Supplementary Material

2,6-Dicyanoaniline based donor-acceptor compounds: the facile synthesis of fluorescent 3,5-diaryl/hetaryl-2,6-dicyanoanilines

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Experimental Section

Optical Spectra Analysis

All spectrophotometric measurements were performed in thermostated quartz sample cells (pathlength ℓ = 1 cm) at 25 °C in spectral-grade DMSO solvent. Ultraviolet-visible (UV-vis) absorption spectra were recorded on Analytik Jena Specord 200 spectrophotometer at the wavelength of maximum absorption (λ_{max}, in nm) in 350-600 nm scan range. Fluorescence emission spectra were recorded with a HITACHI F-7000 FL Spectrofluorophotometer . The slit width was 2.5 nm for excitation and 2.5 nm emission. The PMT voltage was 700 V for each measurement. Relative quantum efficiencies of fluorescence of dicyanoaniline derivatives were obtained by comparing the areas under the corrected emission spectrum of the test sample in EtOH of Coumarin 153 (0.38 in EtOH).[1,2] The spectral range of emission for compounds **1** and **1-I** are exception to spectral range of Coumarin 153. All compounds are solved for measurements in spectral grade DMSO. Dilute solutions (0.1<A<0.3) were used to minimize the reabsorption effects. The relative fluorescence quantum yields, Φ_s, were determined by the standard method and using following equation 1.

$$\Phi_s = [(A_r I_s n_s^{\ 2}) / (A_s I_r n_r^{\ 2})]\ \Phi_r \qquad \textbf{(1)}$$

where the subscript s refers to the sample and the subscript r refers to the reference standard; is quantum yield, A is the absorbance at the excitation wavelength, I is the emission intensity height, and n is the index of refraction of the solvent containing the sample (n_{DMSO}: 1.479 and the reference Standard ($n_{Ethanol}$:1.362). The molar extinction coefficient was calculated using by equation 2 of Beer-Lambert law,

$$A = \varepsilon . l. C \qquad (2)$$

where the A shows absorbance, ℓ the pathlength of quartz cells, C the concentration of the solutions.

2-(2-Thienylmethylene)malononitrile (1d). The compound was prepared from commercially available 2-thiophenecarboxaldehyde and malononitrile by using known procedure. The formed pale orange solid was filtered off and recyrstallized from ethanol to afford pure compound (6.40 g, Yield 90 %, mp 95-96° C).[3]

2-(2-Furanylmethylene)malononitrile (1e). The compound was prepared from commercially available Furan-2-carboxaldehyde and malononitrile by using known procedure. The grey solid crystals were obtained from ethanol (6.12 g, yield 85 %, mp 119-120 °C).[3]

2-(Pyridin-3-ylmethylene)malononitrile (1f). The compound was prepared commercially available 3-pyridinecarboxaldehyde and malononitrile by using known procedure. The formed light yellow solid was filtered off and recyrstallized from ethanol to afford pure compound (1.47 g, yield 95 %, mp 162-164) according the literature.[4]

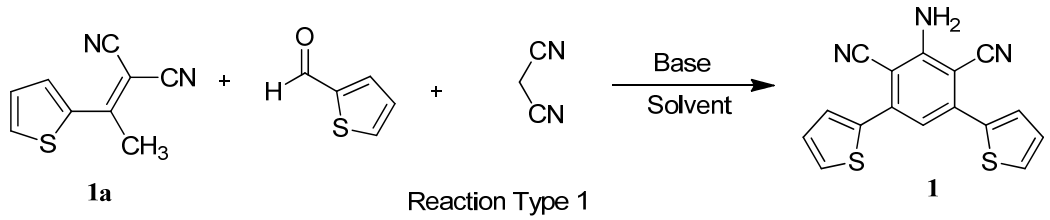
2-(4-Chlorobenzylidene)malononitrile (1g). The compound was prepared commercially available 4-chlorobenzaldehyde and malononitrile by using known procedure. The white needle crystals were obtained from ethanol (1800 mg, yield 96%, mp 161 °C).[3]

2-(4-Nitrobenzylidene)malononitrile (1h). The compound was prepared commercially available 4-nitrobenzaldehyde and malononitrile by using known procedure. The colourless cyristals were obtained from ethanol (1950 mg, yield 96%, mp 161 °C).[5]

Benzylidenemalonitrile (1i). The compound was prepared commercially available benzaldehyde and malononitrile by using known procedure. The white needle crystals were obtained from ethanol (1.20 g, yield 66 %, mp 82 °C).[5]

2-(4-methoxybenzylidene)malononitrile (1j). The compound was prepared commercially available p-anisaldehyde and malononitrile by using known procedure. The formed white solid was filtered off and recyrstallized from ethanol to afford pure compound (1310 mg, yield 71 %, mp 116 °C).[5]

4-(2,2-dicyanovinyl)benzoic acid (1k). The compound was prepared commercially available 4-carboxybenzaldehyde and malononitrile by using known procedure. The yellow crystals were obtained from ethanol (1.28 g, yield 65 %, mp 288-290 ^{o}C).[6]



Scheme S1. Reaction Type 1.

Table S1. Optimization of solvent, temperature and time by using different amount piperidine for the synthesis of **1** via Reaction Type 1

Solvents	Piperidine	Temp. (^{O}C)	Time	Yield (%)
Acetonitrile	cat.	rt	10 min.	62
Acetonitrile	***equiv.***	***rt***	***10 min.***	***64***
Acetonitrile	cat.	80	18 h	54
Acetonitrile	equiv.	80	18 h	59
Ethanol	equiv.	rt	10 min.	18
Ethanol	equiv.	rt	10 min.	31
Ethanol	cat.	80	18 h	38
Ethanol	equiv.	80	18 h	47
Methanol	equiv.	rt	10 min.	31
Methanol	equiv.	80	18 h	51
Toluene	equiv.	rt	10 min.	25
Toluene	equiv.	80	18 h	34
DMF	equiv.	rt	10 min.	48
DMF	equiv.	80	18 h	47

rt:Room Temperature

Table S2. Optimization of base for the synthesis of **1** in acetonitrile via Reaction Type 1

Solvent	Base	Temp. (^{O}C)	Time	Yield (%)
Acetonitrile	-	rt	10 min.	No reaction
Acetonitrile	-	80	18 h	No reaction
Acetonitrile	Piperidine(cat.)	rt	10 min.	62
Acetonitrile	***Piperidine(equiv.)***	***rt***	***10 min.***	***64***
Acetonitrile	Piperidine(cat.)	80	18 h	54
Acetonitrile	Piperidine(equiv.)	80	18 h	59
Acetonitrile	Pyridine(cat.)	rt	10 min.	Trace
Acetonitrile	Pyridine(equiv.)	rt	10 min.	Trace
Acetonitrile	Pyridine(cat.)	80	18 h	Trace
Acetonitrile	Pyridine(equiv.)	80	18 h	Trace
Acetonitrile	Pyrrolidine (cat.)	rt	10 min.	44
Acetonitrile	Pyrrolidine (equiv.)	rt	10 min.	51
Acetonitrile	Pyrrolidine (cat.)	80	18 h	60
Acetonitrile	Pyrrolidine (equiv.)	80	18 h	60
Acetonitrile	Morpholine(cat.)	rt	10 min.	Trace
Acetonitrile	Morpholine(equiv.)	rt	10 min.	Trace
Acetonitrile	Morpholine(cat.)	80	18 h	63
Acetonitrile	Morpholine(equiv.)	80	18 h	47
Acetonitrile	Triethylamine(cat.)	rt	10 min.	8
Acetonitrile	Triethylamine(equiv.)	rt	10 min.	44
Acetonitrile	Triethylamine(cat.)	80	18 h	18
Acetonitrile	Triethylamine(equiv.)	80	18 h	18
Acetonitrile	Diethylamine(cat.)	rt	10 min.	47
Acetonitrile	Diethylamine(equiv.)	rt	10 min.	47
Acetonitrile	Diethylamine(cat.)	80	18 h	8
Acetonitrile	Diethylamine(equiv.)	80	18 h	44
Acetonitrile	DMAP(cat.)	rt	10 min.	18
Acetonitrile	DMAP(equiv.)	rt	10 min.	38
Acetonitrile	DMAP(cat.)	80	18 h	28
Acetonitrile	DMAP(equiv.)	80	18 h	28

rt:room temperature, cat..:catalytic, equiv.:equivalent

Table S3. Optimization of base for the synthesis of **1** in acetonitrile via Reaction Type 2

Solvent	Base	Temp. (^{O}C)	Time	Yield (%)
Acetonitrile	-	rt	10 min.	No reaction
Acetonitrile	-	80	18 h	No reaction
Acetonitrile	Piperidine(cat.)	rt	10 min.	60
Acetonitrile	***Piperidine(equiv.)***	***rt***	***10 min.***	***68***
Acetonitrile	Piperidine(cat.)	80	18 h	54
Acetonitrile	Piperidine(equiv.)	80	18 h	47
Acetonitrile	Pyridine(cat.)	rt	10 min.	Trace
Acetonitrile	Pyridine(equiv.)	rt	10 min.	Trace
Acetonitrile	Pyridine(cat.)	80	18 h	Trace
Acetonitrile	Pyridine(equiv.)	80	18 h	Trace
Acetonitrile	Pyrrolidine (cat.)	rt	10 min.	64
Acetonitrile	Pyrrolidine (equiv.)	rt	10 min.	60
Acetonitrile	Pyrrolidine (cat.)	80	18 h	63
Acetonitrile	Pyrrolidine (equiv.)	80	18 h	63
Acetonitrile	Morpholine(cat.)	rt	10 min.	34
Acetonitrile	Morpholine(equiv.)	rt	10 min.	21
Acetonitrile	Morpholine(cat.)	80	18 h	44
Acetonitrile	Morpholine(equiv.)	80	18 h	47
Acetonitrile	Triethylamine(cat.)	rt	10 min.	21
Acetonitrile	Triethylamine(equiv.)	rt	10 min.	31
Acetonitrile	Triethylamine(cat.)	80	18 h	11
Acetonitrile	Triethylamine(equiv.)	80	18 h	15
Acetonitrile	Diethylamine(cat.)	rt	10 min.	60
Acetonitrile	Diethylamine(equiv.)	rt	10 min.	53
Acetonitrile	Diethylamine(cat.)	80	18 h	37
Acetonitrile	Diethylamine(equiv.)	80	18 h	47
Acetonitrile	DMAP(cat.)	rt	10 min.	31
Acetonitrile	DMAP(equiv.)	rt	10 min.	40
Acetonitrile	DMAP(cat.)	80	18 h	21
Acetonitrile	DMAP(equiv.)	80	18 h	34

Table S4. The photograph of synthesized 3,5-disubstituted-2,6-dicyanoanilines under ambient and UV light (365 nm) irradiation

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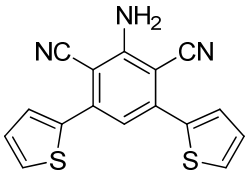
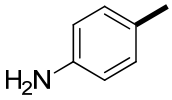
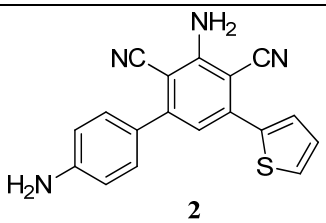
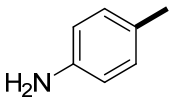
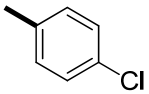
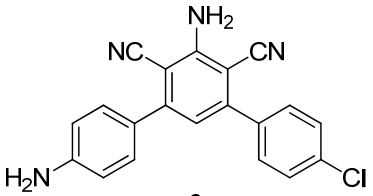
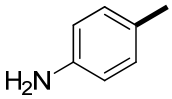
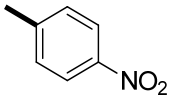
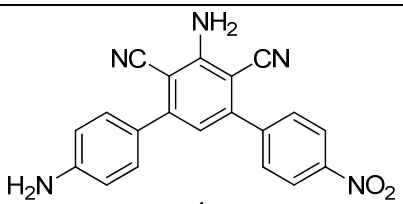
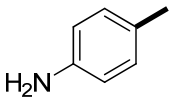
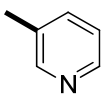
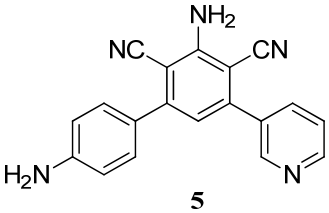
			Ambient Light	UV Light
		 **1**		
		 **2**		
		 **3**		
		 **4**		
		 **5**		

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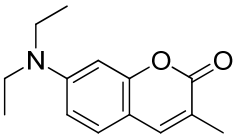
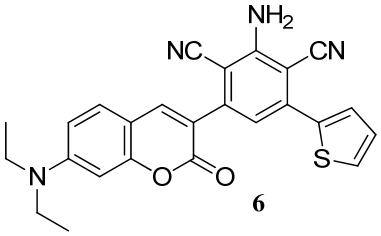
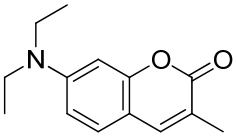
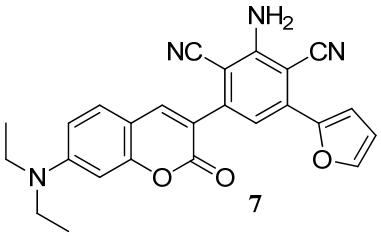
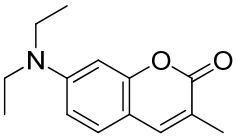
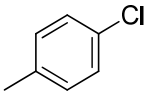
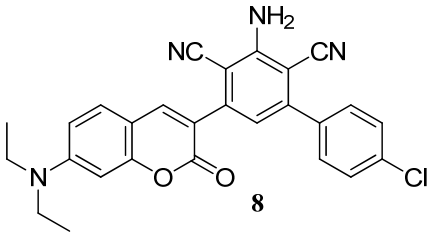
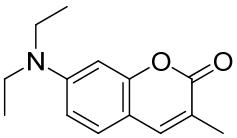
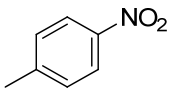
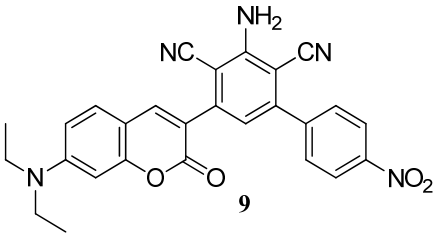
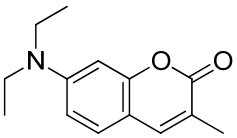
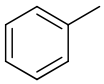
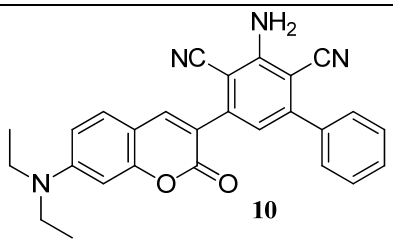
			Ambient Light	UV Light
		 **6**		
		 **7**		
		 **8**		
		 **9**		
		 **10**		

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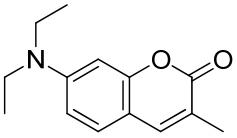
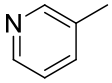
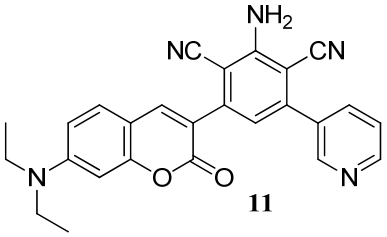
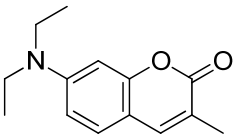
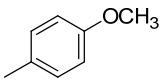
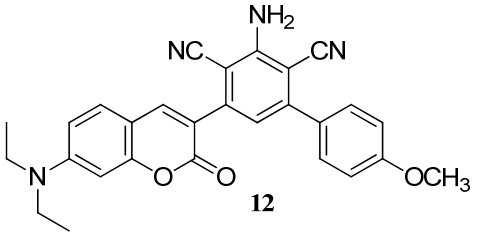
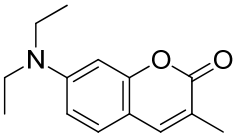
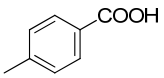
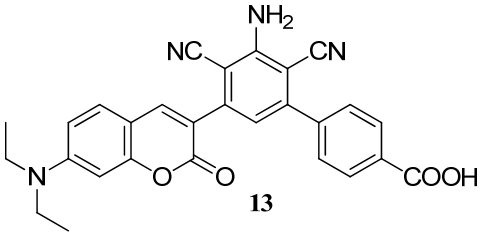
		 **11**		
		 **12**		
		 **13**		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Department of Chemistry
Ataturk University
25240 Erzurum Turkey

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Please consider this CIF for submission to the Cambridge
Crystallographic
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Data Centre. I certify that all authors have seen and approved of
this
submission, that all have made significant scientific contributions
to the
work reported, and that all share responsibility and accountability
for
the results.

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Sahin, ertan.
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 'Sahin, ertan'                  #<--'Last name, first name'
; ?
;
;
Department of Chemistry
Ataturk University
25240 Erzurum Turkey

;

#------------------  SECTION 2. COMPOUND(S) DETAILS ---------------
---------#

data_shelxlzeynel-rxn128-son3

_audit_creation_date                    2013-12-26T10:24:45-00:00
_audit_creation_method                  'WinGX routine CIF_UPDATE'
```



```
#------------------------------------------------------------------
---------#
#                   CHEMICAL INFORMATION
#
#------------------------------------------------------------------
---------#

_chemical_name_systematic
;
 ?
;
_chemical_formula_moiety                'C20 H17 N3 S2'
_chemical_formula_sum                   'C20 H17 N3 S2'
_chemical_formula_weight                363.49
_chemical_compound_source               'synthesis as described'

#------------------------------------------------------------------
---------#
#                   UNIT CELL INFORMATION
#
#------------------------------------------------------------------
---------#

_symmetry_cell_setting                  monoclinic
_symmetry_space_group_name_H-M          'P 21/a'
_symmetry_space_group_name_Hall         '-P 2yab'
_symmetry_Int_Tables_number             14
loop_
    _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x+1/2, y+1/2, -z'
 '-x, -y, -z'
 'x-1/2, -y-1/2, z'

_cell_length_a                           8.6608(3)
_cell_length_b                           12.1142(7)
_cell_length_c                           17.8406(7)
_cell_angle_alpha                        90.0000(0)
_cell_angle_beta                         95.3794(27)
_cell_angle_gamma                        90.0000(0)
_cell_volume                            1863.6(14)
_cell_formula_units_Z                   4
_cell_measurement_temperature           293(2)
_cell_measurement_reflns_used           0
_cell_measurement_theta_min             0
_cell_measurement_theta_max             0
_cell_measurement_wavelength            0.71073

#------------------------------------------------------------------
---------#
#                   CRYSTAL INFORMATION
#
#------------------------------------------------------------------
---------#

_exptl_crystal_description              prism
```



```
_exptl_crystal_colour                   colourless
_exptl_crystal_size_max                 0.3
_exptl_crystal_size_mid                 0.2
_exptl_crystal_size_min                 0.1
_exptl_crystal_density_diffrn           1.296
_exptl_crystal_density_method           'not measured'
_exptl_crystal_F_000                    760
_exptl_special_details
;
 ?
;

#------------------------------------------------------------------------
---------#
#                   ABSORPTION CORRECTION
#
#------------------------------------------------------------------------
---------#

_exptl_absorpt_coefficient_mu           0.293
_exptl_absorpt_correction_type          'Multi-scan'
_exptl_absorpt_correction_T_max         0.971
_exptl_absorpt_correction_T_min         0.932

#------------------------------------------------------------------------
---------#
#                   DATA COLLECTION
#
#------------------------------------------------------------------------
---------#

_diffrn_ambient_temperature             293(2)
_diffrn_radiation_wavelength            0.71073
_diffrn_radiation_type                  MoK\a
_diffrn_radiation_monochromator         graphite
_diffrn_radiation_probe                 x-ray
_diffrn_reflns_av_R_equivalents         0.1149
_diffrn_reflns_av_unetI/netI            0.1135
_diffrn_reflns_number                   38231
_diffrn_reflns_limit_h_min              -10
_diffrn_reflns_limit_h_max              10
_diffrn_reflns_limit_k_min              -15
_diffrn_reflns_limit_k_max              15
_diffrn_reflns_limit_l_min              -22
_diffrn_reflns_limit_l_max              22
_diffrn_reflns_theta_min                2.29
_diffrn_reflns_theta_max                26.6
_diffrn_reflns_theta_full               26.6
_diffrn_measured_fraction_theta_full
                                        0.984
_diffrn_measured_fraction_theta_max
                                        0.984
_reflns_number_total                    3842
_reflns_number_gt                       2591
_reflns_threshold_expression            >2\s(I)
_diffrn_radiation_detector              'RX'
```



```
_diffrn_measurement_device
;
RAXIS conversion
;
_diffrn_detector_area_resol_mean        10.0000
_diffrn_measurement_method              'dtprofit.ref'


#---------------------------------------------------------------------
---------#
#                   COMPUTER PROGRAMS USED
#
#---------------------------------------------------------------------
---------#

_computing_structure_refinement         'SHELXL-97 (Sheldrick,
2008)'
_computing_molecular_graphics           'Ortep-3 for Windows
(Farrugia, 1997)'
_computing_publication_material
                                    'WinGX publication routines
(Farrugia, 1999)'

#---------------------------------------------------------------------
---------#
#                   STRUCTURE SOLUTION
#---------------------------------------------------------------------
---------#

_atom_sites_solution_primary            direct
_atom_sites_solution_secondary          difmap
_atom_sites_solution_hydrogens          geom

#---------------------------------------------------------------------
---------#
#                   REFINEMENT INFORMATION
#
#---------------------------------------------------------------------
---------#

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor
wR and
 goodness of fit S are based on F^2^, conventional R-factors R are
based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2\s(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
;
```



```
_refine_ls_structure_factor_coef        Fsqd
_refine_ls_matrix_type                  full
_refine_ls_weighting_scheme             calc
_refine_ls_weighting_details
         'calc w=1/[\s^2^(Fo^2^)+(0.2000P)^2^+0.0000P] where
P=(Fo^2^+2Fc^2^)/3'
_refine_ls_hydrogen_treatment           constr
_refine_ls_extinction_method            SHELXL
_refine_ls_extinction_expression

Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^
_refine_ls_extinction_coef              0
_refine_ls_number_reflns                3842
_refine_ls_number_parameters            229
_refine_ls_number_restraints            3
_refine_ls_R_factor_all                 0.2169
_refine_ls_R_factor_gt                  0.108
_refine_ls_wR_factor_ref                0.2896
_refine_ls_wR_factor_gt                 0.1033
_refine_ls_goodness_of_fit_ref          1.057
_refine_ls_restrained_S_all             1.063
_refine_ls_shift/su_max                 0
_refine_ls_shift/su_mean                0
_refine_diff_density_max                0.703
_refine_diff_density_min                -0.49
_refine_diff_density_rms                0.085

#-------------------------------------------------------------------
---------#
#                   ATOMIC TYPES, COORDINATES AND THERMAL PARAMETERS
#
#-------------------------------------------------------------------
---------#

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    _atom_type_description
    _atom_type_scat_dispersion_real
    _atom_type_scat_dispersion_imag
    _atom_type_scat_source
C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and
6.1.1.4'
H H 0 0 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
N N 0.0061 0.0033 'International Tables Vol C Tables 4.2.6.8 and
6.1.1.4'
S S 0.1246 0.1234 'International Tables Vol C Tables 4.2.6.8 and
6.1.1.4'

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    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
    _atom_site_adp_type
```



```
    _atom_site_occupancy
    _atom_site_symmetry_multiplicity
    _atom_site_calc_flag
    _atom_site_refinement_flags
    _atom_site_disorder_assembly
    _atom_site_disorder_group
S1 S 0.2891(2) -0.03341(17) 0.52311(11) 0.0829(8) Uani 1 1 d . . .
S2 S 0.4822(3) 0.3646(2) 0.65394(16) 0.04838(18) Uani 1 1 d . . .
C15 C 0.2834(9) -0.1537(7) 0.7492(4) 0.078(2) Uani 1 1 d . . .
C16 C 0.3410(9) 0.2155(6) 0.8610(5) 0.079(2) Uani 1 1 d . . .
C8 C 0.3370(8) 0.1449(5) 0.7967(4) 0.0659(18) Uani 1 1 d . . .
C5 C 0.3637(7) 0.0032(5) 0.6747(4) 0.0629(17) Uani 1 1 d . . .
C9 C 0.3594(7) 0.1896(5) 0.7267(4) 0.0606(17) Uani 1 1 d . . .
C7 C 0.3196(8) 0.0298(5) 0.8072(4) 0.0637(17) Uani 1 1 d . . .
N3 N 0.2973(7) -0.0074(5) 0.8771(3) 0.0762(18) Uani 1 1 d . . .
C10 C 0.3644(7) 0.3110(5) 0.7135(4) 0.0671(18) Uani 1 1 d D . .
C4 C 0.3763(8) -0.0677(6) 0.6097(4) 0.0699(19) Uani 1 1 d . . .
N2 N 0.2401(9) -0.2415(5) 0.7530(4) 0.100(2) Uani 1 1 d . . .
C3 C 0.4570(9) -0.1676(6) 0.6064(4) 0.077(2) Uani 1 1 d . . .
H3 H 0.5143 -0.2002 0.6471 0.093 Uiso 1 1 calc R . .
C14 C 0.3760(7) 0.1187(5) 0.6691(4) 0.0646(18) Uani 1 1 d . . .
H14 H 0.3969 0.1483 0.623 0.078 Uiso 1 1 calc R . .
C6 C 0.3328(8) -0.0377(5) 0.7451(4) 0.0641(17) Uani 1 1 d . . .
C19 C 0.1550(10) 0.0234(7) 0.9116(5) 0.094(3) Uani 1 1 d . . .
H19A H 0.1154 0.092 0.8892 0.113 Uiso 1 1 calc R . .
H19B H 0.1811 0.0365 0.9649 0.113 Uiso 1 1 calc R . .
C2 C 0.4395(10) -0.2123(6) 0.5327(5) 0.085(2) Uani 1 1 d . . .
H2 H 0.4829 -0.279 0.5198 0.101 Uiso 1 1 calc R . .
C17 C 0.3840(11) -0.1025(7) 0.9122(5) 0.094(3) Uani 1 1 d . . .
H17A H 0.3663 -0.1048 0.9651 0.113 Uiso 1 1 calc R . .
H17B H 0.3411 -0.1696 0.8892 0.113 Uiso 1 1 calc R . .
N1 N 0.3501(11) 0.2699(6) 0.9152(4) 0.111(3) Uani 1 1 d . . .
C1 C 0.3549(9) -0.1491(6) 0.4842(4) 0.079(2) Uani 1 1 d . . .
H1 H 0.3337 -0.1668 0.4336 0.095 Uiso 1 1 calc R . .
C20 C 0.0268(10) -0.0640(7) 0.9020(5) 0.107(3) Uani 1 1 d . . .
H20A H 0.0134 -0.0876 0.8504 0.16 Uiso 1 1 calc R . .
H20B H -0.0685 -0.0331 0.9159 0.16 Uiso 1 1 calc R . .
H20C H 0.0553 -0.1262 0.9337 0.16 Uiso 1 1 calc R . .
C18 C 0.5502(10) -0.1027(8) 0.9068(6) 0.111(3) Uani 1 1 d . . .
H18A H 0.5701 -0.1098 0.855 0.167 Uiso 1 1 calc R . .
H18B H 0.5964 -0.1636 0.9351 0.167 Uiso 1 1 calc R . .
H18C H 0.5939 -0.0348 0.9267 0.167 Uiso 1 1 calc R . .
C11 C 0.2694(6) 0.3993(4) 0.7467(3) 0.0769(17) Uani 1 1 d D . .
H11 H 0.1987 0.3893 0.7822 0.043 Uiso 1 1 calc R . .
C12 C 0.3070(13) 0.4970(9) 0.7146(6) 0.0769(17) Uani 1 1 d D . .
H12 H 0.2584 0.5631 0.7245 0.166 Uiso 1 1 calc R . .
C13 C 0.4186(14) 0.4904(6) 0.6680(6) 0.0744(16) Uani 1 1 d . . .
H13 H 0.4575 0.5522 0.6452 0.149 Uiso 1 1 calc R . .

loop_
    _atom_site_aniso_label
    _atom_site_aniso_U_11
    _atom_site_aniso_U_22
    _atom_site_aniso_U_33
    _atom_site_aniso_U_23
    _atom_site_aniso_U_13
```



```
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S1 0.0843(15) 0.0895(15) 0.0738(14) -0.0091(10) 0.0016(10)
0.0091(10)
S2 0.0528(4) 0.0614(4) 0.0341(3) 0.0017(3) -0.0133(3) -0.0120(3)
C15 0.090(5) 0.081(5) 0.064(5) -0.010(4) 0.017(4) 0.007(4)
C16 0.097(6) 0.067(5) 0.074(5) -0.004(4) 0.018(4) -0.003(4)
C8 0.068(4) 0.057(4) 0.073(5) -0.009(3) 0.010(3) 0.005(3)
C5 0.062(4) 0.061(4) 0.066(5) -0.006(3) 0.002(3) 0.007(3)
C9 0.054(4) 0.057(4) 0.072(5) 0.005(3) 0.008(3) 0.000(3)
C7 0.068(4) 0.051(4) 0.073(5) 0.005(4) 0.013(3) 0.008(3)
N3 0.098(5) 0.057(3) 0.075(4) 0.005(3) 0.021(3) 0.008(3)
C10 0.066(4) 0.066(4) 0.067(4) -0.009(3) -0.001(3) -0.004(3)
C4 0.072(4) 0.059(4) 0.078(5) -0.006(4) 0.008(3) -0.001(3)
N2 0.138(6) 0.057(4) 0.107(6) -0.008(4) 0.028(5) -0.022(4)
C3 0.098(6) 0.069(5) 0.066(5) -0.002(4) 0.012(4) 0.011(4)
C14 0.067(4) 0.061(4) 0.065(4) -0.001(3) 0.004(3) 0.005(3)
C6 0.077(4) 0.047(4) 0.068(5) -0.002(3) 0.006(3) 0.001(3)
C19 0.099(6) 0.097(6) 0.092(6) -0.008(5) 0.041(5) -0.001(5)
C2 0.114(6) 0.065(5) 0.075(5) -0.017(4) 0.014(5) 0.014(4)
C17 0.129(8) 0.079(5) 0.075(6) 0.003(4) 0.014(5) -0.009(5)
N1 0.172(7) 0.085(5) 0.080(5) -0.011(4) 0.026(5) -0.012(5)
C1 0.082(5) 0.094(6) 0.062(5) -0.028(4) 0.003(4) 0.002(4)
C20 0.096(7) 0.101(6) 0.124(8) 0.000(6) 0.018(6) -0.002(5)
C18 0.094(7) 0.106(7) 0.129(8) 0.012(6) -0.010(6) 0.005(5)
C11 0.072(4) 0.086(4) 0.068(3) -0.004(3) 0.021(3) 0.001(3)
C12  0.083(4) 0.080(4) 0.070(3) -0.009(3) 0.031(3) -0.013(3)
C13 0.088(4) 0.072(3) 0.066(3) 0.003(3) 0.032(3) -0.001(3)



#------------------------------------------------------------------
---------#
#                   MOLECULAR GEOMETRY
#
#------------------------------------------------------------------
---------#

_geom_special_details
;
 All s.u.'s (except the s.u. in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell s.u.'s
are taken
 into account individually in the estimation of s.u.'s in distances,
angles
 and torsion angles; correlations between s.u.'s in cell parameters
are only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s involving
l.s. planes.
;
loop_
    _geom_bond_atom_site_label_1
    _geom_bond_atom_site_label_2
    _geom_bond_distance
```



```
    _geom_bond_site_symmetry_2
    _geom_bond_publ_flag
S1 C1 1.686(7) . ?
S1 C4 1.706(8) . ?
S2 C13 1.648(10) . ?
S2 C10 1.672(7) . ?
C15 N2 1.132(9) . ?
C15 C6 1.473(10) . ?
C16 N1 1.168(9) . ?
C16 C8 1.428(10) . ?
C8 C9 1.392(9) . ?
C8 C7 1.417(9) . ?
C5 C6 1.400(9) . ?
C5 C14 1.407(9) . ?
C5 C4 1.456(9) . ?
C9 C14 1.358(9) . ?
C9 C10 1.491(9) . ?
C7 N3 1.357(8) . ?
C7 C6 1.389(9) . ?
N3 C19 1.475(9) . ?
N3 C17 1.482(10) . ?
C10 C11 1.504(7) . ?
C4 C3 1.401(9) . ?
C3 C2 1.416(10) . ?
C3 H3 0.93 . ?
C14 H14 0.93 . ?
C19 C20 1.532(11) . ?
C19 H19A 0.97 . ?
C19 H19B 0.97 . ?
C2 C1 1.324(10) . ?
C2 H2 0.93 . ?
C17 C18 1.451(11) . ?
C17 H17A 0.97 . ?
C17 H17B 0.97 . ?
C1 H1 0.93 . ?
C20 H20A 0.96 . ?
C20 H20B 0.96 . ?
C20 H20C 0.96 . ?
C18 H18A 0.96 . ?
C18 H18B 0.96 . ?
C18 H18C 0.96 . ?
C11 C12 1.367(10) . ?
C11 H11 0.93 . ?
C12 C13 1.336(15) . ?
C12 H12 0.93 . ?
C13 H13 0.93 . ?

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    _geom_angle_atom_site_label_3
    _geom_angle
    _geom_angle_site_symmetry_1
    _geom_angle_site_symmetry_3
    _geom_angle_publ_flag
C1 S1 C4 91.8(4) . . ?
```



```
C13 S2 C10 91.7(5) . . ?
N2 C15 C6 177.4(8) . . ?
N1 C16 C8 176.5(9) . . ?
C9 C8 C7 121.8(6) . . ?
C9 C8 C16 119.5(6) . . ?
C7 C8 C16 118.6(6) . . ?
C6 C5 C14 115.9(6) . . ?
C6 C5 C4 122.8(6) . . ?
C14 C5 C4 121.2(6) . . ?
C14 C9 C8 117.9(6) . . ?
C14 C9 C10 119.9(6) . . ?
C8 C9 C10 122.3(6) . . ?
N3 C7 C6 124.5(6) . . ?
N3 C7 C8 118.3(6) . . ?
C6 C7 C8 117.2(6) . . ?
C7 N3 C19 119.7(6) . . ?
C7 N3 C17 122.4(6) . . ?
C19 N3 C17 115.5(6) . . ?
C9 C10 C11 127.9(6) . . ?
C9 C10 S2 120.8(5) . . ?
C11 C10 S2 111.3(4) . . ?
C3 C4 C5 128.2(7) . . ?
C3 C4 S1 110.6(5) . . ?
C5 C4 S1 121.2(5) . . ?
C4 C3 C2 111.0(7) . . ?
C4 C3 H3 124.5 . . ?
C2 C3 H3 124.5 . . ?
C9 C14 C5 124.1(6) . . ?
C9 C14 H14 117.9 . . ?
C5 C14 H14 117.9 . . ?
C7 C6 C5 123.0(6) . . ?
C7 C6 C15 118.4(6) . . ?
C5 C6 C15 117.6(6) . . ?
N3 C19 C20 113.8(7) . . ?
N3 C19 H19A 108.8 . . ?
C20 C19 H19A 108.8 . . ?
N3 C19 H19B 108.8 . . ?
C20 C19 H19B 108.8 . . ?
H19A C19 H19B 107.7 . . ?
C1 C2 C3 112.9(7) . . ?
C1 C2 H2 123.5 . . ?
C3 C2 H2 123.5 . . ?
C18 C17 N3 116.1(7) . . ?
C18 C17 H17A 108.3 . . ?
N3 C17 H17A 108.3 . . ?
C18 C17 H17B 108.3 . . ?
N3 C17 H17B 108.3 . . ?
H17A C17 H17B 107.4 . . ?
C2 C1 S1 113.5(6) . . ?
C2 C1 H1 123.2 . . ?
S1 C1 H1 123.2 . . ?
C19 C20 H20A 109.5 . . ?
C19 C20 H20B 109.5 . . ?
H20A C20 H20B 109.5 . . ?
C19 C20 H20C 109.5 . . ?
H20A C20 H20C 109.5 . . ?
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H20B C20 H20C 109.5 . . ?
C17 C18 H18A 109.5 . . ?
C17 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
C17 C18 H18C 109.5 . . ?
H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?
C12 C11 C10 106.9(6) . . ?
C12 C11 H11 126.6 . . ?
C10 C11 H11 126.6 . . ?
C13 C12 C11 115.1(8) . . ?
C13 C12 H12 122.5 . . ?
C11 C12 H12 122.5 . . ?
C12 C13 S2 114.9(8) . . ?
C12 C13 H13 122.5 . . ?
S2 C13 H13 122.5 . . ?

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    _geom_torsion_atom_site_label_3
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    _geom_torsion_site_symmetry_2
    _geom_torsion_site_symmetry_3
    _geom_torsion_site_symmetry_4
    _geom_torsion_publ_flag
N1 C16 C8 C9 -124(14) . . . . ?
N1 C16 C8 C7 52(14) . . . . ?
C7 C8 C9 C14 -4.9(10) . . . . ?
C16 C8 C9 C14 171.2(6) . . . . ?
C7 C8 C9 C10 174.7(6) . . . . ?
C16 C8 C9 C10 -9.2(10) . . . . ?
C9 C8 C7 N3 -179.6(6) . . . . ?
C16 C8 C7 N3 4.2(9) . . . . ?
C9 C8 C7 C6 2.9(10) . . . . ?
C16 C8 C7 C6 -173.3(7) . . . . ?
C6 C7 N3 C19 -117.8(8) . . . . ?
C8 C7 N3 C19 64.9(9) . . . . ?
C6 C7 N3 C17 43.9(11) . . . . ?
C8 C7 N3 C17 -133.4(7) . . . . ?
C14 C9 C10 C11 142.5(6) . . . . ?
C8 C9 C10 C11 -37.1(10) . . . . ?
C14 C9 C10 S2 -35.7(9) . . . . ?
C8 C9 C10 S2 144.7(6) . . . . ?
C13 S2 C10 C9 178.2(6) . . . . ?
C13 S2 C10 C11 -0.3(5) . . . . ?
C6 C5 C4 C3 -45.3(11) . . . . ?
C14 C5 C4 C3 137.3(7) . . . . ?
C6 C5 C4 S1 135.5(6) . . . . ?
C14 C5 C4 S1 -41.9(9) . . . . ?
C1 S1 C4 C3 1.0(6) . . . . ?
C1 S1 C4 C5 -179.8(6) . . . . ?
C5 C4 C3 C2 179.3(7) . . . . ?
S1 C4 C3 C2 -1.4(8) . . . . ?
```



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C8 C9 C14 C5 3.6(10) . . . . ?
C10 C9 C14 C5 -176.0(6) . . . . ?
C6 C5 C14 C9 -0.3(9) . . . . ?
C4 C5 C14 C9 177.3(7) . . . . ?
N3 C7 C6 C5 -176.6(7) . . . . ?
C8 C7 C6 C5 0.7(10) . . . . ?
N3 C7 C6 C15 15.4(10) . . . . ?
C8 C7 C6 C15 -167.3(6) . . . . ?
C14 C5 C6 C7 -2.0(10) . . . . ?
C4 C5 C6 C7 -179.5(6) . . . . ?
C14 C5 C6 C15 166.1(6) . . . . ?
C4 C5 C6 C15 -11.4(10) . . . . ?
N2 C15 C6 C7 55(19) . . . . ?
N2 C15 C6 C5 -113(19) . . . . ?
C7 N3 C19 C20 96.6(9) . . . . ?
C17 N3 C19 C20 -66.4(10) . . . . ?
C4 C3 C2 C1 1.3(10) . . . . ?
C7 N3 C17 C18 46.3(11) . . . . ?
C19 N3 C17 C18 -151.3(8) . . . . ?
C3 C2 C1 S1 -0.6(10) . . . . ?
C4 S1 C1 C2 -0.2(7) . . . . ?
C9 C10 C11 C12 -176.2(7) . . . . ?
S2 C10 C11 C12 2.1(7) . . . . ?
C10 C11 C12 C13 -3.5(11) . . . . ?
C11 C12 C13 S2 3.6(13) . . . . ?
C10 S2 C13 C12 -1.8(9) . . . . ?

# The following lines are used to test the character set of files
sent by
# network email or other means. They are not part of the CIF data
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# abcdefghijklmnopqrstuvwxyzABCDEFGHIJKLMNOPQRSTUVWXYZ0123456789
# !@#$%^&*()_+{}:"~<>?|\-=[];'`,./

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References

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2. Valeur, B. *Molecular Fluorescence*, Wiley-VCH Verlag GmbH, Weinheim, **2002**.

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4. Dieskau, A. P.; Holzwarth, M. S. and Plietker, B. *Chem A Eur J.* **2012**, S1-S74.

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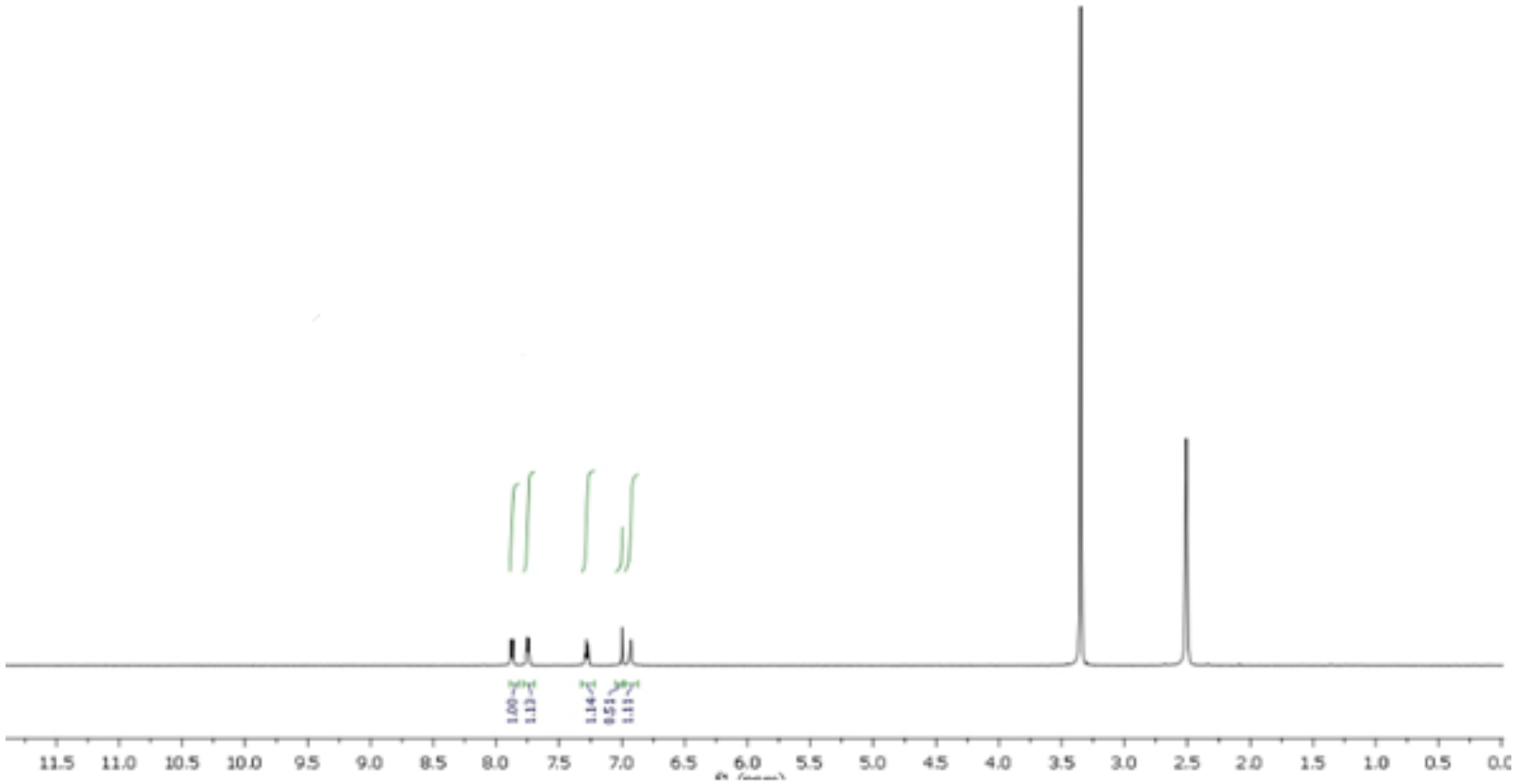
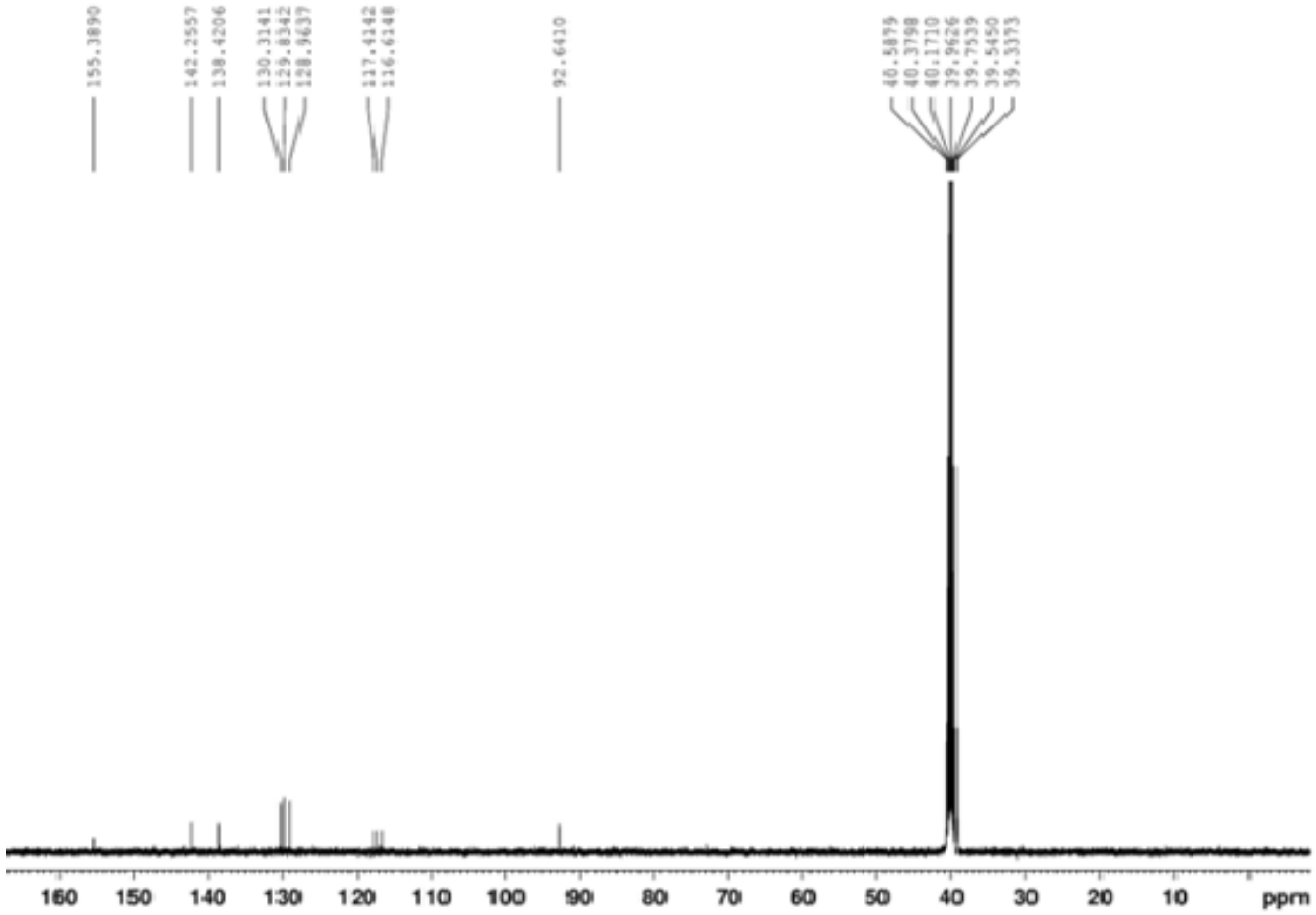
^{1}H NMR Spectra and ^{13}C NMR/^{13}C APT Spectra of Synthesized Compounds:

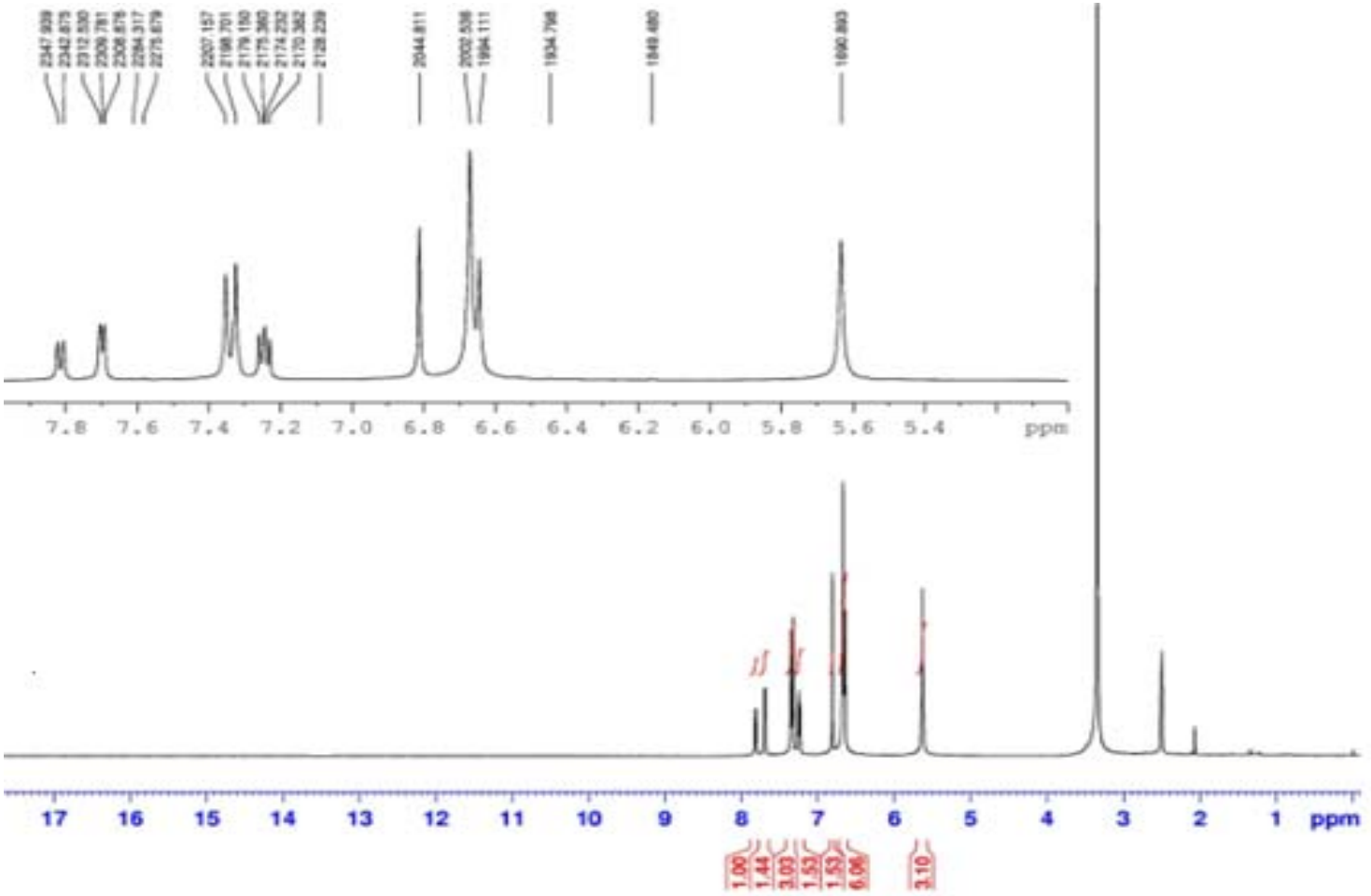
^{1}H NMR Spectrum of Compound 1



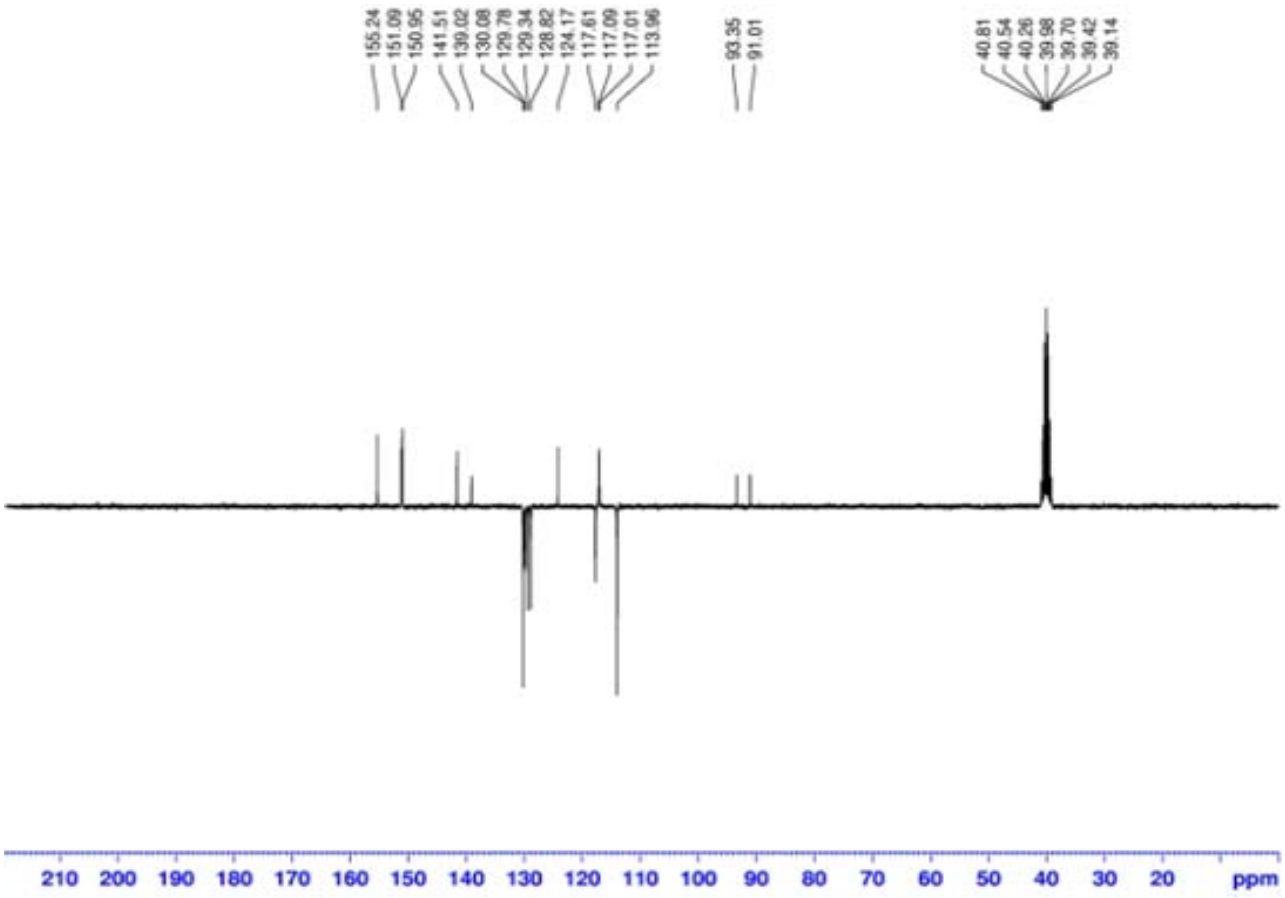
^{13}C NMR Spectrum of Compound 1



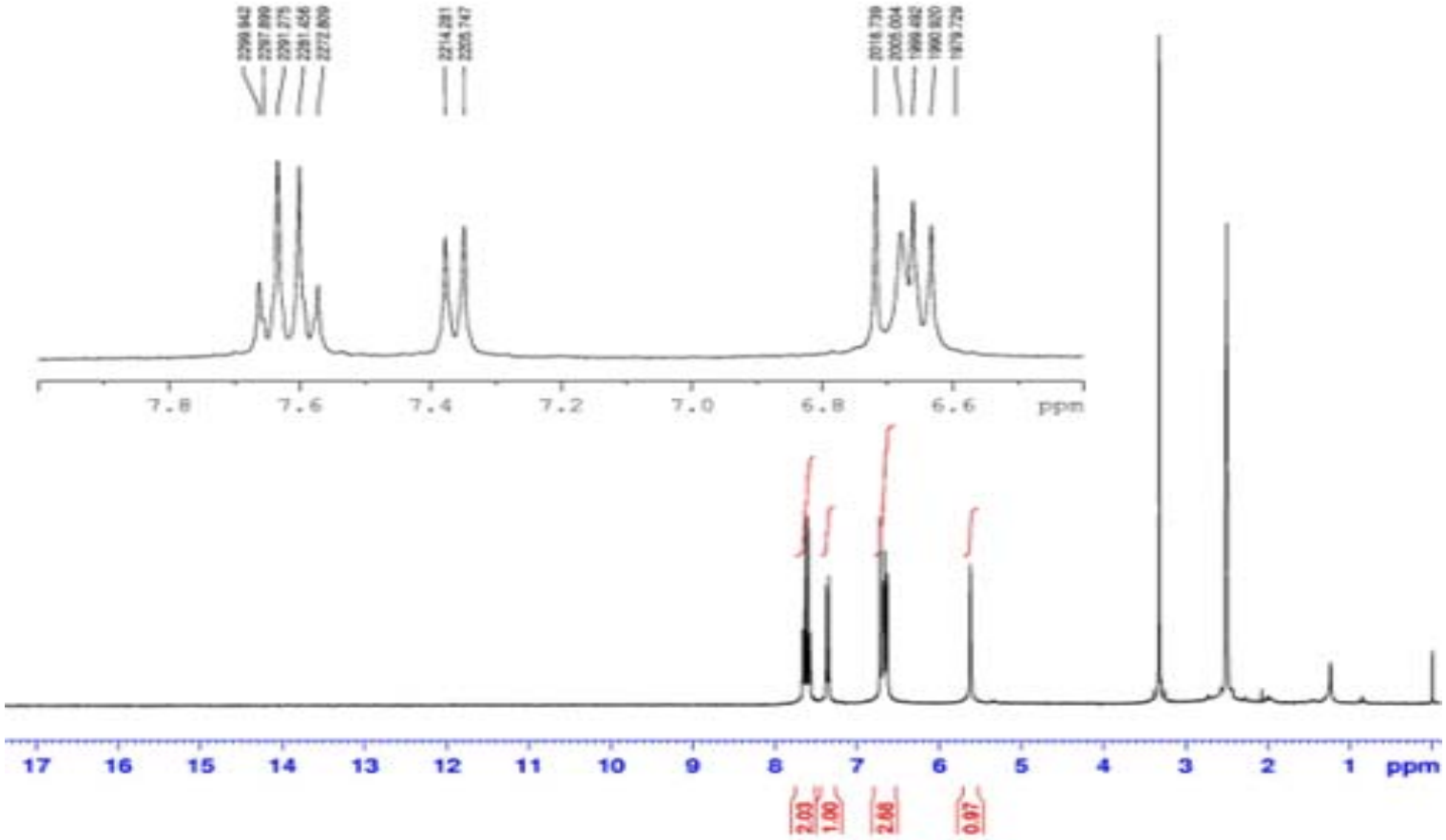
^{1}H NMR Spectrum of Compound 2



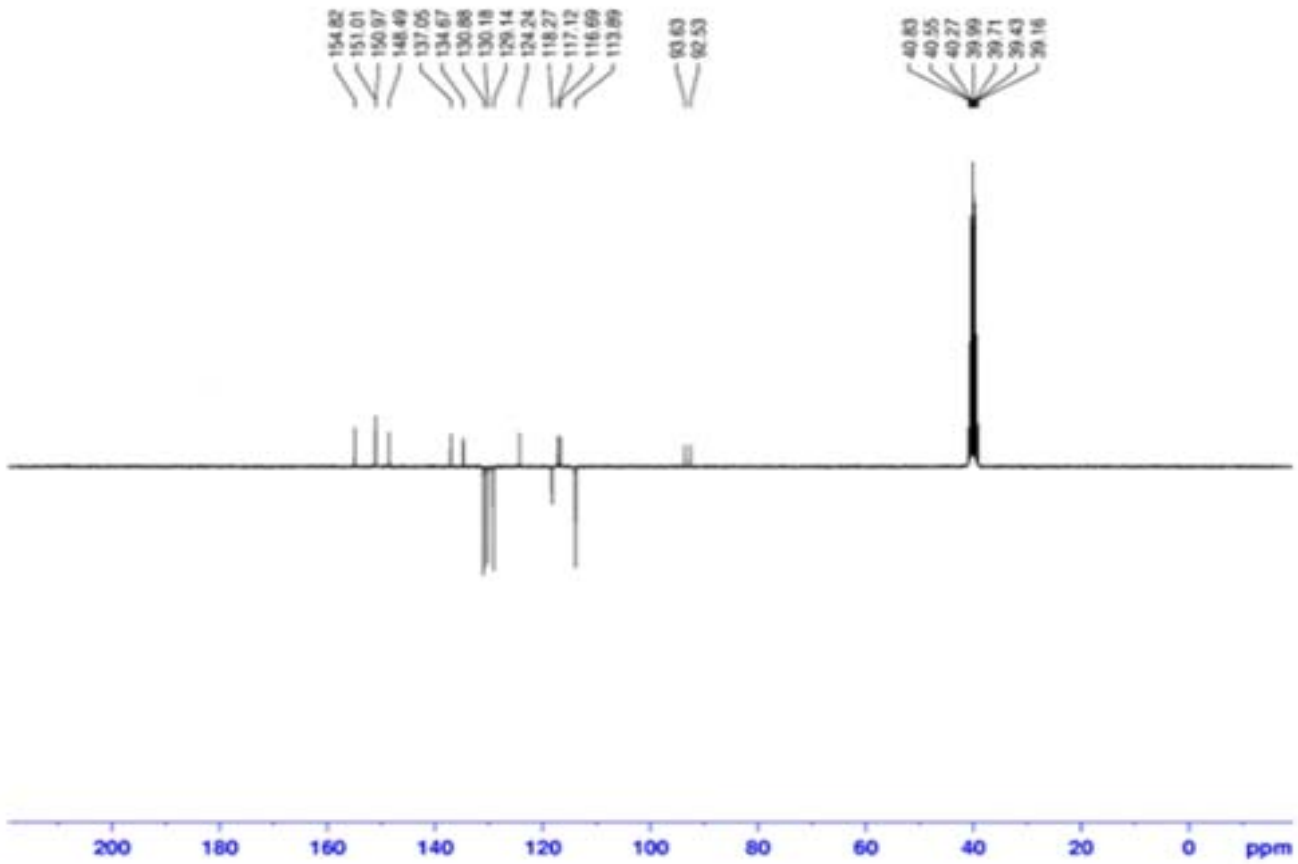
^{13}C APT Spectrum of Compound 2



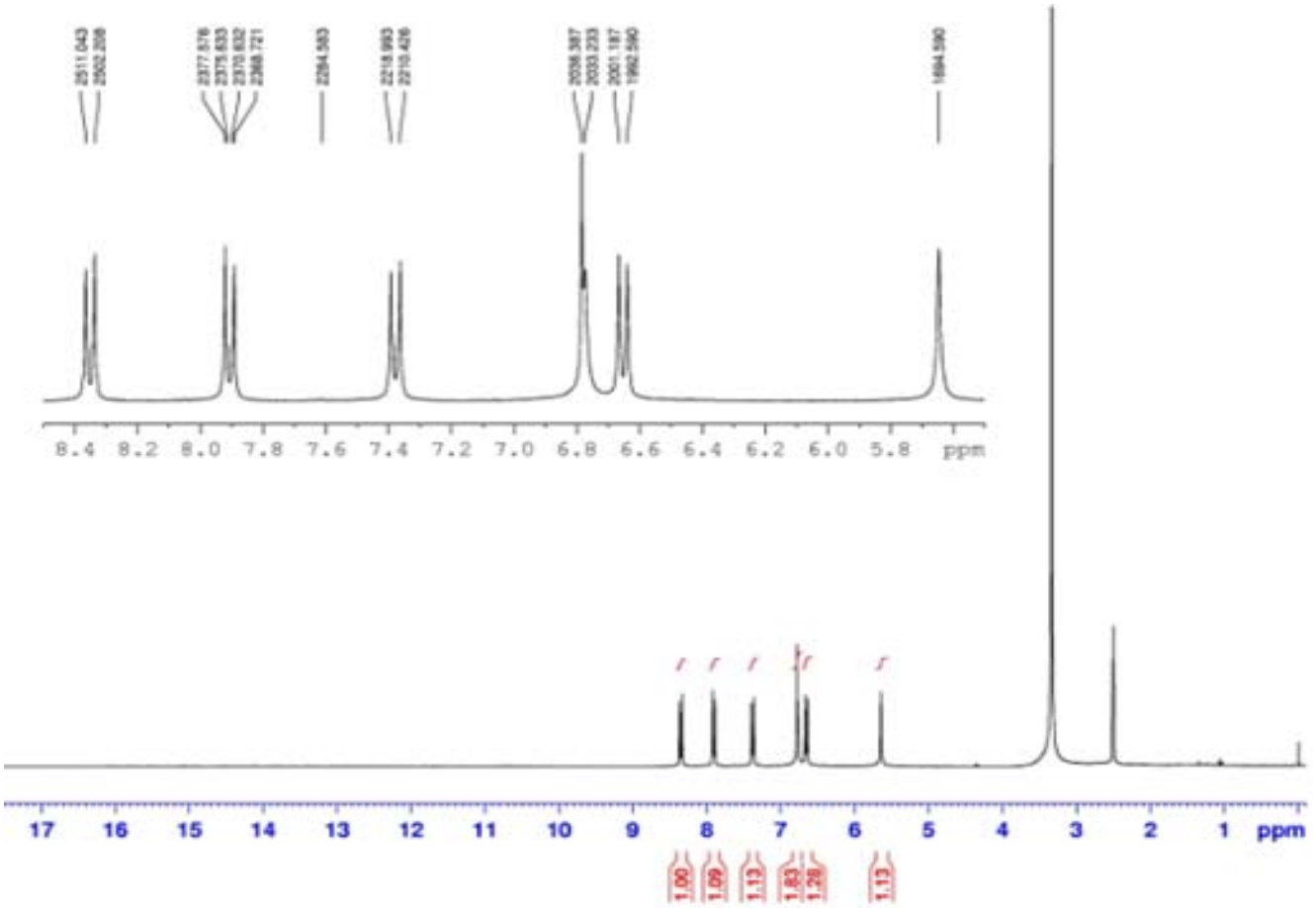
^{1}H NMR Spectrum of Compound 3



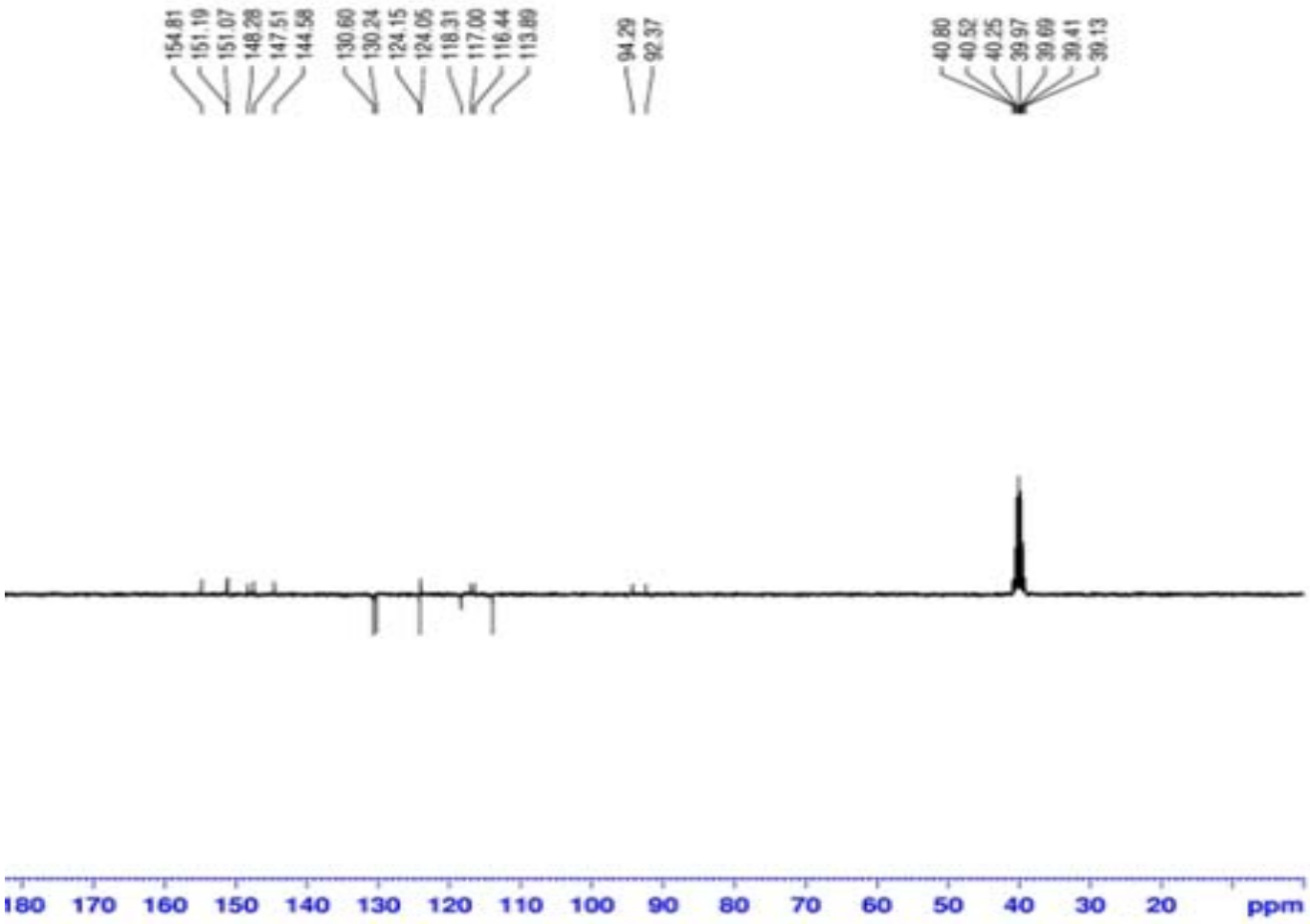
^{13}C APT Spectrum of Compound 3



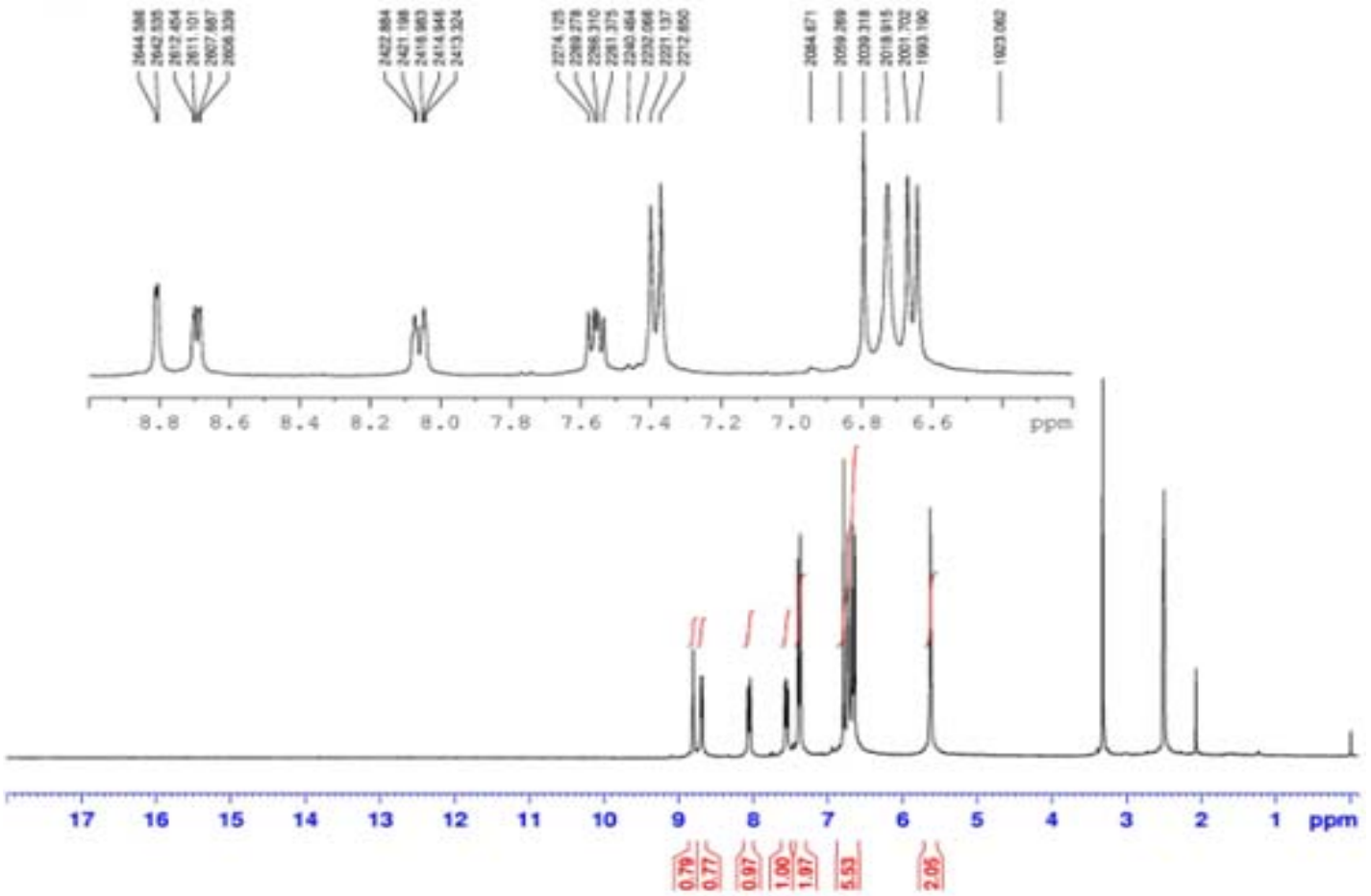
^{1}H NMR Spectrum of Compound 4



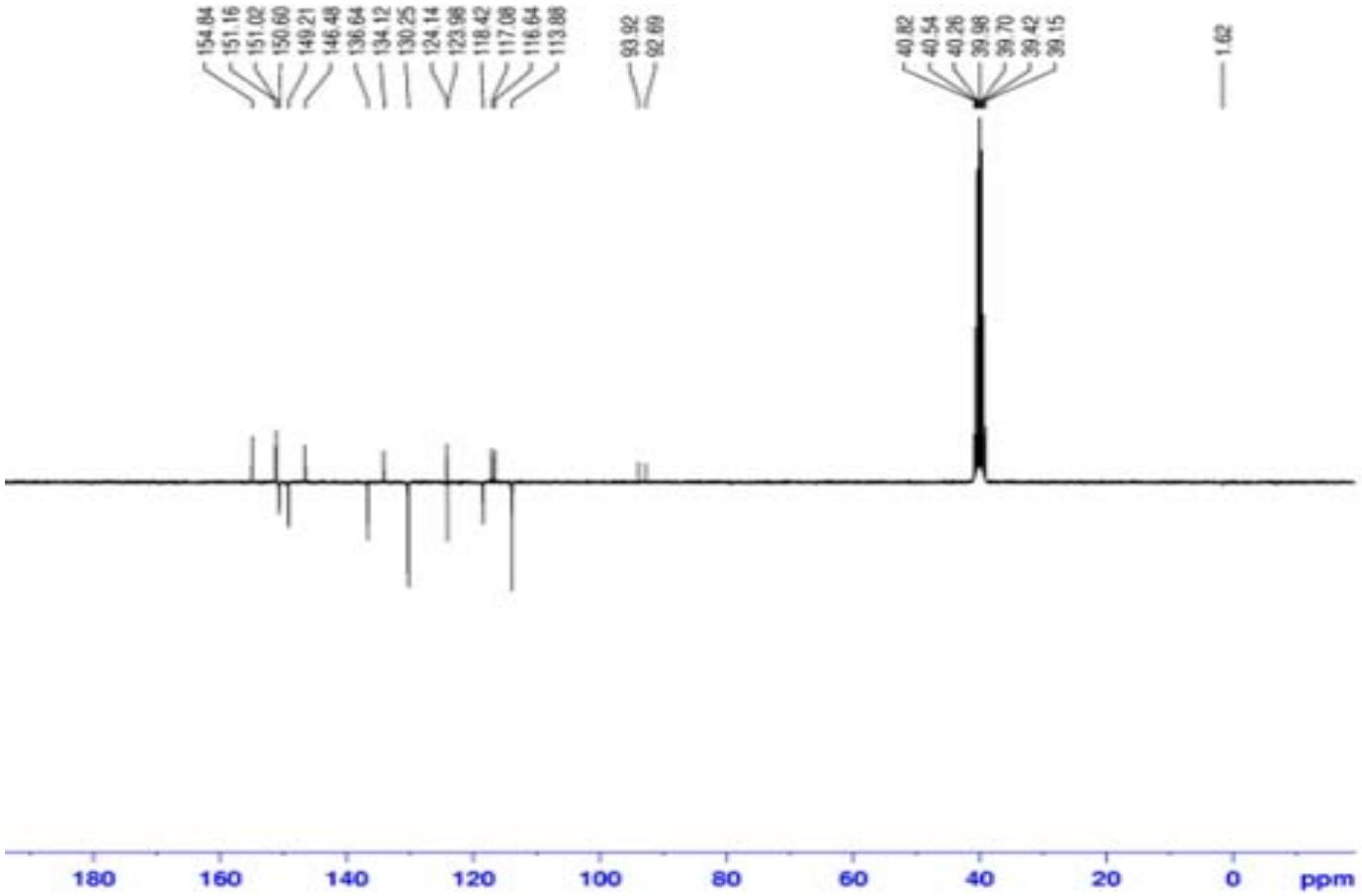
^{13}C APT Spectrum of Compound 4



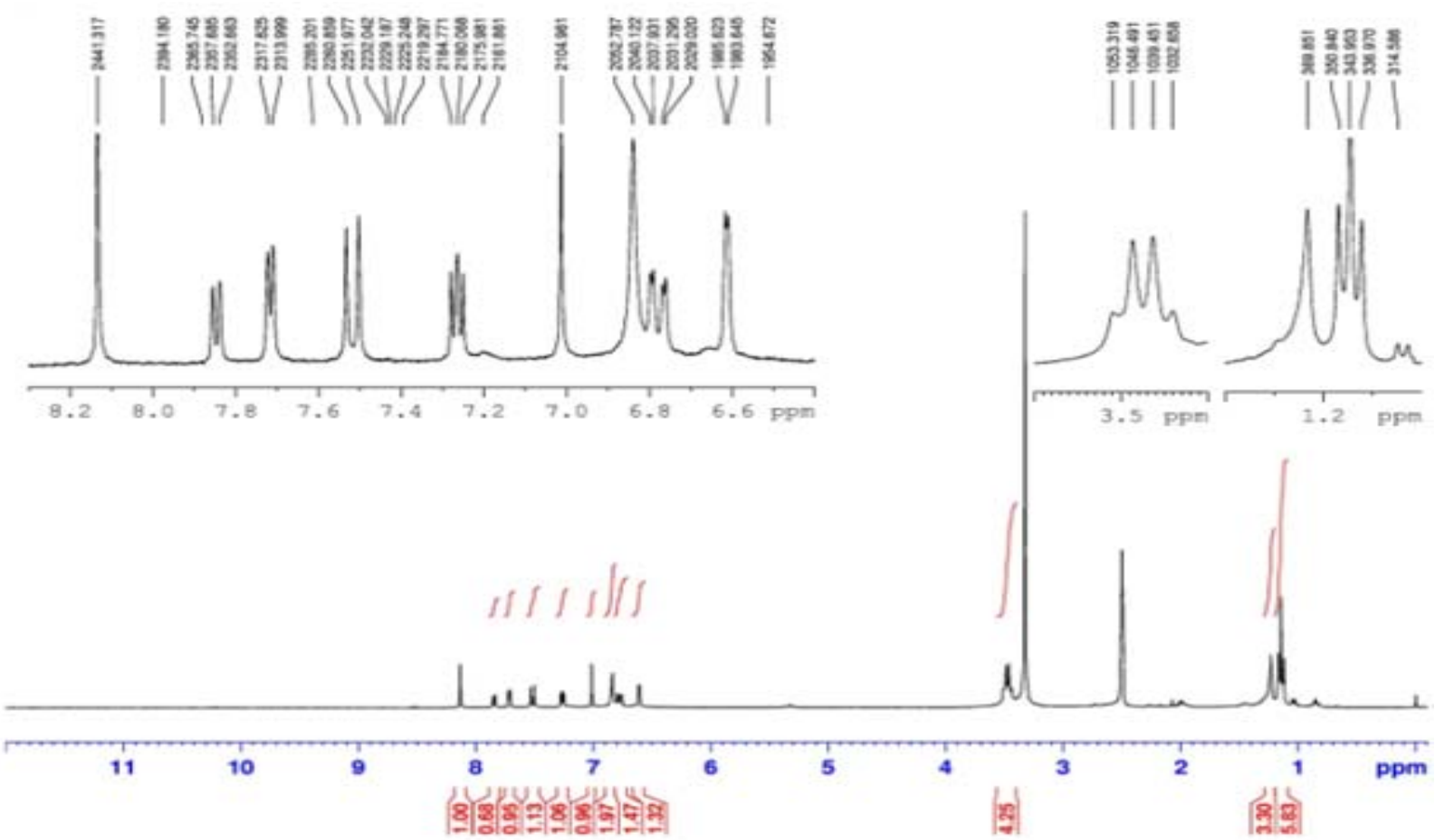
^{1}H NMR Spectrum of Compound 5



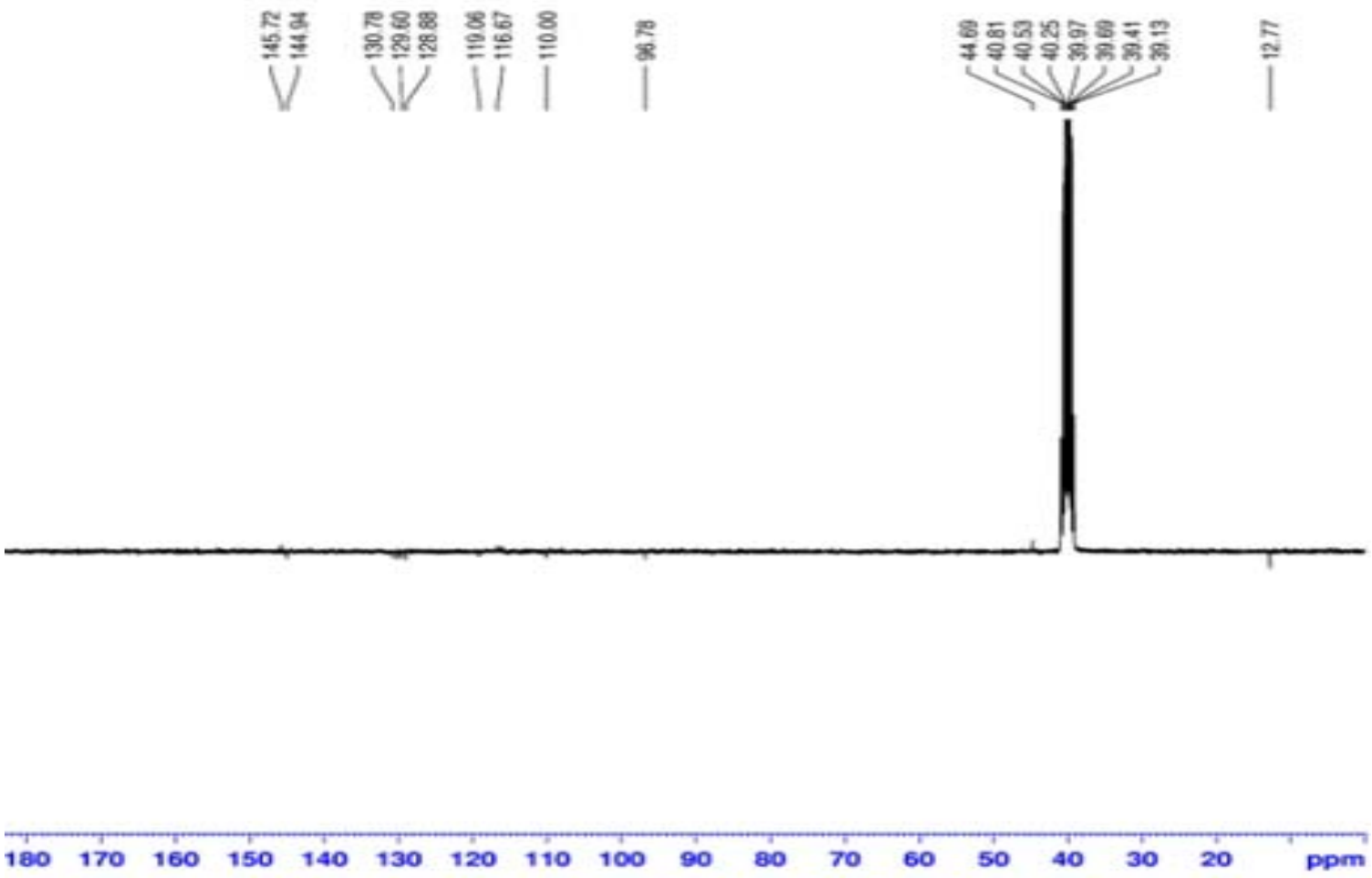
^{13}C APT Spectrum of Compound 5



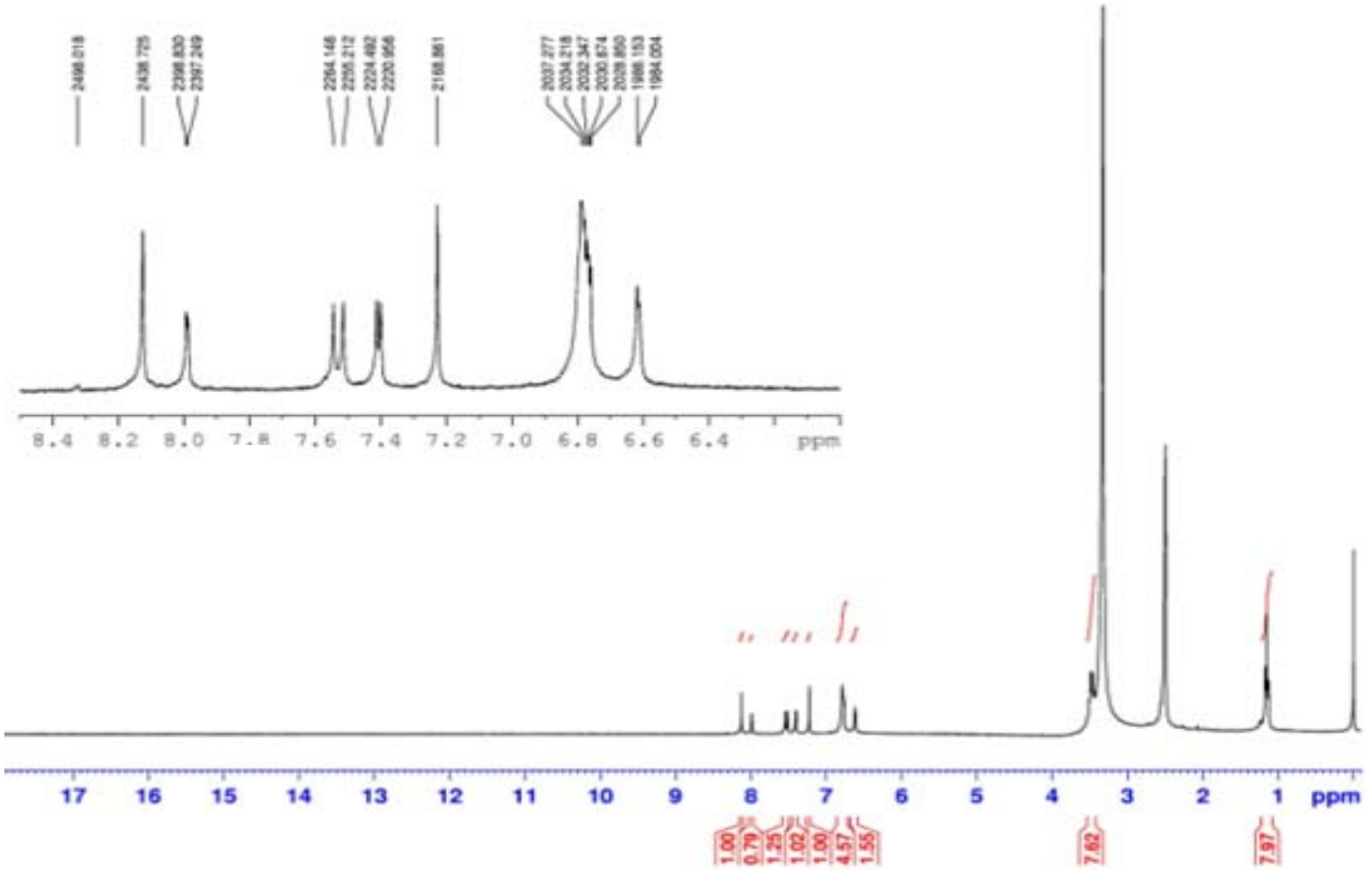
^{1}H NMR Spectrum of Compound 6



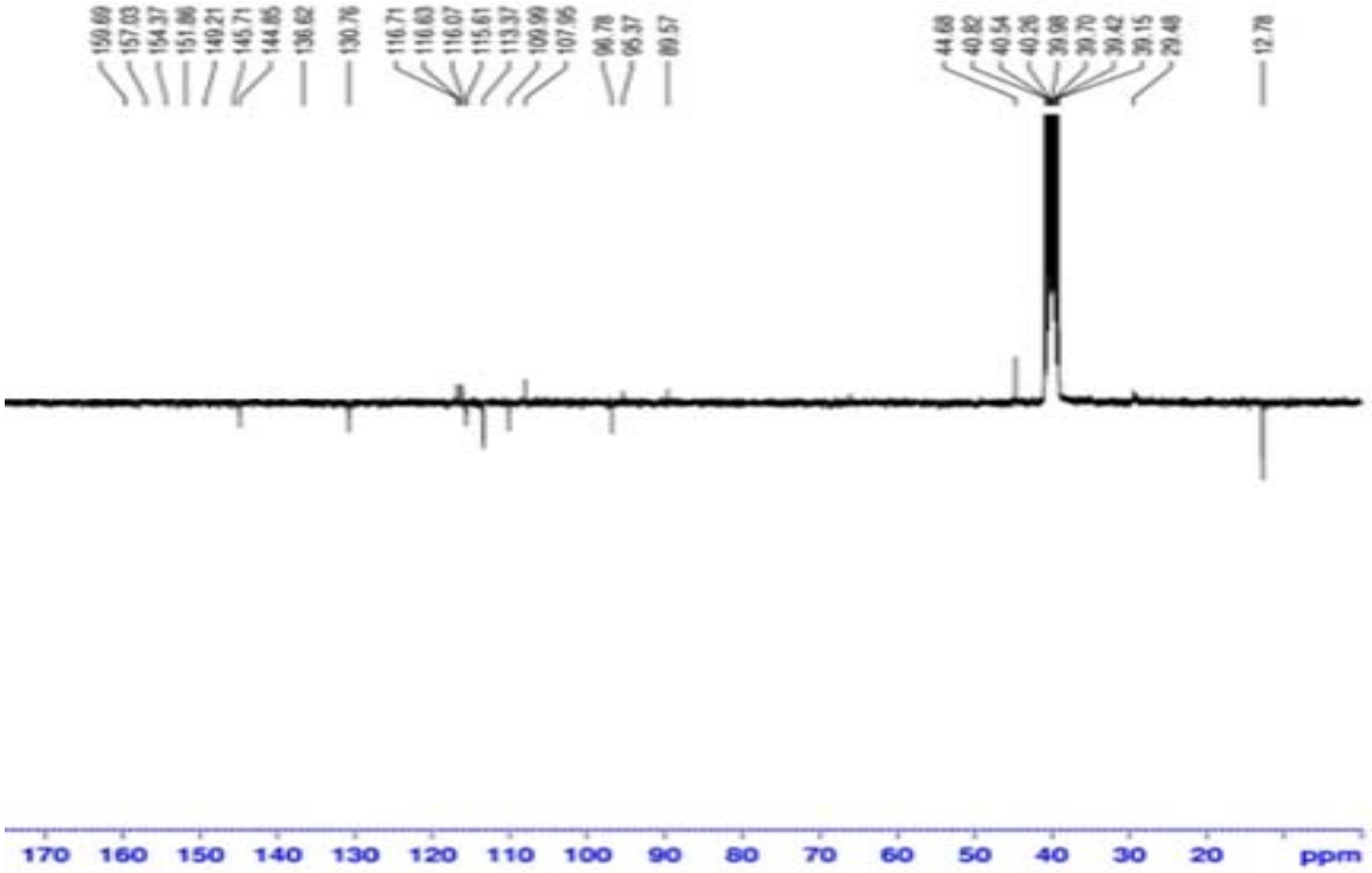
^{13}C APT Spectrum of Compound 6



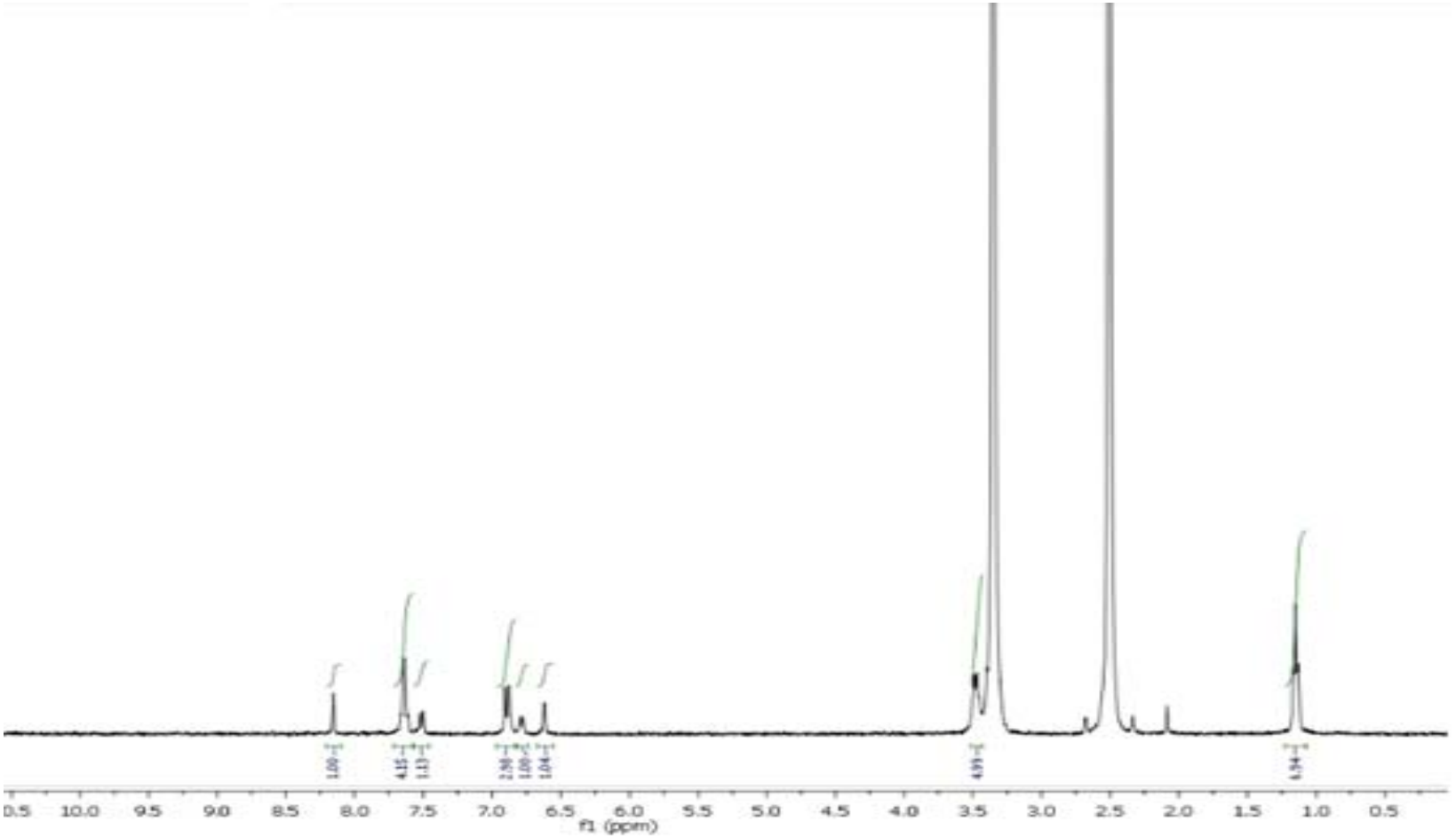
^{1}H NMR Spectrum of Compound 7



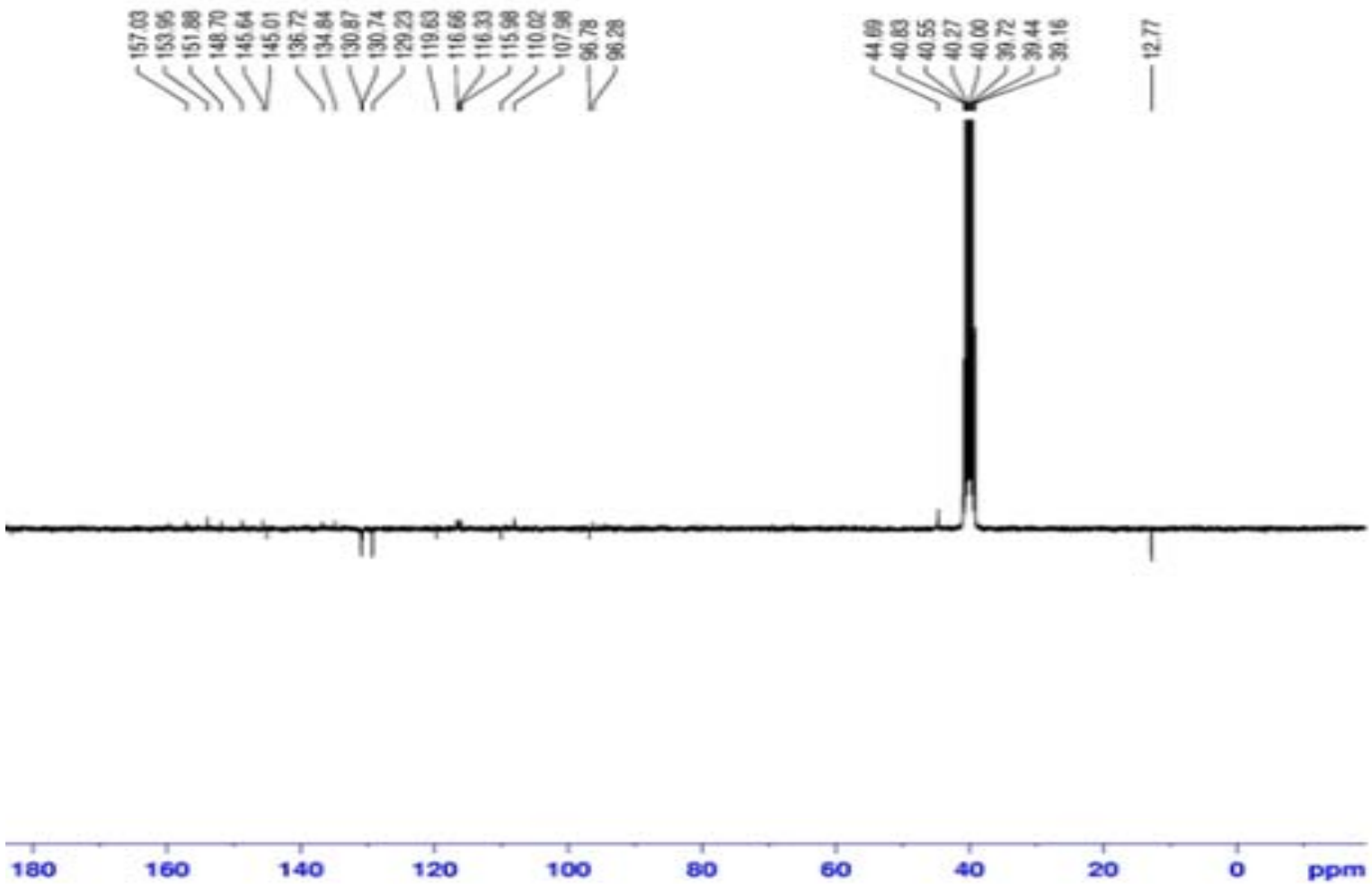
^{13}C APT Spectrum of Compound 7



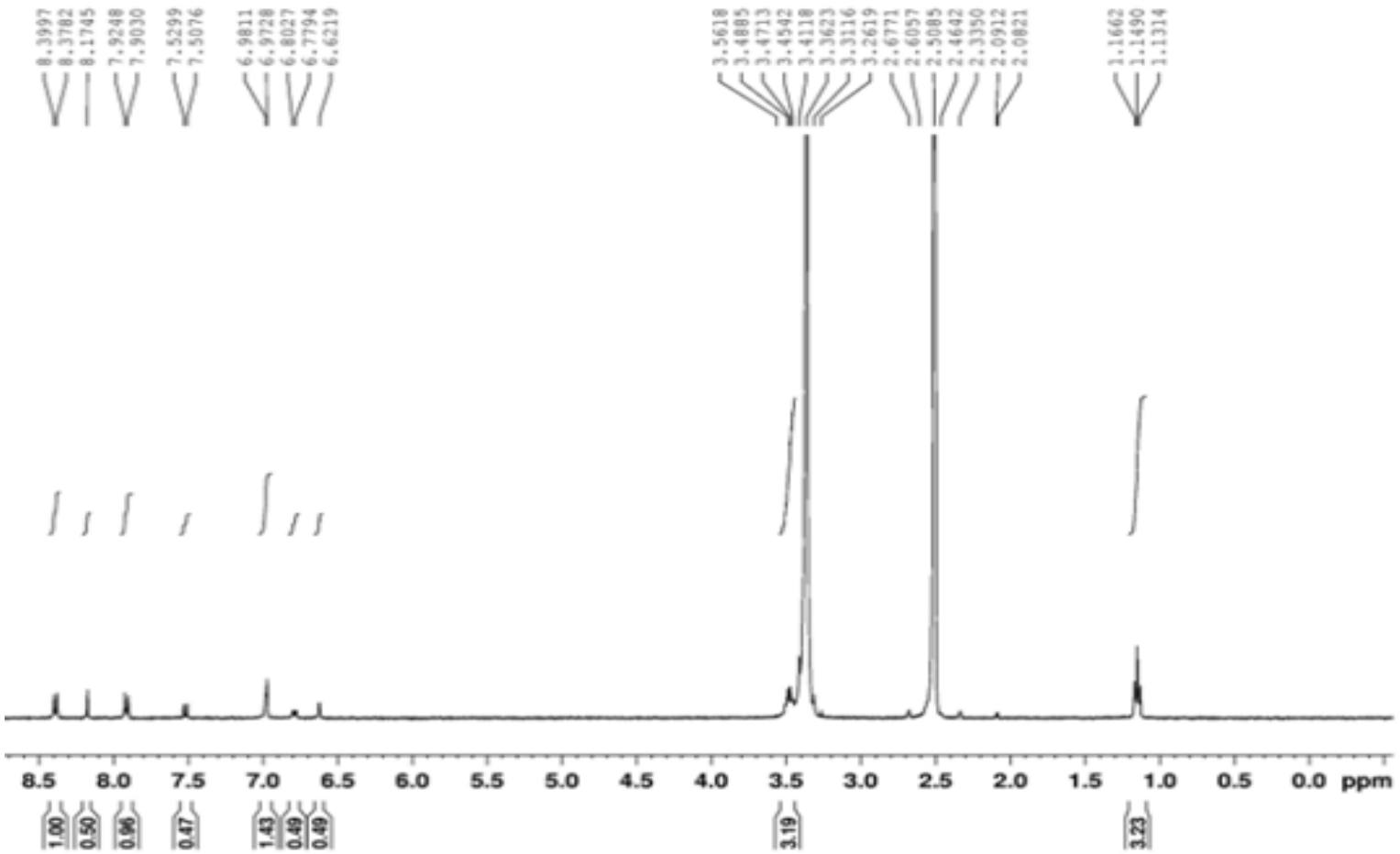
^{1}H NMR Spectrum of Compound 8



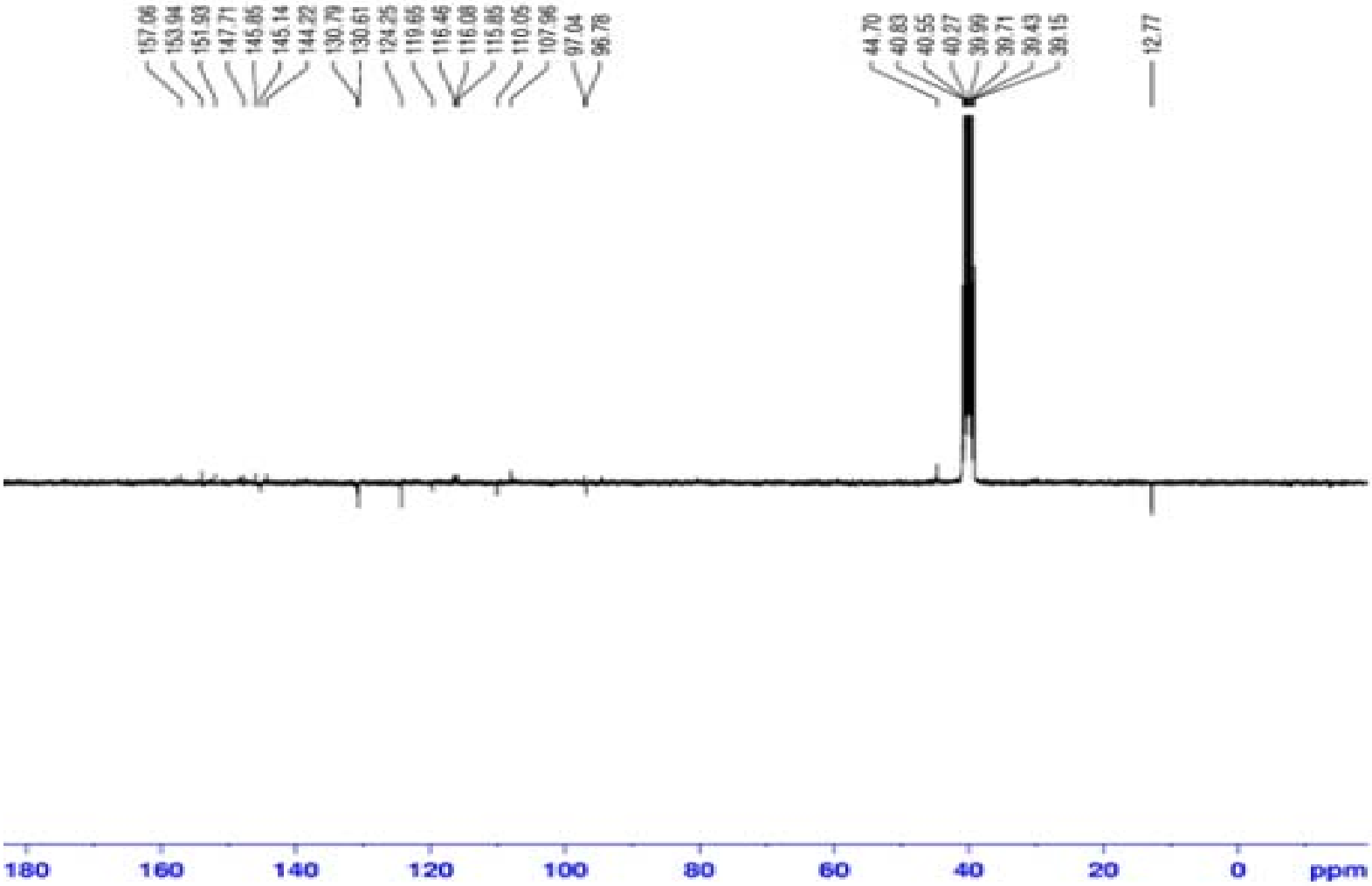
^{13}C APT Spectrum of Compound 8



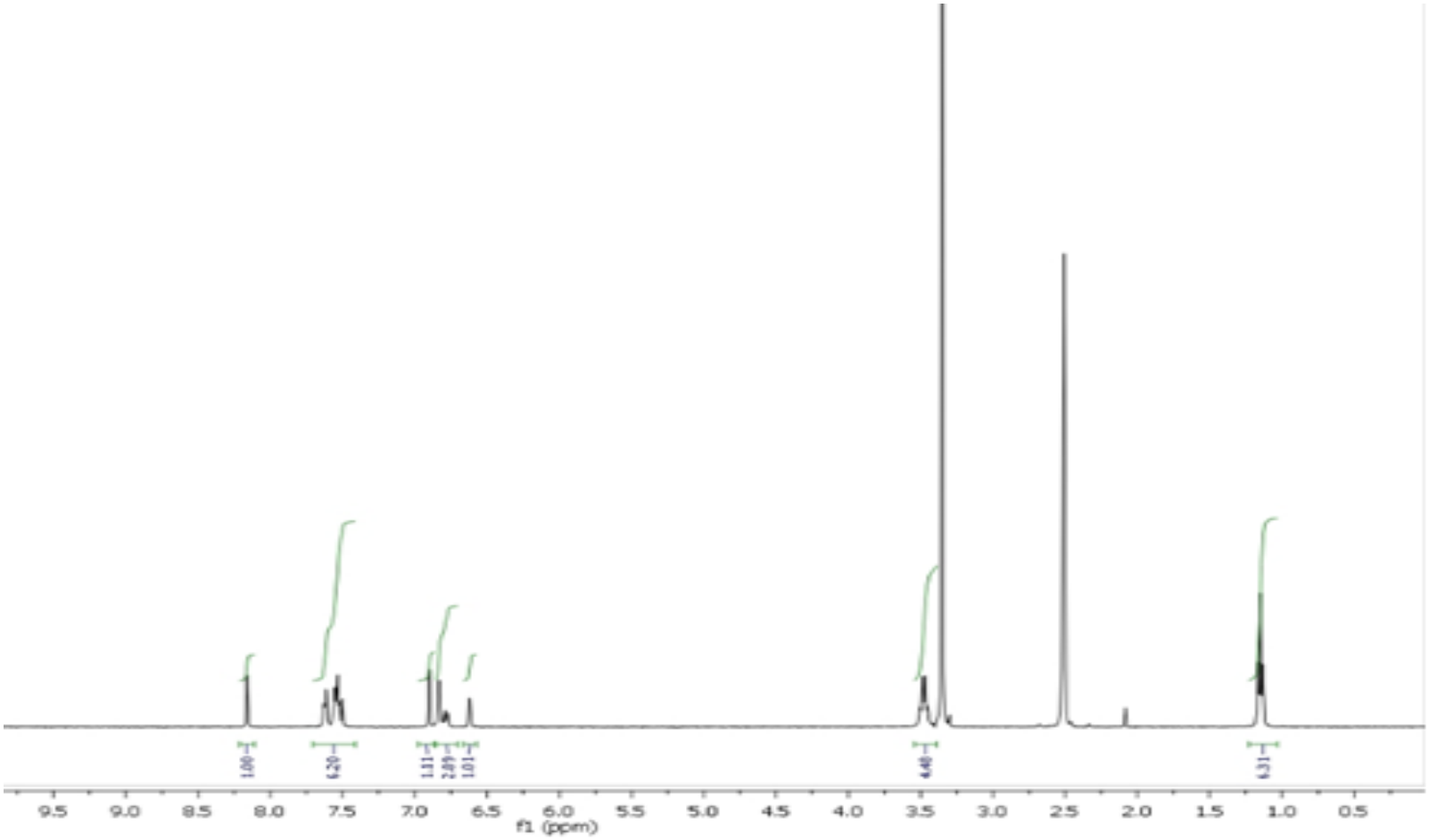
^{1}H NMR Spectrum of Compound 9



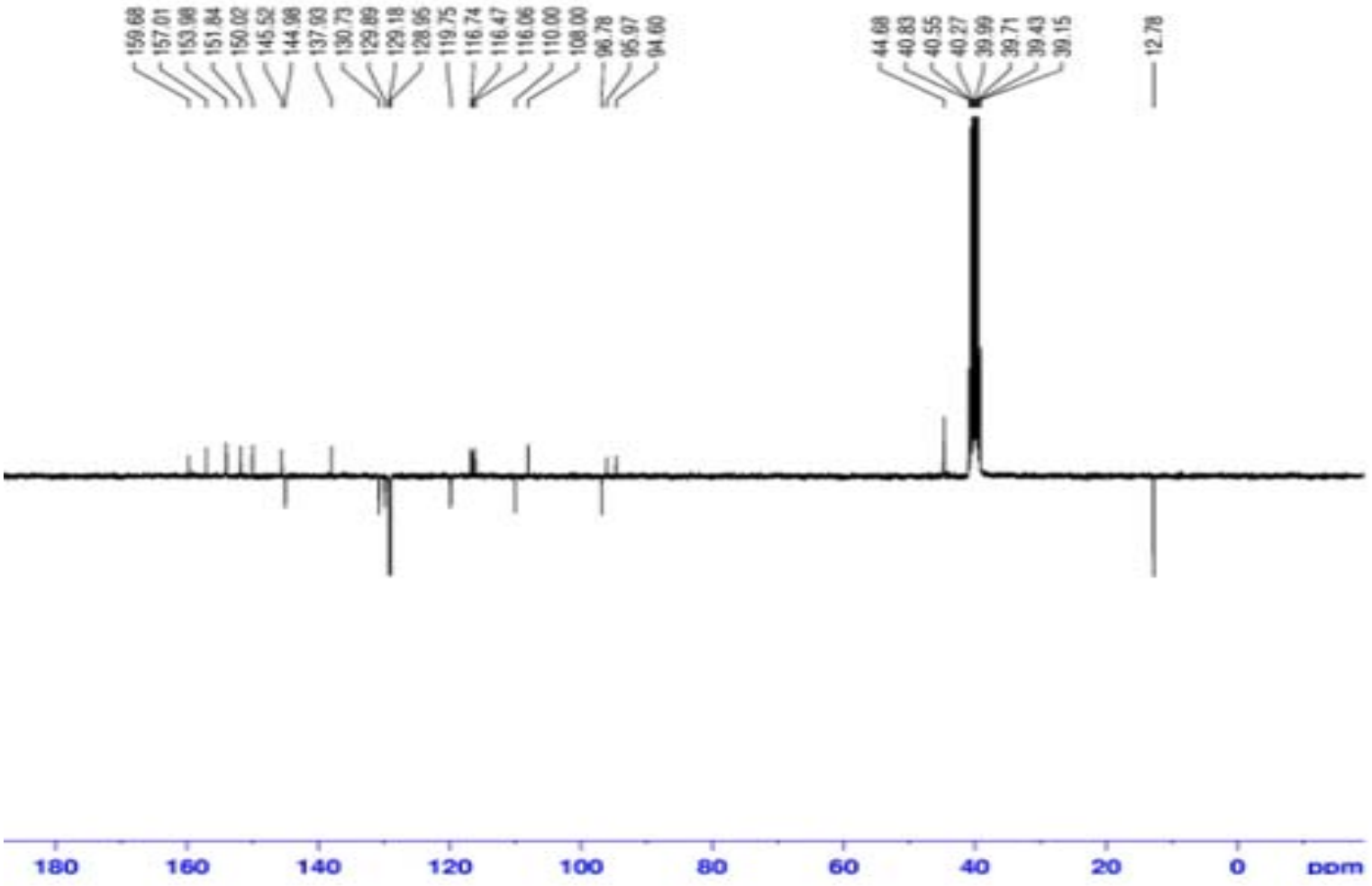
^{13}C APT Spectrum of Compound 9



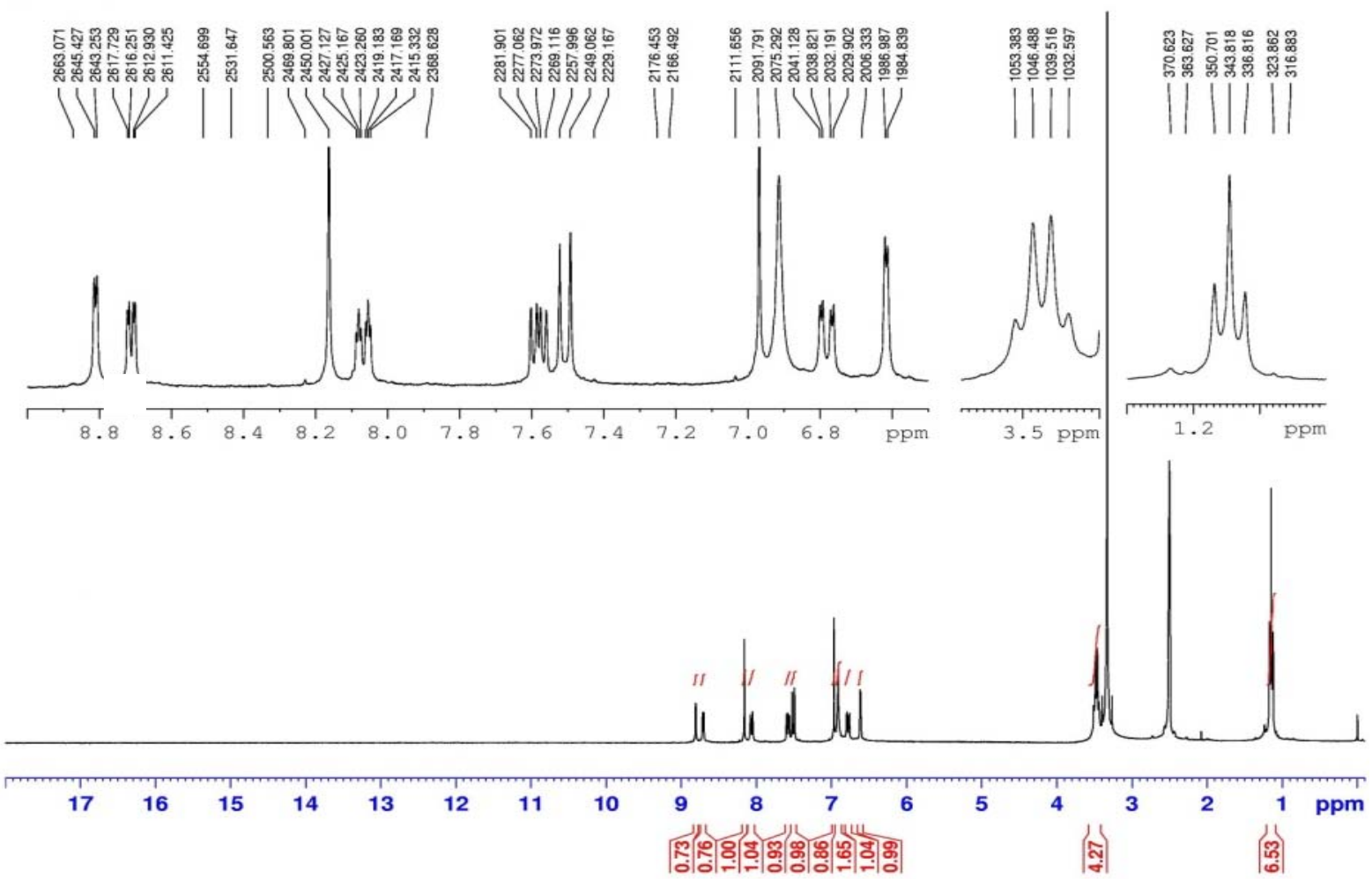
^{1}H NMR Spectrum of Compound 10



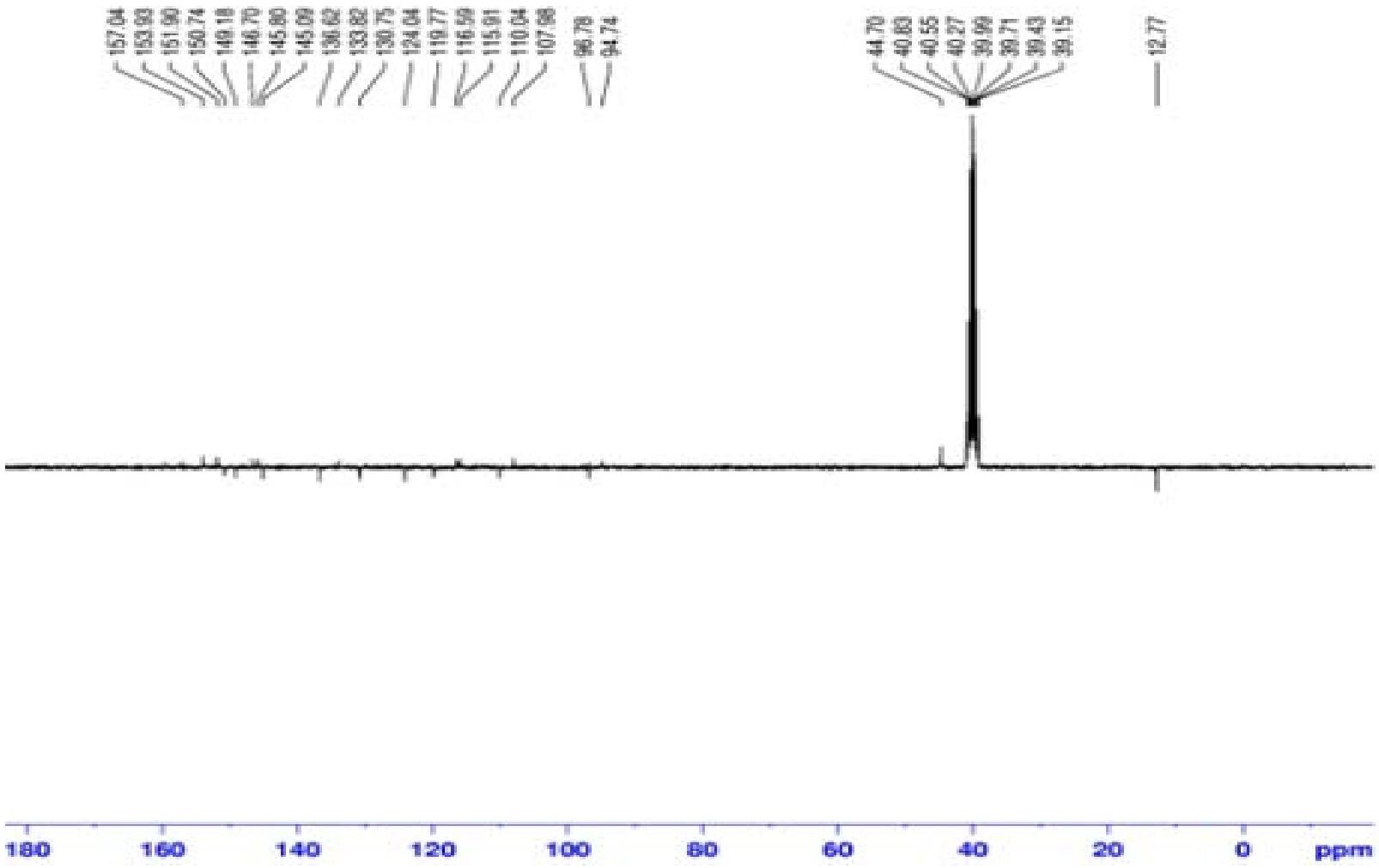
^{13}C APT Spectrum of Compound 10



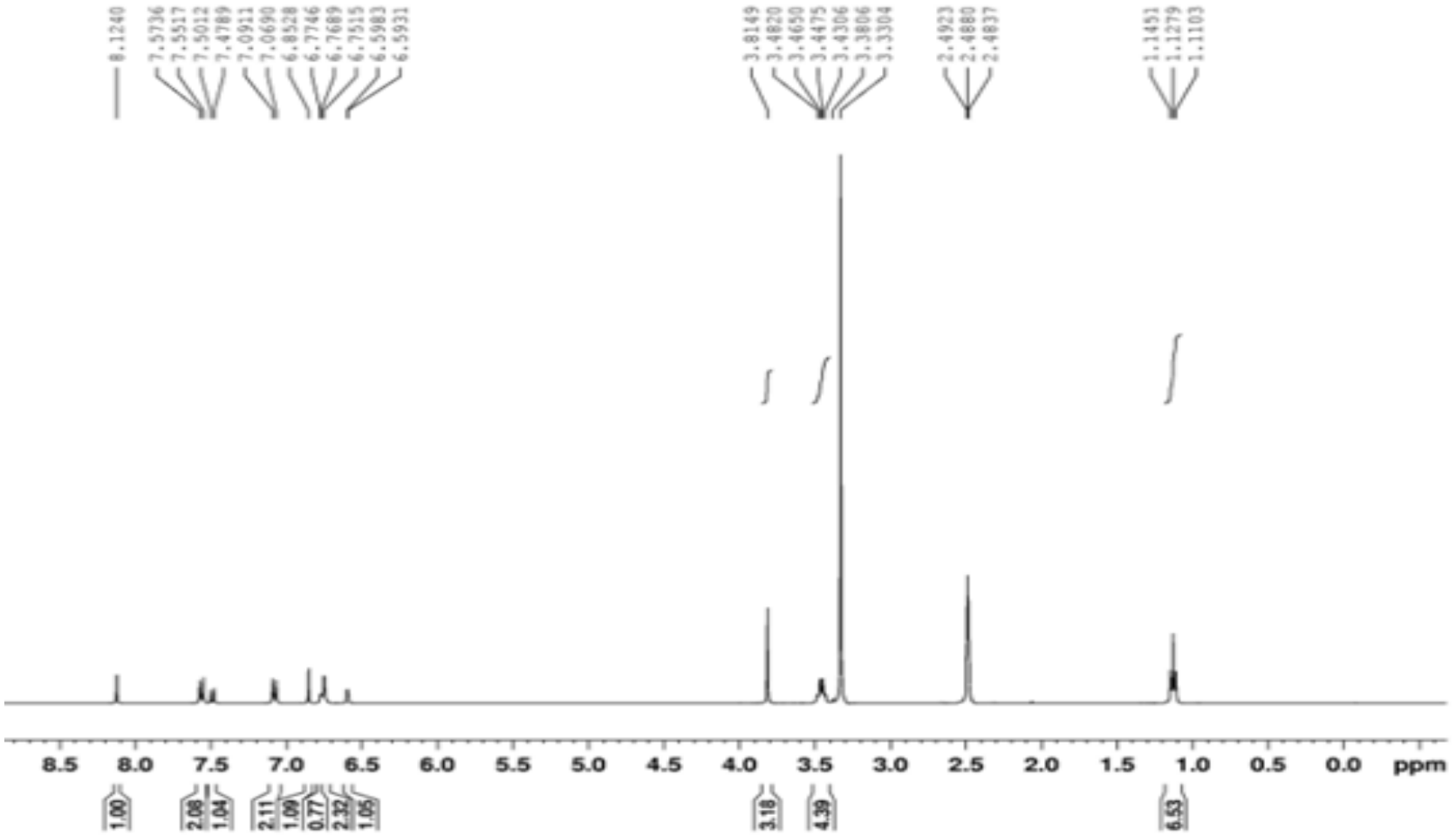
^{1}H NMR Spectrum of Compound 11



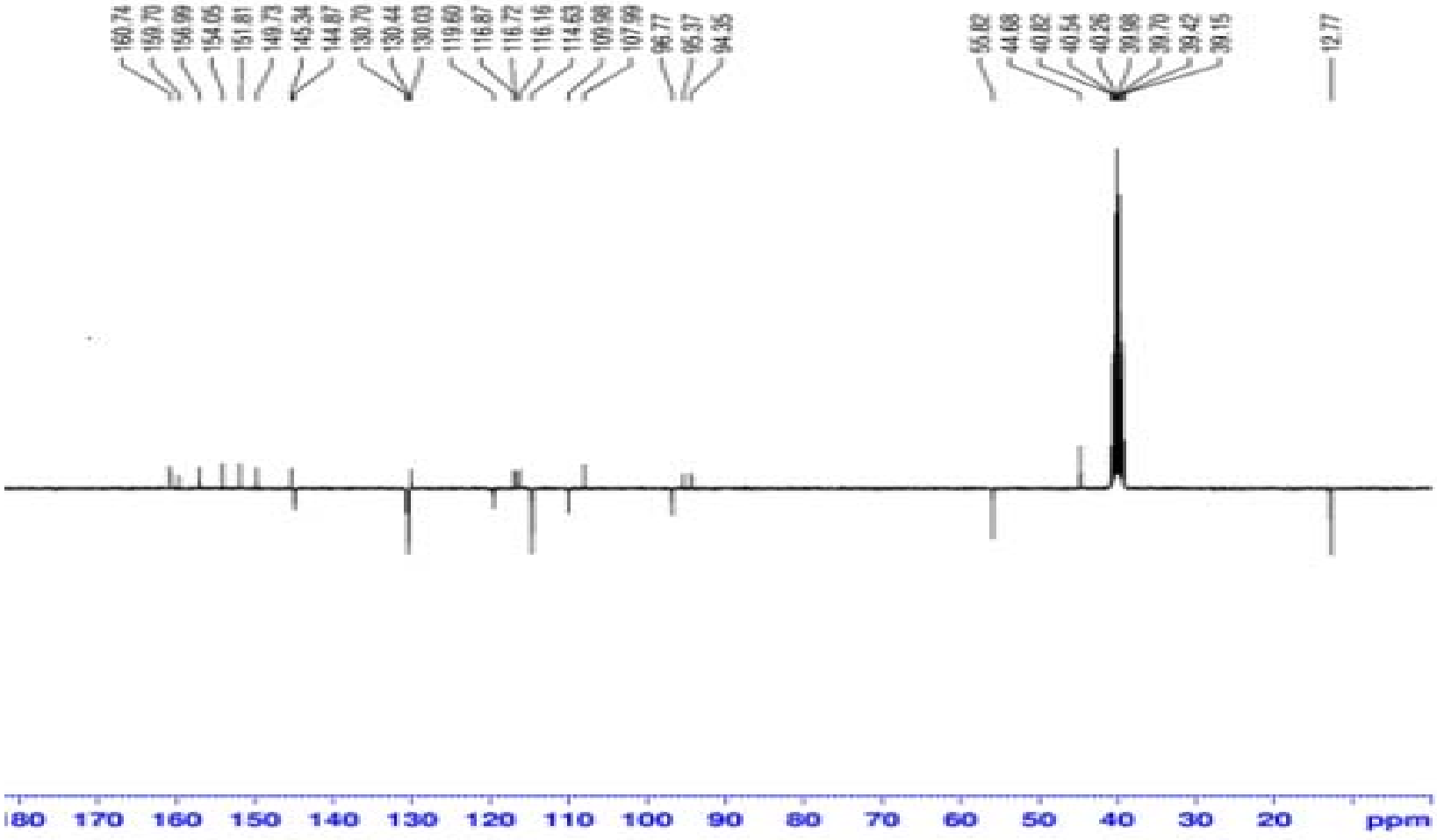
^{13}C NMR Spectrum of Compound 11



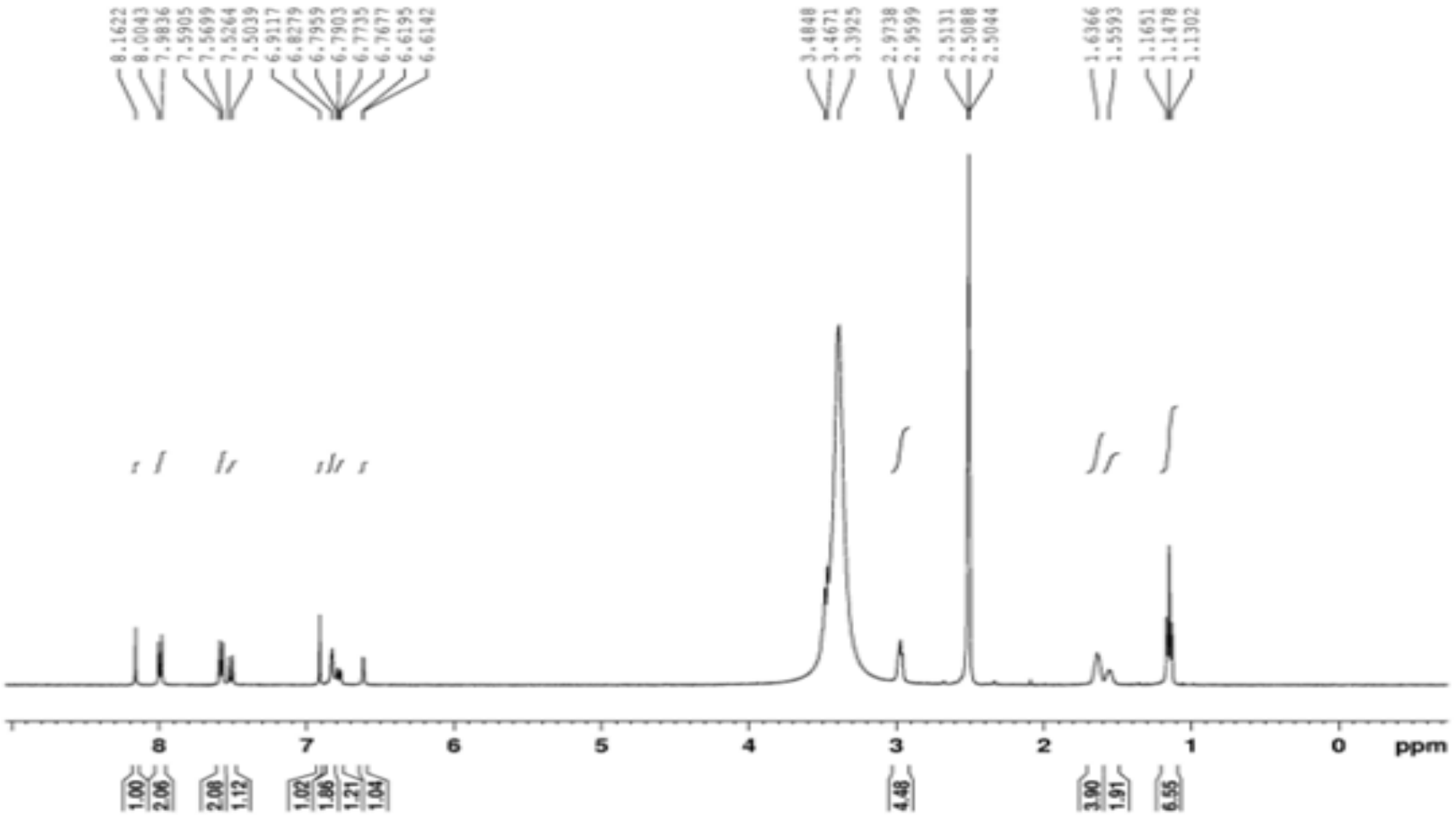
^{1}H NMR Spectrum of Compound 12



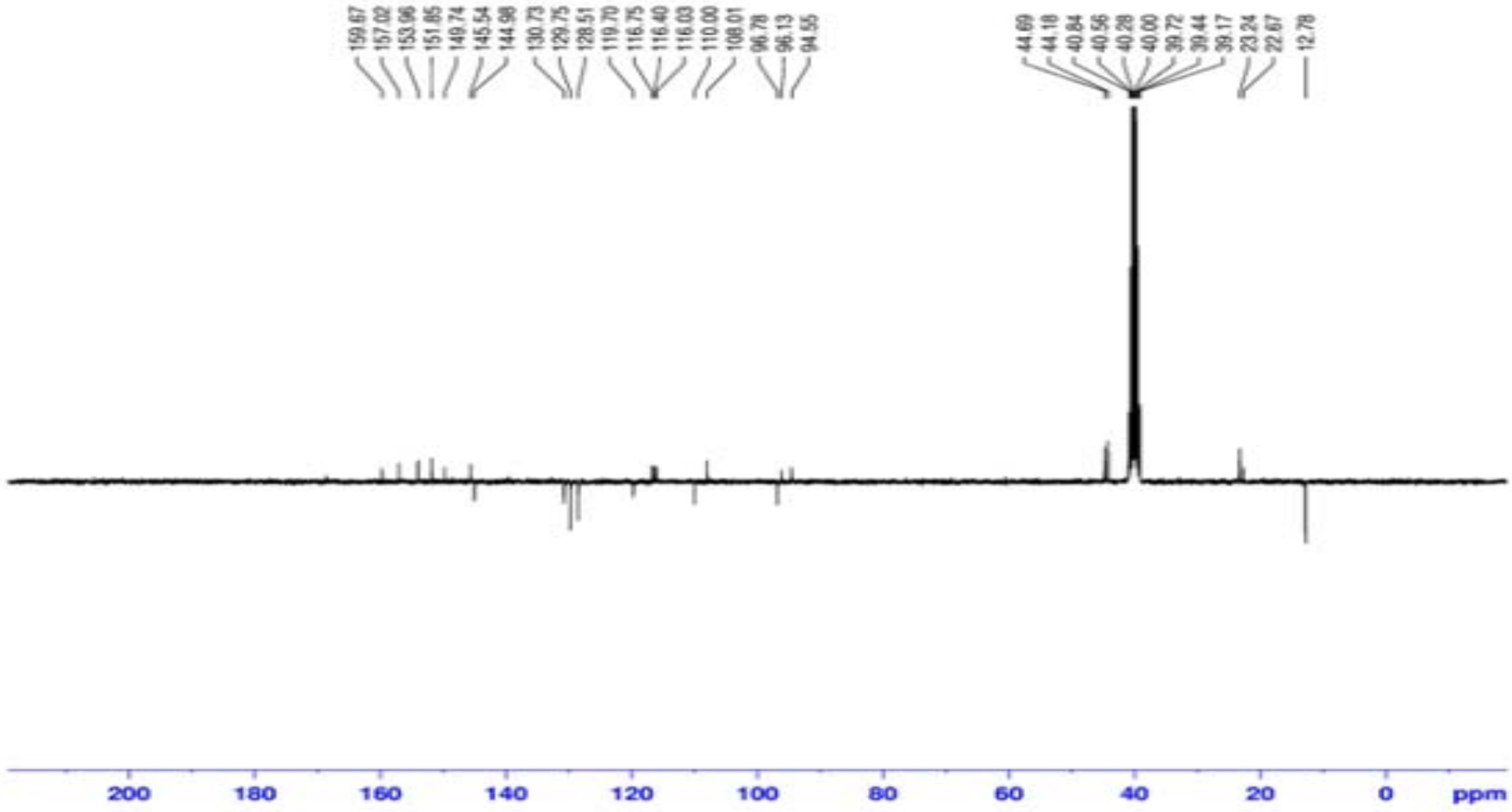
^{13}C APT Spectrum of Compound 12



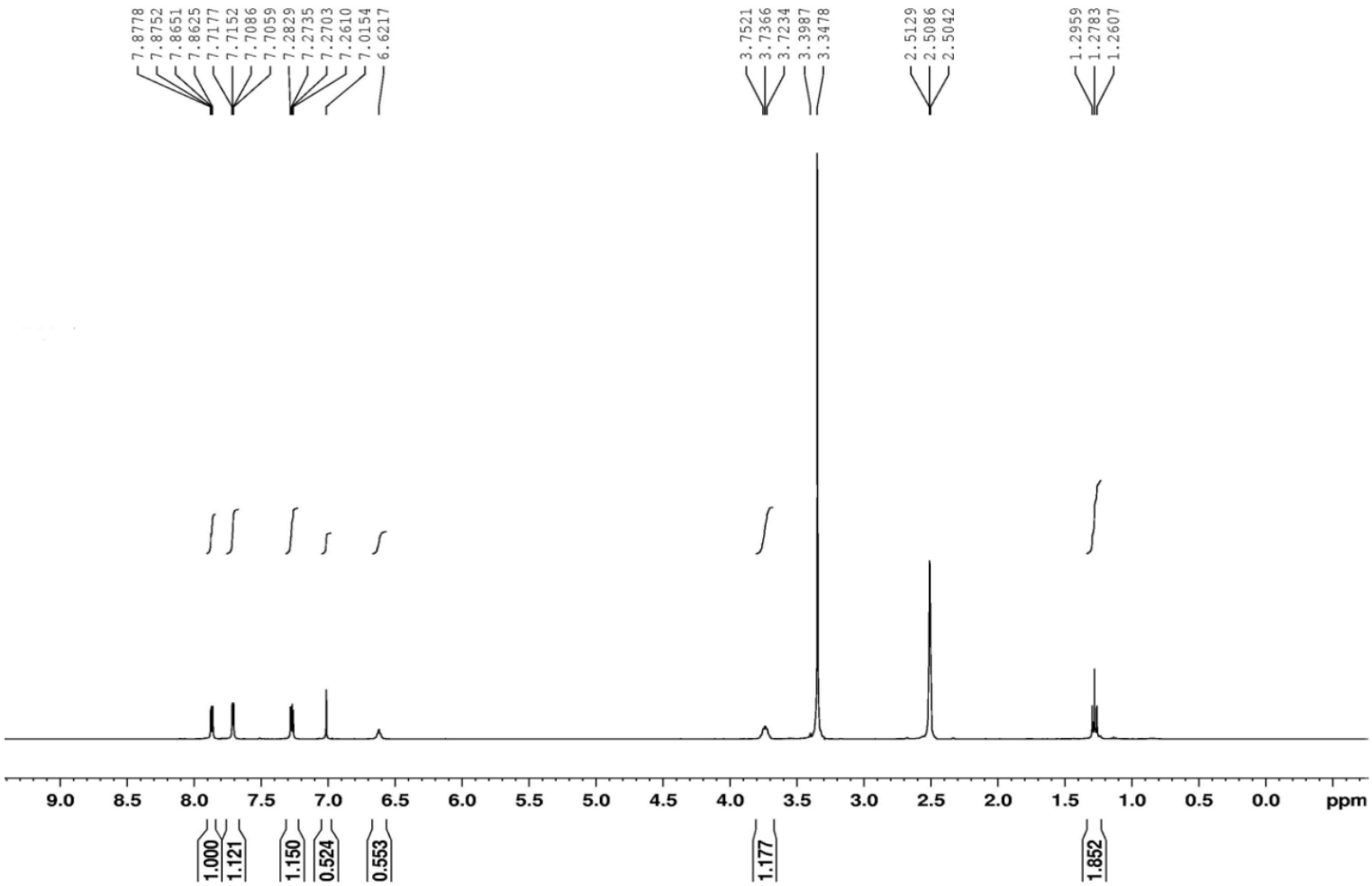
^{1}H NMR Spectrum of Compound 13



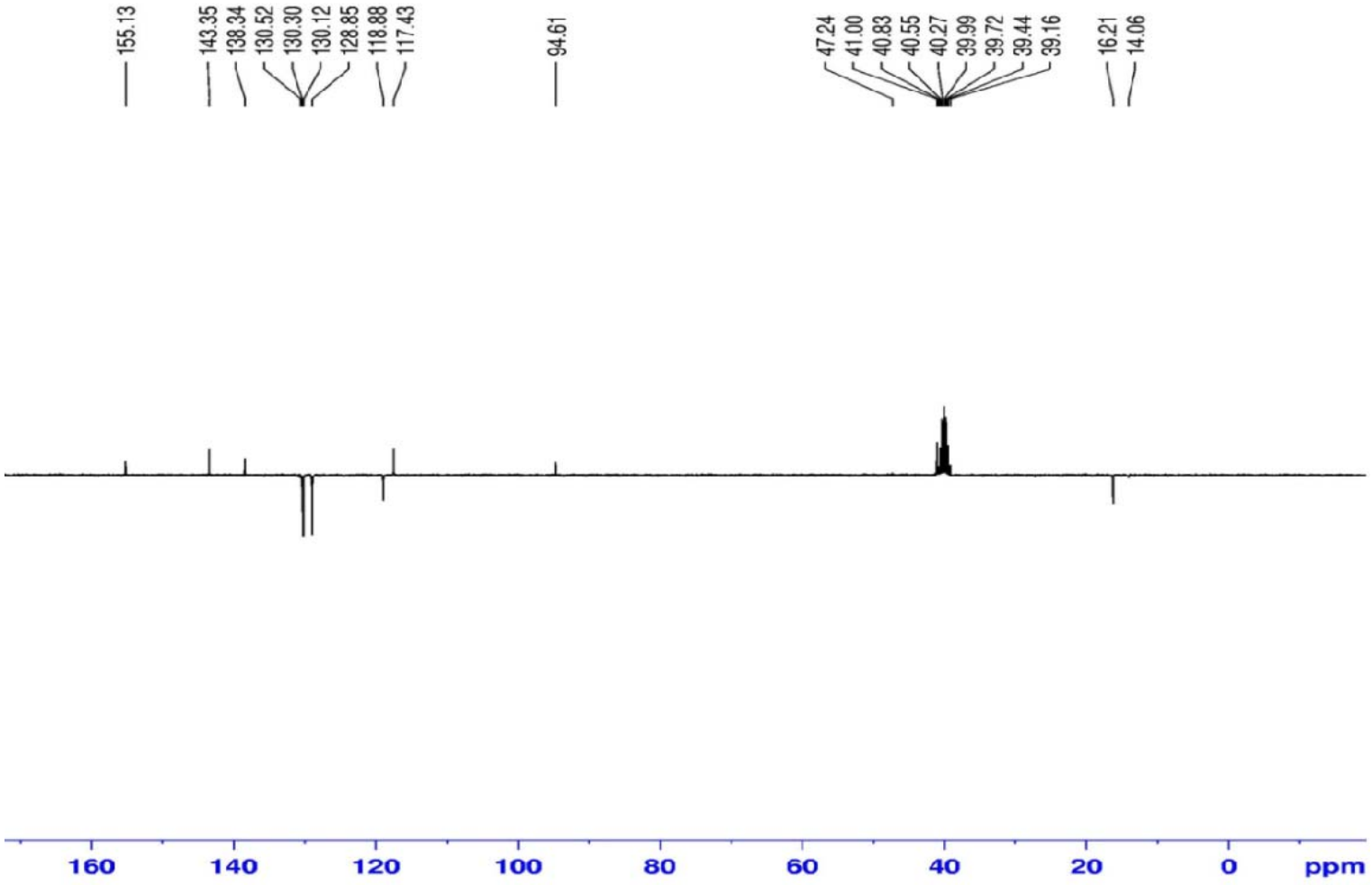
^{13}C APT Spectrum of Compound 13



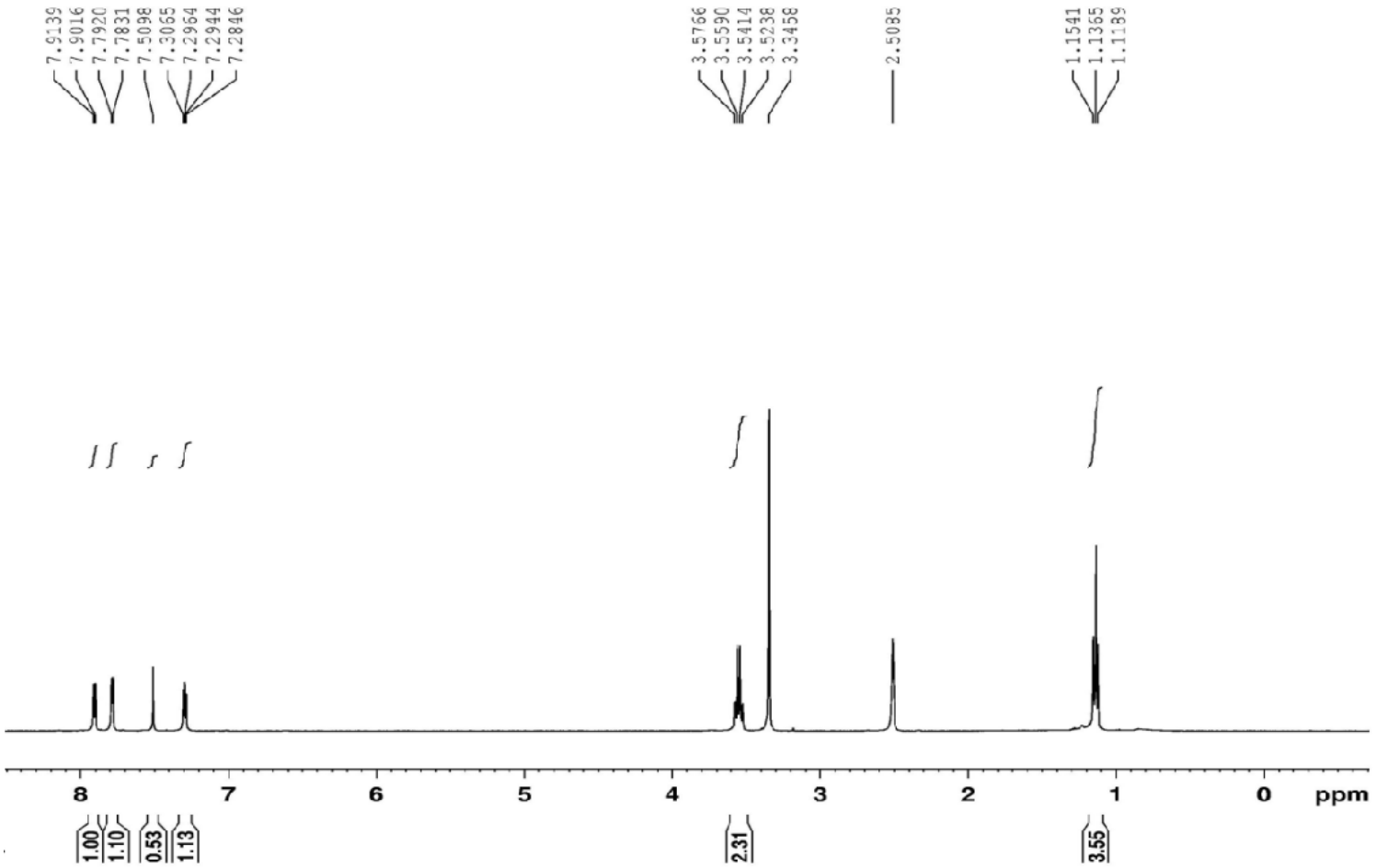
[1]H NMR Spectrum of Compound 1-I



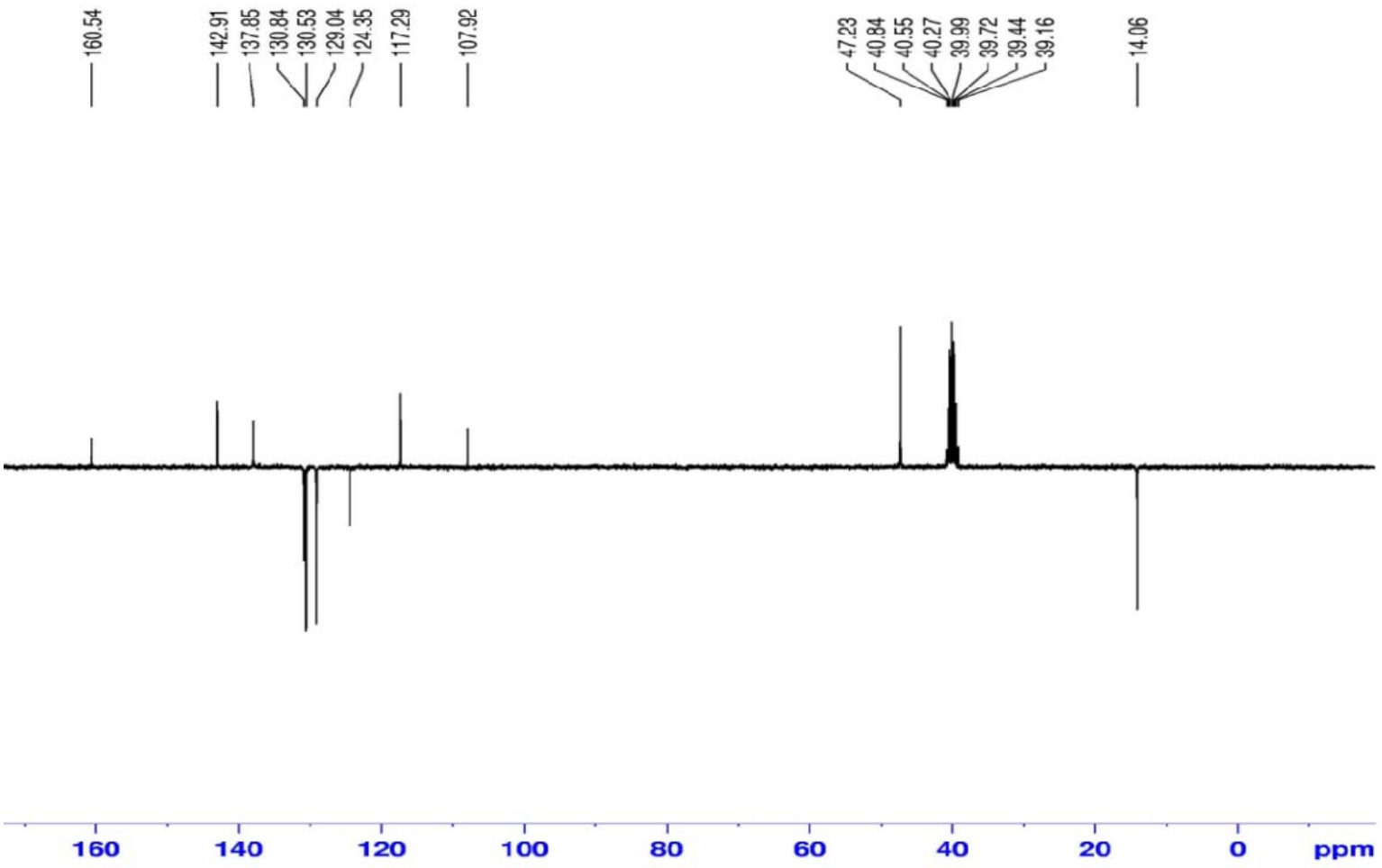
^{13}C APT Spectrum of Compound 1-I



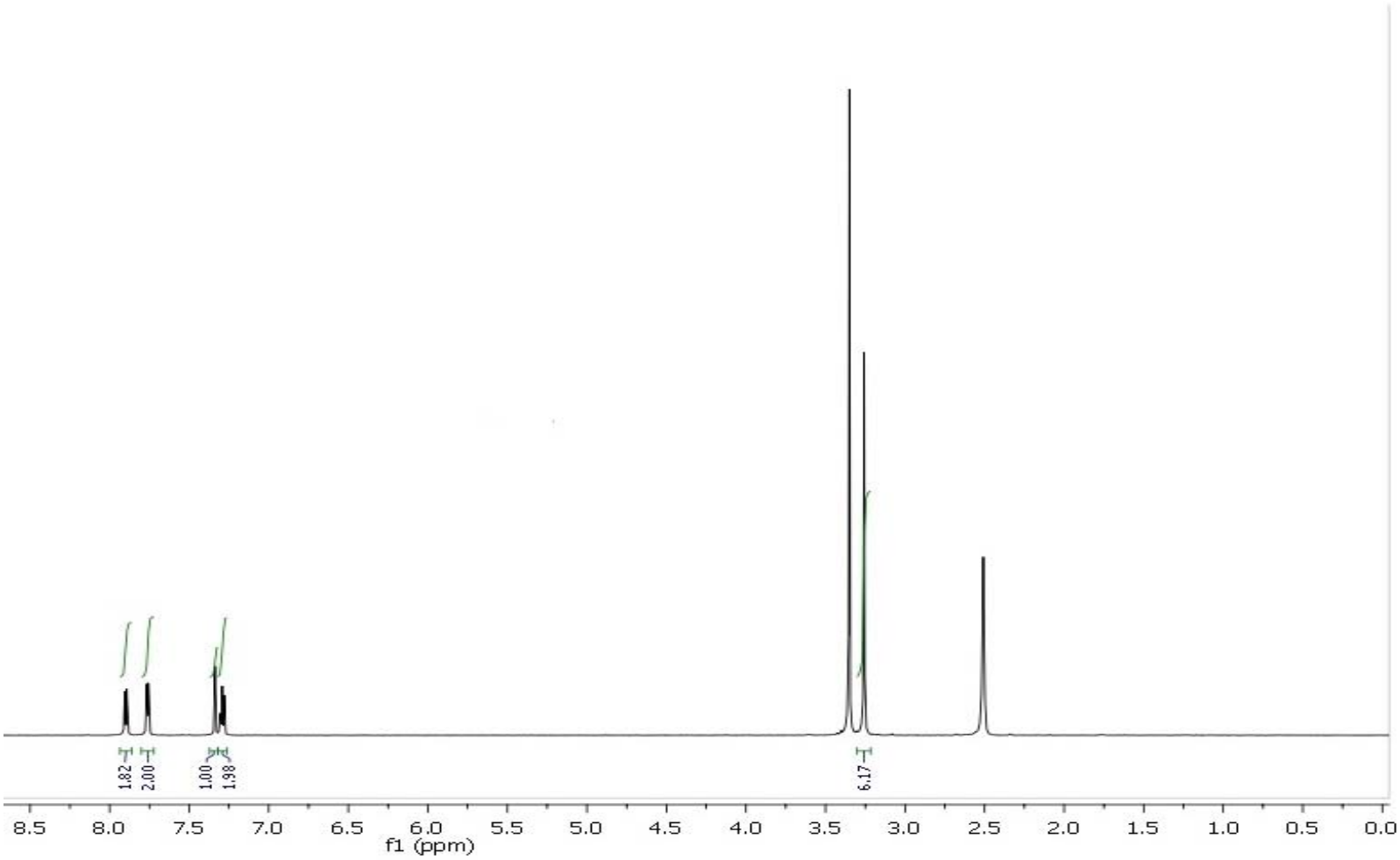
^{1}H NMR Spectrum of Compound 1-II



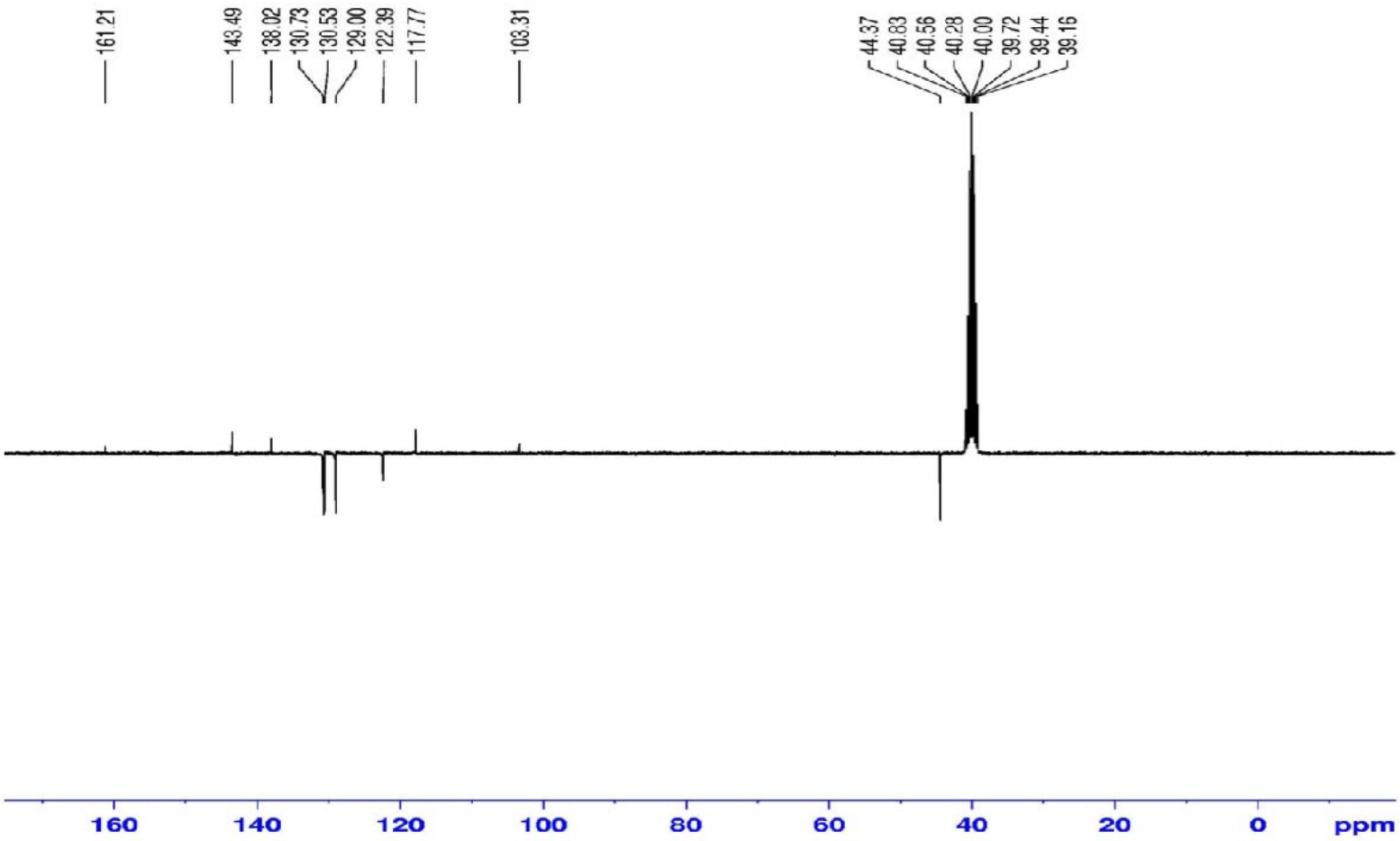
^{13}C APT Spectrum of Compound 1-II



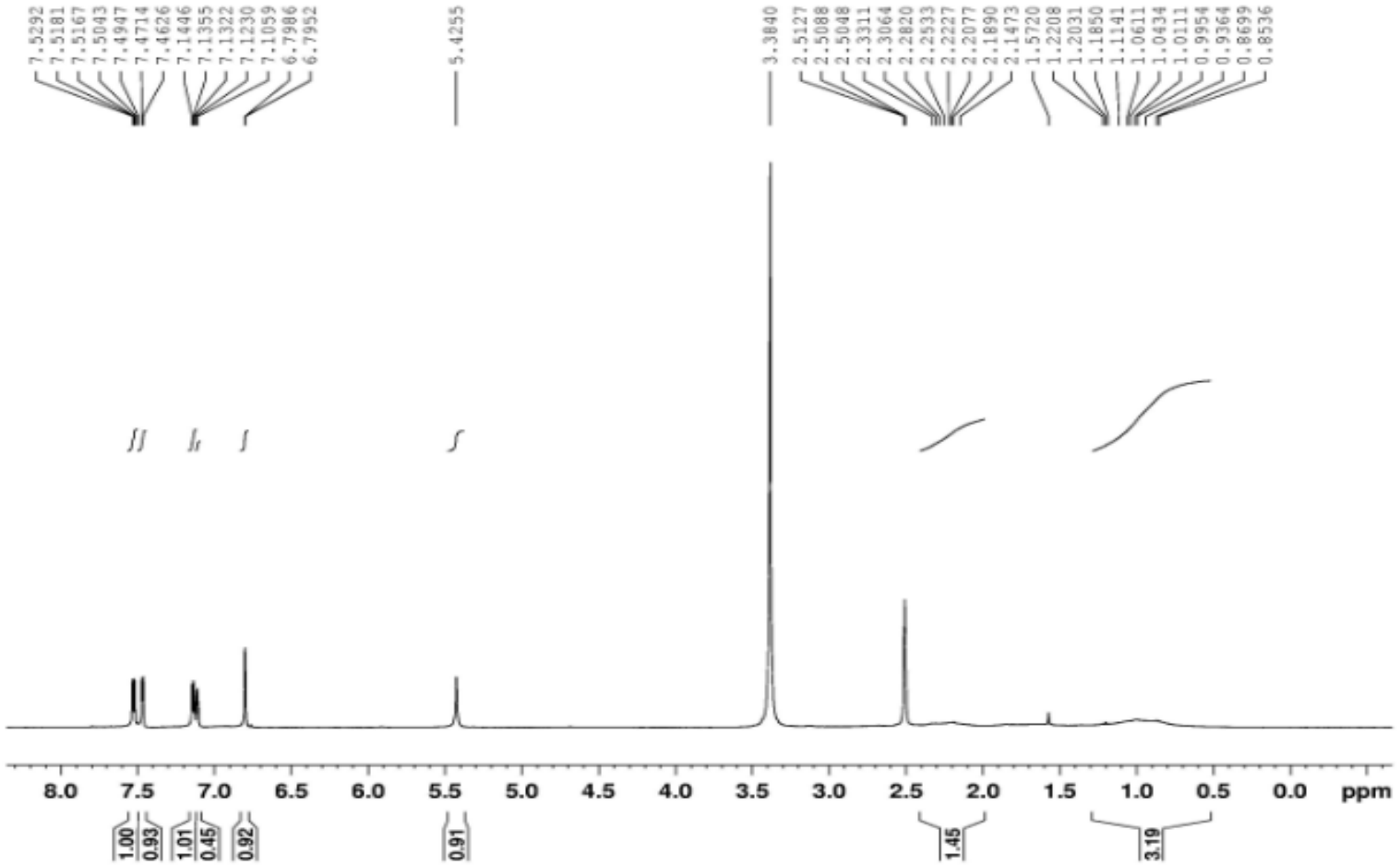
^{1}H NMR Spectrum of Compound 1-III



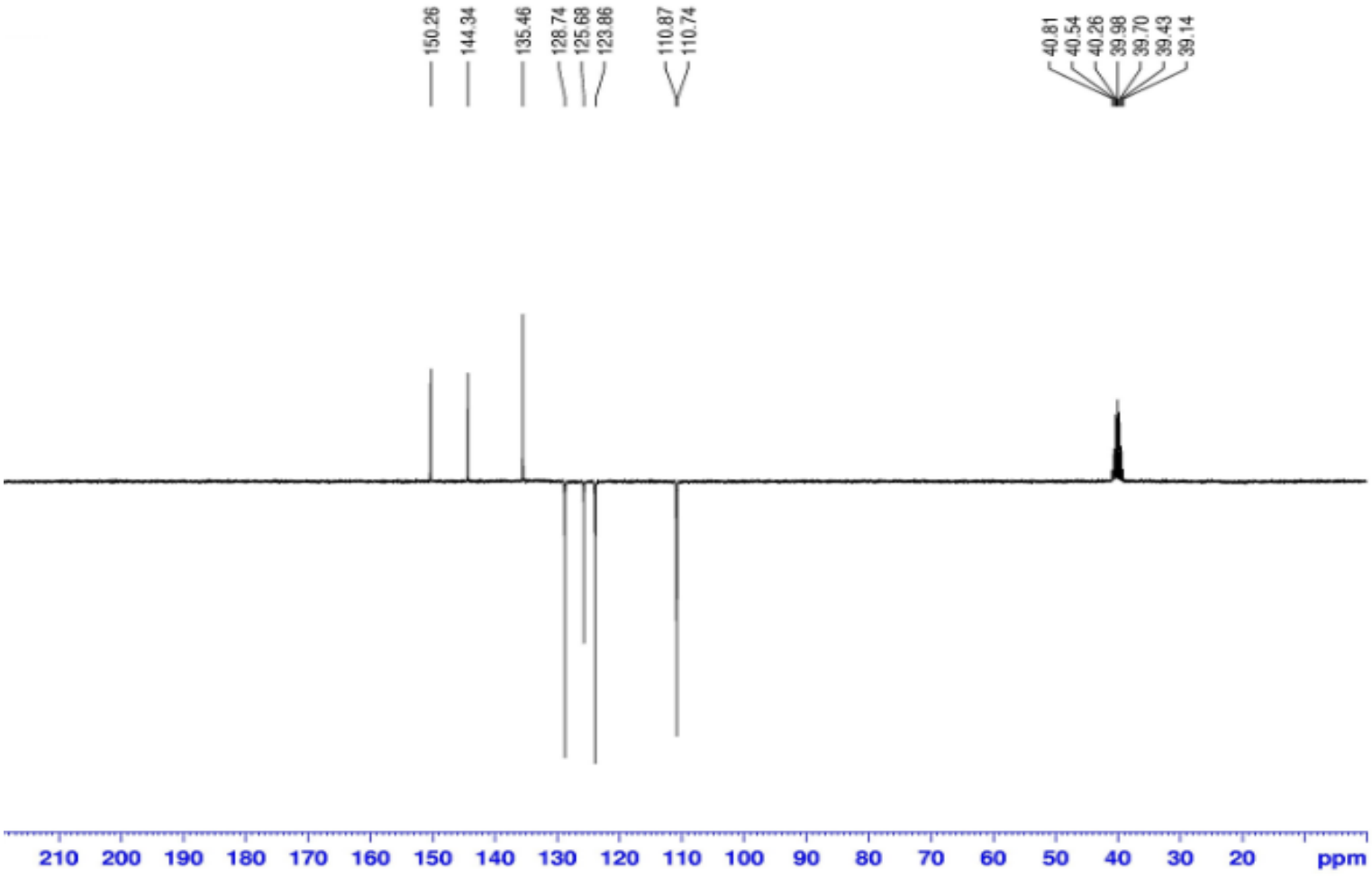
^{13}C APT Spectrum of Compound 1-III



^{1}H NMR Spectrum of compound 1-IV

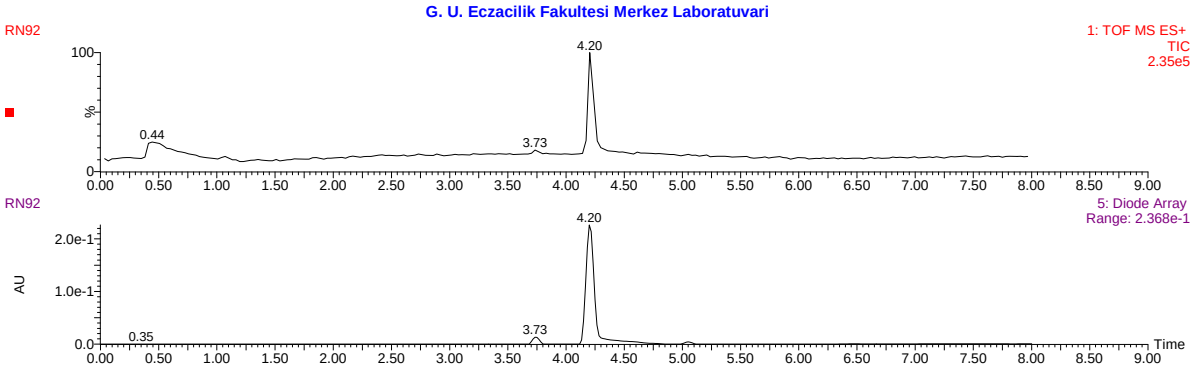


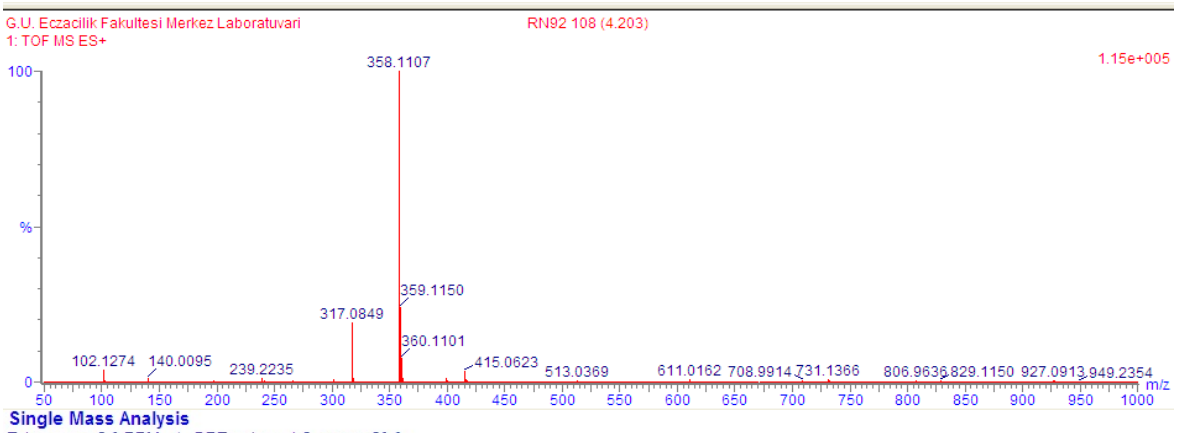
^{13}C APT Spectrum of Compound 1-IV



The HRMS spectra with chromotograms of all synthesized new compounds

Compound 2





Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

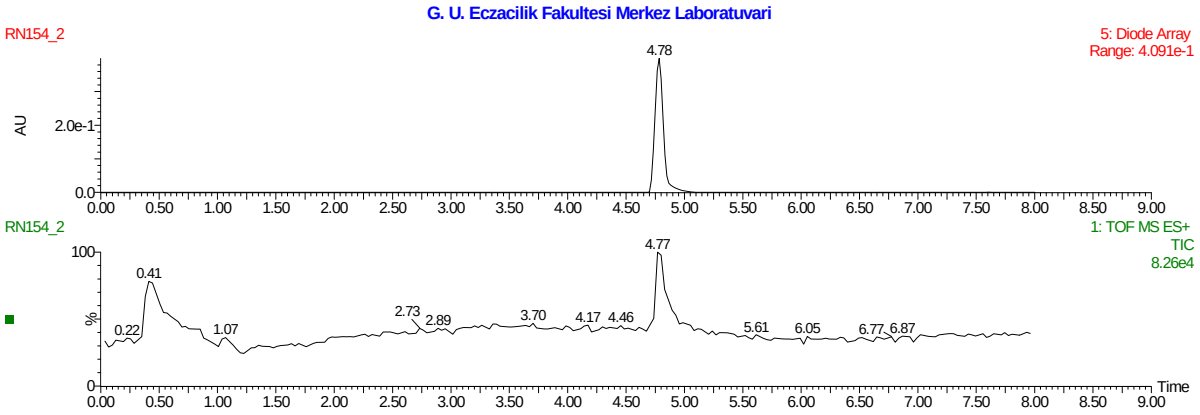
Monoisotopic Mass, Even Electron Ions

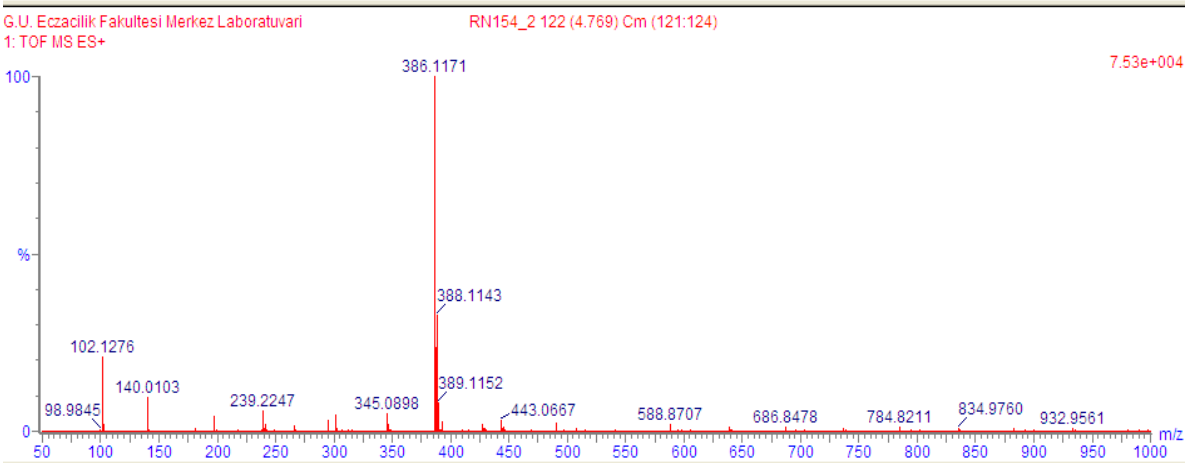
19 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N	S
317.0849	317.0861	-1.2	-3.8	14.5	C18 H13 N4 S	45.3	0.0	18	13	4	1

Compound 3





Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

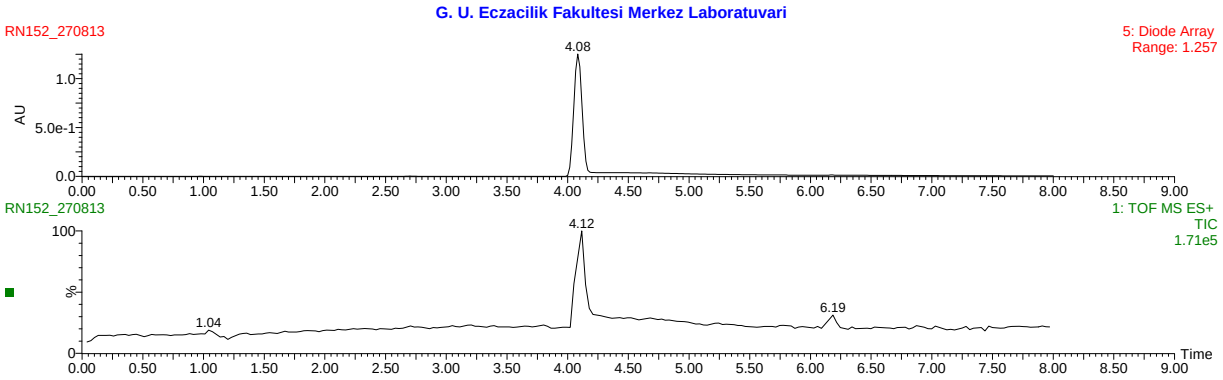
Monoisotopic Mass, Even Electron Ions

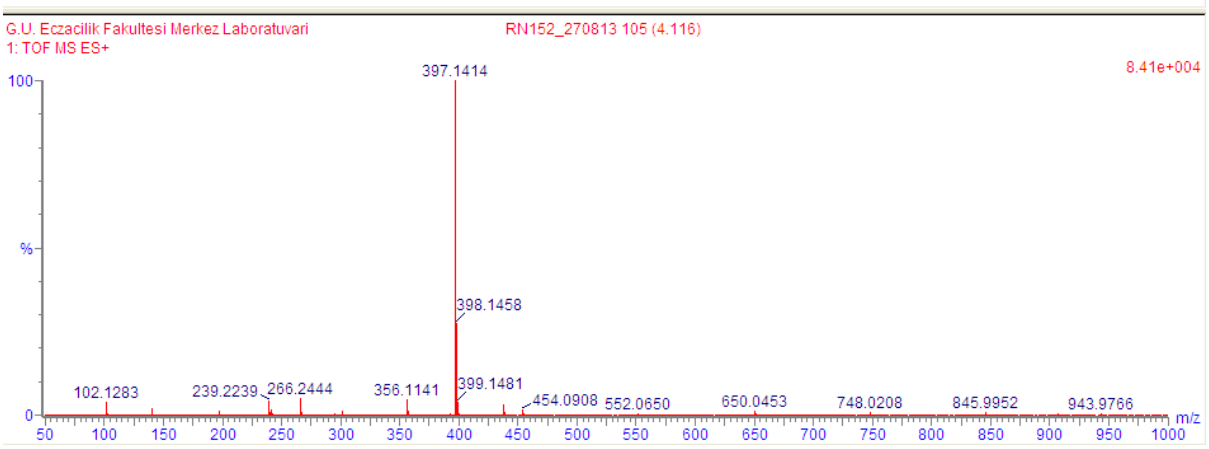
11 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N	Cl
386.1171	386.1172	-0.1	-0.3	16.5	C22 H17 N5 Cl	197.3	0.0	22	17	5	1

Compound 4





Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

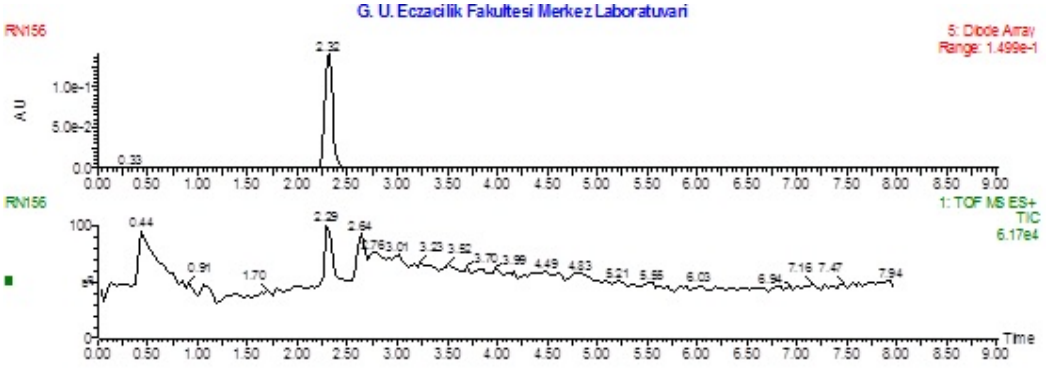
Monoisotopic Mass, Even Electron Ions

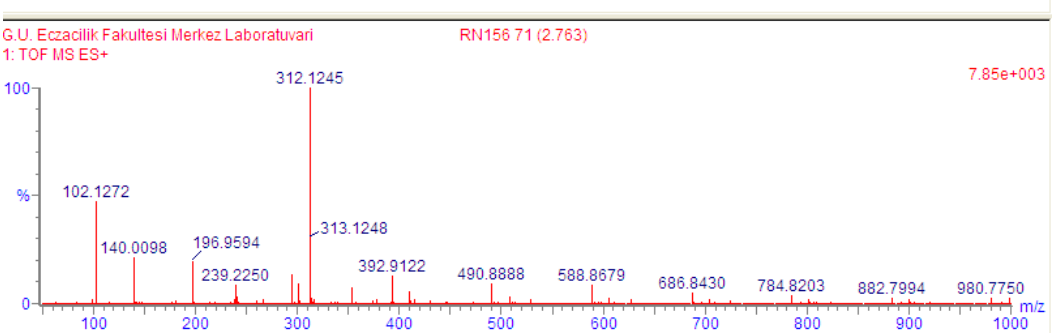
30 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N	O
397.1414	397.1413	0.1	0.3	17.5	C22 H17 N6 O2	256.9	0.0	22	17	6	2

Compound 5





Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

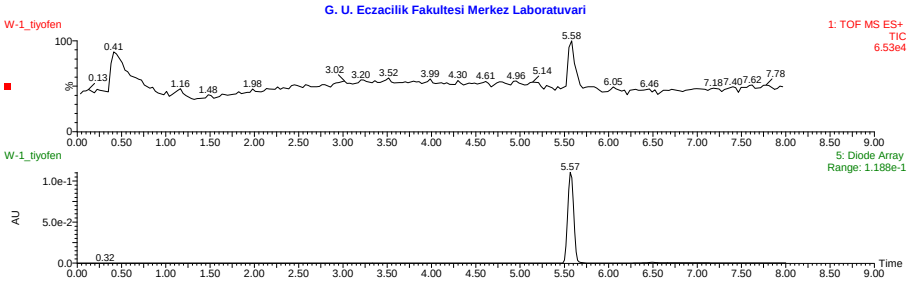
Monoisotopic Mass, Even Electron Ions

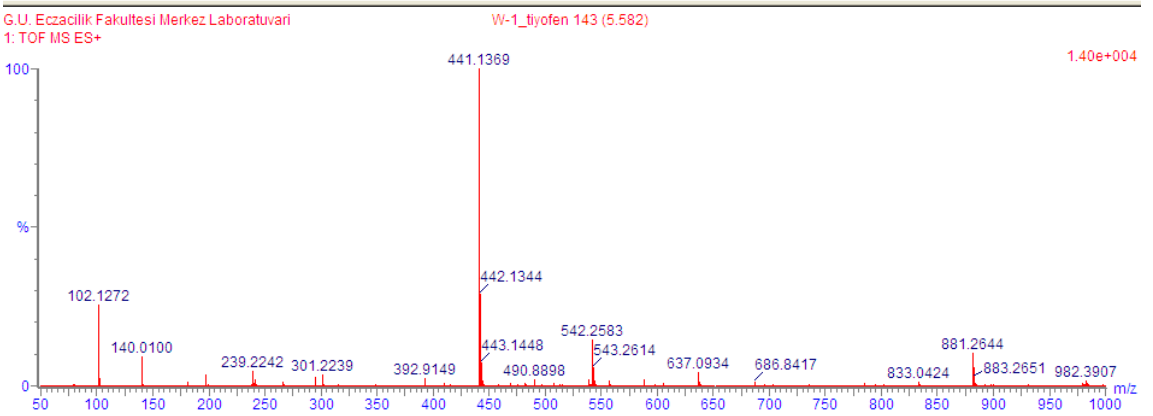
17 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N
312.1245	312.1249	-0.4	-1.3	15.5	C19 H14 N5	115.6	0.0	19	14	5

Compound 6





Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

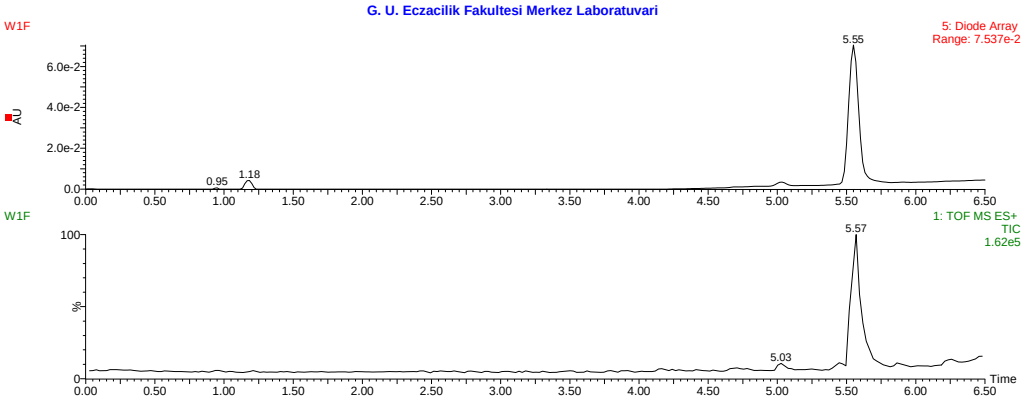
Monoisotopic Mass, Even Electron Ions

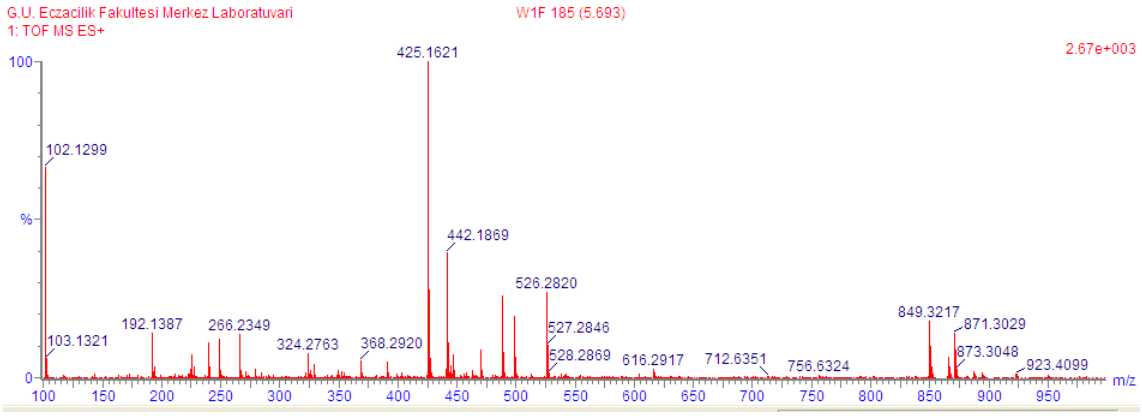
118 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N	O	S
441.1369	441.1385	-1.6	-3.6	17.5	C25 H21 N4 O2 S	55.6	0.0	25	21	4	2	1

Compound 7

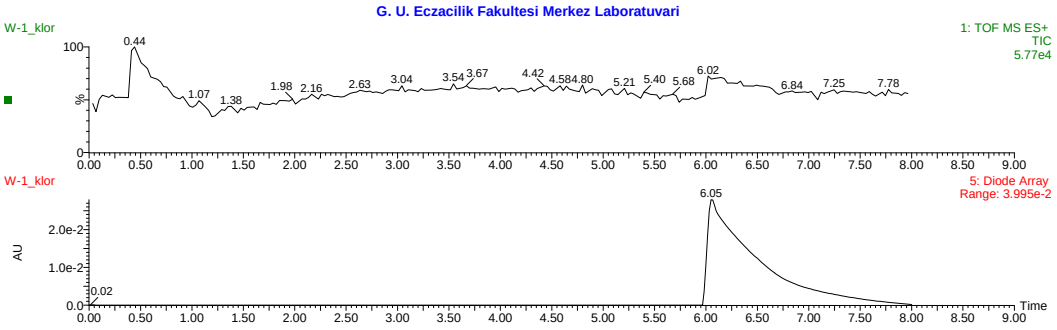


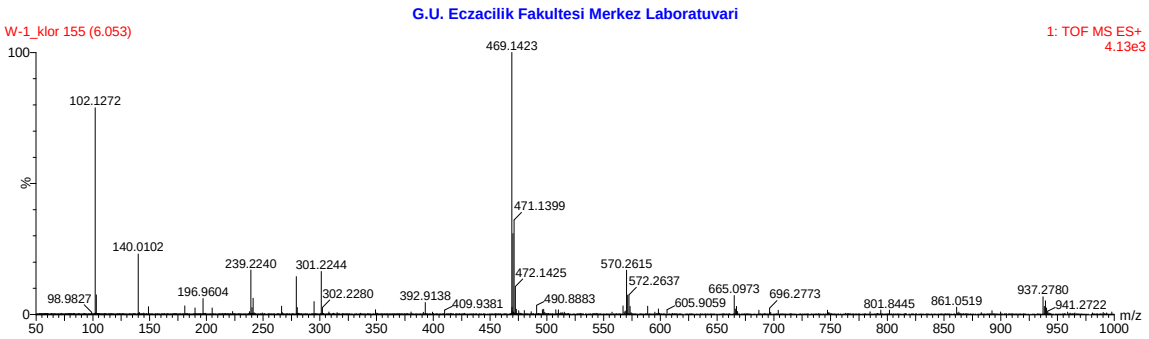


Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
21 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N	O
425.1621	425.1614	0.7	1.6	17.5	C25 H21 N4 O3	80.5	0.0	25	21	4	3

Compound 8





Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

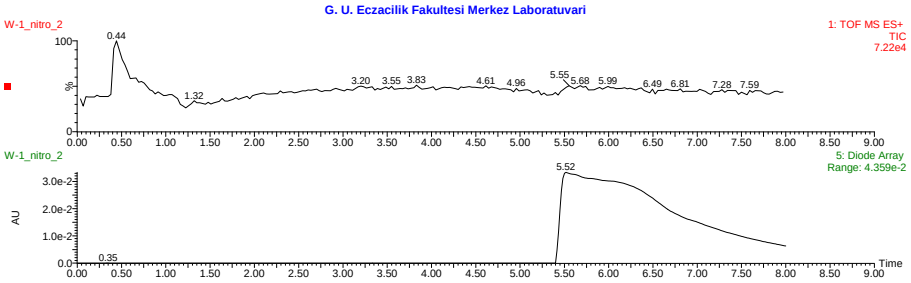
Monoisotopic Mass, Even Electron Ions

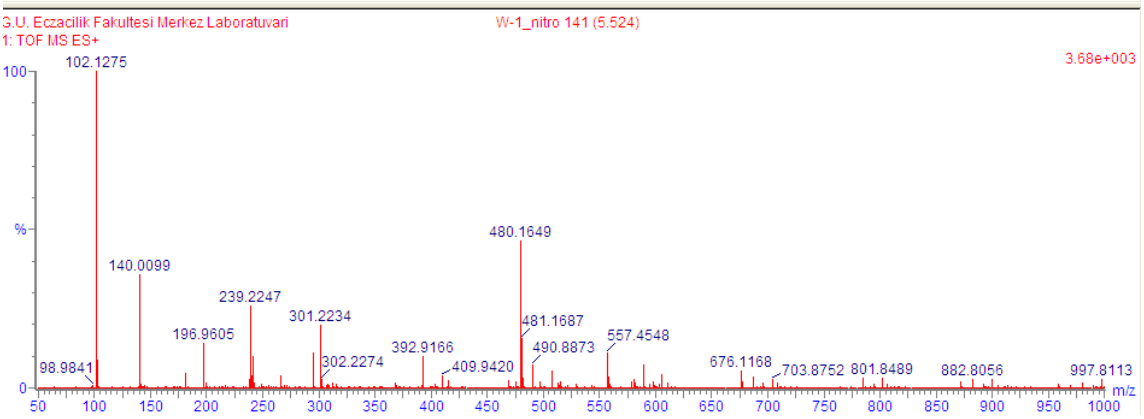
34 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N	O	Cl
469.1423	469.1431	-0.8	-1.7	18.5	C27 H22 N4 O2 Cl	117.2	0.0	27	22	4	2	1

Compound 9

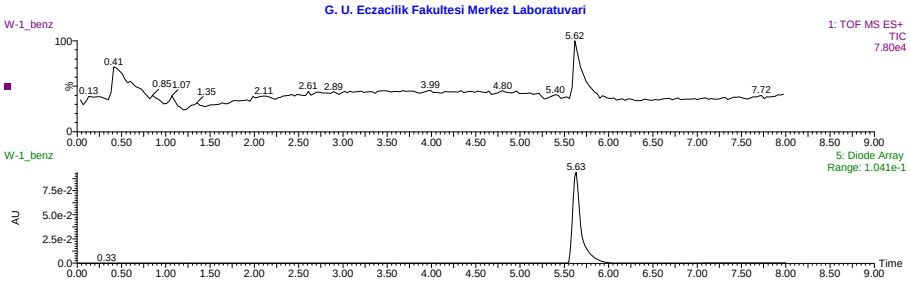


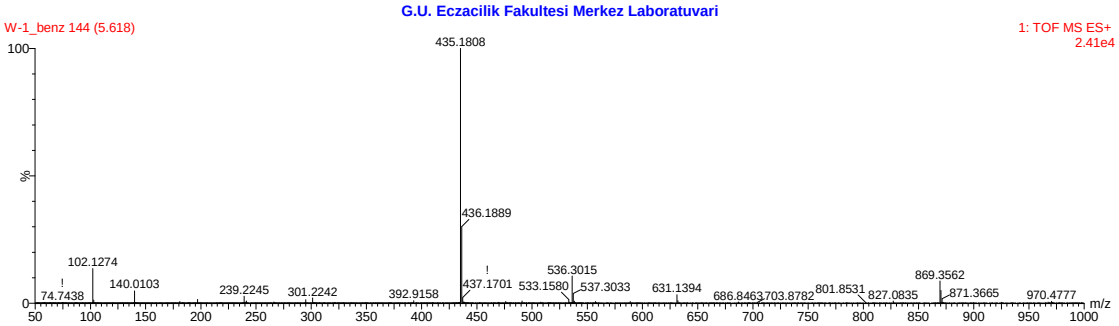


Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
21 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N	O
480.1649	480.1672	-2.3	-4.8	19.5	C27 H22 N5 O4	82.3	0.0	27	22	5	4

Compound 10





Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

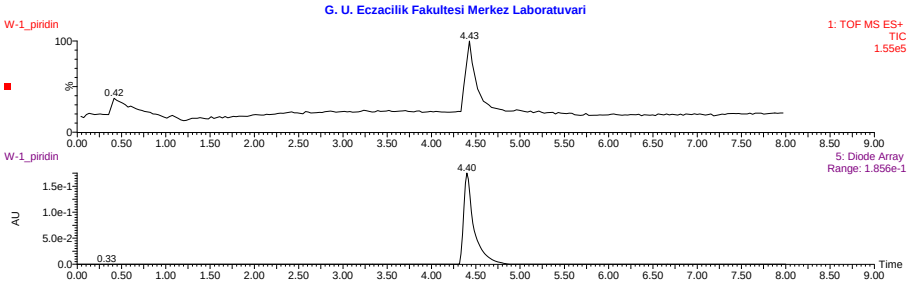
Monoisotopic Mass, Even Electron Ions

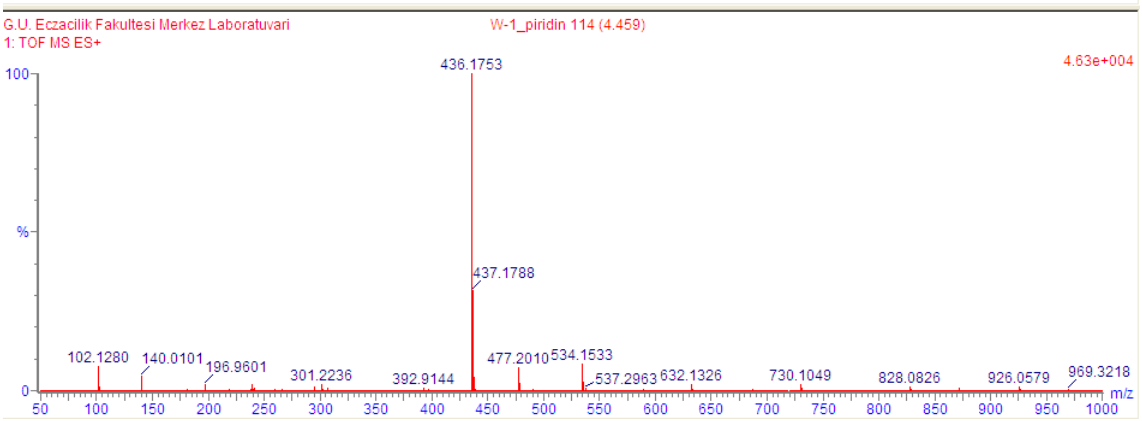
18 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N	O
435.1808	435.1821	-1.3	-3.0	18.5	C27 H23 N4 O2	58.2	0.0	27	23	4	2

Compound 11

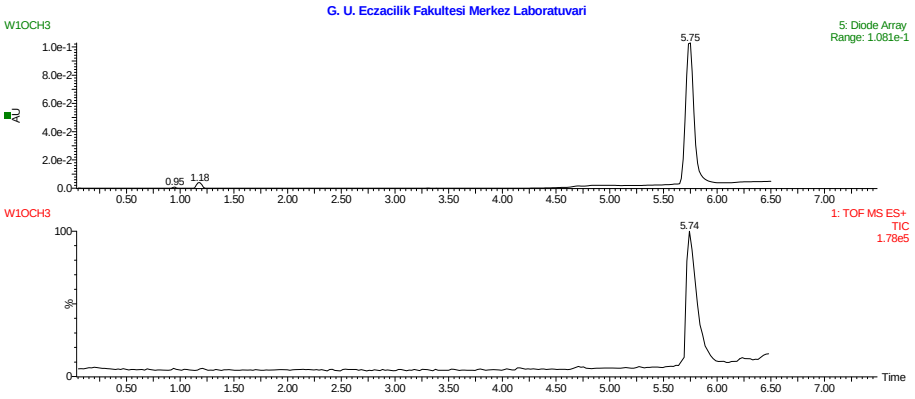


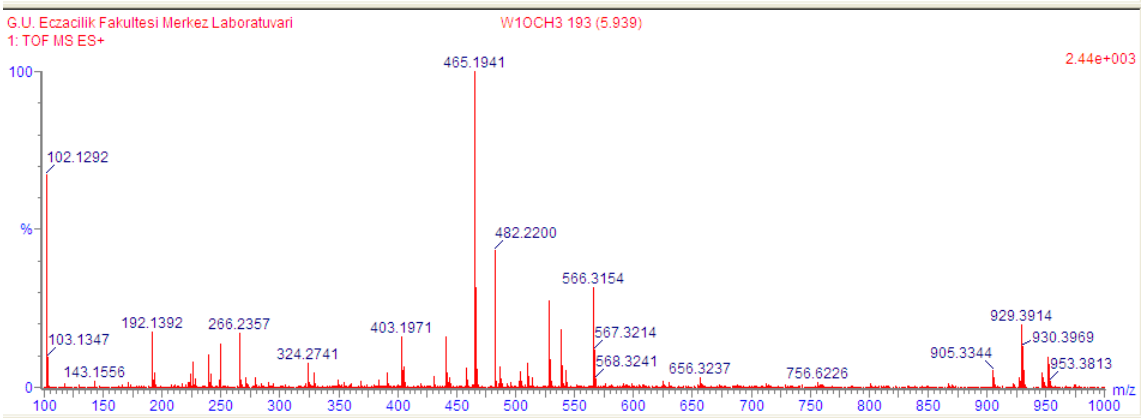


Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
33 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N	O
436.1753	436.1774	-2.1	-4.8	18.5	C26 H22 N5 O2	60.6	0.0	26	22	5	2

Compound 12

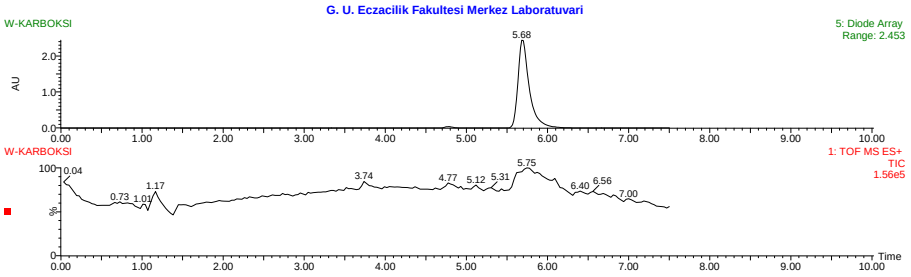


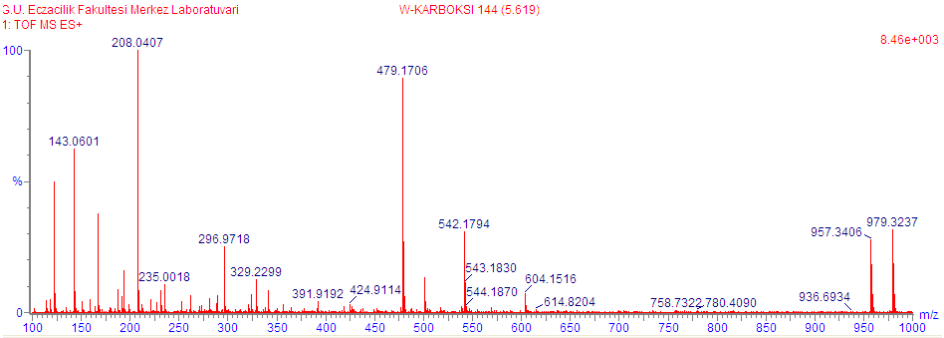


Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N	O
465.1941	465.1927	1.4	3.0	18.5	C28 H25 N4 O3	58.0	0.0	28	25	4	3

Compound 13





Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

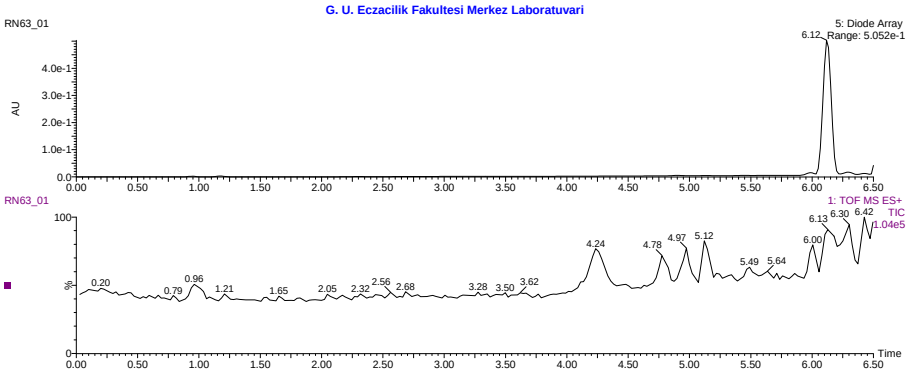
Monoisotopic Mass, Even Electron Ions

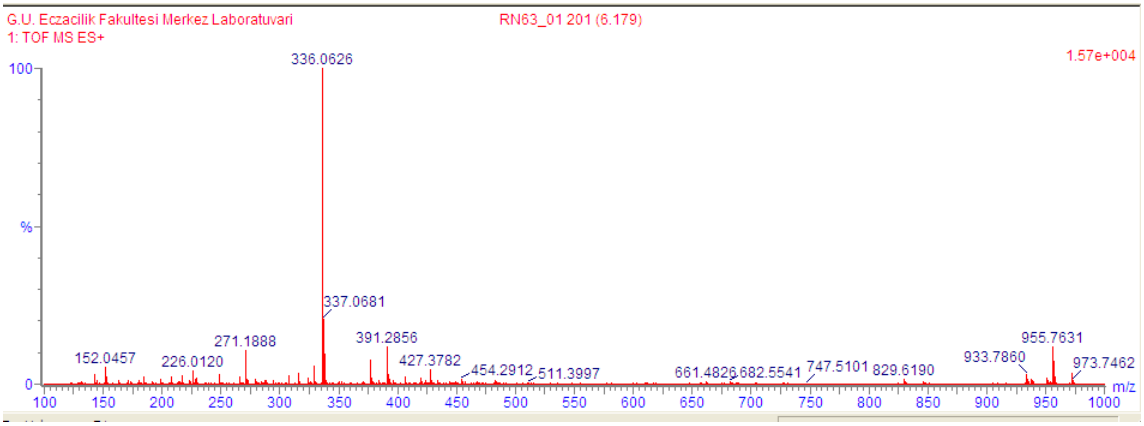
16 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N	O
479.1706	479.1719	-1.3	-2.7	19.5	C28 H23 N4 O4	60.5	0.0	28	23	4	4

Compound I-1





Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

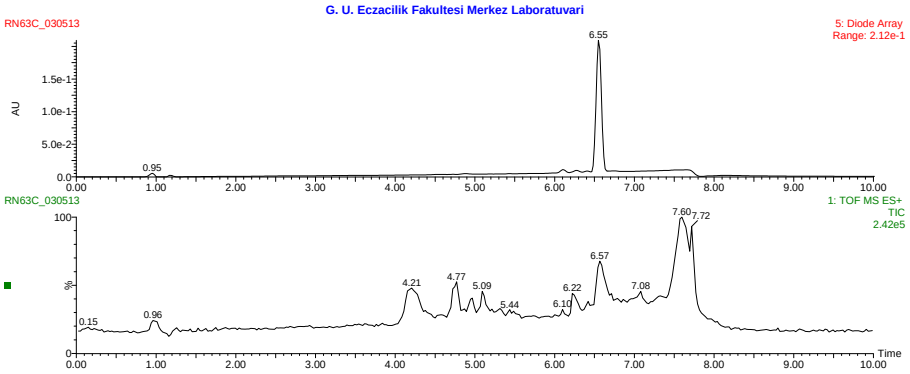
Monoisotopic Mass, Even Electron Ions

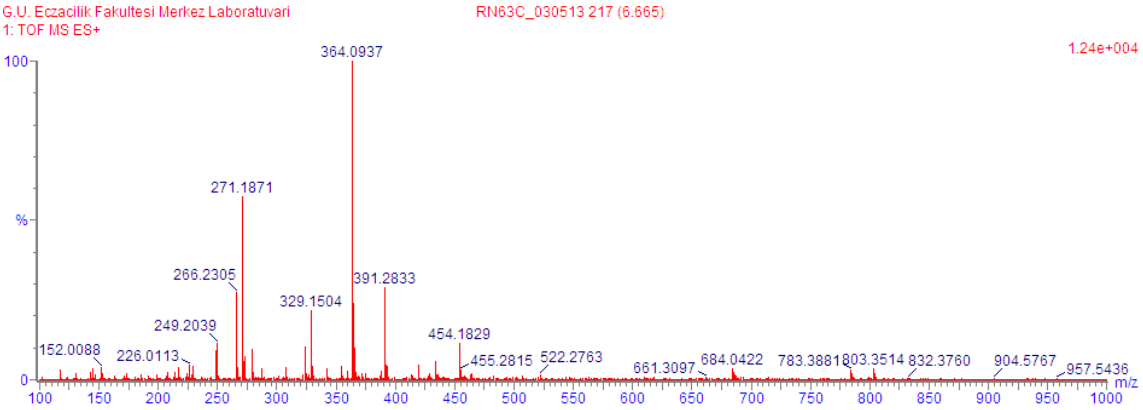
9 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N	S
336.0626	336.0629	-0.3	-0.9	13.5	C18 H14 N3 S2	50.5	0.0	18	14	3	2

Compound 1-II





Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

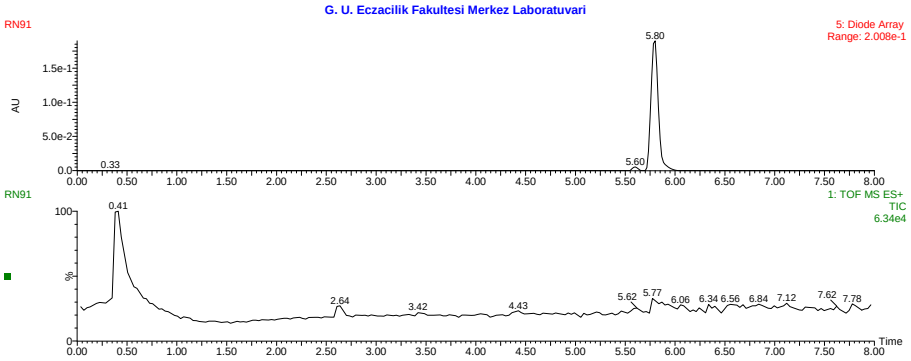
Monoisotopic Mass, Even Electron Ions

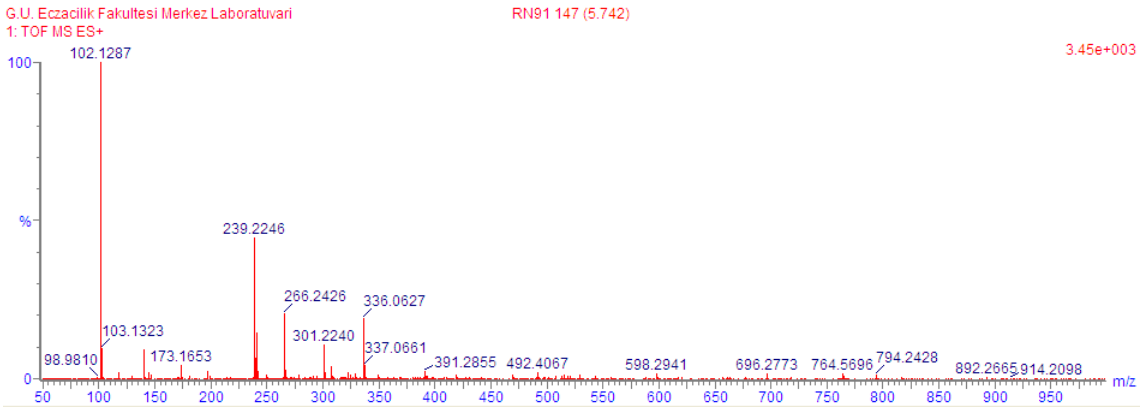
9 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N	S
364.0937	364.0942	-0.5	-1.4	13.5	C20 H18 N3 S2	34.0	0.0	20	18	3	2

Compound 1-III

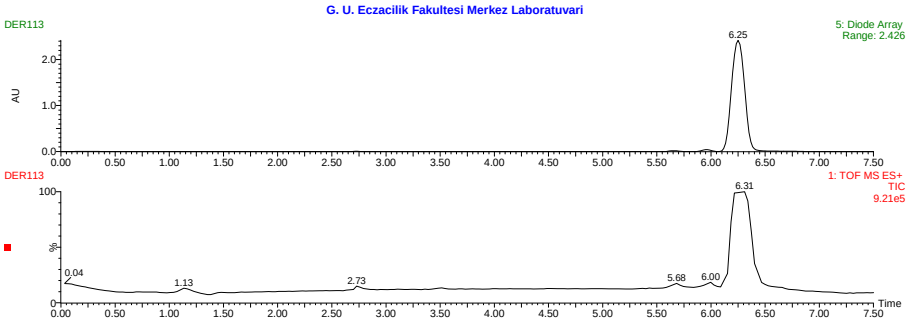


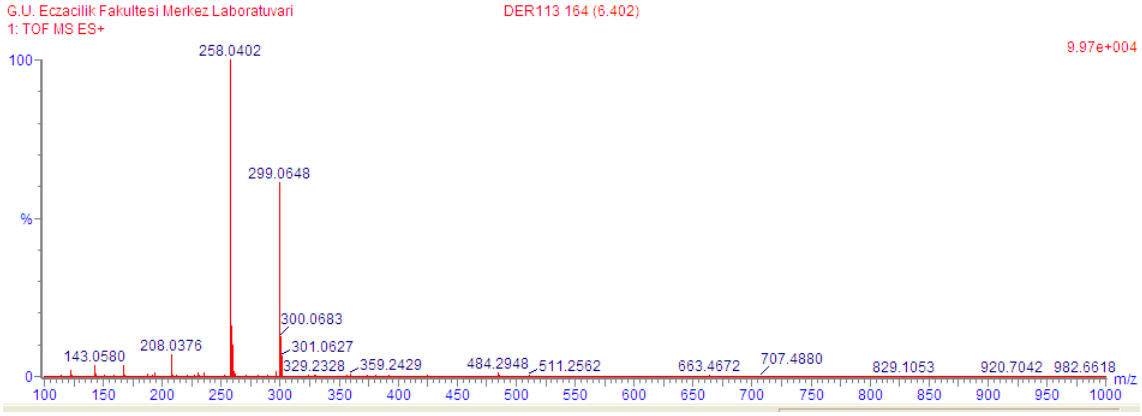


Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
9 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N	S
336.0627	336.0629	-0.2	-0.6	13.5	C18 H14 N3 S2	26.7	0.0	18	14	3	2

Compound 1-IV





Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N	S
258.0402	258.0411	-0.9	-3.5	9.5	C14 H12 N S2	394.5	0.0	14	12	1	2