMR spectrum (400 MHz, DMSO-d_6) of of phenylhydrazone 5x and minor isomer - 4,5-dihydro-1H-pyrazole 6a



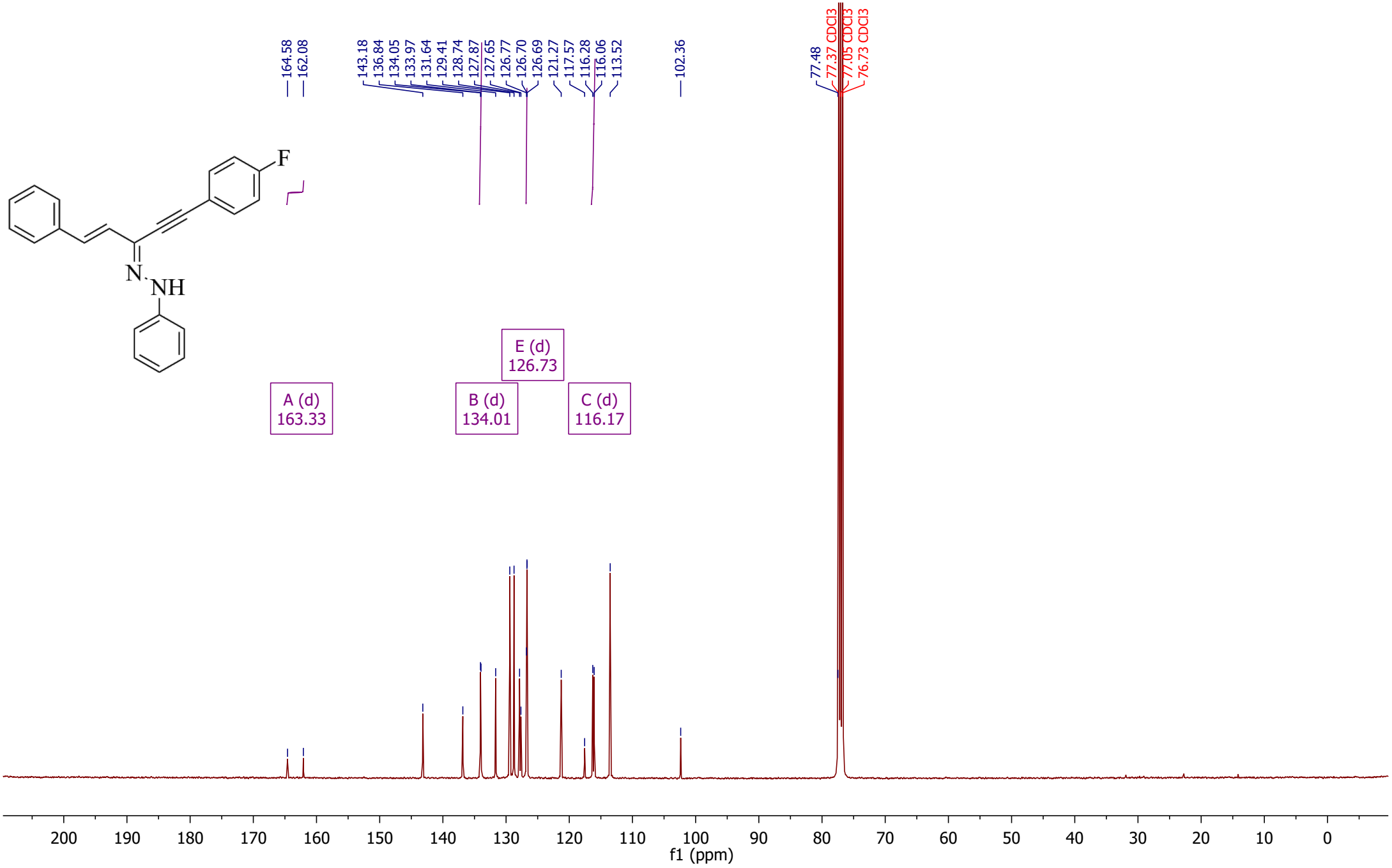
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, DMSO-d_6) of of phenylhydrazone 5x and minor isomer - 4,5-dihydro-1H-pyrazole 6a



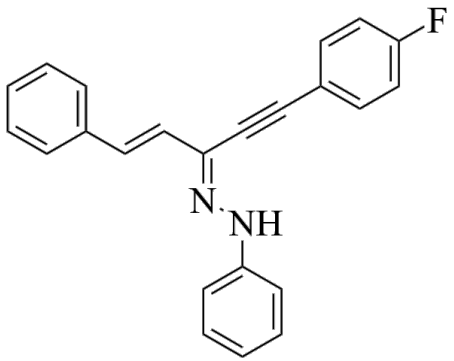
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of phenylhydrazone 5y



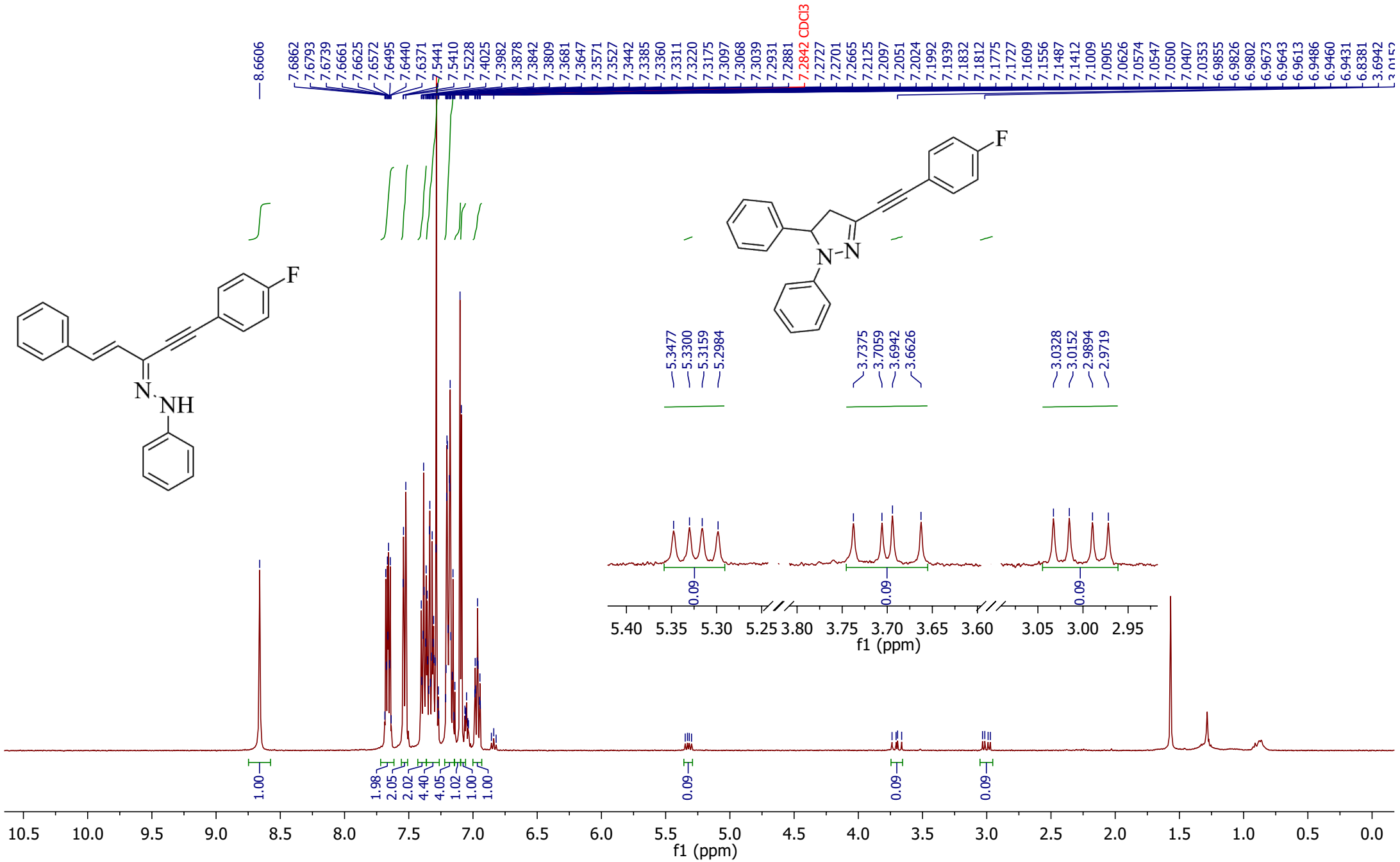
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of phenylhydrazone 5y



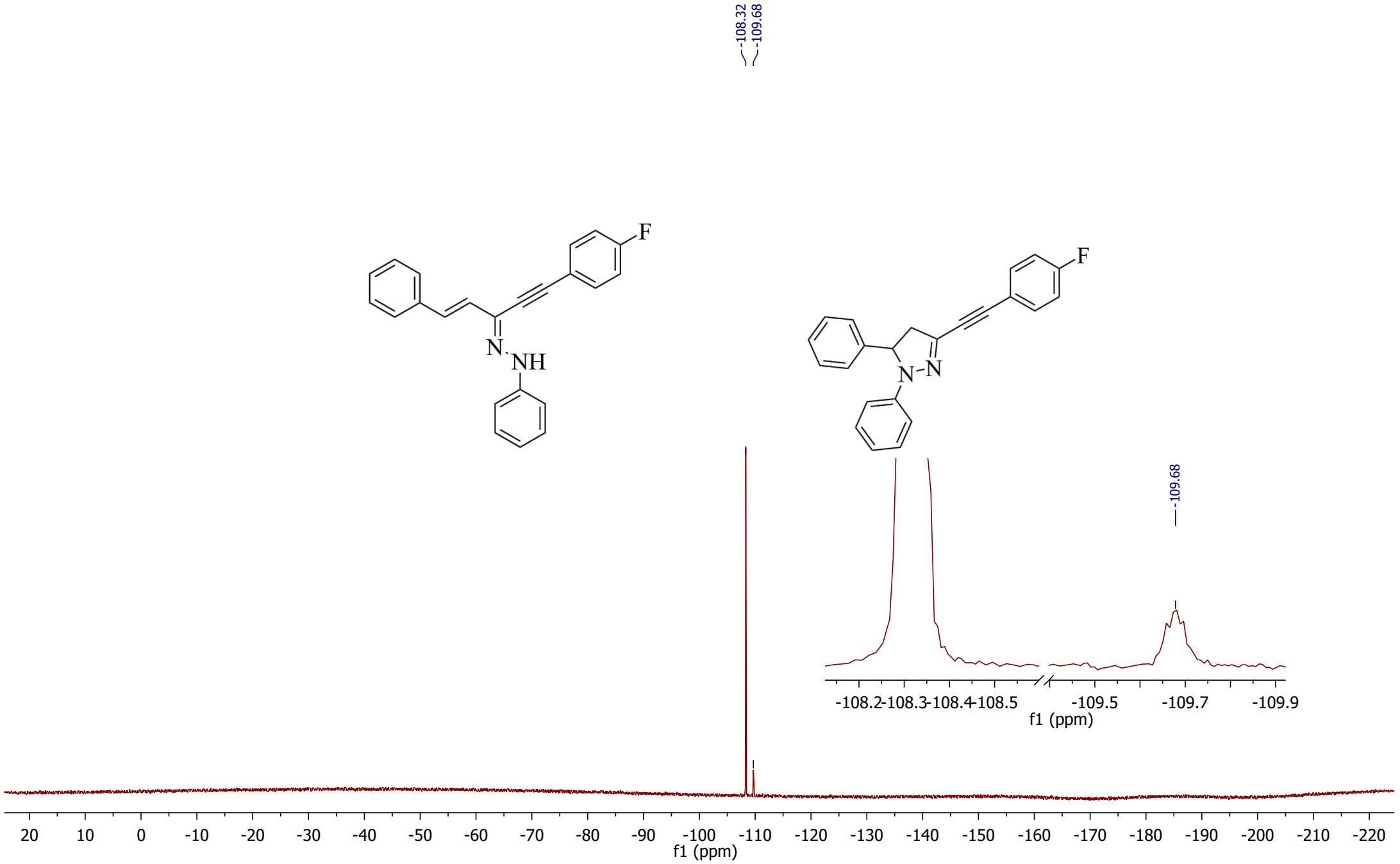
^{19}F NMR spectrum (376 MHz, $CDCl_3$) of phenylhydrazone 5y



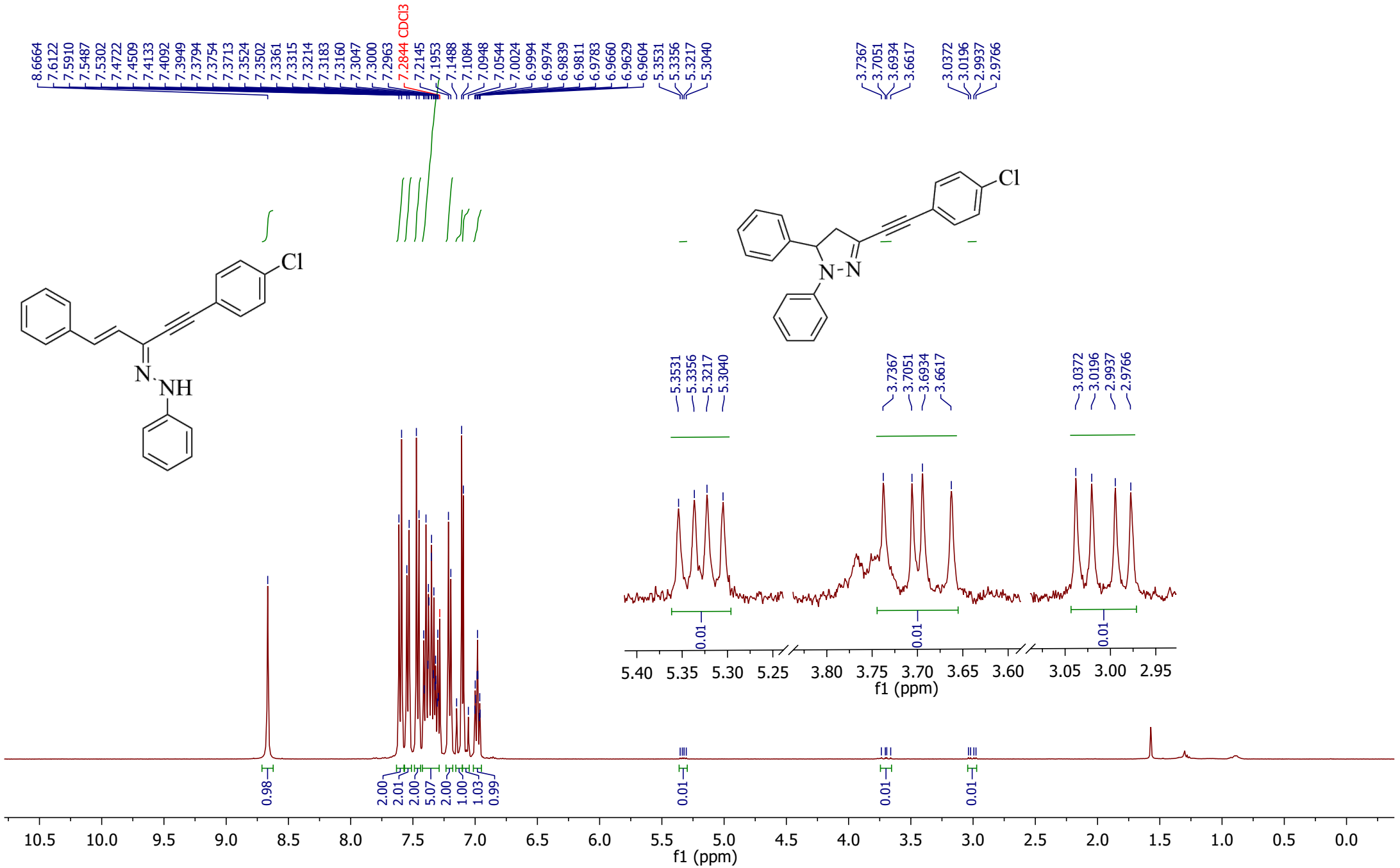
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of phenylhydrazone 5y and minor isomer - 4,5-dihydro-*1H*-pyrazole 6b



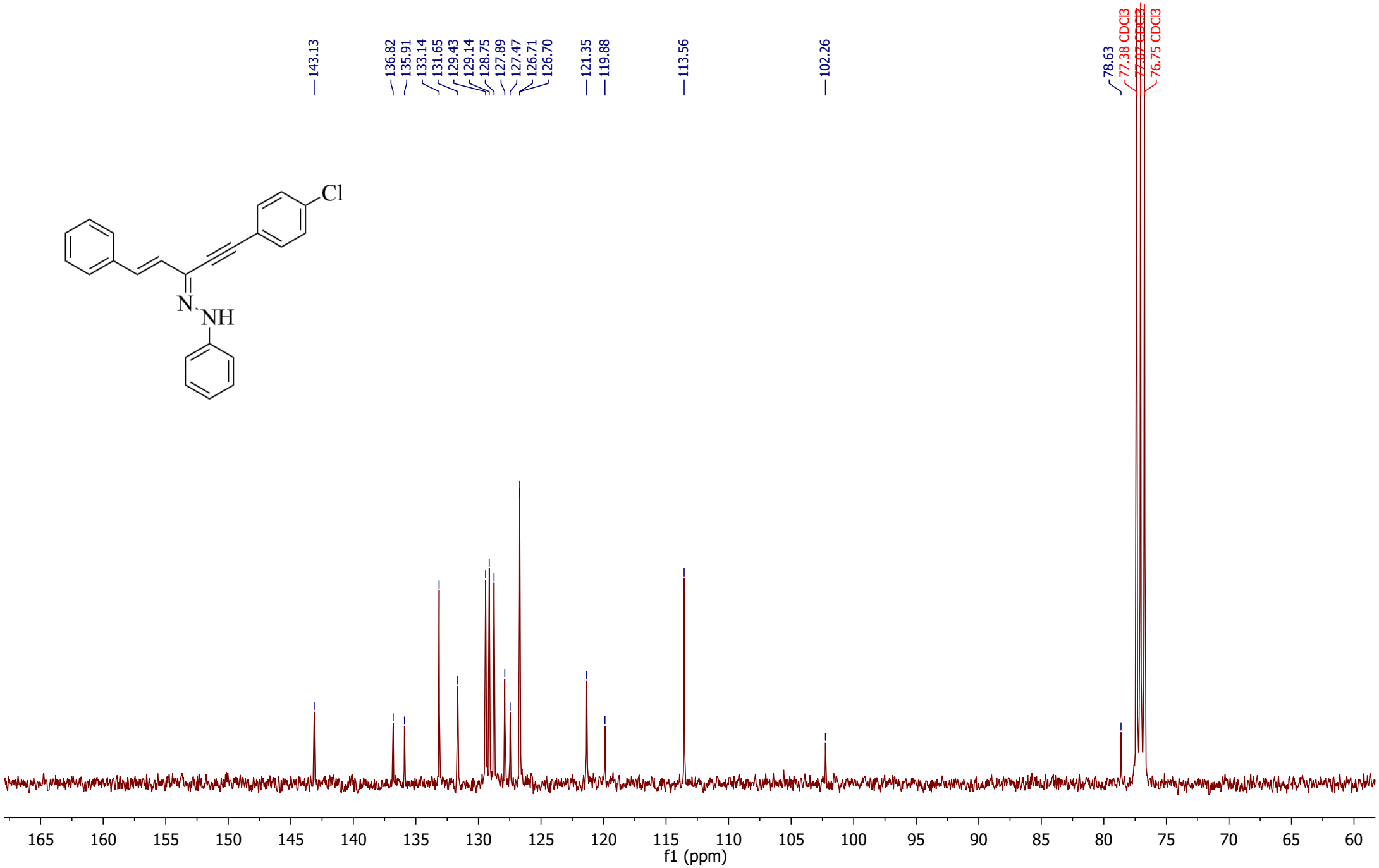
^{19}F NMR spectrum (376 MHz, $CDCl_3$) of phenylhydrazone 5y and minor isomer - 4,5-dihydro-*1H*-pyrazole 6b



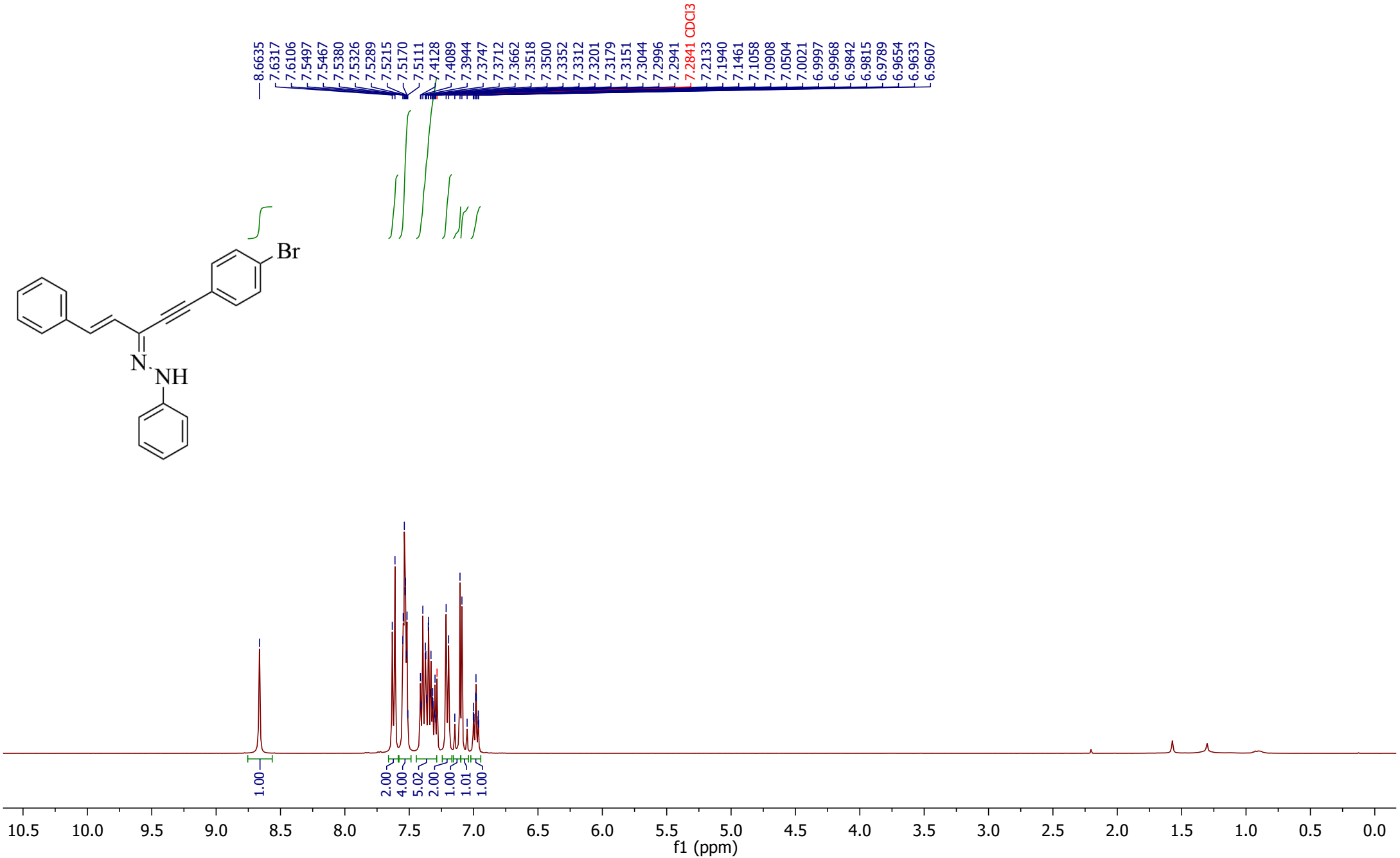
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of phenylhydrazone 5z and minor isomer - 4,5-dihydro-1*H*-pyrazole 6c



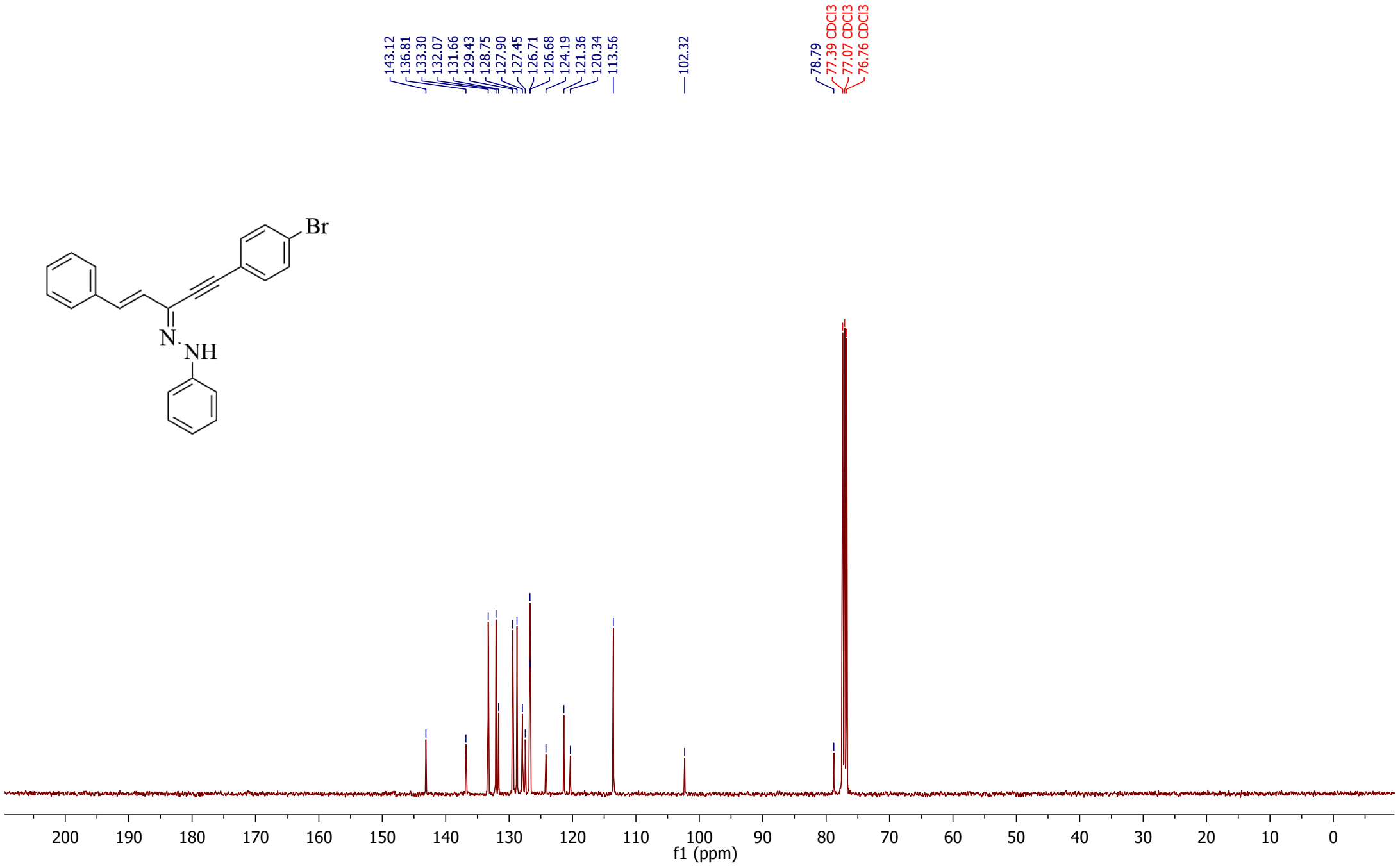
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of phenylhydrazone 5z



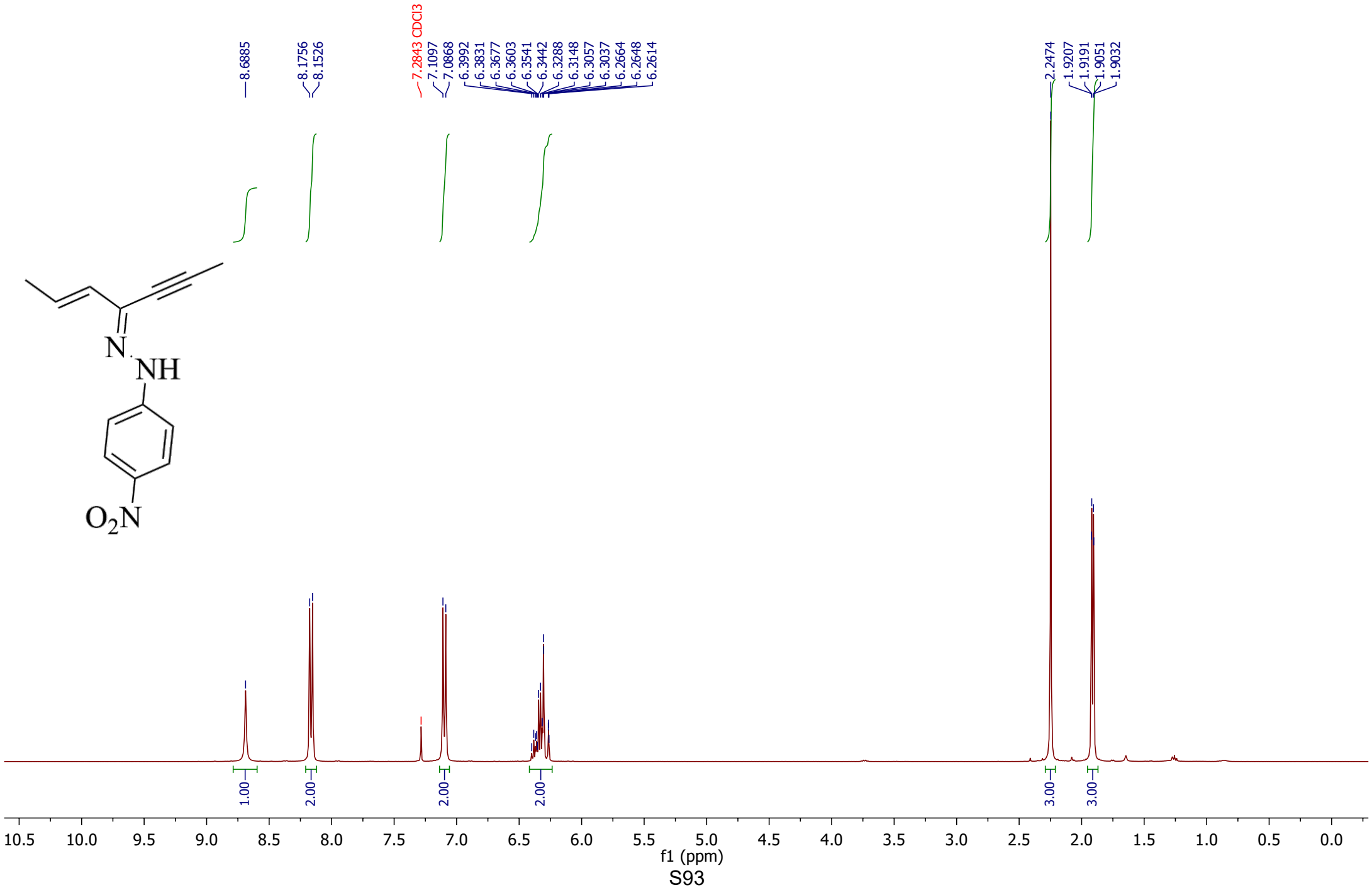
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of phenylhydrazone 5aa



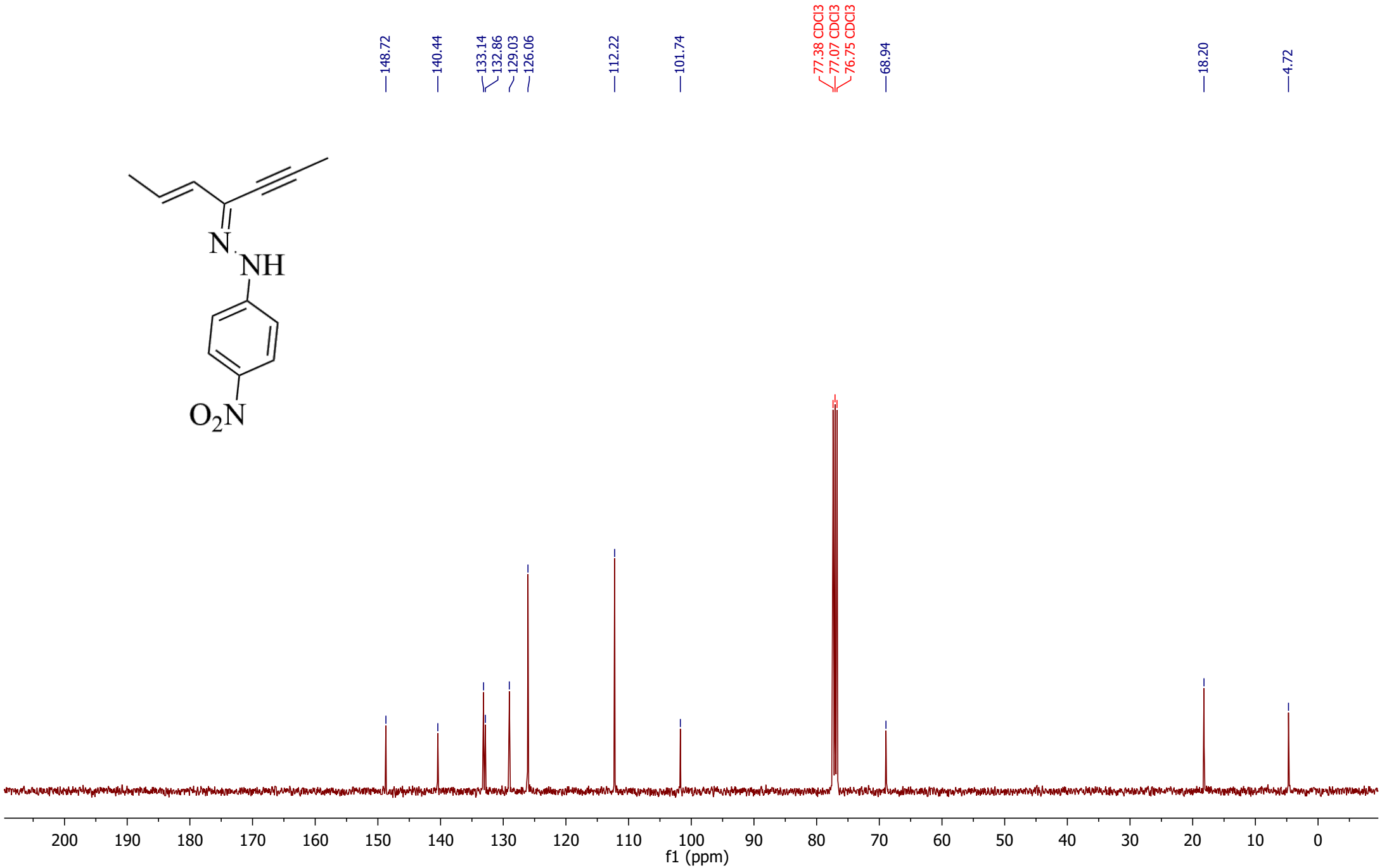
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of phenylhydrazone 5aa



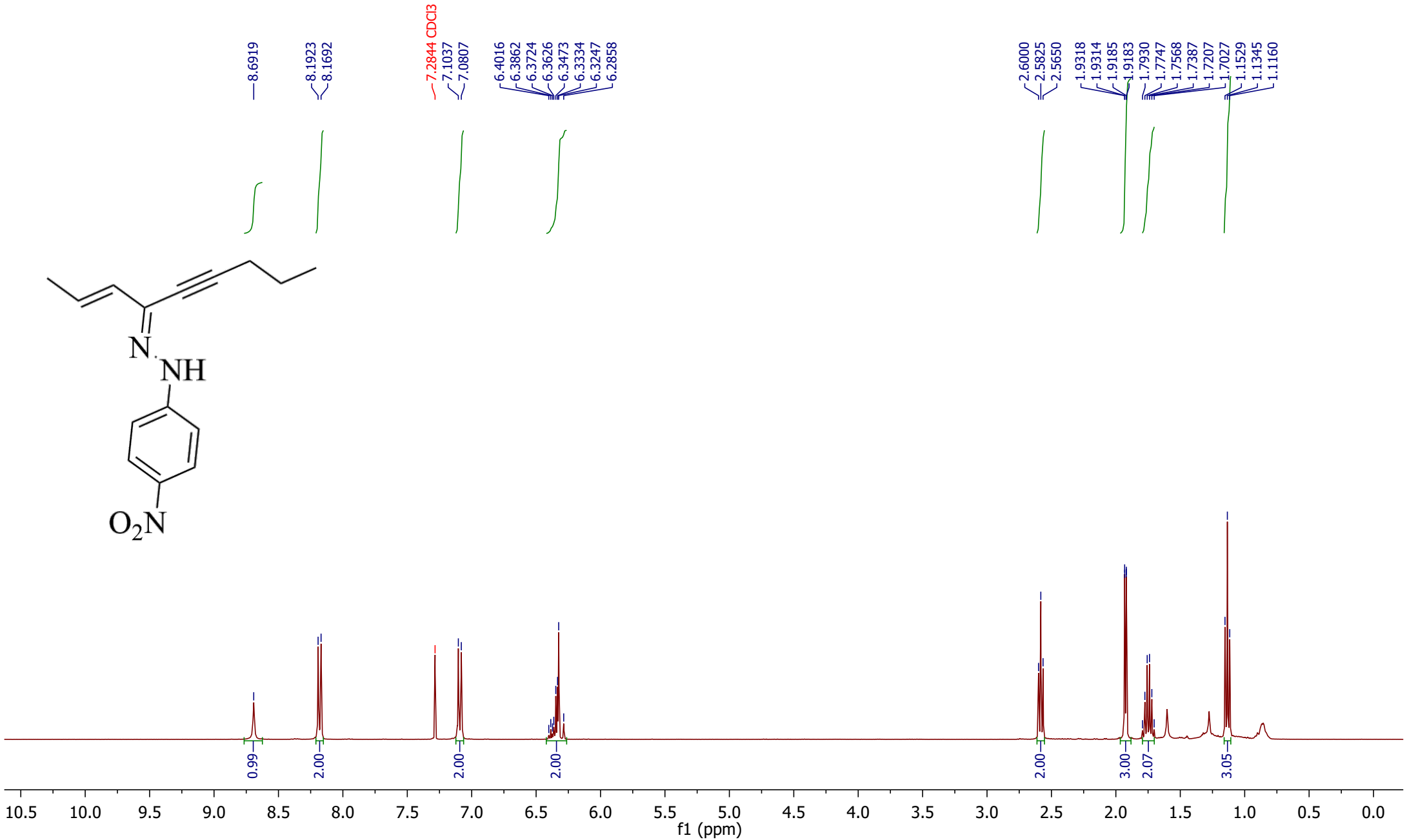
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4-nitrophenylhydrazone 5ab



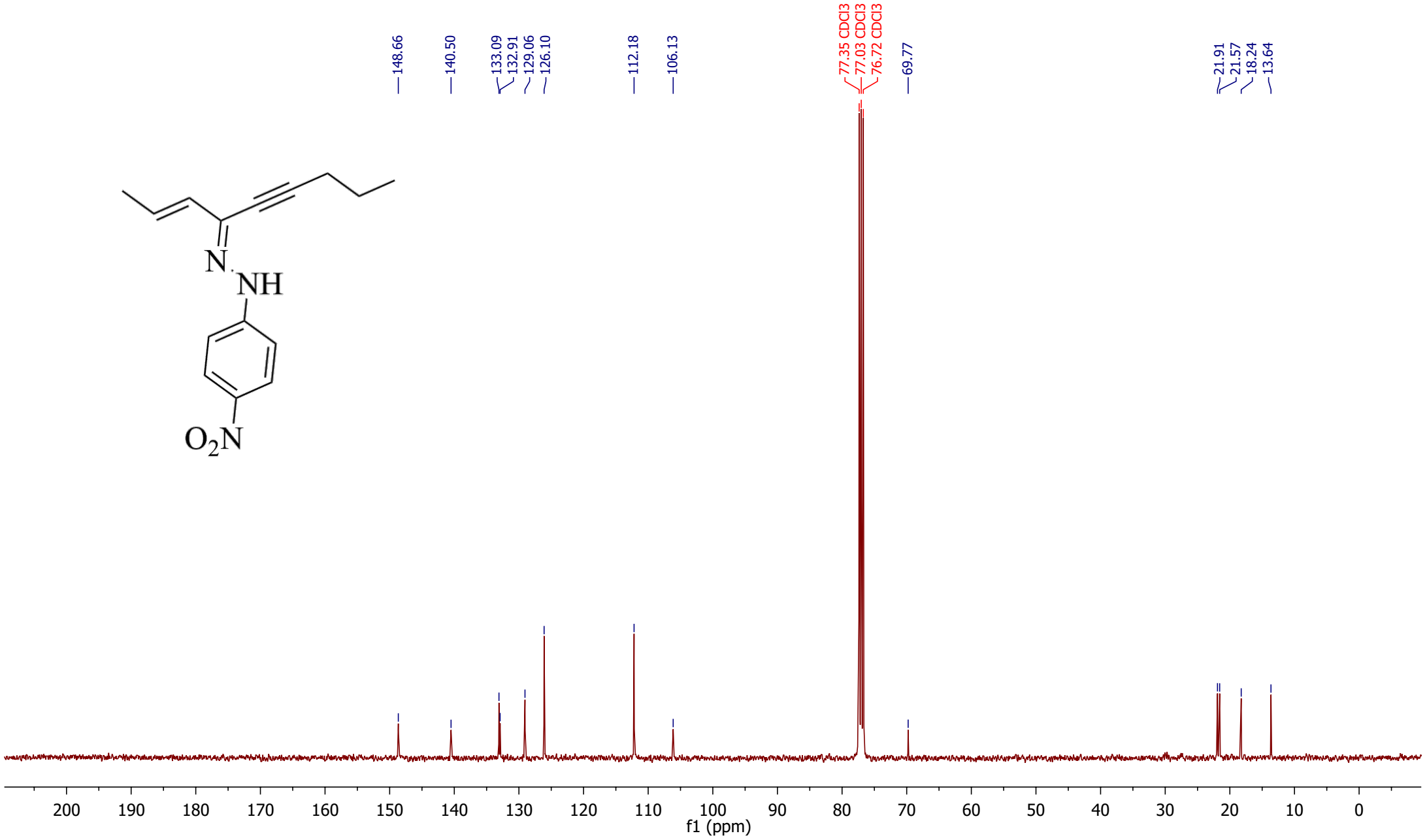
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 4-nitrophenylhydrazone 5ab



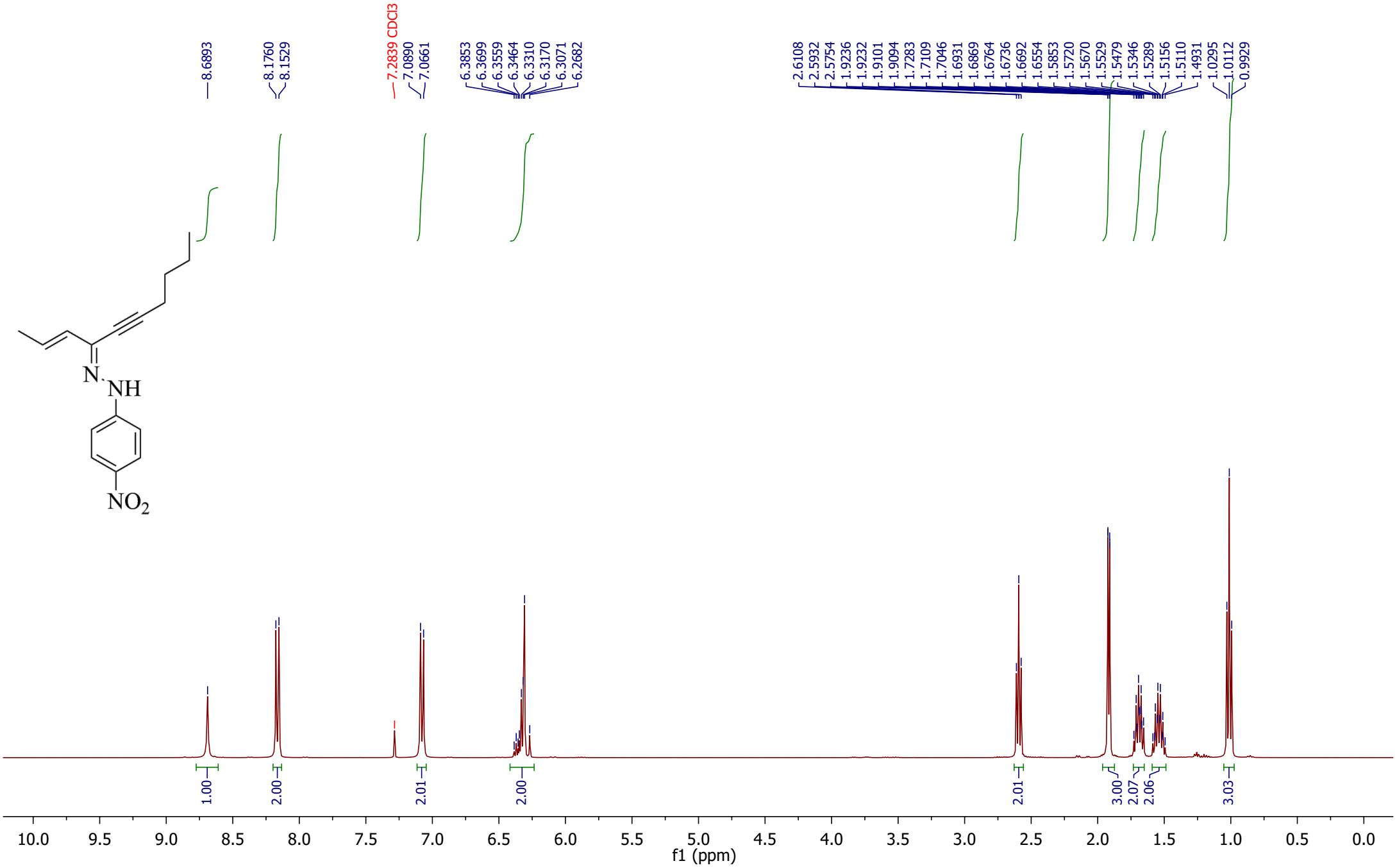
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4-nitrophenylhydrazone 5ac



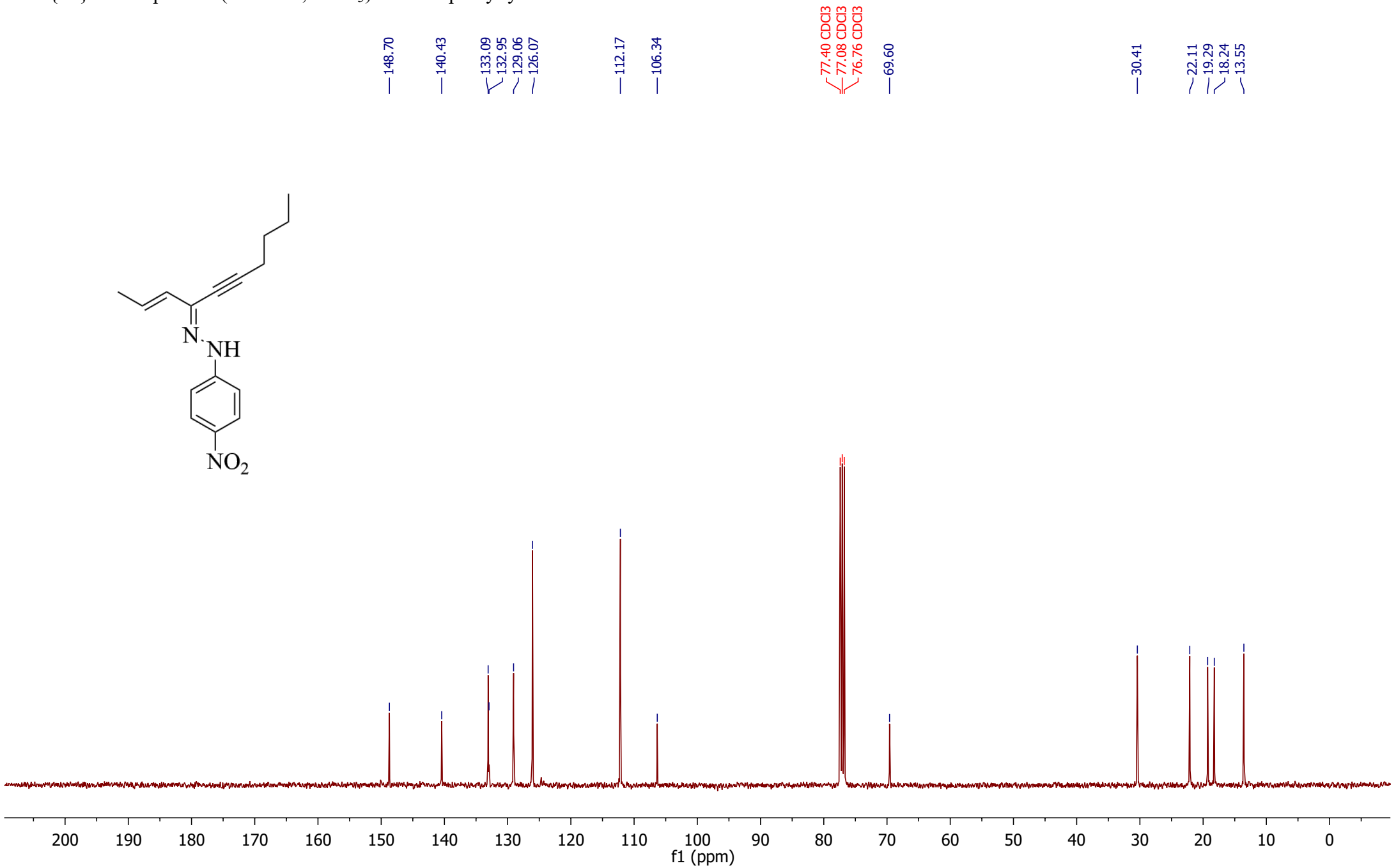
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 4-nitrophenylhydrazone 5ac



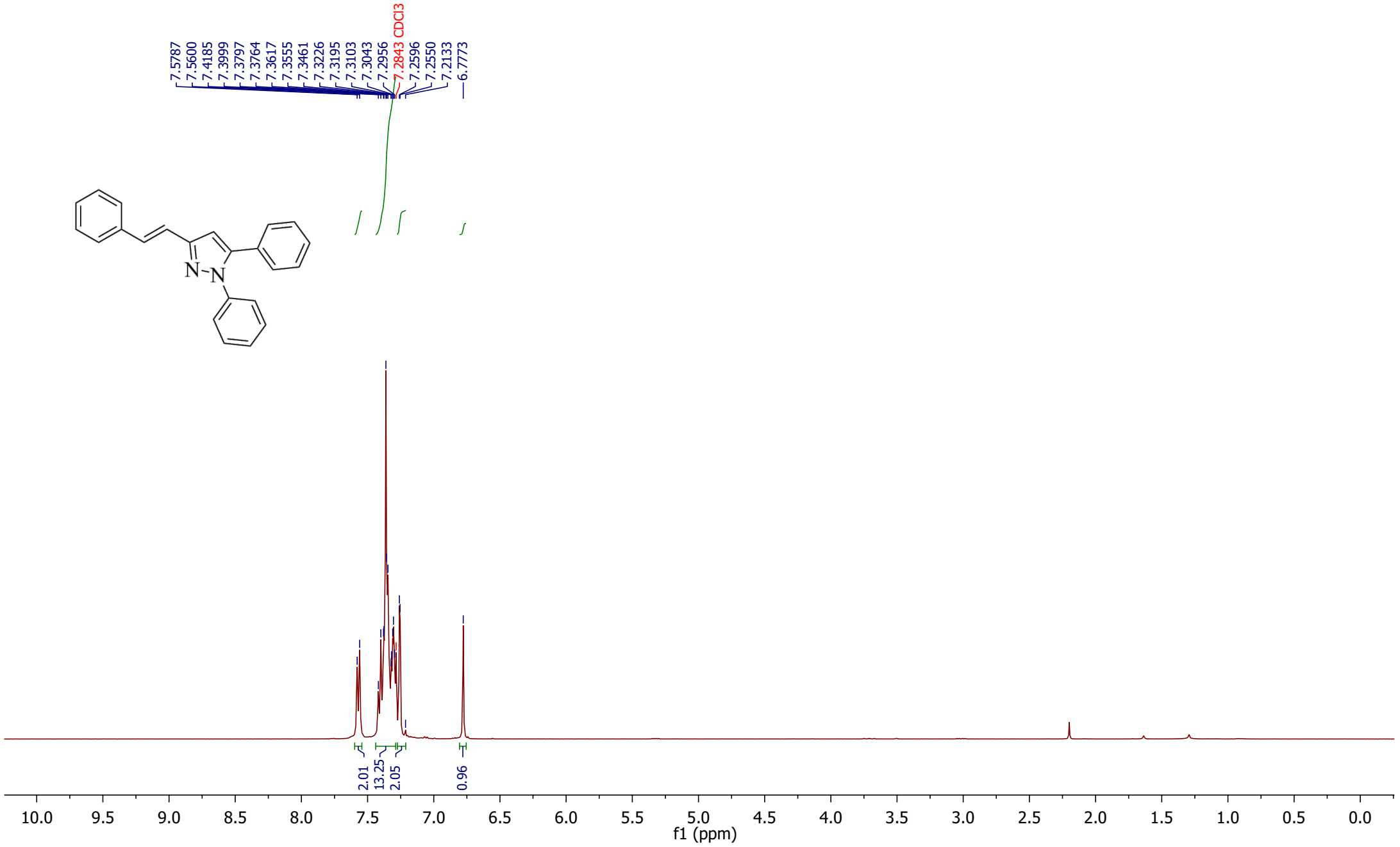
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4-nitrophenylhydrazone 5ad



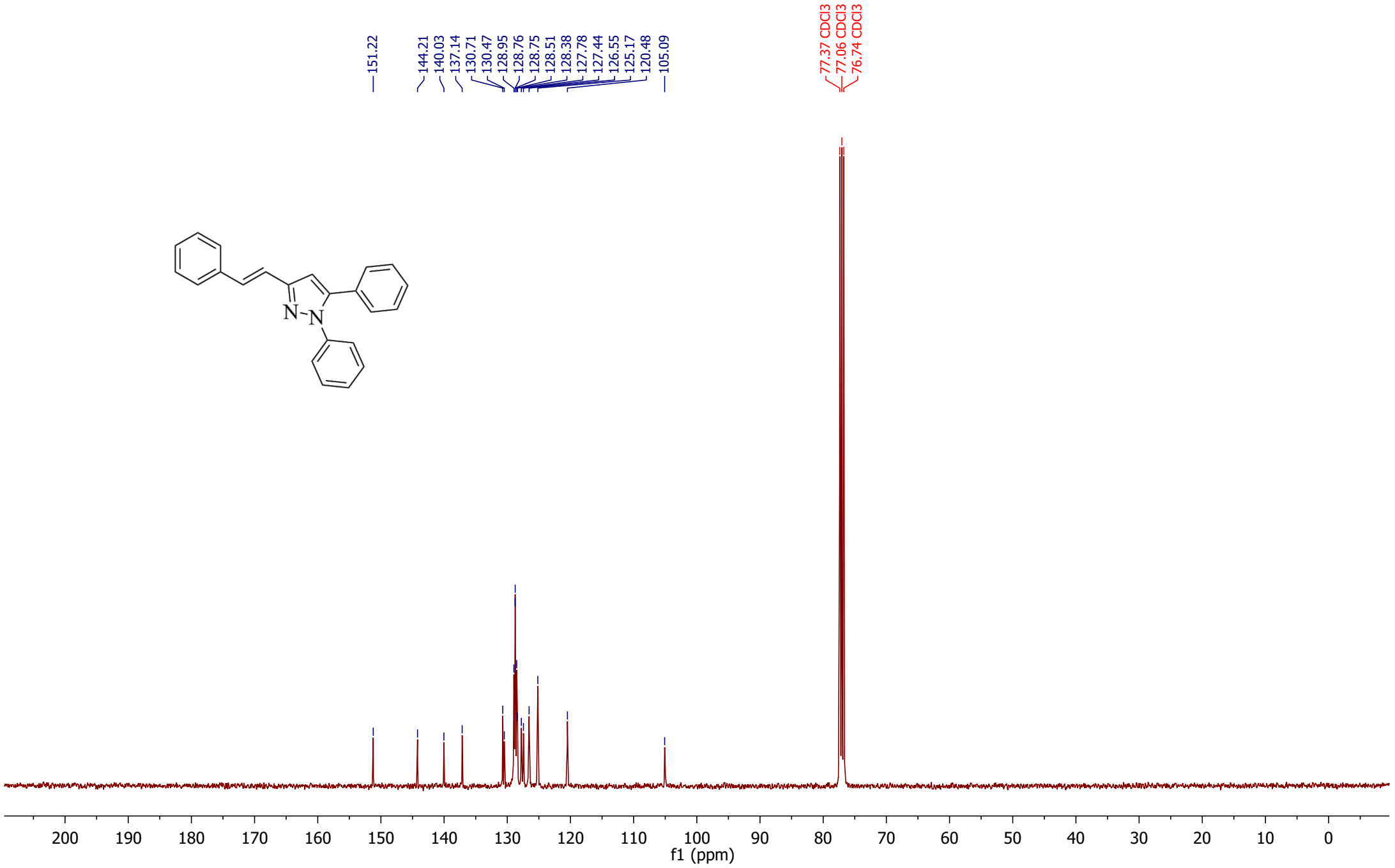
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 4-nitrophenylhydrazone 5ad



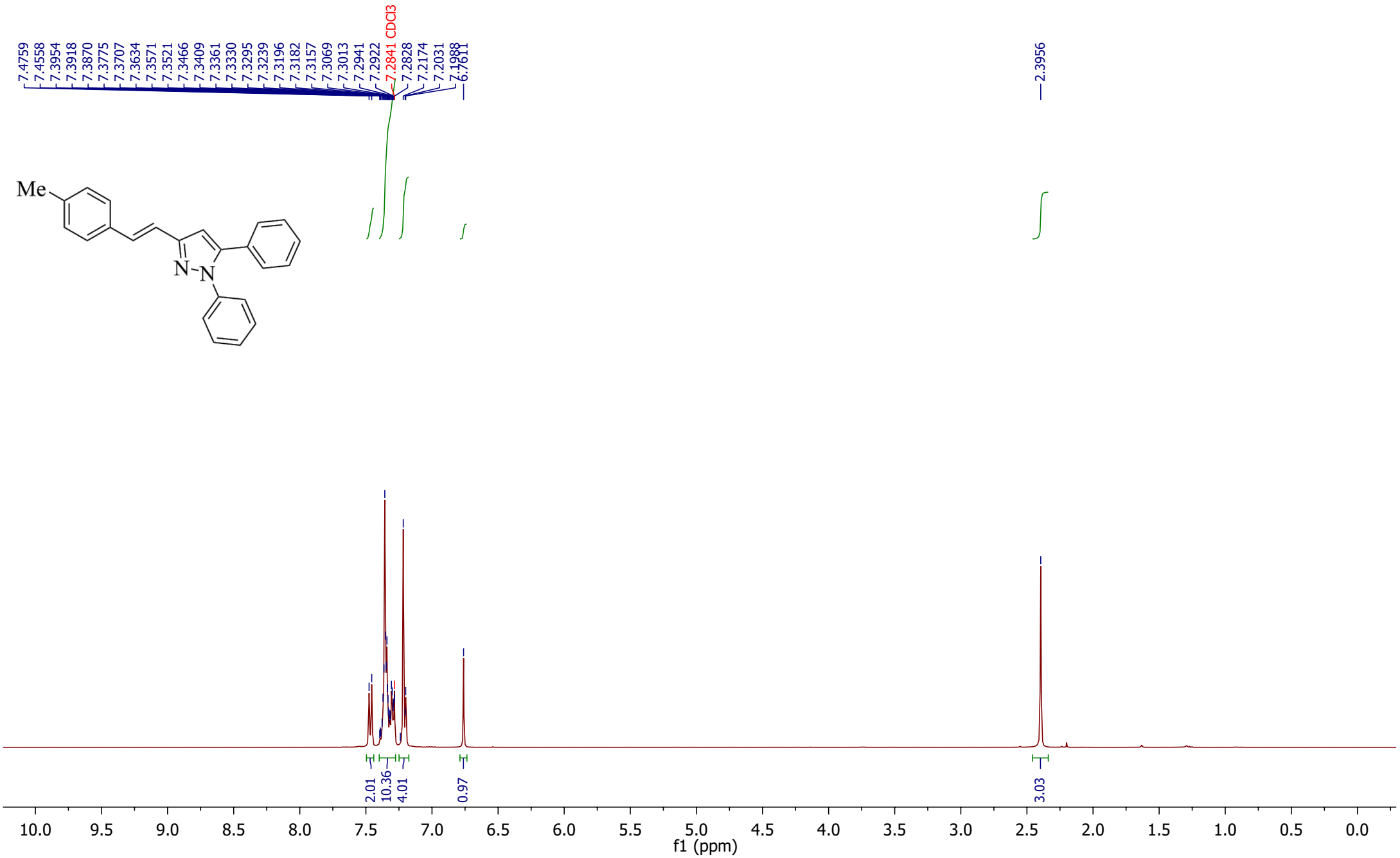
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4a



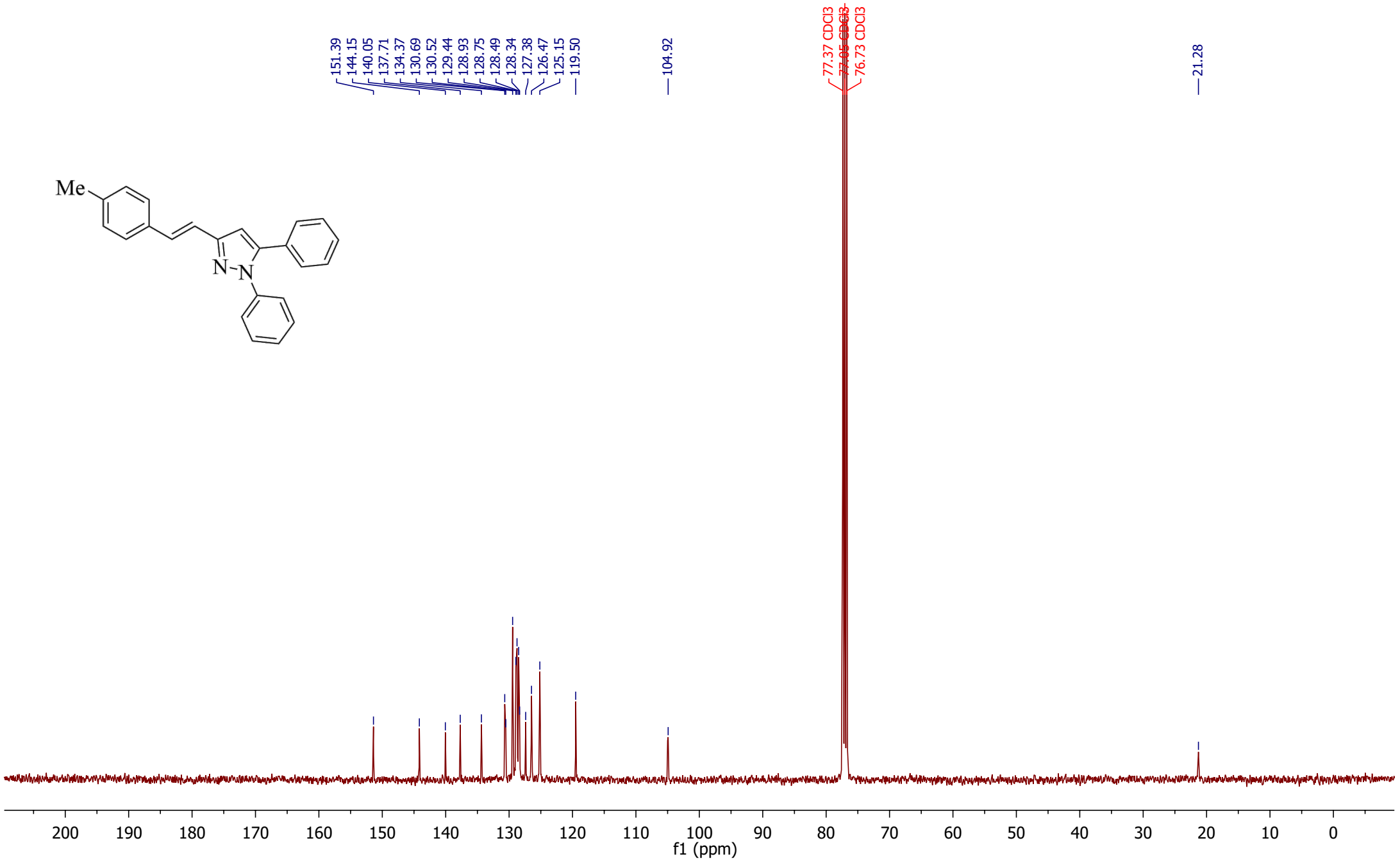
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4a



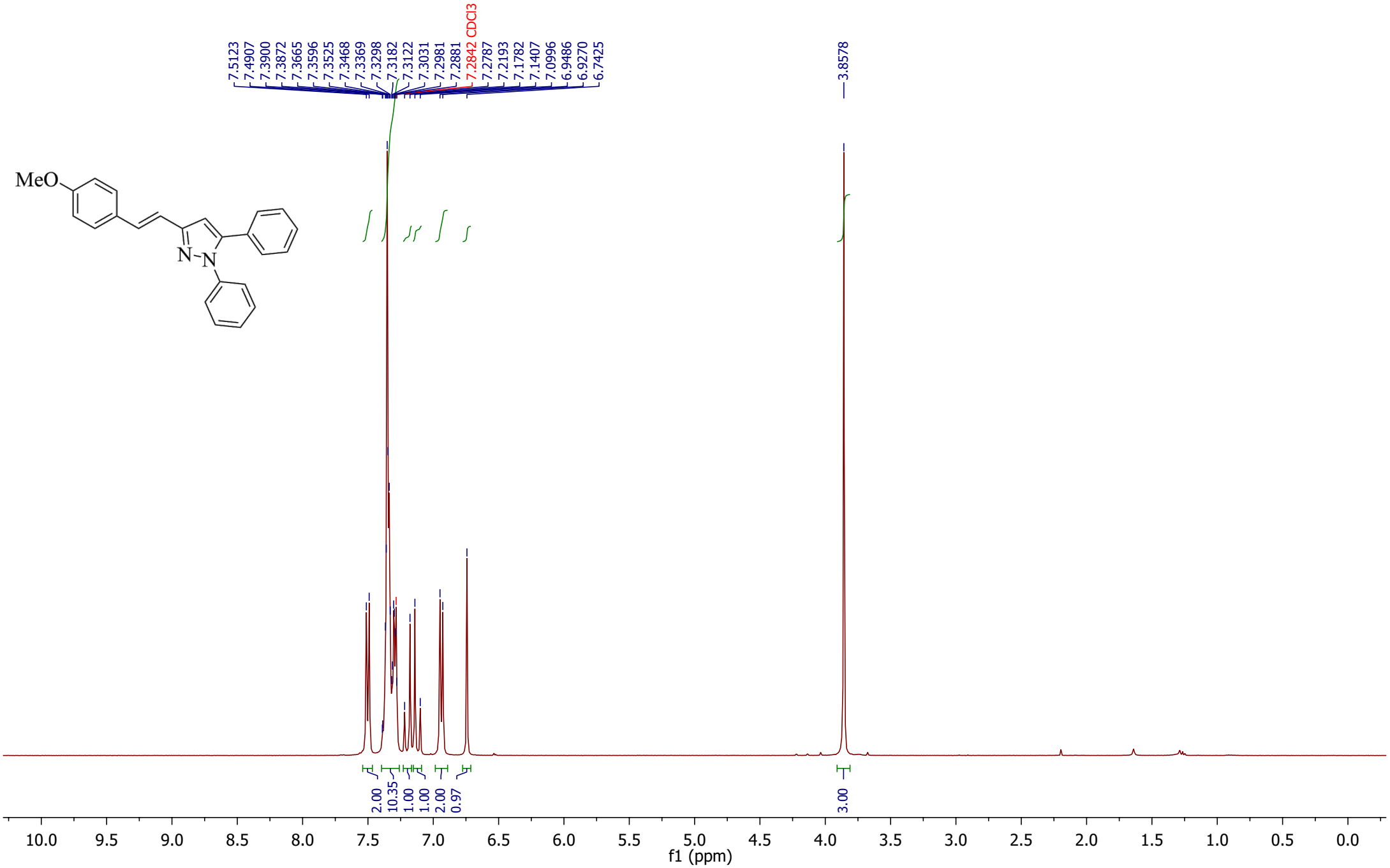
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4b



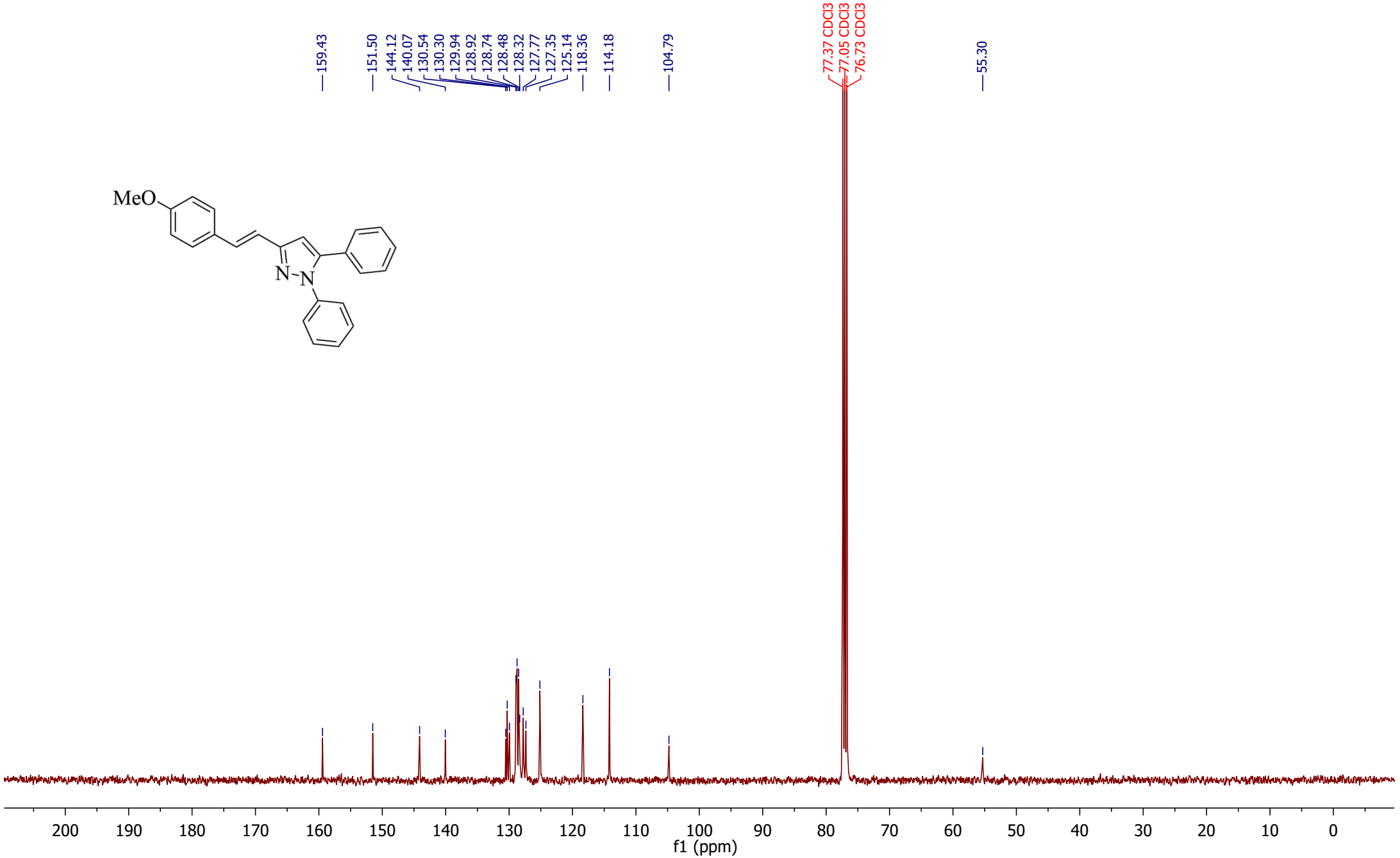
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4b



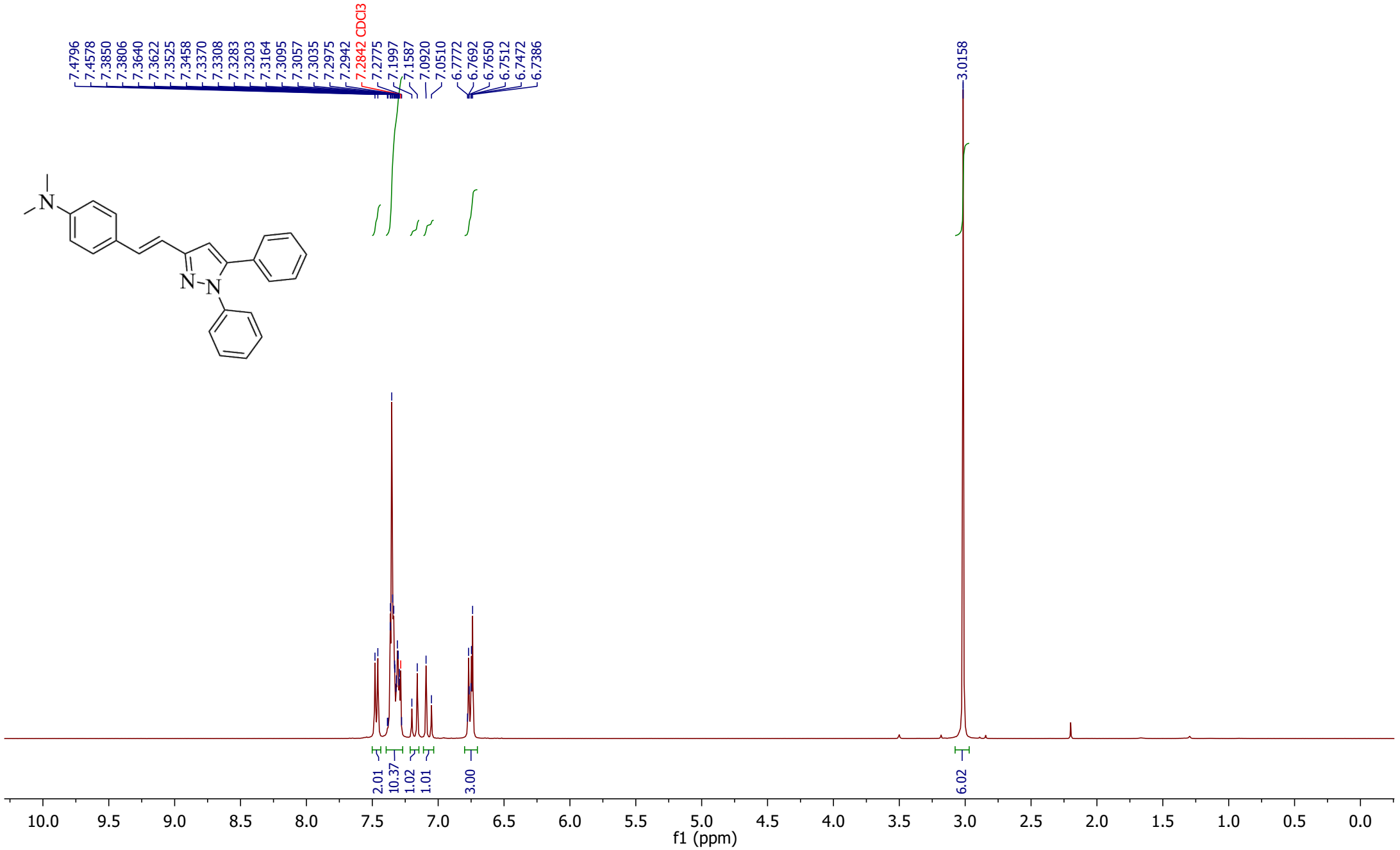
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4c



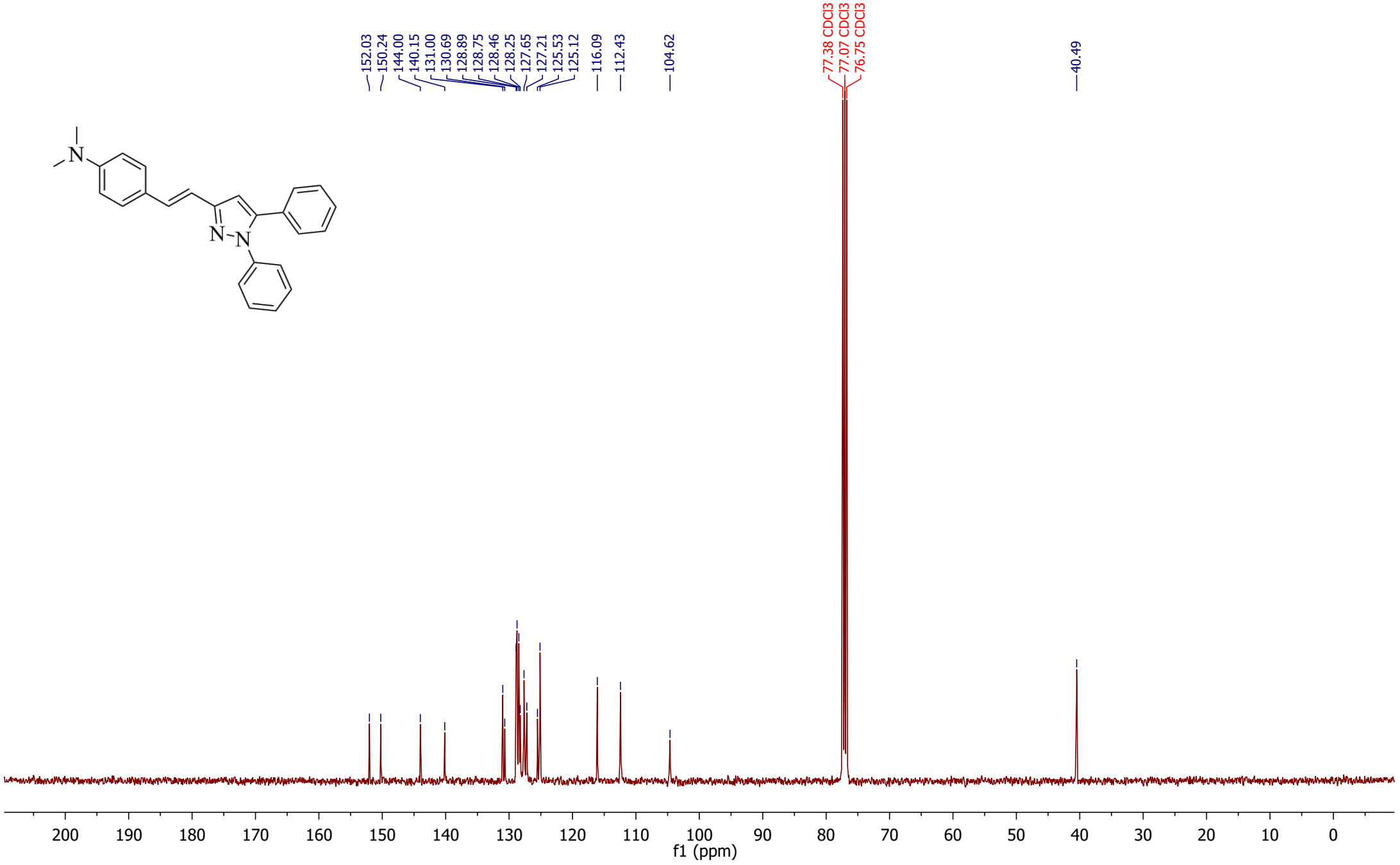
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4c



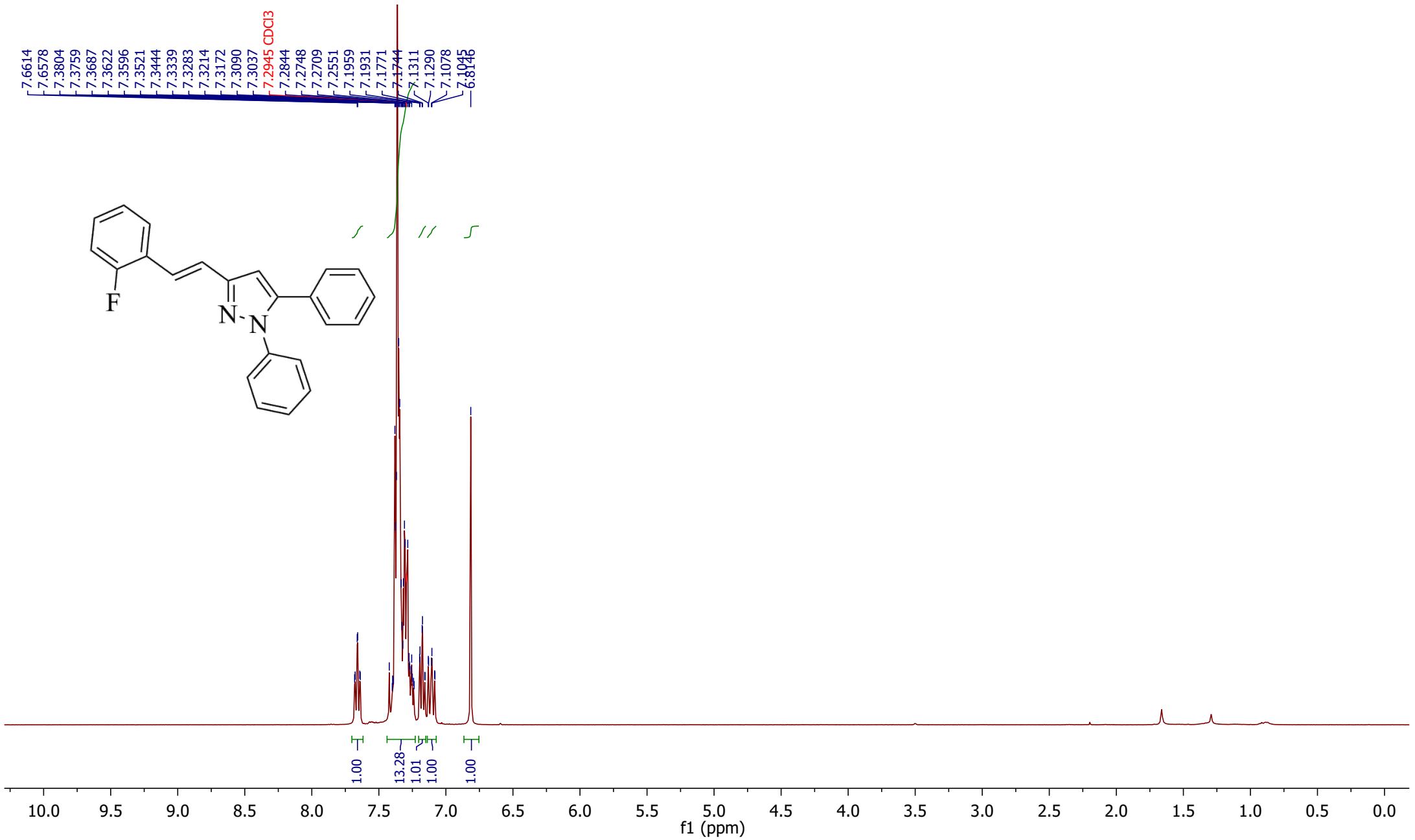
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4d



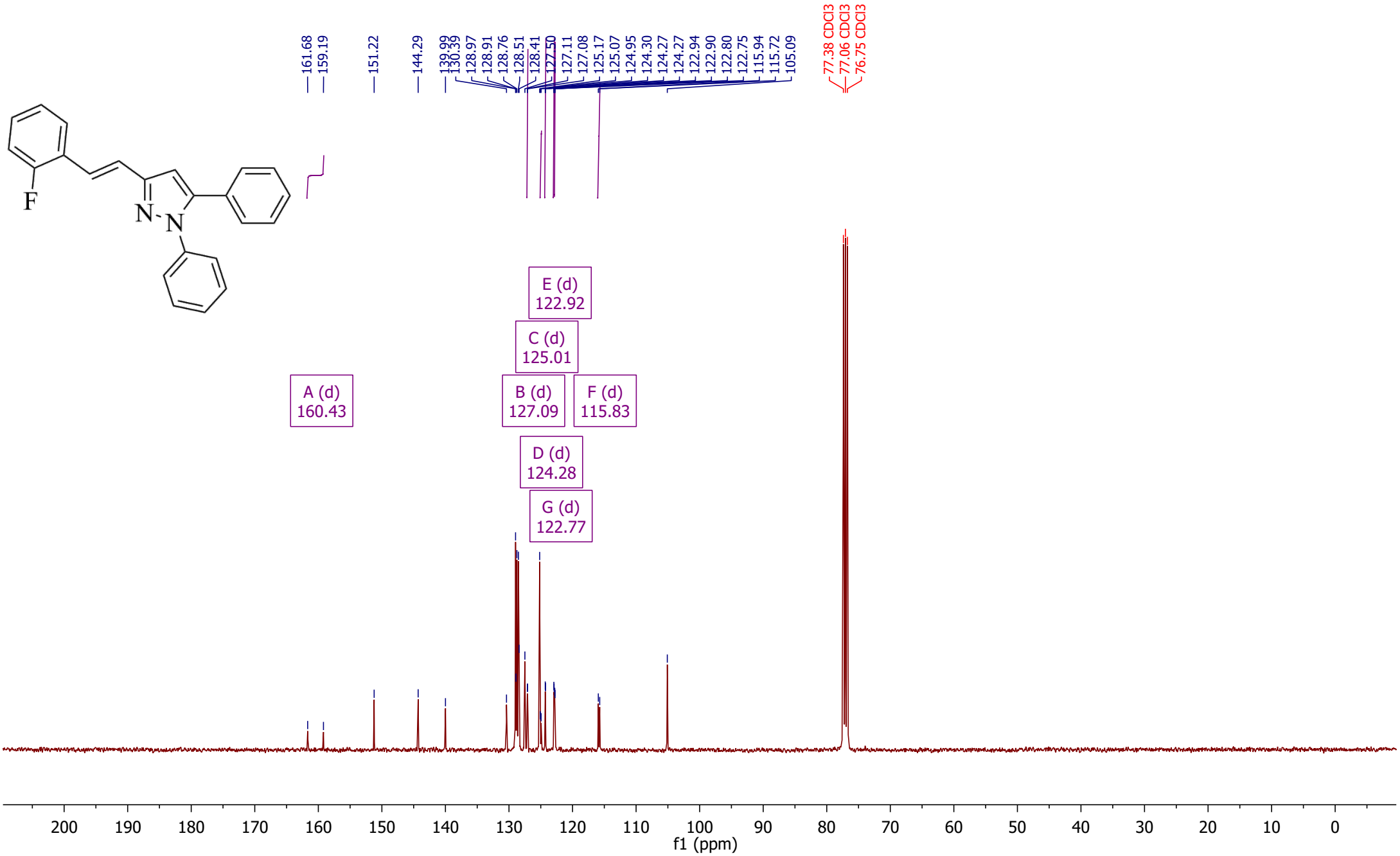
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4d



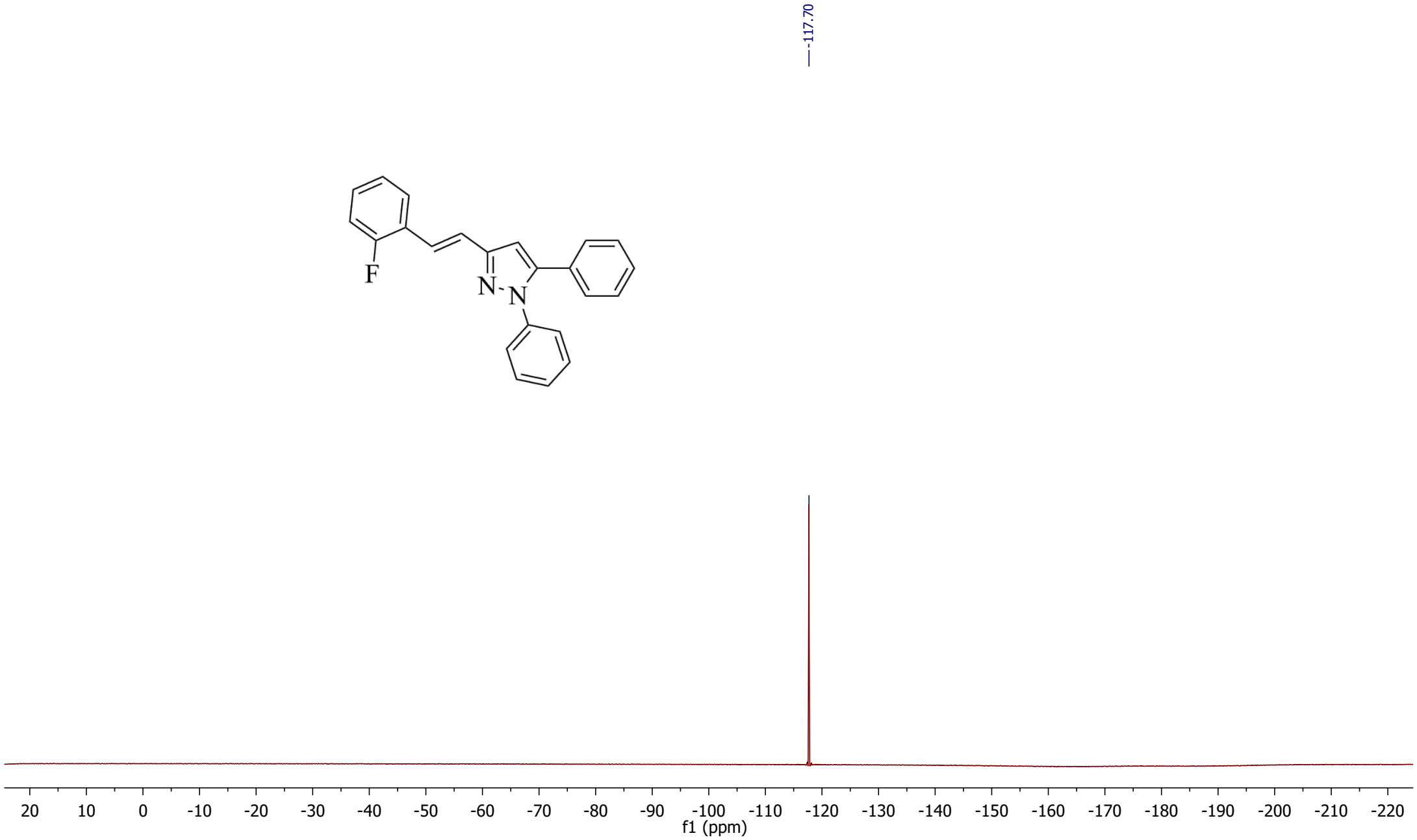
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4e



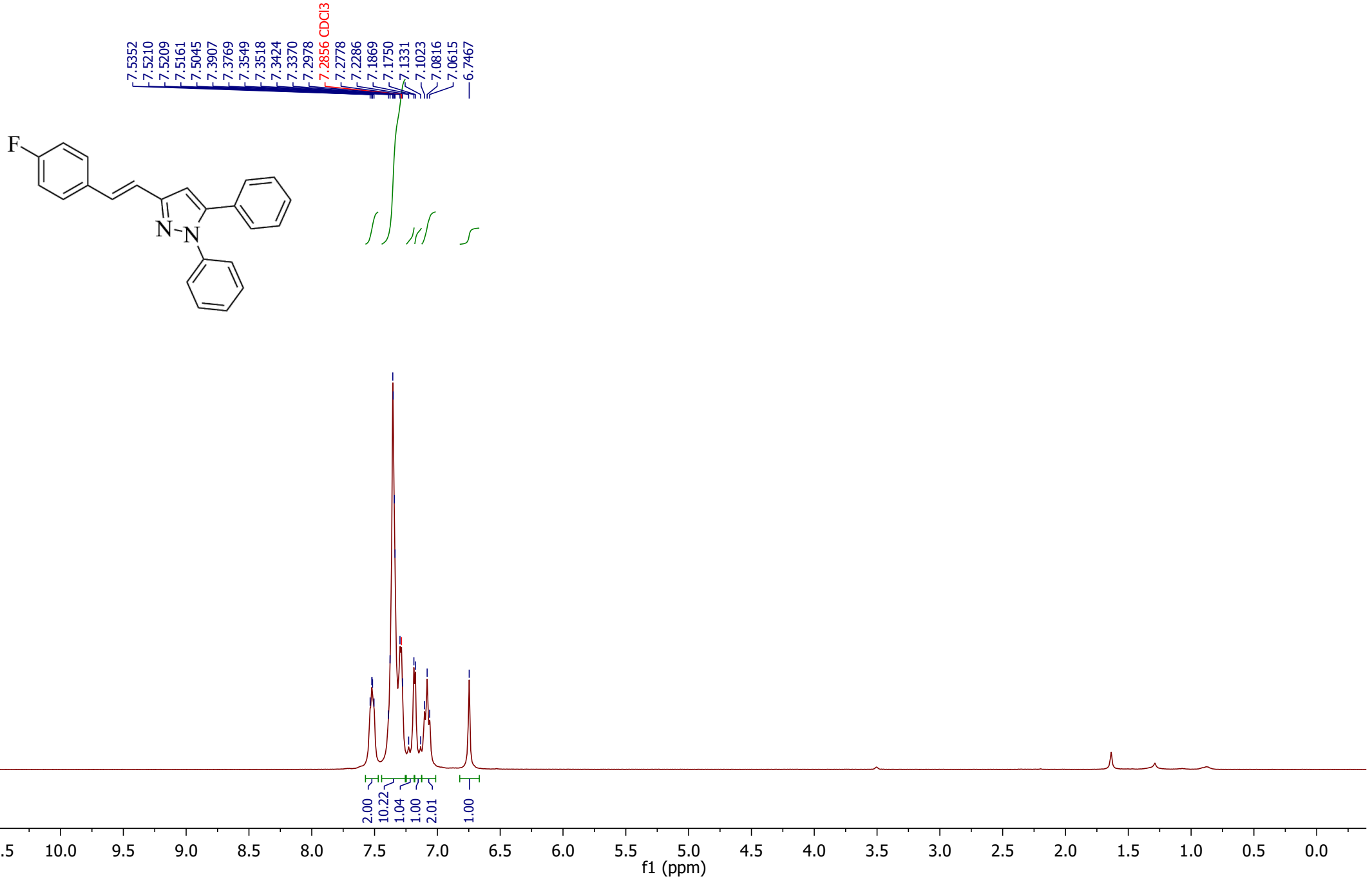
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4e



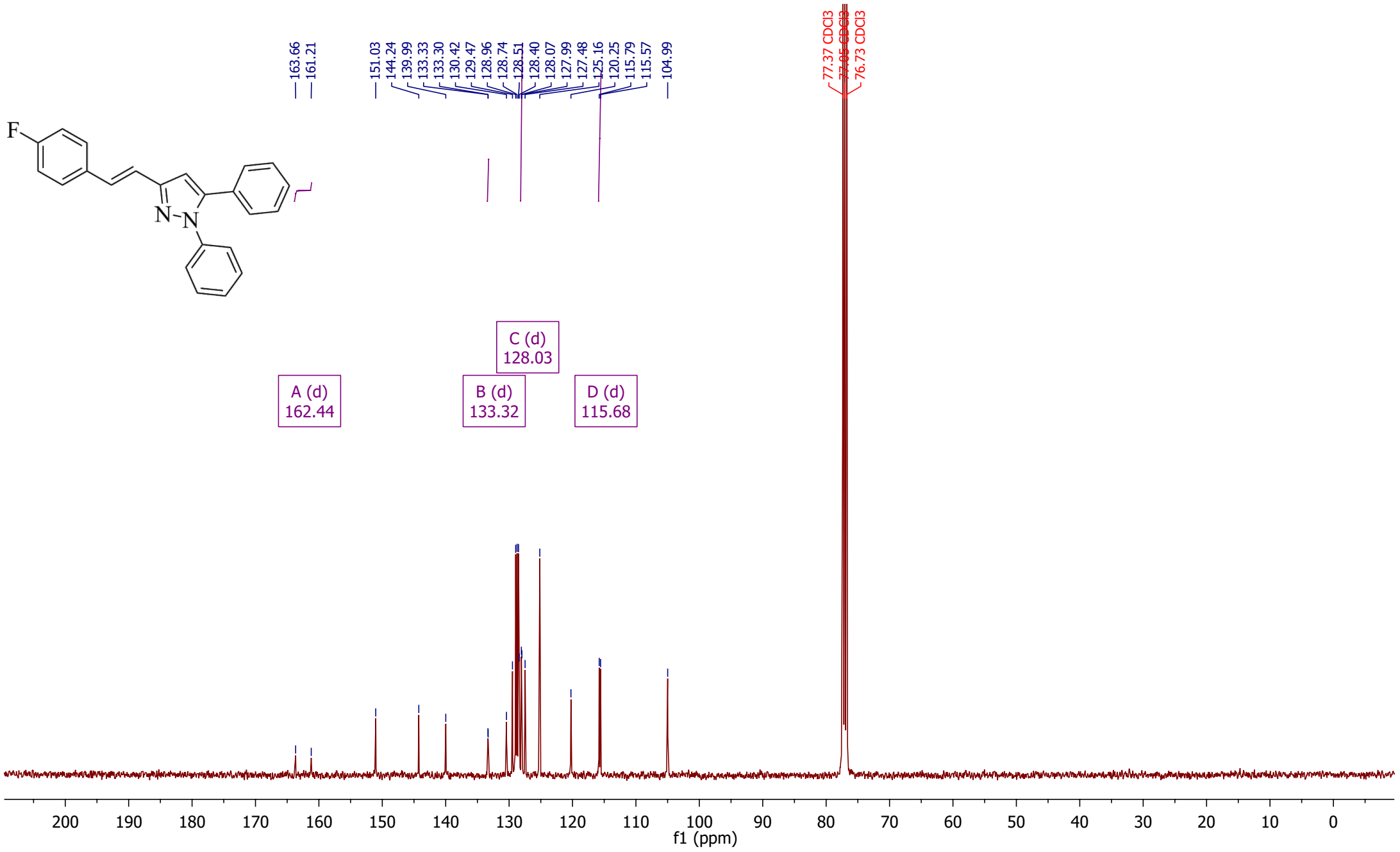
^{19}F NMR spectrum (376 MHz, $CDCl_3$) of 1*H*-pyrazole 4e



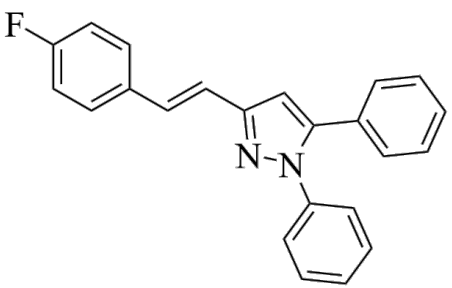
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4f



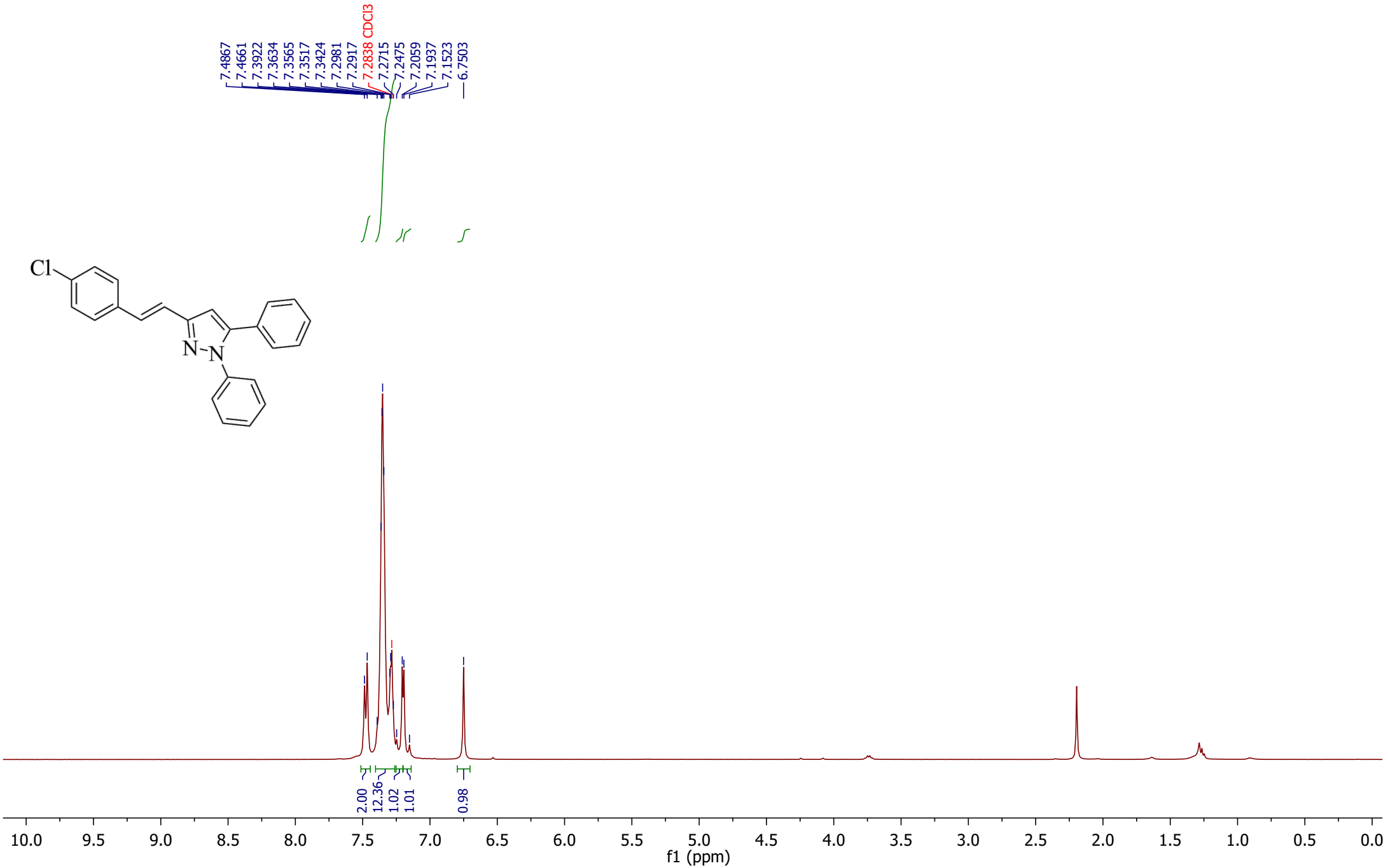
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4f



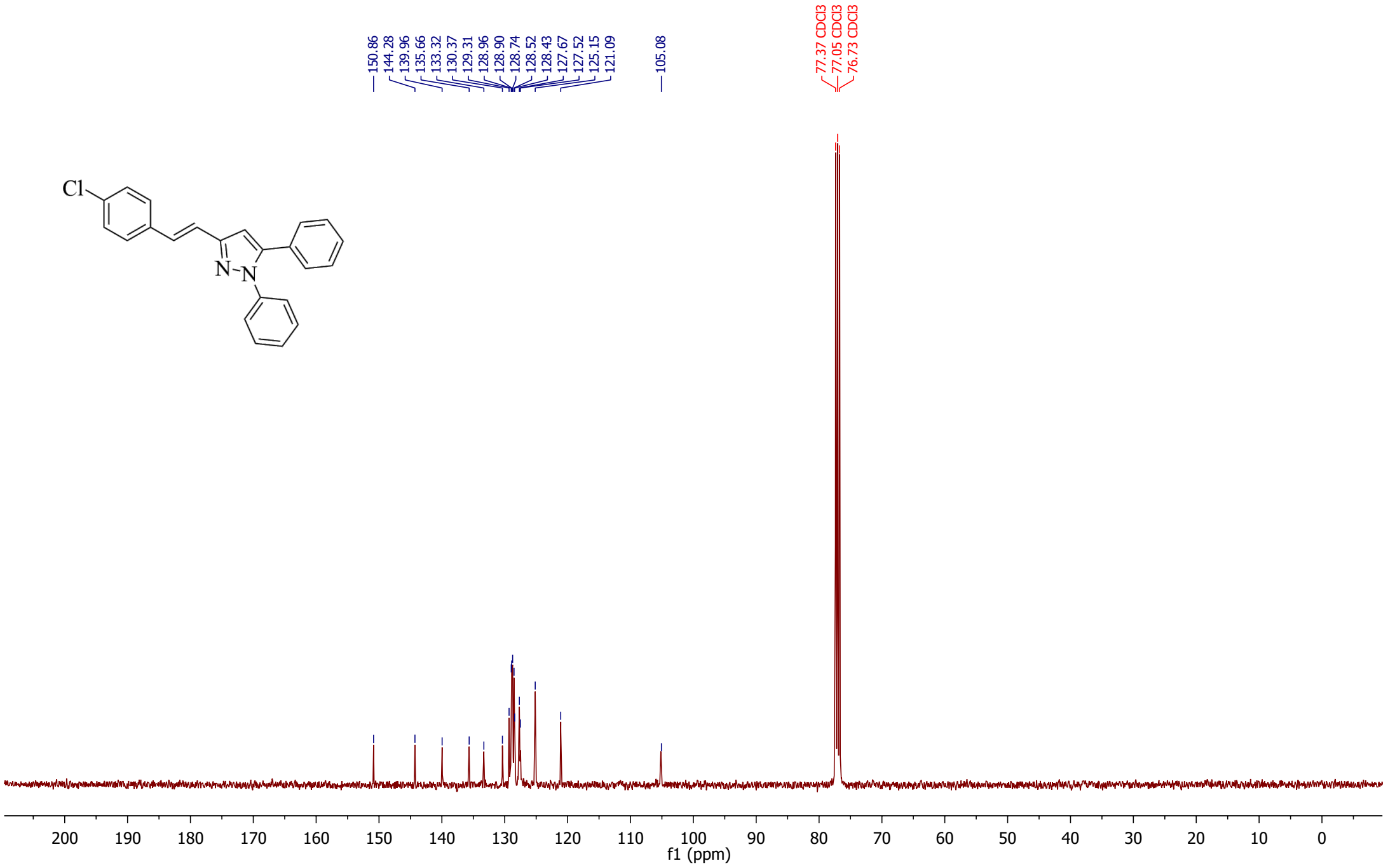
^{19}F NMR spectrum (376 MHz, CDCl3) of 1*H*-pyrazole 4f



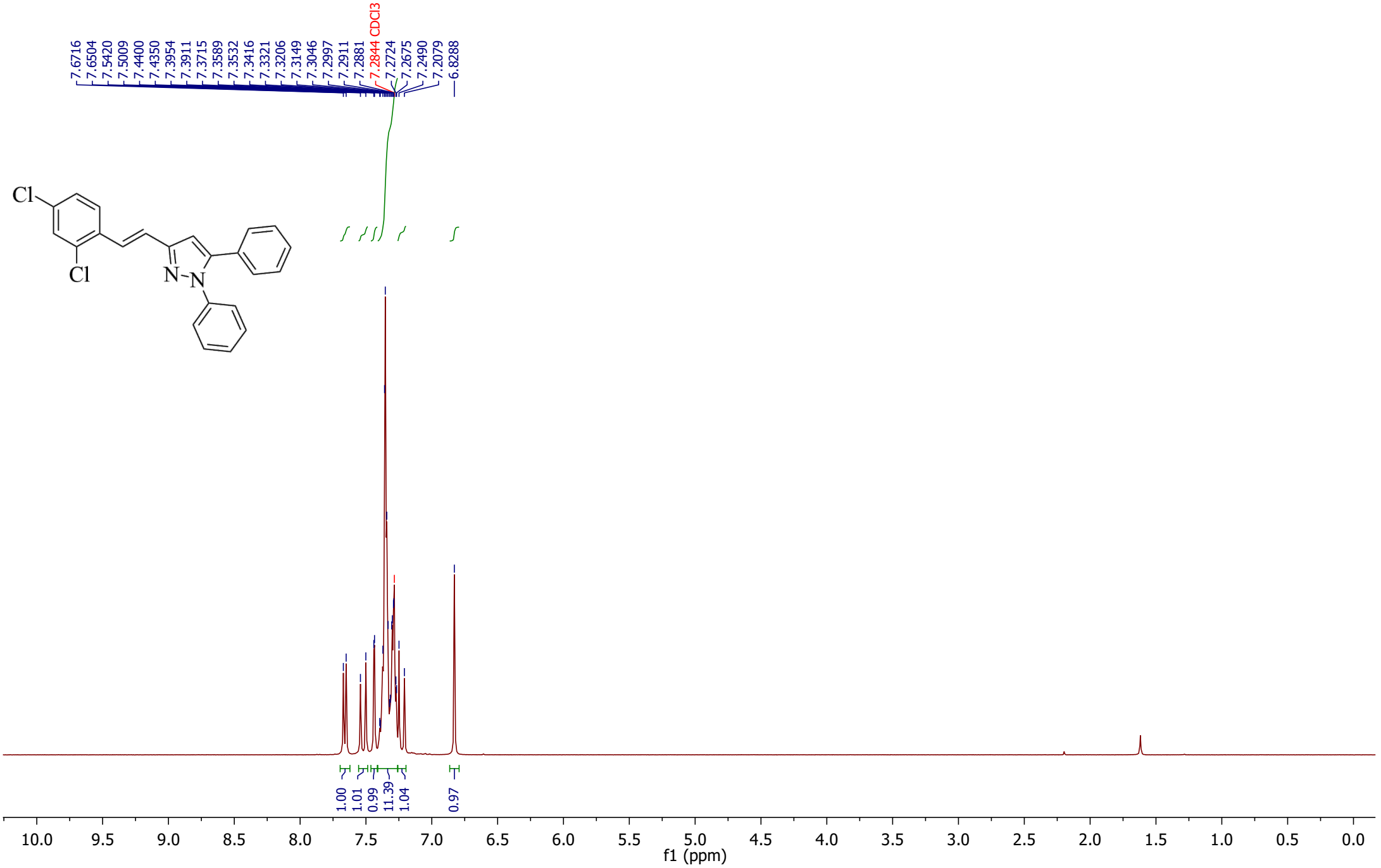
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4g



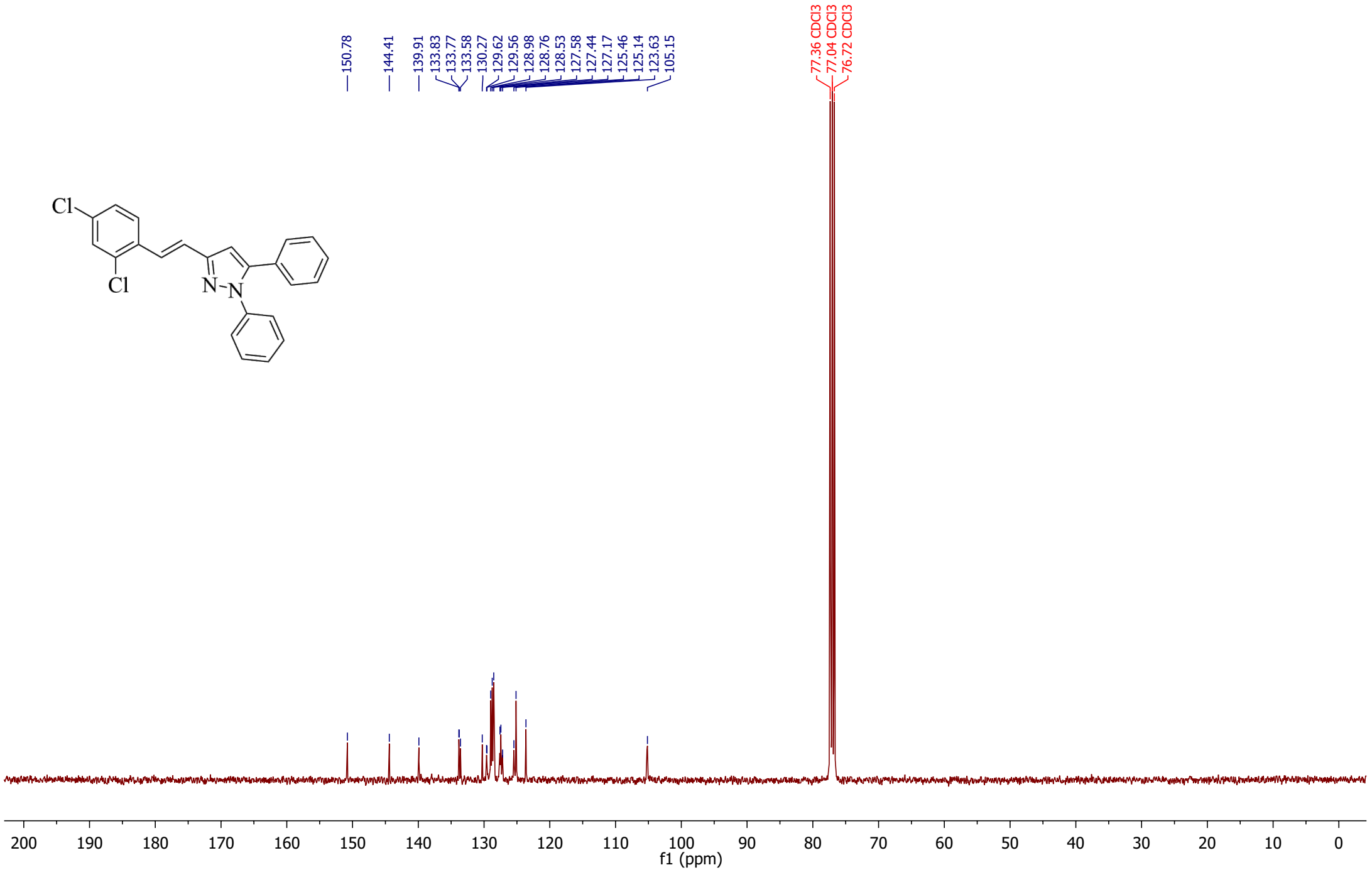
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4g



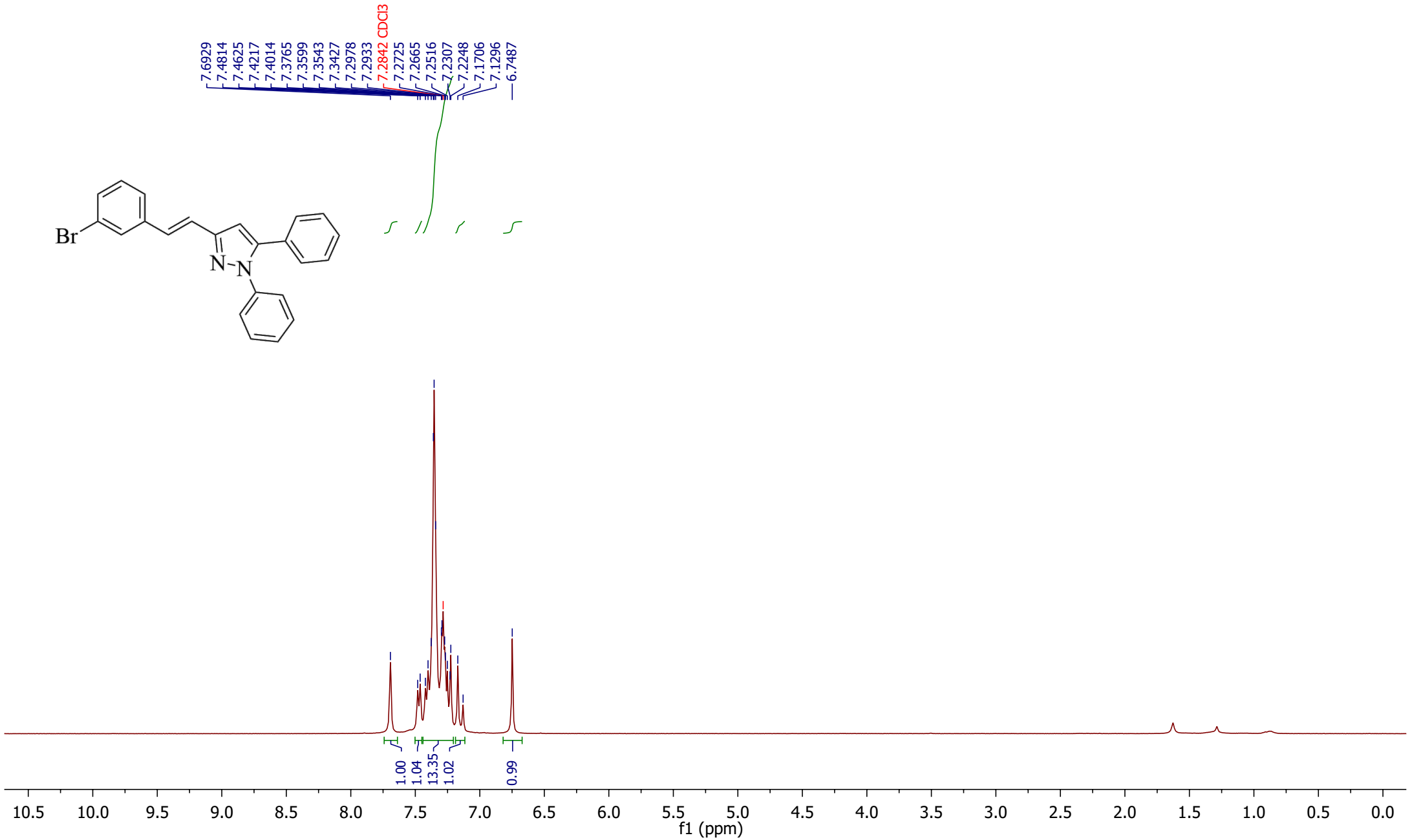
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4h



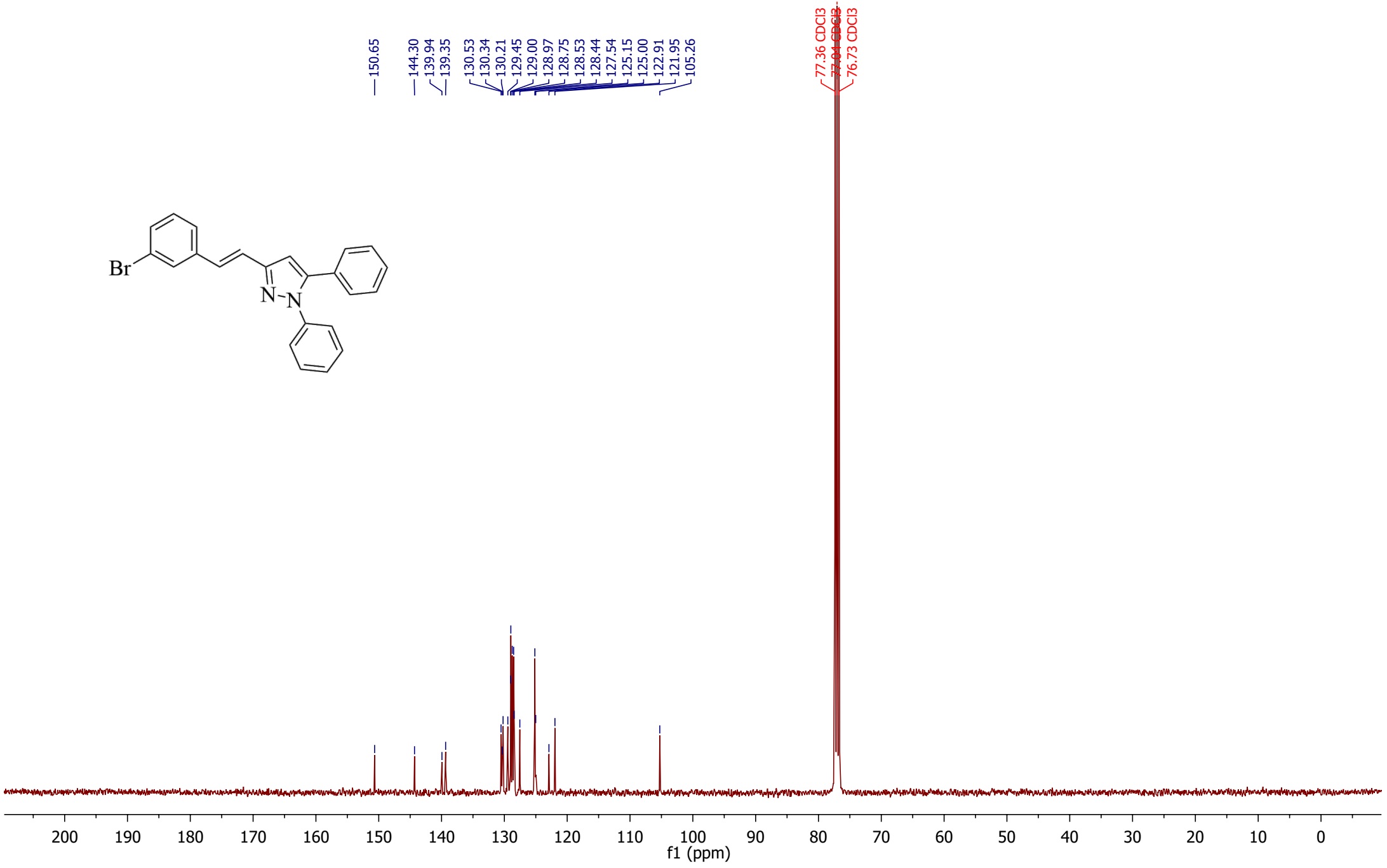
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4h



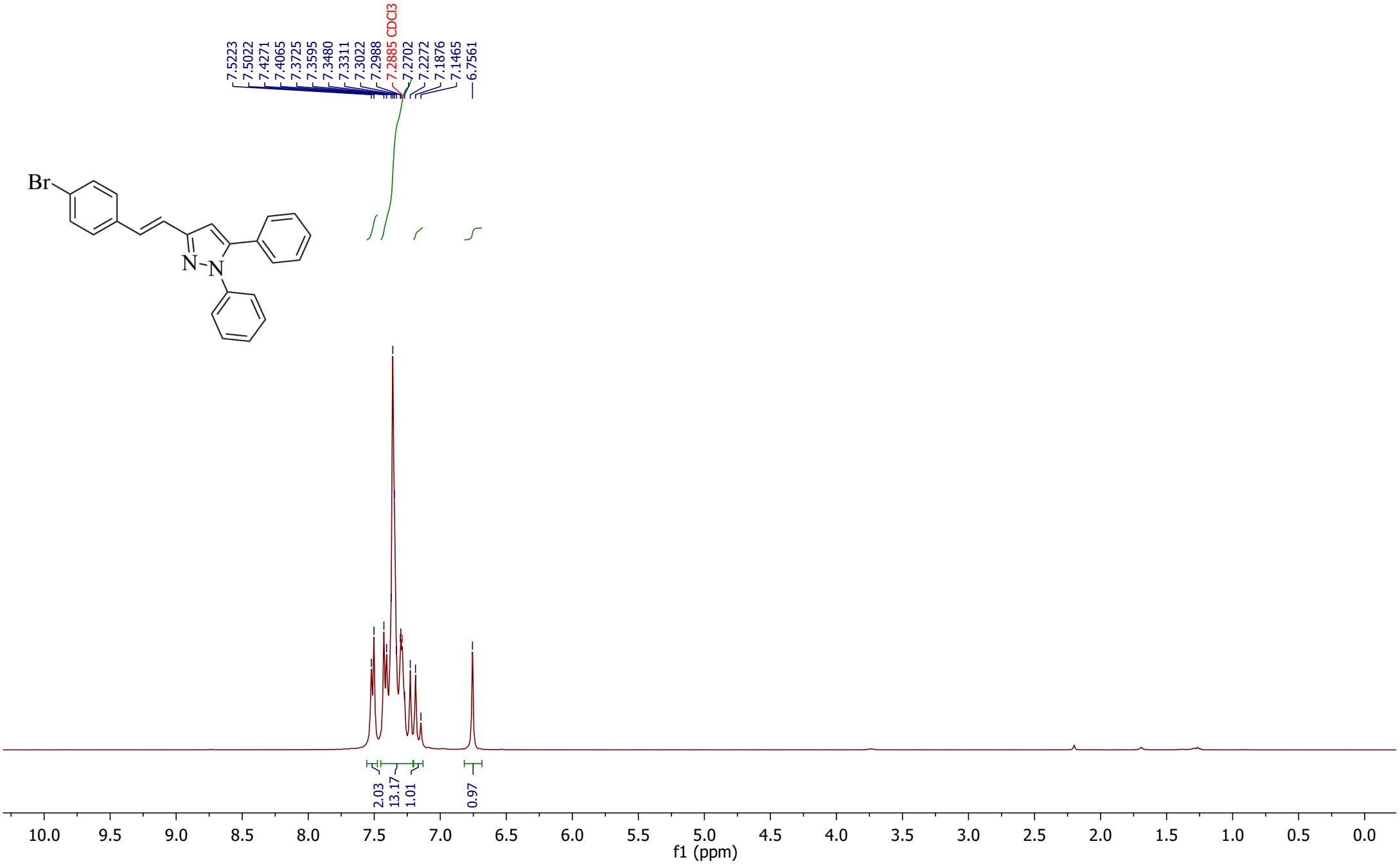
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4i



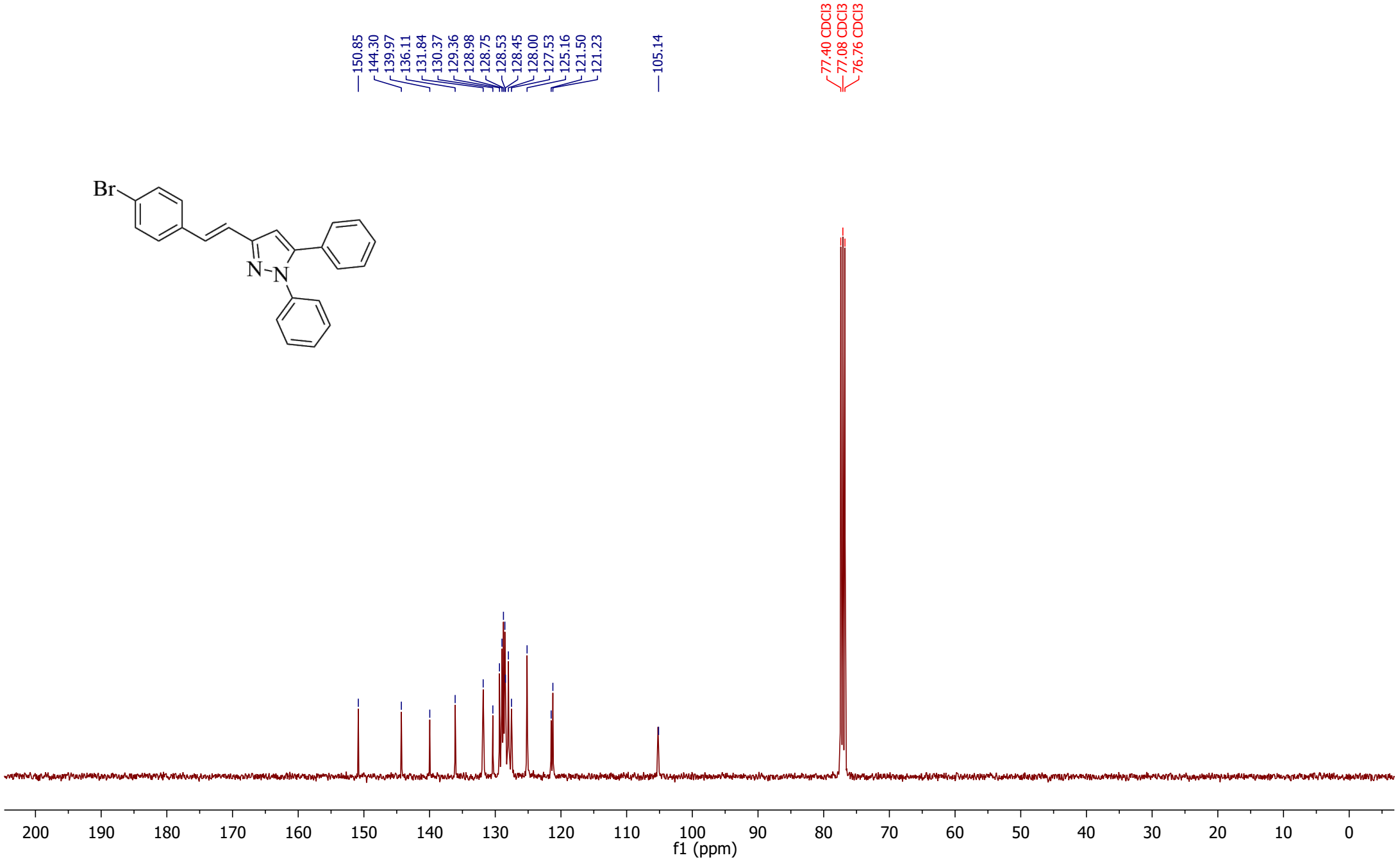
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4i



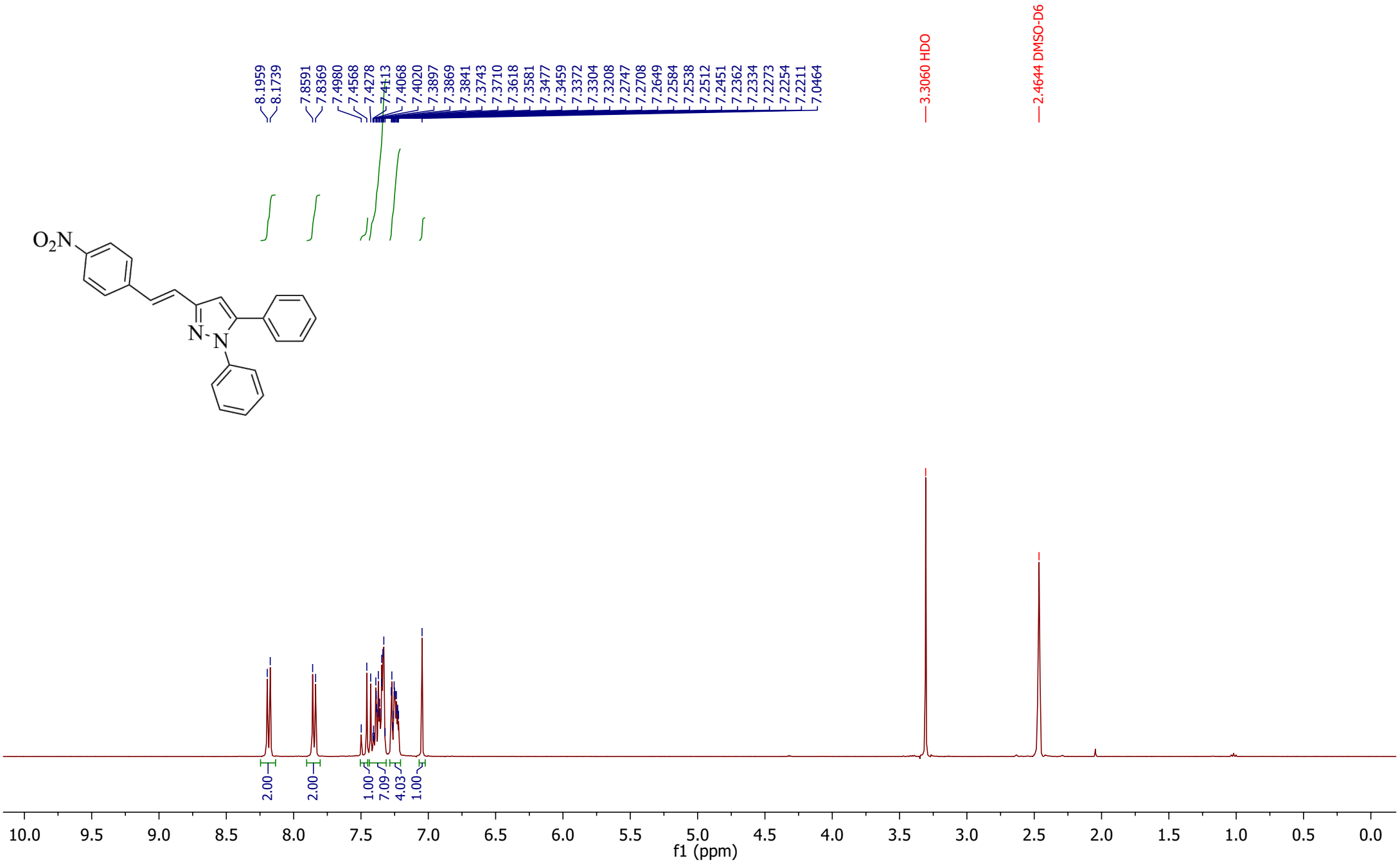
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4j



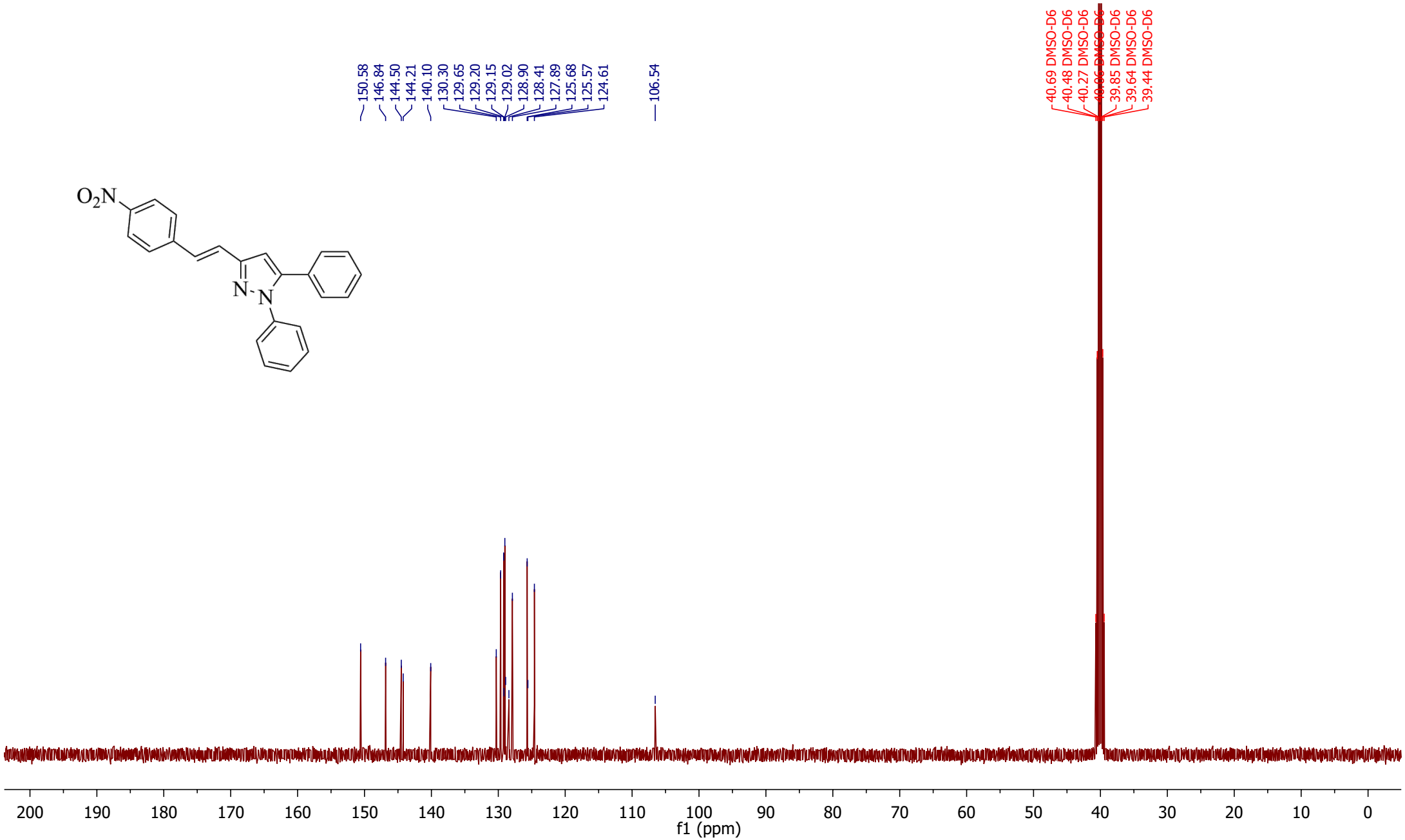
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4j



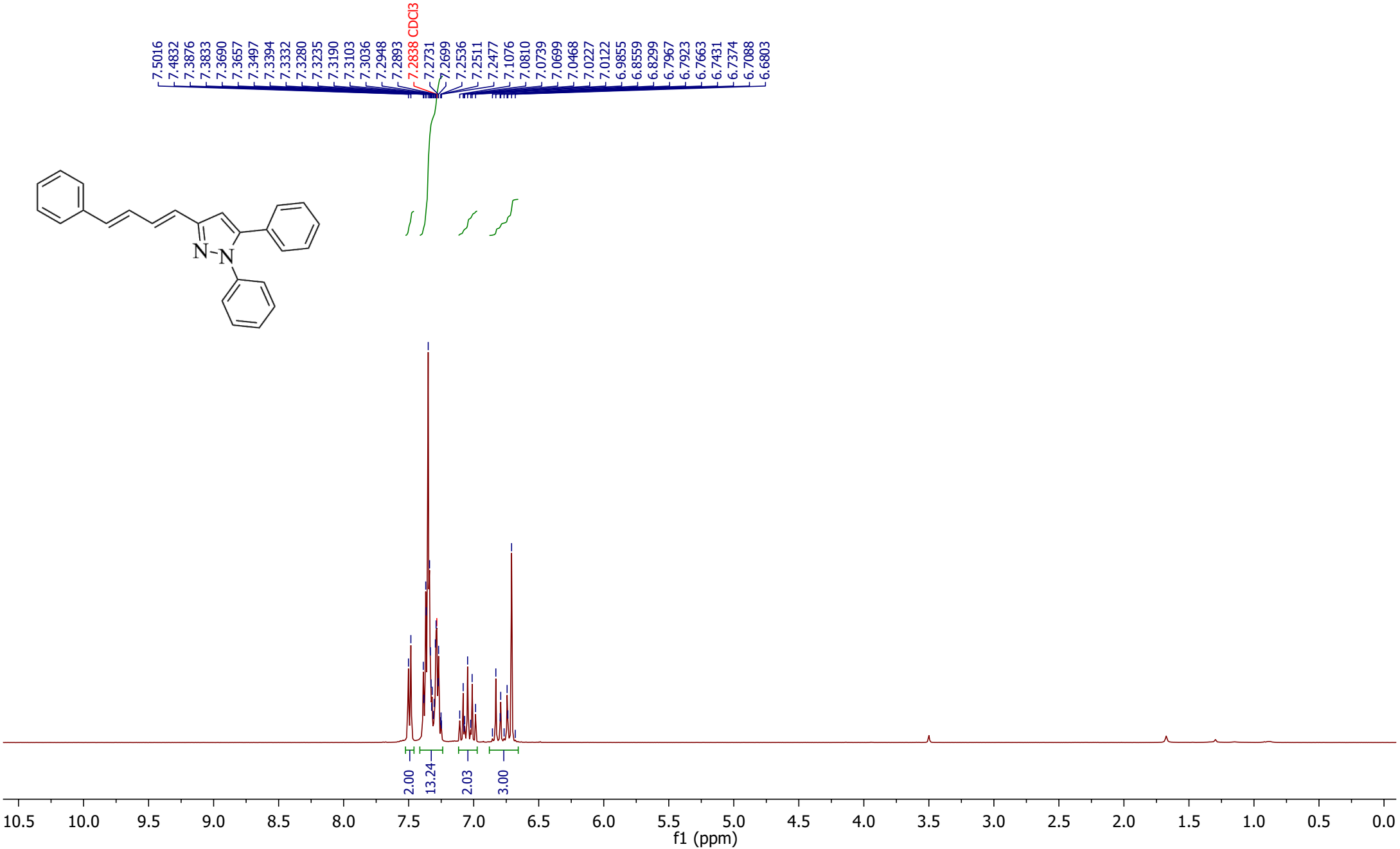
^{1}H NMR spectrum (400 MHz, DMSO-d_6) of 1*H*-pyrazole 4k



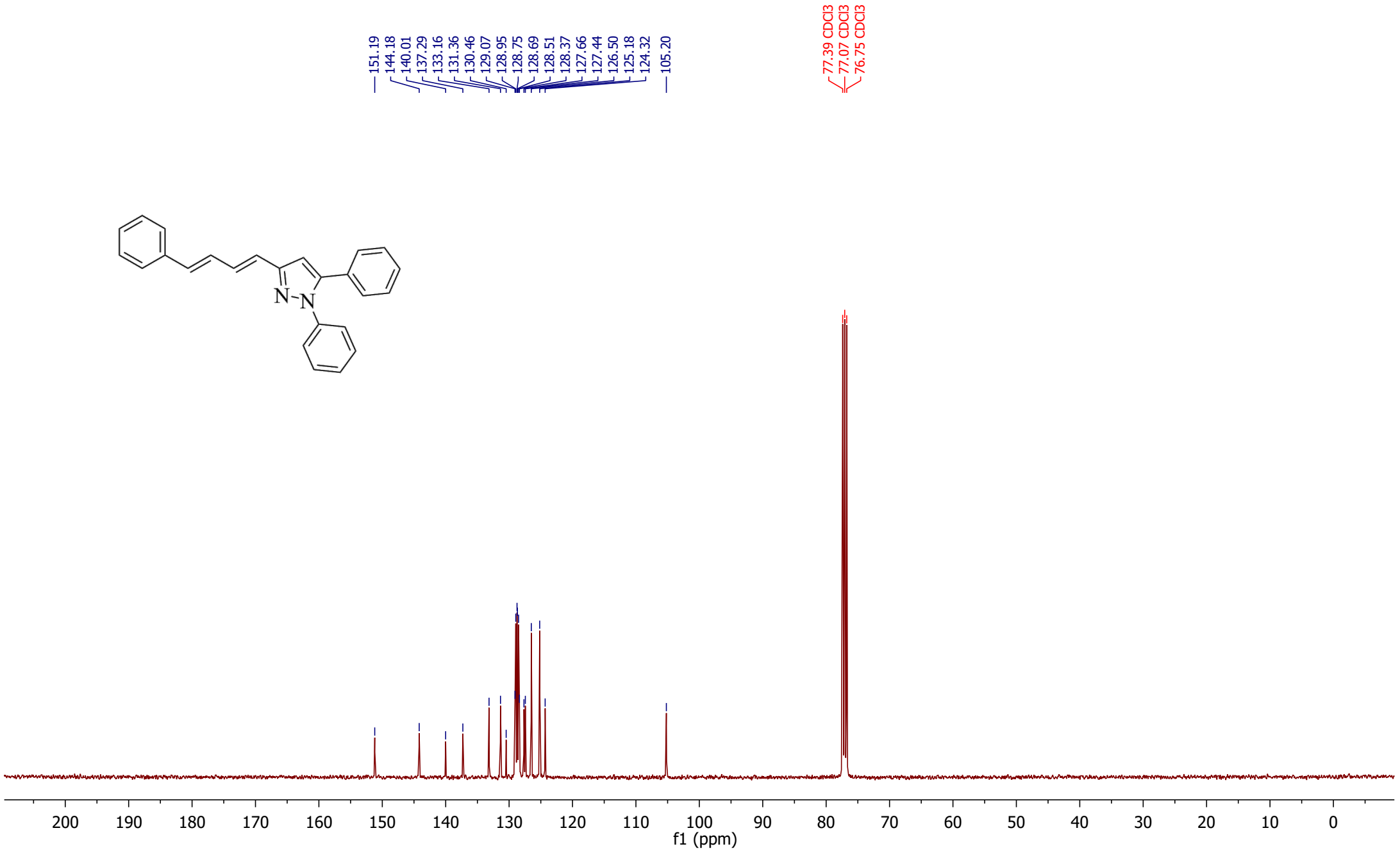
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, DMSO-d_6) of 1*H*-pyrazole 4k



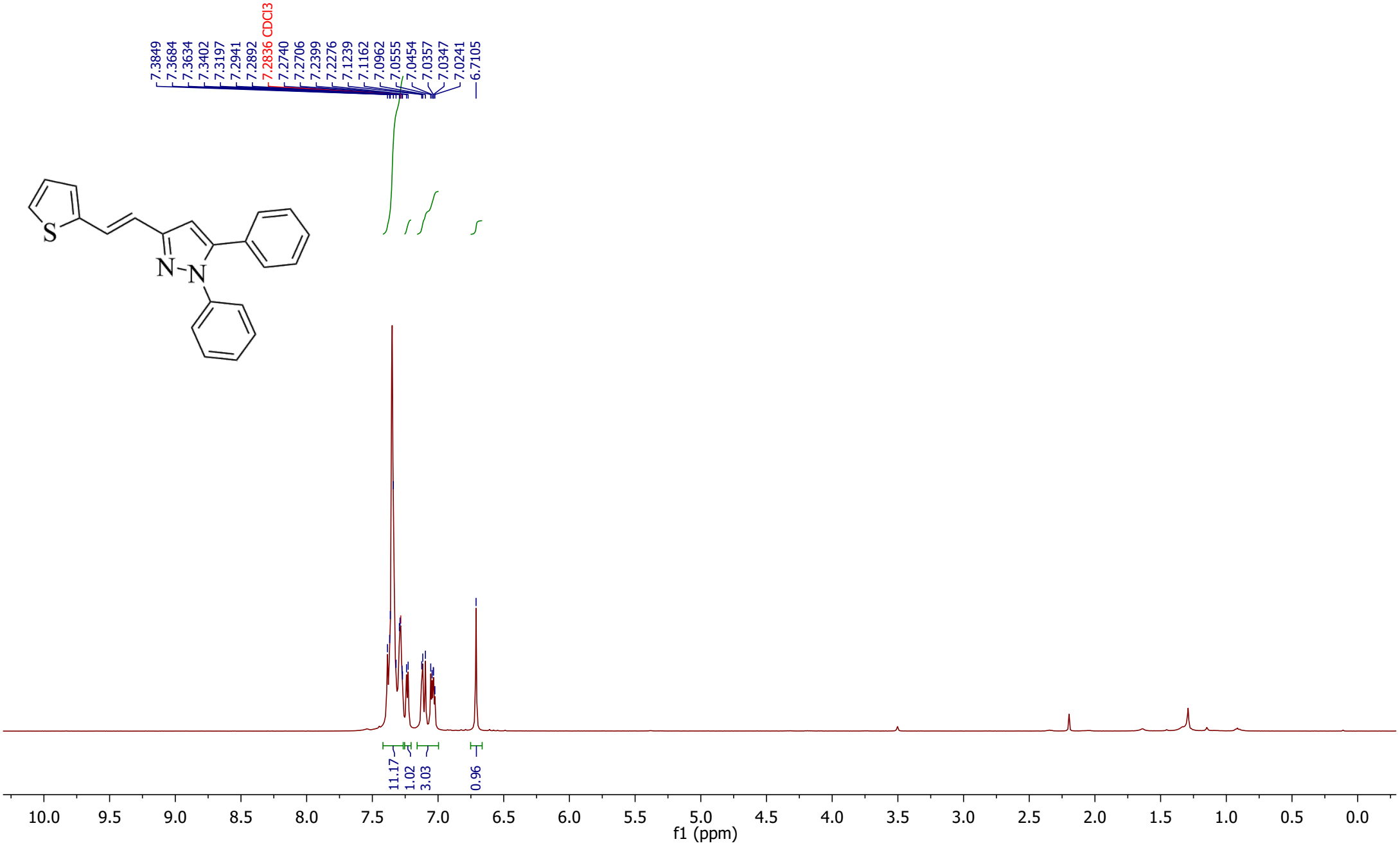
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4l



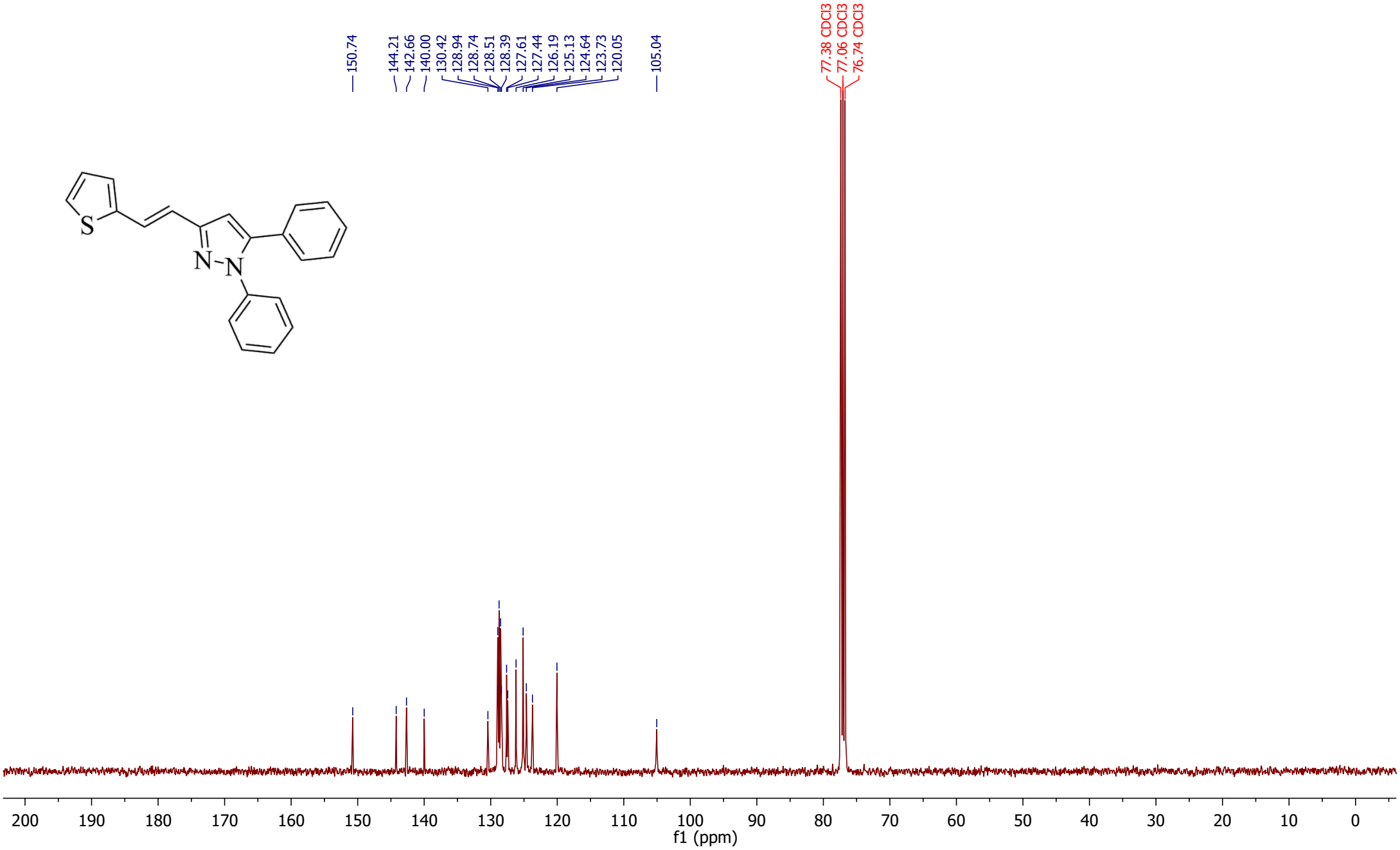
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4l



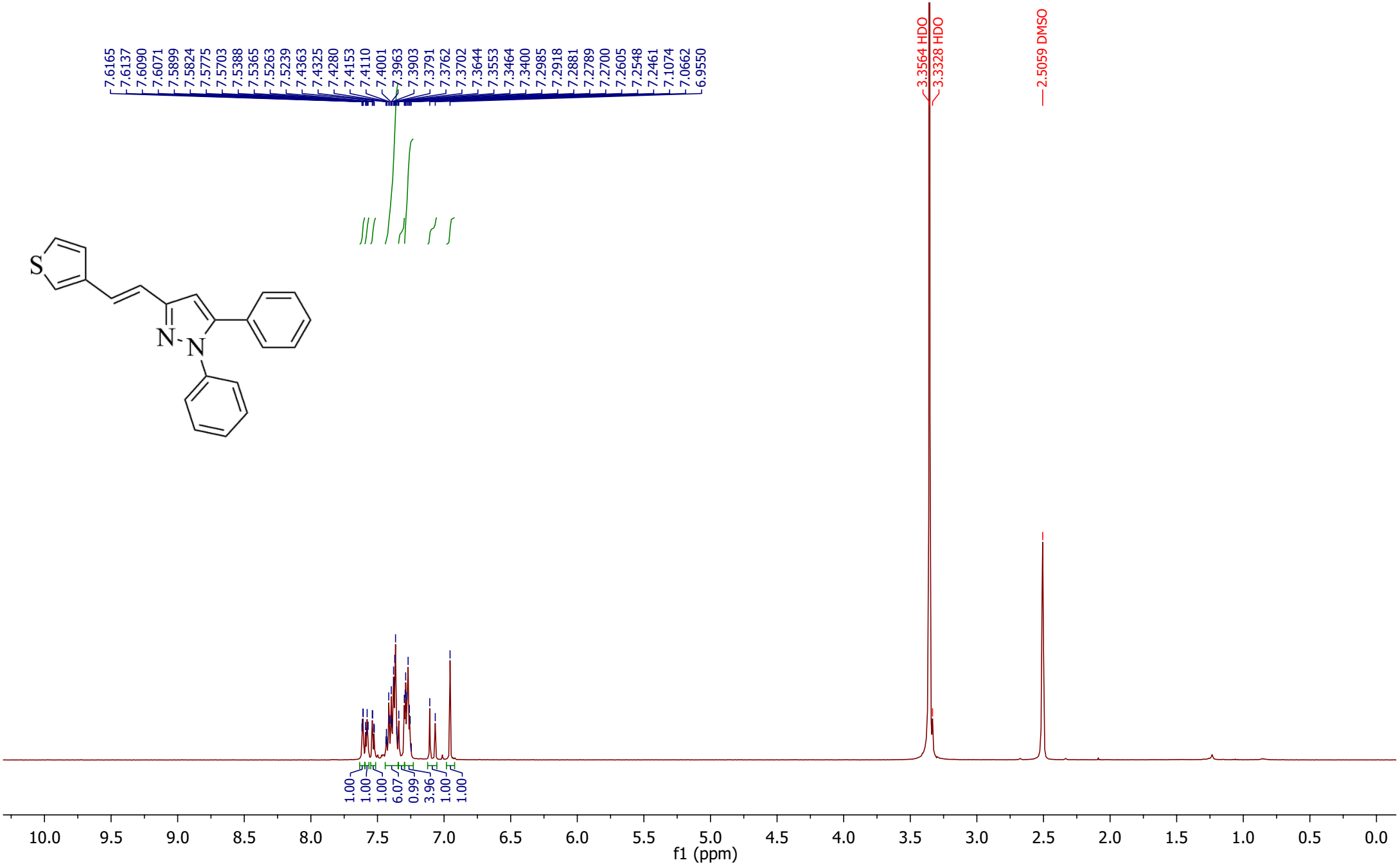
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4m



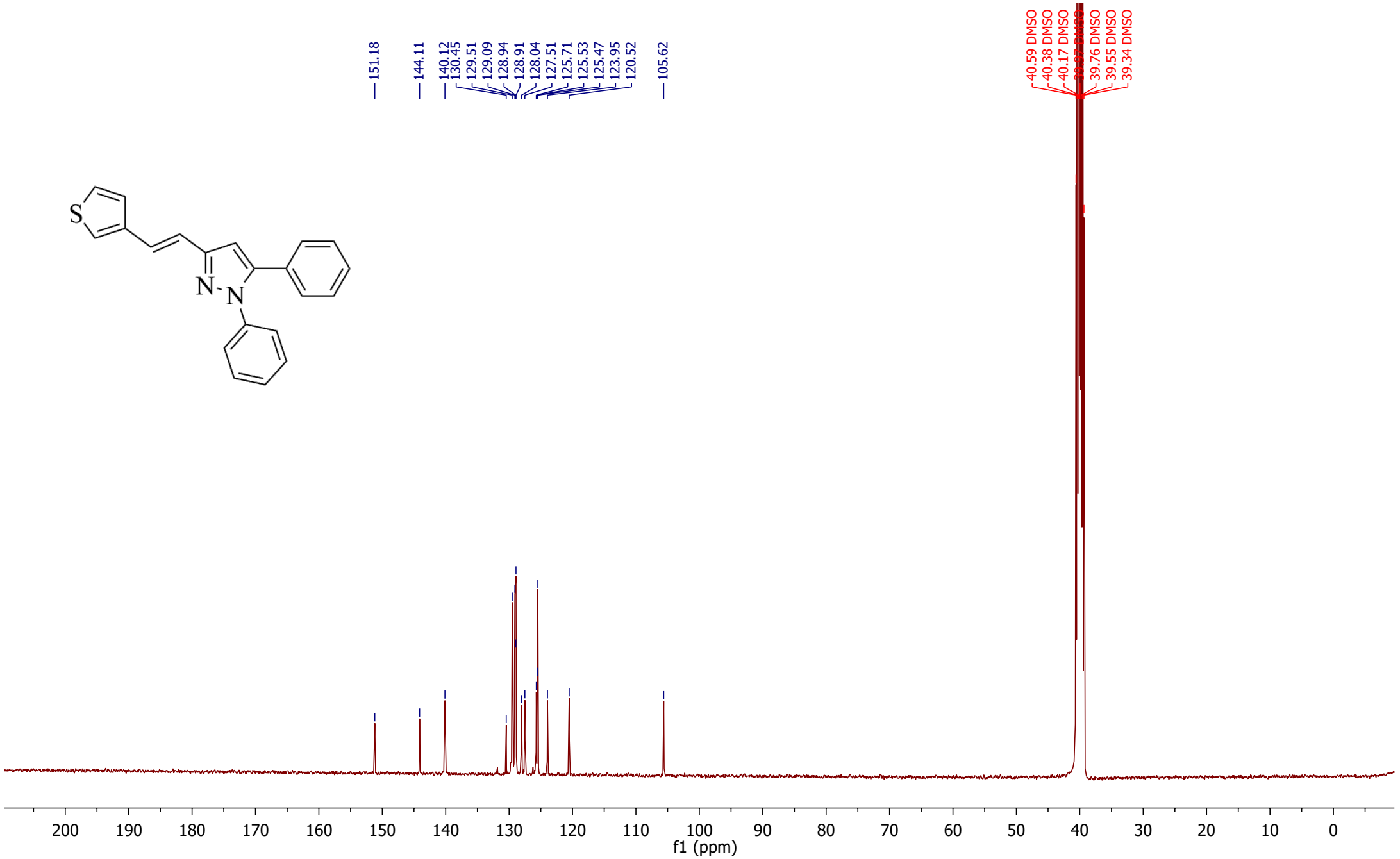
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4m



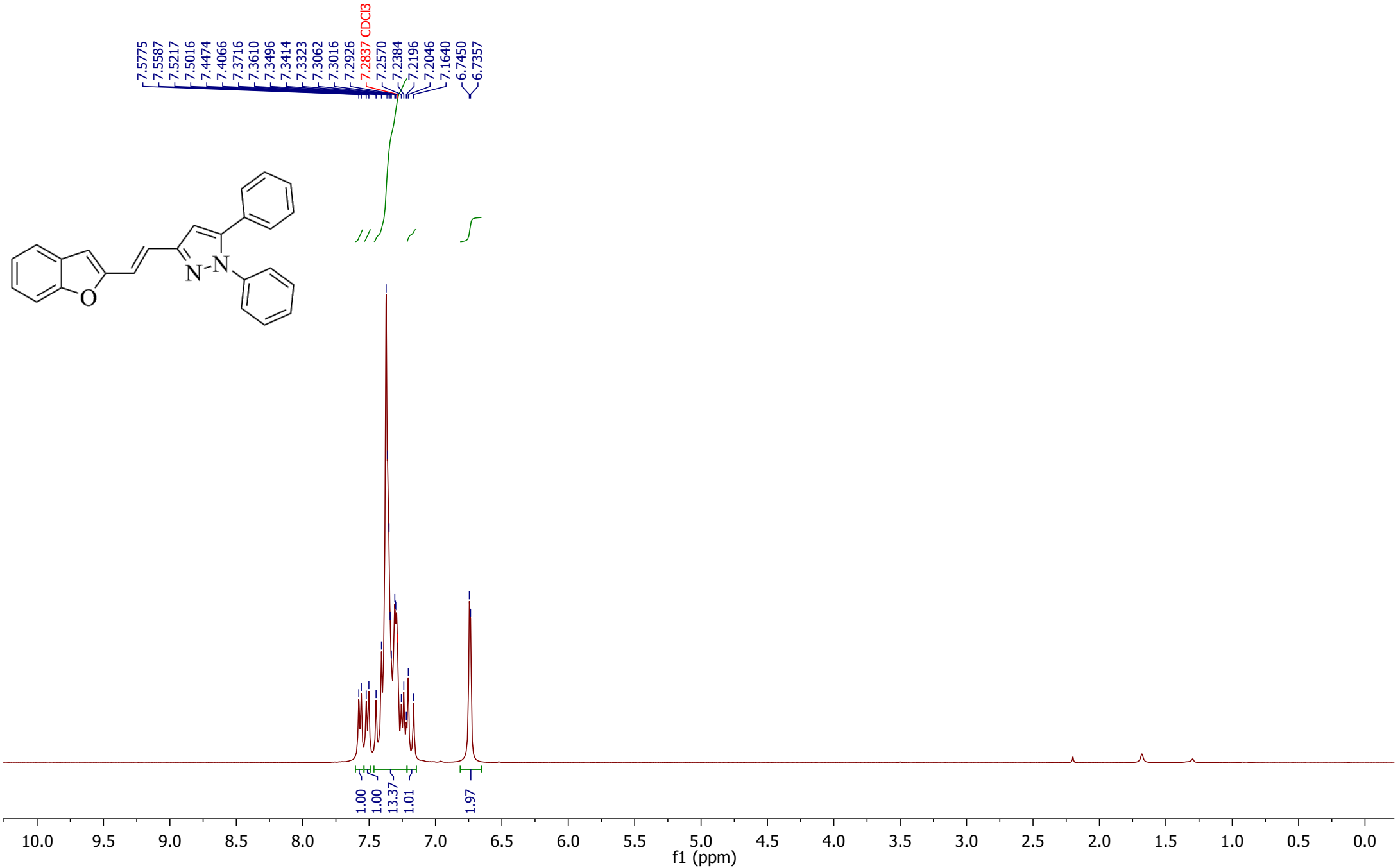
^{1}H NMR spectrum (400 MHz, DMSO-d_6) of 1*H*-pyrazole 4n



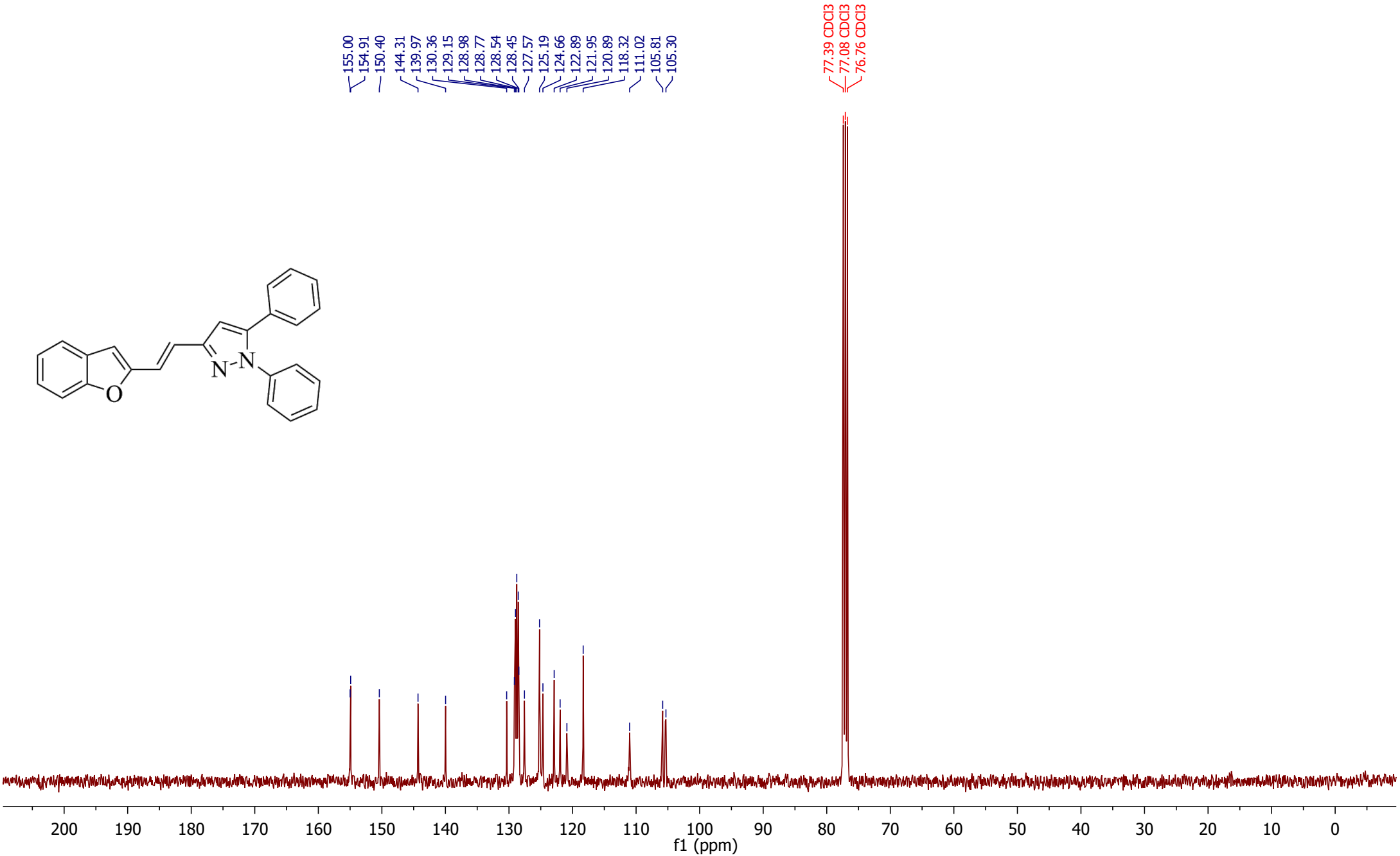
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, DMSO-d_6) of 1*H*-pyrazole 4n



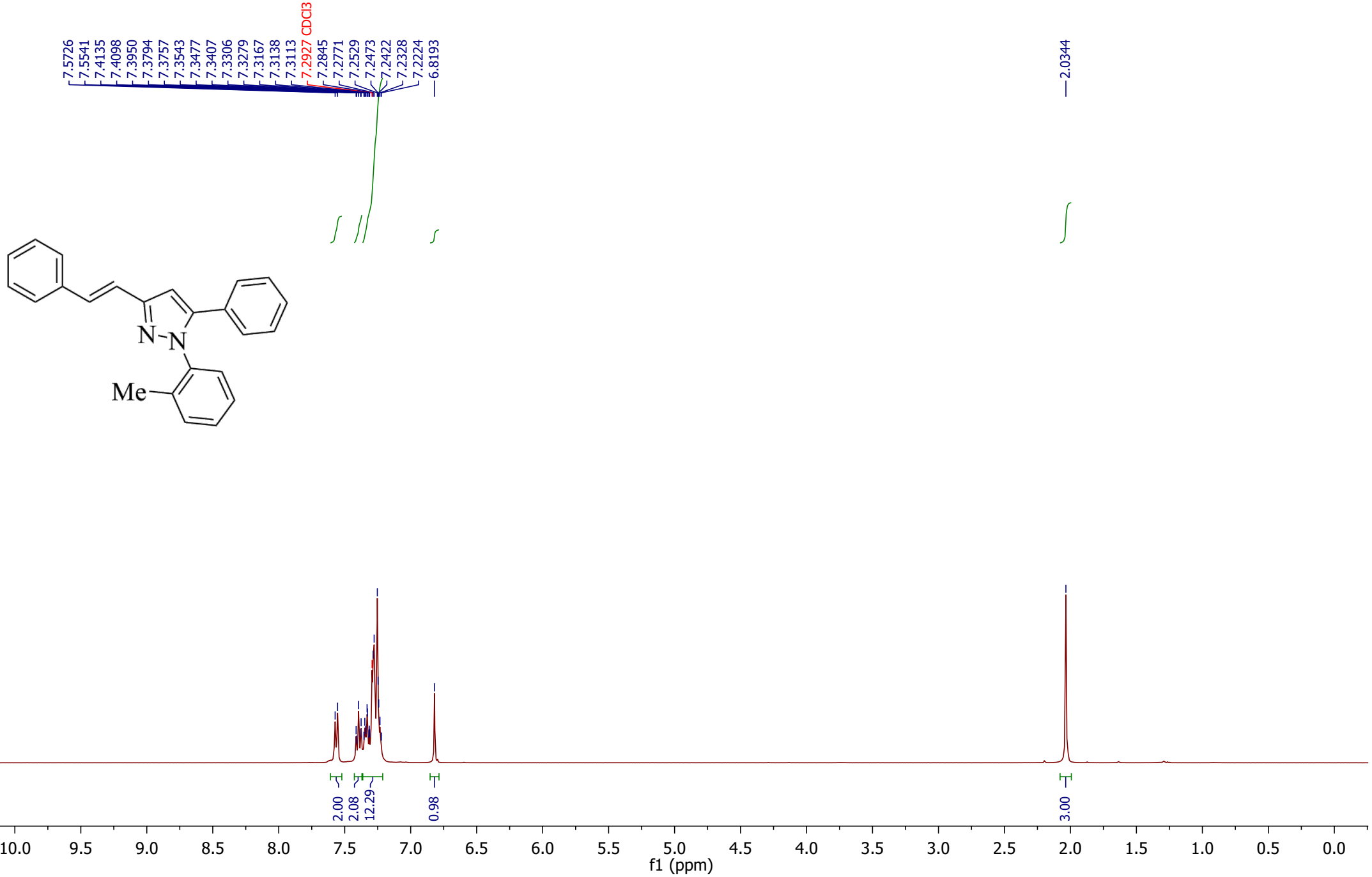
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4o



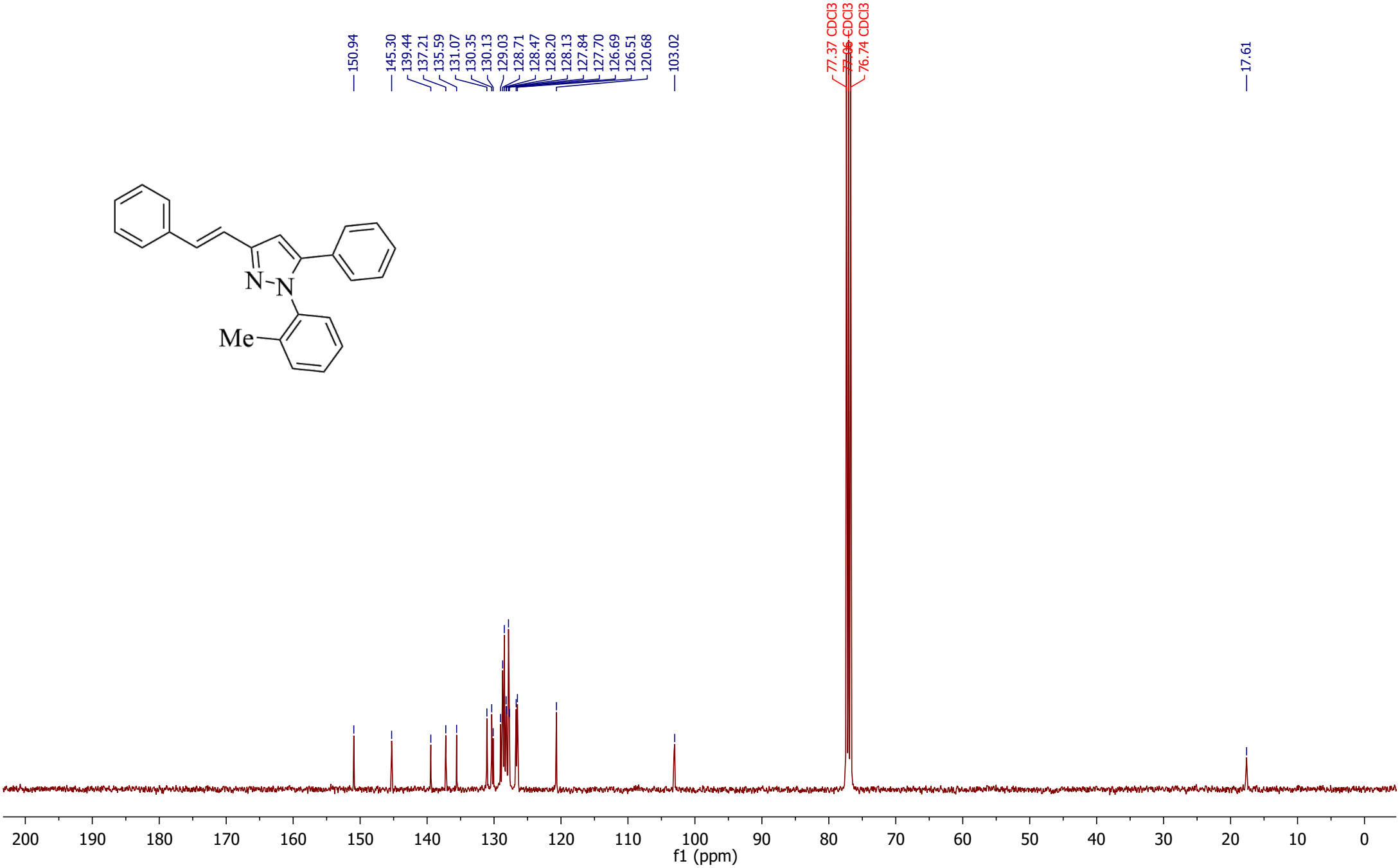
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4o



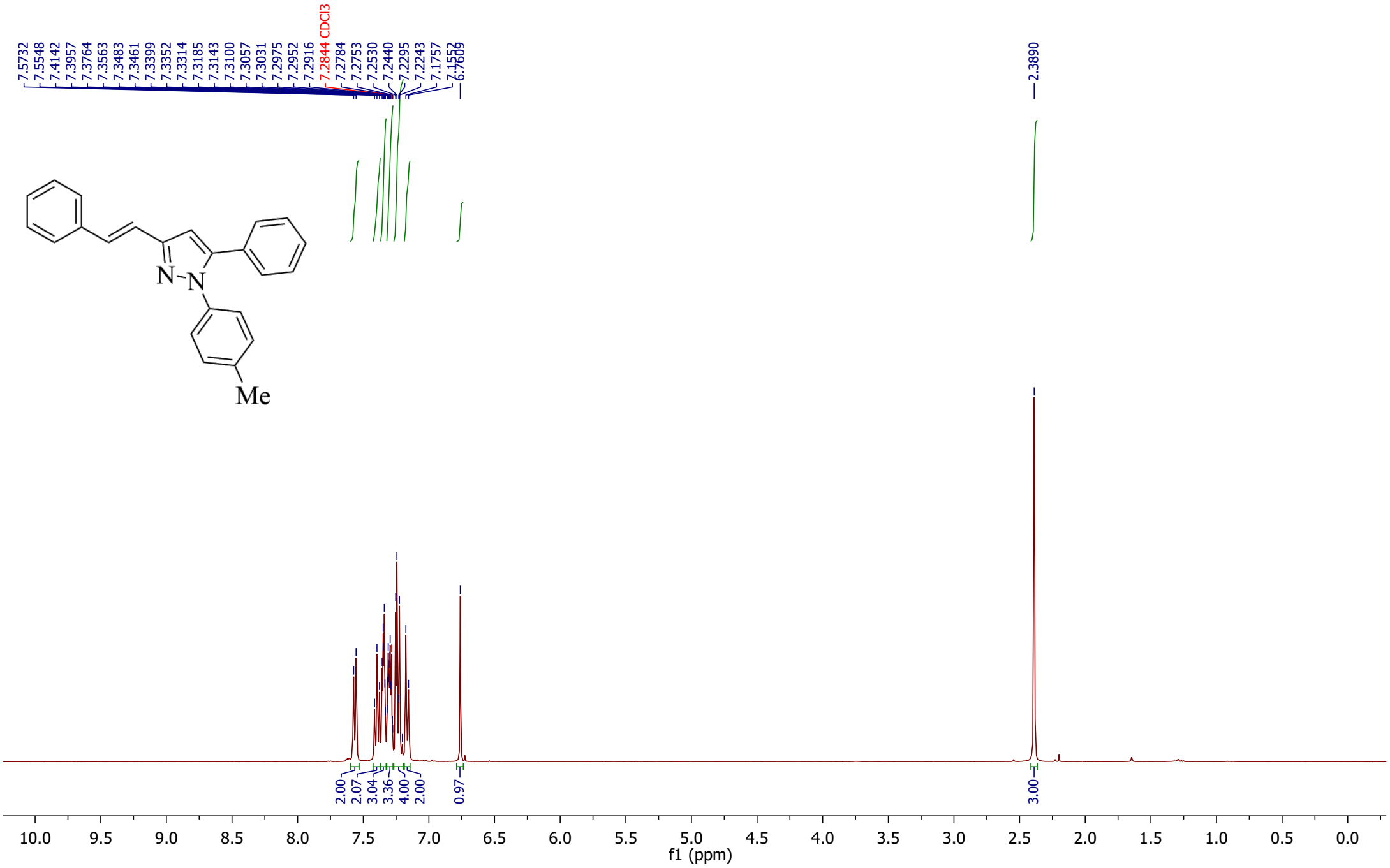
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4p



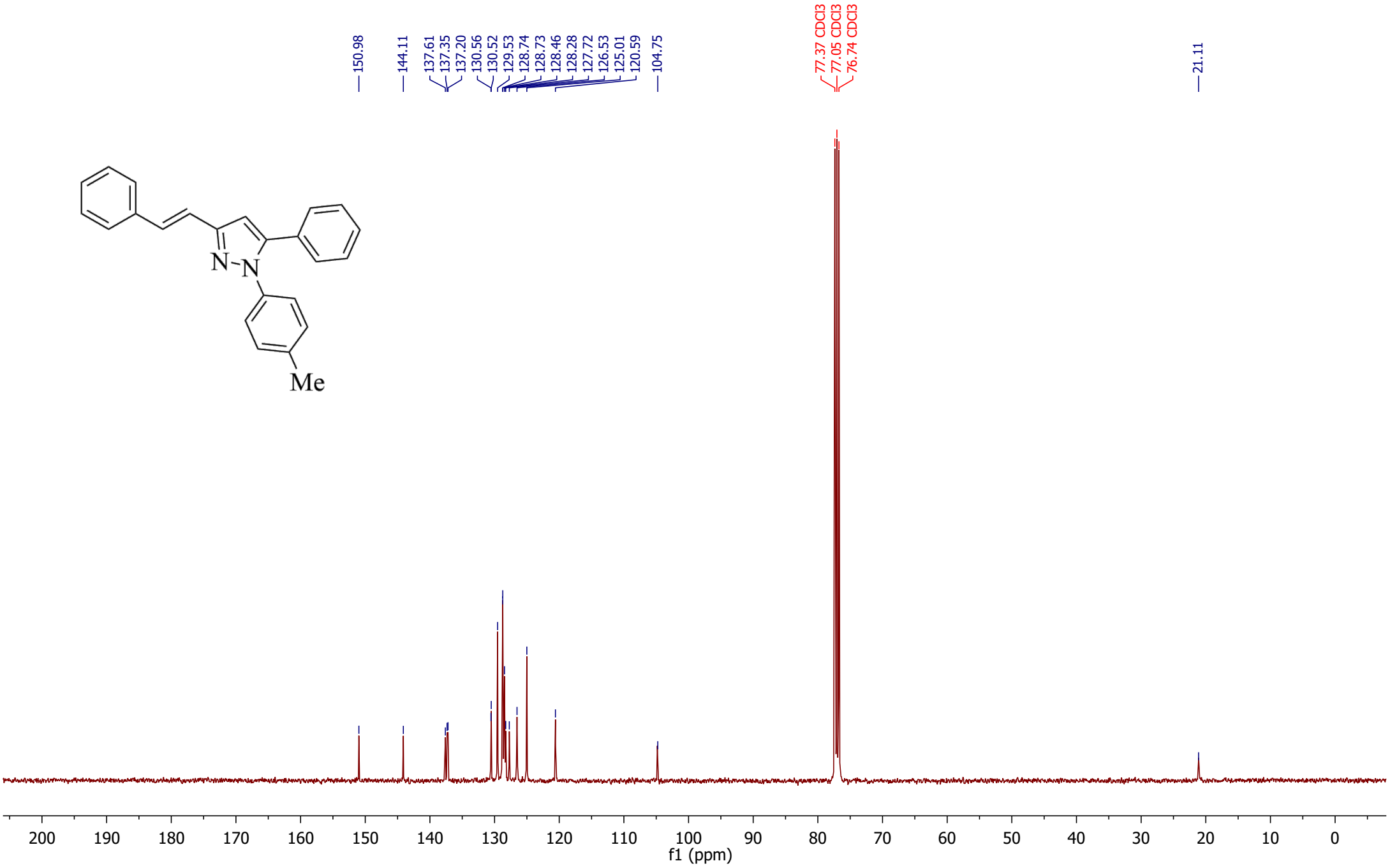
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4p



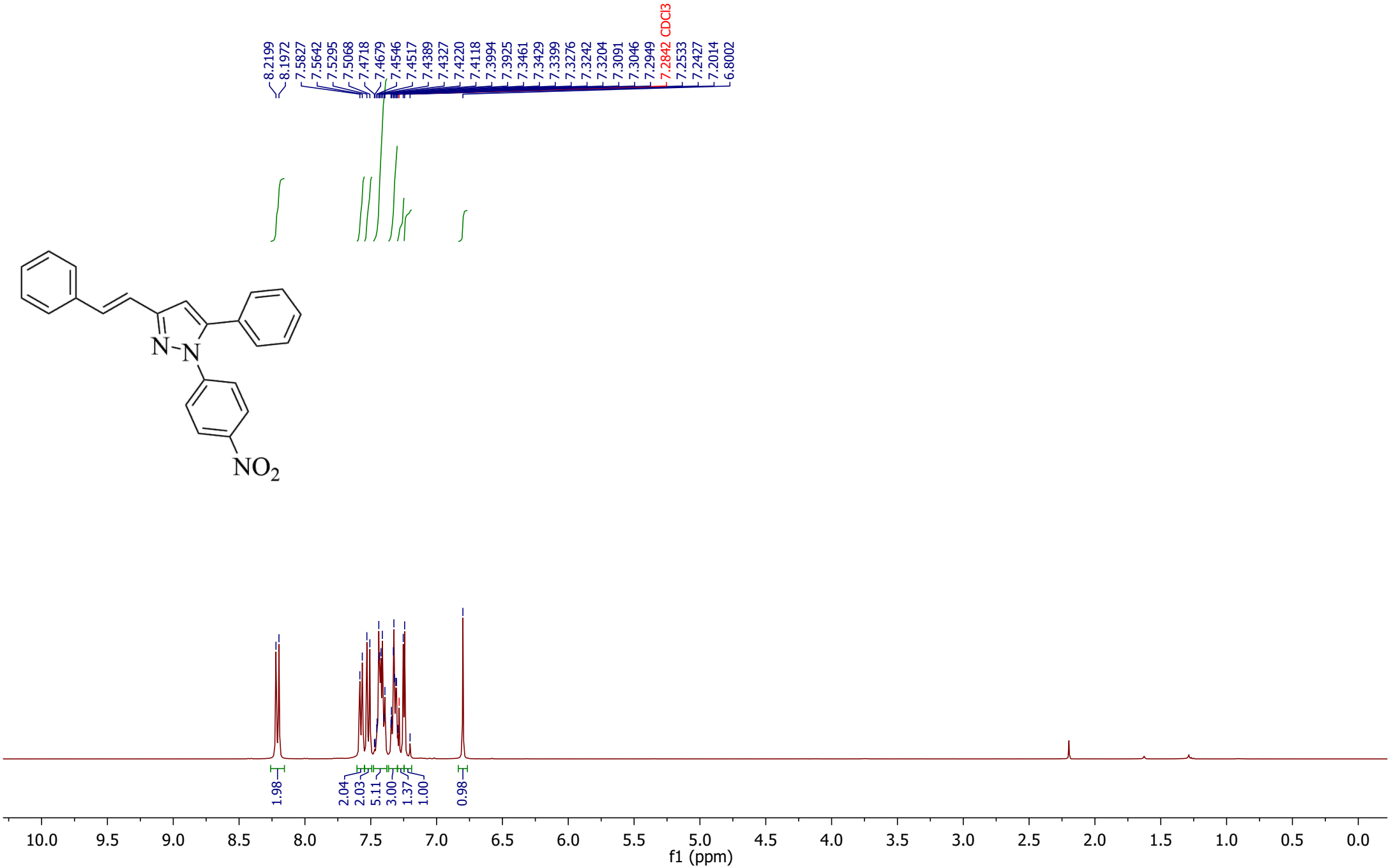
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4q



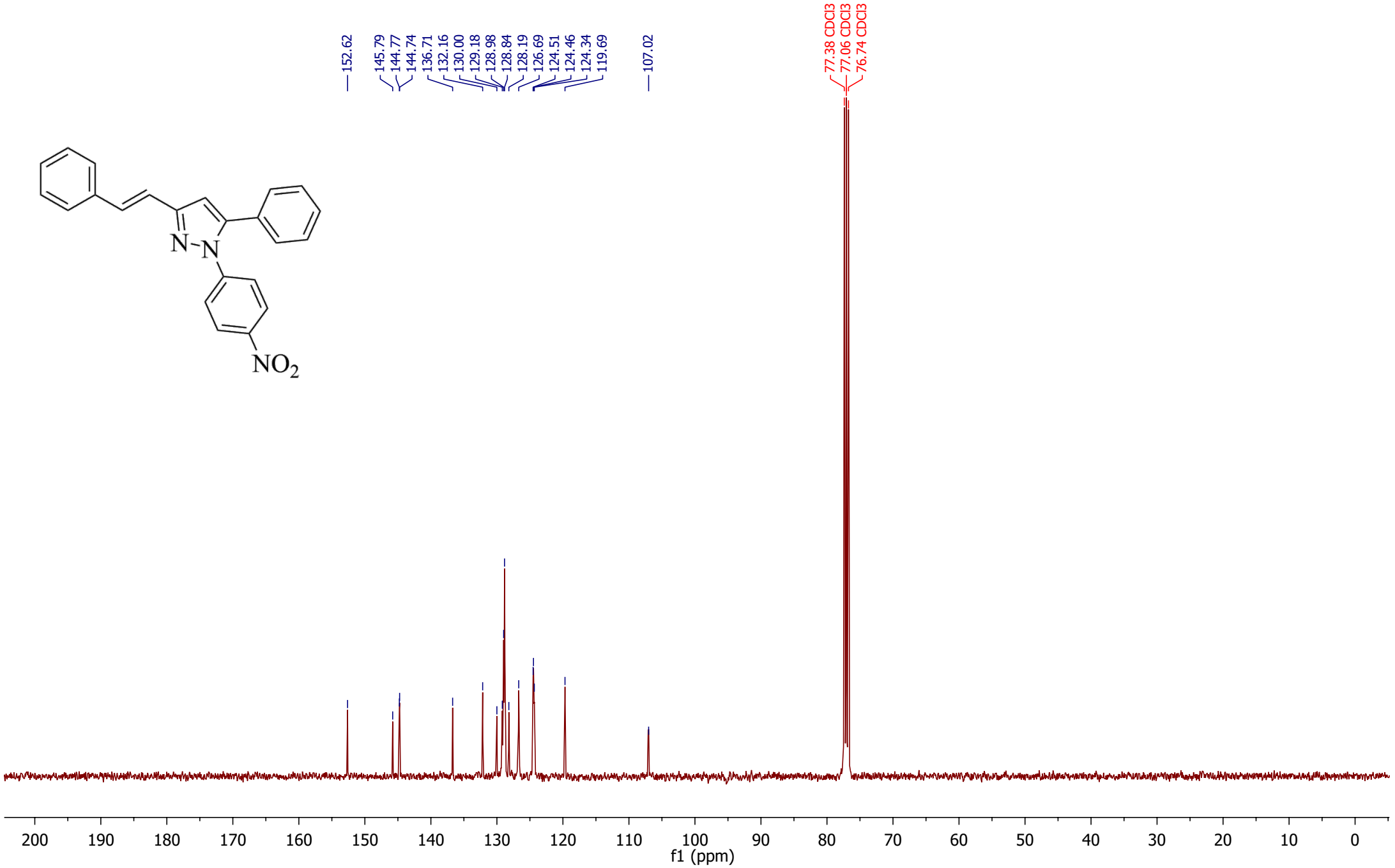
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4q



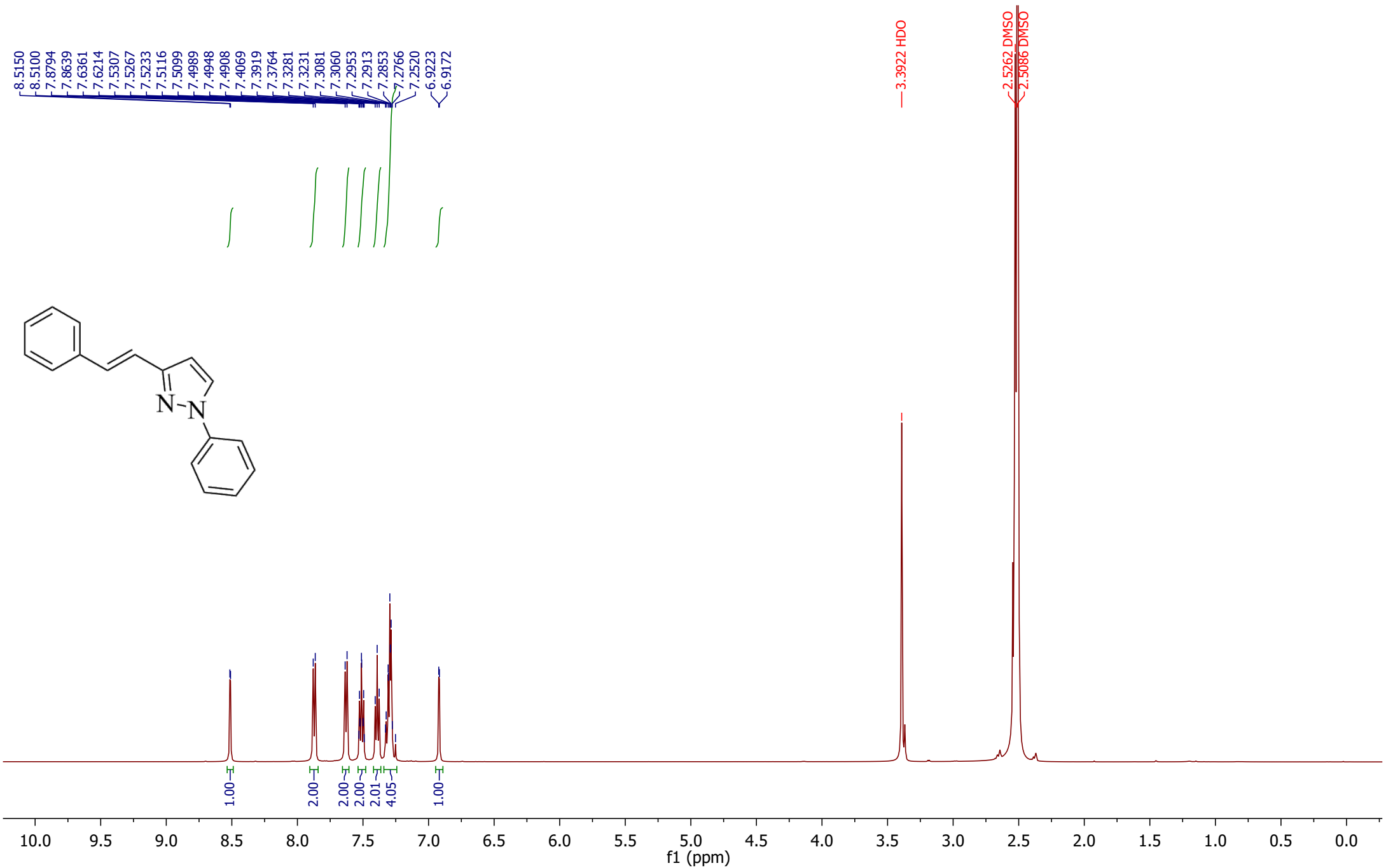
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4r



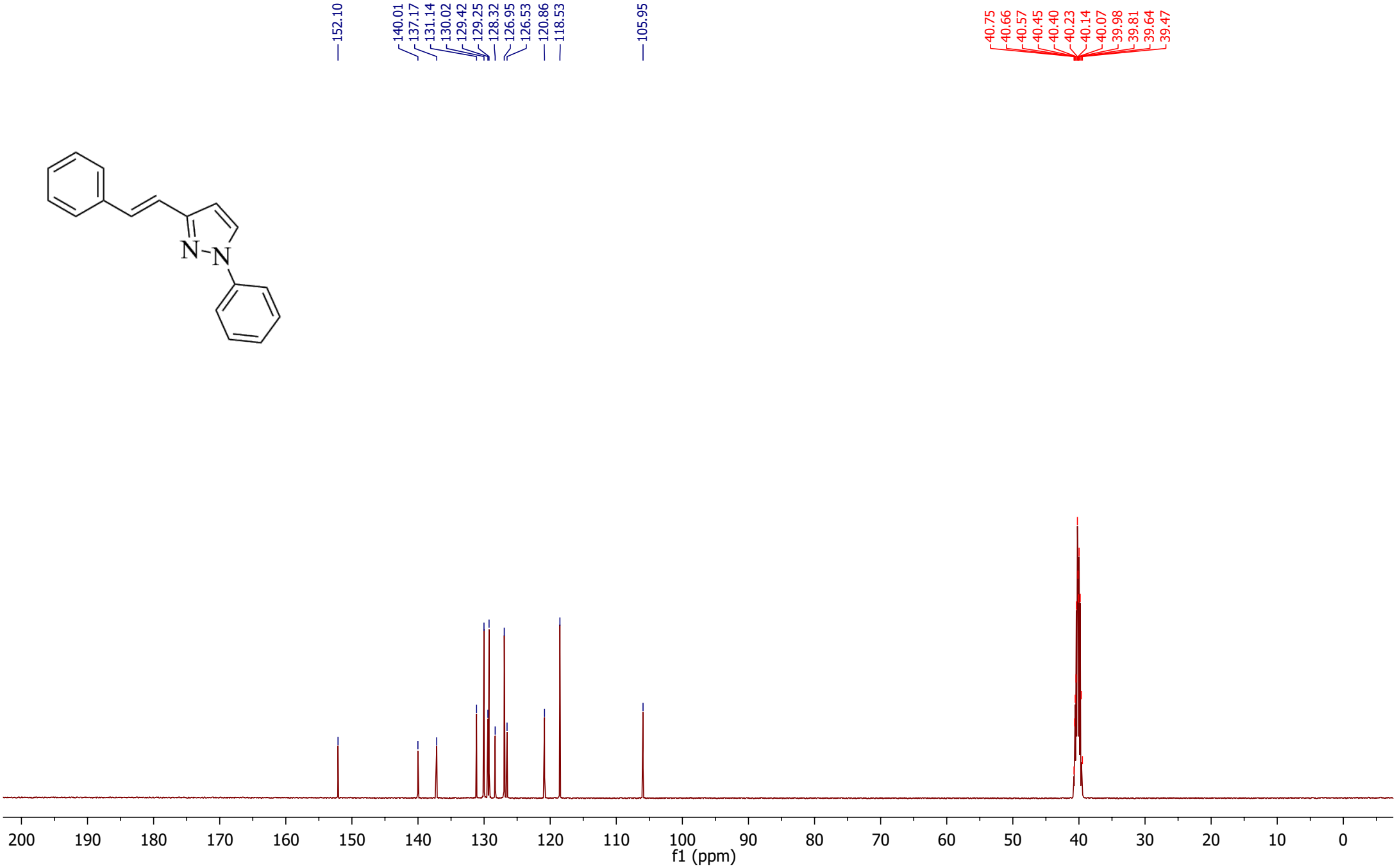
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4r



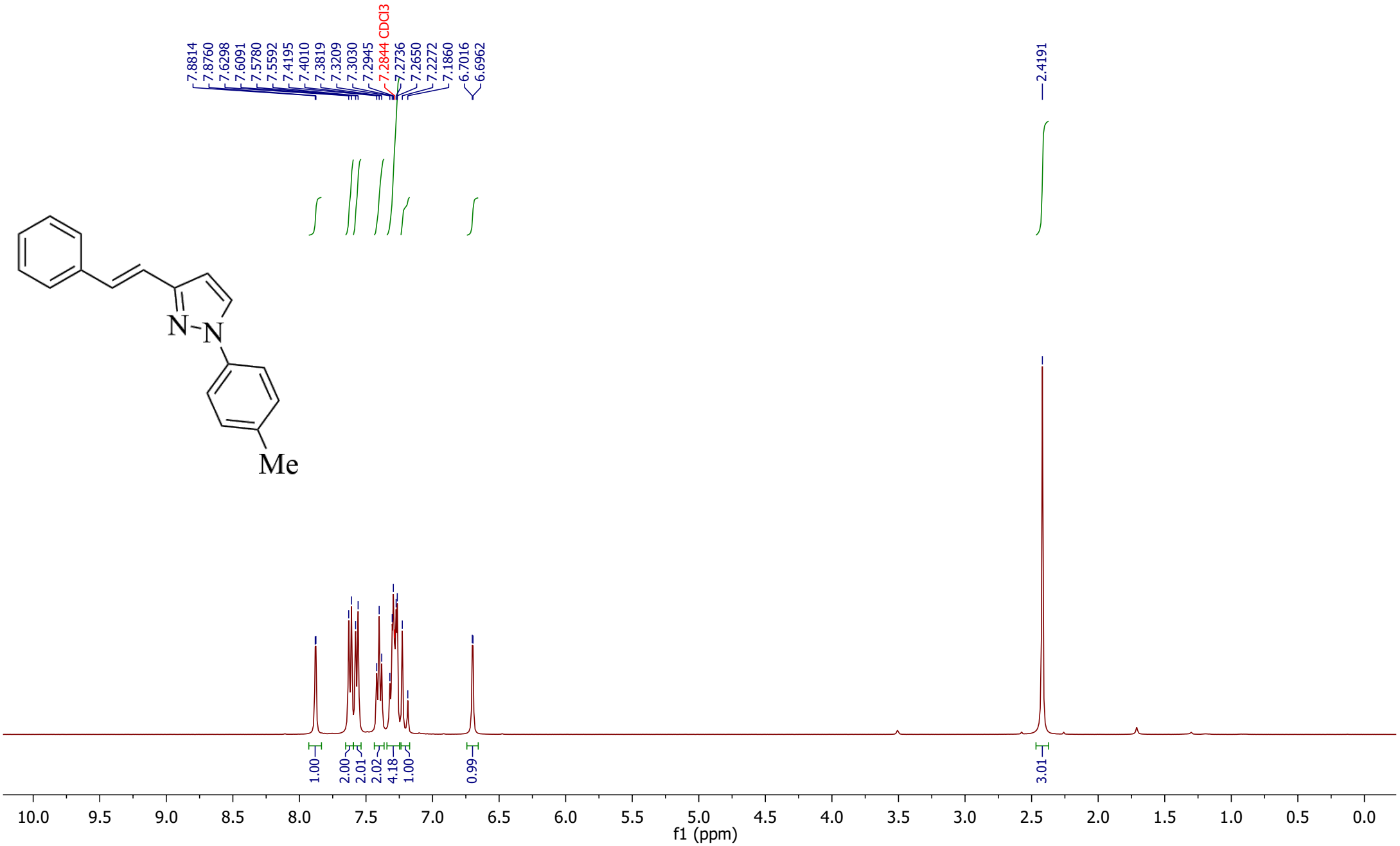
^{1}H NMR spectrum (500 MHz, DMSO-d_6) of 1*H*-pyrazole 4s



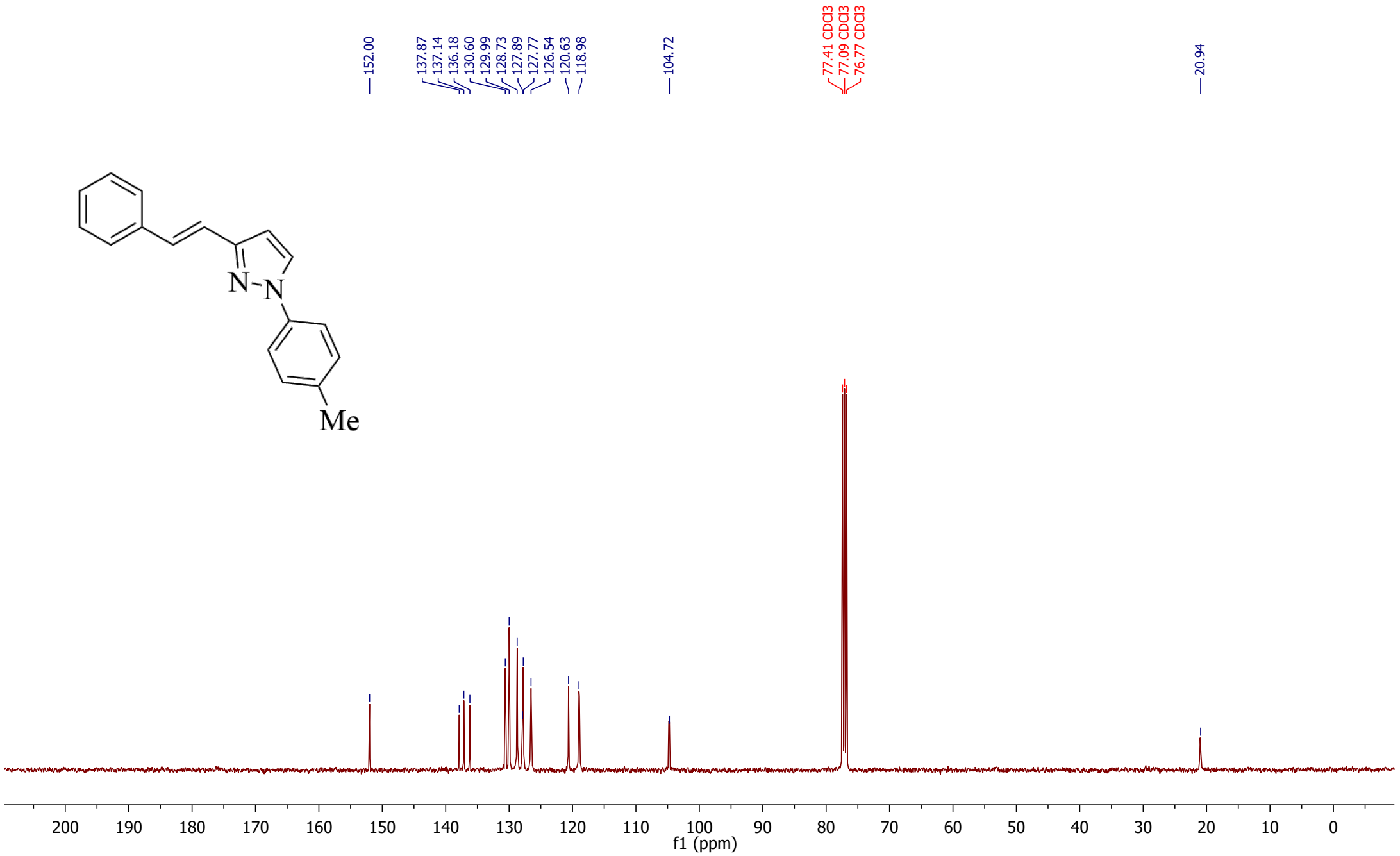
$^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, DMSO-d_6) of 1*H*-pyrazole 4s



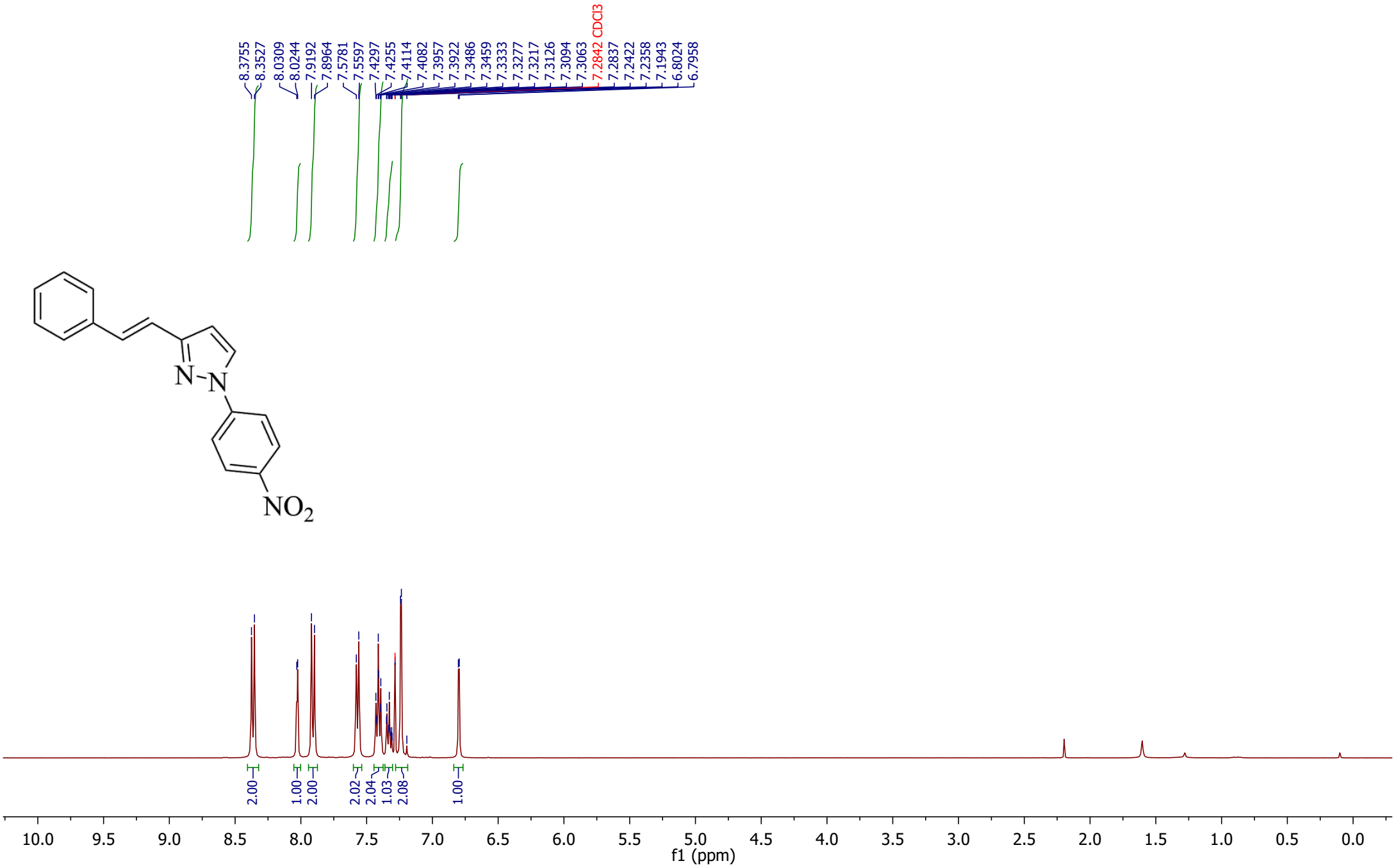
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4t



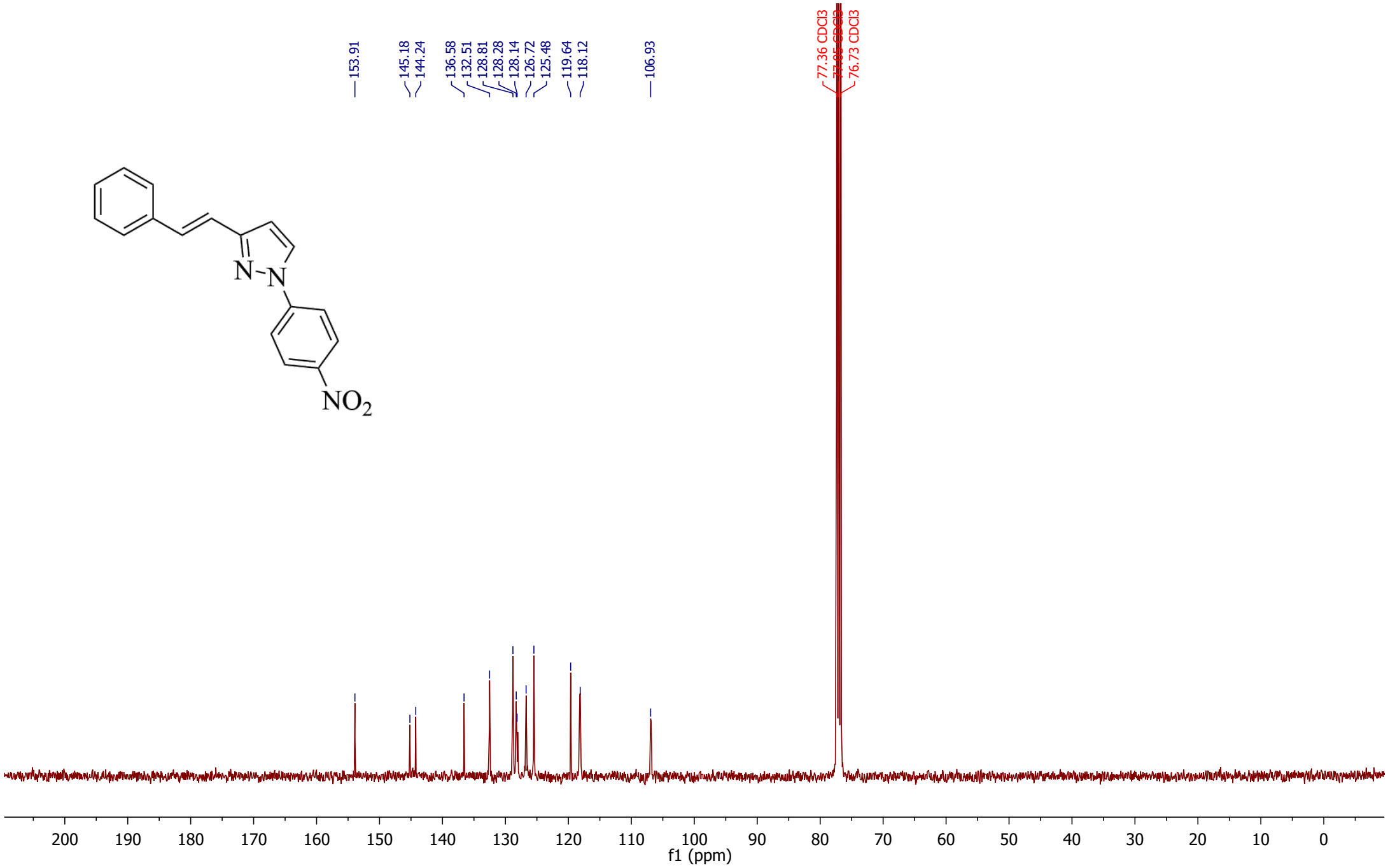
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4t



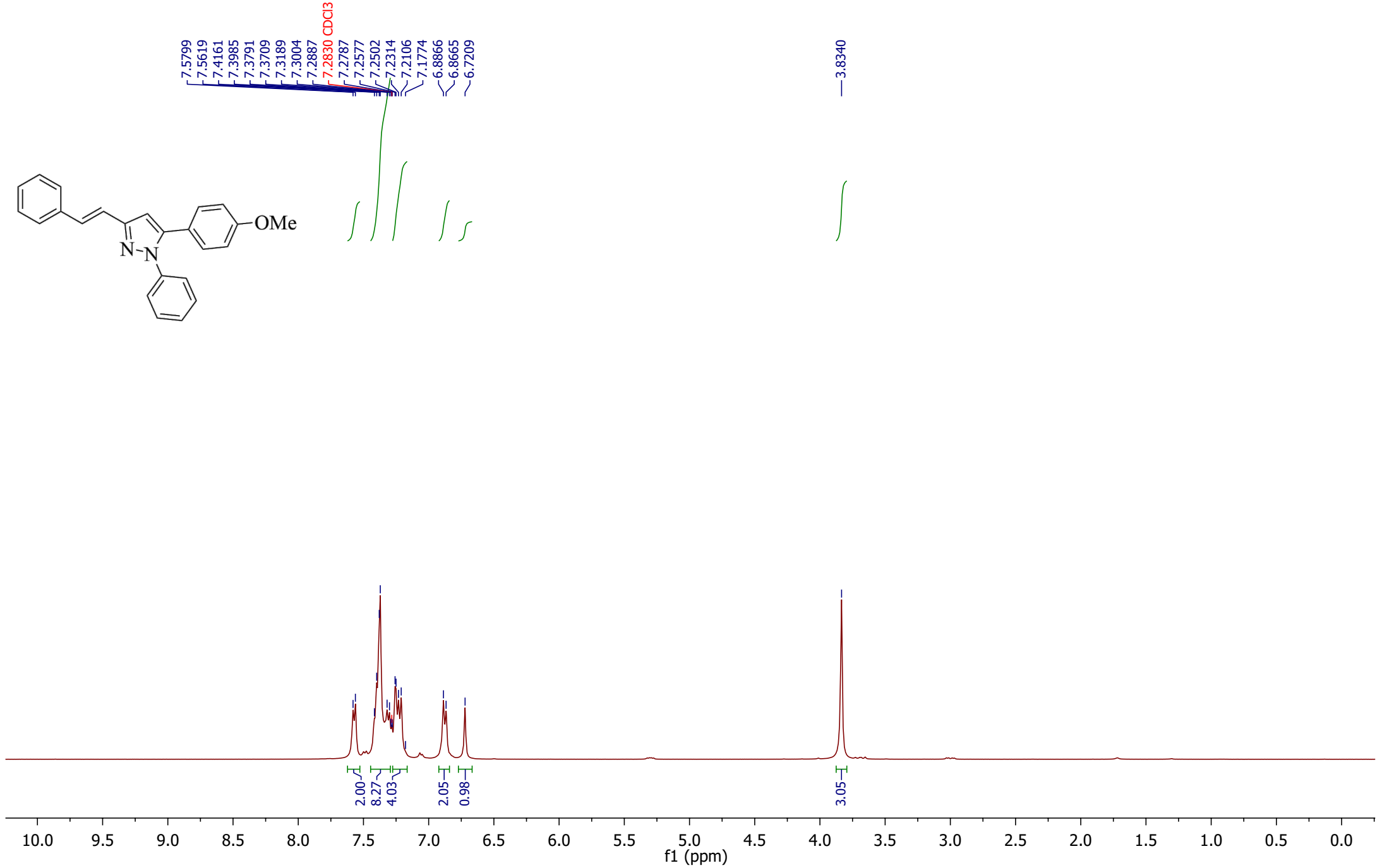
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4u



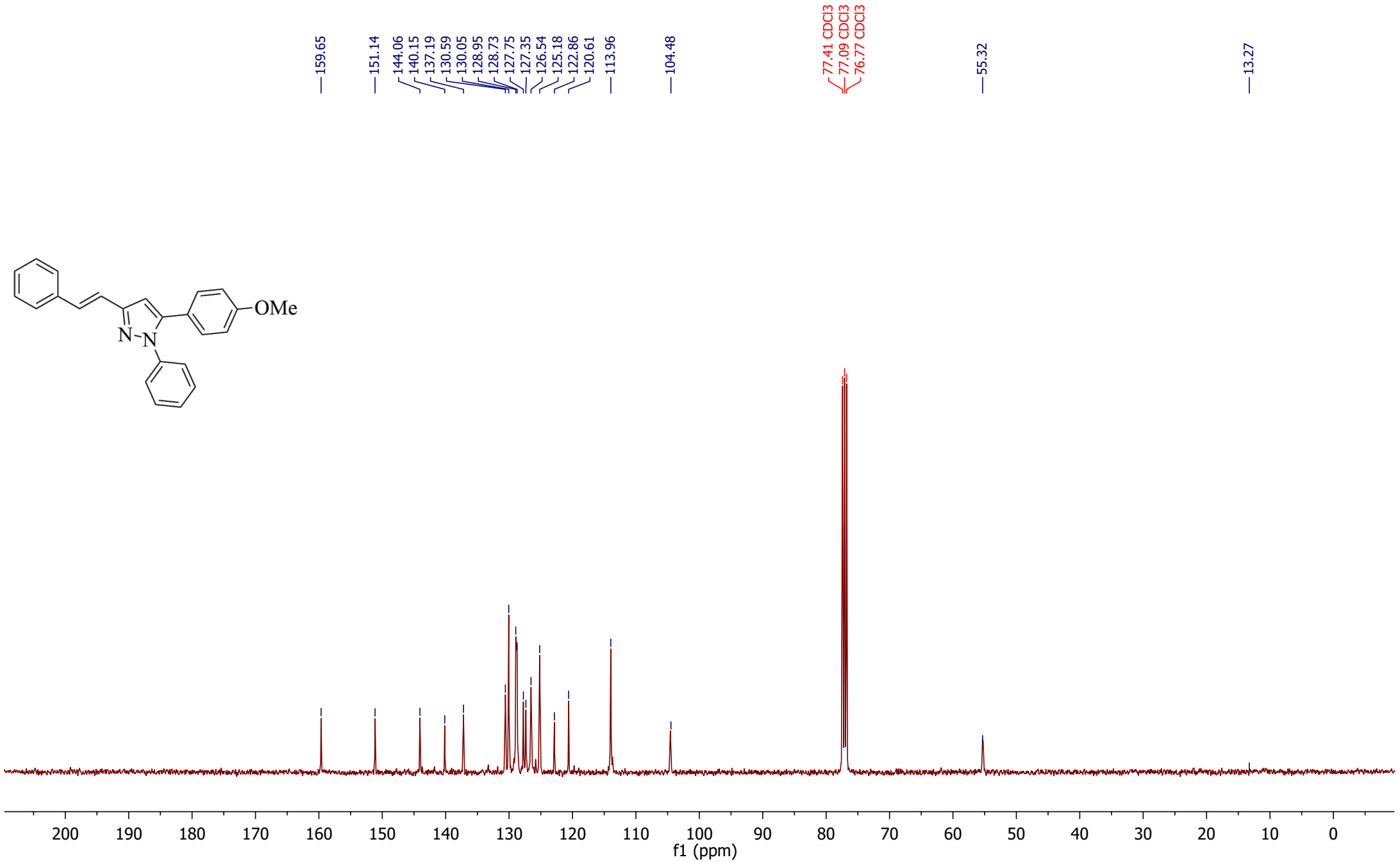
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4u



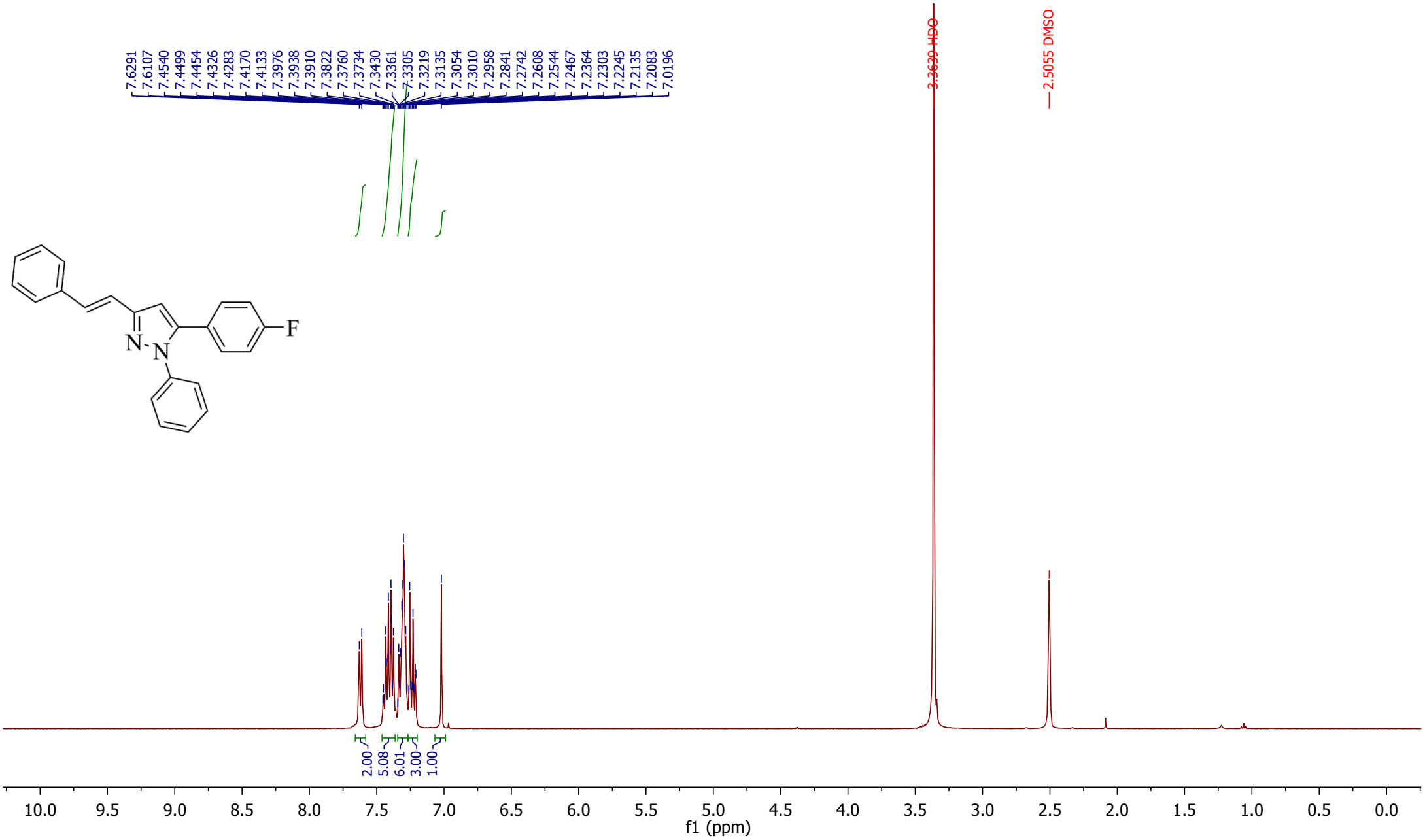
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4v



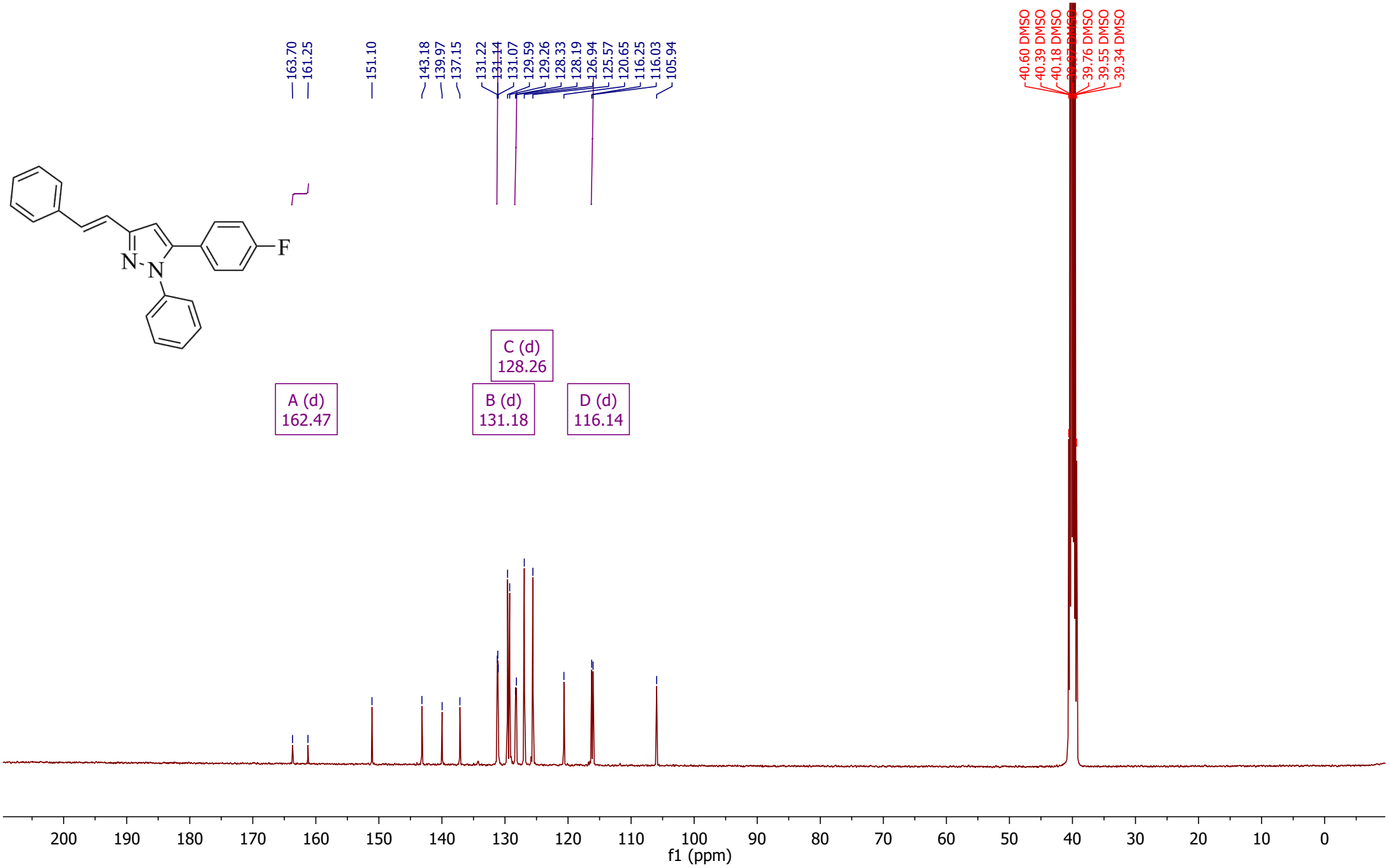
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4v



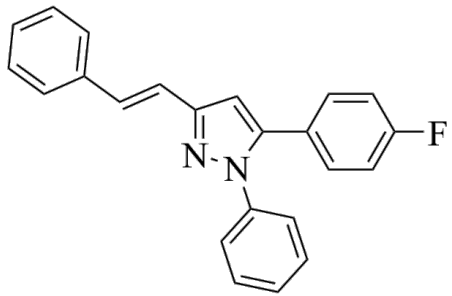
^{1}H NMR spectrum (400 MHz, DMSO-d_6) of 1*H*-pyrazole 4w



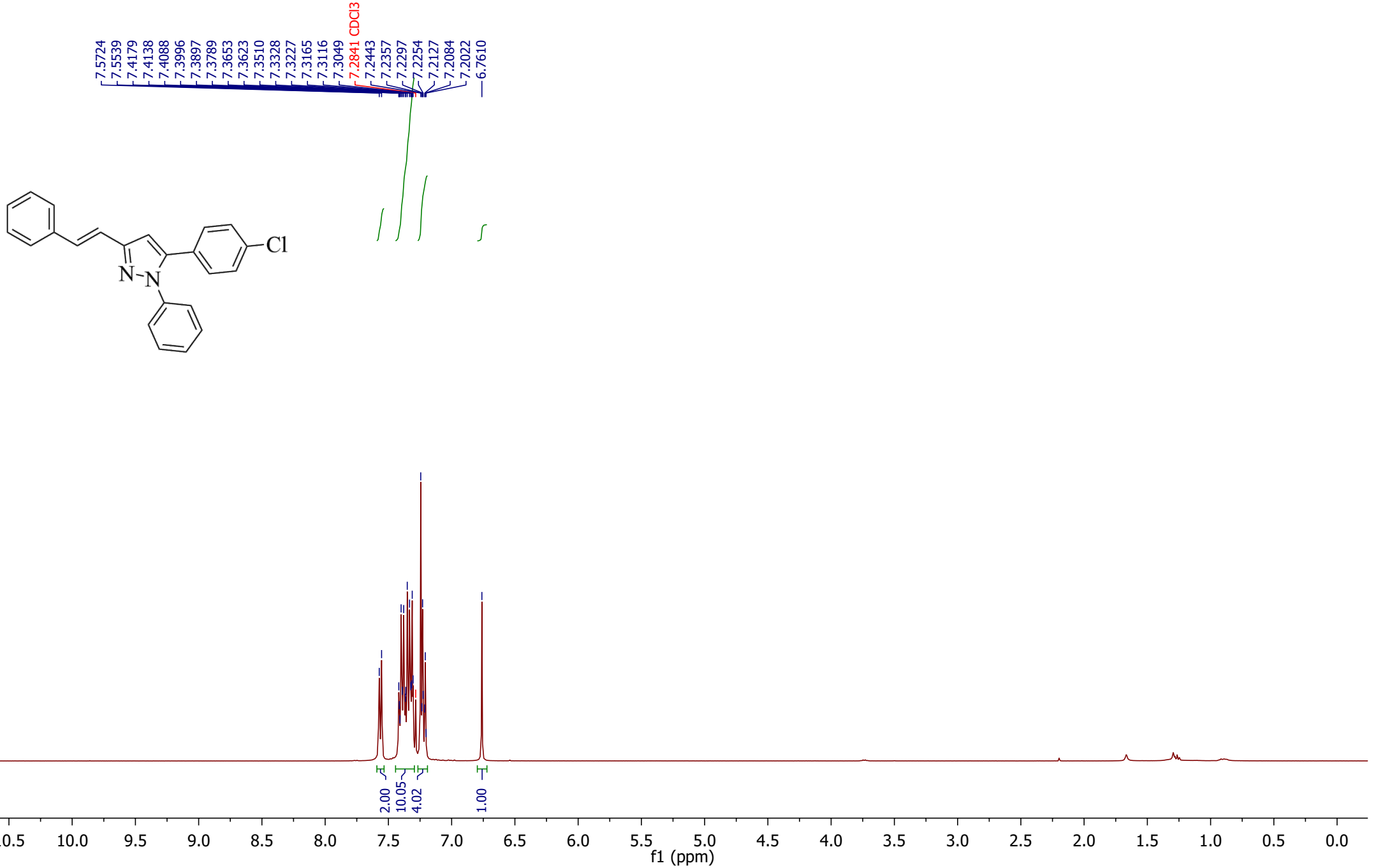
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, DMSO-d_6) of 1*H*-pyrazole 4w



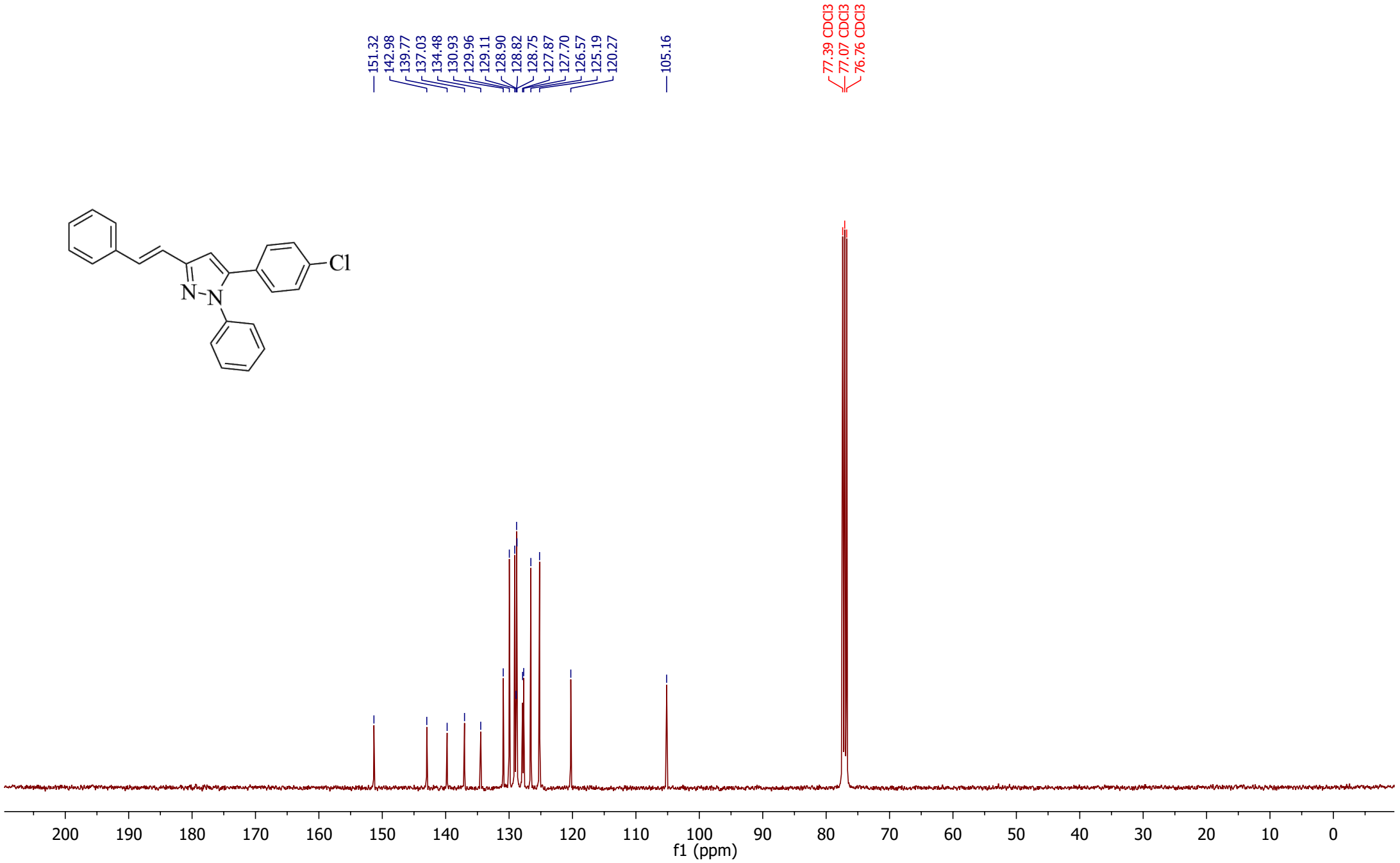
^{19}F NMR (376 MHz, DMSO-d_6) of 1*H*-pyrazole 4w



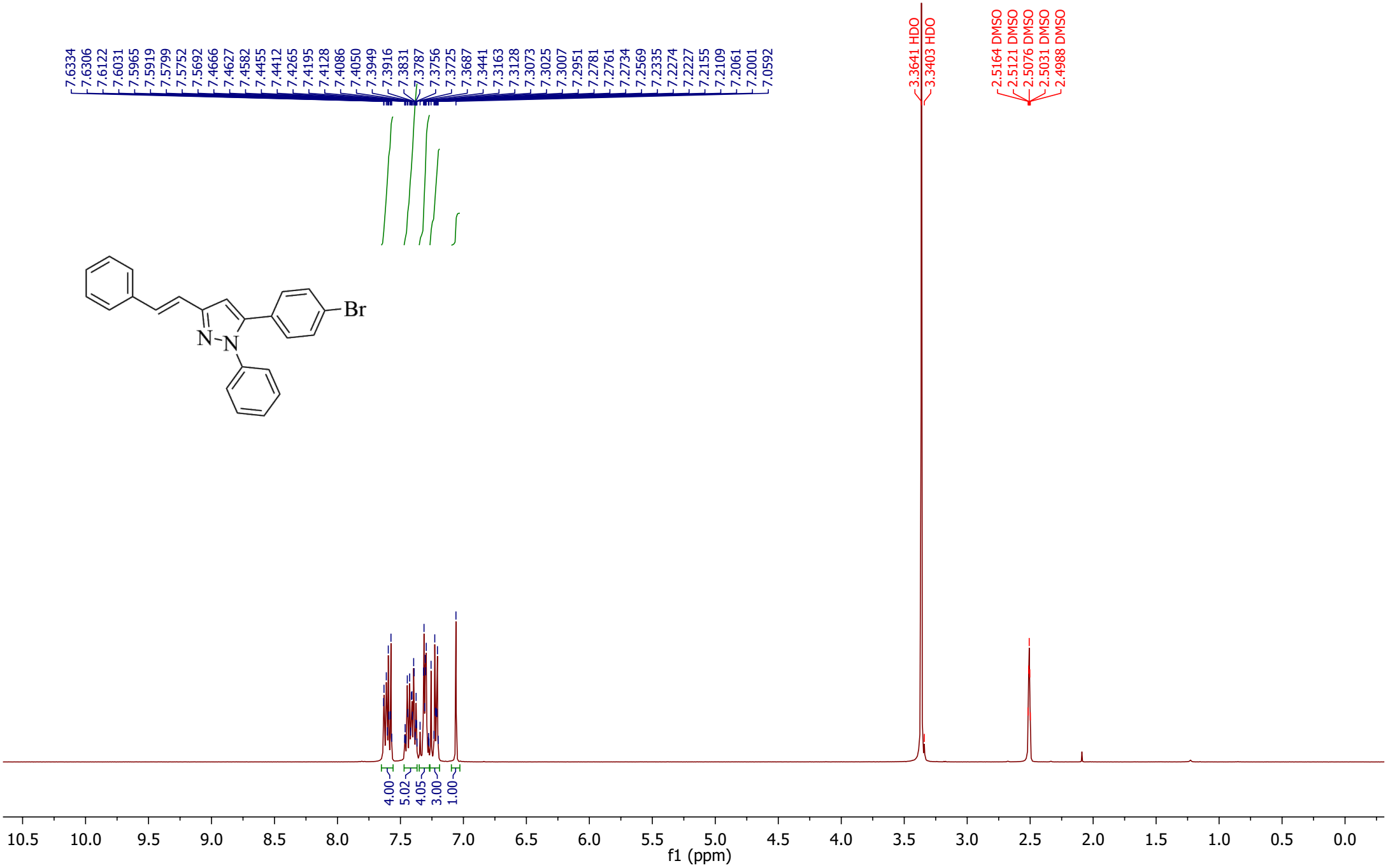
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4x



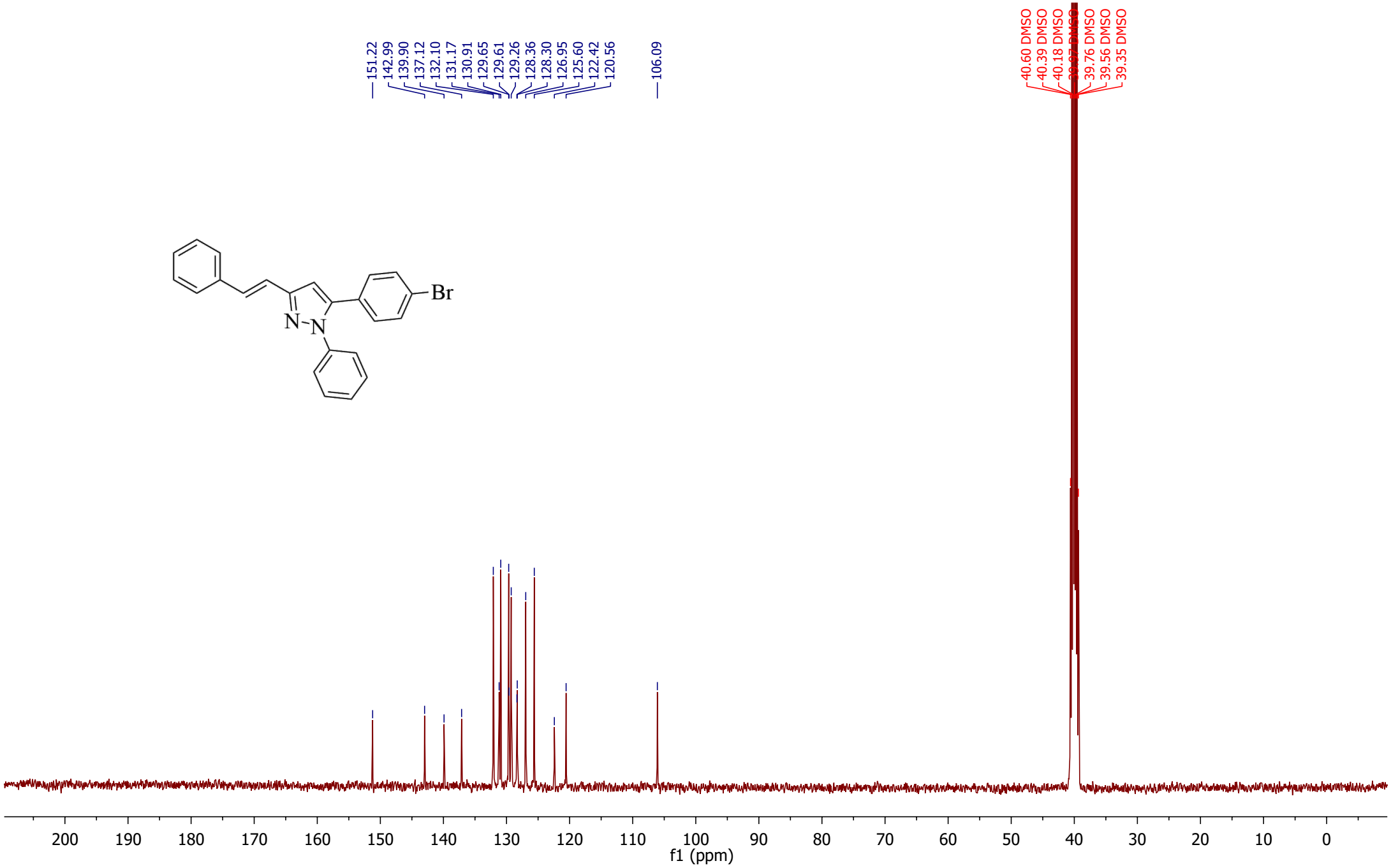
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4x



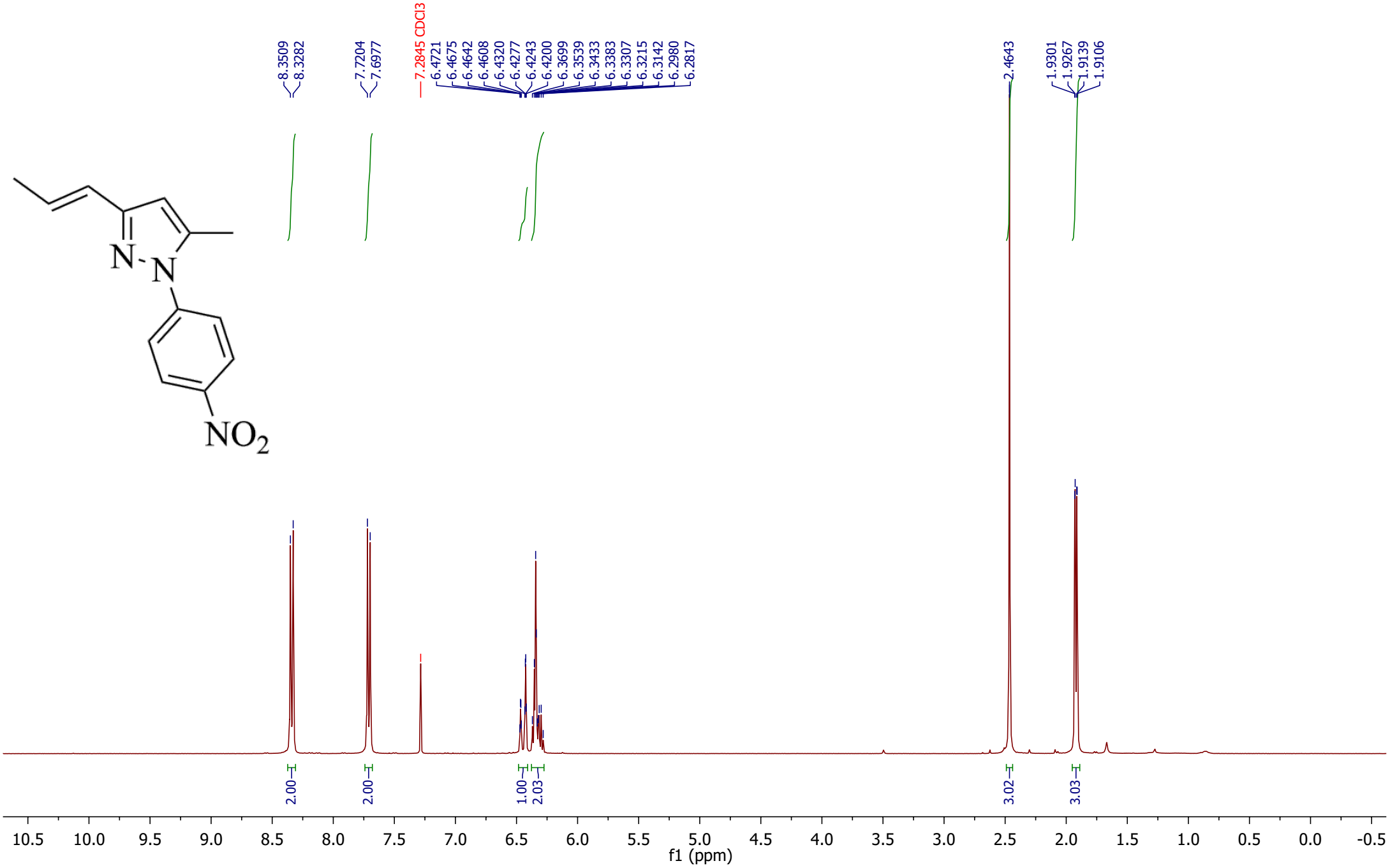
^{1}H NMR spectrum (400 MHz, DMSO-d_6) of 1*H*-pyrazole 4y



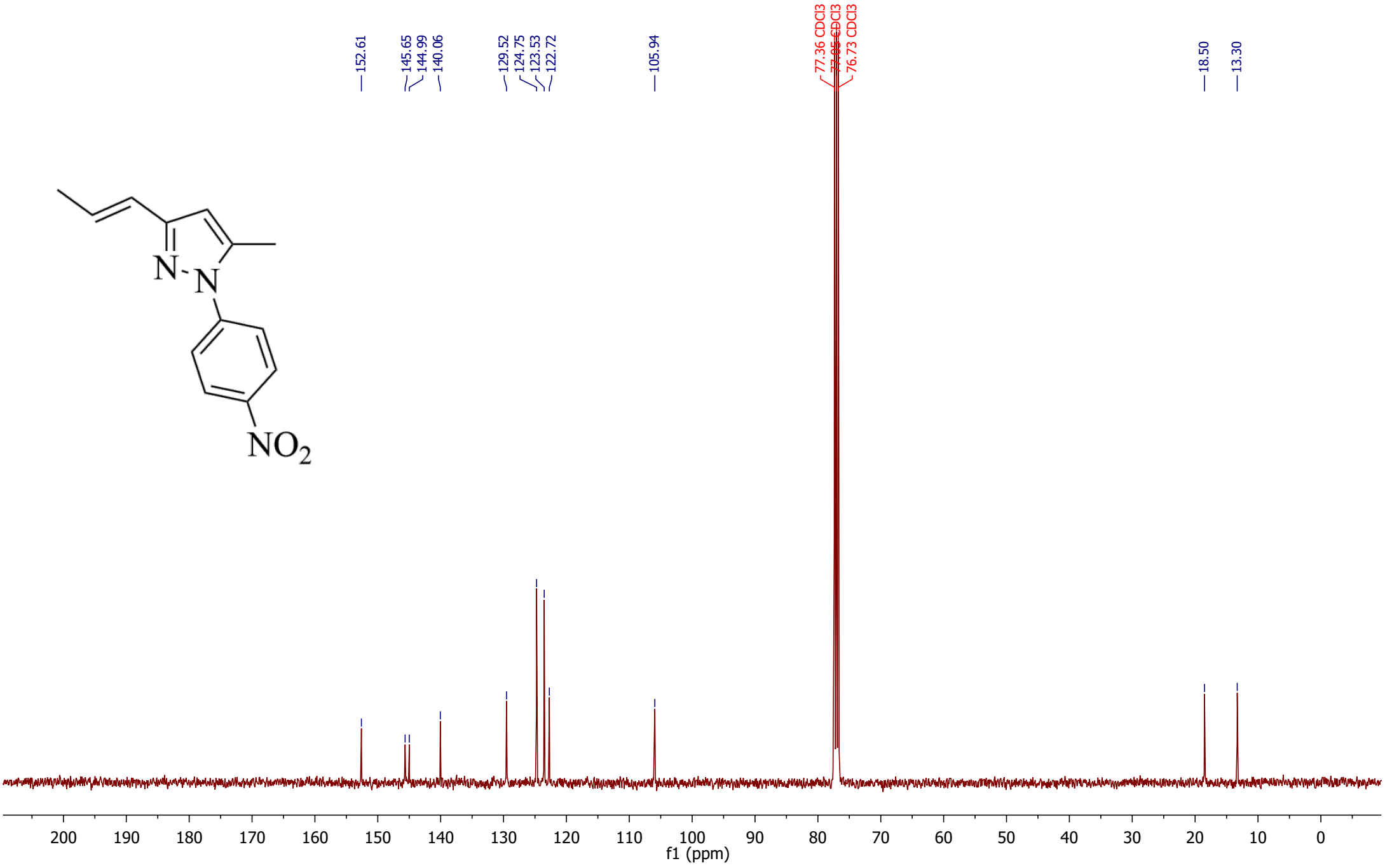
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, DMSO-d_6) of 1*H*-pyrazole 4y



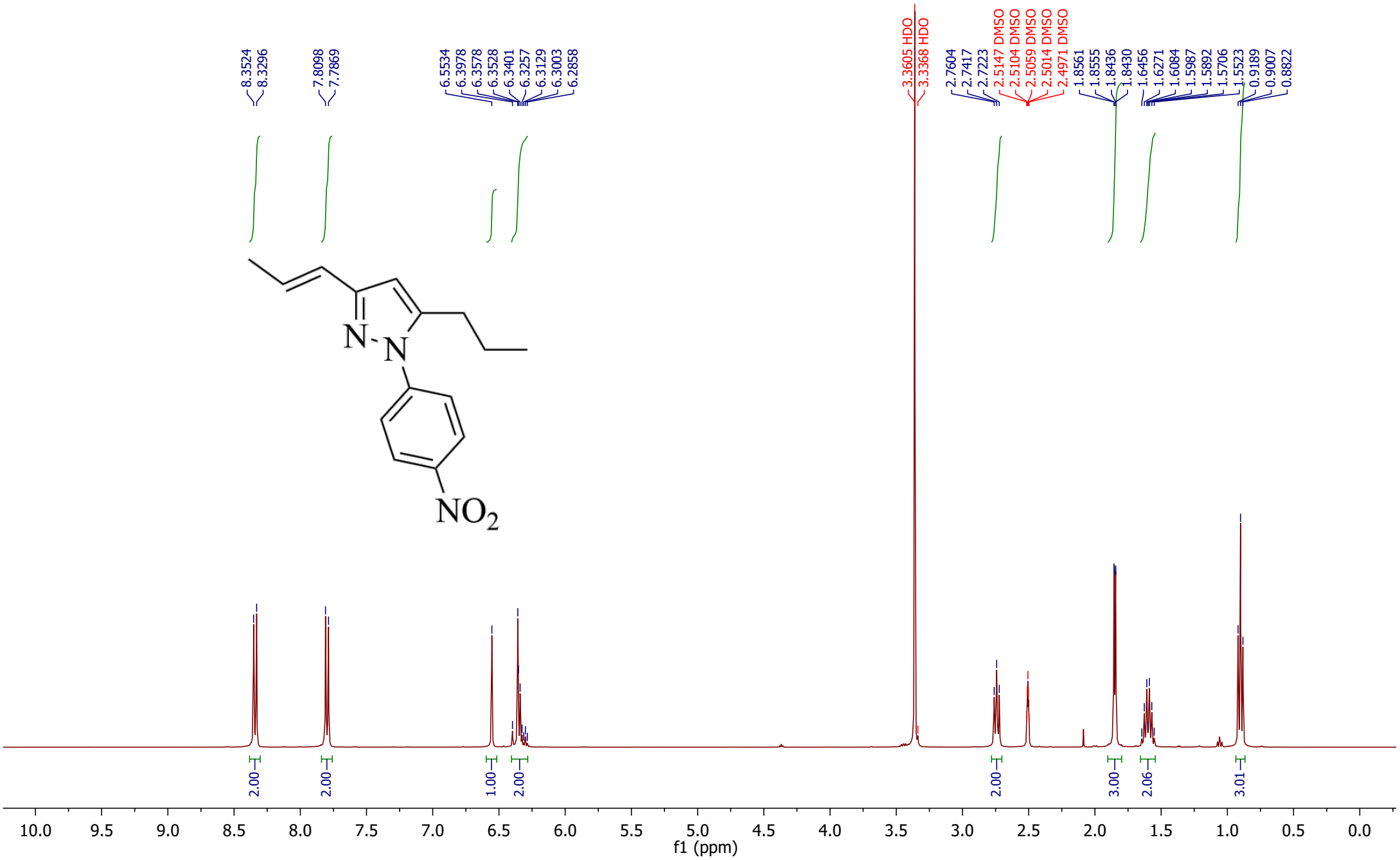
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4z



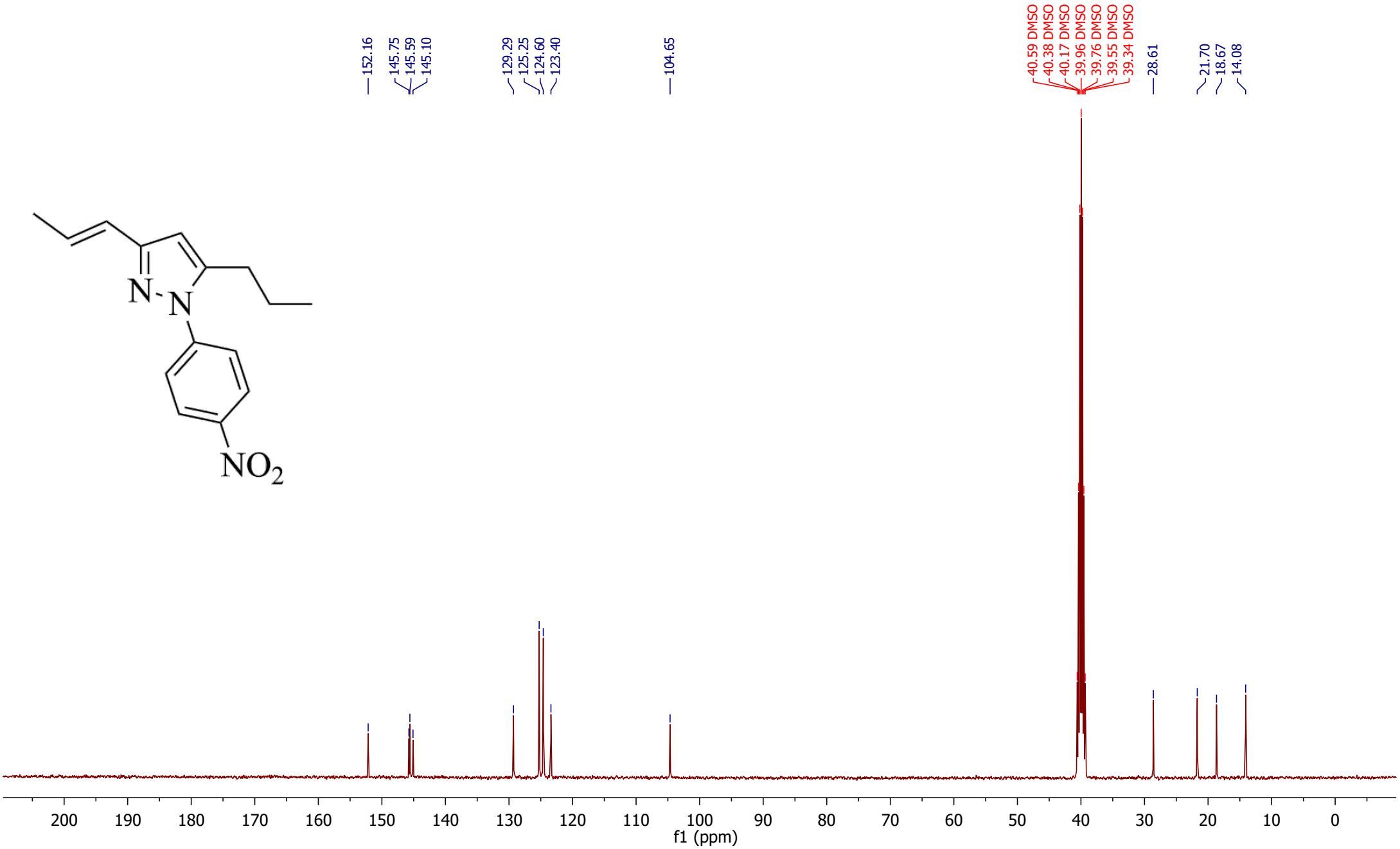
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4z



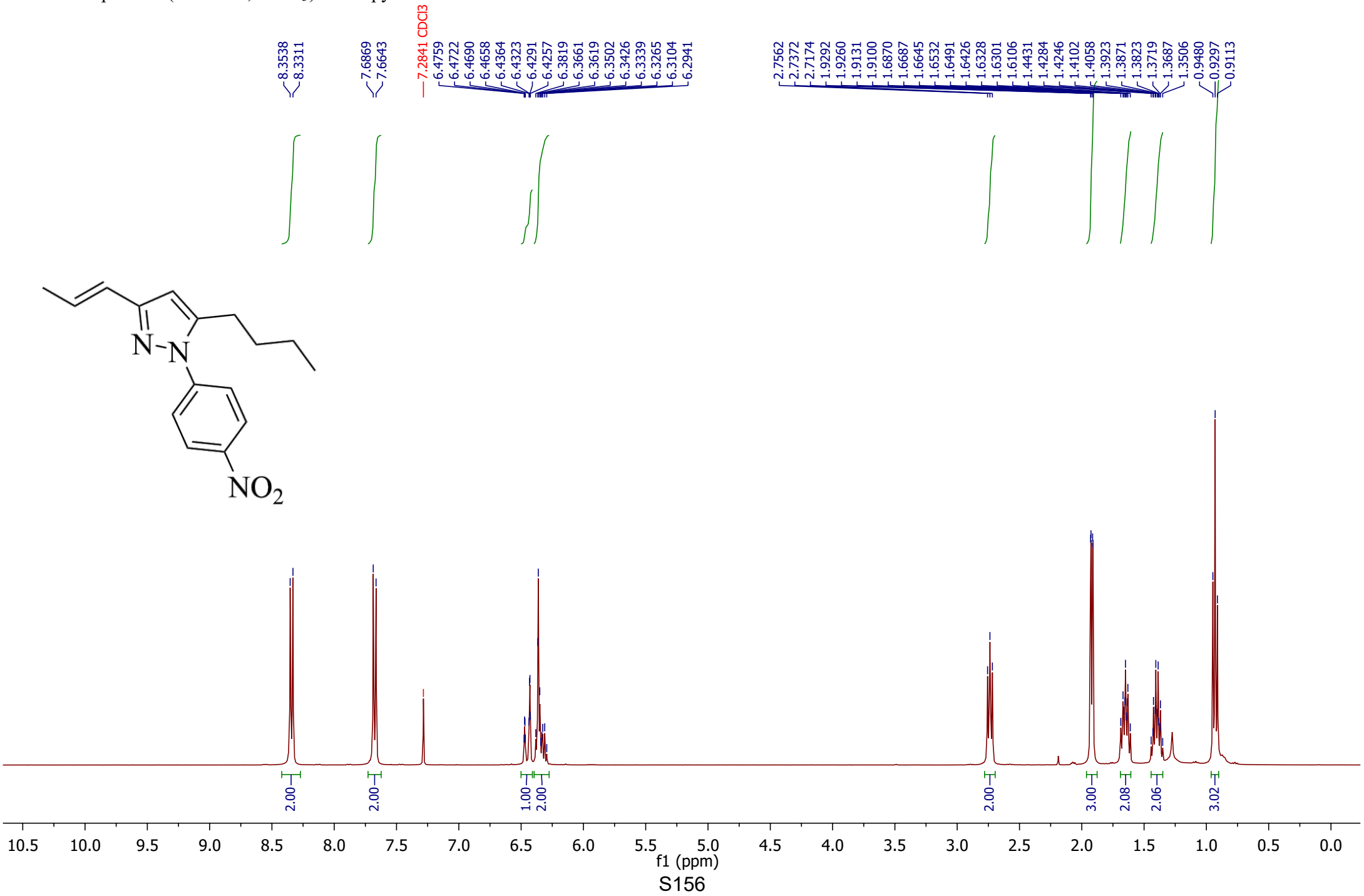
^{1}H NMR spectrum (400 MHz, DMSO-d_6) of 1*H*-pyrazole 4aa



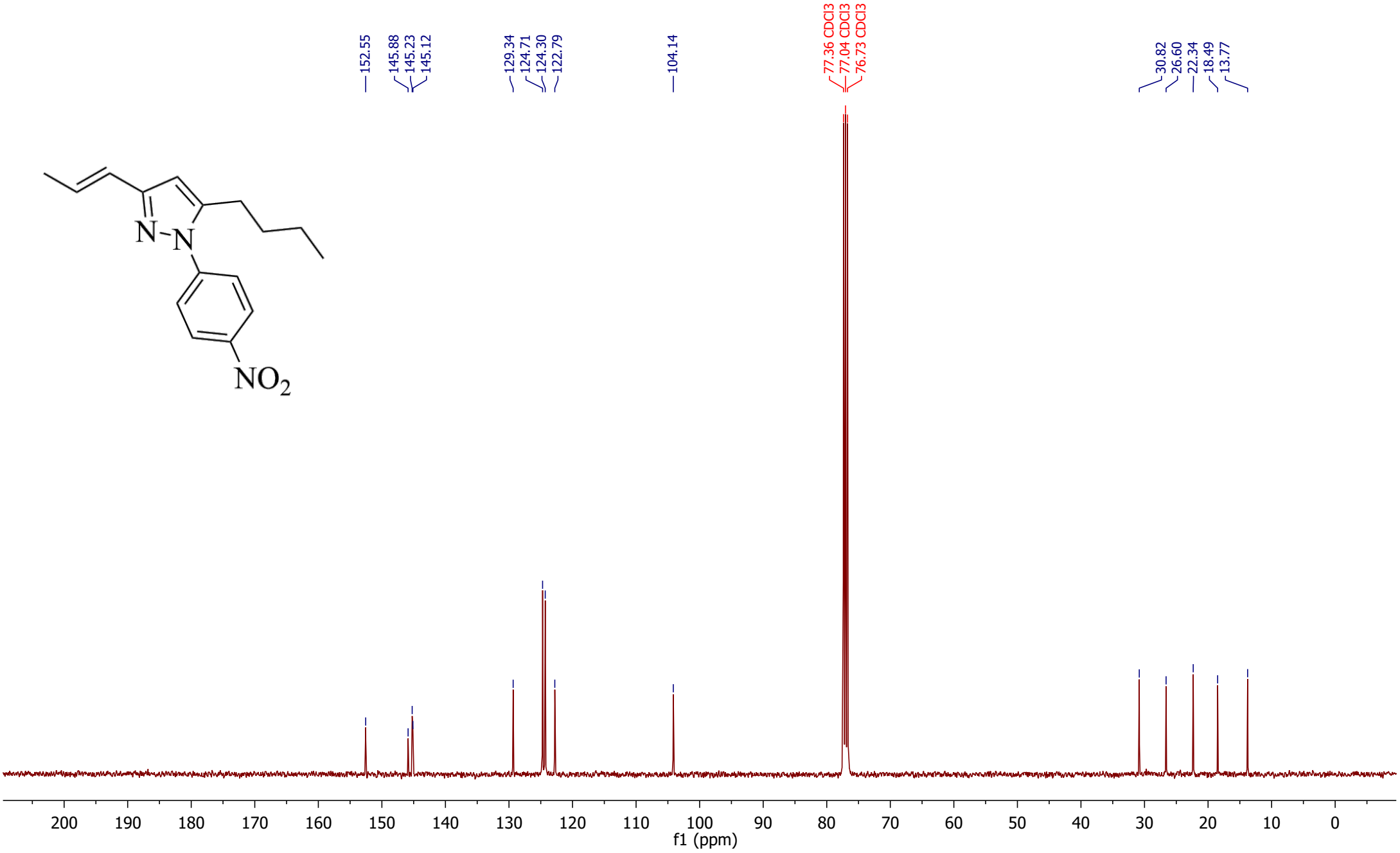
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, DMSO-d_6) of 1*H*-pyrazole 4aa



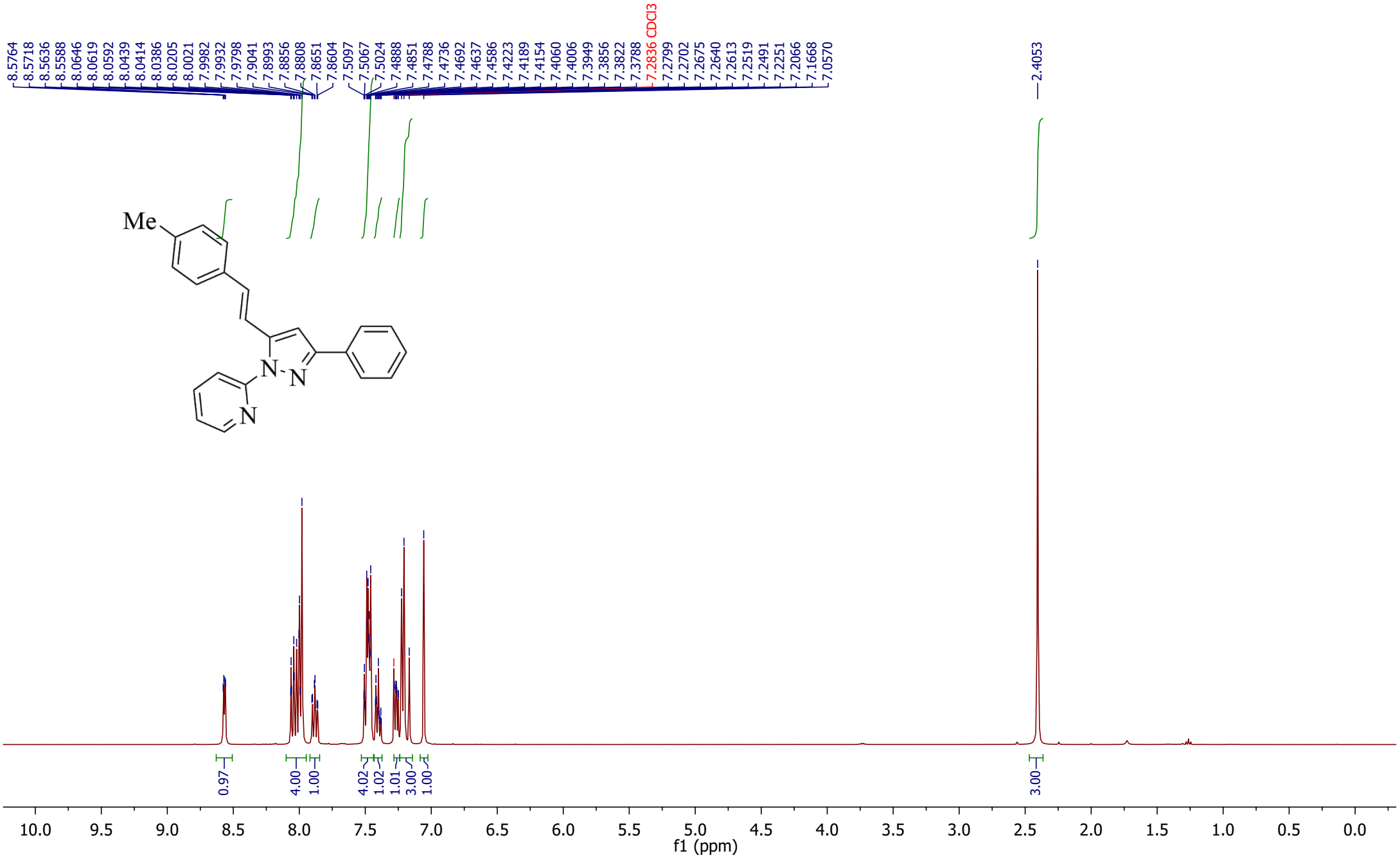
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 4ab



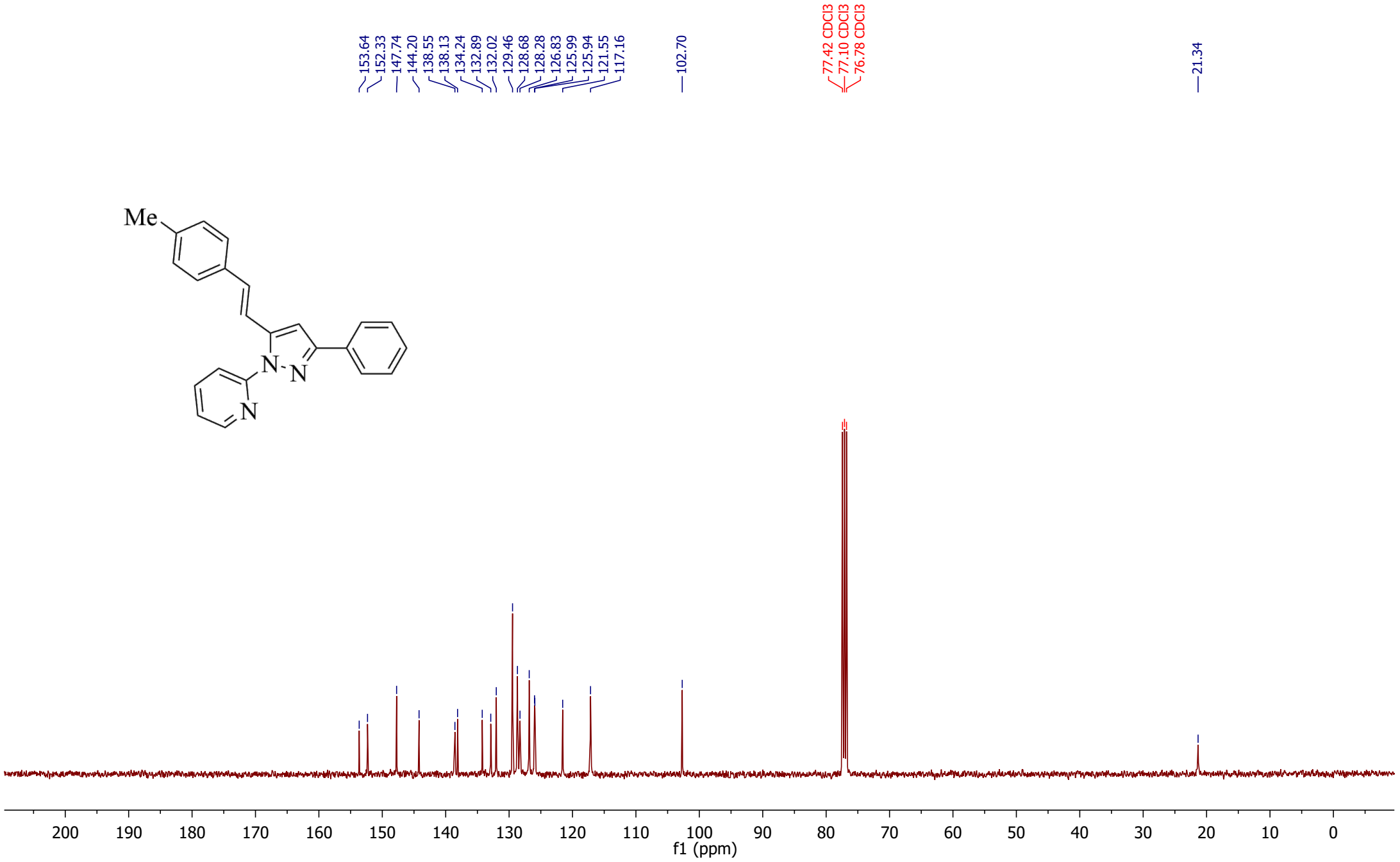
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 4ab



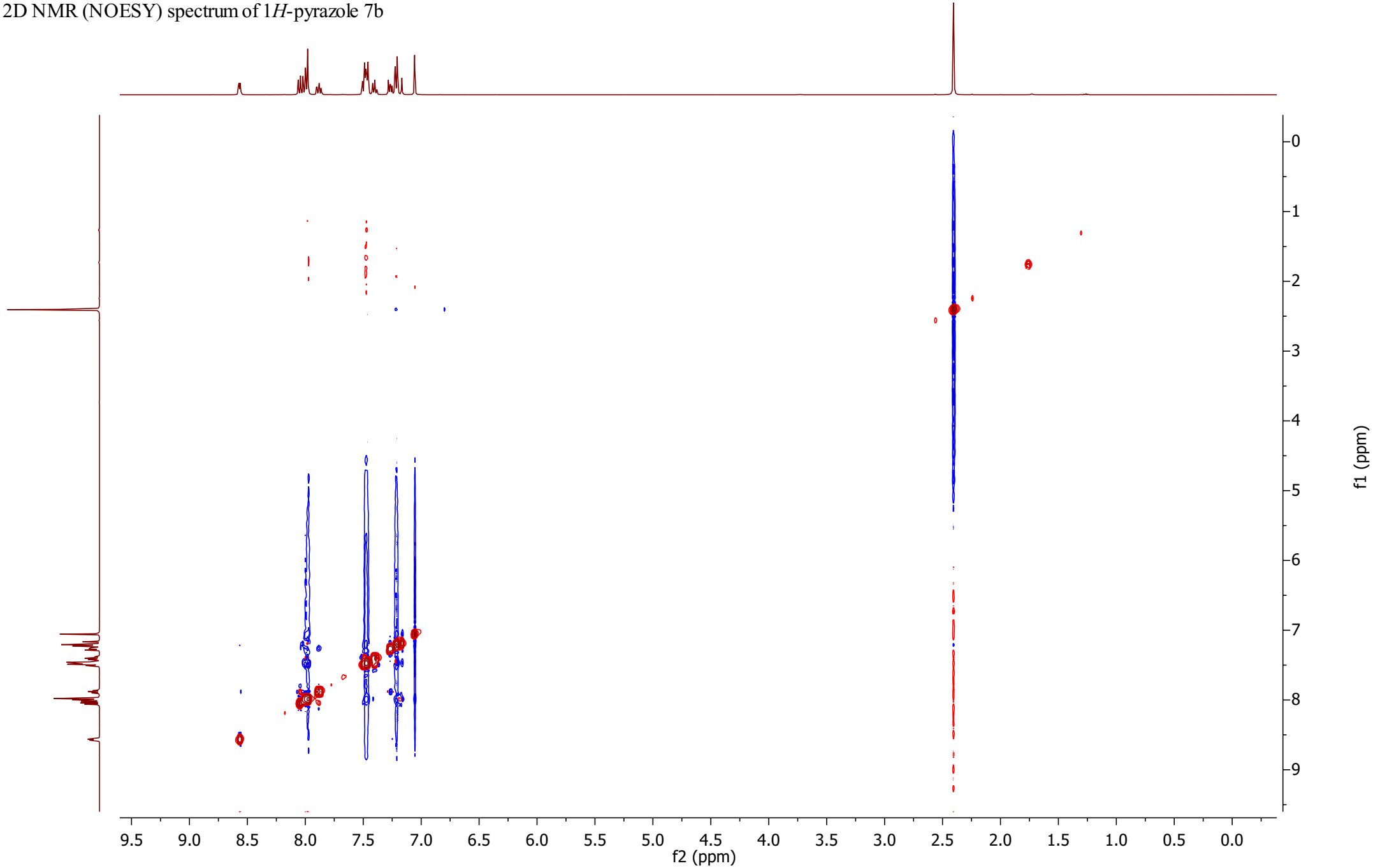
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 7b



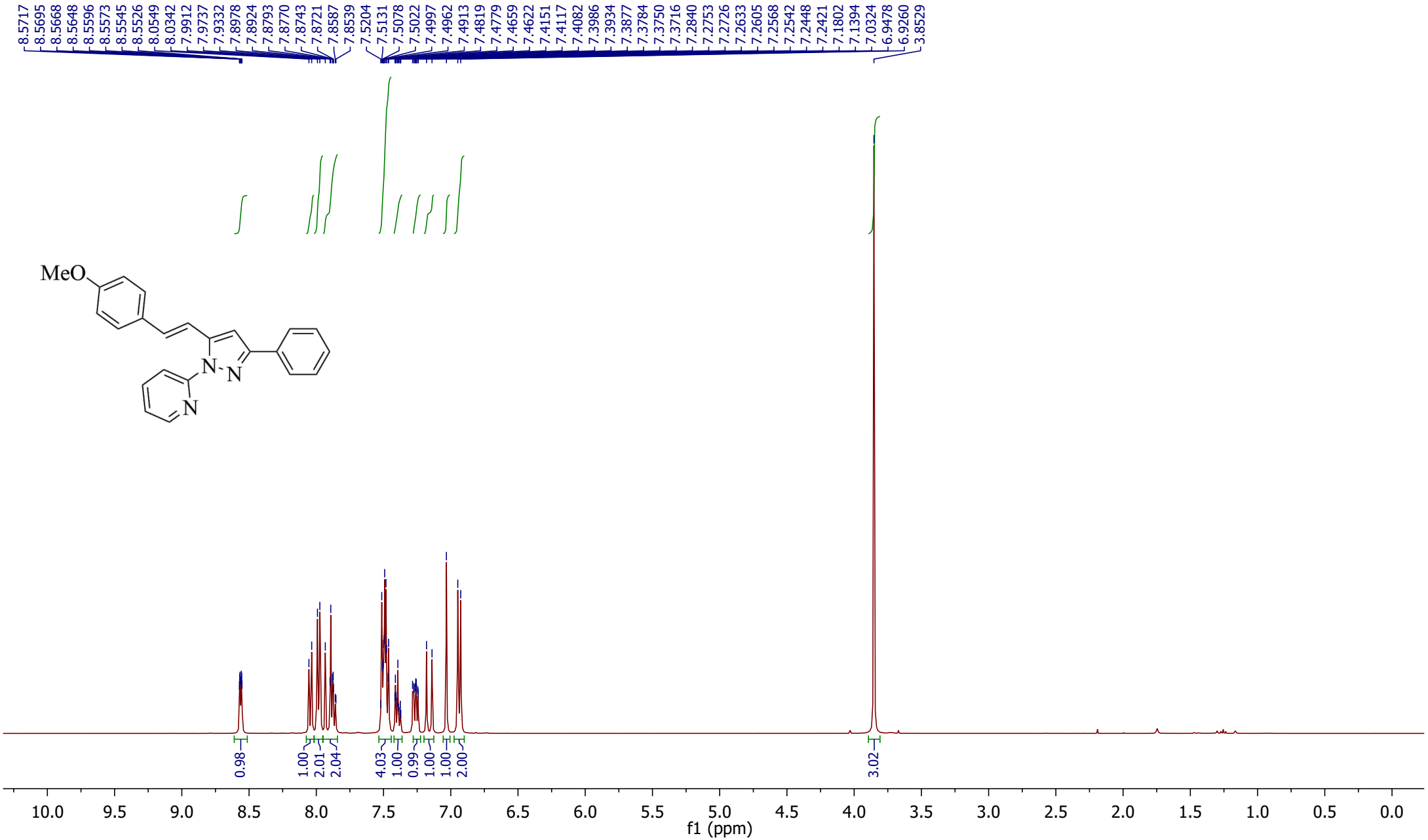
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 7b



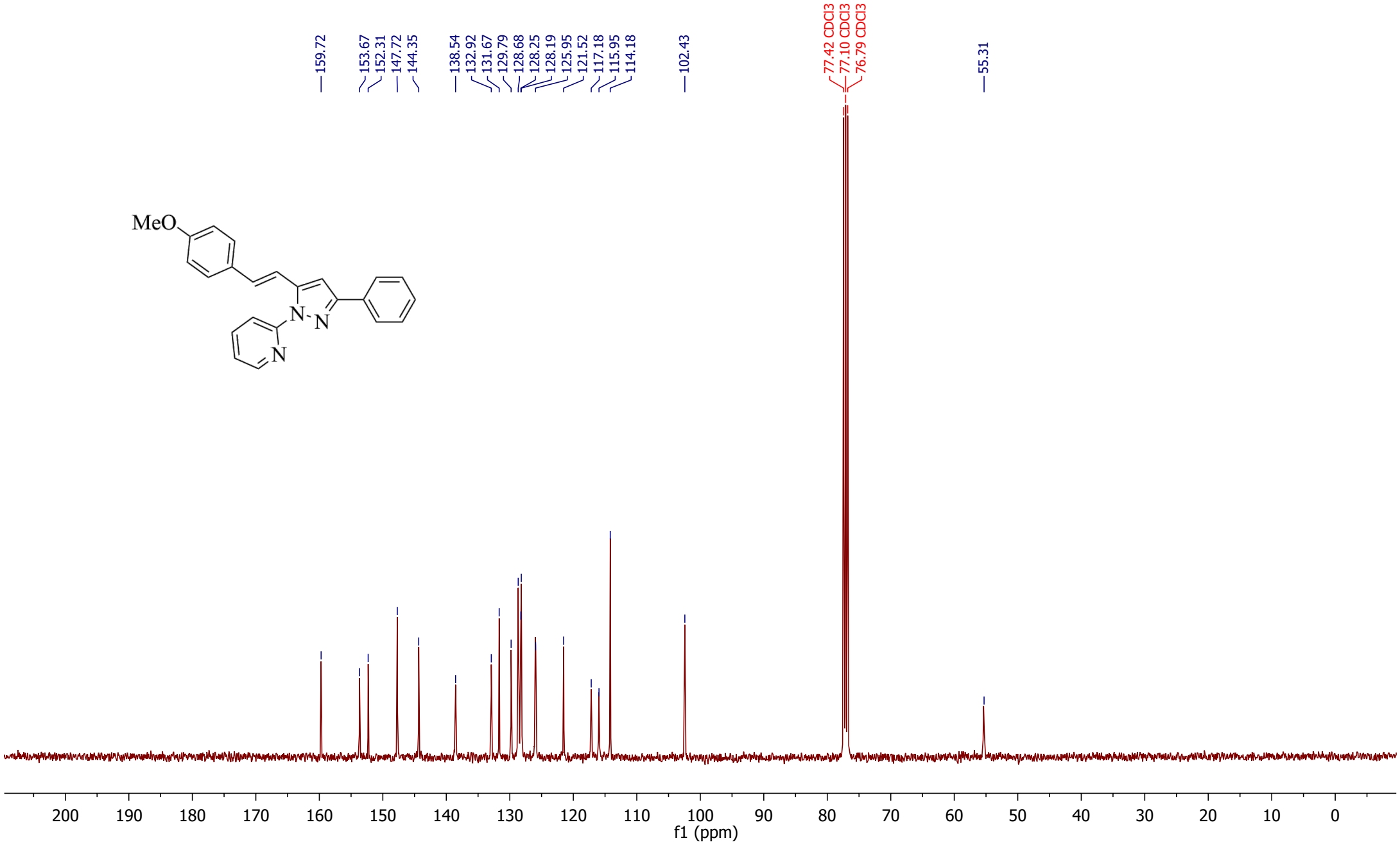
2D NMR (NOESY) spectrum of 1*H*-pyrazole 7b



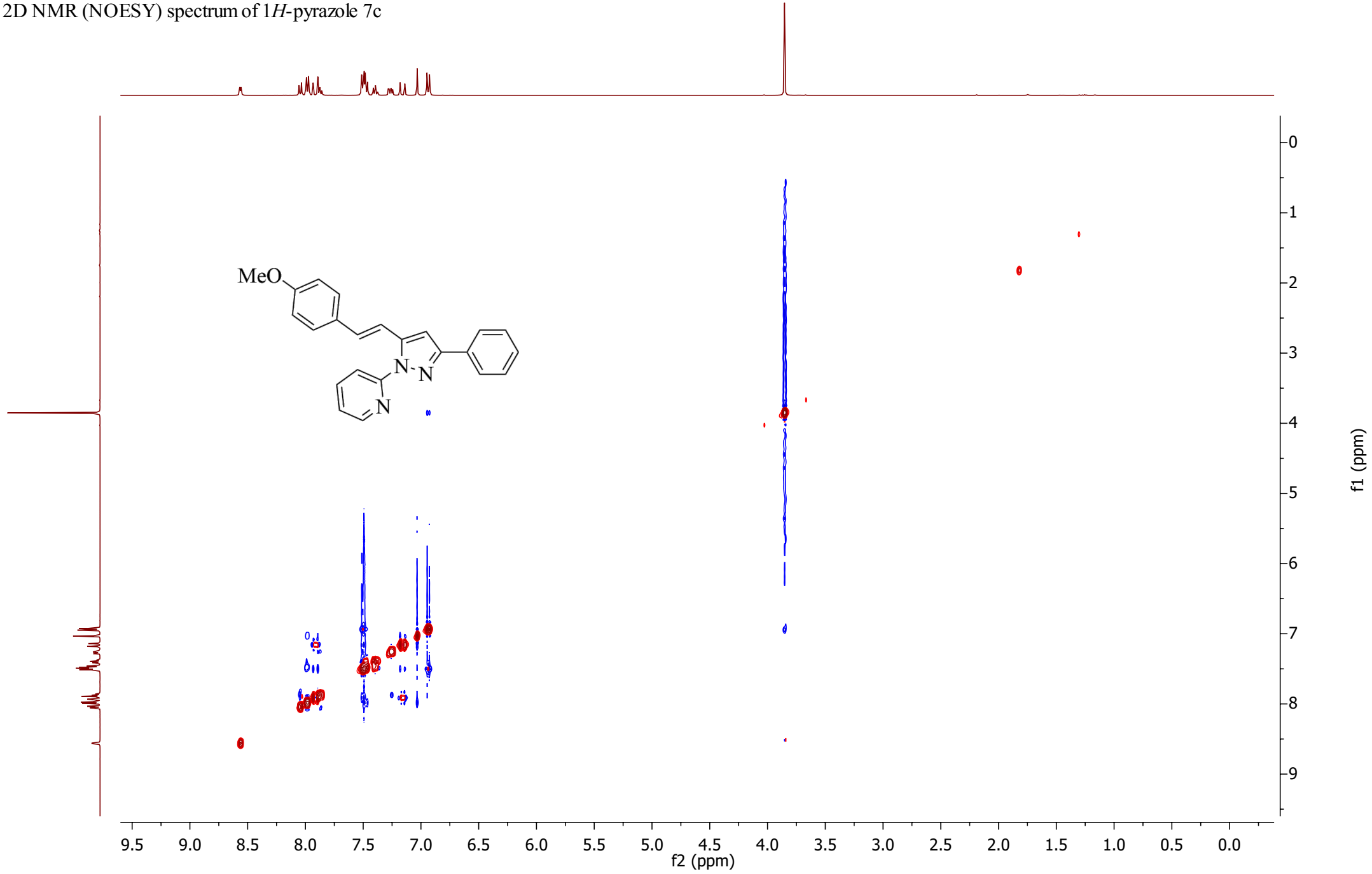
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 7c



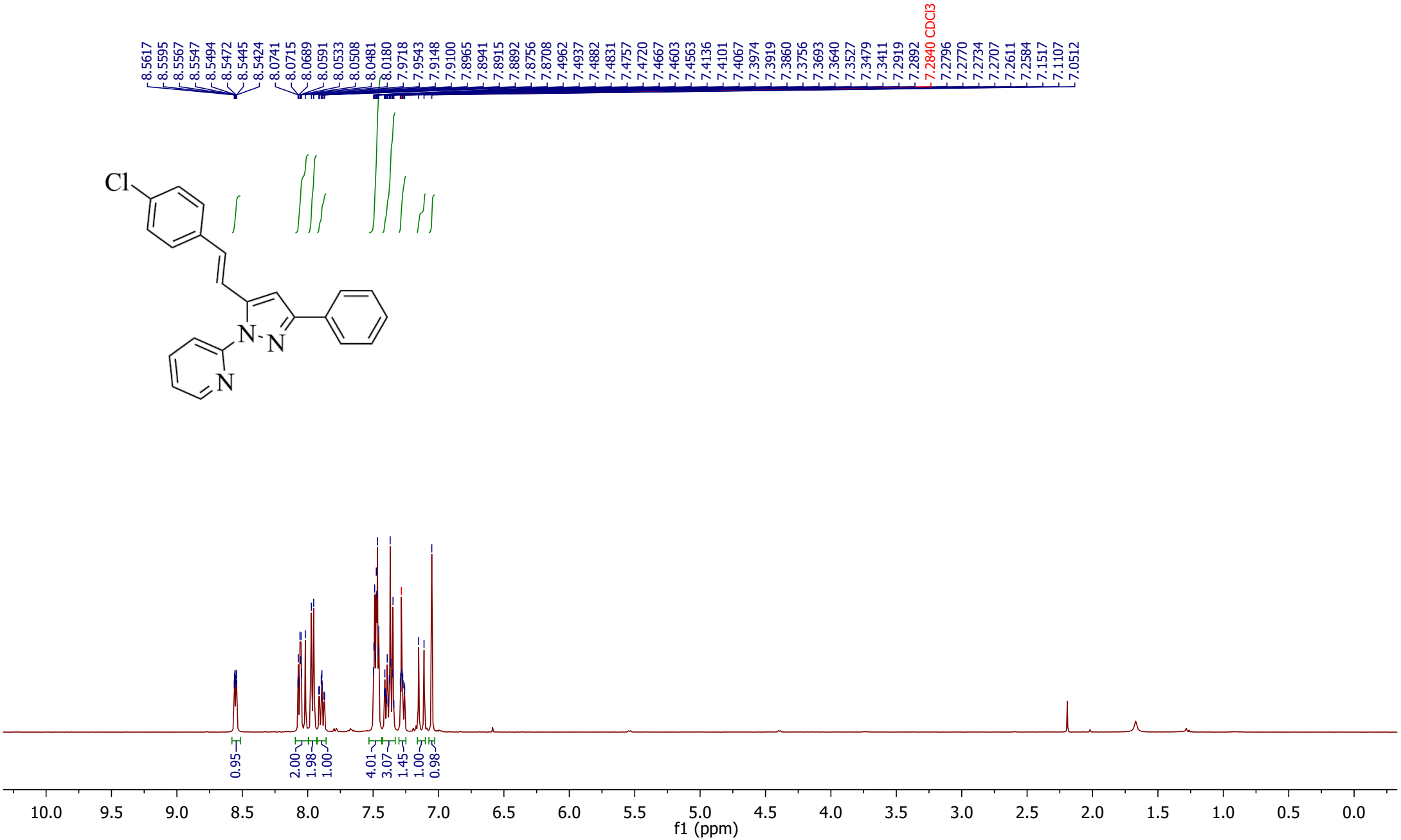
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 7c



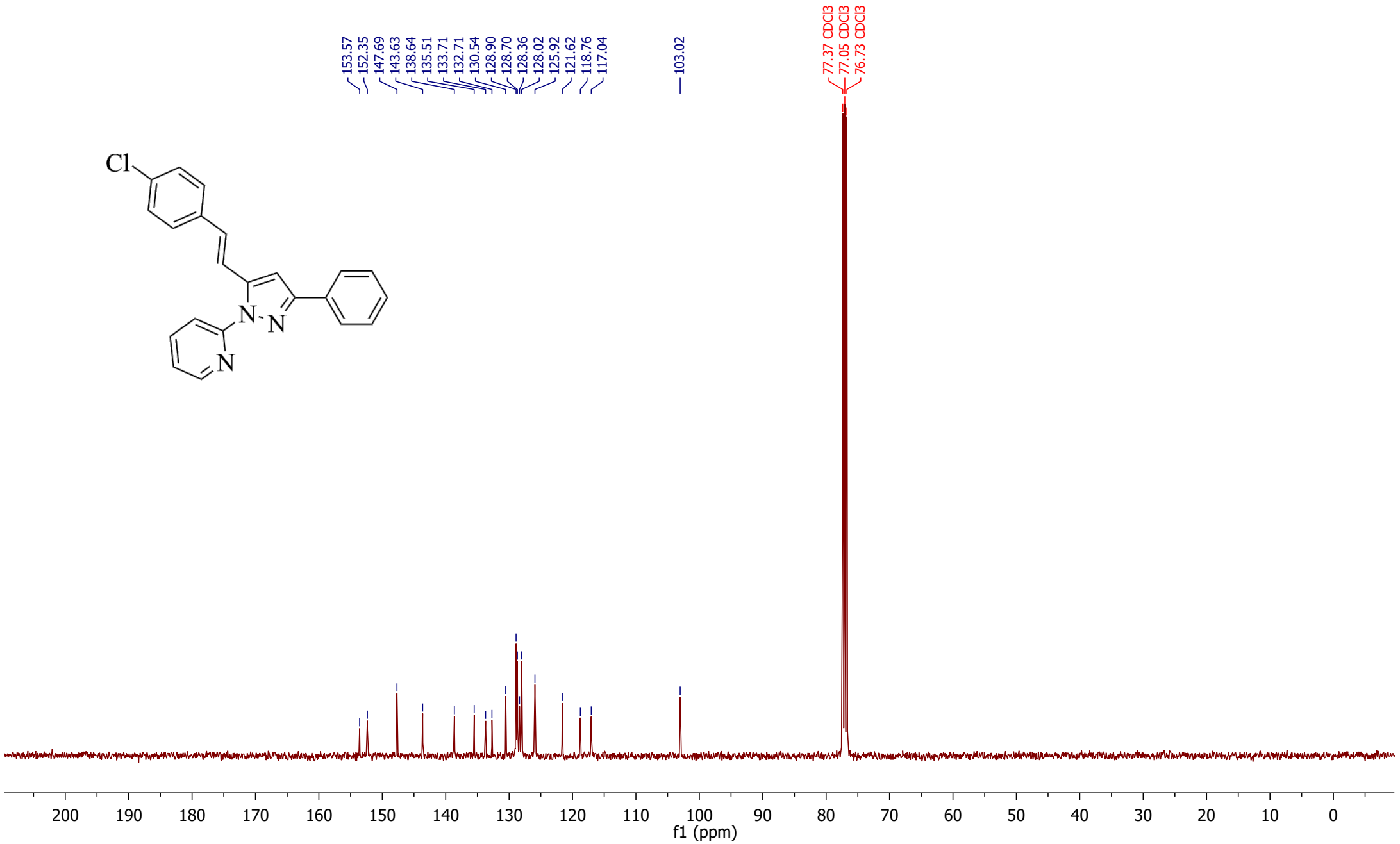
2D NMR (NOESY) spectrum of 1*H*-pyrazole 7c



^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1*H*-pyrazole 7d



$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of 1*H*-pyrazole 7d



2D NMR (NOESY) spectrum of 1*H*-pyrazole 7d

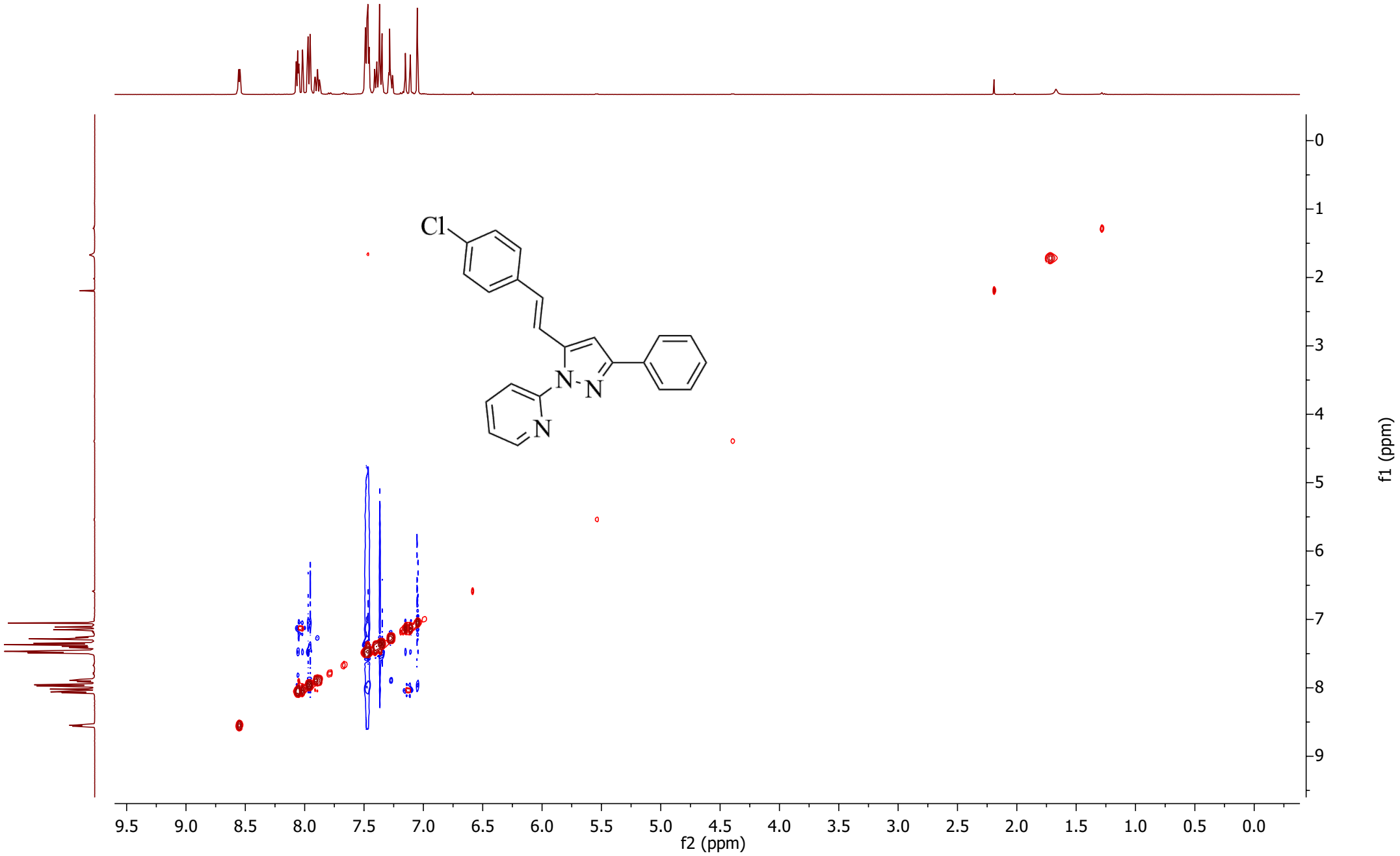
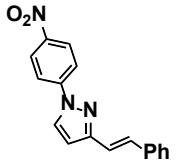
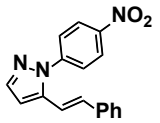


Table 1. Melting points and parameters for ^{1}H and ^{13}C NMR spectra of (*E*)-1-(4-nitrophenyl)-3-styryl-1*H*-pyrazole synthesized in present work (the substance **4u**) and in the report[1] (Miller's compound **I**), and its isomer (Miller's compound **II**) in $CDCl_3$



Miller's compound **I**
mp 184-186 °C



Miller's compound **II**
mp 138-140 °C

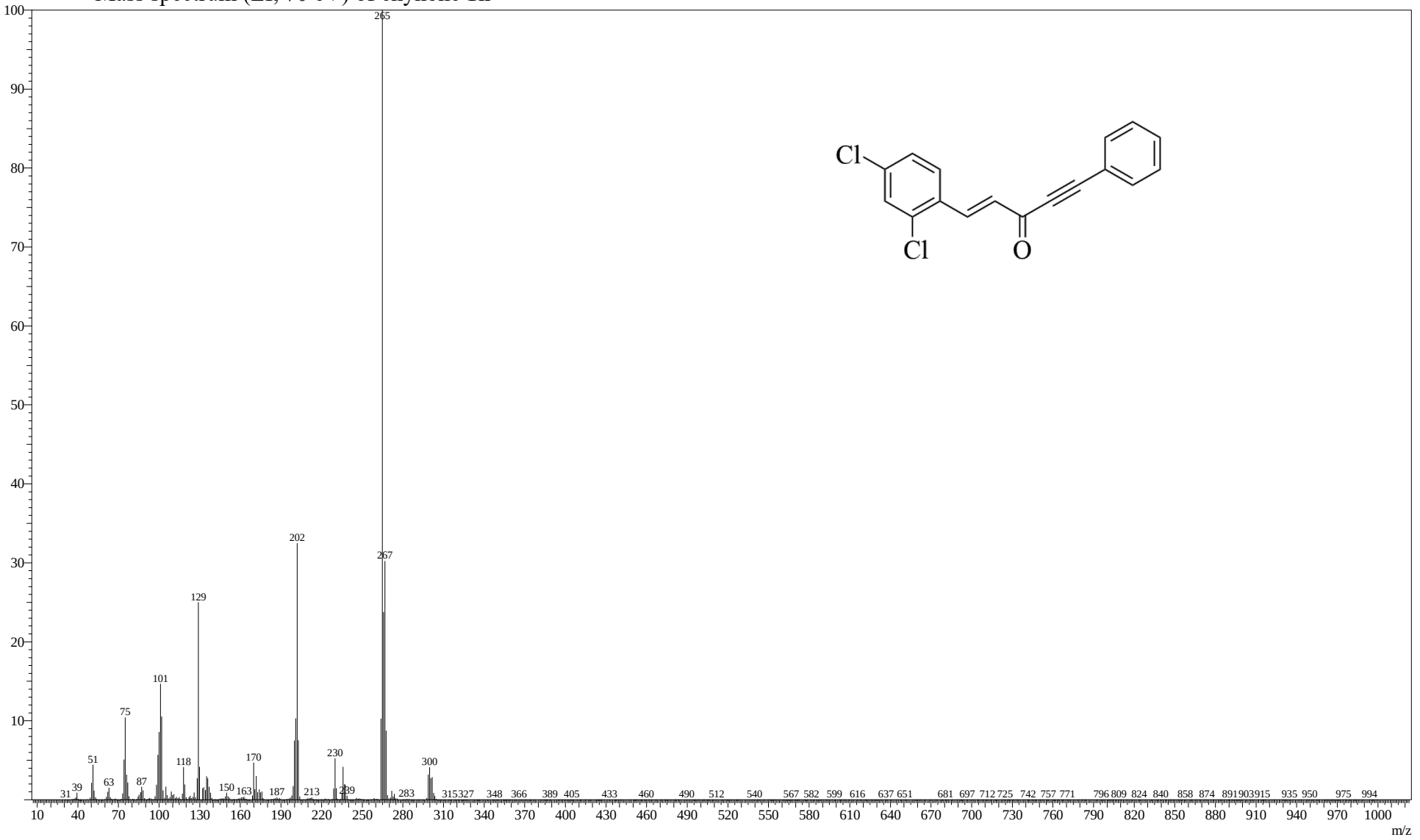
Structure	Operating frequency	^{1}H NMR, δ					
Miller's compound **I**	250 Hz	8.34 (d, *J* = 9.2 Hz, 2H)	7.99 (d, *J* = 2.8 Hz, 2H)	7.88 (d, *J* = 9.2 Hz, 2H)	7.56 (d, *J* = 8.0 Hz, 2H)	7.16–7.47 (m, 5H)	6.78 (d, *J* = 2.8 Hz, 1H)
Our substance **4u**	400 Hz	8.36 (d, *J* = 9.1 Hz, 2H)	8.03 (d, *J* = 2.6 Hz, 1H)	7.91 (d, *J* = 9.1 Hz, 2H)	7.57 (d, J = 7.4 Hz, 2H)	7.43–7.39 (m, 2H) 7.35–7.31 (m, 1H) 7.28–7.19 (m, 2H)	6.78 (d, *J* = 2.6 Hz, 1H)
Miller's compound **II**	250 Hz	8.40 (d, *J* = 9.2 Hz, 2H)	7.65–8.77 (m, 3H)	7.29–7.51 (m, 3H)	7.18 (d, *J* = 16.2 Hz, 1H)	6.92 (d, *J* = 16.2 Hz, 1H)	6.71 (d, *J* = 1.8 Hz, 1H)

Structure	Operating frequency	^{13}C {^{1}H} NMR, δ												
Miller's compound **I**	62.9 Hz	153.7	144.9	143.7	136.6	132.3	128.6	128.0	127.8	126.5	125.2	119.4	117.9	106.6
Our substance **4u**	100 Hz	153.9	145.2	144.2	136.6	132.5	128.8	128.3	128.1	126.7	125.5	119.6	118.1	106.9
Miller's compound **II**	62.9 Hz	146.3	144.5	141.7	141.6	135.8	133.5	128.8	128.7	126.7	124.9	124.8	114.7	105.9

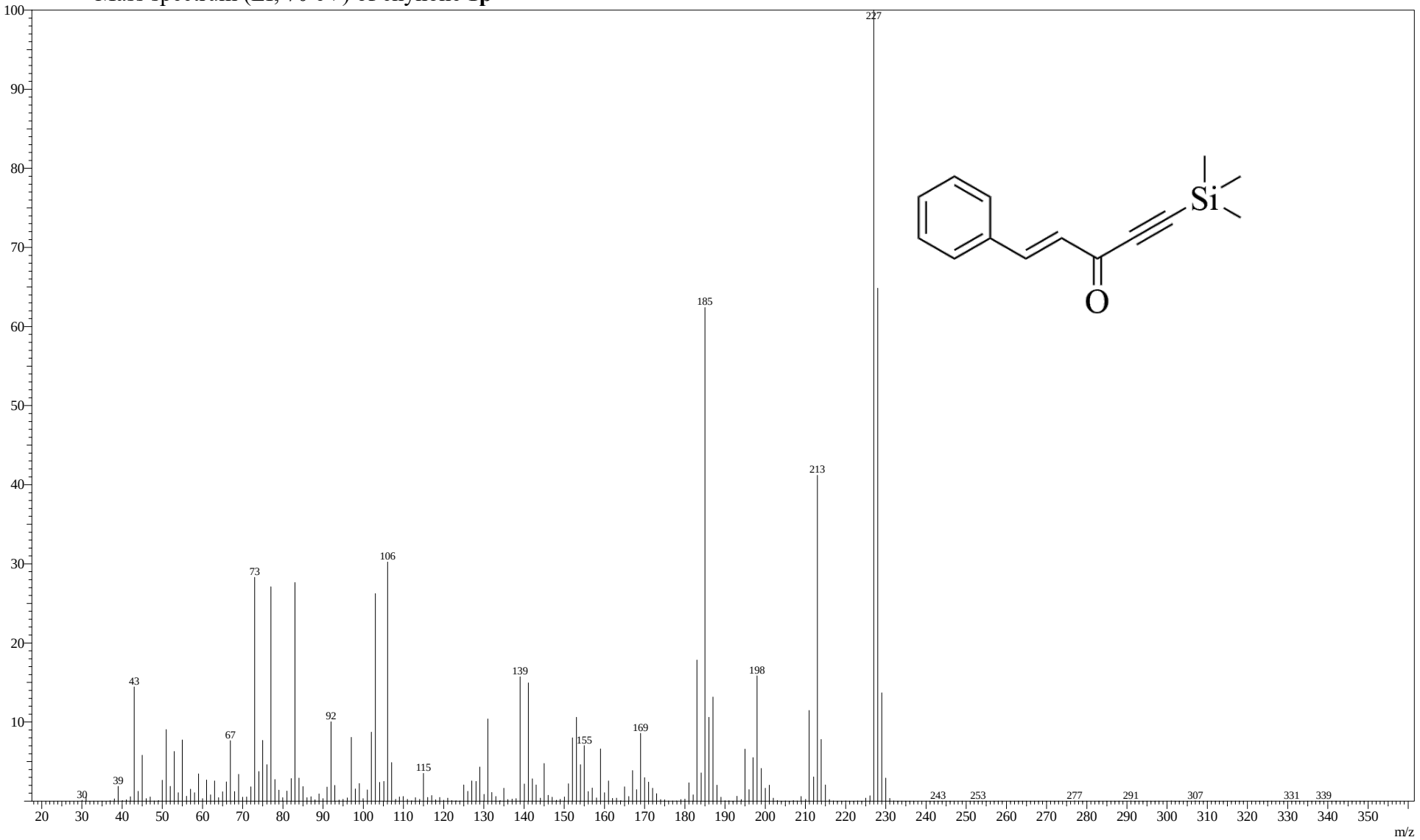
References

1. Miller, R. D.; Reiser, O. The Synthesis of Electron Donor-Acceptor Substituted Pyrazoles. *J. Heterocycl. Chem.* **1993**, *30*, 755–763.

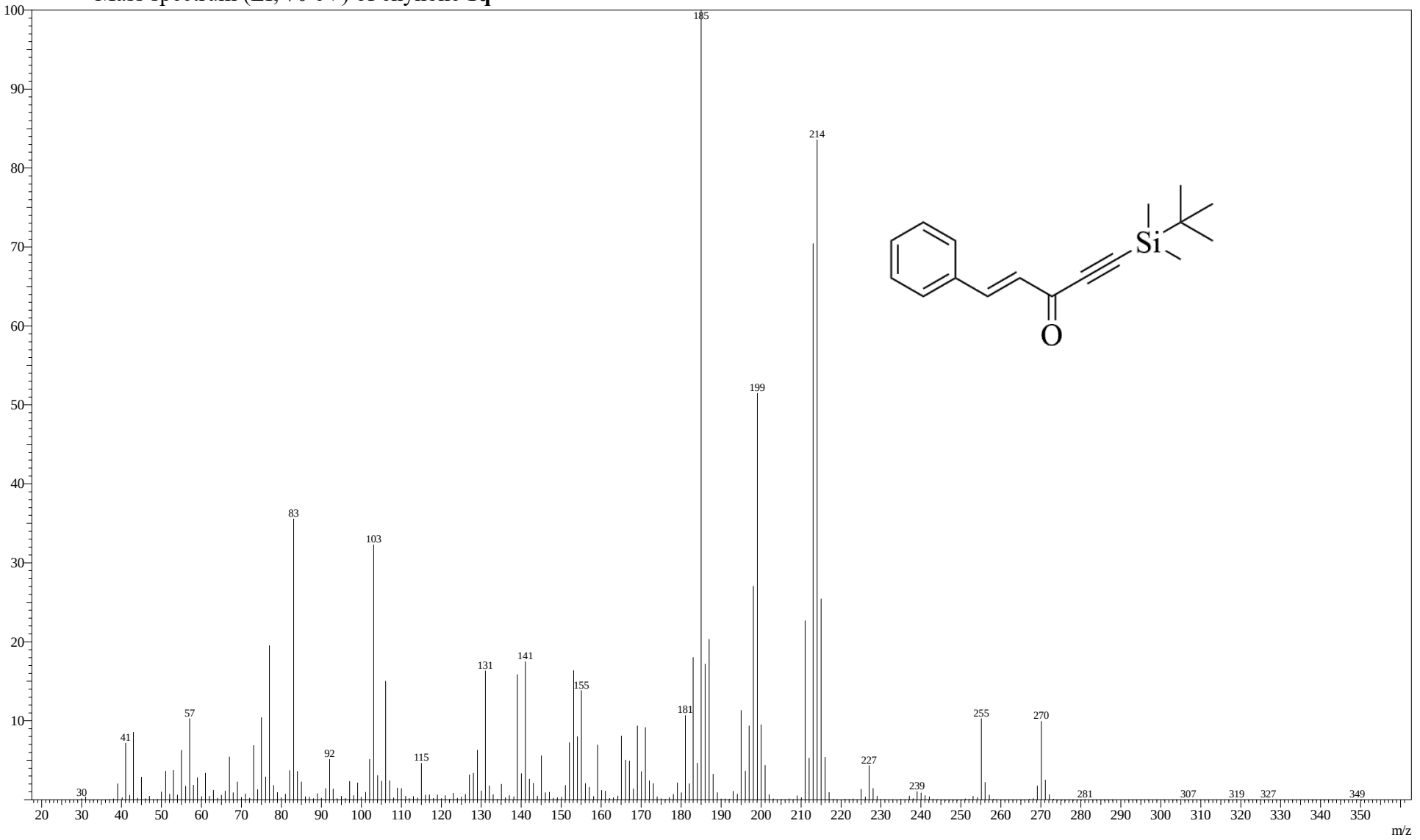
Mass spectrum (EI, 70 eV) of enynone **1h**



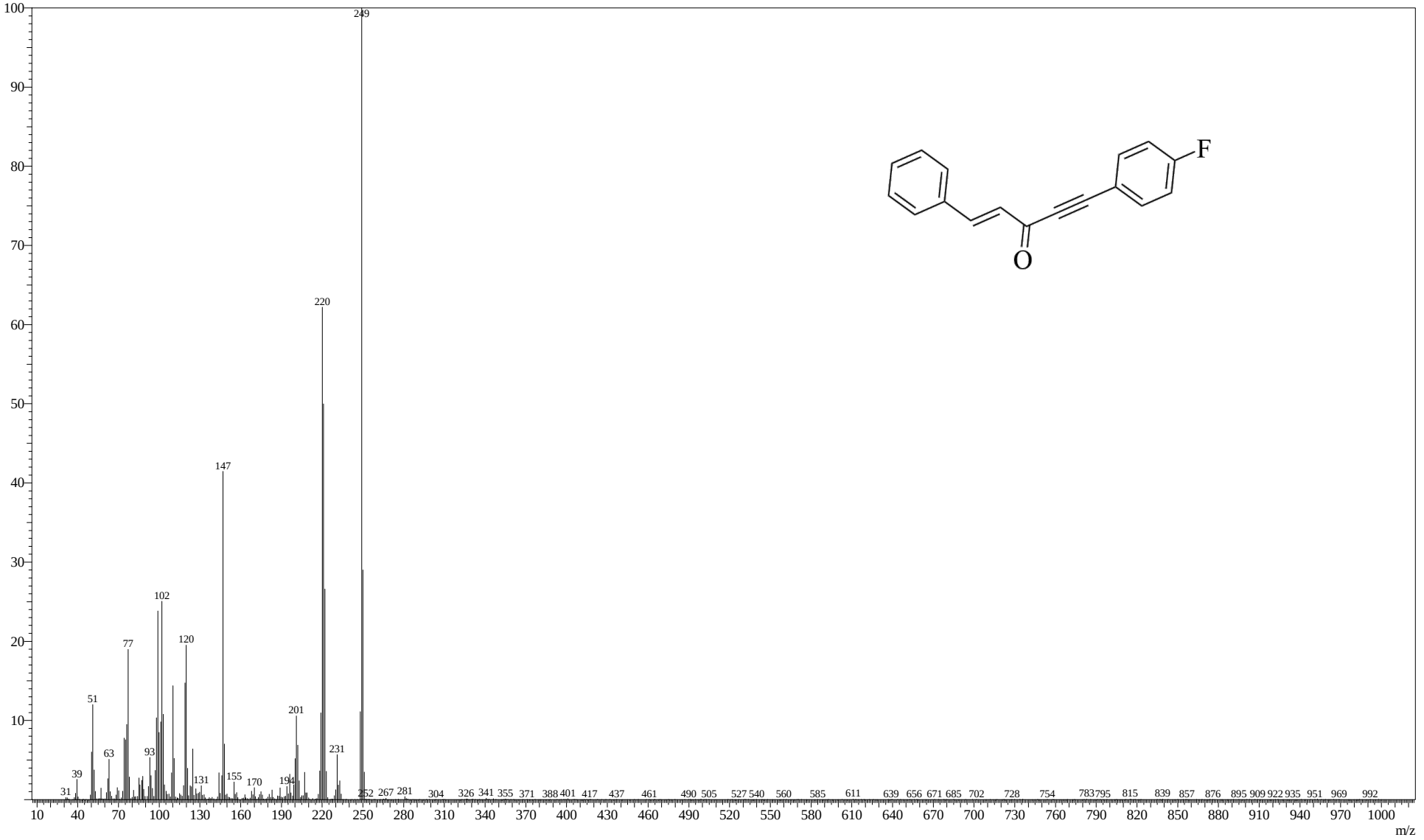
Mass spectrum (EI, 70 eV) of enynone **1p**



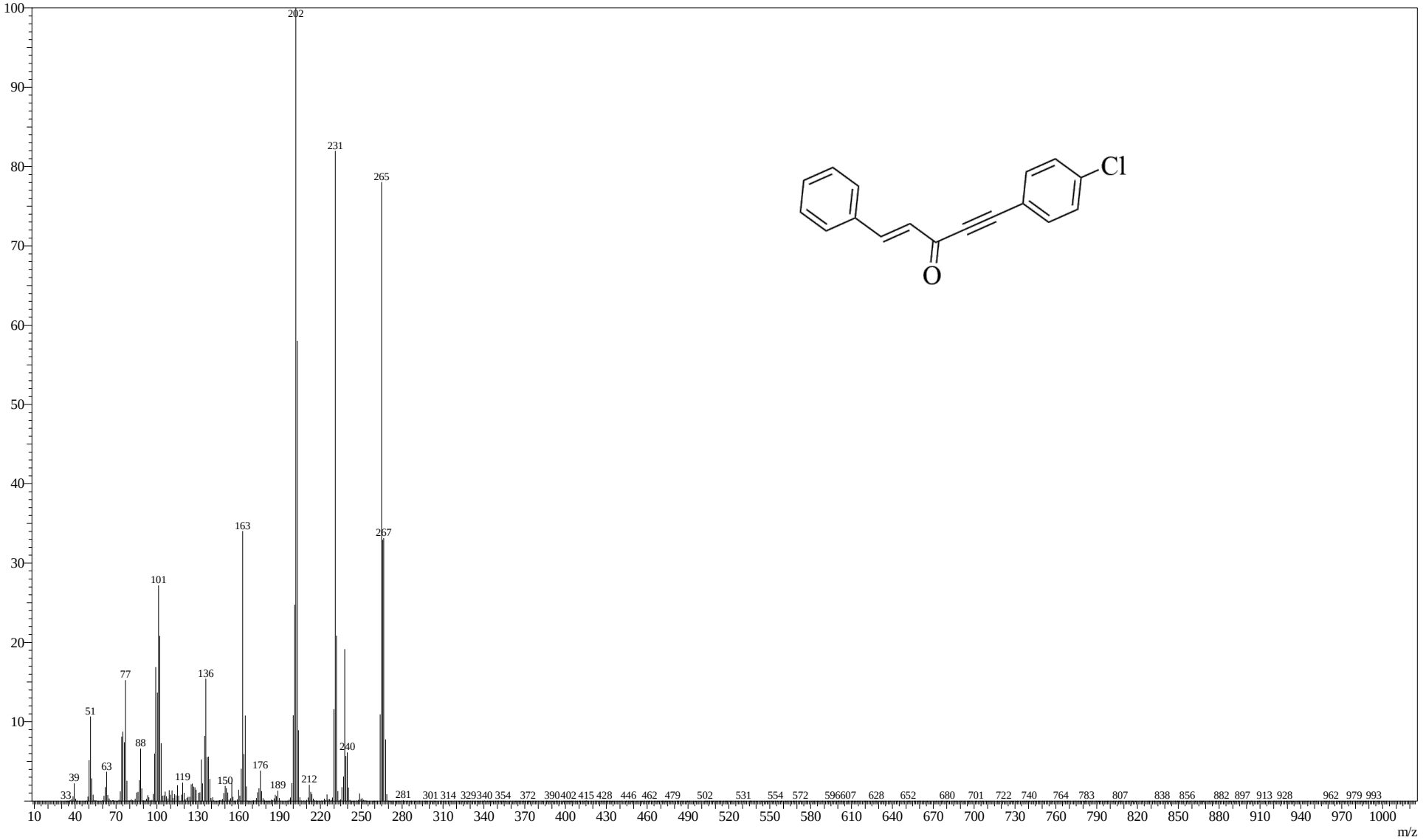
Mass spectrum (EI, 70 eV) of enynone **1q**



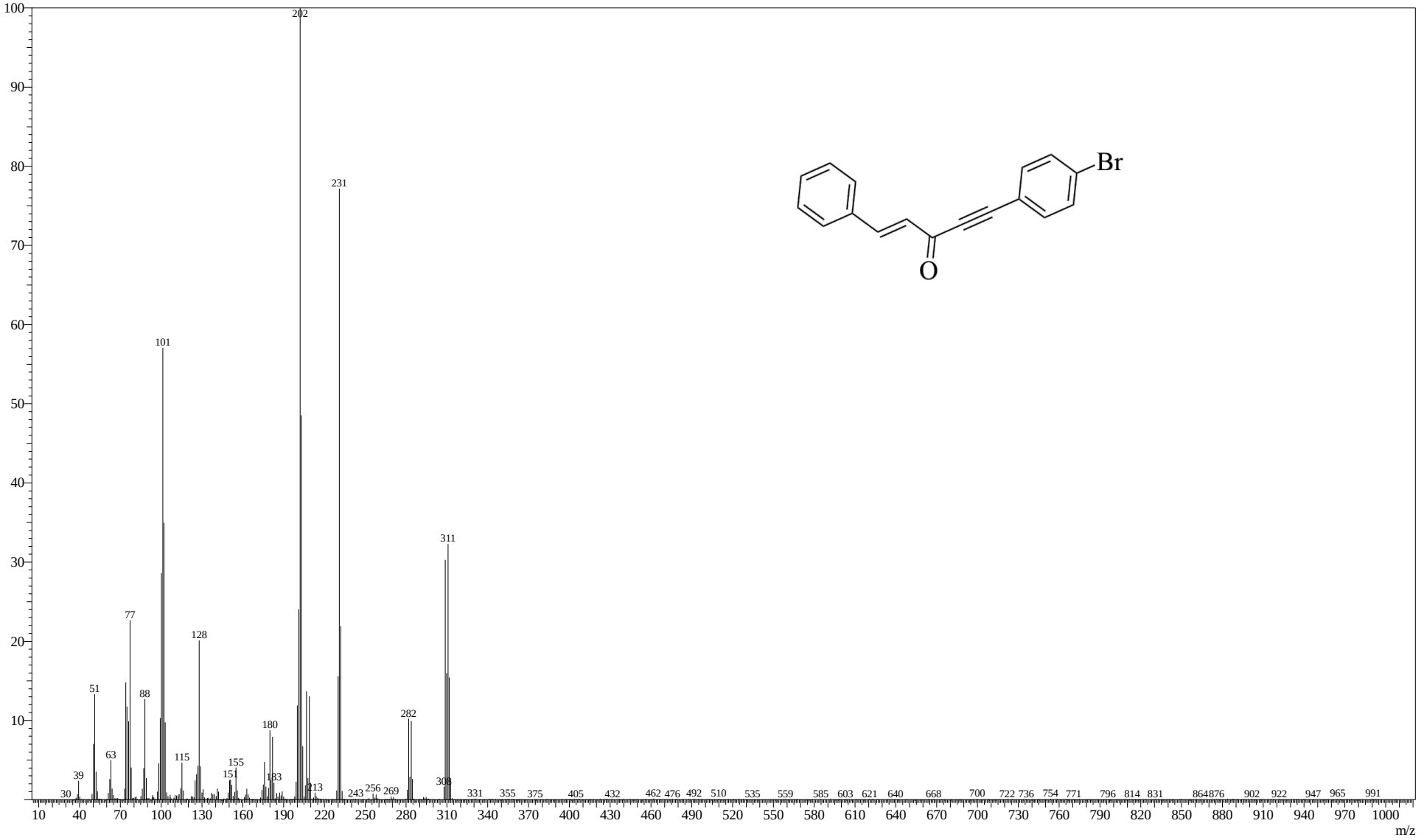
Mass spectrum (EI, 70 eV) of enynone **1t**



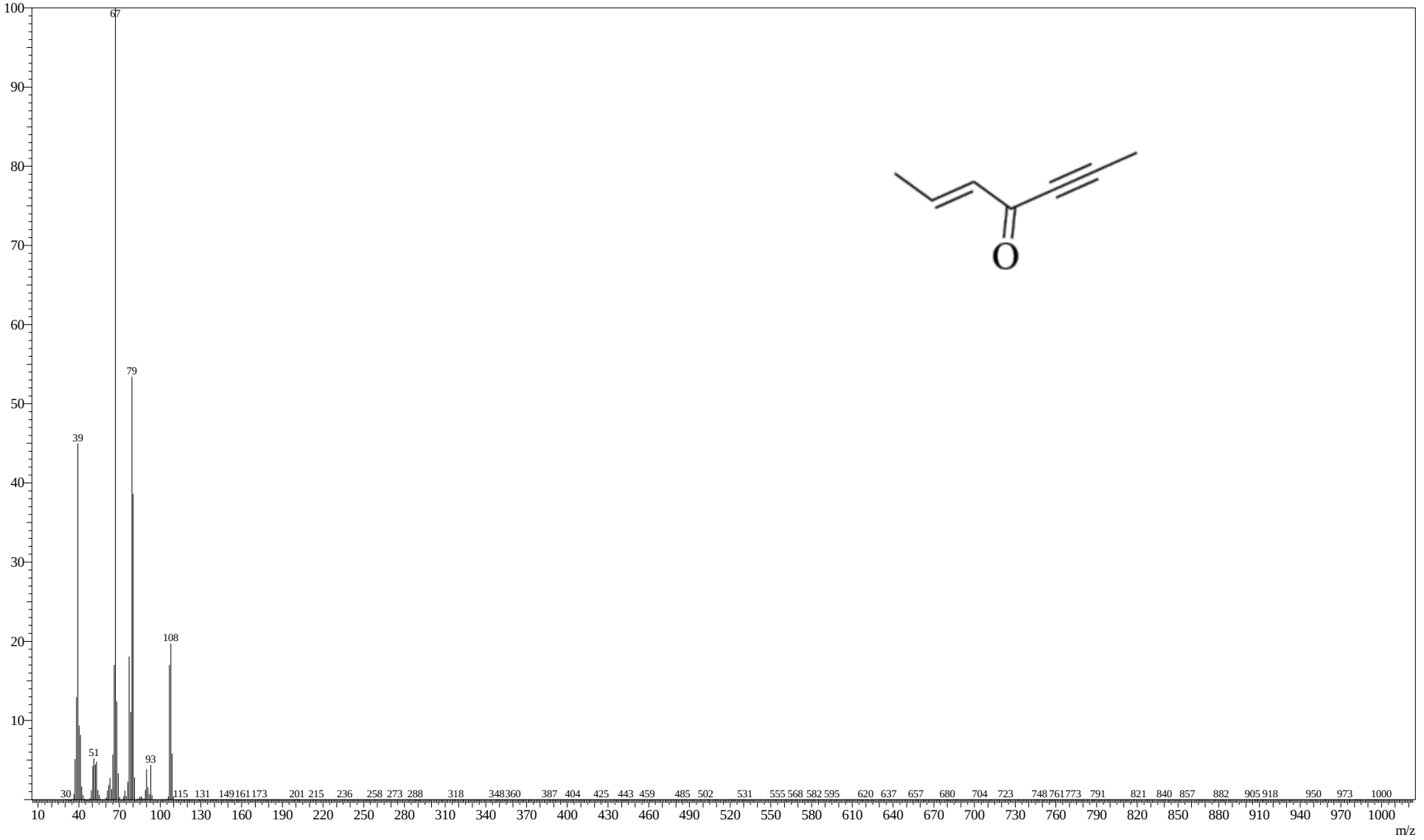
Mass spectrum (EI, 70 eV) of enynone **1u**



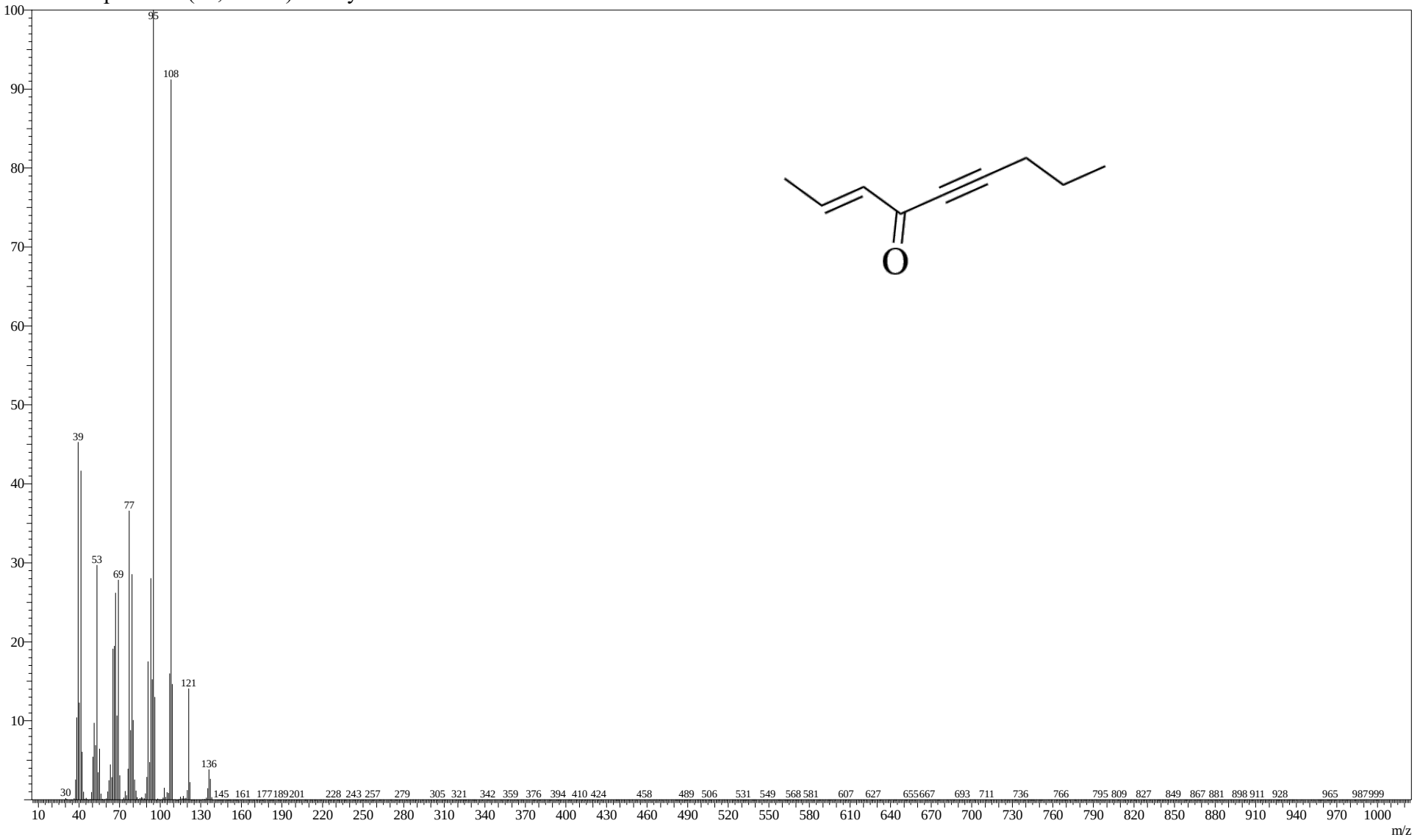
Mass spectrum (EI, 70 eV) of enynone **1v**



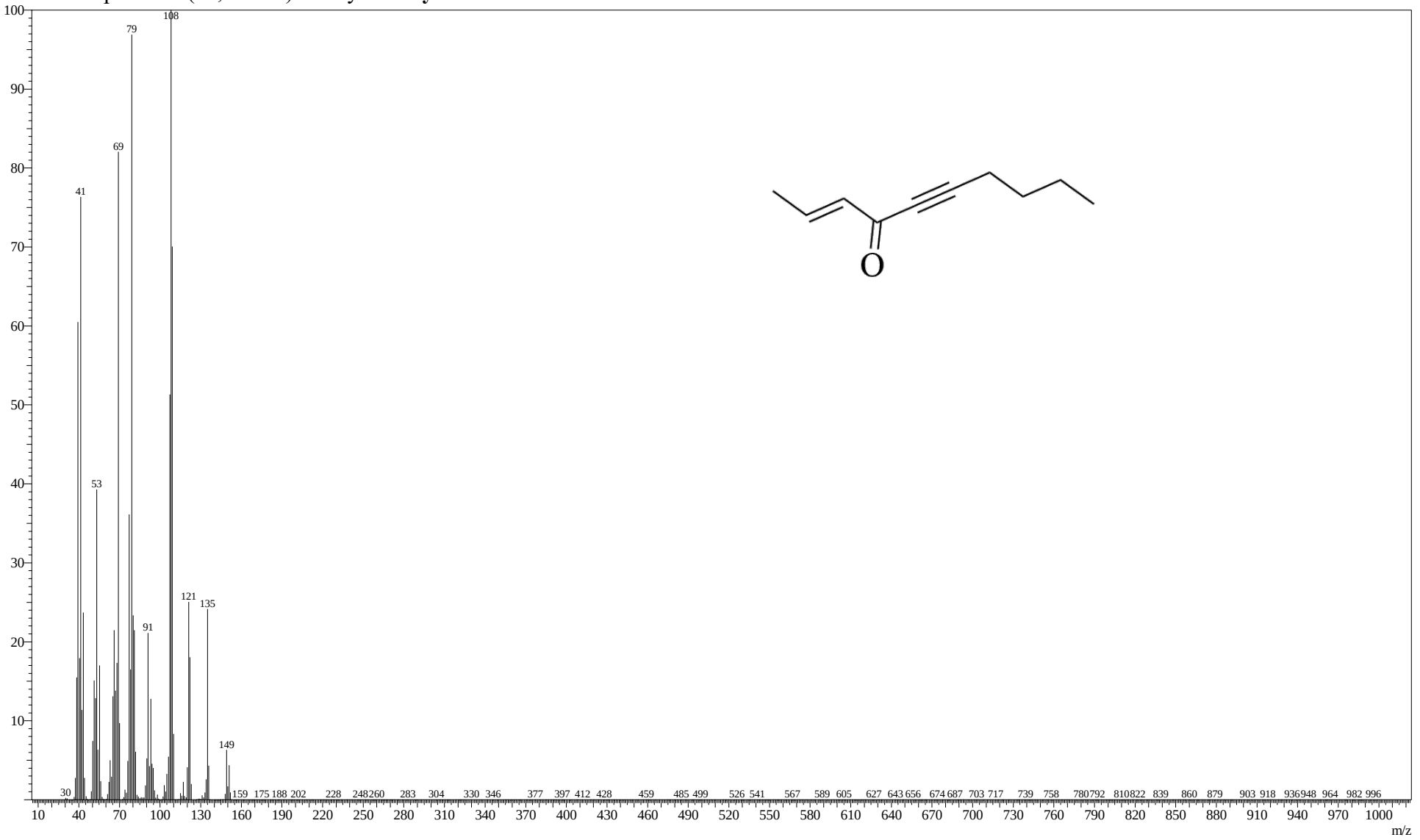
Mass spectrum (EI, 70 eV) of enynone **1w**



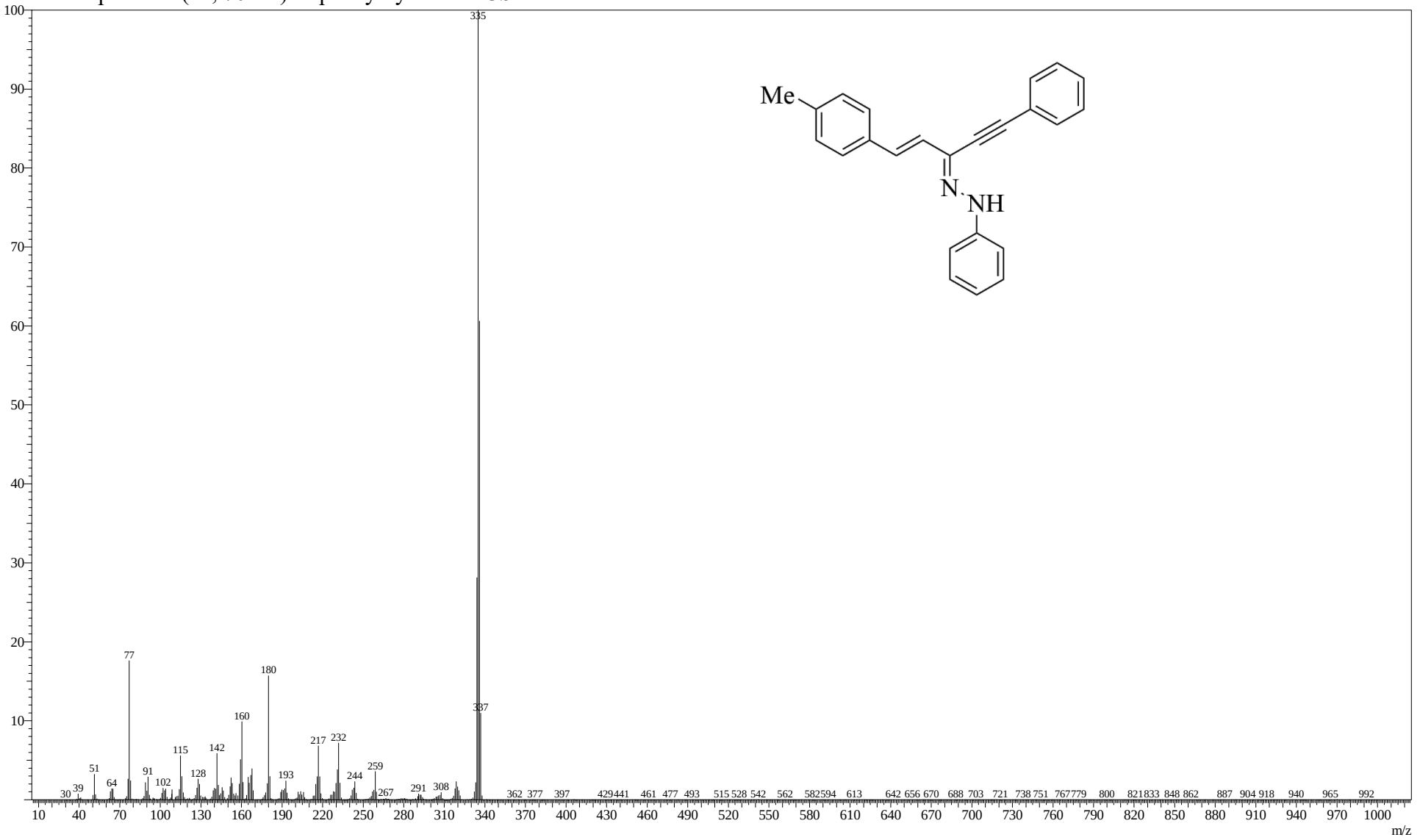
Mass spectrum (EI, 70 eV) of enynone **1x**



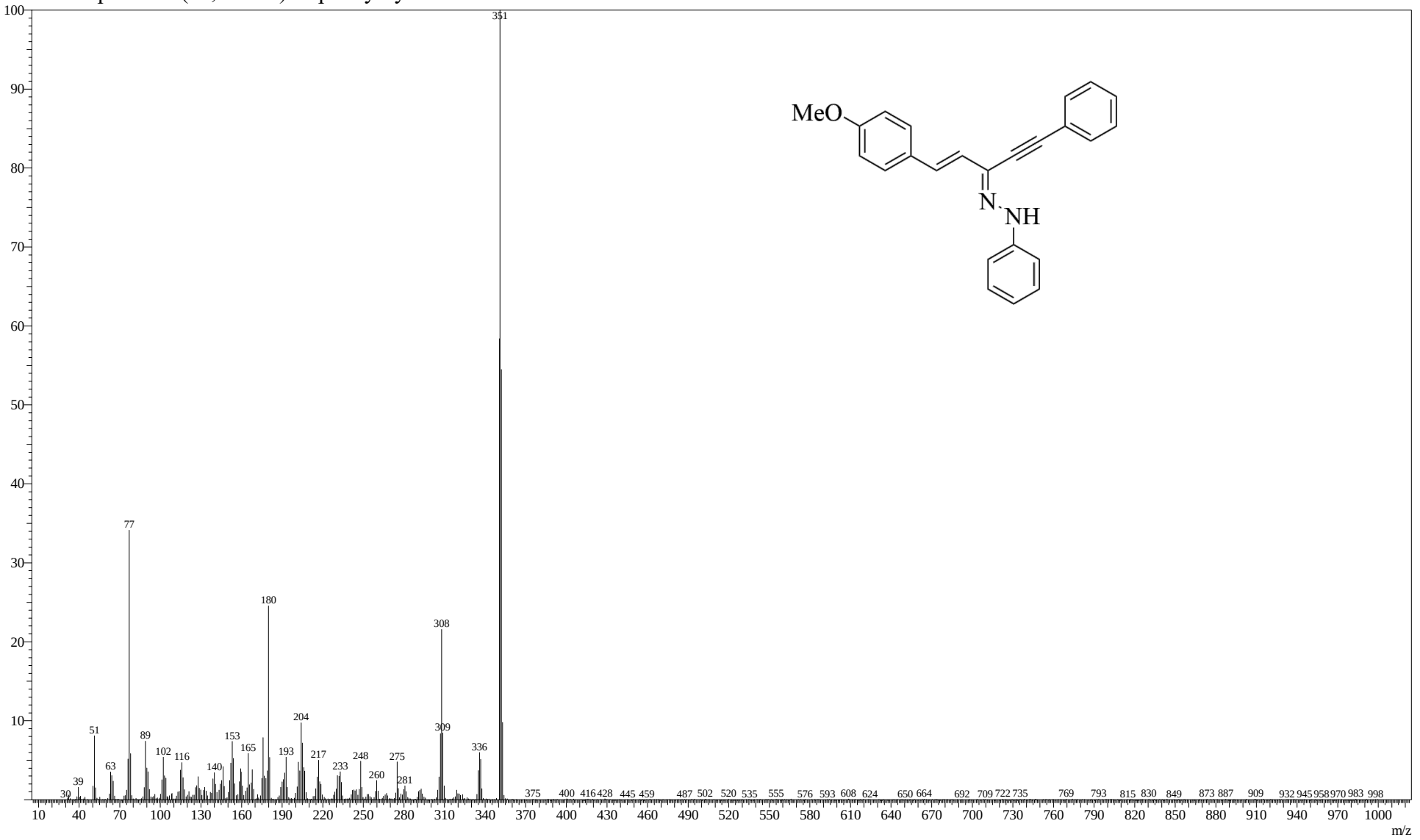
Mass spectrum (EI, 70 eV) of enynone **1y**



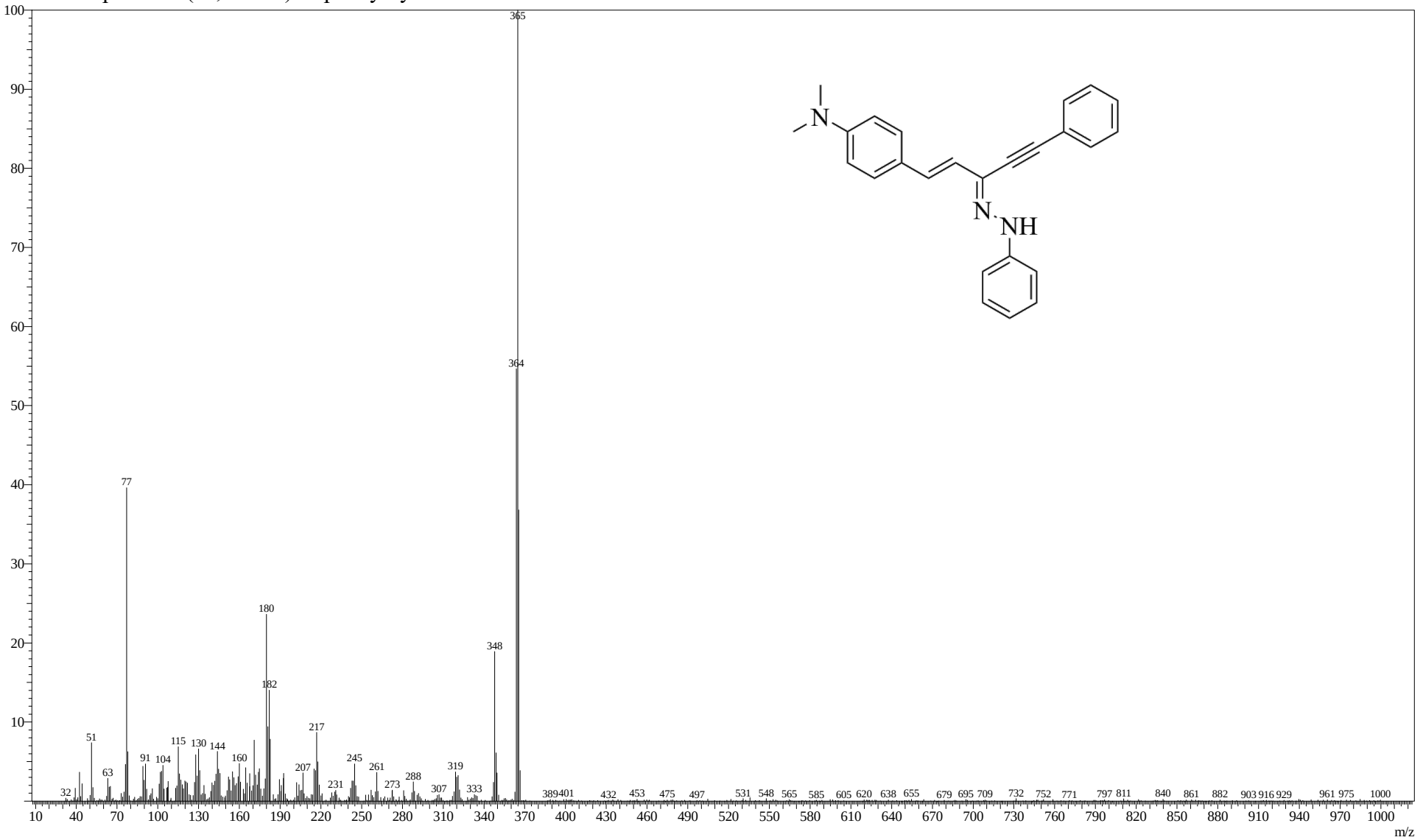
Mass spectrum (EI, 70 eV) of phenylhydrazone **5b**



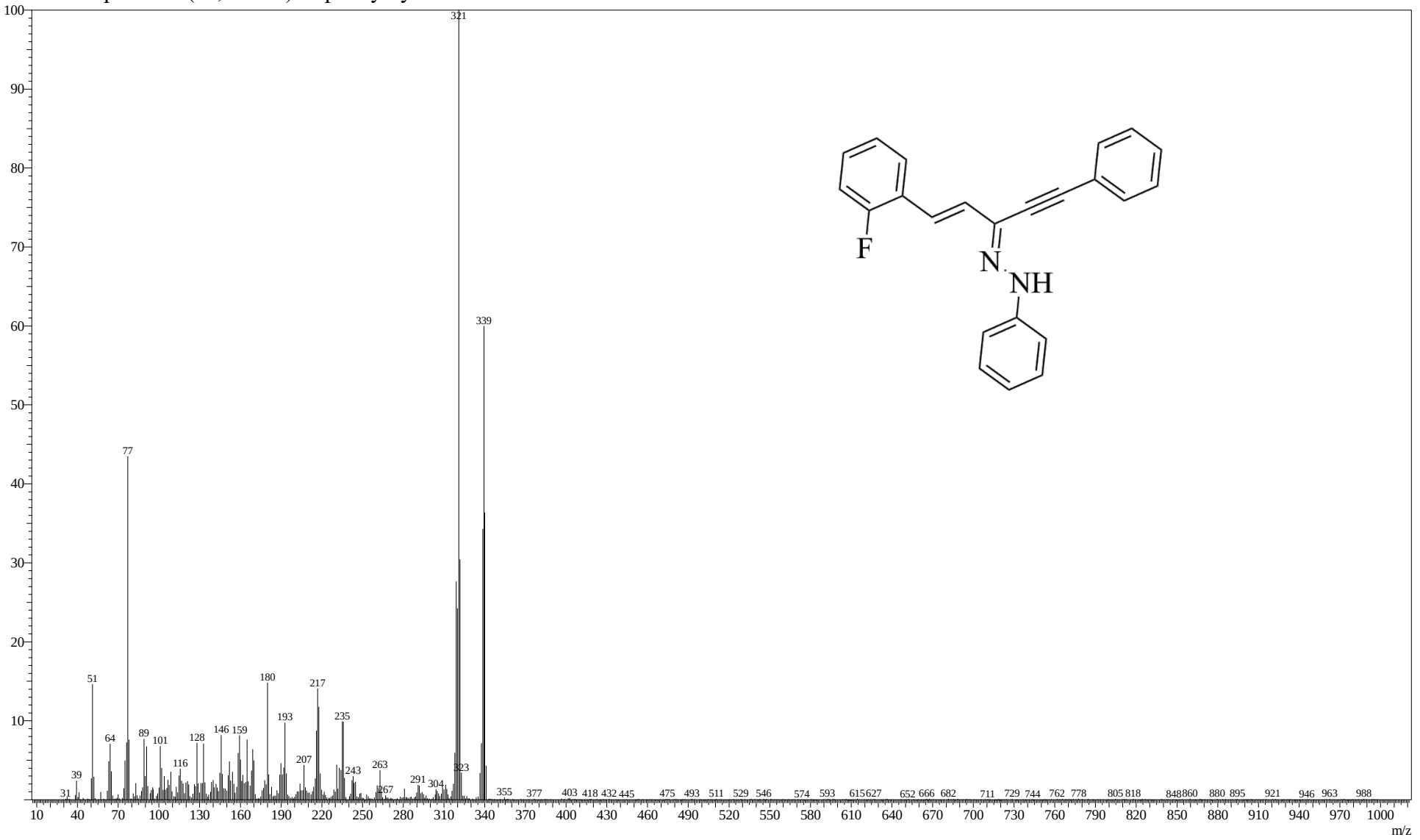
Mass spectrum (EI, 70 eV) of phenylhydrazone **5c**



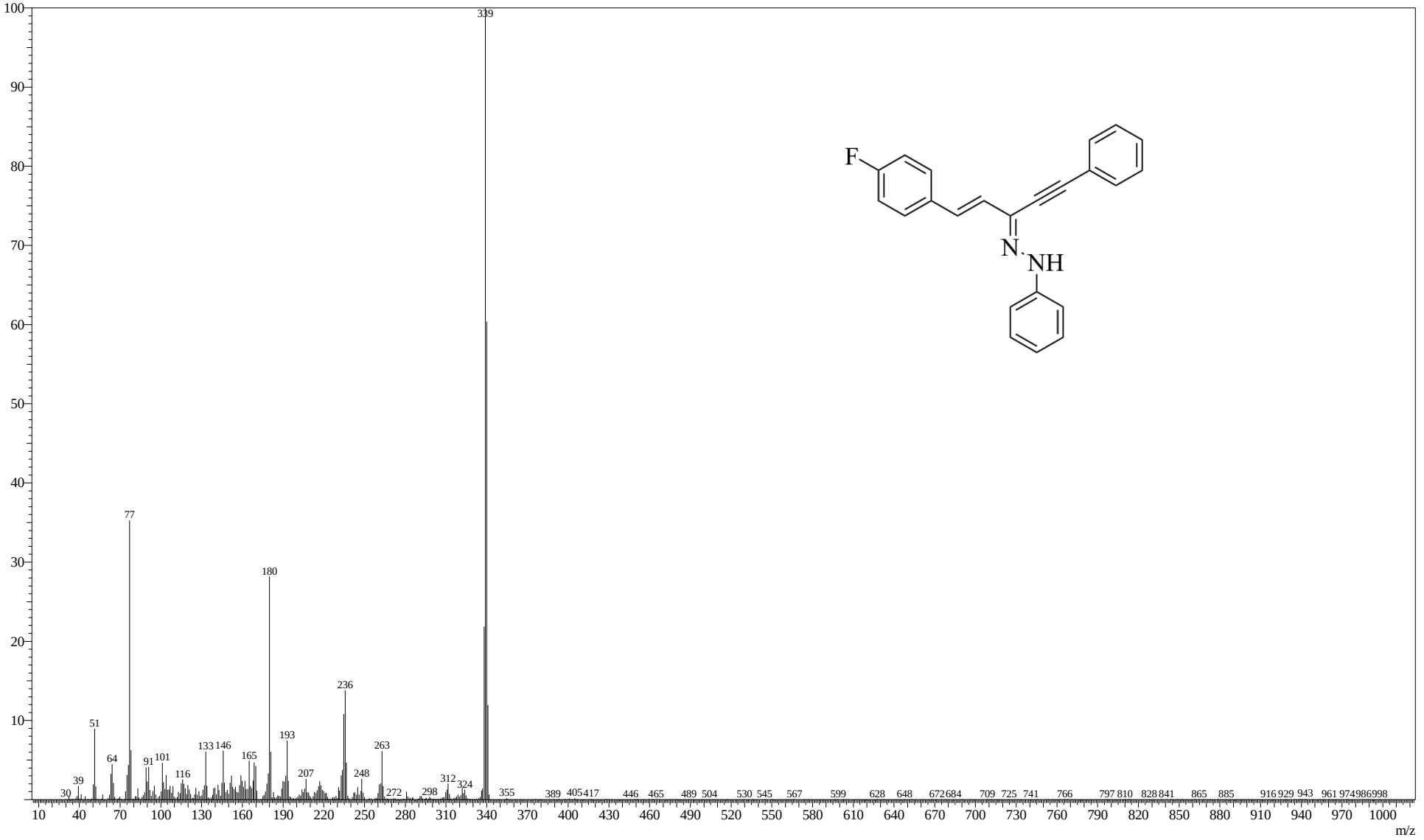
Mass spectrum (EI, 70 eV) of phenylhydrazone **5d**



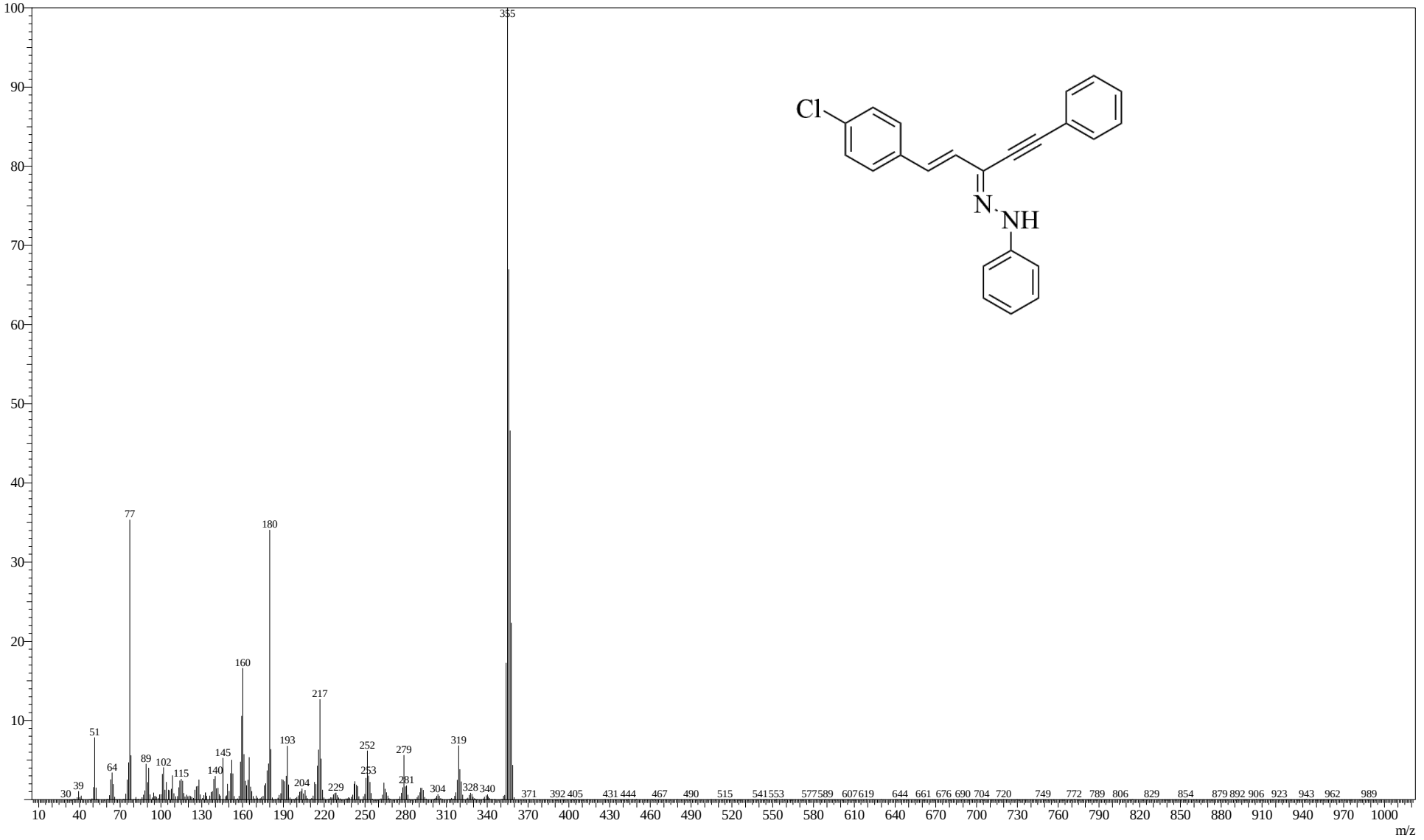
Mass spectrum (EI, 70 eV) of phenylhydrazone **5e**



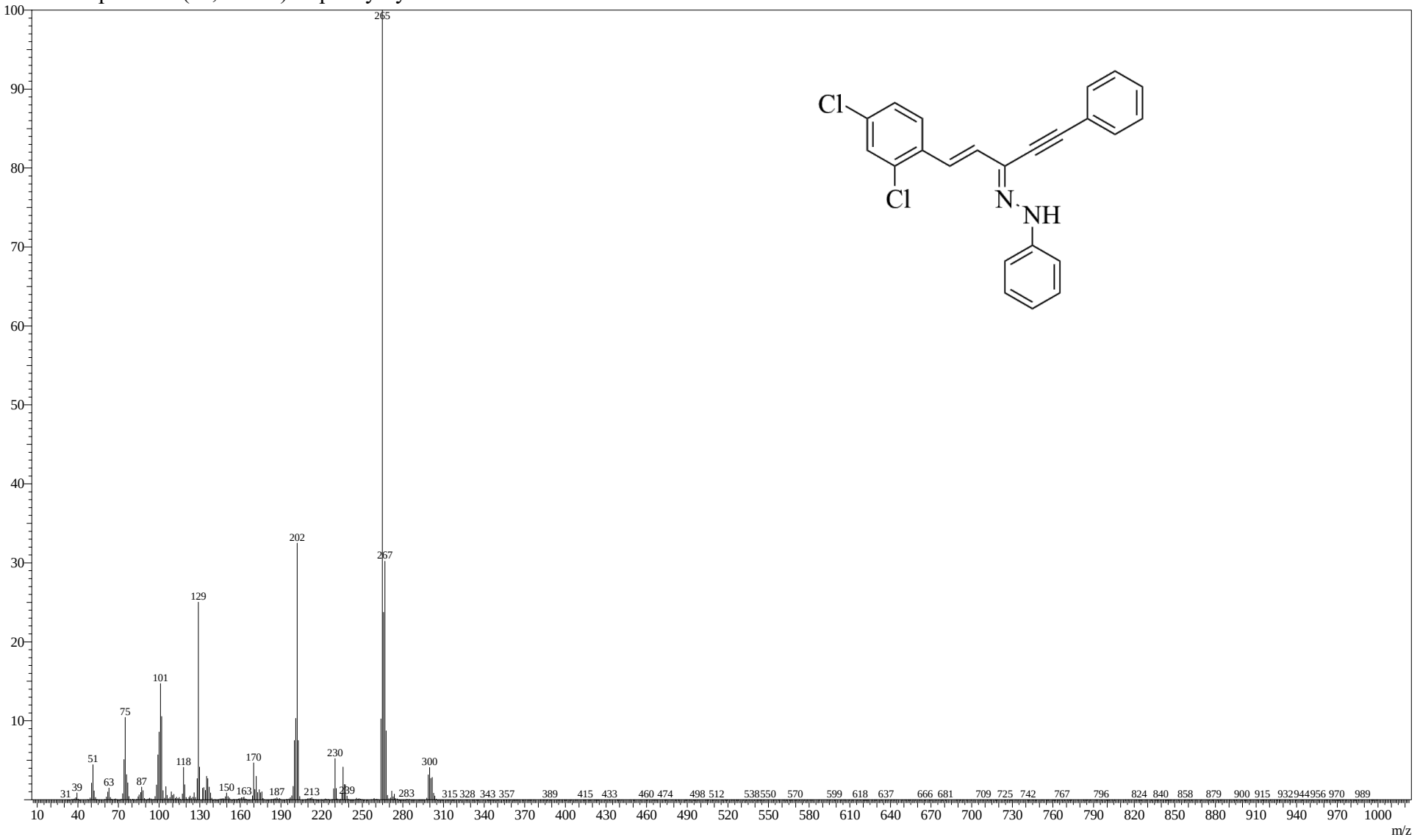
Mass spectrum (EI, 70 eV) of phenylhydrazone **5f**



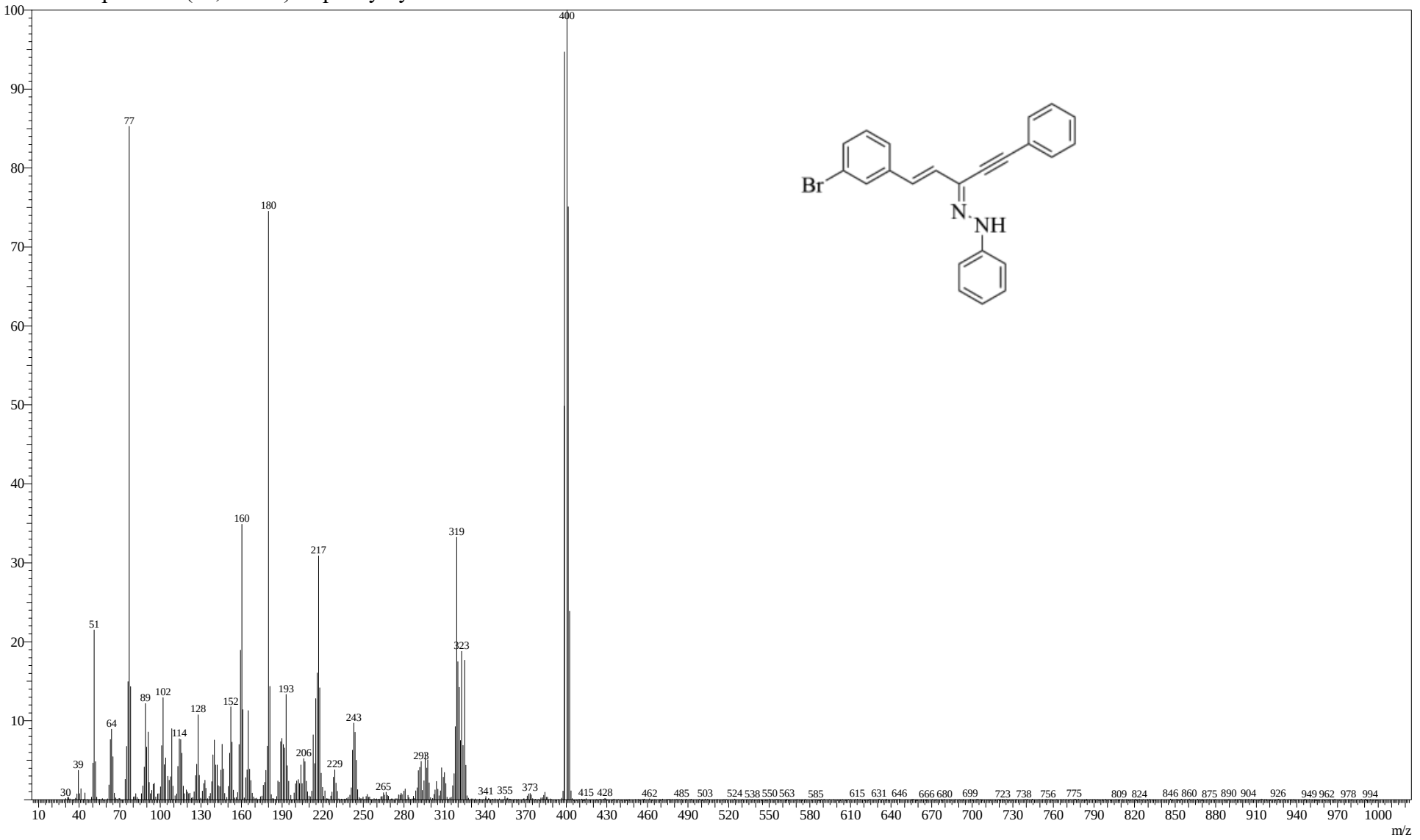
Mass spectrum (EI, 70 eV) of phenylhydrazone **5g**



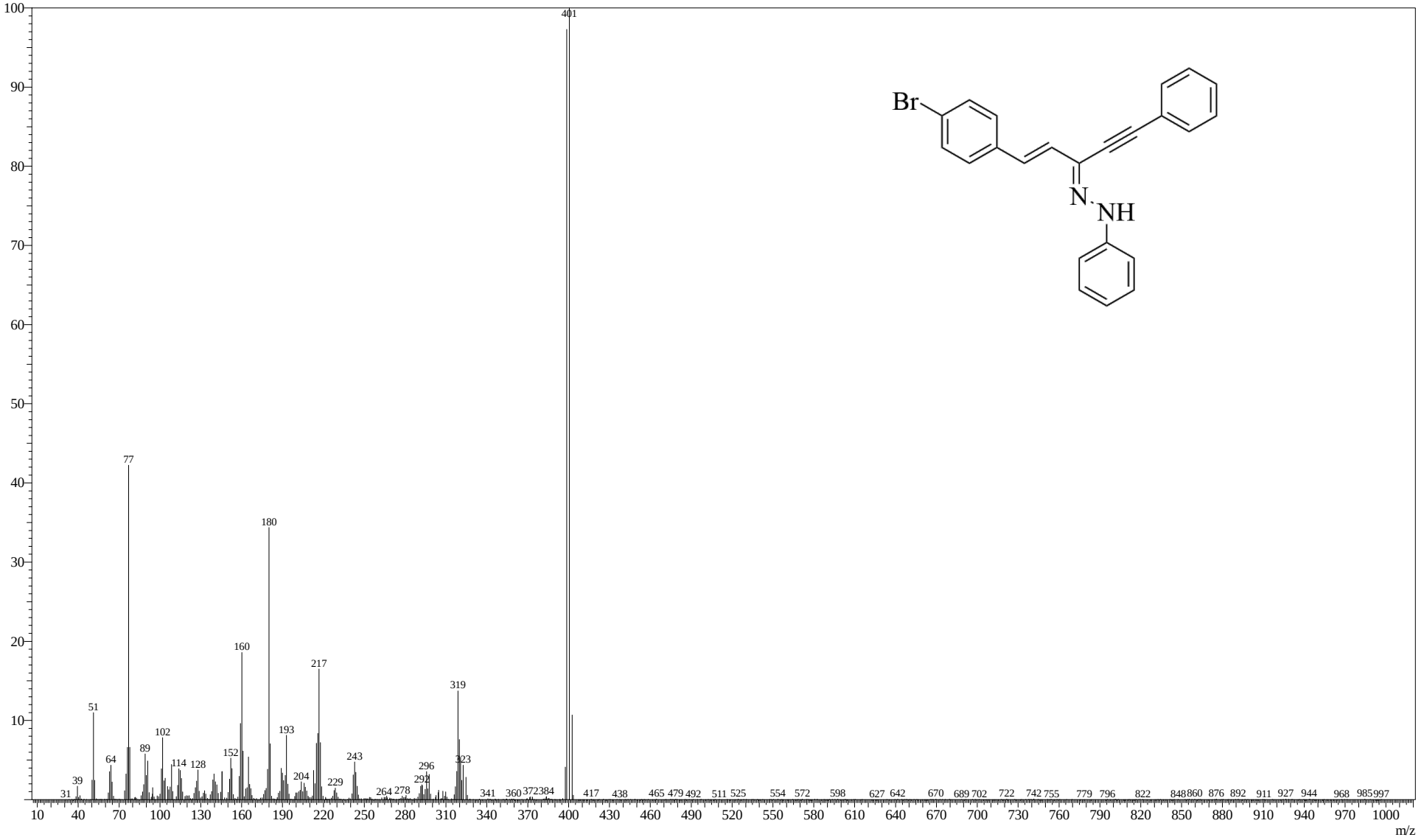
Mass spectrum (EI, 70 eV) of phenylhydrazone **5h**



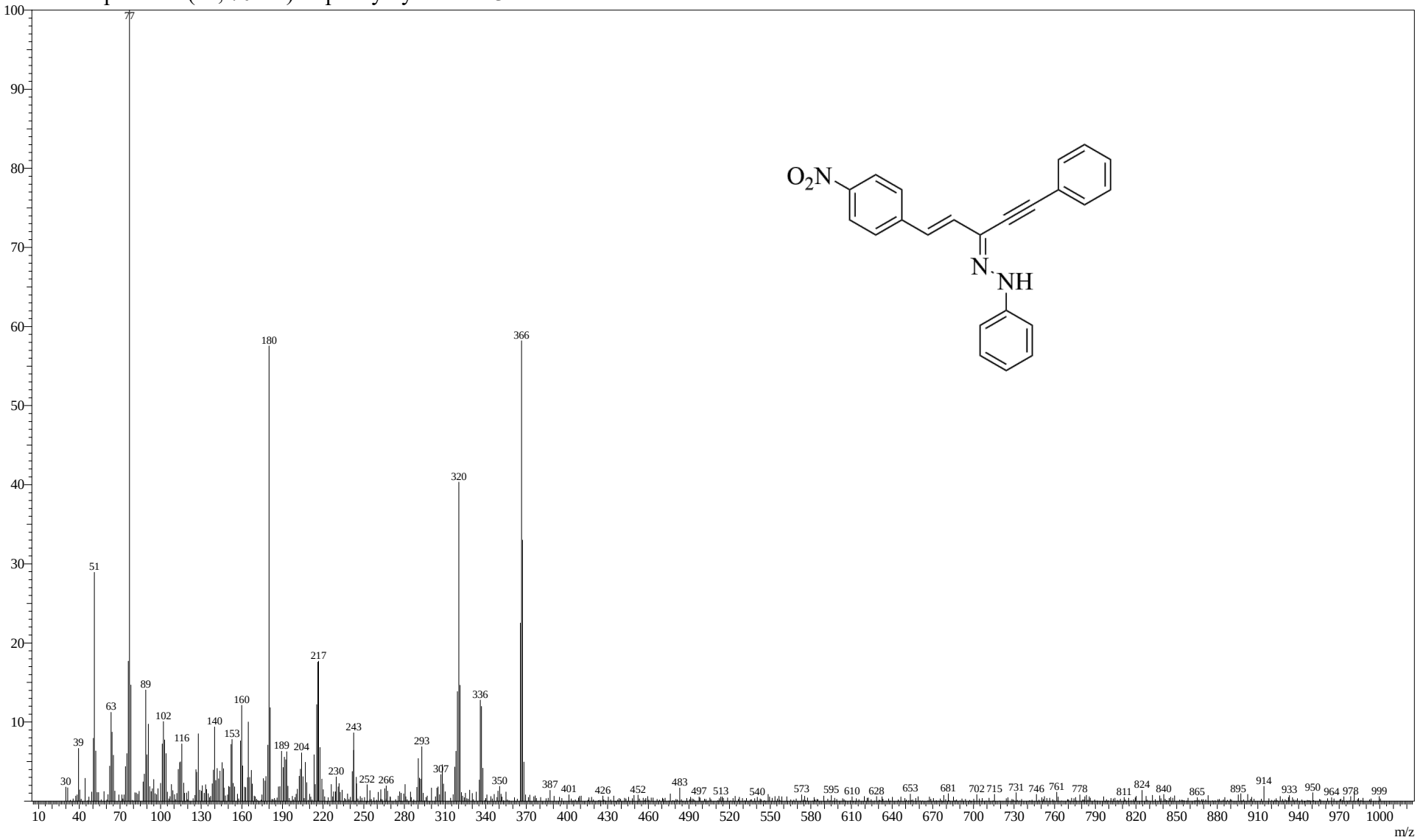
Mass spectrum (EI, 70 eV) of phenylhydrazone **5i**



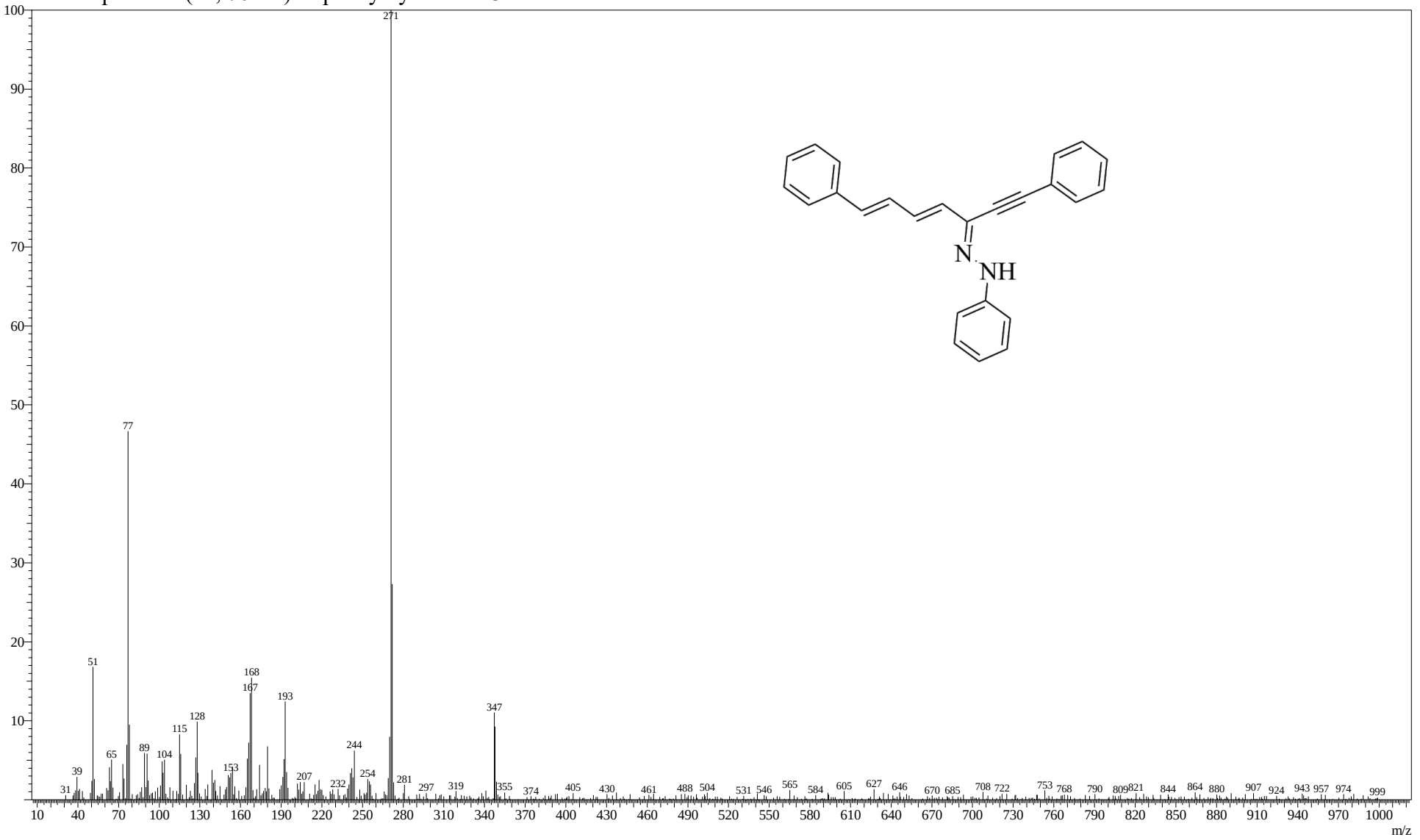
Mass spectrum (EI, 70 eV) of phenylhydrazone **5j**



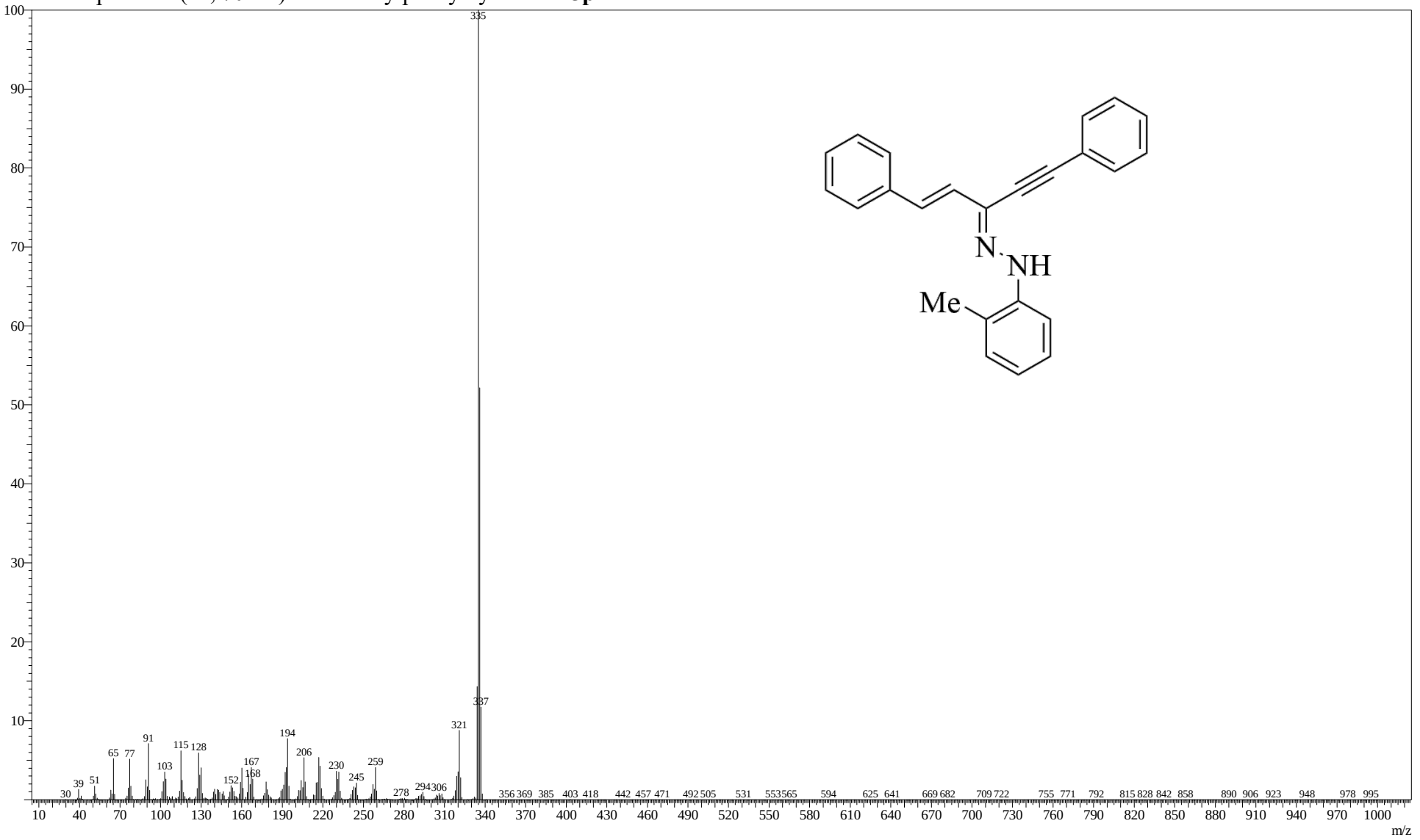
Mass spectrum (EI, 70 eV) of phenylhydrazone **5k**



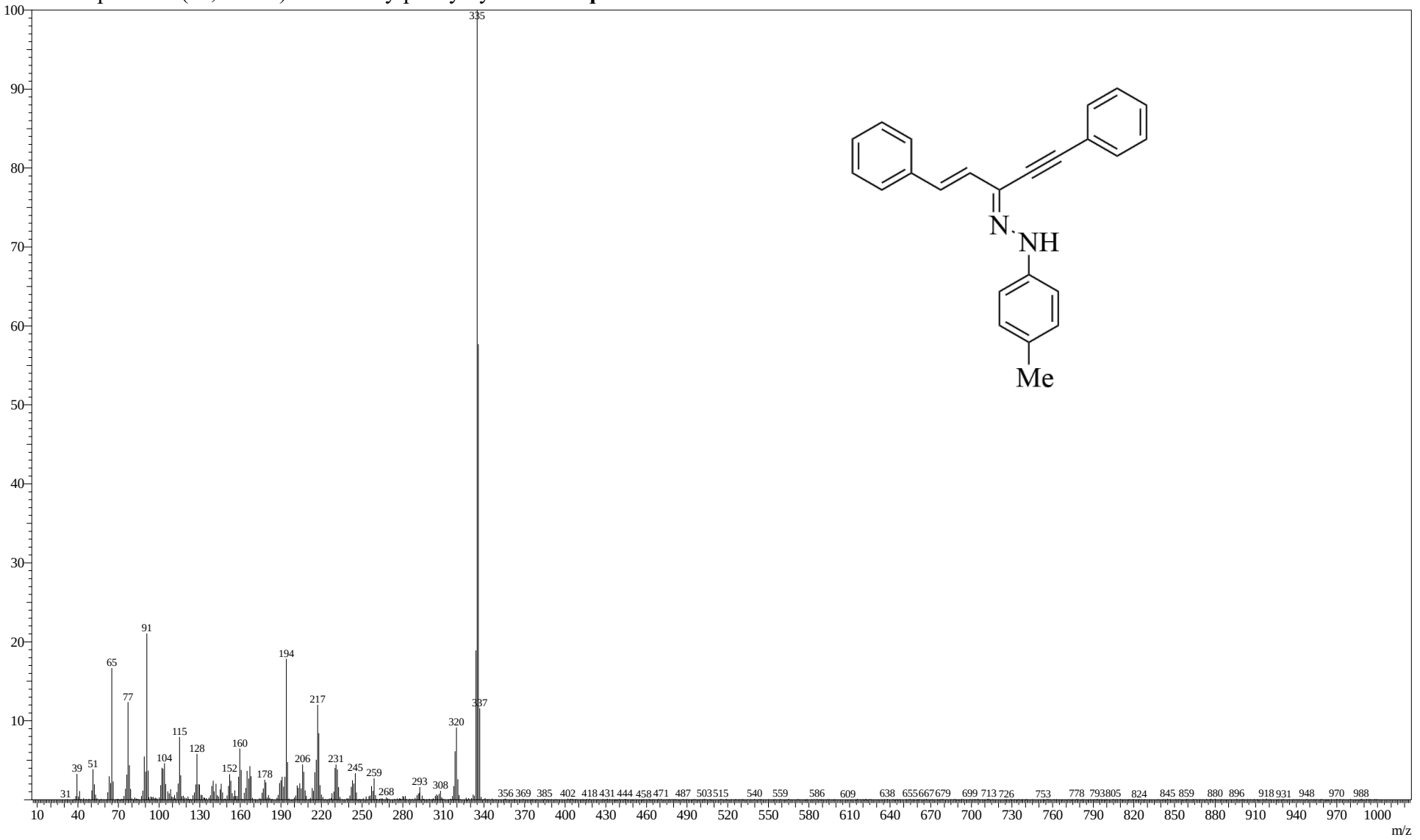
Mass spectrum (EI, 70 eV) of phenylhydrazone **5l**



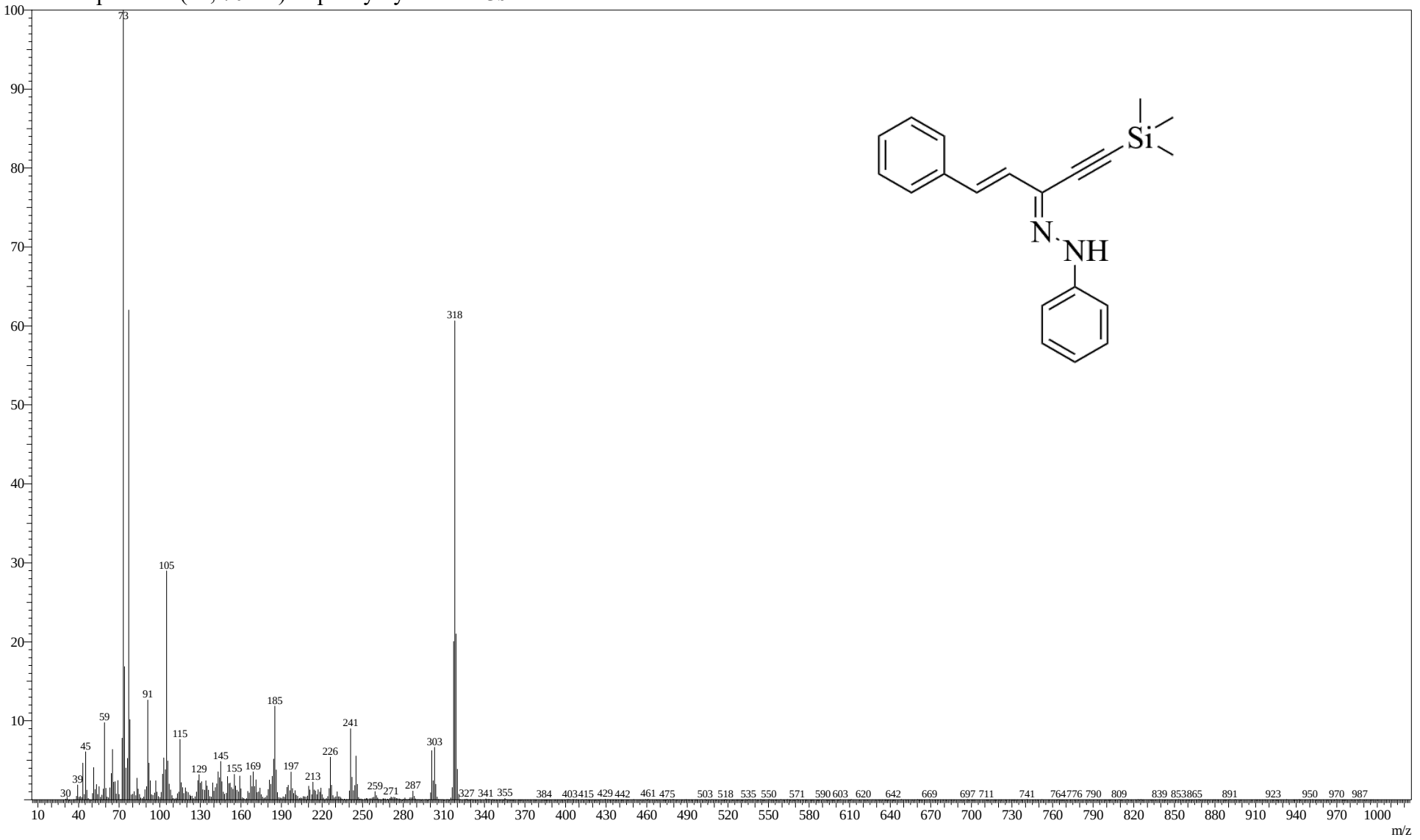
Mass spectrum (EI, 70 eV) of 2-methylphenylhydrazone **5p**



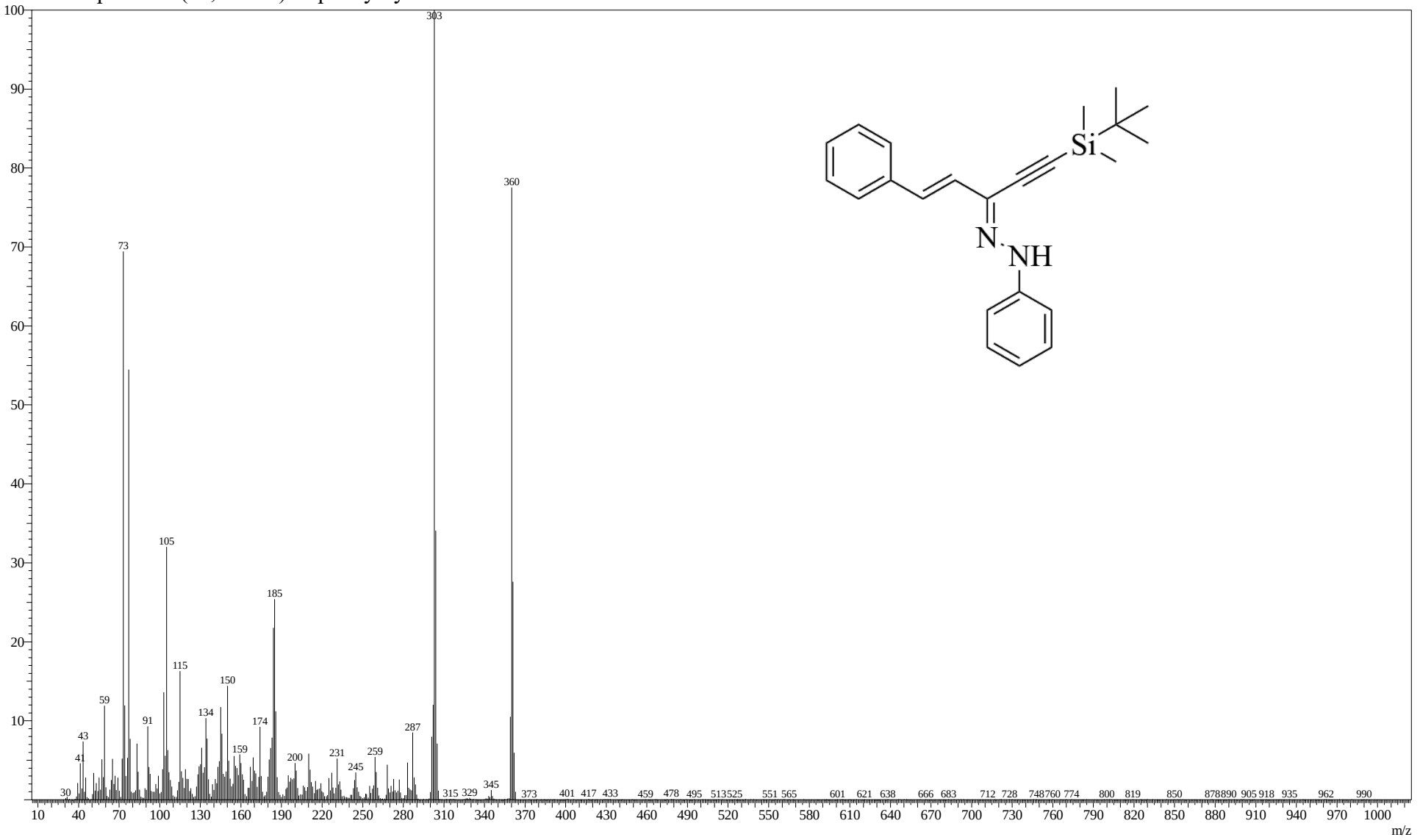
Mass spectrum (EI, 70 eV) of 4-methylphenylhydrazone **5q**



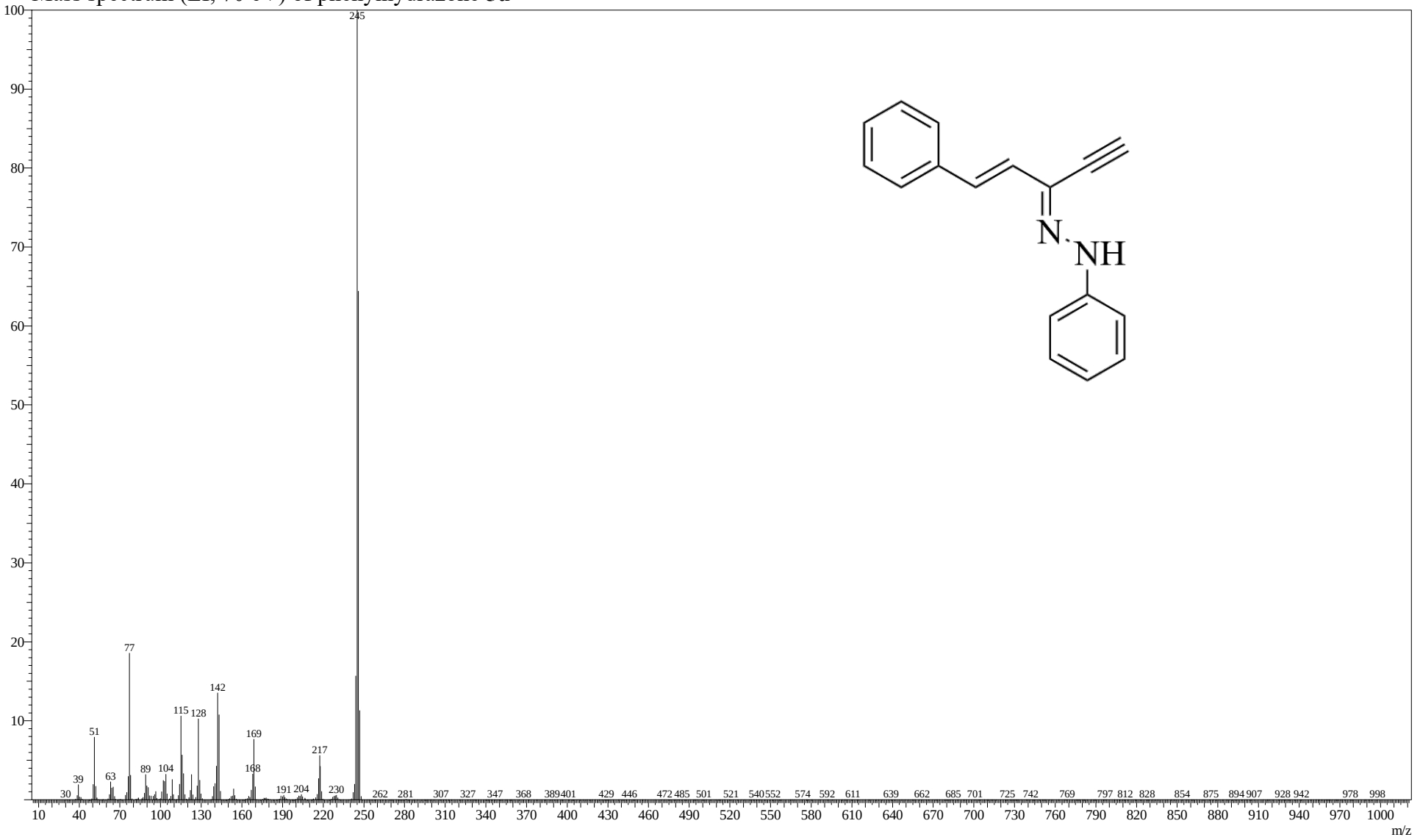
Mass spectrum (EI, 70 eV) of phenylhydrazone **5s**



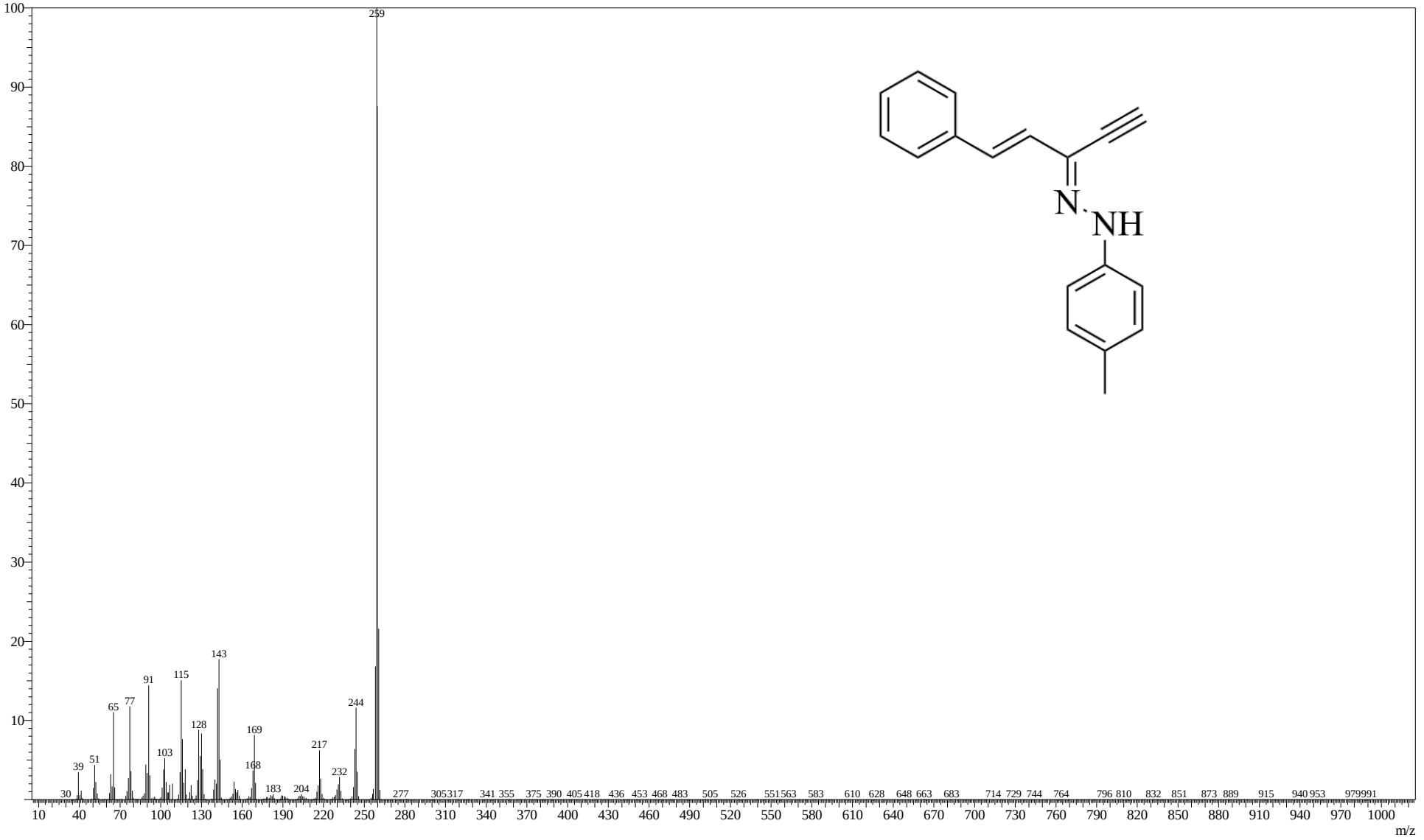
Mass spectrum (EI, 70 eV) of phenylhydrazone **5t**



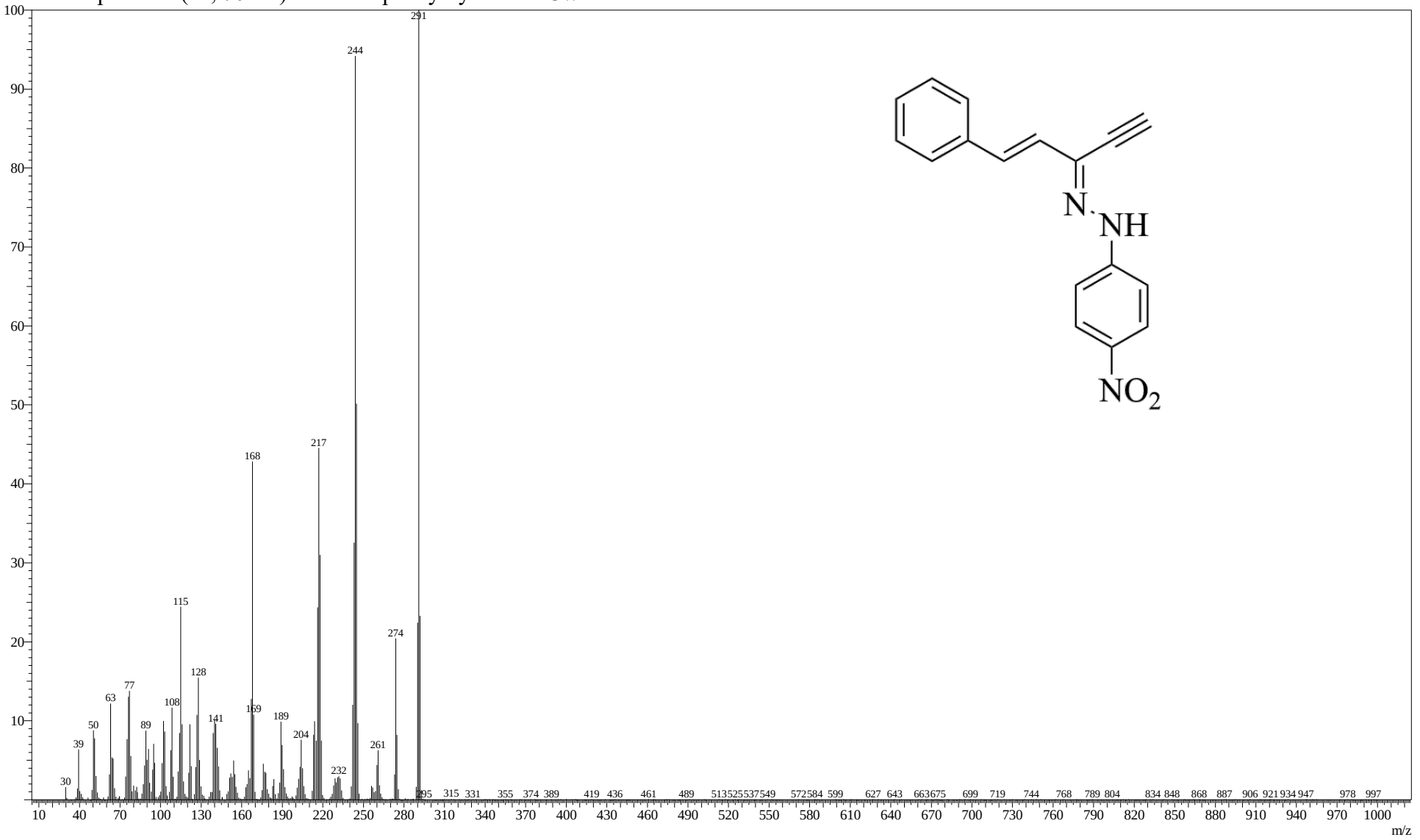
Mass spectrum (EI, 70 eV) of phenylhydrazone **5u**



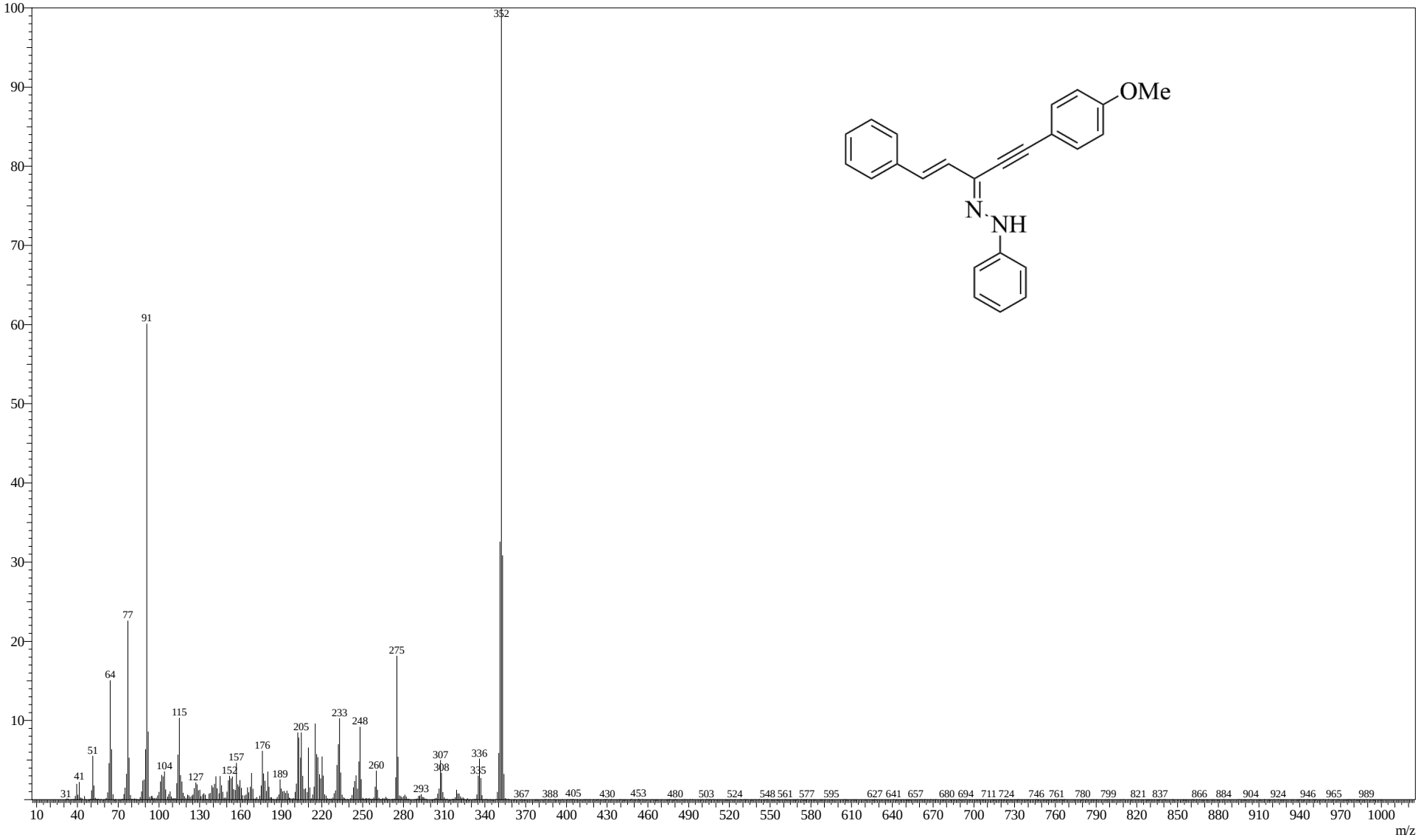
Mass spectrum (EI, 70 eV) of 4-methylphenylhydrazone **5v**



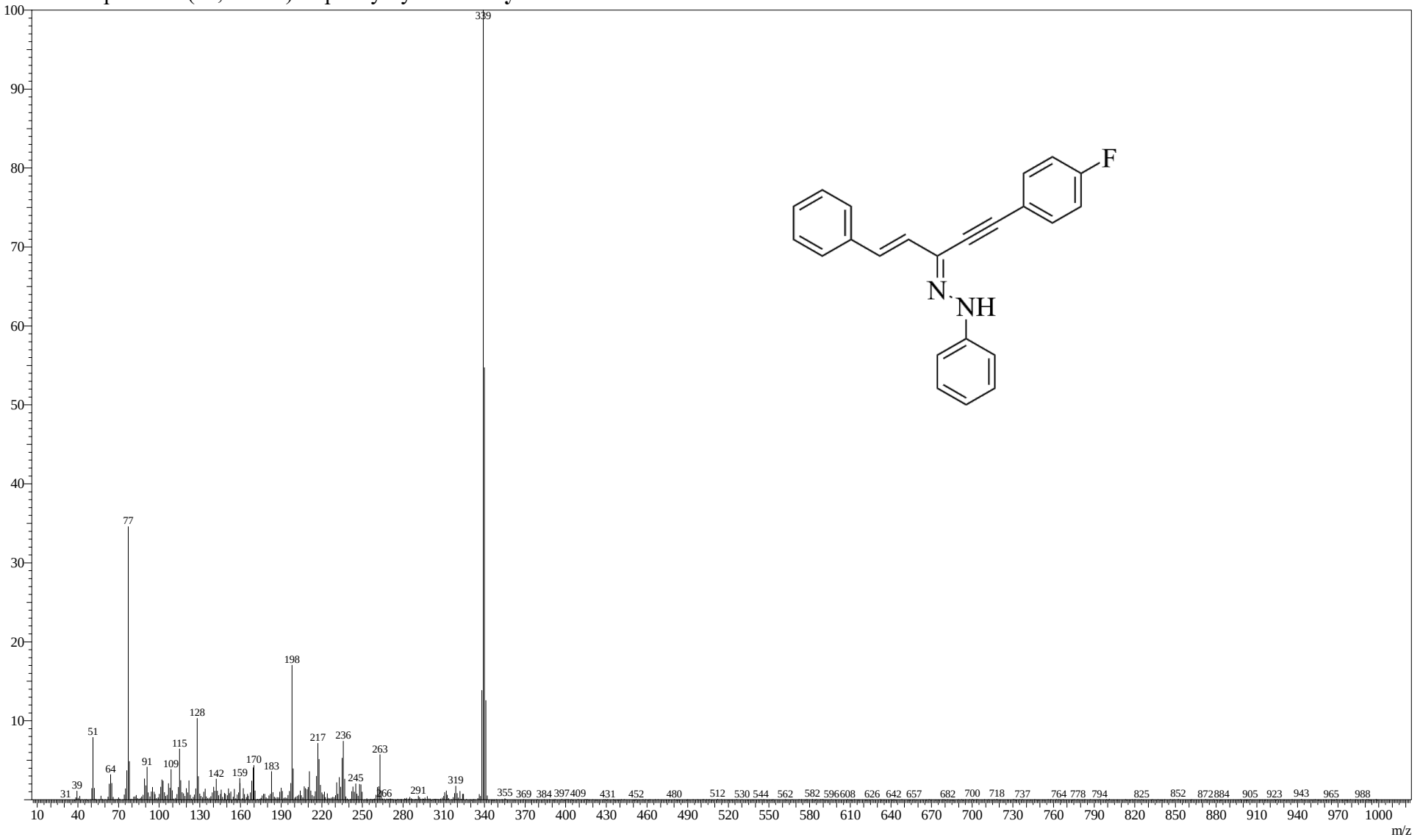
Mass spectrum (EI, 70 eV) of 4-nitrophenylhydrazone **5w**



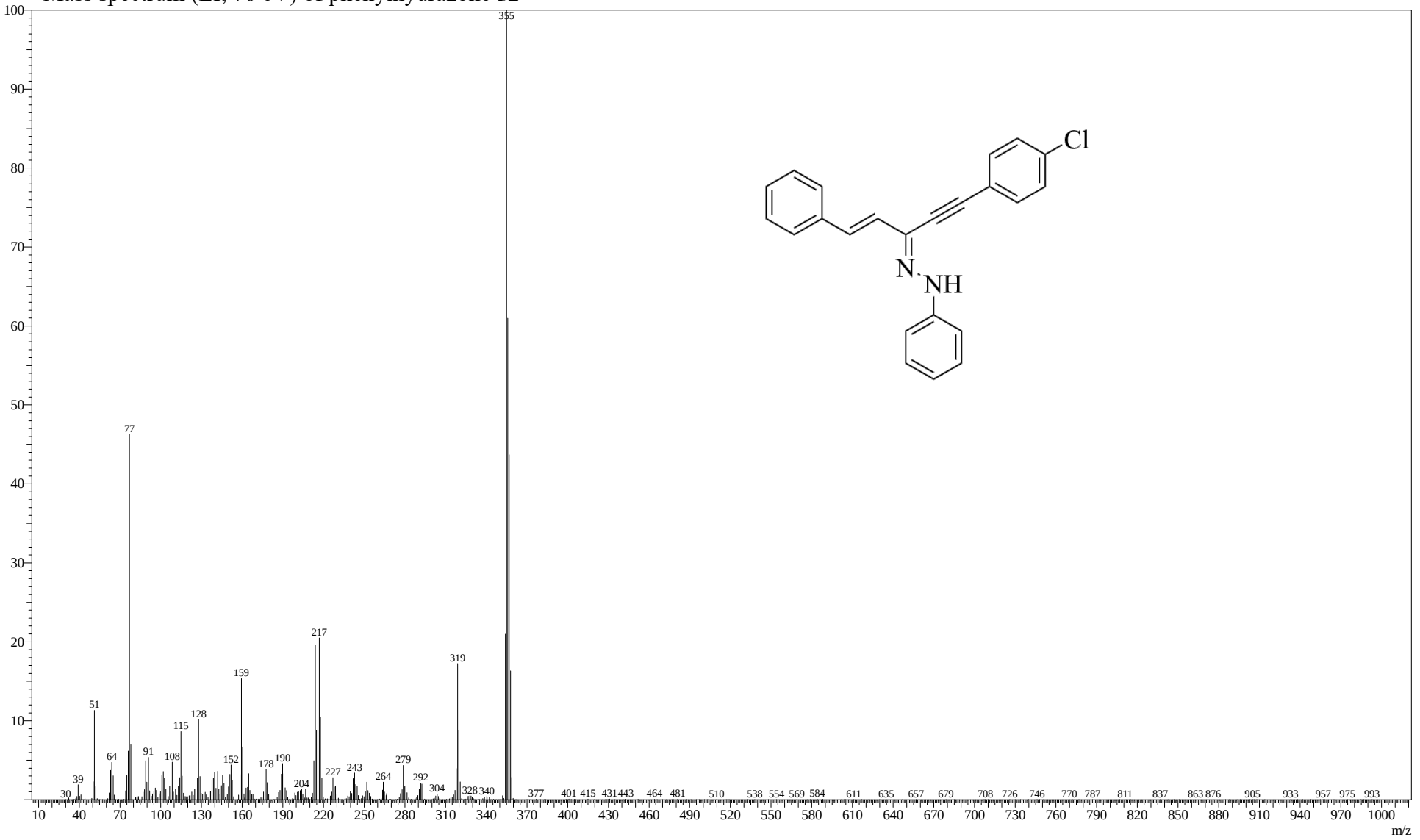
Mass spectrum (EI, 70 eV) of phenylhydrazone **5x**



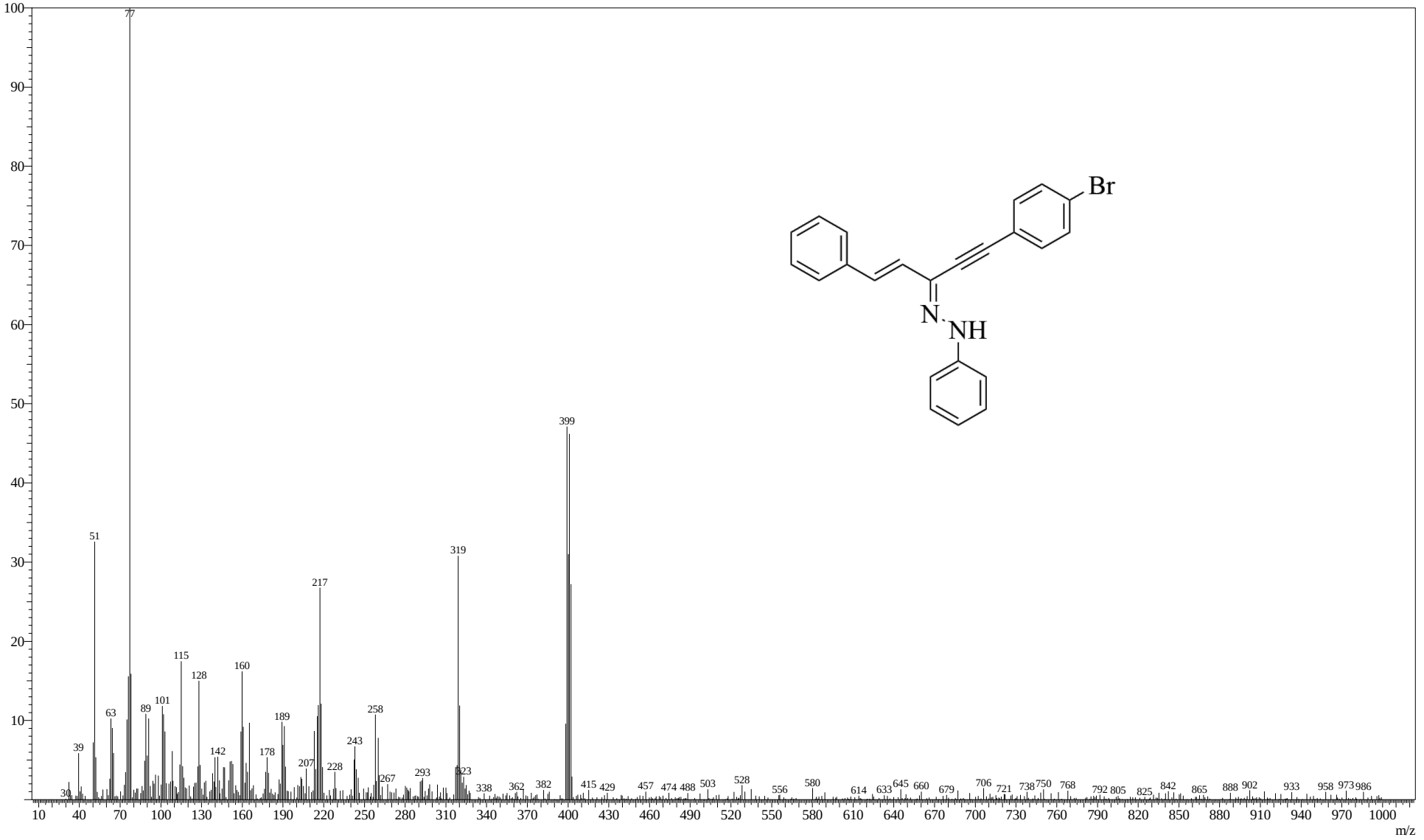
Mass spectrum (EI, 70 eV) of phenylhydrazone **5y**



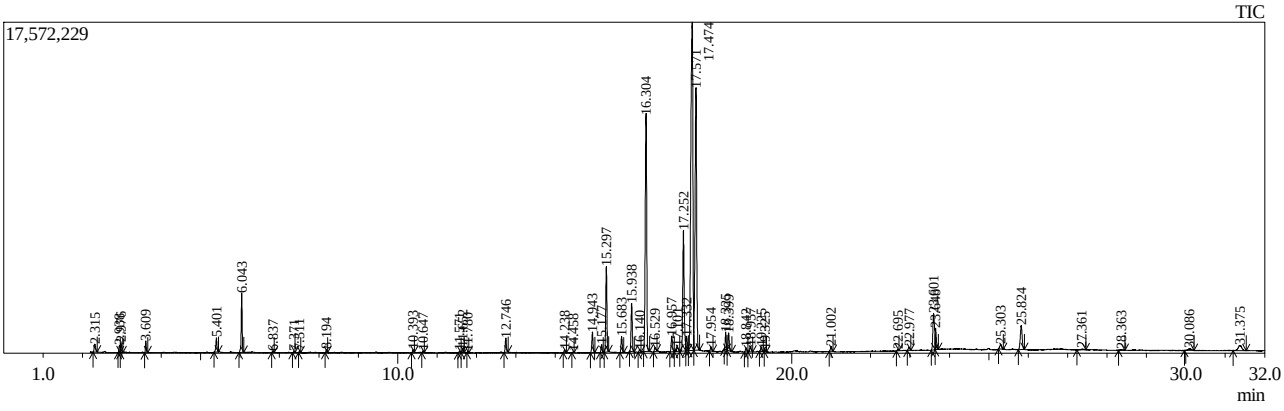
Mass spectrum (EI, 70 eV) of phenylhydrazone **5z**



Mass spectrum (EI, 70 eV) of phenylhydrazone **5aa**



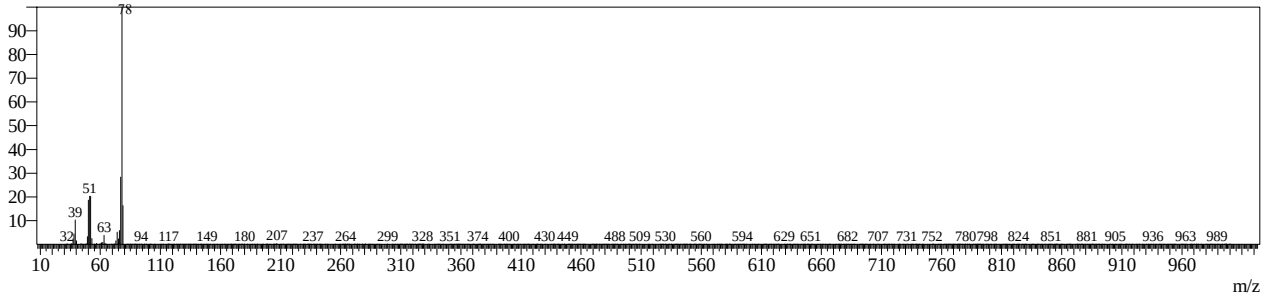
Reaction mixture of enynone **1w** with phenylhydrazine 2**a**



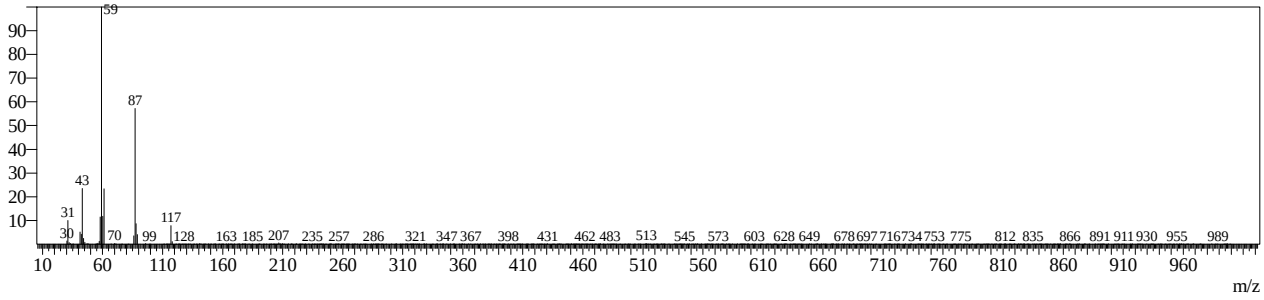
Peak Report TIC

Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark	Name
1	2.315	2.272	2.372	1124513	0.52	424271	0.54	2.65		
2	2.938	2.902	2.958	765657	0.36	366837	0.47	2.09		
3	2.976	2.958	3.028	1102023	0.51	506637	0.65	2.18	V	
4	3.609	3.575	3.658	976424	0.45	608641	0.78	1.60		
5	5.401	5.342	5.455	1550684	0.72	755315	0.97	2.05		
6	6.043	5.972	6.095	5448107	2.53	3116707	4.00	1.75		
7	6.837	6.800	6.868	112983	0.05	60126	0.08	1.88	MI	
8	7.371	7.333	7.393	63544	0.03	42350	0.05	1.50	MI	
9	7.511	7.487	7.542	146346	0.07	91113	0.12	1.61	MI	
10	8.194	8.155	8.222	283148	0.13	172056	0.22	1.65	MI	
11	10.393	10.353	10.425	292330	0.14	154615	0.20	1.89	MI	
12	10.647	10.613	10.677	162371	0.08	92085	0.12	1.76	MI	
13	11.571	11.532	11.607	179734	0.08	94026	0.12	1.91	MI	
14	11.652	11.608	11.688	430182	0.20	230464	0.30	1.87	MI	
15	11.780	11.753	11.807	82928	0.04	51122	0.07	1.62	MI	
16	12.746	12.698	12.805	1571687	0.73	750893	0.96	2.09		
17	14.238	14.198	14.278	304743	0.14	156409	0.20	1.95	MI	
18	14.458	14.417	14.480	57982	0.03	39317	0.05	1.47	MI	
19	14.943	14.892	15.005	2278493	1.06	1073990	1.38	2.12		
20	15.177	15.135	15.218	844112	0.39	419708	0.54	2.01		
21	15.297	15.238	15.352	9399890	4.37	4501870	5.77	2.09		
22	15.683	15.635	15.738	1753365	0.81	850380	1.09	2.06		
23	15.938	15.882	16.002	5402390	2.51	2545559	3.26	2.12		
24	16.140	16.103	16.175	332211	0.15	163334	0.21	2.03	MI	
25	16.304	16.238	16.395	33126842	15.39	12583515	16.13	2.63		
26	16.529	16.492	16.582	576174	0.27	214963	0.28	2.68	MI	
27	16.957	16.905	17.022	1926323	0.90	816787	1.05	2.36		
28	17.101	17.022	17.155	768675	0.36	240029	0.31	3.20	V	
29	17.252	17.155	17.308	16145547	7.50	6378531	8.18	2.53	V	
30	17.332	17.308	17.378	1829820	0.85	762718	0.98	2.40	V	
31	17.474	17.378	17.515	63419813	29.47	17406600	22.32	3.64	V	
32	17.571	17.515	17.658	39772804	18.48	13901176	17.82	2.86	V	
33	17.954	17.912	17.998	503694	0.23	228748	0.29	2.20		
34	18.325	18.285	18.358	1643556	0.76	910077	1.17	1.81		
35	18.399	18.362	18.478	1922504	0.89	926401	1.19	2.08		
36	18.842	18.798	18.888	517525	0.24	224611	0.29	2.30		
37	18.957	18.888	19.008	662855	0.31	283280	0.36	2.34	V	
38	19.225	19.182	19.275	514604	0.24	228033	0.29	2.26		
39	19.325	19.298	19.358	174745	0.08	90570	0.12	1.93	MI	
40	21.002	20.952	21.052	596905	0.28	253760	0.33	2.35		
41	22.695	22.655	22.718	114487	0.05	61008	0.08	1.88	MI	
42	22.977	22.930	23.022	455430	0.21	176304	0.23	2.58	MI	
43	23.601	23.538	23.635	5601272	2.60	1925230	2.47	2.91		
44	23.648	23.635	23.718	2427892	1.13	1142721	1.47	2.12	V	
45	25.303	25.248	25.365	802207	0.37	252756	0.32	3.17		
46	25.824	25.748	25.902	4212909	1.96	1263668	1.62	3.33		
47	27.361	27.238	27.460	244824	0.11	46842	0.06	5.23	MI	
48	28.363	28.295	28.457	171364	0.08	37681	0.05	4.55	MI	
49	30.086	29.962	30.208	534331	0.25	91533	0.12	5.84	MI	
50	31.375	31.203	31.533	1854168	0.86	280806	0.36	6.60	MI	
				215187117	100.00	77996173	100.00			

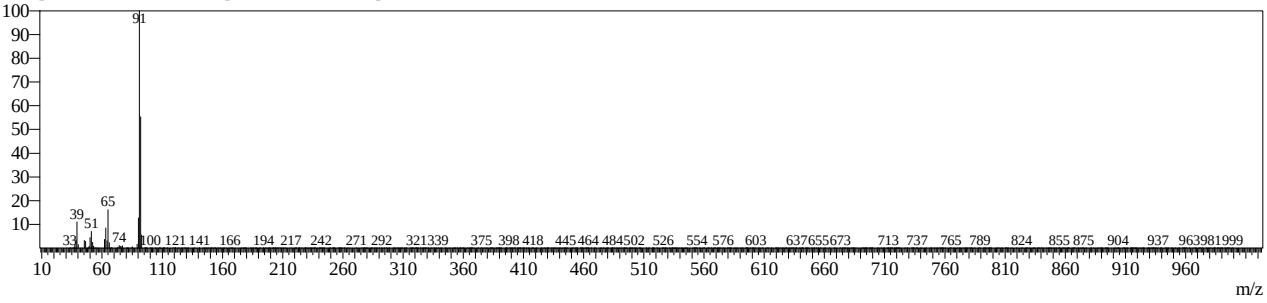
Line#:1 R.Time:2.315(Scan#:70)
MassPeaks:481
RawMode:Averaged 2.313-2.317(69-71)
BasePeak:78(169297) 100



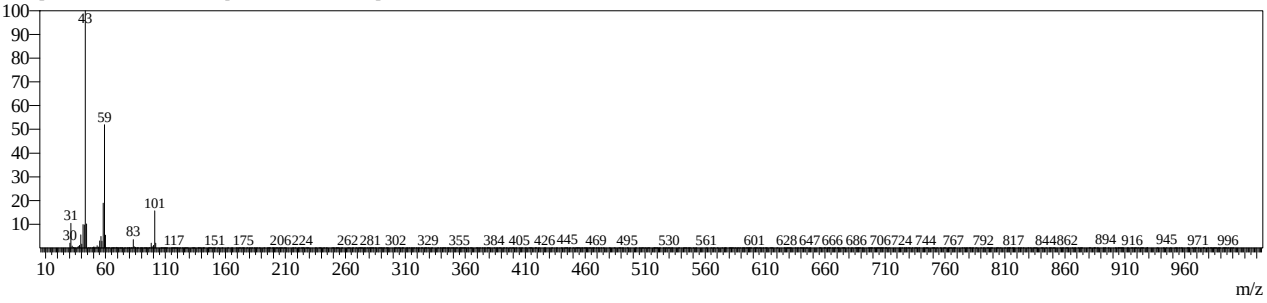
Line#:2 R.Time:2.938(Scan#:444)
MassPeaks:473
RawMode:Averaged 2.937-2.940(443-445)
BasePeak:59(82982) 100



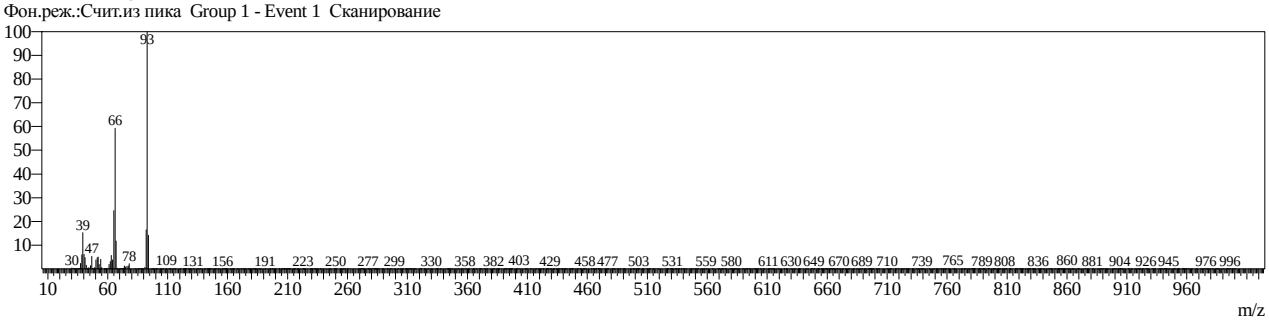
Line#:3 R.Time:2.977(Scan#:467)
MassPeaks:506
RawMode:Averaged 2.975-2.978(466-468) BasePeak:91(136589)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



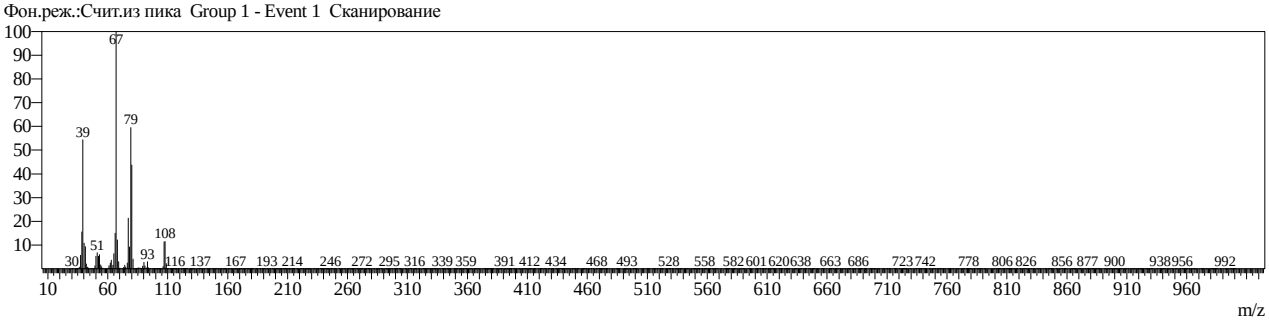
Line#:4 R.Time:3.608(Scan#:846)
MassPeaks:494
RawMode:Averaged 3.607-3.610(845-847) BasePeak:43(224047)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



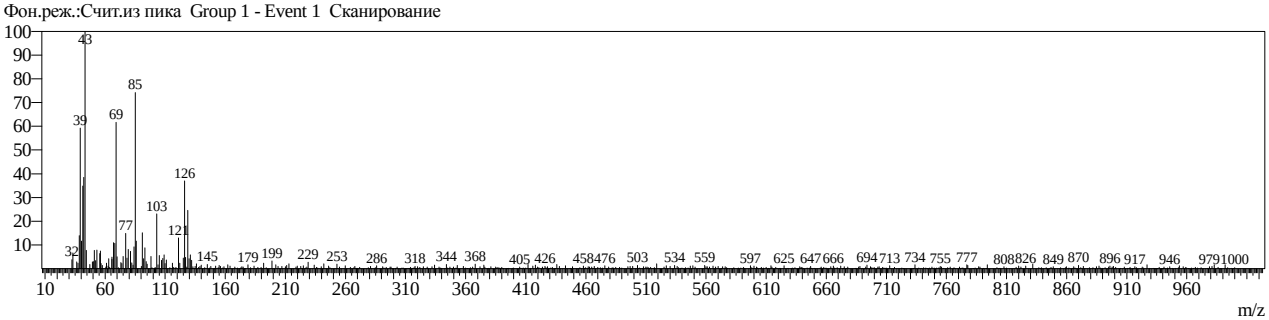
Line#:5 R.Time:5.402(Scan#:1922)
MassPeaks:465
RawMode:Averaged 5.400-5.403(1921-1923) BasePeak:93(238639)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



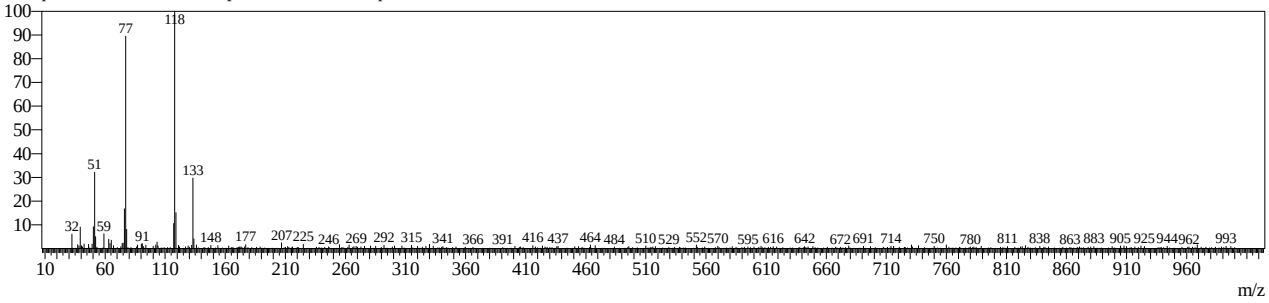
Line#:6 R.Time:6.043(Scan#:2307)
MassPeaks:515
RawMode:Averaged 6.042-6.045(2306-2308) BasePeak:67(690040)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



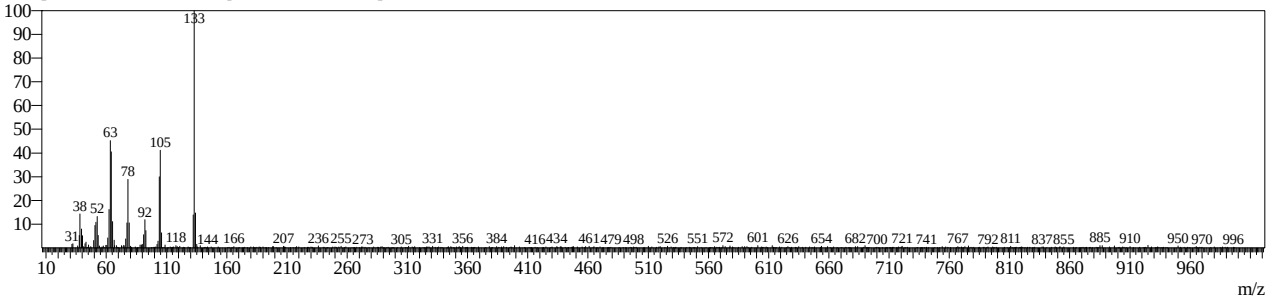
Line#:7 R.Time:6.837(Scan#:2783)
MassPeaks:480
RawMode:Averaged 6.835-6.838(2782-2784) BasePeak:43(7869)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



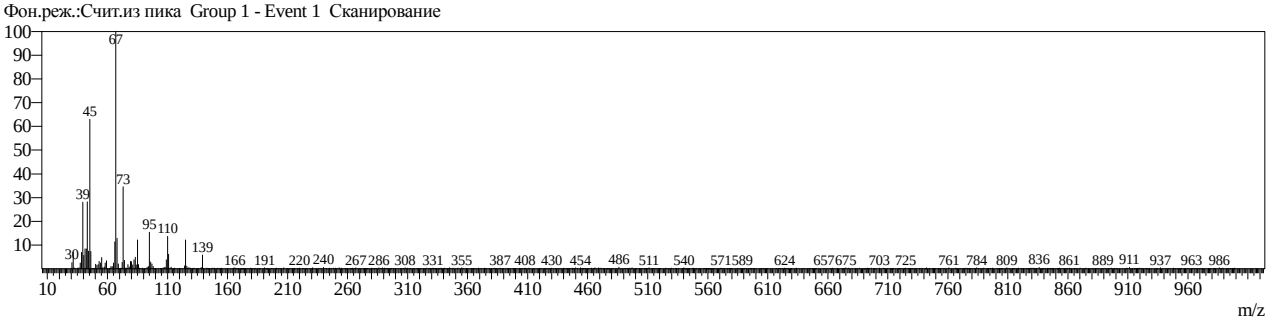
Line#:8 R.Time:7.370(Scan#:3103)
MassPeaks:461
RawMode:Averaged 7.368-7.372(3102-3104) BasePeak:118(11391)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



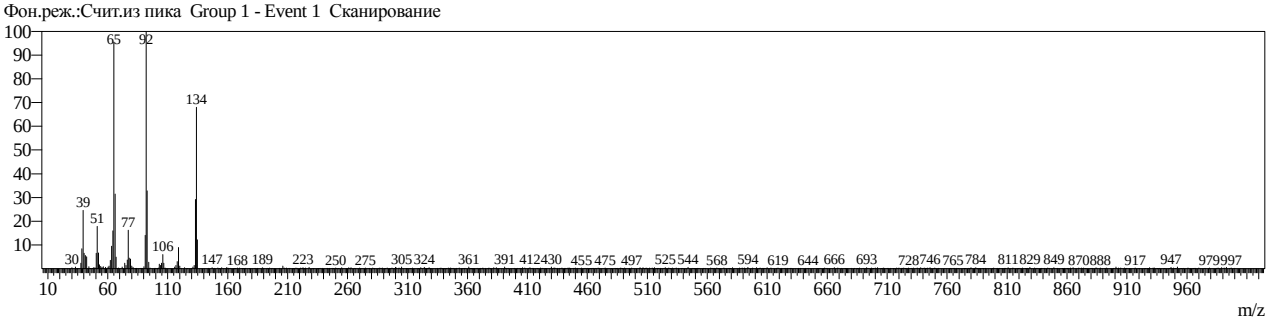
Line#:9 R.Time:7.512(Scan#:3188)
MassPeaks:470
RawMode:Averaged 7.510-7.513(3187-3189) BasePeak:133(17951)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



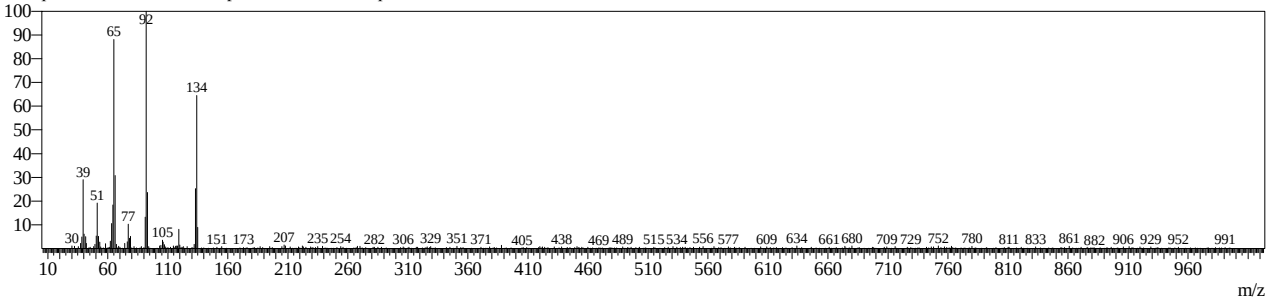
Line#:10 R.Time:8.193(Scan#:3597)
MassPeaks:485
RawMode:Averaged 8.192-8.195(3596-3598) BasePeak:67(35474)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



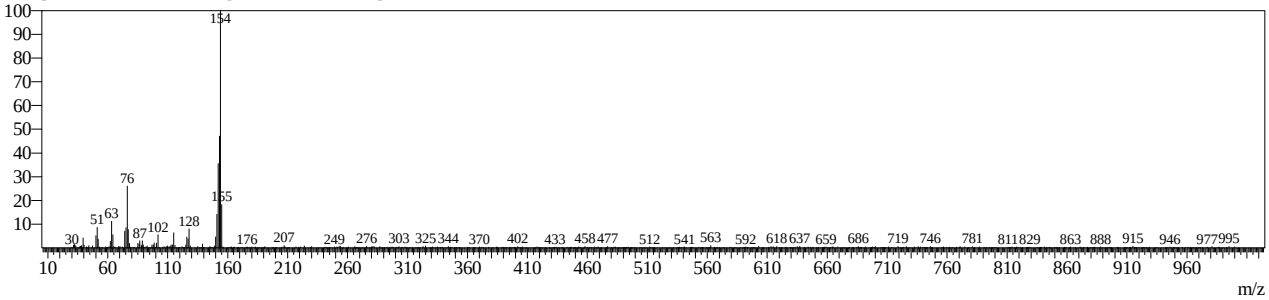
Line#:11 R.Time:10.393(Scan#:4917)
MassPeaks:474
RawMode:Averaged 10.392-10.395(4916-4918) BasePeak:92(27152)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



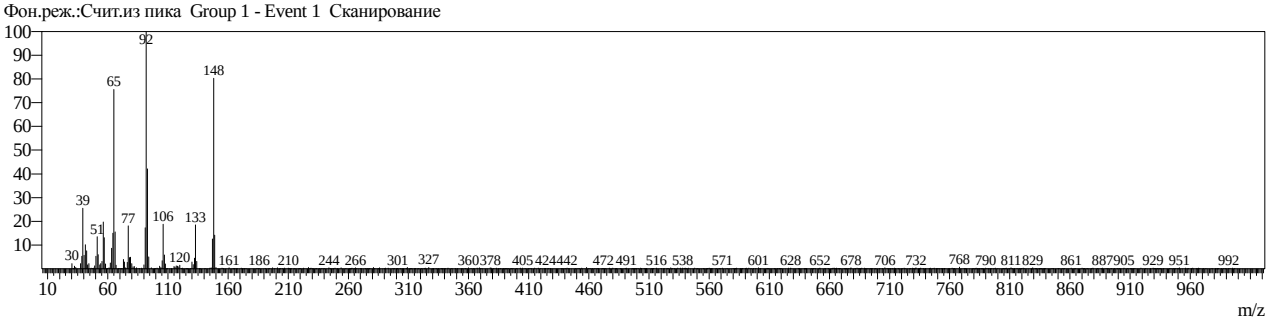
Line#:12 R.Time:10.647(Scan#:5069)
MassPeaks:464
RawMode:Averaged 10.645-10.648(5068-5070) BasePeak:92(16362)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



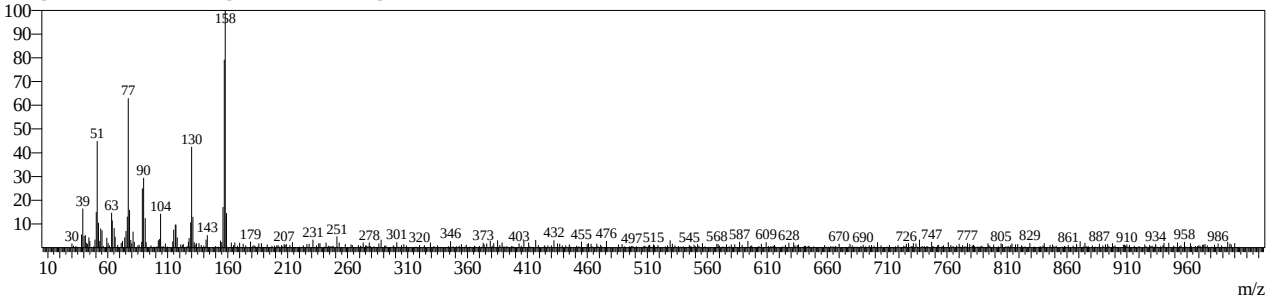
Line#:13 R.Time:11.572(Scan#:5624)
MassPeaks:499
RawMode:Averaged 11.570-11.573(5623-5625) BasePeak:154(23660)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



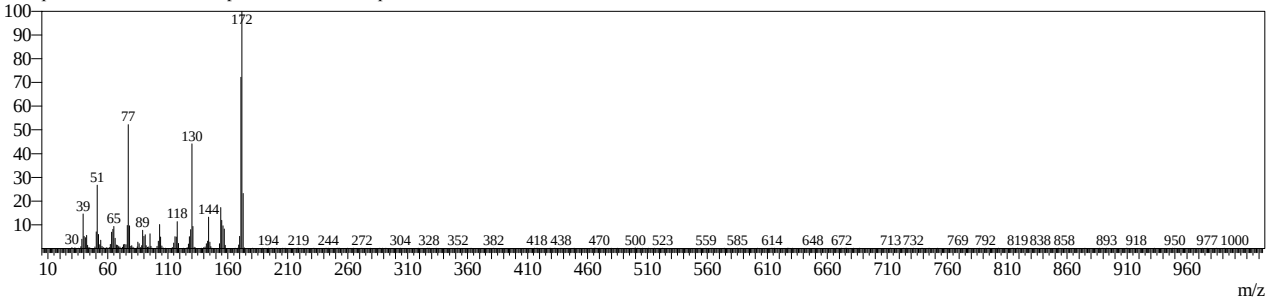
Line#:14 R.Time:11.652(Scan#:5672)
MassPeaks:492
RawMode:Averaged 11.650-11.653(5671-5673) BasePeak:92(35771)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



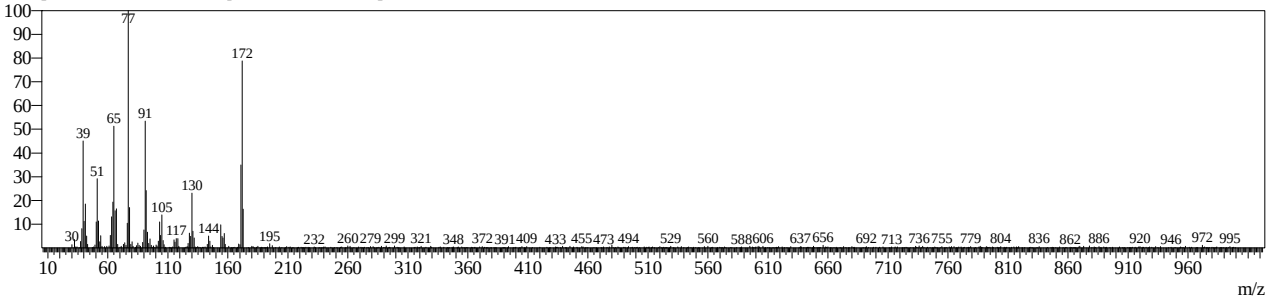
Line#:15 R.Time:11.780(Scan#:5749)
MassPeaks:517
RawMode:Averaged 11.778-11.782(5748-5750) BasePeak:158(5972)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



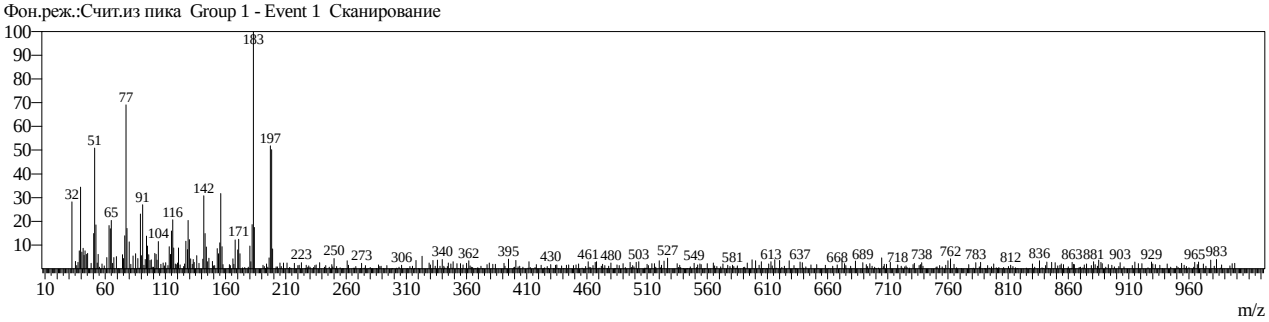
Line#:16 R.Time:12.745(Scan#:6328)
MassPeaks:532
RawMode:Averaged 12.743-12.747(6327-6329) BasePeak:172(118974)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



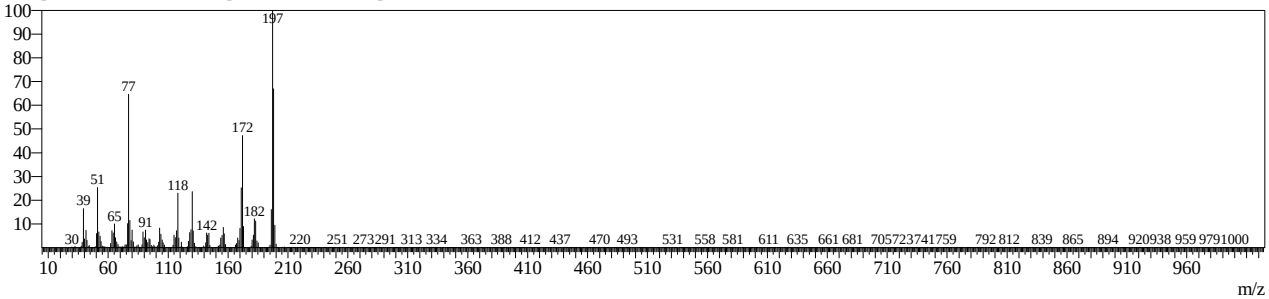
Line#:17 R.Time:14.238(Scan#:7224)
MassPeaks:515
RawMode:Averaged 14.237-14.240(7223-7225) BasePeak:77(18864)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



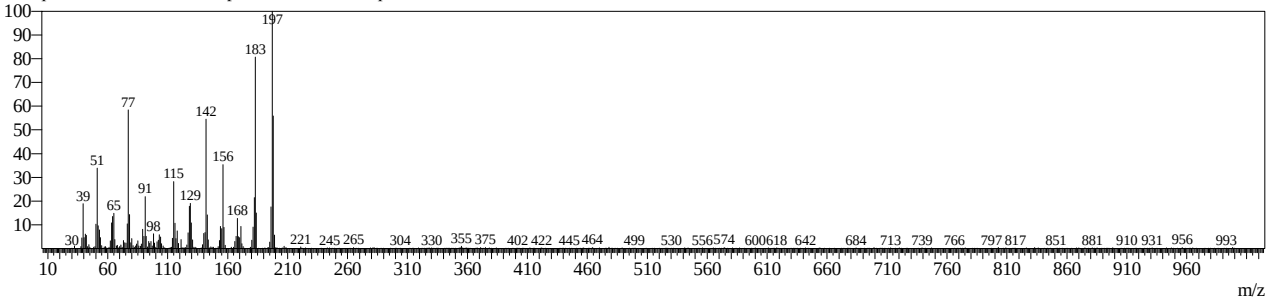
Line#:18 R.Time:14.458(Scan#:7356)
MassPeaks:485
RawMode:Averaged 14.457-14.460(7355-7357) BasePeak:183(3576)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



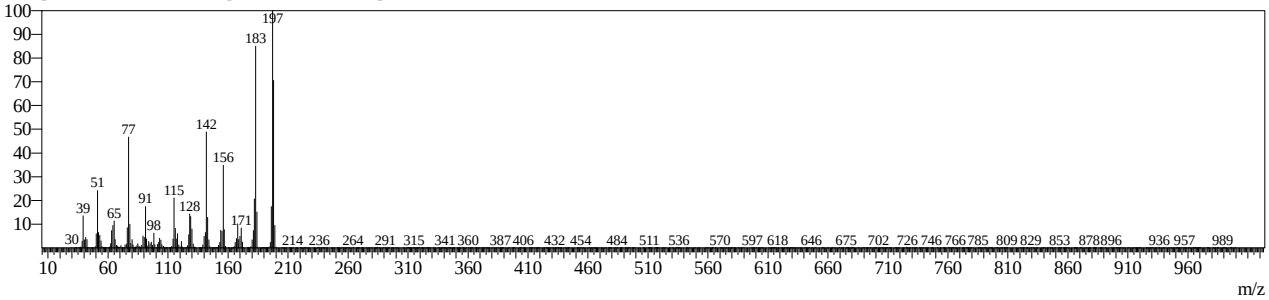
Line#:19 R.Time:14.943(Scan#:7647)
MassPeaks:521
RawMode:Averaged 14.942-14.945(7646-7648) BasePeak:197(139551)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



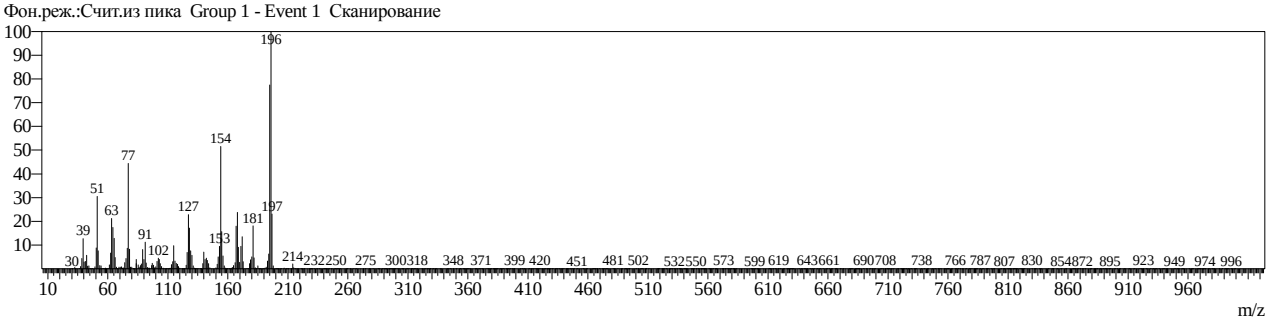
Line#:20 R.Time:15.177(Scan#:7787)
MassPeaks:531
RawMode:Averaged 15.175-15.178(7786-7788) BasePeak:197(41768)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



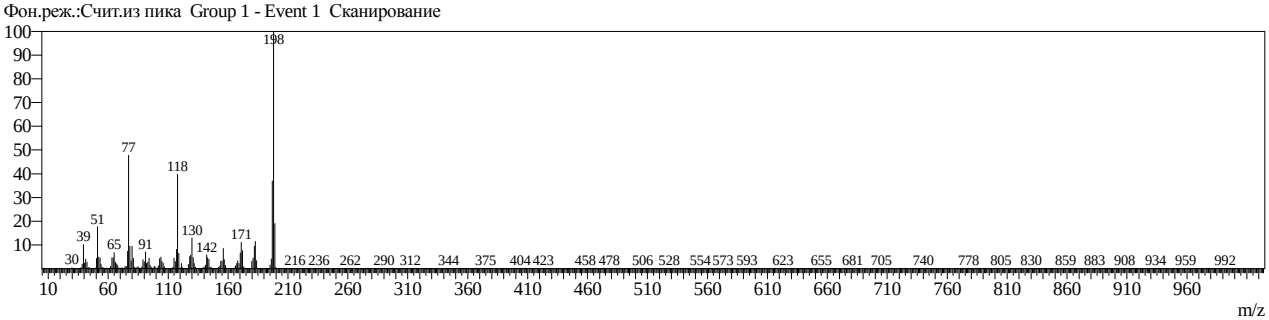
Line#:21 R.Time:15.297(Scan#:7859)
MassPeaks:545
RawMode:Averaged 15.295-15.298(7858-7860) BasePeak:197(526103)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



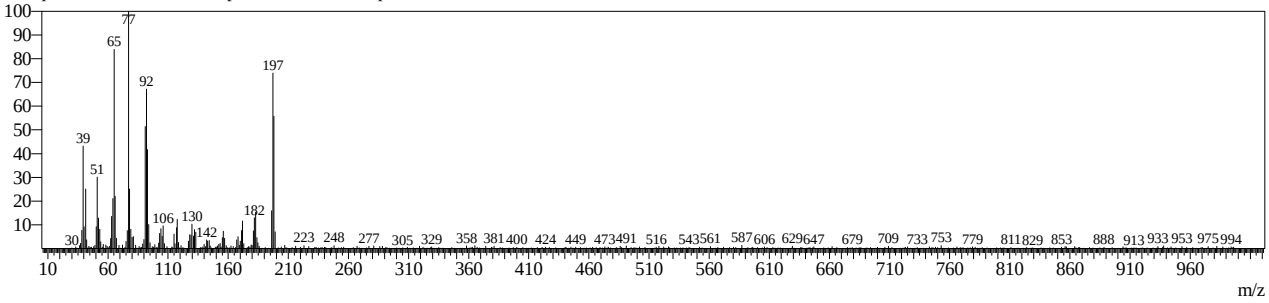
Line#:22 R.Time:15.683(Scan#:8091)
MassPeaks:528
RawMode:Averaged 15.682-15.685(8090-8092) BasePeak:196(104270)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



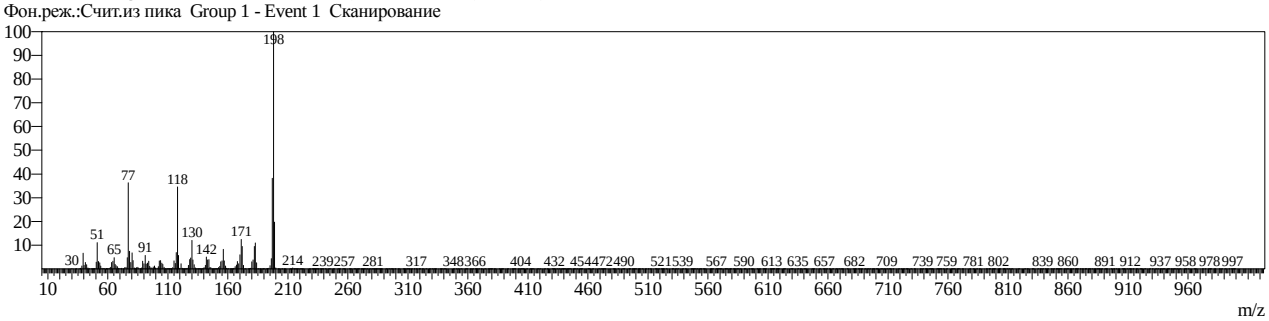
Line#:23 R.Time:15.938(Scan#:8244)
MassPeaks:540
RawMode:Averaged 15.937-15.940(8243-8245) BasePeak:198(436631)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



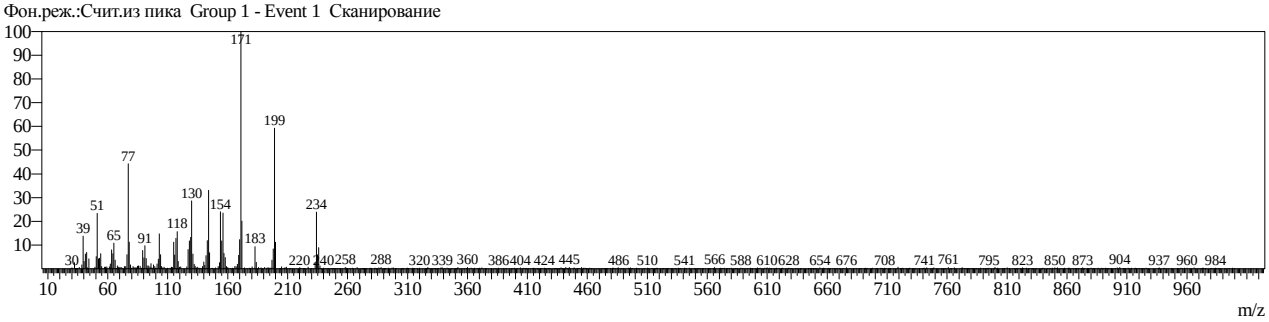
Line#:24 R.Time:16.140(Scan#:8365)
MassPeaks:506
RawMode:Averaged 16.138-16.142(8364-8366) BasePeak:77(15462)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



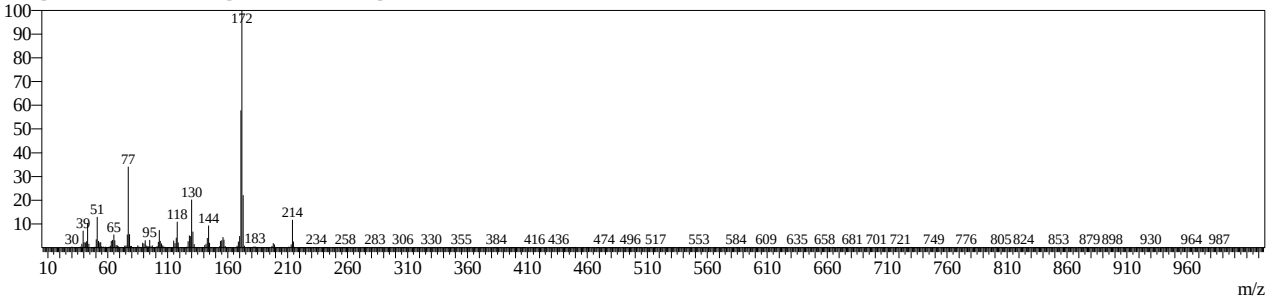
Line#:25 R.Time:16.303(Scan#:8463)
MassPeaks:547
RawMode:Averaged 16.302-16.305(8462-8464) BasePeak:198(2473096)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



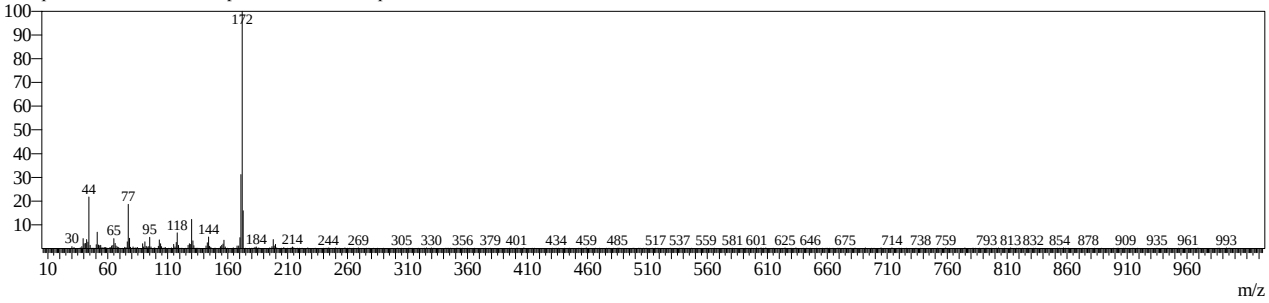
Line#:26 R.Time:16.530(Scan#:8599)
MassPeaks:517
RawMode:Averaged 16.528-16.532(8598-8600) BasePeak:171(26797)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



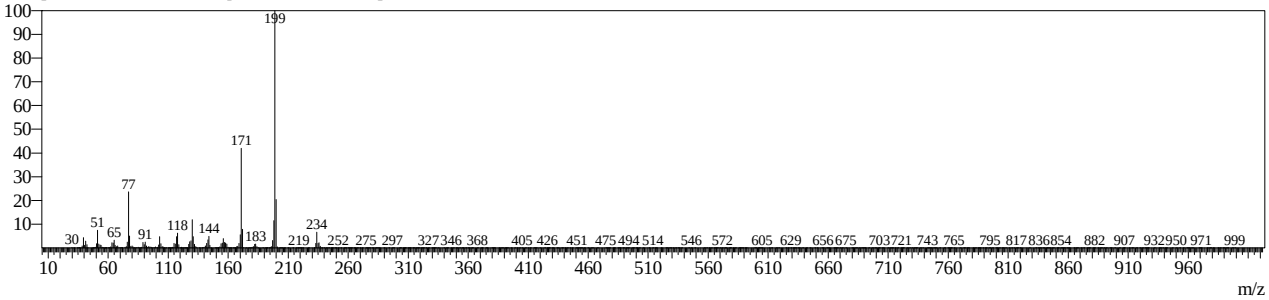
Line#:27 R.Time:16.957(Scan#:8855)
MassPeaks:523
RawMode:Averaged 16.955-16.958(8854-8856) BasePeak:172(178715)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



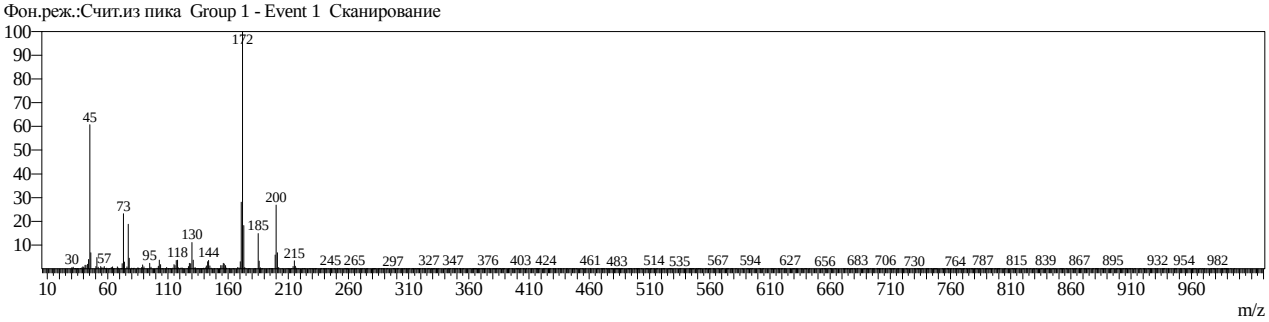
Line#:28 R.Time:17.102(Scan#:8942)
MassPeaks:534
RawMode:Averaged 17.100-17.103(8941-8943) BasePeak:172(62156)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



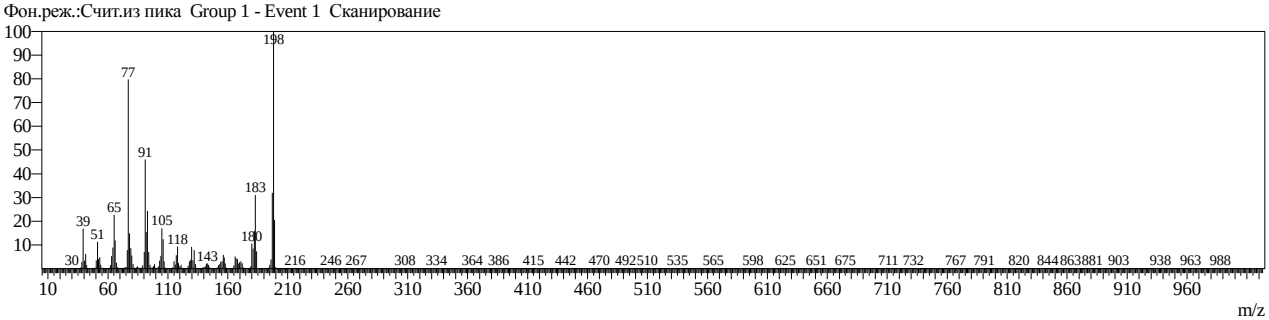
Line#:29 R.Time:17.252(Scan#:9032)
MassPeaks:550
RawMode:Averaged 17.250-17.253(9031-9033) BasePeak:199(1639568)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



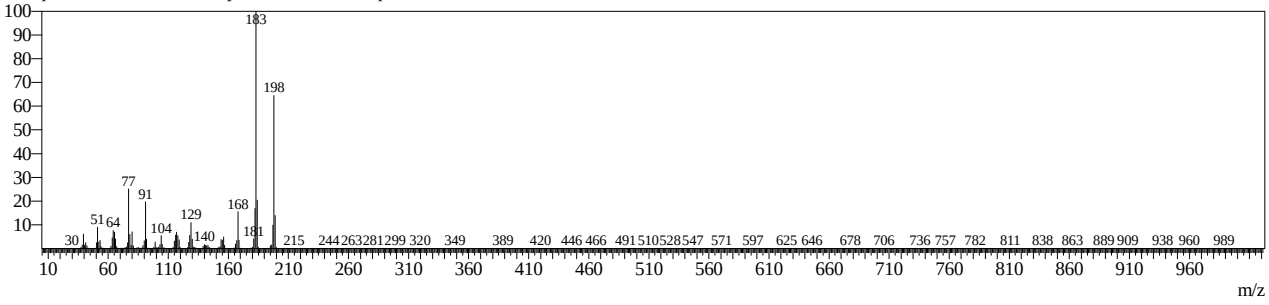
Line#:30 R.Time:17.332(Scan#:9080)
MassPeaks:487
RawMode:Averaged 17.330-17.333(9079-9081) BasePeak:172(109176)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



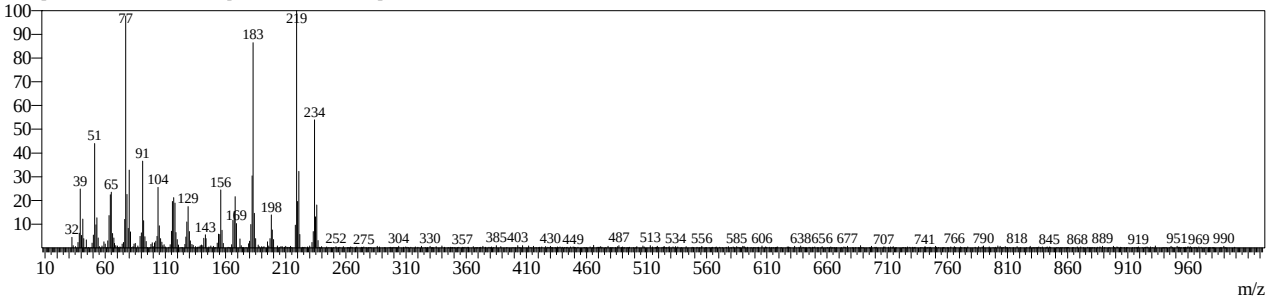
Line#:31 R.Time:17.475(Scan#:9166)
MassPeaks:546
RawMode:Averaged 17.473-17.477(9165-9167) BasePeak:198(2310826)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



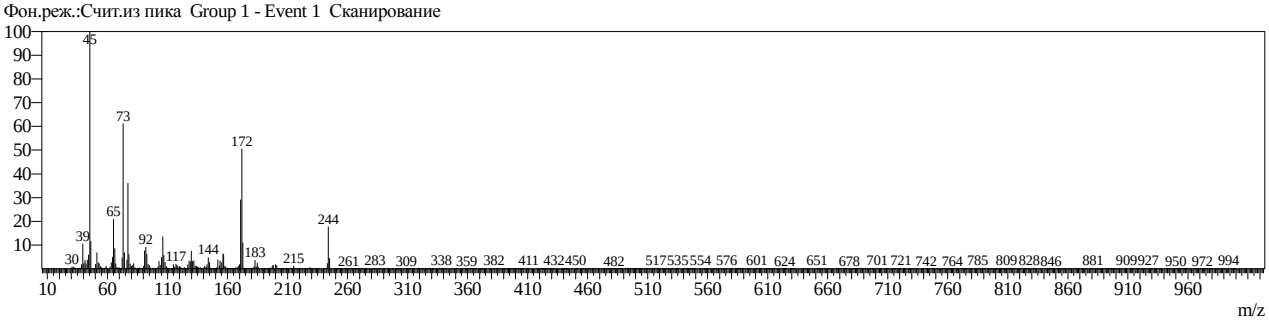
Line#:32 R.Time:17.570(Scan#:9223)
MassPeaks:558
RawMode:Averaged 17.568-17.572(9222-9224) BasePeak:183(2795211)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



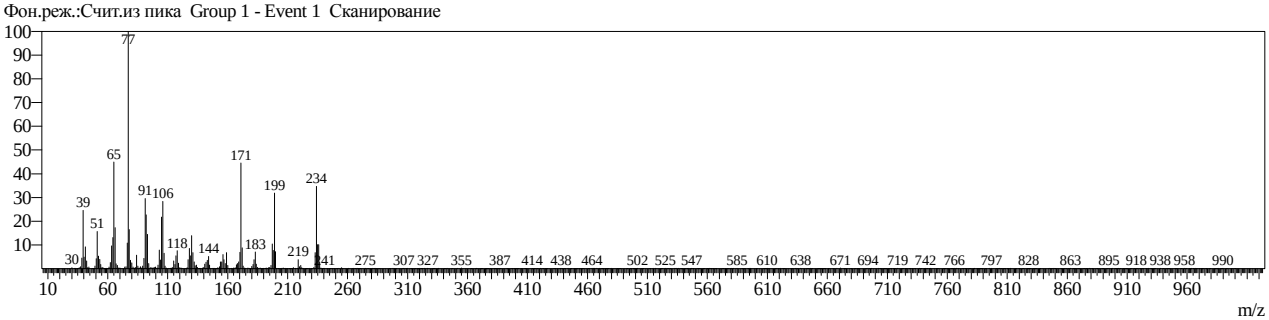
Line#:33 R.Time:17.953(Scan#:9453)
MassPeaks:543
RawMode:Averaged 17.952-17.955(9452-9454) BasePeak:219(18094)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



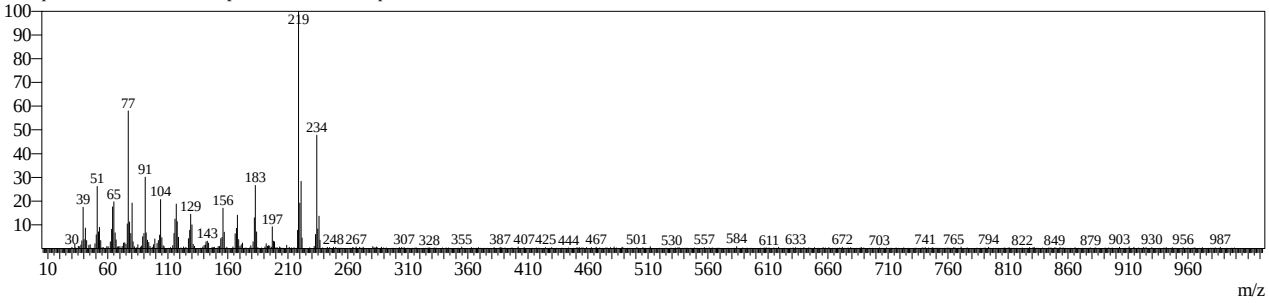
Line#:34 R.Time:18.325(Scan#:9676)
MassPeaks:539
RawMode:Averaged 18.323-18.327(9675-9677) BasePeak:45(152333)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



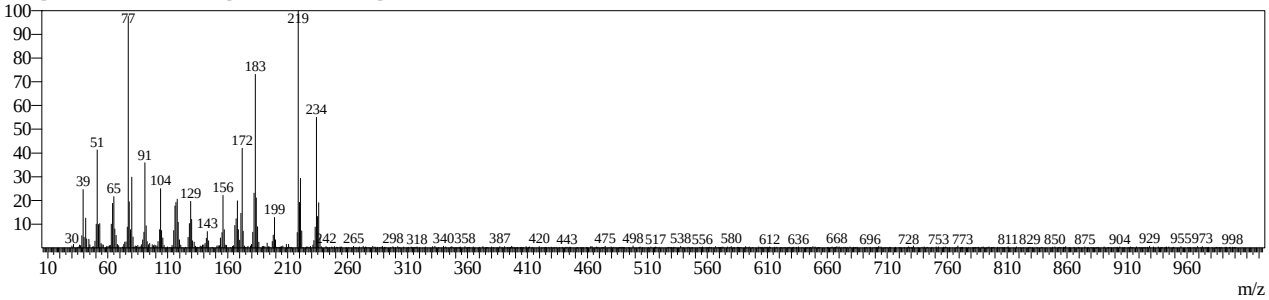
Line#:35 R.Time:18.400(Scan#:9721)
MassPeaks:544
RawMode:Averaged 18.398-18.402(9720-9722) BasePeak:77(115630)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



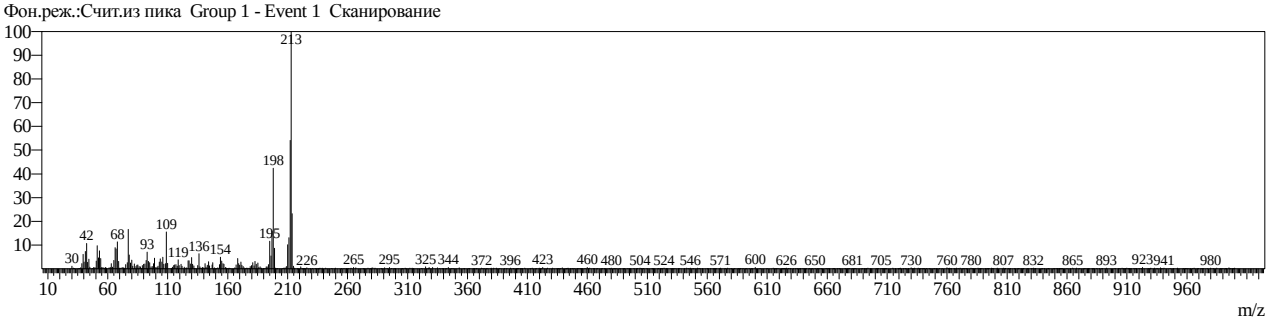
Line#:36 R.Time:18.842(Scan#:9986)
MassPeaks:543
RawMode:Averaged 18.840-18.843(9985-9987) BasePeak:219(24662)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



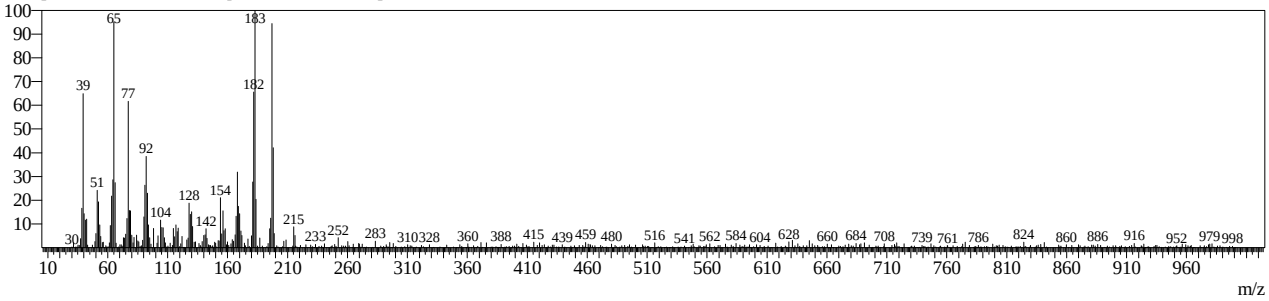
Line#:37 R.Time:18.957(Scan#:10055)
MassPeaks:536
RawMode:Averaged 18.955-18.958(10054-10056) BasePeak:219(22128)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



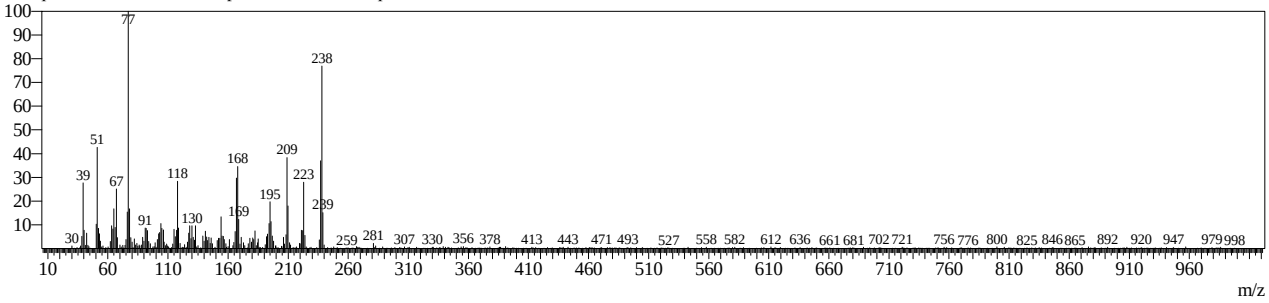
Line#:38 R.Time:19.225(Scan#:10216)
MassPeaks:535
RawMode:Averaged 19.223-19.227(10215-10217) BasePeak:213(37231)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



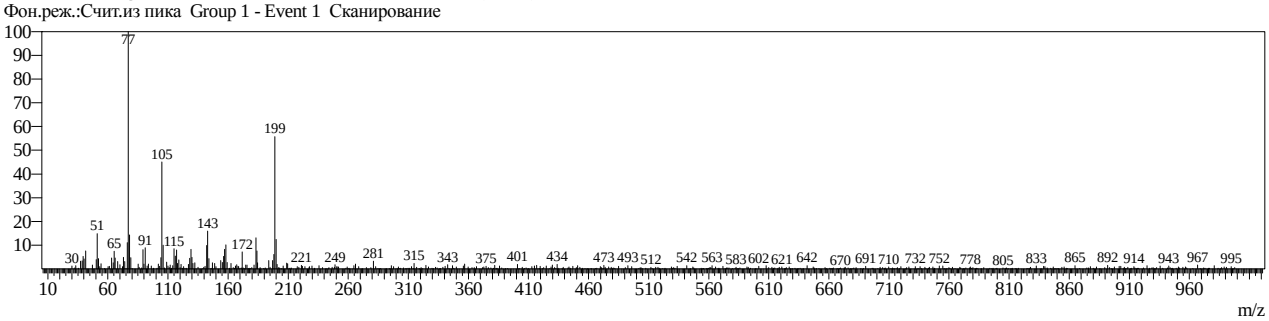
Line#:39 R.Time:19.325(Scan#:10276)
MassPeaks:536
RawMode:Averaged 19.323-19.327(10275-10277) BasePeak:183(6260)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



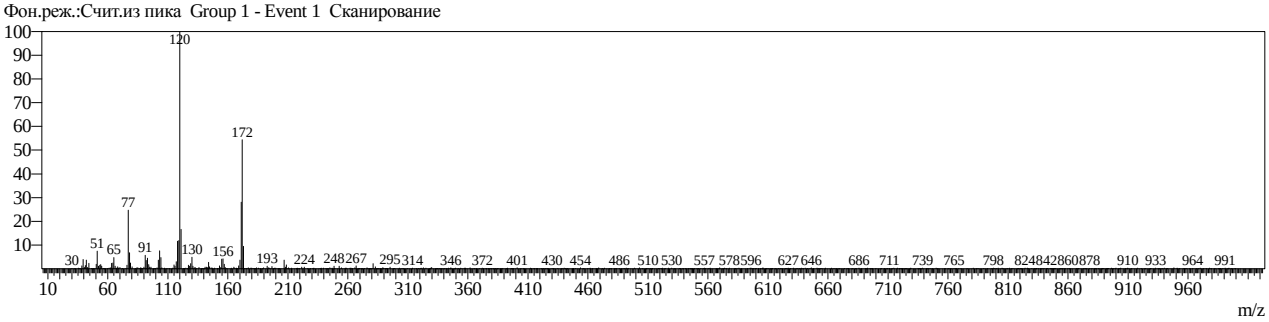
Line#:40 R.Time:21.002(Scan#:11282)
MassPeaks:560
RawMode:Averaged 21.000-21.003(11281-11283) BasePeak:77(22176)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



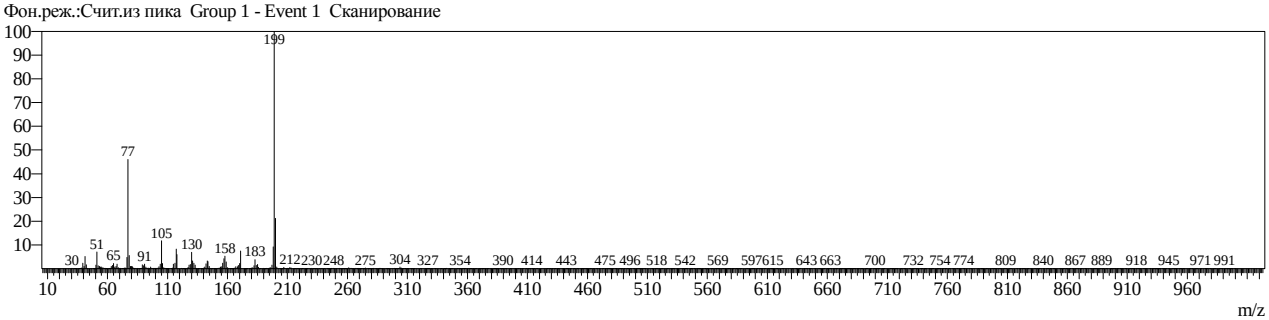
Line#:41 R.Time:22.695(Scan#:12298)
MassPeaks:507
RawMode:Averaged 22.693-22.697(12297-12299) BasePeak:77(10518)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



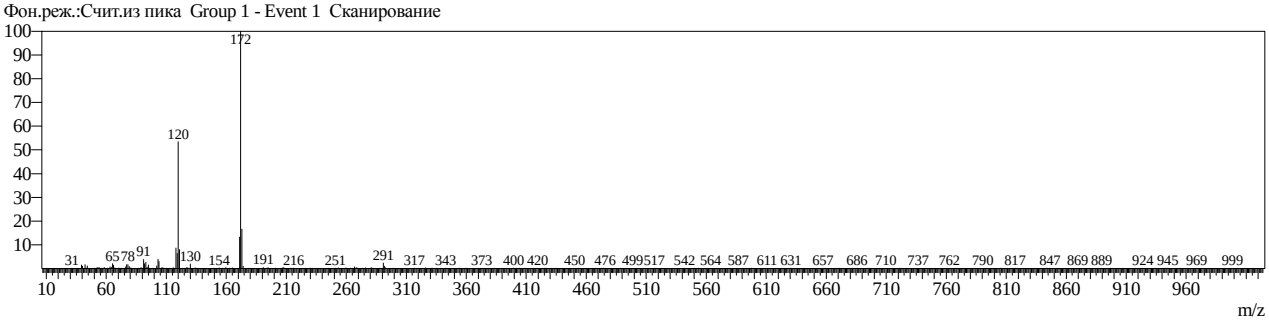
Line#:42 R.Time:22.977(Scan#:12467)
MassPeaks:533
RawMode:Averaged 22.975-22.978(12466-12468) BasePeak:120(43271)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



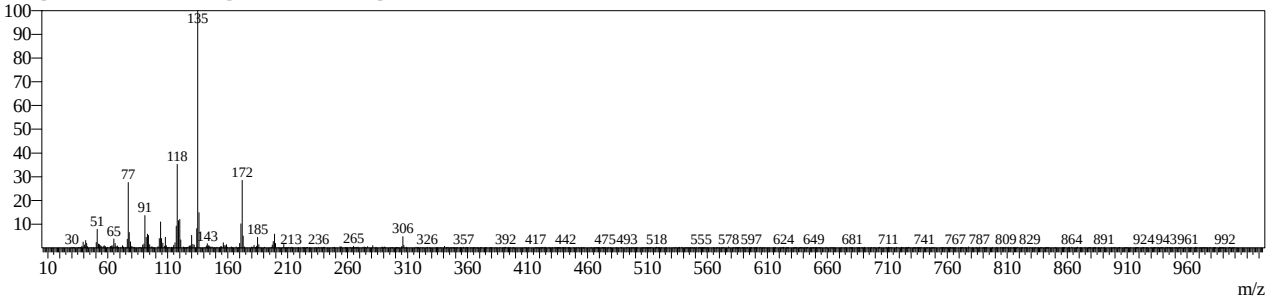
Line#:43 R.Time:23.600(Scan#:12841)
MassPeaks:563
RawMode:Averaged 23.598-23.602(12840-12842) BasePeak:199(432724)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



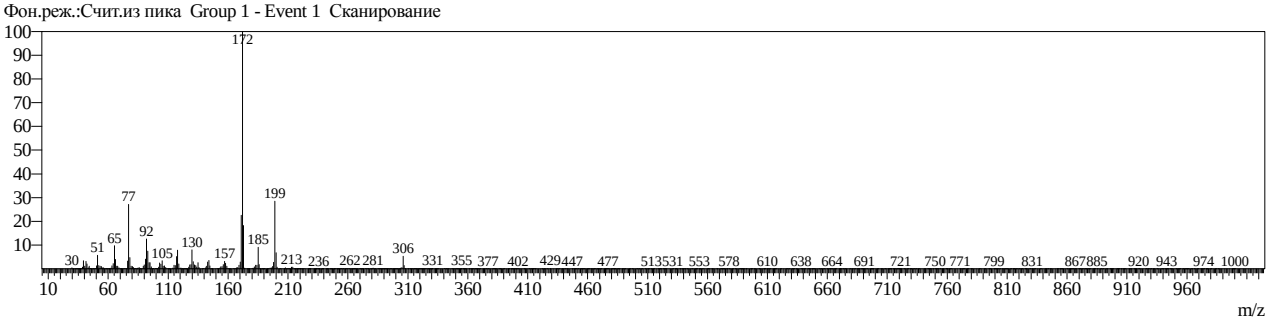
Line#:44 R.Time:23.648(Scan#:12870)
MassPeaks:522
RawMode:Averaged 23.647-23.650(12869-12871) BasePeak:172(125278)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



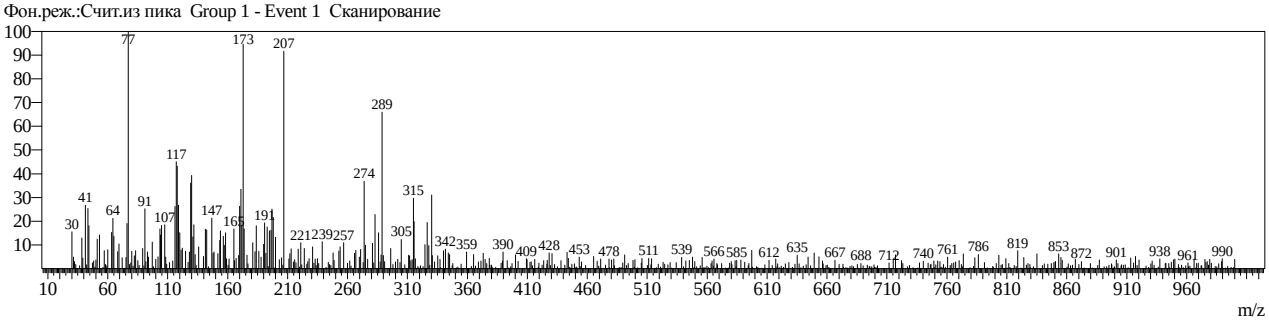
Line#:45 R.Time:25.303(Scan#:13863)
MassPeaks:514
RawMode:Averaged 25.302-25.305(13862-13864) BasePeak:135(58397)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



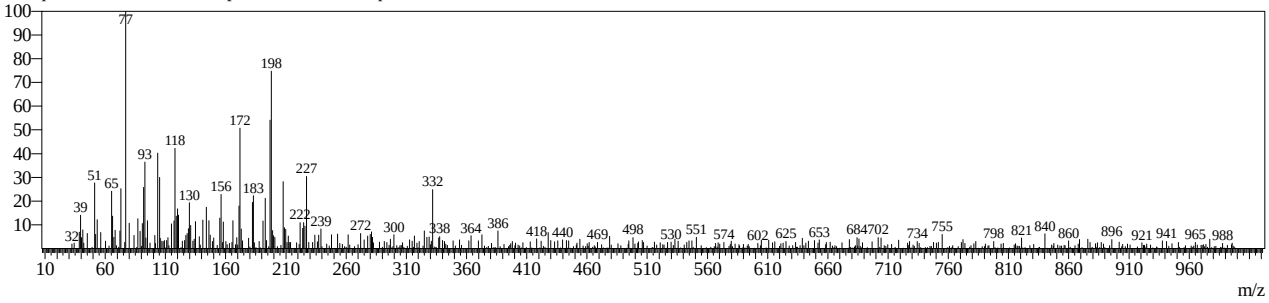
Line#:46 R.Time:25.823(Scan#:14175)
MassPeaks:574
RawMode:Averaged 25.822-25.825(14174-14176) BasePeak:172(311050)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



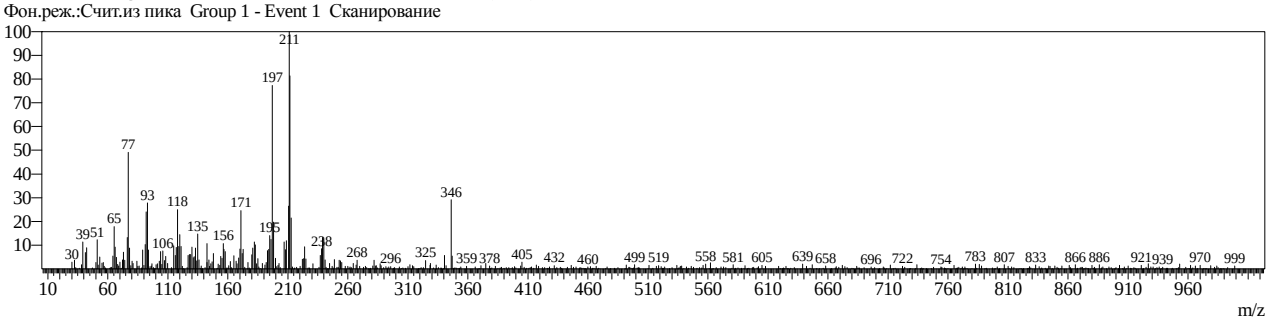
Line#:47 R.Time:27.362(Scan#:15098)
MassPeaks:562
RawMode:Averaged 27.360-27.363(15097-15099) BasePeak:77(2254)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



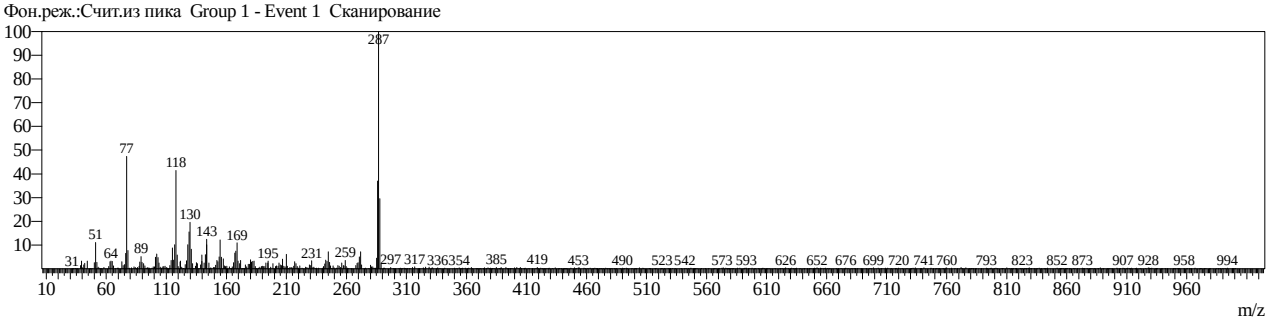
Line#:48 R.Time:28.363(Scan#:15699)
MassPeaks:515
RawMode:Averaged 28.362-28.365(15698-15700) BasePeak:77(2819)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



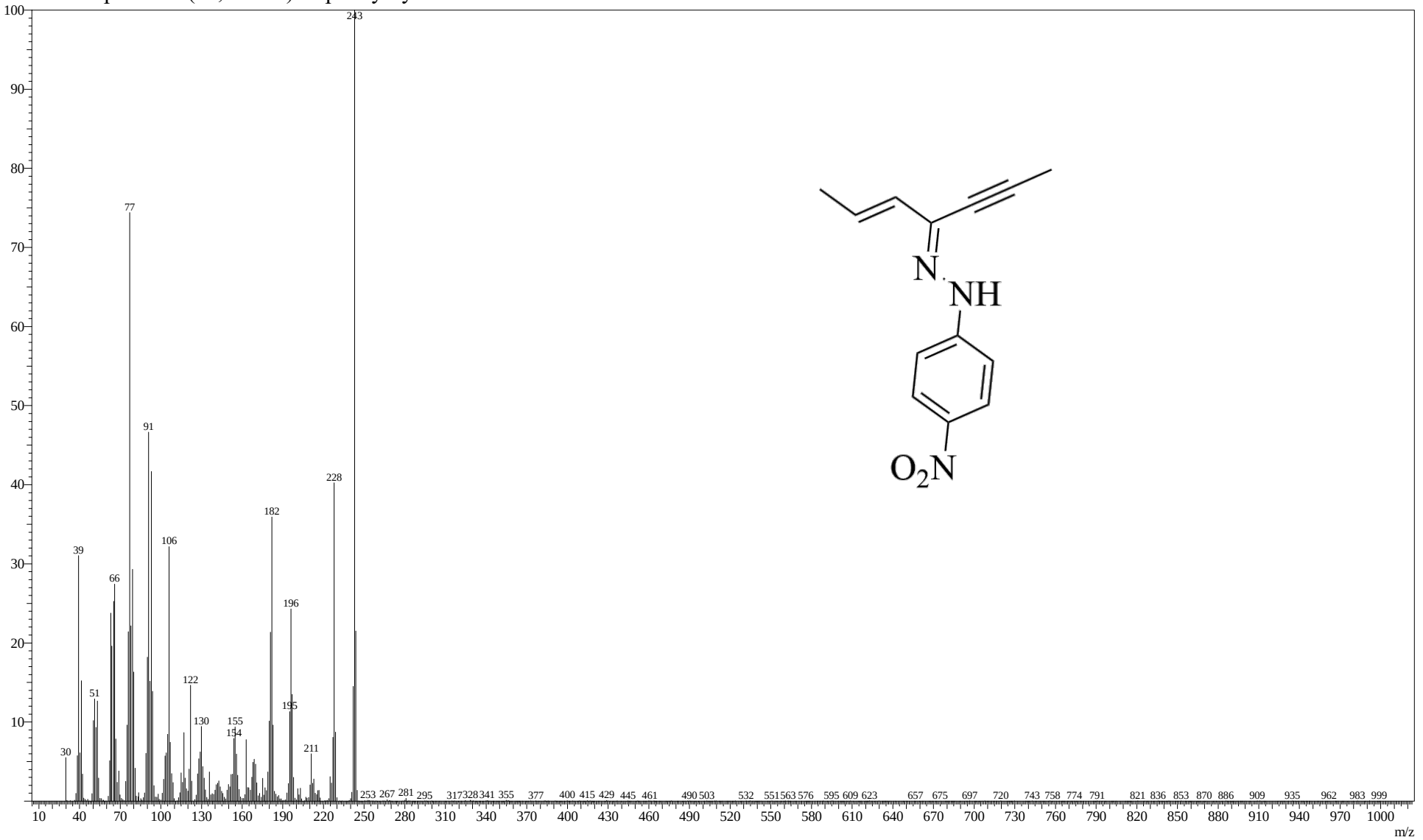
Line#:49 R.Time:30.087(Scan#:16733)
MassPeaks:527
RawMode:Averaged 30.085-30.088(16732-16734) BasePeak:211(7749)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



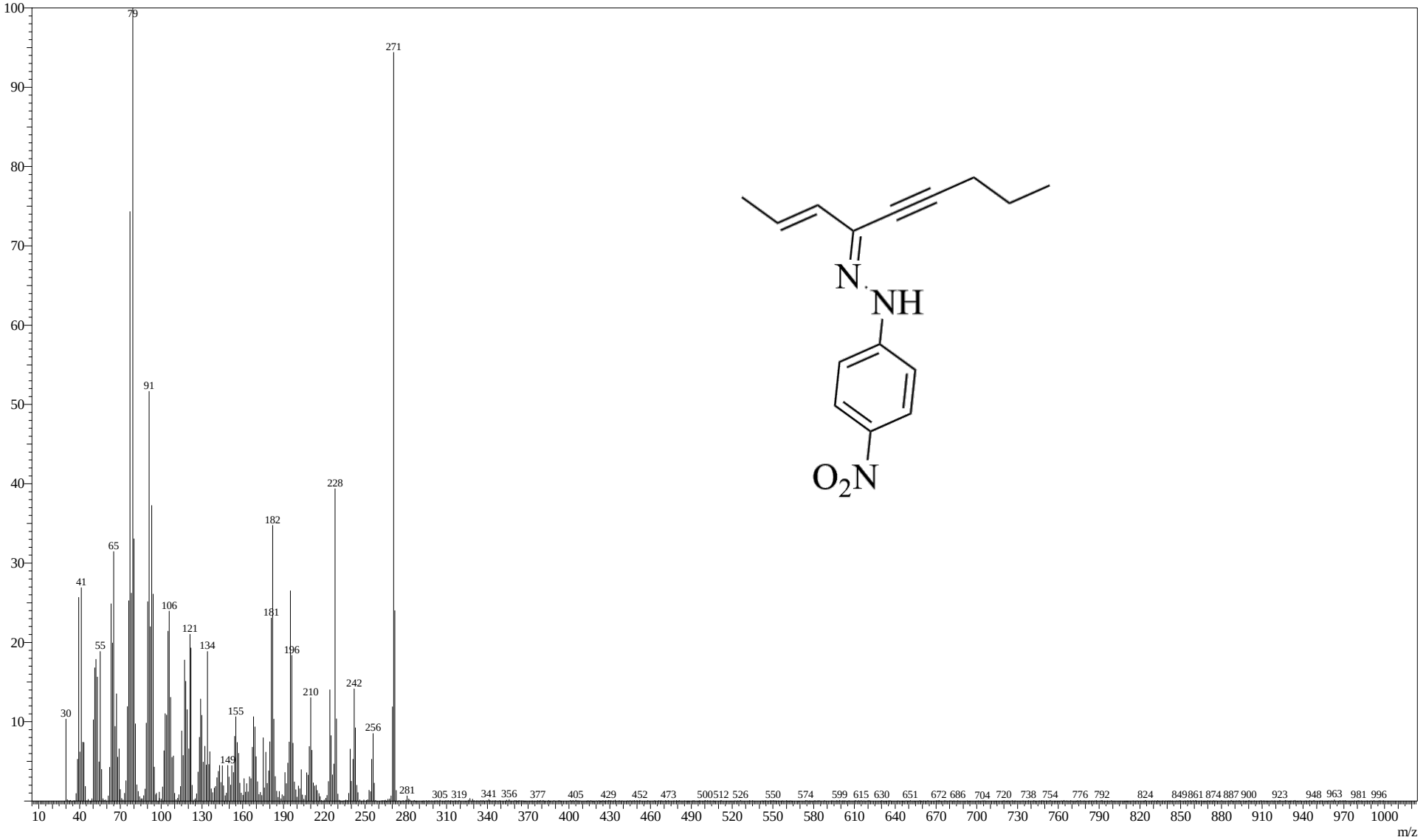
Line#:50 R.Time:31.375(Scan#:17506)
MassPeaks:567
RawMode:Averaged 31.373-31.377(17505-17507) BasePeak:287(37236)
Фон.реж.:Счит.из пика Group 1 - Event 1 Сканирование



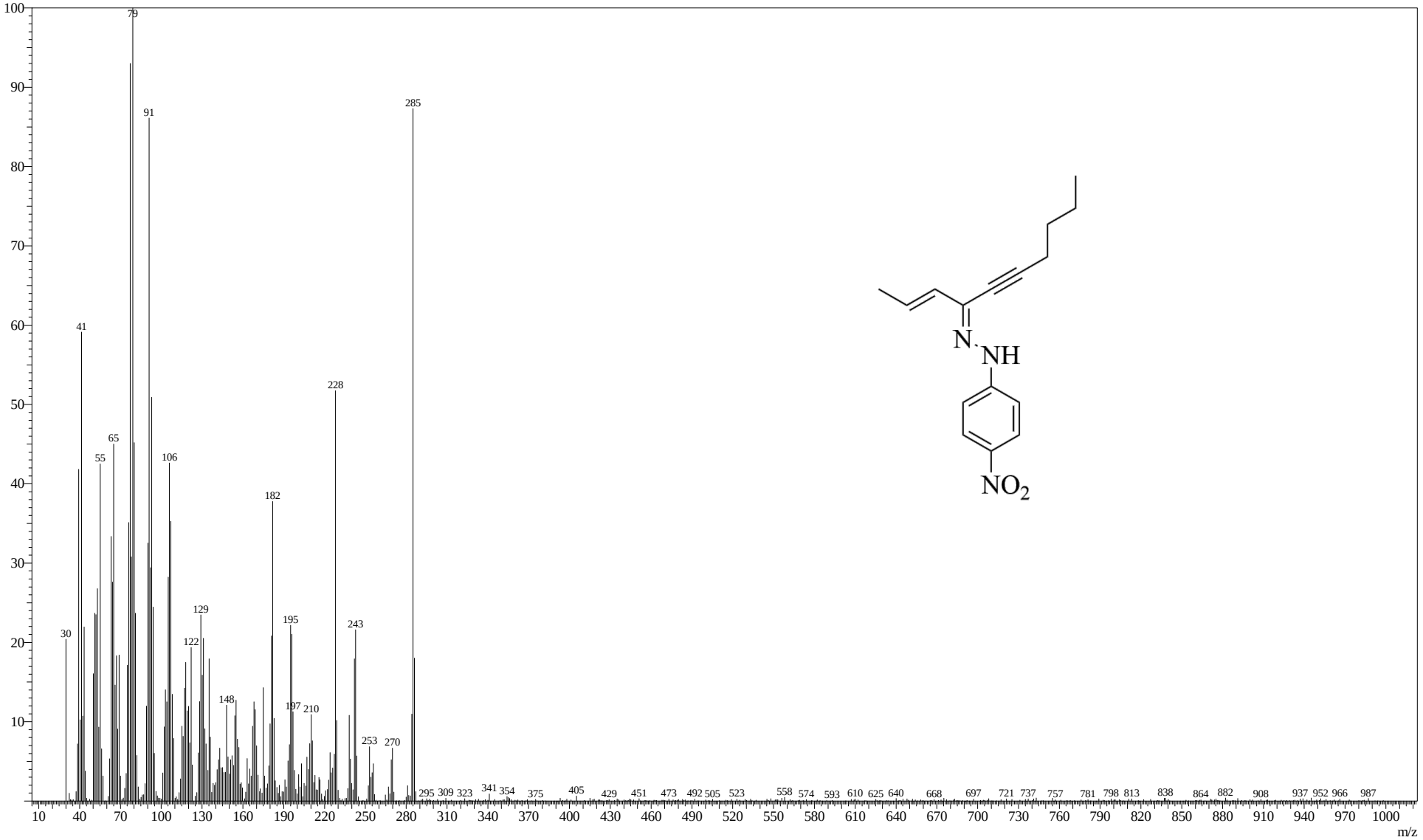
Mass spectrum (EI, 70 eV) of phenylhydrazone **5ab**



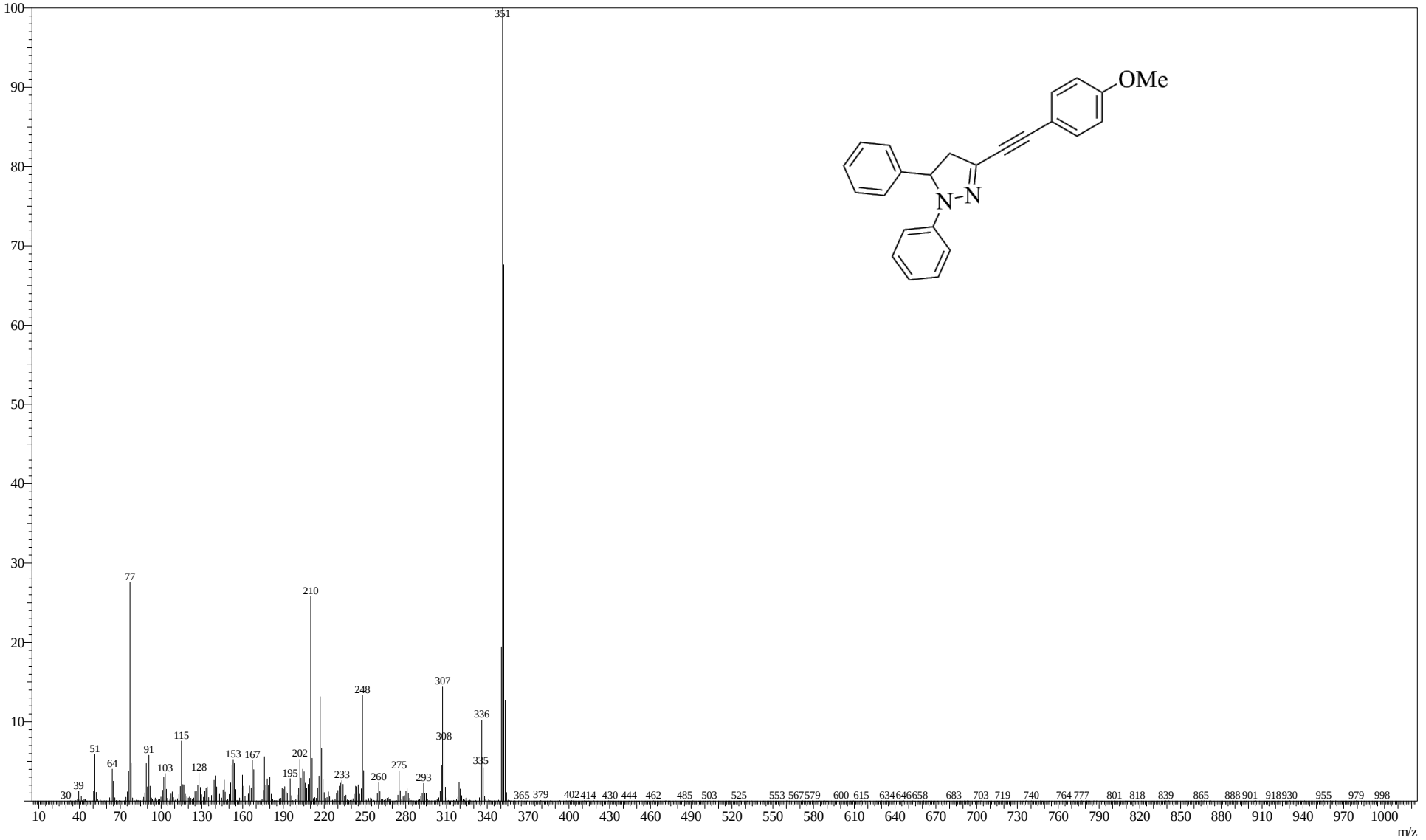
Mass spectrum (EI, 70 eV) of 4-nitrophenylhydrazone **5ac**



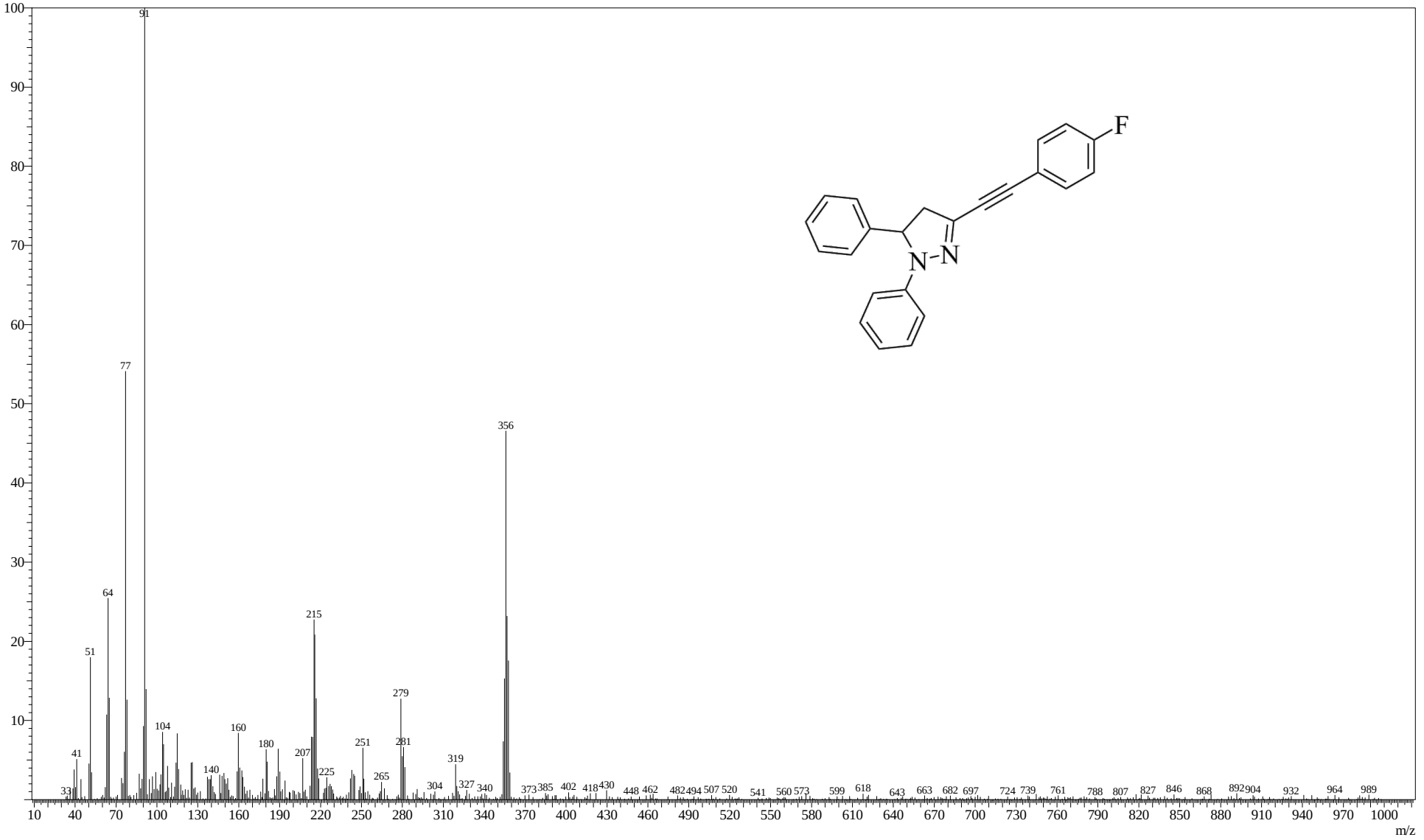
Mass spectrum (EI, 70 eV) of 4-nitrophenylhydrazone **5ad**



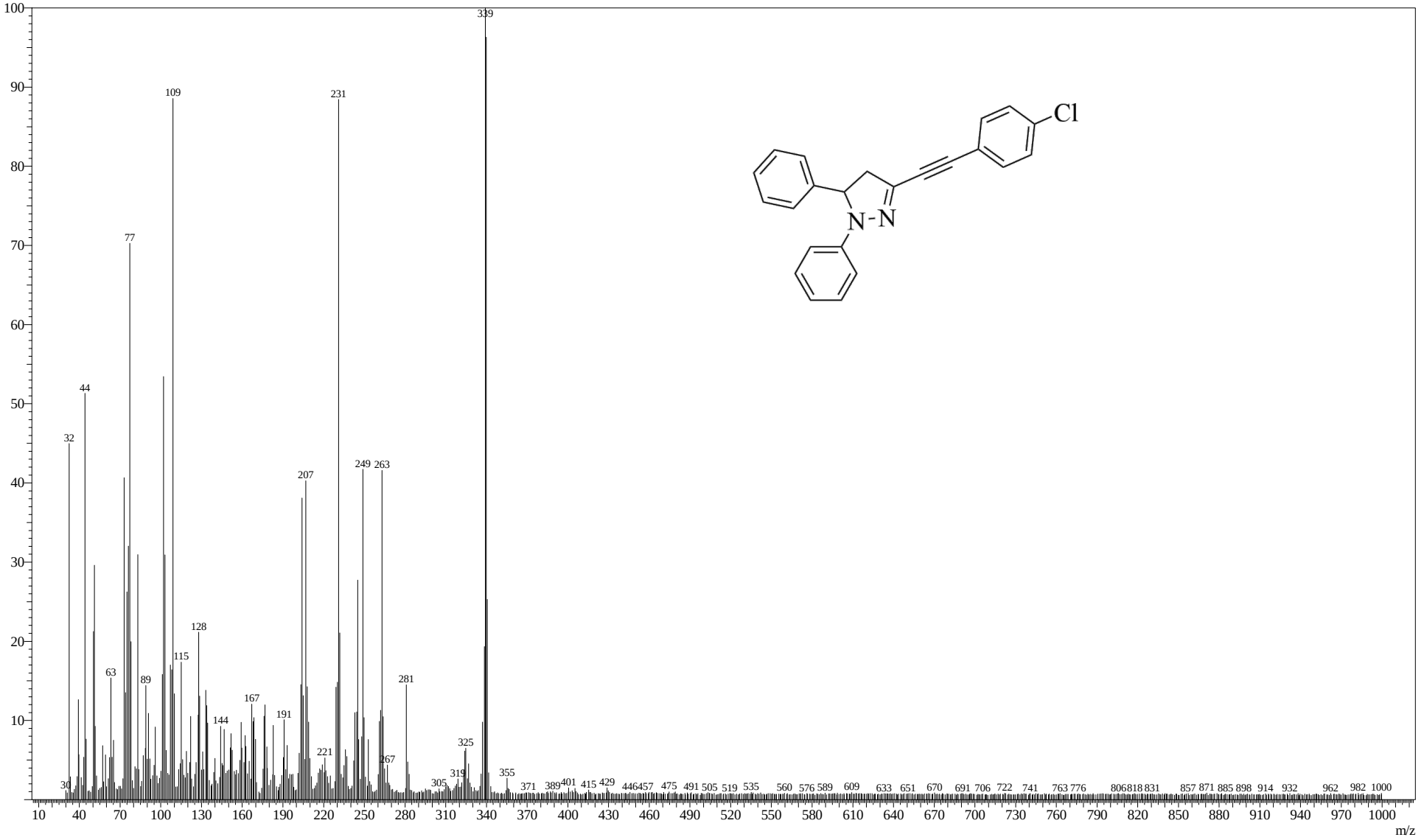
Mass spectrum (EI, 70 eV) of 4,5-dihydro-1*H*-pyrazole **6a**



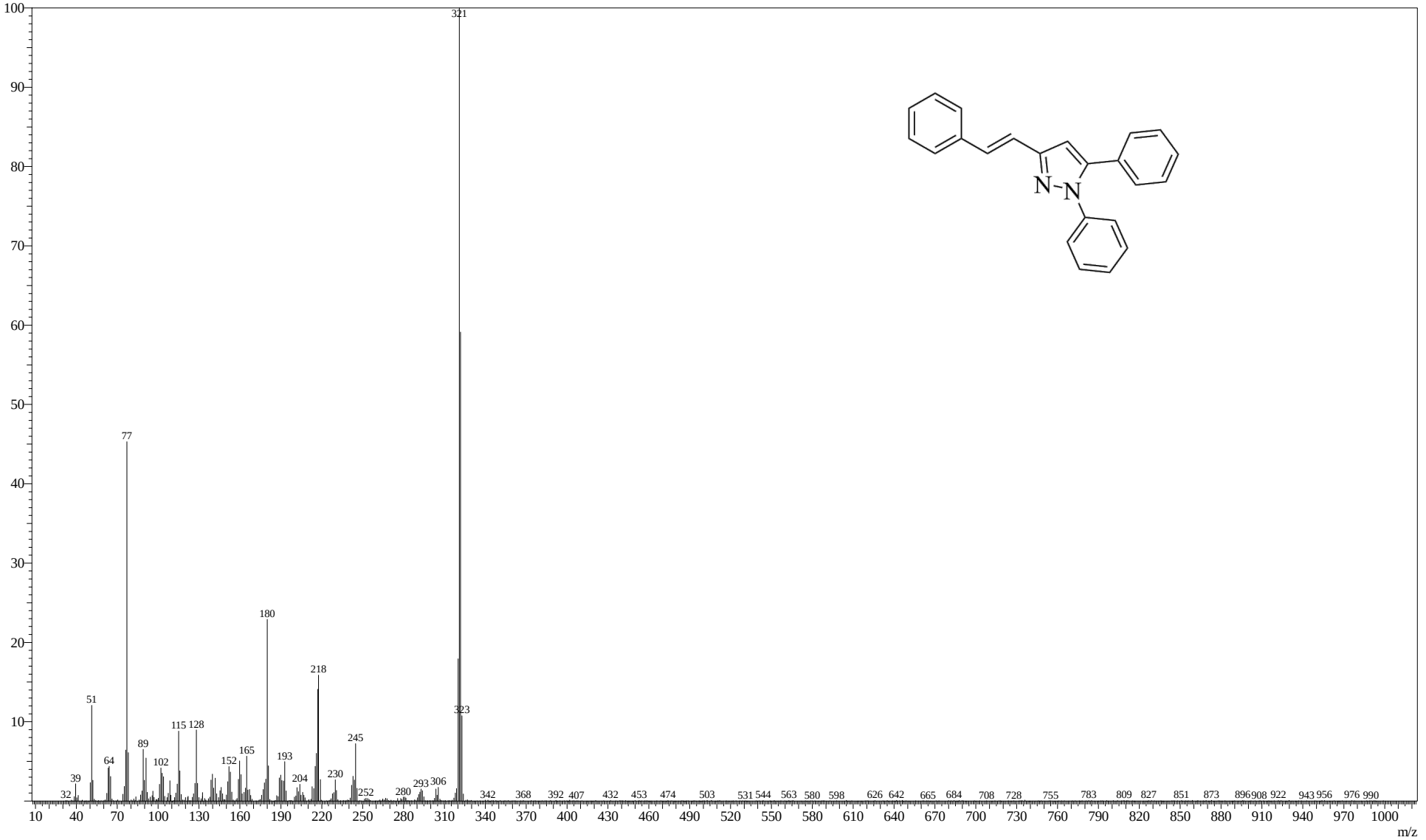
Mass spectrum (EI, 70 eV) of 4,5-dihydro-1*H*-pyrazole **6b**



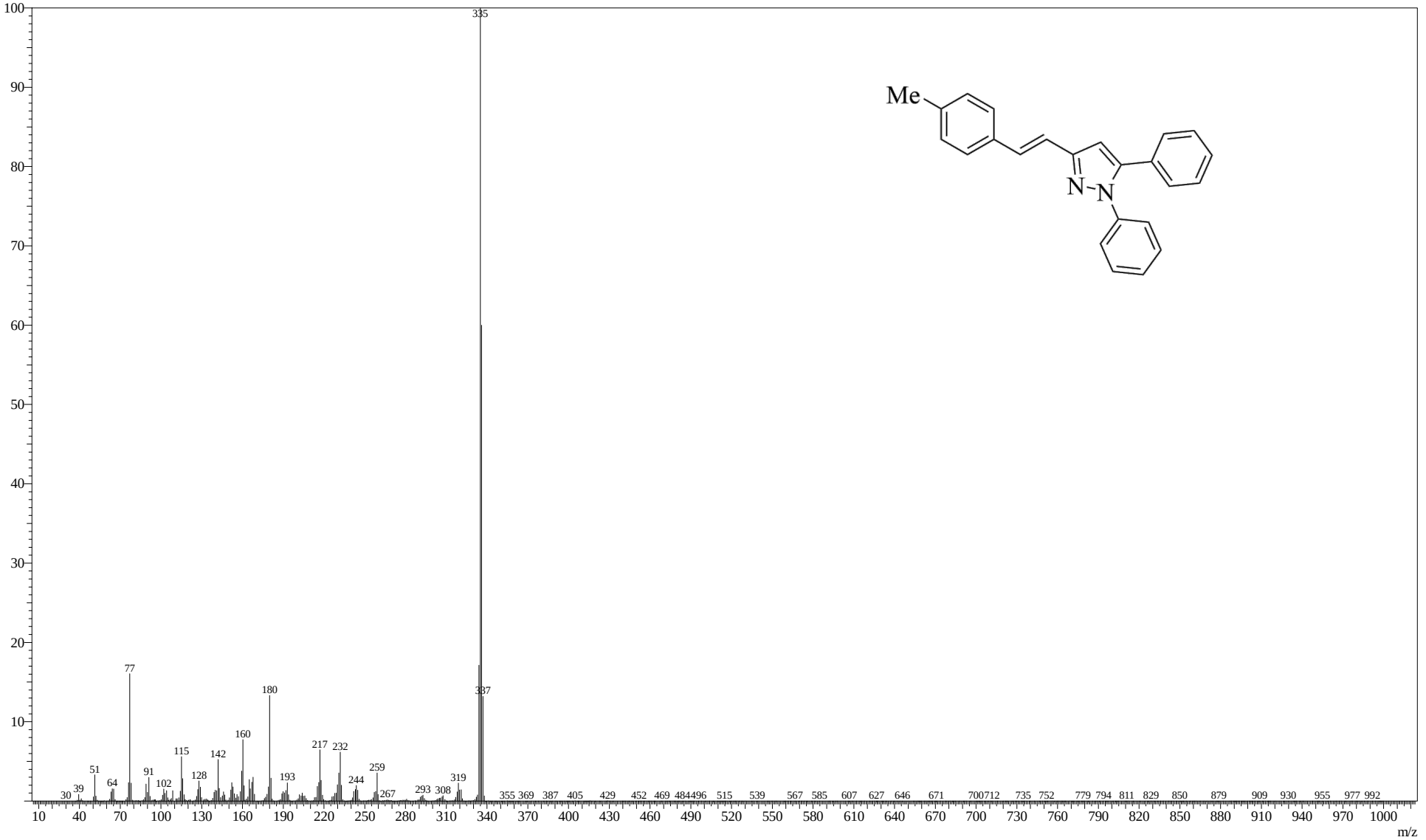
Mass spectrum (EI, 70 eV) of enynone **6c**



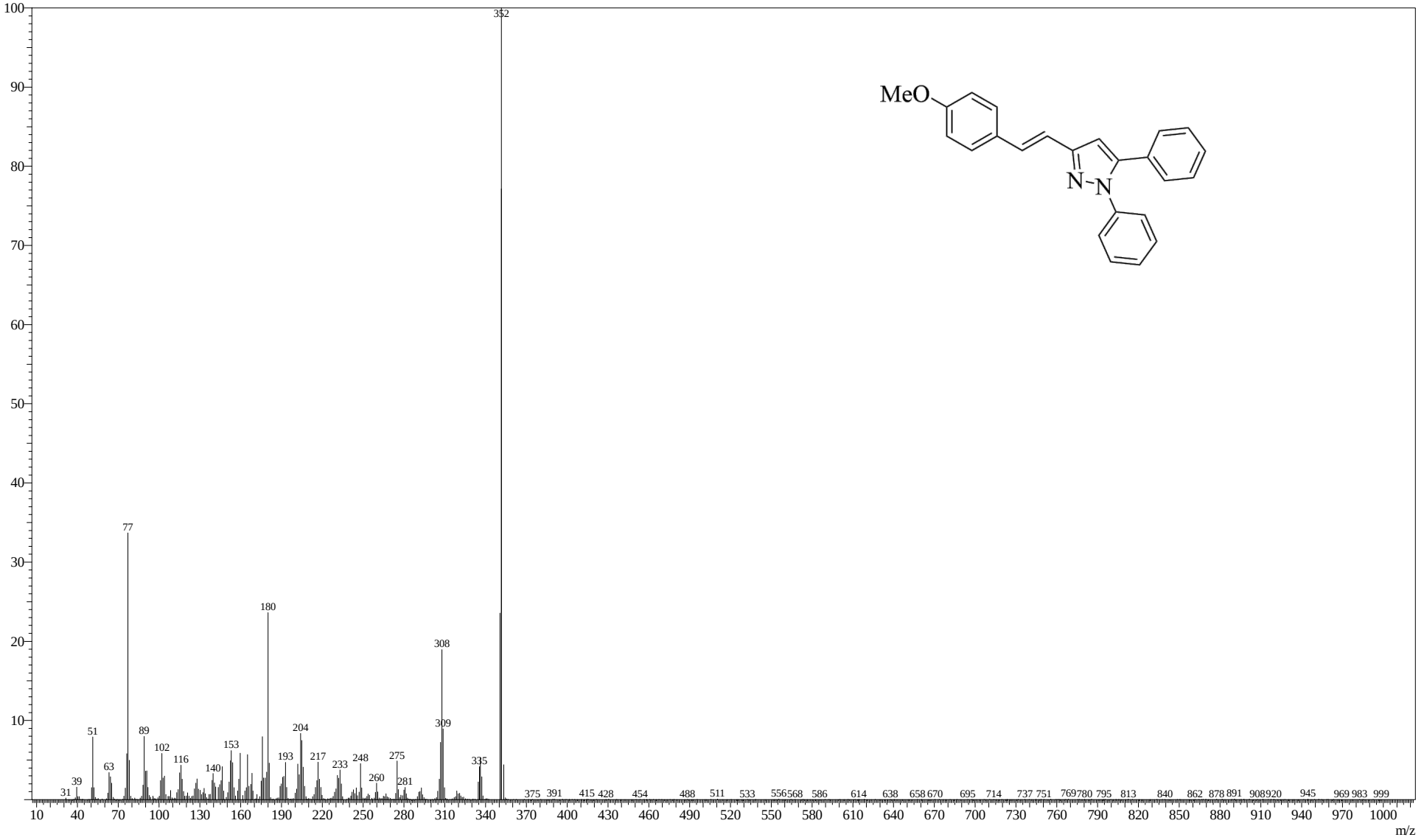
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4a**



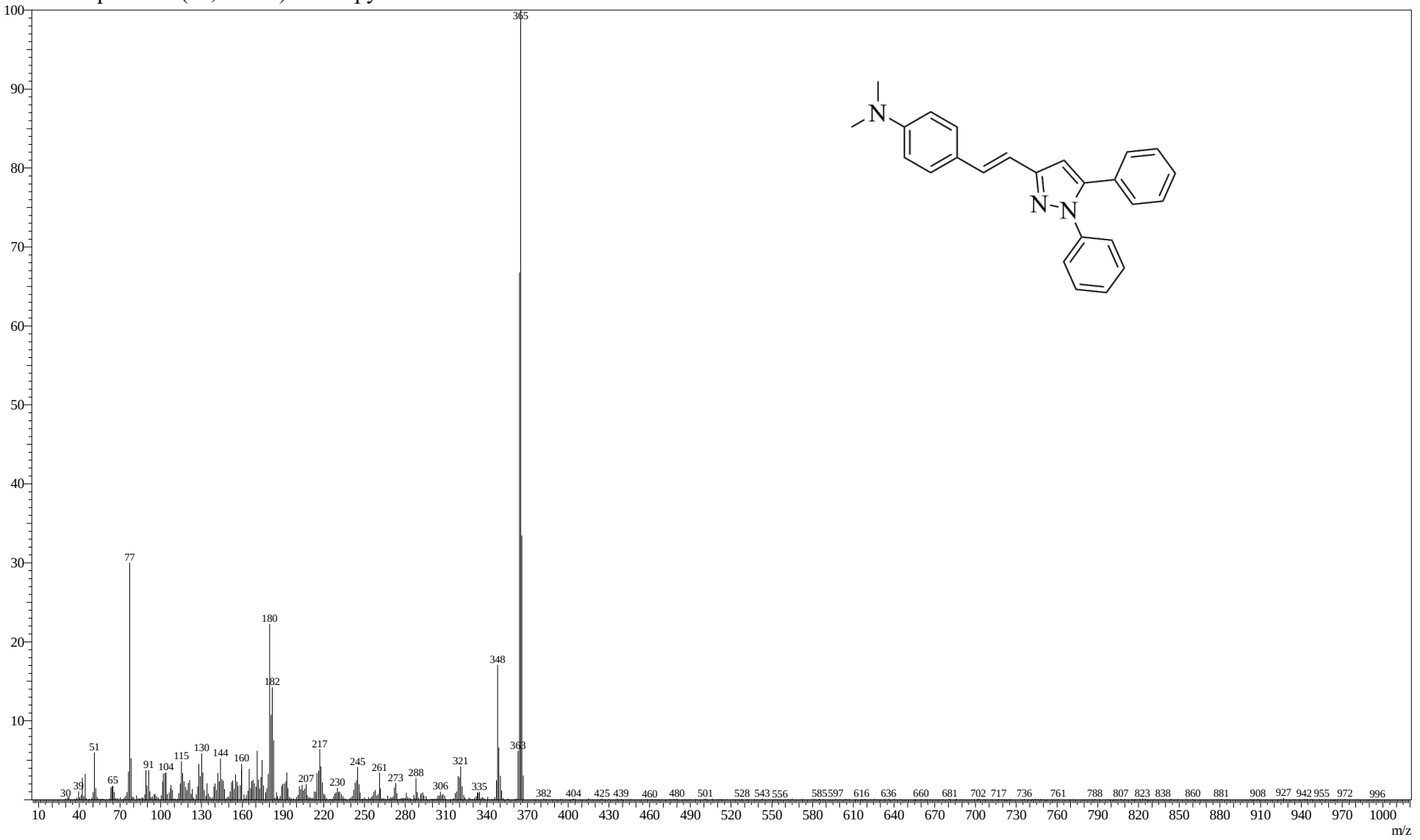
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4b**



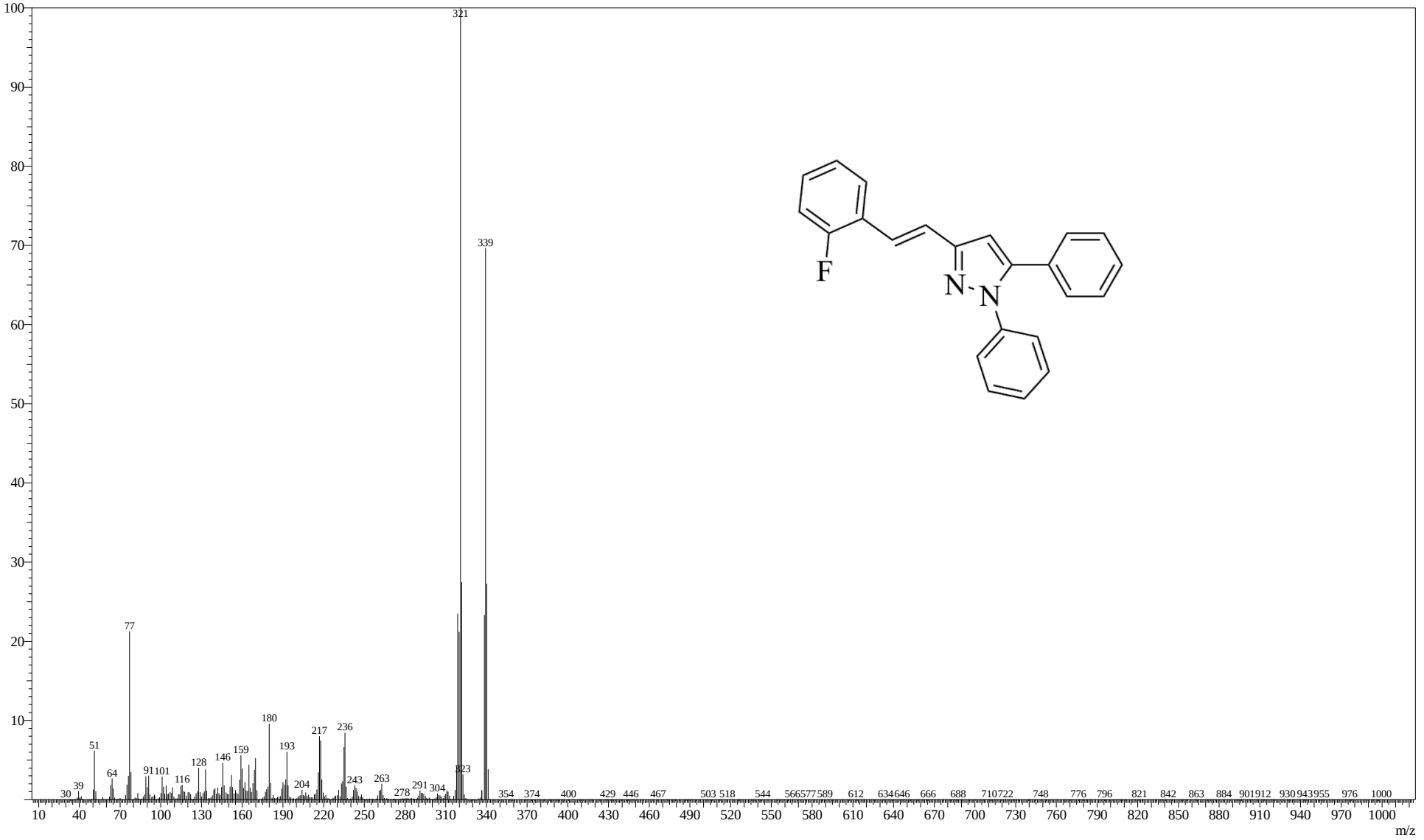
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4c**



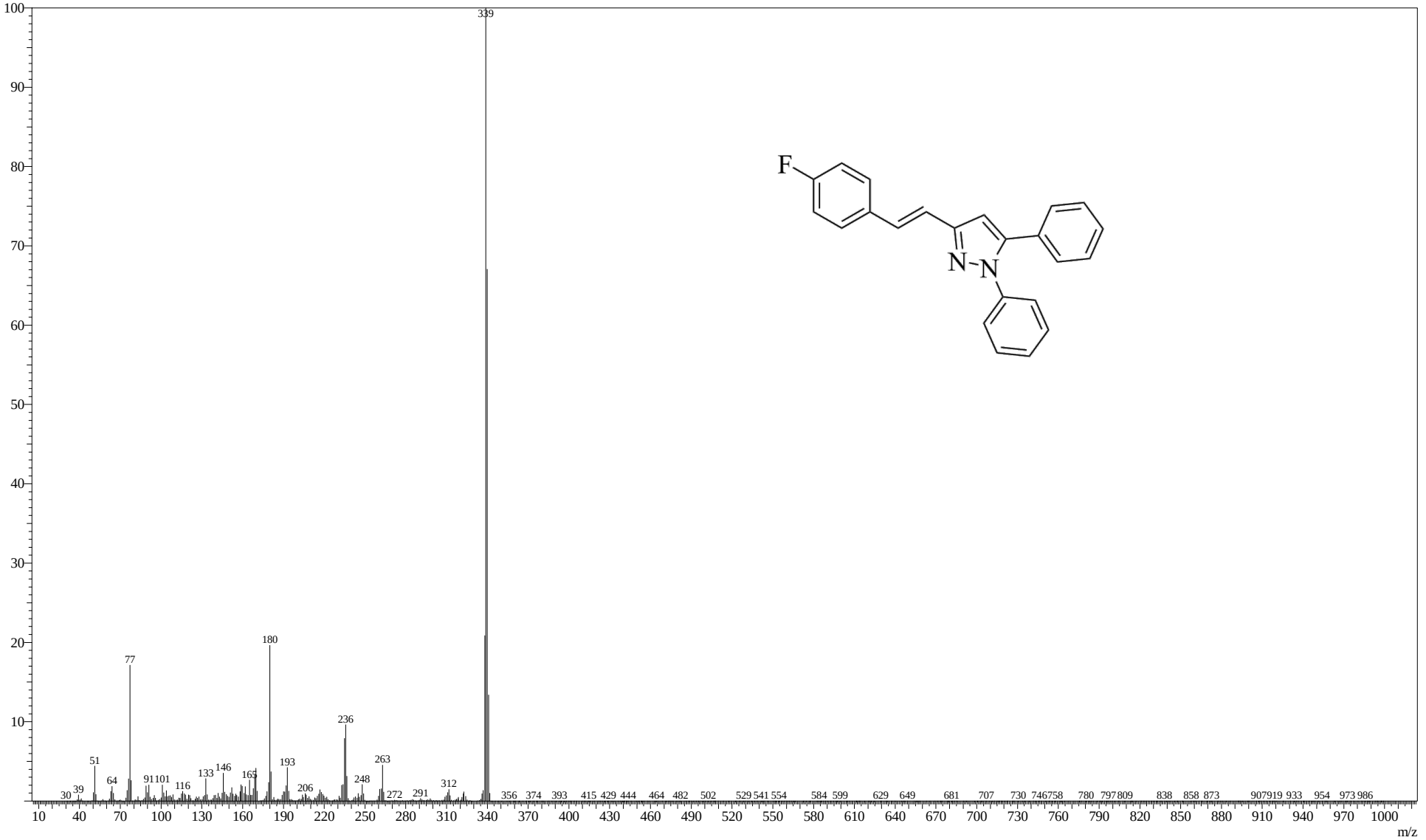
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4d**



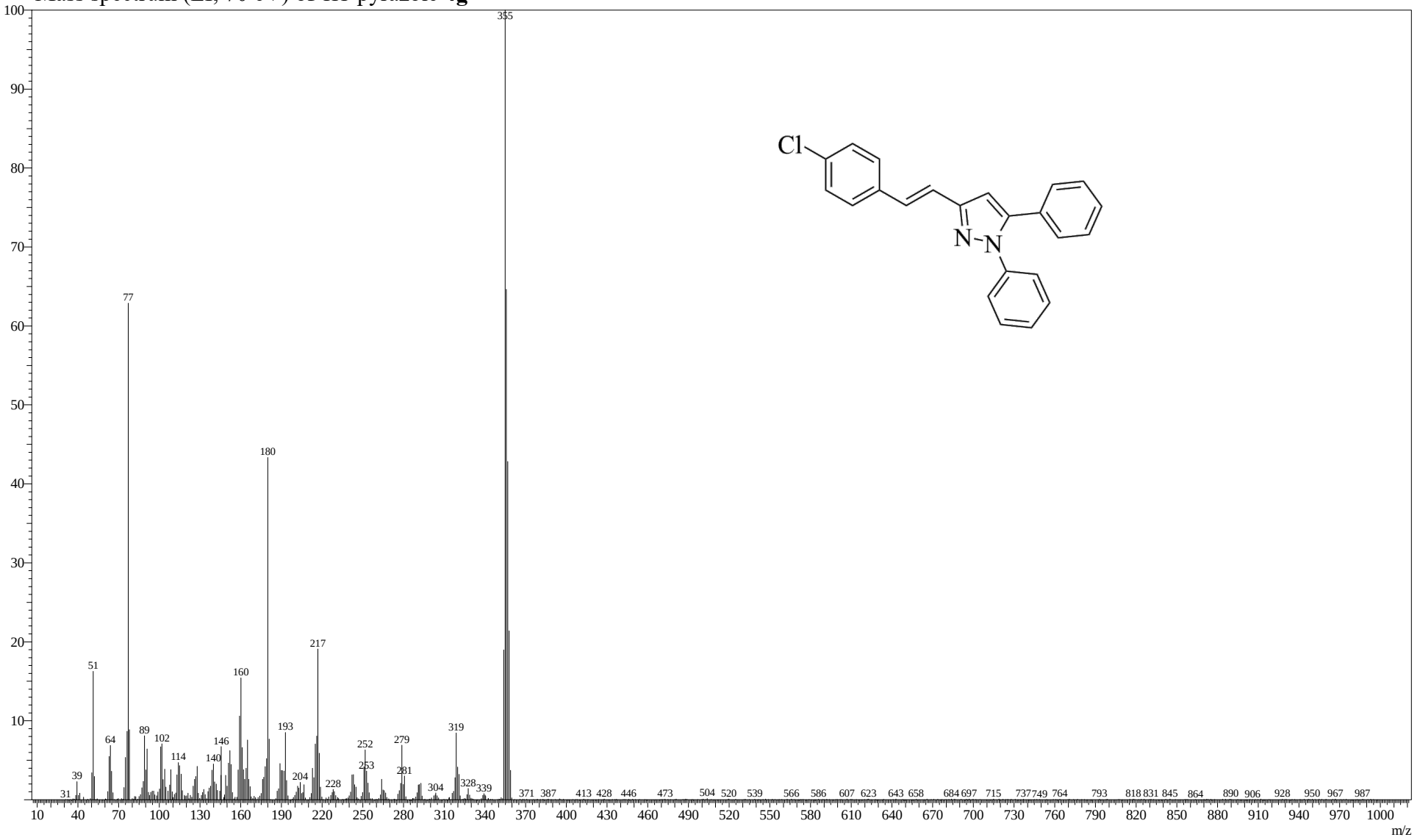
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4e**



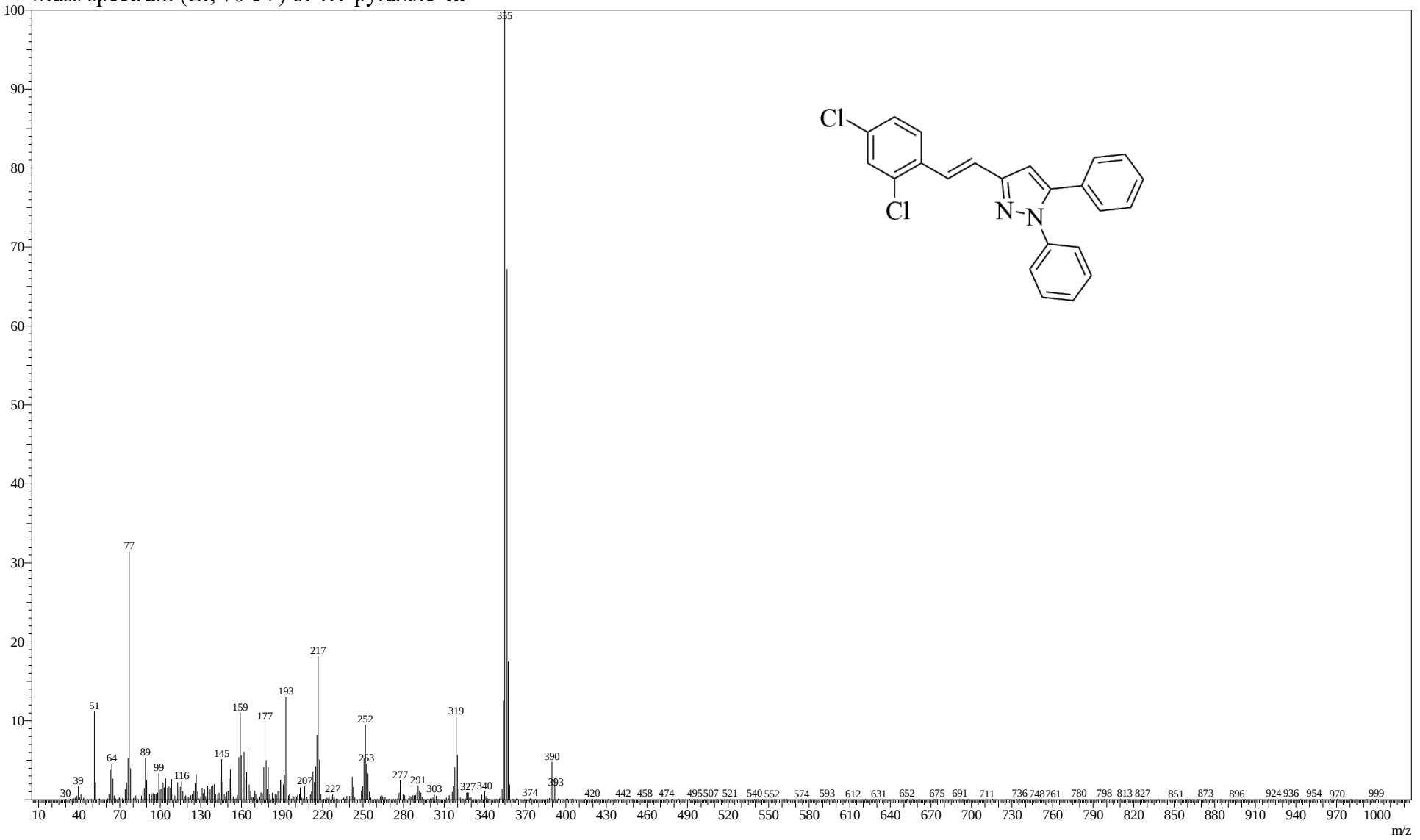
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4f**



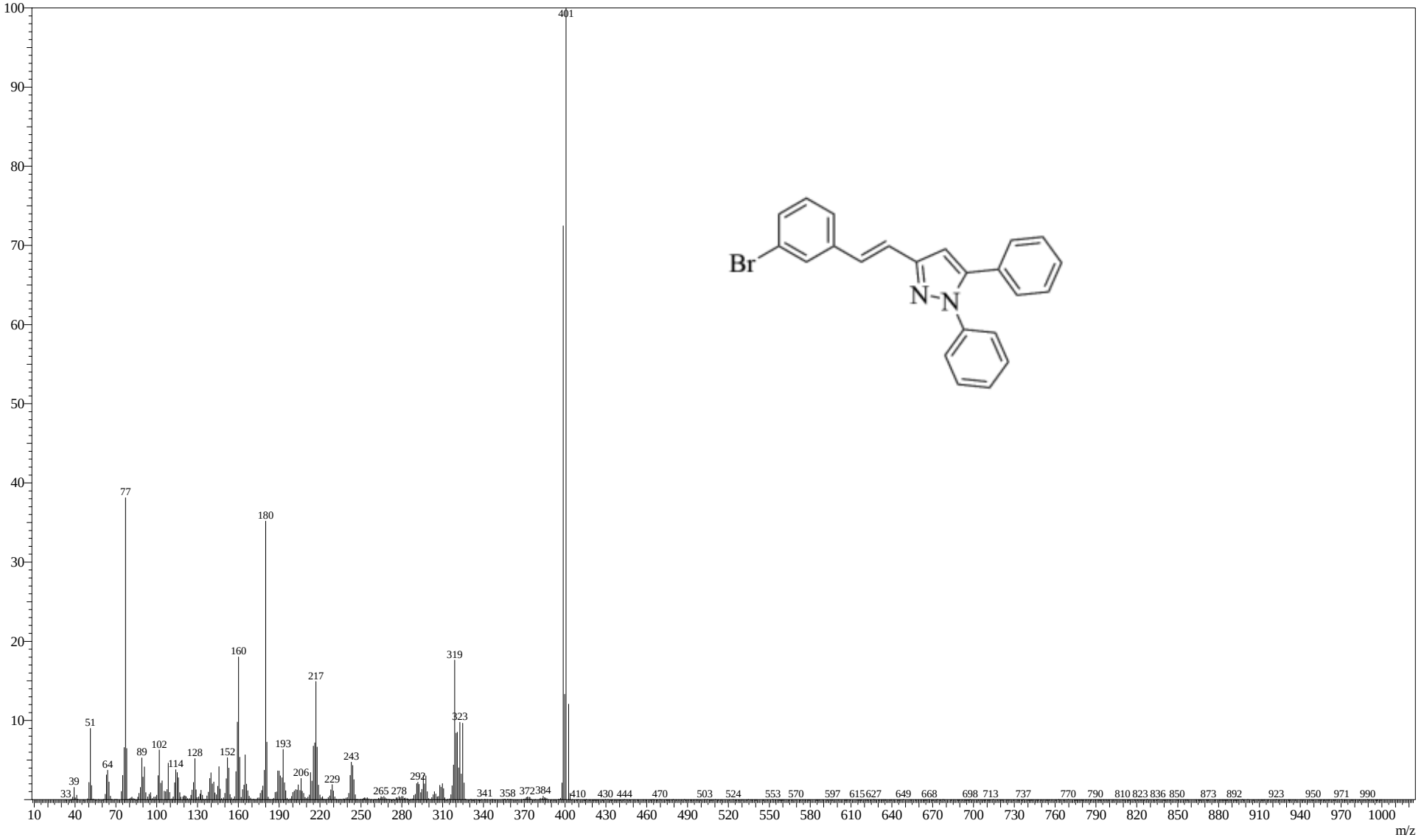
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4g**



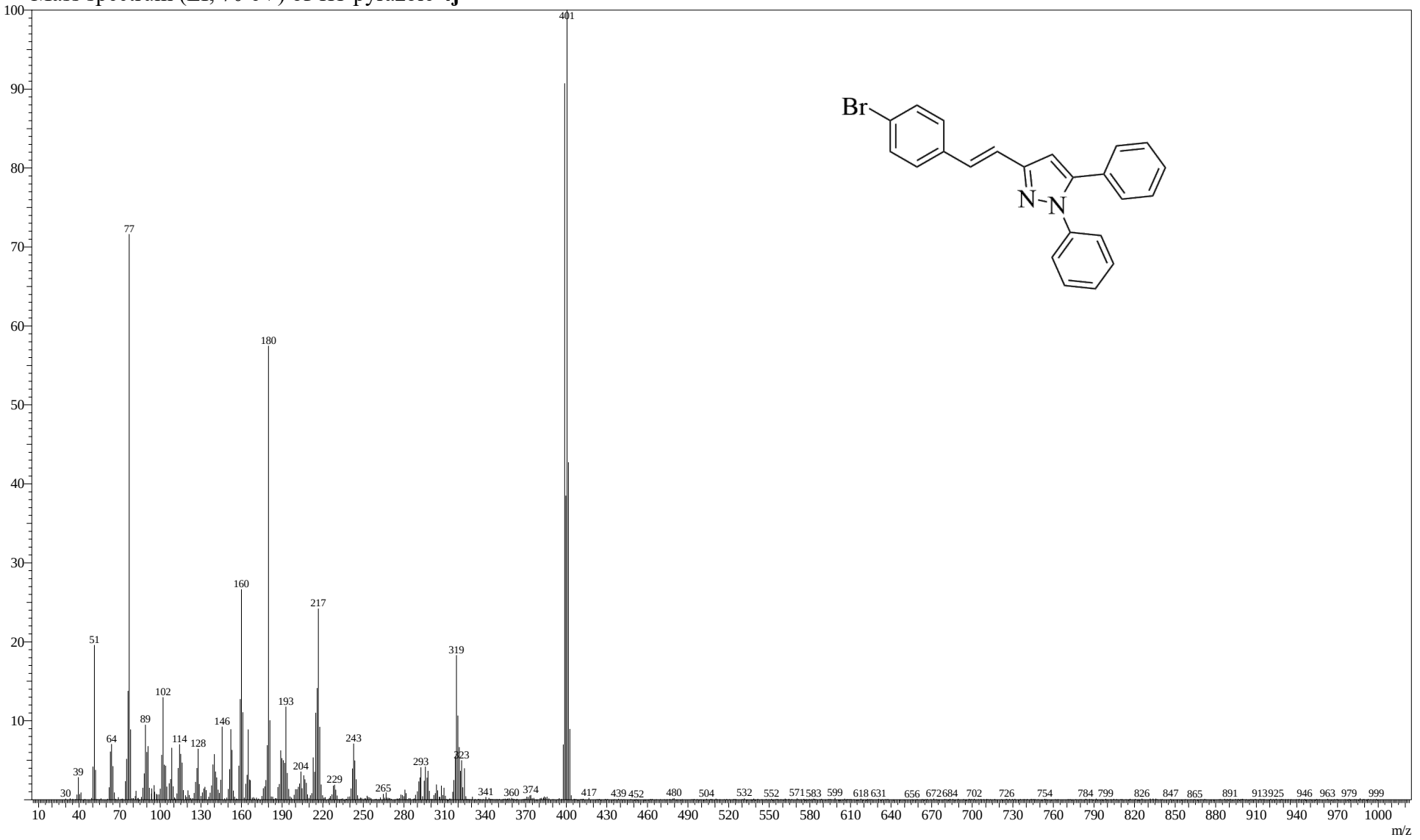
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4h**



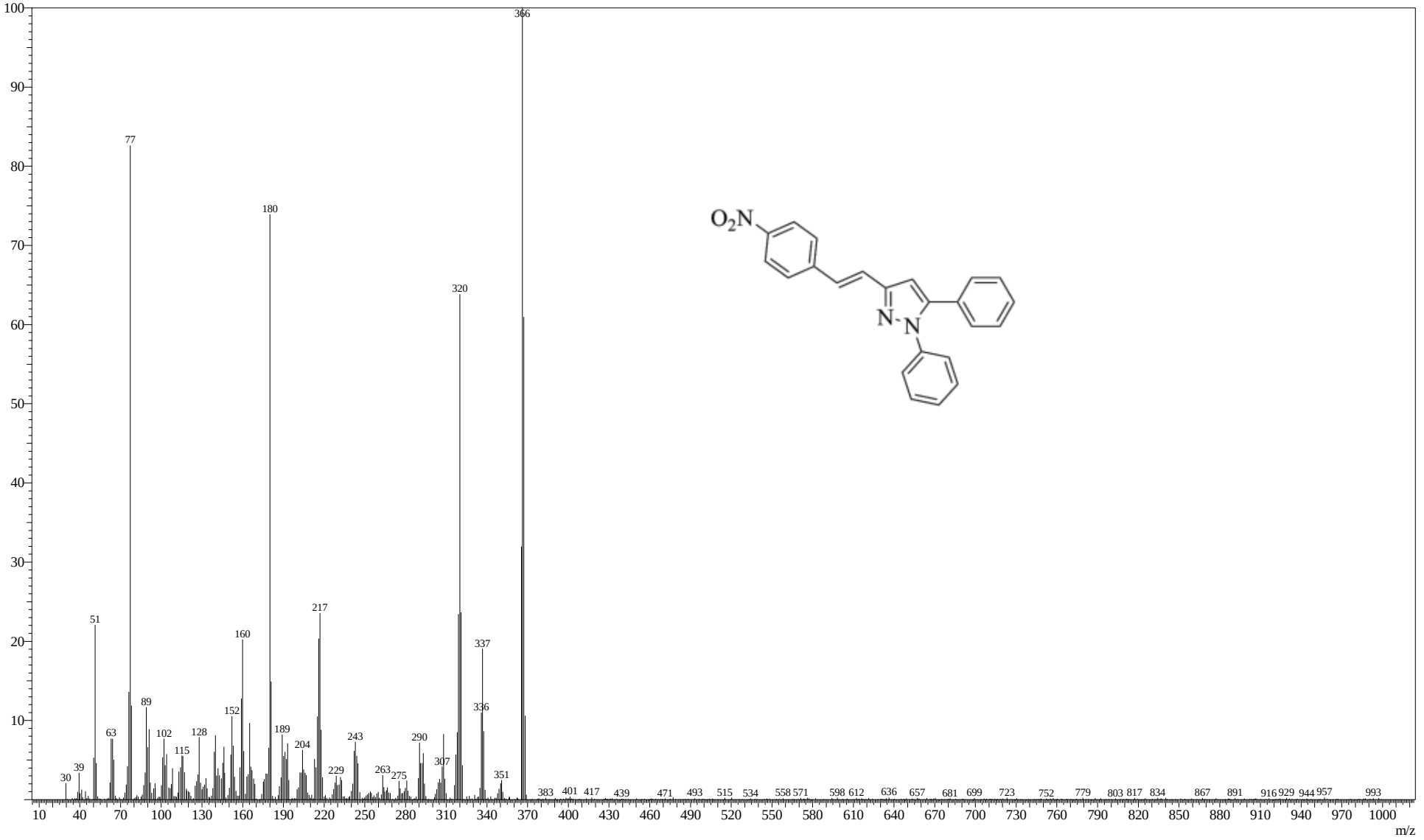
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4i**



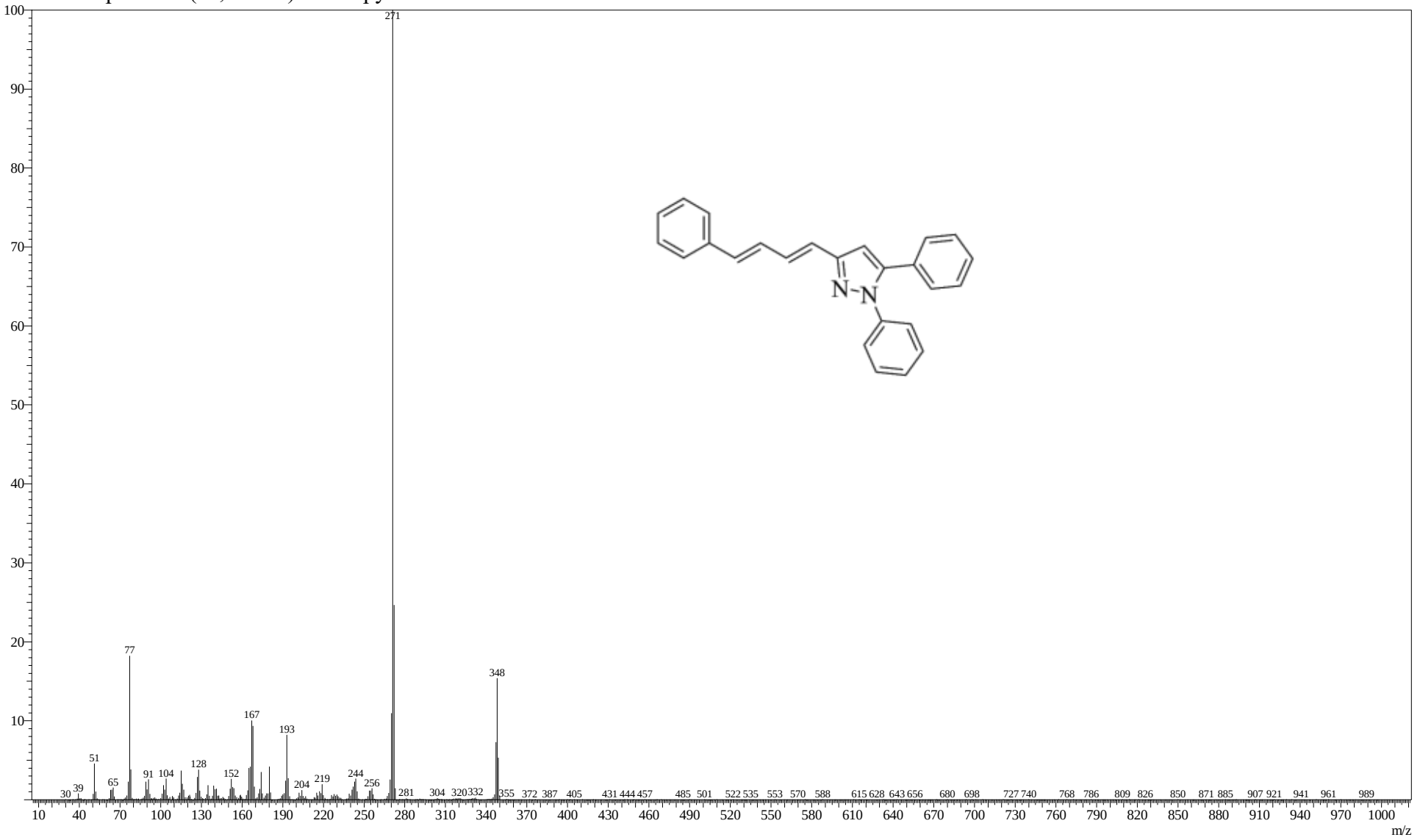
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4j**



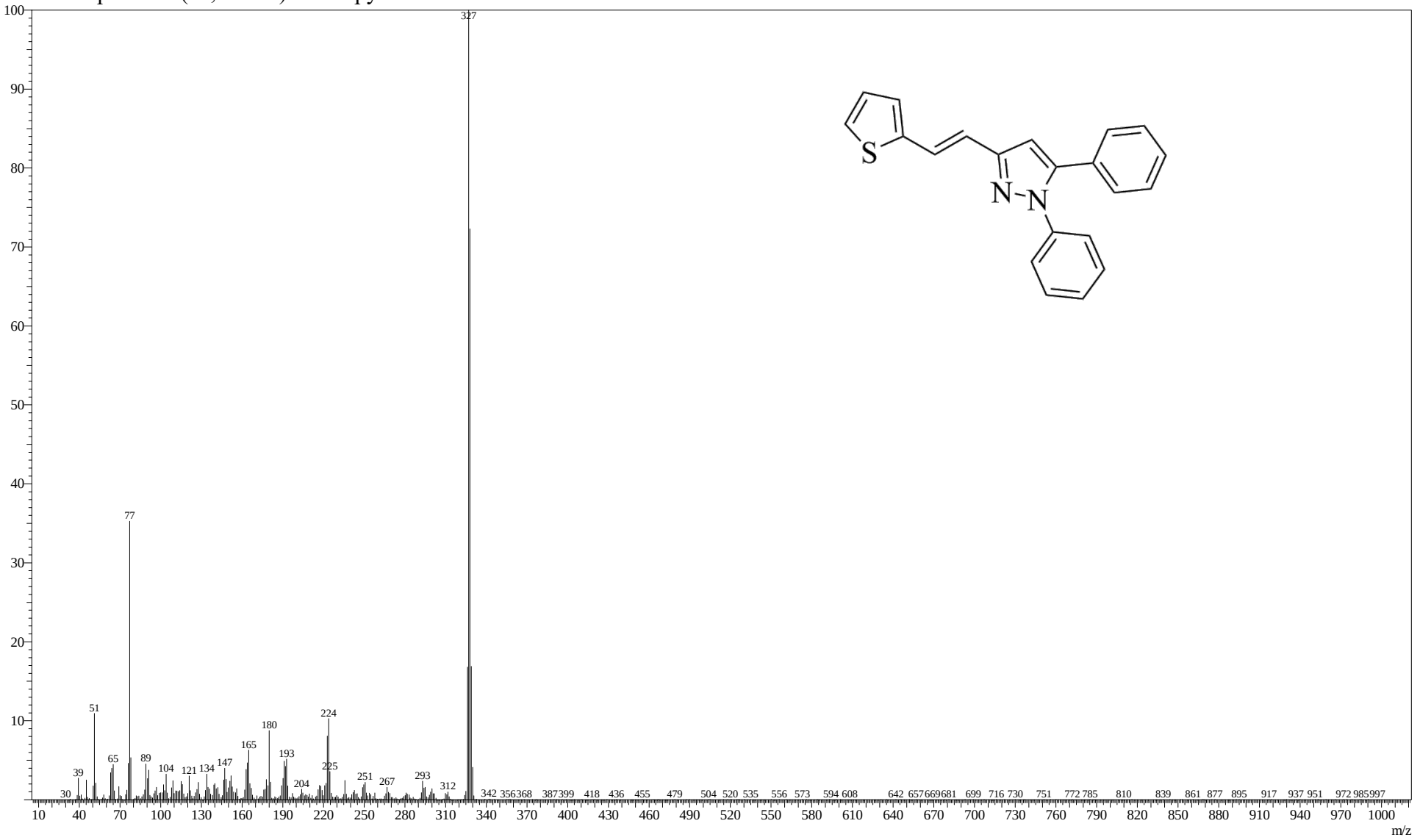
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4k**



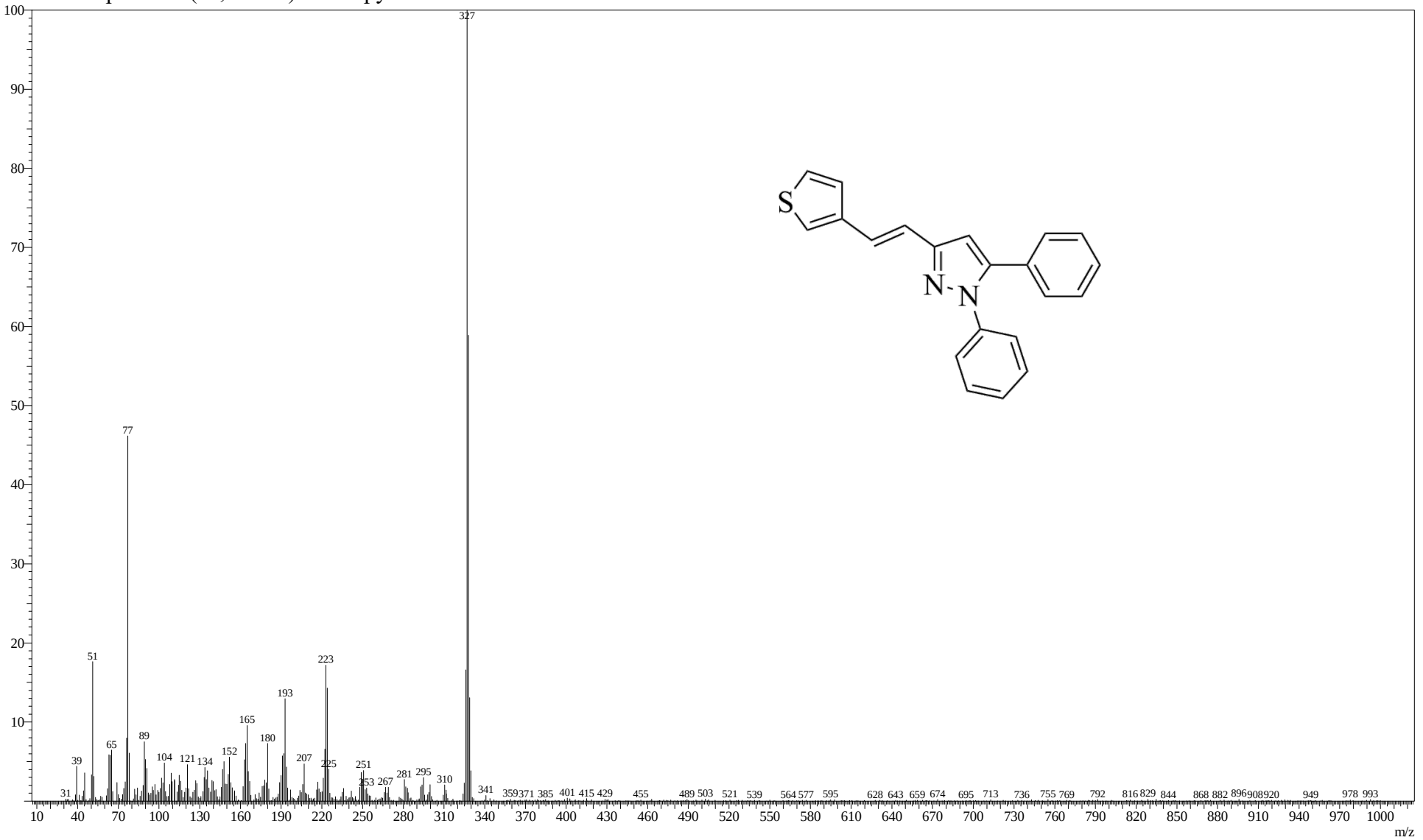
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4l**



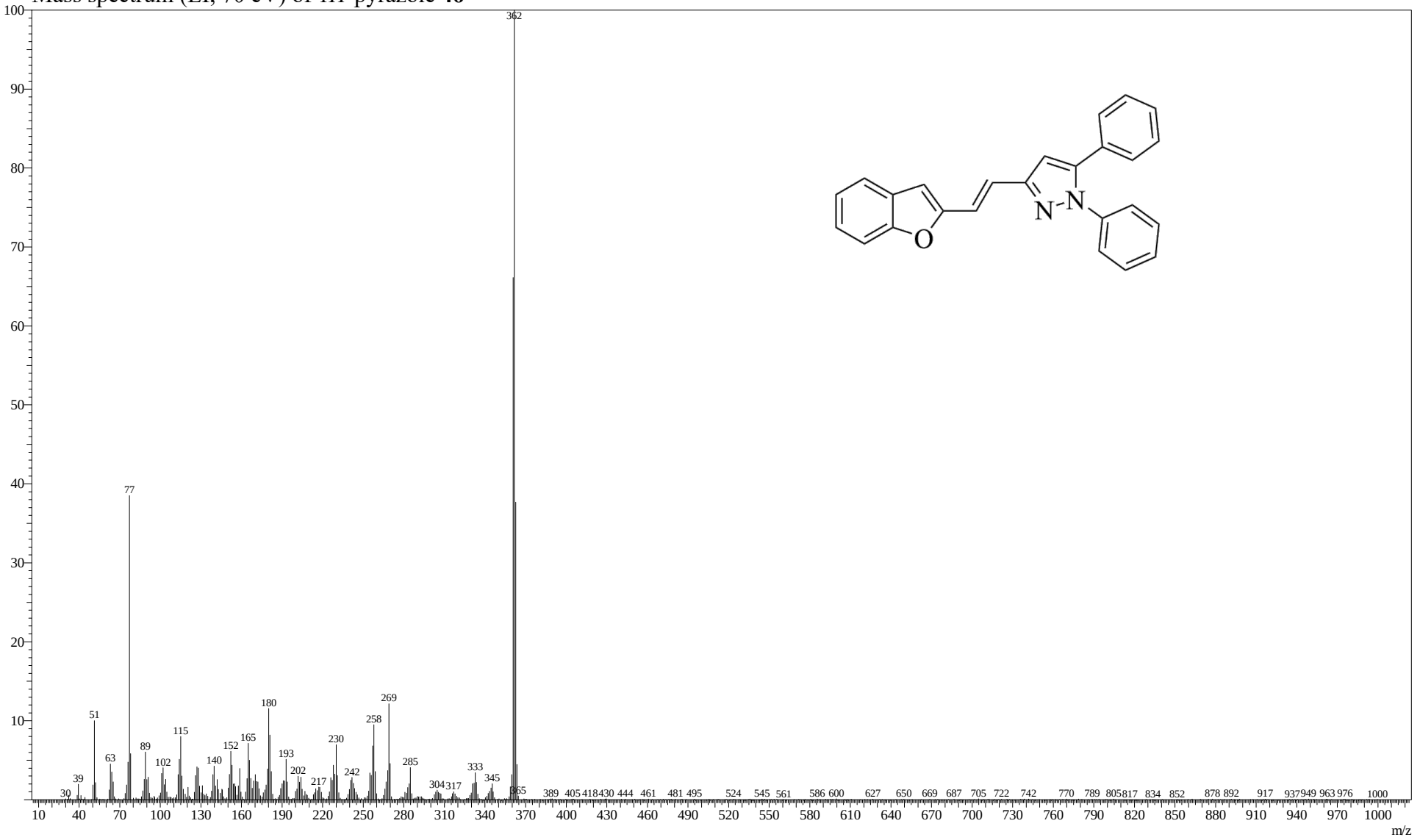
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4m**



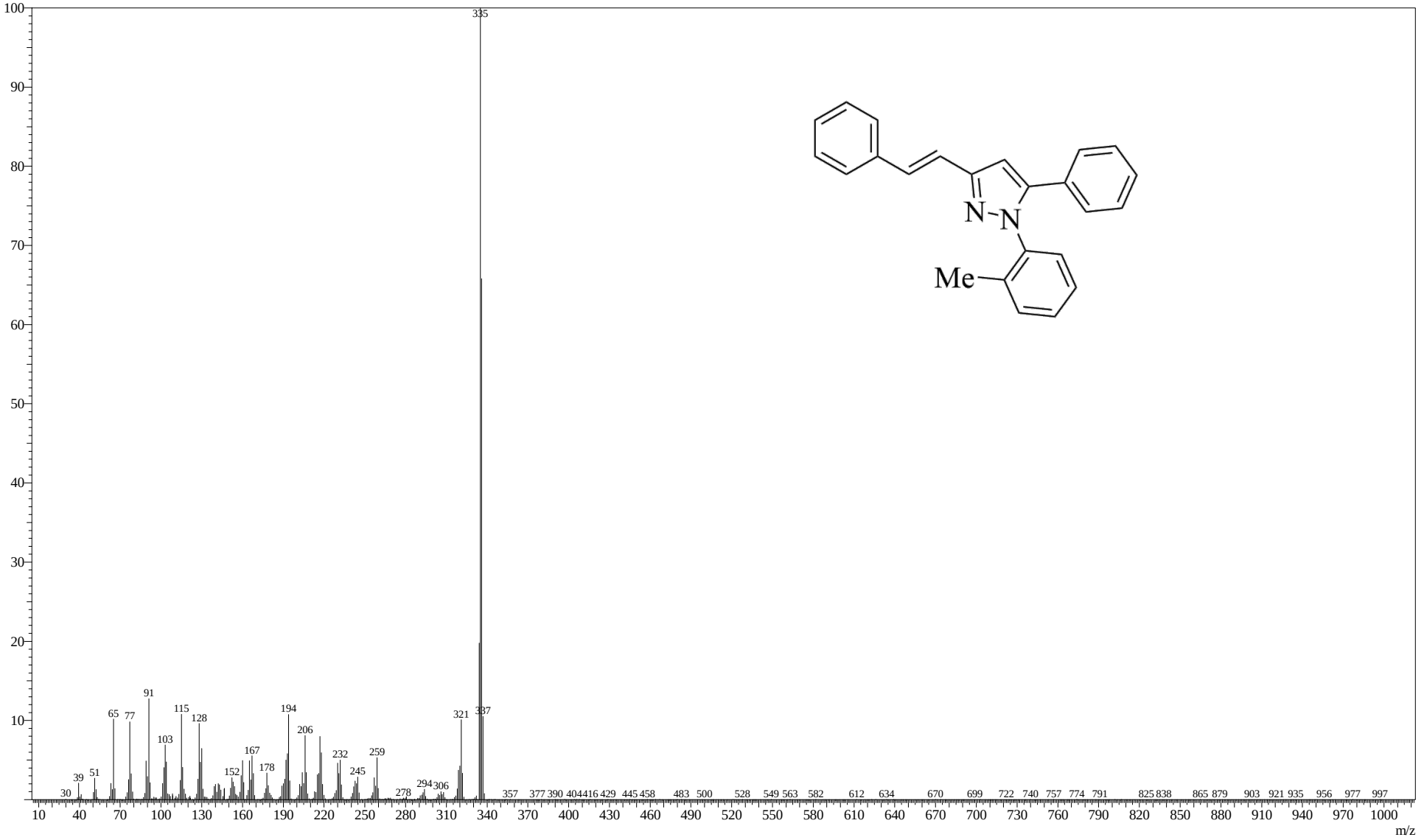
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4n**



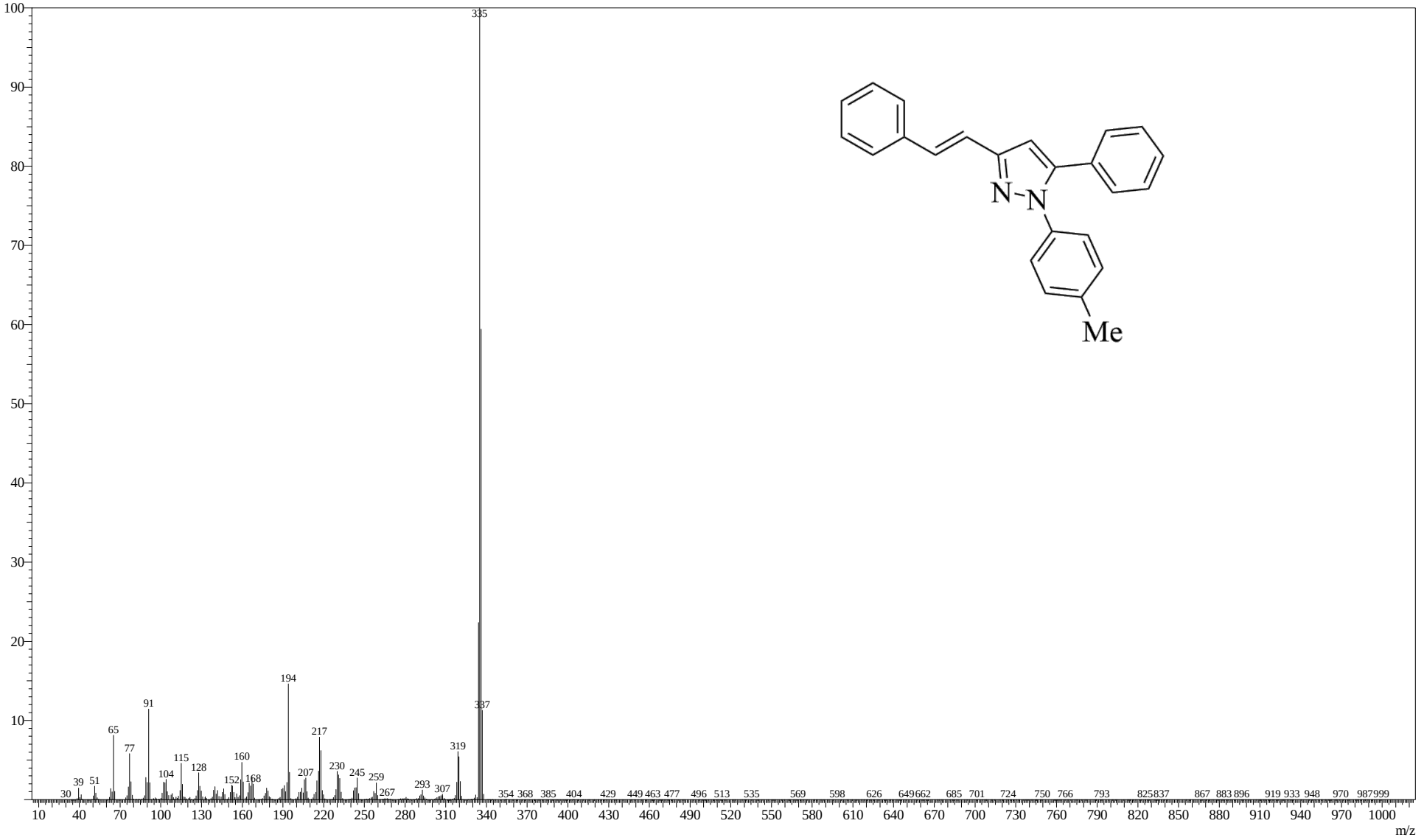
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4o**



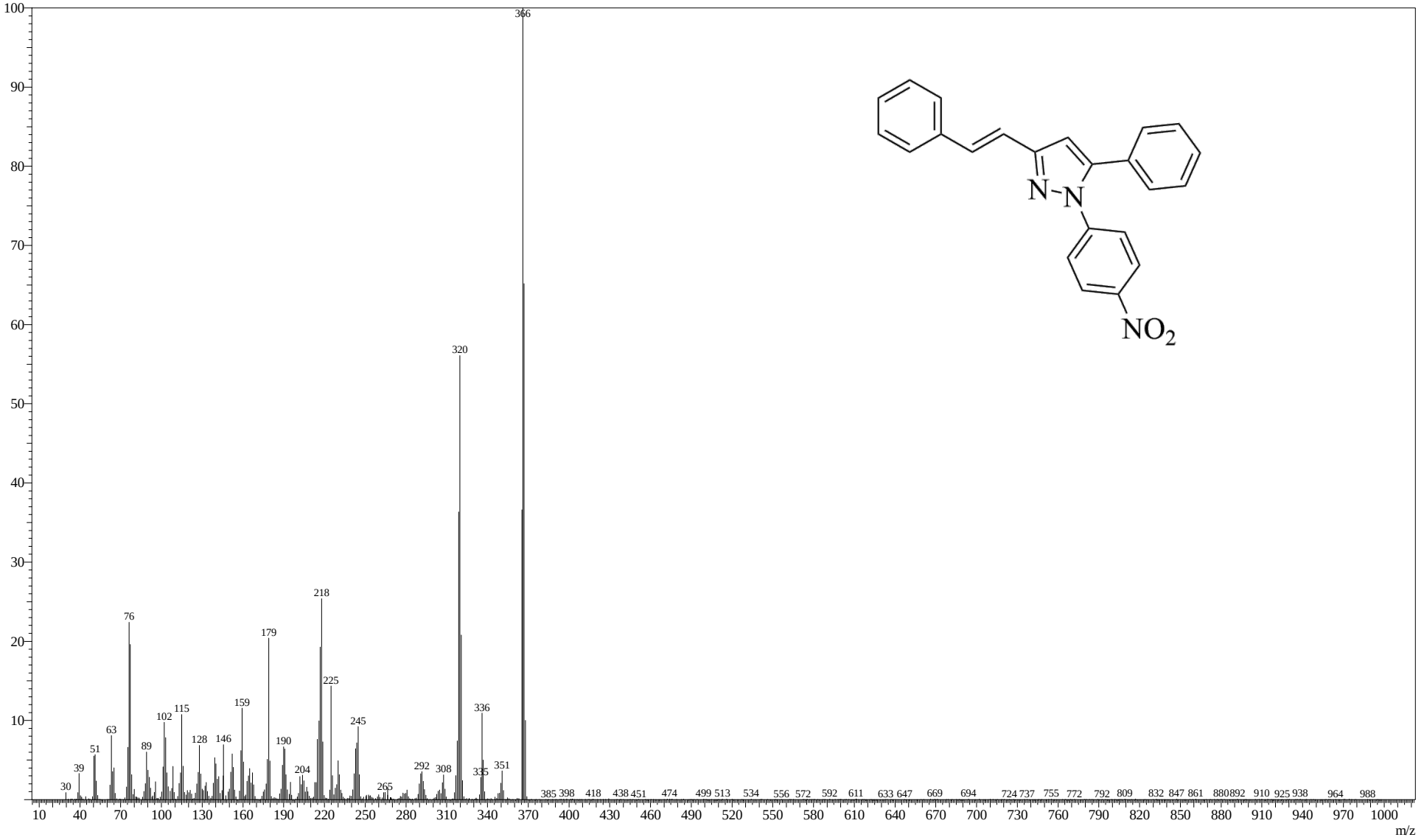
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4p**



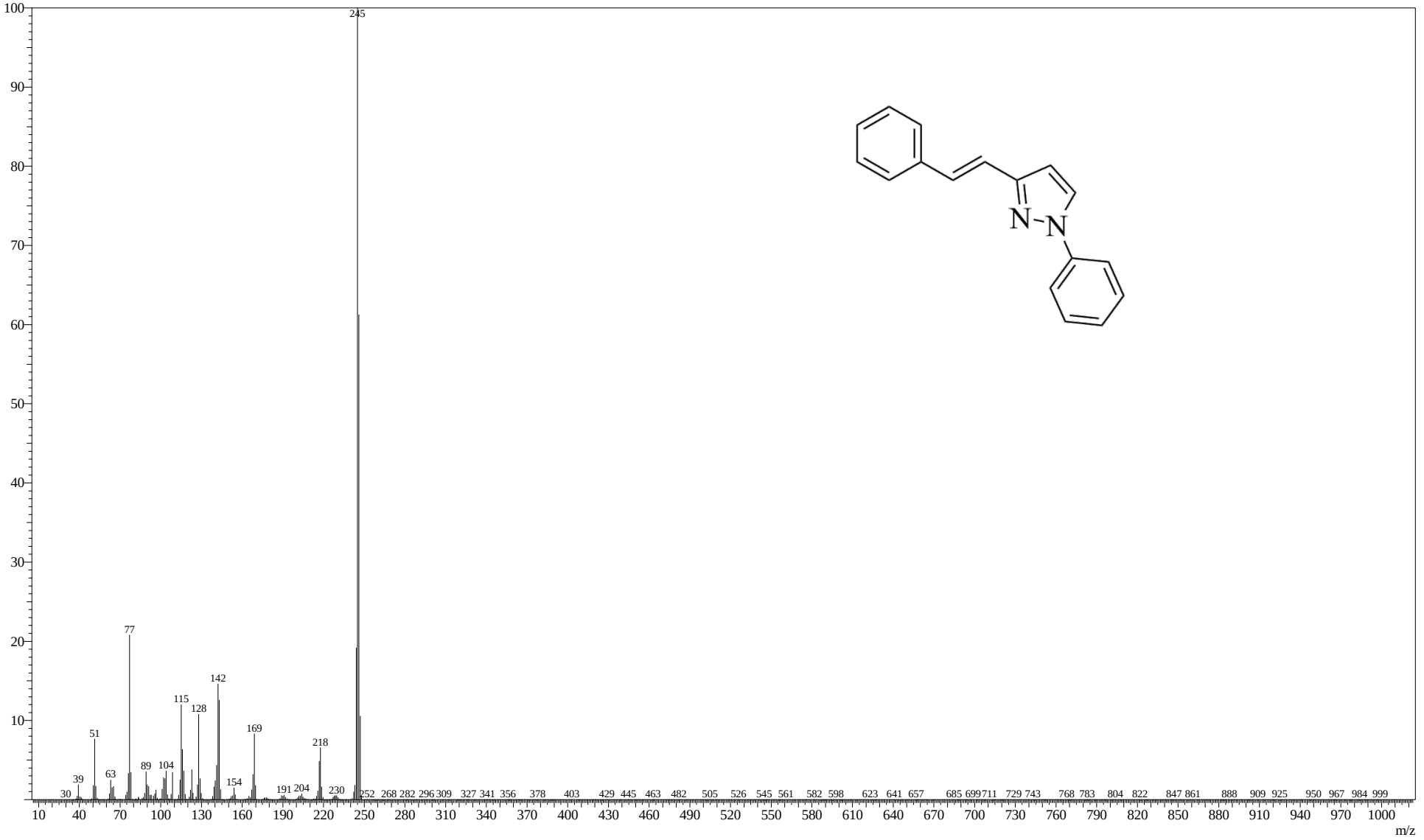
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4q**



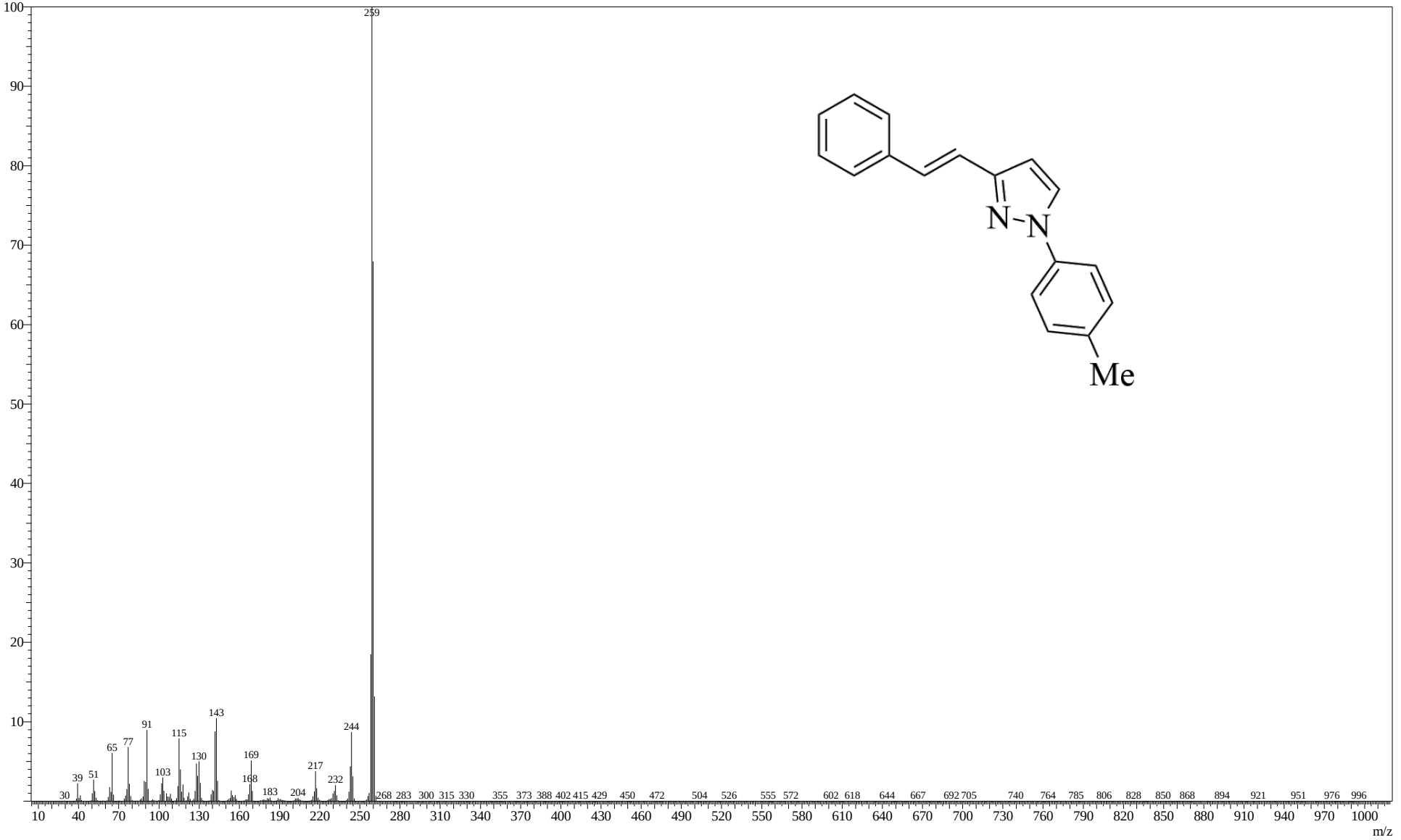
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4r**



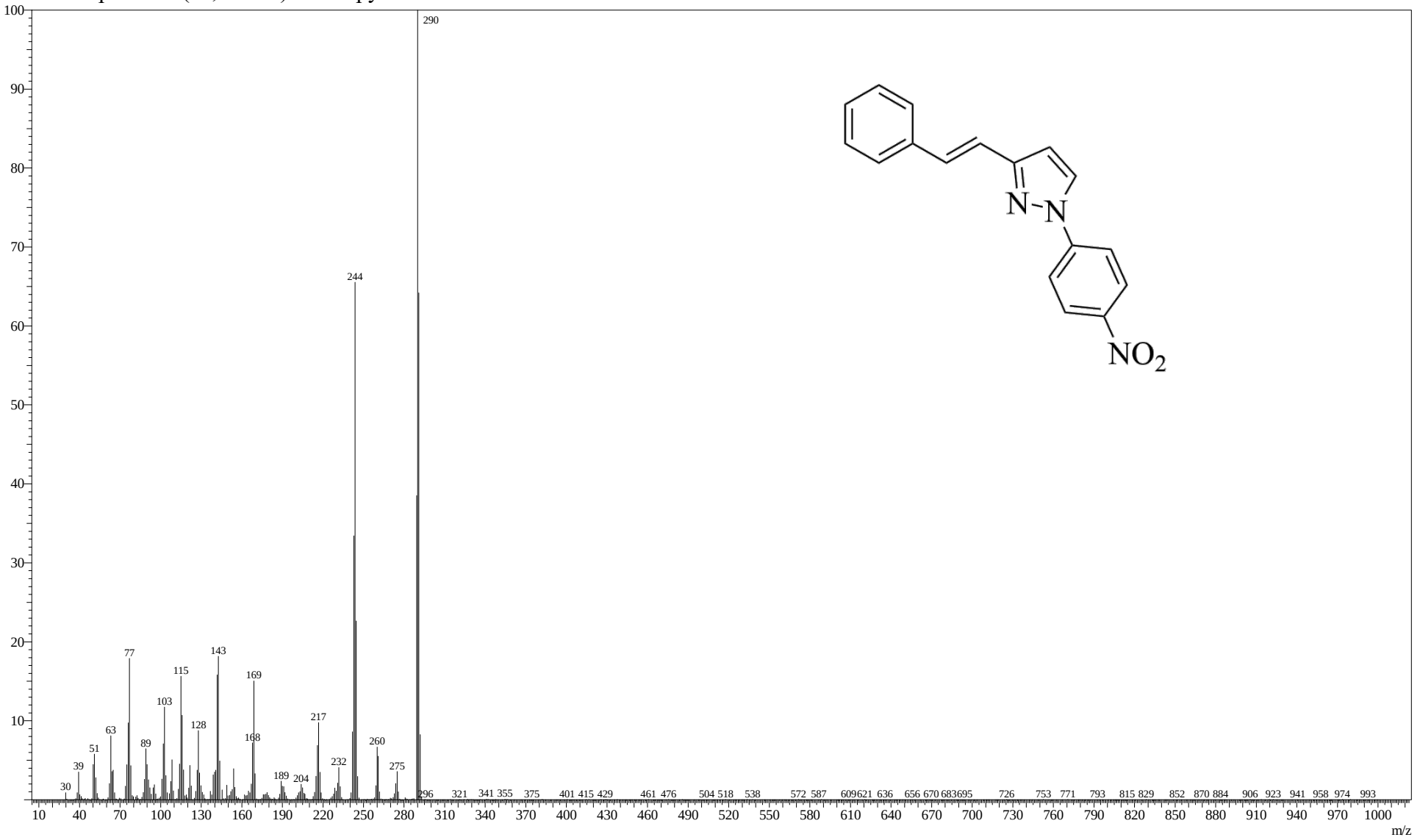
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4s**



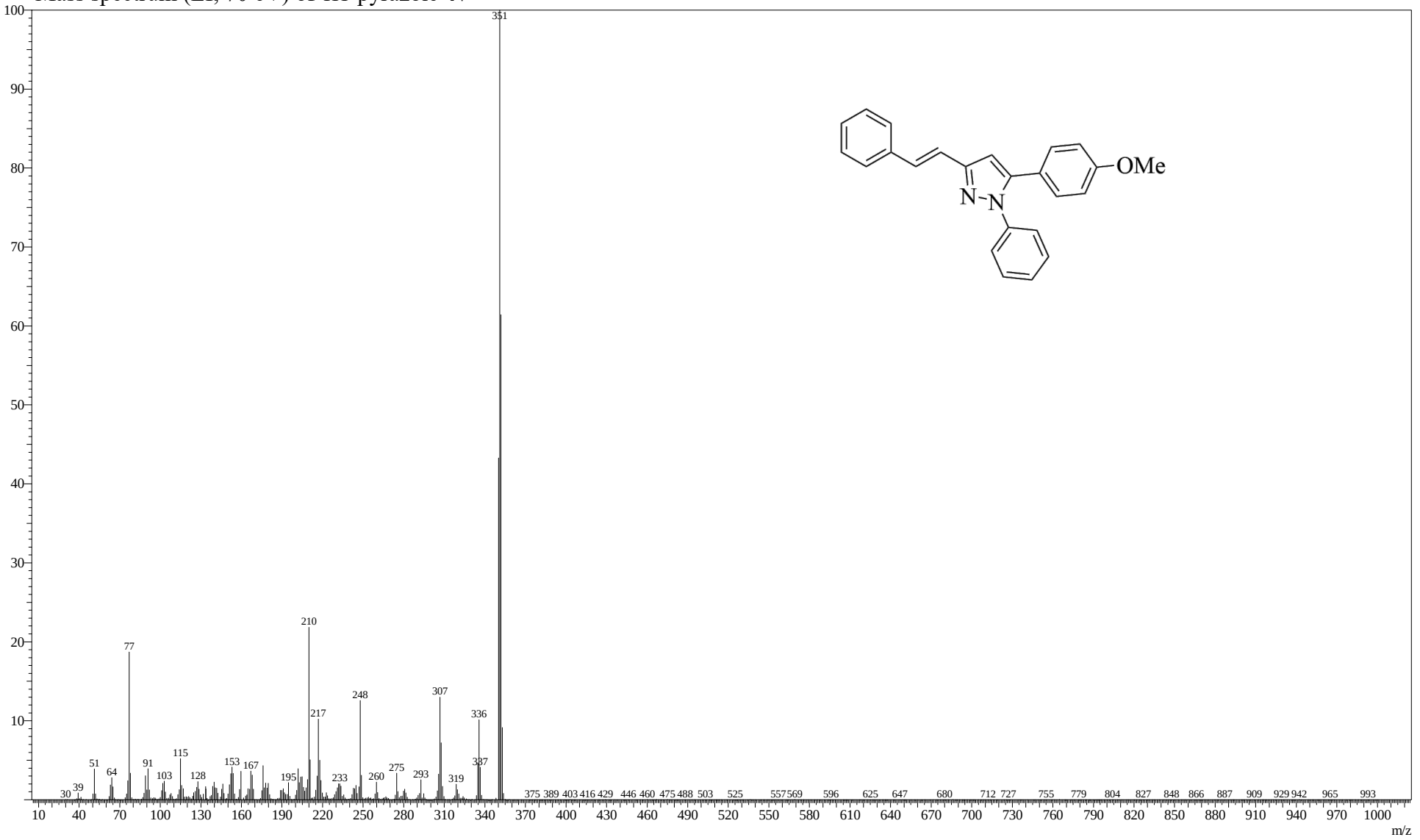
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4t**



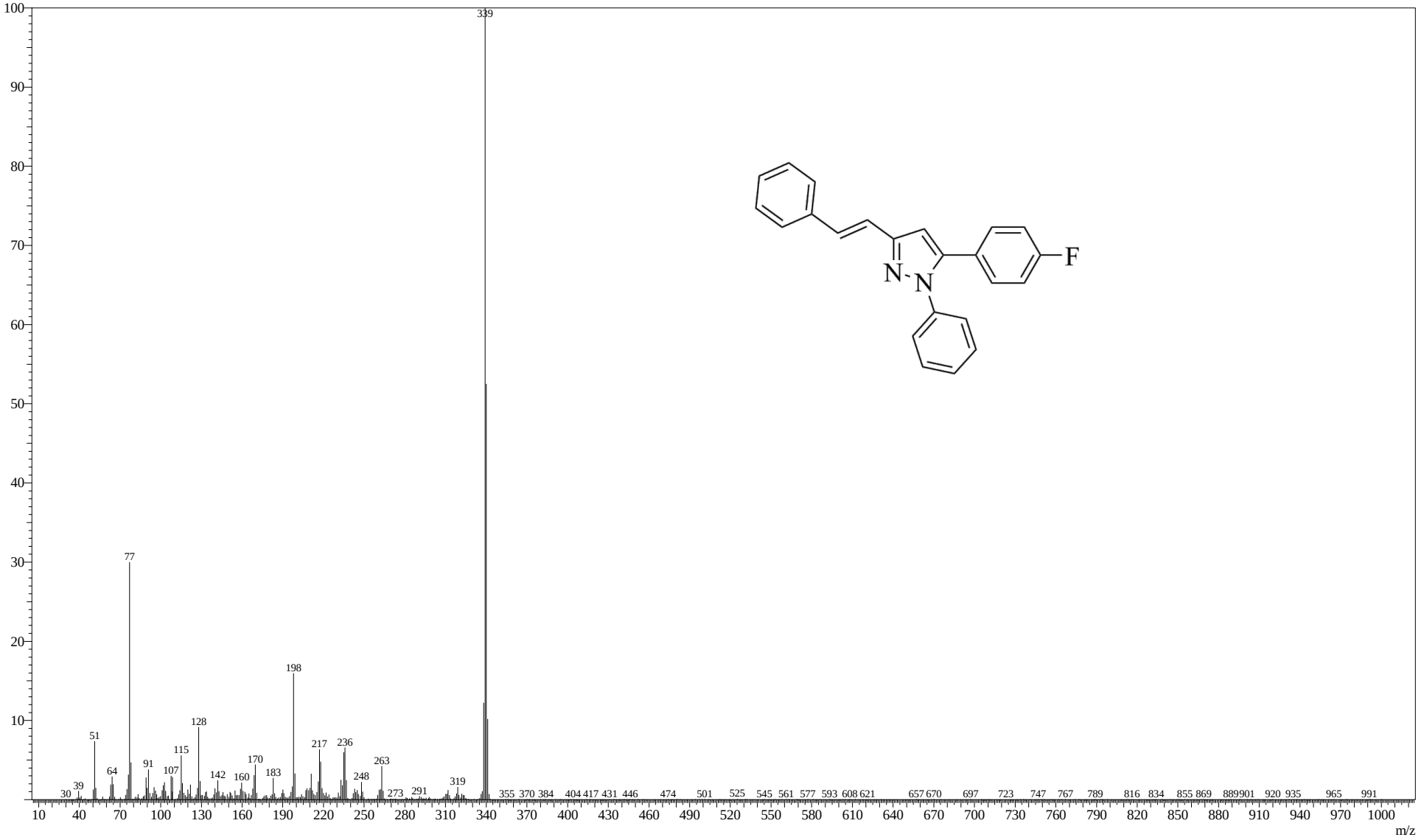
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4u**



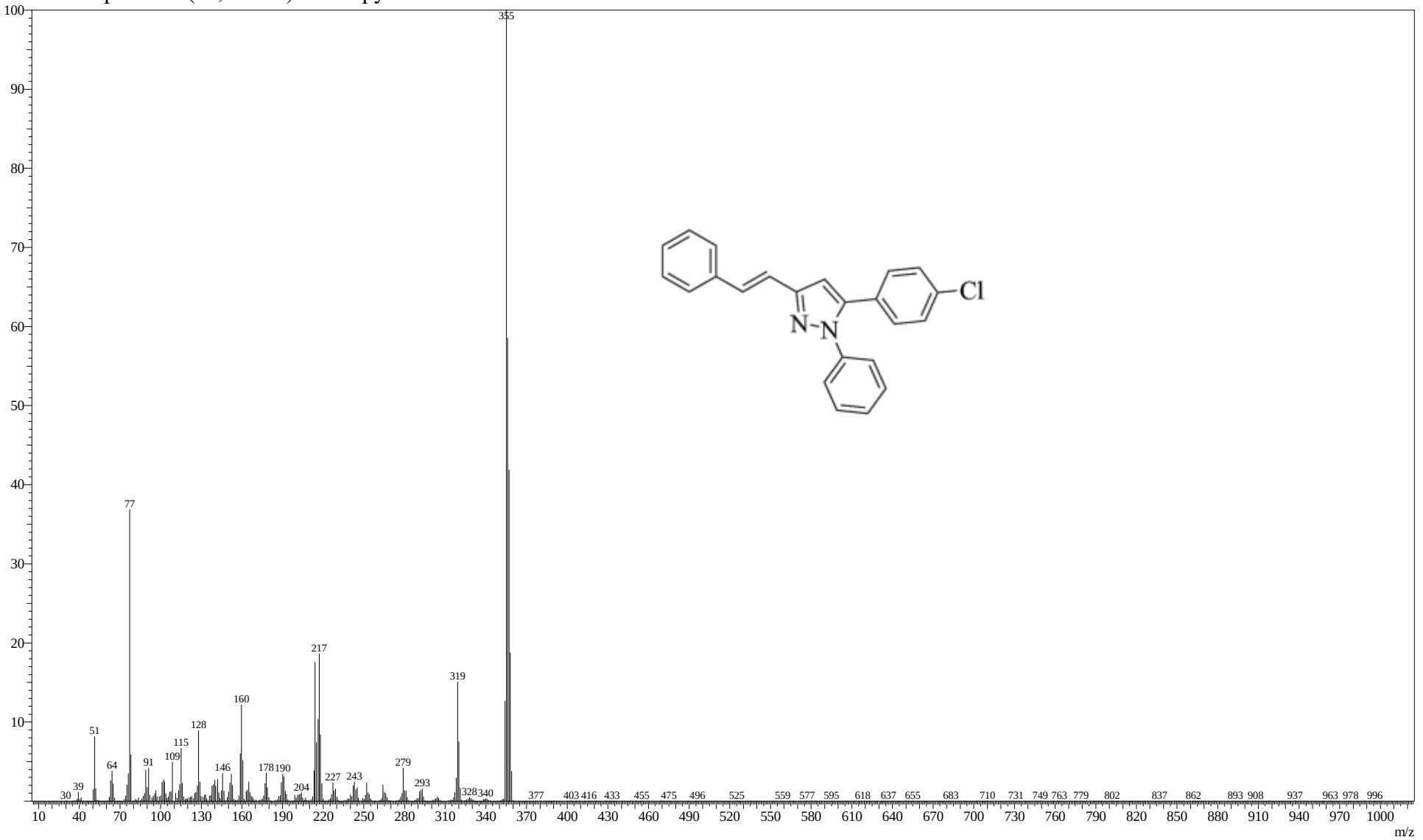
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4v**



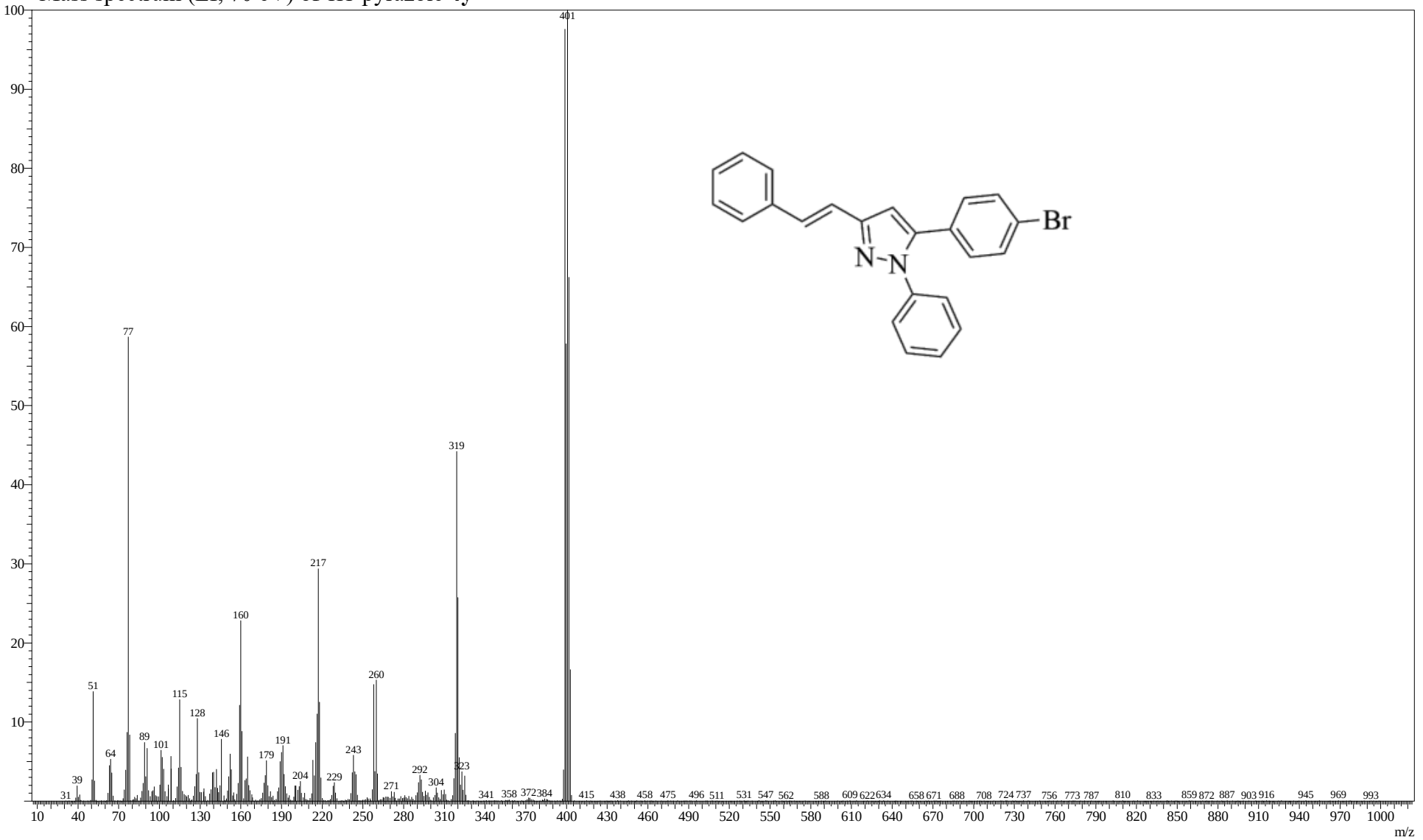
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4w**



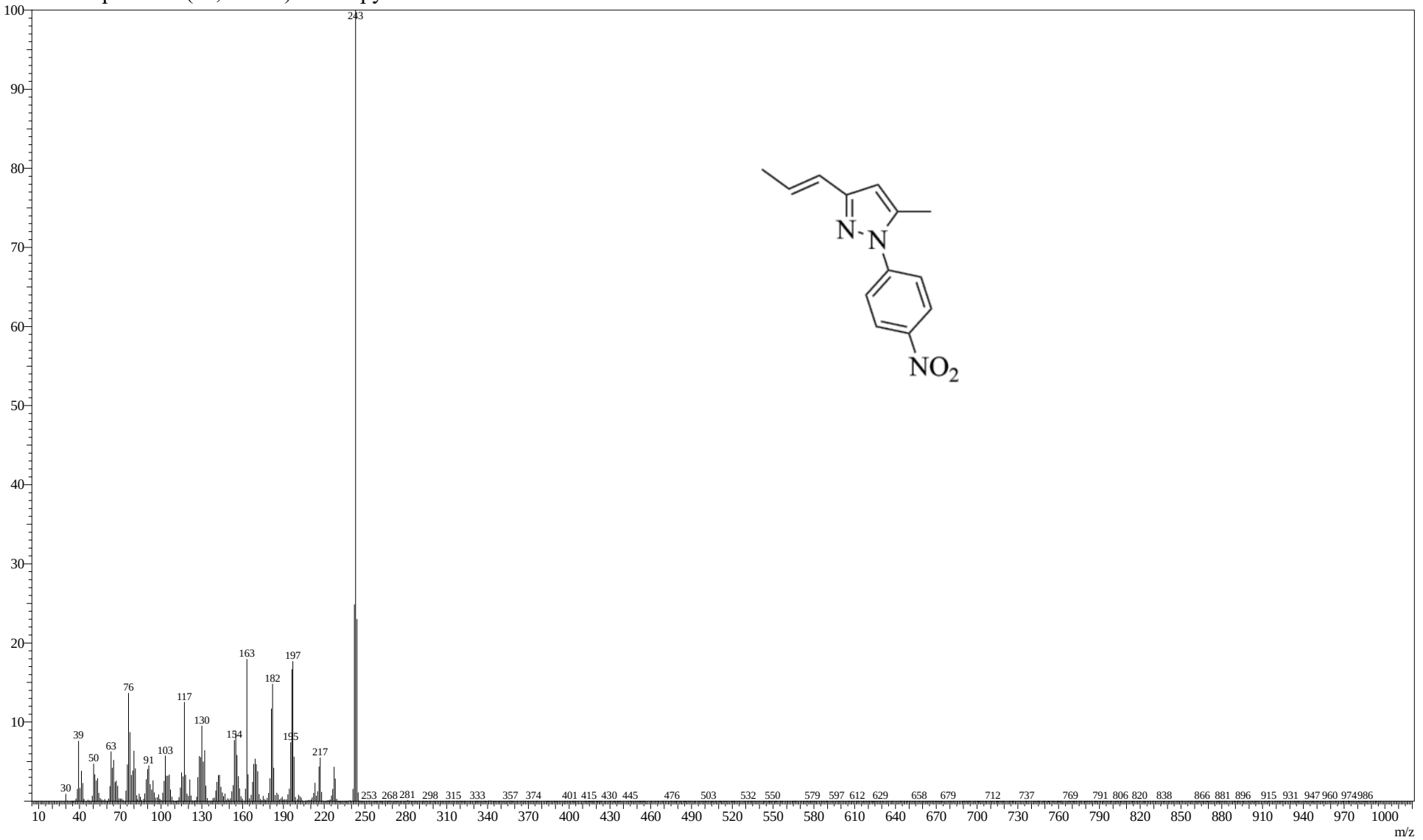
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4x**



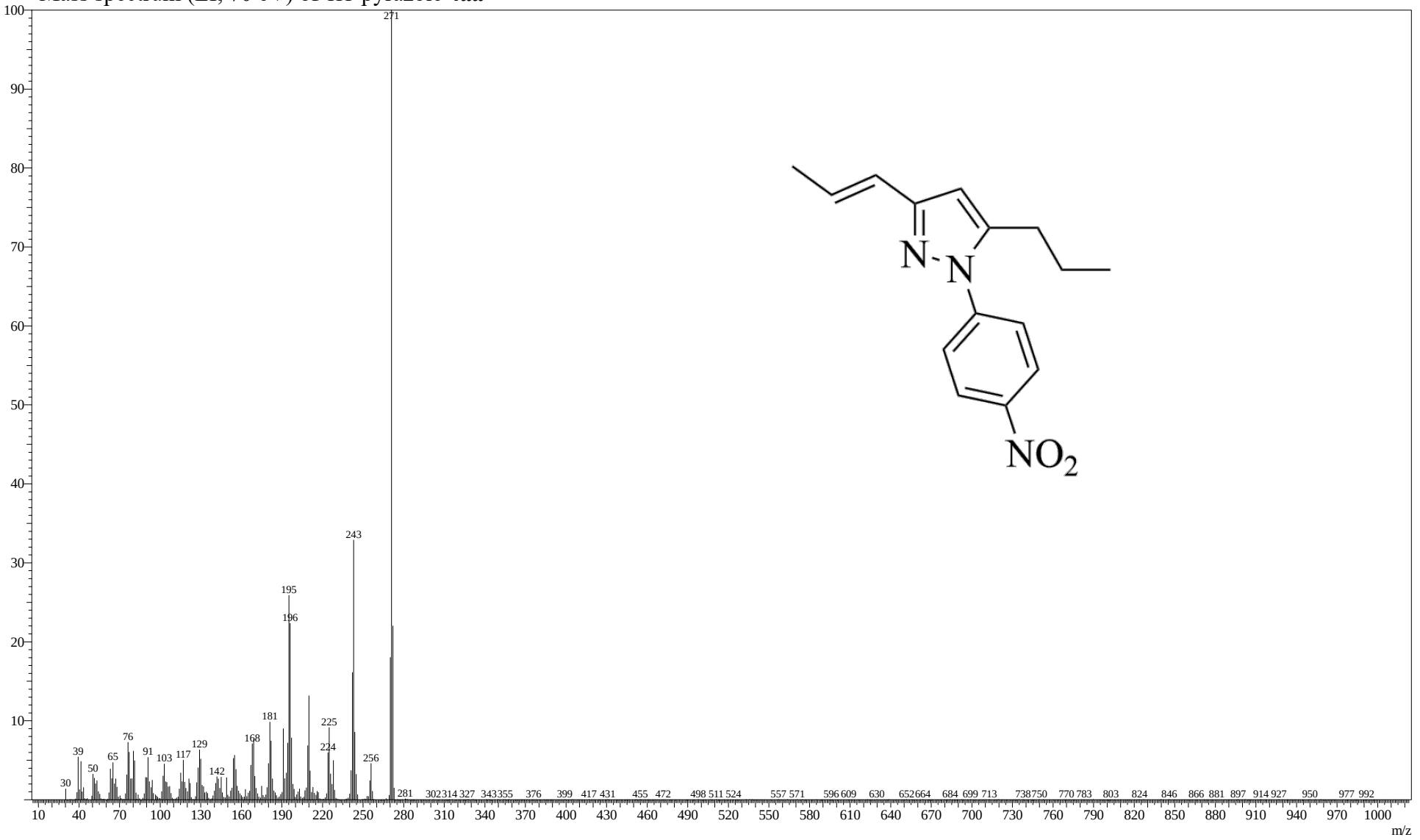
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4y**



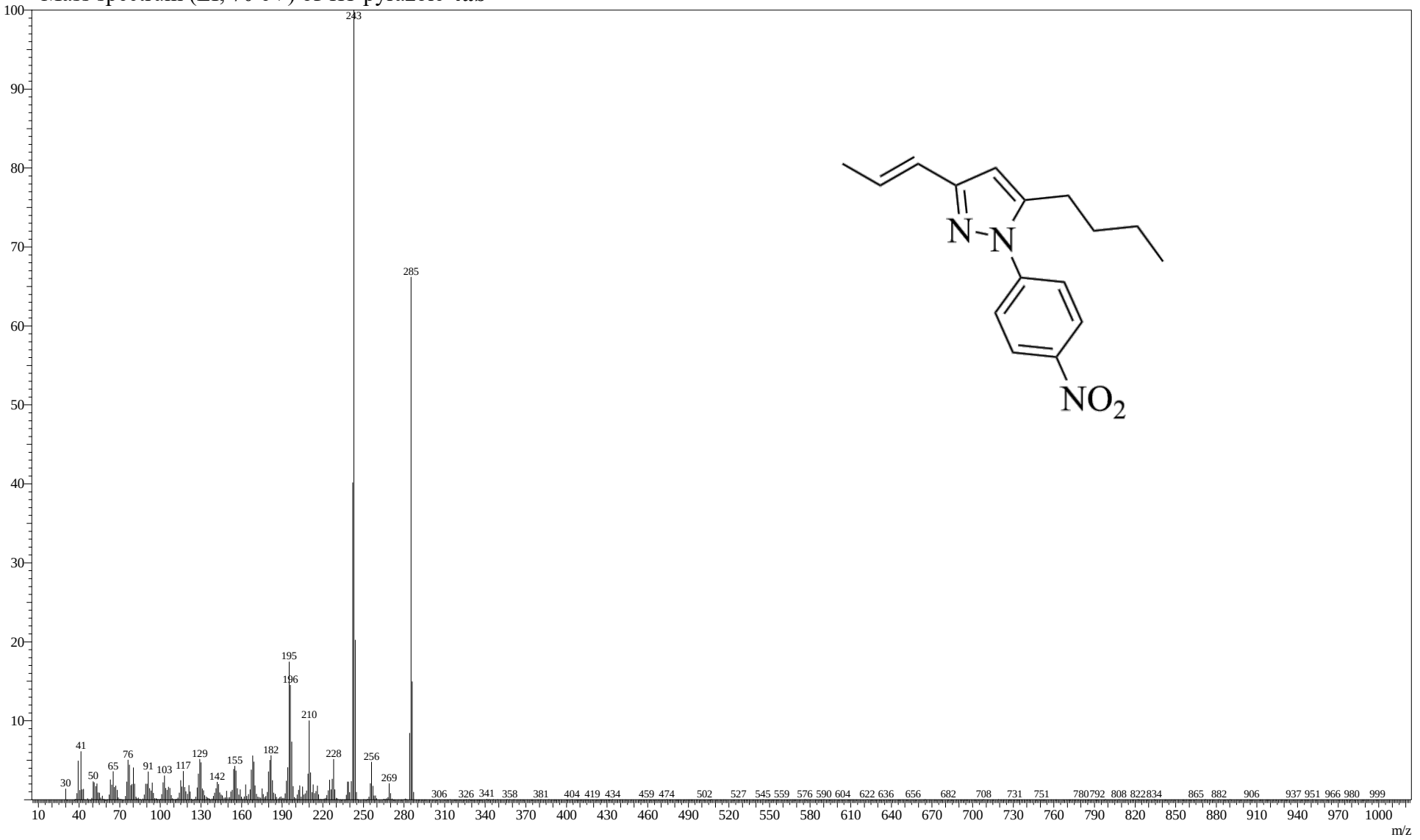
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4z**



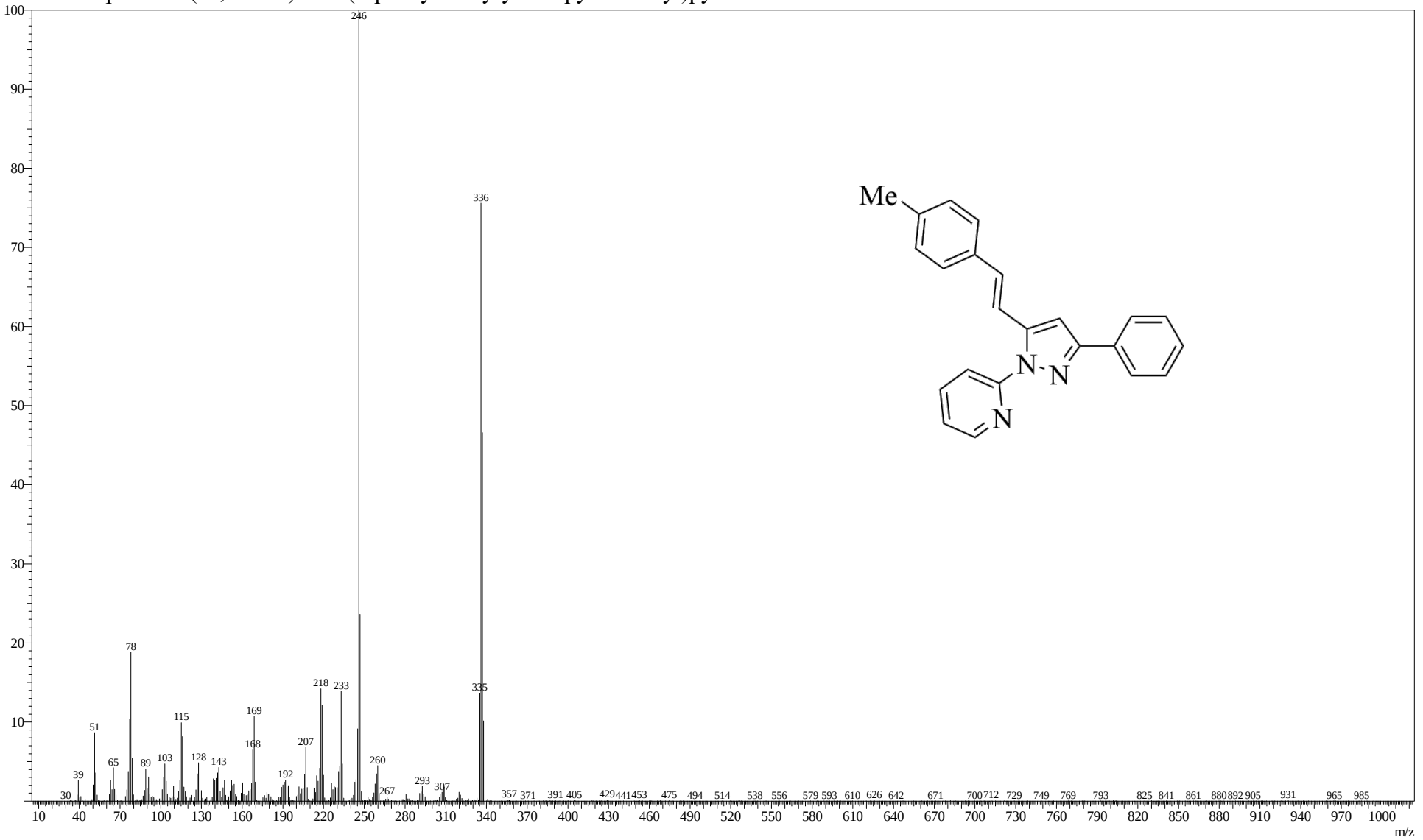
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4aa**



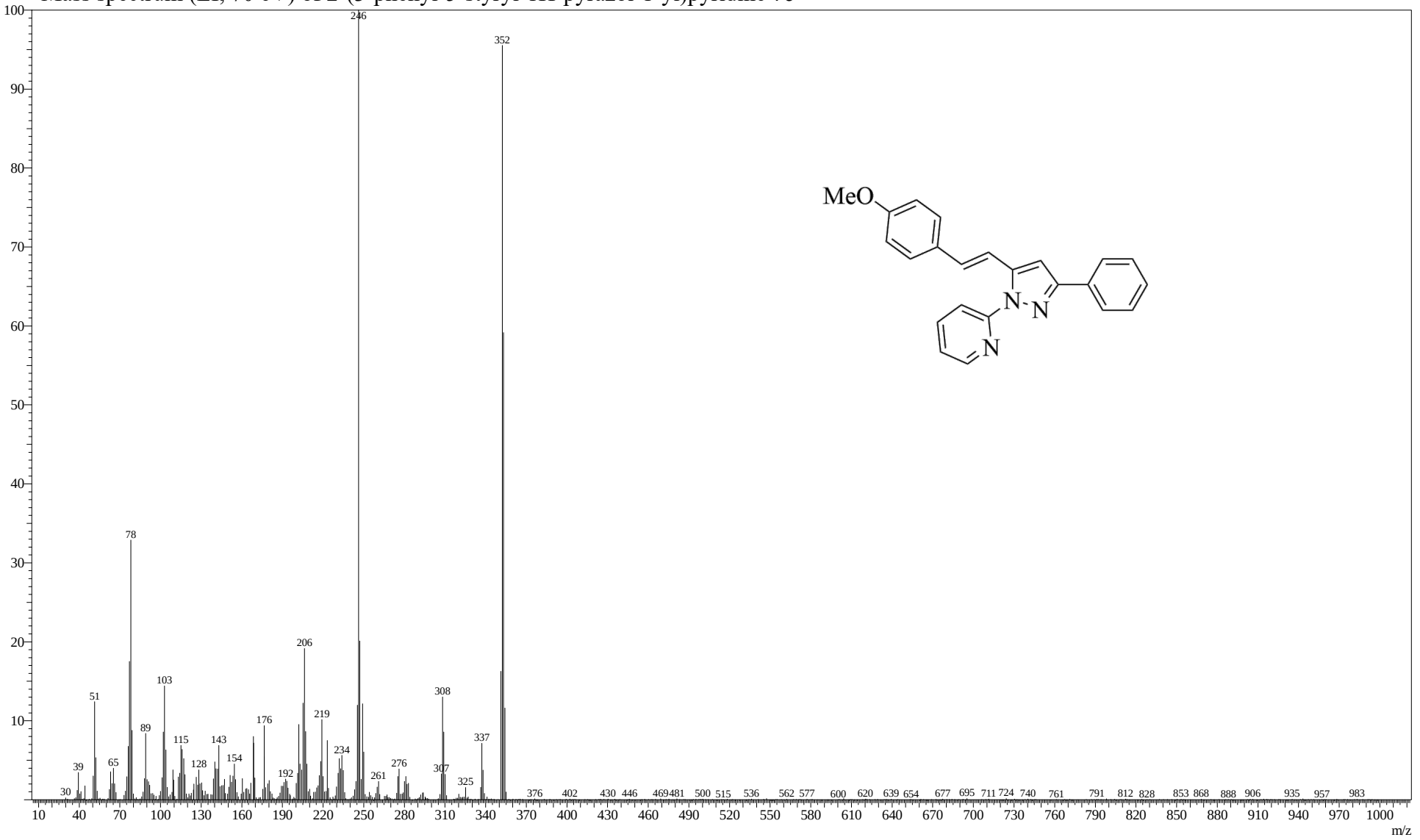
Mass spectrum (EI, 70 eV) of 1*H*-pyrazole **4ab**



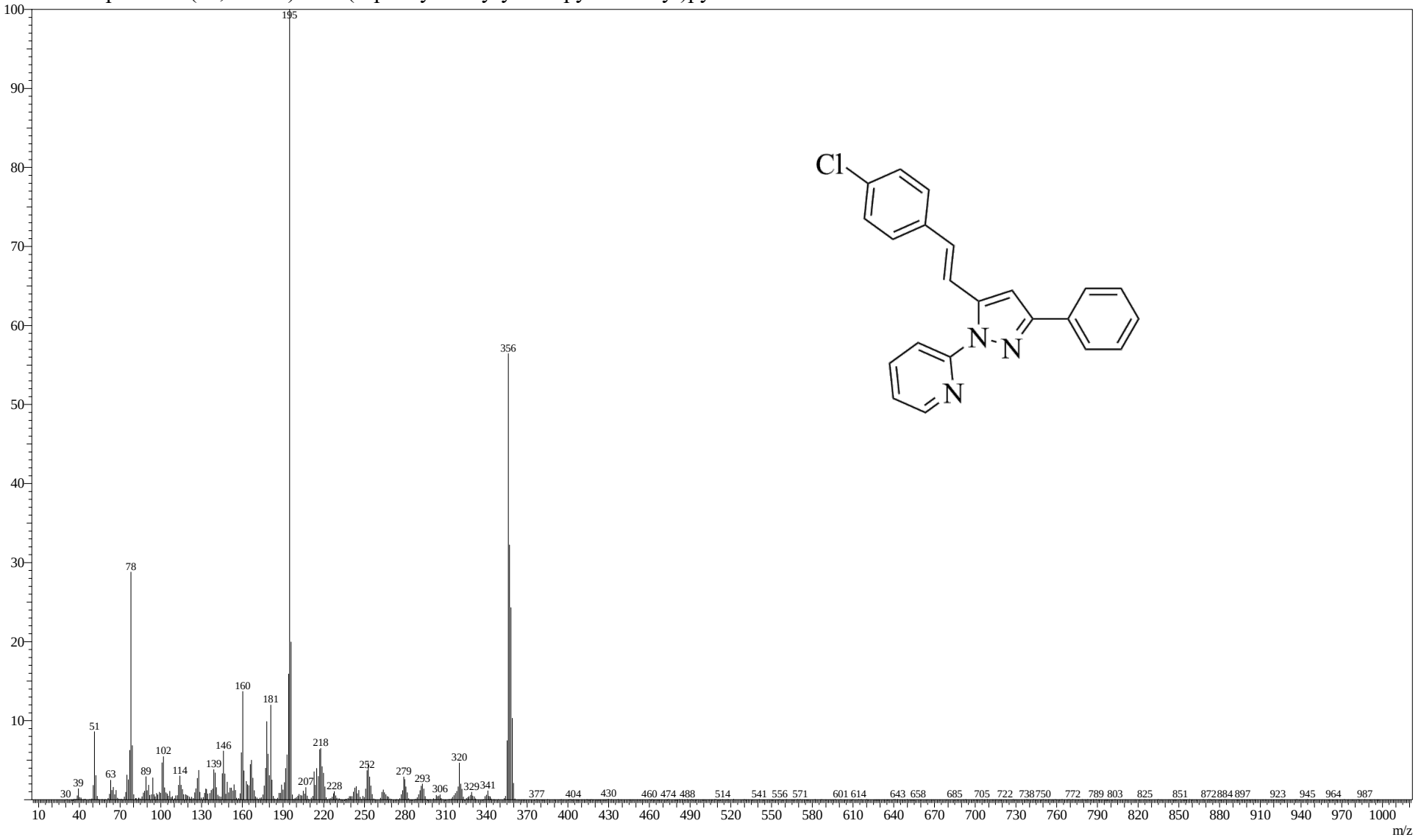
Mass spectrum (EI, 70 eV) of 2-(3-phenyl-5-styryl-1H-pyrazol-1-yl)pyridine **7b**

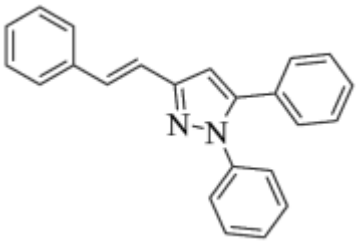


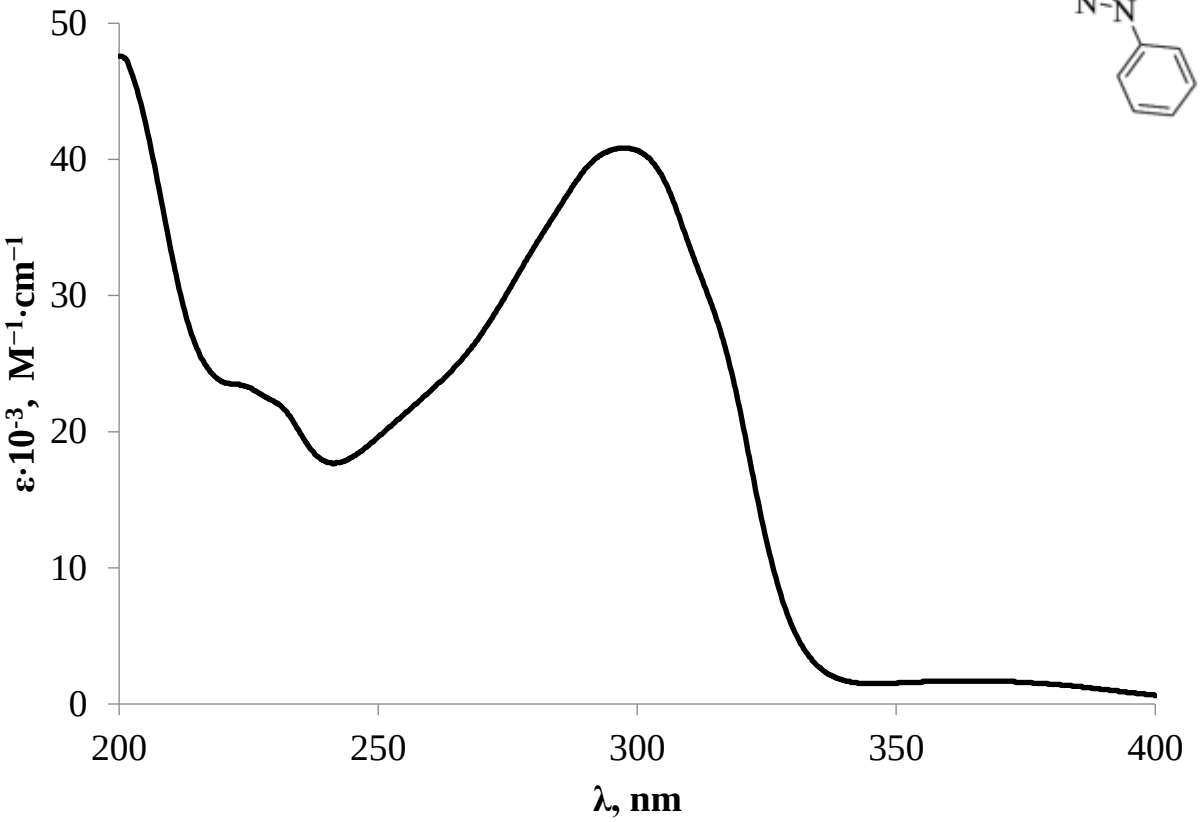
Mass spectrum (EI, 70 eV) of 2-(3-phenyl-5-styryl-1H-pyrazol-1-yl)pyridine **7c**



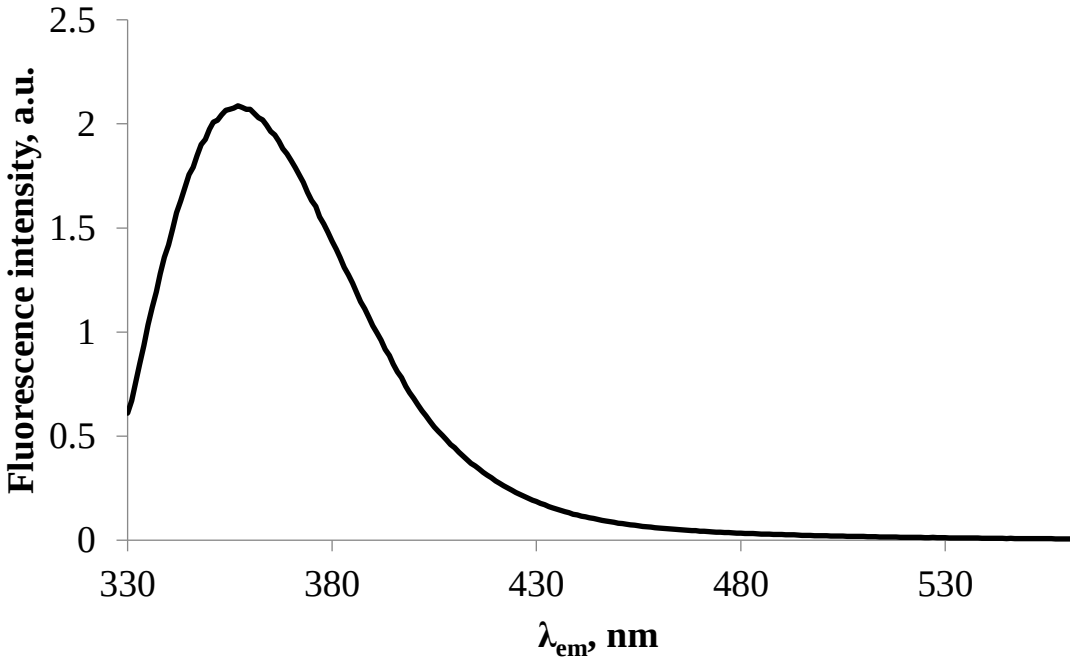
Mass spectrum (EI, 70 eV) of 2-(3-phenyl-5-styryl-1H-pyrazol-1-yl)pyridine **7d**



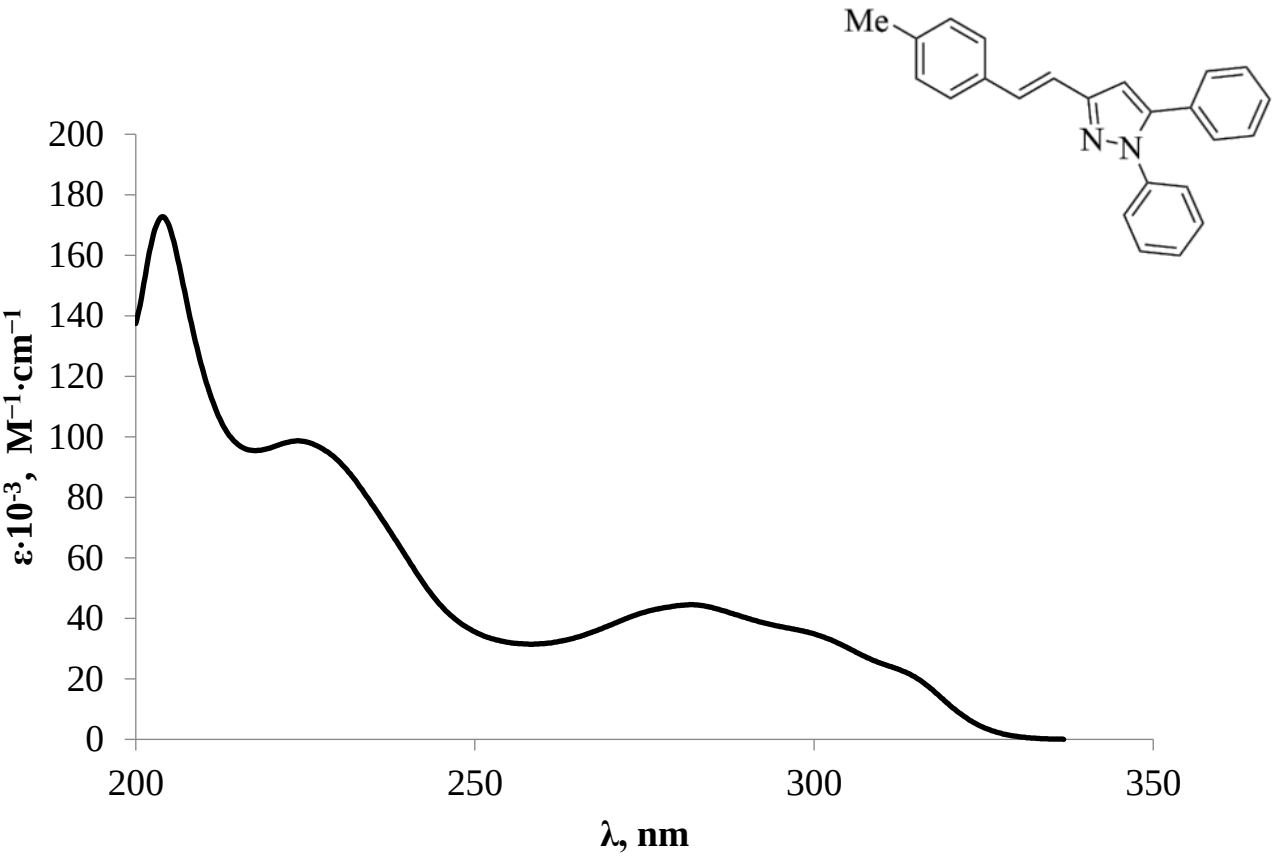




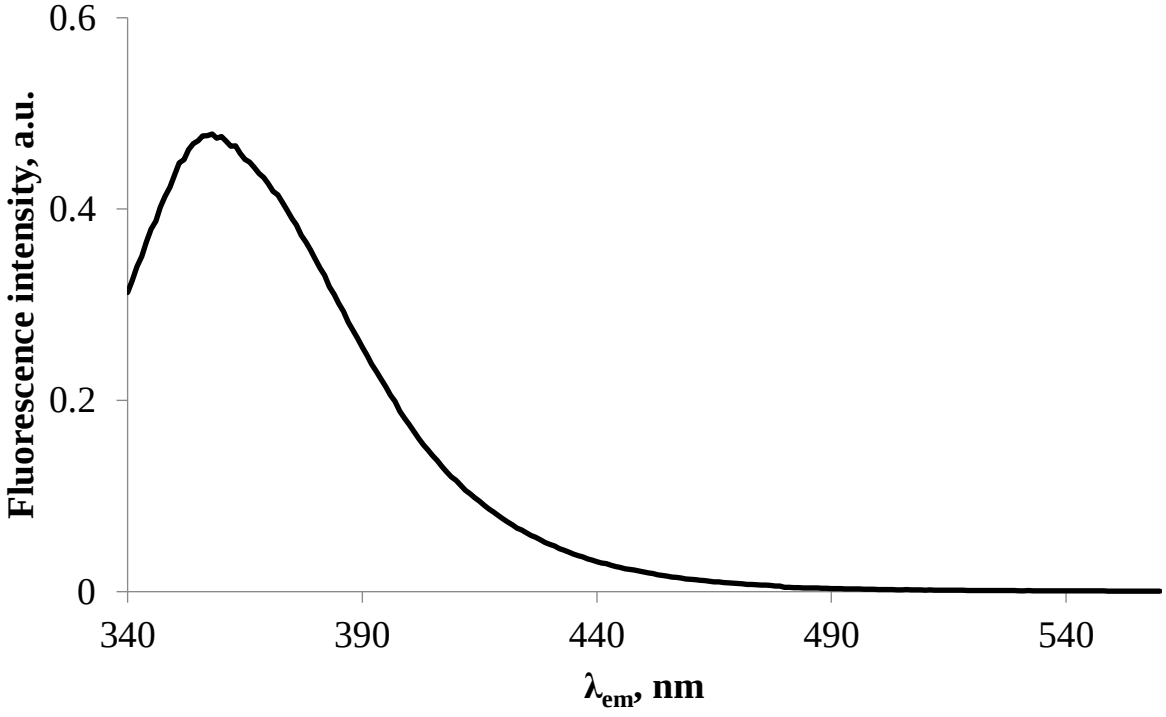
Absorption spectrum of pyrazole **4a**



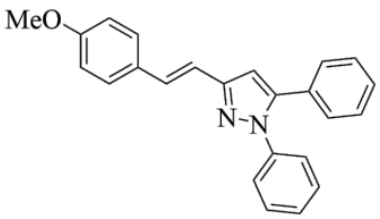
Emission spectrum of pyrazole **4a** (EX wavelength is 307 nm)

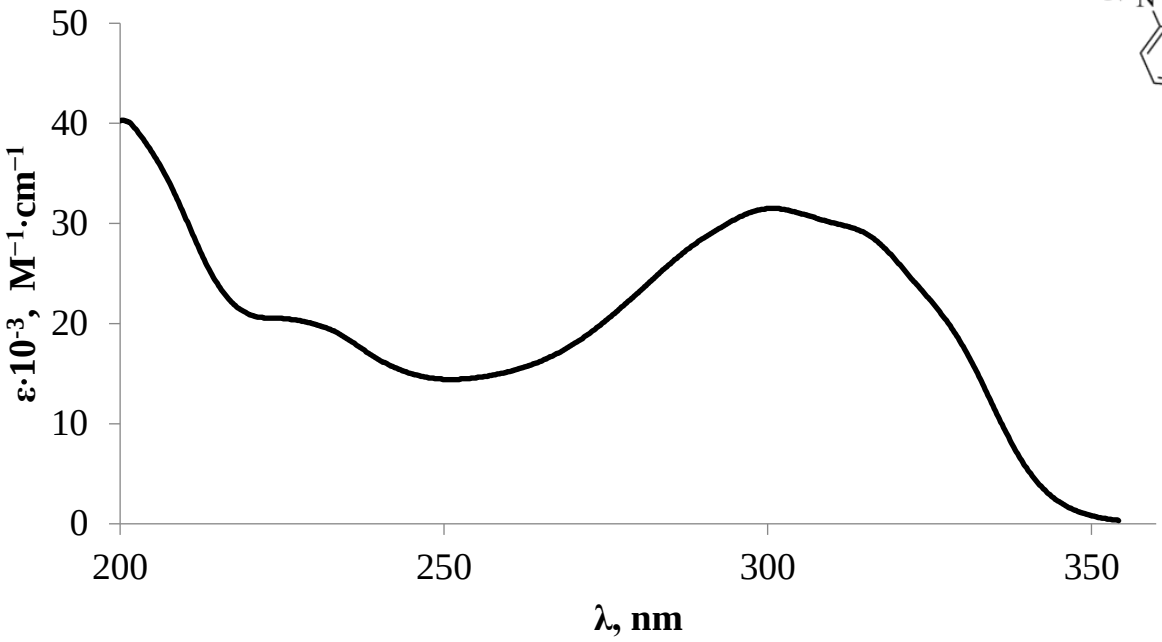


Absorption spectrum of pyrazole **4b**

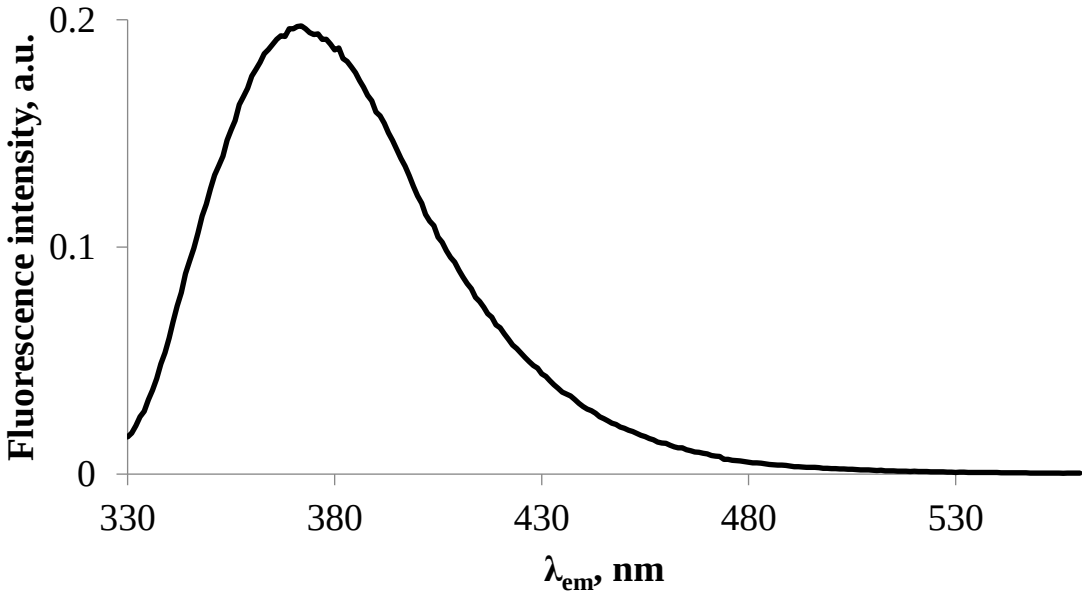


Emission spectrum of pyrazole **4b** (EX wavelength is 309 nm)

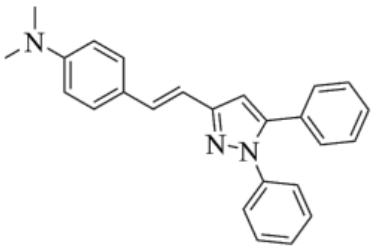


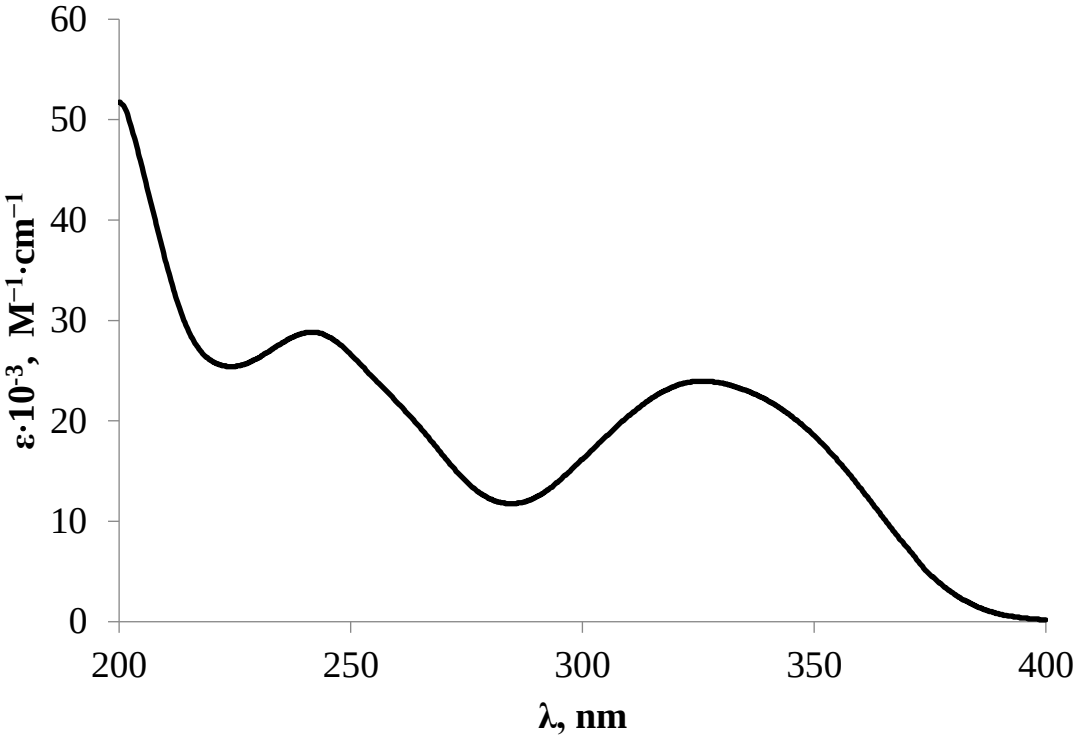


Absorption spectrum of pyrazole **4c**

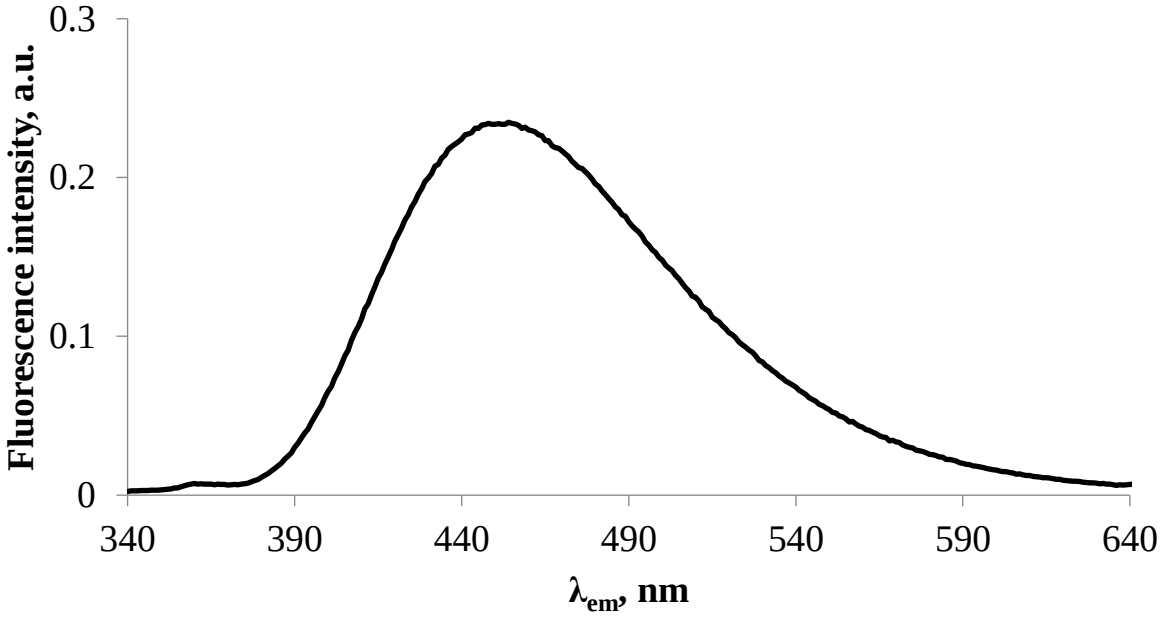


Emission spectrum of pyrazole **4c** (EX wavelength is 301 nm)

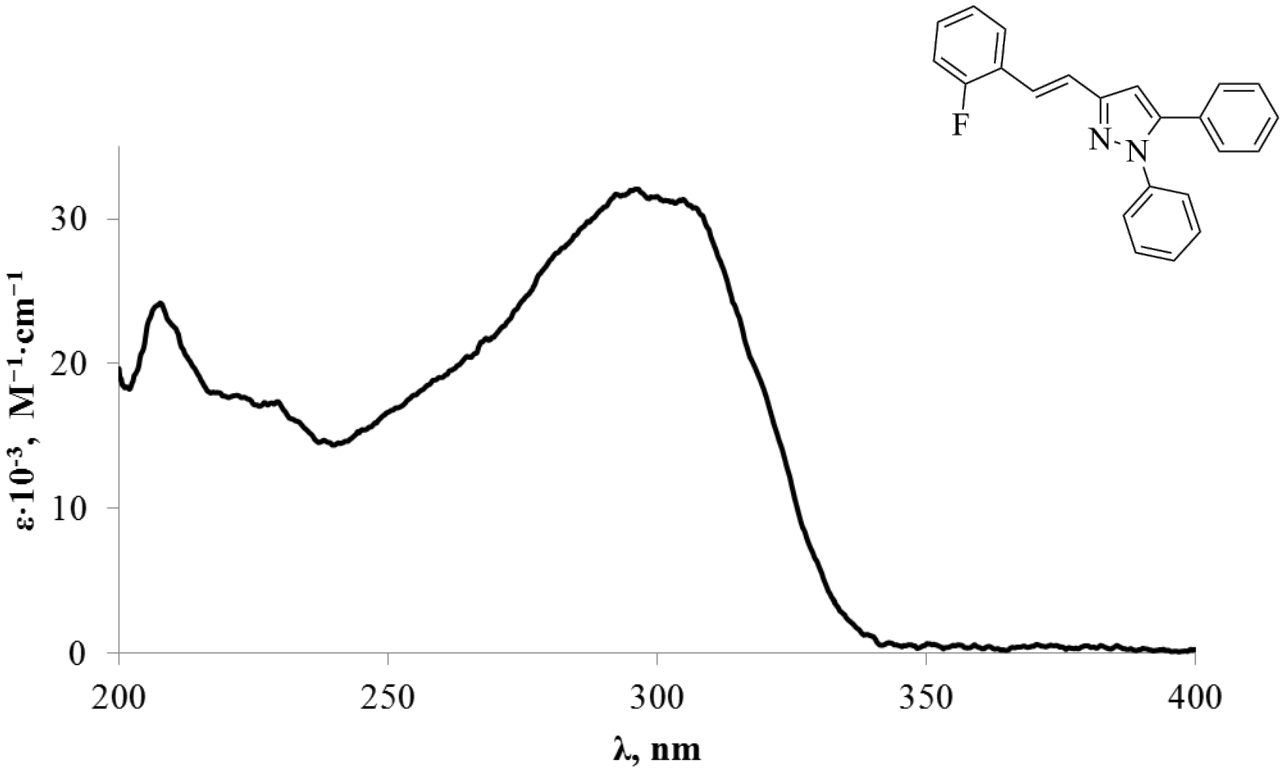




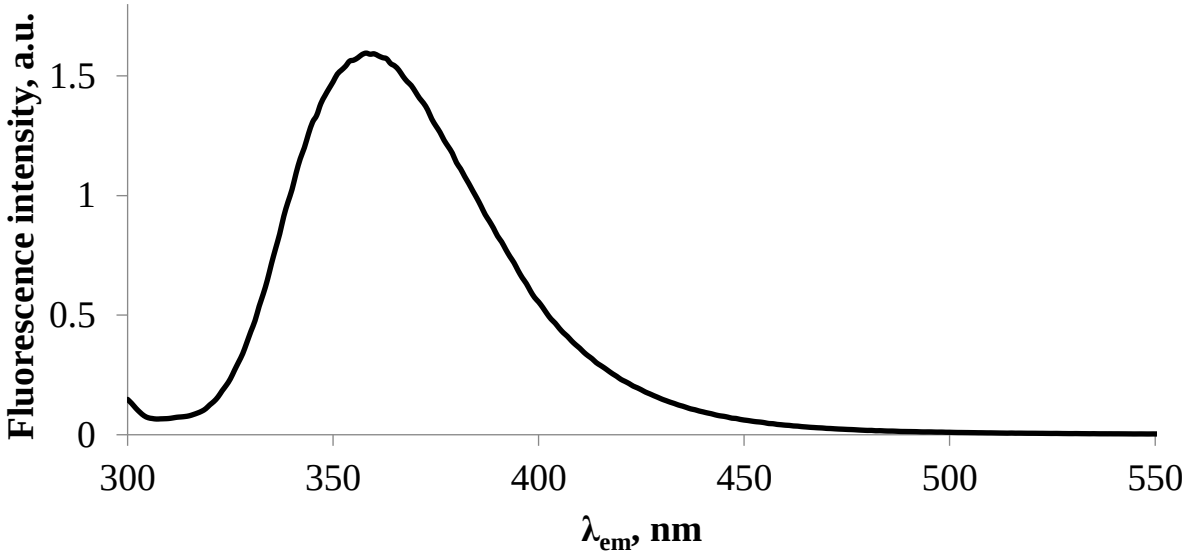
Absorption spectrum of pyrazole **4d**



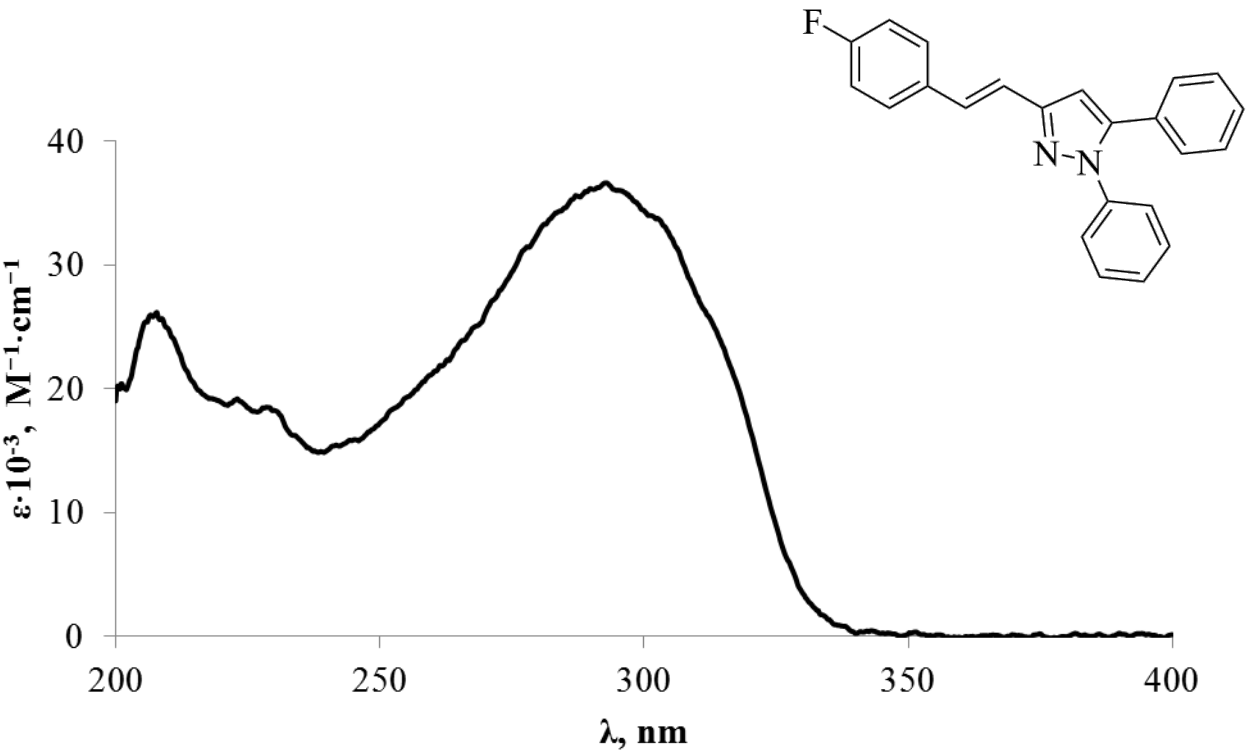
Emission spectrum of pyrazole **4d** (EX wavelength is 326 nm)



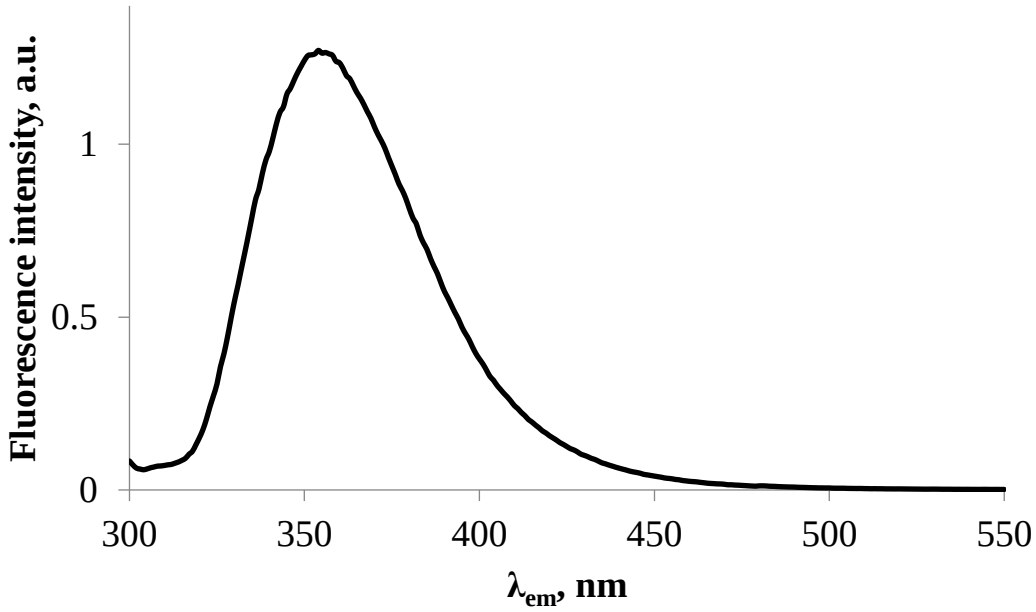
Absorption spectrum of pyrazole **4e**



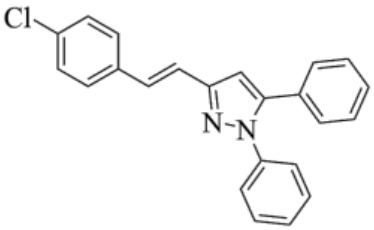
Emission spectrum of pyrazole **4e** (EX wavelength is 296 nm)

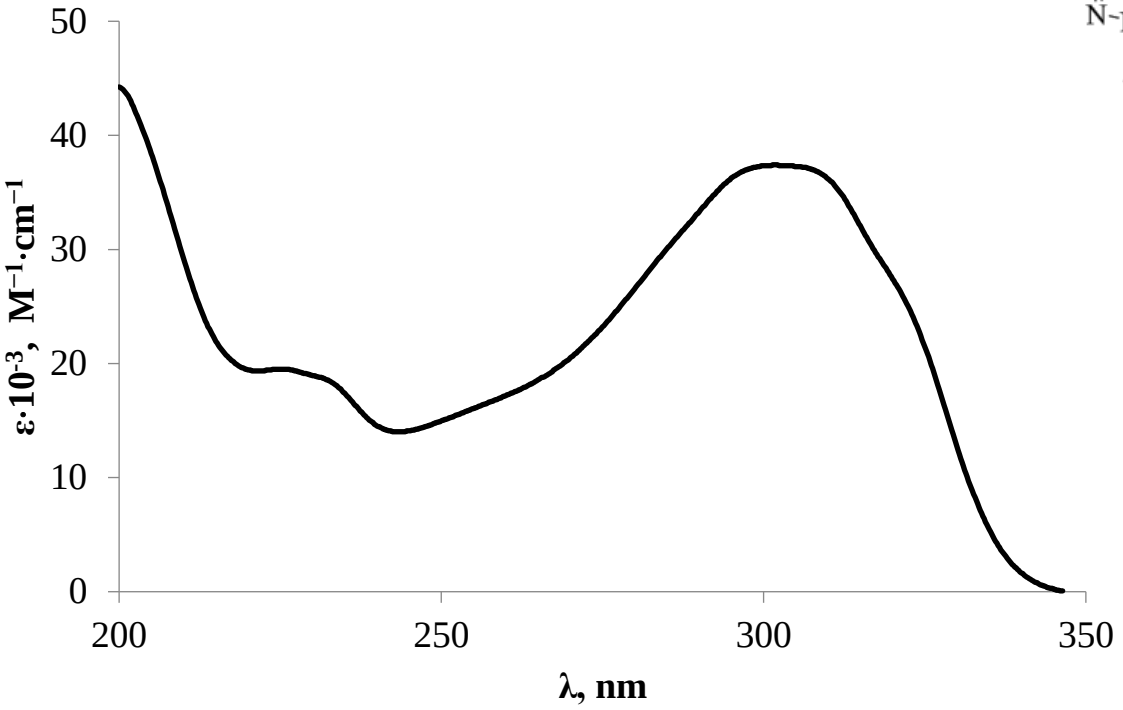


Absorption spectrum of pyrazole **4f**

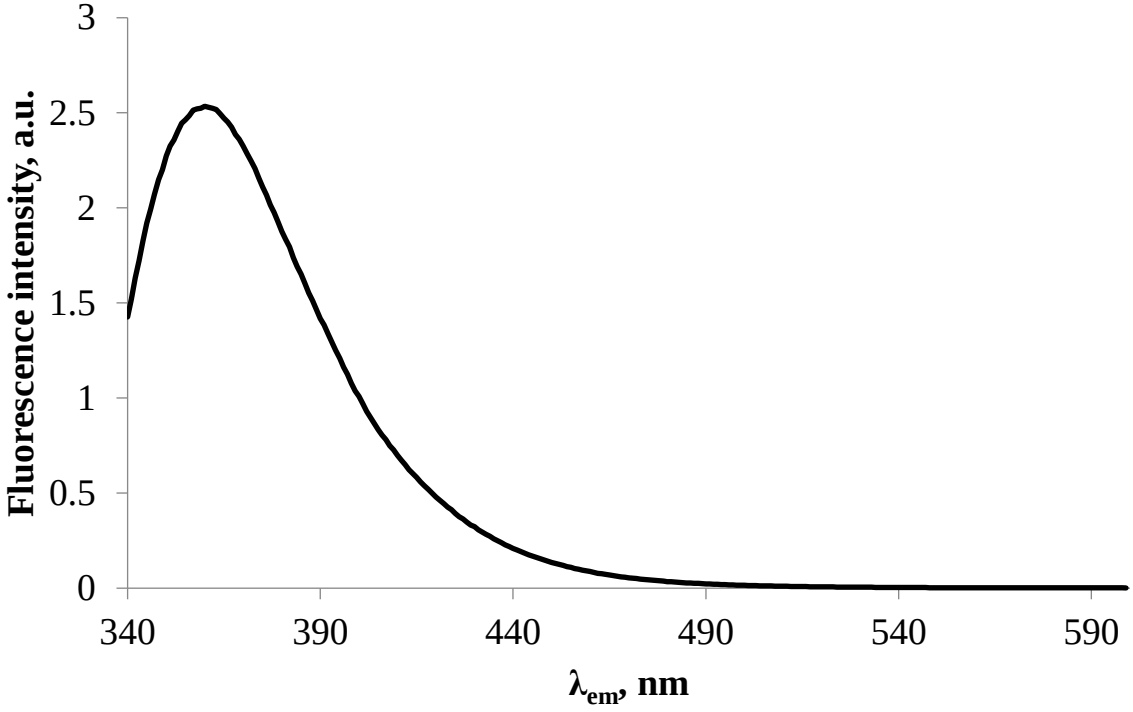


Emission spectrum of pyrazole **4f** (EX wavelength is 293 nm)

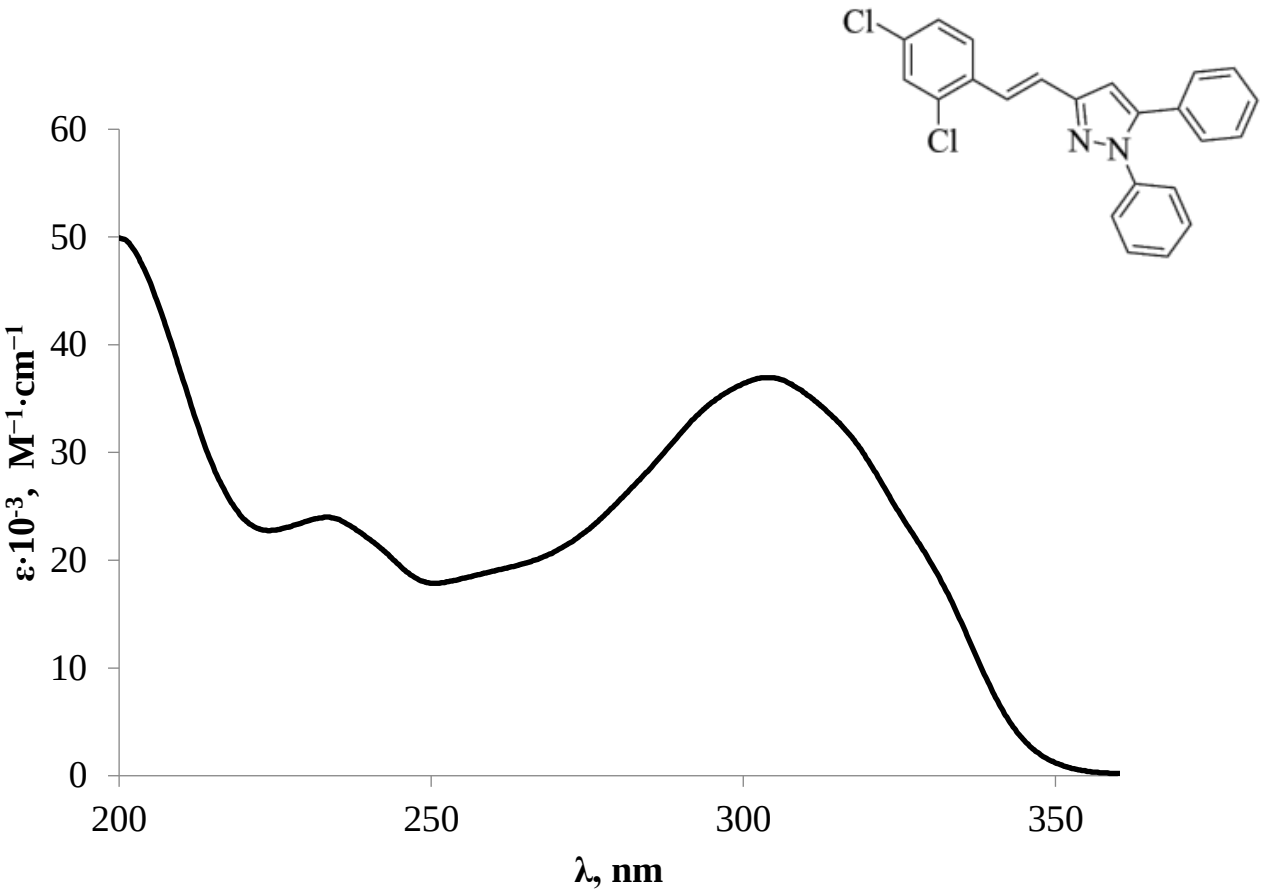




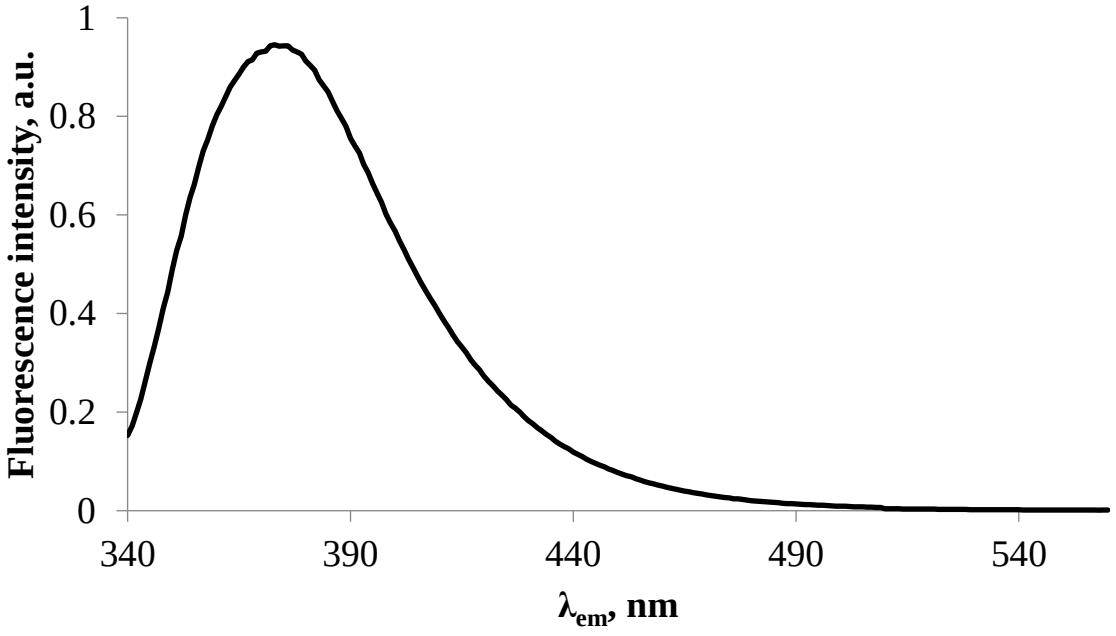
Absorption spectrum of pyrazole **4g**



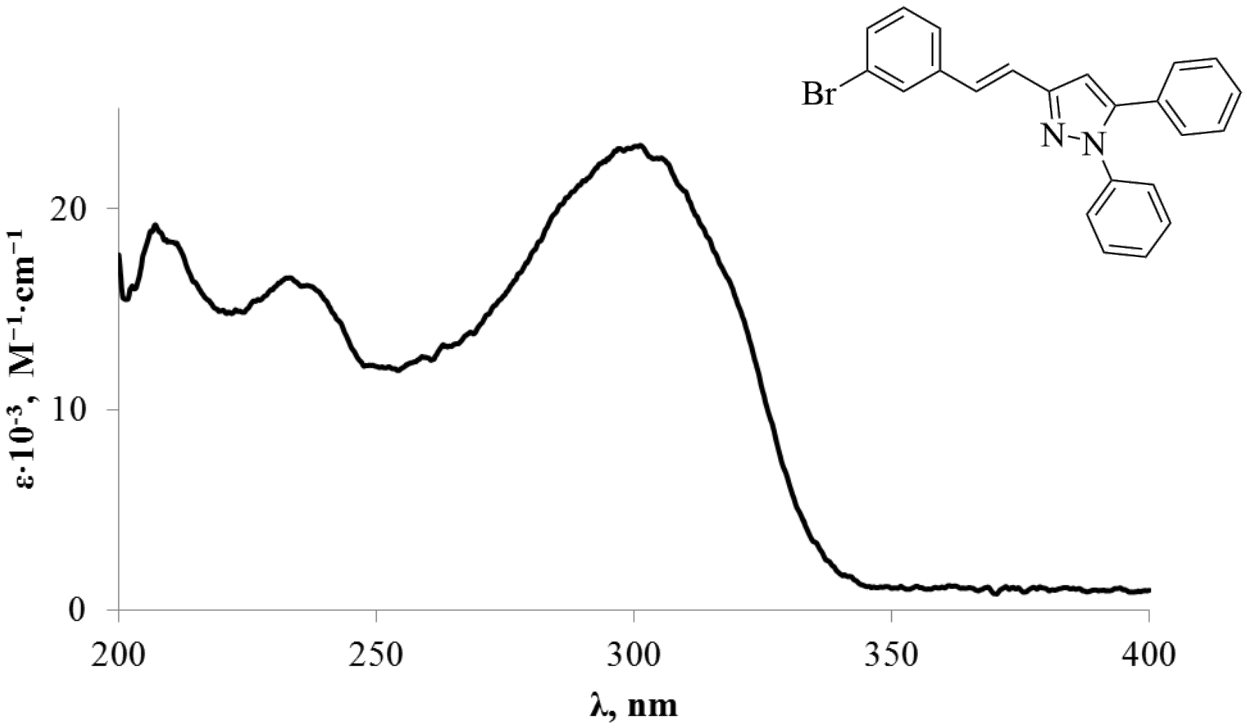
Emission spectrum of pyrazole **4g** (EX wavelength is 312 nm)



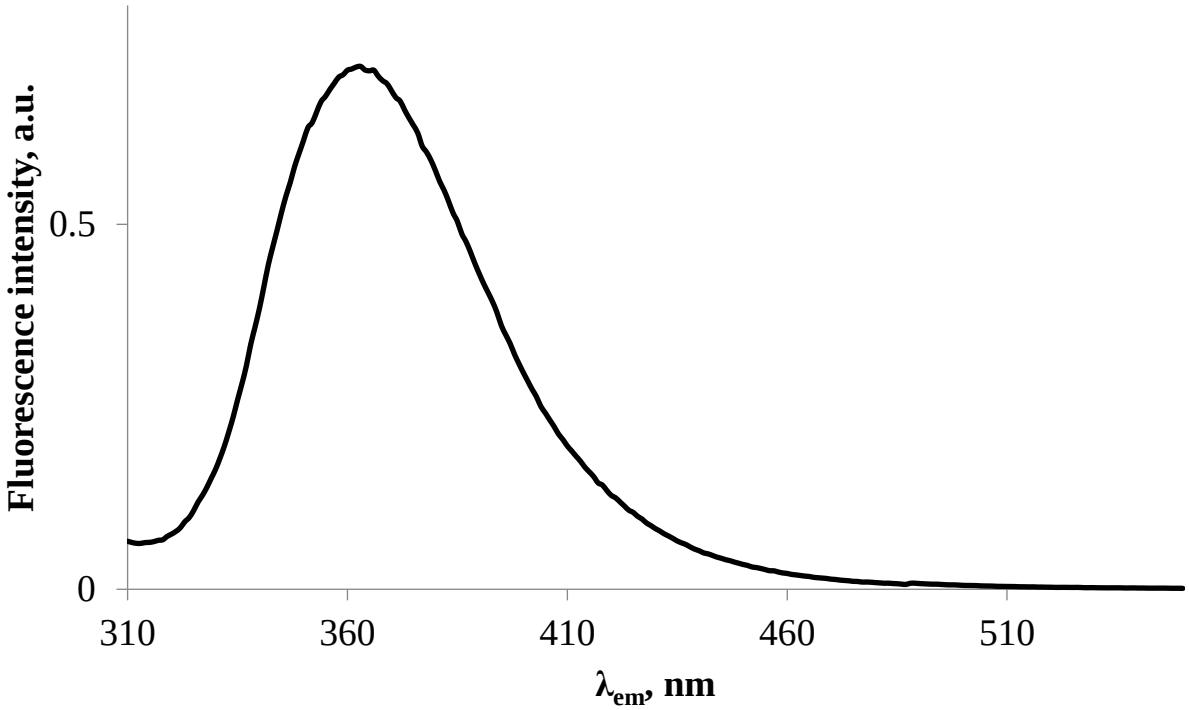
Absorption spectrum of pyrazole **4h**



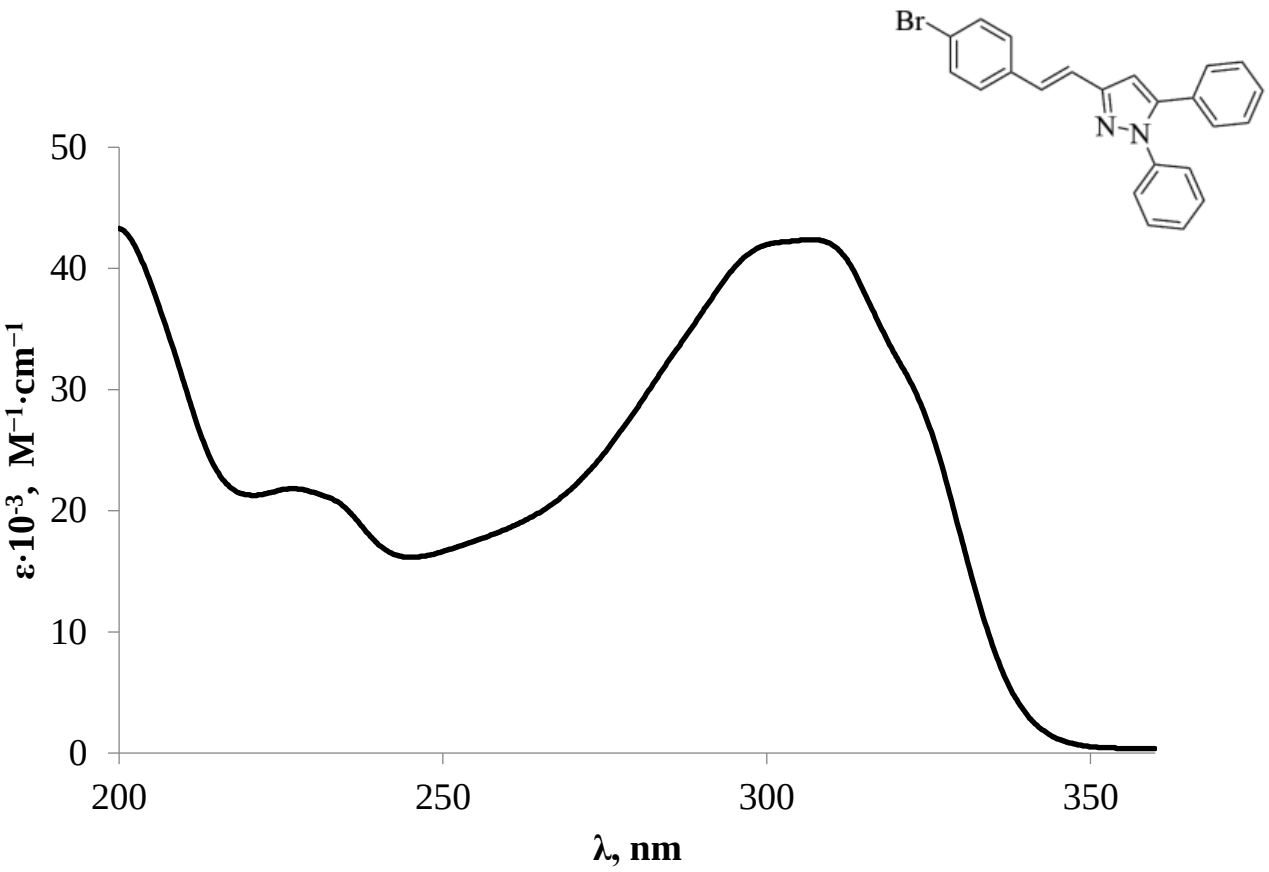
Emission spectrum of pyrazole **4h** (EX wavelength is 304 nm)



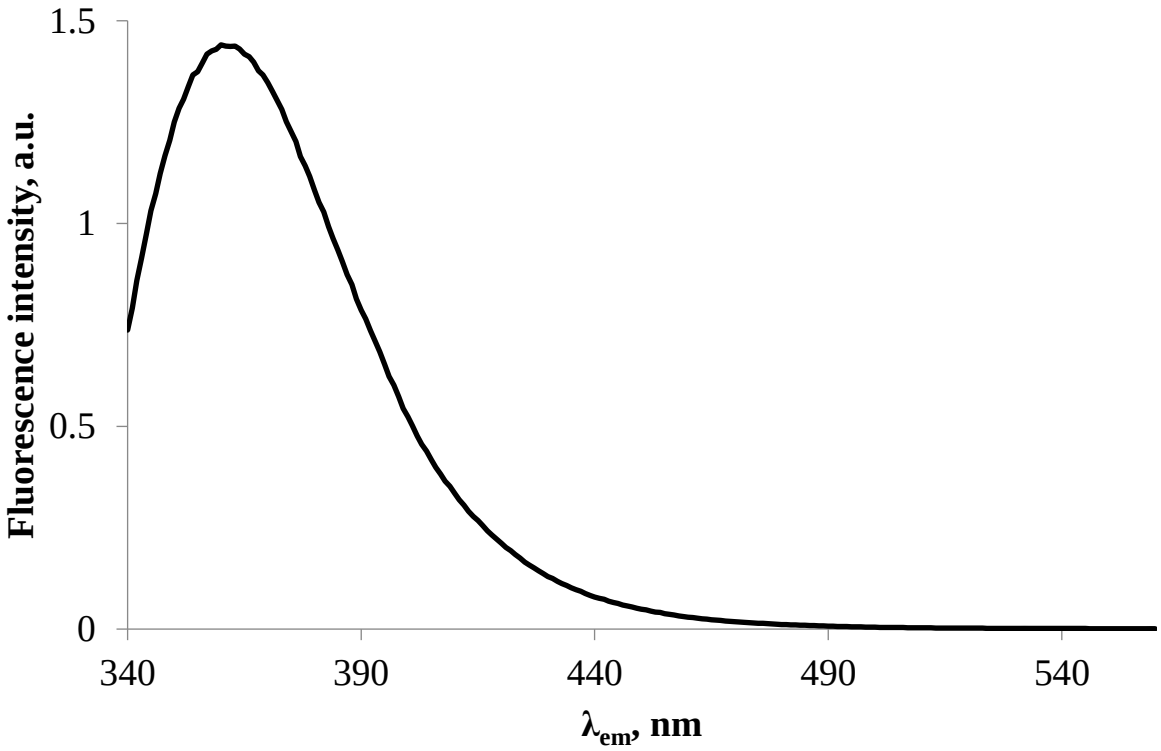
Absorption spectrum of pyrazole **4i**



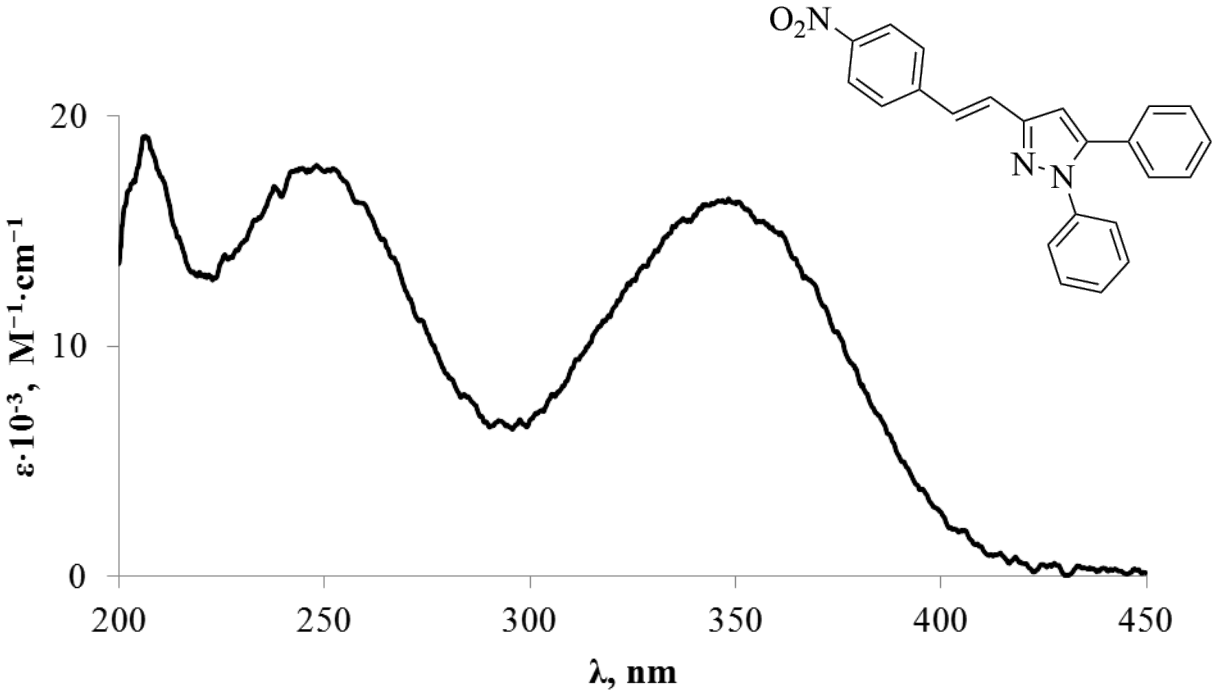
Emission spectrum of pyrazole **4i** (EX wavelength is 300 nm)



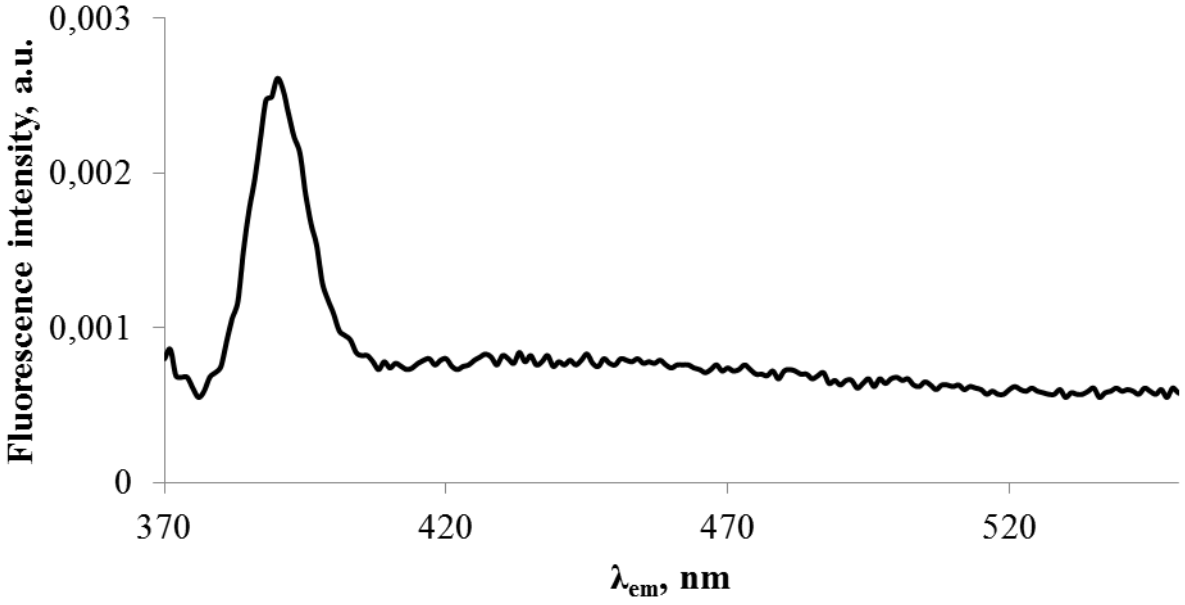
Absorption spectrum of pyrazole **4j**



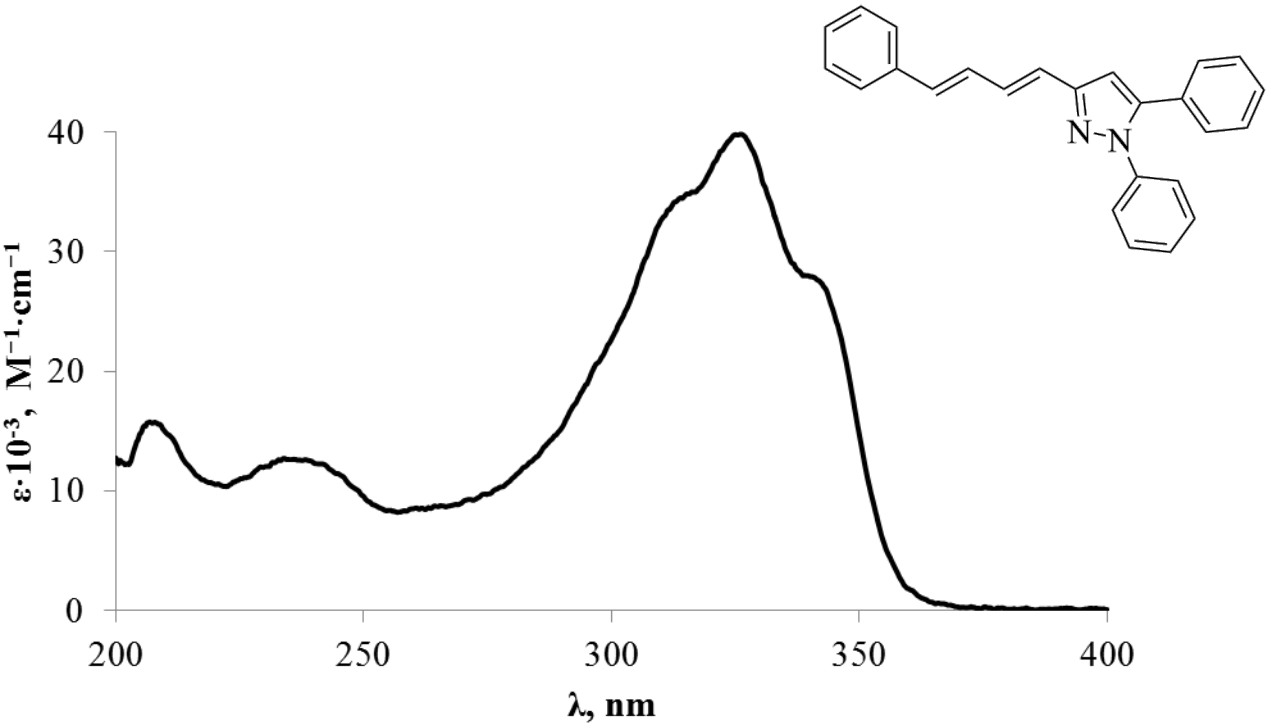
Emission spectrum of pyrazole **4j** (EX wavelength is 307 nm)



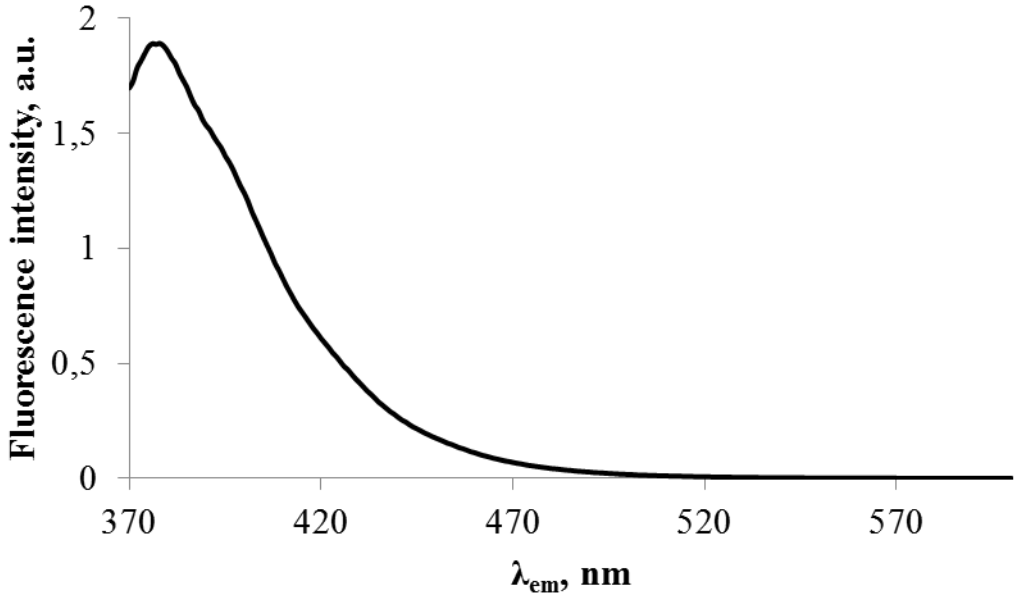
Absorption spectrum of pyrazole **4k**



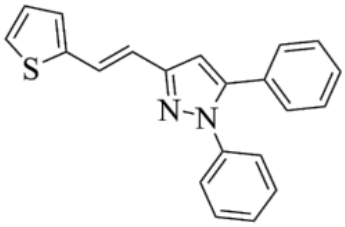
Emission spectrum of pyrazole **4k** (EX wavelength is 350 nm)

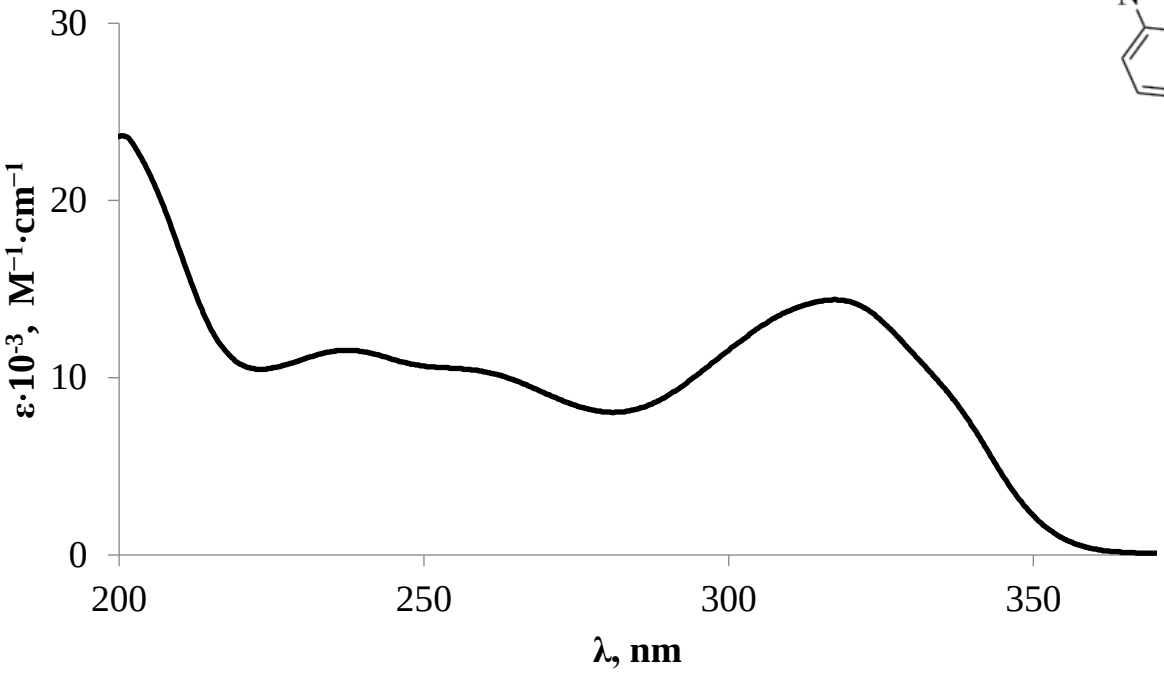


Absorption spectrum of pyrazole **4l**

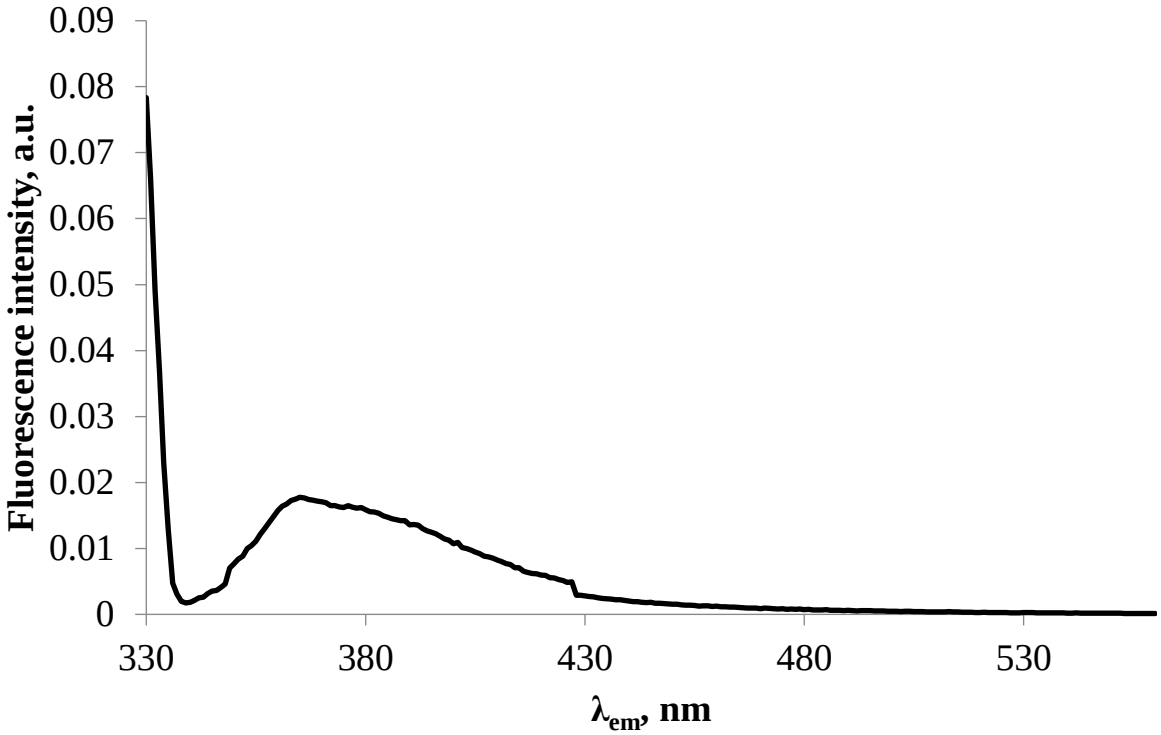


Emission spectrum of pyrazole **4l** (EX wavelength is 325 nm)

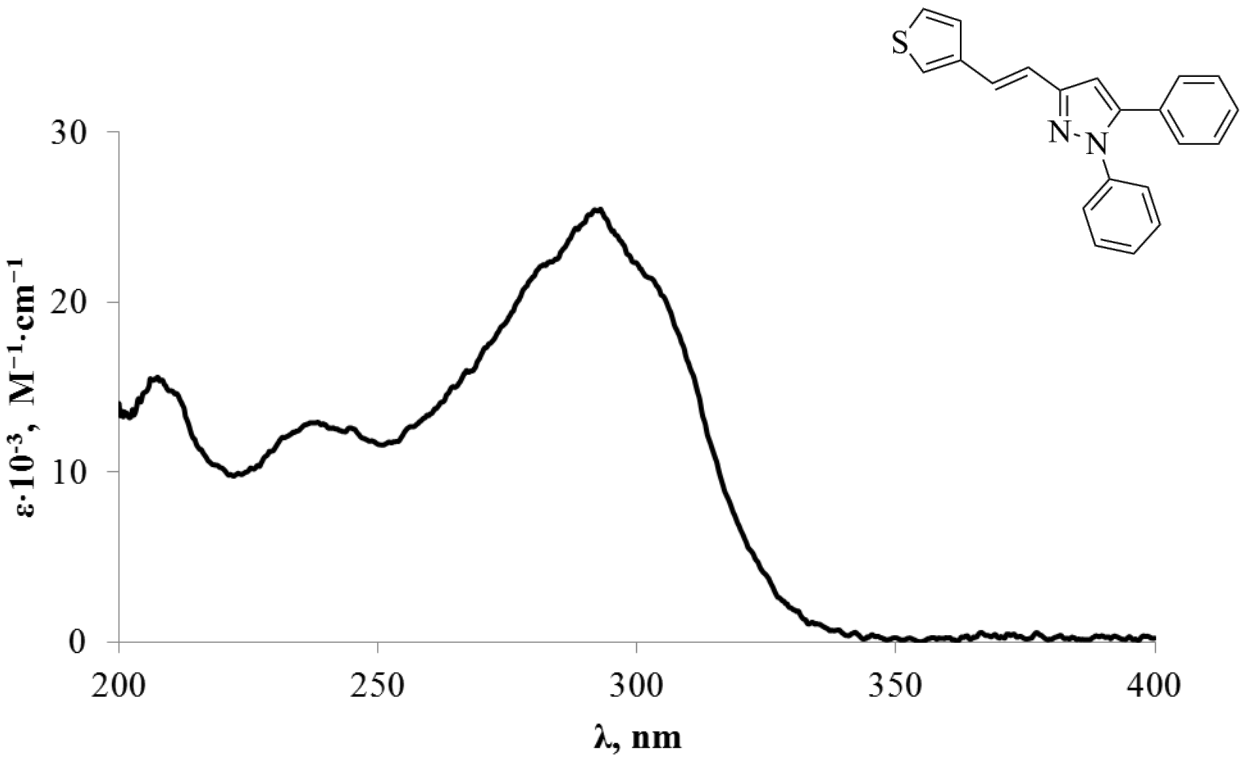




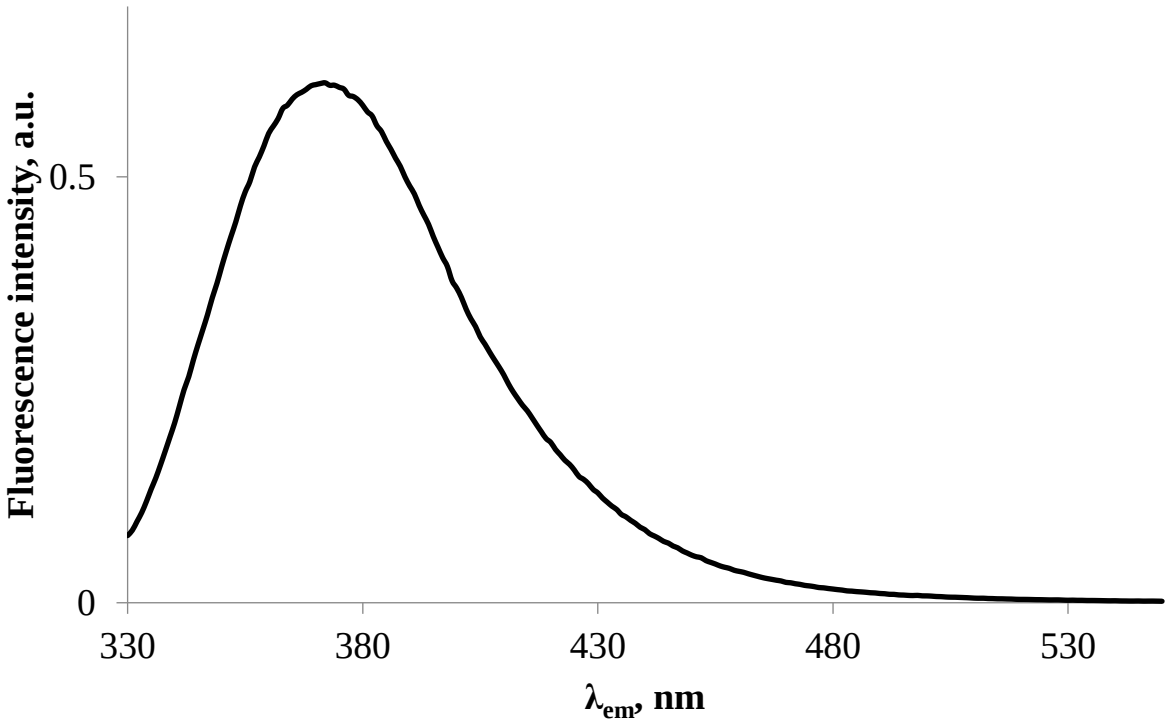
Absorption spectrum of pyrazole **4m**



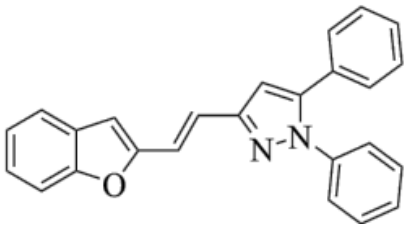
Emission spectrum of pyrazole **4m** (EX wavelength is 327 nm)

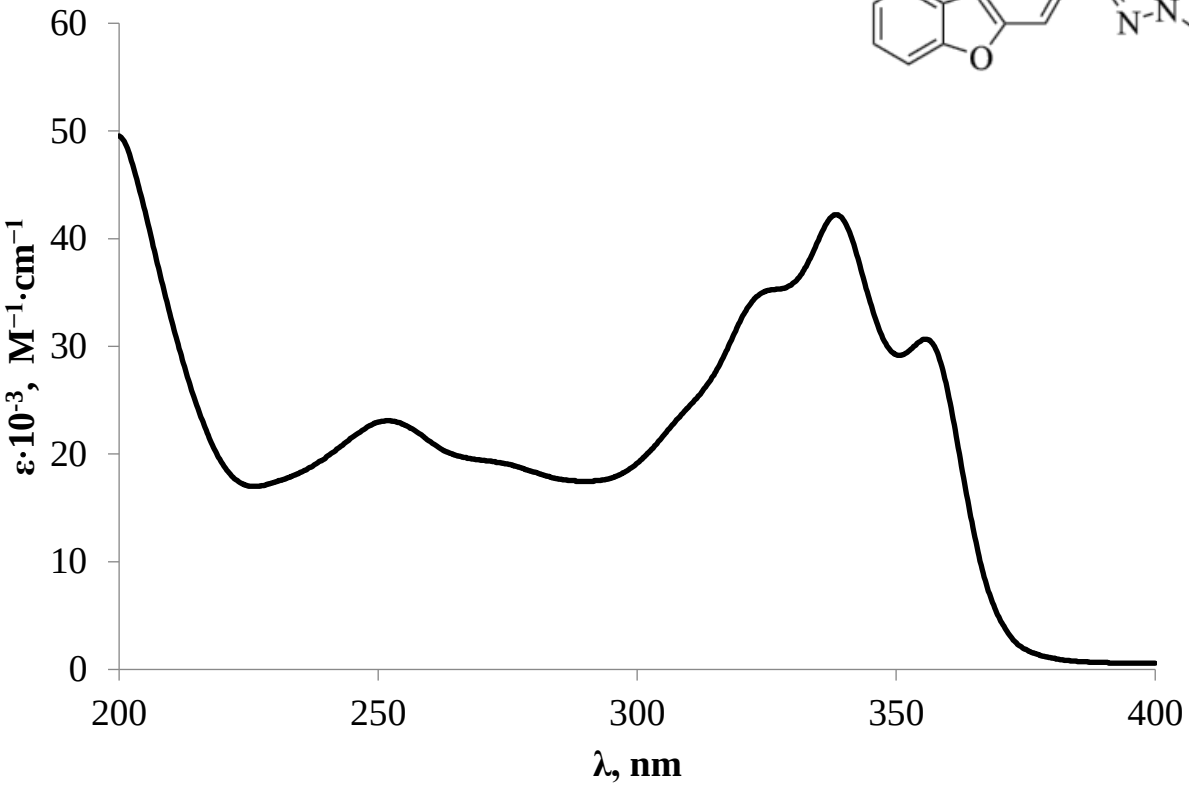


Absorption spectrum of pyrazole **4n**

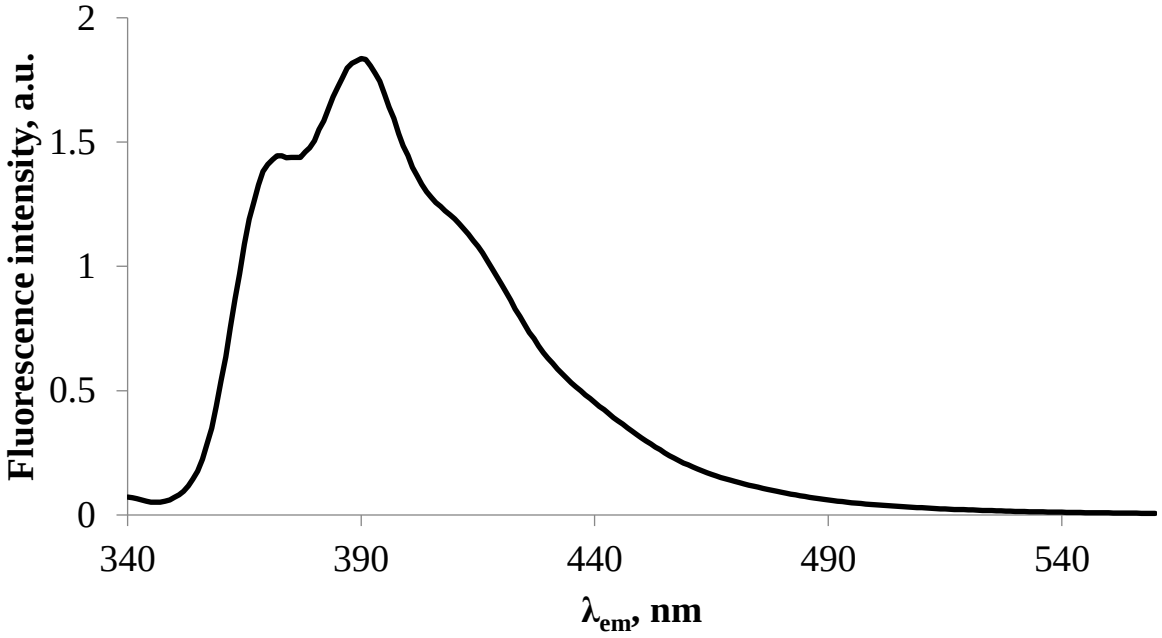


Emission spectrum of pyrazole **4n** (EX wavelength is 292 nm)

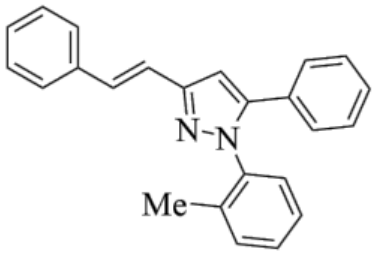


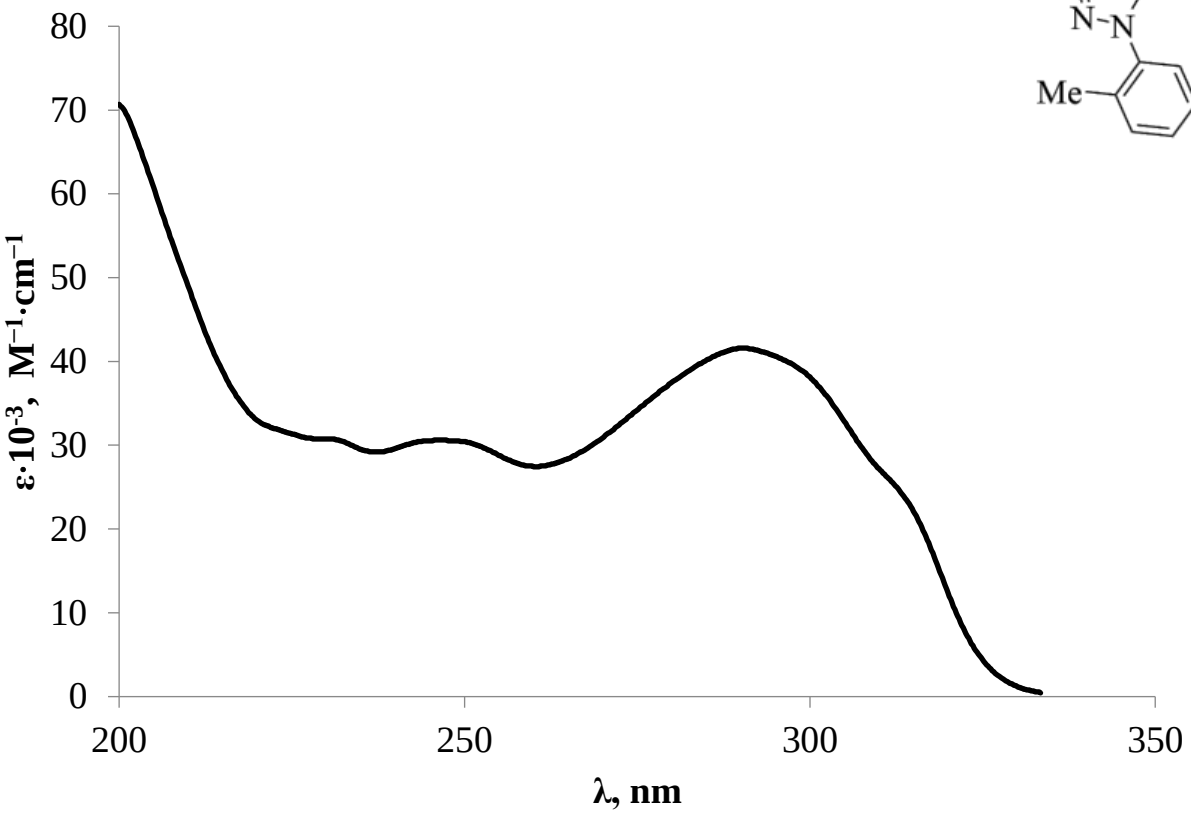


Absorption spectrum of pyrazole **4o**

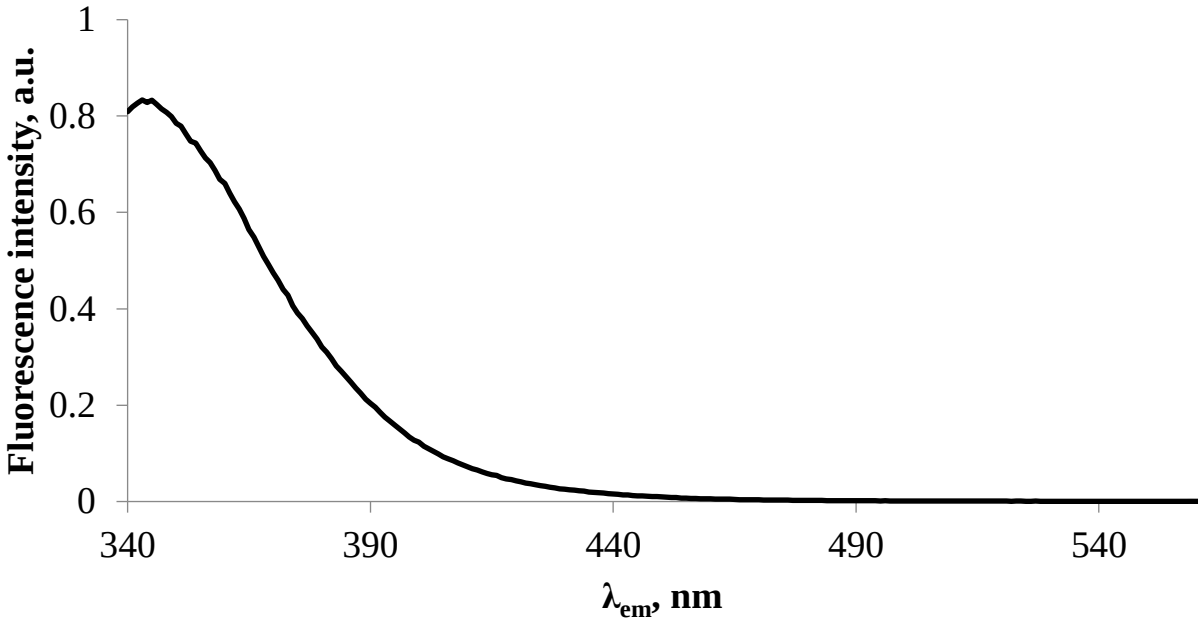


Emission spectrum of pyrazole **4o** (EX wavelength is 338 nm)

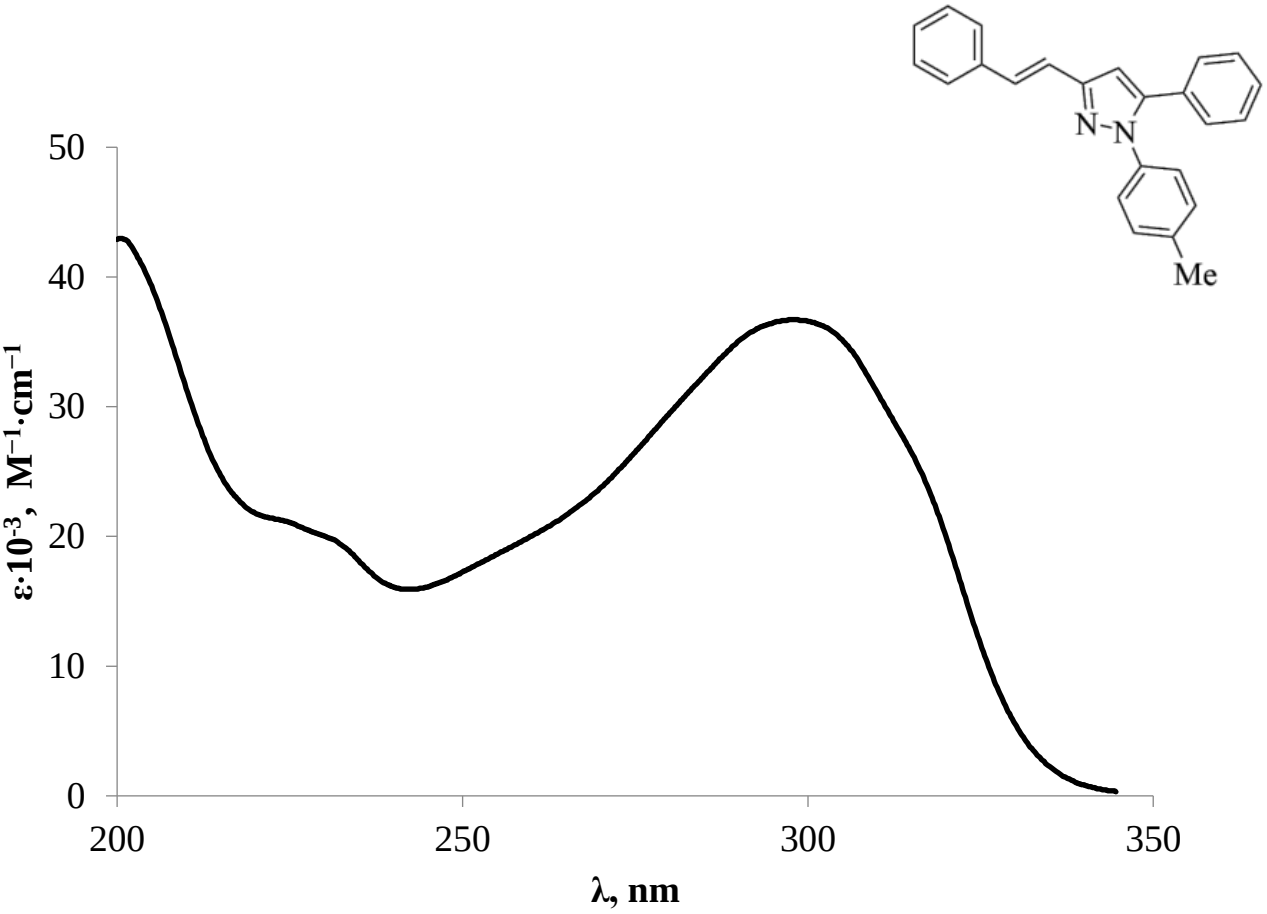




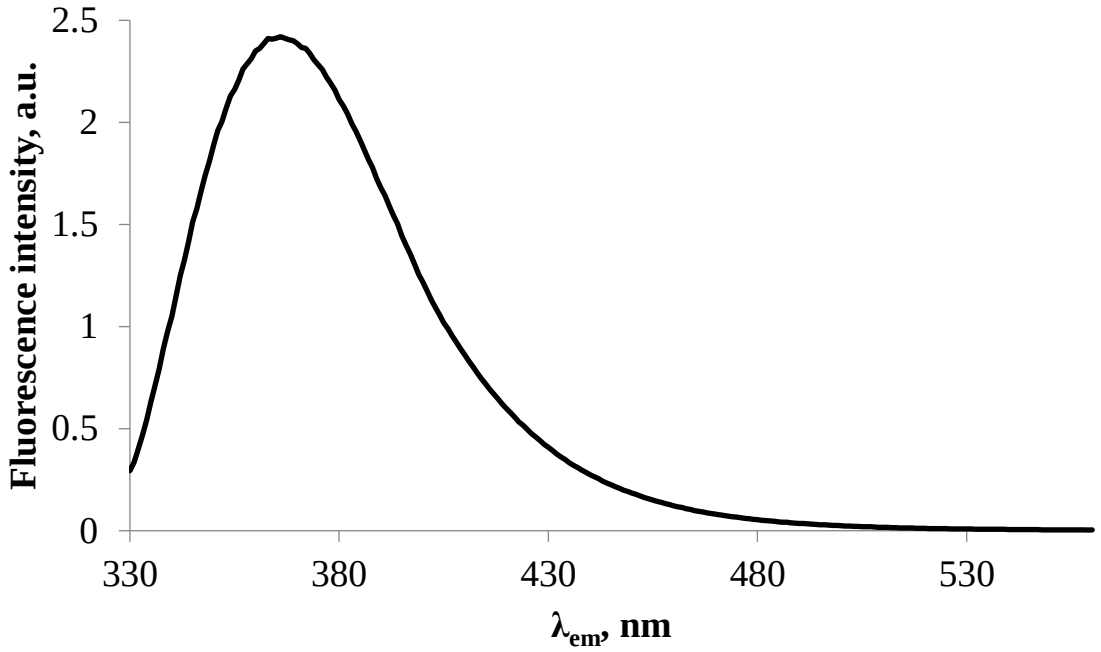
Absorption spectrum of pyrazole **4p**



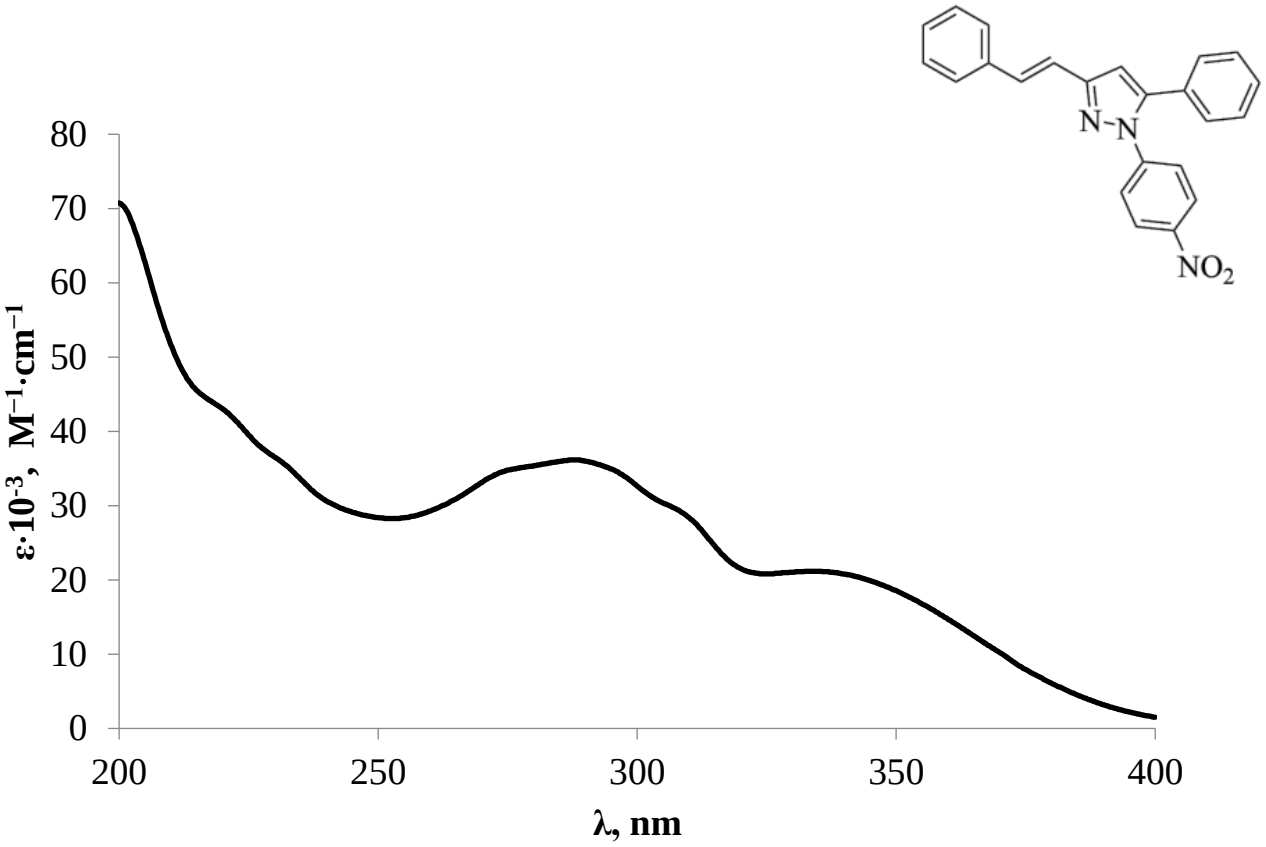
Emission spectrum of pyrazole **4p** (EX wavelength is 290 nm)



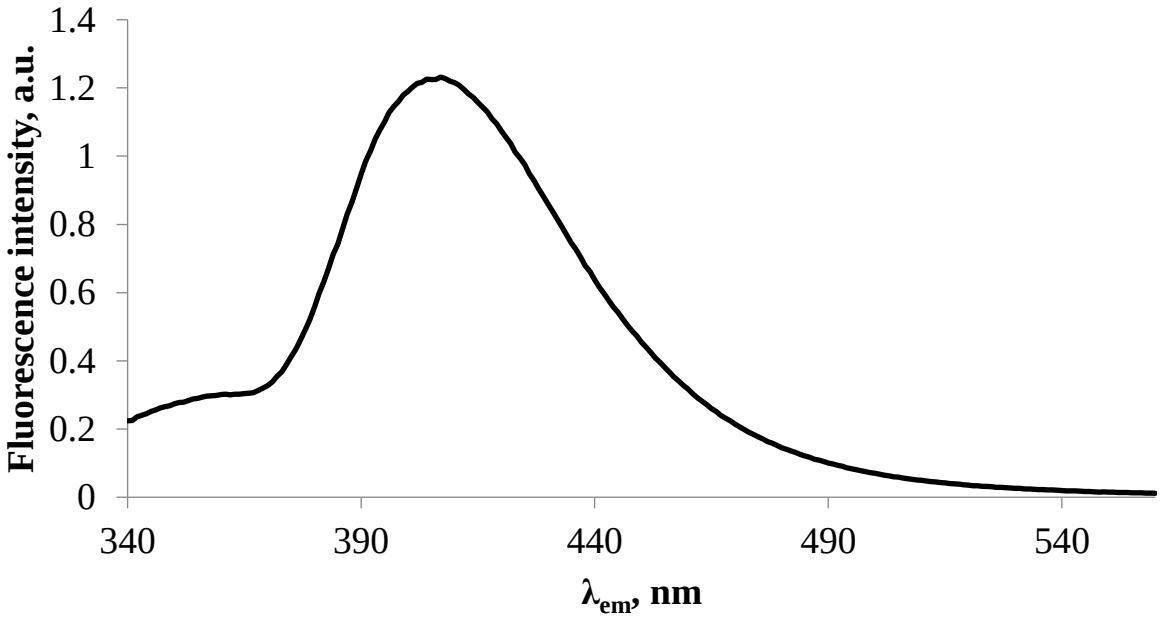
Absorption spectrum of pyrazole **4q**



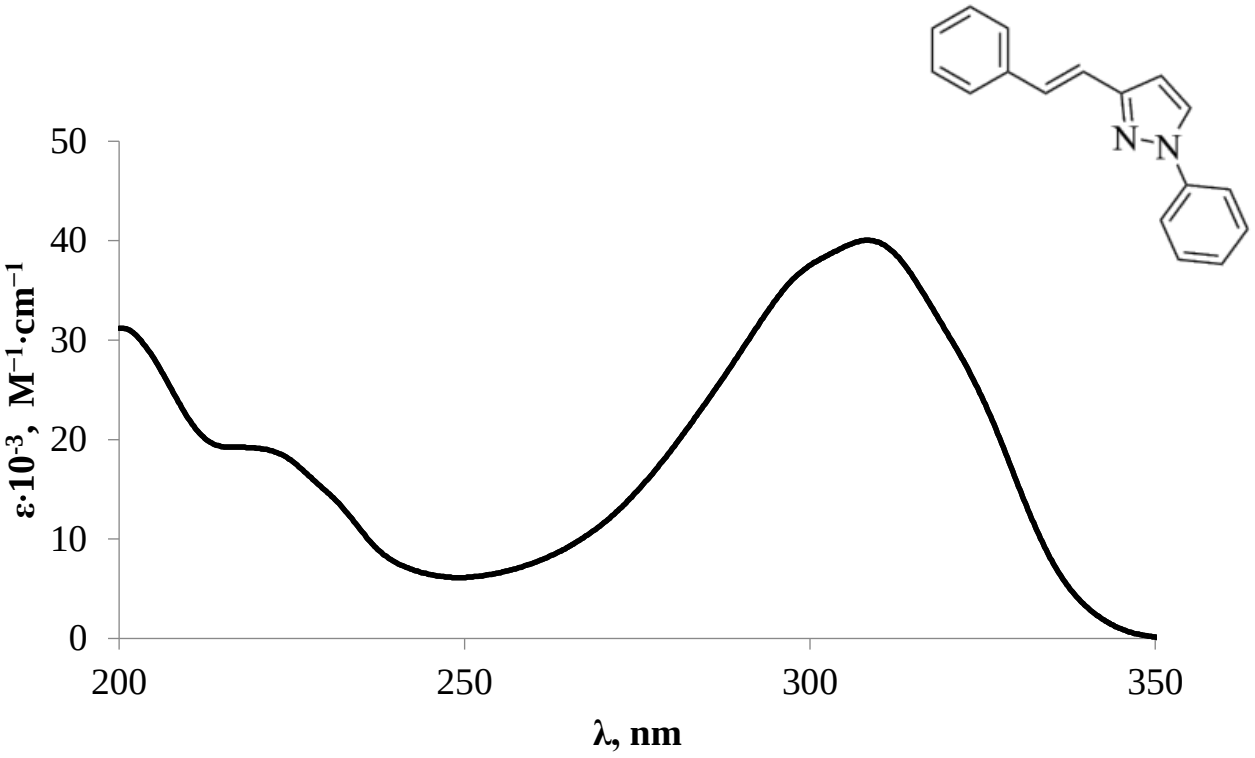
Emission spectrum of pyrazole **4q** (EX wavelength is 308 nm)



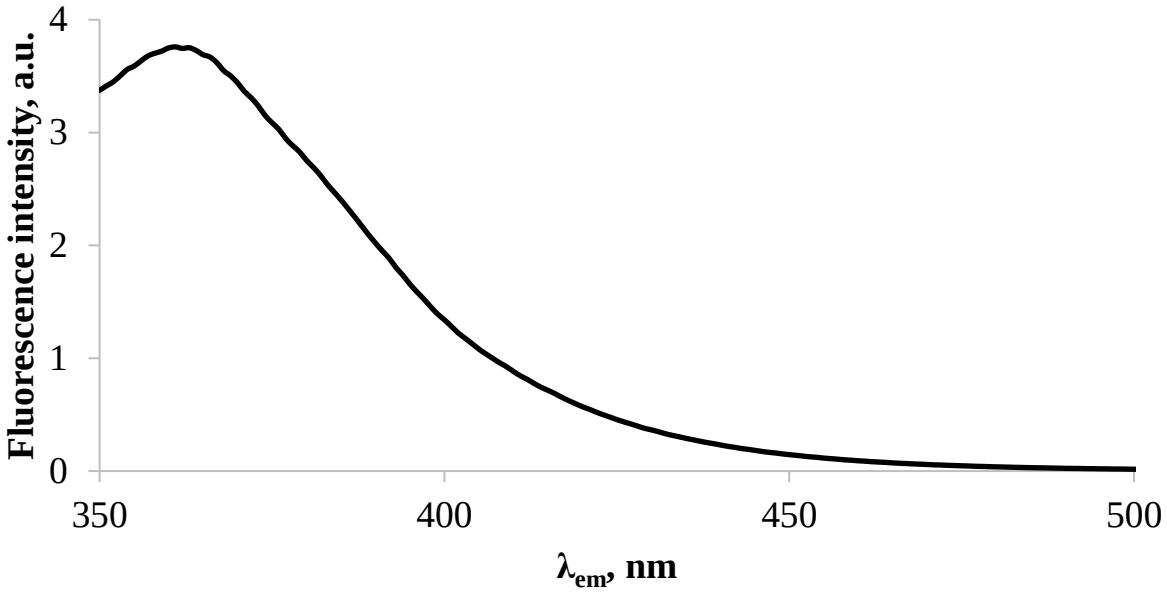
Absorption spectrum of pyrazole **4r**



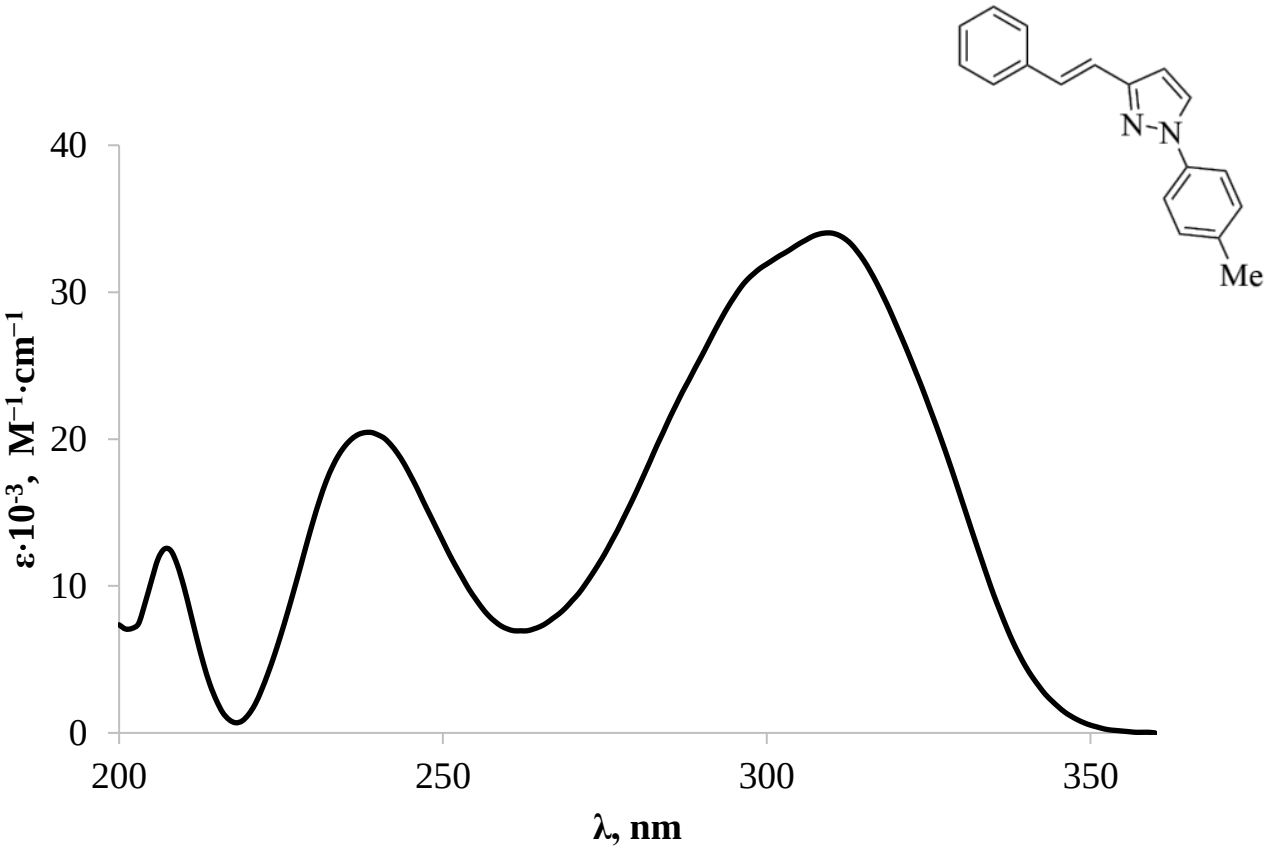
Emission spectrum of pyrazole **4r** (EX wavelength is 298 nm)



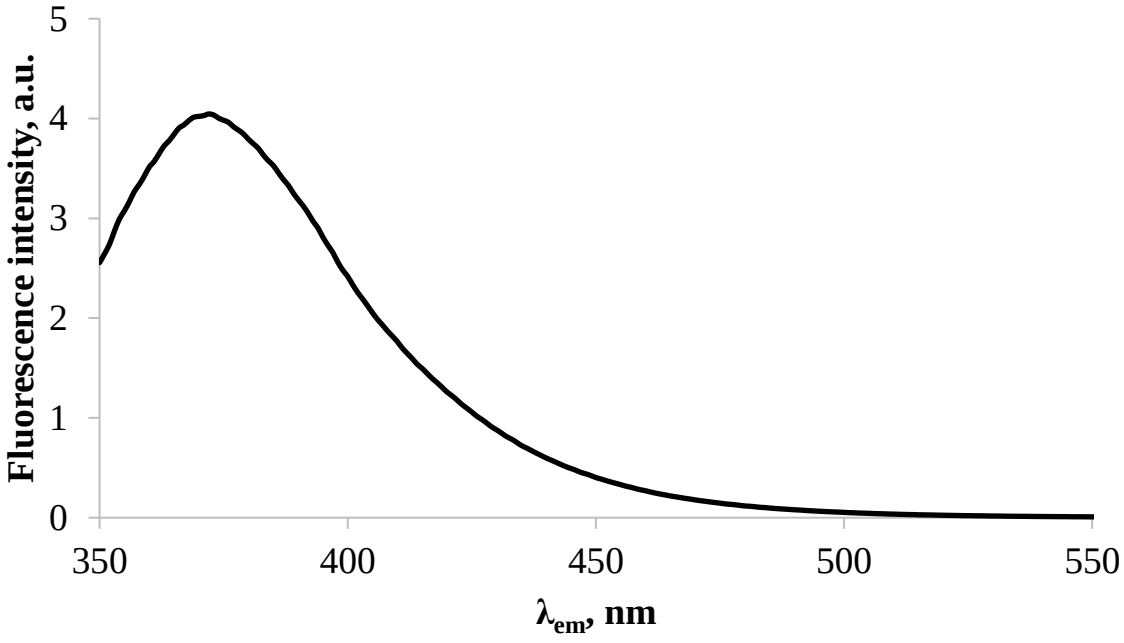
Absorption spectrum of pyrazole **4s**



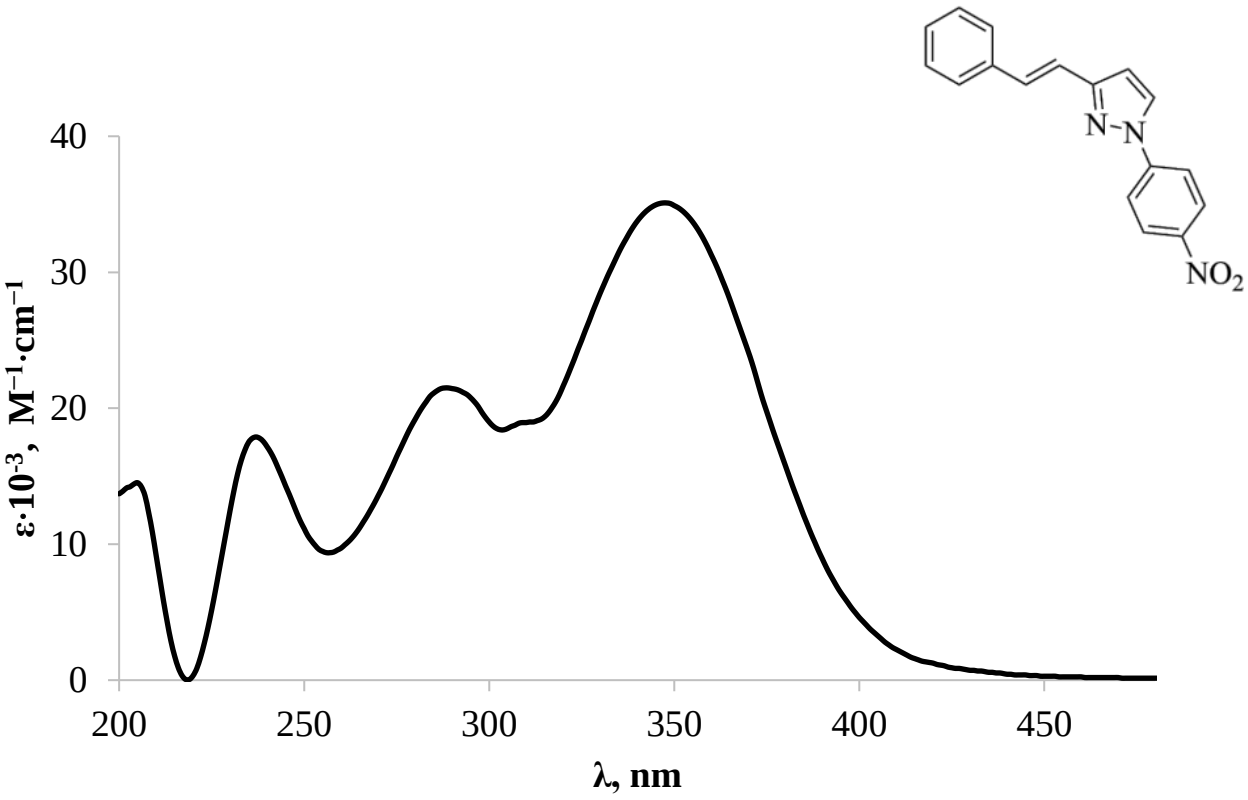
Emission spectrum of pyrazole **4s** (EX wavelength is 308 nm)



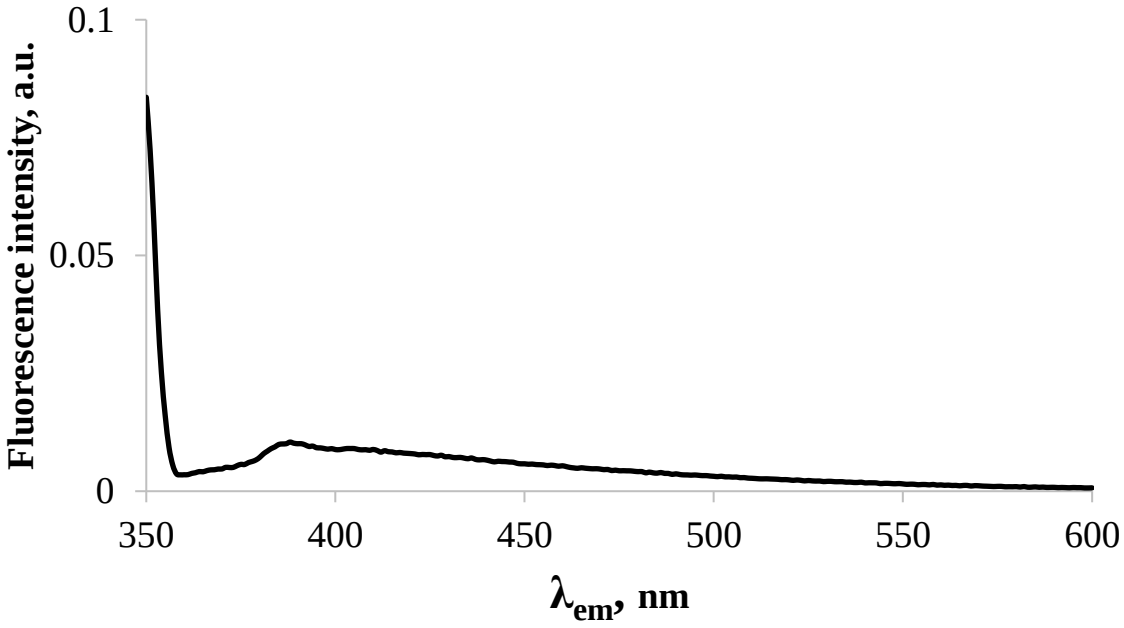
Absorption spectrum of pyrazole **4t**



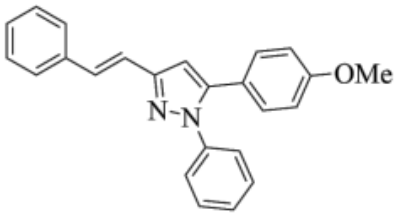
Emission spectrum of pyrazole **4t** (EX wavelength is 309 nm)

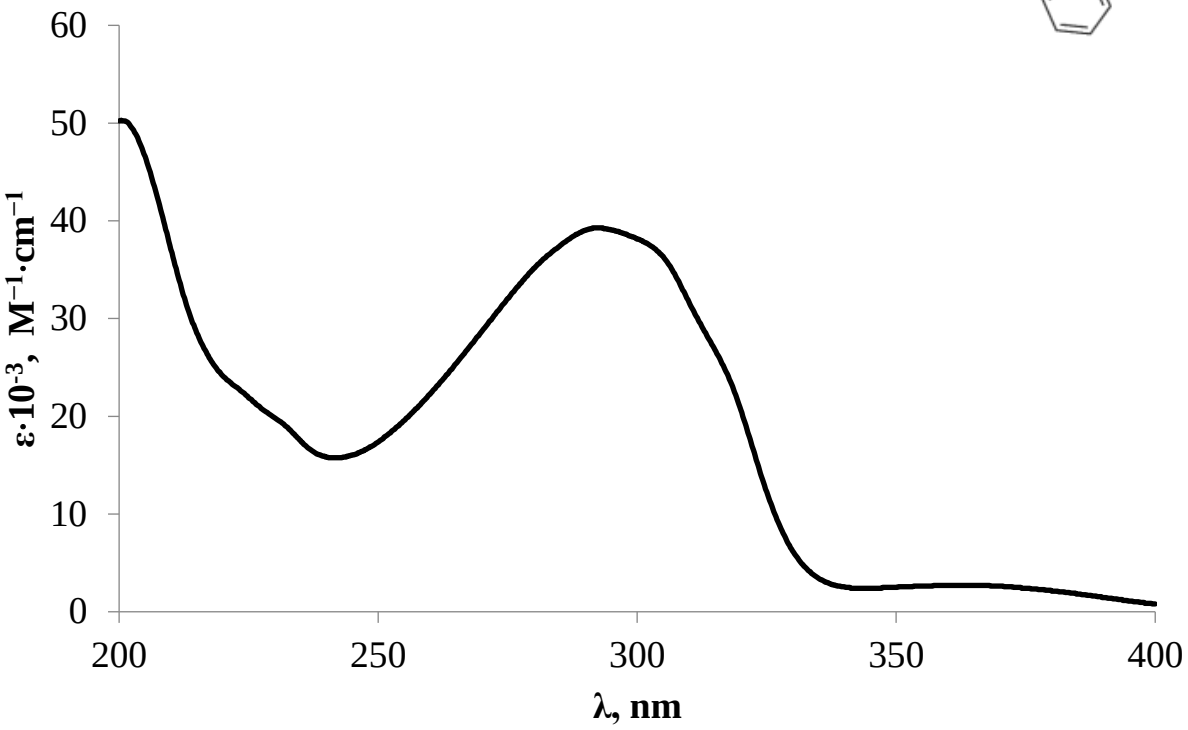


Absorption spectrum of pyrazole **4u**

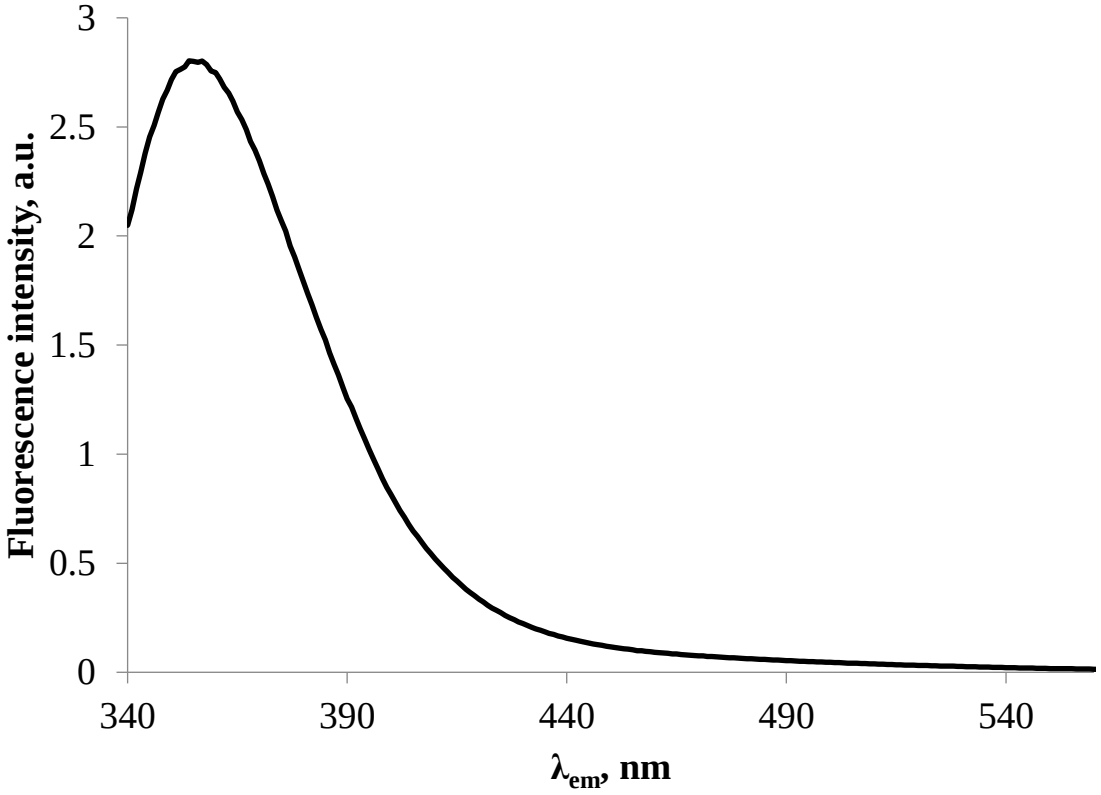


Emission spectrum of pyrazole **4u** (EX wavelength is 347 nm)

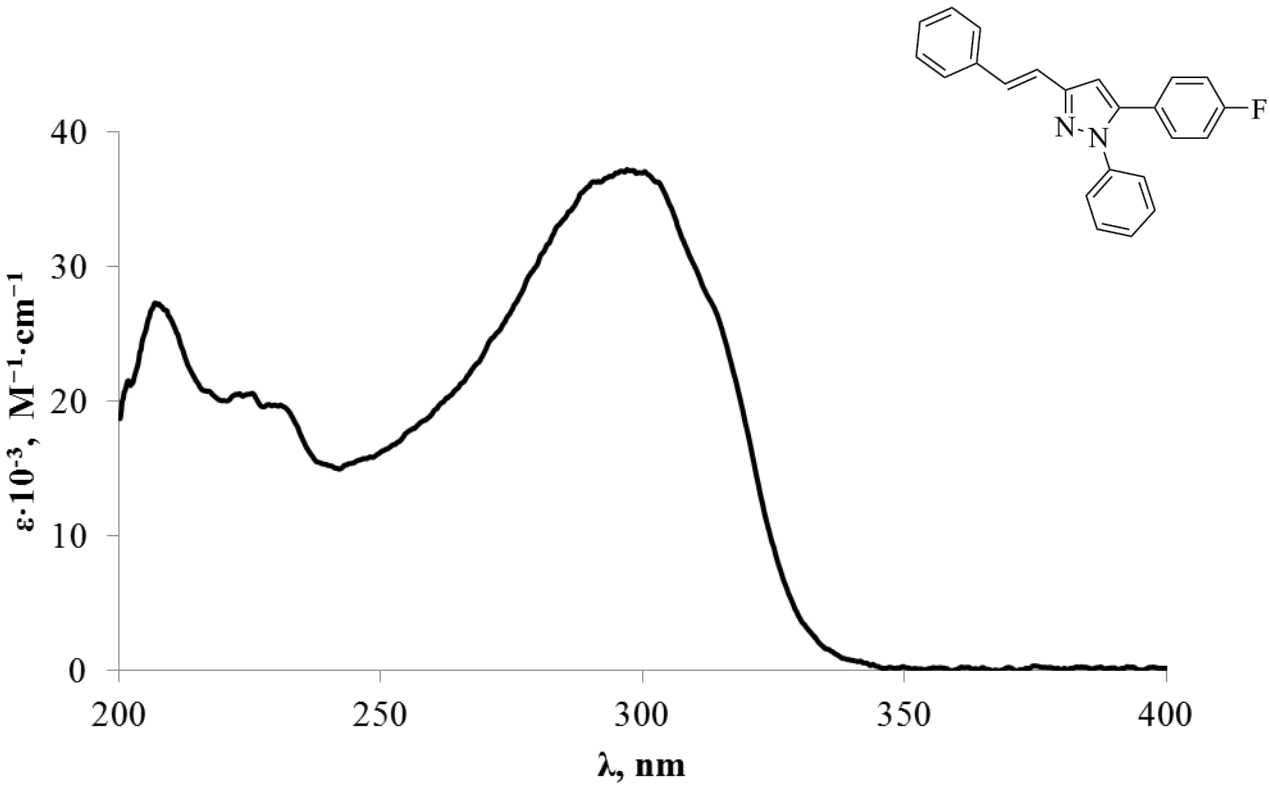




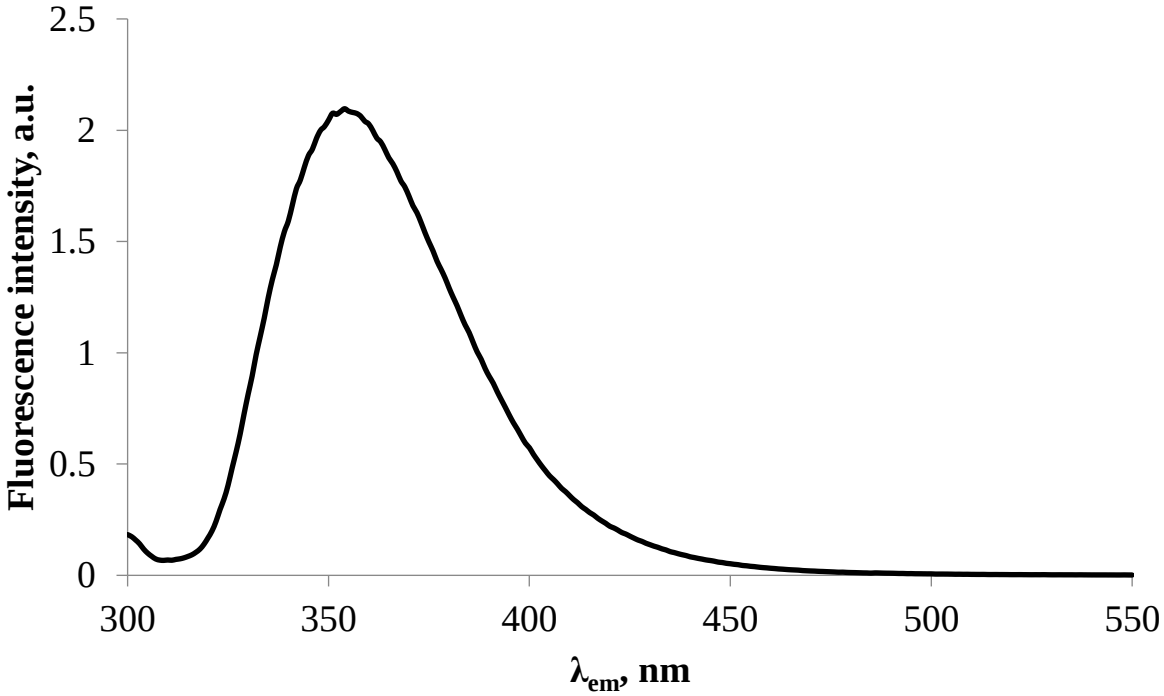
Absorption spectrum of pyrazole **4v**



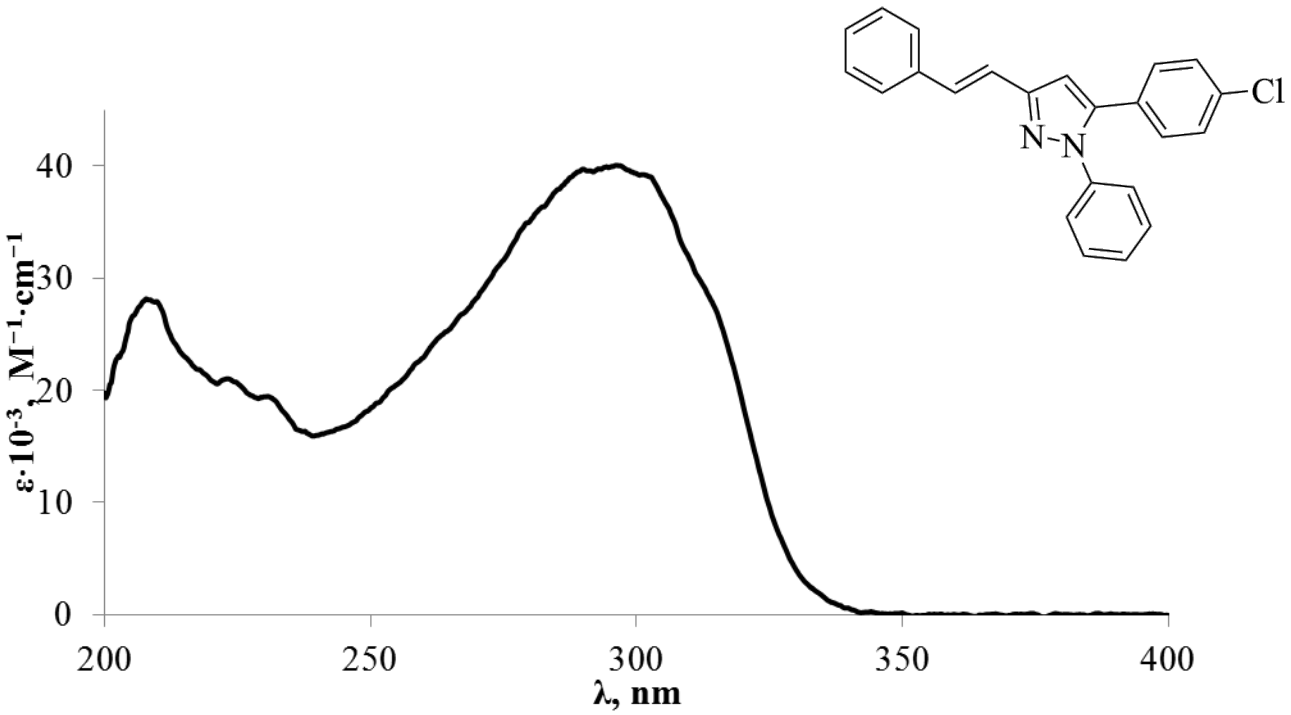
Emission spectrum of pyrazole **4v** (EX wavelength is 292 nm)



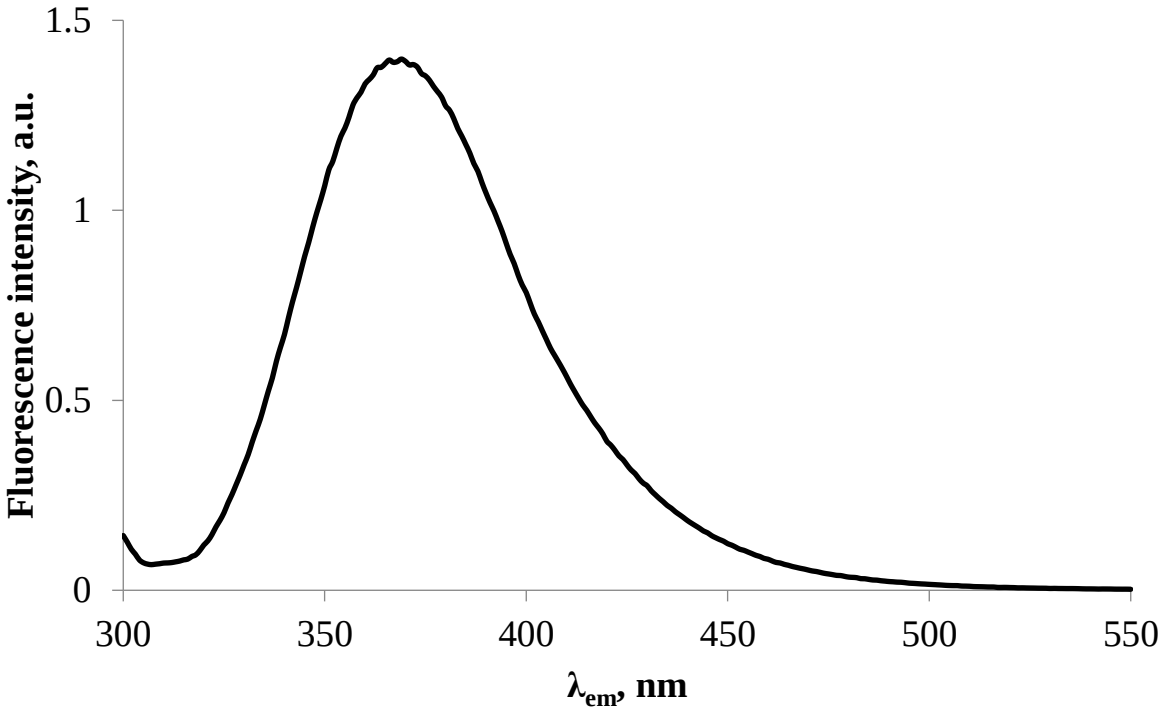
Absorption spectrum of pyrazole **4w**



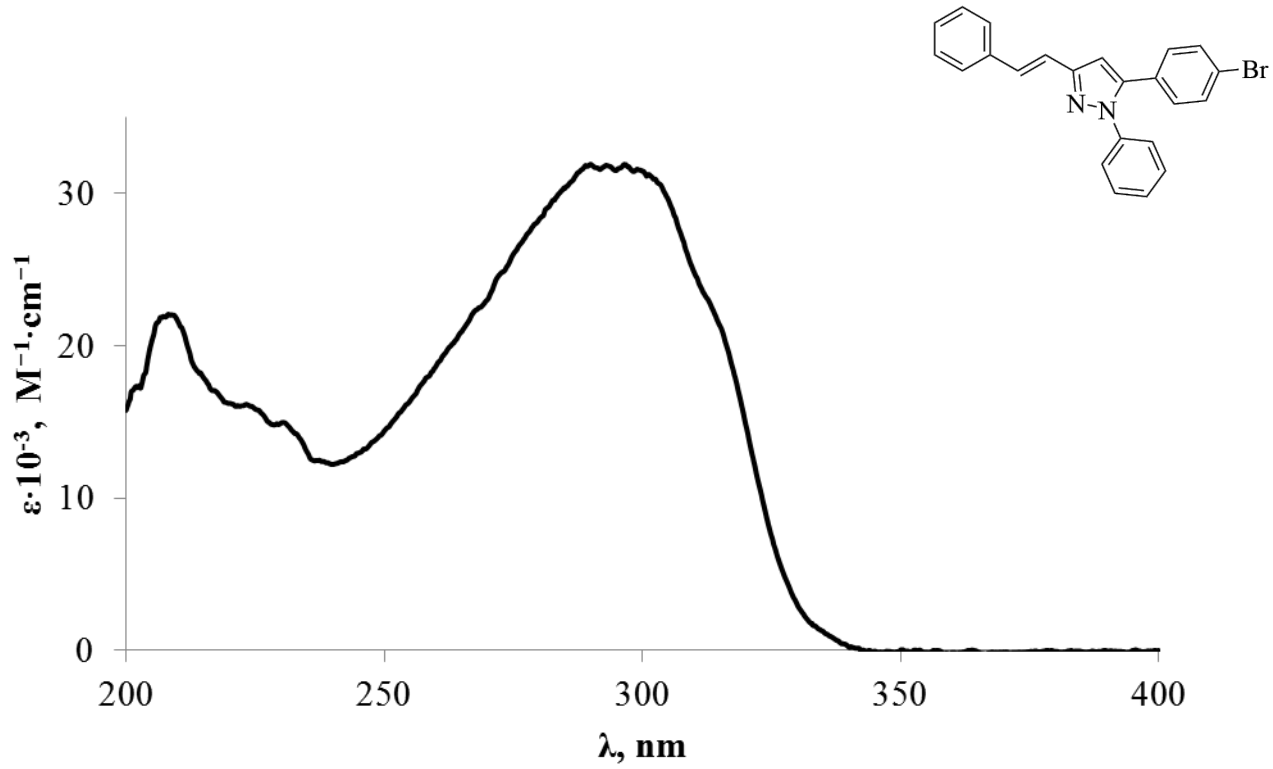
Emission spectrum of pyrazole **4w** (EX wavelength is 298 nm)



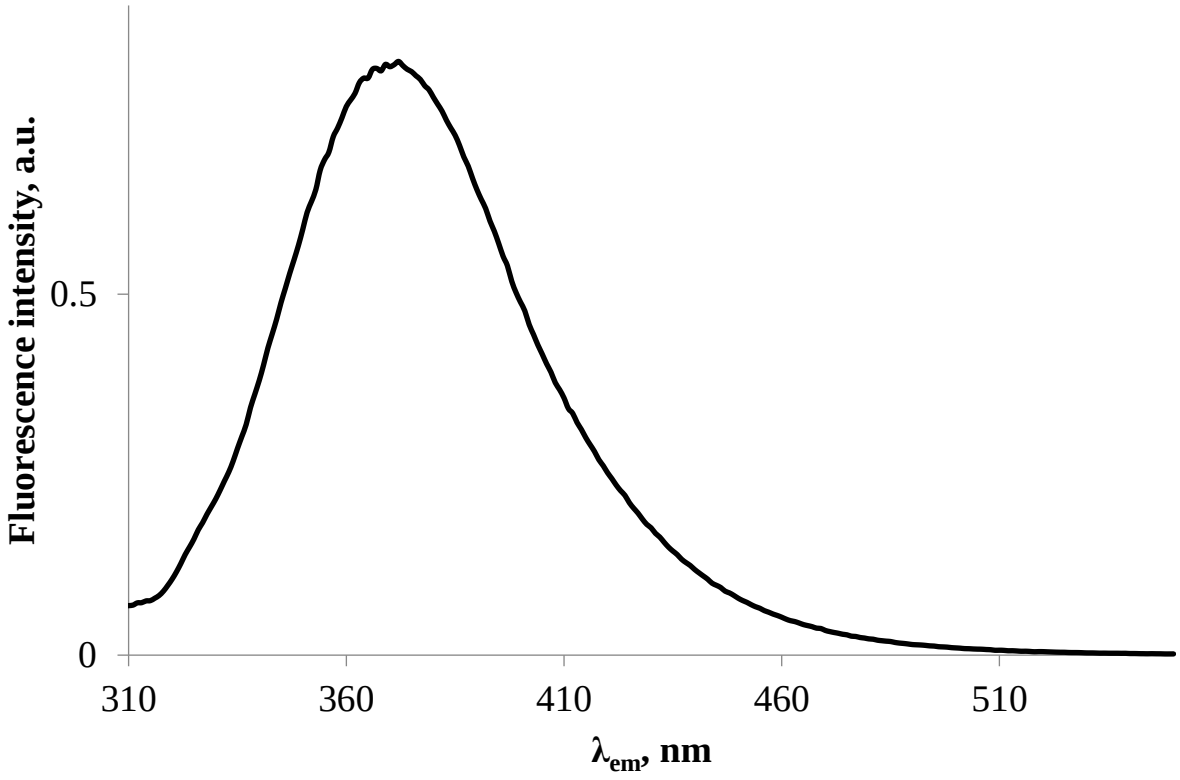
Absorption spectrum of pyrazole **4x**



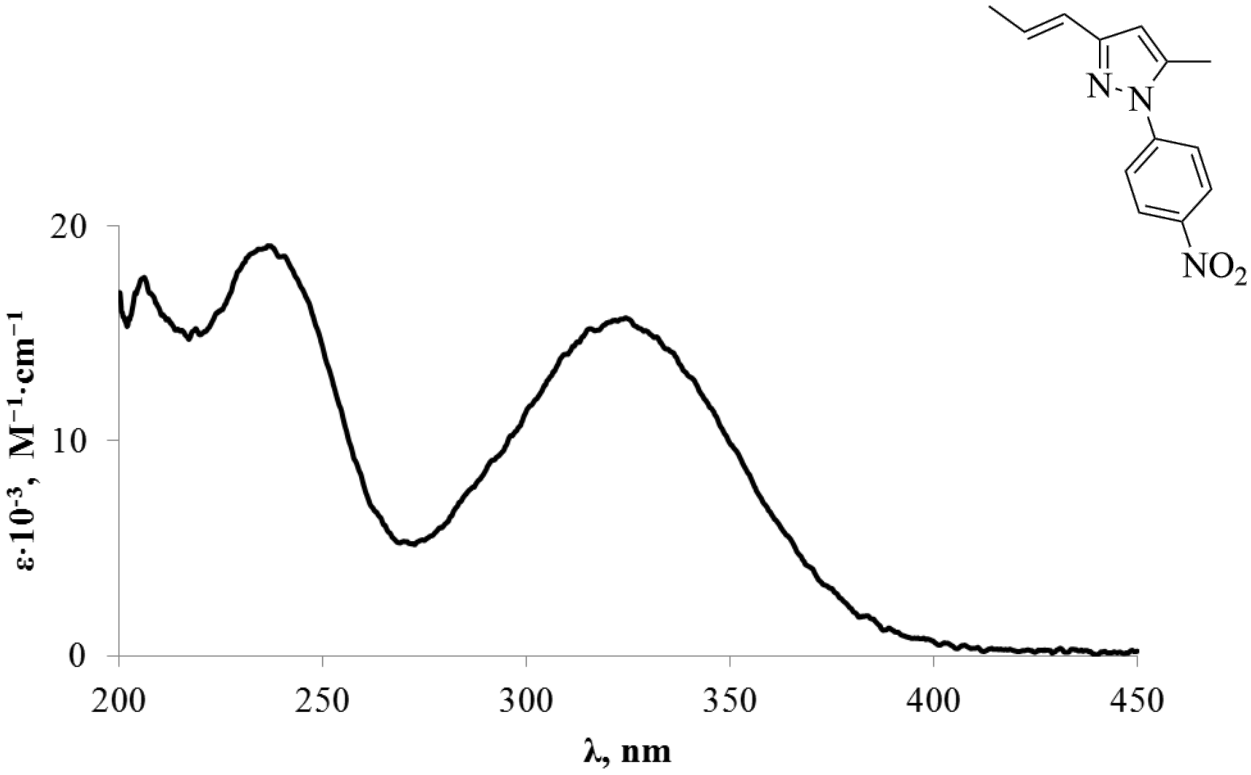
Emission spectrum of pyrazole **4x** (EX wavelength is 296 nm)



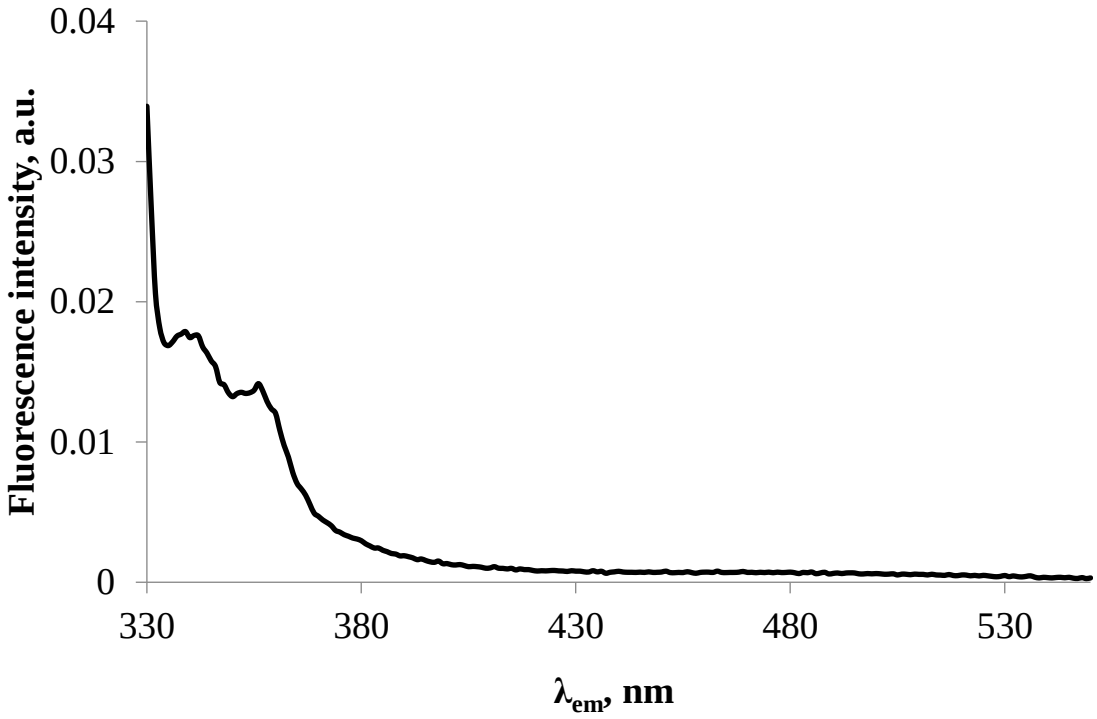
Absorption spectrum of pyrazole **4y**



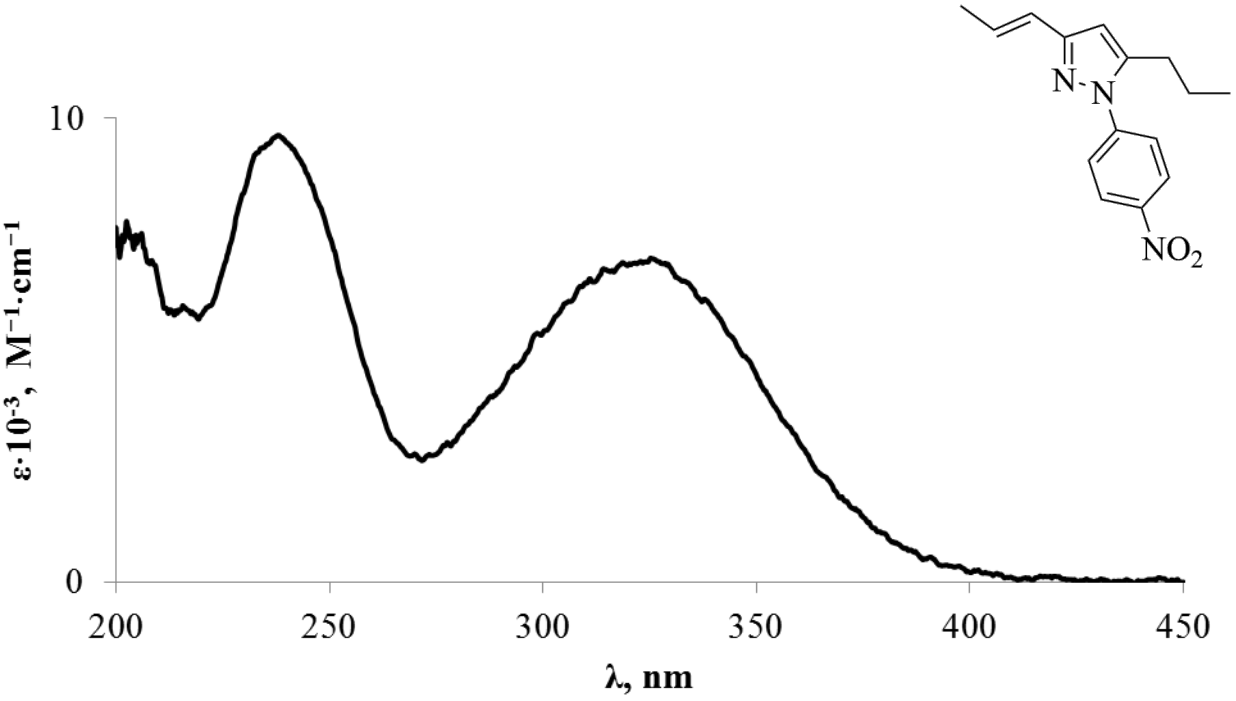
Emission spectrum of pyrazole **4y** (EX wavelength is 295 nm)



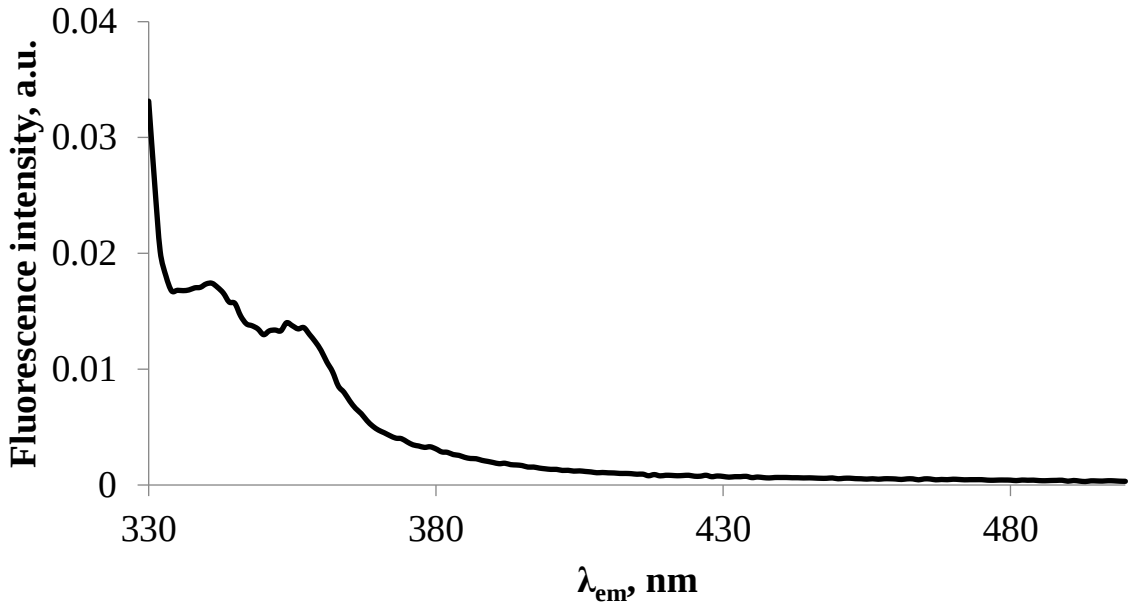
Absorption spectrum of pyrazole **4z**



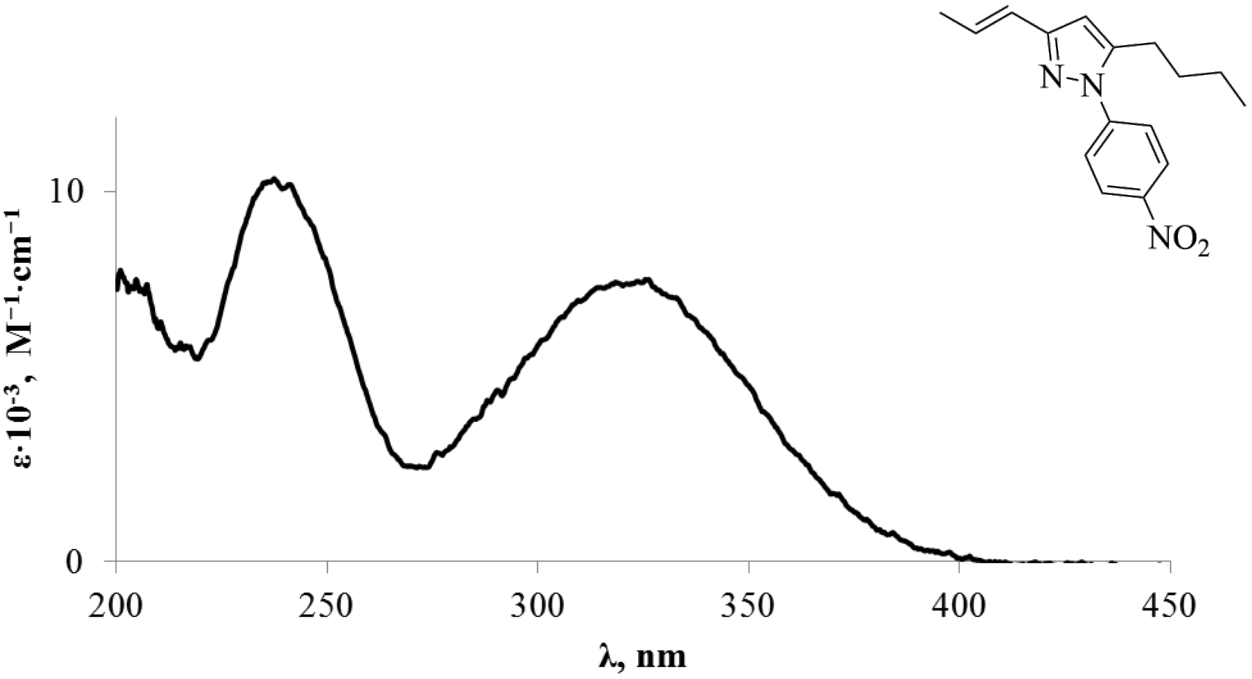
Emission spectrum of pyrazole **4z** (EX wavelength is 322 nm)



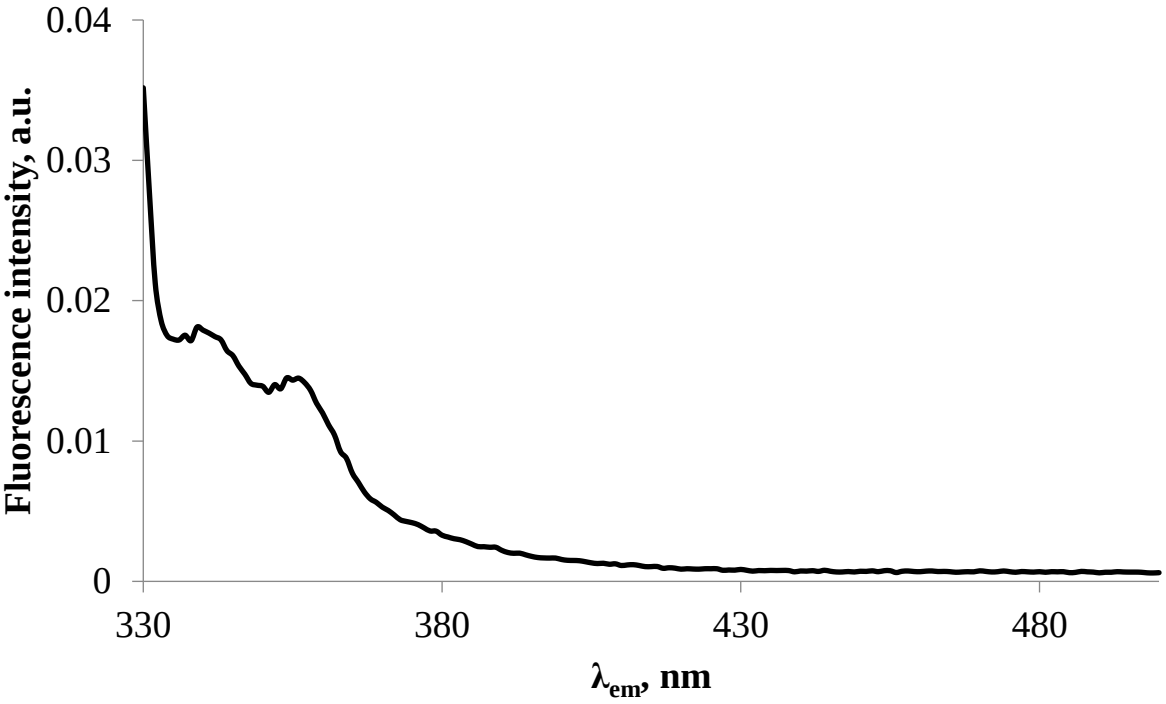
Absorption spectrum of pyrazole **4aa**



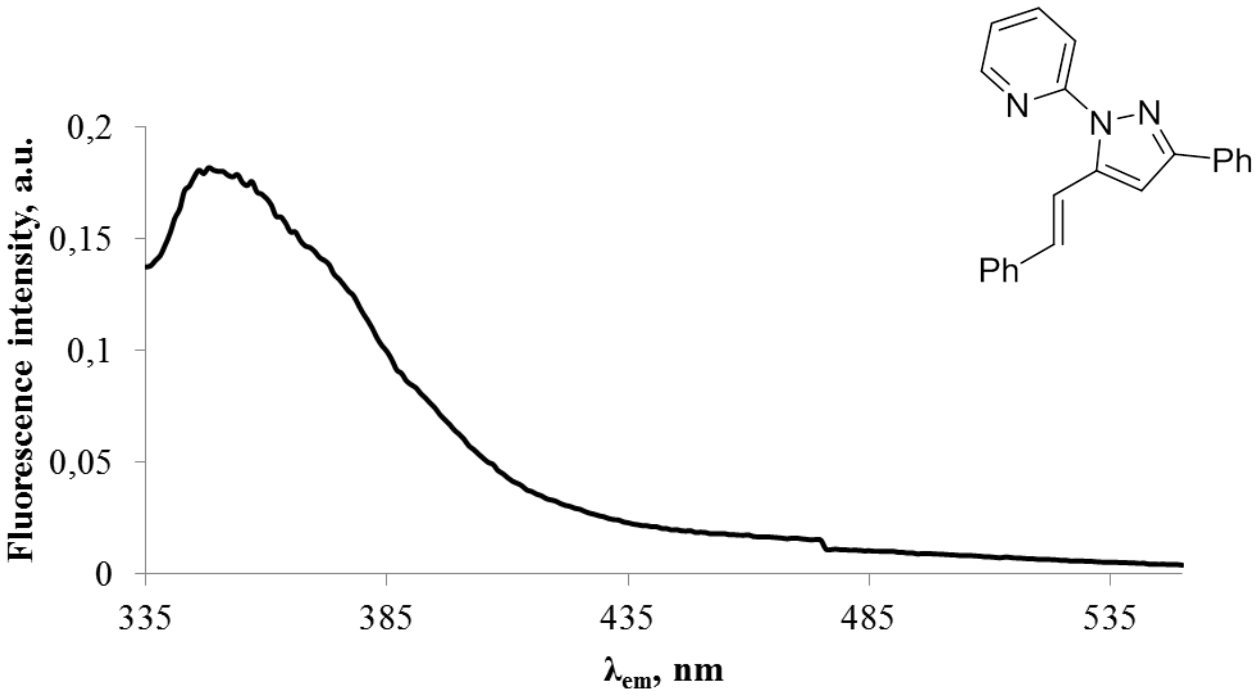
Emission spectrum of pyrazole **4aa** (EX wavelength is 322 nm)



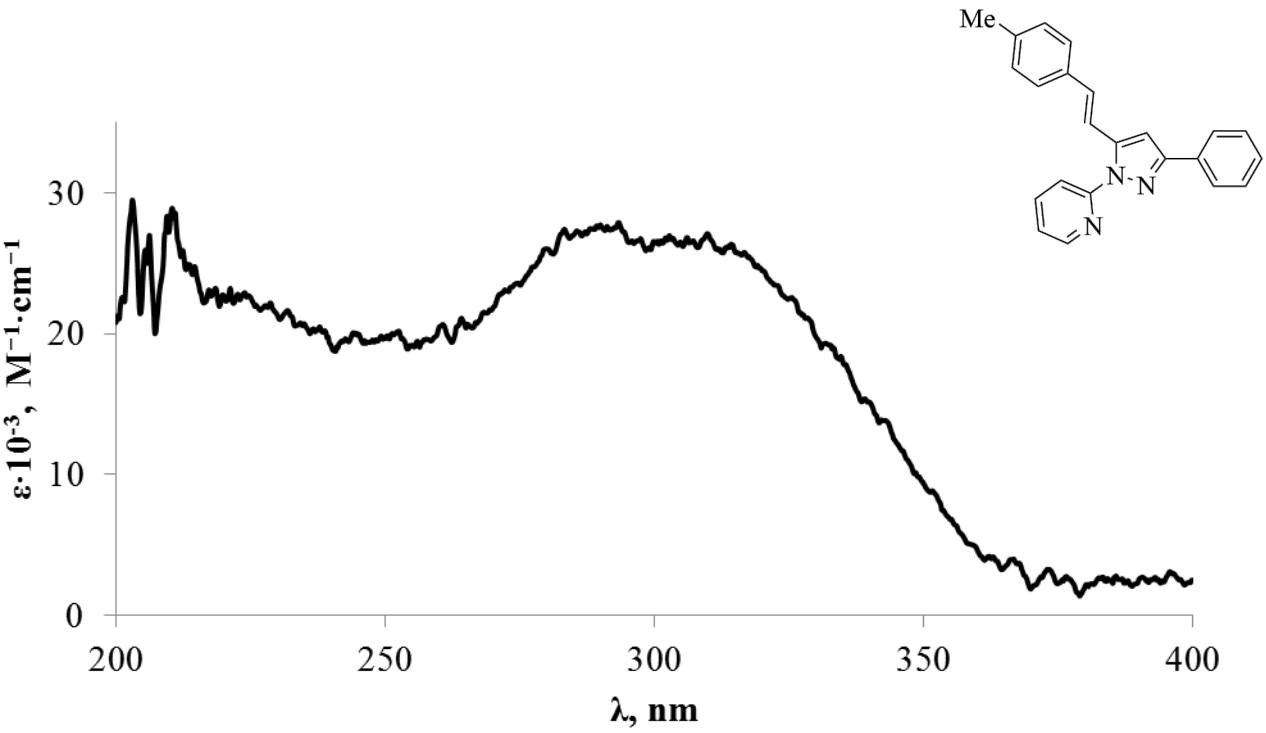
Absorption spectrum of pyrazole **4ab**



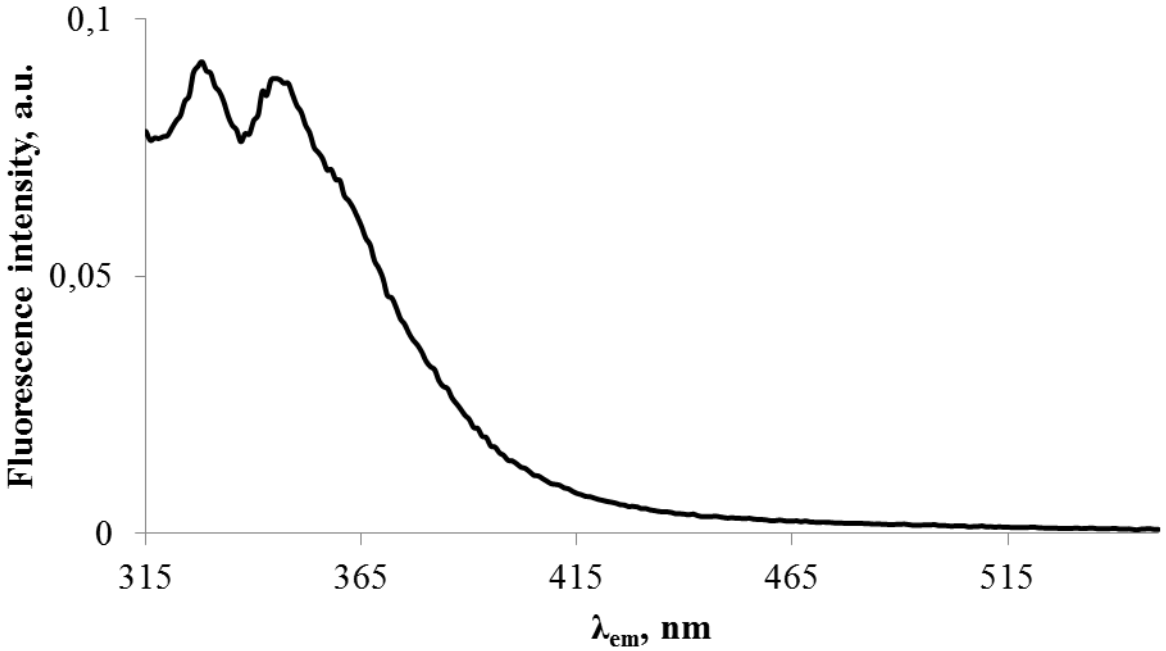
Emission spectrum of pyrazole **4ab** (EX wavelength is 322 nm)



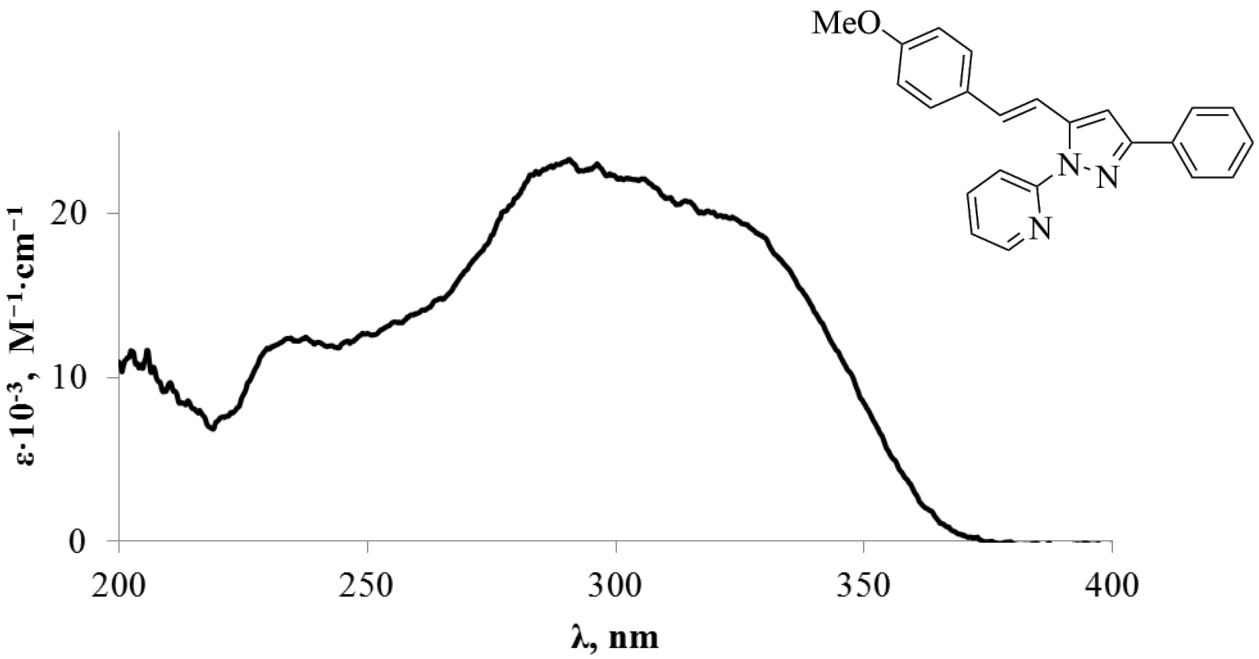
Emission spectrum of pyrazole **7a** (EX wavelength is 309 nm)



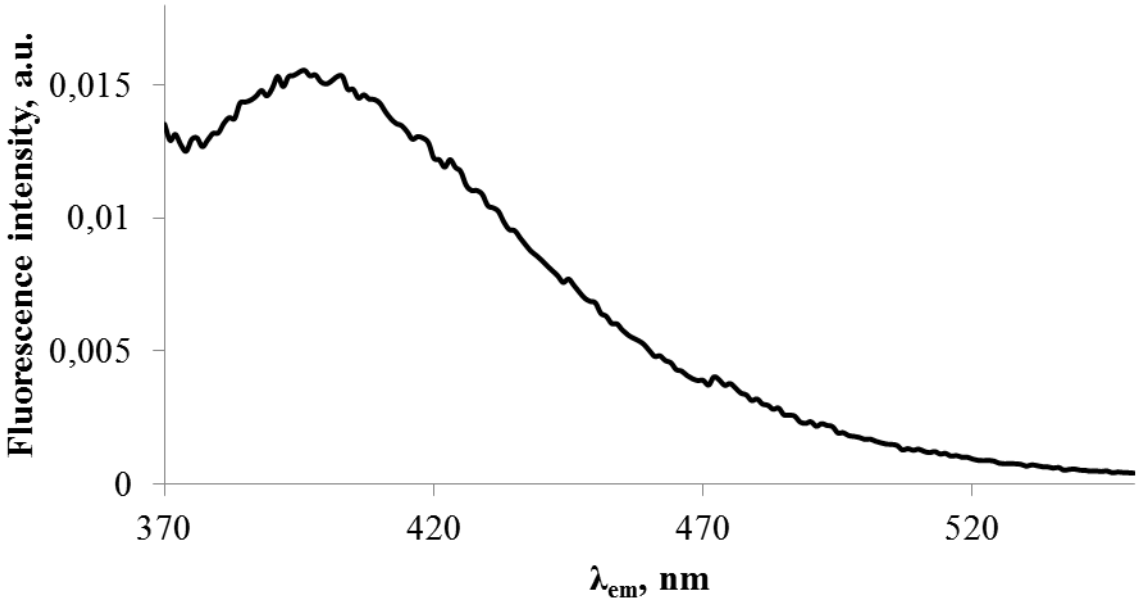
Absorption spectrum of pyrazole **7b**



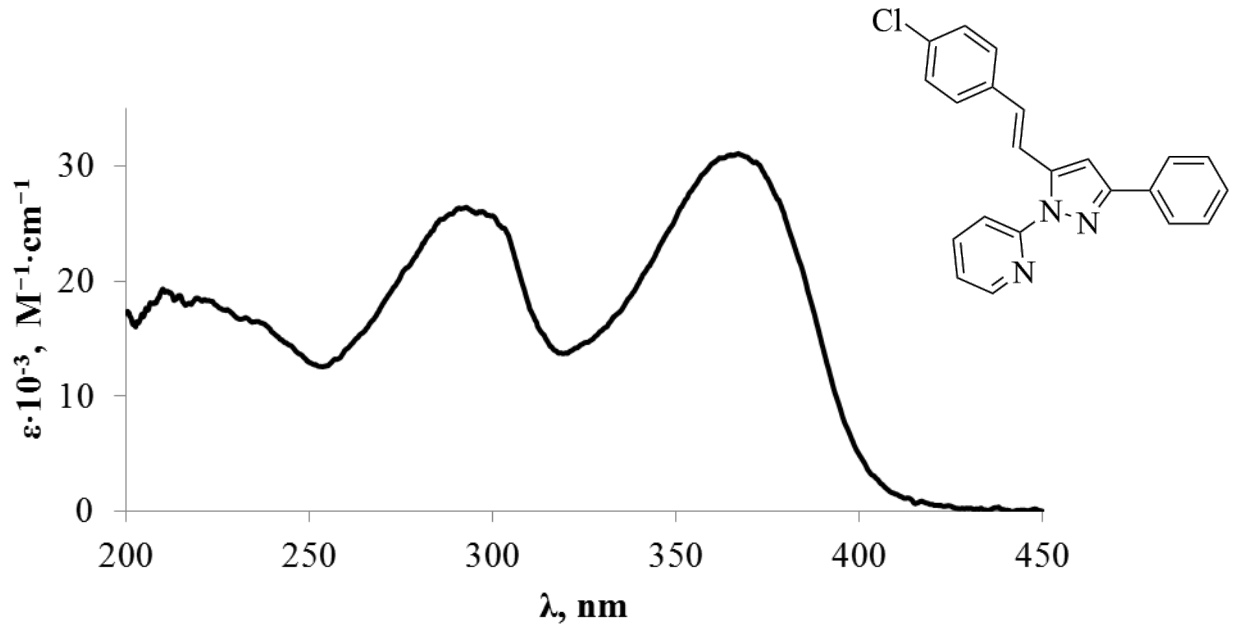
Emission spectrum of pyrazole **7b** (EX wavelength is 309 nm)



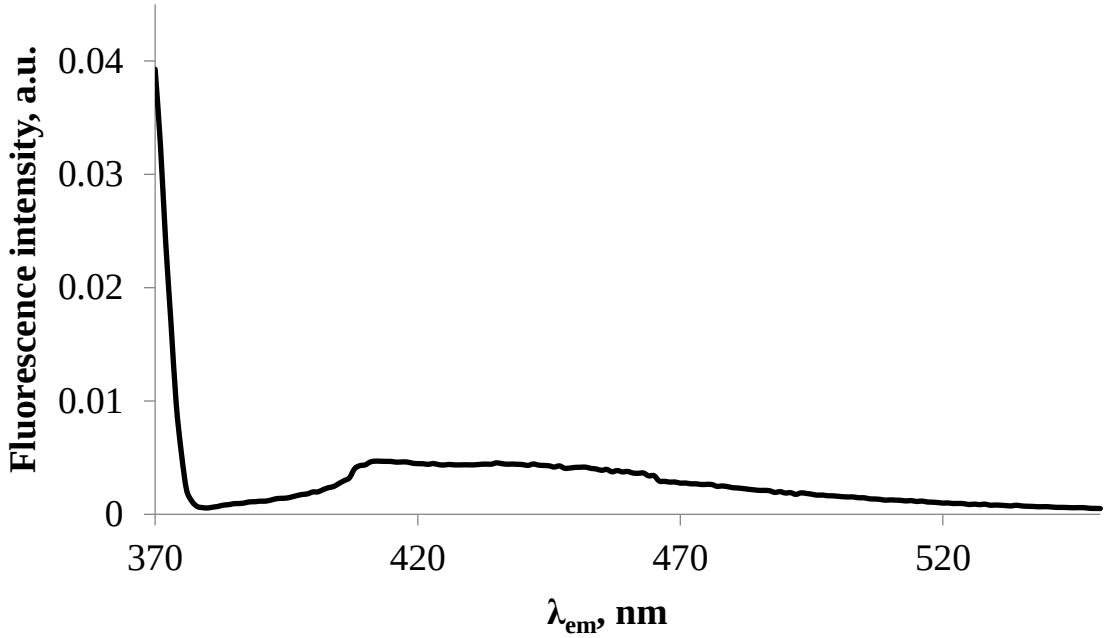
Absorption spectrum of pyrazole **7c**



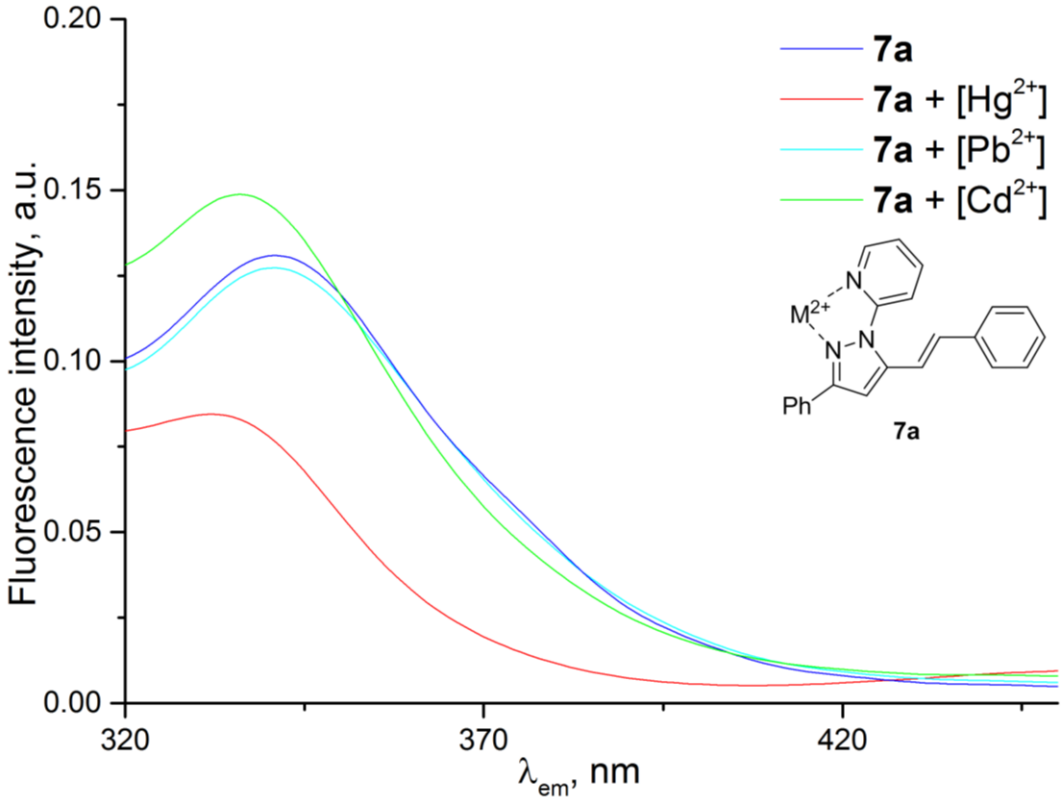
Emission spectrum of pyrazole **7c** (EX wavelength is 329 nm)



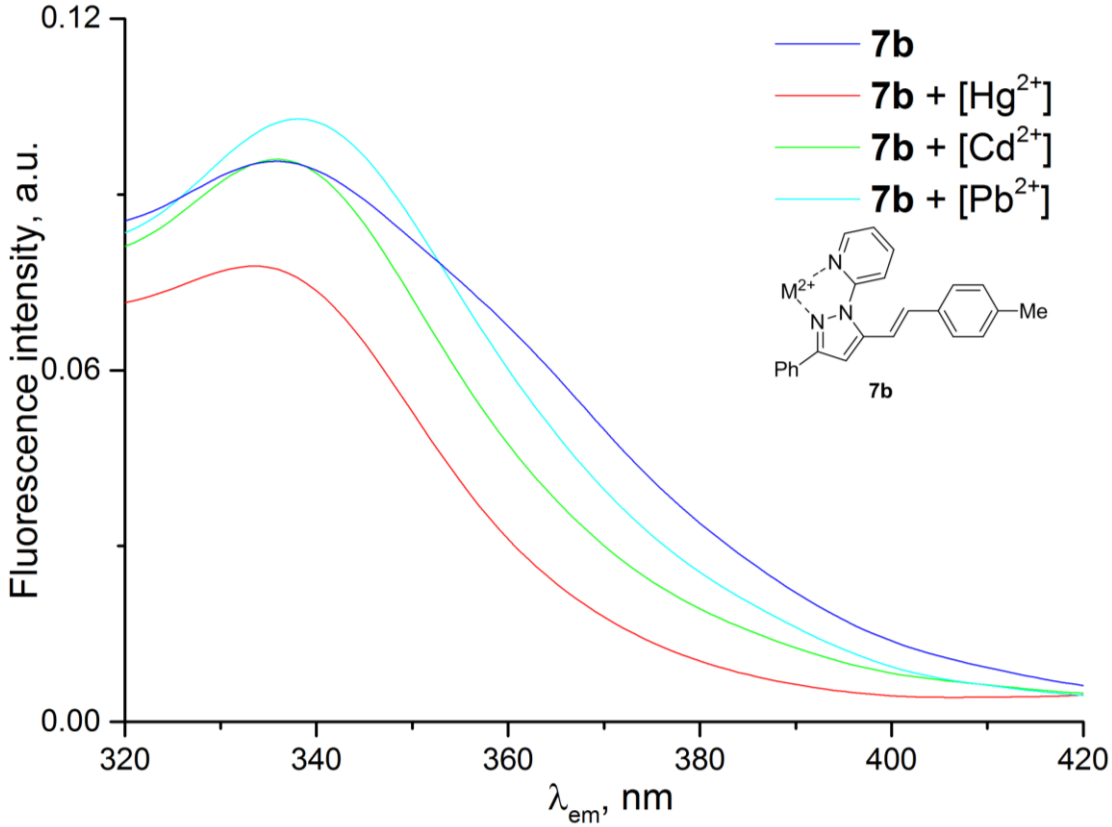
Absorption spectrum of pyrazole **7d**



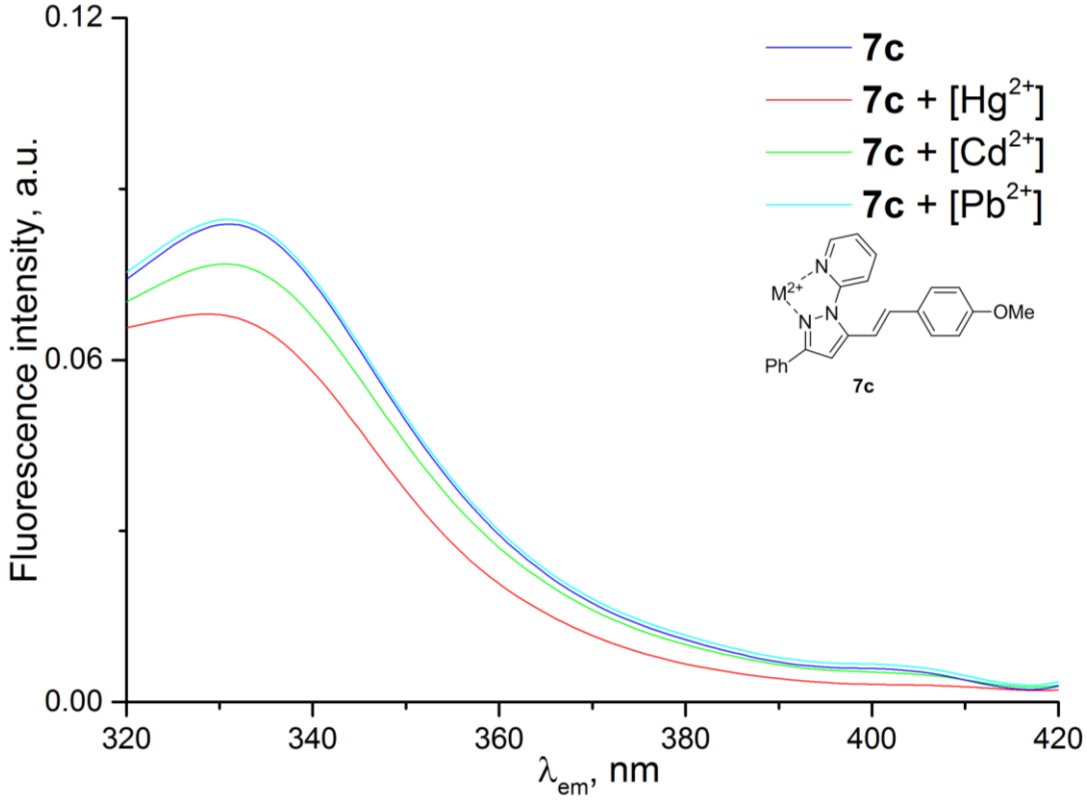
Emission spectrum of pyrazole **7d** (EX wavelength is 367 nm)



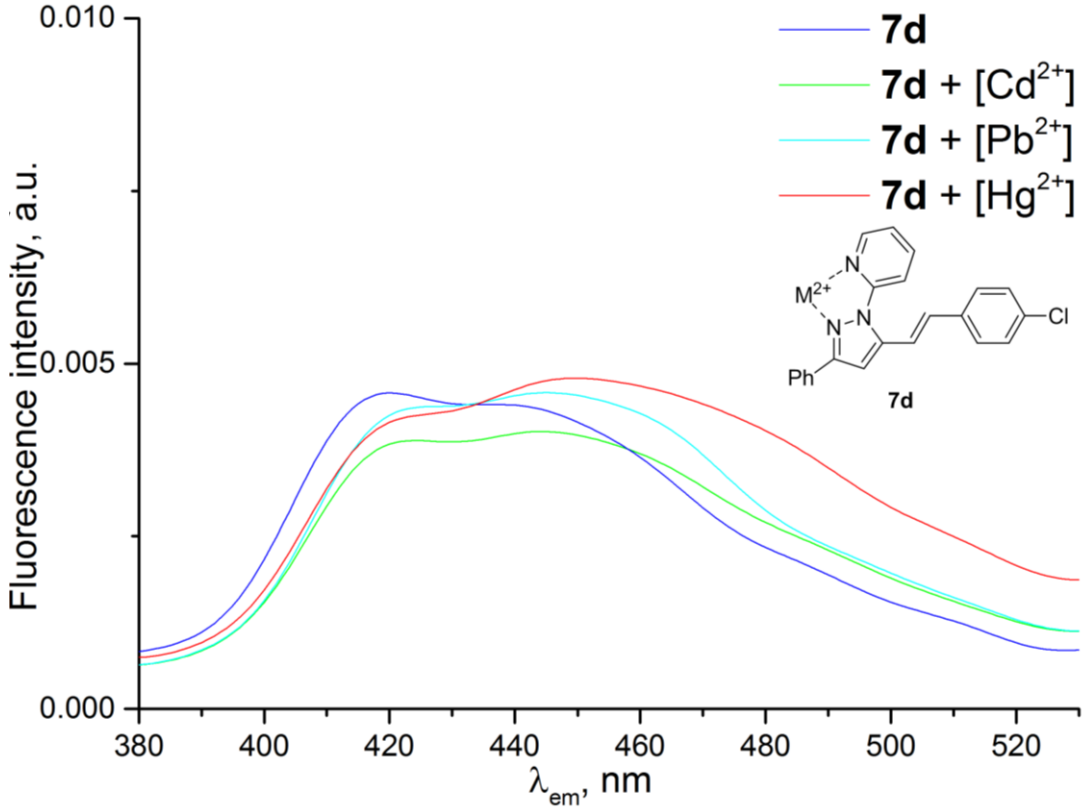
Emission spectrum of pyrazole **7a** complexes (at EX wavelength of zonde **7a** 309 nm)



Emission spectrum of pyrazole **7b** complexes (at EX wavelength of zonde **7b** 309 nm)



Emission spectrum of pyrazole **7c** complexes (at EX wavelength of zonde **7c** 329 nm)



Emission spectrum of pyrazole **7d** complexes (at EX wavelength of zonde **7d** 367 nm)