

# Supplementary Materials

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## Part 1: X-ray Crystallographic Data Collection

Table S1. Crystallographic data for **7k** and **15e**.

Compound	7k	15e
Empirical formula	C <sub>20</sub> H <sub>19</sub> BrO	C <sub>21</sub> H <sub>21</sub> BrO
Formula weight	355.26	369.29
Crystal system	Orthorhombic	Monoclinic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	P2 <sub>1</sub> /c
Unit Cell Dimensions, (Å, °)	<i>a</i> = 7.2662(1)	<i>a</i> = 14.0033(3)
	<i>b</i> = 12.8517(2)	<i>b</i> = 7.7072(2)
	<i>c</i> = 16.8476(3)	<i>c</i> = 15.9479(3)
		β = 105.606(2)
V, Å <sup>3</sup>	1573.28(4)	1657.74(6)
Z	4	4
ρ calc., Mg m <sup>−3</sup>	1.500	1.480
μ, mm <sup>−1</sup>	3.538	3.379
F(000)	728	760
θ-max, °	65.79	66.481
Index ranges	−8 ≤ <i>h</i> ≤ 8,	−16 ≤ <i>h</i> ≤ 16,
	−14 ≤ <i>k</i> ≤ 15,	−8 ≤ <i>k</i> ≤ 8,
	−19 ≤ <i>l</i> ≤ 19	−18 ≤ <i>l</i> ≤ 18
Reflections collected	25884	61561
Independent reflections	2620 [R(int) = 0.0429]	2893 [R(int) = 0.0670]
Completeness to θ-max, %	97.1	96.5
Refinement method	Full-matrix least-squares on F <sup>2</sup>	Full-matrix least-squares on F <sup>2</sup>
Data/restraints/ parameters	2620 / 0 / 200	2893 / 0 / 209
Goodness-of-fit on F <sup>2</sup>	1.114	1.080
Final R indices [I > 2σ(I)]	R1 = 0.0216, wR2 = 0.0510	R1 = 0.0297, wR2 = 0.0635
R indices (all data)	R1 = 0.0240, wR2 = 0.0525	R1 = 0.0406, wR2 = 0.0689
Absolute structure parameter	−0.041(8)	
Largest diff. peak and hole, e.Å <sup>−3</sup>	0.224 and −0.355	0.436 and −0.283

## Part 2: Cartesian Coordinates for Optimized Geometries and Thermochemical data

## 1. Thermochemical Data

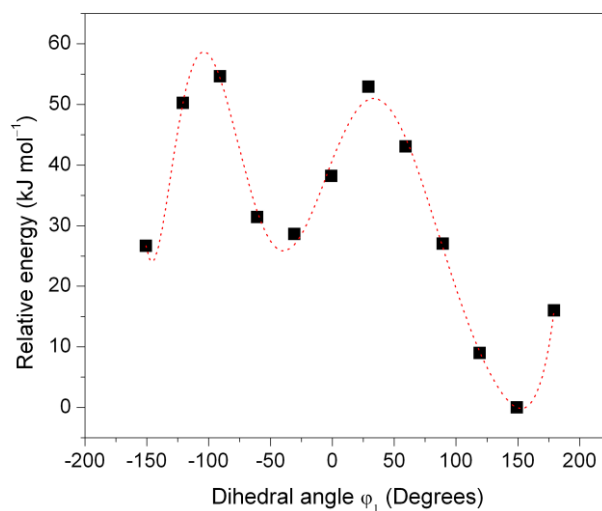
**Table S2.** Free energy ( $G$  + ZPE + thermal corrections at 298.15 K) in Hartrees for all compounds studied determined at the DFT B3LYP/6-31+G(d,p) level, changes in free energy ( $\Delta G^0$ ) for different processes, activation energy ( $\Delta G^\ddagger$ ) and relative energies ( $\Delta G^{0,\text{rel}}$ ).<sup>a</sup>

REAGENTS	$G^0$ (Hartrees)	$G^0$ (Hartrees)	$\Delta G^{0,E/Z}$ (kJ mol <sup>-1</sup> )	$\Delta G^{0,\text{rel}}$ (kJ mol <sup>-1</sup> )
(E)-3h, A	-849.49142			0
(Z)-3h, A	-849.47487		43	43
(E)-3h, B_2	-849.49210			
(Z)-3h, B_2	-849.47645		41	
(E)-3h, B	-849.48584			15
(Z)-3h, B	-849.47245			50
TS			$\Delta G^\ddagger$ (kJ mol <sup>-1</sup> )	
(E)-3h, A $\rightarrow$ <i>cis</i> -4h, A	-849.48408		19	
(Z)-3h, A $\rightarrow$ <i>trans</i> -4h, A	-849.46937		14	
INTERMEDIATES			$\Delta G^{0,R-I}$ (kJ mol <sup>-1</sup> )	$\Delta G^{0,\text{rel}}$ (kJ mol <sup>-1</sup> )
<i>cis</i> -4h, A	-849.49182		-1	0
<i>trans</i> -4h, A	-849.48516		-27	17
<i>cis</i> -4h, B	-849.47772		21	37
<i>trans</i> -4h, B	-849.47804		-15	36
PRODUCTS			$\Delta G^{0,7h-12h}$ (kJ mol <sup>-1</sup> )	
<i>cis</i> , A	-849.14799	-849.138025	-26	
<i>trans</i> , A	-849.14685	-849.132352	-38	
<i>cis</i> , B	-849.14691	-849.140602	-17	
<i>trans</i> , B	-849.14513	-849.137892	-19	
	7s	12s	$\Delta G^{0,7s-12s}$ (kJ mol <sup>-1</sup> )	$K$ , Boltzmann
	-775.311037	-775.310585	-1.2	1.6

<sup>a</sup> All compounds have no imaginary frequencies, except those corresponding to transition states (TS), which have one negative (imaginary) frequency corresponding to the reaction coordinate.

## 2. Energy Surface Scan

**Figure S1.** Change in energy resulting from the rotation around the dihedral angle formed between the 1,2-dihydronaphthalene ring and the benzylidene(propyl)oxonium moiety ( $\text{Me}-\text{CH}-(\text{C}=\text{C})$ ,  $\phi_1$ ) of compound (*E*)-3h, A, determined by a relaxed potential energy surface scan at the B3LYP/6-31G(d) level.



## 3. Cartesian Coordinates for Optimized geometries

### Reagents

(*E*)-3h, A

symmetry c1

C	-4.283592000	-1.508947000	-1.143037000
C	-3.568098000	-2.001736000	-0.048264000
C	-2.556013000	-1.250802000	0.552221000
C	-2.242845000	0.036178000	0.040823000
C	-2.987242000	0.524962000	-1.051061000
C	-3.994433000	-0.238057000	-1.641832000
H	-5.067248000	-2.109336000	-1.594399000
H	-3.807682000	-2.982805000	0.353133000
H	-2.798696000	1.515540000	-1.451139000
H	-4.552556000	0.162267000	-2.482171000
C	1.289091000	0.562286000	-0.887981000
C	-0.960575000	2.283842000	0.338441000
H	-1.940813000	2.703454000	0.083442000
C	-0.132985000	2.446623000	-0.959966000
H	0.071639000	3.494712000	-1.178166000
H	-0.606374000	1.970045000	-1.821832000
O	1.191226000	1.848323000	-0.793883000
C	2.512108000	-0.108818000	-0.609865000
C	2.579464000	-1.498251000	-0.880967000
C	3.646619000	0.571119000	-0.098551000
C	3.758913000	-2.192922000	-0.643569000
H	1.711839000	-2.013376000	-1.283657000
C	4.817030000	-0.133900000	0.132205000

H	3.591088000	1.635431000	0.102892000
C	4.873350000	-1.512106000	-0.137836000
H	3.817589000	-3.255525000	-0.853377000
H	5.691757000	0.377384000	0.519989000
H	5.795352000	-2.055417000	0.045629000
C	-0.388980000	-1.285918000	1.845627000
C	-1.849296000	-1.747506000	1.794096000
C	-1.147206000	0.809369000	0.674158000
H	-1.911476000	-2.837691000	1.859918000
H	0.222022000	-1.880272000	1.144999000
H	0.036241000	-1.469634000	2.837383000
H	-2.376103000	-1.351560000	2.674773000
C	-0.269032000	0.172569000	1.497360000
H	0.534997000	0.733602000	1.964007000
C	-0.376927000	3.145681000	1.472065000
H	-0.400747000	4.202389000	1.188239000
H	-0.966654000	3.028647000	2.384437000
H	0.660760000	2.891276000	1.704540000
H	0.449160000	0.012281000	-1.311983000

(Z)-3h, A

symmetry c1

C	0.934339000	3.572147000	-0.947600000
C	0.918136000	3.220170000	0.404813000
C	1.110214000	1.898501000	0.811015000
C	1.320754000	0.889078000	-0.165542000
C	1.350964000	1.265837000	-1.523797000
C	1.157008000	2.590016000	-1.914535000
H	0.788305000	4.606956000	-1.241481000
H	0.766758000	3.988302000	1.158489000
H	1.541586000	0.529828000	-2.297818000
H	1.190596000	2.853628000	-2.967012000
C	-0.944806000	-2.257988000	0.174932000
C	2.023247000	-1.556282000	-0.698240000
H	2.627631000	-1.051815000	-1.461283000
C	0.841210000	-2.159736000	-1.503709000
H	1.179746000	-2.958436000	-2.164105000
H	0.305132000	-1.406839000	-2.074201000
O	-0.051934000	-2.831286000	-0.568644000
C	-1.840113000	-1.167161000	-0.052558000
C	-2.691919000	-0.869940000	1.047853000
C	-2.006766000	-0.437773000	-1.259862000
C	-3.649604000	0.130460000	0.955770000
H	-2.597552000	-1.442965000	1.965828000
C	-2.981160000	0.545147000	-1.346176000
H	-1.416272000	-0.661110000	-2.137226000
C	-3.794523000	0.839765000	-0.241770000
H	-4.291799000	0.347823000	1.802551000
H	-3.116028000	1.085660000	-2.276974000
H	-4.551094000	1.614112000	-0.322806000
C	0.640435000	0.135194000	2.547892000
C	1.189582000	1.539554000	2.277716000

C	1.517760000	-0.508699000	0.281268000
H	0.661520000	2.282158000	2.883047000
H	-0.460907000	0.152637000	2.478369000
H	0.876523000	-0.181967000	3.568385000
H	2.244092000	1.576100000	2.588509000
C	1.182833000	-0.856612000	1.556112000
H	1.358441000	-1.871133000	1.901939000
C	2.897701000	-2.665055000	-0.087269000
H	3.308851000	-3.296482000	-0.880896000
H	3.735390000	-2.229553000	0.462851000
H	2.343836000	-3.315256000	0.594643000
H	-1.131027000	-2.851099000	1.070461000

(E)-3h, B\_2

symmetry c1

C	-4.237654000	-1.607939000	-1.140190000
C	-3.292698000	-2.156218000	-0.269218000
C	-2.322576000	-1.358622000	0.341547000
C	-2.290940000	0.035484000	0.076468000
C	-3.254873000	0.571679000	-0.799681000
C	-4.218036000	-0.237762000	-1.402748000
H	-4.987926000	-2.243981000	-1.599306000
H	-3.313894000	-3.221430000	-0.054066000
H	-3.287009000	1.637150000	-1.001632000
H	-4.955440000	0.204696000	-2.065027000
C	1.269729000	0.417519000	-0.857044000
C	-0.994802000	2.283527000	0.241727000
H	-1.955909000	2.746545000	-0.014449000
C	-0.253013000	2.229780000	-1.108752000
H	-0.080267000	3.224298000	-1.519654000
H	-0.765274000	1.600087000	-1.840576000
O	1.102132000	1.692060000	-0.921695000
C	2.546165000	-0.143428000	-0.580574000
C	2.679415000	-1.553158000	-0.644786000
C	3.672196000	0.664344000	-0.277375000
C	3.914346000	-2.142089000	-0.410617000
H	1.814922000	-2.167291000	-0.880776000
C	4.898767000	0.063450000	-0.044435000
H	3.565187000	1.742750000	-0.234363000
C	5.019862000	-1.335049000	-0.110089000
H	4.023764000	-3.219994000	-0.461549000
H	5.766933000	0.671446000	0.186715000
H	5.985376000	-1.796721000	0.073387000
C	-1.284197000	-1.966312000	1.260510000
C	-0.873513000	-0.998547000	2.374488000
C	-0.597696000	0.372881000	1.823228000
C	-1.266498000	0.874735000	0.755114000
H	-1.679055000	-0.919224000	3.121791000
H	0.000619000	-1.378423000	2.913224000
H	-0.389822000	-2.228330000	0.672092000
H	-1.654508000	-2.905927000	1.680957000
H	0.106528000	0.997832000	2.363671000

C	-0.292889000	3.233719000	1.225020000
H	-0.226771000	4.237211000	0.793571000
H	-0.858697000	3.307198000	2.156984000
H	0.723573000	2.912918000	1.470129000
H	0.424052000	-0.225258000	-1.103132000

## (Z)-3h, B\_2

symmetry c1

C	1.385325000	3.382441000	-0.922980000
C	1.170288000	2.985104000	0.399962000
C	1.280230000	1.645890000	0.782284000
C	1.619485000	0.664644000	-0.185032000
C	1.842141000	1.083130000	-1.511221000
C	1.725138000	2.425554000	-1.880222000
H	1.306290000	4.429907000	-1.197394000
H	0.921962000	3.729992000	1.151788000
H	2.143591000	0.371035000	-2.272932000
H	1.917852000	2.720553000	-2.907165000
C	-1.588236000	-2.123833000	0.024117000
C	1.768410000	-1.853497000	-0.811756000
H	2.412336000	-1.519899000	-1.636743000
C	0.399193000	-2.018097000	-1.496642000
H	0.448916000	-2.770768000	-2.285630000
H	-0.005981000	-1.091553000	-1.891701000
O	-0.557079000	-2.620536000	-0.546375000
C	-2.271291000	-0.873095000	-0.049684000
C	-3.526167000	-0.883047000	0.627705000
C	-1.859331000	0.316486000	-0.712955000
C	-4.350463000	0.231473000	0.612326000
H	-3.845591000	-1.779994000	1.150348000
C	-2.690306000	1.425783000	-0.711961000
H	-0.890218000	0.400011000	-1.183331000
C	-3.933661000	1.385626000	-0.061638000
H	-5.307688000	0.208432000	1.121736000
H	-2.367251000	2.333510000	-1.209837000
H	-4.573482000	2.262902000	-0.073332000
C	1.016692000	1.214350000	2.208438000
C	1.915917000	0.042655000	2.613758000
C	1.894829000	-1.033167000	1.560825000
C	1.750709000	-0.754983000	0.246686000
H	2.952697000	0.388527000	2.749583000
H	1.602703000	-0.363684000	3.580762000
H	-0.035112000	0.898724000	2.298143000
H	1.146412000	2.059427000	2.891183000
H	2.058489000	-2.055492000	1.887286000
C	2.319923000	-3.213526000	-0.354117000
H	2.370029000	-3.904582000	-1.201412000
H	3.331063000	-3.098251000	0.042910000
H	1.701704000	-3.679917000	0.417518000
H	-2.045047000	-2.873932000	0.671856000

## (E)-3h, B

## symmetry c1

C	2.741286000	-2.588619000	-1.363417000
C	2.404522000	-2.666718000	-0.009231000
C	1.928764000	-1.552880000	0.684210000
C	1.781931000	-0.312716000	0.005846000
C	2.132119000	-0.253172000	-1.357353000
C	2.604401000	-1.375168000	-2.038170000
H	3.112768000	-3.466476000	-1.882875000
H	2.519246000	-3.608937000	0.519967000
H	2.046075000	0.674241000	-1.909009000
H	2.869189000	-1.297411000	-3.087984000
C	-1.453158000	1.526500000	-0.191104000
C	1.375412000	2.287358000	0.269538000
H	0.968940000	2.903742000	1.079502000
C	0.518550000	2.602883000	-0.990425000
H	1.064794000	2.488021000	-1.924289000
H	0.108844000	3.615963000	-0.944964000
O	-0.609922000	1.677098000	-1.154233000
C	-2.463798000	0.531760000	-0.250102000
C	-3.439678000	0.509141000	0.778731000
C	-2.521272000	-0.412722000	-1.307565000
C	-4.457641000	-0.433360000	0.743959000
H	-3.390396000	1.233262000	1.587300000
C	-3.542185000	-1.349676000	-1.327804000
H	-1.767829000	-0.392383000	-2.087183000
C	-4.507888000	-1.359242000	-0.307470000
H	-5.210783000	-0.452846000	1.524259000
H	-3.597094000	-2.075984000	-2.131695000
H	-5.305378000	-2.095702000	-0.333693000
C	1.628464000	-1.631565000	2.164490000
C	0.452462000	-0.727349000	2.548370000
C	0.622149000	0.638462000	1.943976000
C	1.259149000	0.848828000	0.761737000
H	-0.493902000	-1.167629000	2.192326000
H	0.363520000	-0.651901000	3.636636000
H	2.519747000	-1.309640000	2.723255000
H	1.432534000	-2.666693000	2.458967000
H	0.241229000	1.491993000	2.502923000
C	2.817346000	2.782215000	0.030449000
H	2.818464000	3.835180000	-0.271533000
H	3.393472000	2.701416000	0.955482000
H	3.331780000	2.203784000	-0.739855000
H	-1.431470000	2.237464000	0.634323000

## (Z)-3h, B

## symmetry c1

C	-4.952870000	-0.164819000	-0.957945000
C	-4.474611000	1.000269000	-0.353209000
C	-3.182073000	1.067765000	0.170023000
C	-2.329845000	-0.065672000	0.090665000
C	-2.832163000	-1.230605000	-0.518547000
C	-4.125286000	-1.284445000	-1.039406000

H	-5.960991000	-0.196139000	-1.359274000
H	-5.118088000	1.873253000	-0.283182000
H	-2.220770000	-2.120385000	-0.600227000
H	-4.481141000	-2.198130000	-1.505152000
C	1.730217000	-0.286787000	-1.481544000
C	-0.090351000	-1.159186000	1.000502000
H	0.788256000	-0.741310000	1.503456000
C	0.435072000	-1.978600000	-0.202137000
H	-0.317709000	-2.636581000	-0.628776000
H	1.310894000	-2.576749000	0.056710000
O	0.769050000	-1.121145000	-1.350194000
C	2.932157000	-0.051465000	-0.749036000
C	3.746118000	0.981752000	-1.293584000
C	3.392808000	-0.754930000	0.397959000
C	4.964949000	1.304397000	-0.714290000
H	3.407999000	1.520301000	-2.174069000
C	4.616330000	-0.430734000	0.960700000
H	2.808329000	-1.546873000	0.843614000
C	5.400744000	0.597486000	0.411911000
H	5.576219000	2.094880000	-1.135960000
H	4.968633000	-0.973081000	1.831632000
H	6.355502000	0.843559000	0.866645000
C	-2.693616000	2.315788000	0.871445000
C	-1.200376000	2.546635000	0.620763000
C	-0.432801000	1.276255000	0.872815000
C	-0.954936000	0.047787000	0.644221000
H	-1.040538000	2.876350000	-0.418499000
H	-0.823226000	3.351211000	1.260014000
H	-2.857346000	2.201441000	1.953664000
H	-3.279213000	3.184188000	0.555592000
H	0.574481000	1.362956000	1.277223000
C	-0.738739000	-2.146990000	1.996087000
H	-0.042175000	-2.948767000	2.265895000
H	-1.005586000	-1.614703000	2.912374000
H	-1.647491000	-2.602150000	1.597155000
H	1.587192000	0.312489000	-2.381645000

**TS**

(*E*)-3h, A → *cis*-4h, A  
symmetry c1

C	-2.033770000	-3.266068000	-0.666258000
C	-1.748057000	-2.860648000	0.639761000
C	-1.486235000	-1.522708000	0.936128000
C	-1.519054000	-0.558978000	-0.112617000
C	-1.828648000	-0.987324000	-1.425533000
C	-2.073429000	-2.326008000	-1.703013000
H	-2.233838000	-4.312643000	-0.874631000
H	-1.735130000	-3.594786000	1.440181000
H	-1.870709000	-0.273887000	-2.241600000
H	-2.302369000	-2.638159000	-2.716645000
C	1.194630000	1.782956000	0.316088000
C	-1.619120000	1.955513000	-0.734366000

H	-2.284303000	1.574260000	-1.512881000
C	-0.313187000	2.398684000	-1.472243000
H	-0.484099000	3.329468000	-2.014712000
H	0.036306000	1.637985000	-2.171192000
O	0.682554000	2.712960000	-0.497591000
C	1.963249000	0.593207000	-0.054004000
C	2.972417000	0.227834000	0.867997000
C	1.819211000	-0.175963000	-1.230054000
C	3.818124000	-0.849540000	0.618269000
H	3.111377000	0.815412000	1.771315000
C	2.673595000	-1.245640000	-1.478663000
H	1.052143000	0.047352000	-1.957520000
C	3.671705000	-1.587775000	-0.558659000
H	4.594481000	-1.103547000	1.332489000
H	2.559591000	-1.818759000	-2.393058000
H	4.332349000	-2.424706000	-0.761922000
C	-0.249327000	0.090757000	2.415309000
C	-1.254195000	-1.066215000	2.357289000
C	-1.268532000	0.838941000	0.217967000
H	-0.905563000	-1.901174000	2.971675000
H	0.757641000	-0.304562000	2.226411000
H	-0.230584000	0.531226000	3.416203000
H	-2.215522000	-0.746553000	2.784616000
C	-0.588429000	1.156725000	1.394372000
H	-0.660546000	2.177970000	1.754373000
C	-2.311441000	3.167774000	-0.078290000
H	-2.652039000	3.857597000	-0.855915000
H	-3.186386000	2.852734000	0.496277000
H	-1.642606000	3.721943000	0.584586000
H	1.582331000	2.275995000	1.205796000

(Z)-3h, A → *trans*-4h, A  
symmetry c1

C	-4.467599000	-1.562995000	-0.716525000
C	-3.535860000	-2.065653000	0.195960000
C	-2.428155000	-1.310088000	0.579122000
C	-2.259331000	-0.001193000	0.039497000
C	-3.222026000	0.495367000	-0.872156000
C	-4.307580000	-0.281077000	-1.256251000
H	-5.320674000	-2.169658000	-1.004582000
H	-3.674912000	-3.057841000	0.615485000
H	-3.116909000	1.487085000	-1.298197000
H	-5.030155000	0.108005000	-1.965858000
C	1.144294000	0.537699000	-0.749143000
C	2.671692000	-1.381132000	-1.035874000
H	-2.027393000	2.649920000	-0.027911000
C	-0.129280000	2.493269000	-0.999759000
H	0.075626000	3.554646000	-1.144792000
H	-0.590253000	2.079320000	-1.903907000
O	1.141100000	1.875234000	-0.785145000
C	2.434568000	-0.099546000	-0.502069000
C	0.020721000	0.131152000	0.975005000

C	3.448190000	0.550904000	0.230531000
C	3.904484000	-2.002028000	-0.842346000
H	1.903099000	-1.876766000	-1.622528000
C	4.675746000	-0.074330000	0.418221000
H	3.272382000	1.543542000	0.632054000
C	4.904435000	-1.351277000	-0.113949000
H	4.088205000	-2.984462000	-1.264792000
H	5.459073000	0.429434000	0.975243000
H	5.865015000	-1.834196000	0.036126000
C	-0.015597000	-1.363505000	1.240393000
C	-1.435313000	-1.818981000	1.596782000
C	-1.115220000	0.784621000	0.479098000
H	0.719324000	0.716262000	1.563527000
H	-1.713050000	-1.438970000	2.590393000
H	0.686184000	-1.614791000	2.039682000
H	0.320565000	-1.914431000	0.352448000
C	-1.040600000	2.271572000	0.249659000
H	-1.480299000	-2.910039000	1.658115000
C	-0.542482000	3.091764000	1.455547000
H	-0.635099000	4.159195000	1.234764000
H	-1.142871000	2.880334000	2.344399000
H	0.505234000	2.891764000	1.691968000
H	0.477596000	0.032523000	-1.450934000

## INTERMEDIATES

*cis*-4h, A

symmetry c1

C	-4.792629000	-1.449483000	-0.276856000
C	-3.671000000	-2.073346000	0.274457000
C	-2.459527000	-1.395919000	0.389585000
C	-2.382033000	-0.025619000	-0.047024000
C	-3.554187000	0.590289000	-0.591005000
C	-4.733023000	-0.115337000	-0.718200000
H	-5.722539000	-2.003459000	-0.366598000
H	-3.740732000	-3.101837000	0.615175000
H	-3.518471000	1.613578000	-0.943269000
H	-5.608298000	0.354697000	-1.153248000
C	1.216661000	0.529938000	-0.645258000
C	-1.079269000	2.179146000	0.064765000
H	-2.008832000	2.605186000	-0.316572000
C	0.065222000	2.563183000	-0.924648000
H	0.234804000	3.641367000	-0.879805000
H	-0.217748000	2.292910000	-1.952481000
O	1.274368000	1.938843000	-0.559365000
C	2.575684000	-0.055703000	-0.362875000
C	3.135041000	-0.984618000	-1.249687000
C	3.295808000	0.325202000	0.779520000
C	4.395845000	-1.532284000	-0.997783000
H	2.593096000	-1.274096000	-2.146542000
C	4.556518000	-0.216470000	1.027358000
H	2.884938000	1.065145000	1.460577000
C	5.106884000	-1.149999000	0.141266000

H	4.822671000	-2.247309000	-1.694070000
H	5.113323000	0.092475000	1.906582000
H	6.088063000	-1.571139000	0.337158000
C	0.024559000	-1.549887000	0.348319000
C	-1.256452000	-2.047105000	1.013387000
C	-1.167911000	0.689950000	0.137948000
H	-1.339591000	-3.135128000	0.937943000
H	0.039977000	-1.886109000	-0.696392000
H	0.905073000	-1.979536000	0.830511000
H	-1.243089000	-1.814679000	2.089381000
C	0.114532000	-0.019271000	0.391332000
H	0.494989000	0.316291000	1.366608000
C	-0.820532000	2.801139000	1.465636000
H	-0.892446000	3.888911000	1.379974000
H	-1.564284000	2.469221000	2.195254000
H	0.176677000	2.553076000	1.833671000
H	0.886334000	0.226854000	-1.650358000

*trans*-4h, A  
symmetry c1

C	-4.191931000	-1.684774000	-0.620147000
C	-3.520184000	-1.721713000	0.603542000
C	-2.397307000	-0.928395000	0.830189000
C	-1.947913000	-0.044004000	-0.213936000
C	-2.667205000	-0.018763000	-1.450916000
C	-3.761679000	-0.833824000	-1.654034000
H	-5.055716000	-2.324599000	-0.775597000
H	-3.872191000	-2.382000000	1.390280000
H	-2.338210000	0.623175000	-2.258507000
H	-4.286133000	-0.820012000	-2.603281000
C	1.538801000	0.948742000	0.939129000
C	-0.551912000	2.018863000	-0.816362000
H	-0.989027000	1.901993000	-1.810656000
C	0.975806000	2.244384000	-0.978243000
H	1.153351000	3.240073000	-1.390157000
H	1.398090000	1.502713000	-1.667485000
O	1.627772000	2.208563000	0.274428000
C	2.320535000	-0.153354000	0.243149000
C	3.672007000	-0.310717000	0.588890000
C	1.787080000	-0.974141000	-0.761436000
C	4.471679000	-1.250499000	-0.062770000
H	4.103532000	0.315440000	1.365283000
C	2.584413000	-1.914775000	-1.418520000
H	0.737046000	-0.904137000	-1.035944000
C	3.929722000	-2.053982000	-1.069658000
H	5.515410000	-1.355713000	0.216256000
H	2.153768000	-2.541292000	-2.193517000
H	4.549112000	-2.789140000	-1.573820000
C	-0.205510000	-0.671356000	1.996567000
C	-1.698892000	-0.940779000	2.162856000
C	-0.844118000	0.820622000	0.030009000
H	-1.873421000	-1.896640000	2.665117000

H	0.261298000	-1.501386000	1.457443000
H	0.284340000	-0.610296000	2.973019000
H	-2.155061000	-0.170185000	2.804501000
C	0.018507000	0.638856000	1.233966000
H	-0.265847000	1.480419000	1.891705000
C	-1.217138000	3.273838000	-0.164967000
H	-1.121239000	4.110038000	-0.862741000
H	-2.280381000	3.113457000	0.032239000
H	-0.713177000	3.542974000	0.765638000
H	2.003717000	1.131256000	1.910958000

*cis*-4h, B

symmetry c1

C	-4.752716000	-1.560628000	0.061510000
C	-3.520052000	-2.188765000	0.248667000
C	-2.325729000	-1.481152000	0.121869000
C	-2.383942000	-0.079517000	-0.195006000
C	-3.662333000	0.543064000	-0.353323000
C	-4.826051000	-0.189361000	-0.244543000
H	-5.667283000	-2.137554000	0.162897000
H	-3.489079000	-3.241992000	0.511530000
H	-3.722839000	1.593275000	-0.612178000
H	-5.789253000	0.285670000	-0.395674000
C	1.377603000	0.773470000	-0.760260000
C	-1.155796000	2.149299000	-0.147456000
H	-1.991997000	2.600162000	-0.695155000
C	0.168990000	2.770531000	-0.618573000
H	0.263196000	3.788203000	-0.233268000
H	0.217936000	2.814610000	-1.717076000
O	1.259294000	2.028564000	-0.104187000
C	2.667034000	0.097811000	-0.344151000
C	3.285834000	-0.796411000	-1.228315000
C	3.244636000	0.333885000	0.909952000
C	4.456883000	-1.462418000	-0.858181000
H	2.864983000	-0.963403000	-2.217746000
C	4.420822000	-0.326017000	1.275254000
H	2.789076000	1.048744000	1.586869000
C	5.025477000	-1.229341000	0.396797000
H	4.931444000	-2.147240000	-1.554215000
H	4.868642000	-0.128176000	2.244412000
H	5.941147000	-1.737591000	0.682586000
C	-1.005259000	-2.166099000	0.369061000
C	0.154602000	-1.191084000	0.581919000
C	0.096213000	-0.103960000	-0.532269000
C	-1.176589000	0.663122000	-0.322380000
H	0.110826000	-0.731378000	1.575637000
H	1.110938000	-1.711394000	0.509069000
H	-0.782104000	-2.791598000	-0.510302000
H	-1.103653000	-2.856228000	1.213201000
H	-0.057229000	-0.673862000	-1.464814000
C	-1.377781000	2.464319000	1.371666000
H	-1.422535000	3.550899000	1.485051000

H	-2.307812000	2.033225000	1.746240000
H	-0.542089000	2.091326000	1.967589000
H	1.432241000	0.961295000	-1.844577000

*trans*-4h, B  
symmetry c1

C	-4.927067000	-1.087482000	-0.487774000
C	-3.896664000	-1.859630000	0.050893000
C	-2.609408000	-1.344023000	0.191064000
C	-2.353760000	0.012745000	-0.218796000
C	-3.431594000	0.773054000	-0.779259000
C	-4.693096000	0.233754000	-0.911597000
H	-5.921388000	-1.514098000	-0.582895000
H	-4.098432000	-2.878346000	0.367774000
H	-3.259593000	1.786520000	-1.118681000
H	-5.498216000	0.820331000	-1.340442000
C	1.388329000	0.417651000	0.837321000
C	-0.775188000	2.010879000	-0.425903000
H	-1.252107000	2.256105000	-1.382677000
C	0.739139000	2.245207000	-0.526031000
H	0.949593000	3.310492000	-0.642395000
H	1.178987000	1.713342000	-1.381676000
O	1.331724000	1.835687000	0.694791000
C	2.669868000	-0.145445000	0.209001000
C	3.818396000	0.661450000	0.209631000
C	2.768731000	-1.449099000	-0.299006000
C	5.025841000	0.183274000	-0.301981000
H	3.760014000	1.668906000	0.606994000
C	3.979253000	-1.929823000	-0.808706000
H	1.915451000	-2.121866000	-0.297282000
C	5.111005000	-1.113929000	-0.814421000
H	5.901291000	0.825436000	-0.297210000
H	4.033294000	-2.941834000	-1.198229000
H	6.050617000	-1.486016000	-1.210551000
C	-1.503911000	-2.209452000	0.730584000
C	-0.369335000	-1.388276000	1.335237000
C	0.083399000	-0.290821000	0.353279000
C	-1.056498000	0.578846000	-0.080658000
H	-0.693388000	-0.915160000	2.270614000
H	0.479689000	-2.030846000	1.581813000
H	-1.111276000	-2.810999000	-0.105824000
H	-1.909216000	-2.924235000	1.453193000
H	0.325229000	-0.790222000	-0.609661000
C	-1.373281000	2.950844000	0.672085000
H	-1.205046000	3.985163000	0.359130000
H	-2.444251000	2.797233000	0.812148000
H	-0.863221000	2.794907000	1.624382000
H	1.443231000	0.271345000	1.923377000

**PRODUCTS***cis*-7h, A

symmetry c1

C	-4.740495000	-1.468807000	0.264218000
C	-3.526189000	-2.147210000	0.123616000
C	-2.325333000	-1.454020000	-0.038705000
C	-2.324889000	-0.037469000	-0.066565000
C	-3.554306000	0.629482000	0.080635000
C	-4.749674000	-0.074008000	0.243286000
H	-5.665610000	-2.024536000	0.386932000
H	-3.509912000	-3.234630000	0.140588000
H	-3.590567000	1.713240000	0.064632000
H	-5.683680000	0.470110000	0.350911000
C	1.389513000	0.716690000	-0.920912000
C	-0.982008000	2.188711000	-0.000011000
H	-1.877593000	2.647974000	-0.439861000
C	0.214174000	2.772523000	-0.756055000
H	0.400242000	3.811124000	-0.466271000
H	0.029803000	2.743768000	-1.842468000
O	1.408984000	2.063310000	-0.446987000
C	2.569551000	0.008246000	-0.270254000
C	3.651604000	-0.426637000	-1.042158000
C	2.598474000	-0.199606000	1.115821000
C	4.744217000	-1.065317000	-0.445868000
H	3.643668000	-0.261365000	-2.116885000
C	3.688062000	-0.831626000	1.715348000
H	1.764344000	0.139789000	1.722604000
C	4.764387000	-1.269186000	0.934973000
H	5.577149000	-1.397064000	-1.059310000
H	3.699087000	-0.984047000	2.791014000
H	5.611850000	-1.762753000	1.402076000
C	-0.032884000	-1.439594000	-1.064242000
C	-1.004415000	-2.180908000	-0.143352000
C	-1.040047000	0.688001000	-0.248078000
H	-1.160431000	-3.207950000	-0.490748000
H	-0.377342000	-1.518077000	-2.108357000
H	0.952956000	-1.912135000	-1.024633000
H	-0.555275000	-2.250626000	0.859525000
C	0.056595000	0.023488000	-0.682299000
C	-0.946143000	2.546978000	1.498964000
H	-1.031826000	3.630867000	1.639595000
H	-1.765102000	2.068530000	2.044504000
H	-0.002505000	2.220258000	1.945923000
H	1.567702000	0.722648000	-2.014060000

*trans*-7h, A

symmetry c1

C	4.714000000	-1.326016000	0.617308000
C	3.806529000	-1.819519000	-0.325092000
C	2.582110000	-1.187270000	-0.548343000
C	2.243046000	-0.025327000	0.188028000
C	3.167177000	0.459734000	1.129758000

C	4.389228000	-0.181174000	1.345440000
H	5.661071000	-1.832307000	0.779990000
H	4.053725000	-2.710802000	-0.897407000
H	2.935230000	1.345004000	1.712523000
H	5.081848000	0.214482000	2.082818000
C	-1.413024000	0.547526000	-0.958129000
C	0.702480000	2.060850000	0.409277000
H	1.082570000	2.168888000	1.434481000
C	-0.800105000	2.352333000	0.474133000
H	-0.988544000	3.424868000	0.578236000
H	-1.255846000	1.841098000	1.334792000
O	-1.452317000	1.962798000	-0.732326000
C	-2.562118000	-0.150087000	-0.223630000
C	-3.840868000	-0.137334000	-0.800360000
C	-2.398474000	-0.755527000	1.029829000
C	-4.930659000	-0.708534000	-0.141858000
H	-3.981399000	0.332531000	-1.770795000
C	-3.487953000	-1.327168000	1.694656000
H	-1.413320000	-0.788642000	1.486577000
C	-4.756470000	-1.305334000	1.111052000
H	-5.913177000	-0.690283000	-0.605120000
H	-3.342954000	-1.792461000	2.665683000
H	-5.602275000	-1.752942000	1.625127000
C	0.163342000	-1.481036000	-1.143705000
C	1.611934000	-1.685904000	-1.594975000
C	0.929914000	0.628231000	-0.052390000
H	1.803087000	-2.740159000	-1.822148000
H	-0.075653000	-2.178552000	-0.326570000
H	-0.526398000	-1.724140000	-1.960377000
H	1.776135000	-1.124320000	-2.527837000
C	-0.053428000	-0.055030000	-0.681495000
C	1.443201000	3.073508000	-0.488122000
H	1.359052000	4.086540000	-0.077686000
H	2.506274000	2.829735000	-0.574246000
H	1.011139000	3.074523000	-1.493590000
H	-1.611189000	0.453019000	-2.034145000

*cis*-7h, B

symmetry c1

C	-4.762351000	-1.281285000	0.619633000
C	-3.729557000	-1.980874000	-0.011824000
C	-2.516184000	-1.360460000	-0.315194000
C	-2.313620000	-0.001161000	0.027413000
C	-3.369321000	0.694238000	0.643491000
C	-4.579675000	0.063994000	0.940654000
H	-5.698348000	-1.781116000	0.851612000
H	-3.870609000	-3.025308000	-0.280825000
H	-3.251990000	1.740360000	0.902569000
H	-5.374239000	0.625436000	1.423863000
C	1.401300000	0.486545000	-0.994507000
C	-0.893839000	2.163642000	-0.274800000
H	-1.819662000	2.589091000	-0.686489000

C	0.252284000	2.562237000	-1.209955000
H	0.468087000	3.632975000	-1.145008000
H	-0.000628000	2.319713000	-2.254482000
O	1.457934000	1.903787000	-0.828919000
C	2.567092000	-0.102561000	-0.211997000
C	3.667855000	-0.644508000	-0.883623000
C	2.567832000	-0.090641000	1.189878000
C	4.751294000	-1.171255000	-0.172946000
H	3.681542000	-0.649521000	-1.970904000
C	3.648031000	-0.610997000	1.903066000
H	1.718544000	0.329160000	1.721124000
C	4.743219000	-1.155335000	1.222889000
H	5.598676000	-1.588320000	-0.709717000
H	3.636245000	-0.594346000	2.989310000
H	5.582989000	-1.562532000	1.778745000
C	-1.431898000	-2.084637000	-1.080587000
C	-0.035377000	-1.623022000	-0.659992000
C	0.056379000	-0.112821000	-0.619771000
C	-1.015443000	0.645313000	-0.293329000
H	0.214558000	-2.026004000	0.333205000
H	0.717745000	-2.030338000	-1.344623000
H	-1.566217000	-1.875712000	-2.153665000
H	-1.534734000	-3.168232000	-0.957491000
C	-0.664724000	2.749551000	1.136072000
H	0.333088000	2.483120000	1.495618000
H	-0.734431000	3.843482000	1.111719000
H	-1.393217000	2.380361000	1.862626000
H	1.569353000	0.251664000	-2.063264000

*trans*-7h, B

symmetry c1

C	4.745150000	-1.417921000	0.337440000
C	3.603933000	-2.079827000	-0.124621000
C	2.380983000	-1.416785000	-0.244609000
C	2.285525000	-0.044252000	0.094287000
C	3.438335000	0.601304000	0.577329000
C	4.655380000	-0.072791000	0.696270000
H	5.688781000	-1.949306000	0.420532000
H	3.661545000	-3.132846000	-0.391111000
H	3.395359000	1.645474000	0.864958000
H	5.529058000	0.455823000	1.066744000
C	-1.388785000	0.723605000	-0.886258000
C	0.800048000	2.050045000	0.541438000
H	1.289577000	2.092885000	1.524262000
C	-0.692925000	2.311480000	0.760099000
H	-0.877086000	3.357136000	1.023818000
H	-1.086467000	1.679316000	1.569199000
O	-1.420514000	2.088730000	-0.446961000
C	-2.544328000	-0.057776000	-0.250979000
C	-3.814381000	0.015935000	-0.841284000
C	-2.398191000	-0.792801000	0.933708000
C	-4.913100000	-0.622409000	-0.263541000

H	-3.941727000	0.585699000	-1.758583000
C	-3.496391000	-1.431581000	1.517753000
H	-1.419836000	-0.874523000	1.398401000
C	-4.756626000	-1.348579000	0.921097000
H	-5.888566000	-0.555257000	-0.737073000
H	-3.364923000	-1.997152000	2.436096000
H	-5.609000000	-1.848330000	1.372408000
C	1.128270000	-2.159926000	-0.652579000
C	0.153410000	-1.260760000	-1.413439000
C	-0.036222000	0.067204000	-0.712123000
C	0.980292000	0.653183000	-0.038954000
H	0.536243000	-1.066708000	-2.428761000
H	-0.807398000	-1.770947000	-1.538707000
H	0.630683000	-2.529520000	0.257697000
H	1.385031000	-3.043437000	-1.247023000
C	1.403413000	3.145316000	-0.367440000
H	1.380466000	4.117574000	0.138910000
H	2.438373000	2.932263000	-0.645983000
H	0.818495000	3.227339000	-1.288174000
H	-1.597234000	0.788690000	-1.963478000

*cis*-12h, A

symmetry c1

C	4.708180000	-1.721093000	0.162062000
C	3.516731000	-2.242237000	-0.341304000
C	2.354081000	-1.467756000	-0.420857000
C	2.375037000	-0.107885000	-0.013351000
C	3.572325000	0.374762000	0.560037000
C	4.722184000	-0.409115000	0.638205000
H	5.599425000	-2.339654000	0.214763000
H	3.475679000	-3.280229000	-0.663410000
H	3.605298000	1.366113000	0.987605000
H	5.622186000	0.003562000	1.085364000
C	-1.311696000	0.744126000	0.393218000
C	1.100148000	2.080281000	-0.114641000
C	-0.219815000	2.822513000	-0.100478000
H	-0.264677000	3.520929000	-0.946733000
H	-0.243329000	3.442364000	0.816308000
O	-1.406285000	2.051379000	-0.178686000
C	-2.677540000	0.101596000	0.273810000
C	-3.221605000	-0.613090000	1.348043000
C	-3.410367000	0.191278000	-0.918448000
C	-4.466063000	-1.239762000	1.233559000
H	-2.670630000	-0.677853000	2.283317000
C	-4.655560000	-0.429668000	-1.034229000
H	-3.008637000	0.766240000	-1.746649000
C	-5.186476000	-1.150691000	0.040235000
H	-4.873851000	-1.788814000	2.077673000
H	-5.214453000	-0.347052000	-1.962322000
H	-6.155993000	-1.632216000	-0.050231000
C	-0.102770000	-1.507616000	-0.039239000
C	1.052601000	-2.104899000	-0.848061000

C	1.146595000	0.724353000	-0.140526000
H	1.112419000	-3.189929000	-0.709552000
H	0.071171000	-1.679198000	1.031936000
H	-1.047900000	-1.993619000	-0.298389000
H	0.863505000	-1.935904000	-1.918953000
C	-0.189313000	-0.011814000	-0.348803000
H	-0.450436000	0.064690000	-1.415893000
C	2.260304000	3.050744000	-0.088843000
H	2.588126000	3.292801000	0.931126000
H	3.125975000	2.674902000	-0.638750000
H	1.960339000	3.999068000	-0.550553000
H	-1.045825000	0.818615000	1.460496000

*trans*-12h, A

symmetry c1

C	-4.414364000	-1.133933000	-0.868750000
C	-3.804459000	-1.416694000	0.353024000
C	-2.608047000	-0.800568000	0.736760000
C	-1.999972000	0.162039000	-0.113987000
C	-2.599596000	0.379044000	-1.374560000
C	-3.789284000	-0.245740000	-1.745097000
H	-5.342889000	-1.624868000	-1.145368000
H	-4.252919000	-2.147544000	1.022074000
H	-2.116893000	1.019630000	-2.098092000
H	-4.216051000	-0.047431000	-2.724240000
C	1.540404000	0.417236000	1.355176000
C	-0.232808000	1.985340000	-0.208864000
C	1.136900000	2.490164000	0.201416000
H	1.071011000	3.542690000	0.503827000
H	1.784633000	2.459931000	-0.694985000
O	1.776817000	1.834364000	1.284157000
C	2.306814000	-0.335133000	0.267984000
C	3.695802000	-0.463736000	0.436793000
C	1.728294000	-0.879798000	-0.887126000
C	4.485039000	-1.109896000	-0.514899000
H	4.160725000	-0.044733000	1.325888000
C	2.515020000	-1.533087000	-1.842119000
H	0.660234000	-0.799659000	-1.052072000
C	3.894302000	-1.649394000	-1.661790000
H	5.556866000	-1.196698000	-0.359929000
H	2.044164000	-1.951352000	-2.727474000
H	4.502912000	-2.157828000	-2.404188000
C	-0.405127000	-1.221133000	1.814050000
C	-1.923532000	-1.227999000	2.016221000
C	-0.743599000	0.840002000	0.309635000
H	-2.280447000	-2.221945000	2.307183000
H	-0.136769000	-1.921539000	1.014921000
H	0.109561000	-1.554362000	2.723428000
H	-2.179469000	-0.548565000	2.843193000
C	0.025419000	0.209726000	1.483117000
H	-0.236606000	0.801561000	2.373592000
C	-0.857442000	2.891154000	-1.246342000

H	-0.609138000	2.591007000	-2.273639000
H	-1.945998000	2.927714000	-1.161963000
H	-0.480446000	3.913046000	-1.122694000
H	1.994393000	0.140459000	2.313427000

*cis*-12h, B

symmetry c1

C	4.637695000	-1.804954000	0.130106000
C	3.443655000	-2.211785000	-0.464511000
C	2.300729000	-1.400814000	-0.445931000
C	2.370970000	-0.127121000	0.167204000
C	3.571355000	0.254982000	0.797045000
C	4.695728000	-0.568470000	0.778900000
H	5.509063000	-2.452980000	0.101851000
H	3.390520000	-3.184126000	-0.950068000
H	3.612192000	1.196953000	1.332829000
H	5.608114000	-0.250423000	1.275269000
C	-1.354120000	0.829437000	0.477742000
C	1.125178000	2.063264000	-0.039160000
C	-0.204330000	2.784944000	-0.143148000
H	-0.171359000	3.497720000	-0.974519000
H	-0.394182000	3.370509000	0.776843000
O	-1.313350000	1.941782000	-0.410423000
C	-2.689849000	0.125138000	0.341407000
C	-3.109013000	-0.757567000	1.347193000
C	-3.515381000	0.322213000	-0.772246000
C	-4.322441000	-1.440166000	1.238530000
H	-2.486564000	-0.907780000	2.226640000
C	-4.732415000	-0.357505000	-0.880166000
H	-3.203056000	1.016591000	-1.544154000
C	-5.139290000	-1.242632000	0.121162000
H	-4.632829000	-2.118147000	2.028698000
H	-5.364270000	-0.191810000	-1.748472000
H	-6.085864000	-1.768657000	0.036186000
C	1.007297000	-1.939153000	-1.041735000
C	-0.178707000	-0.957257000	-1.035159000
C	-0.132271000	-0.082454000	0.232808000
C	1.155833000	0.726965000	0.160273000
H	-0.144700000	-0.303395000	-1.913848000
H	-1.115762000	-1.520643000	-1.088698000
H	0.728488000	-2.831837000	-0.463402000
H	1.194289000	-2.295842000	-2.062296000
H	-0.066189000	-0.755454000	1.101418000
C	2.321065000	2.966746000	-0.225796000
H	2.582794000	3.496623000	0.700559000
H	3.206857000	2.420427000	-0.555150000
H	2.102005000	3.736956000	-0.975260000
H	-1.272879000	1.208200000	1.511844000

*trans*-12h, B

symmetry c1

C	4.629398000	-0.841572000	-1.114439000
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C	4.072633000	0.434230000	-1.197821000
C	2.805299000	0.717742000	-0.670672000
C	2.087135000	-0.308628000	-0.012515000
C	2.645158000	-1.601460000	0.030345000
C	3.901897000	-1.869845000	-0.509077000
H	5.613338000	-1.035506000	-1.531828000
H	4.627857000	1.230645000	-1.689171000
H	2.072167000	-2.411372000	0.468318000
H	4.306571000	-2.876947000	-0.464462000
C	-1.445202000	1.271197000	0.215503000
C	0.268281000	-0.434926000	1.738905000
C	-1.075609000	0.055221000	2.235183000
H	-1.019992000	0.257722000	3.310149000
H	-1.841874000	-0.727711000	2.092639000
O	-1.504395000	1.277554000	1.651587000
C	-2.487851000	0.318126000	-0.369184000
C	-3.837256000	0.700633000	-0.298634000
C	-2.178026000	-0.922988000	-0.941665000
C	-4.848560000	-0.127660000	-0.785938000
H	-4.092780000	1.658453000	0.147875000
C	-3.188813000	-1.757399000	-1.431519000
H	-1.145492000	-1.250642000	-1.007286000
C	-4.525850000	-1.363501000	-1.356021000
H	-5.885350000	0.191347000	-0.725487000
H	-2.927180000	-2.715359000	-1.872337000
H	-5.309493000	-2.010324000	-1.740126000
C	2.222330000	2.109807000	-0.869950000
C	0.852595000	2.343942000	-0.208809000
C	0.001871000	1.057200000	-0.253701000
C	0.752382000	0.009731000	0.557869000
H	0.970375000	2.647725000	0.837418000
H	0.336602000	3.162638000	-0.725871000
H	2.124524000	2.270405000	-1.953214000
H	2.941497000	2.862556000	-0.523692000
H	-0.033231000	0.728050000	-1.302276000
C	0.958322000	-1.385982000	2.687401000
H	0.560457000	-2.406836000	2.602096000
H	2.035624000	-1.435491000	2.520005000
H	0.791500000	-1.071861000	3.724845000
H	-1.750762000	2.288869000	-0.051855000

7s

symmetry c1

C	-4.638861000	-0.602377000	0.249785000
C	-3.619592000	-1.556802000	0.194321000
C	-2.285369000	-1.181133000	0.026817000
C	-1.941776000	0.188538000	-0.094722000
C	-2.981637000	1.135538000	-0.031429000
C	-4.312543000	0.749445000	0.137208000
C	-0.515793000	0.578481000	-0.252809000
C	0.424267000	-0.358087000	-0.543328000
H	-5.672000000	-0.912239000	0.377481000

H	-3.863155000	-2.613364000	0.280947000
H	-2.760629000	2.193752000	-0.113678000
H	-5.090353000	1.506621000	0.178953000
C	-1.179166000	-2.209140000	0.000186000
H	-0.785107000	-2.343874000	1.020289000
H	-1.570860000	-3.181269000	-0.318730000
C	-0.046092000	-1.754029000	-0.918683000
H	-0.417306000	-1.719076000	-1.956180000
H	0.763451000	-2.480826000	-0.913478000
C	1.899165000	-0.025408000	-0.708299000
H	2.193547000	-0.369568000	-1.720603000
C	-0.140373000	2.051666000	-0.217562000
H	-0.929836000	2.611315000	-0.736862000
C	1.122418000	2.229442000	-1.062046000
H	1.519135000	3.246665000	-0.980667000
H	0.894934000	2.030551000	-2.122029000
O	2.162165000	1.378063000	-0.610814000
C	-0.001287000	2.638480000	1.199420000
H	0.169242000	3.720676000	1.153899000
H	-0.906269000	2.463325000	1.789635000
H	0.839077000	2.182522000	1.728512000
C	2.926448000	-0.683372000	0.295485000
C	2.924784000	-2.224280000	0.239652000
H	3.785844000	-2.602148000	0.802216000
H	2.030574000	-2.660500000	0.693503000
H	3.016977000	-2.599671000	-0.786455000
C	2.638875000	-0.238295000	1.741313000
H	1.631130000	-0.528402000	2.057856000
H	3.354379000	-0.706812000	2.426922000
H	2.732126000	0.845449000	1.844091000
C	4.339091000	-0.207855000	-0.116033000
H	5.087698000	-0.641828000	0.556516000
H	4.580634000	-0.530004000	-1.136587000
H	4.424084000	0.879333000	-0.074700000

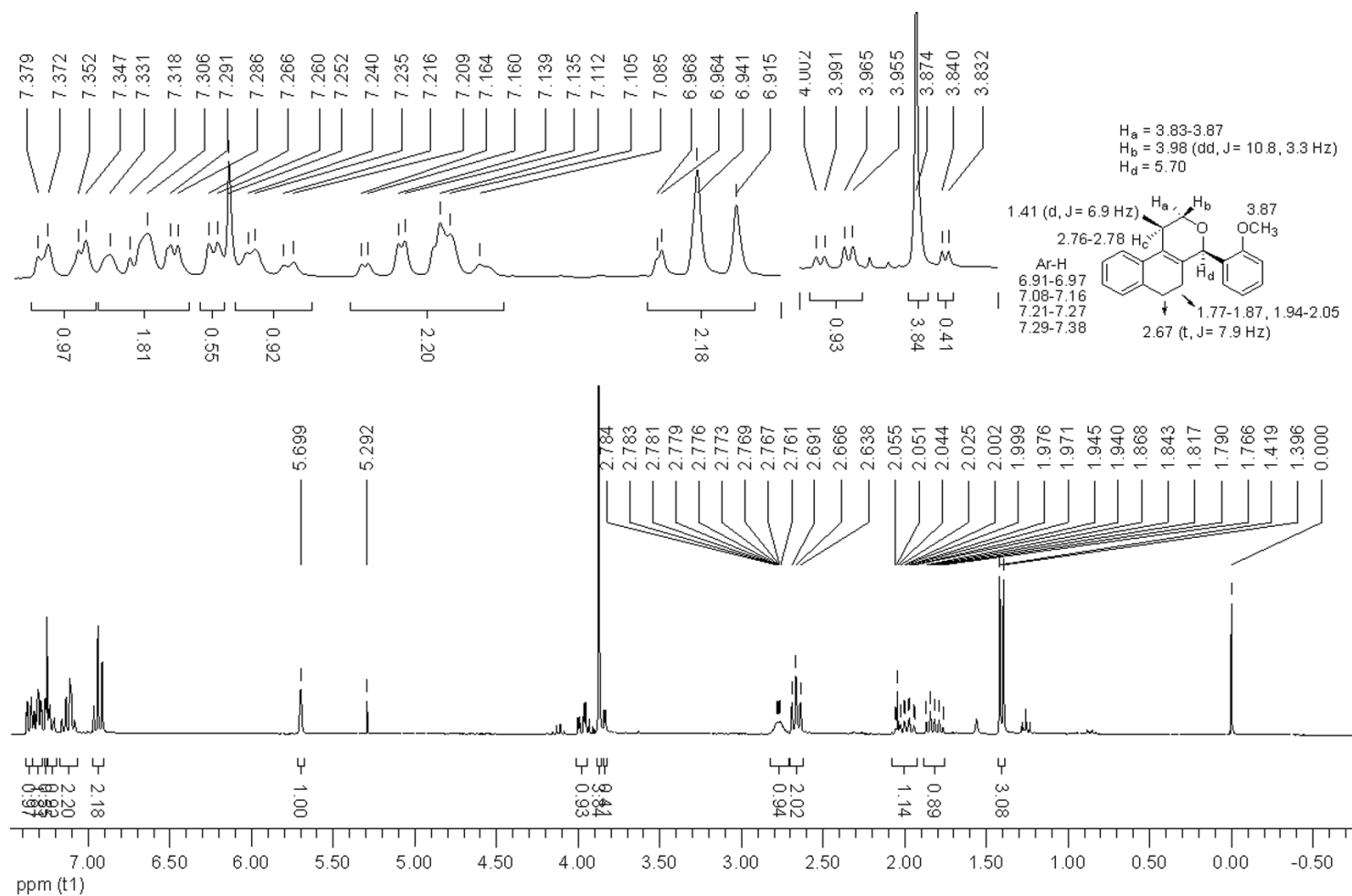
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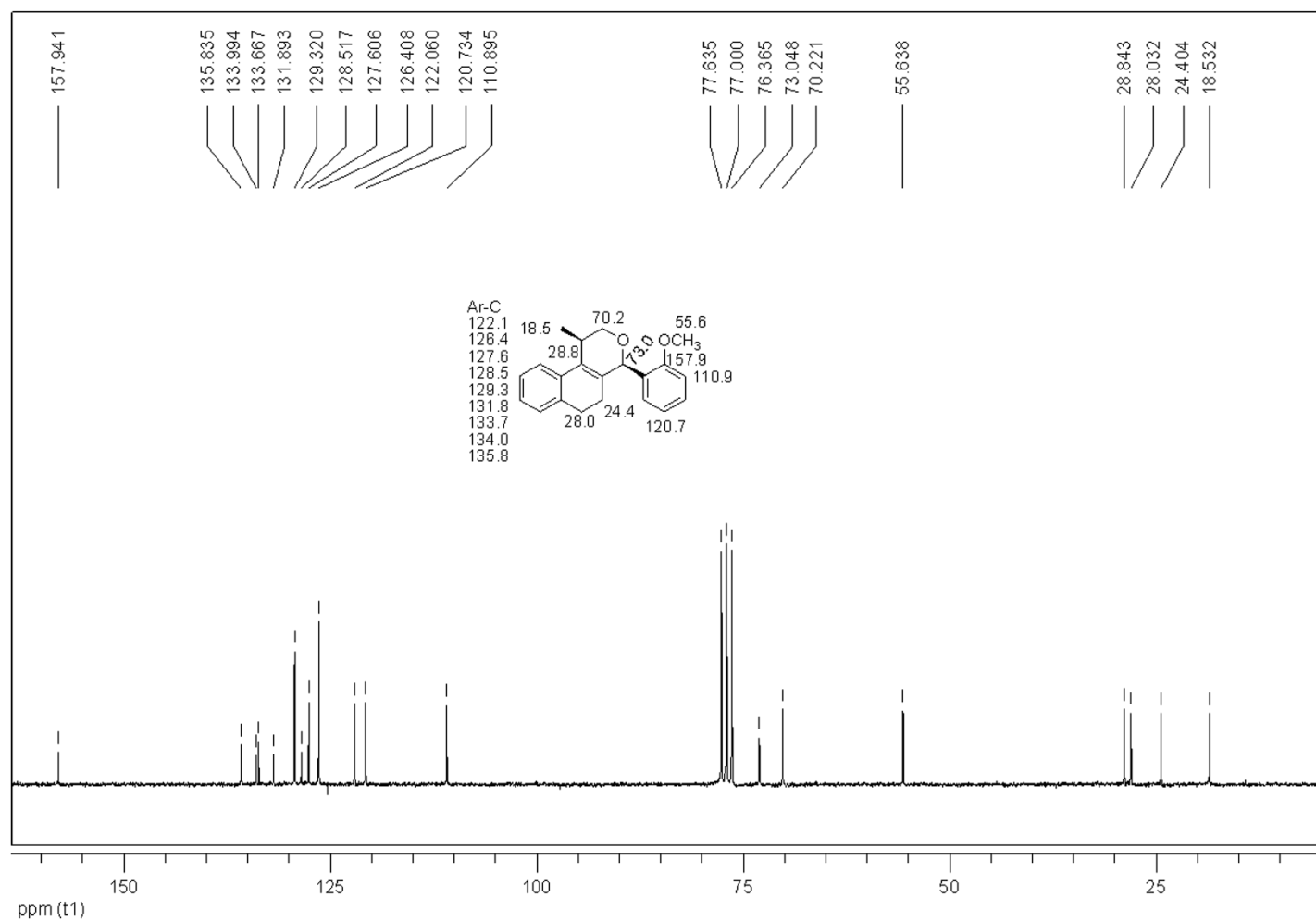
symmetry c1

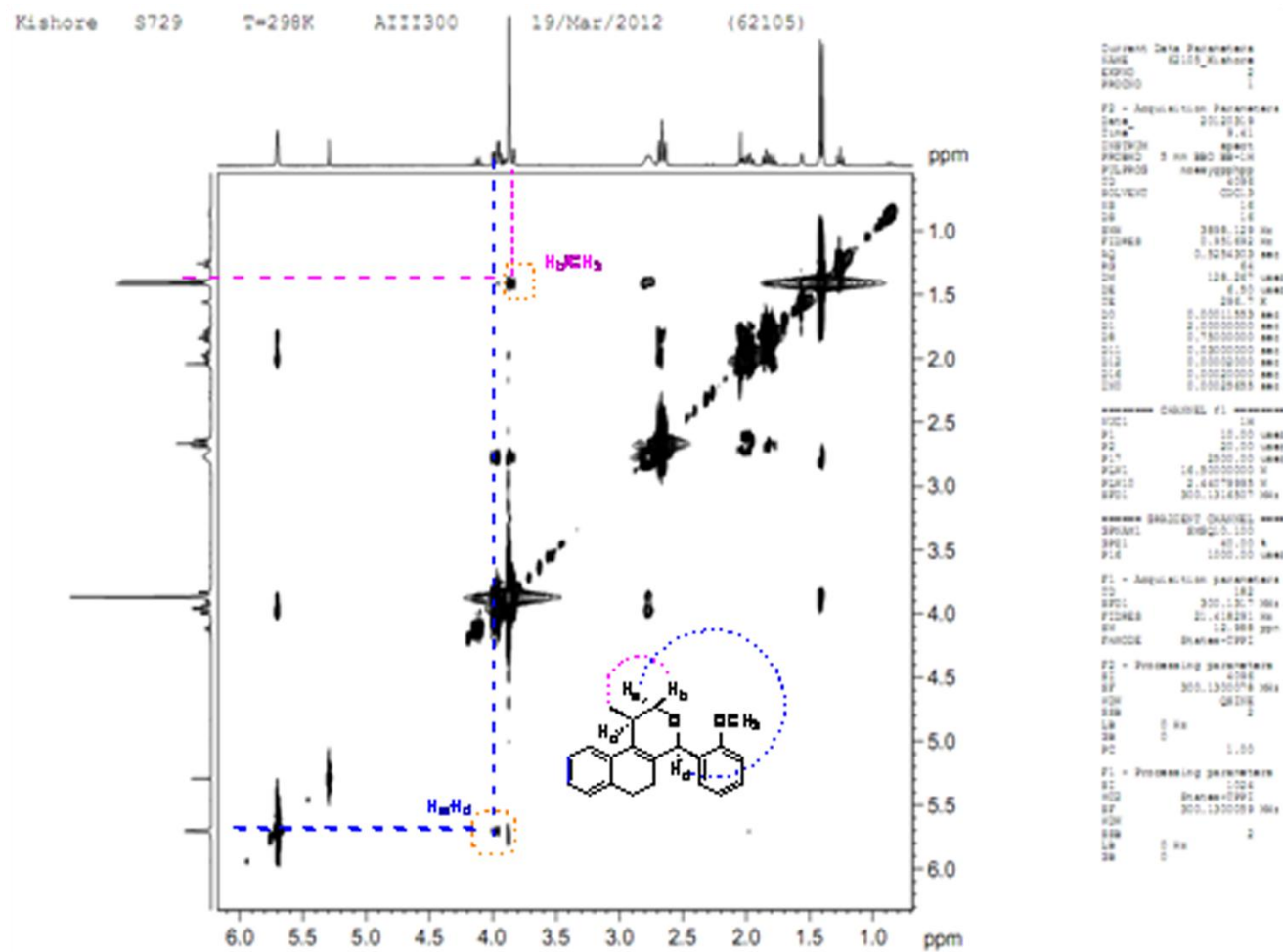
C	-4.510766000	-0.952518000	0.553385000
C	-3.534499000	-1.699876000	-0.103471000
C	-2.244715000	-1.194151000	-0.315750000
C	-1.930380000	0.113494000	0.120196000
C	-2.916288000	0.840849000	0.817352000
C	-4.191940000	0.322925000	1.029090000
H	-5.503513000	-1.365705000	0.707381000
H	-3.770579000	-2.701768000	-0.456261000
H	-2.665333000	1.814103000	1.224213000
H	-4.929659000	0.906651000	1.572343000
C	-1.199461000	-2.080428000	-0.968271000
H	-0.992399000	-2.918139000	-0.286016000
H	-1.611826000	-2.533800000	-1.878538000
C	0.115889000	-1.360814000	-1.286590000
H	0.006903000	-0.761664000	-2.200186000

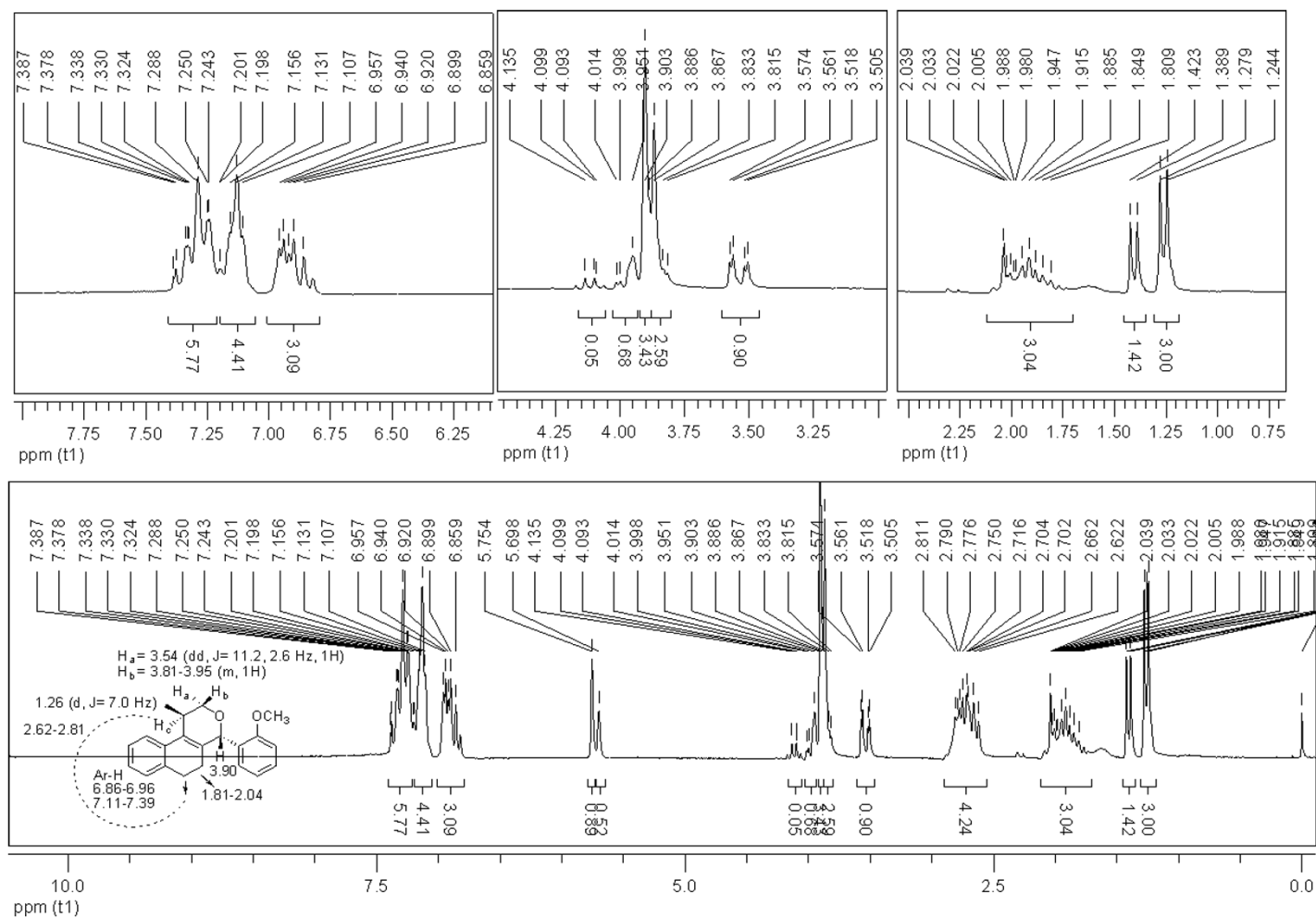
H	0.893920000	-2.101858000	-1.487185000
C	1.956340000	0.155907000	-0.323565000
H	2.173126000	0.174709000	-1.408318000
C	1.157519000	2.385091000	-0.467739000
H	1.289378000	3.350980000	0.035816000
H	1.446873000	2.533117000	-1.526890000
O	2.050249000	1.495289000	0.165785000
C	-1.268386000	3.063389000	-0.650612000
H	-0.896109000	3.686011000	-1.475503000
H	-2.256849000	2.694181000	-0.929353000
H	-1.384991000	3.732922000	0.212868000
C	3.110467000	-0.630696000	0.373822000
C	3.115590000	-2.113272000	-0.047044000
H	3.980146000	-2.616578000	0.400125000
H	2.220203000	-2.644847000	0.290847000
H	3.196086000	-2.227667000	-1.134420000
C	2.990654000	-0.540674000	1.909858000
H	2.073510000	-1.012348000	2.278958000
H	3.835530000	-1.057656000	2.379111000
H	2.995311000	0.499727000	2.243562000
C	4.450934000	0.000819000	-0.062072000
H	5.289886000	-0.530591000	0.401571000
H	4.579146000	-0.058704000	-1.150037000
H	4.504704000	1.052434000	0.229387000
H	0.480061000	-0.973596000	0.806796000
C	0.524742000	-0.408181000	-0.134500000
C	-0.285840000	1.953048000	-0.373796000
C	-0.565780000	0.661384000	-0.099718000

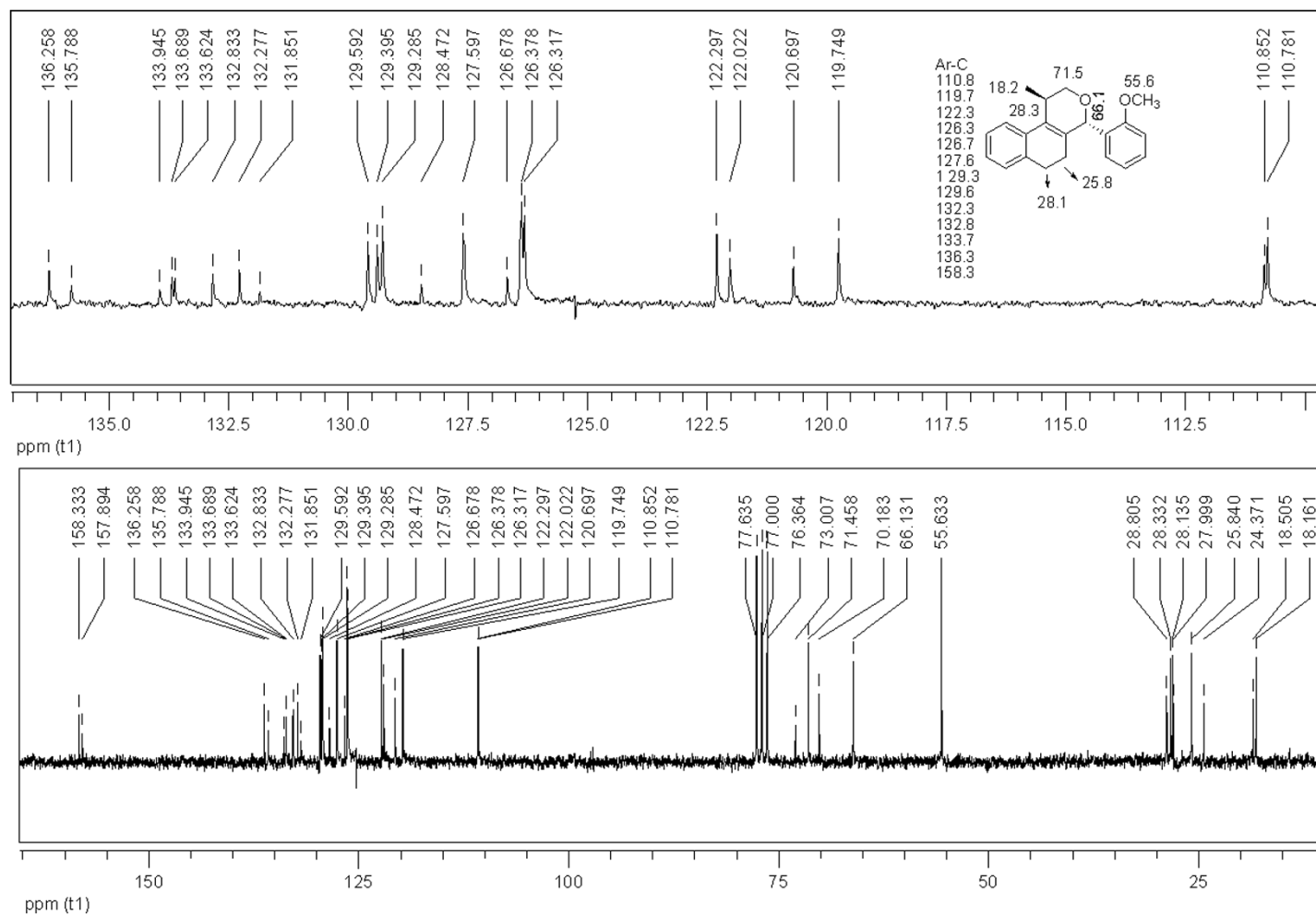
## Part 3: Selected-NMR Spectra

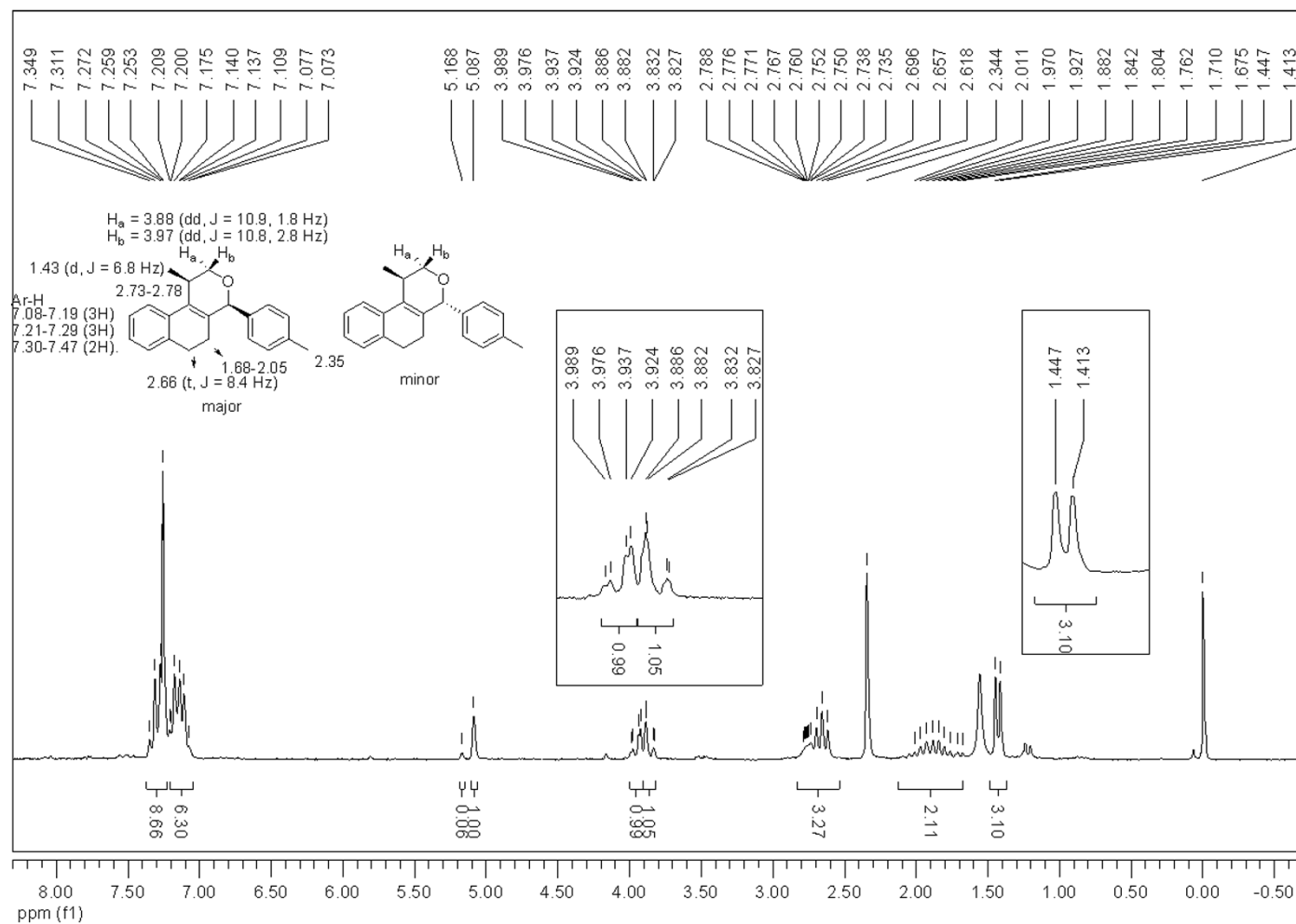
 $^1\text{H}$ -NMR of compound *cis-7c* (300 MHz,  $\text{CDCl}_3$ )

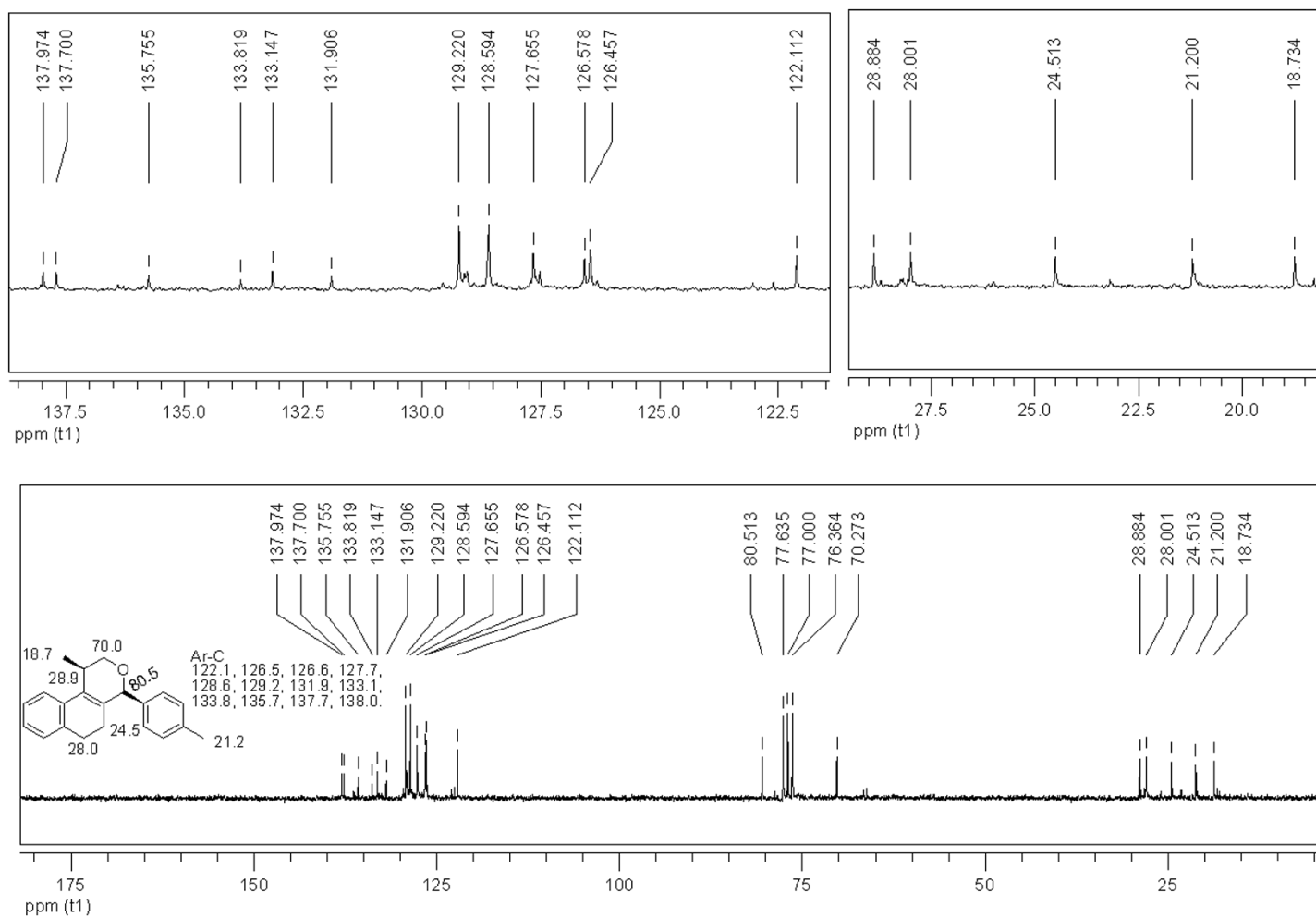
$^{13}\text{C}$ -NMR of compound *cis*-7c (75 MHz,  $\text{CDCl}_3$ )

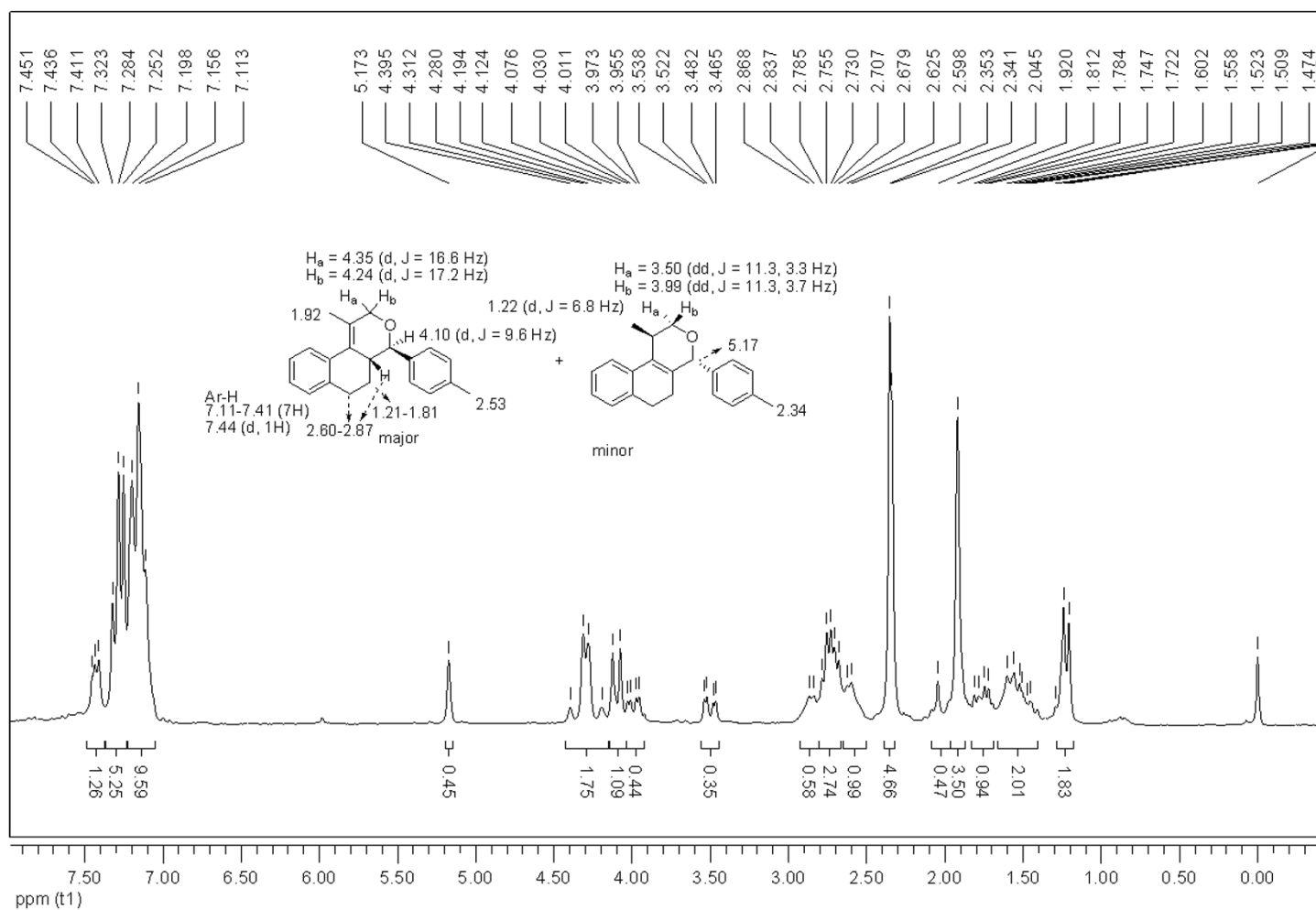
2D NOESY-NMR of compound *cis-7c* (300 MHz, CDCl<sub>3</sub>)

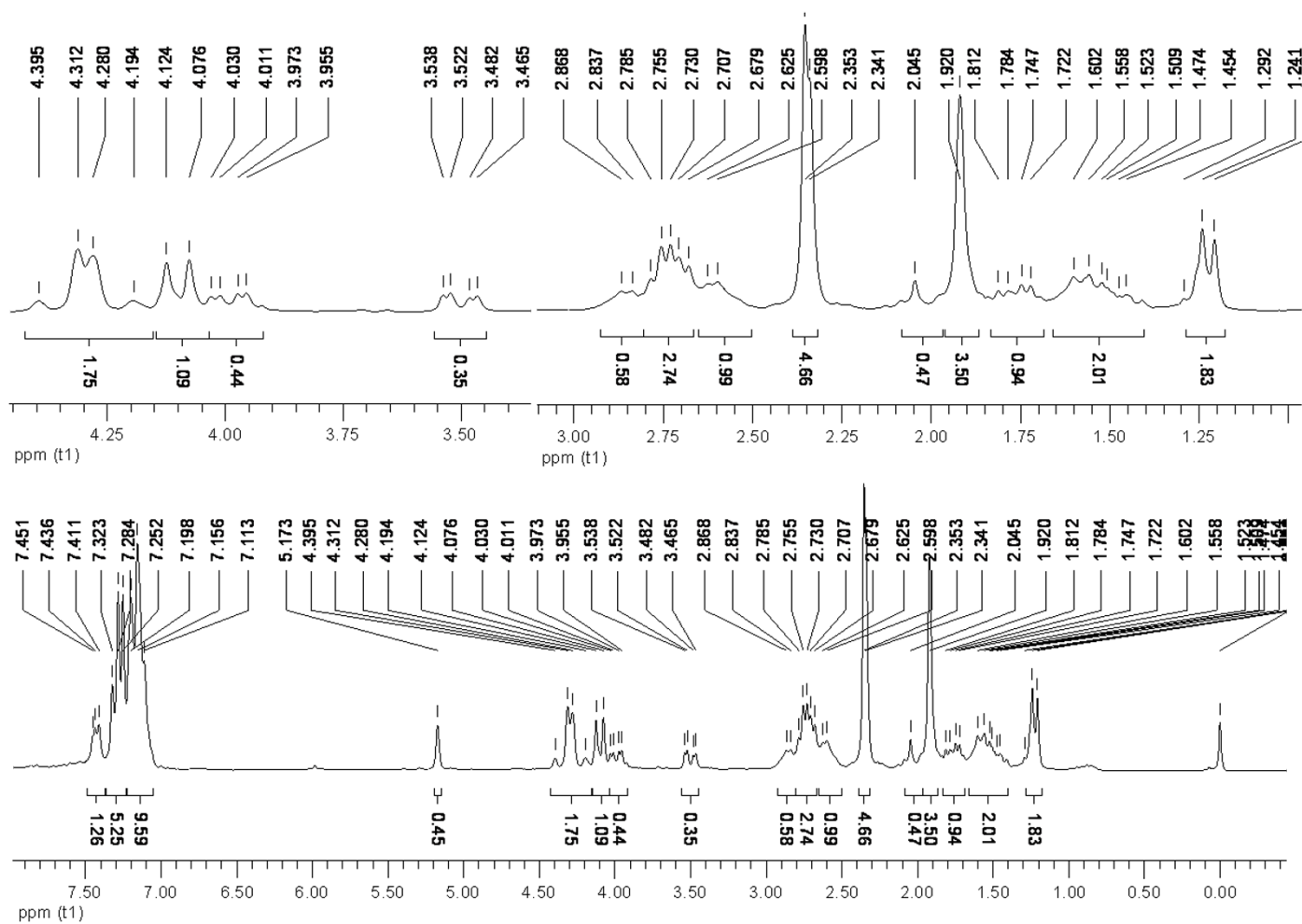
$^1\text{H}$ -NMR of compound *trans*-7c (300 MHz,  $\text{CDCl}_3$ )

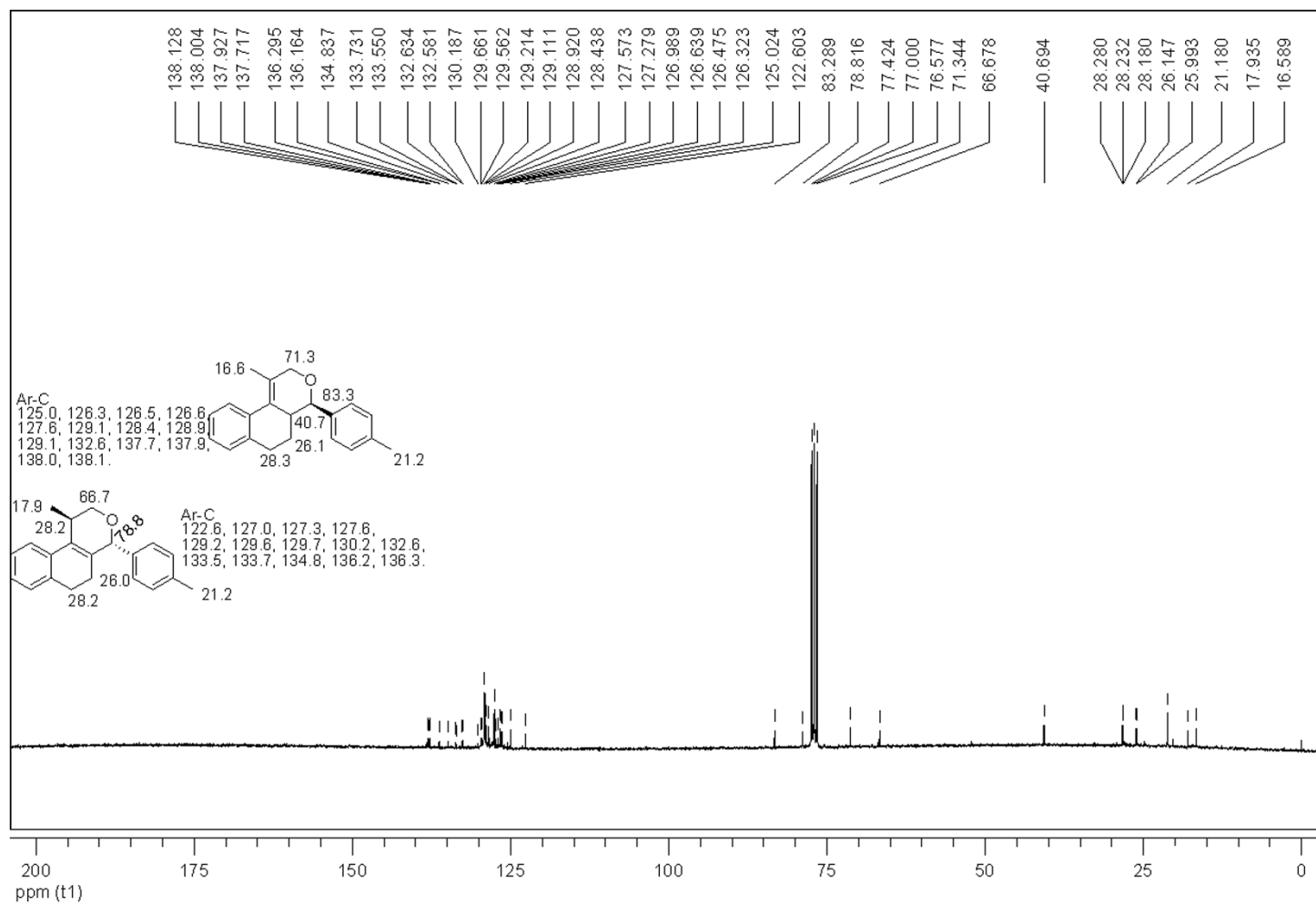
$^{13}\text{C}$ -NMR of compound *trans*-7c (75 MHz,  $\text{CDCl}_3$ )

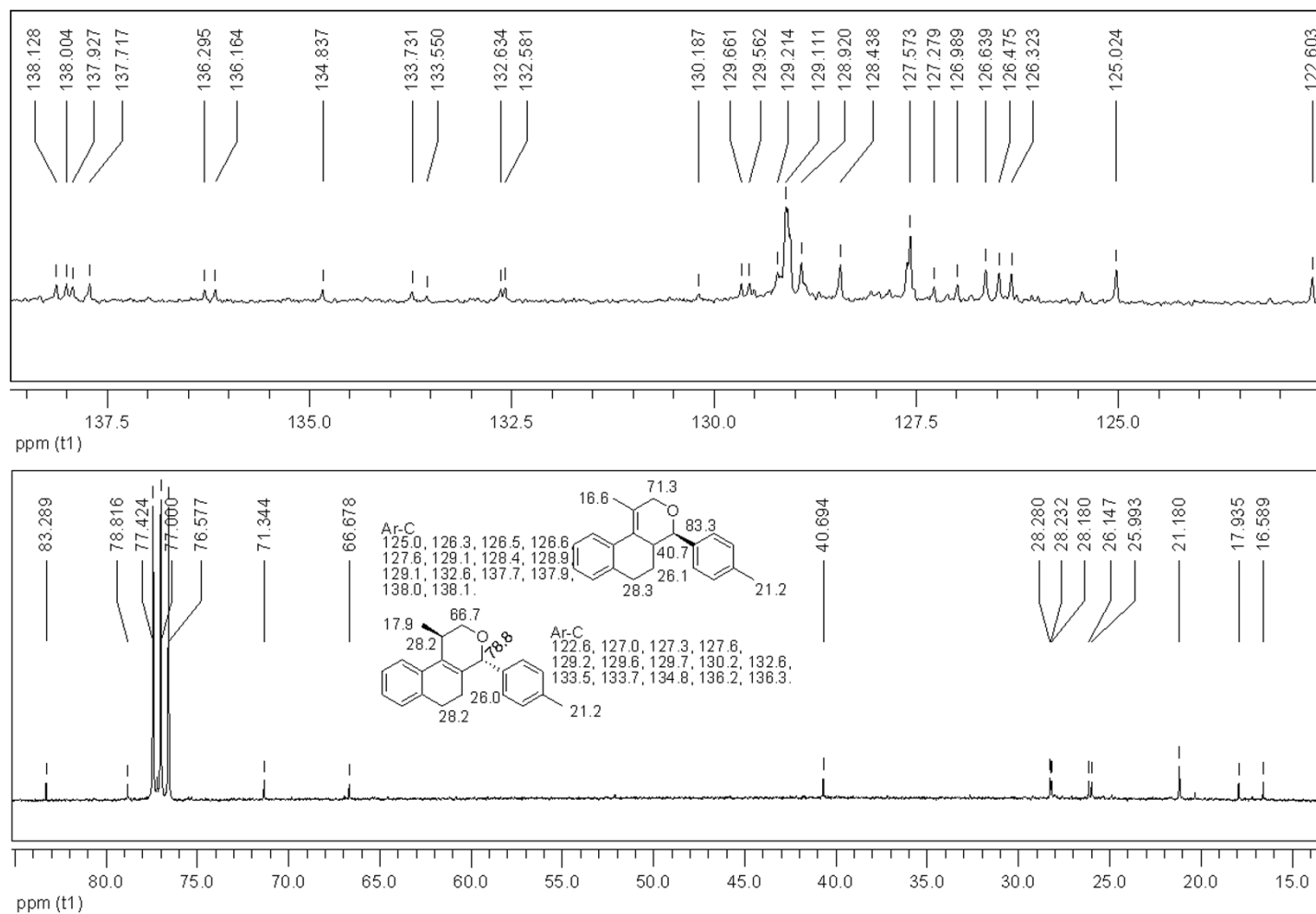
$^1\text{H}$ -NMR of compound *trans*-7d (200 MHz,  $\text{CDCl}_3$ )

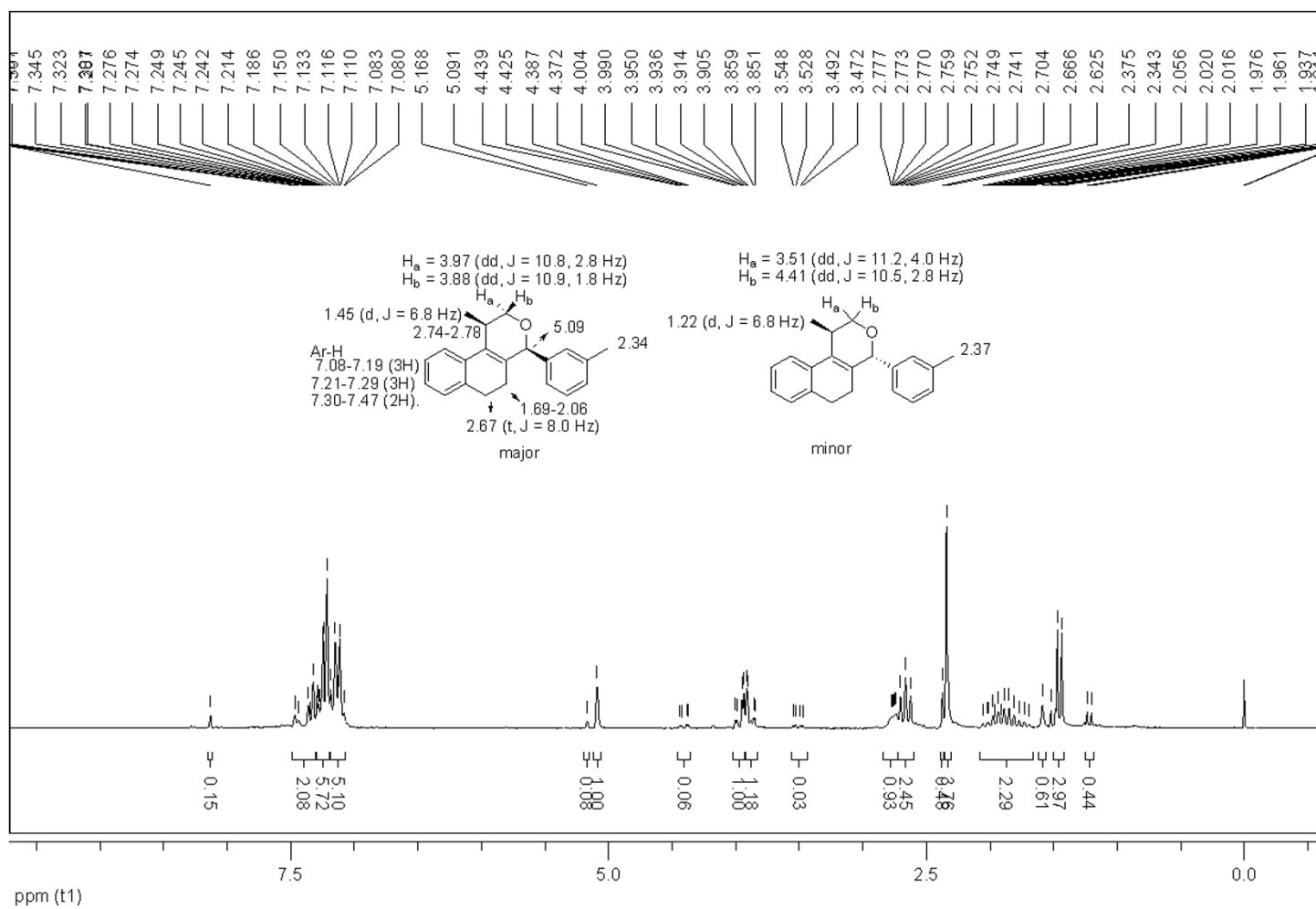
$^{13}\text{C}$ -NMR of compound *cis*-7d (50 MHz,  $\text{CDCl}_3$ )

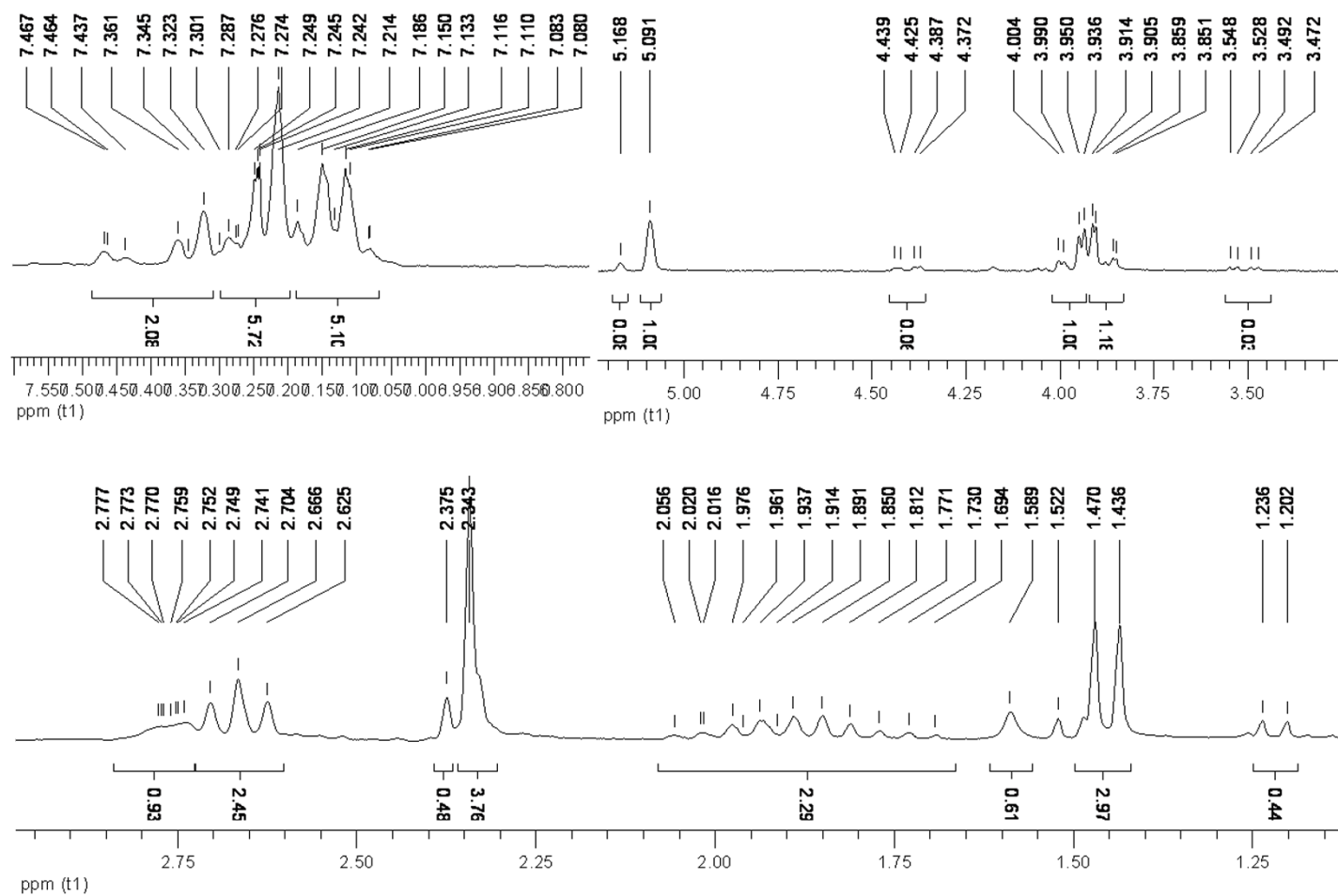
<sup>1</sup>H-NMR of compounds **12d** and *trans*-**7d** (200 MHz, CDCl<sub>3</sub>)

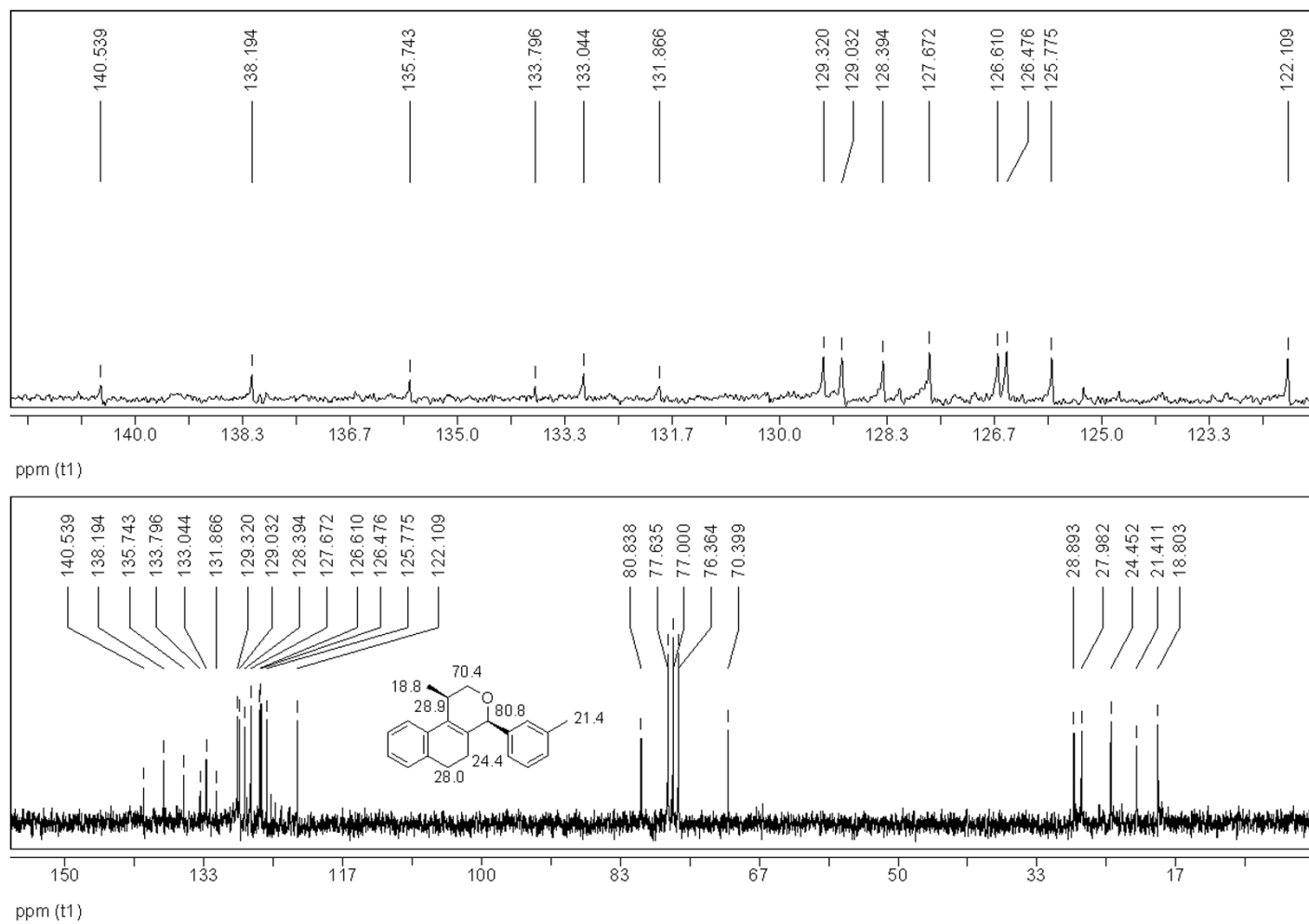
<sup>1</sup>H-NMR of compounds **12d** and *trans*-**7d** (200 MHz, CDCl<sub>3</sub>, selected expansions)

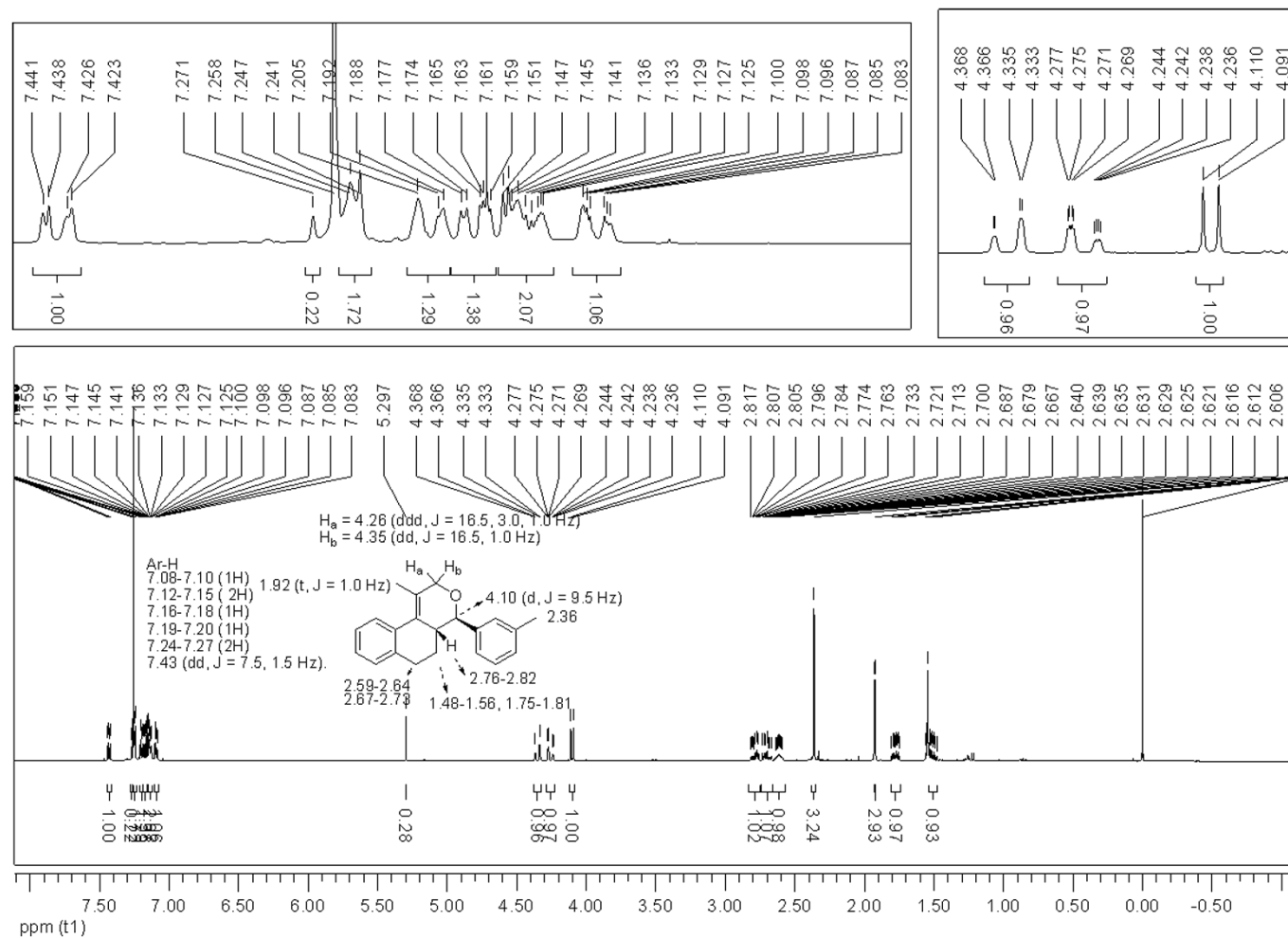
$^{13}\text{C}$ -NMR of compounds **12d** and *trans*-**7d** (75 MHz,  $\text{CDCl}_3$ )

$^{13}\text{C}$ -NMR of compounds **12d** and *trans*-**7d** (75 MHz,  $\text{CDCl}_3$ , selected expansions)

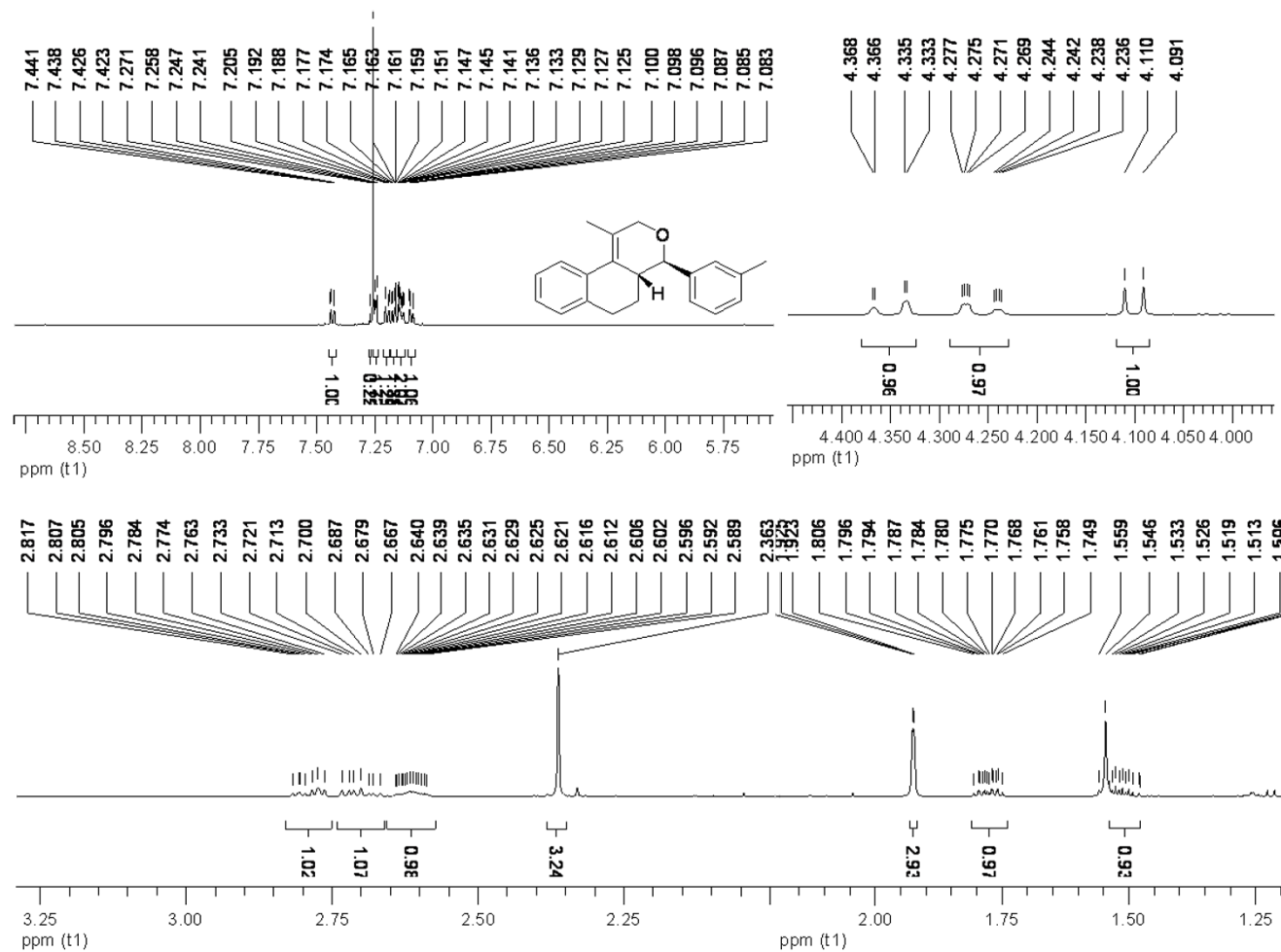
$^1\text{H}$ -NMR of compounds *cis*-7e and *trans*-7e (200 MHz,  $\text{CDCl}_3$ )

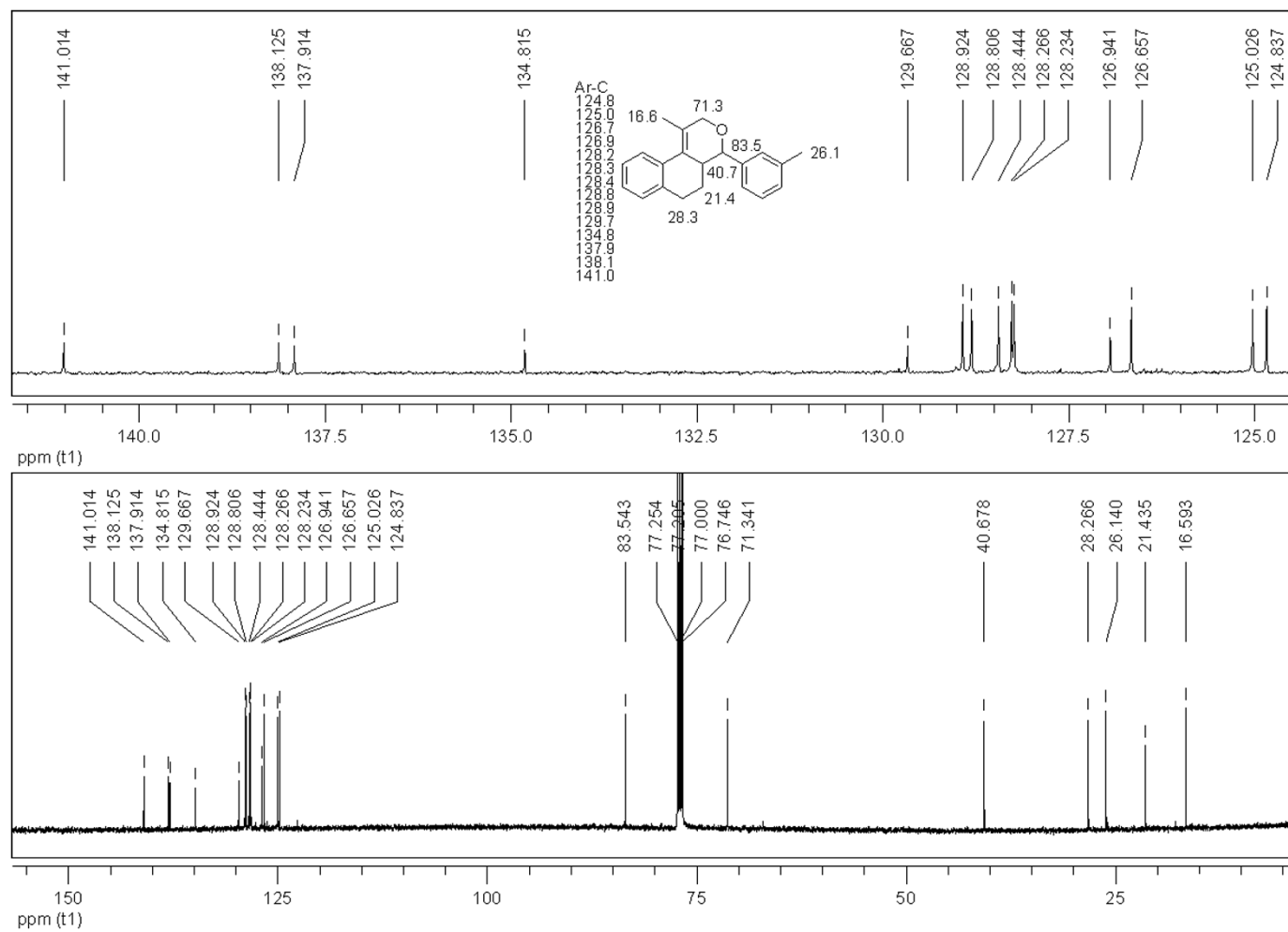
$^1\text{H}$ -NMR of compounds *cis*-7e and *trans*-7e (200 MHz,  $\text{CDCl}_3$ )

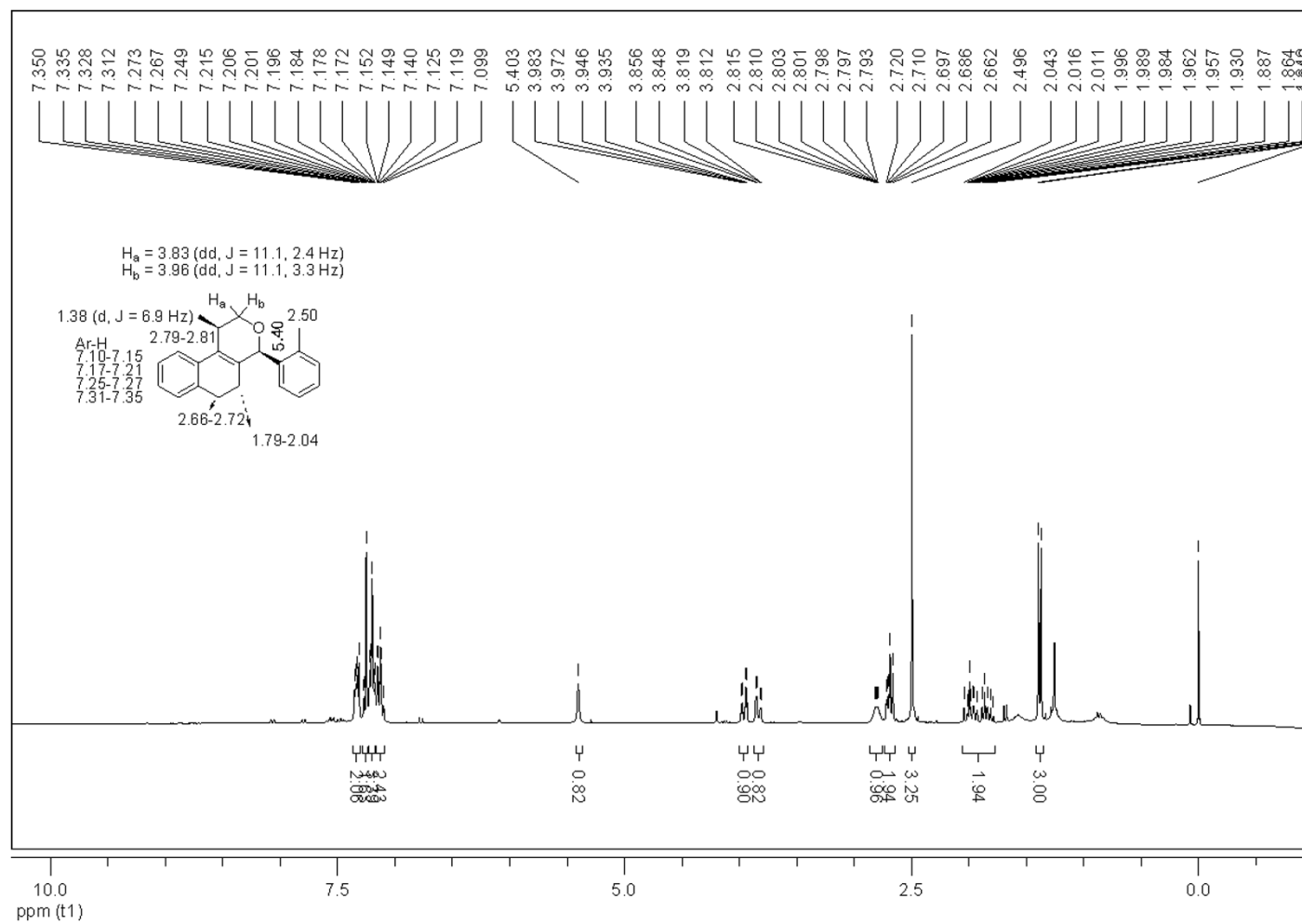
$^{13}\text{C}$ -NMR of compound *cis*-7e (50 MHz,  $\text{CDCl}_3$ )

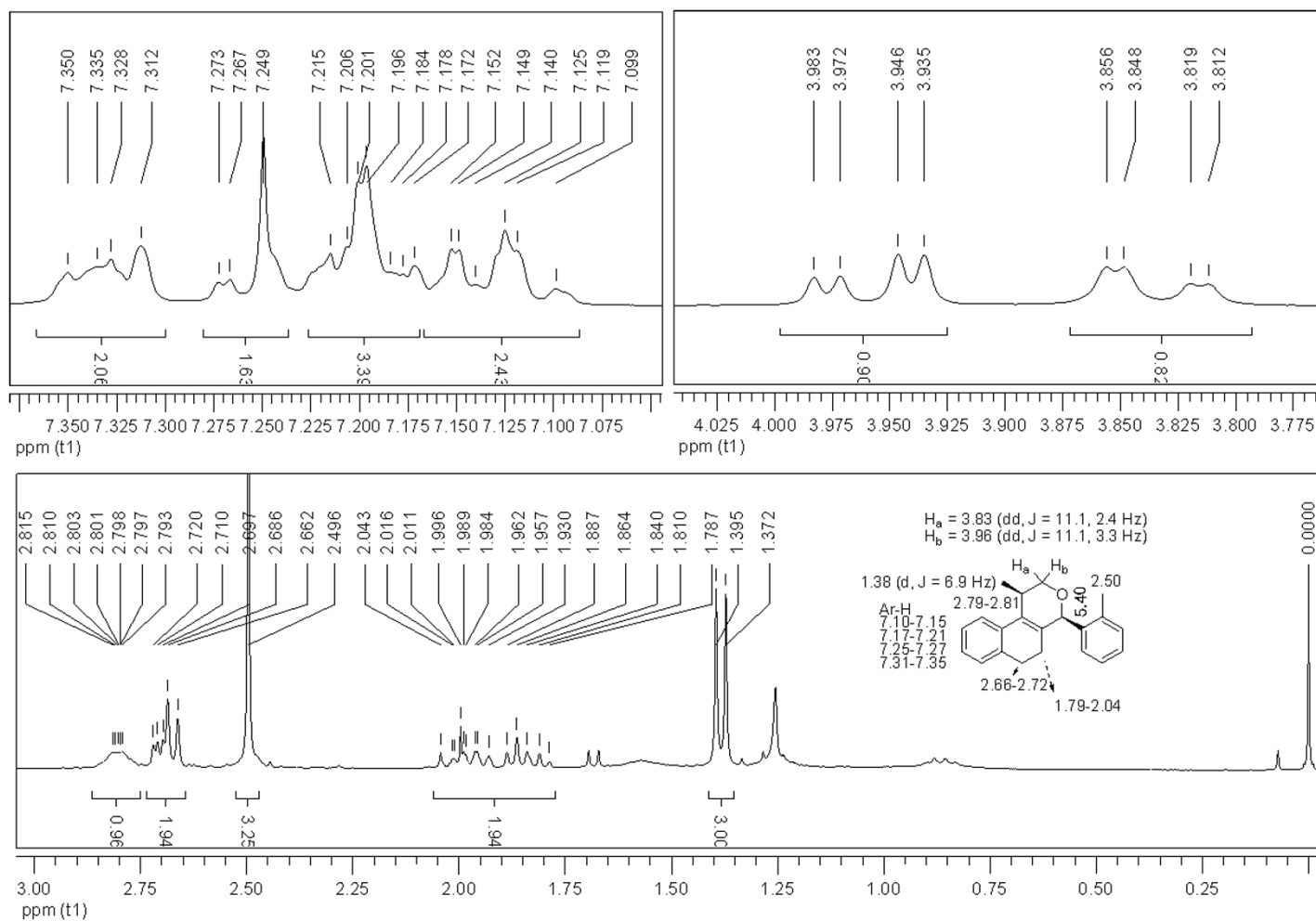
<sup>1</sup>H-NMR of compound **12e** (500 MHz, CDCl<sub>3</sub>)

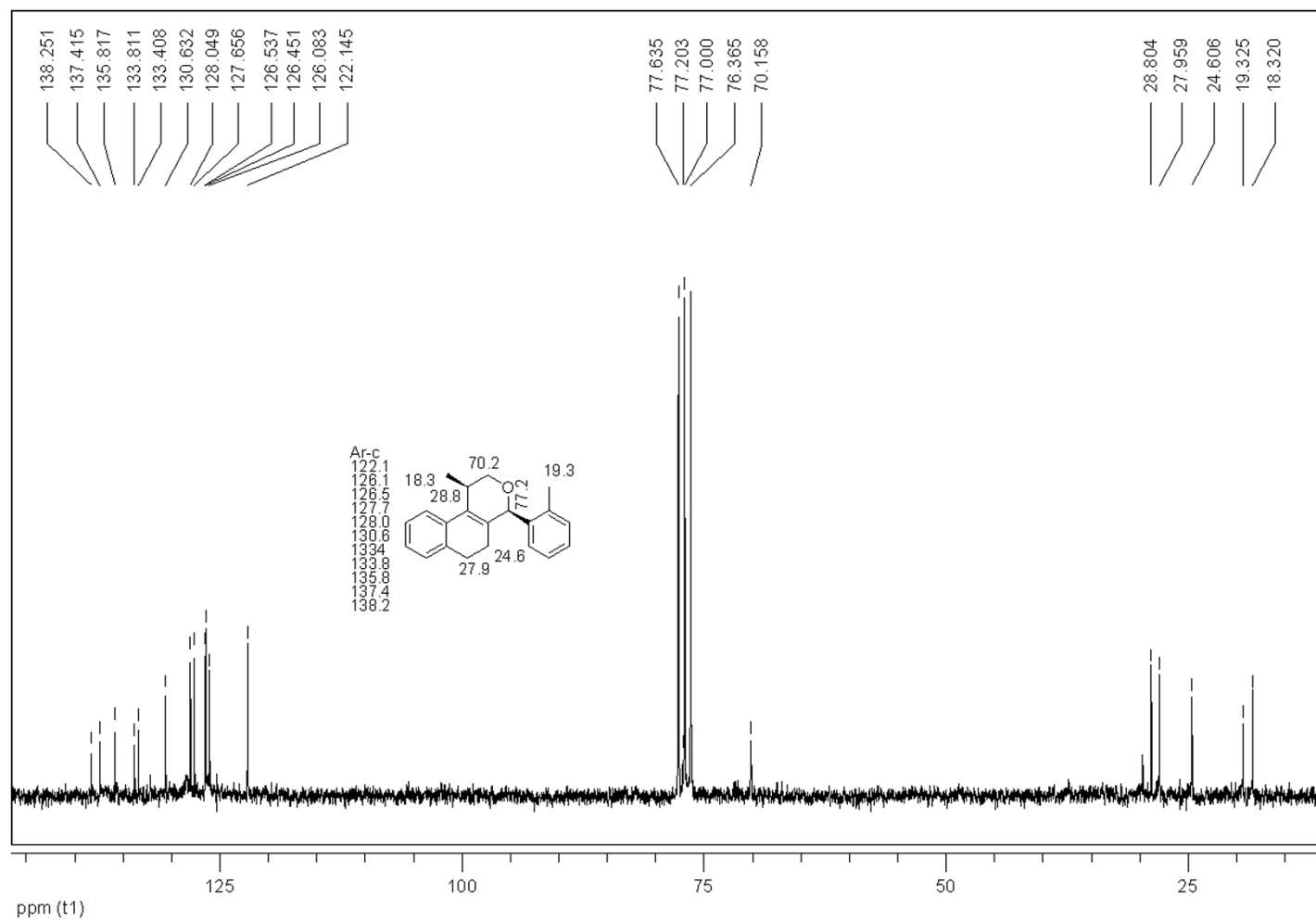
<sup>1</sup>H-NMR of compound **12e** (300 MHz, CDCl<sub>3</sub>)

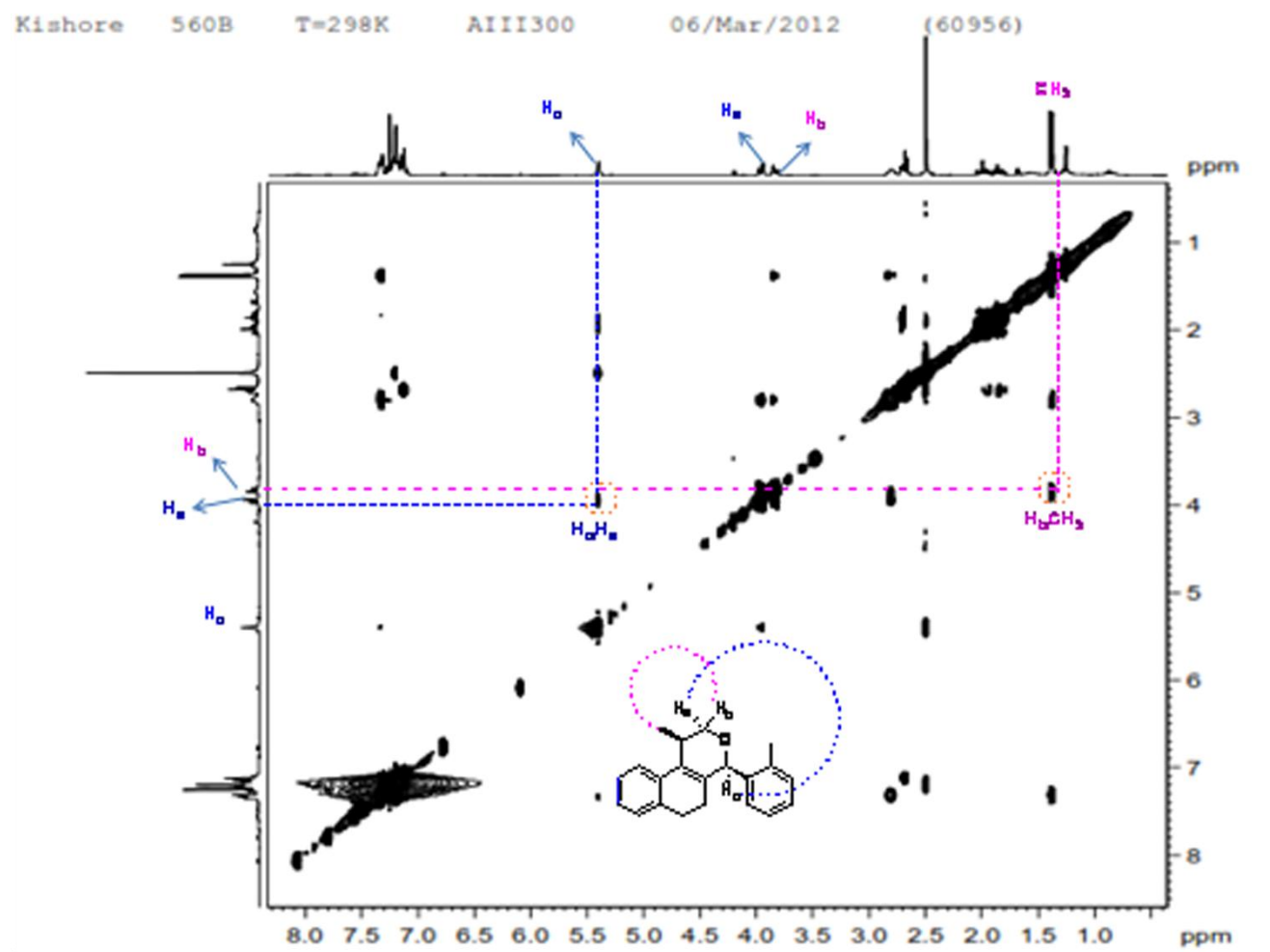


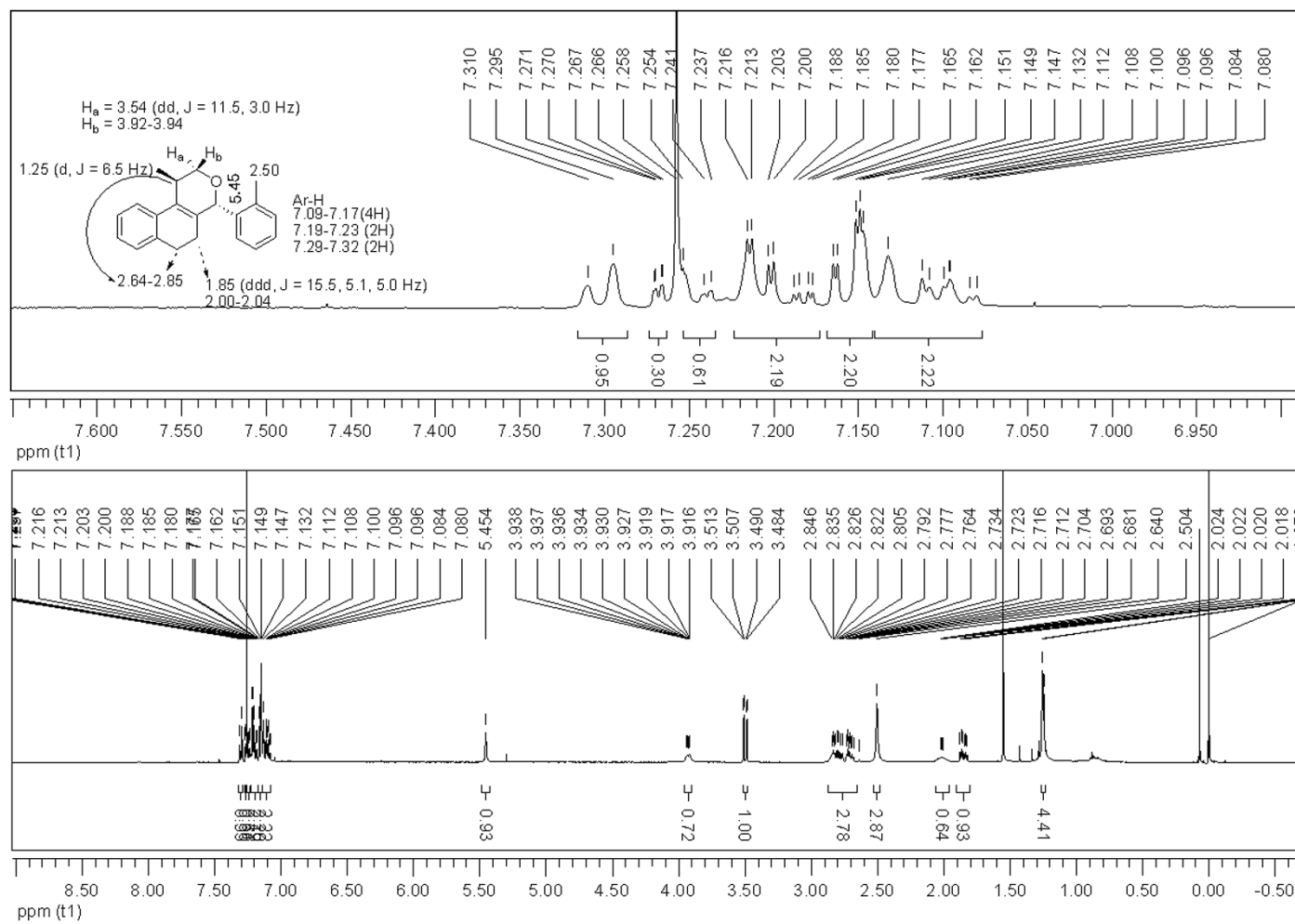
$^{13}\text{C}$ -NMR of compound **12e** (75 MHz,  $\text{CDCl}_3$ )

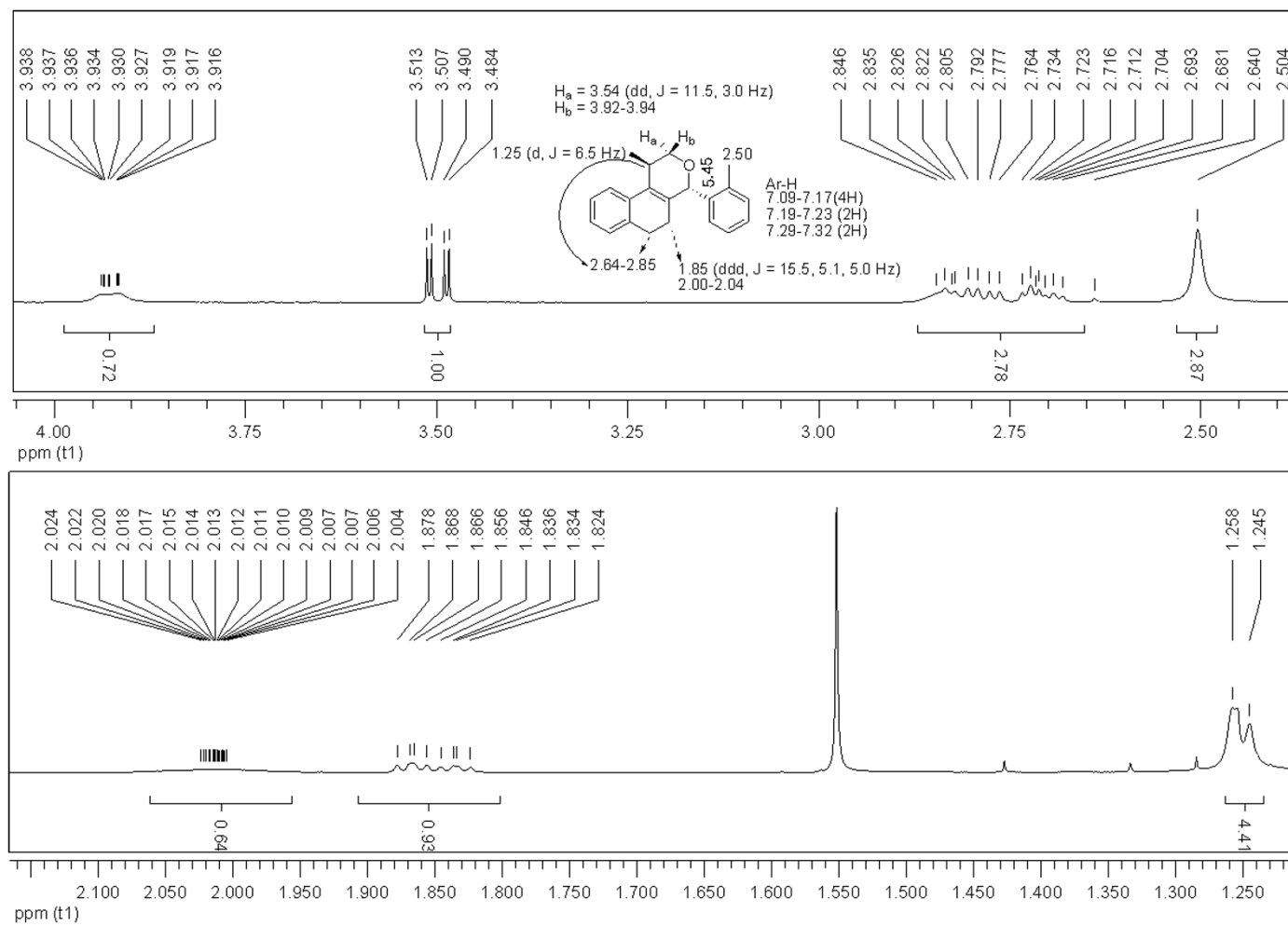
<sup>1</sup>H-NMR of compound *cis-7f* (300 MHz, CDCl<sub>3</sub>)

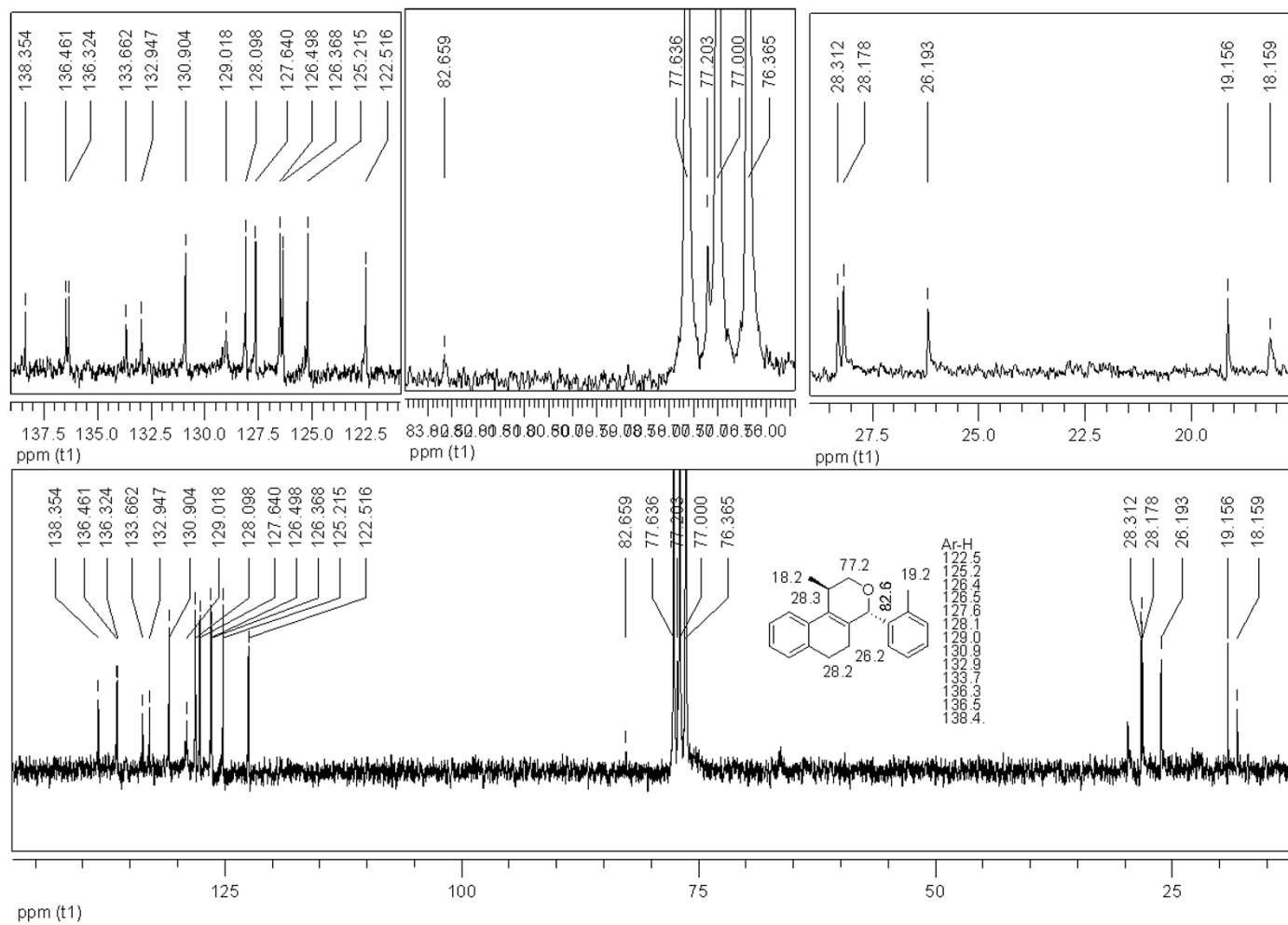
$^1\text{H}$ -NMR of compound *cis*-7f (300 MHz,  $\text{CDCl}_3$ )

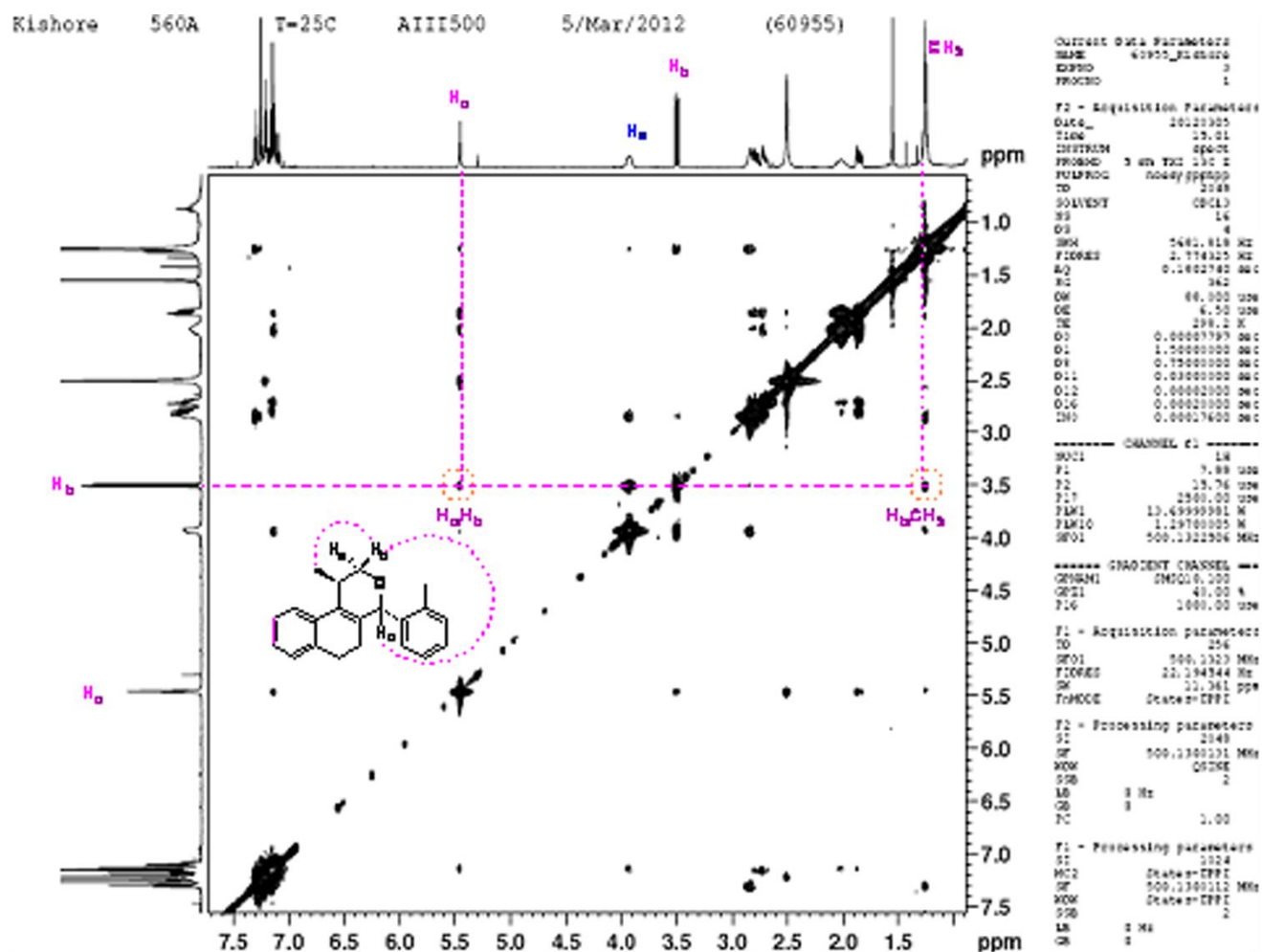
$^{13}\text{C}$ -NMR of compound *cis*-7f (75 MHz,  $\text{CDCl}_3$ )

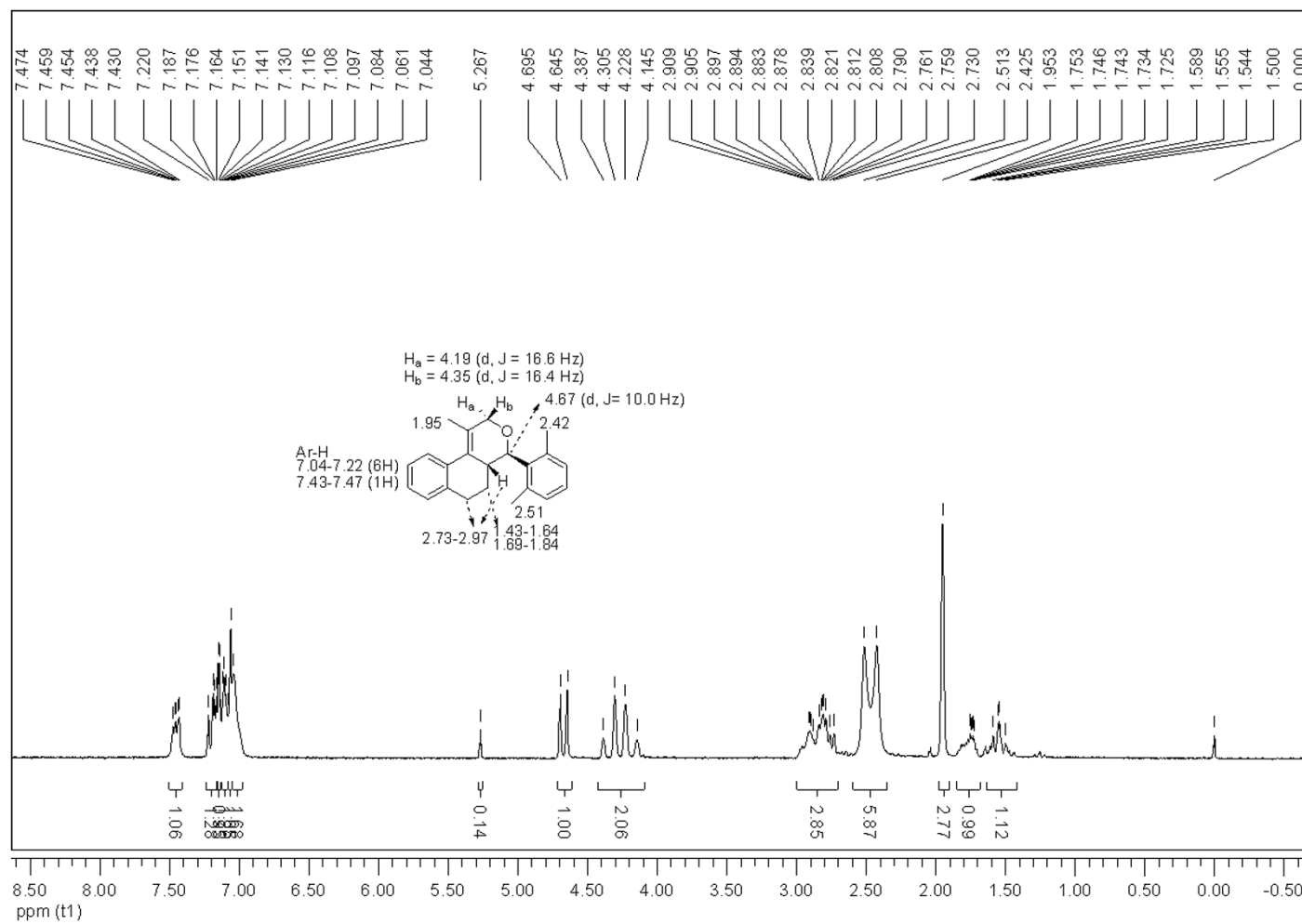
2D NOESY NMR of compound *cis-7f* (300 MHz, CDCl<sub>3</sub>)

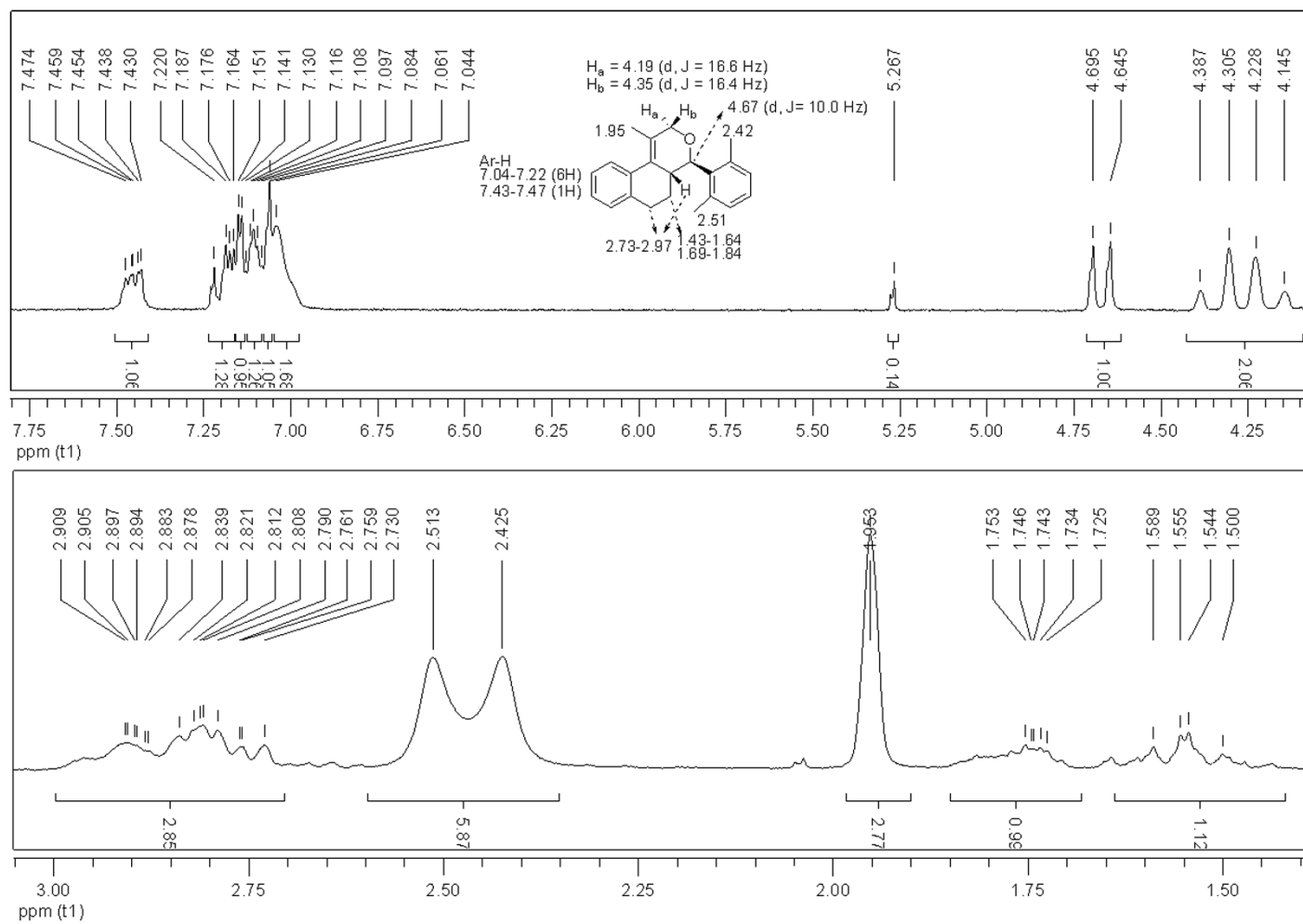
<sup>1</sup>H-NMR of compound *trans*-7f (500 MHz, CDCl<sub>3</sub>)

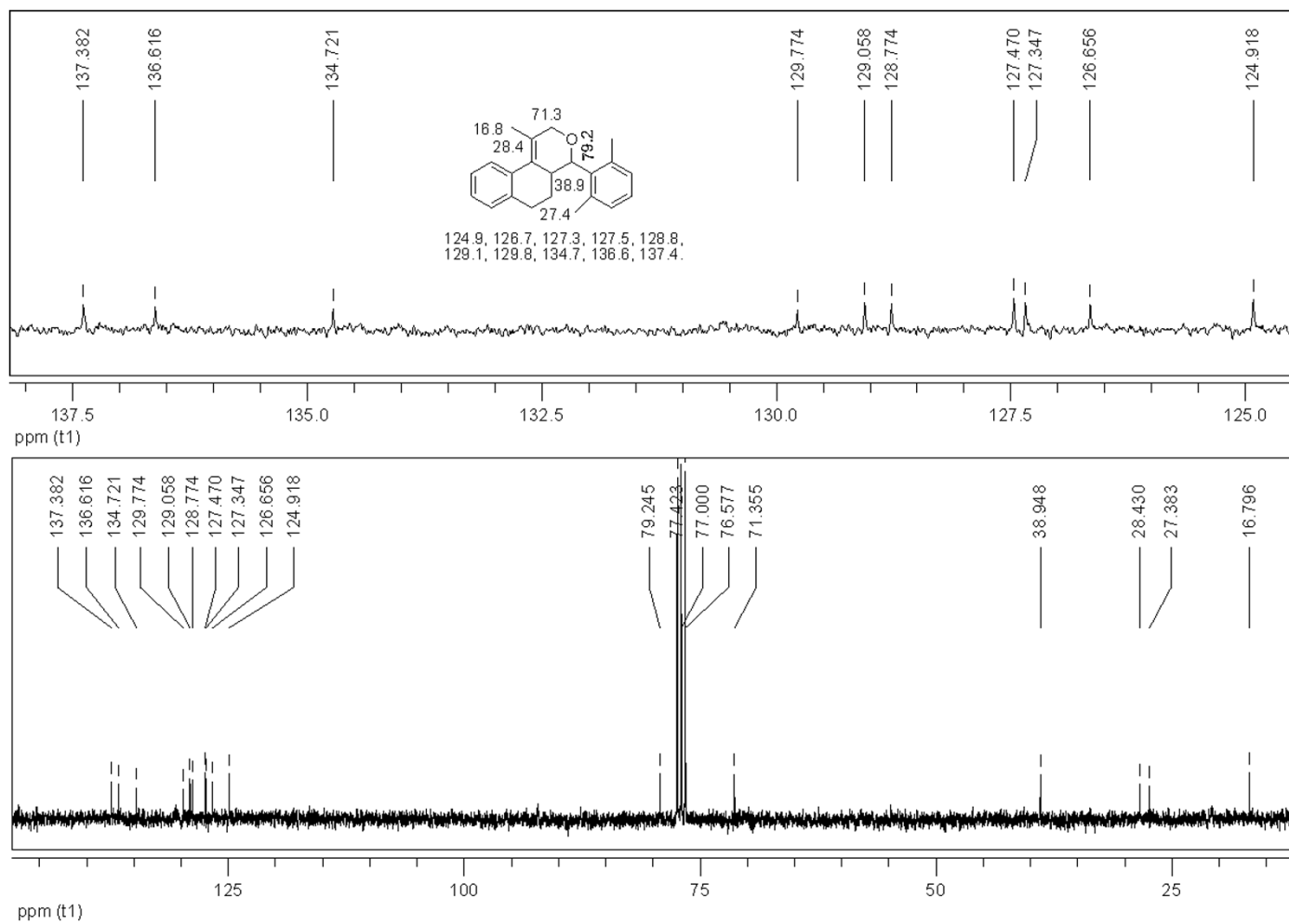
<sup>1</sup>H-NMR of compound *trans*-7f (500 MHz, CDCl<sub>3</sub>)

$^{13}\text{C}$ -NMR of compound *trans*-7f (75 MHz,  $\text{CDCl}_3$ )

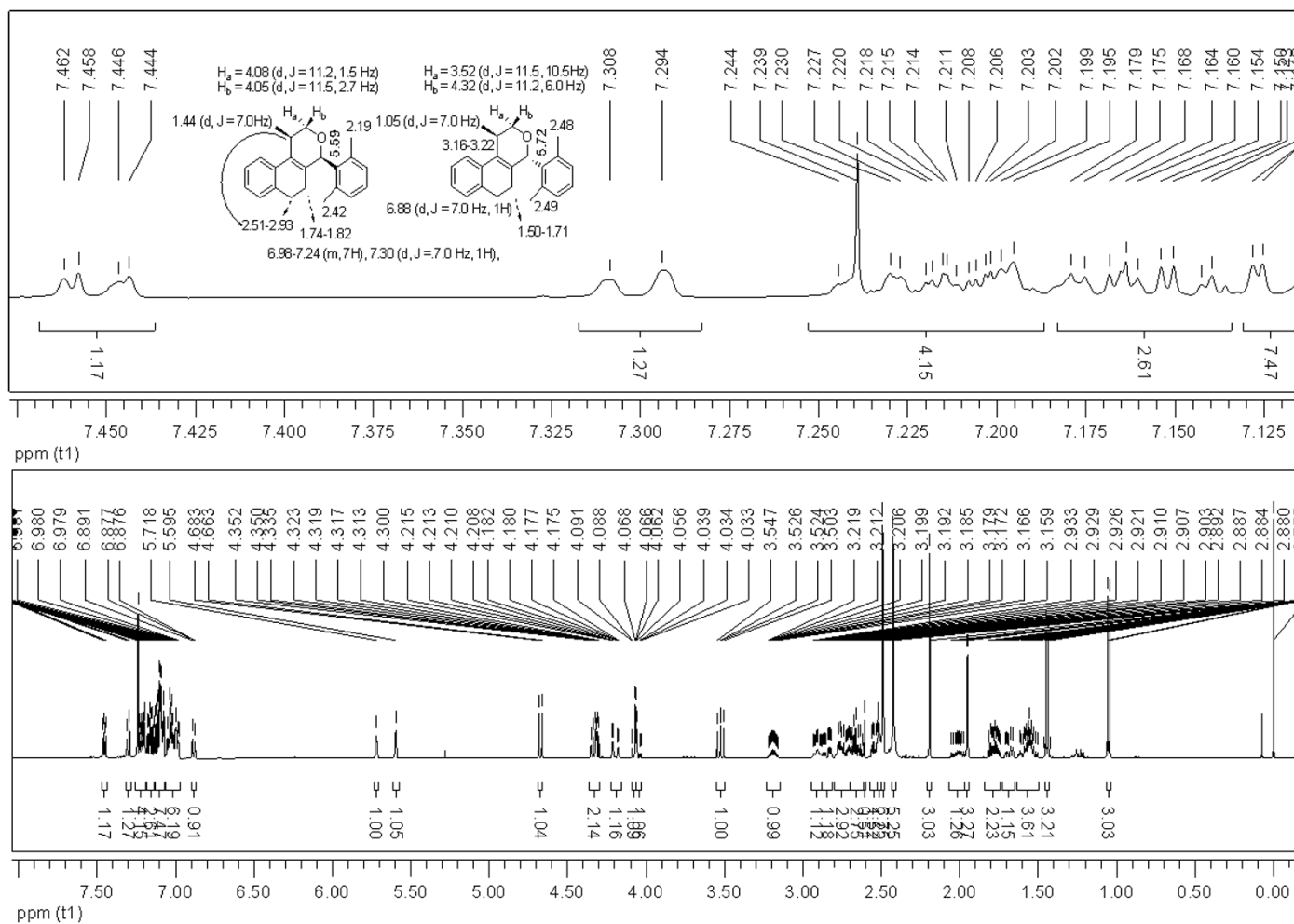
2D NOESY NMR of compound *trans*-7f (500 MHz, CDCl<sub>3</sub>)

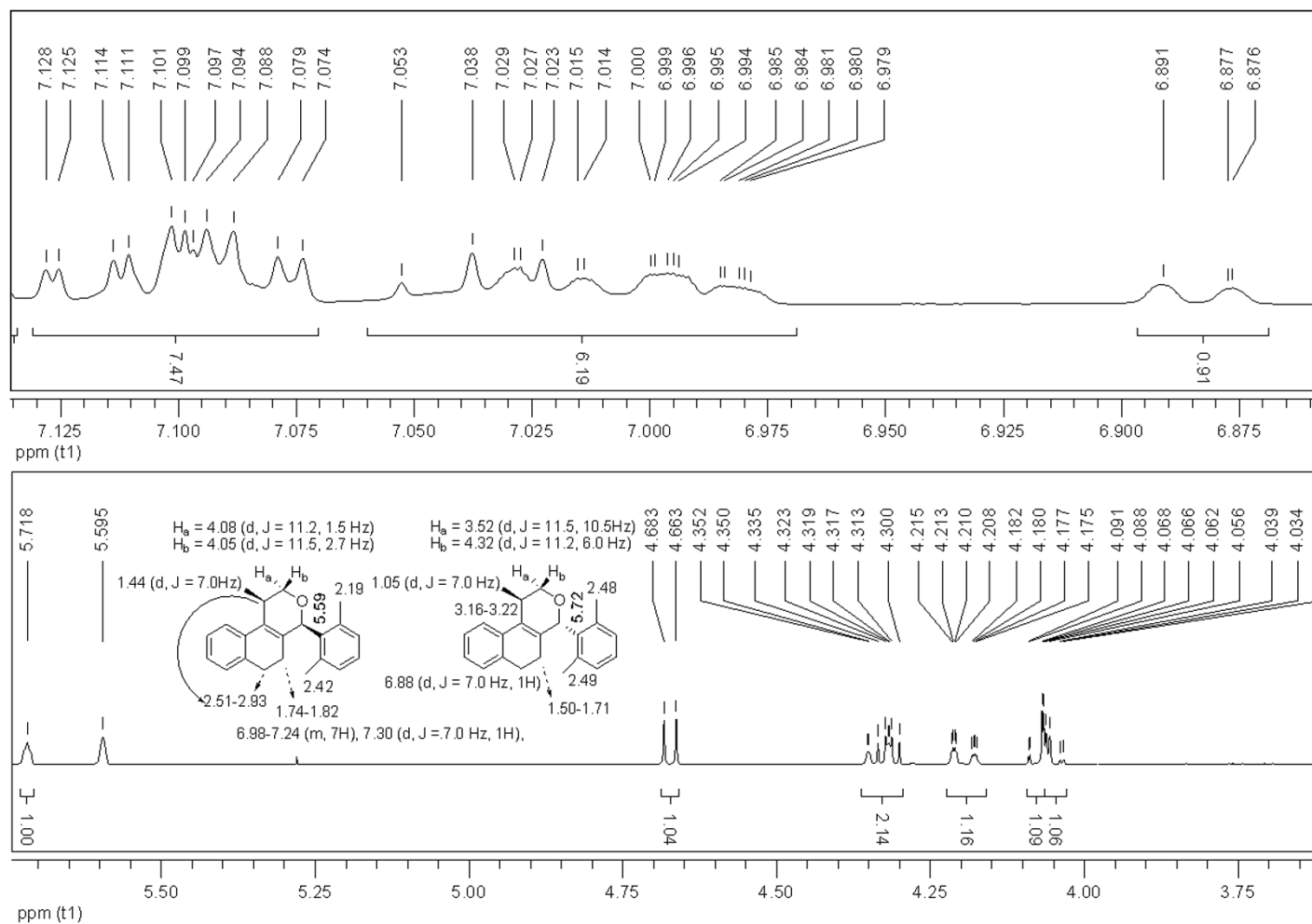
<sup>1</sup>H-NMR of compound **12g** (200 MHz, CDCl<sub>3</sub>)

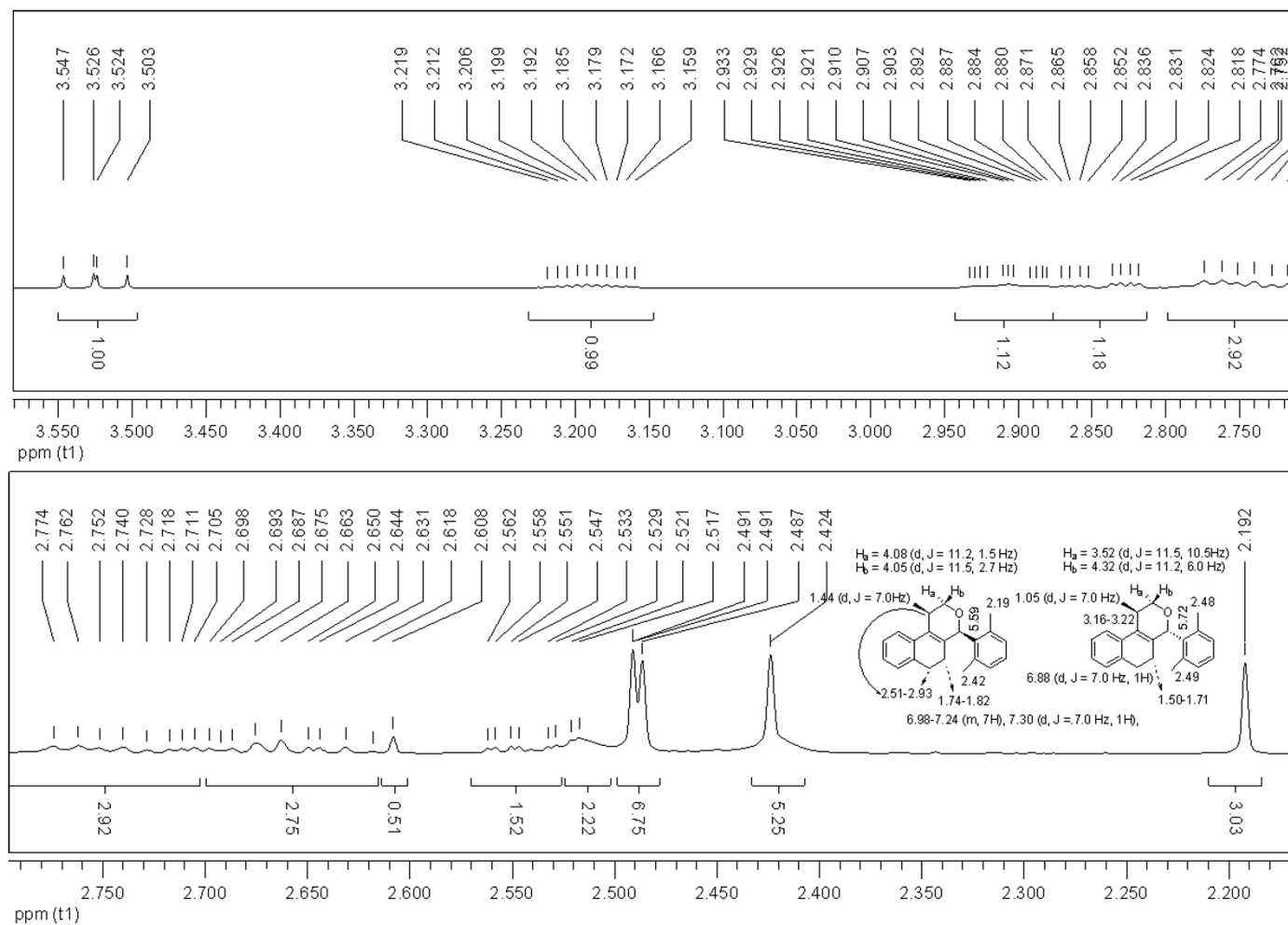
$^1\text{H}$ -NMR of compound **12g** (200 MHz,  $\text{CDCl}_3$ )

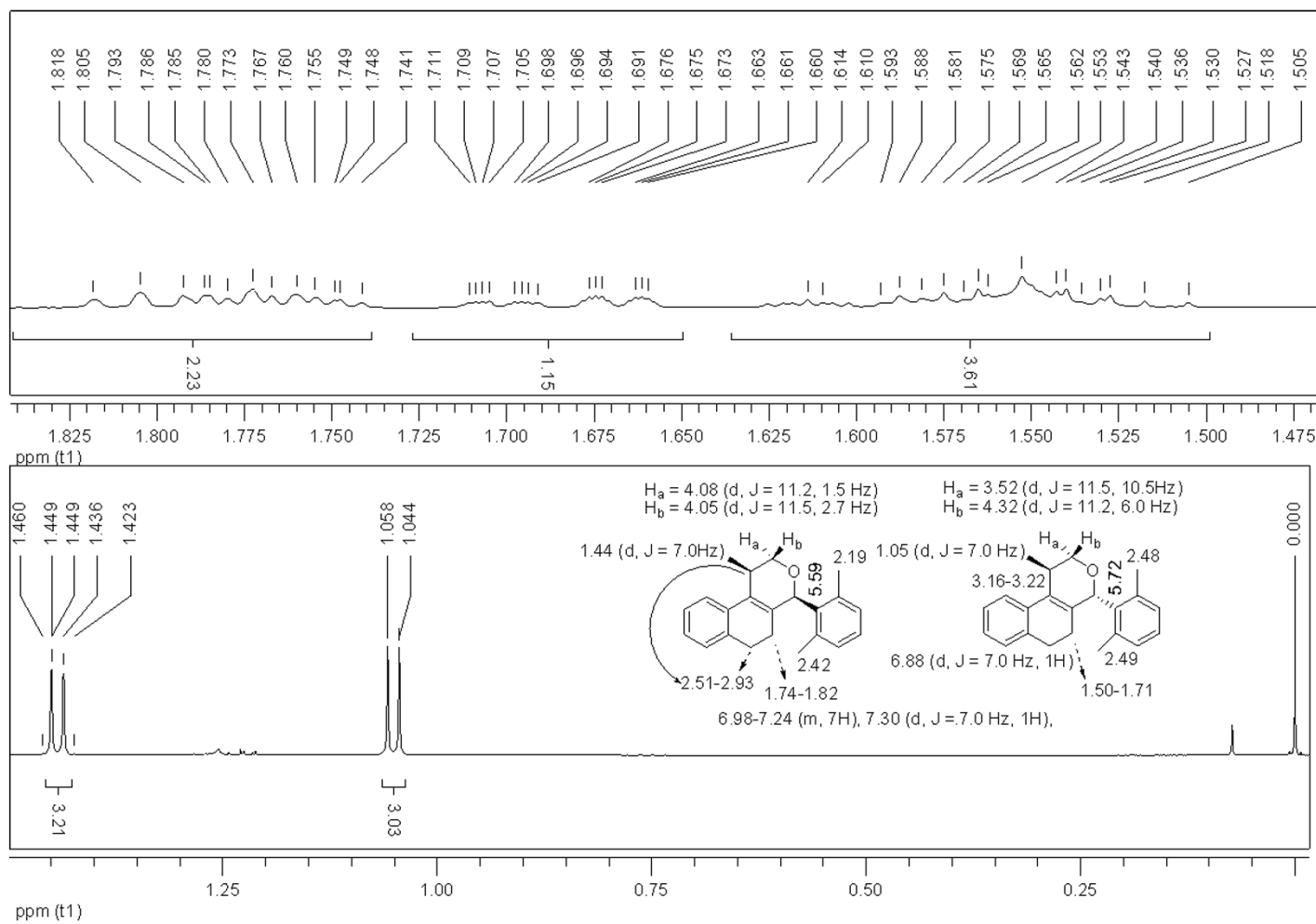
$^{13}\text{C}$ -NMR of compound **12g** (75 MHz,  $\text{CDCl}_3$ )

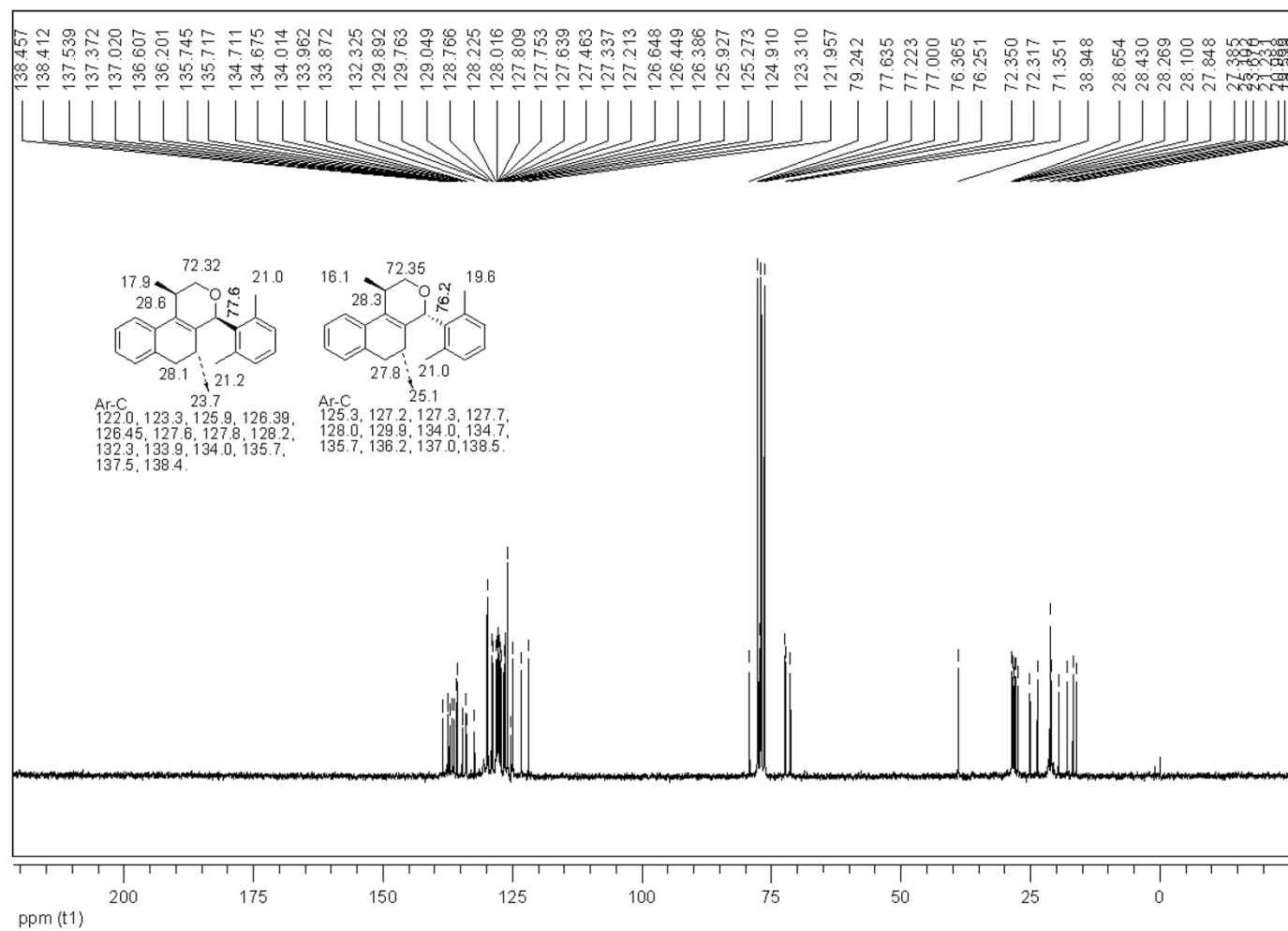
<sup>1</sup>H-NMR of compounds *cis*-**7g** and *trans*-**7g** (500 MHz, CDCl<sub>3</sub>)

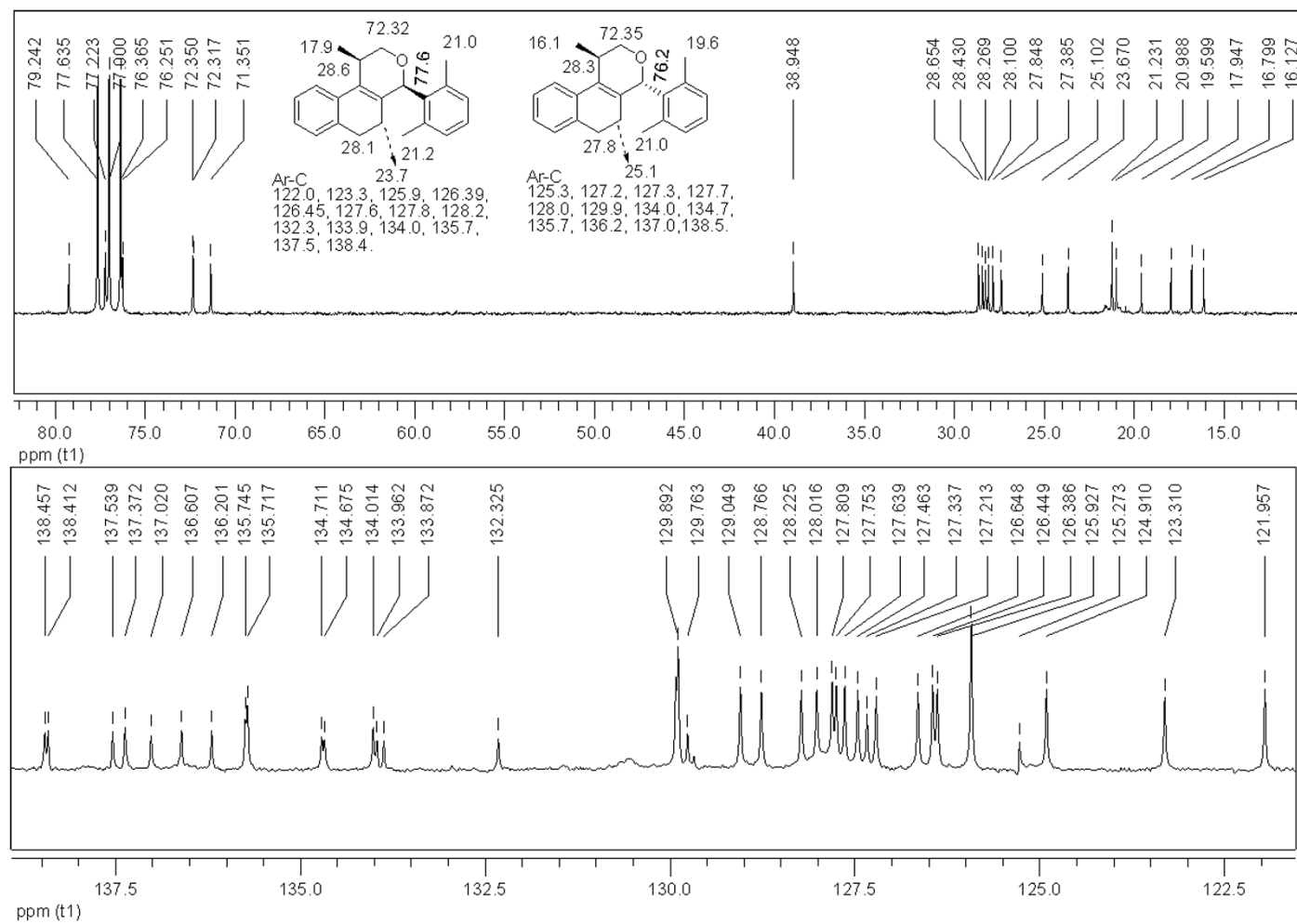


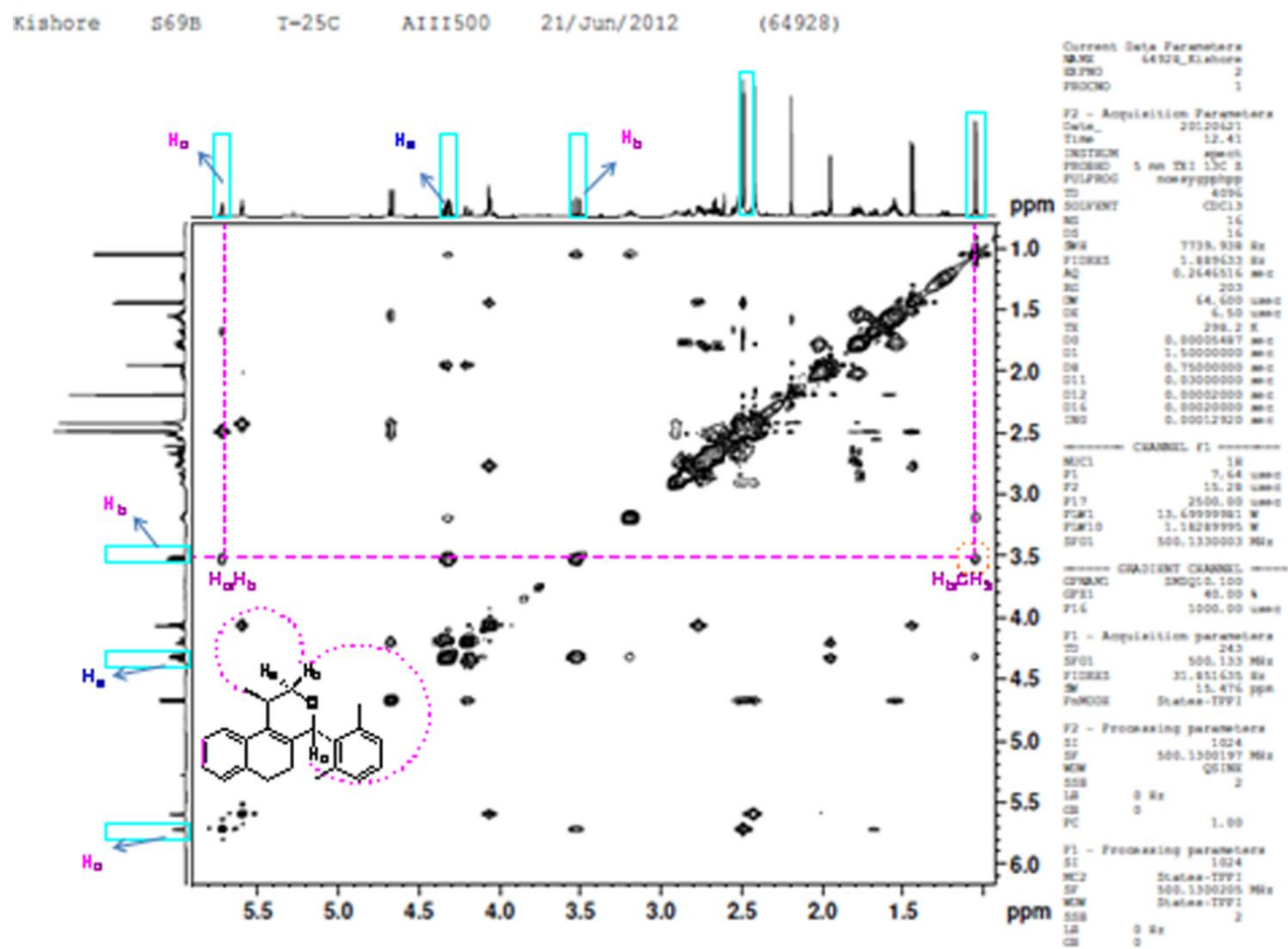
$^1\text{H}$ -NMR of compounds *cis*-**7g** and *trans*-**7g** (300 MHz,  $\text{CDCl}_3$ )

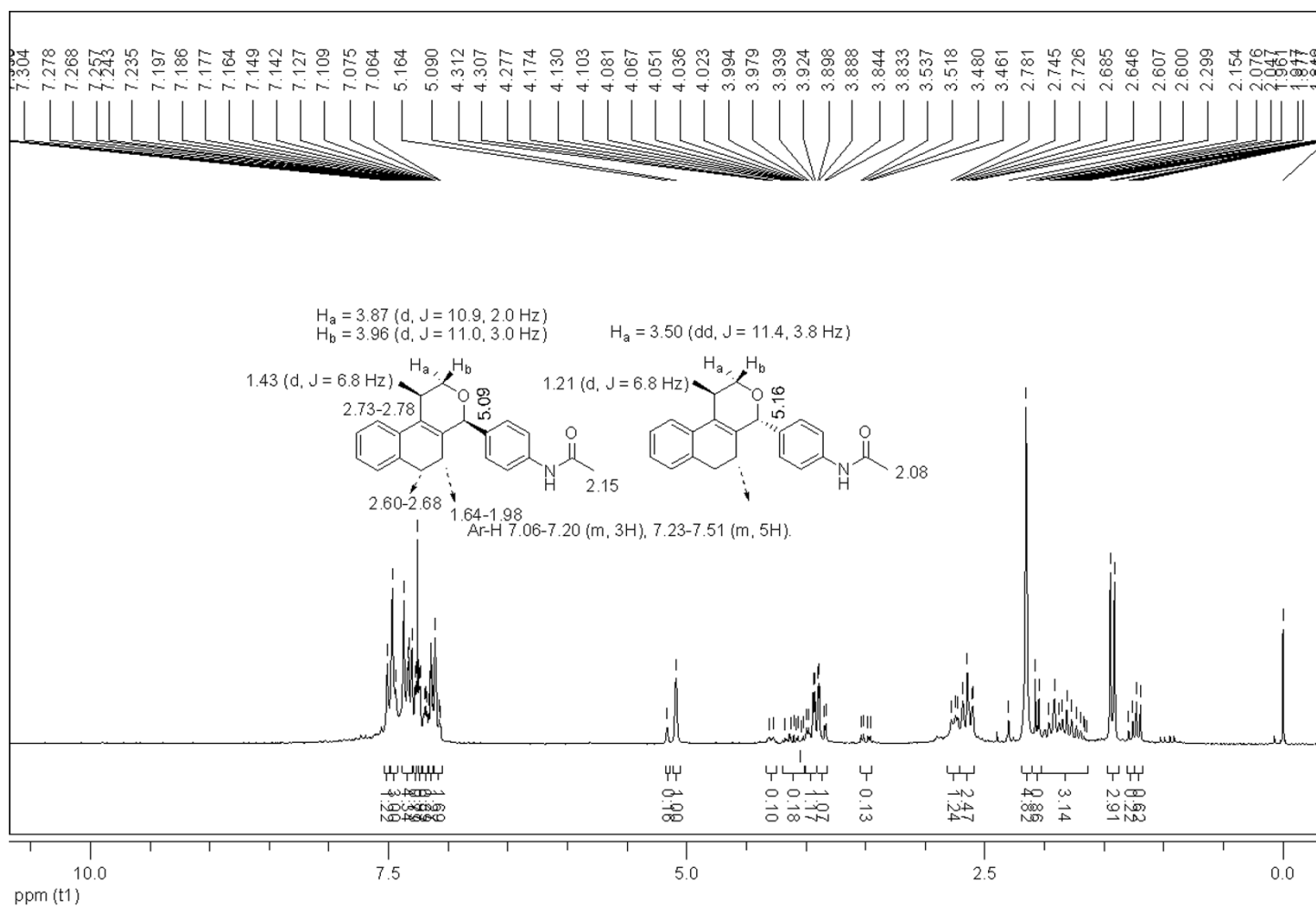
$^1\text{H}$ -NMR of compounds *cis*-**7g** and *trans*-**7g** (500 MHz,  $\text{CDCl}_3$ )

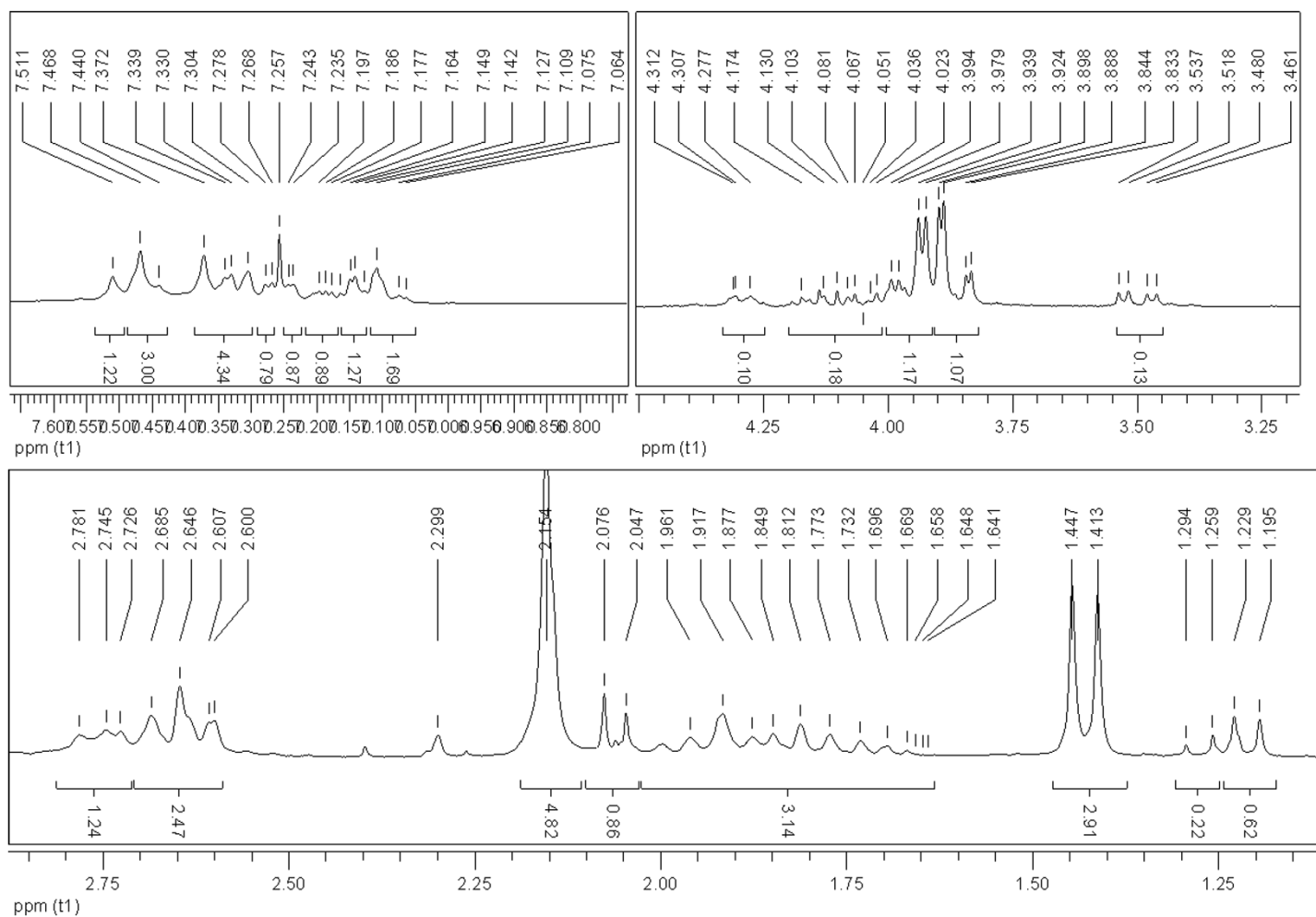
$^1\text{H}$ -NMR of compounds *cis*-**7g** and *trans*-**7g** (500 MHz,  $\text{CDCl}_3$ )

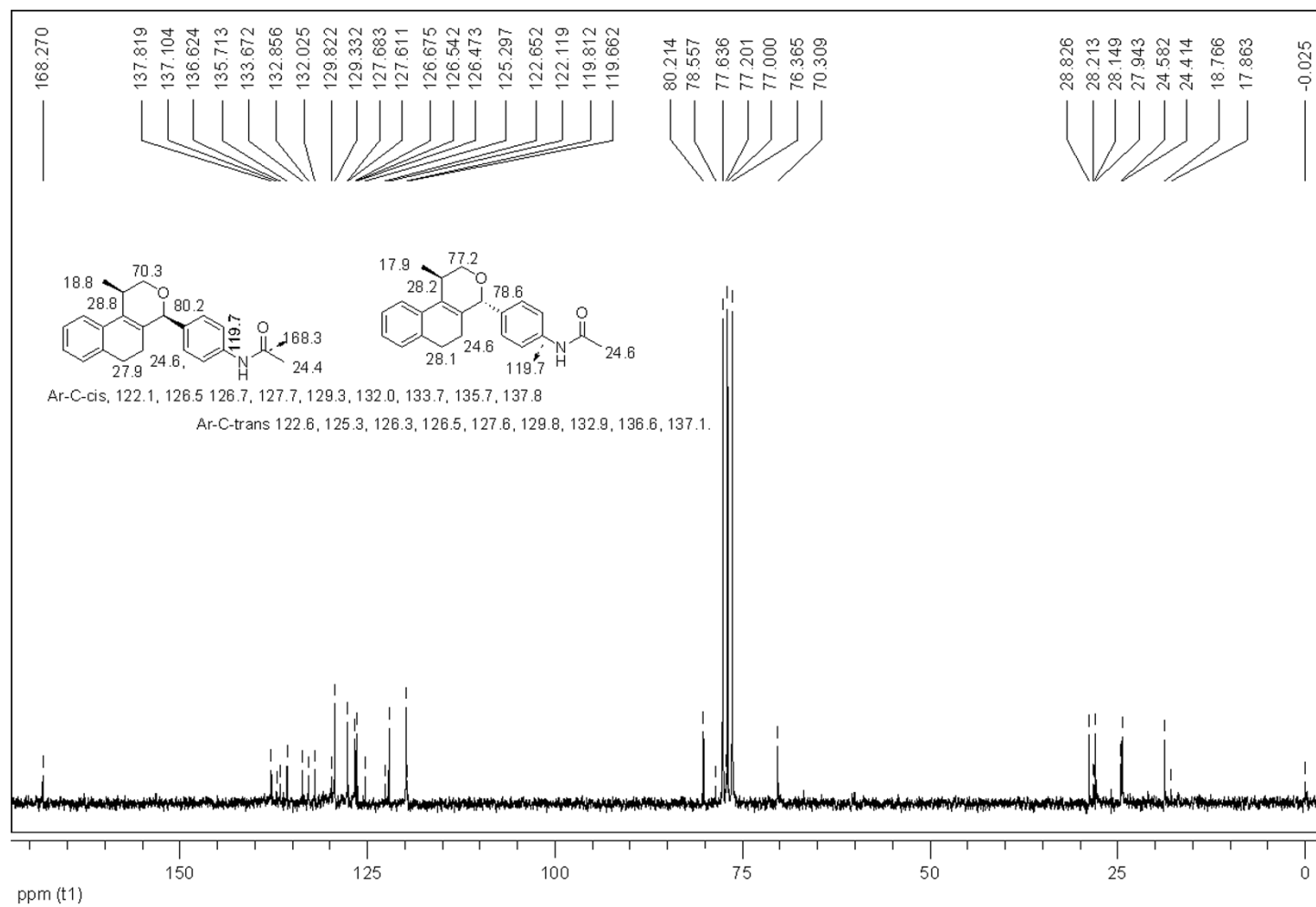
$^{13}\text{C}$ -NMR of compounds *cis*-7g and *trans*-7g (50 MHz,  $\text{CDCl}_3$ )

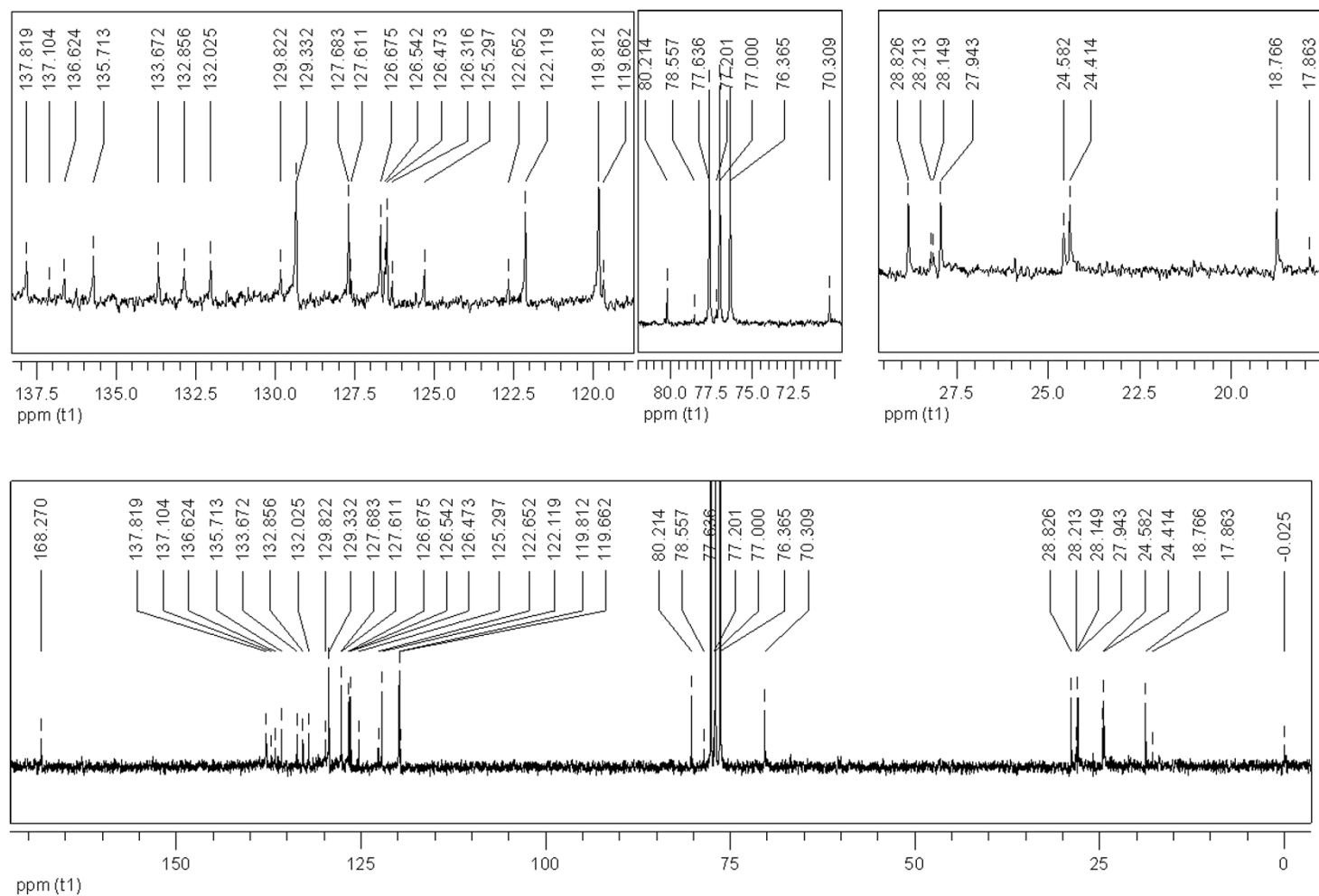
$^{13}\text{C}$ -NMR of compounds *cis*-7g and *trans*-7g (50 MHz,  $\text{CDCl}_3$ )

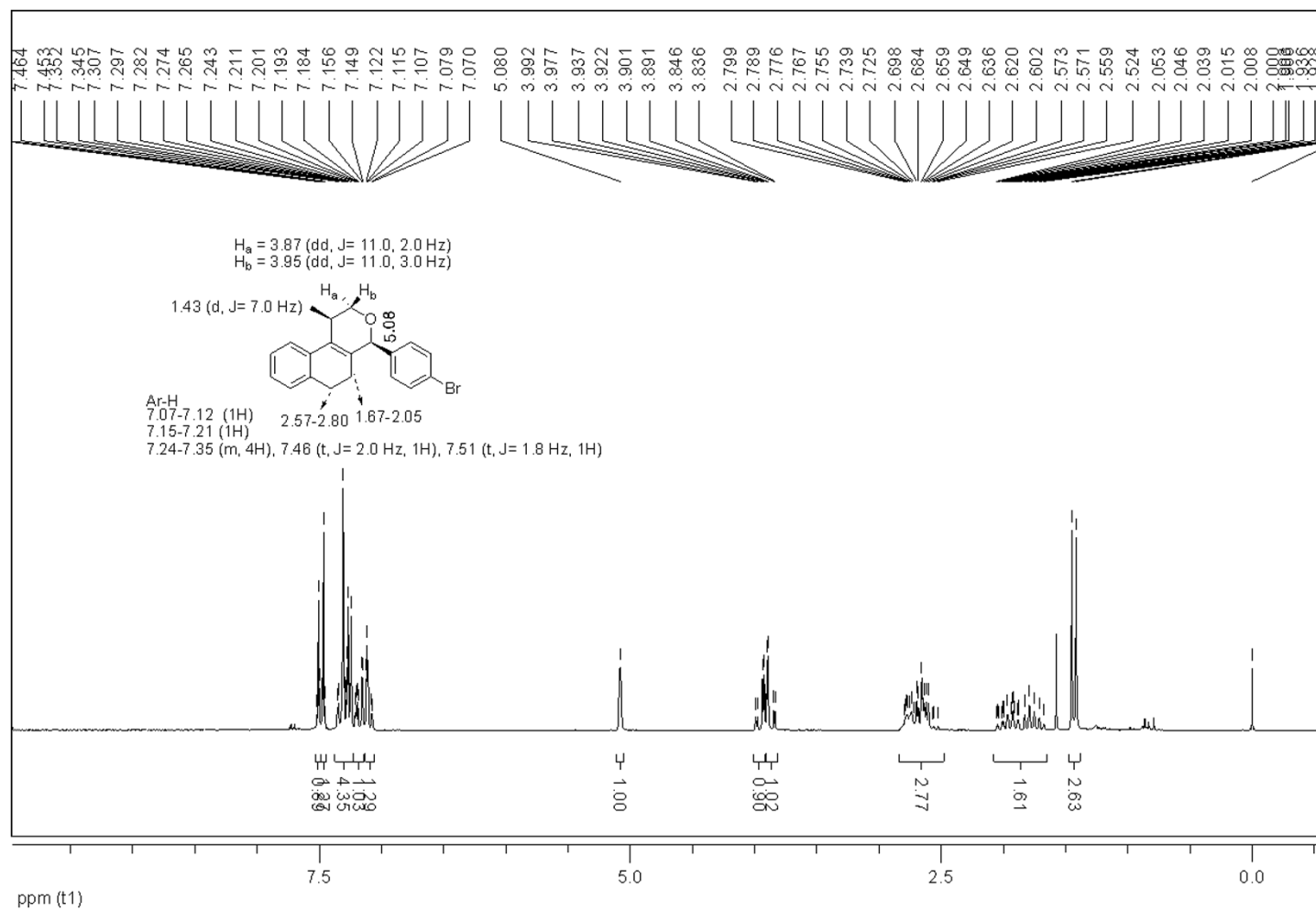
2D NOESY NMR of compound *cis*-7g (500 MHz, CDCl<sub>3</sub>)

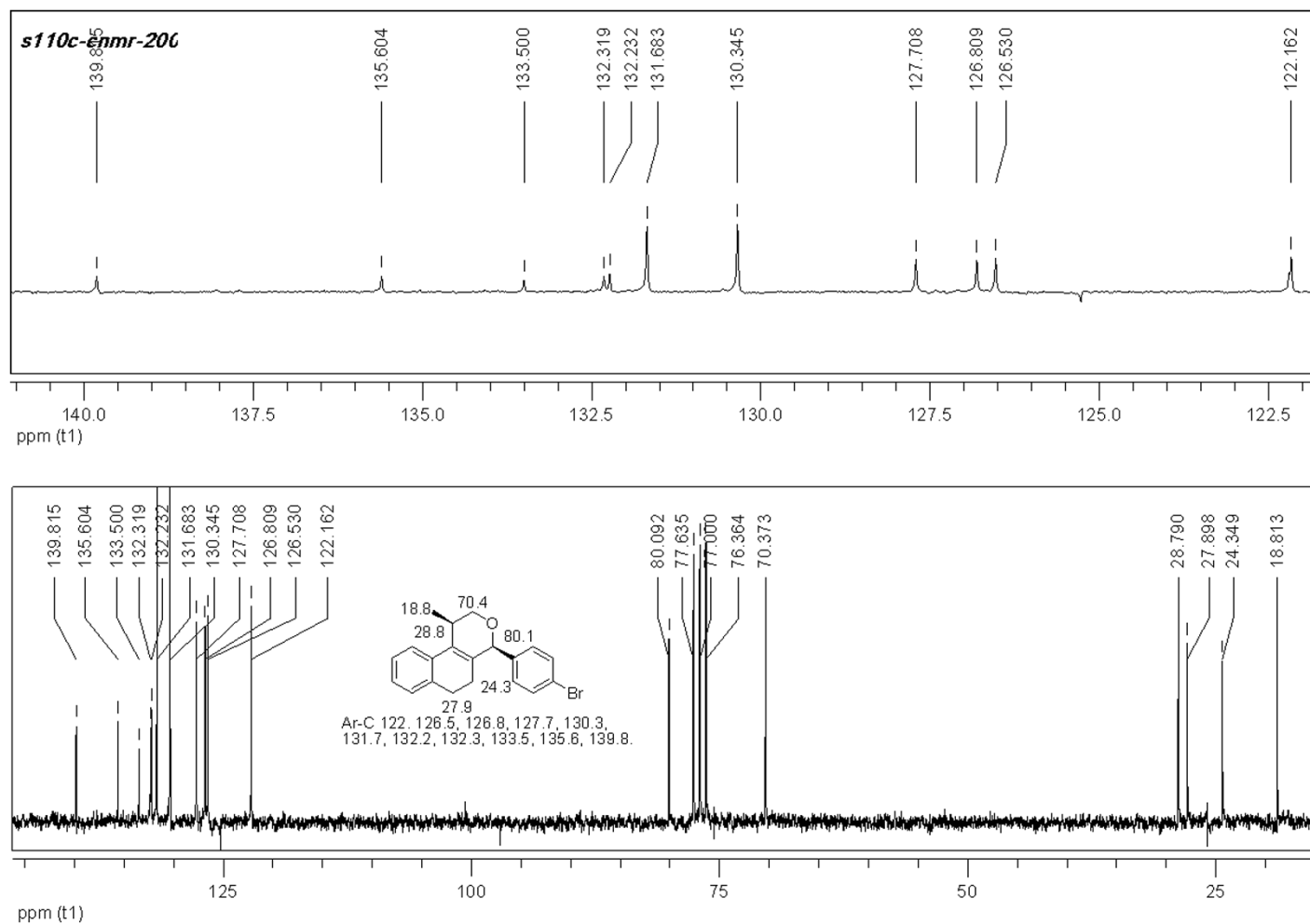
$^1\text{H}$ -NMR of compounds *cis*-**7i** and *trans*-**7i** (200 MHz,  $\text{CDCl}_3$ )

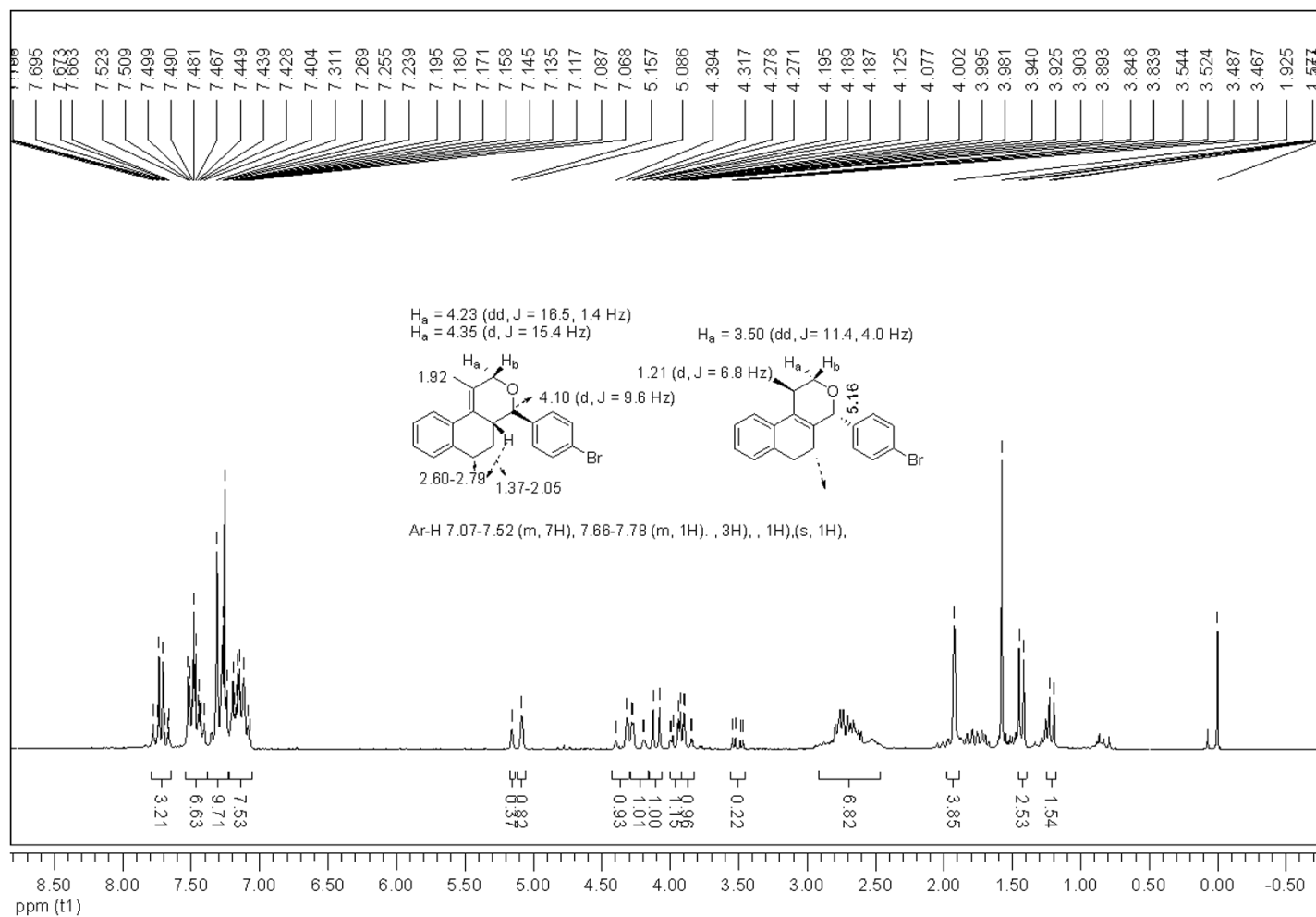
<sup>1</sup>H-NMR of compounds *cis-7i* and *trans-7i* (200 MHz, CDCl<sub>3</sub>)

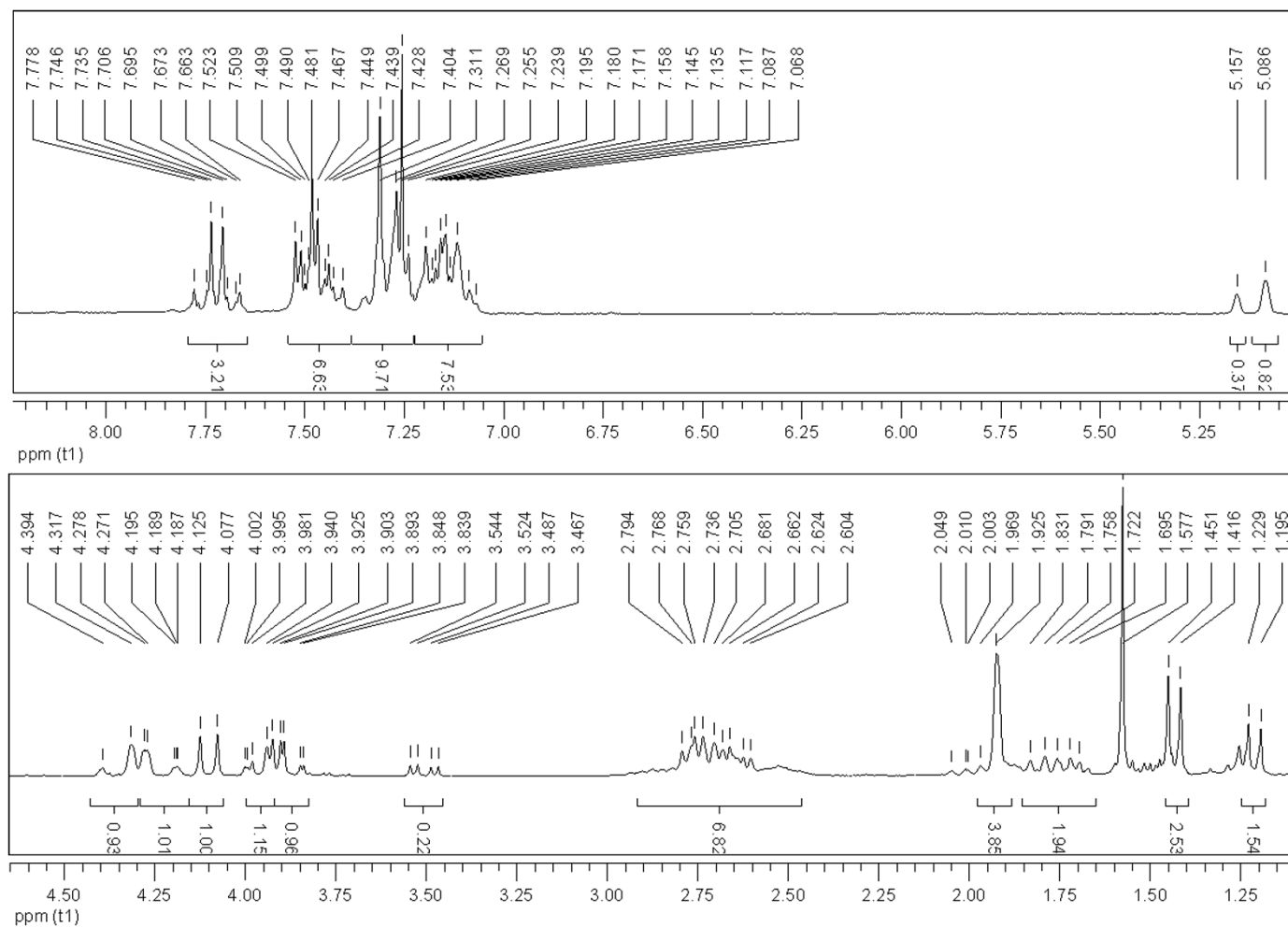
$^{13}\text{C}$ -NMR of compounds *cis*-**7i** and *trans*-**7i** (75 MHz,  $\text{CDCl}_3$ )

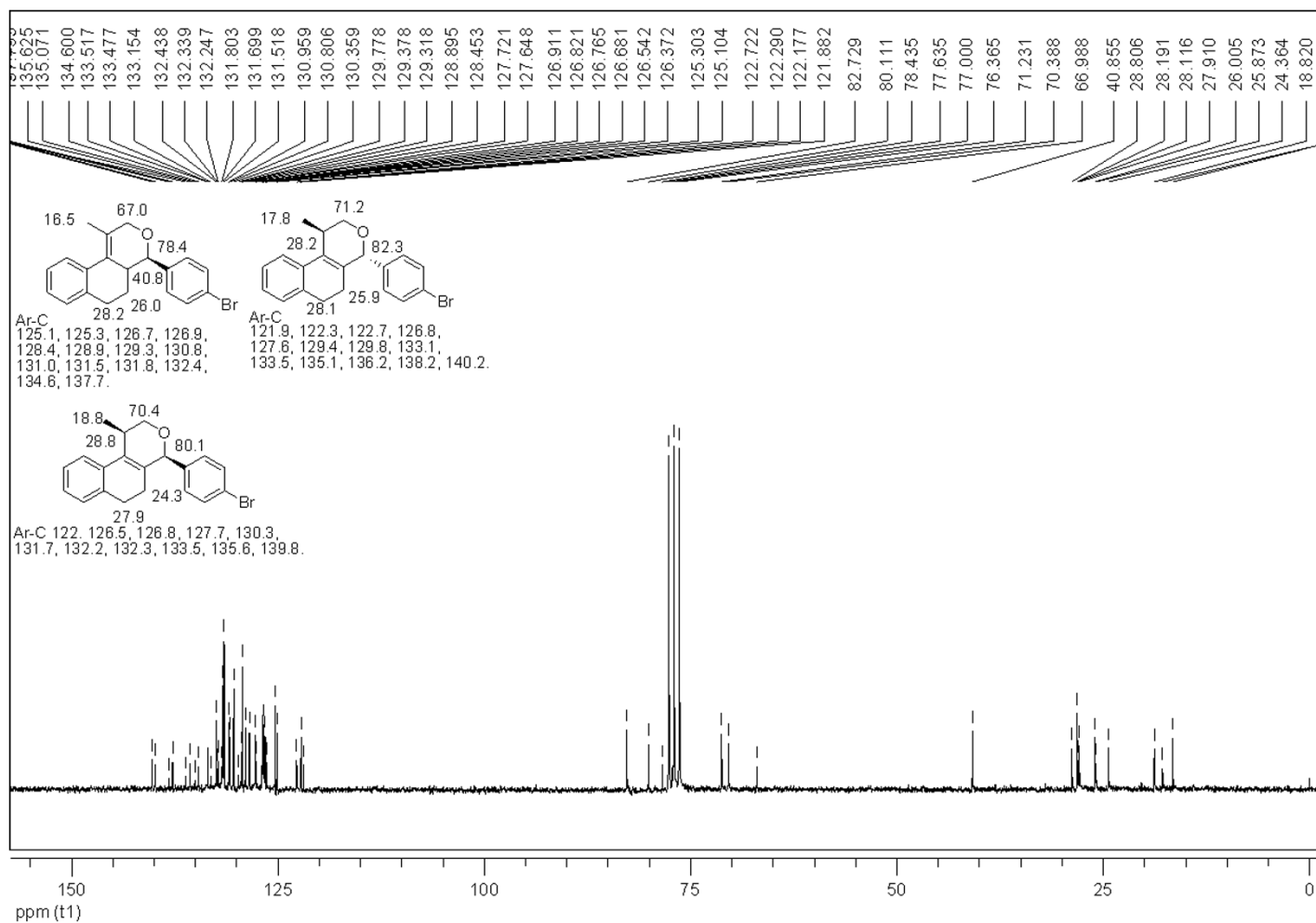
$^{13}\text{C}$ -NMR of compounds *cis*-**7i** and *trans*-**7i** (75 MHz,  $\text{CDCl}_3$ )

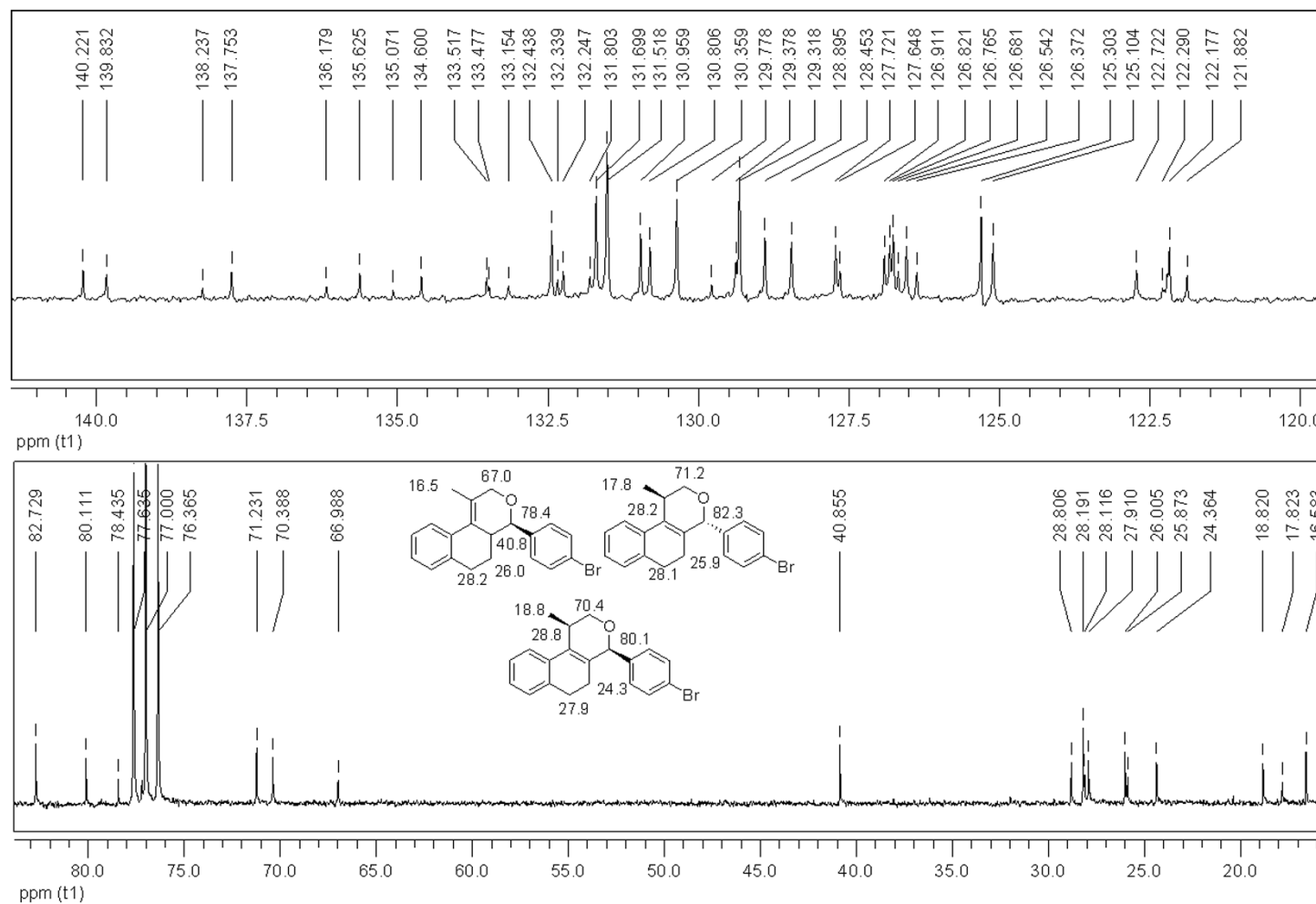
<sup>1</sup>H-NMR of compound *cis*-7j (200 MHz, CDCl<sub>3</sub>)

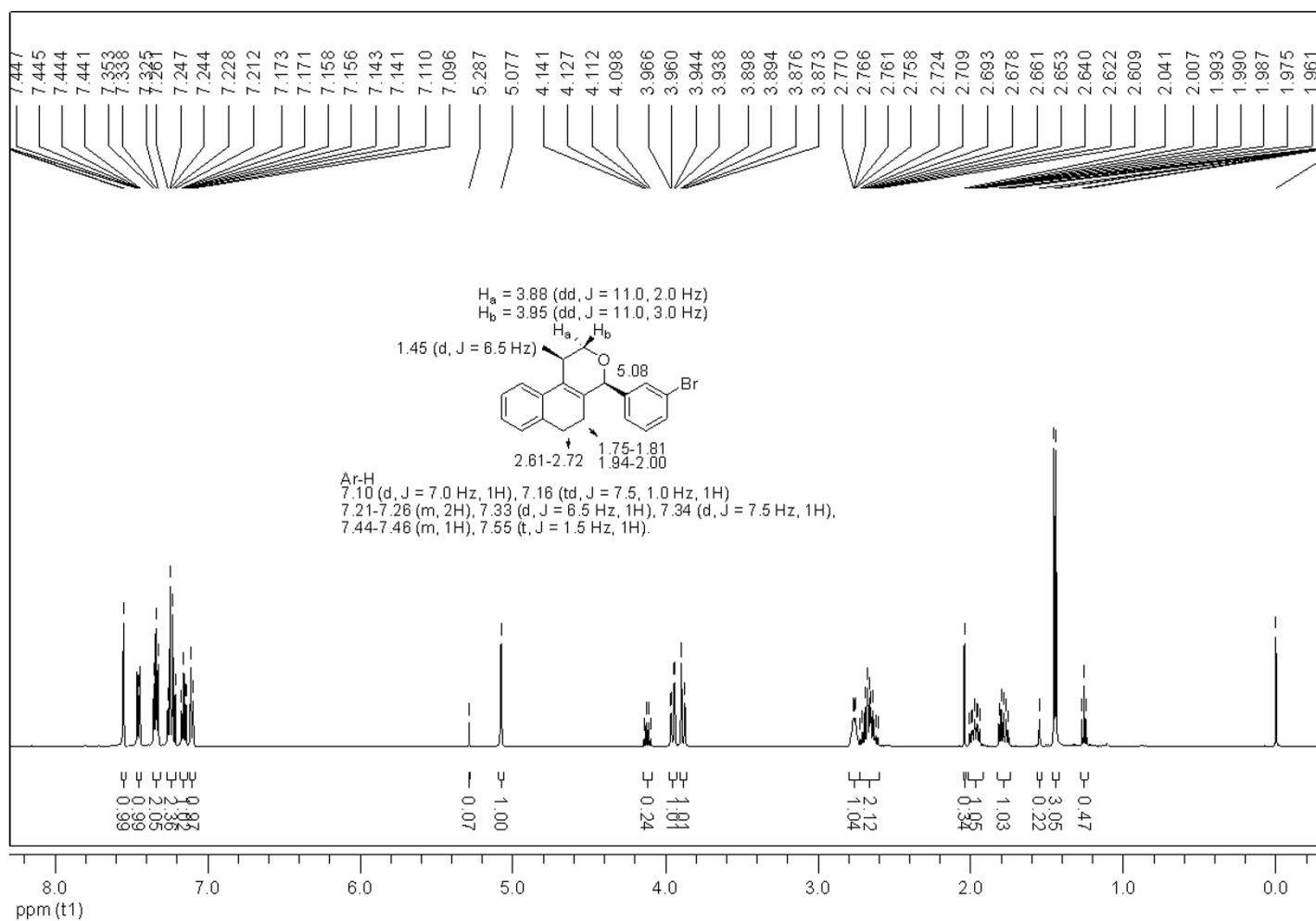
$^{13}\text{C}$ -NMR of compound *cis*-7j (50 MHz,  $\text{CDCl}_3$ )

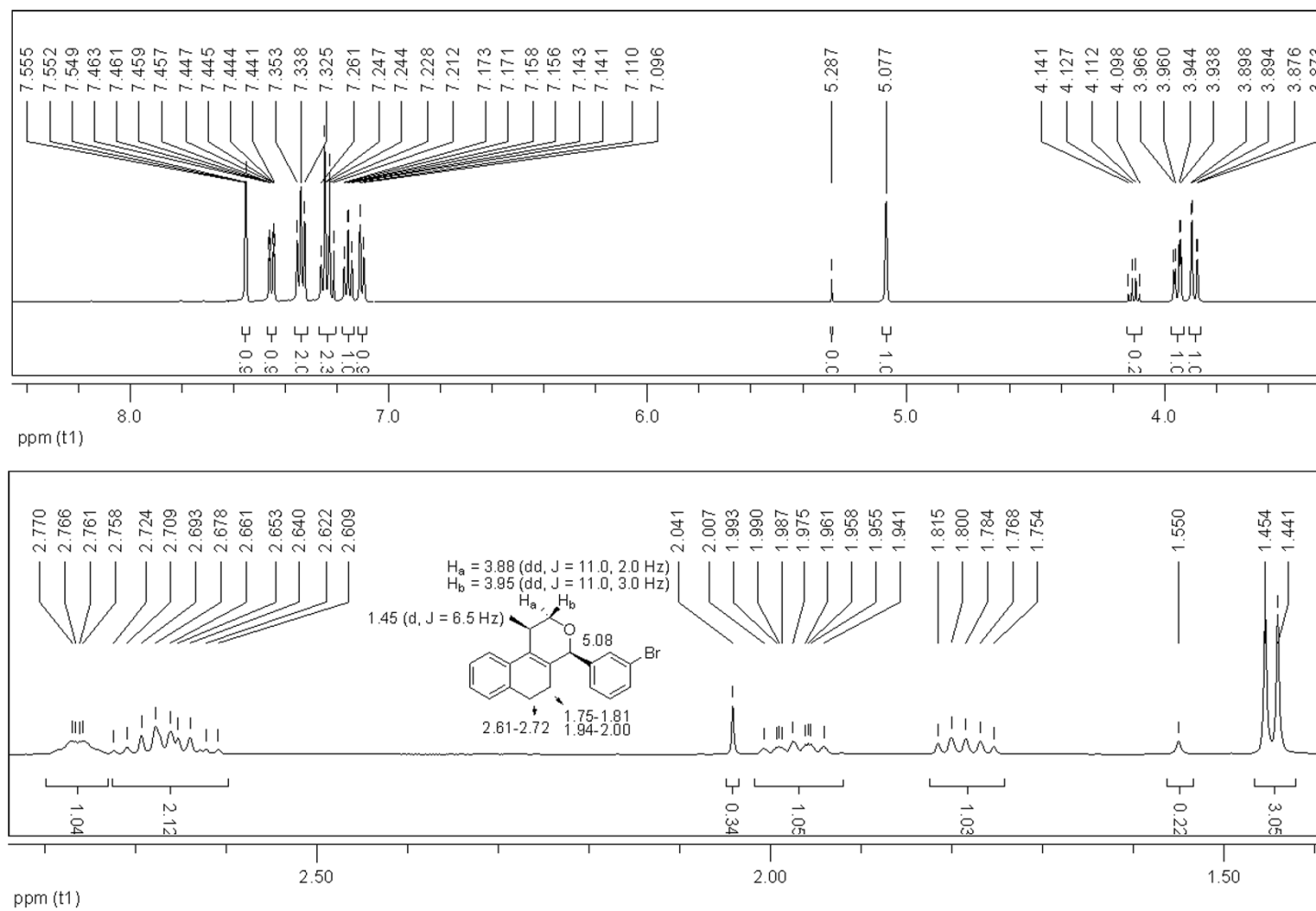
$^1\text{H}$ -NMR of compounds **12j** and *trans*-**7j** (200 MHz,  $\text{CDCl}_3$ )

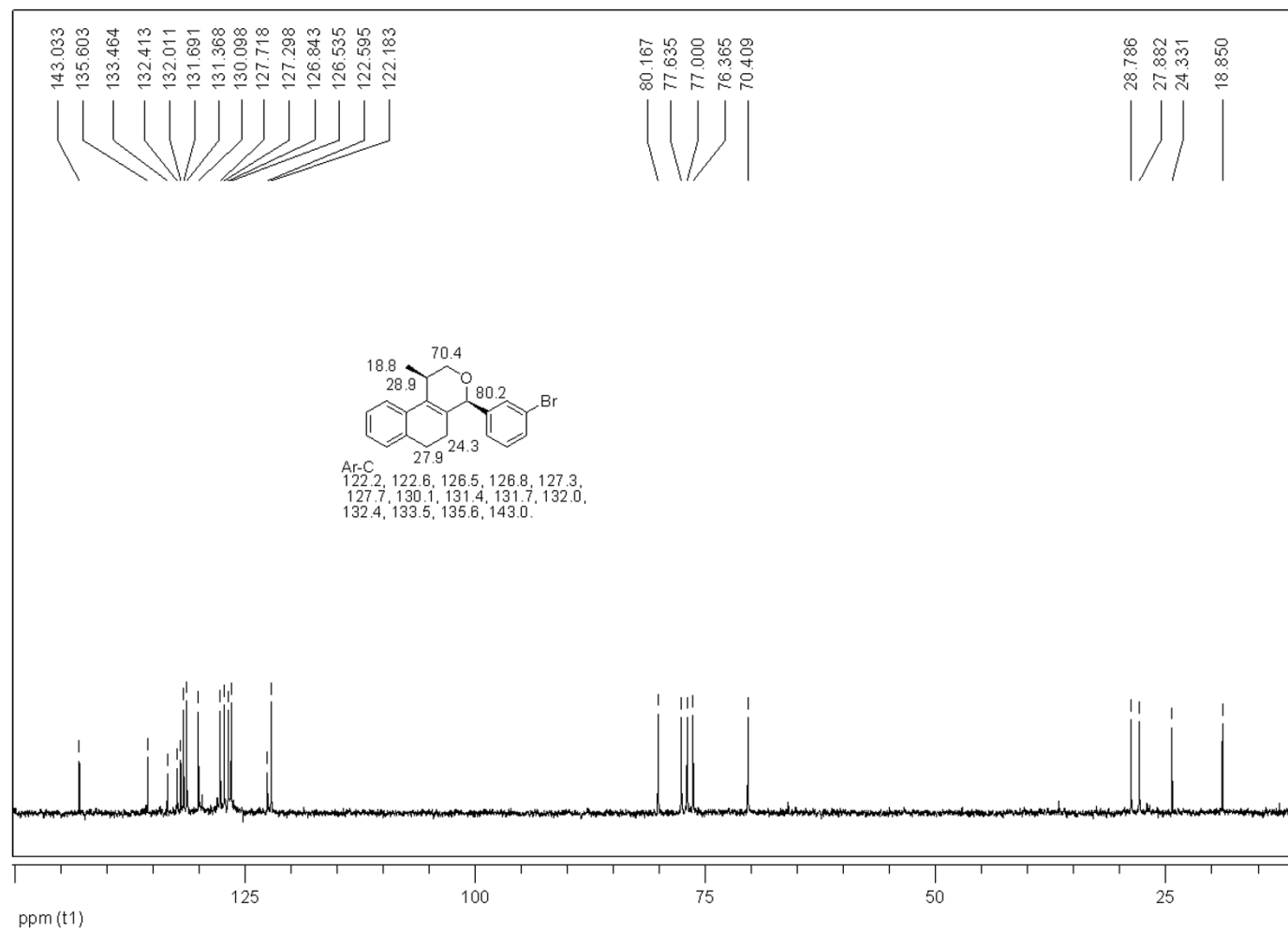
$^1\text{H}$ -NMR of compounds **12j** and *trans*-**7j** (200 MHz,  $\text{CDCl}_3$ )

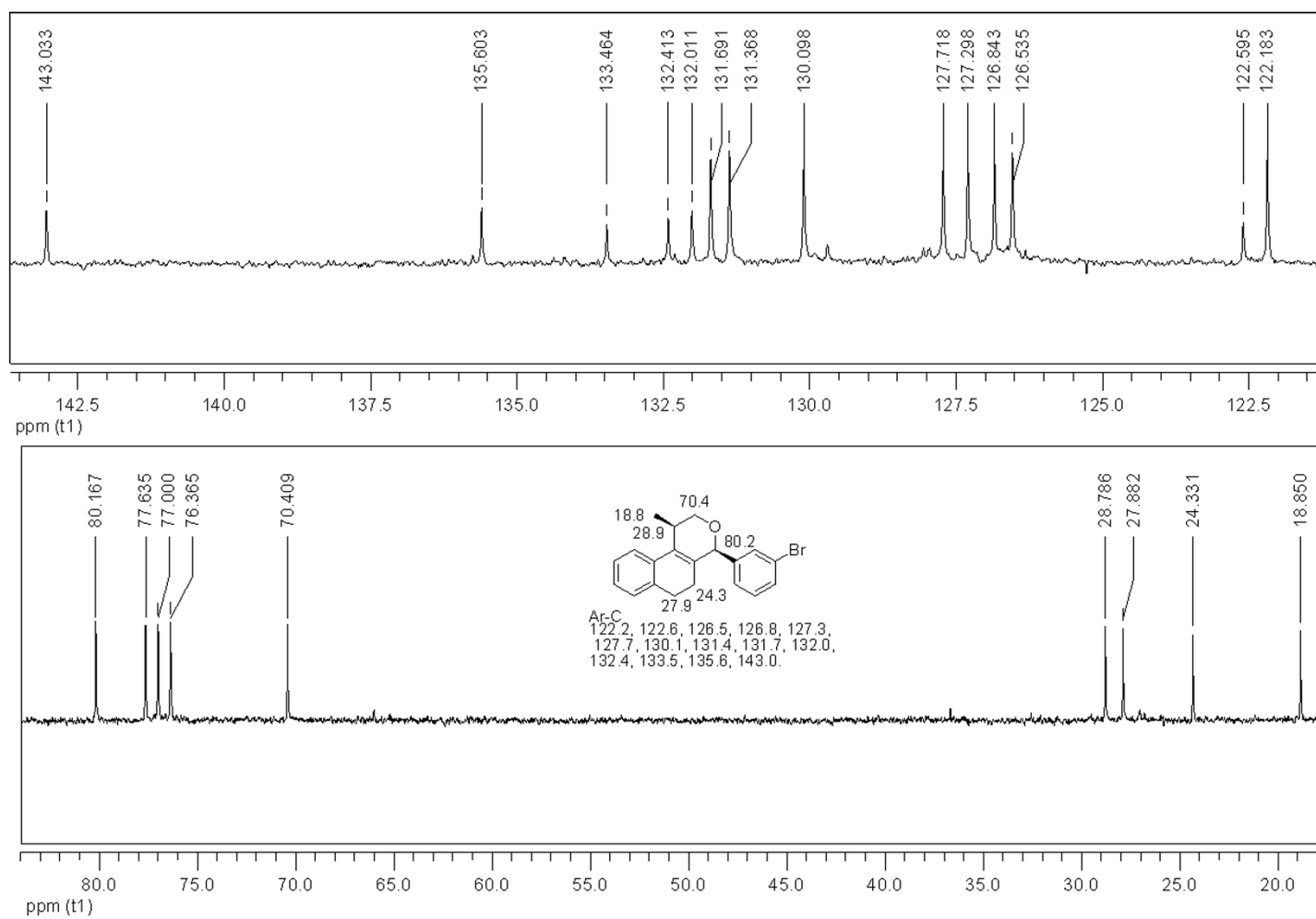
$^{13}\text{C}$ -NMR of compounds **12j** and *trans*-**7j** (50 MHz,  $\text{CDCl}_3$ )

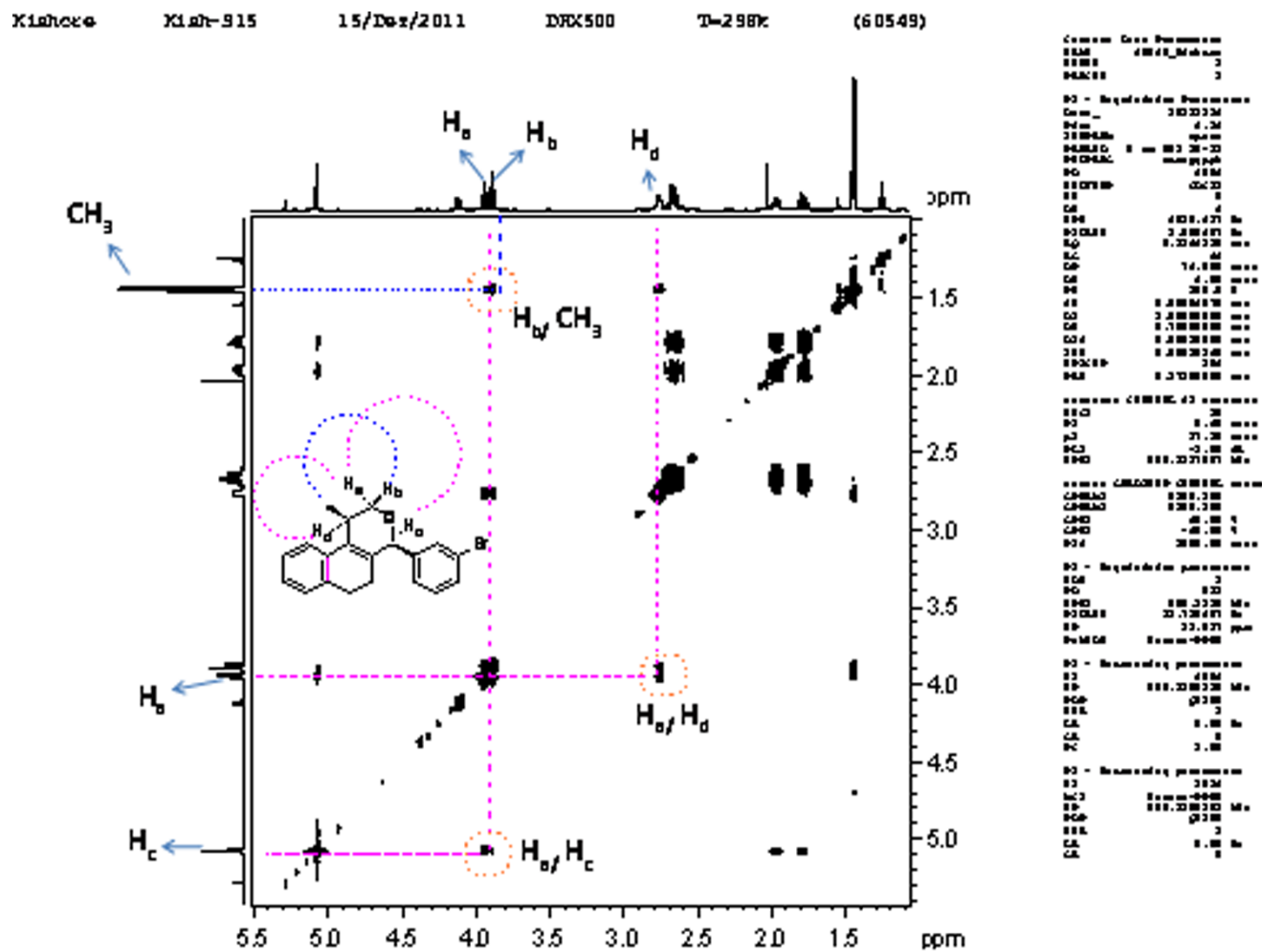
$^{13}\text{C}$ -NMR of compounds **12j** and *trans*-**7j** (50 MHz,  $\text{CDCl}_3$ )

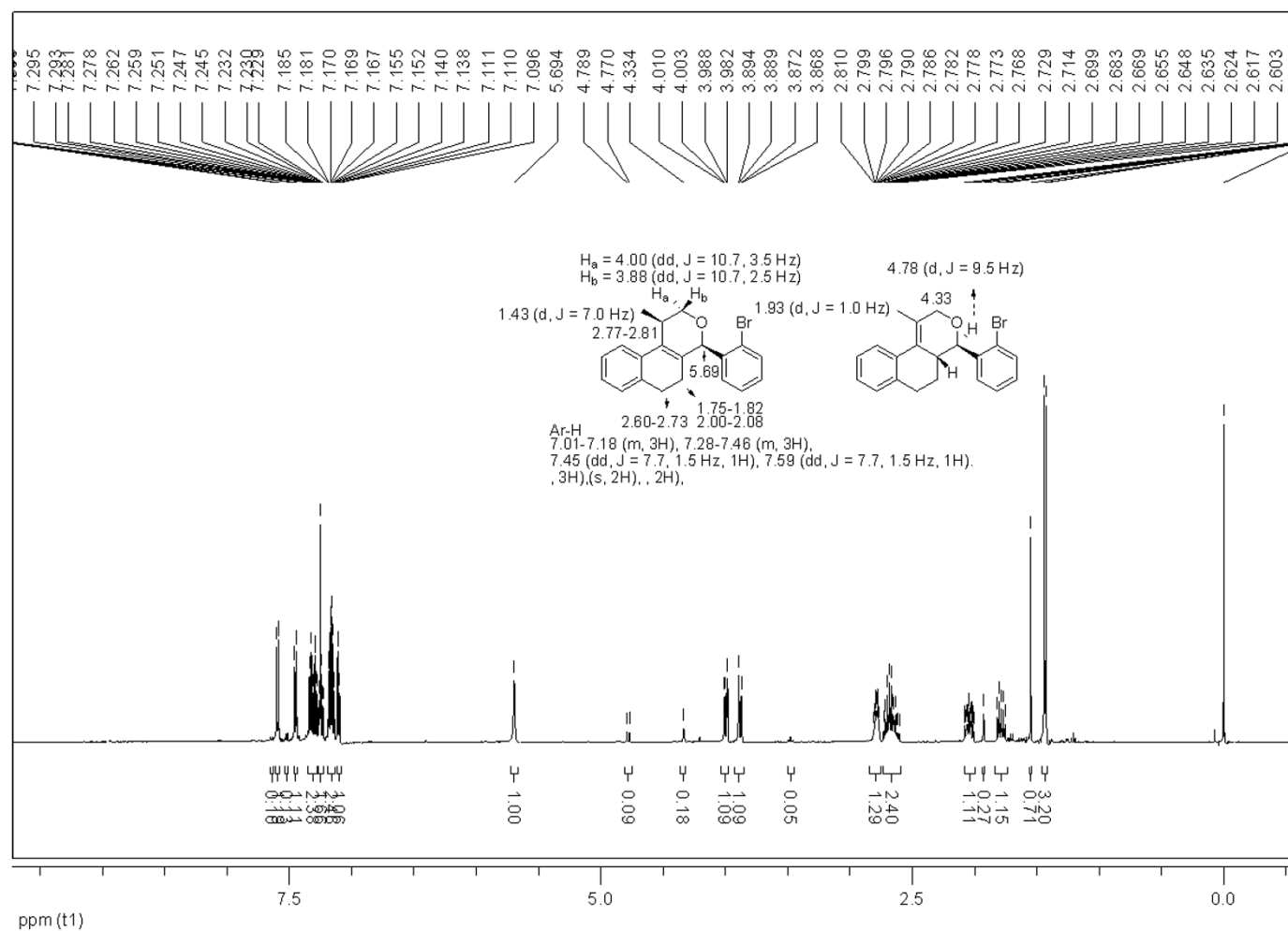
<sup>1</sup>H-NMR of compound *cis*-**7k** (500 MHz, CDCl<sub>3</sub>)

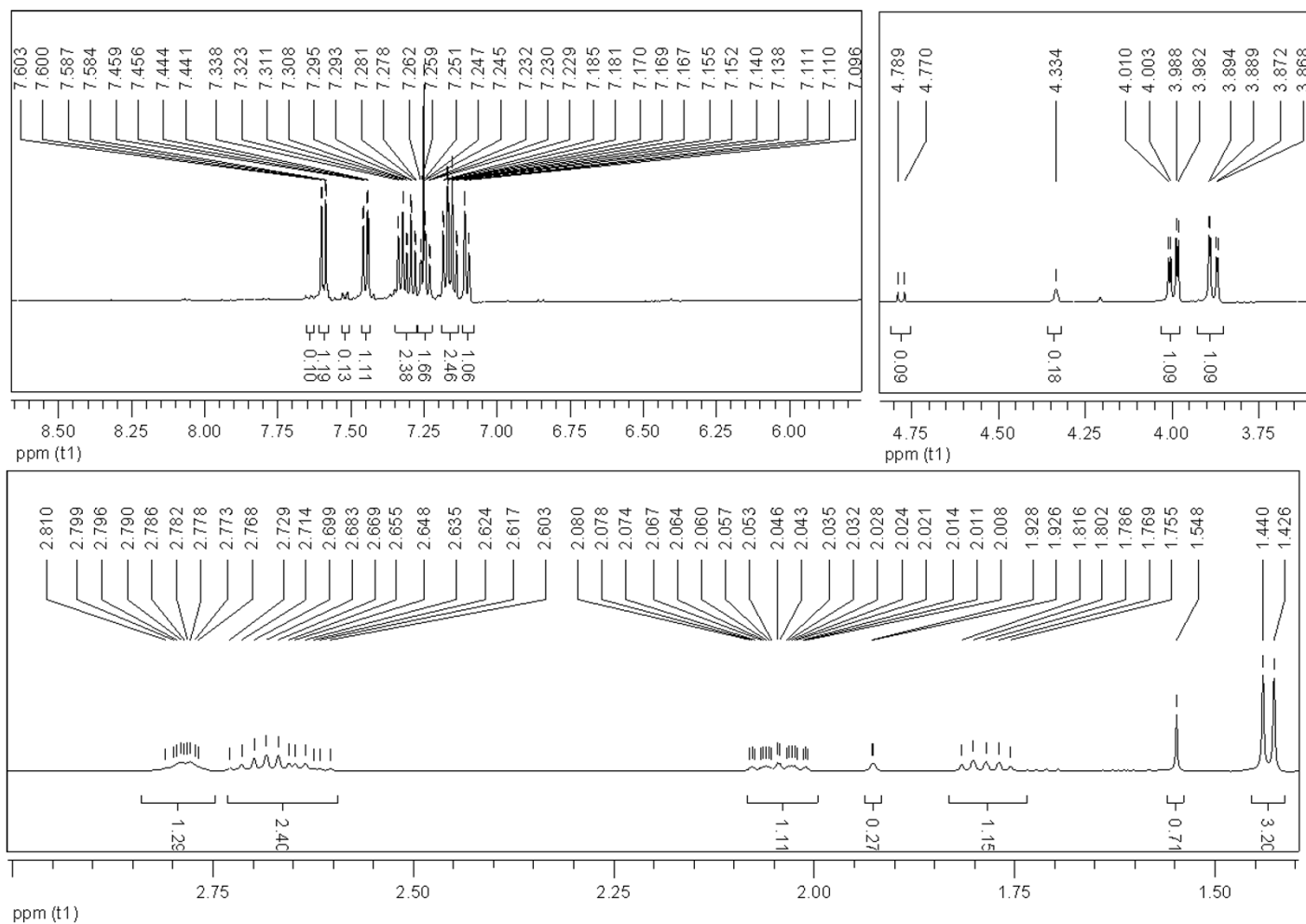
$^1\text{H}$ -NMR of compound *cis*-**7k** (300 MHz,  $\text{CDCl}_3$ )

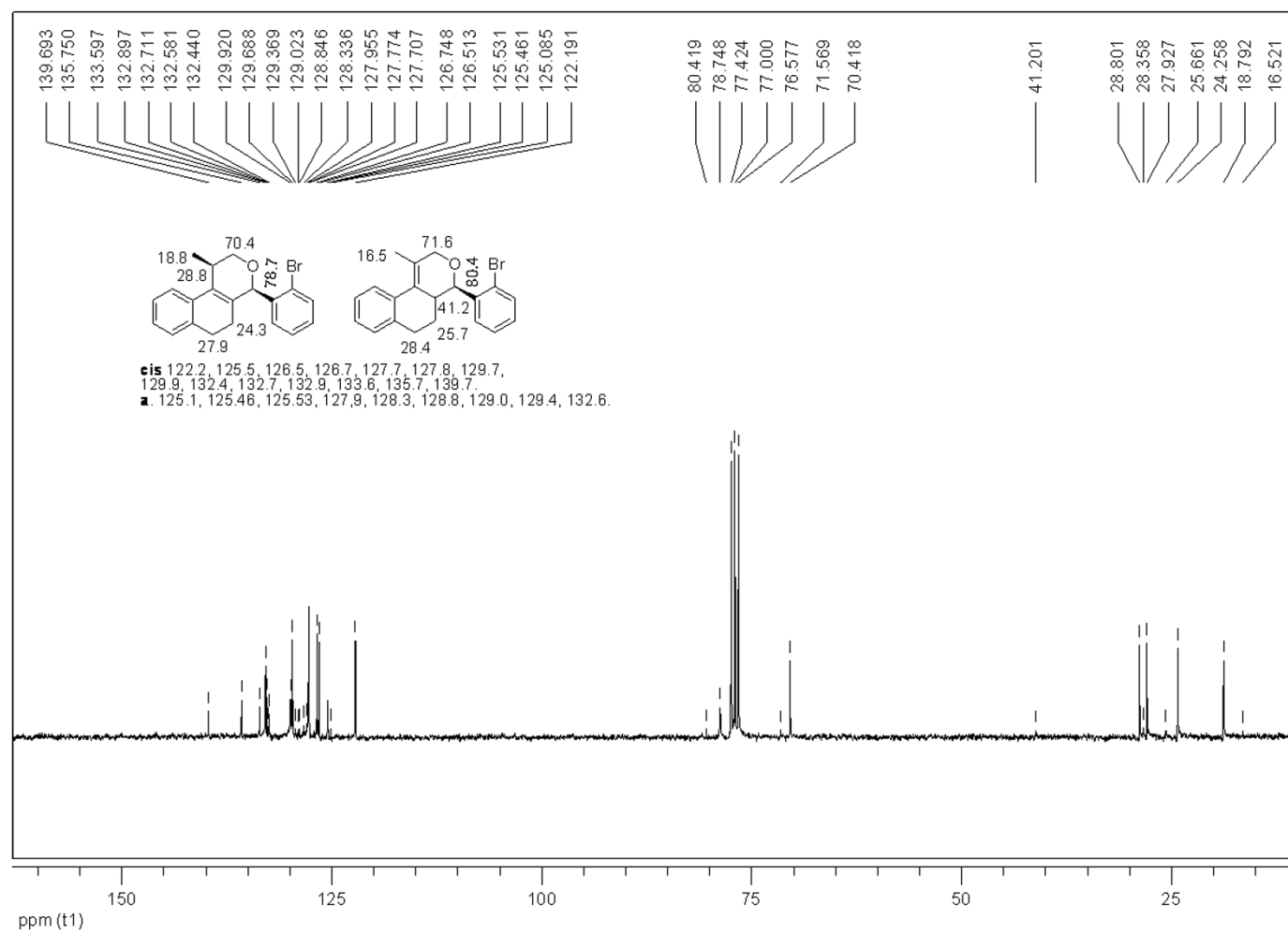
$^{13}\text{C}$ -NMR of compound *cis*-**7k** (75 MHz,  $\text{CDCl}_3$ )

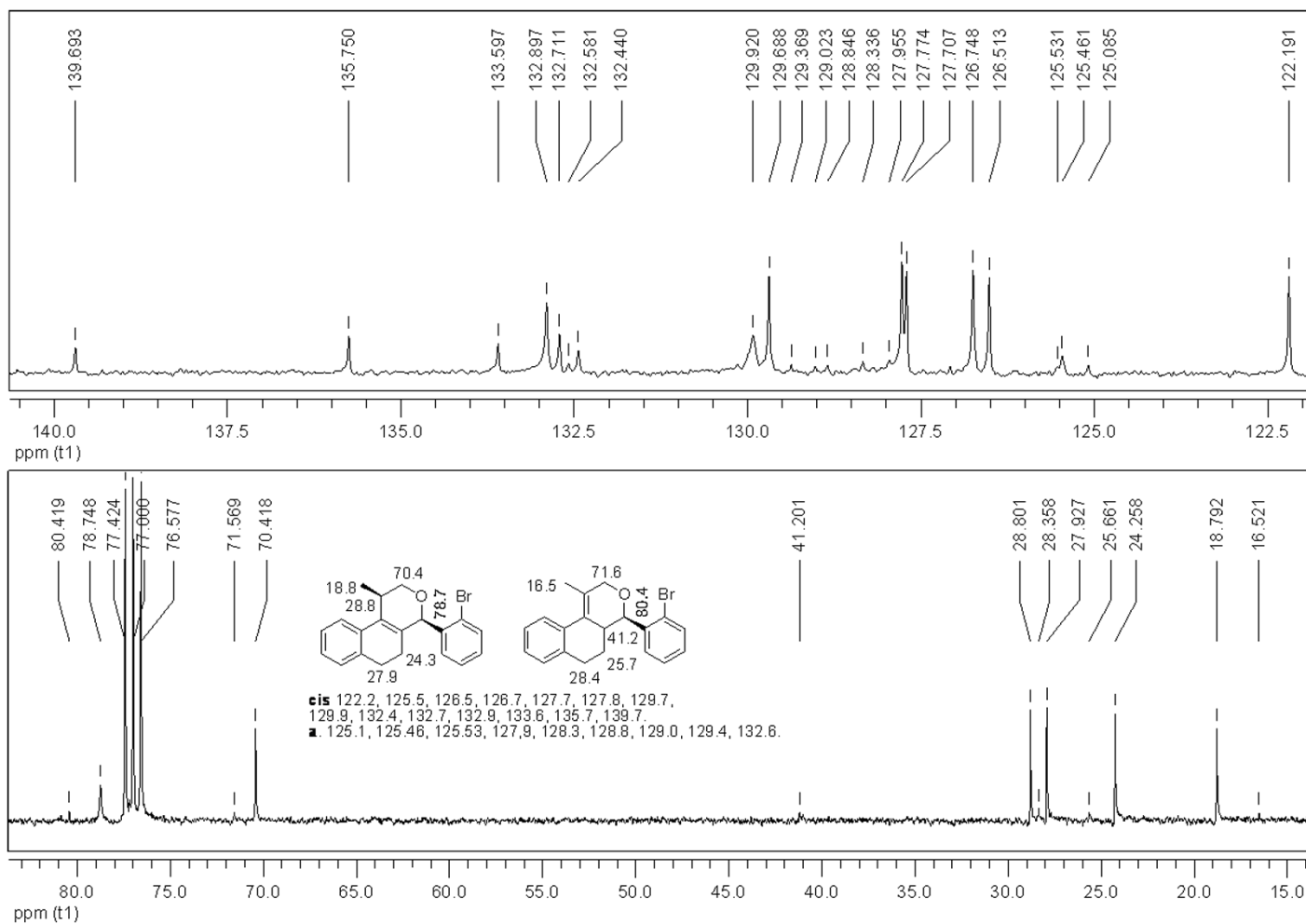
$^{13}\text{C}$ -NMR of compound *cis*-**7k** (75 MHz,  $\text{CDCl}_3$ )

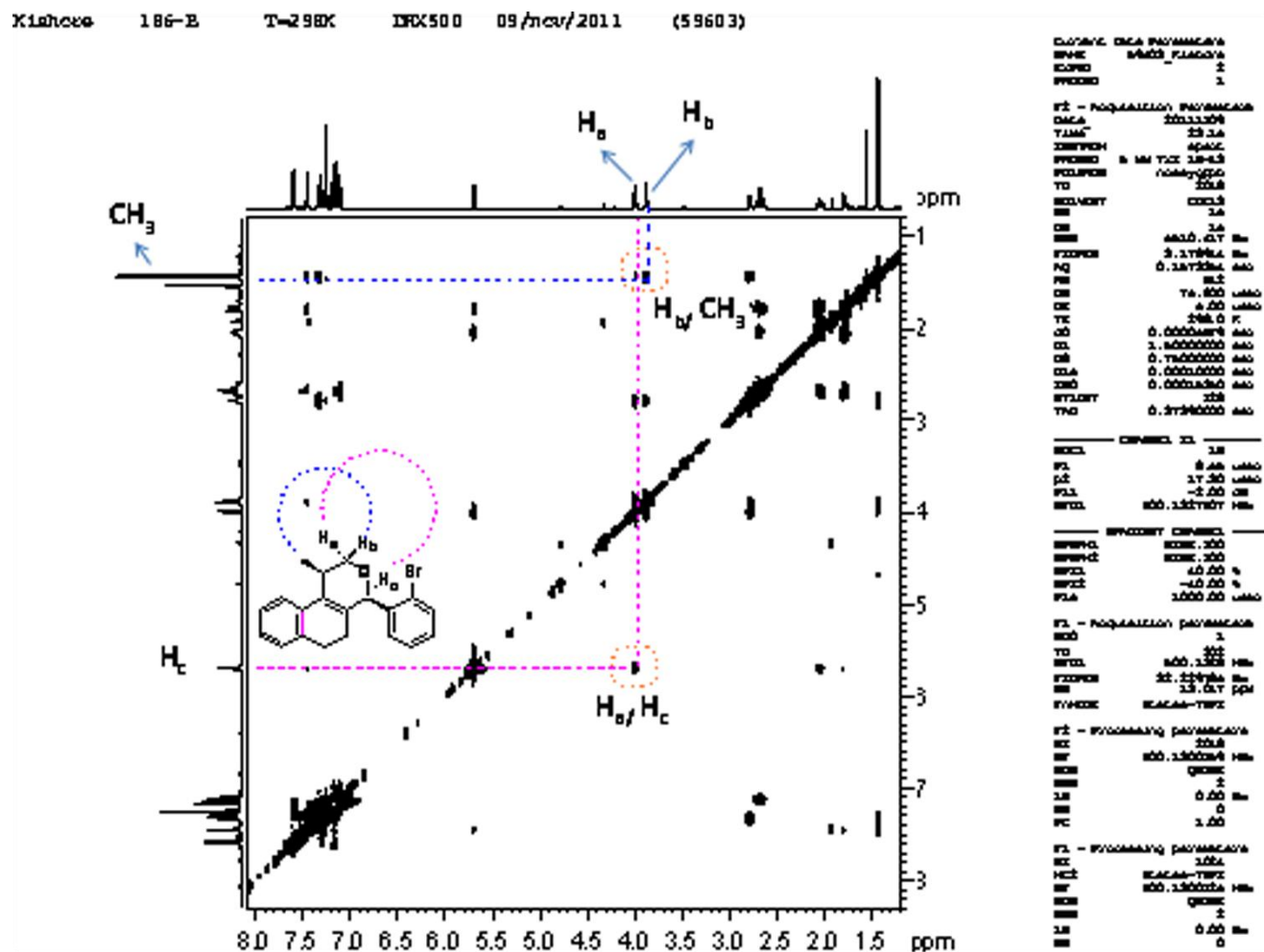
2D NOESY NMR of compound *cis-7k* (500 MHz, CDCl<sub>3</sub>)

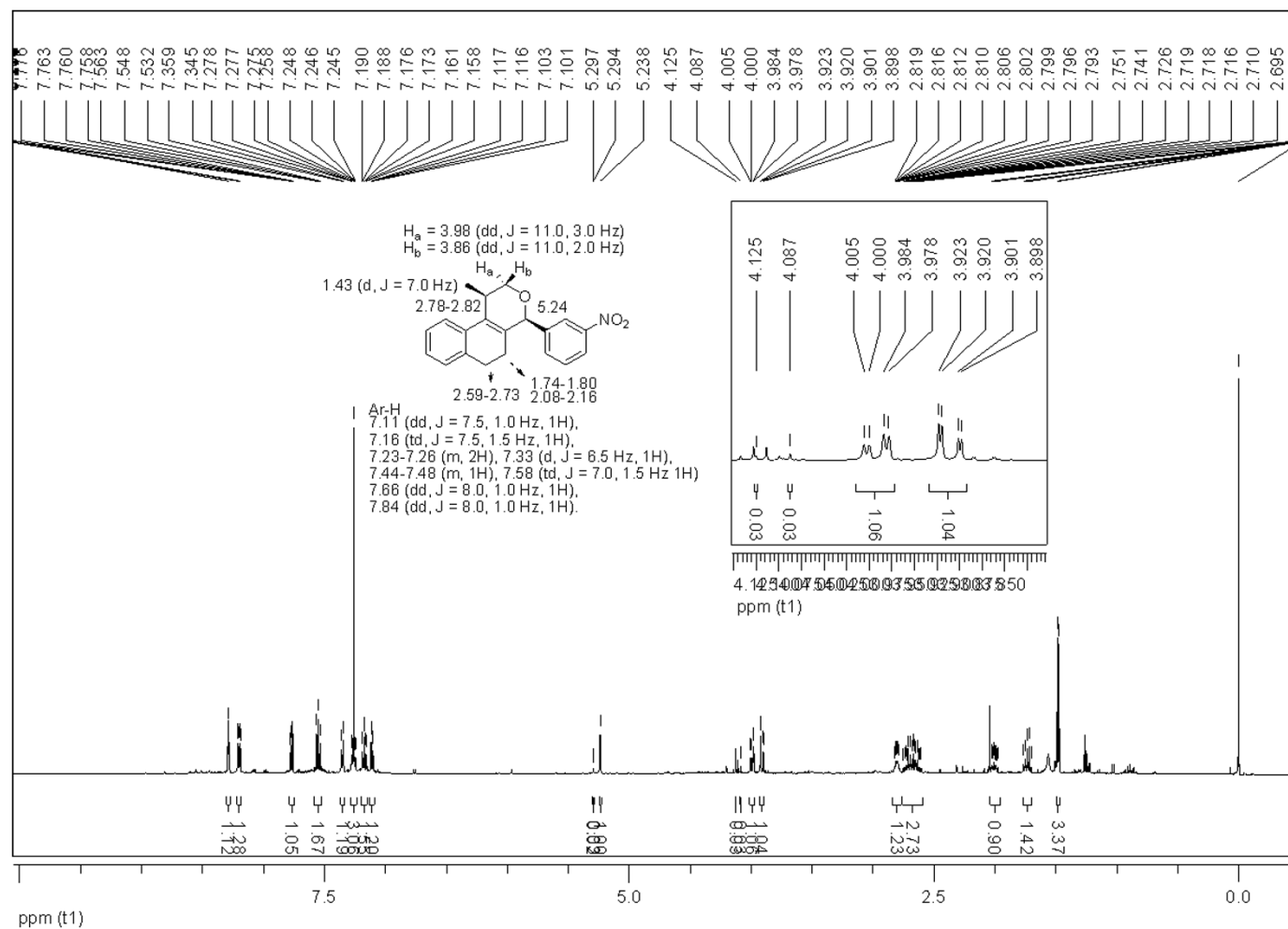
$^1\text{H}$ -NMR of compounds *cis*-**71** and **121** (500 MHz,  $\text{CDCl}_3$ )

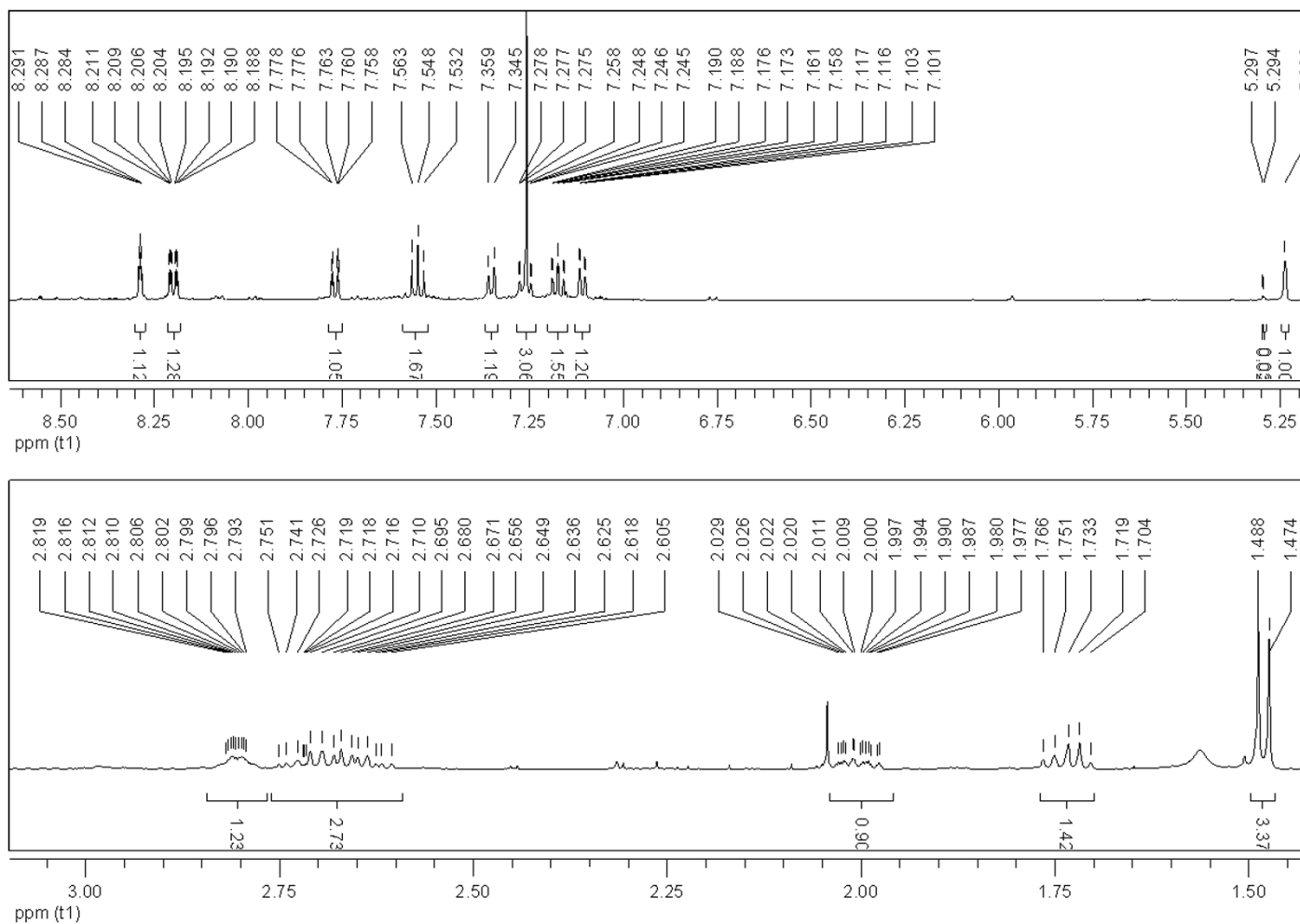
$^1\text{H}$ -NMR of compounds *cis*-**71** and **121** (500 MHz,  $\text{CDCl}_3$ )

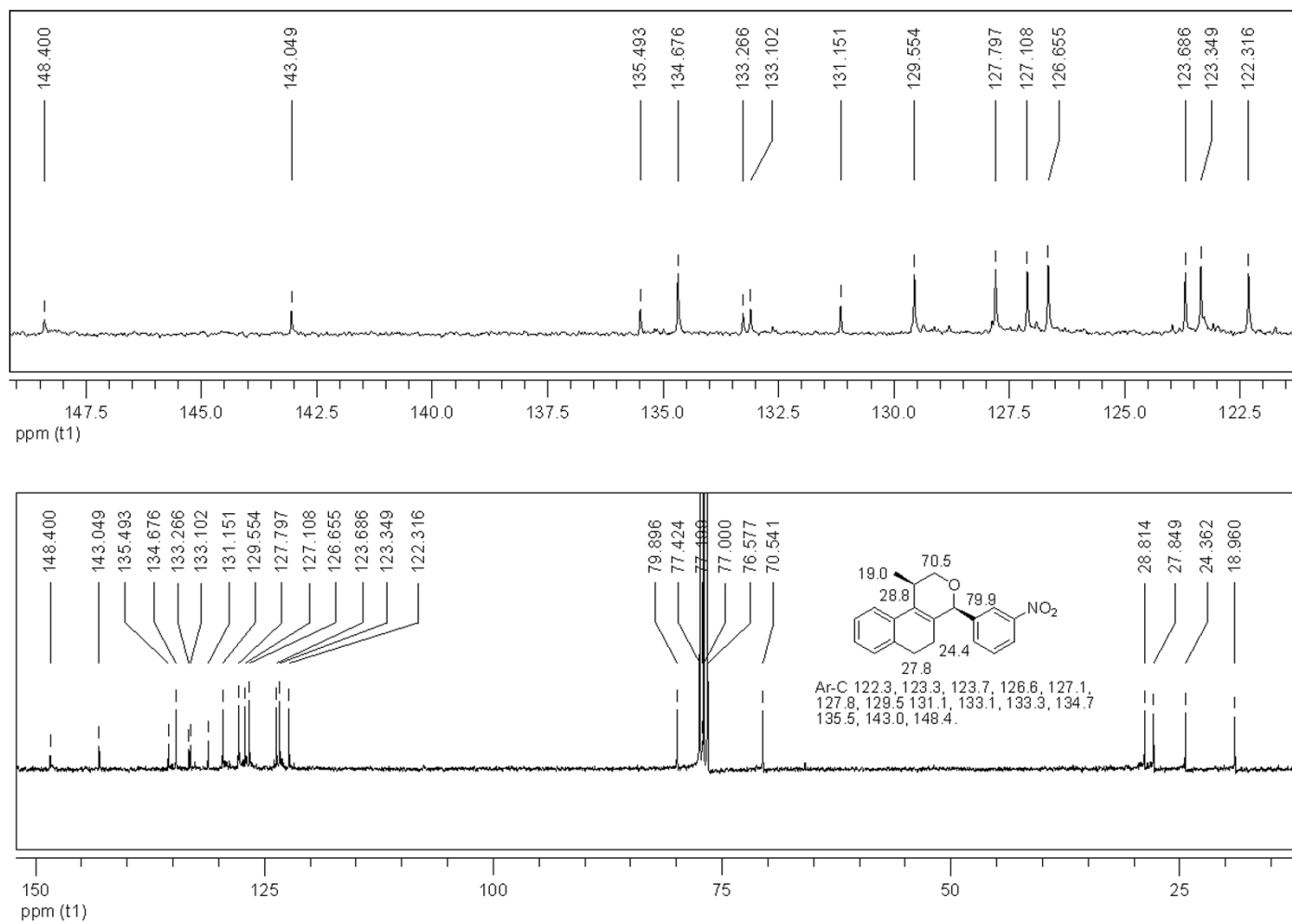
$^{13}\text{C}$ -NMR of compounds *cis*-**71** and **121** (75 MHz,  $\text{CDCl}_3$ )

$^{13}\text{C}$ -NMR of compounds *cis*-**7l** and **12l** (75 MHz,  $\text{CDCl}_3$ )

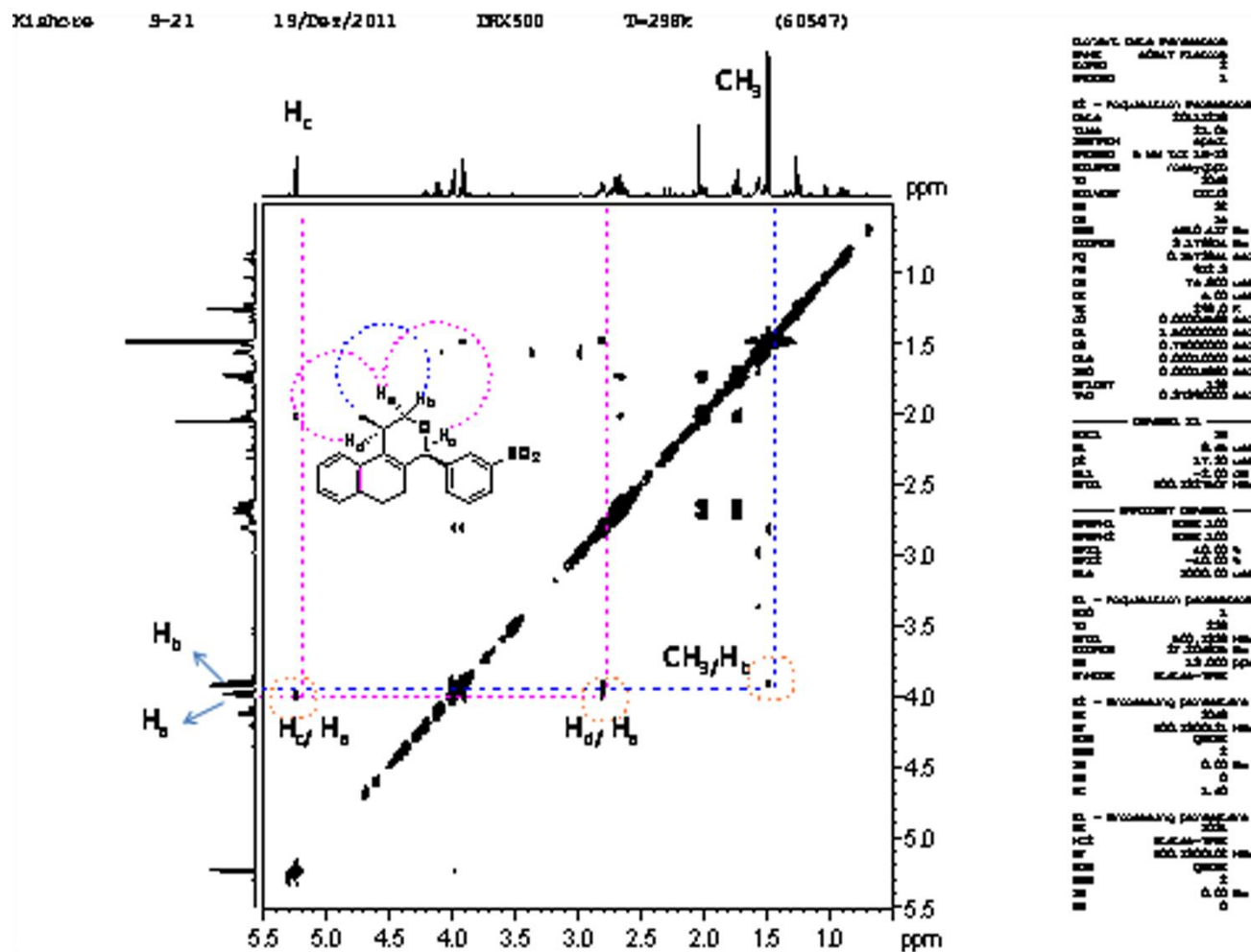
2D NOESY NMR of compound *cis*-71 (500 MHz, CDCl<sub>3</sub>)

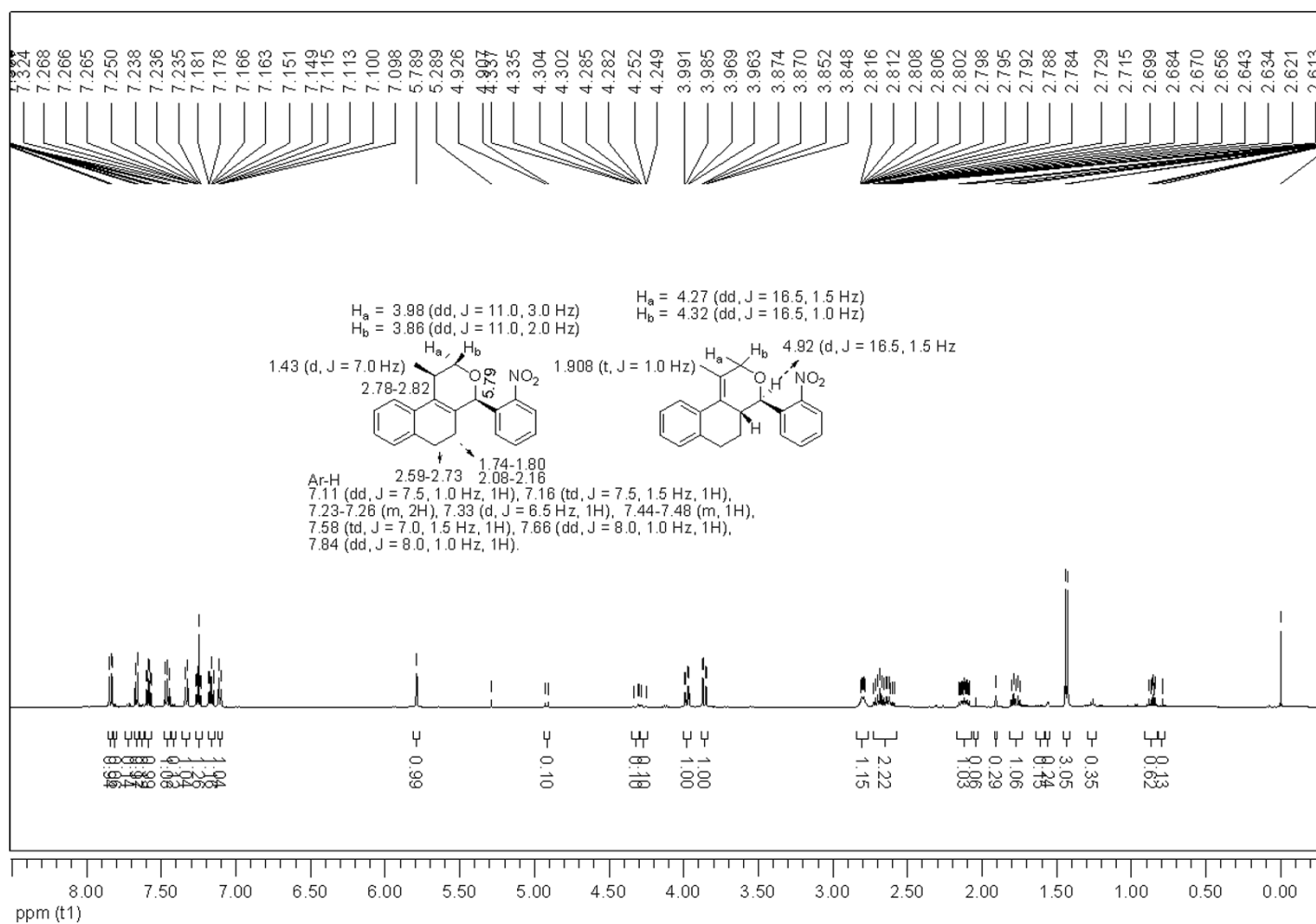
<sup>1</sup>H-NMR of compound *cis*-**7n** (500 MHz, CDCl<sub>3</sub>)

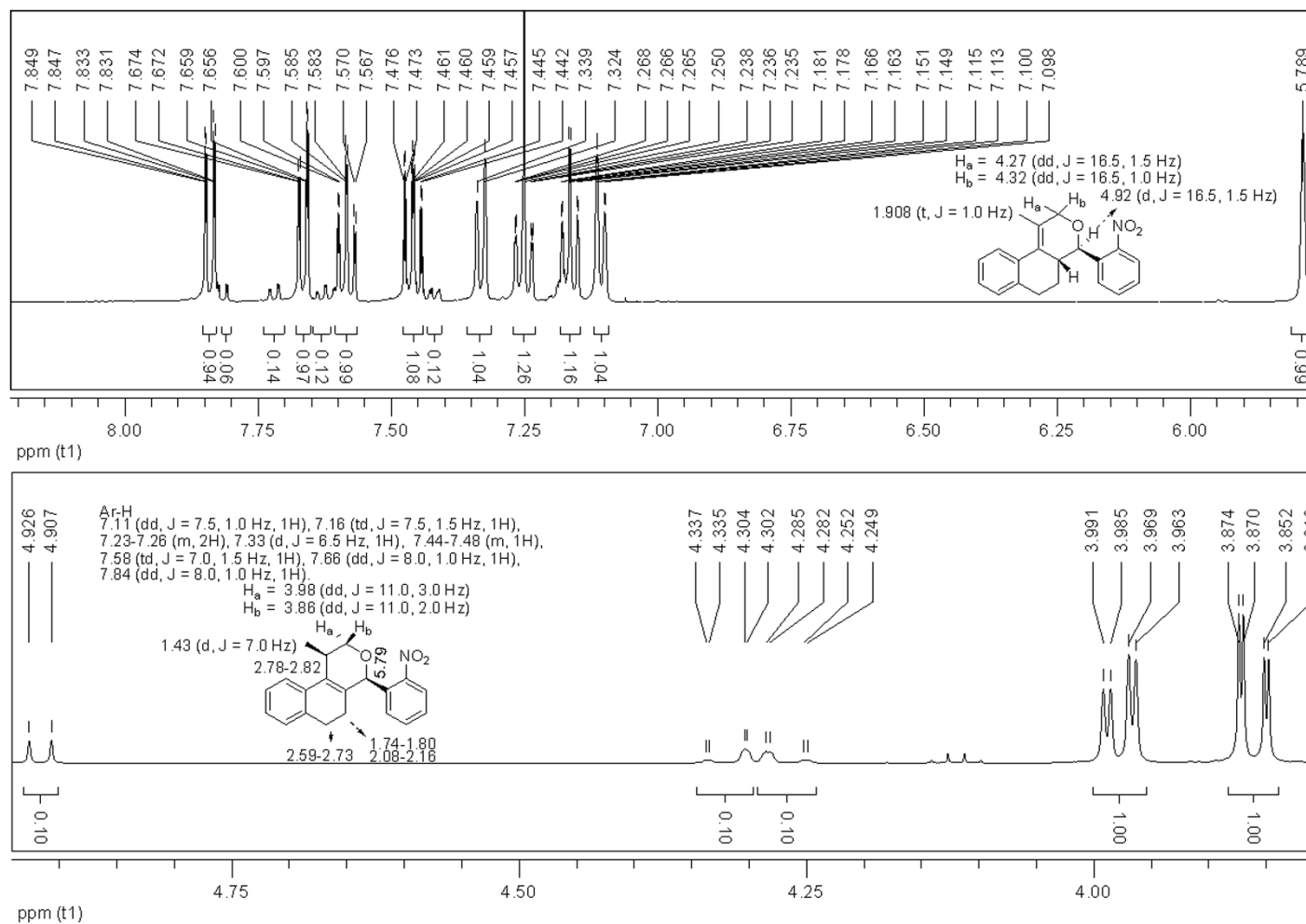
<sup>1</sup>H-NMR of compound *cis*-**7n** (500 MHz, CDCl<sub>3</sub>)

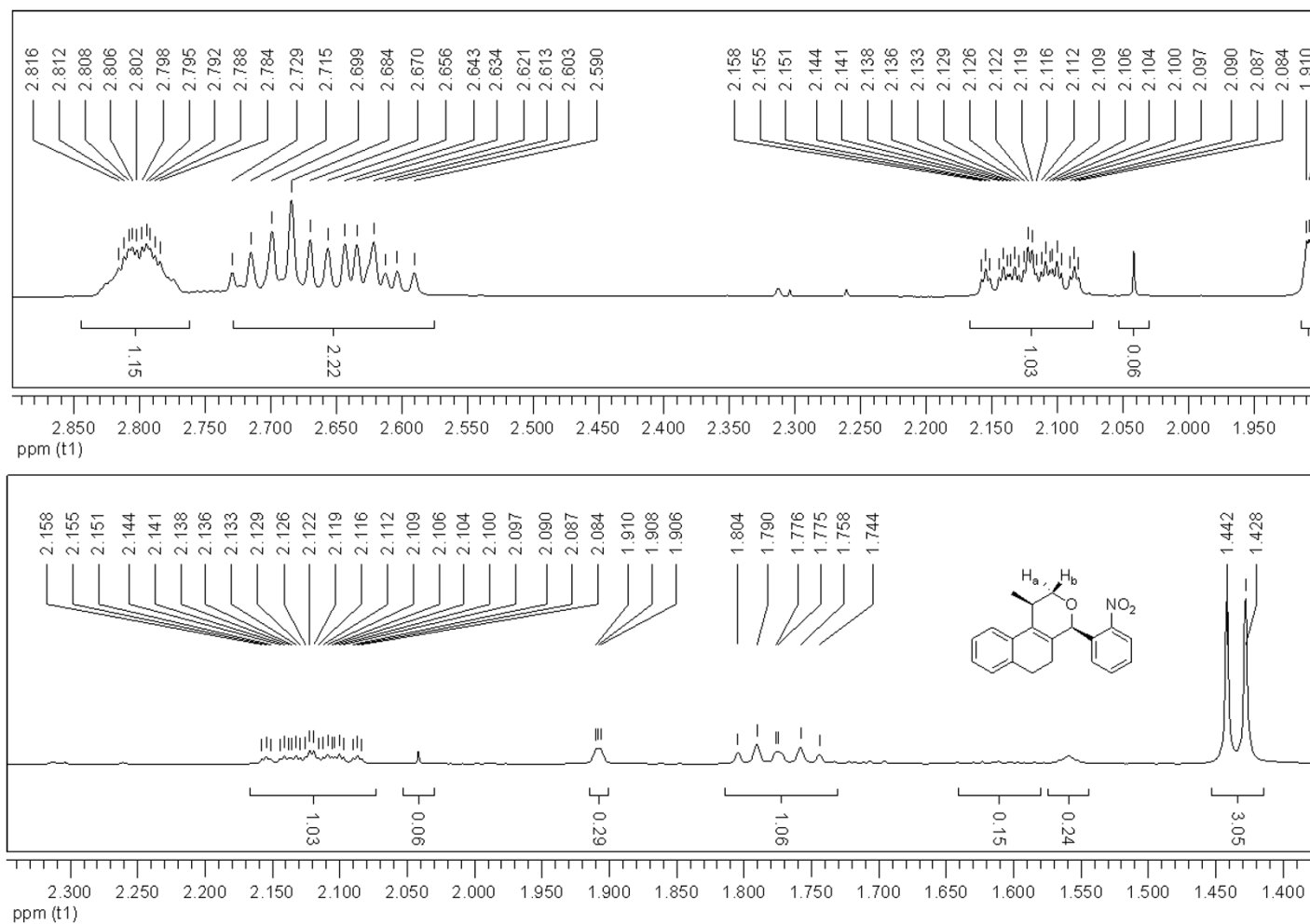
$^{13}\text{C}$ -NMR of compound *cis*-**7n** (50 MHz,  $\text{CDCl}_3$ )

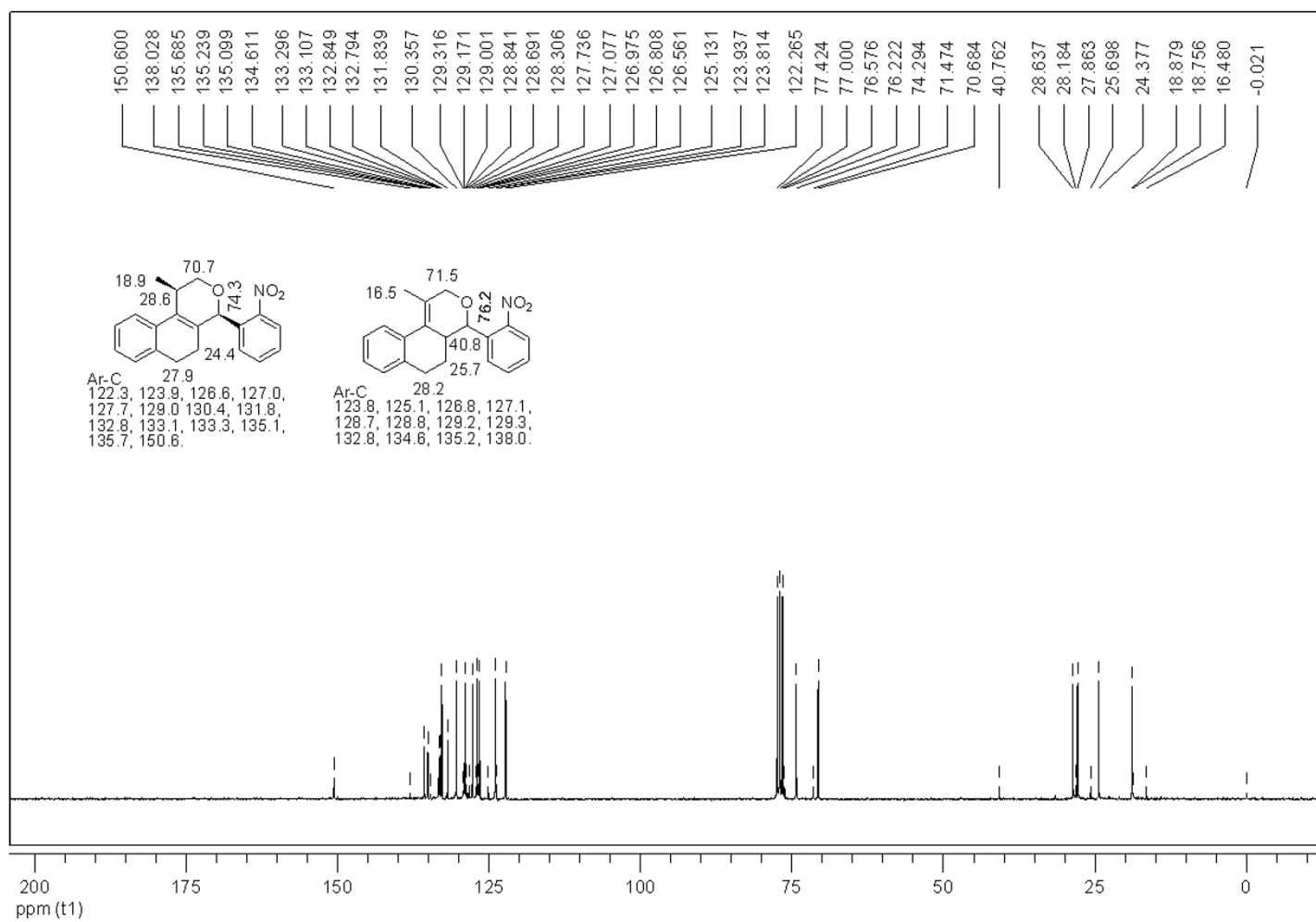
**2D NOESY NMR of compound *cis*-7n (500 MHz, CDCl<sub>3</sub>)**

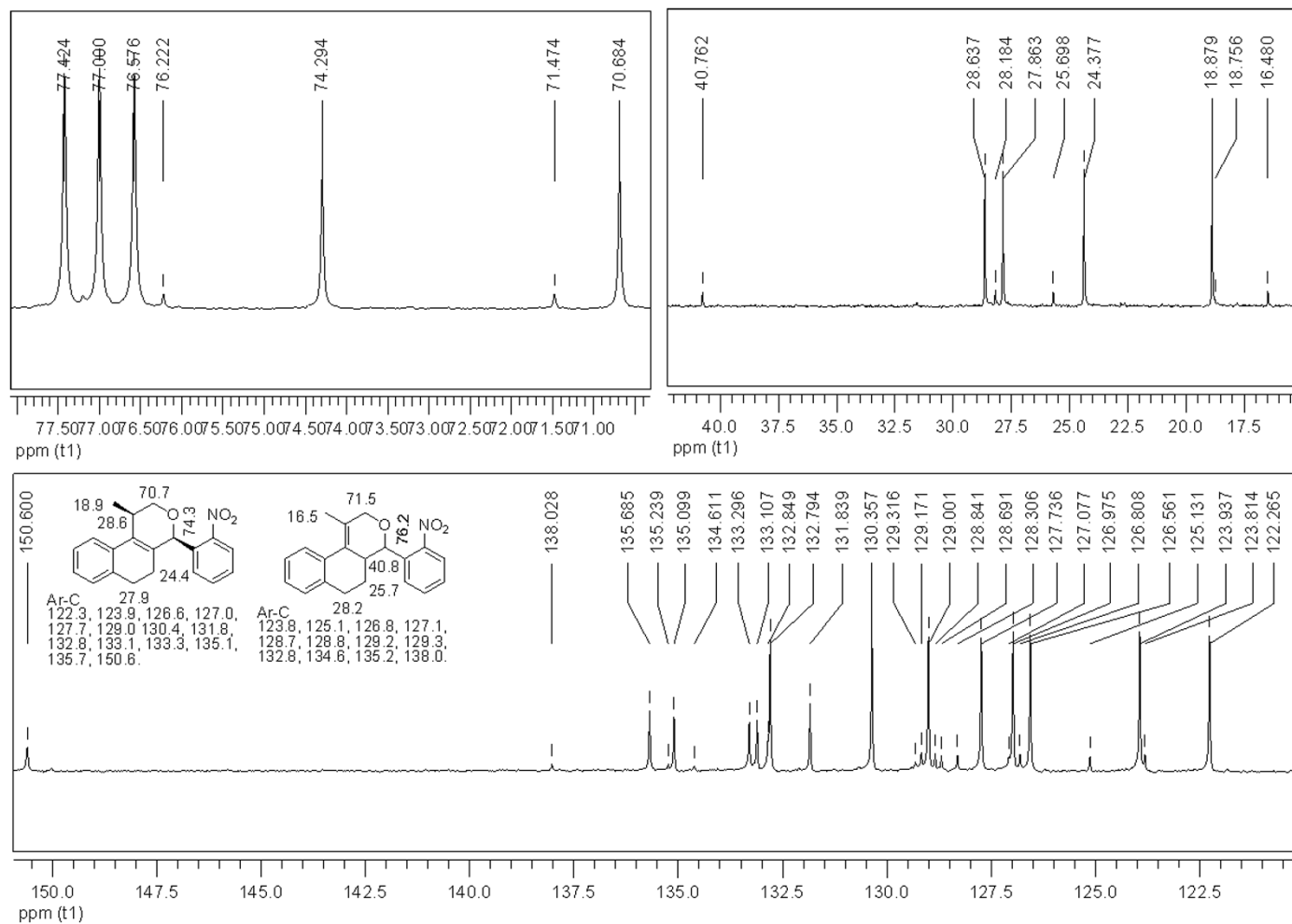


<sup>1</sup>H-NMR of compounds *cis*-**7o** and **12o** (500 MHz, CDCl<sub>3</sub>)

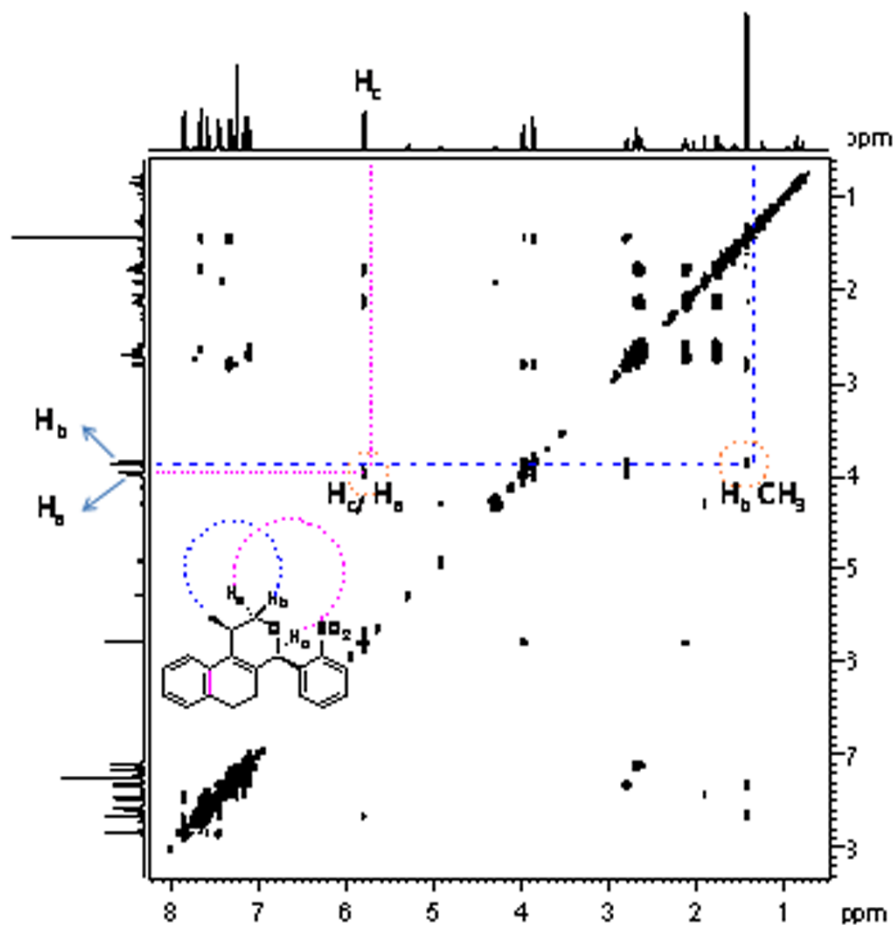
<sup>1</sup>H-NMR of compounds *cis*-**7o** and **12o** (500 MHz, CDCl<sub>3</sub>)

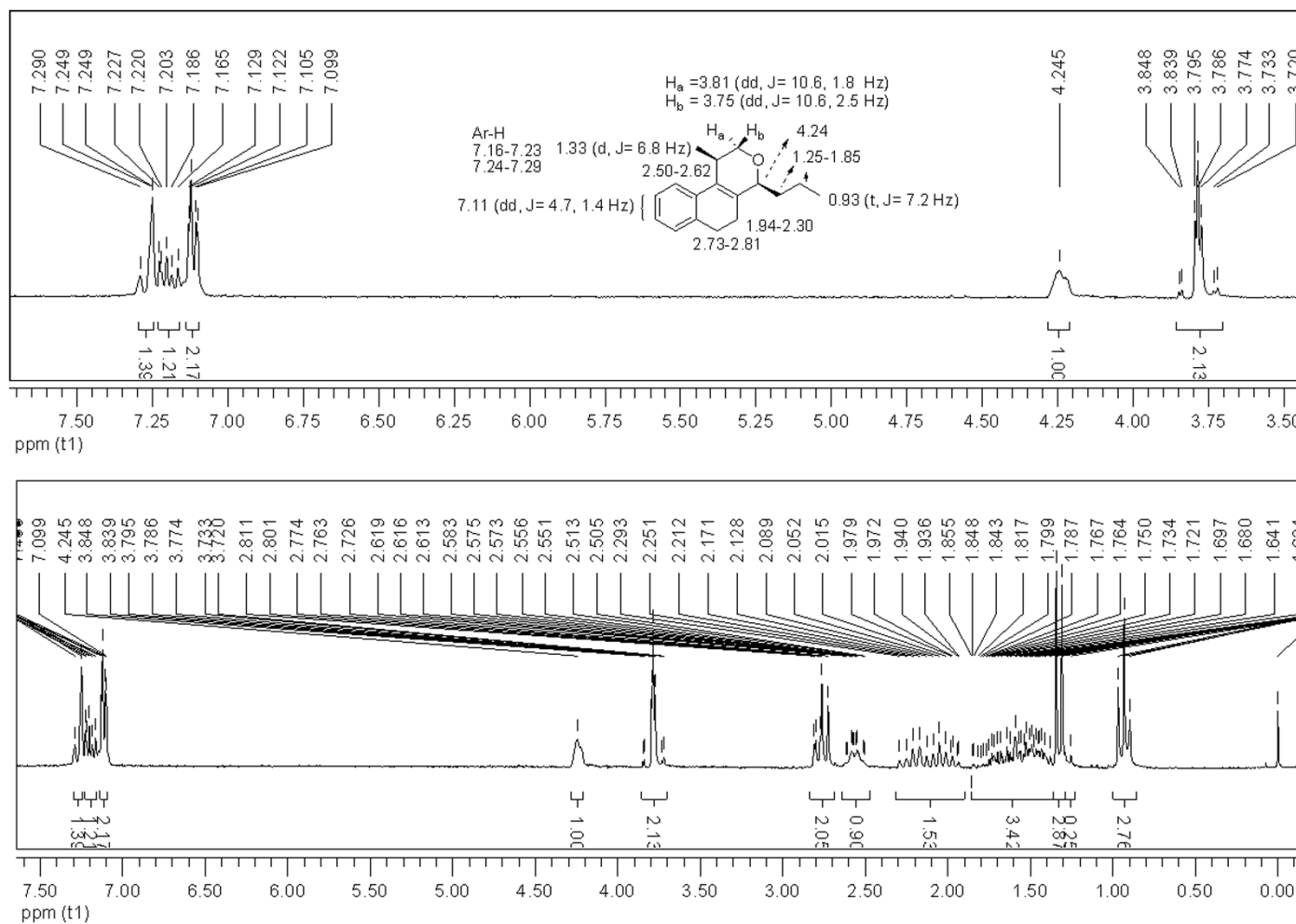
<sup>1</sup>H-NMR of compounds *cis*-**7o** and **12o** (500 MHz, CDCl<sub>3</sub>)

$^{13}\text{C}$ -NMR of compounds *cis*-**7o** and **12o** (75 MHz,  $\text{CDCl}_3$ )

$^{13}\text{C}$ -NMR of compounds *cis*-**7o** and **12o** (75 MHz,  $\text{CDCl}_3$ )

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[illegible]

<sup>1</sup>H-NMR of compound *cis*-7q (200 MHz, CDCl<sub>3</sub>)

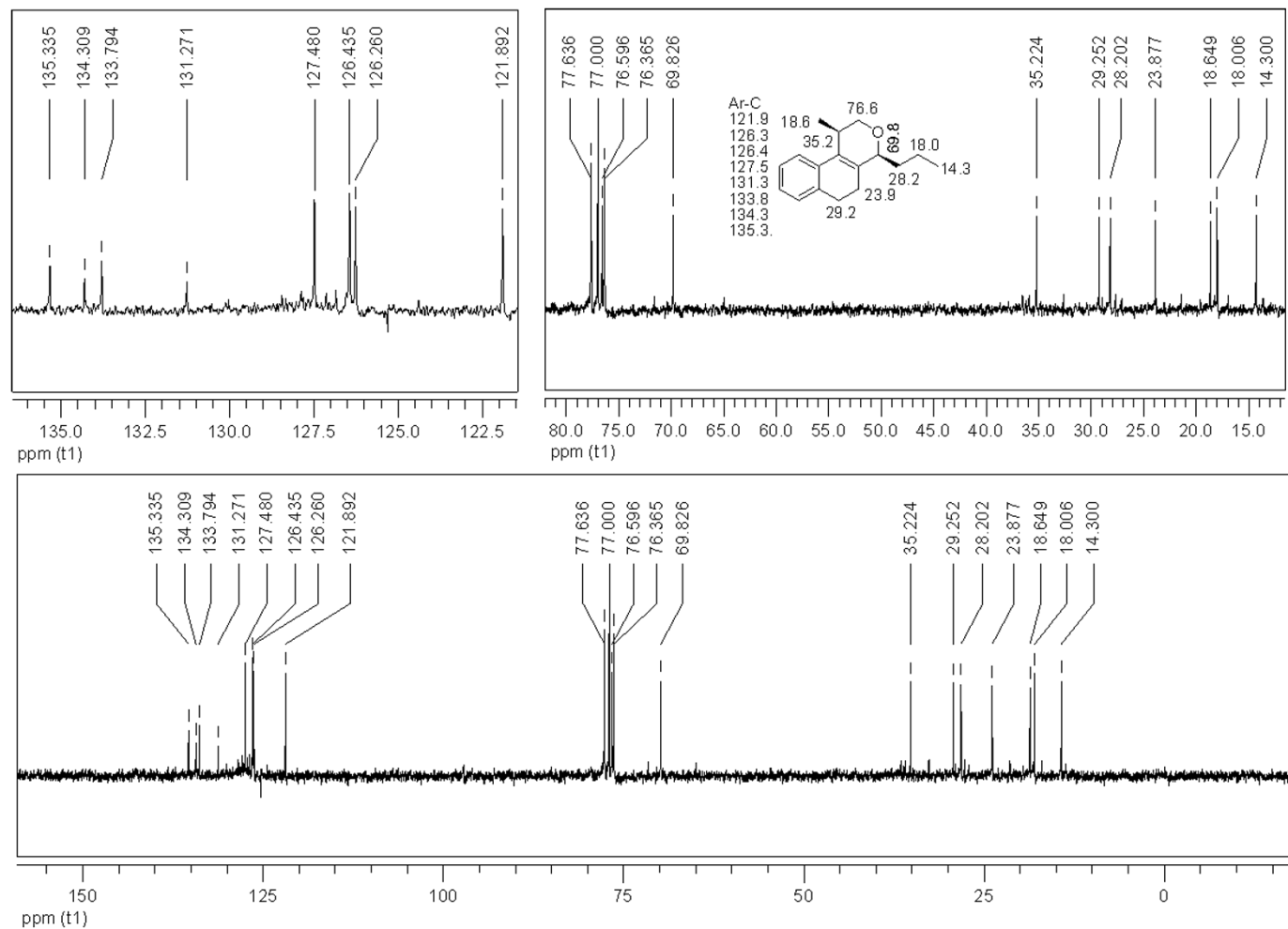
The figure displays two  $^1\text{H}$  NMR spectra of compound **1**. The top spectrum is the  $^1\text{H}$  NMR in  $\text{CDCl}_3$ , and the bottom spectrum is the  $^1\text{H}$  NMR in  $\text{DMSO}-d_6$ . Both spectra include chemical shift values (ppm), integration values, and a chemical structure of compound **1** with proton assignments.

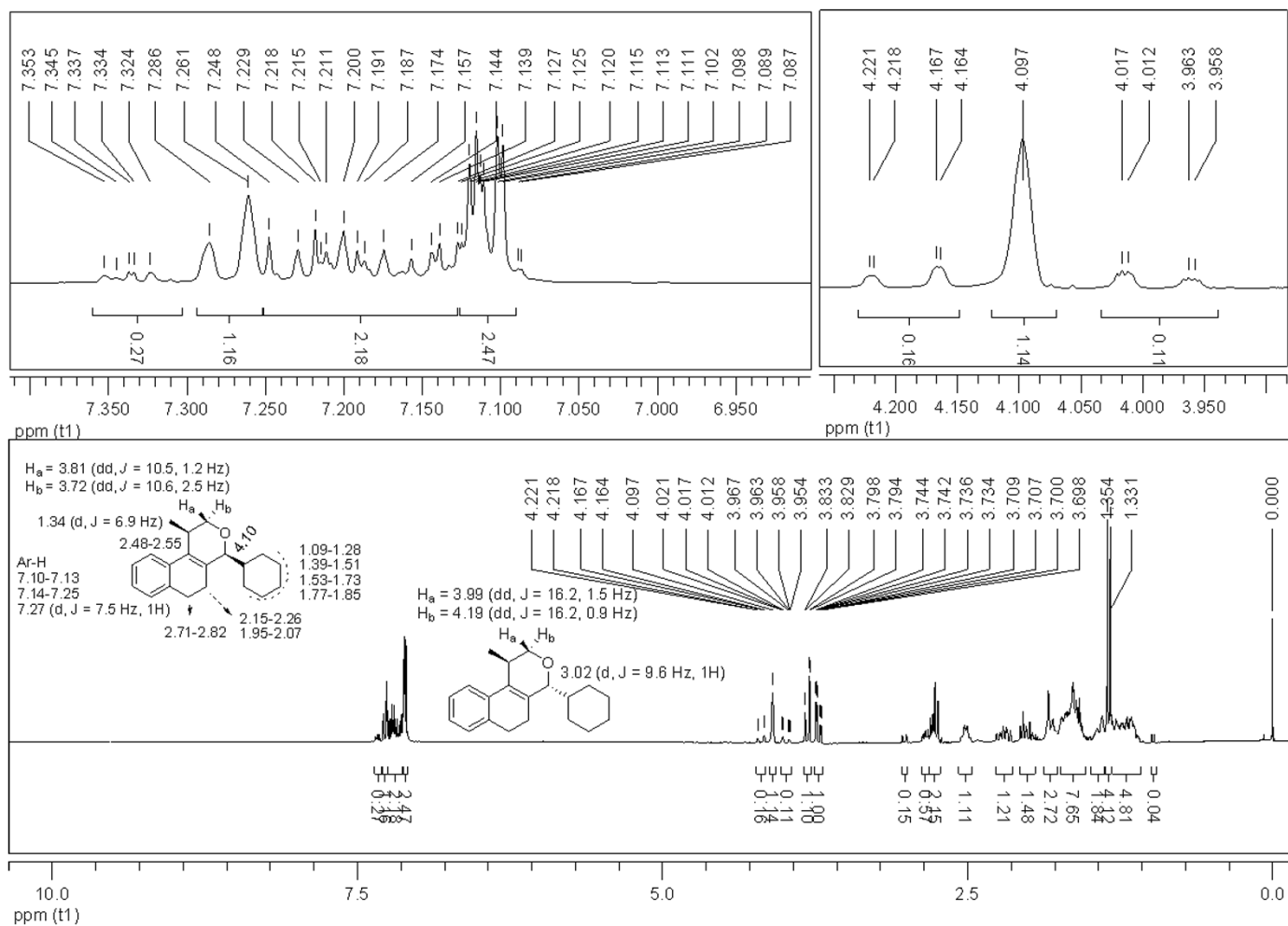
**Top Spectrum ( $^1\text{H}$  NMR in  $\text{CDCl}_3$ ):**

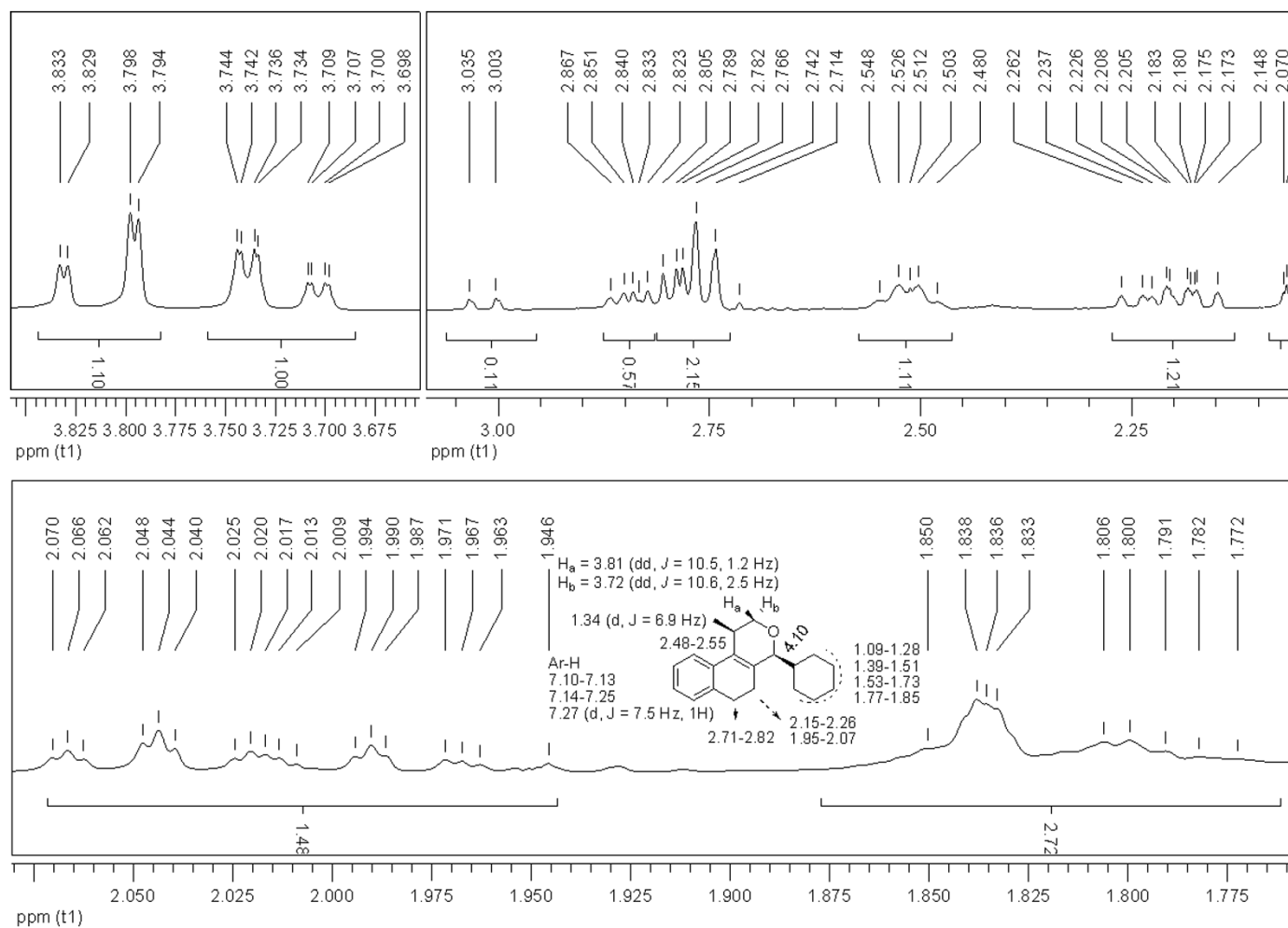
- Chemical shift range: 1.936 to 2.811 ppm.
- Integration values: 2.06, 0.90, 1.53.
- Chemical structure of compound **1** is shown with proton assignments:  $\text{H}_a$ ,  $\text{H}_b$ , and  $\text{H}_c$ .

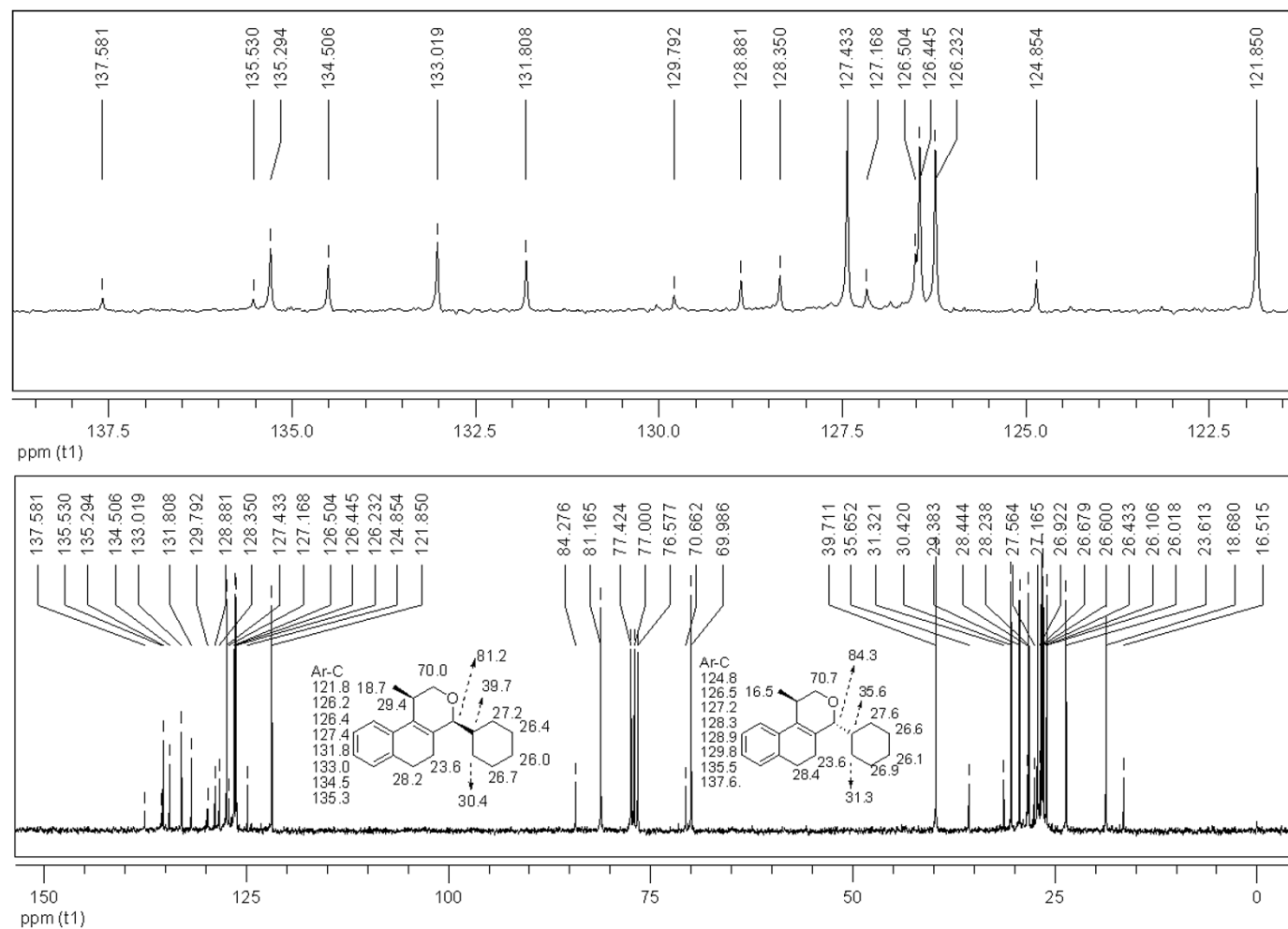
**Bottom Spectrum ( $^1\text{H}$  NMR in  $\text{DMSO}-d_6$ ):**

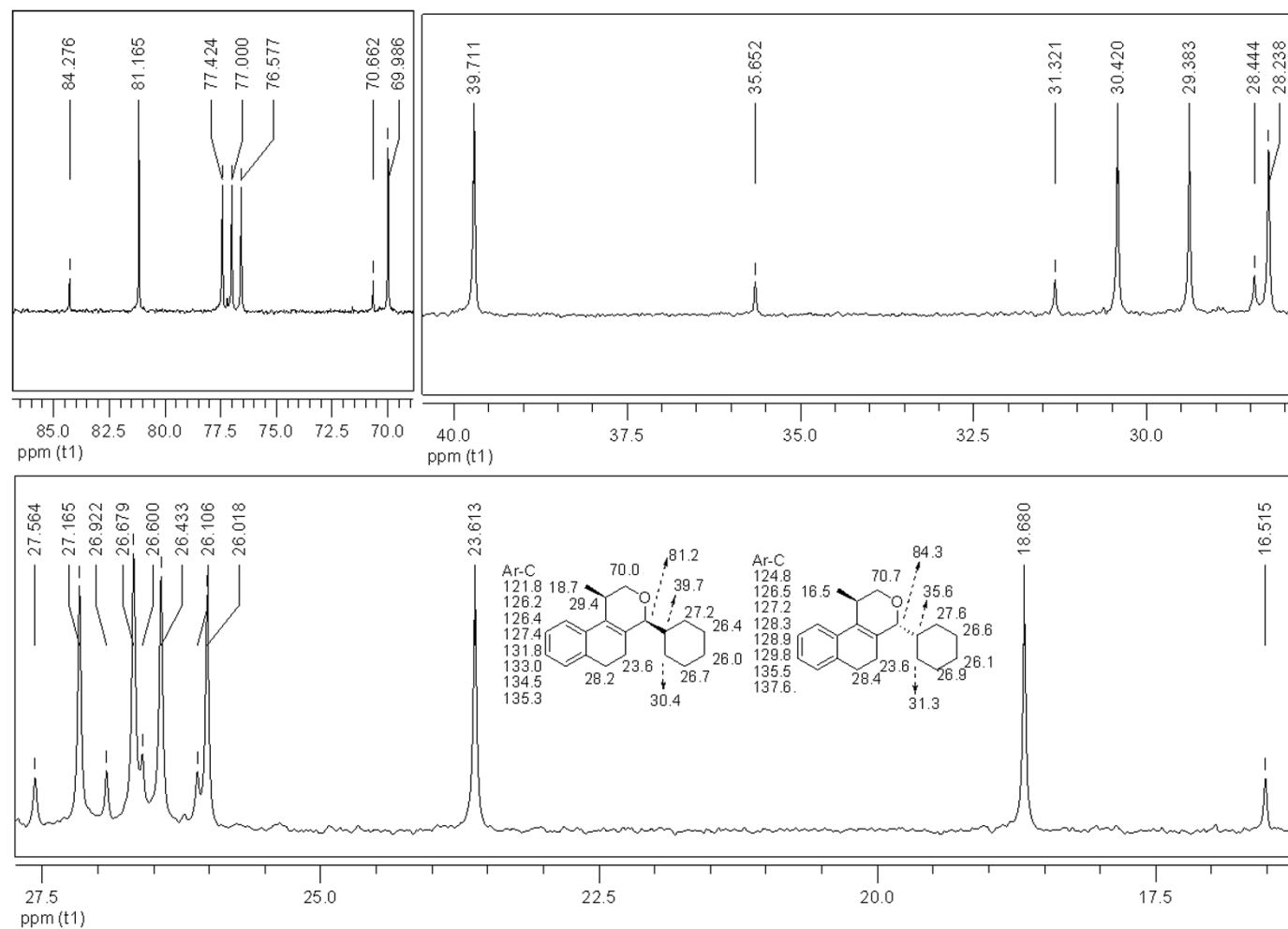
- Chemical shift range: 0.000 to 1.855 ppm.
- Integration values: 1.53, 3.42, 2.87, 0.25, 2.76.
- Chemical structure of compound **1** is shown with proton assignments:  $\text{H}_a$ ,  $\text{H}_b$ , and  $\text{H}_c$ .

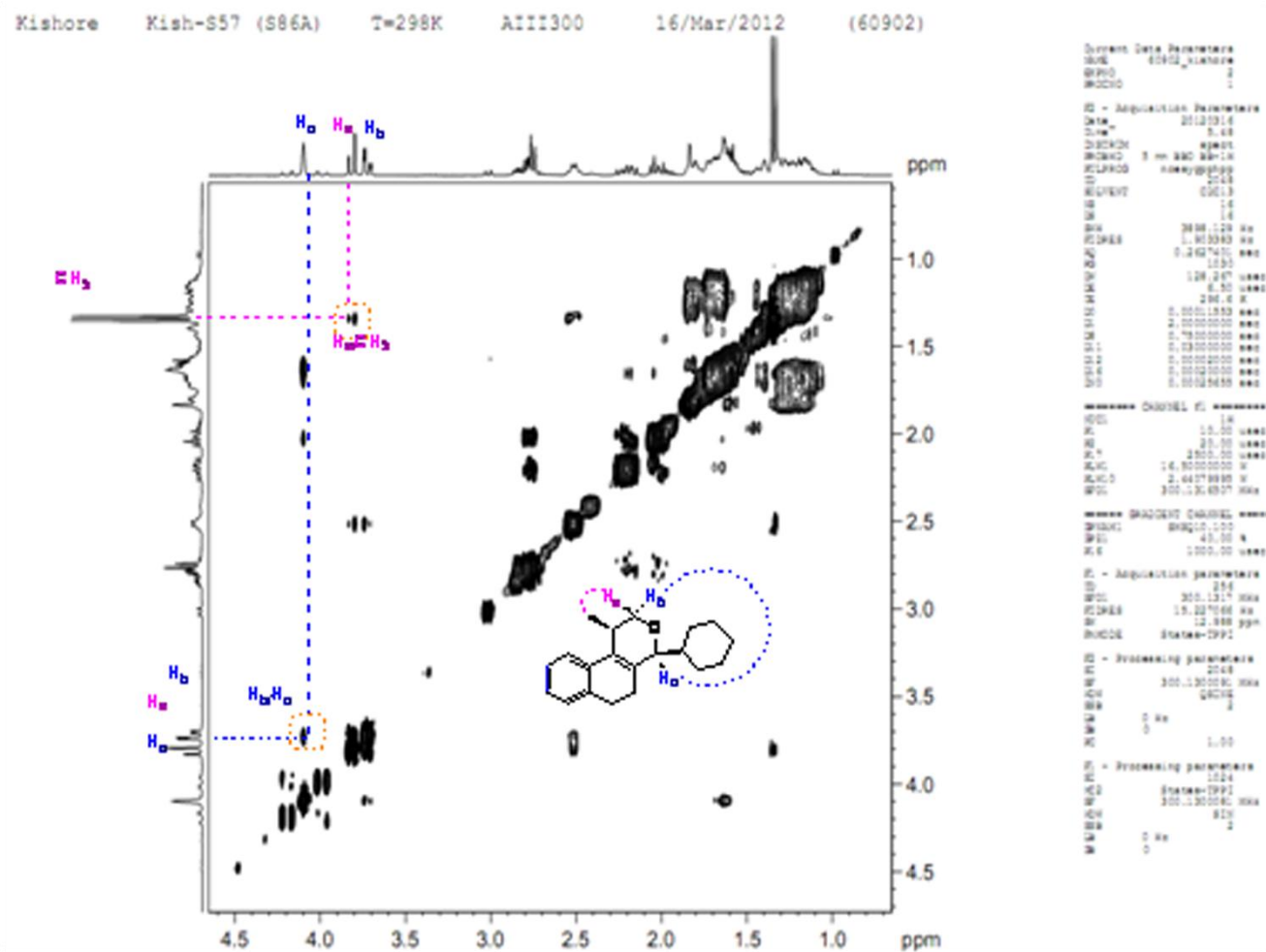
$^{13}\text{C}$ -NMR of compound *cis*-7q (50 MHz,  $\text{CDCl}_3$ )

$^1\text{H}$ -NMR of compound *cis*-**7r** and *trans*-**7r** (300 MHz,  $\text{CDCl}_3$ )

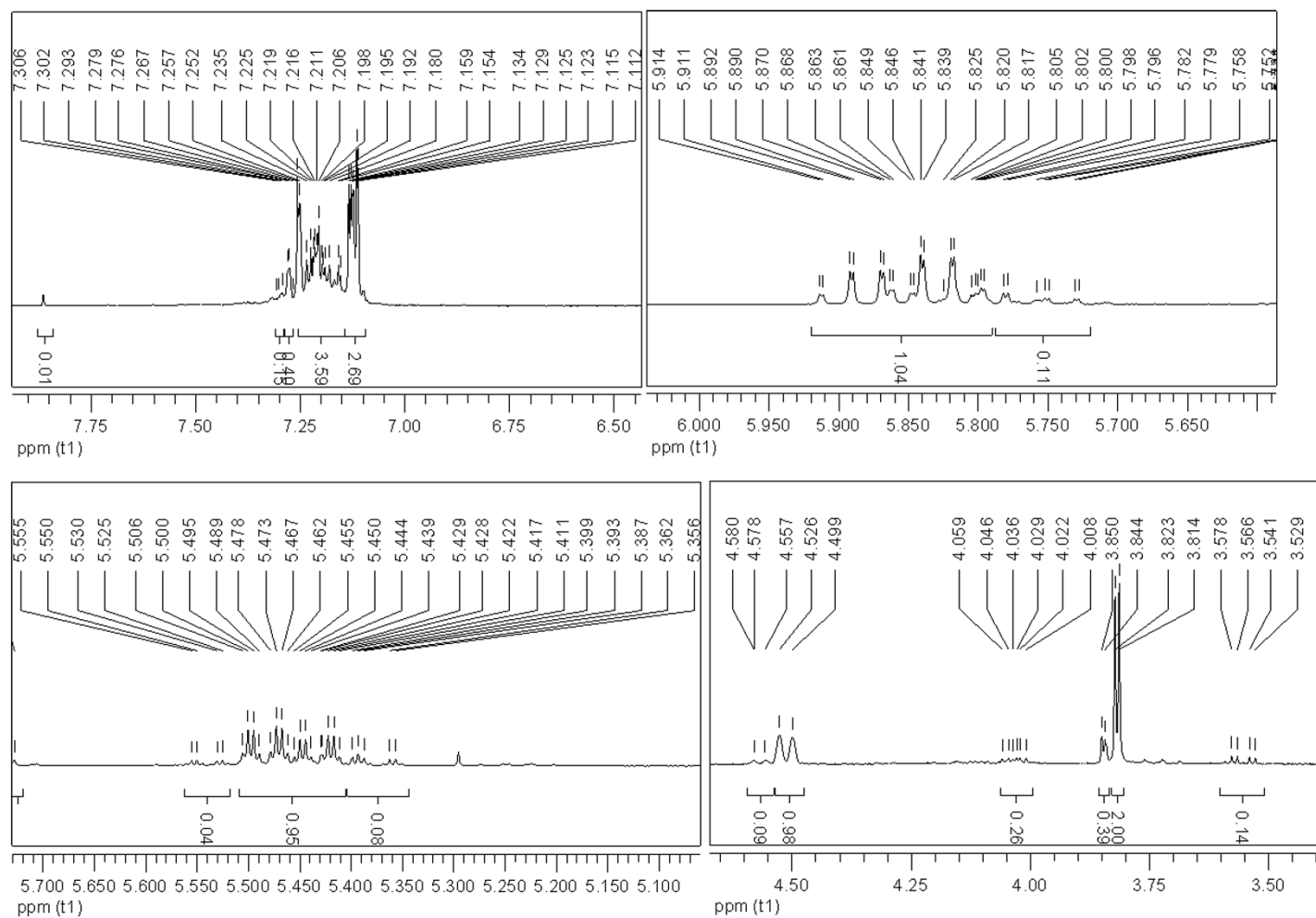
<sup>1</sup>H-NMR of compound *cis*-**7r** and *trans*-**7r** (300 MHz, CDCl<sub>3</sub>)

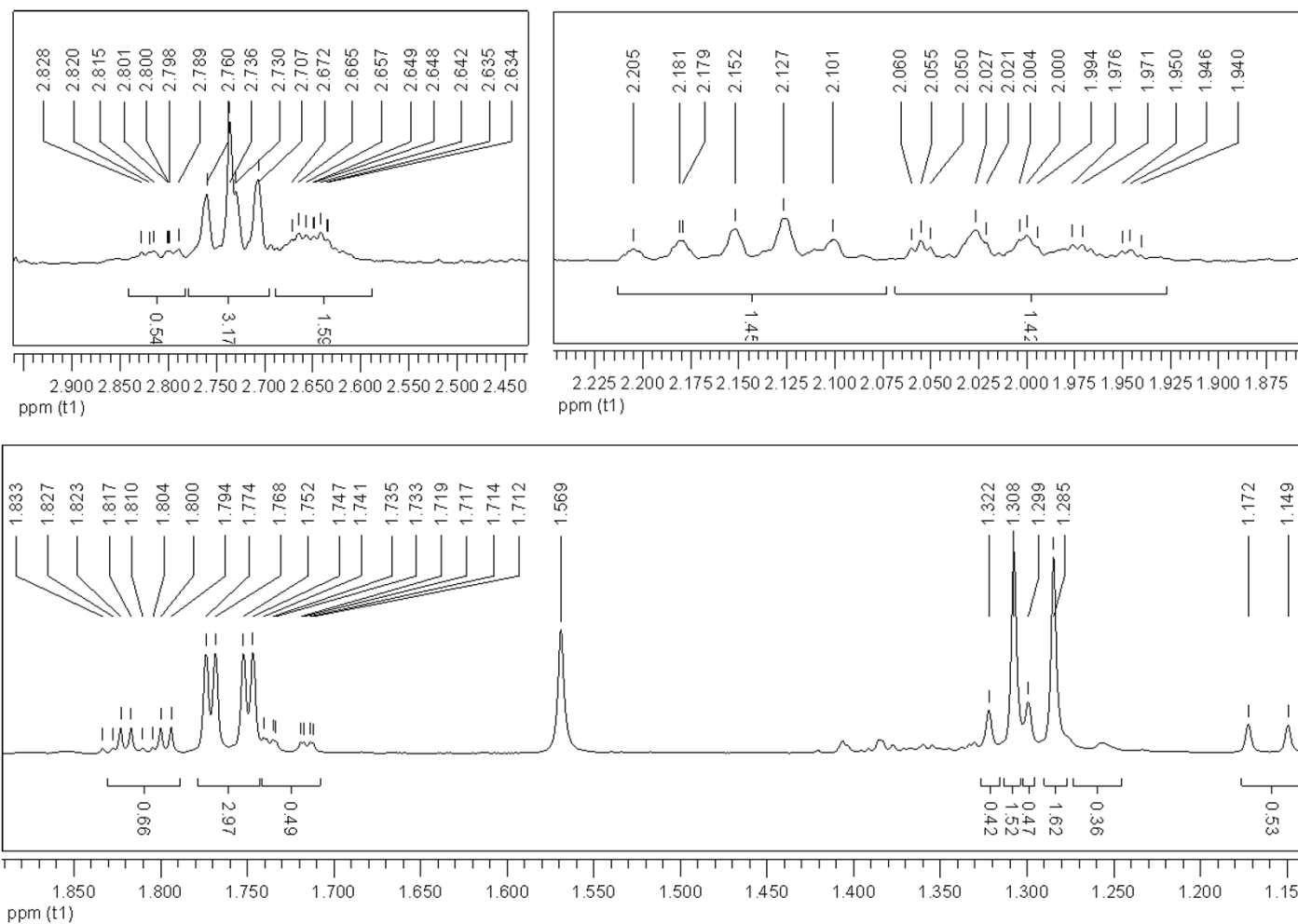
$^{13}\text{C}$ -NMR of compound *cis*-**7r** and *trans*-**7r** (75 MHz,  $\text{CDCl}_3$ )

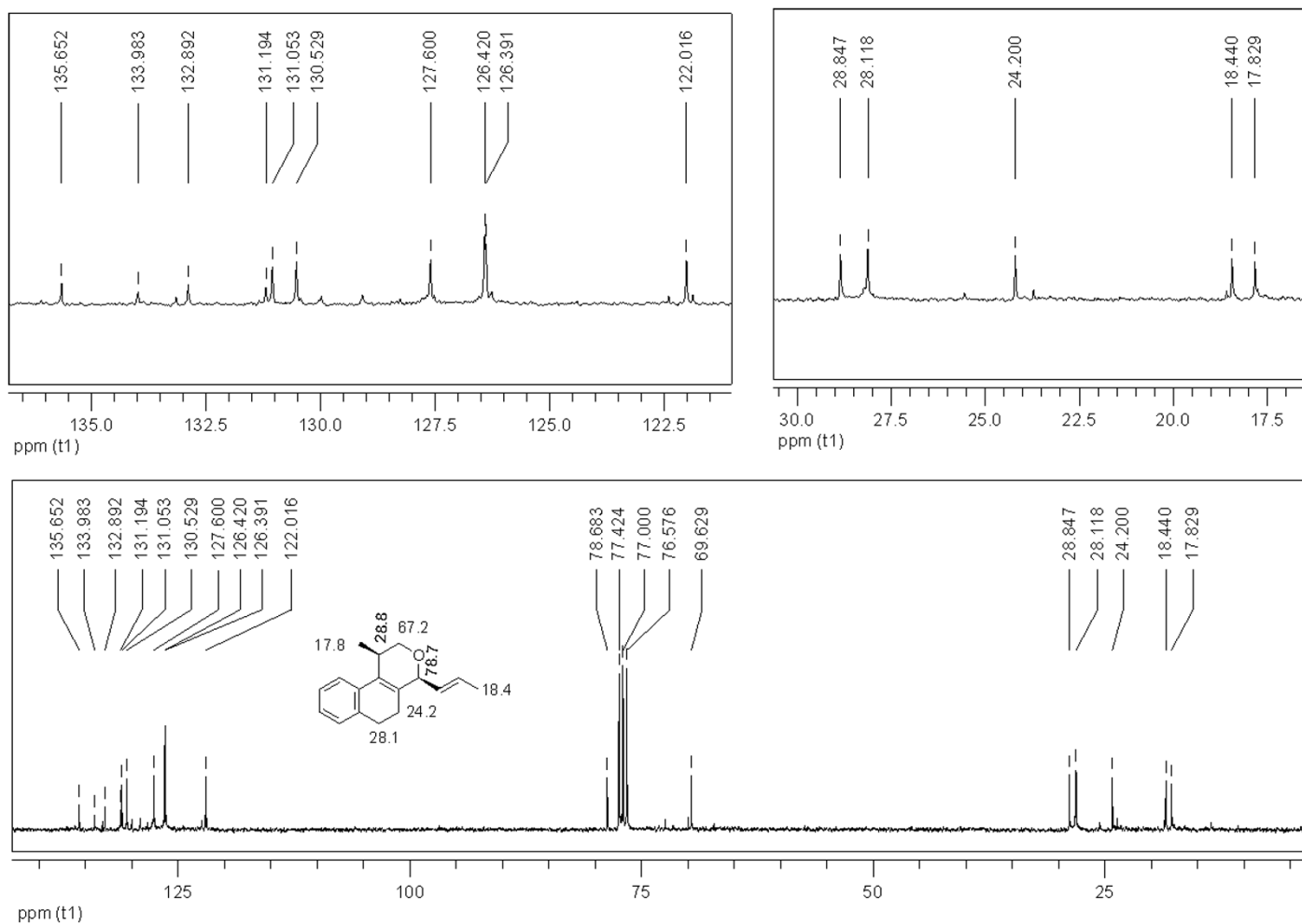
$^{13}\text{C}$ -NMR of compound *cis*-**7r** and *trans*-**7r** (75 MHz,  $\text{CDCl}_3$ )

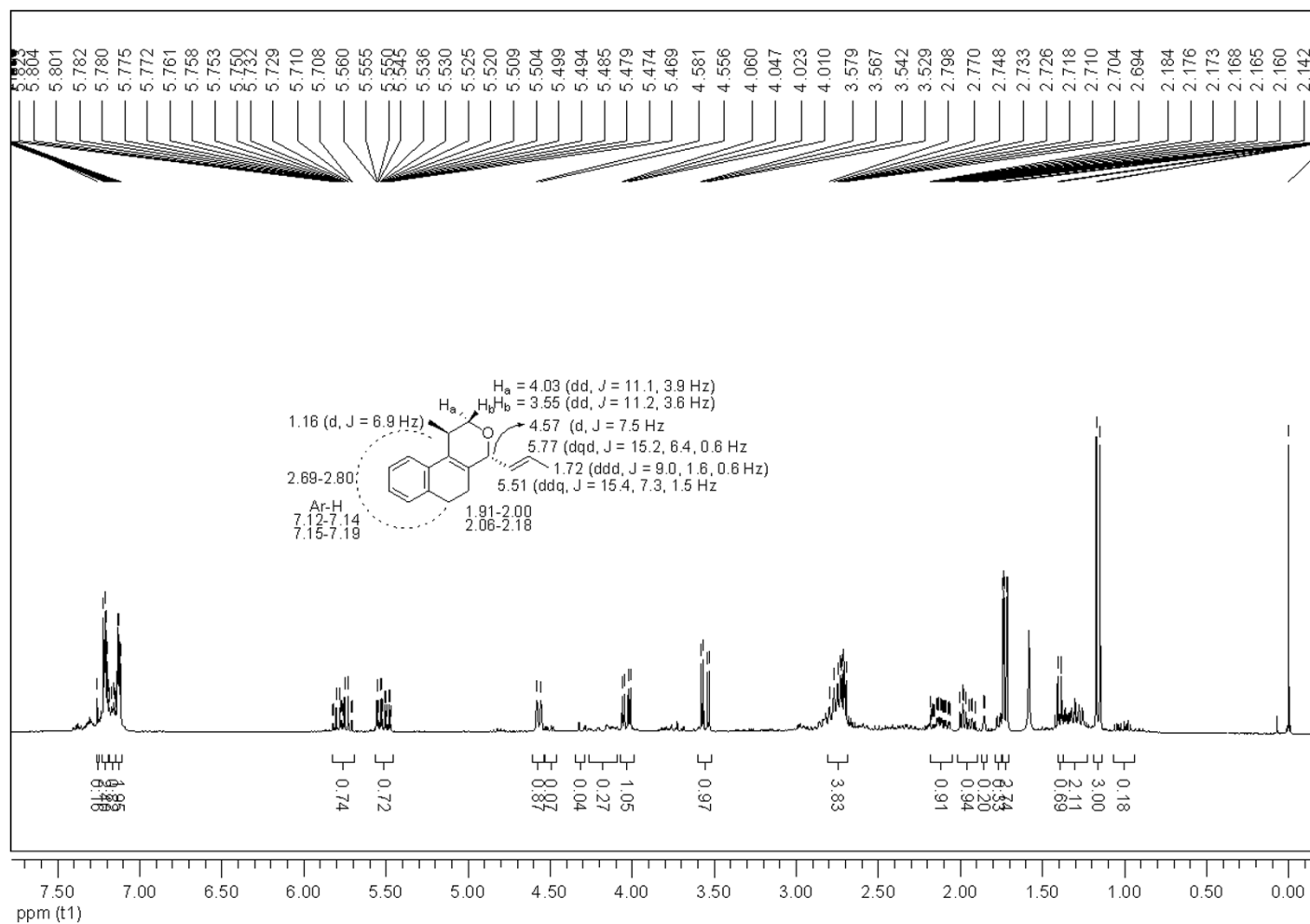
2D NOESY NMR of compound *cis*-7r and *trans*-7r (300 MHz, CDCl<sub>3</sub>)

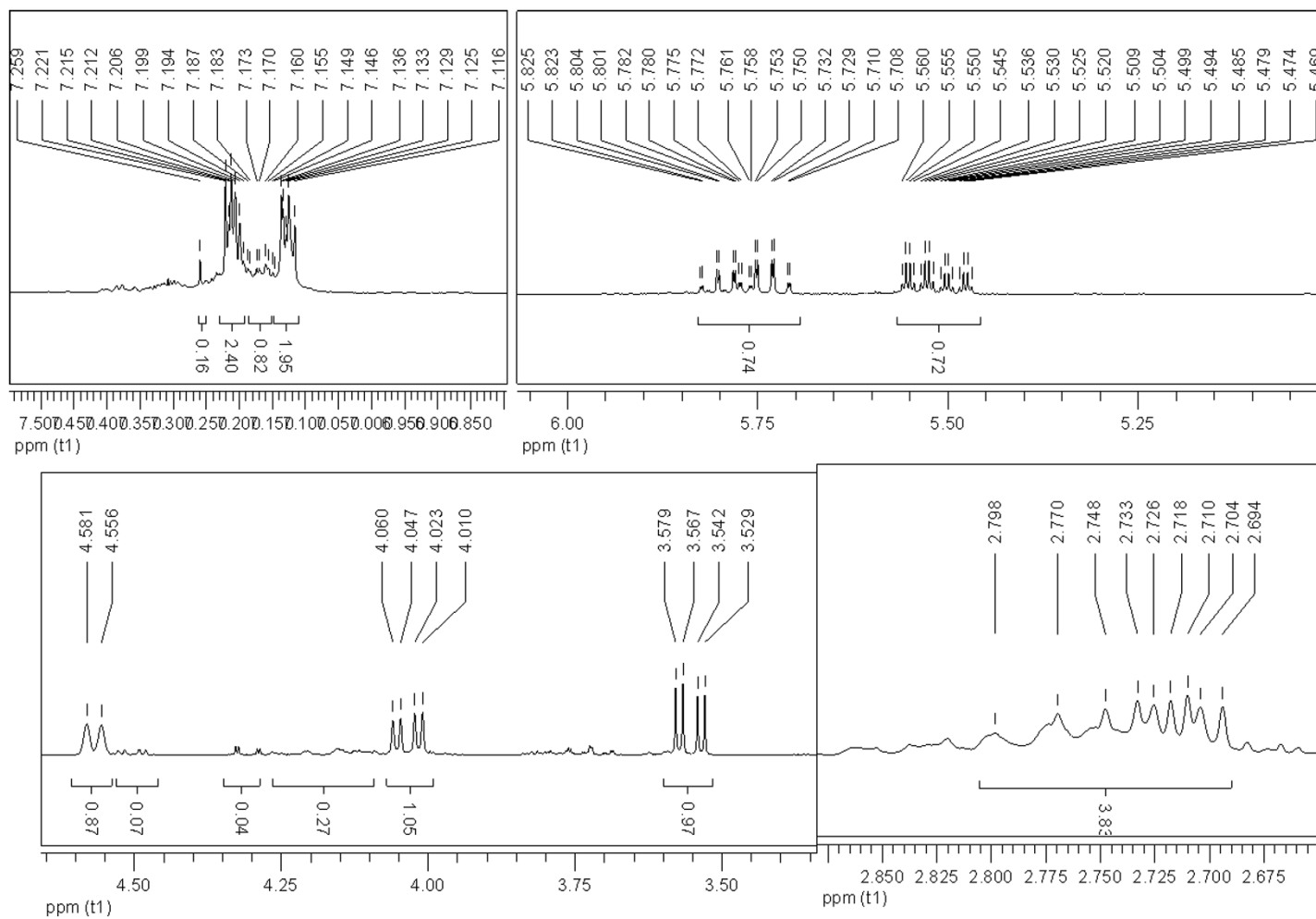
[illegible]

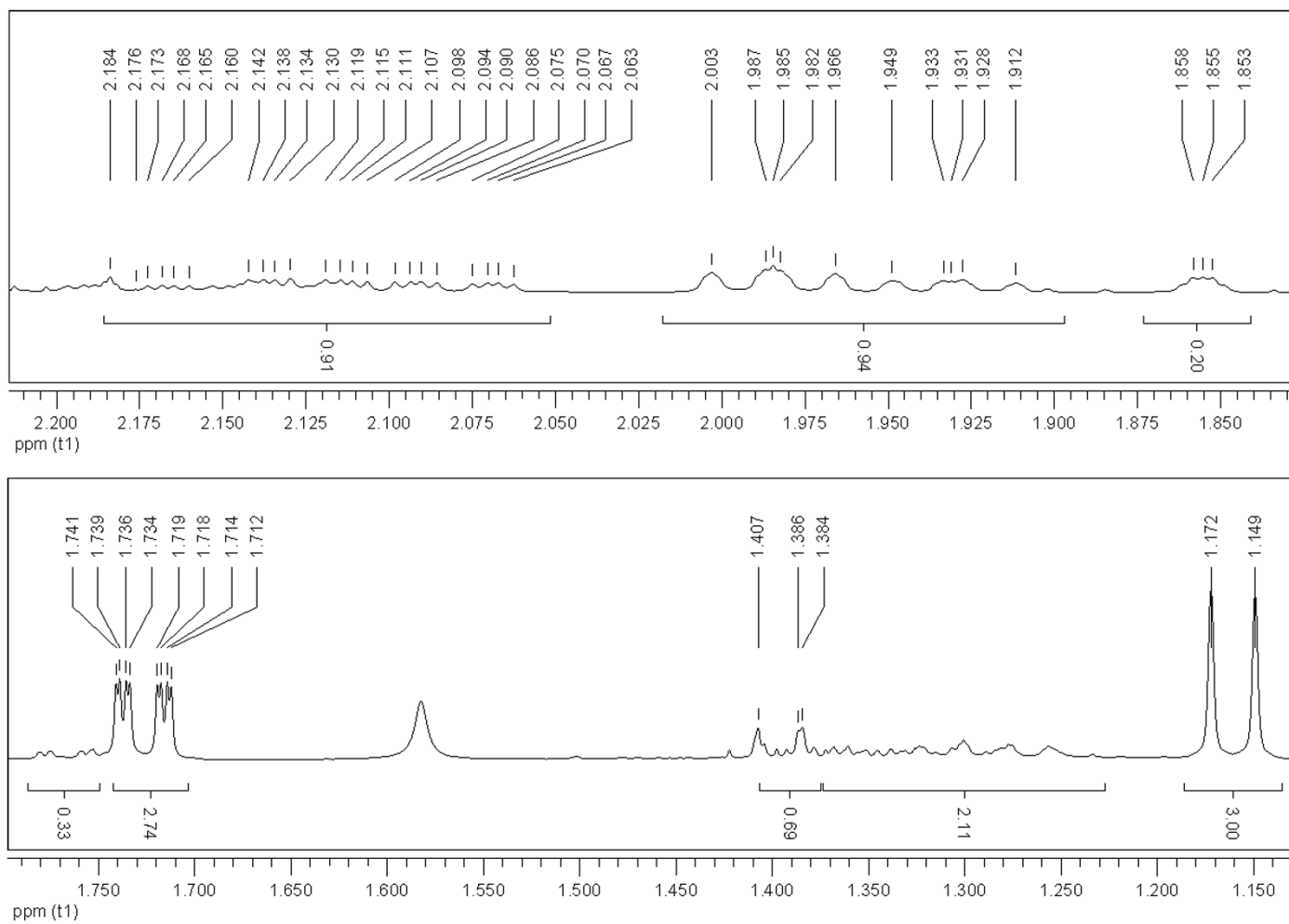
<sup>1</sup>H-NMR of compound *cis-7t* (300 MHz, CDCl<sub>3</sub>)

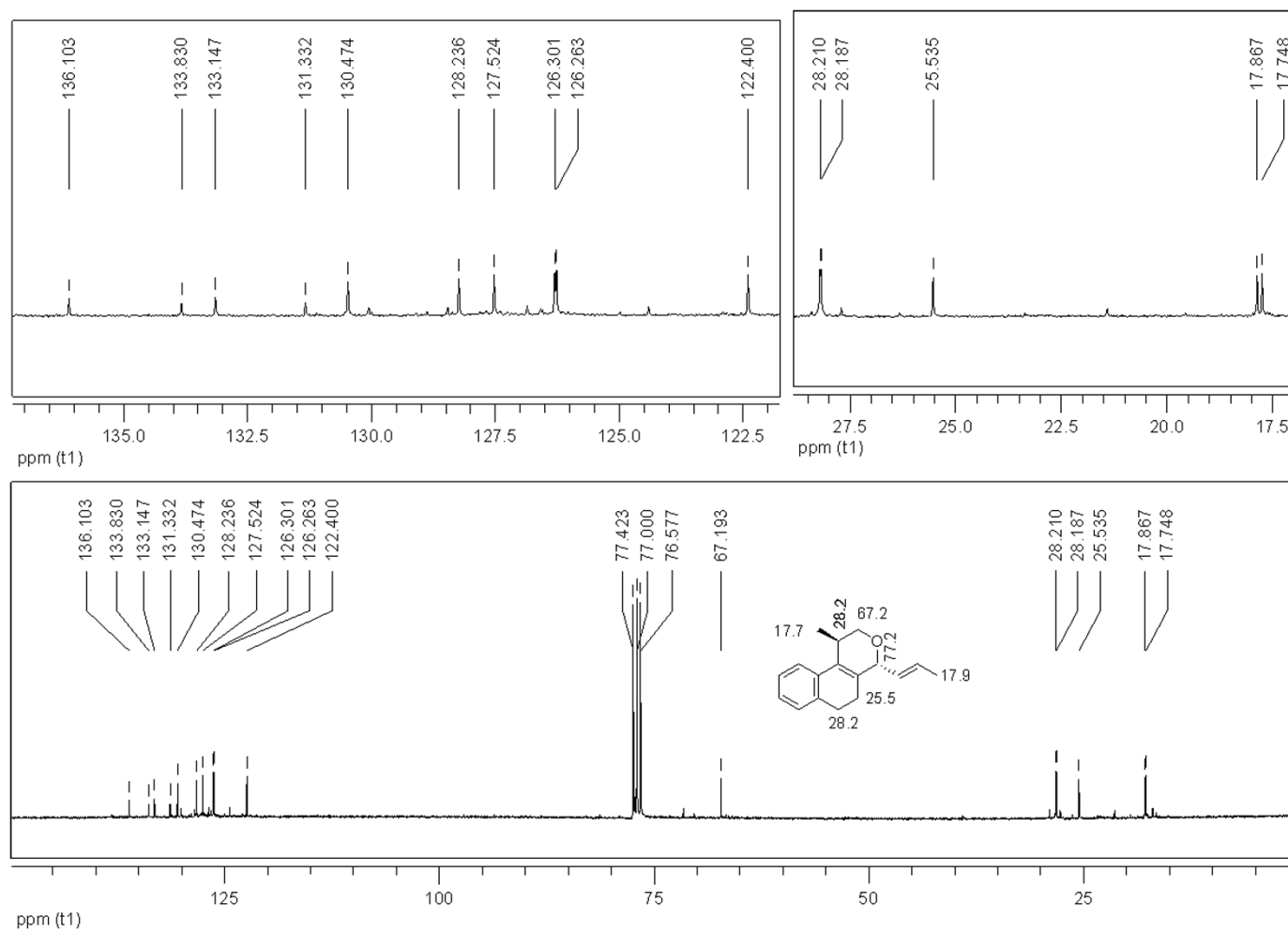
$^1\text{H}$ -NMR of compound *cis*-**7t** (300 MHz,  $\text{CDCl}_3$ )

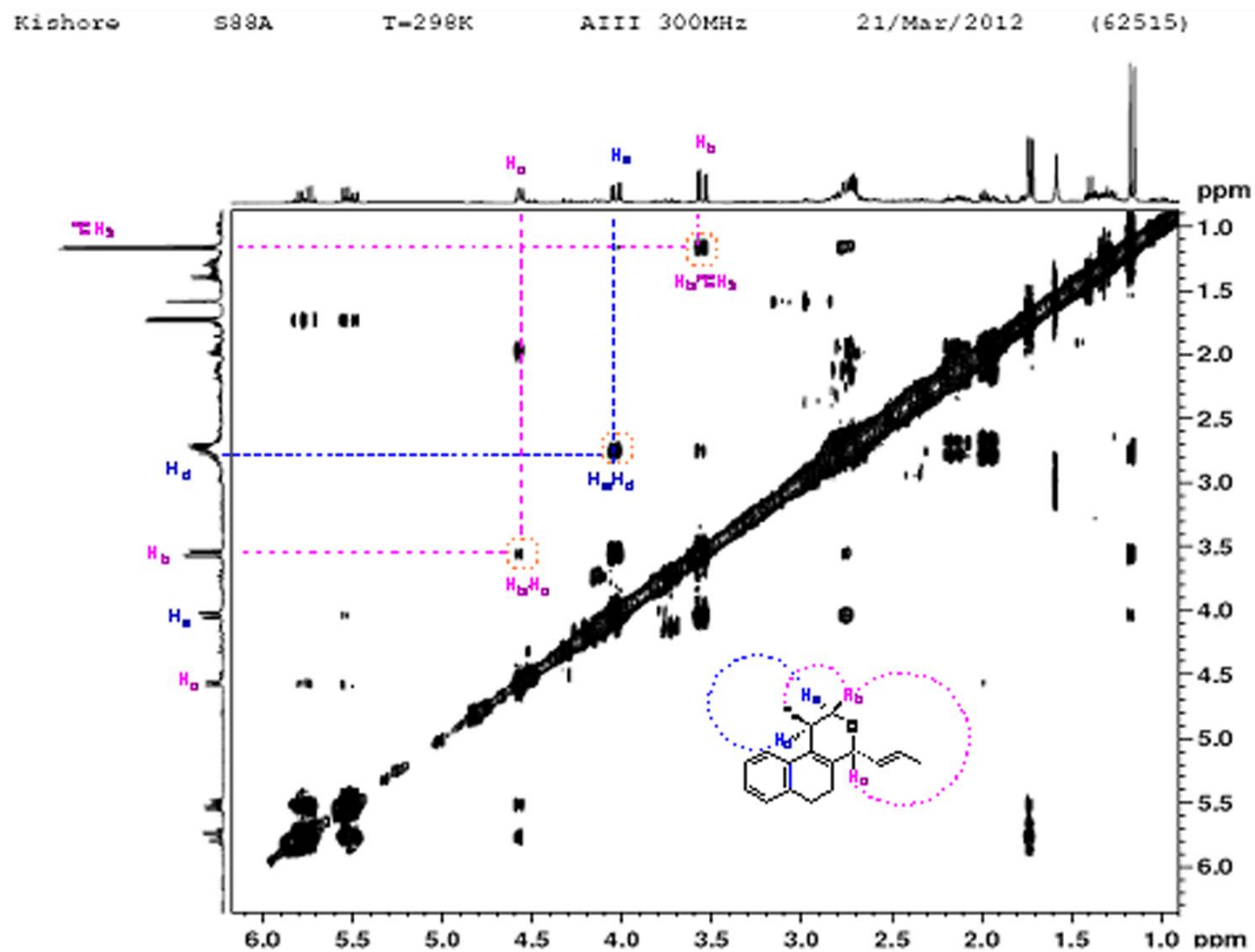
$^{13}\text{C}$ -NMR of compound *cis*-7t (75 MHz,  $\text{CDCl}_3$ )

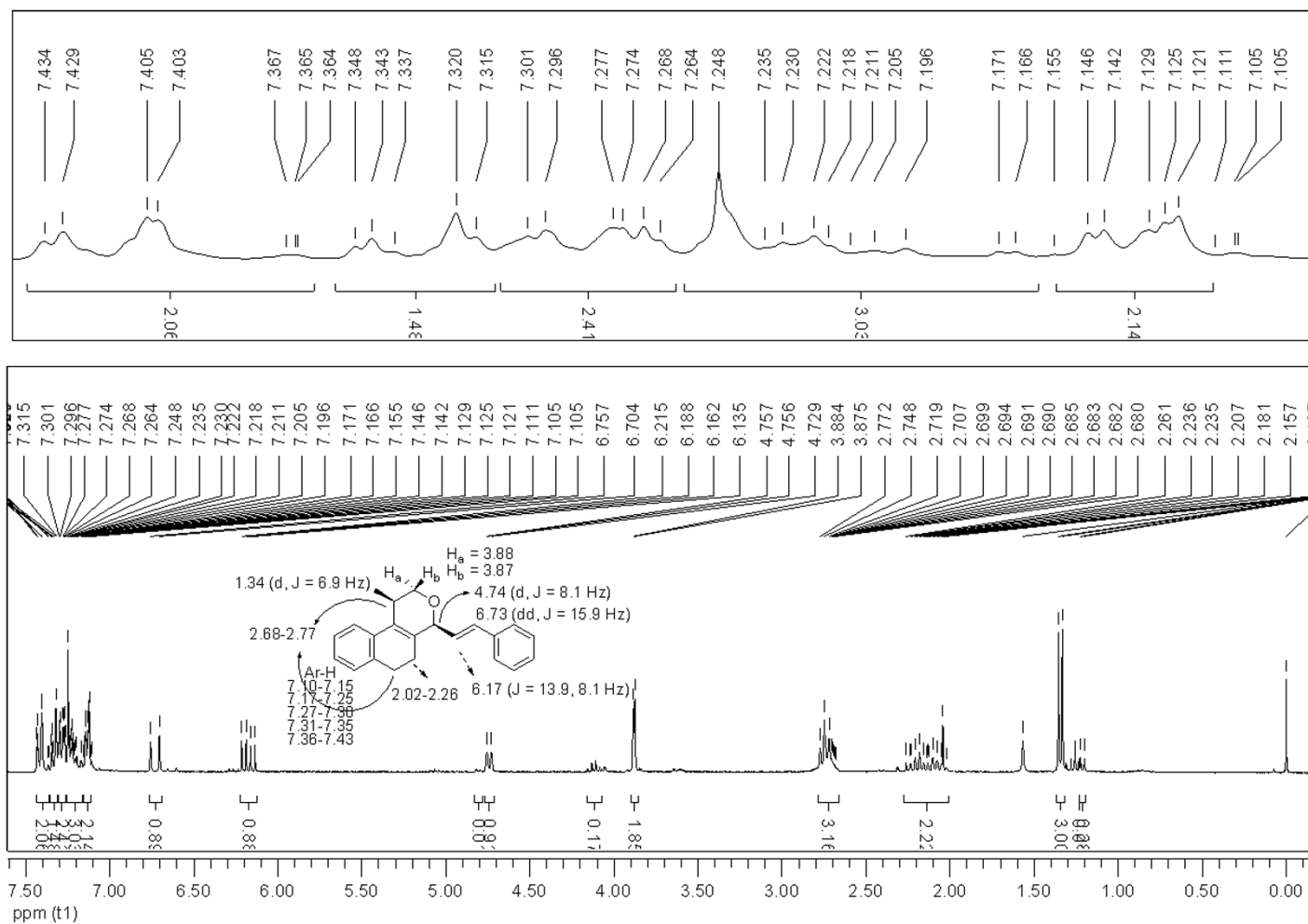
$^1\text{H}$ -NMR of compound *trans*-7t (300 MHz,  $\text{CDCl}_3$ )

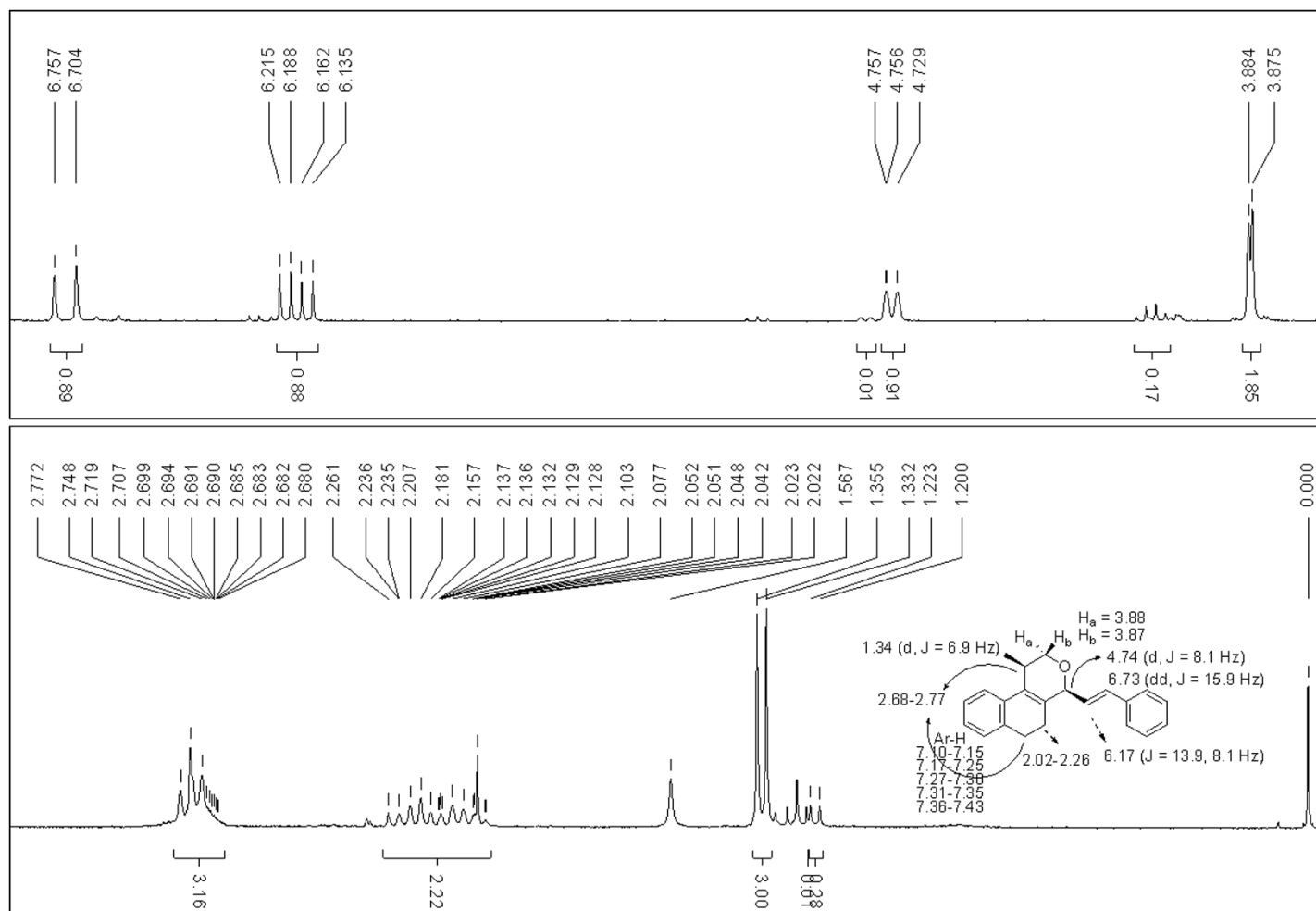
$^1\text{H}$ -NMR of compound *trans*-7t (300 MHz,  $\text{CDCl}_3$ )

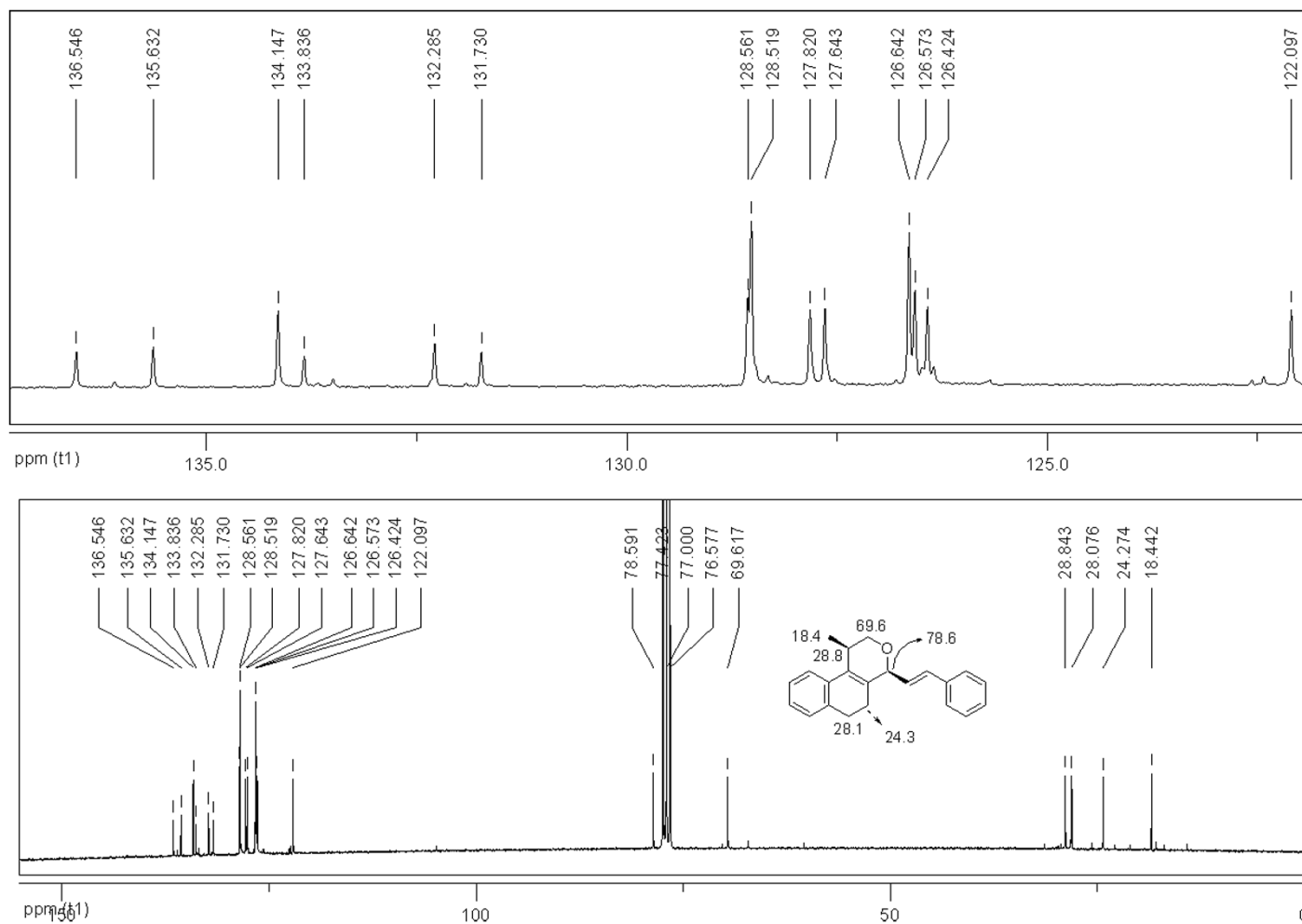
$^1\text{H}$ -NMR of compound *trans*-7t (300 MHz,  $\text{CDCl}_3$ )

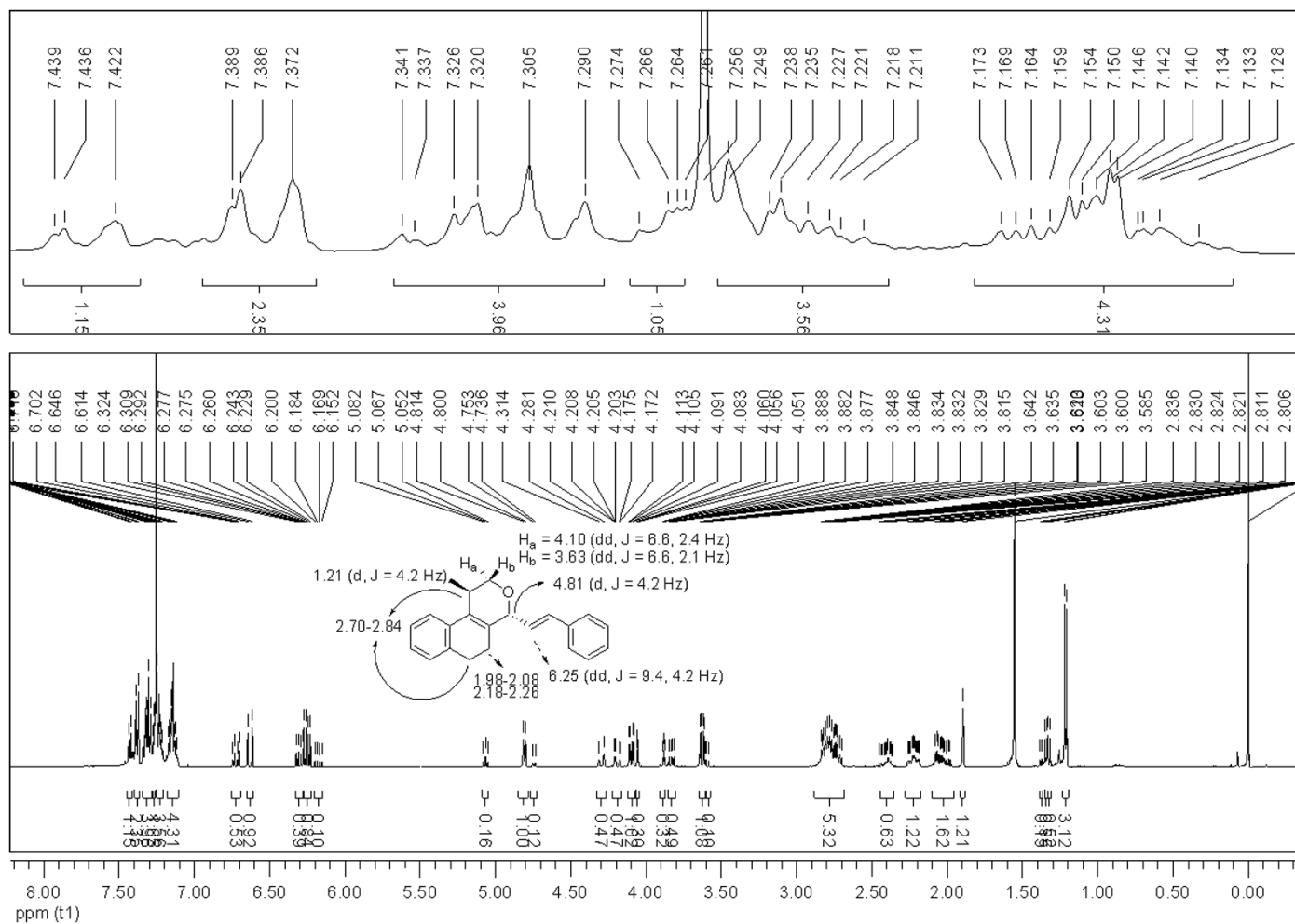
$^{13}\text{C}$ -NMR of compound *trans*-7t (75 MHz,  $\text{CDCl}_3$ )

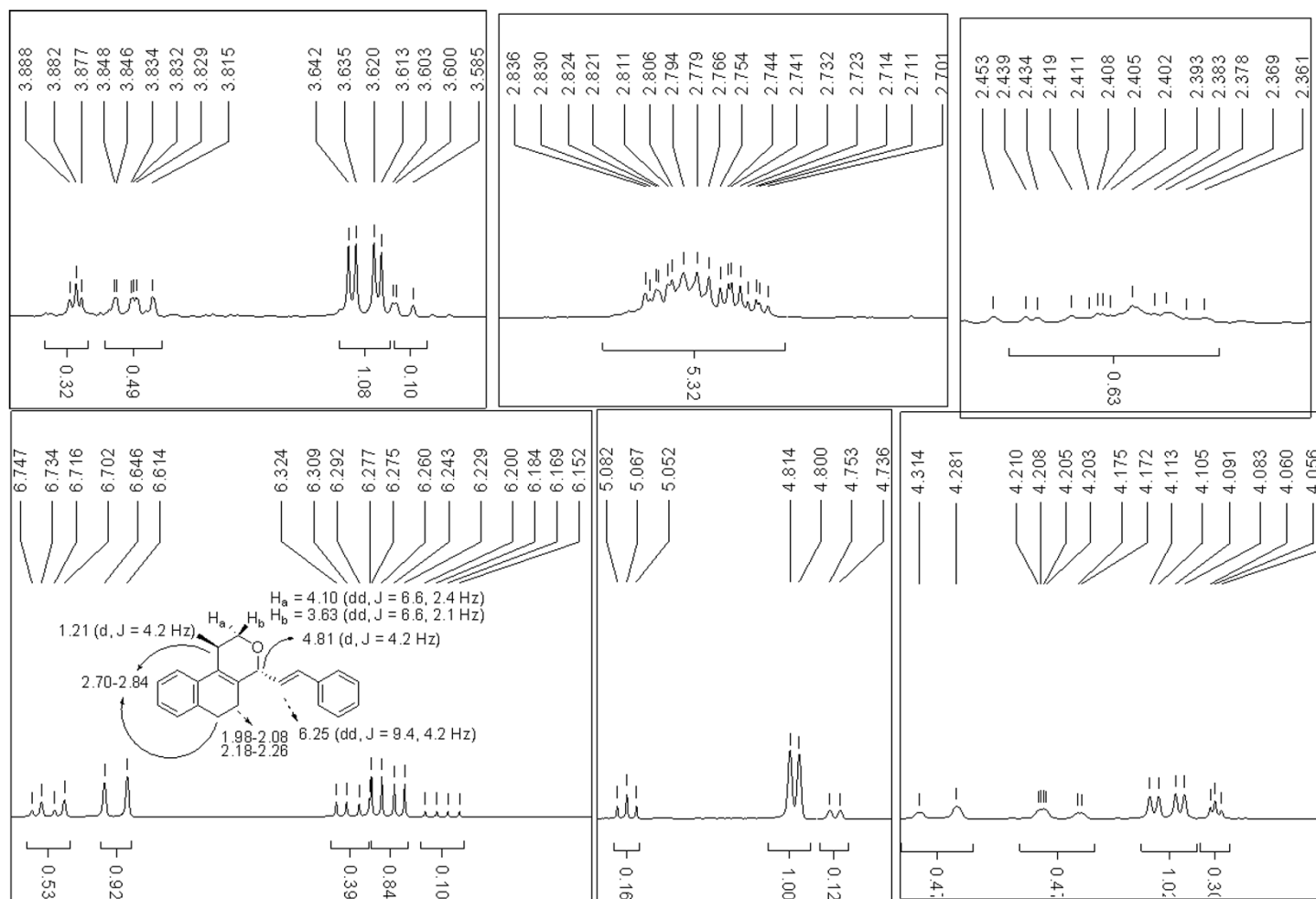
2D NOESY NMR of compound *trans*-7t (300 MHz, CDCl<sub>3</sub>)

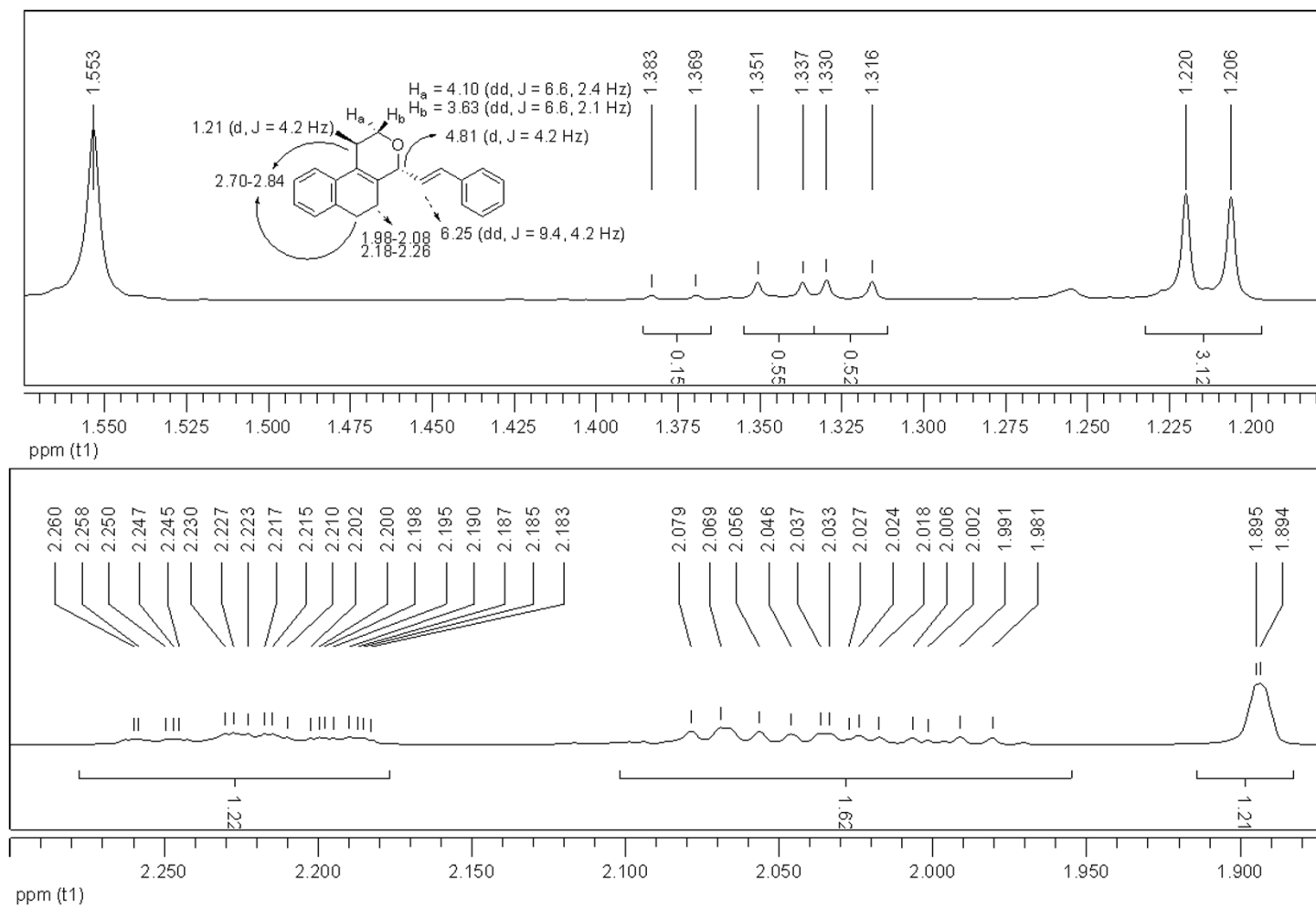
<sup>1</sup>H-NMR of compound *cis*-**7u** (300 MHz, CDCl<sub>3</sub>)

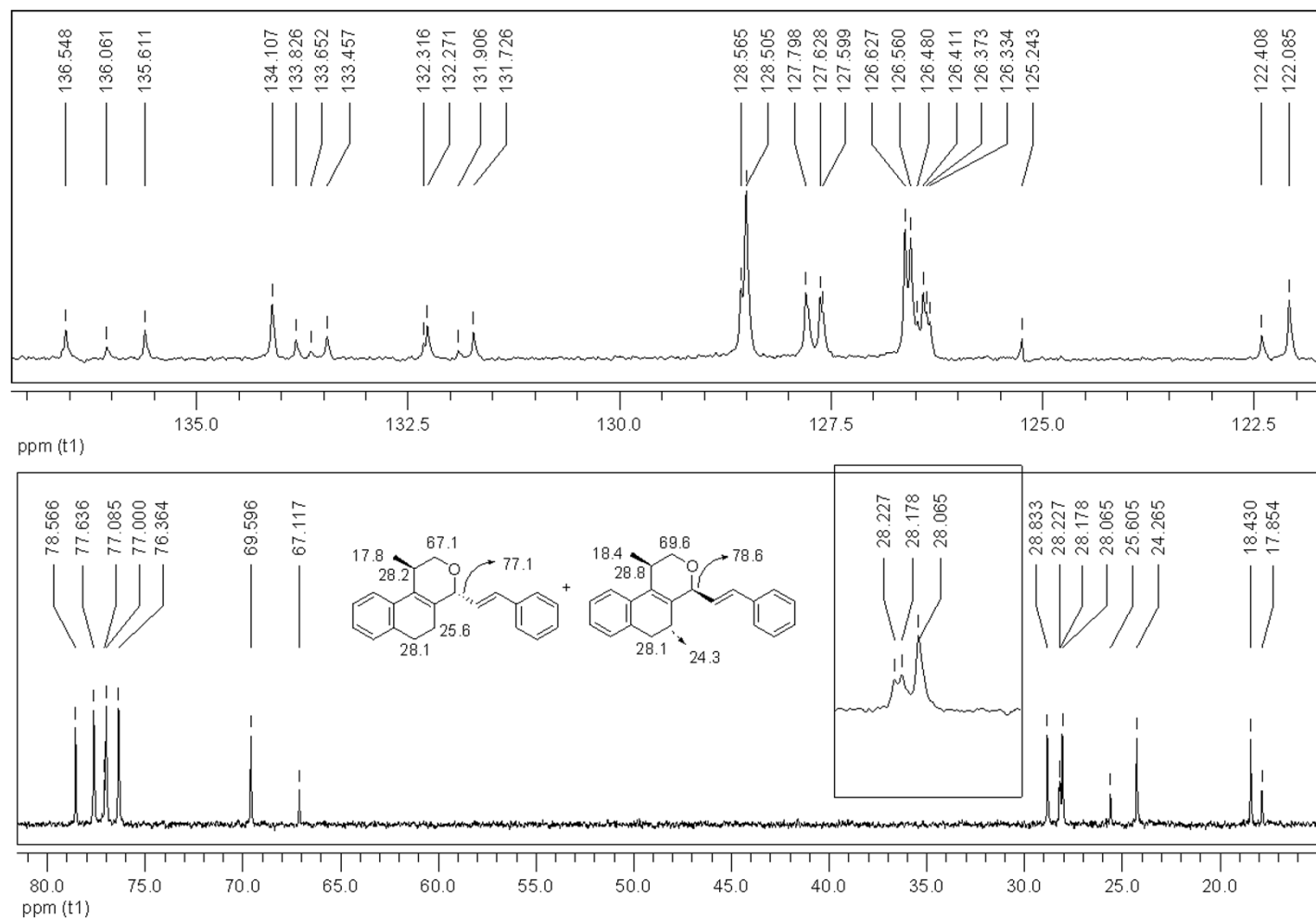
$^1\text{H}$ -NMR of compound *cis*-**7u** (300 MHz,  $\text{CDCl}_3$ )

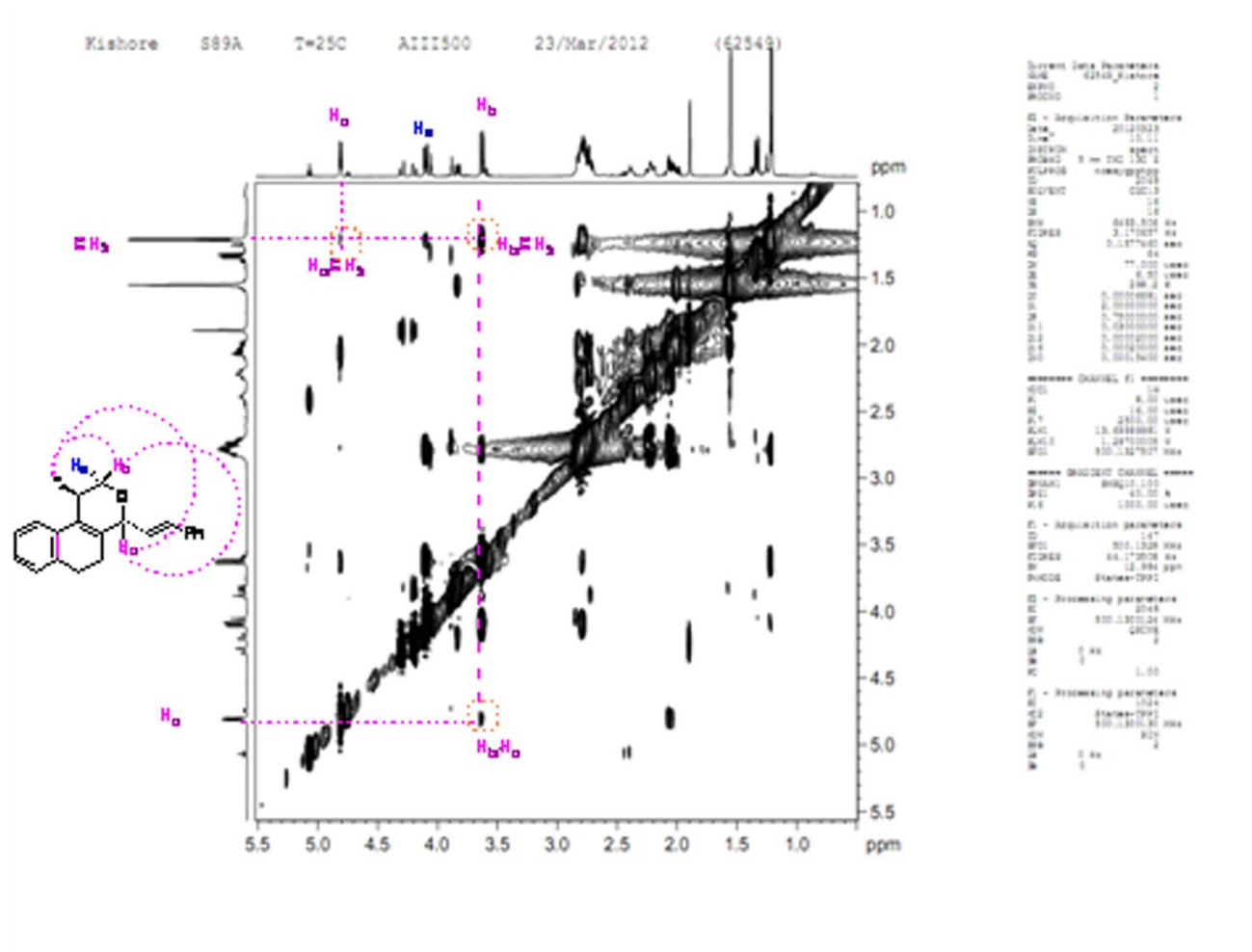
$^{13}\text{C}$ -NMR of compound *cis*-**7u** (75 MHz,  $\text{CDCl}_3$ )

<sup>1</sup>H-NMR of compound *trans*-**7u** (500 MHz, CDCl<sub>3</sub>)

$^1\text{H}$ -NMR of compound *trans*-**7u** (500 MHz,  $\text{CDCl}_3$ )

$^1\text{H}$ -NMR of compound *trans*-**7u** (500 MHz,  $\text{CDCl}_3$ )

$^{13}\text{C}$ -NMR of compound *trans*-**7u** (50 MHz,  $\text{CDCl}_3$ )

2D NOESY NMR of compound *trans*-7u (500 MHz, CDCl<sub>3</sub>)

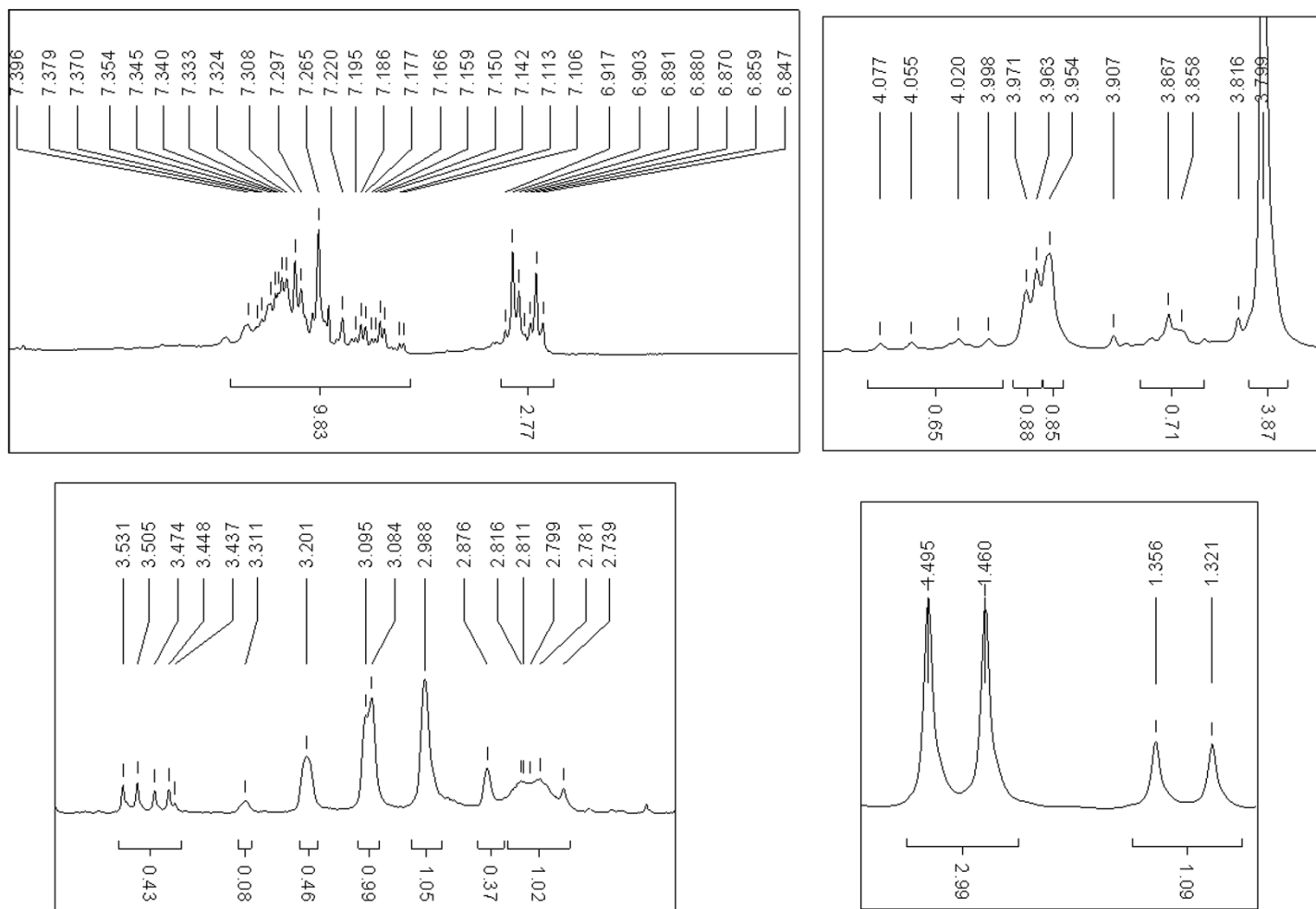
**Chemical Structure 1 (Left):** COc1ccc(cc1)[C@H]2C=C(c3ccccc3)C(OC)[C@H]2C  
Protons labeled: H<sub>a</sub>, H<sub>b</sub>, H<sub>c</sub>, H<sub>d</sub>.  
Coupling constants: 1.48 (d, J = 7.0 Hz), 2.74, 2.82.  
Peak assignments: 3.94, 3.97, 5.43, 3.09, 2.99, 3.80.

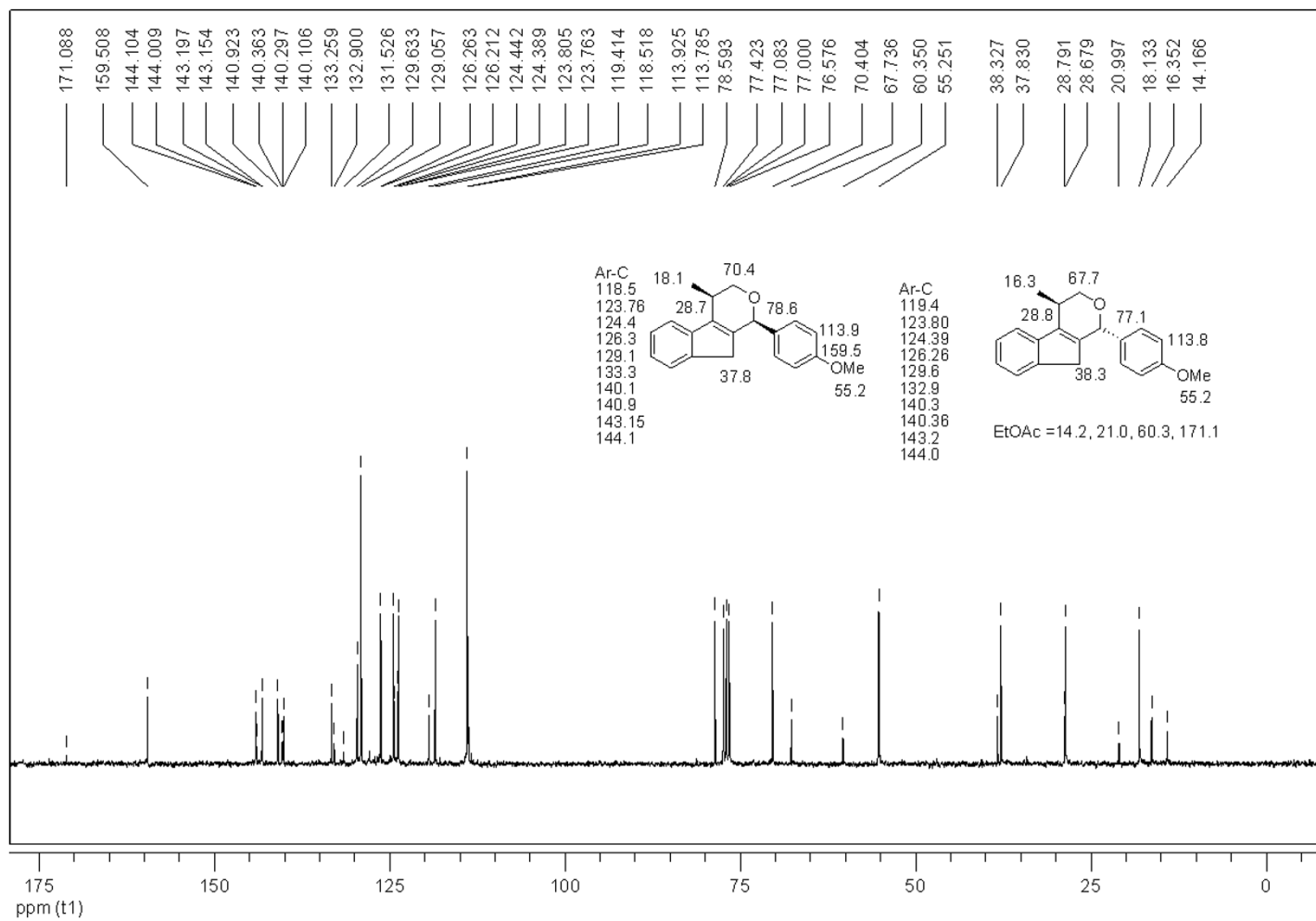
**Chemical Structure 2 (Right):** COc1ccc(cc1)[C@H]2C=C(c3ccccc3)C(OC)[C@H]2C  
Protons labeled: H<sub>a</sub>, H<sub>b</sub>, H<sub>c</sub>, H<sub>d</sub>.  
Coupling constants: 1.34 (d, J = 7.0 Hz), 3.49.  
Peak assignments: 3.86, 4.04, 5.50, 3.20, 2.88, 3.80.

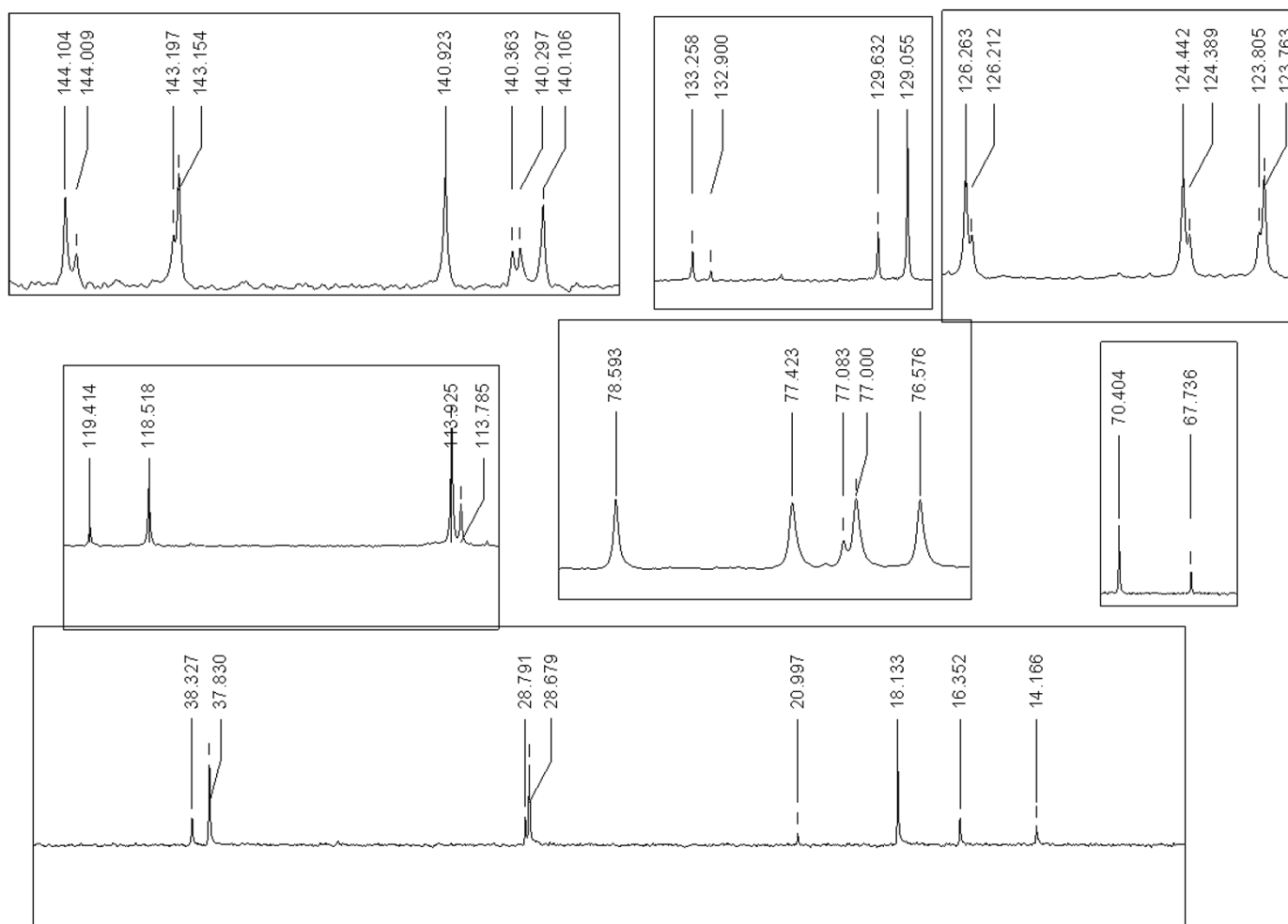
**1H NMR Spectrum Data:**

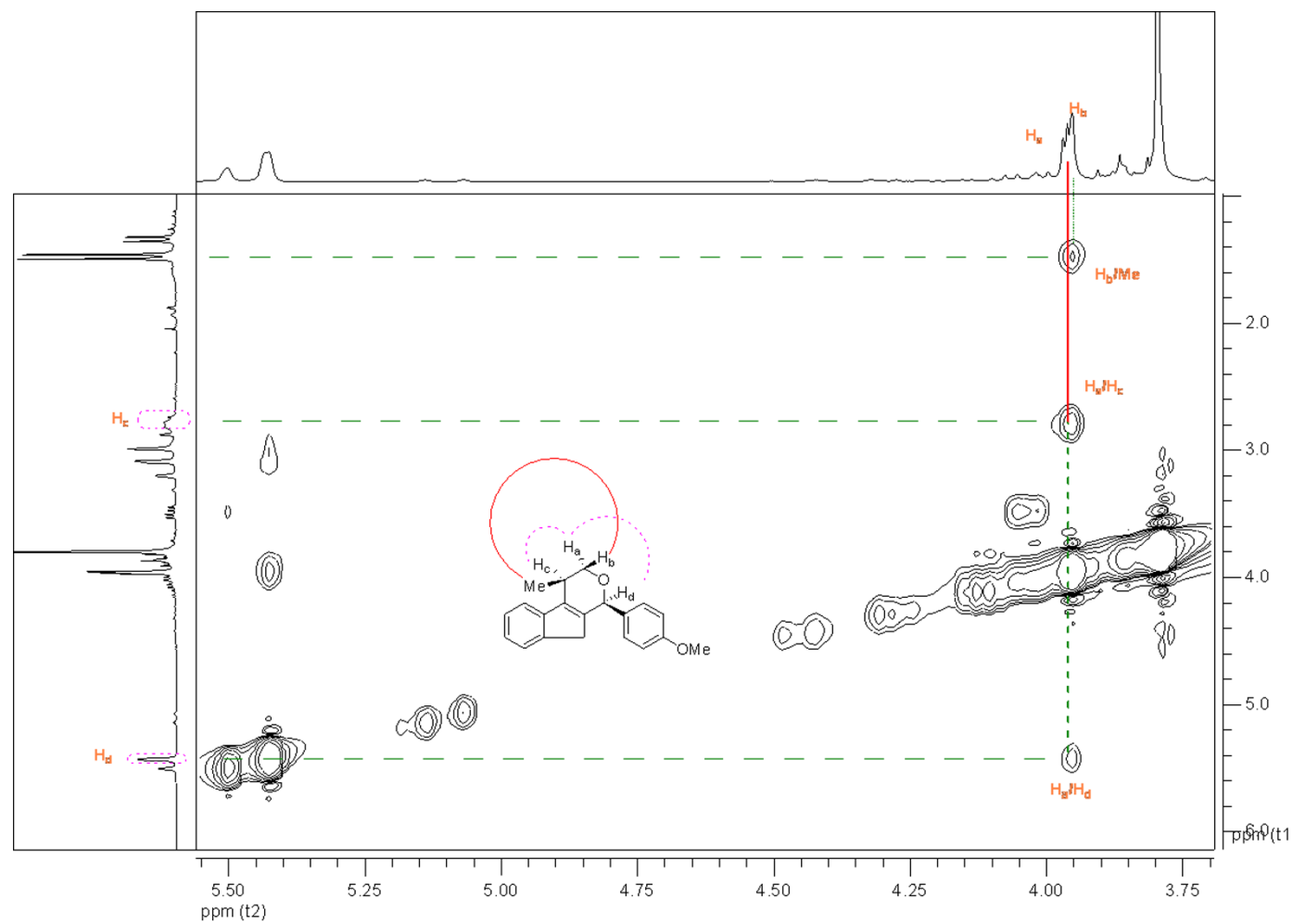
Chemical Shift (ppm)	Integration
7.396 - 7.324	9.83
7.297 - 7.252	2.77
6.917 - 6.847	0.66
5.503 - 5.427	0.99
3.971 - 3.858	0.97
3.954 - 3.879	0.42
3.867 - 3.804	0.46
3.799 - 3.701	0.48
3.531 - 3.437	0.43
3.505 - 3.474	0.40
3.448 - 3.437	0.46
3.201 - 3.084	2.99
3.095 - 2.988	1.09
2.876 - 2.816	1.09
2.816 - 2.799	1.09
2.799 - 2.781	1.09
2.781 - 2.739	1.09
2.739 - 2.701	1.09
2.701 - 2.684	1.09
2.684 - 2.667	1.09
2.667 - 2.650	1.09
2.650 - 2.633	1.09
2.633 - 2.616	1.09
2.616 - 2.599	1.09
2.599 - 2.582	1.09
2.582 - 2.565	1.09
2.565 - 2.548	1.09
2.548 - 2.531	1.09
2.531 - 2.514	1.09
2.514 - 2.497	1.09
2.497 - 2.480	1.09
2.480 - 2.463	1.09
2.463 - 2.446	1.09
2.446 - 2.429	1.09
2.429 - 2.412	1.09
2.412 - 2.395	1.09
2.395 - 2.378	1.09
2.378 - 2.361	1.09
2.361 - 2.344	1.09
2.344 - 2.327	1.09
2.327 - 2.310	1.09
2.310 - 2.293	1.09
2.293 - 2.276	1.09
2.276 - 2.259	1.09
2.259 - 2.242	1.09
2.242 - 2.225	1.09
2.225 - 2.208	1.09
2.208 - 2.191	1.09
2.191 - 2.174	1.09
2.174 - 2.157	1.09
2.157 - 2.140	1.09
2.140 - 2.123	1.09
2.123 - 2.106	1.09
2.106 - 2.089	1.09
2.089 - 2.072	1.09
2.072 - 2.055	1.09
2.055 - 2.038	1.09
2.038 - 2.021	1.09
2.021 - 2.004	1.09
2.004 - 1.987	1.09
1.987 - 1.970	1.09
1.970 - 1.953	1.09
1.953 - 1.936	1.09
1.936 - 1.919	1.09
1.919 - 1.902	1.09
1.902 - 1.885	1.09
1.885 - 1.868	1.09
1.868 - 1.851	1.09
1.851 - 1.834	1.09
1.834 - 1.817	1.09
1.817 - 1.800	1.09
1.800 - 1.783	1.09
1.783 - 1.766	1.09
1.766 - 1.749	1.09
1.749 - 1.732	1.09
1.732 - 1.715	1.09
1.715 - 1.698	1.09
1.698 - 1.681	1.09
1.681 - 1.664	1.09
1.664 - 1.647	1.09
1.647 - 1.630	1.09
1.630 - 1.613	1.09
1.613 - 1.596	1.09
1.596 - 1.579	1.09
1.579 - 1.562	1.09
1.562 - 1.545	1.09
1.545 - 1.528	1.09
1.528 - 1.511	1.09
1.511 - 1.494	1.09
1.494 - 1.477	1.09
1.477 - 1.460	1.09
1.460 - 1.443	1.09
1.443 - 1.426	1.09
1.426 - 1.409	1.09
1.409 - 1.392	1.09
1.392 - 1.375	1.09
1.375 - 1.358	1.09
1.358 - 1.341	1.09
1.341 - 1.324	1.09
1.324 - 1.307	1.09
1.307 - 1.290	1.09
1.290 - 1.273	1.09
1.273 - 1.256	1.09
1.256 - 1.239	1.09
1.239 - 1.222	1.09
1.222 - 1.205	1.09
1.205 - 1.188	1.09
1.188 - 1.171	1.09
1.171 - 1.154	1.09
1.154 - 1.137	1.09
1.137 - 1.120	1.09
1.120 - 1.103	1.09
1.103 - 1.086	1.09
1.086 - 1.069	1.09
1.069 - 1.052	1.09
1.052 - 1.035	1.09
1.035 - 1.018	1.09
1.018 - 1.001	1.09
1.001 - 0.984	1.09
0.984 - 0.967	1.09
0.967 - 0.950	1.09
0.950 - 0.933	1.09
0	

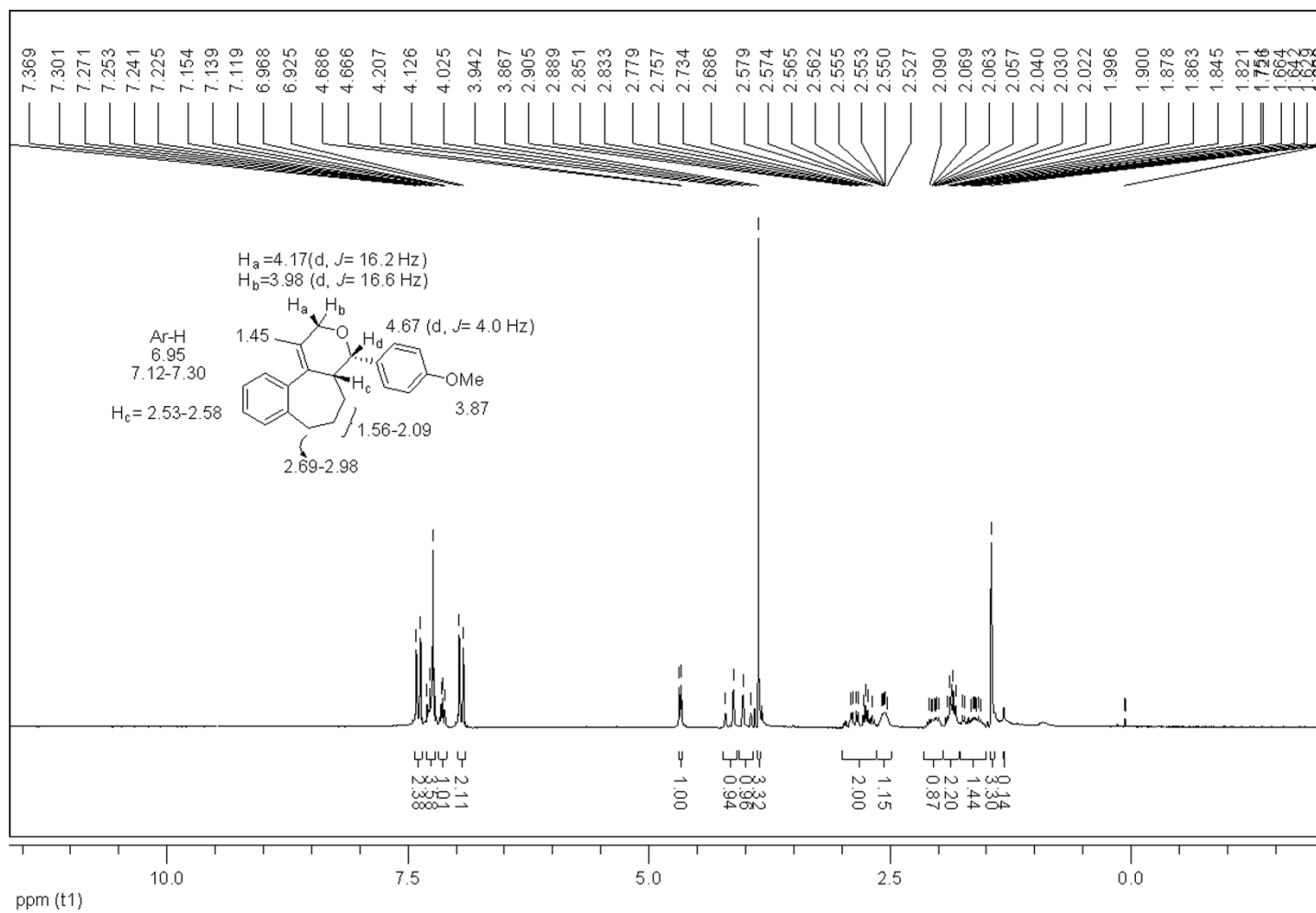
<sup>1</sup>H-NMR of compounds *cis*-**13b** and *trans*-**13b** (300 MHz, CDCl<sub>3</sub>)

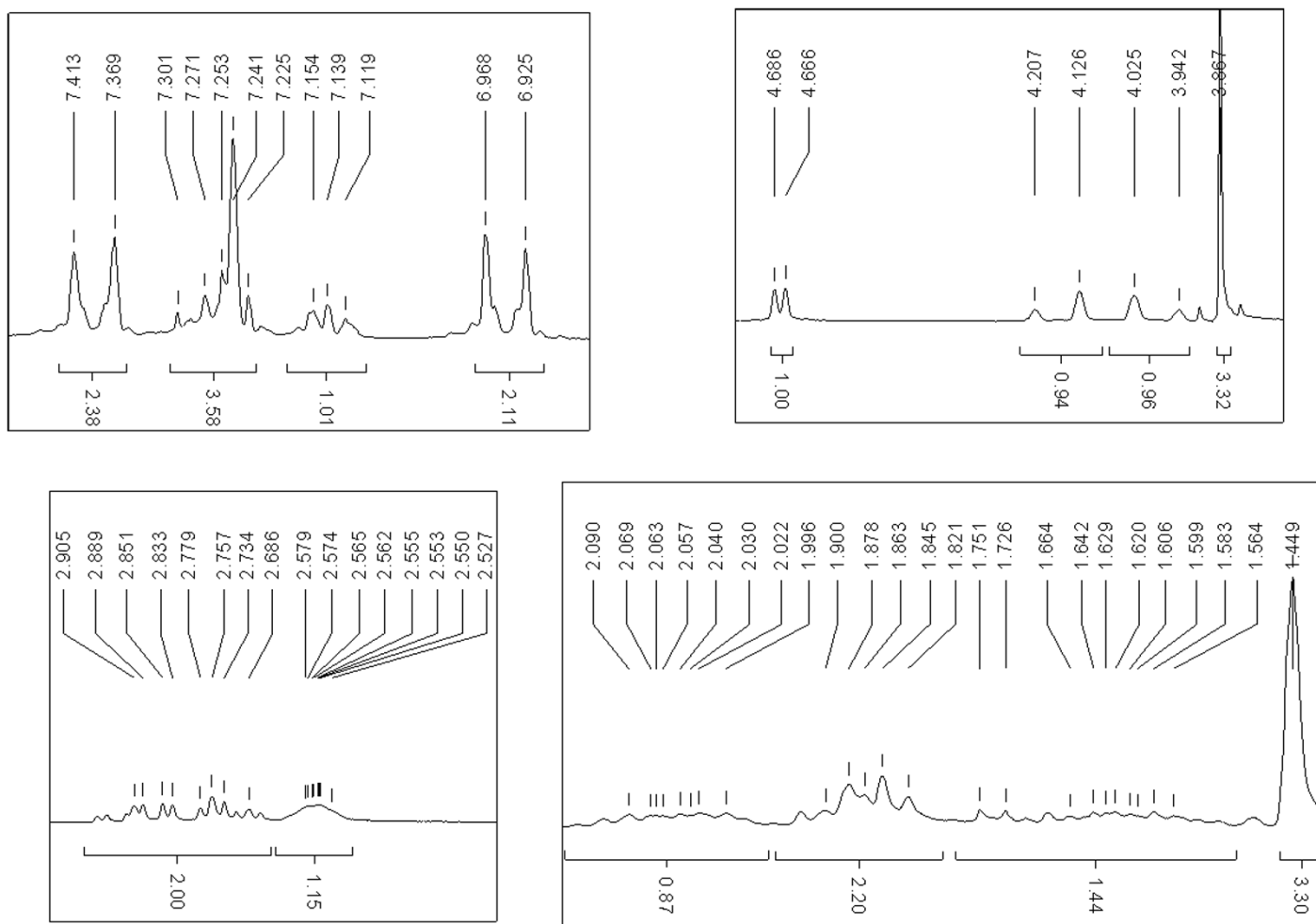


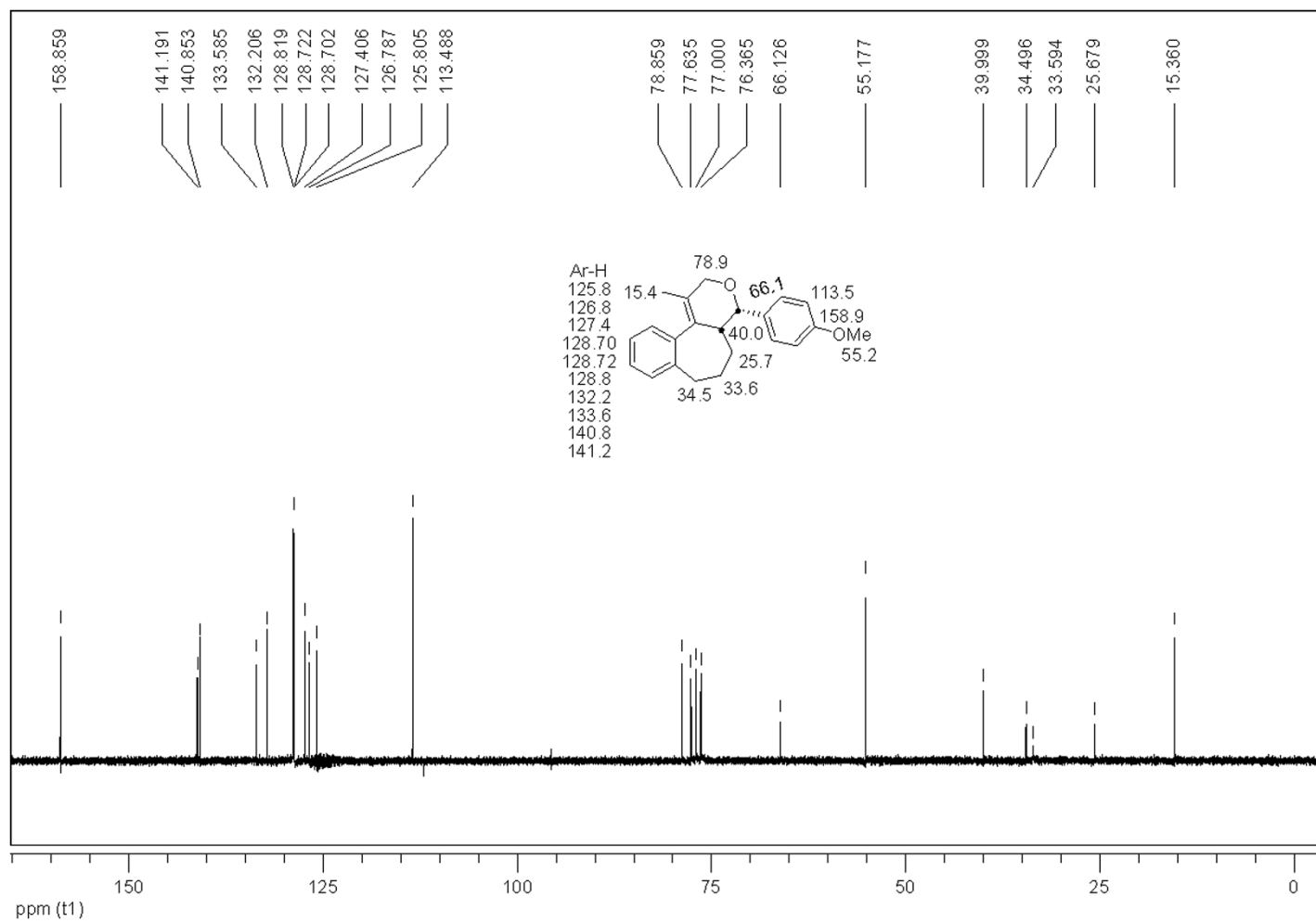
$^{13}\text{C}$ -NMR of compounds *cis*-**13b** and *trans*-**13b** (75 MHz,  $\text{CDCl}_3$ )

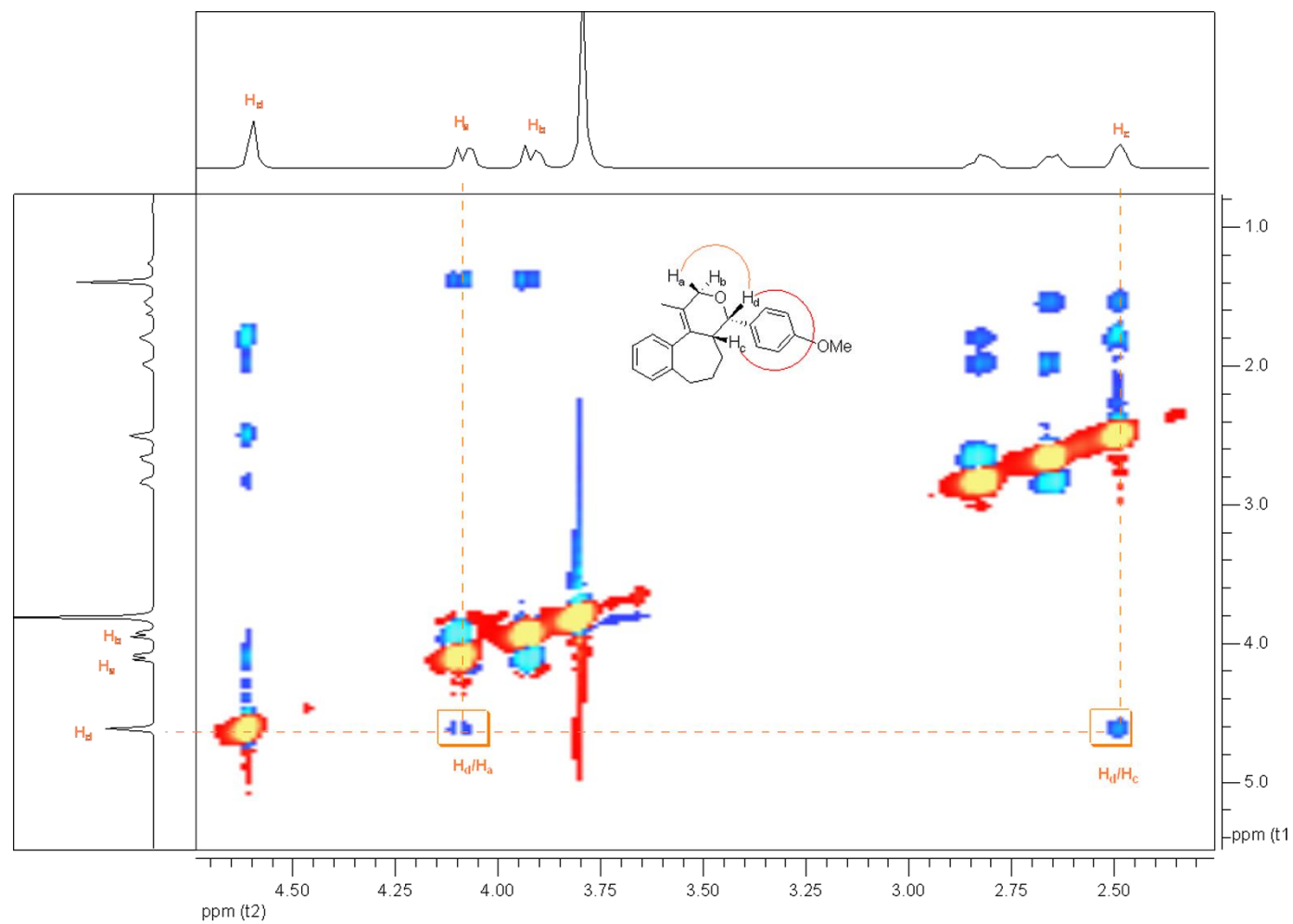
$^{13}\text{C}$ -NMR of compounds *cis*-**13b** and *trans*-**13b** (75 MHz,  $\text{CDCl}_3$ )

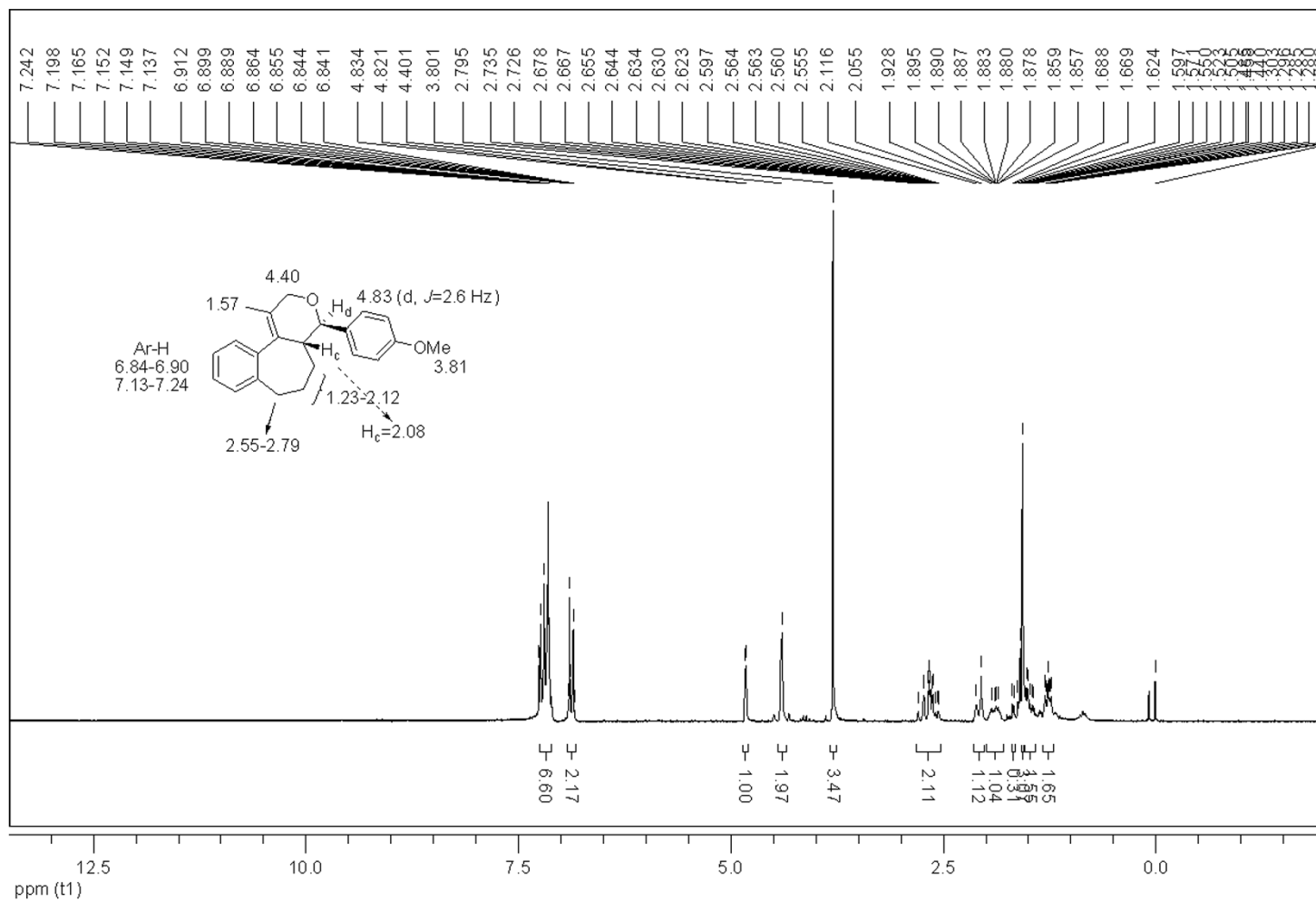
2D NOESY NMR of compound *cis*-**13b** (300 MHz, CDCl<sub>3</sub>)

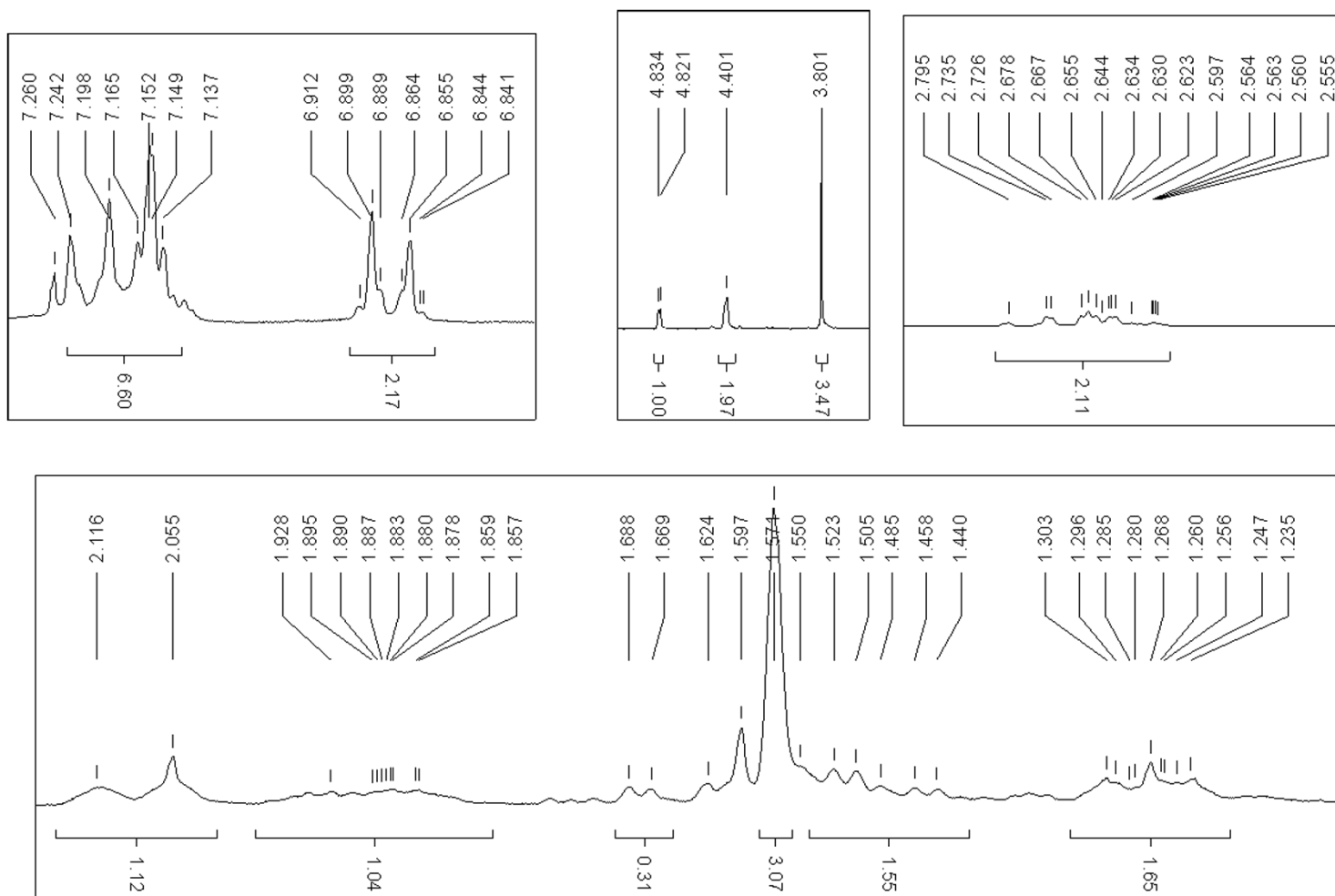
$^1\text{H}$ -NMR of compound *cis*-14c (200 MHz,  $\text{CDCl}_3$ )

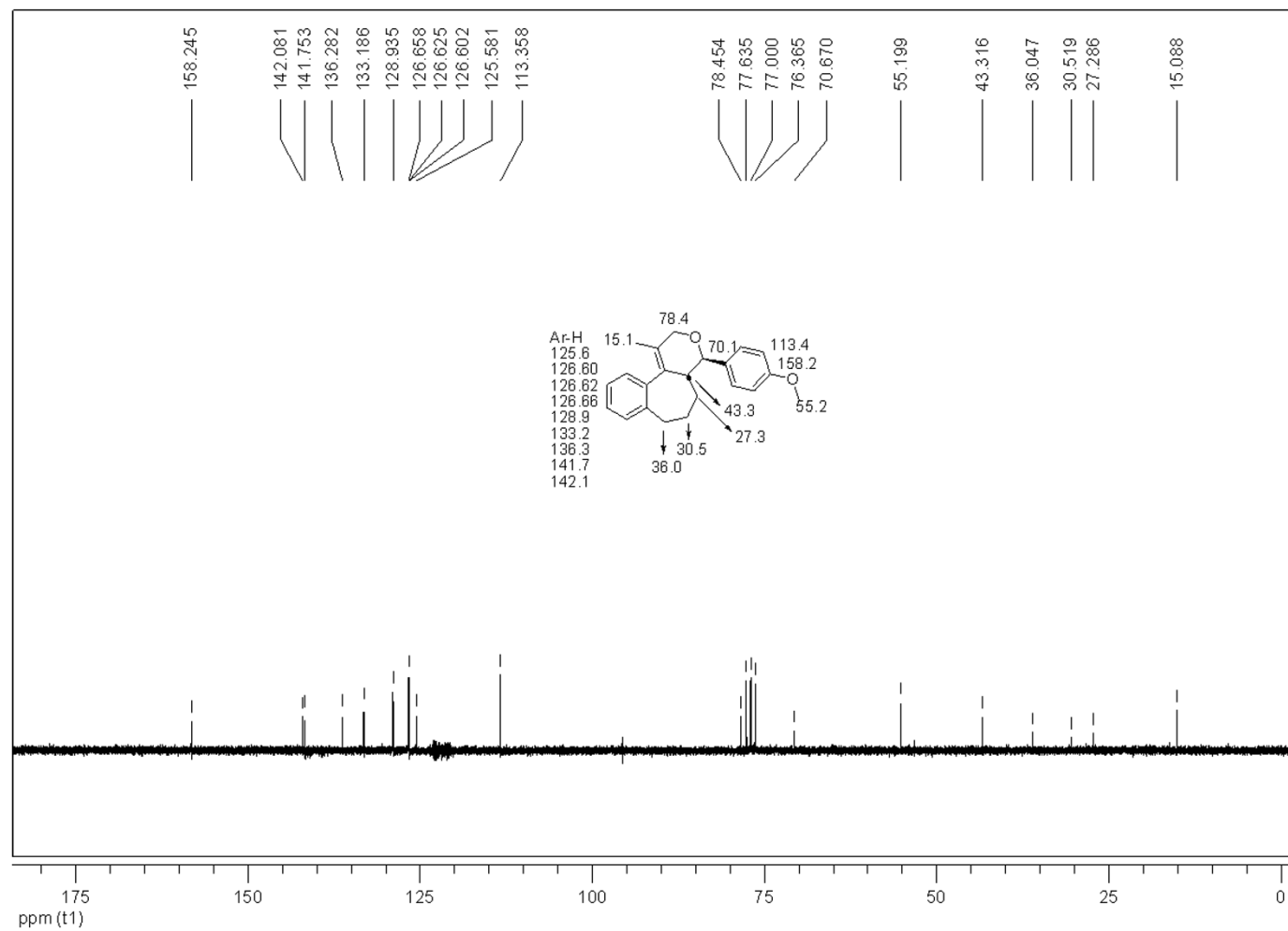
$^1\text{H}$ -NMR of compound *cis*-14c (200 MHz,  $\text{CDCl}_3$ )

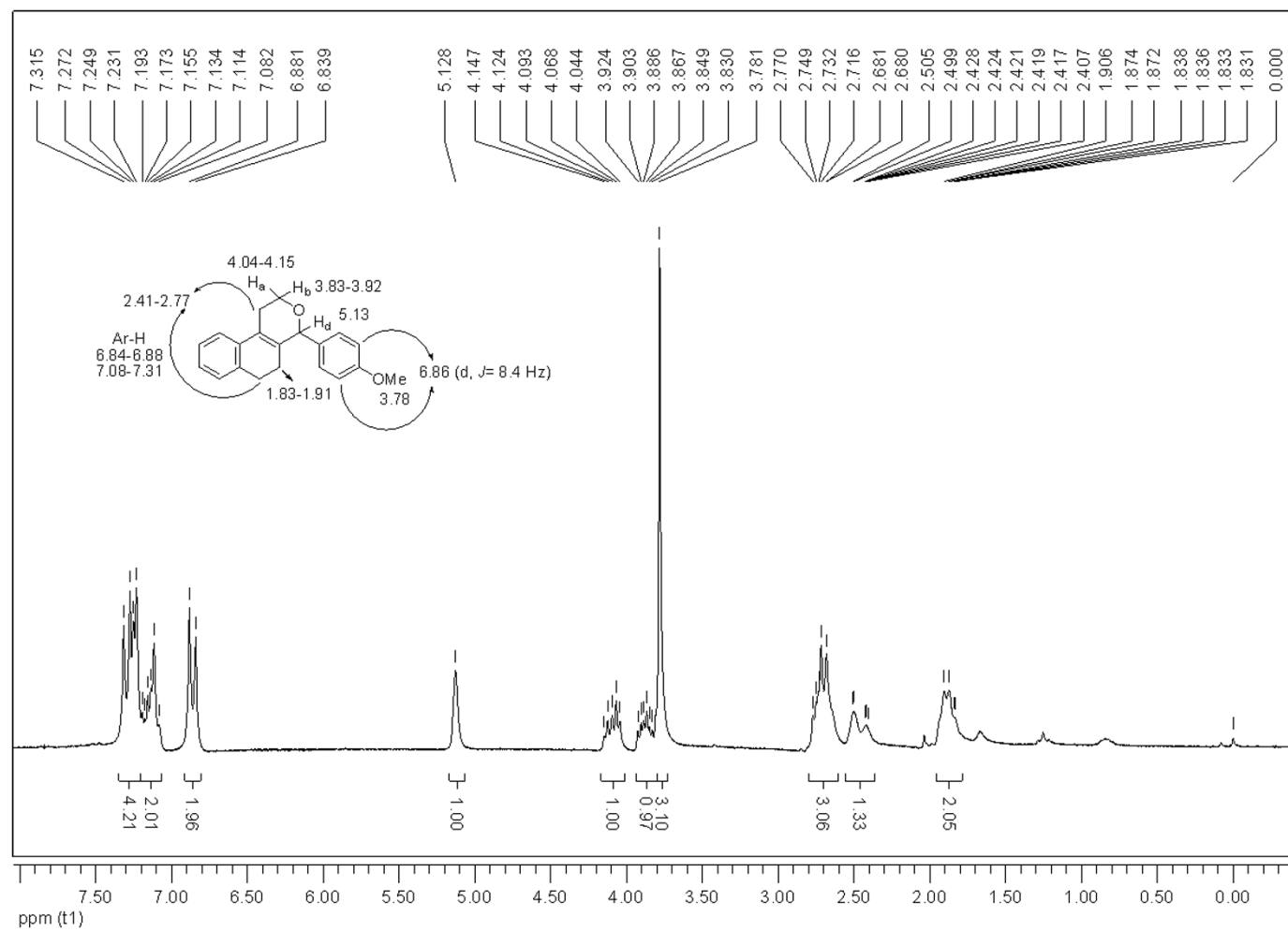
$^{13}\text{C}$ -NMR of compound *cis*-**14c** (50 MHz,  $\text{CDCl}_3$ )

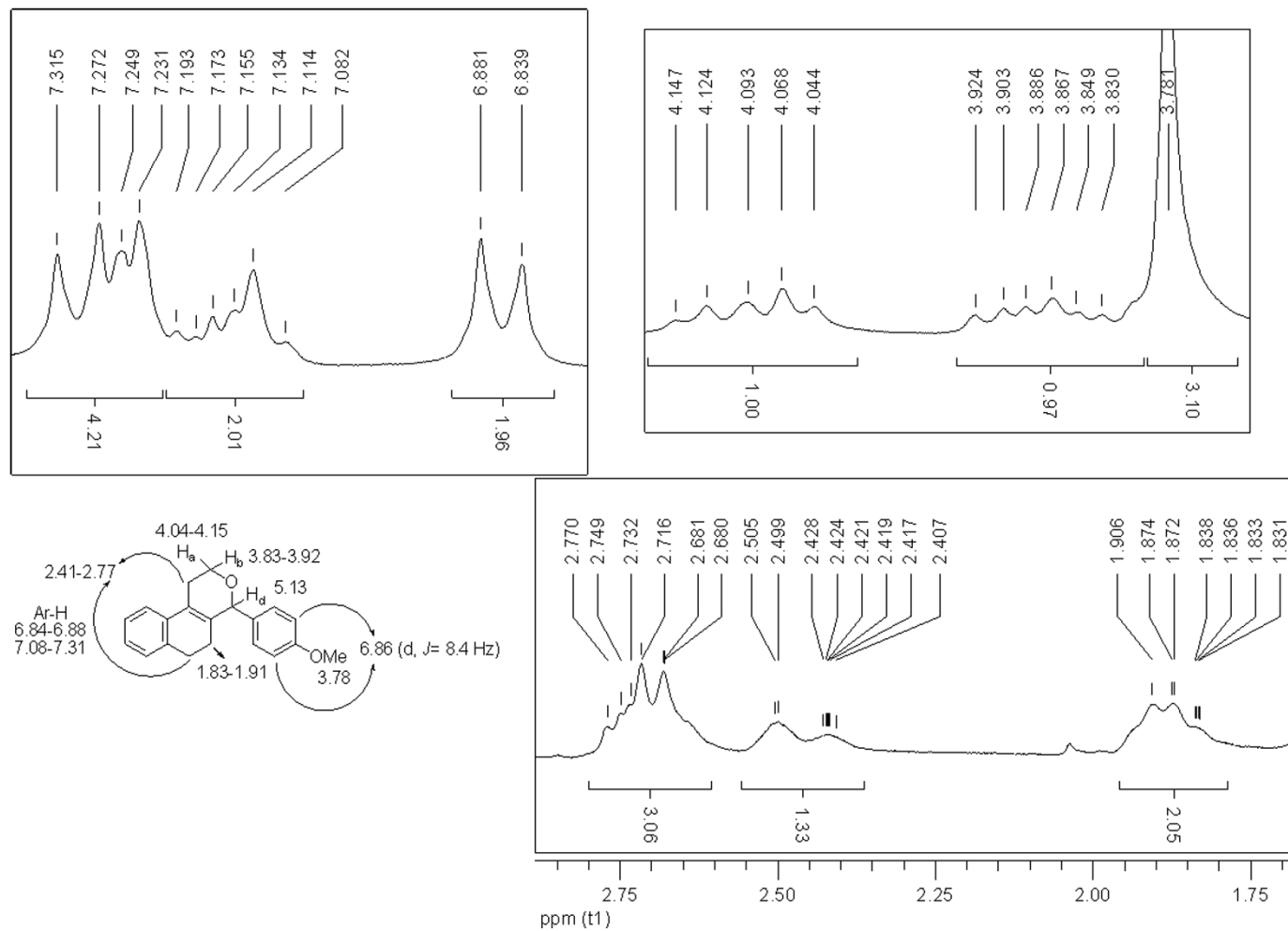
2D NOESY NMR of compound *cis*-**14c** (300 MHz, CDCl<sub>3</sub>)

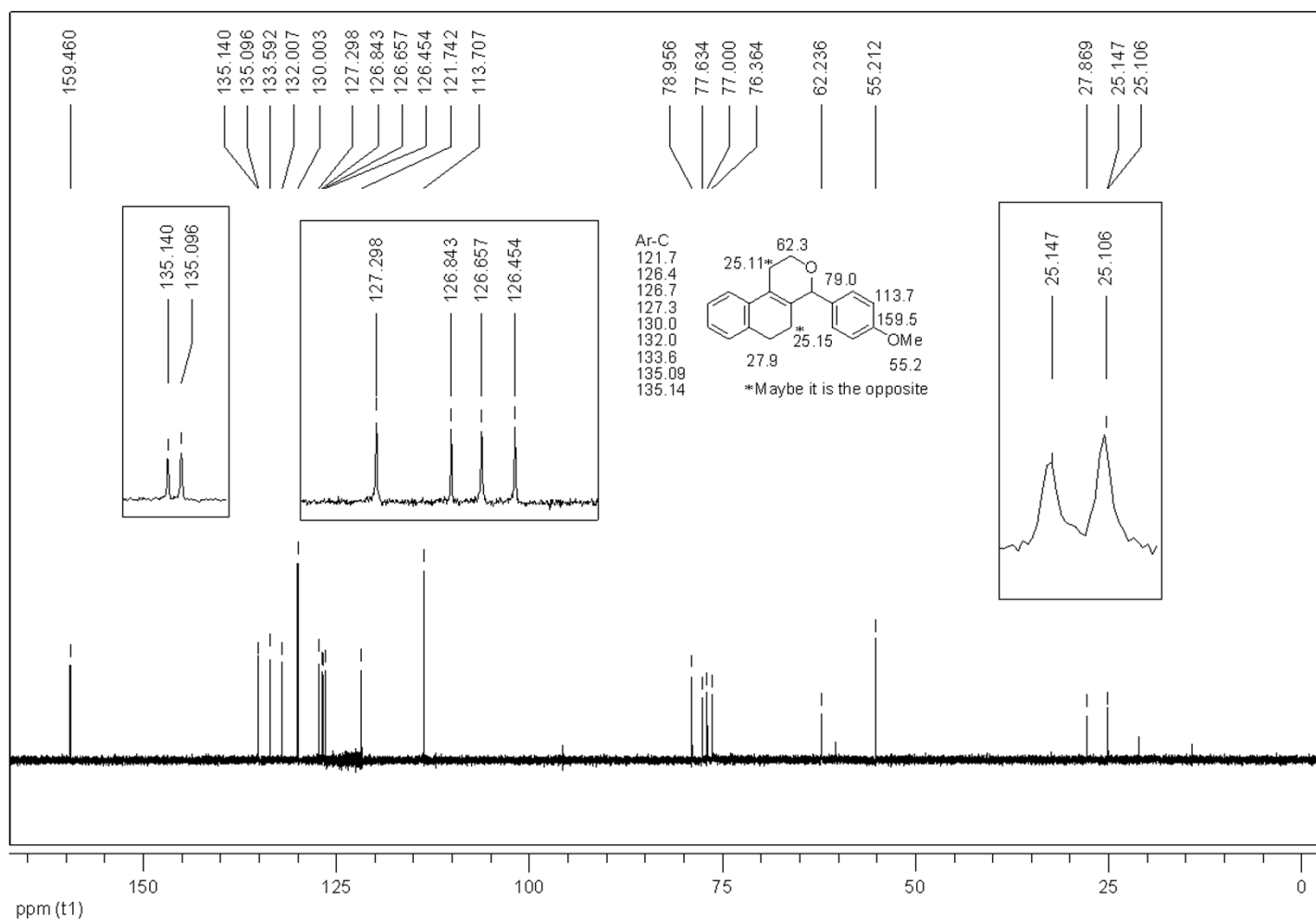
$^1\text{H}$ -NMR of compound *trans*-14c (200 MHz,  $\text{CDCl}_3$ )

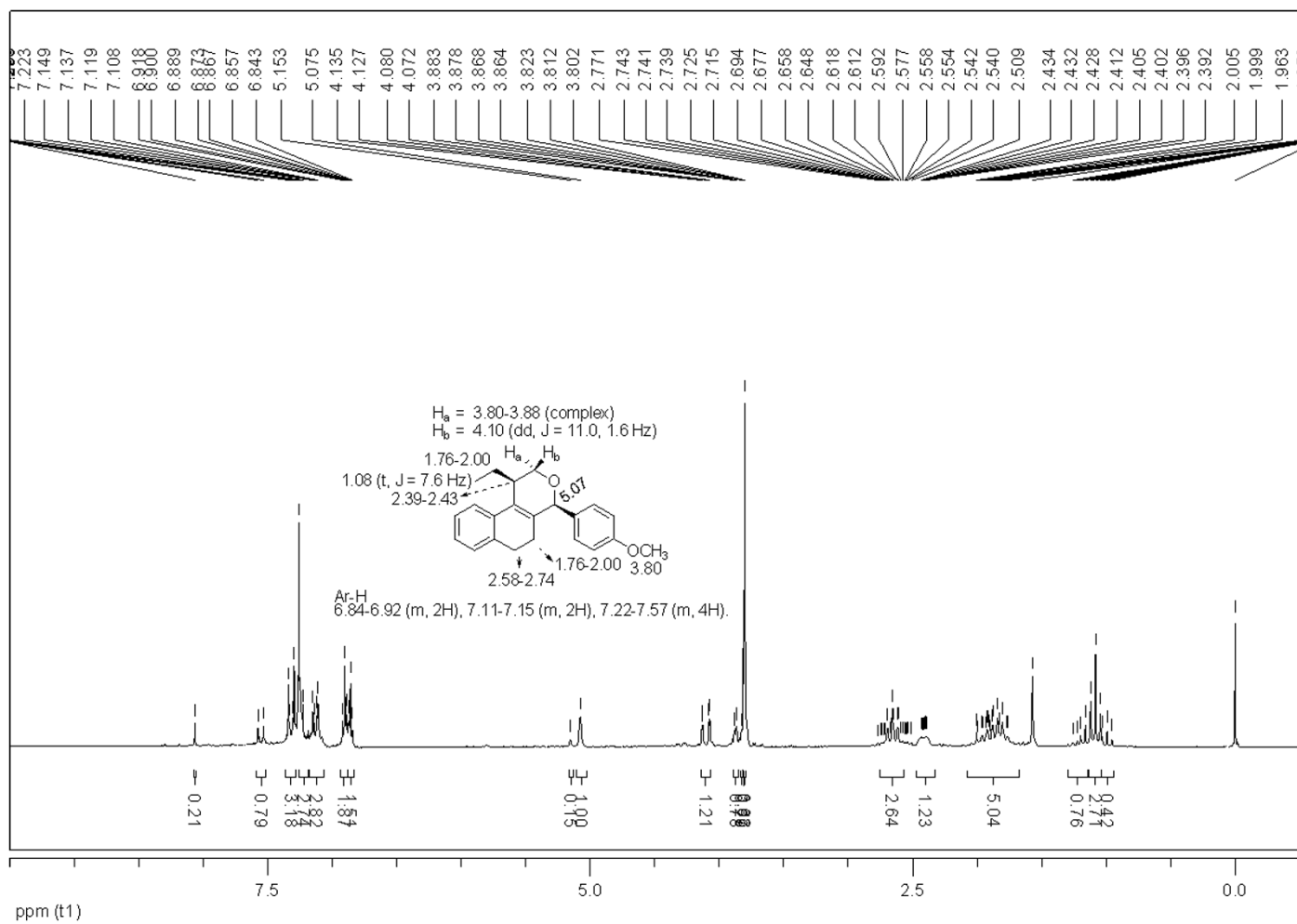
$^1\text{H}$ -NMR of compound *trans*-**14c** (200 MHz,  $\text{CDCl}_3$ )

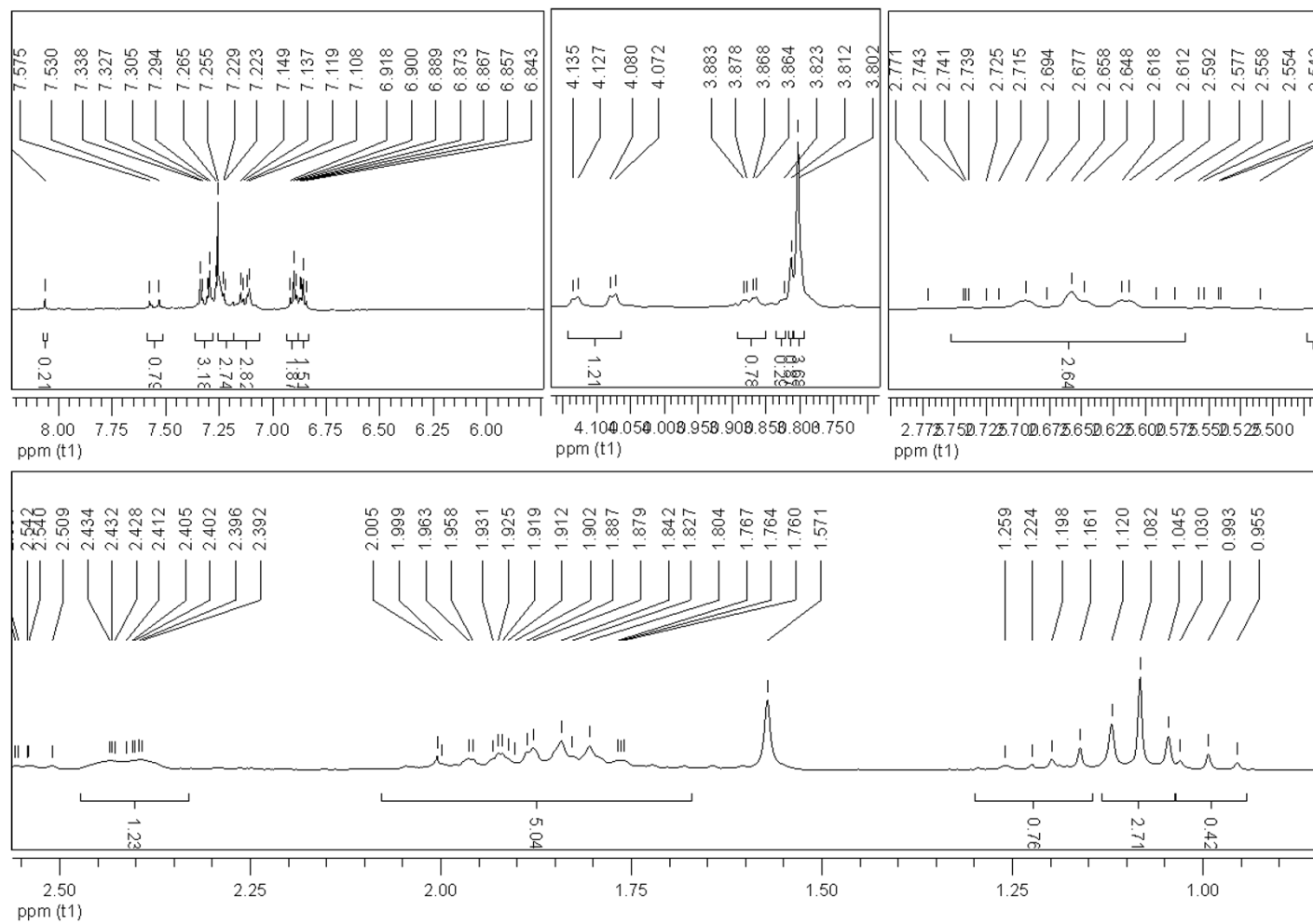
$^{13}\text{C}$ -NMR of compound *trans*-**14c** (50 MHz,  $\text{CDCl}_3$ )

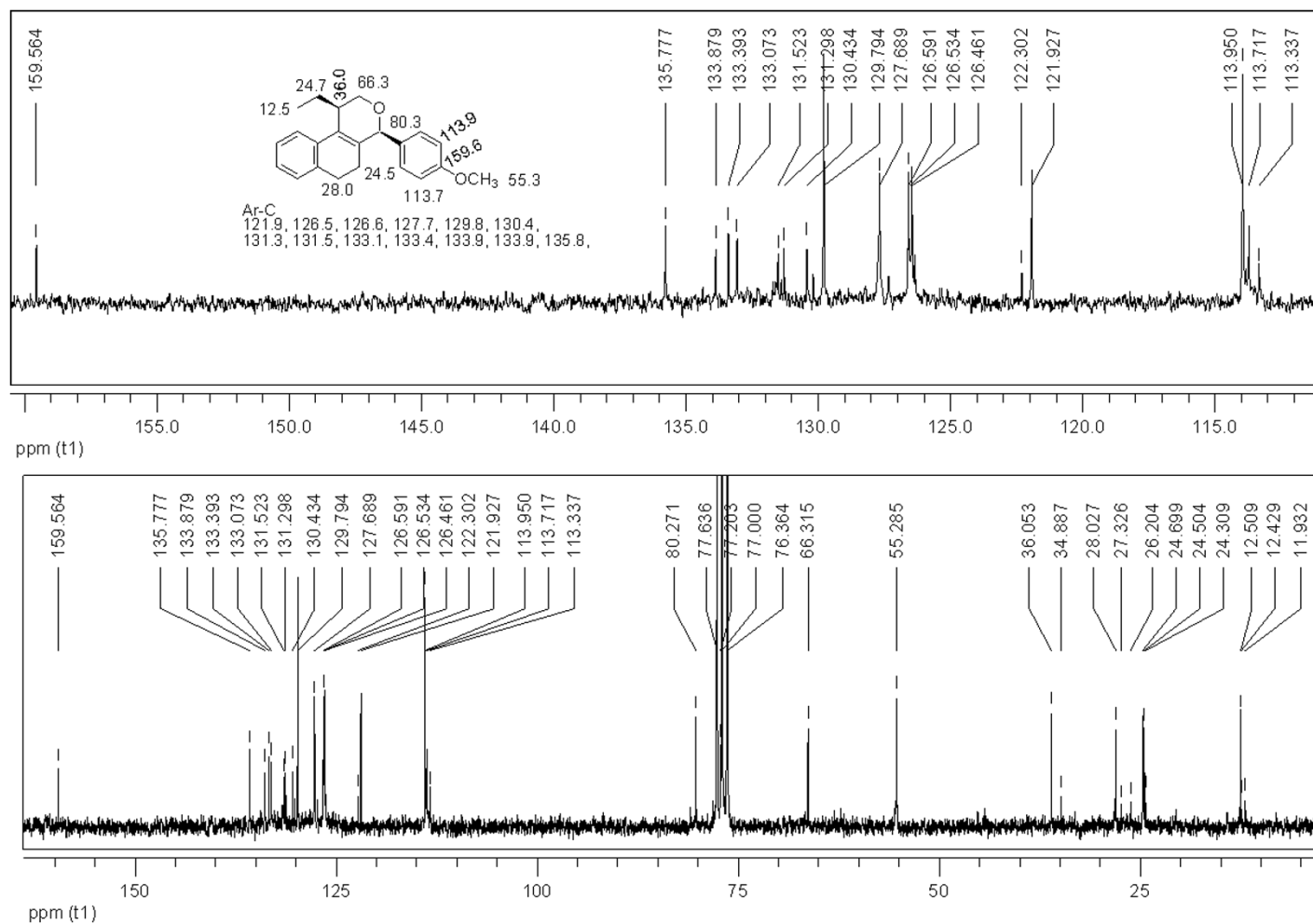
$^1\text{H}$ -NMR of compound **13d** (200 MHz,  $\text{CDCl}_3$ )

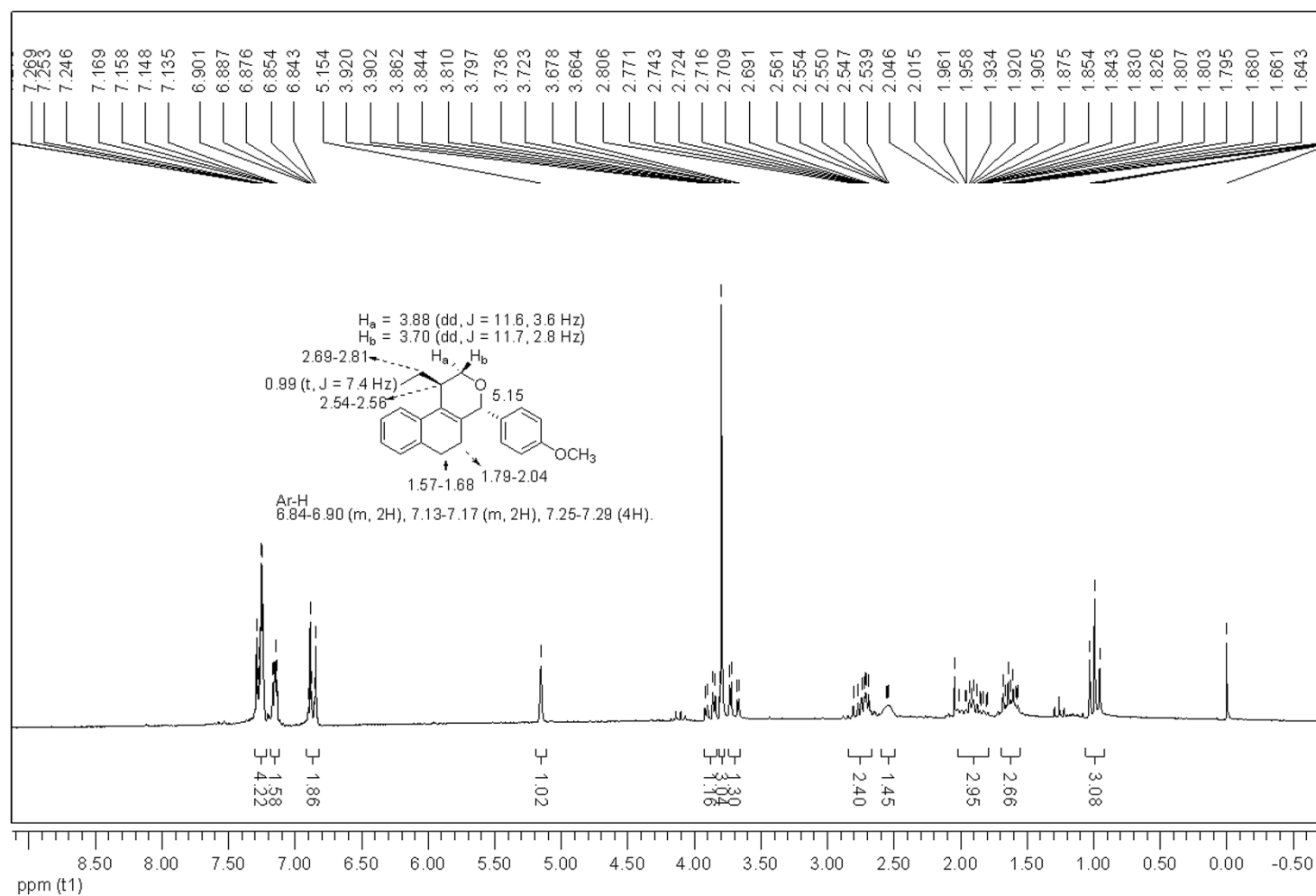
$^1\text{H}$ -NMR of compound **13d** (200 MHz,  $\text{CDCl}_3$ )

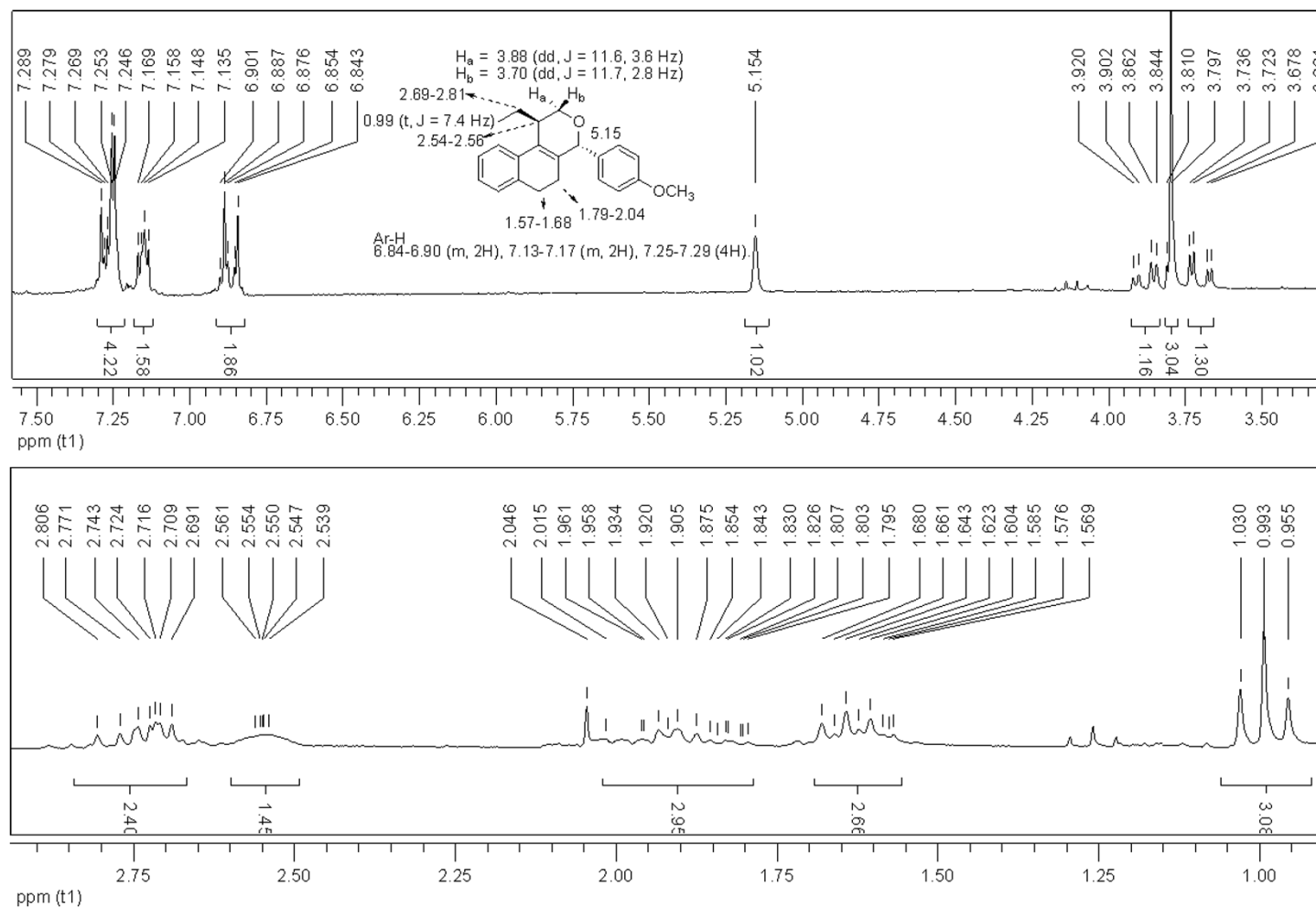
$^{13}\text{C}$ -NMR of compound **13d** (50 MHz,  $\text{CDCl}_3$ )

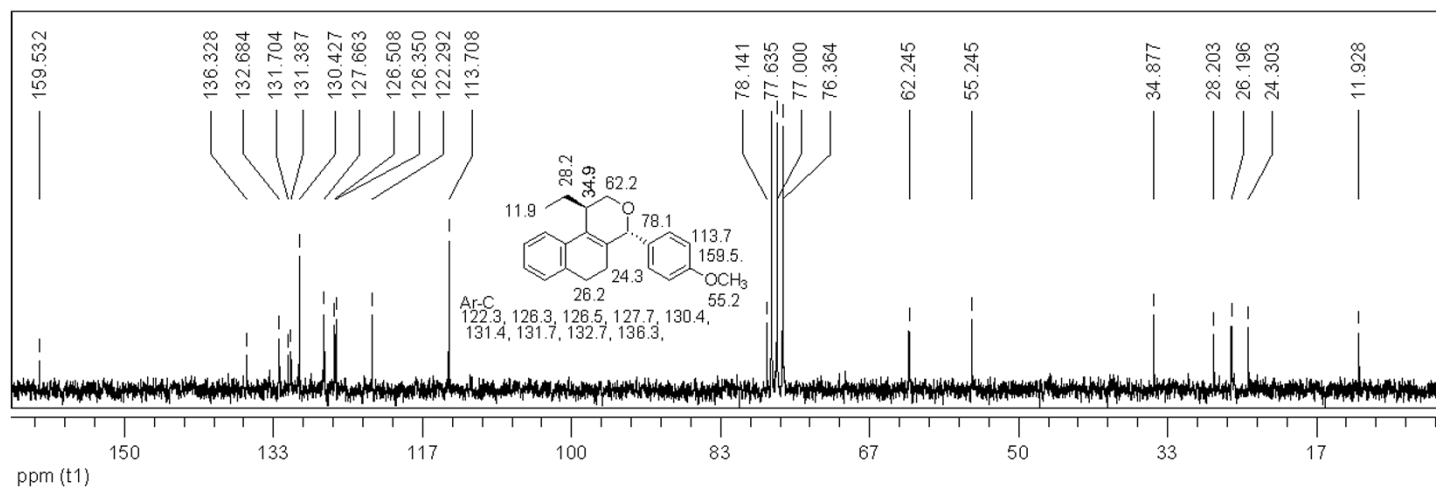
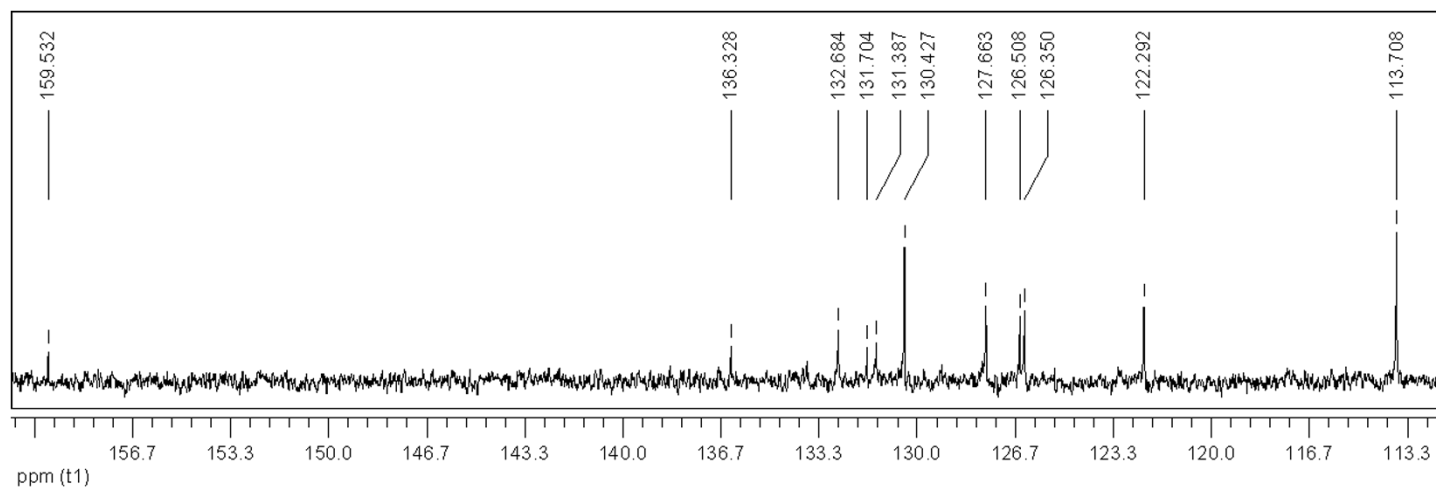
$^1\text{H}$ -NMR of compound *cis*-13e (200 MHz,  $\text{CDCl}_3$ )

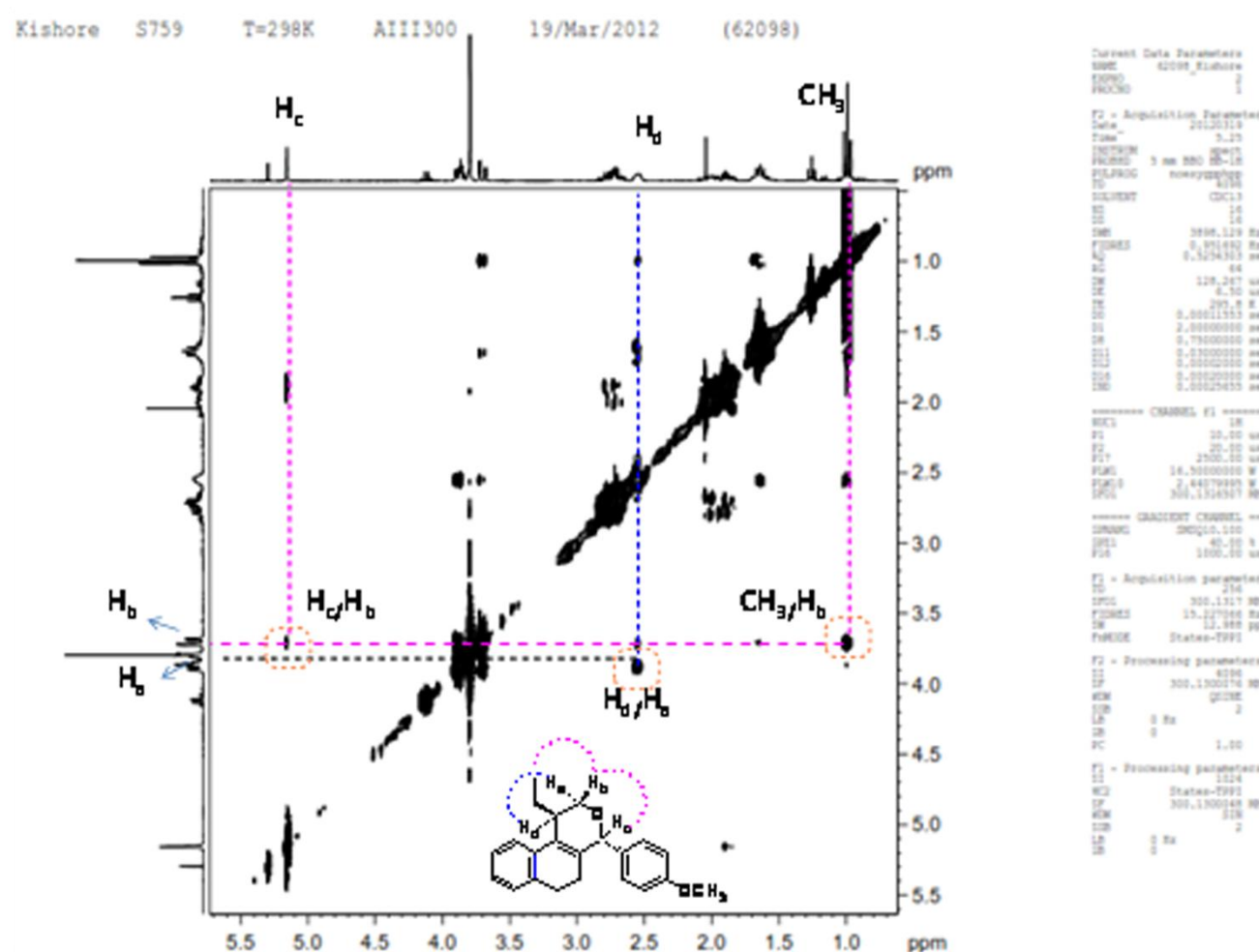
$^1\text{H}$ -NMR of compound *cis*-13e (200 MHz,  $\text{CDCl}_3$ )

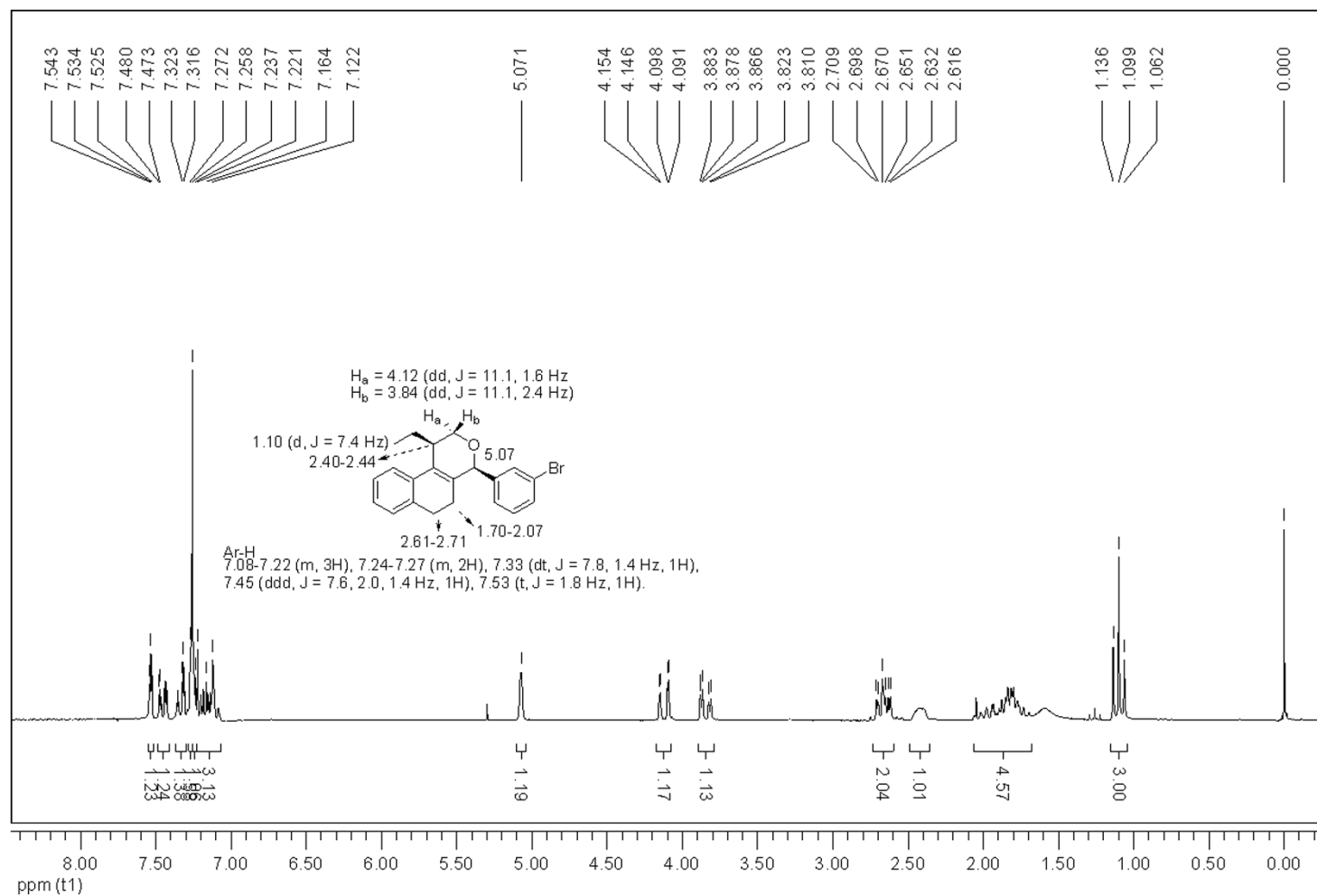
$^{13}\text{C}$ -NMR of compound *cis*-**13e** (50 MHz,  $\text{CDCl}_3$ )

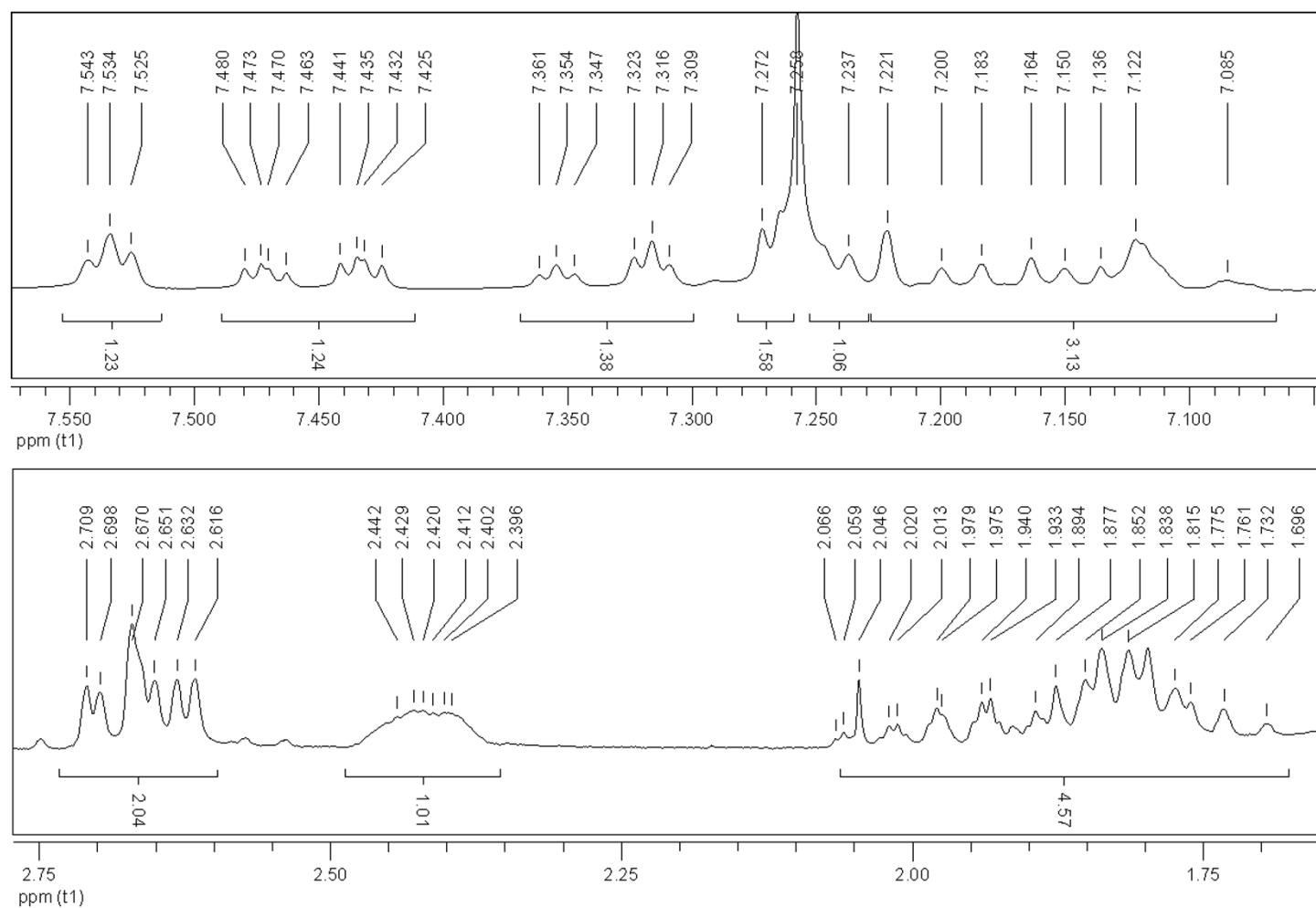
$^1\text{H}$ -NMR of compound *trans*-13e (200 MHz,  $\text{CDCl}_3$ )

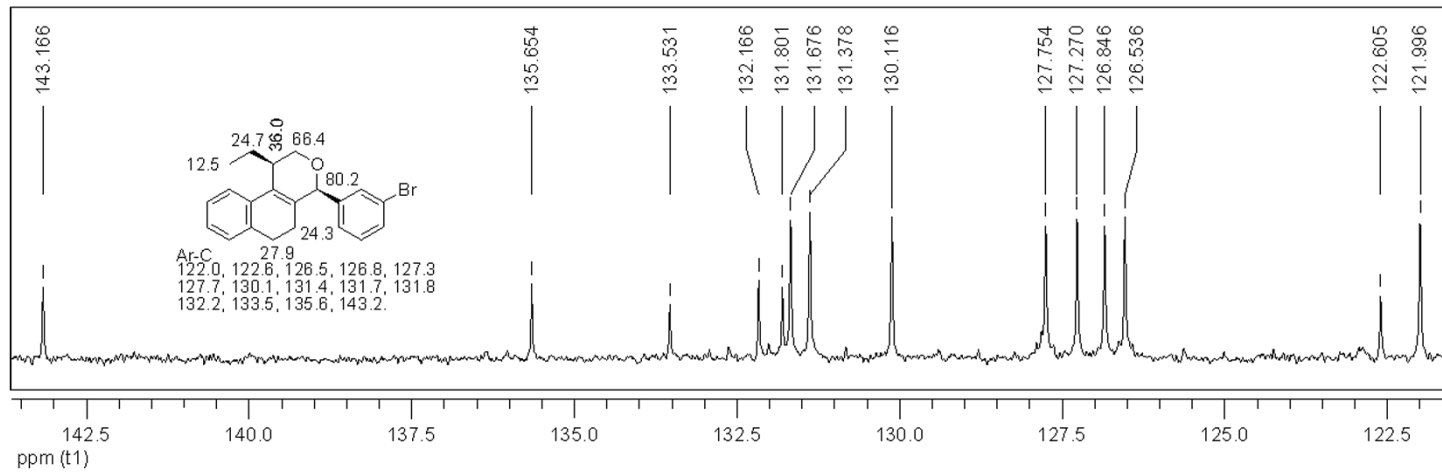
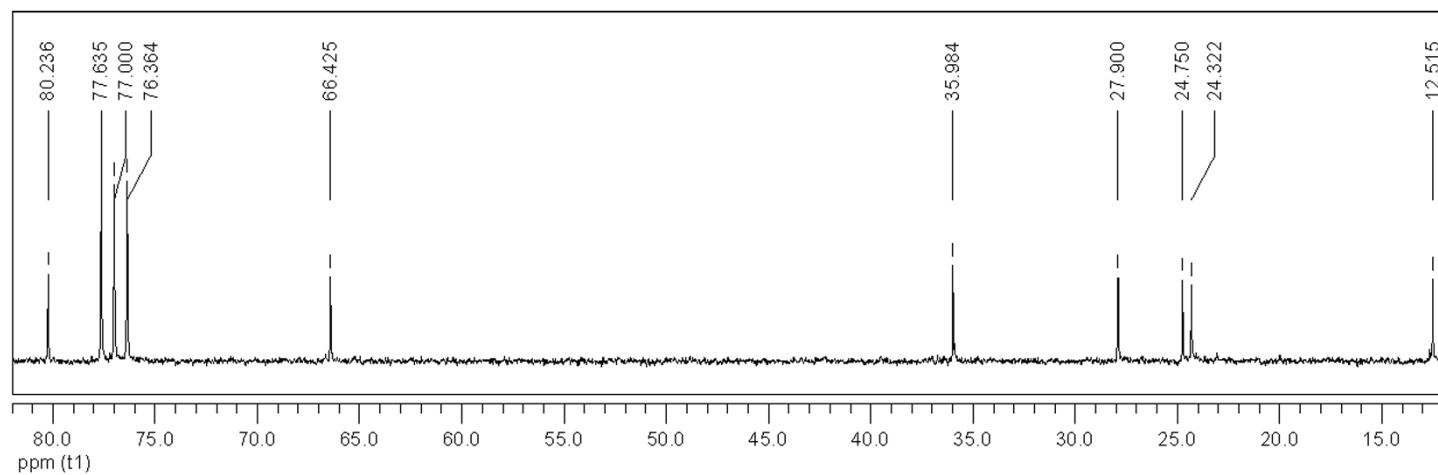
$^1\text{H}$ -NMR of compound *trans*-13e (200 MHz,  $\text{CDCl}_3$ )

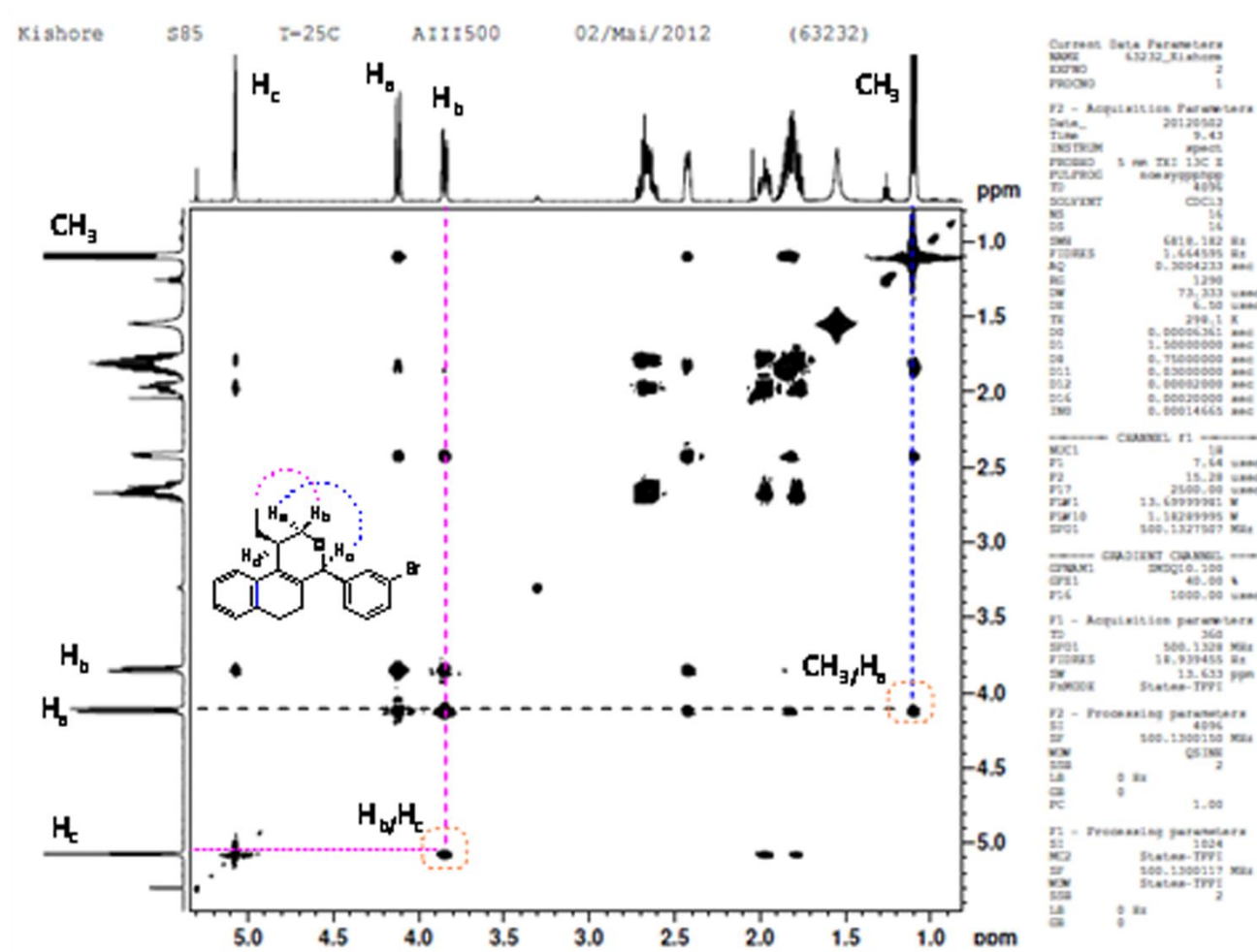
$^{13}\text{C}$ -NMR of compound *trans*-**13e** (50 MHz,  $\text{CDCl}_3$ )

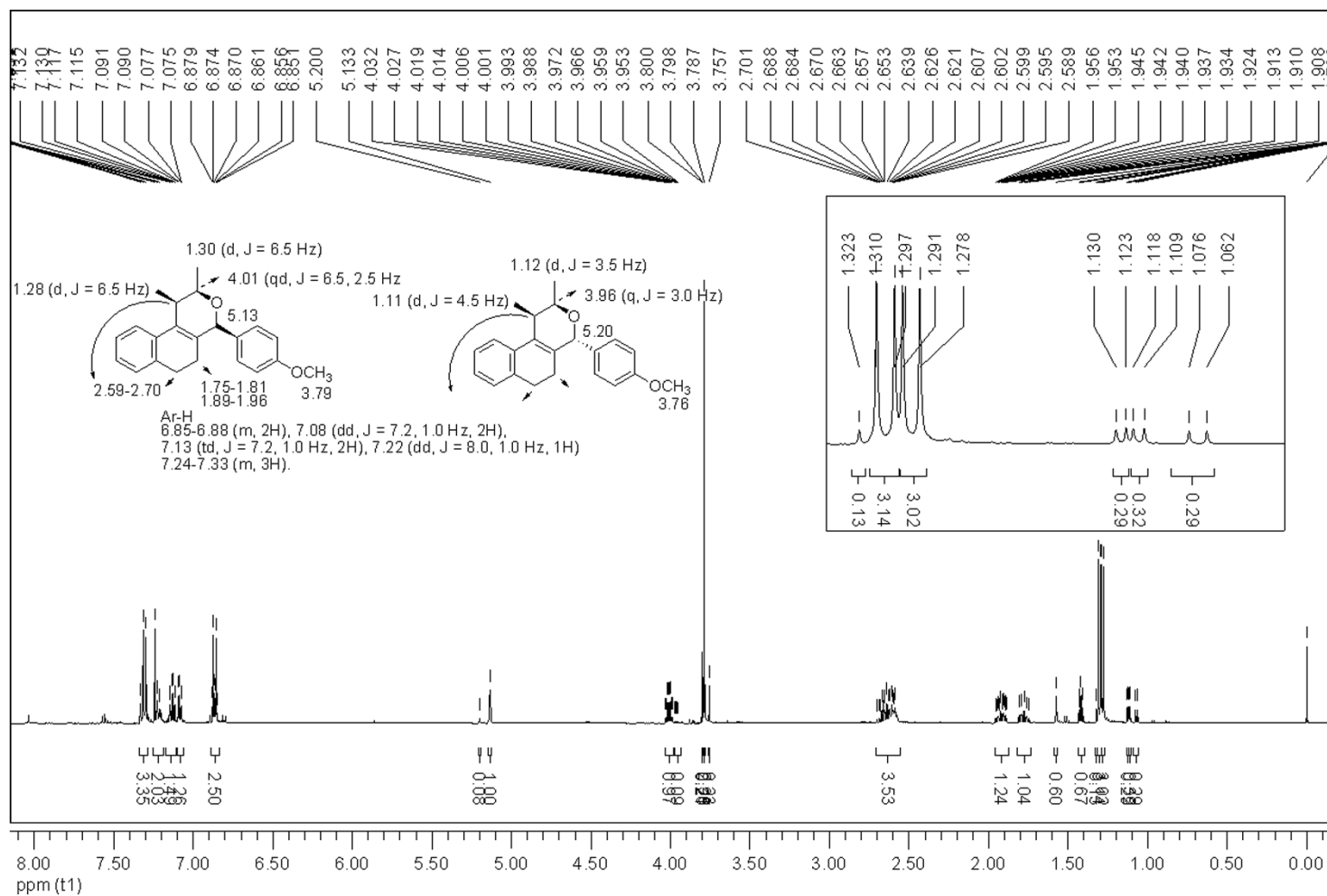
2D NOESY NMR of compound *trans*-13e (300 MHz, CDCl<sub>3</sub>)

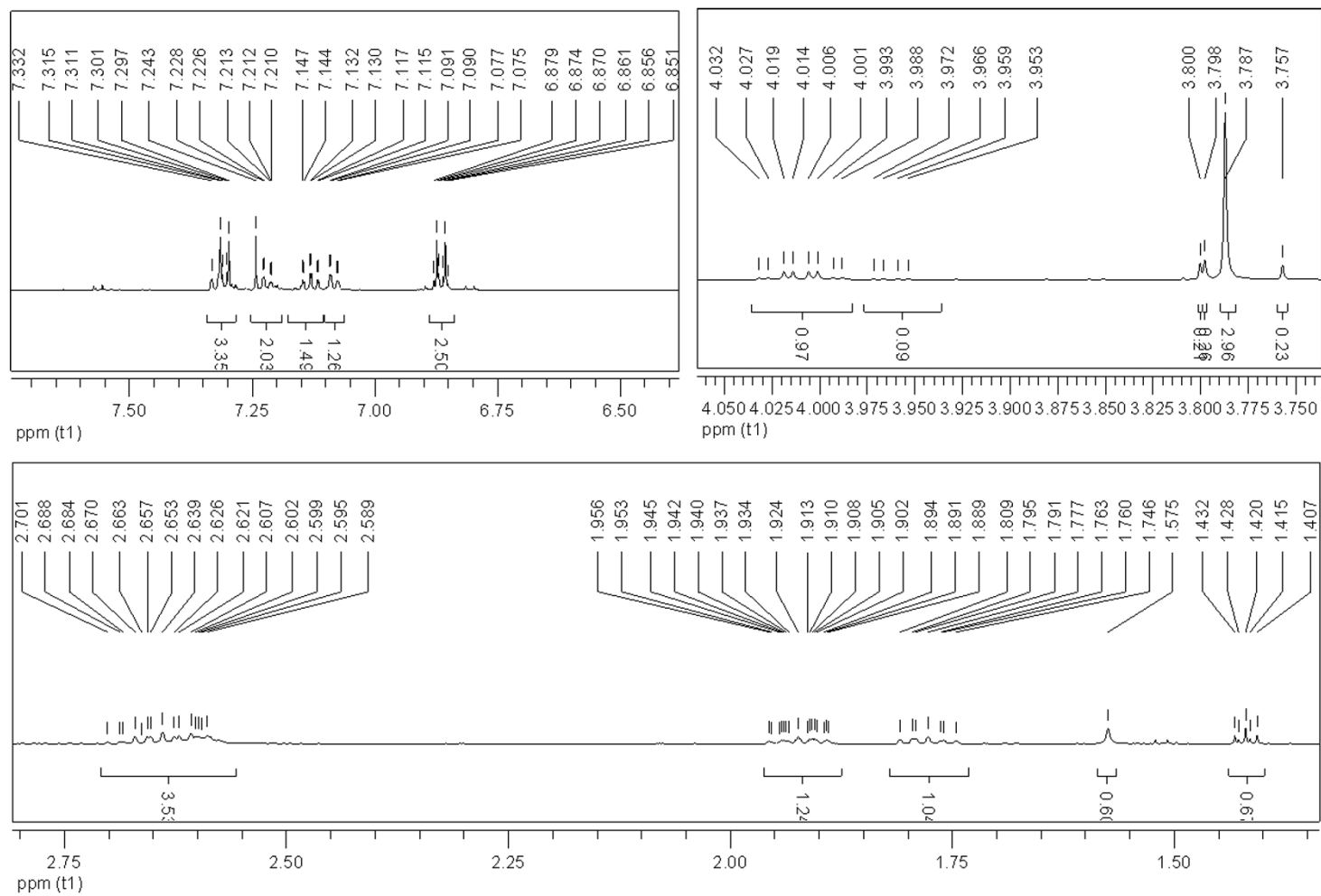
$^1\text{H}$ -NMR of compound *cis*-**15e** (200 MHz,  $\text{CDCl}_3$ )

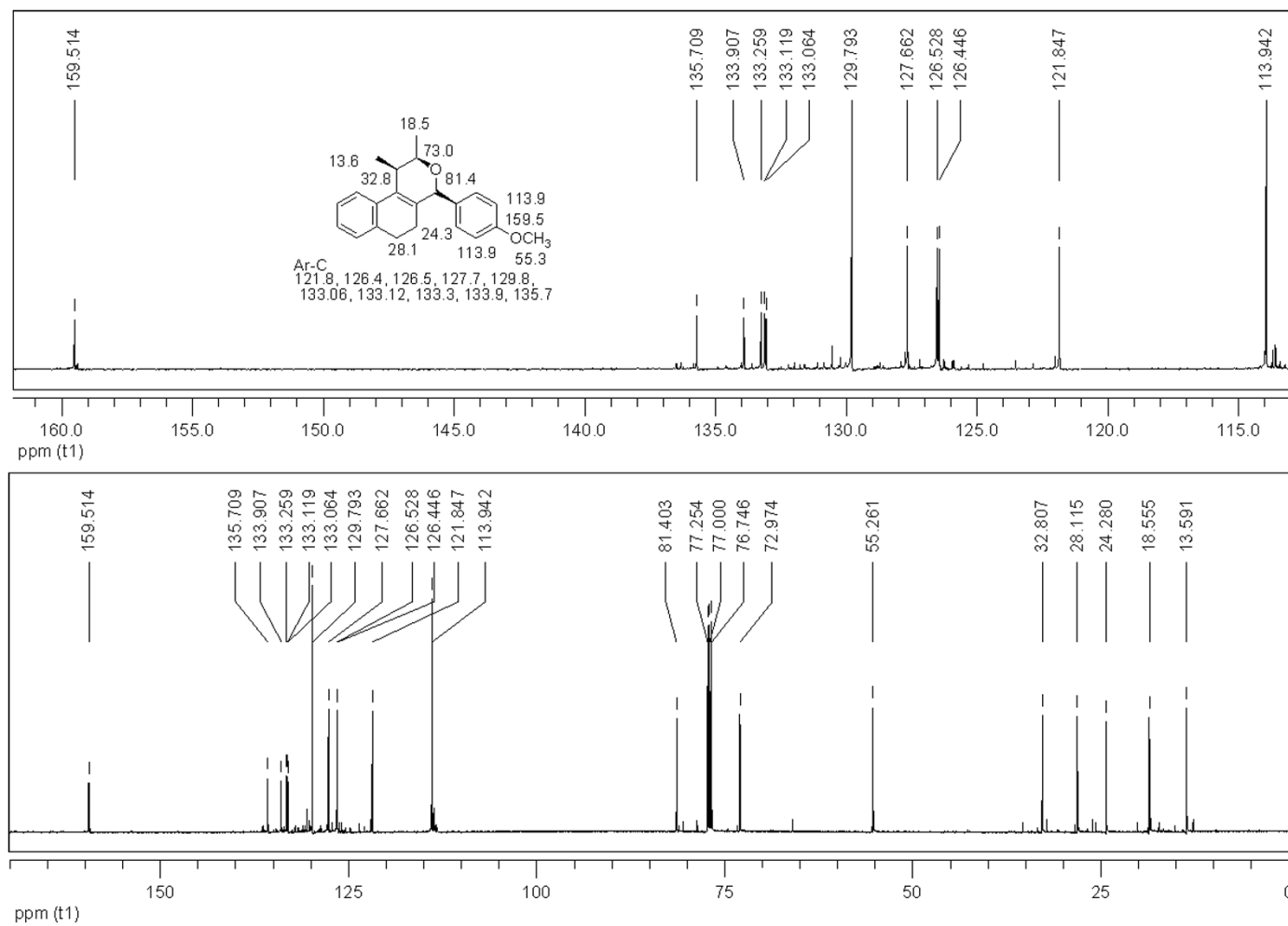
$^1\text{H}$ -NMR of compound *cis*-15e (200 MHz,  $\text{CDCl}_3$ )

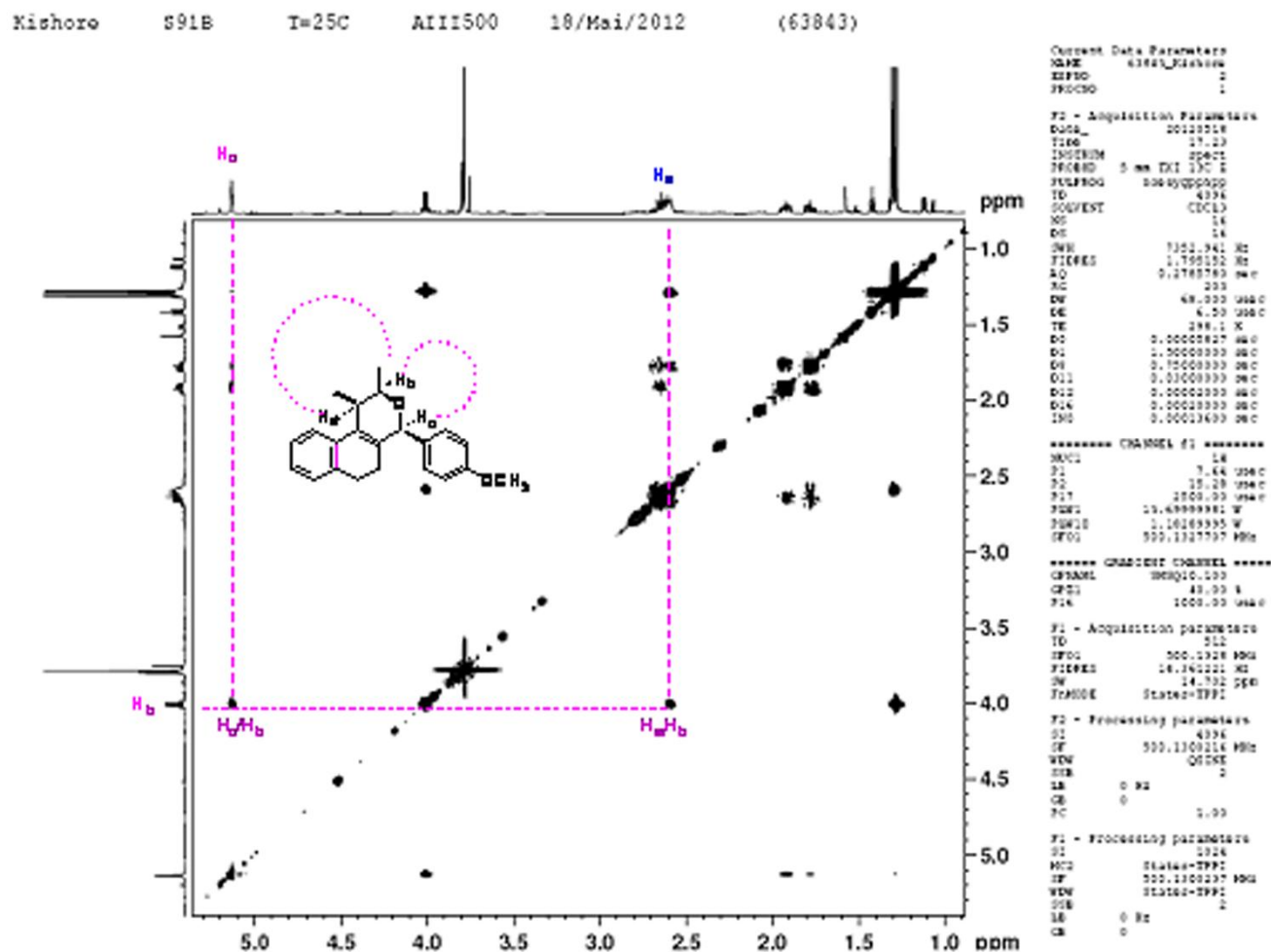
$^{13}\text{C}$ -NMR of compound *cis*-15e (50 MHz,  $\text{CDCl}_3$ )

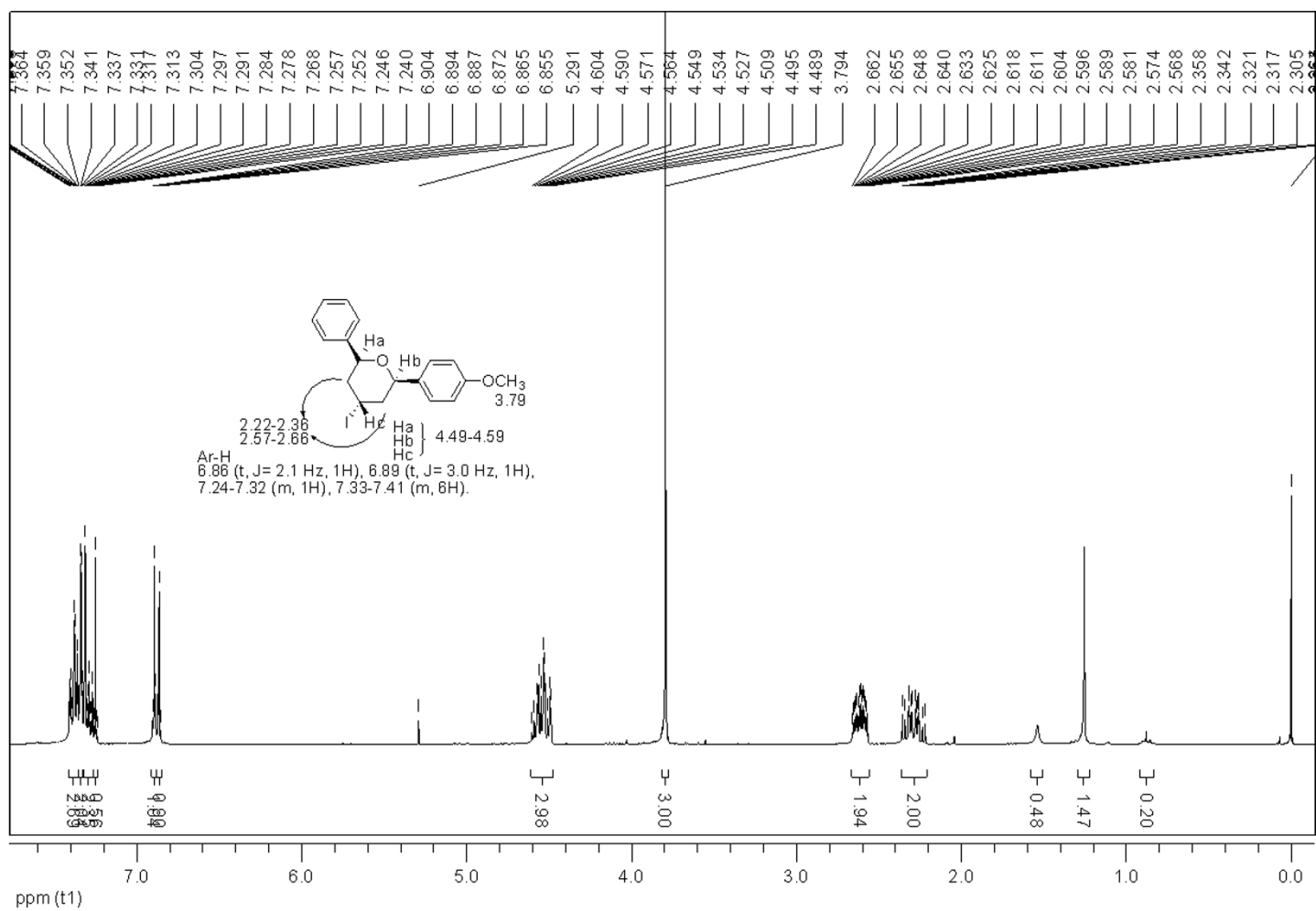
2D NOESY NMR of compound *cis-15e* (500 MHz, CDCl<sub>3</sub>)

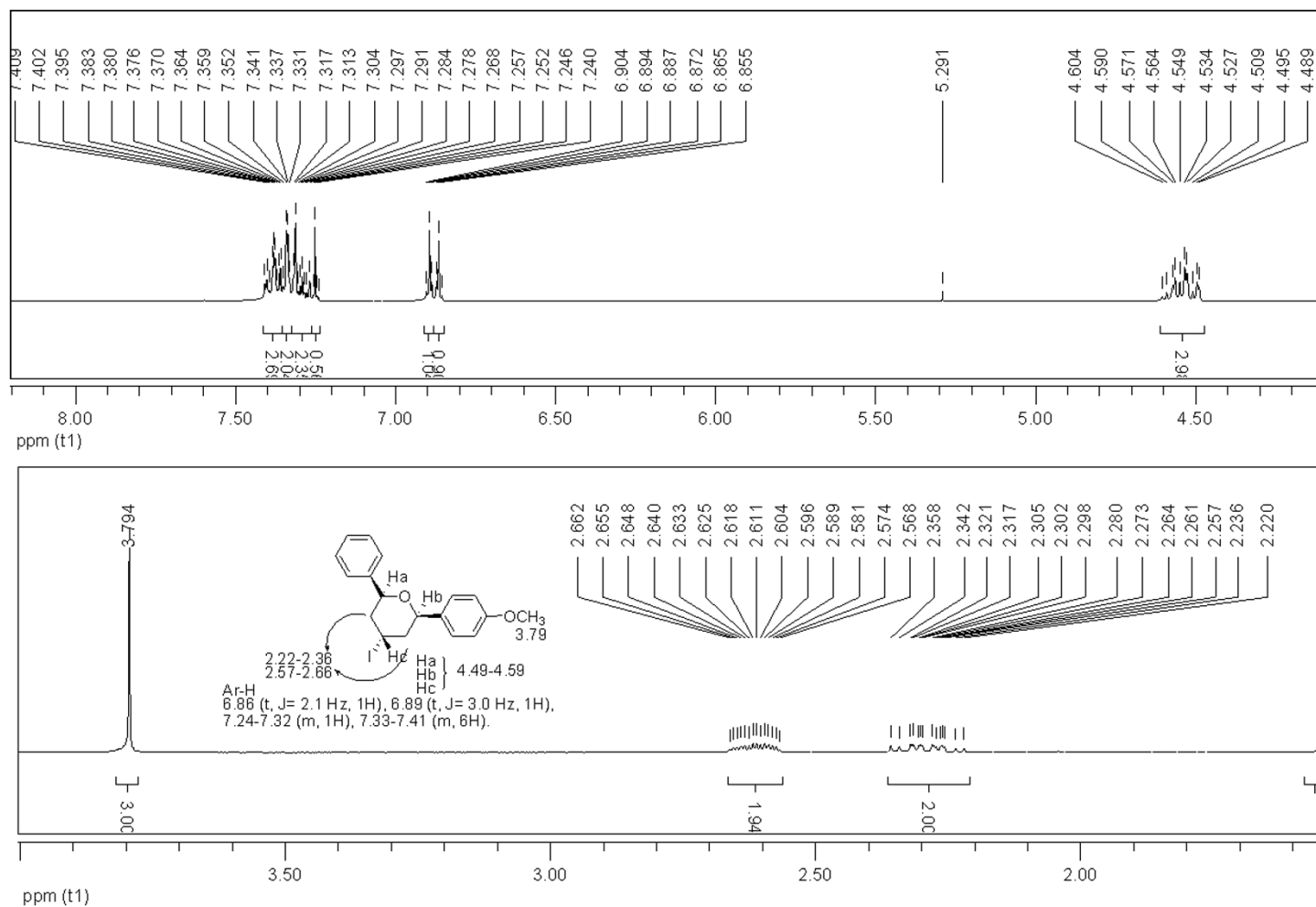
$^1\text{H}$ -NMR of compounds *cis*-**13g** and *trans*-**13g** (500 MHz,  $\text{CDCl}_3$ )

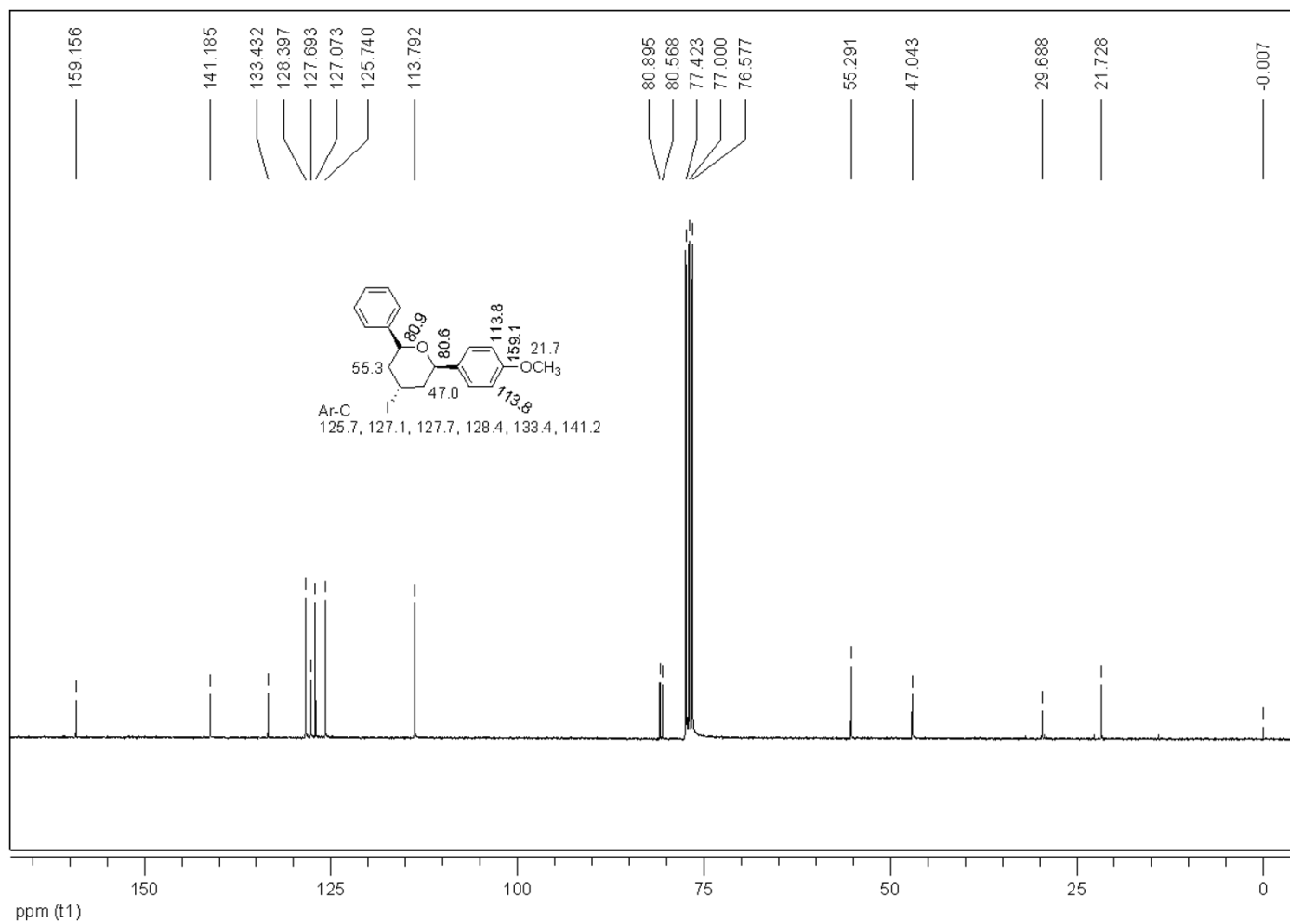
<sup>1</sup>H-NMR of compounds *cis*-**13g** and *trans*-**13g** (300 MHz, CDCl<sub>3</sub>)

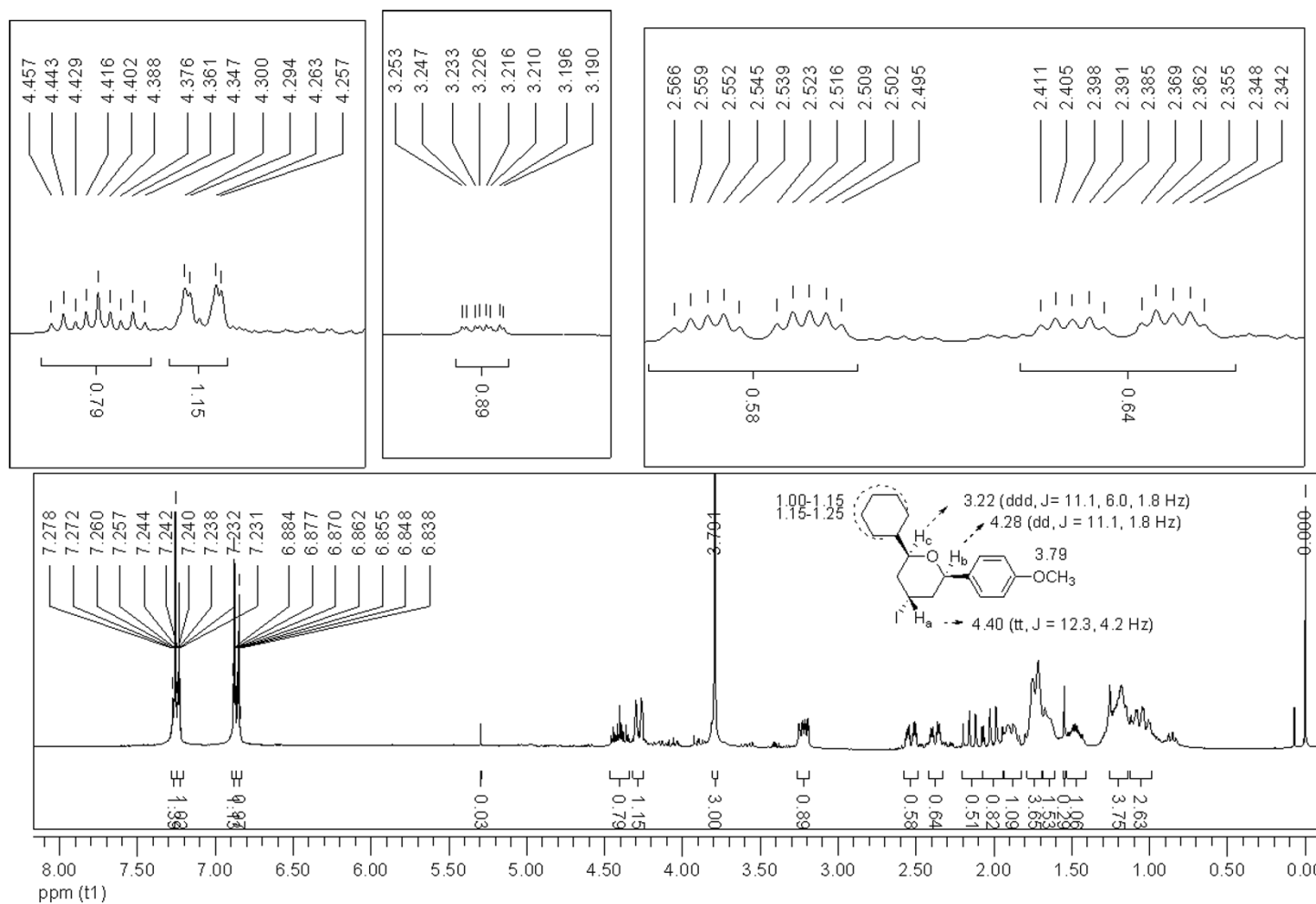
$^{13}\text{C}$ -NMR of compounds *cis*-**13g** and *trans*-**13g** (50 MHz,  $\text{CDCl}_3$ )

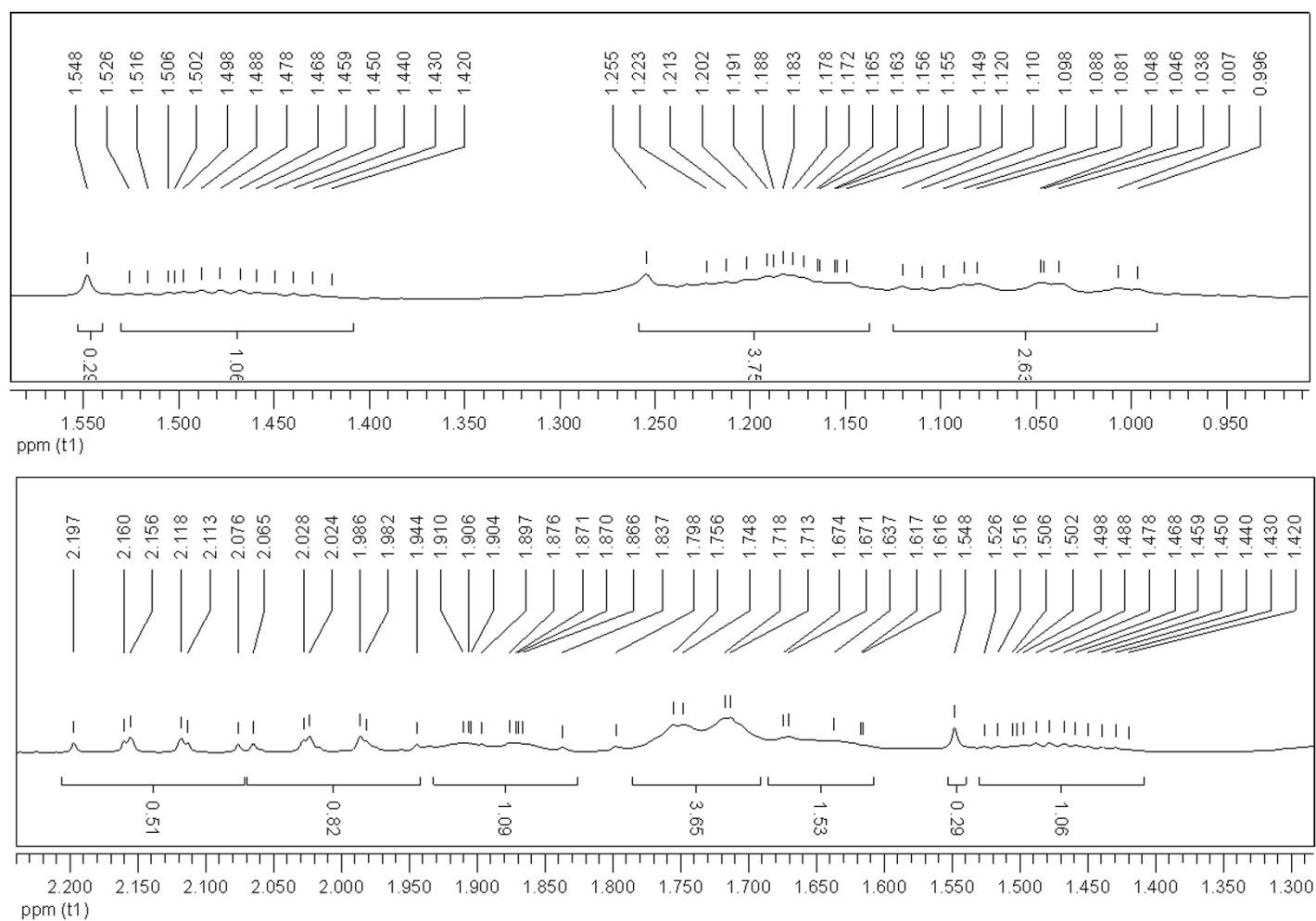
2D NOESY NMR of compound *cis*-13g (500 MHz, CDCl<sub>3</sub>)

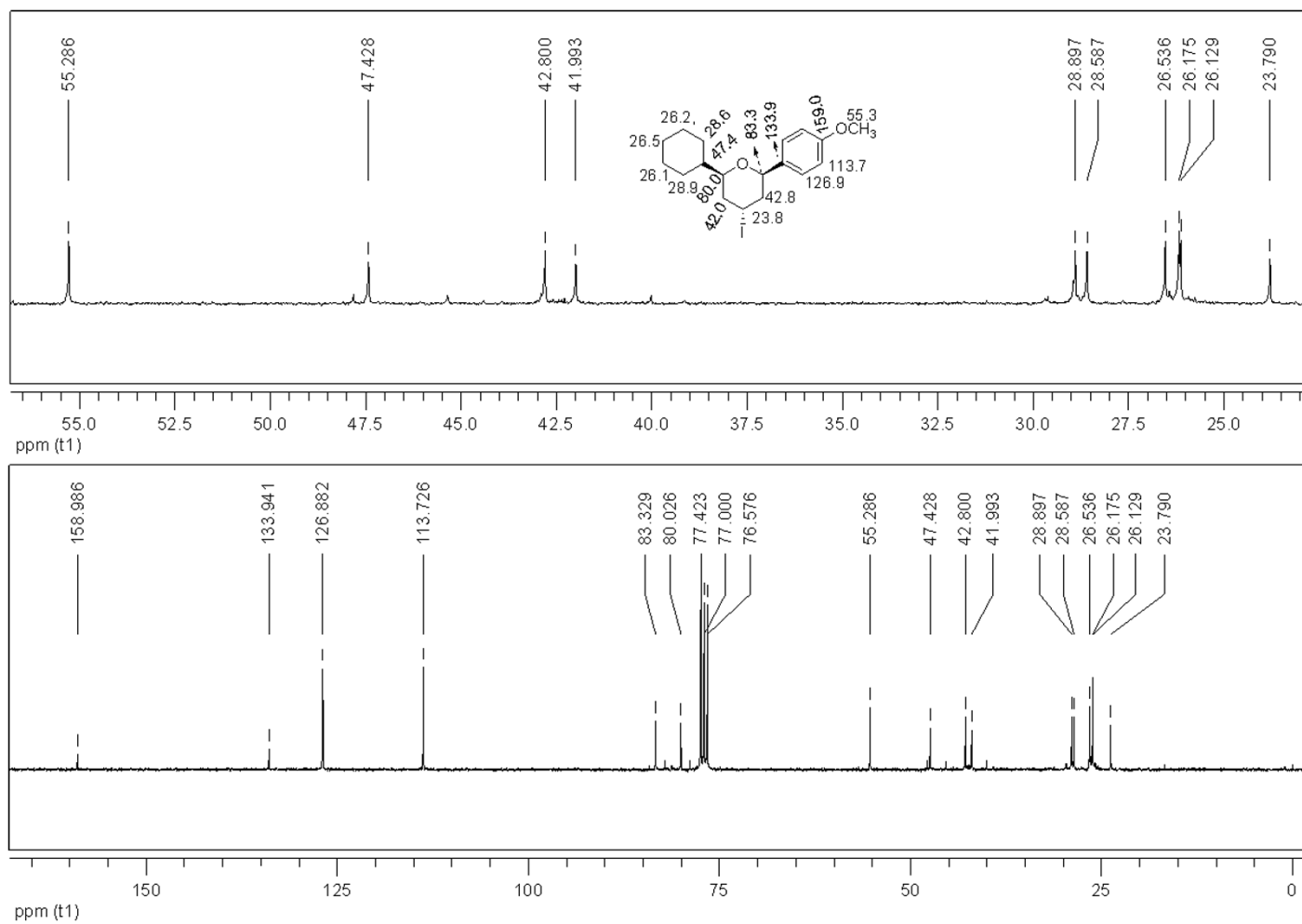
$^1\text{H}$ -NMR of compound **5h** (500 MHz,  $\text{CDCl}_3$ )

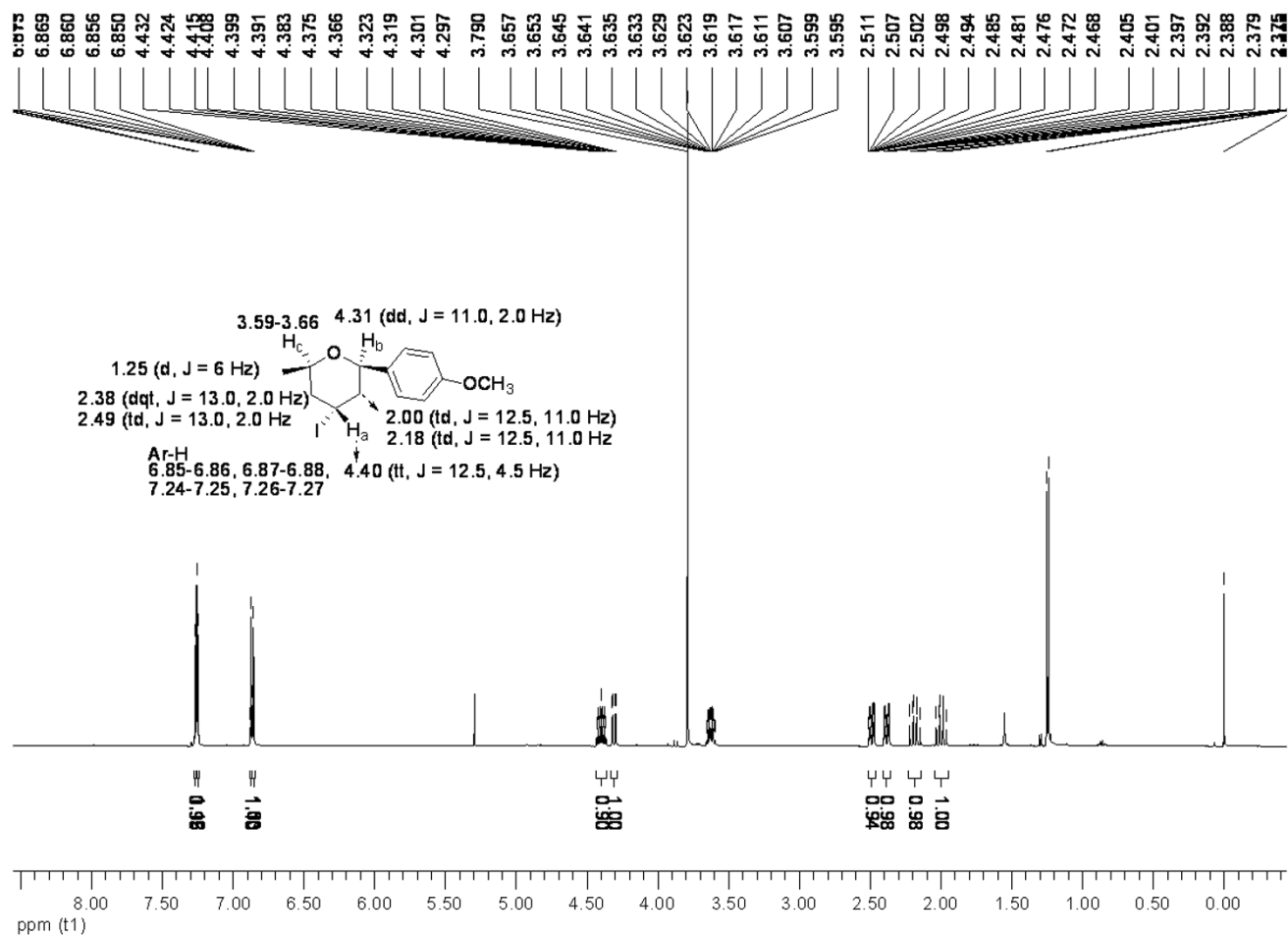
$^1\text{H}$ -NMR of compound **5h** (500 MHz,  $\text{CDCl}_3$ )

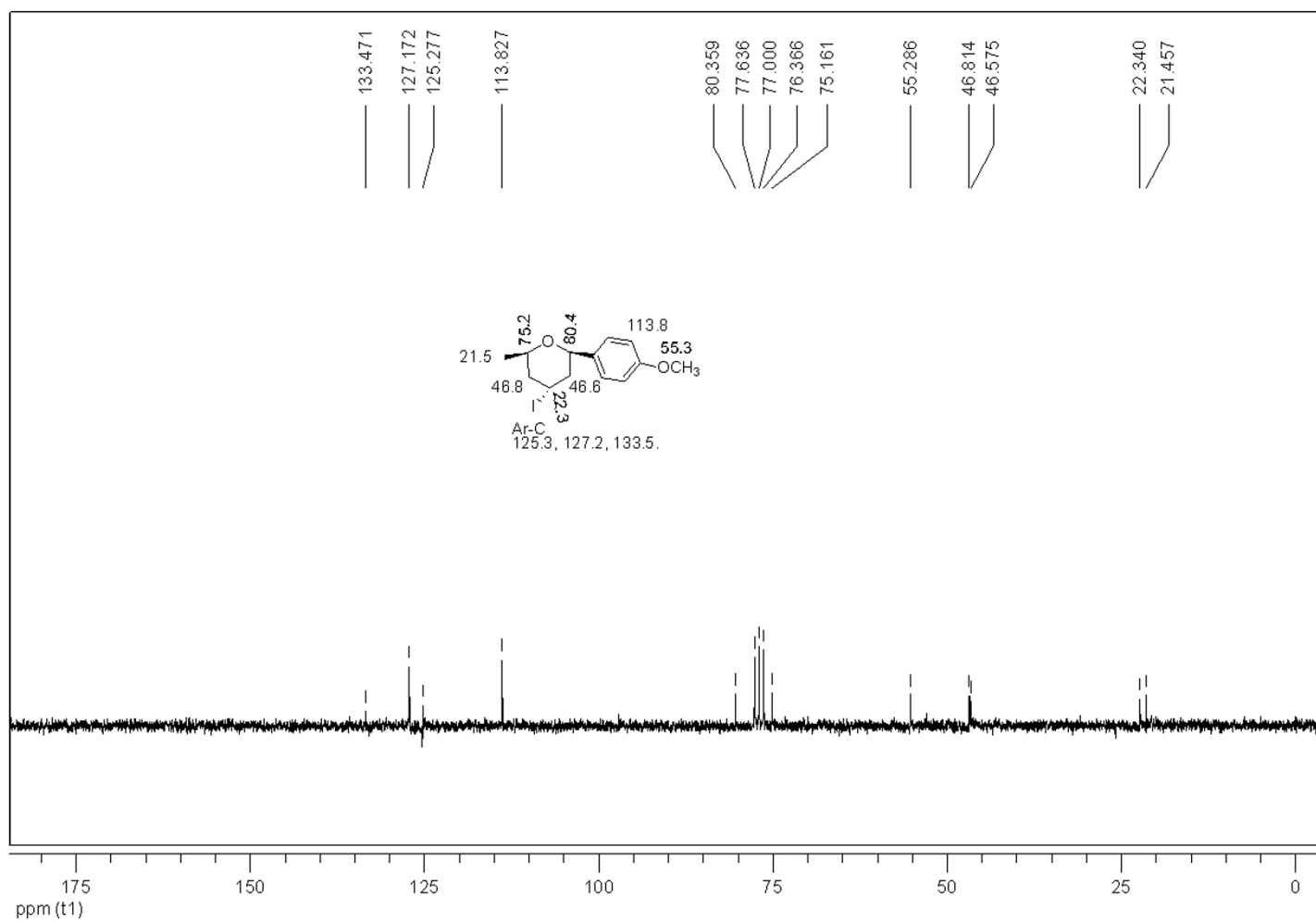
$^{13}\text{C}$ -NMR of compound **5h** (75 MHz,  $\text{CDCl}_3$ )

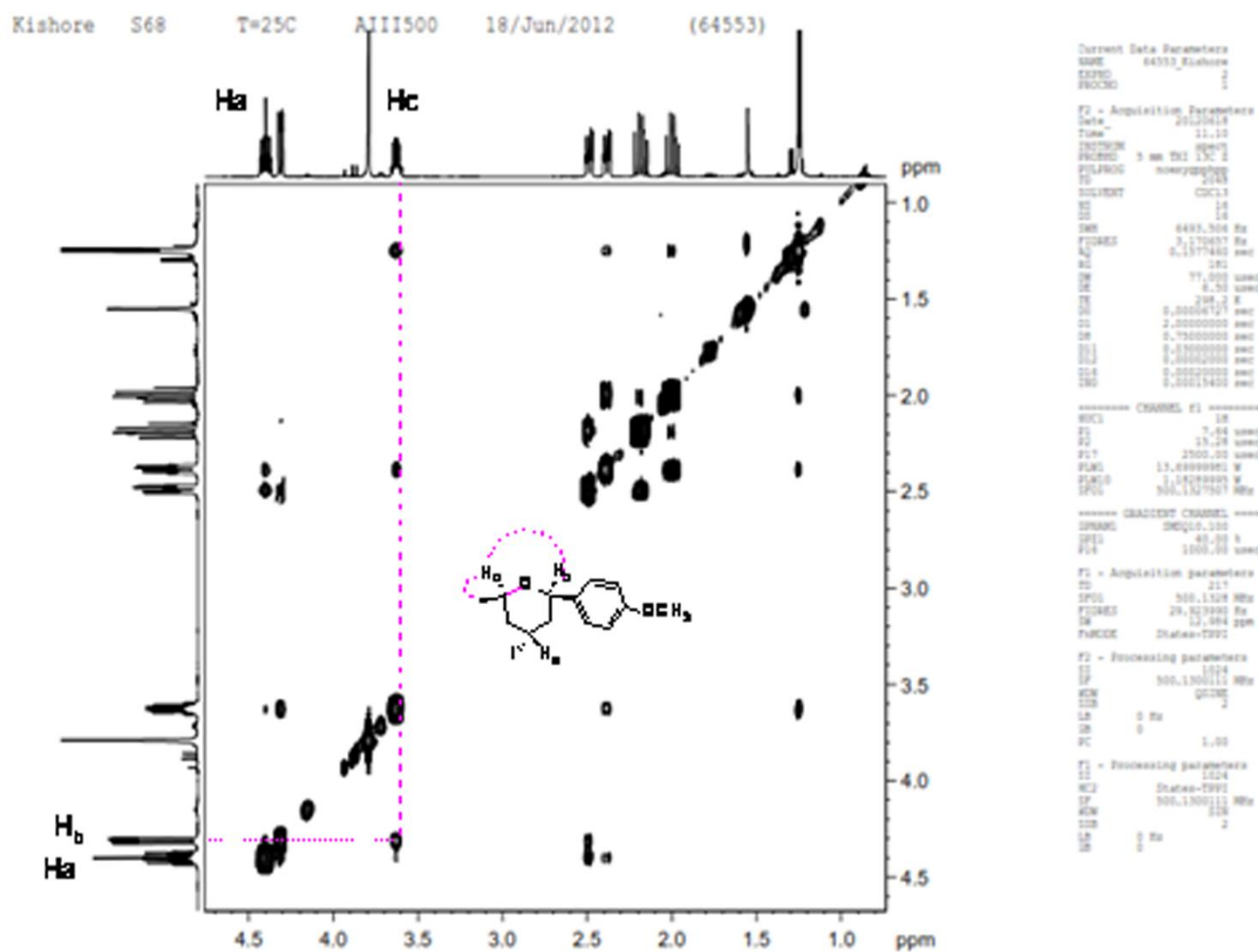
<sup>1</sup>H-NMR of compound **5i** (300 MHz, CDCl<sub>3</sub>)

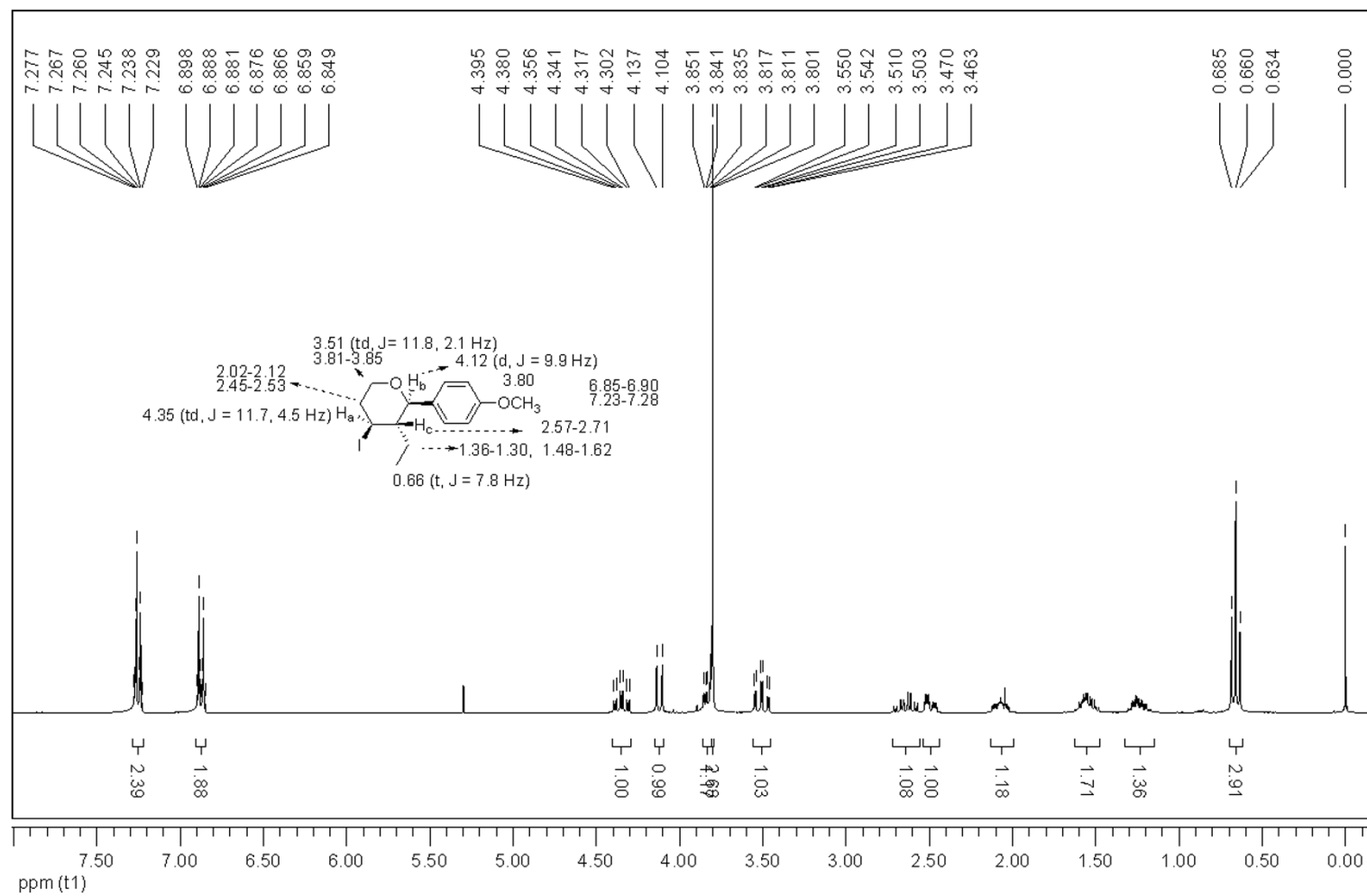
$^1\text{H}$ -NMR of compound **5i** (300 MHz,  $\text{CDCl}_3$ )

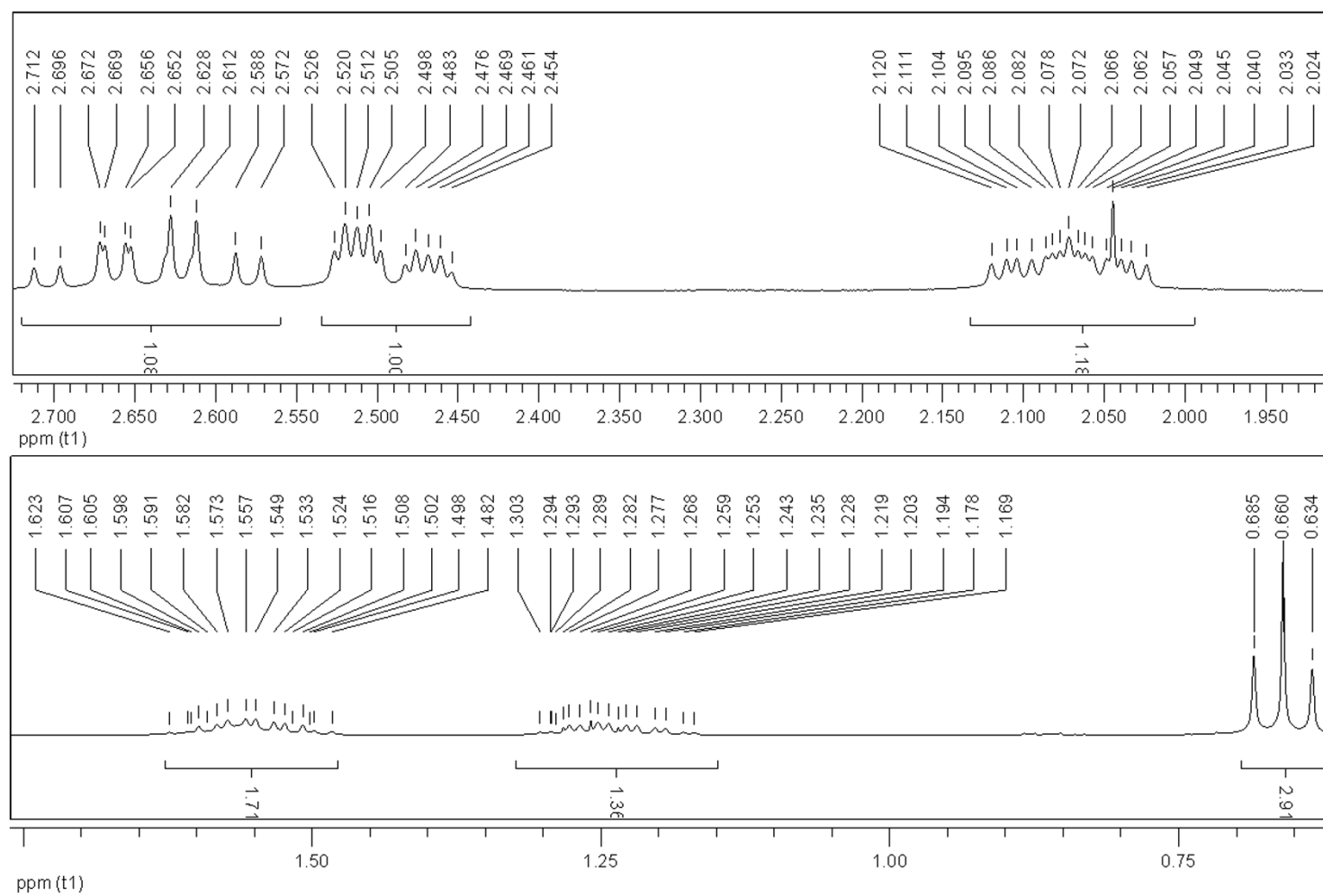
$^{13}\text{C}$ -NMR of compound **5i** (75 MHz,  $\text{CDCl}_3$ )

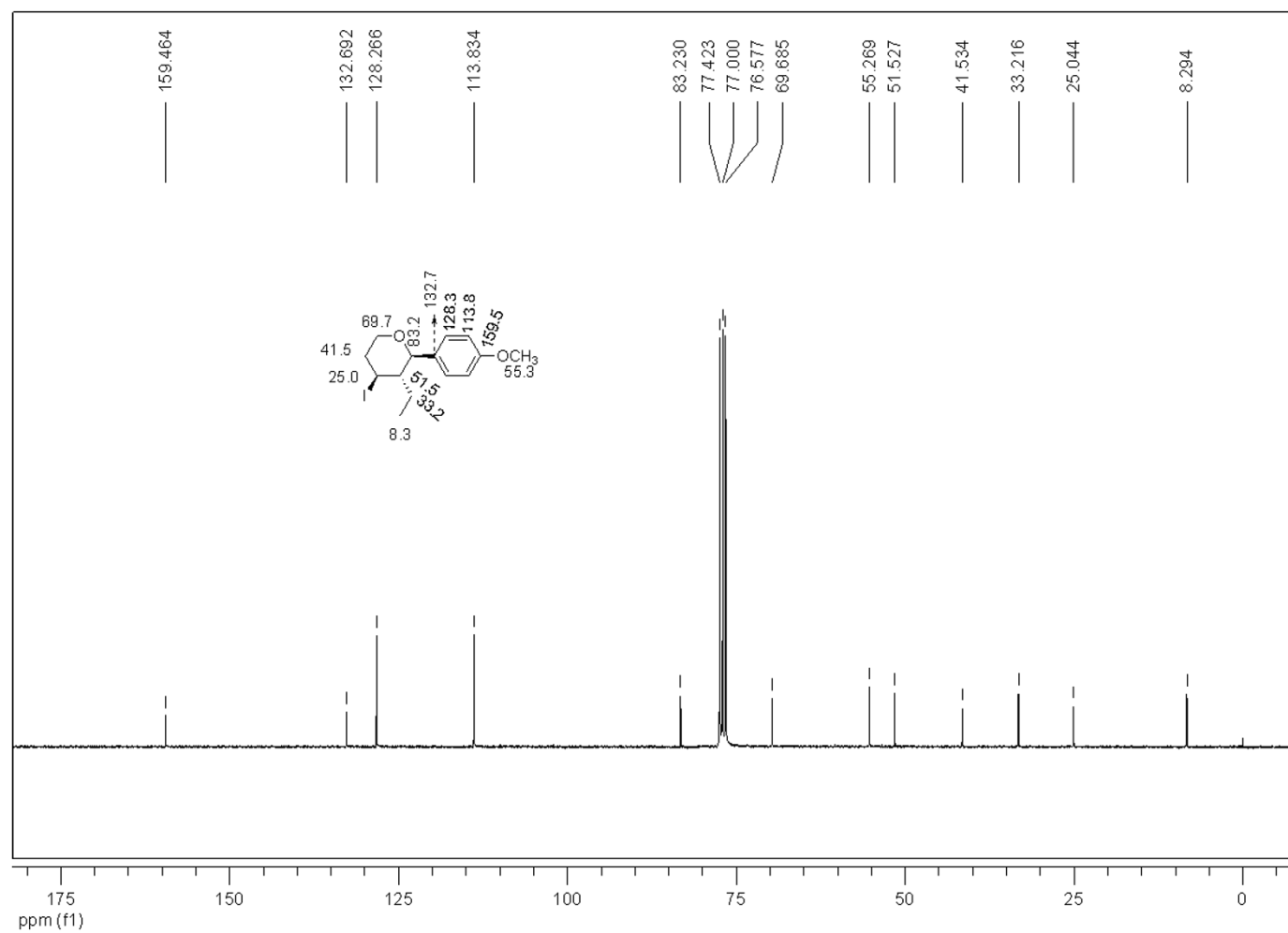
<sup>1</sup>H-NMR of compound **5j** (500 MHz, CDCl<sub>3</sub>)

$^{13}\text{C}$ -NMR of compound **5j** (50 MHz,  $\text{CDCl}_3$ )

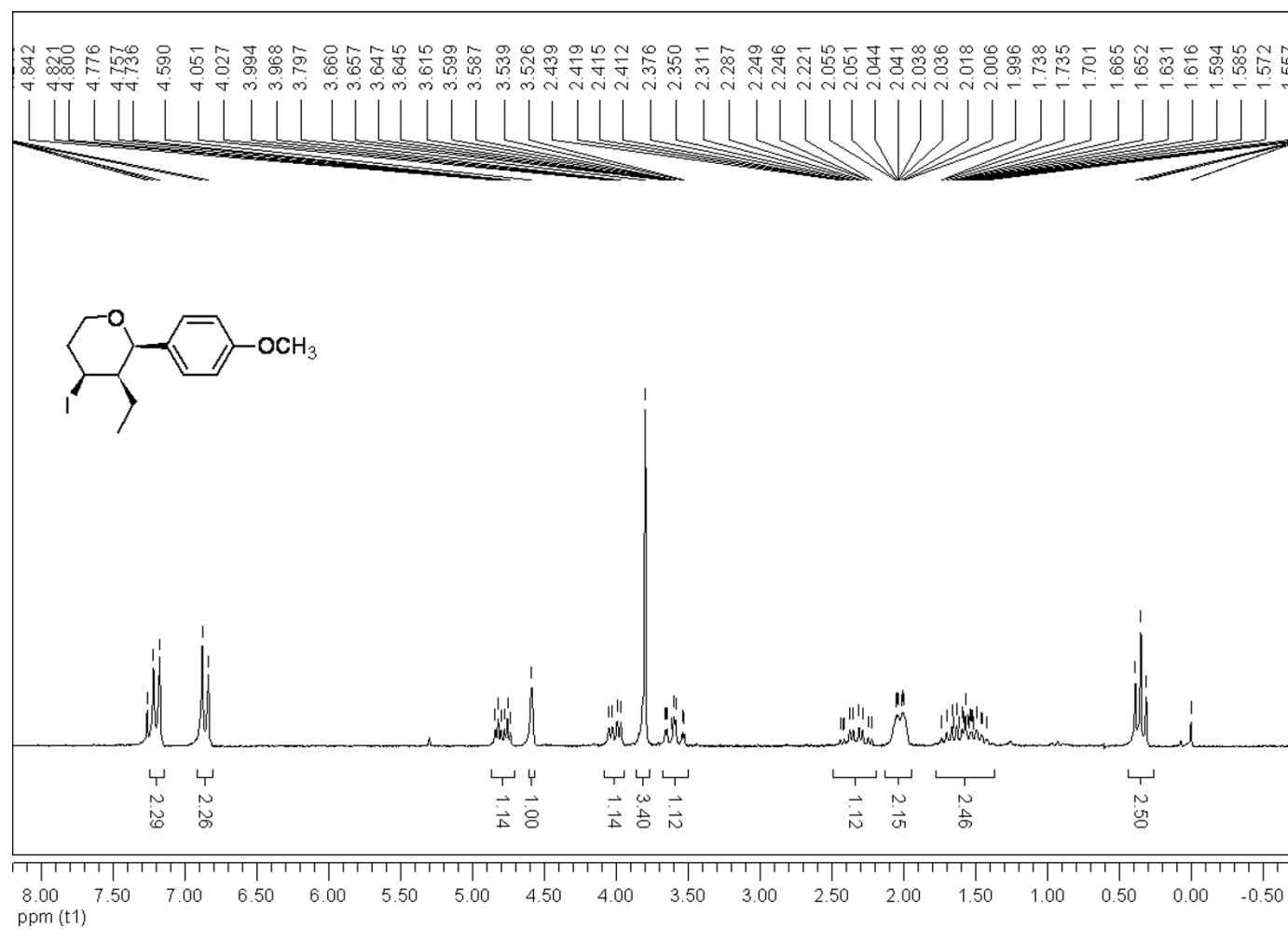
2D NOESY NMR of compound **5j** (500 MHz, CDCl<sub>3</sub>)

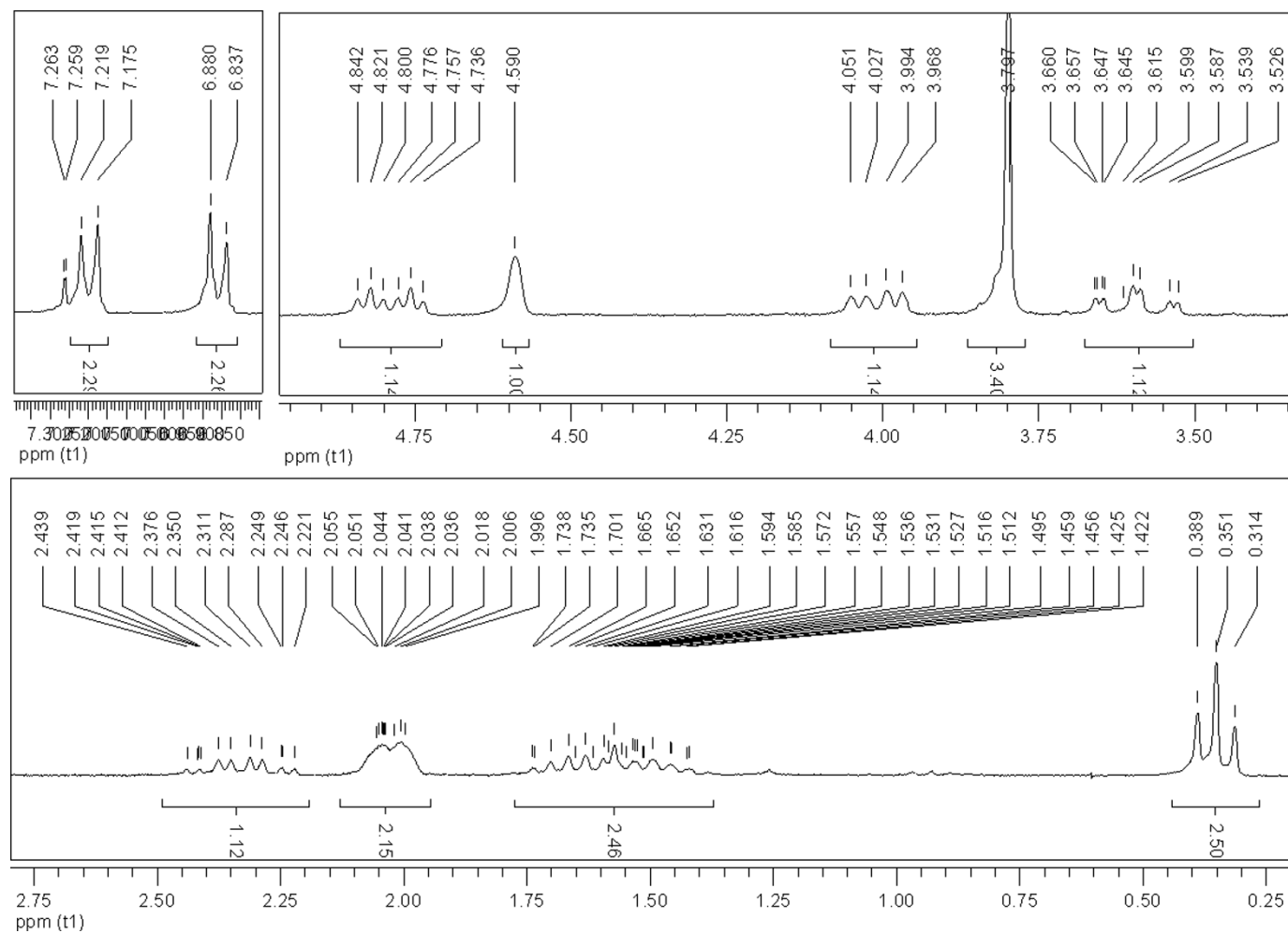
$^1\text{H}$ -NMR of compound **5k** (300 MHz,  $\text{CDCl}_3$ )

$^1\text{H}$ -NMR of compound **5k** (300 MHz,  $\text{CDCl}_3$ )

$^{13}\text{C}$ -NMR of compound **5k** (75 MHz,  $\text{CDCl}_3$ )

2D COSY NMR spectrum of compound 1a. The x-axis is  $^1\text{H}$  NMR (0-8 ppm) and the y-axis is  $^1\text{H}$  NMR (0-7 ppm). The 1D  $^1\text{H}$  NMR spectra are shown along the top and left axes. The 2D plot shows correlations between protons. Key correlations are highlighted: Hc (7.2 ppm) to Ha (7.0 ppm) and Hb (6.8 ppm); Ha (7.0 ppm) to Hc (7.2 ppm) and Hb (6.8 ppm); Hb (6.8 ppm) to Ha (7.0 ppm) and Hc (7.2 ppm). The aromatic region (6.5-7.5 ppm) shows correlations between Hc, Ha, and Hb. The aliphatic region (1.0-4.5 ppm) shows correlations between CH<sub>3</sub>/H<sub>a</sub> (1.0 ppm), H<sub>b</sub>/H<sub>c</sub> (3.5 ppm), and CH<sub>3</sub>/H<sub>b</sub> (4.0 ppm). A chemical structure of 1a is shown in the bottom right, with protons labeled: H<sub>a</sub> (aromatic), H<sub>b</sub> (aromatic), H<sub>c</sub> (aromatic), CH<sub>3</sub> (methyl), and H<sub>b</sub> (methylene).

<sup>1</sup>H-NMR of compound **51** (200 MHz, CDCl<sub>3</sub>)

$^1\text{H}$ -NMR of compound **51** (200 MHz,  $\text{CDCl}_3$ )

$^{13}\text{C}$ -NMR of compound **51** (50 MHz,  $\text{CDCl}_3$ )