[Ag(PcL)]-Catalysed Domino Approach to 6-Substituted Benzoxazino Isoquinolines

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Supporting Information

Table of Contents:

X-ray Single-Crystal Structure Determination	S2
Figure 1S	S2
References	S2
Table 1S. Summary of X-ray single crystal diffraction refinement results for **3e**.	S3
Table 2S. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å2) for **3e**.	S4
Table 3S. Geometric parameters (Å, º) for **3e**.	S5
^{1}H, ^{13}C and two-dimensional NMR spectra of compounds **3**	S7
HPLC spectra of compounds **3** and **3'**	S45

X-ray Single-Crystal Structure Determination.

Crystal data and structure determination results are summarized in Table 1S. X-ray data collection was carried out at 180 K using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) on a Bruker SMART-APEX II diffractometer equipped with an Oxford Cryosystems N_2 gas blower. A ω-scan at three different φ settings and a detector position of -30º in 2θ was performed within the Bragg limits of 1.5 < θ < 27.7°. Determination of the integrated intensities and unit cell refinements were performed using SAINT[1]. The intensity data were corrected for absorption by using SADABS.[1] No *decay correction* was applied. The structures were solved by direct methods (SIR2014)[2] and refined by full-matrix least squares on F^2 (SHELX 2014)[3] with the WINGX interface.[4]

All hydrogen atoms were located from the difference Fourier map and refined as "riding" on the adjacent carbon with individual isotropic temperature factor 1.2 or 1.5 (H-methyl group) times the value of the equivalent temperature factor of the parent atom. All non-hydrogen atoms were *refined with* full occupancy and *anisotropic displacement parameters.* The diagram was drawn using ORTEPIII program.[5]

1. Bruker. *SADABS* and *SAINT* **2009**, Bruker AXS Inc., Madison, Wisconsin, USA.
2. Burla, M. C.; Caliandro, R.; Camalli, M.; Carrozzini, B.; Cascarano, G. L.; De Caro, L.; Giacovazzo, C.; Polidori, G.; Spagna, R. *J. Appl. Crystallogr.* **2005**, *38* (2), 381–388.
3. Sheldrick, G. M. *Acta Crystallogr. Sect. C Struct. Chem.* **2015**, *71*, 3–8.
4. Farrugia, L. J. *J. Appl. Crystallogr.* **2012**, *45* (4), 849–854.
5. M. N. Burnett and C. K. Johnson, ORTEP-III Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA, 1996.

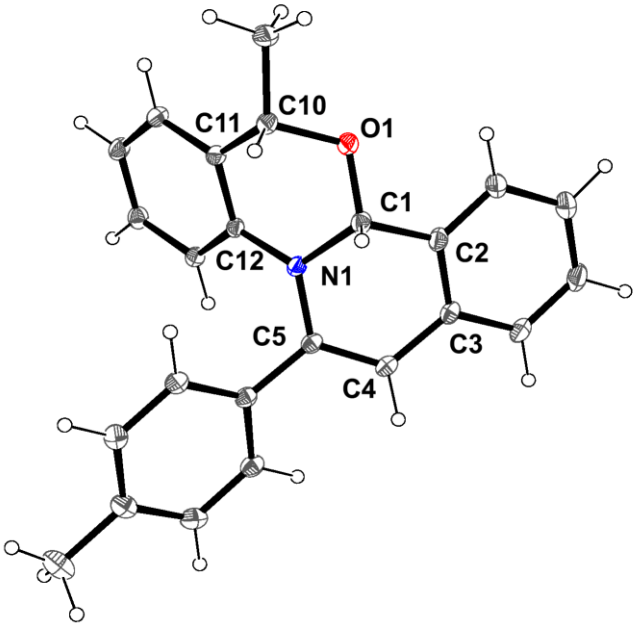


Figure 1S: The molecular structure of compound **3e** showing the numbering schemes for some non-hydrogen atoms. Displacement ellipsoids are plotted at the 40% probability level.

Table 1S. Summary of X-ray single crystal diffraction refinement results for **3e**.

Identification code	**3f**
Empirical formula	$C_{24}H_{21}NO$
Formula weight	339.42
Temperature (K)	180(2)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 14.0503(6) Å
	b = 5.6227(3) Å
	c = 22.727(1) Å
	β = 97.907(1)°
Volume ($Å^3$)	1778.38(14)
Z	4
Density (calculated) (g/cm^3)	1.268
Absorption coefficient μ (mm^{-1})	0.077
F(000)	720
T_{min}, T_{max}	0.692, 0.746
Theta range for data collection	1.5 to 27.7°
Index ranges	-18<=h<=18, -7<=k<=7, -29<=l<=29
$(\sin\theta/\lambda)_{max}$ ($Å^{-1}$)	0.654
Reflections collected	16557
Independent reflections	4171 [R_{int} = 0.0164]
Observed reflections [I>2sigma(I)]	3707
Completeness to theta	100.0 %
Data / restraints / parameters	4171 / 0 / 298
Goodness-of-fit on F^2	1.038
Final R indices [I>2sigma(I)]	R_1 = 0.0406, wR_2 = 0.1103
R indices (all data)	R_1 = 0.0453, wR_2 = 0.1146
Largest diff. peak and hole ($e.Å^{-3}$)	0.285 and -0.223

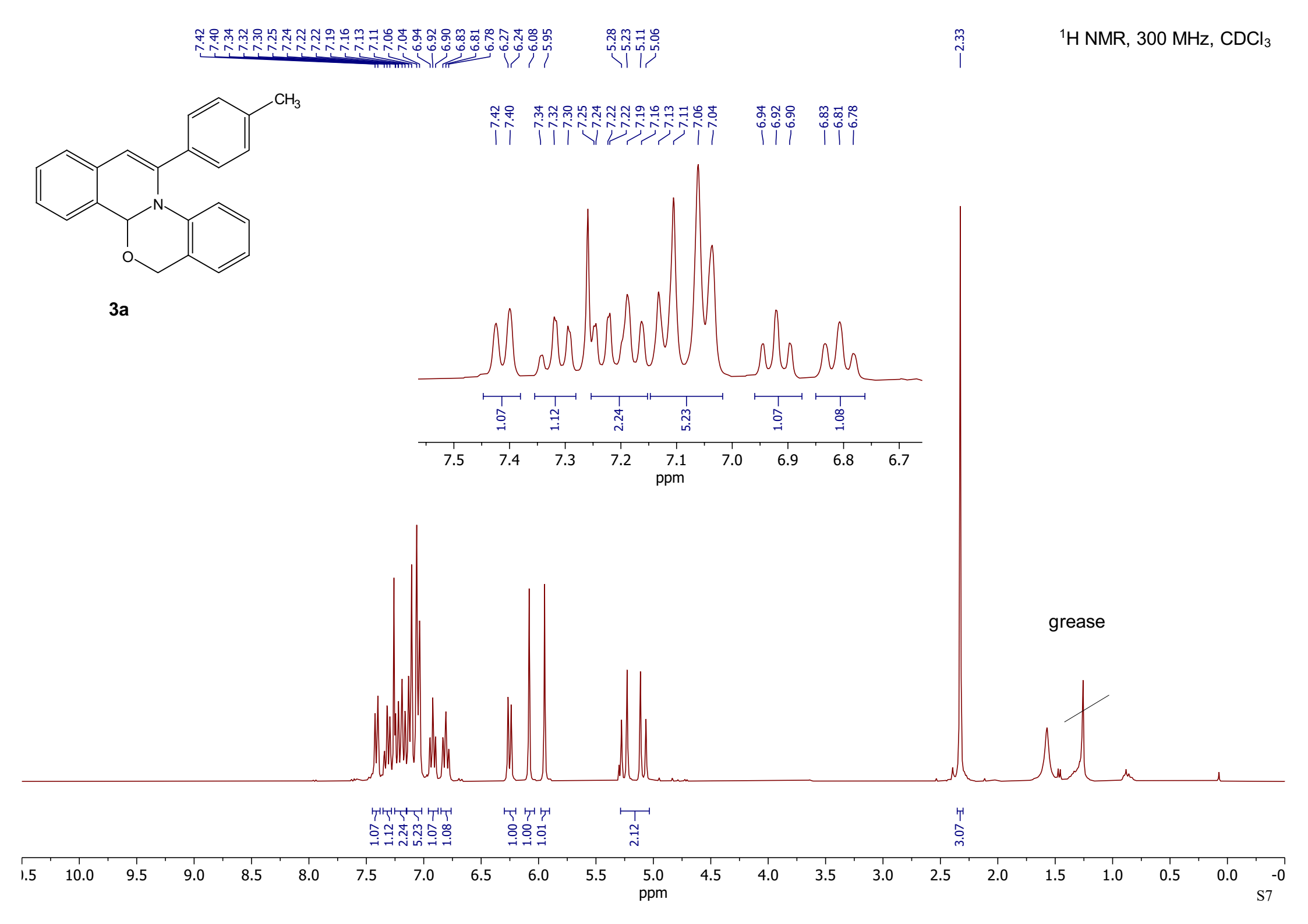
Table 2S. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for **3e**.

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.21375 (6)	0.63809 (17)	0.19670 (4)	0.0230 (2)
O1	0.17875 (6)	0.40750 (15)	0.10828 (4)	0.0287 (2)
C1	0.13916 (8)	0.5172 (2)	0.15433 (5)	0.0253 (2)
C2	0.06474 (8)	0.6931 (2)	0.12756 (5)	0.0267 (2)
C3	0.03840 (8)	0.8714 (2)	0.16491 (5)	0.0248 (2)
C4	0.09069 (8)	0.8867 (2)	0.22471 (5)	0.0256 (2)
C5	0.17794 (7)	0.78327 (19)	0.23913 (5)	0.0223 (2)
C6	0.01980 (10)	0.6743 (3)	0.06960 (6)	0.0400 (3)
C7	-0.05331 (10)	0.8320 (3)	0.04839 (7)	0.0452 (4)
C8	-0.08060 (9)	1.0078 (3)	0.08517 (6)	0.0377 (3)
C9	-0.03530 (8)	1.0283 (2)	0.14297 (6)	0.0311 (3)
C10	0.26151 (8)	0.2645 (2)	0.13047 (5)	0.0255 (2)
C11	0.33939 (8)	0.4391 (2)	0.15364 (5)	0.0226 (2)
C12	0.31030 (7)	0.63101 (19)	0.18691 (4)	0.0199 (2)
C13	0.37697 (8)	0.8051 (2)	0.20842 (5)	0.0224 (2)
C14	0.47168 (8)	0.7882 (2)	0.19727 (5)	0.0265 (2)
C15	0.50018 (8)	0.6015 (2)	0.16393 (5)	0.0297 (3)
C16	0.43391 (8)	0.4283 (2)	0.14223 (5)	0.0277 (2)
C17	0.28193 (10)	0.1062 (2)	0.07995 (6)	0.0330 (3)
C18	0.23168 (7)	0.7978 (2)	0.29997 (5)	0.0227 (2)
C19	0.29163 (8)	0.6131 (2)	0.32340 (5)	0.0254 (2)
C20	0.33734 (8)	0.6221 (2)	0.38174 (5)	0.0287 (3)
C21	0.32416 (9)	0.8139 (2)	0.41854 (5)	0.0302 (3)
C22	0.26370 (9)	0.9975 (2)	0.39517 (5)	0.0305 (3)
C23	0.21894 (8)	0.9919 (2)	0.33688 (5)	0.0273 (2)
C24	0.37368 (13)	0.8251 (3)	0.48164 (6)	0.0459 (4)
H1	0.1097 (13)	0.393 (3)	0.1790 (8)	
H4	0.0619 (13)	0.974 (3)	0.2550 (8)	
H6	0.0394 (13)	0.549 (3)	0.0448 (8)	
H7	-0.0833 (13)	0.818 (3)	0.0061 (8)	
H8	-0.1331 (13)	1.119 (3)	0.0707 (8)	
H9	-0.0539 (13)	1.156 (3)	0.1688 (8)	
H10	0.2425 (13)	0.164 (3)	0.1645 (8)	
H13	0.3577 (13)	0.940 (3)	0.2305 (8)	
H14	0.5178 (13)	0.908 (3)	0.2127 (8)	
H15	0.5656 (13)	0.590 (3)	0.1560 (8)	
H16	0.4533 (13)	0.294 (3)	0.1181 (8)	
H17A	0.2955 (13)	0.203 (3)	0.0457 (8)	
H17B	0.3384 (13)	0.002 (4)	0.0925 (8)	
H17C	0.2260 (13)	0.006 (3)	0.0674 (8)	
H19	0.3017 (13)	0.472 (4)	0.2980 (8)	
H20	0.3798 (13)	0.488 (3)	0.3969 (8)	
H22	0.2542 (13)	1.134 (3)	0.4198 (8)	
H23	0.1784 (13)	1.127 (3)	0.3219 (8)	
H24A	0.4124 (13)	0.969 (4)	0.4892 (8)	
H24B	0.4144 (14)	0.694 (4)	0.4905 (8)	
H24C	0.3257 (13)	0.835 (3)	0.5094 (8)	

Table 3S. Geometric parameters (Å, º) for **3e**.

Bond lengths			
N1—C12	1.4051 (13)	C10—C11	1.5097 (16)
N1—C5	1.4080 (14)	C10—C17	1.5112 (16)
N1—C1	1.4867 (14)	C11—C16	1.3891 (15)
O1—C1	1.3948 (14)	C11—C12	1.4103 (15)
O1—C10	1.4463 (13)	C12—C13	1.3960 (15)
C1—C2	1.5054 (15)	C13—C14	1.3916 (15)
C2—C6	1.3843 (17)	C14—C15	1.3857 (17)
C2—C3	1.3961 (16)	C15—C16	1.3901 (18)
C3—C9	1.3992 (16)	C18—C19	1.3956 (16)
C3—C4	1.4558 (16)	C18—C23	1.4032 (16)
C4—C5	1.3555 (15)	C19—C20	1.3925 (16)
C5—C18	1.4838 (15)	C20—C21	1.3923 (18)
C6—C7	1.3921 (19)	C21—C22	1.3947 (19)
C7—C8	1.382 (2)	C21—C24	1.5068 (18)
C8—C9	1.3835 (18)	C22—C23	1.3864 (17)
Bond angles			
C12—N1—C5	124.65 (9)	C7—C8—C9—C3	-0.1 (2)
C12—N1—C1	119.63 (9)	C2—C3—C9—C8	-0.47 (18)
C5—N1—C1	114.97 (8)	C4—C3—C9—C8	178.37 (12)
C1—O1—C10	111.64 (8)	C1—O1—C10—C11	-70.15 (11)
O1—C1—N1	111.71 (9)	C1—O1—C10—C17	165.35 (10)
O1—C1—C2	108.29 (9)	O1—C10—C11—C16	-133.98 (11)
N1—C1—C2	110.48 (9)	C13—C12—C11	119.63 (10)
C6—C2—C3	120.60 (11)	N1—C12—C11	117.64 (9)
C6—C2—C1	122.34 (11)	C14—C13—C12	120.05 (10)
C3—C2—C1	116.96 (10)	C15—C14—C13	120.46 (11)
C2—C3—C9	118.76 (11)	C14—C15—C16	119.66 (10)
C2—C3—C4	117.91 (10)	C11—C16—C15	120.94 (11)
C9—C3—C4	123.32 (11)	C19—C18—C23	118.09 (10)
C5—C4—C3	121.59 (10)	C19—C18—C5	121.18 (10)
C4—C5—N1	118.66 (10)	C23—C18—C5	120.63 (10)
C4—C5—C18	121.94 (10)	C20—C19—C18	120.74 (11)
N1—C5—C18	119.08 (9)	C21—C20—C19	121.21 (11)
C2—C6—C7	119.95 (13)	C20—C21—C22	117.96 (11)
C8—C7—C6	119.93 (13)	C20—C21—C24	121.47 (13)
C7—C8—C9	120.27 (12)	C22—C21—C24	120.57 (13)
C8—C9—C3	120.48 (12)	C23—C22—C21	121.31 (11)
O1—C10—C11	105.64 (9)	C22—C23—C18	120.68 (11)
O1—C10—C17	106.86 (9)	C17—C10—C11—C16	-15.64 (16)
C11—C10—C17	116.34 (10)	O1—C10—C11—C12	43.00 (12)
C16—C11—C12	119.24 (10)	C17—C10—C11—C12	161.34 (10)
C16—C11—C10	124.90 (10)	C5—N1—C12—C13	-15.18 (16)
C12—C11—C10	115.79 (9)	C1—N1—C12—C13	154.39 (10)
C13—C12—N1	122.73 (9)	C5—N1—C12—C11	165.12 (10)
C10—O1—C1—N1	48.75 (13)	C1—N1—C12—C11	-25.30 (14)
C10—O1—C1—C2	170.64 (9)	C16—C11—C12—C13	-0.77 (15)
C12—N1—C1—O1	0.09 (14)	C10—C11—C12—C13	-177.94 (9)
C5—N1—C1—O1	170.64 (9)	C16—C11—C12—N1	178.94 (10)
C12—N1—C1—C2	-120.53 (11)	C10—C11—C12—N1	1.77 (14)
C5—N1—C1—C2	50.02 (13)	N1—C12—C13—C14	179.97 (10)
O1—C1—C2—C6	22.92 (16)	C11—C12—C13—C14	-0.34 (16)
N1—C1—C2—C6	145.56 (12)	C12—C13—C14—C15	1.20 (17)
O1—C1—C2—C3	-160.56 (10)	C13—C14—C15—C16	-0.93 (17)
N1—C1—C2—C3	-37.92 (14)	C12—C11—C16—C15	1.05 (17)
C6—C2—C3—C9	1.00 (18)	C10—C11—C16—C15	177.93 (11)
C1—C2—C3—C9	-175.58 (10)	C14—C15—C16—C11	-0.20 (18)
C6—C2—C3—C4	-177.90 (12)	C4—C5—C18—C19	148.00 (11)

C1—C2—C3—C4	5.51 (15)	N1—C5—C18—C19	-25.38 (15)
C2—C3—C4—C5	18.77 (17)	C4—C5—C18—C23	-28.10 (16)
C9—C3—C4—C5	-160.08 (12)	N1—C5—C18—C23	158.51 (10)
C3—C4—C5—N1	-6.52 (17)	C23—C18—C19—C20	0.00 (16)
C3—C4—C5—C18	-179.93 (10)	C5—C18—C19—C20	-176.20 (10)
C12—N1—C5—C4	141.11 (11)	C18—C19—C20—C21	0.50 (17)
C1—N1—C5—C4	-28.90 (15)	C19—C20—C21—C22	-0.06 (17)
C12—N1—C5—C18	-45.29 (15)	C19—C20—C21—C24	-179.79 (12)
C1—N1—C5—C18	144.70 (10)	C20—C21—C22—C23	-0.89 (17)
C3—C2—C6—C7	-0.9 (2)	C24—C21—C22—C23	178.84 (12)
C1—C2—C6—C7	175.47 (13)	C21—C22—C23—C18	1.41 (17)
C2—C6—C7—C8	0.3 (2)	C19—C18—C23—C22	-0.93 (16)
C6—C7—C8—C9	0.2 (2)	C5—C18—C23—C22	175.28 (10)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5.28 5.23 5.11 5.06
2.33
CH3
N
O
3a
1.07 1.12 2.24 5.23 1.07 1.08
7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7
ppm
grease
1.07 1.12 2.24 5.23 1.07 1.08 1.00 1.00 1.01 2.12 3.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

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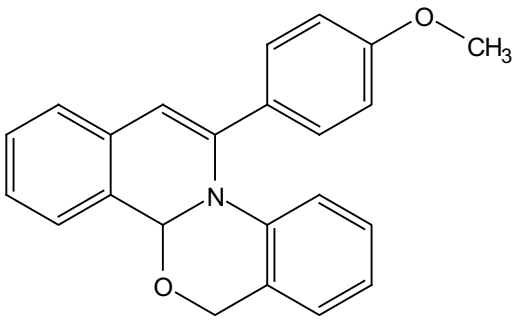
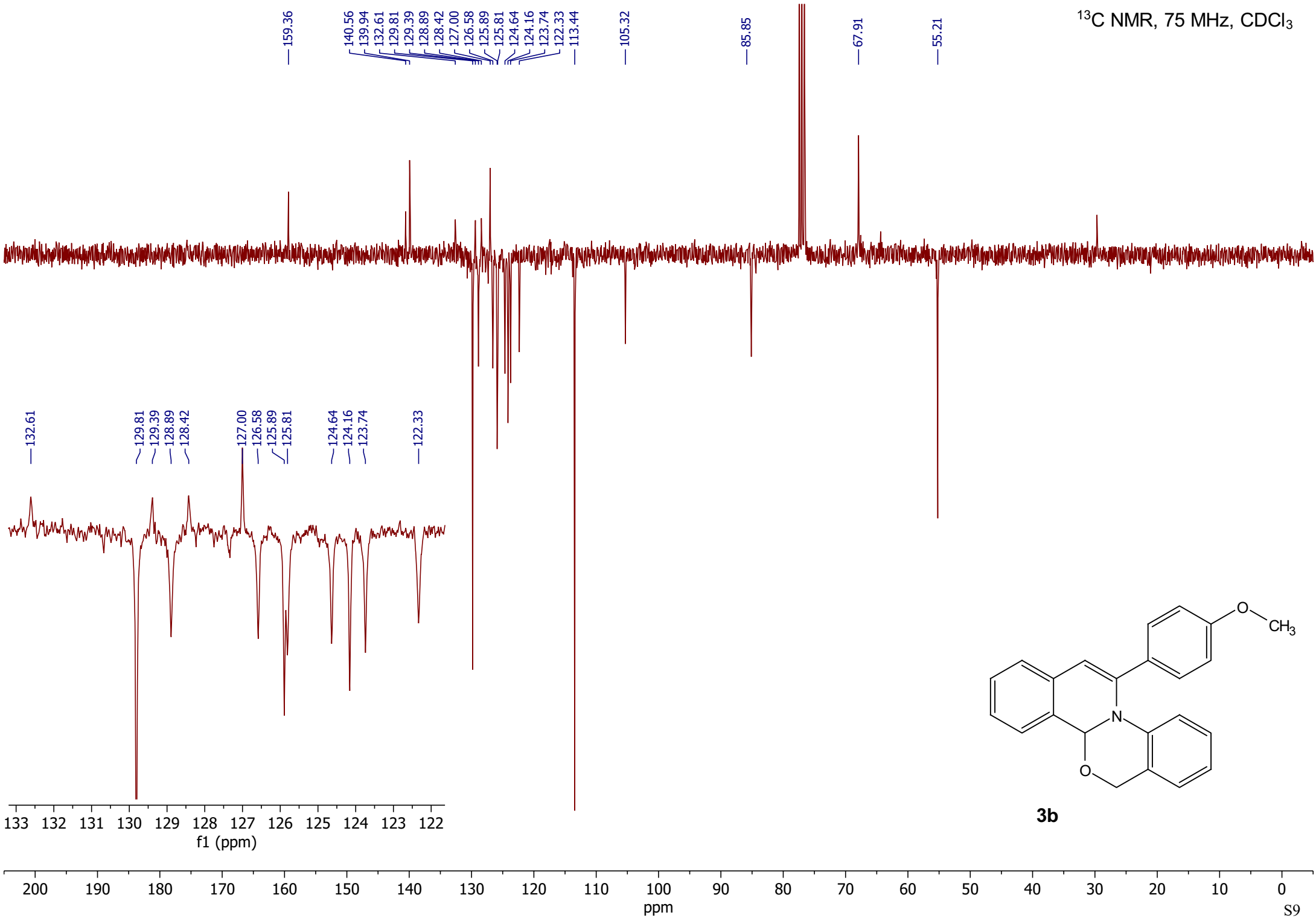


3b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124.16
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113.44
105.32
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O
3b

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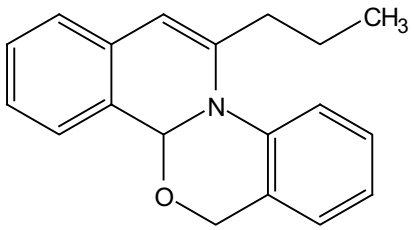

3c

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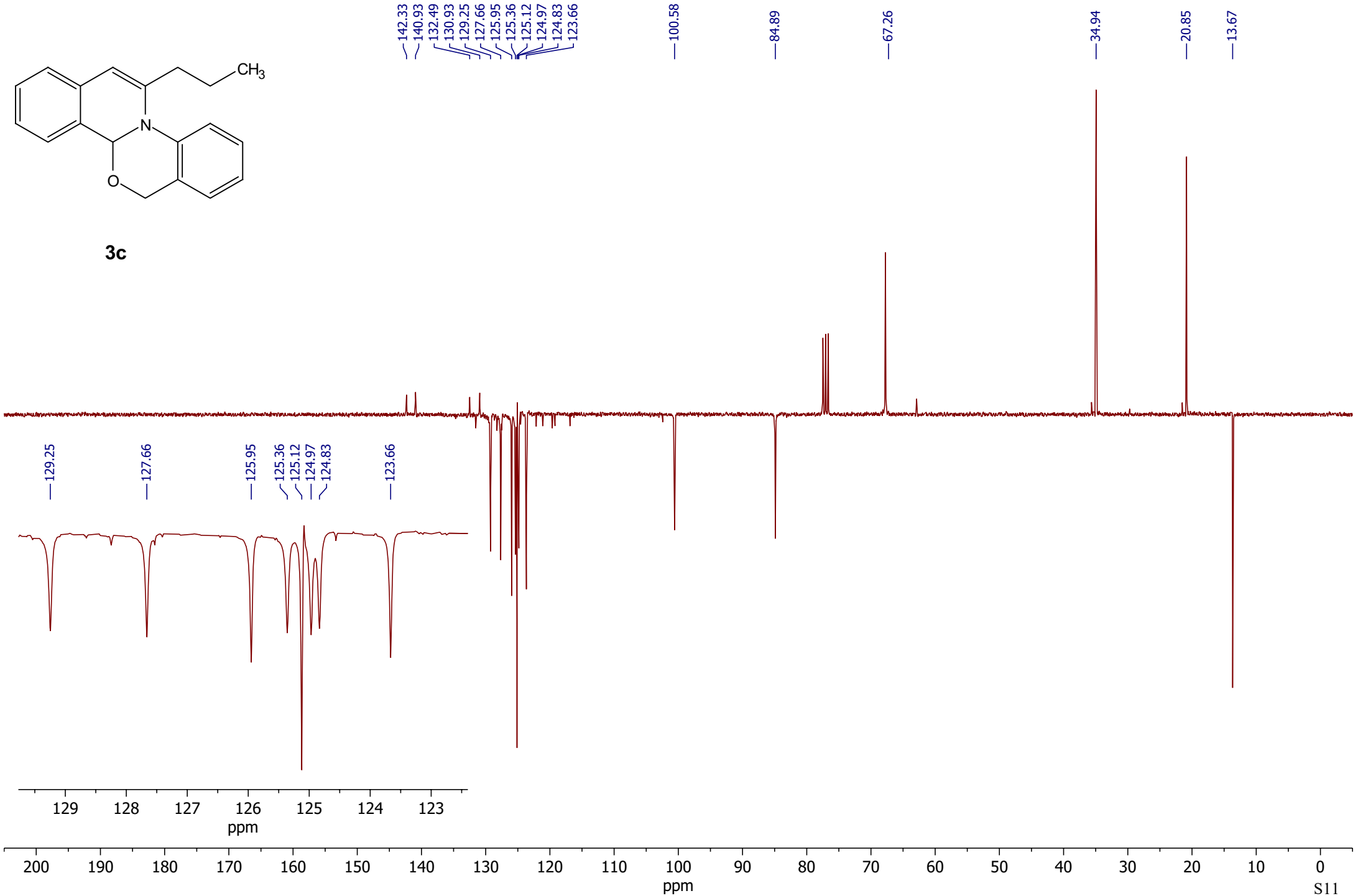
3c



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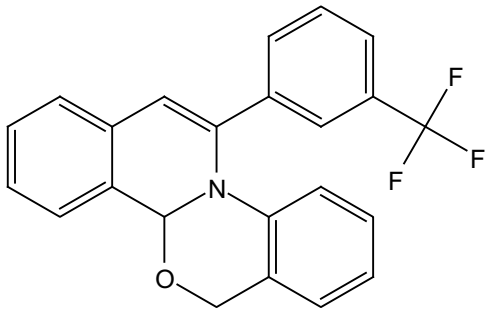
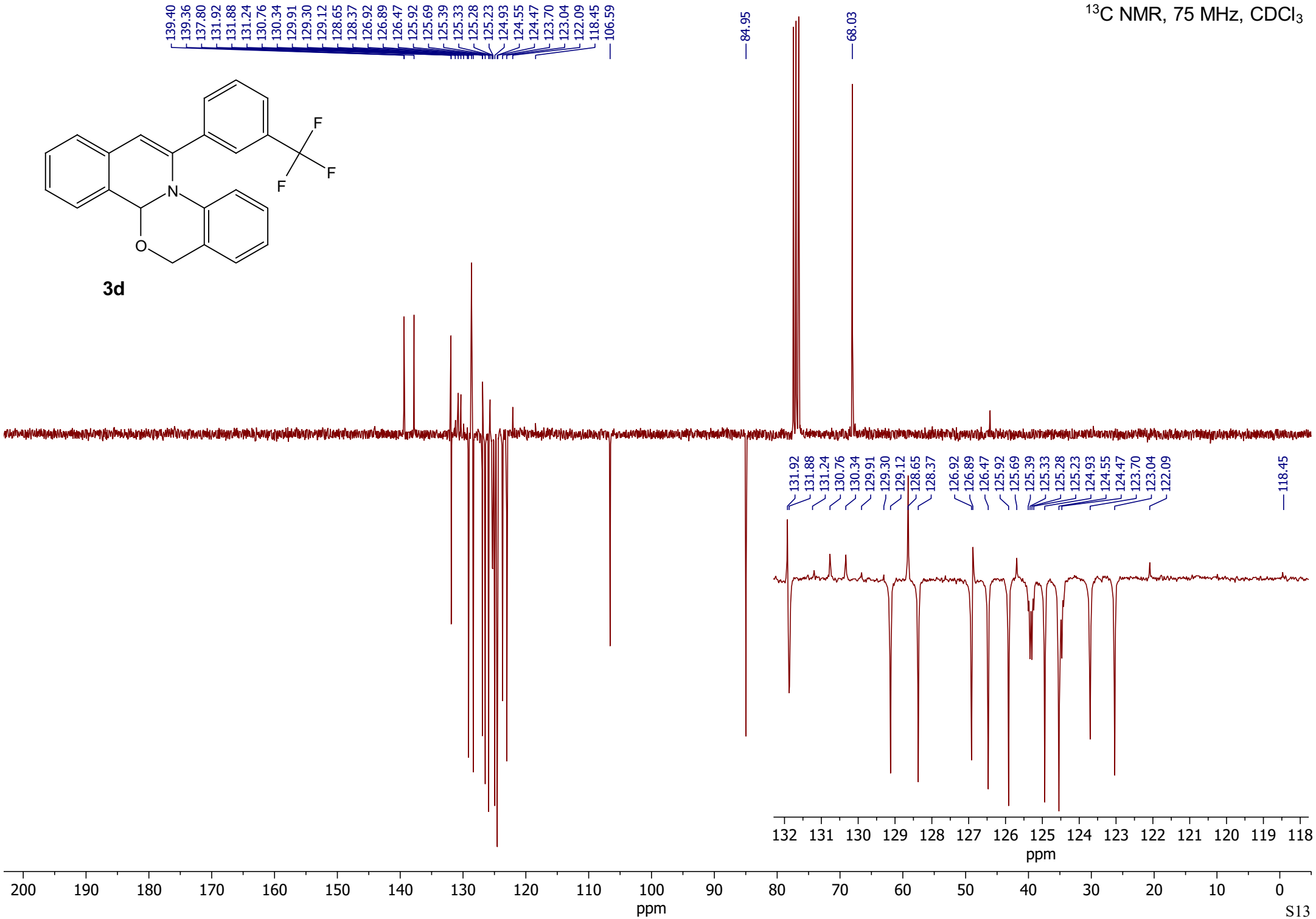


3d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129.12
128.65
128.37
126.92
126.89
126.47
125.92
125.69
125.39
125.33
125.28
125.23
124.93
124.55
124.47
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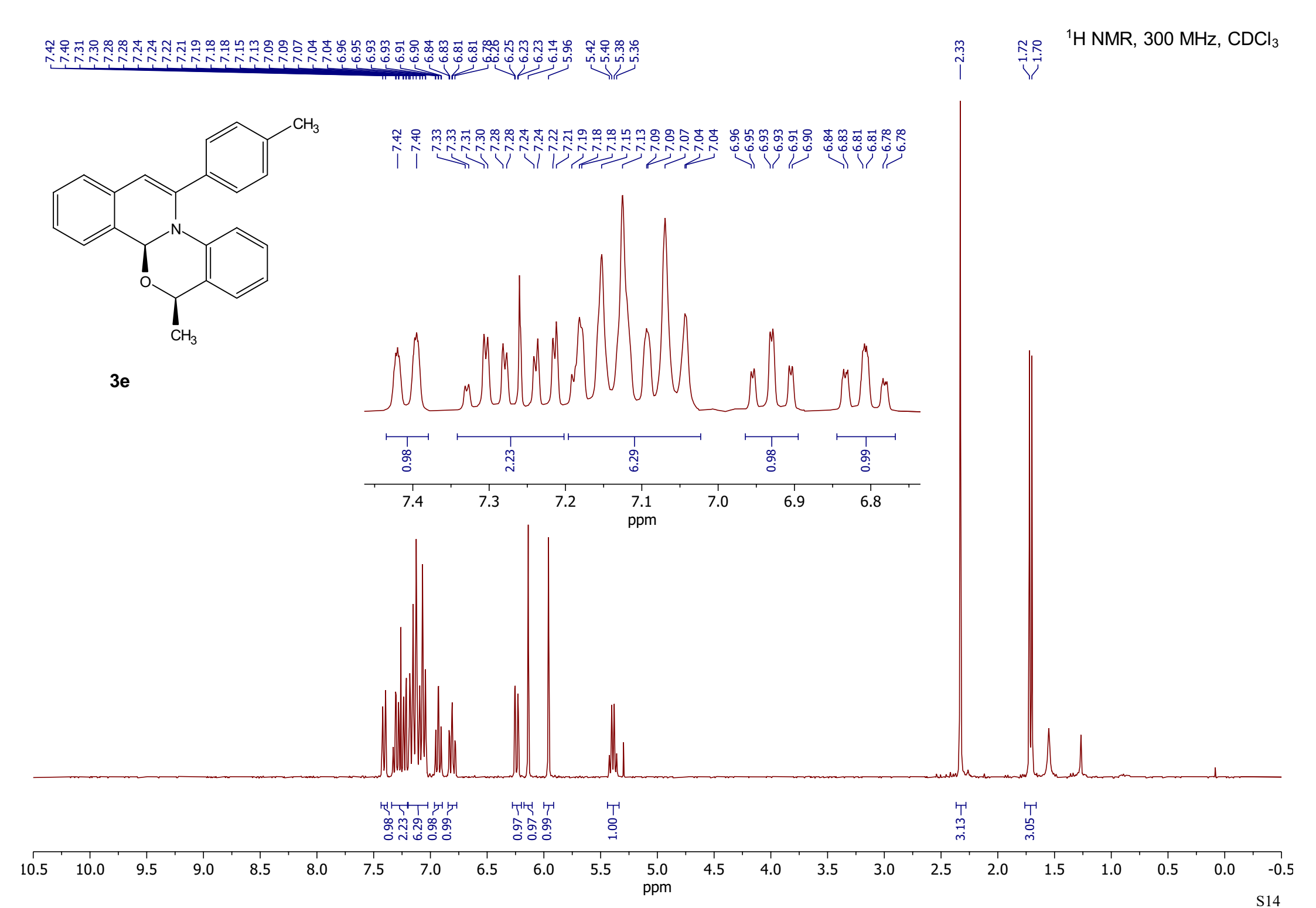
F
F
F
N
O
3d
ppm
S13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CH3
N
O
CH3
3e
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ppm
0.98 2.23 6.29 0.98 0.99 0.97 0.97 0.99 1.00 3.13 3.05
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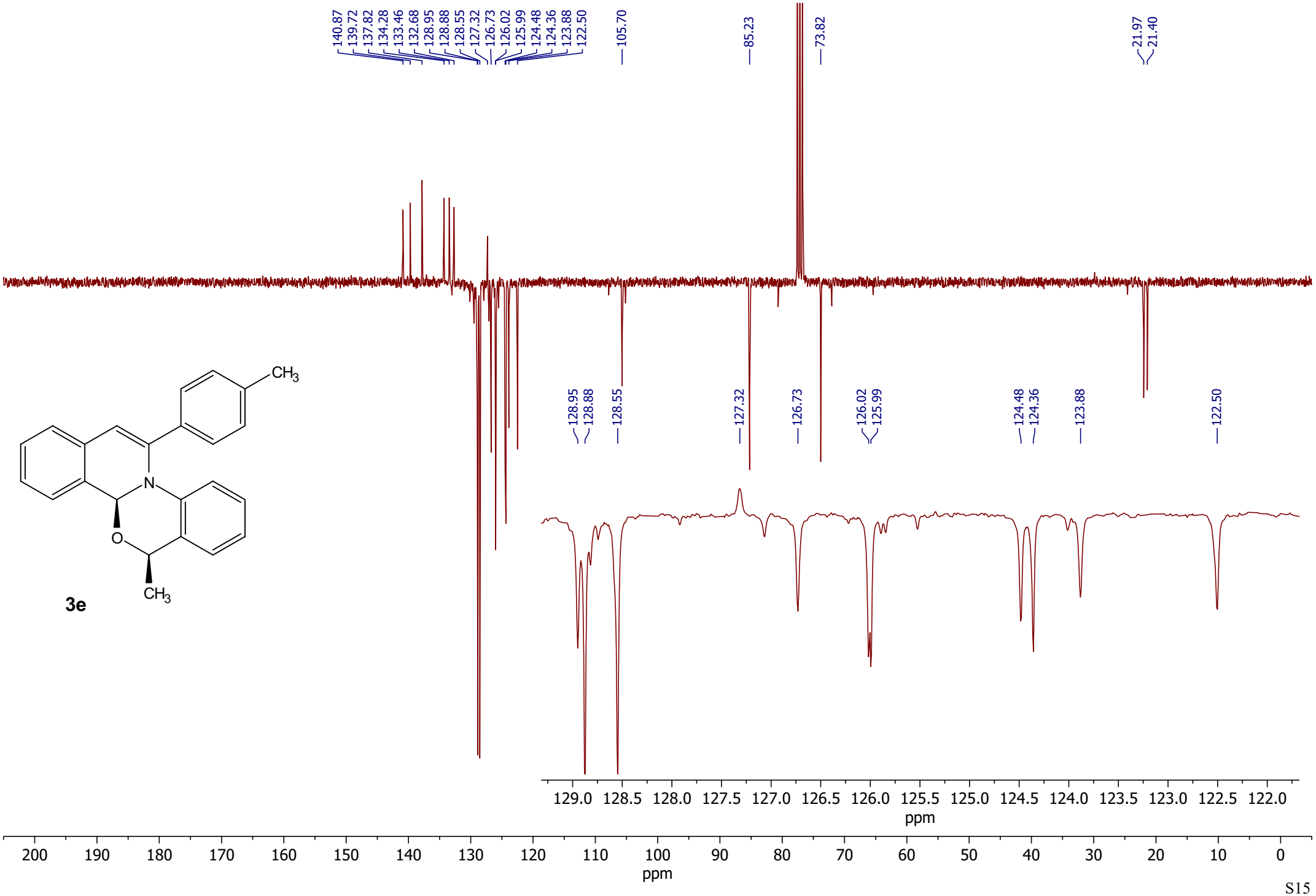
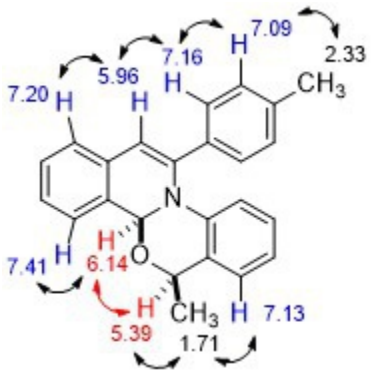
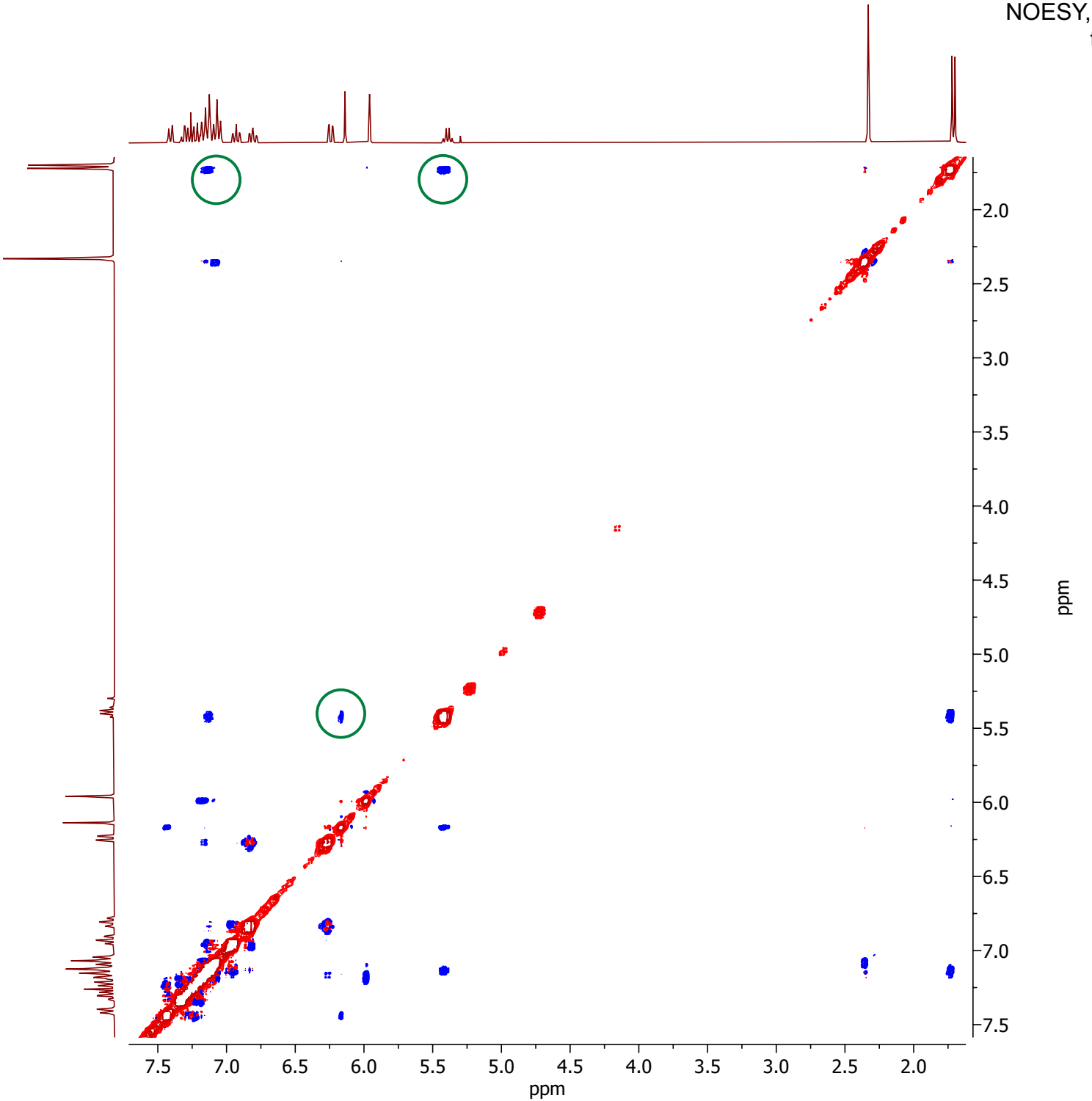
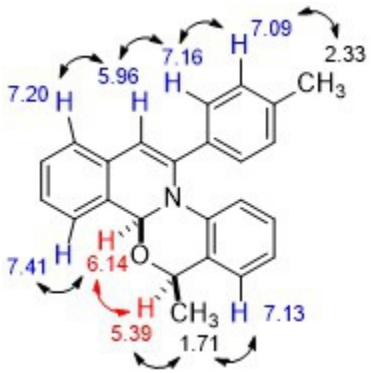




3e

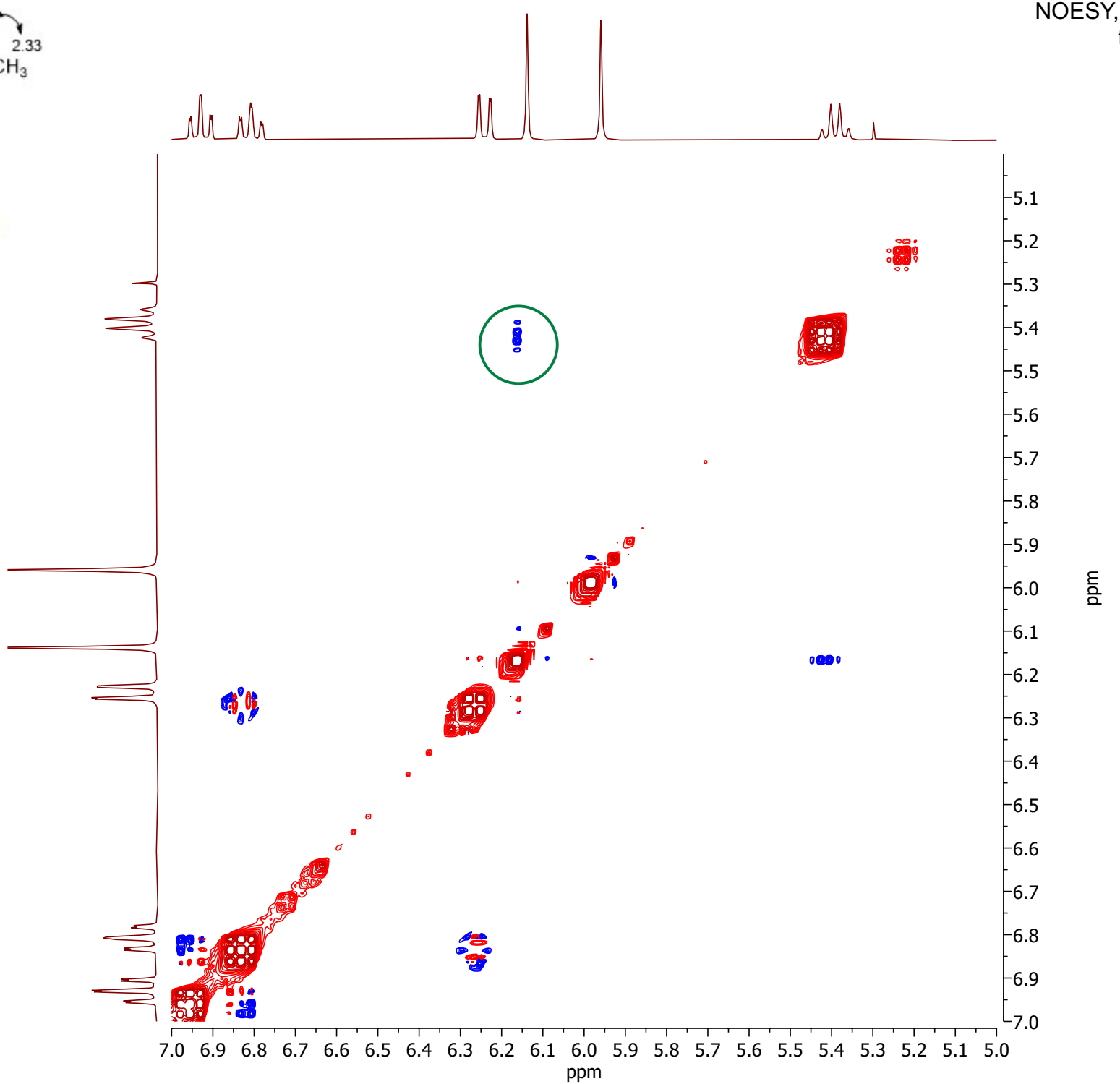
NOESY, 300 MHz, $CDCl_3$
tmix = 1s

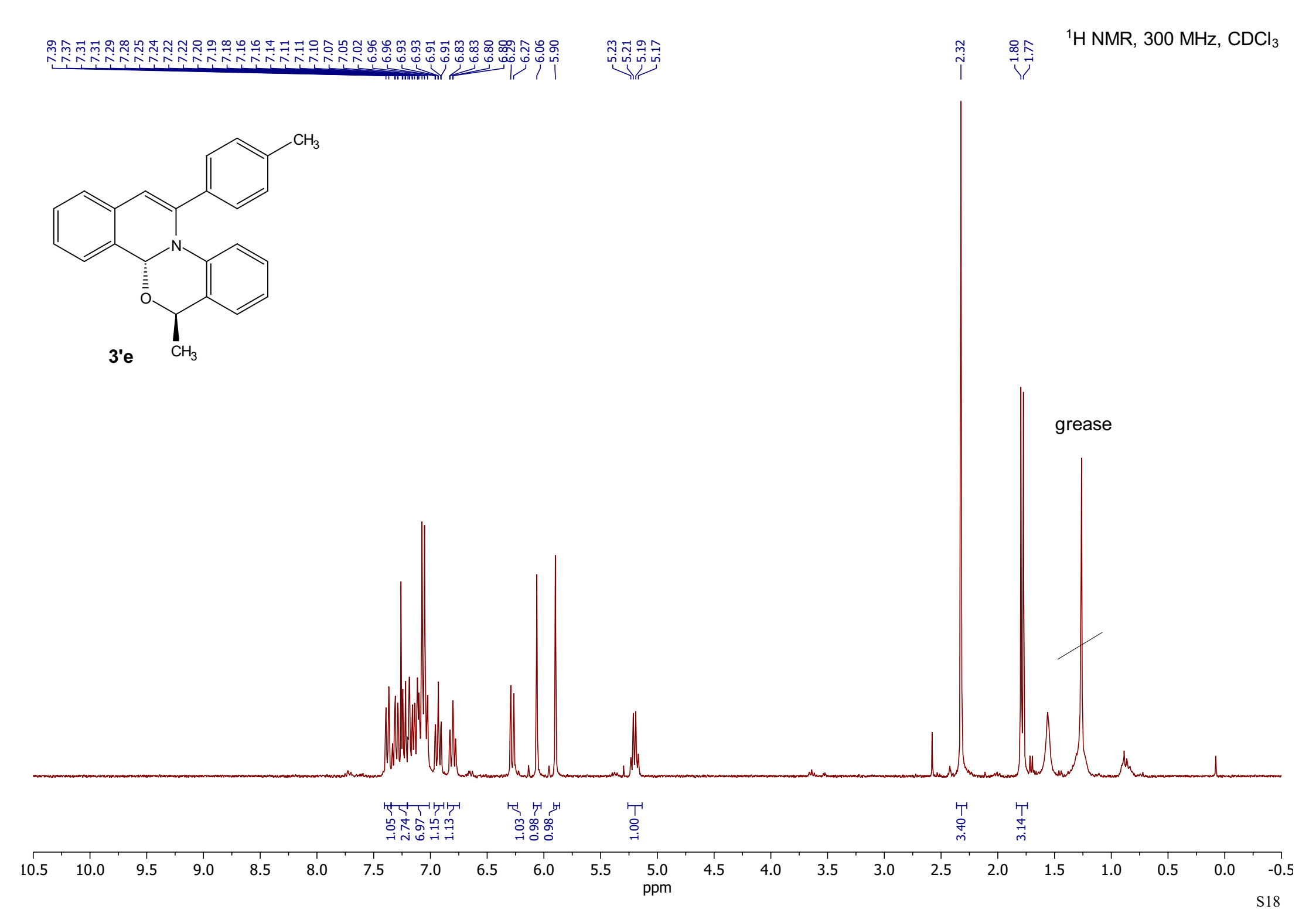




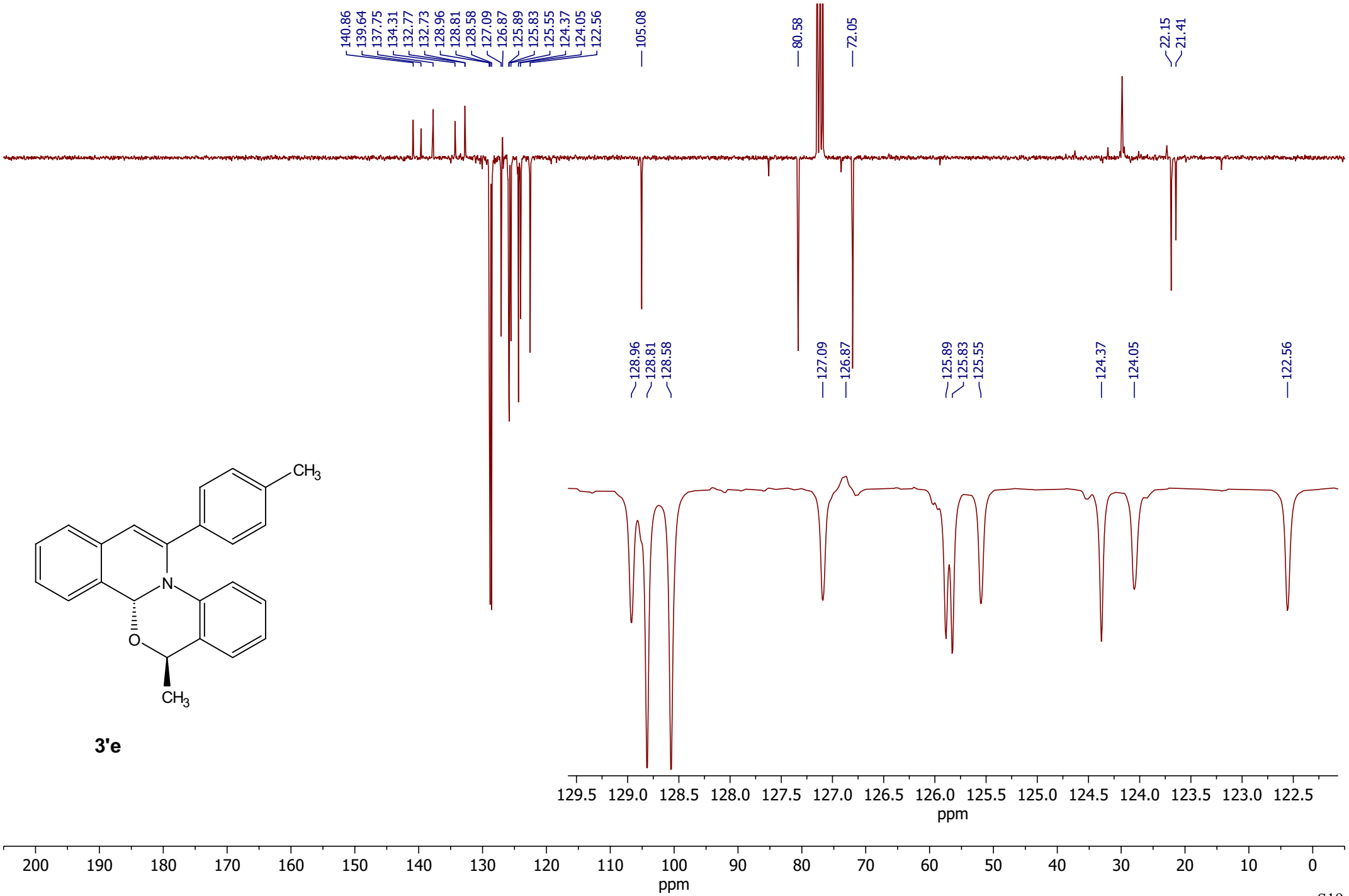
3e

NOESY, 300 MHz, $CDCl_3$
tmix = 1s

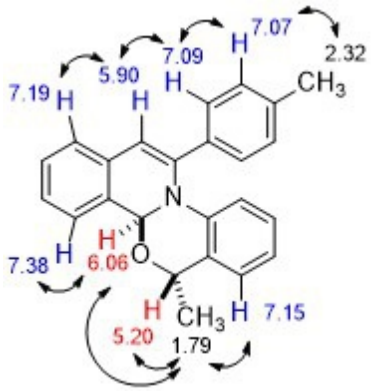



^{1}H NMR, 300 MHz, $CDCl_3$
7.39 7.37 7.31 7.31 7.29 7.28 7.25 7.24 7.22 7.22 7.20 7.19 7.18 7.16 7.16 7.14 7.11 7.11 7.10 7.07 7.05 7.02 6.96 6.96 6.93 6.93 6.91 6.91 6.83 6.83 6.80 6.80 6.29 6.27 6.06 5.90
5.23 5.21 5.19 5.17
2.32
1.80 1.77
CH3
N
O
CH3
3'e
grease
1.05 2.74 6.97 1.15 1.13 1.03 0.98 0.98 1.00 3.40 3.14
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
ppm

^{13}C NMR, 75 MHz, $CDCl_3$

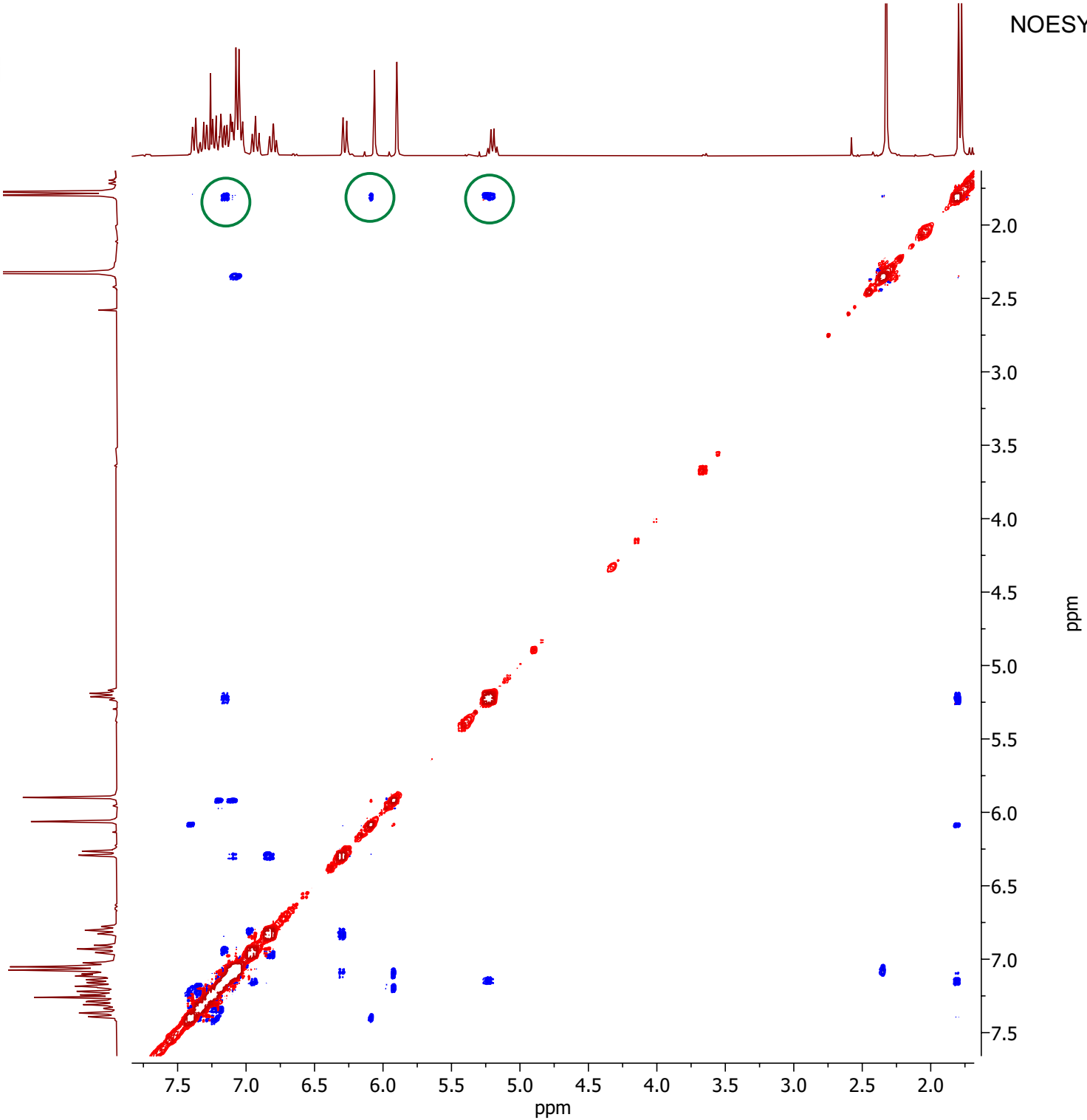


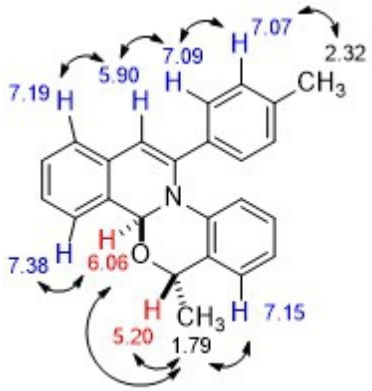
3'e



3'e

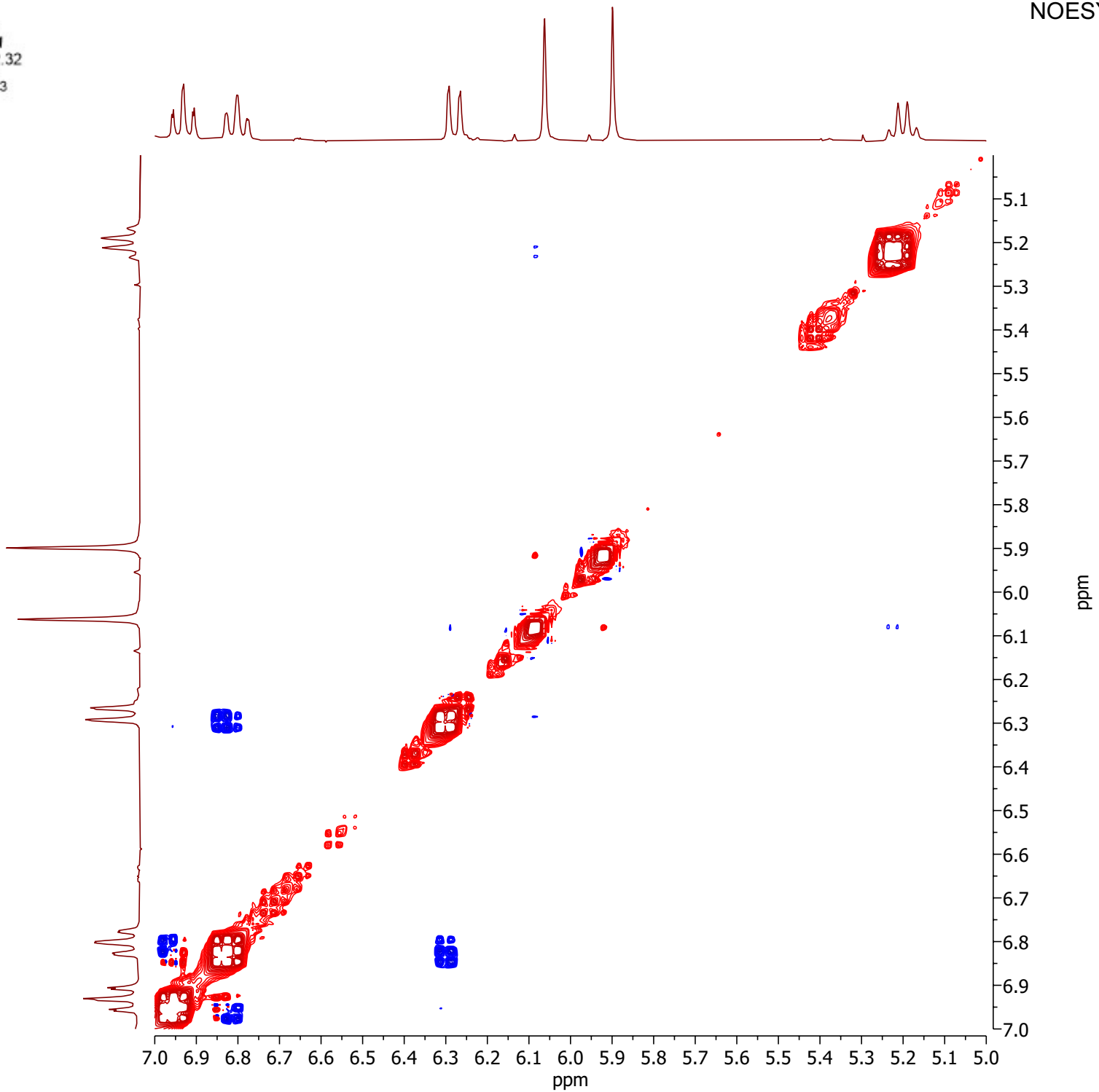
NOESY, 300 MHz, $CDCl_3$
tmix = 1s



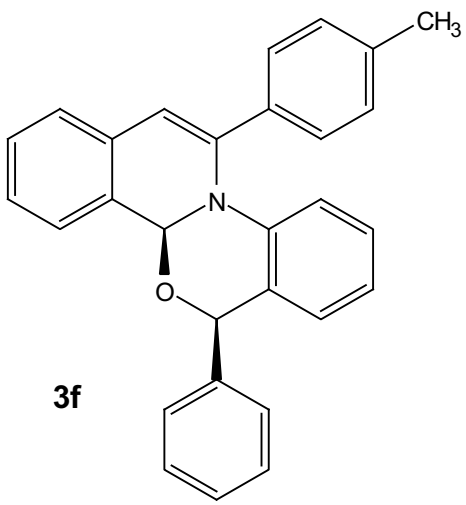


3'e

NOESY, 300 MHz, $CDCl_3$
tmix = 1s



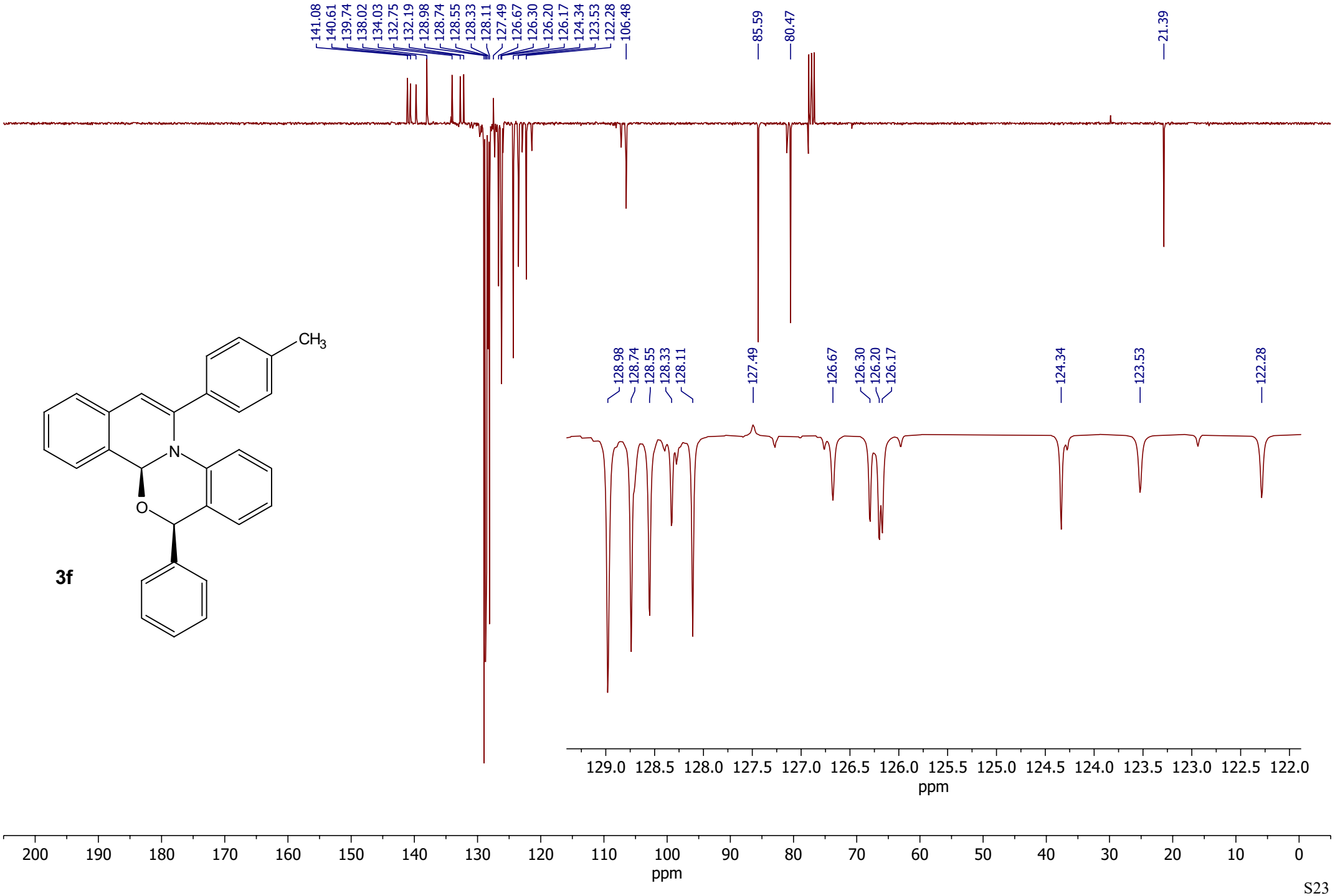
^{1}H NMR, 300 MHz, $CDCl_3$

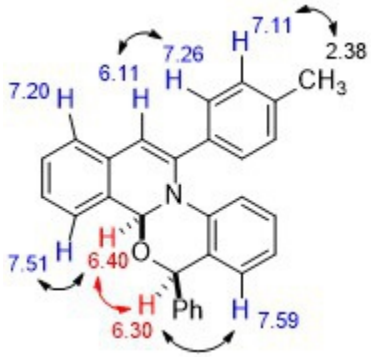


3f

13C NMR, 75 MHz, $CDCl_3$

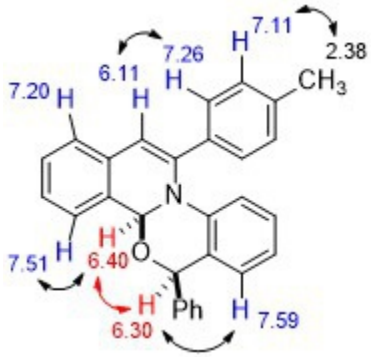
^{13}C NMR, 75 MHz, $CDCl_3$





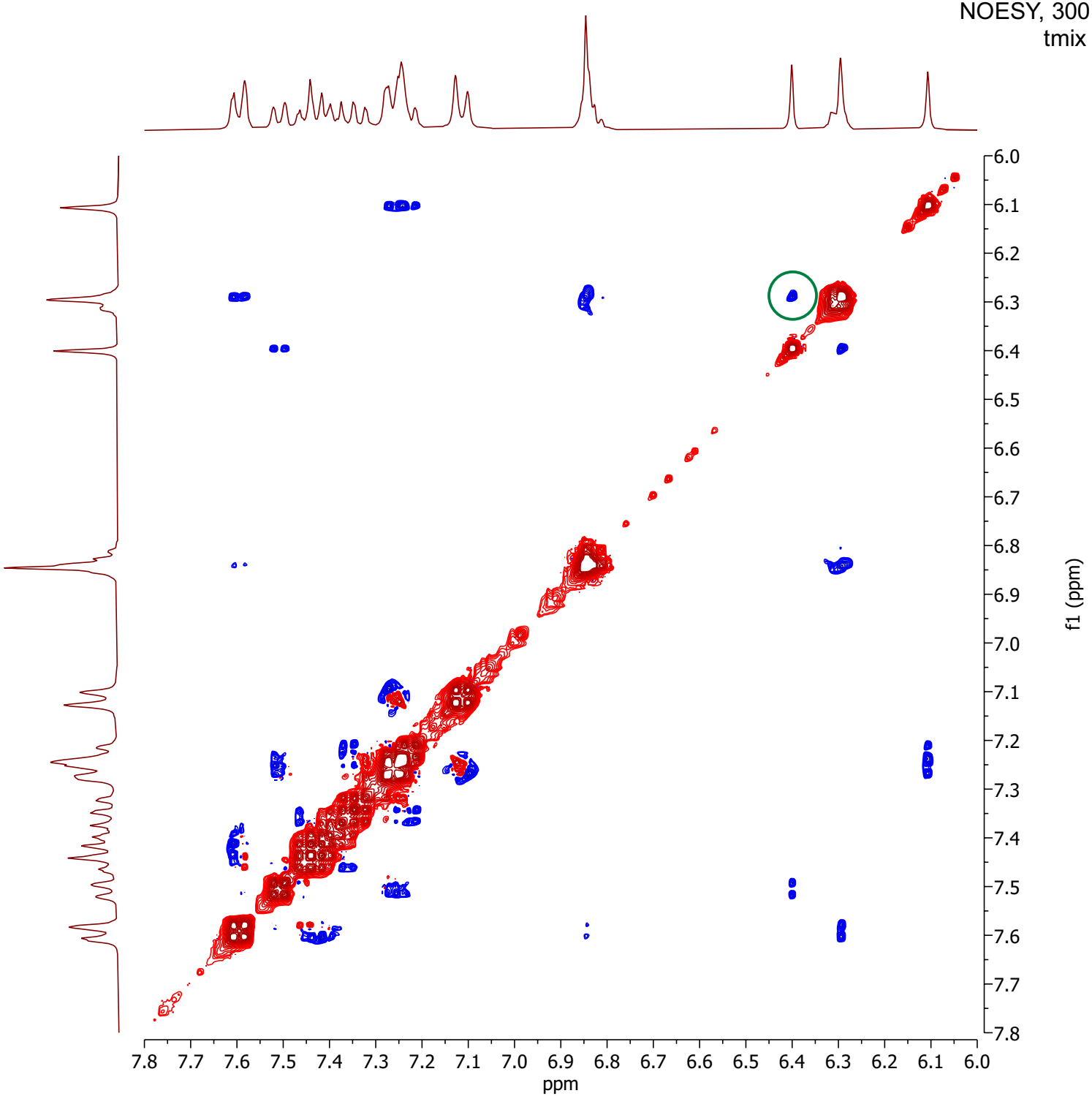
3f

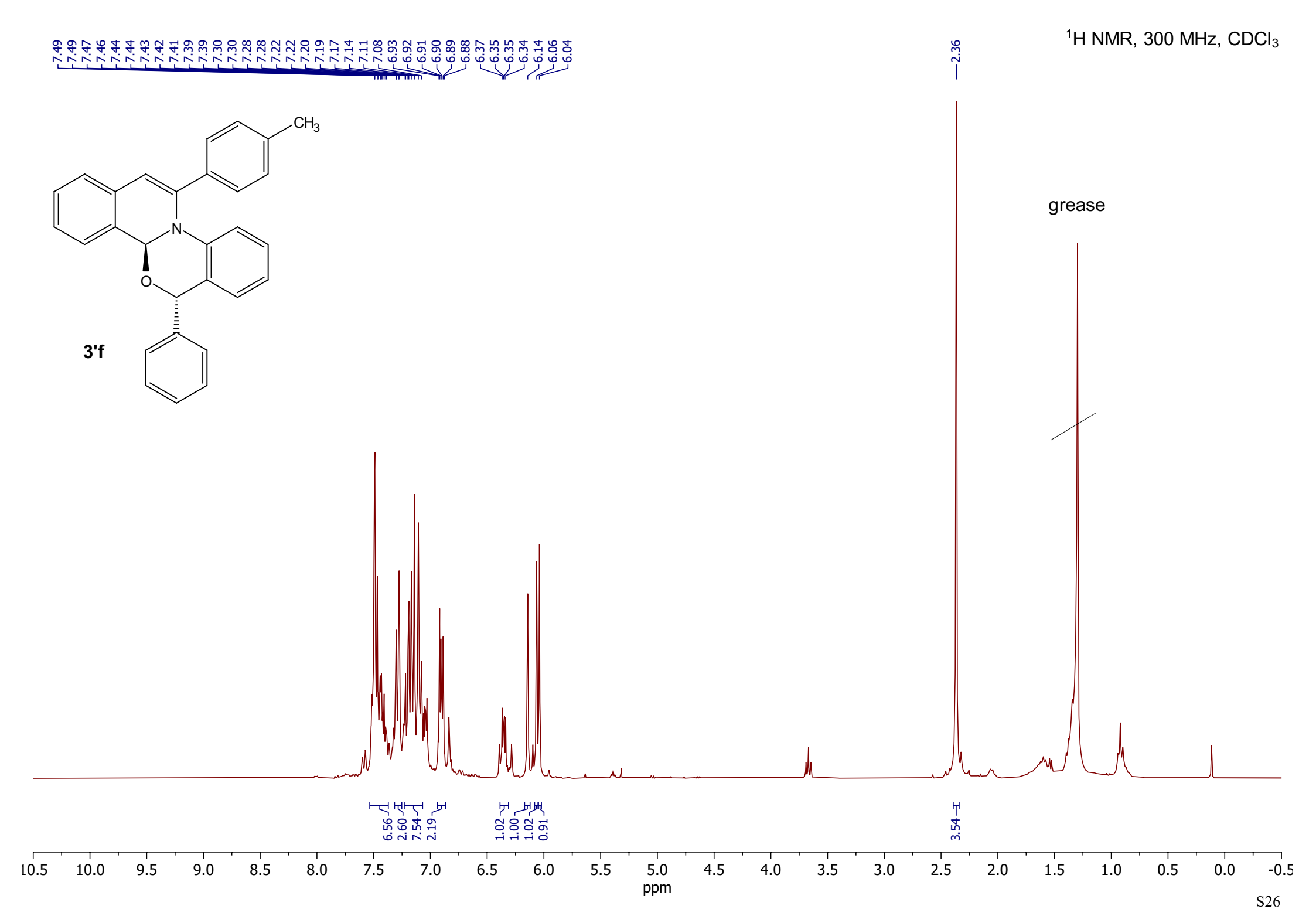
NOESY, 300 MHz, $CDCl_3$
tmix = 1s



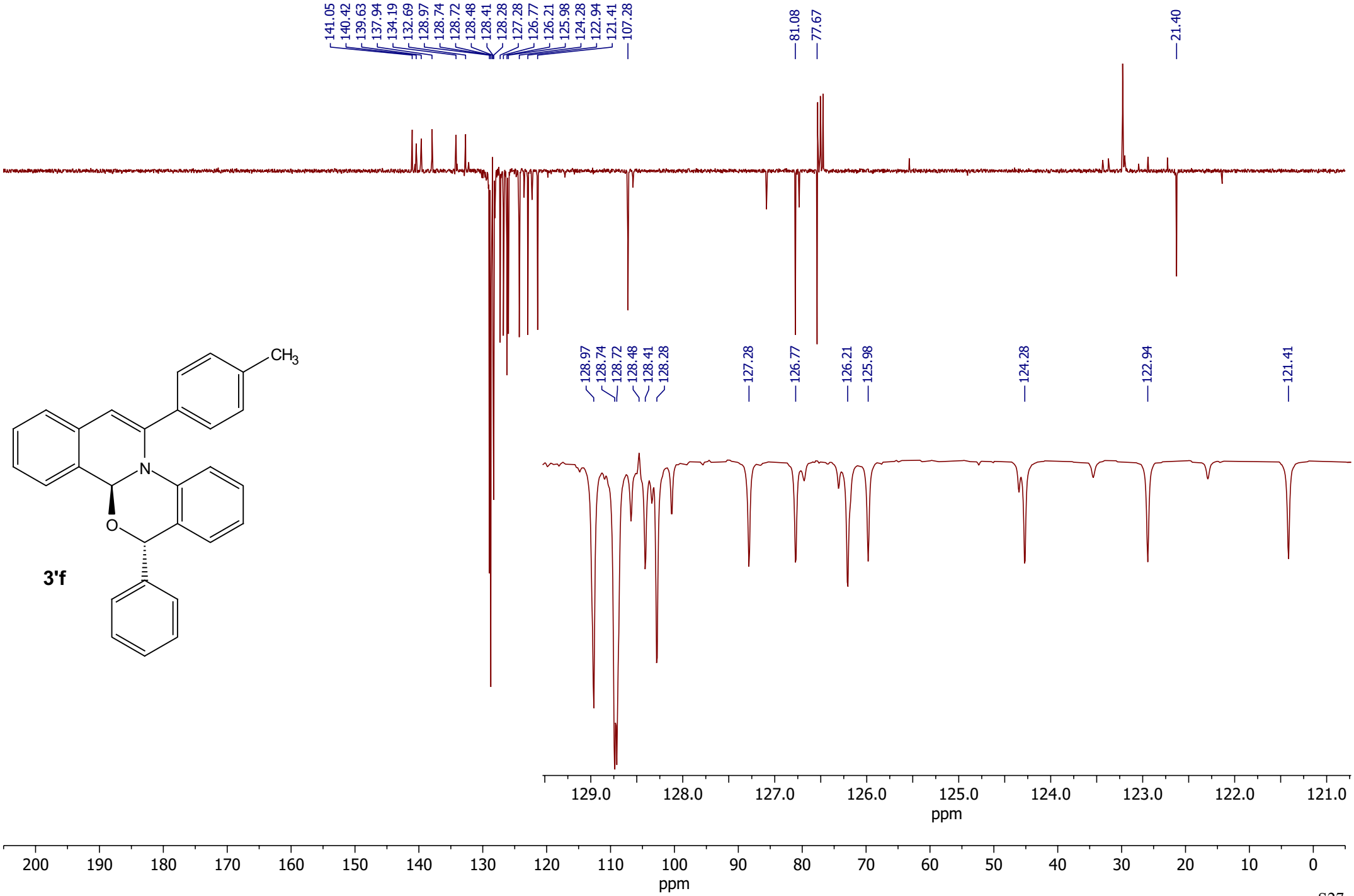
3f

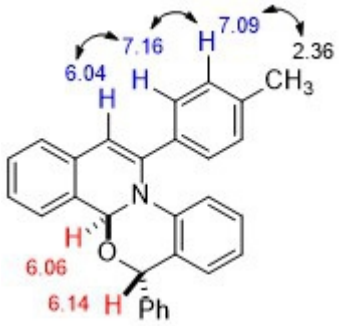
NOESY, 300 MHz, $CDCl_3$
tmix = 1s




^{1}H NMR, 300 MHz, $CDCl_3$
7.49 7.49 7.47 7.46 7.44 7.44 7.43 7.42 7.41 7.39 7.39 7.30 7.30 7.28 7.28 7.22 7.22 7.20 7.19 7.17 7.14 7.11 7.08 6.93 6.92 6.91 6.90 6.89 6.88 6.37 6.35 6.35 6.34 6.14 6.06 6.04
2.36
CH_3
N
O
3'f
grease
6.56 2.60 7.54 2.19 1.02 1.00 1.02 0.91 3.54
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
ppm

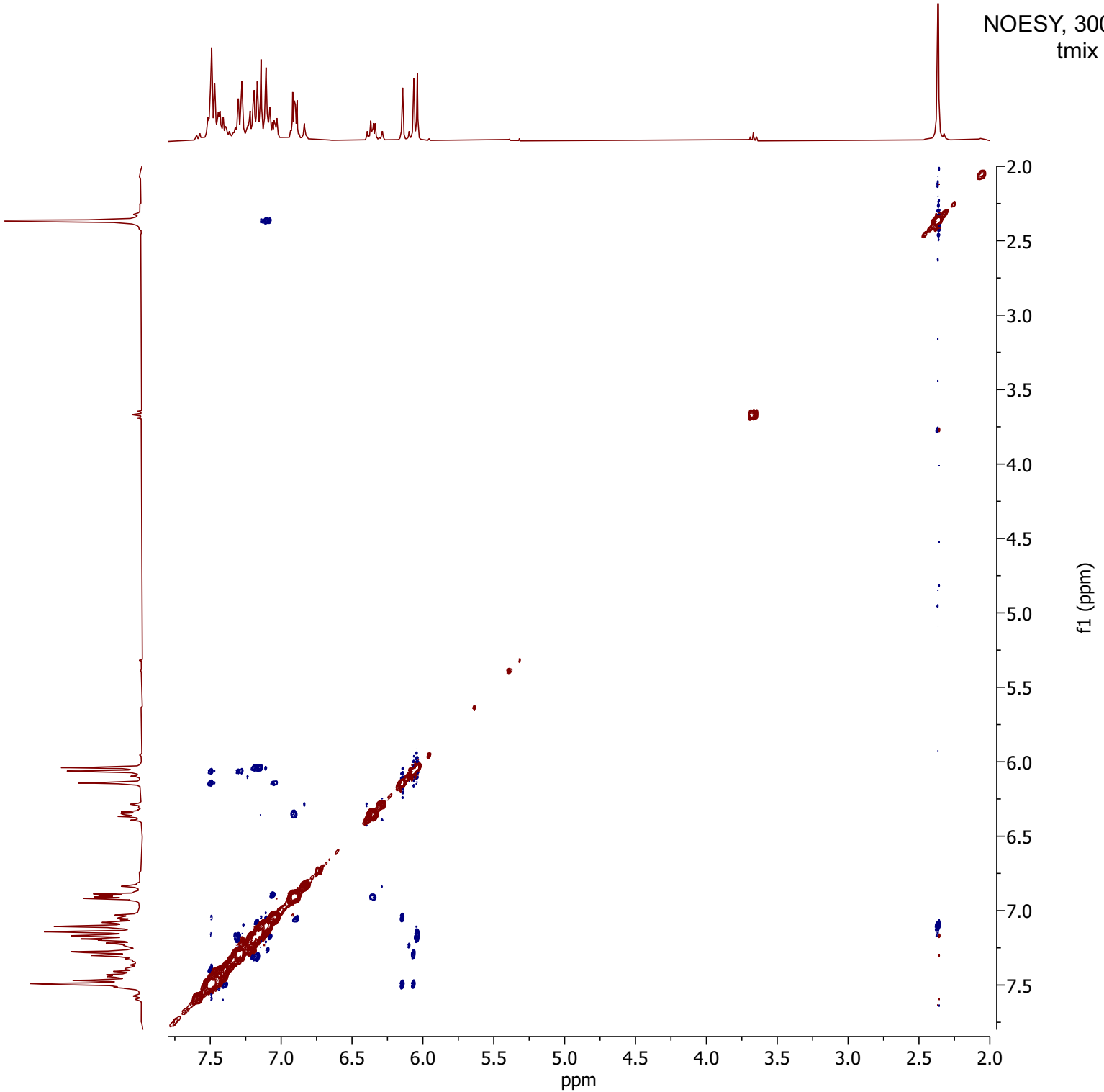
^{13}C NMR, 75 MHz, $CDCl_3$

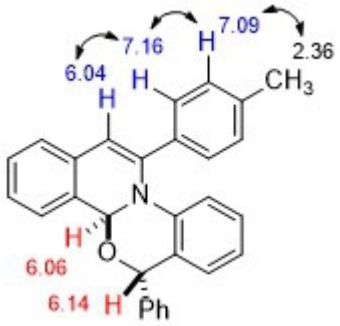




3'f

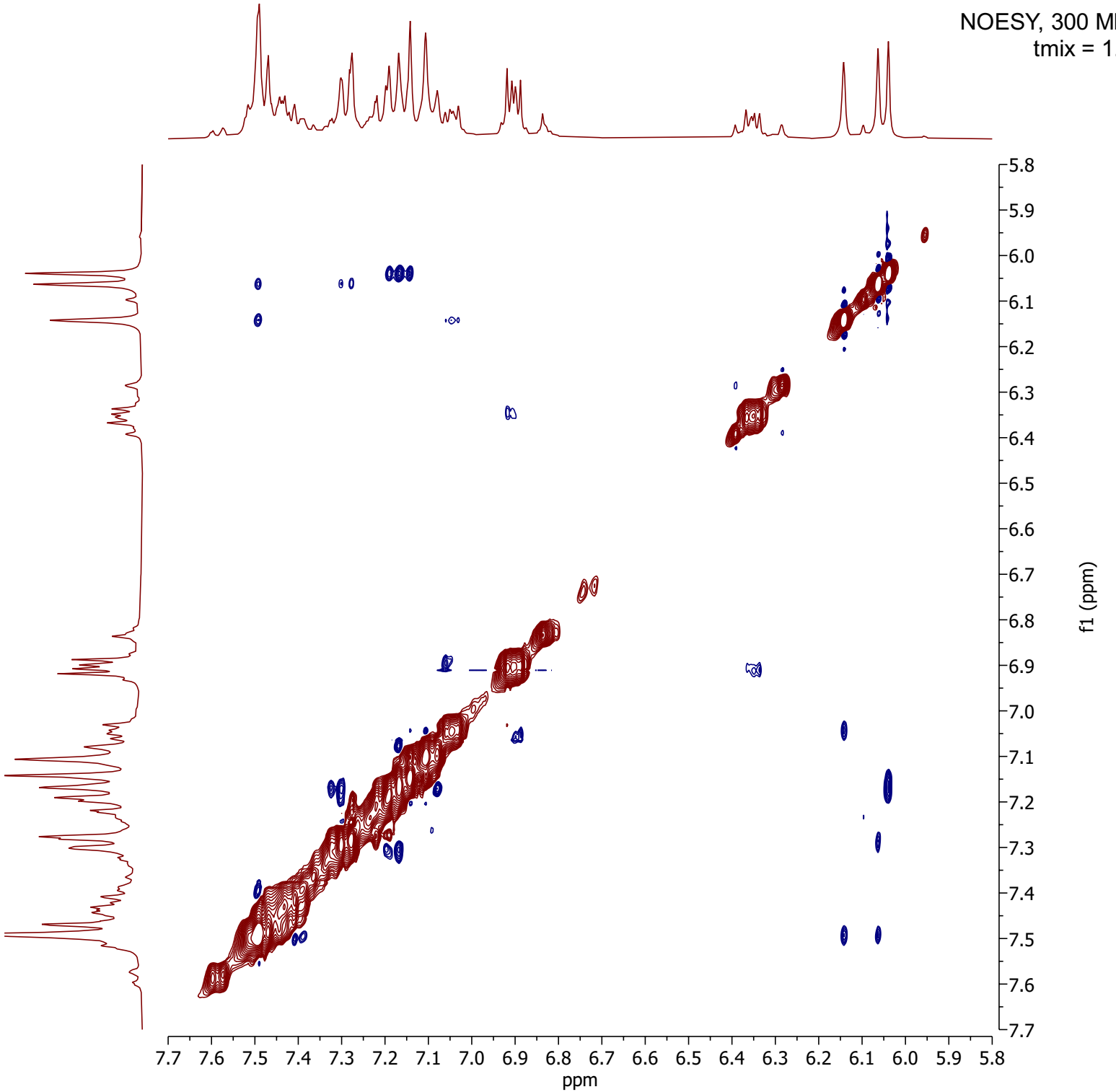
NOESY, 300 MHz, $CDCl_3$
tmix = 1.3s



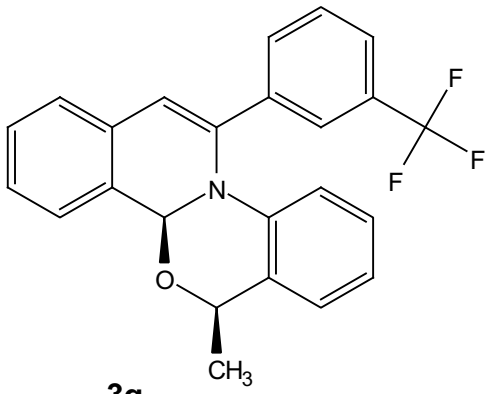


3'f

NOESY, 300 MHz, $CDCl_3$
tmix = 1.3s

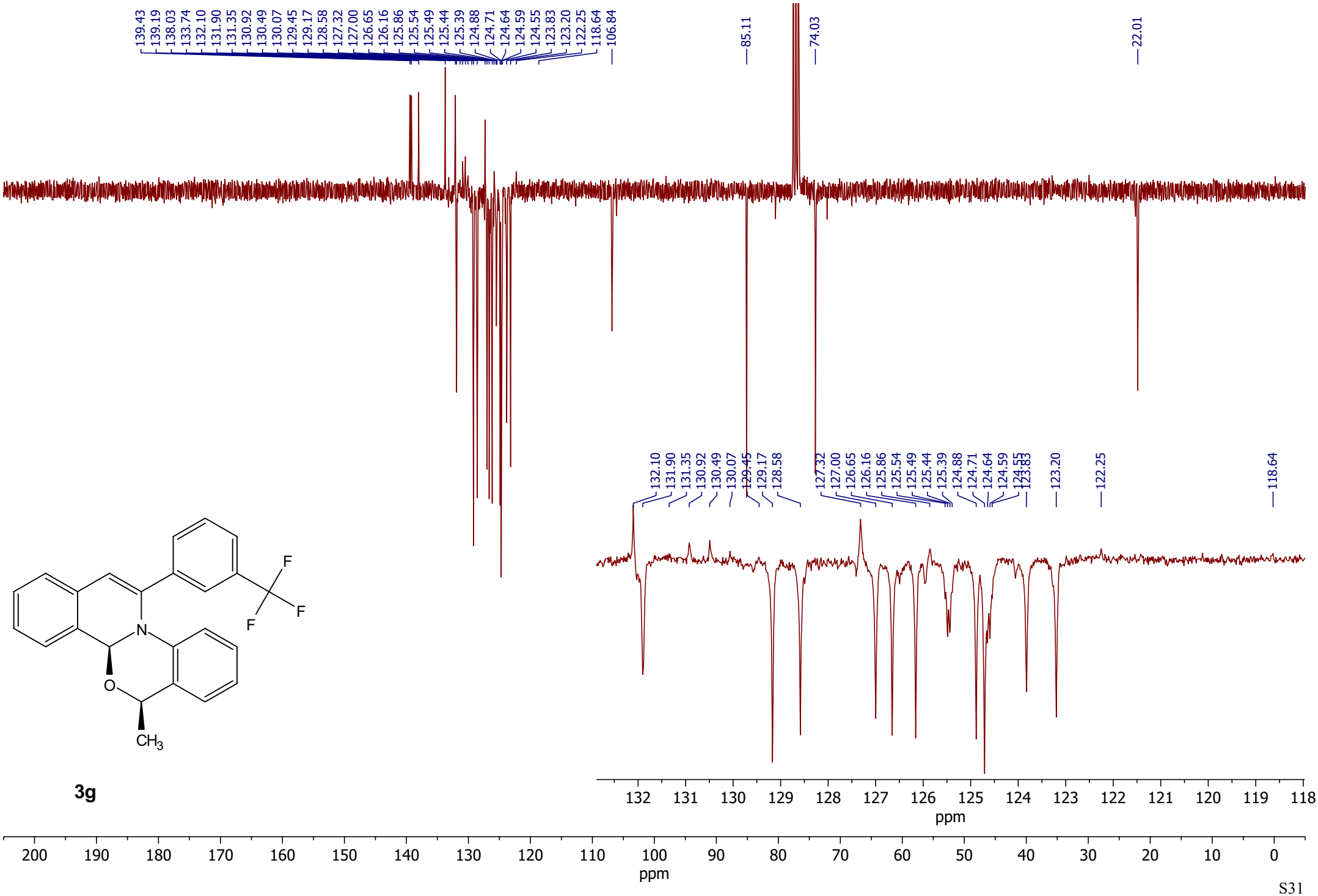


^{1}H NMR, 300 MHz, $CDCl_3$

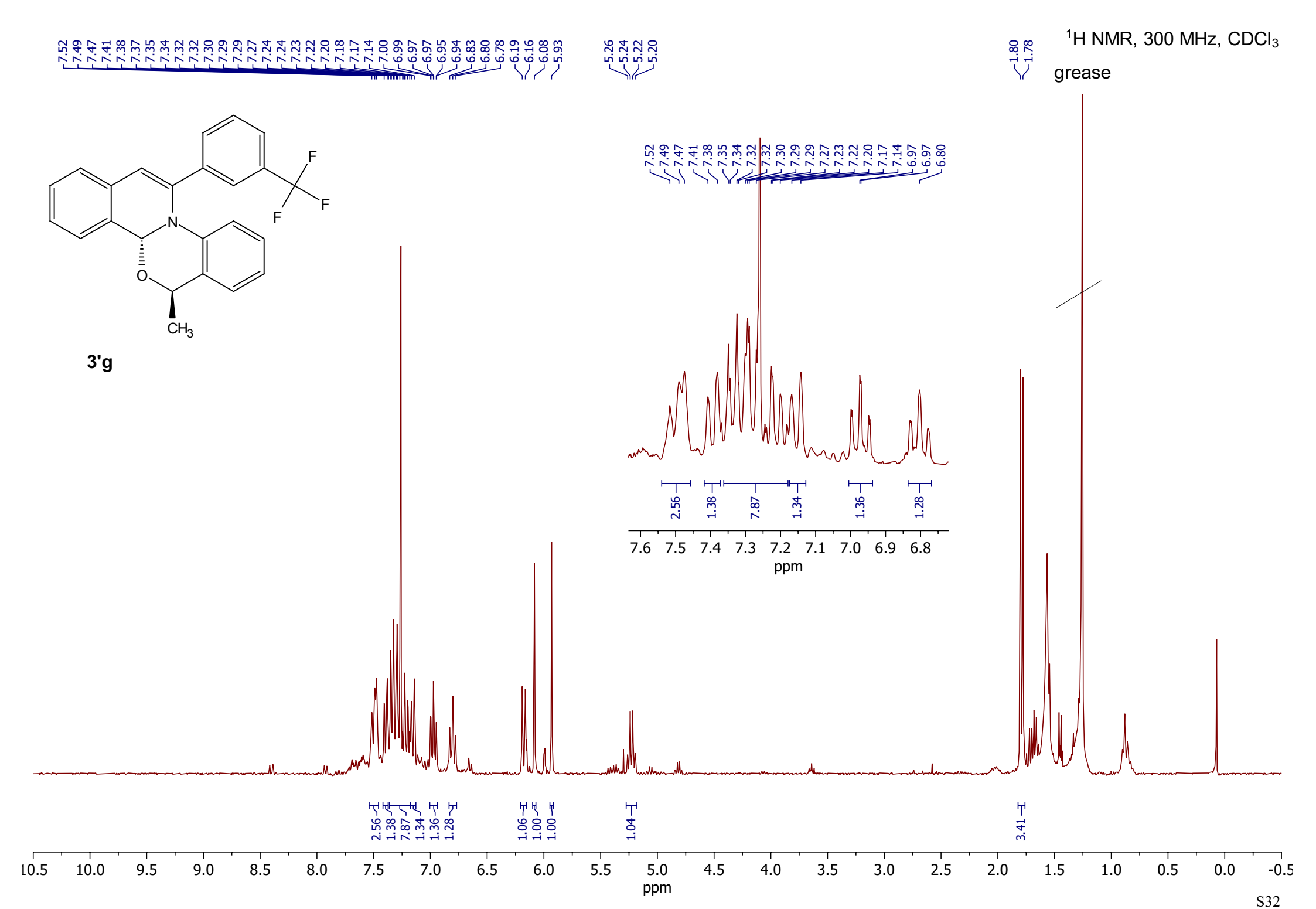


3g

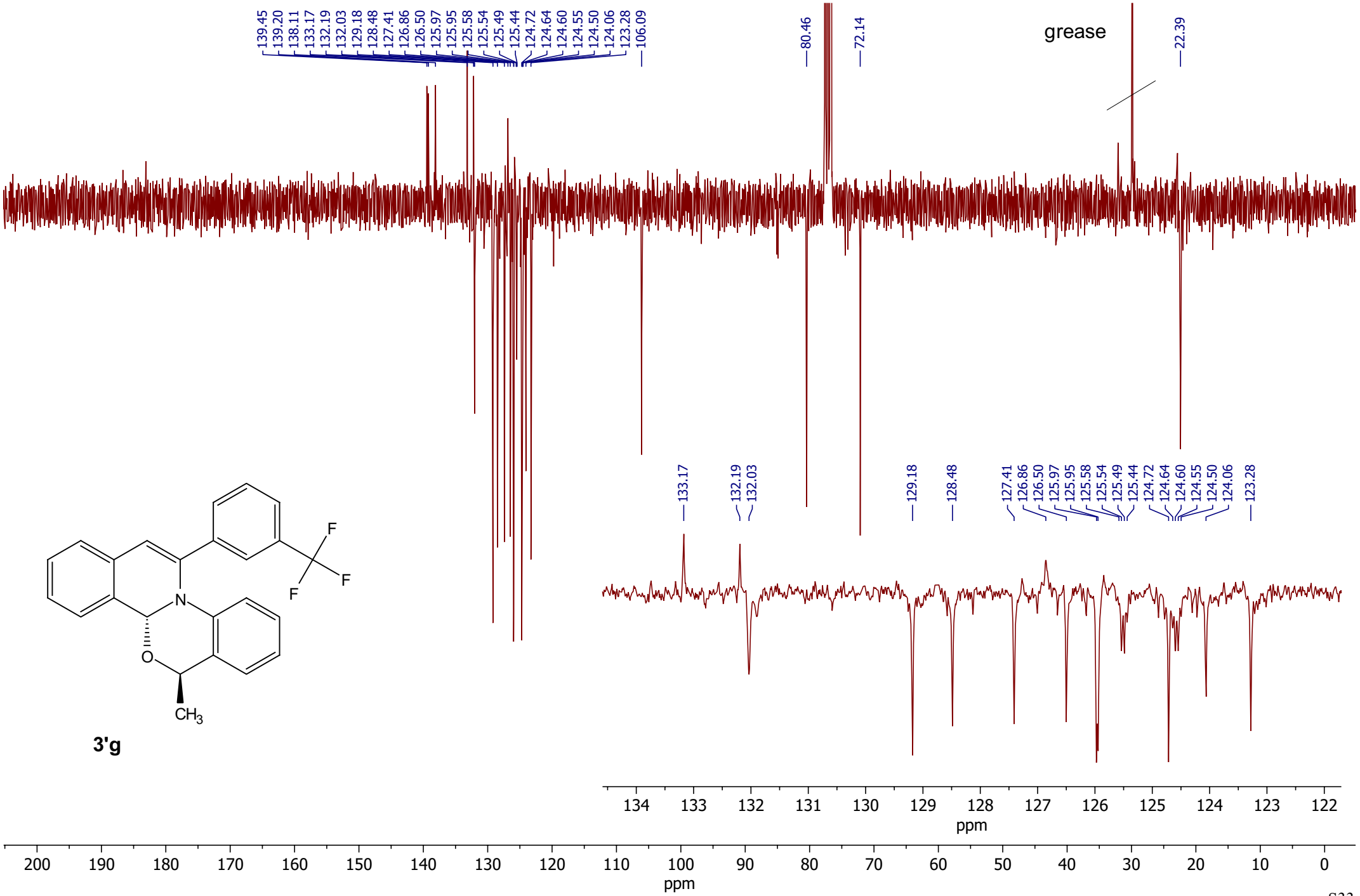
^{13}C NMR, 75 MHz, $CDCl_3$



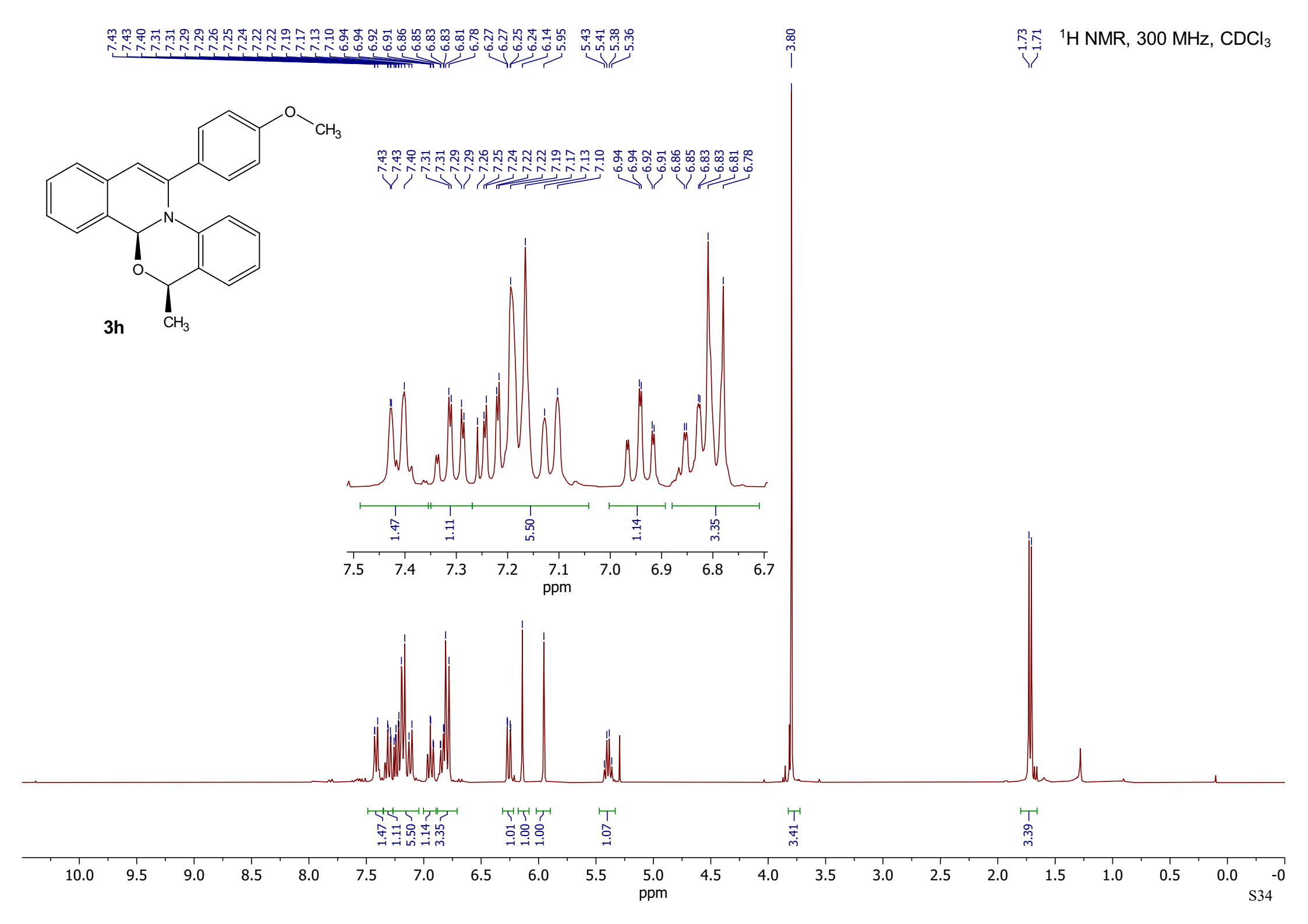
3g


^{1}H NMR, 300 MHz, $CDCl_3$
grease
3'g
F
F
F
N
O
CH_3
ppm

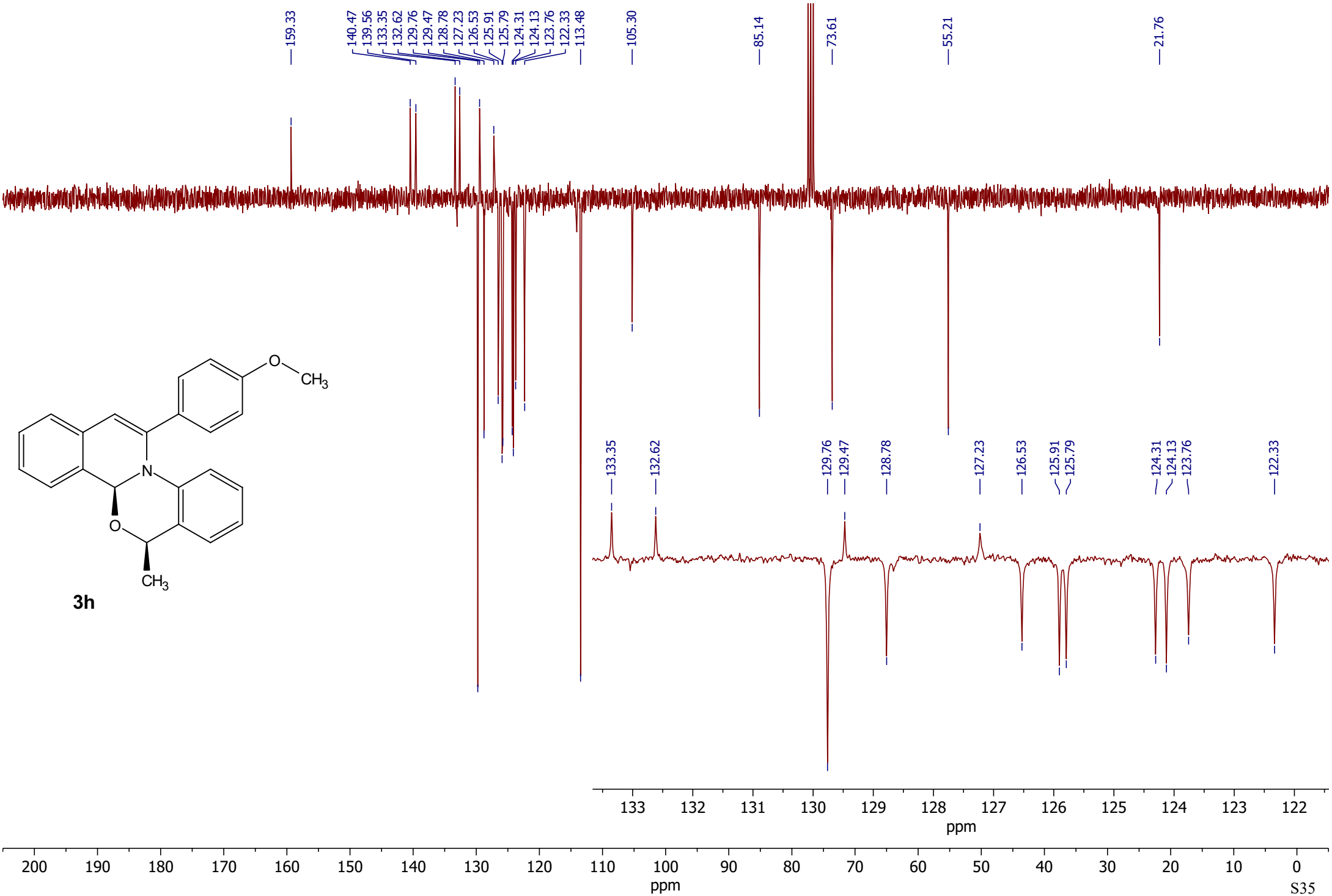
^{13}C NMR, 75 MHz, $CDCl_3$

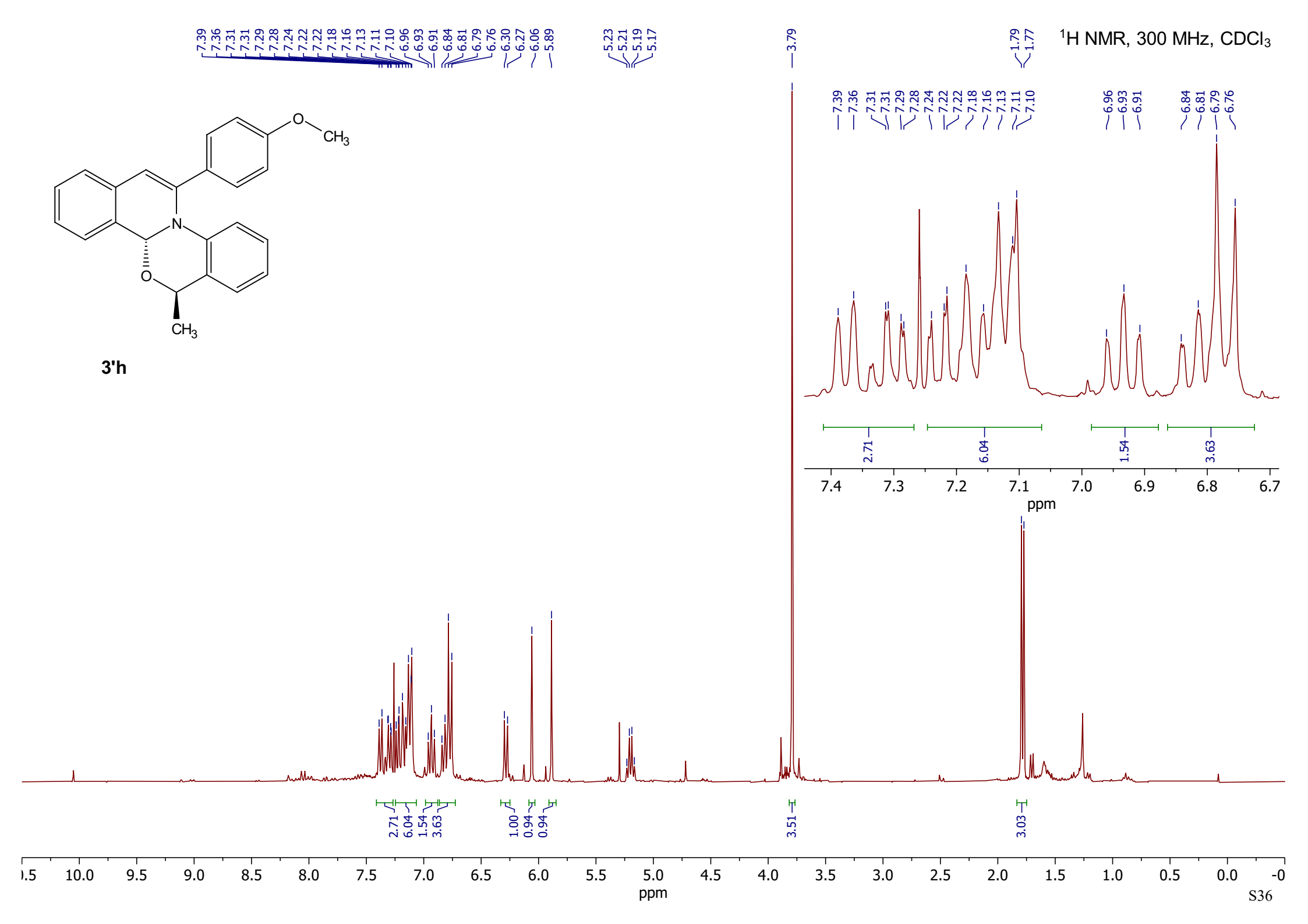


3'g

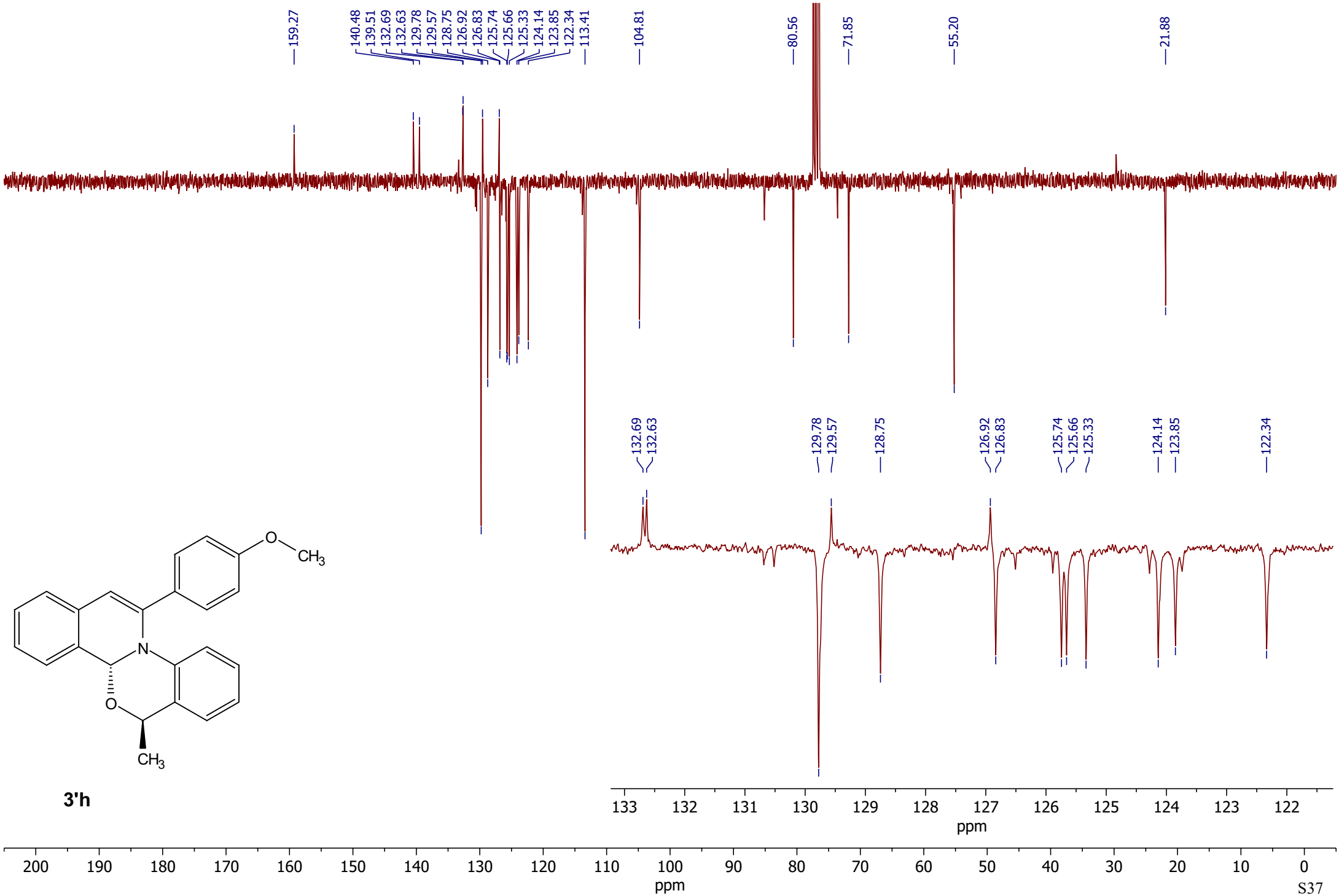

^{1}H NMR, 300 MHz, $CDCl_3$
3h
ppm
S34

^{13}C NMR, 75 MHz, $CDCl_3$

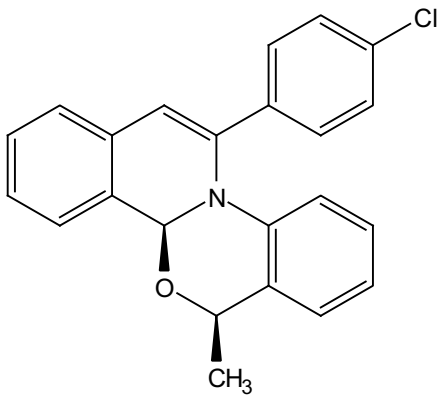



^{1}H NMR, 300 MHz, $CDCl_3$
7.39 7.36 7.31 7.31 7.29 7.28 7.24 7.22 7.22 7.18 7.16 7.13 7.11 7.10 6.96 6.93 6.91 6.84 6.81 6.79 6.76 6.30 6.27 6.06 5.89 5.23 5.21 5.19 5.17 3.79 1.79 1.77
O
CH3
N
O
CH3
3'h
2.71 6.04 1.54 3.63
7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7
ppm
1.00 0.94 0.94 3.51 3.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
ppm

^{13}C NMR, 75 MHz, $CDCl_3$

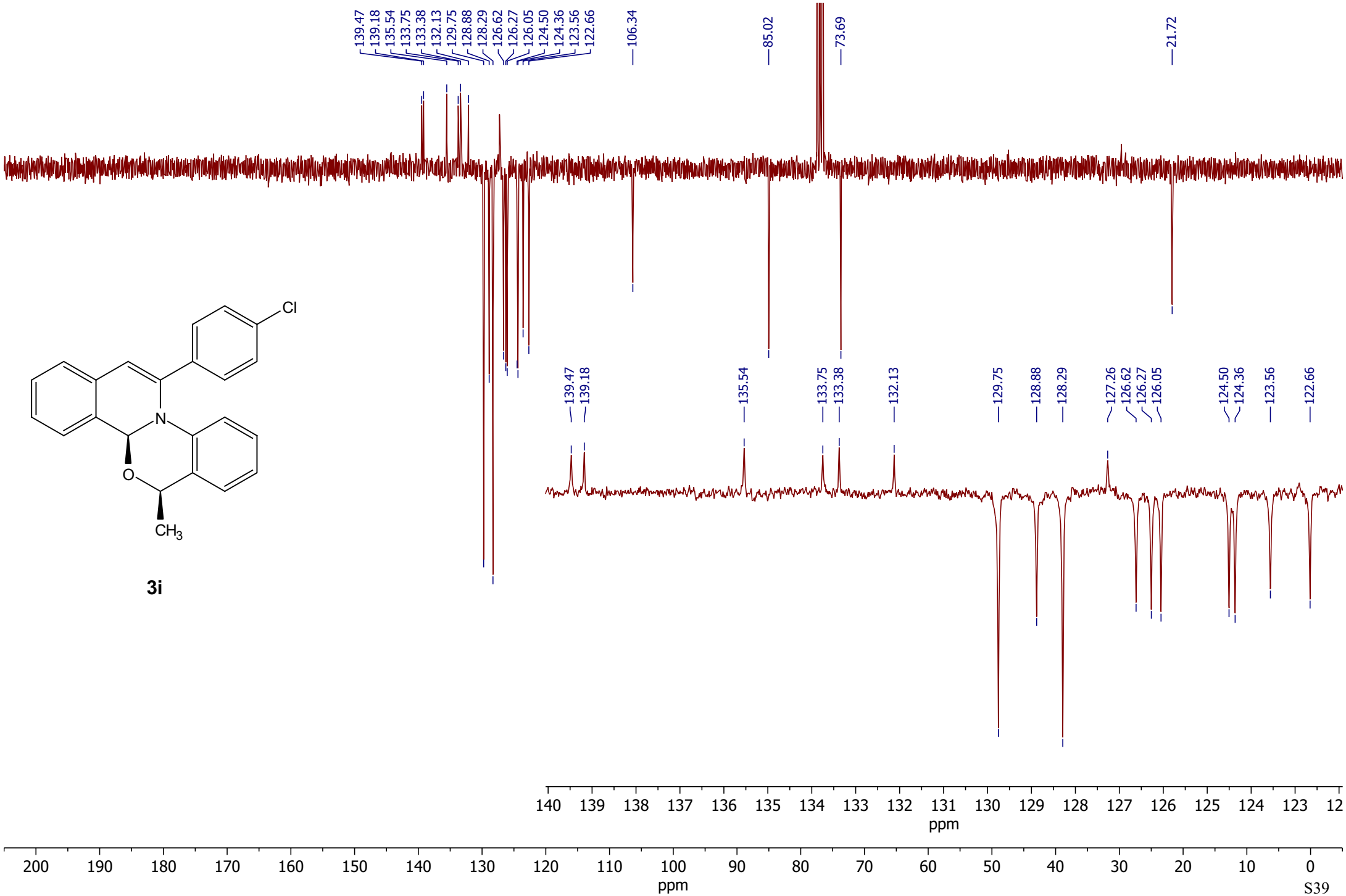


^{1}H NMR, 300 MHz, $CDCl_3$

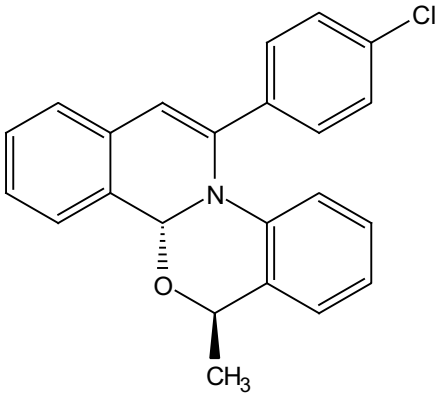


3i

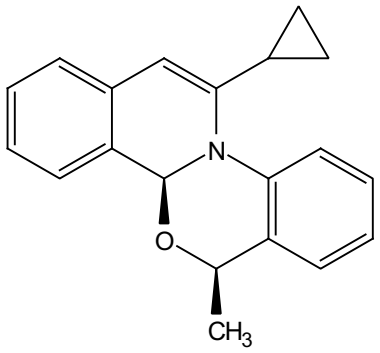
^{13}C NMR, 75 MHz, $CDCl_3$



^{1}H NMR, 300 MHz, $CDCl_3$



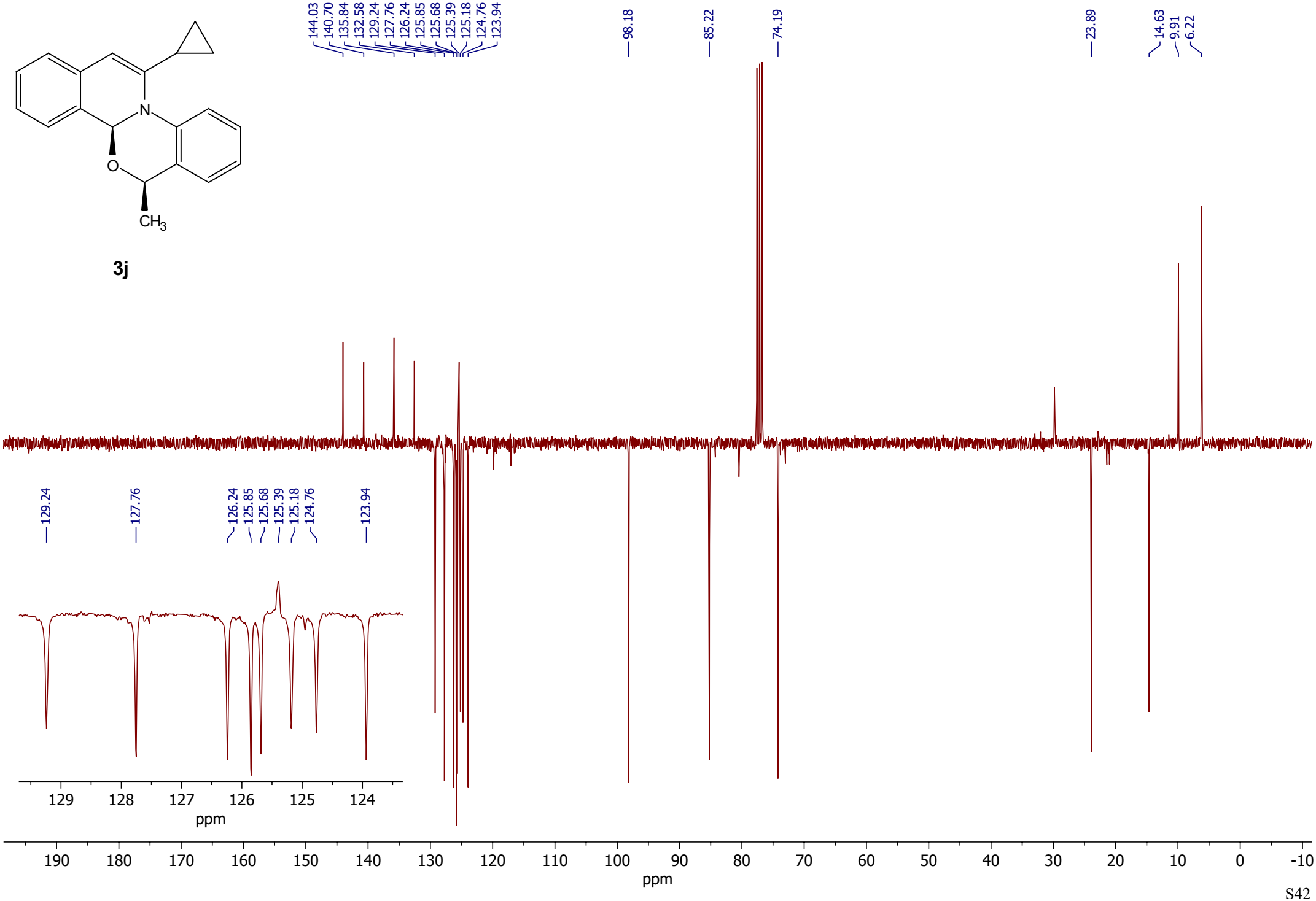
3'i



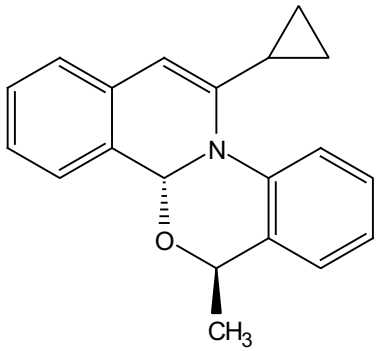
3j

^{13}C NMR, 75 MHz, $CDCl_3$

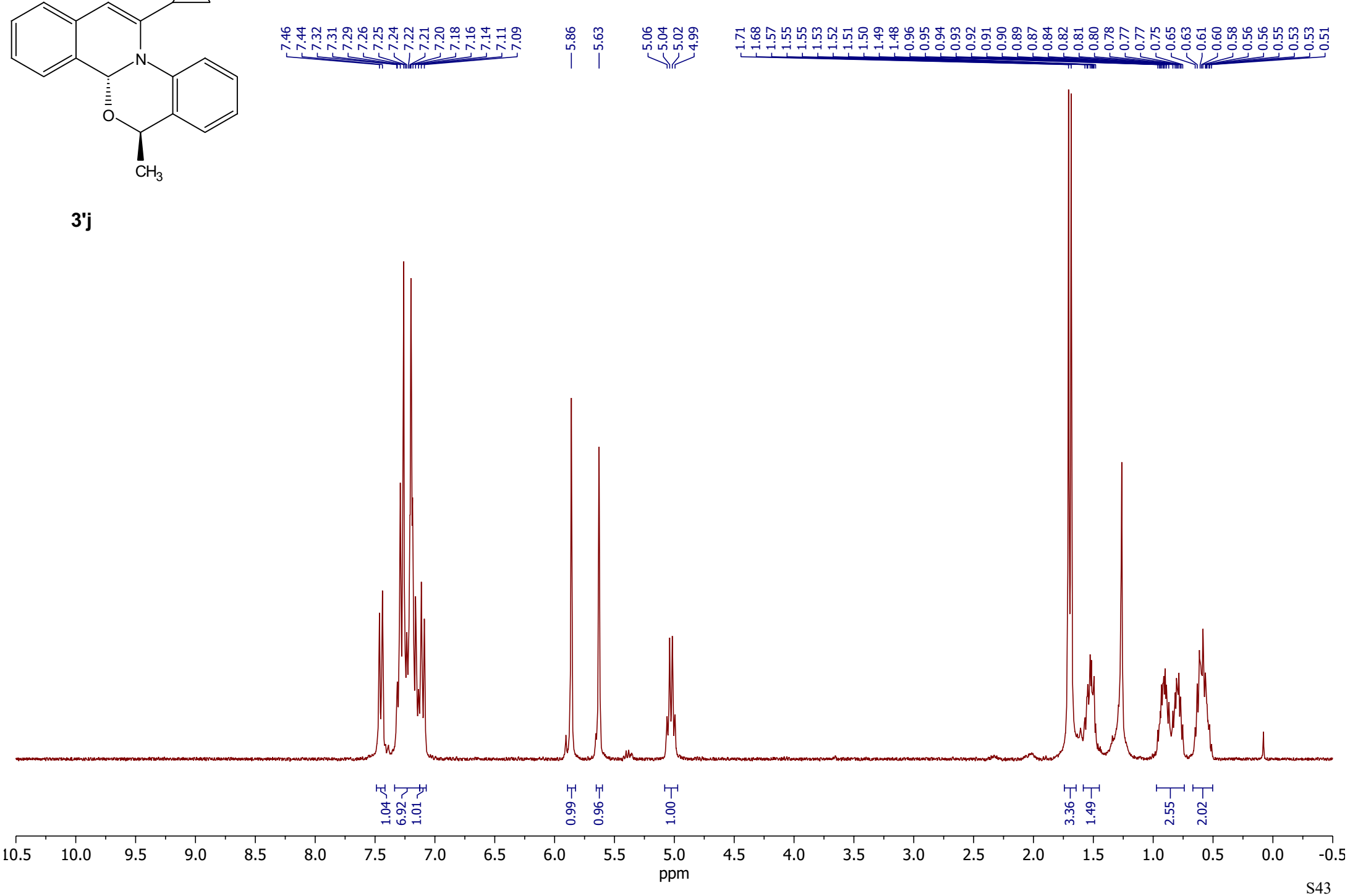
3j

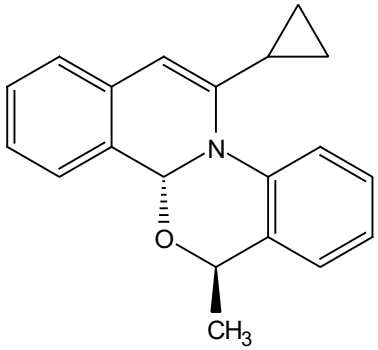


^{1}H NMR, 300 MHz, $CDCl_3$



3'j





3'j

143.73
140.80
135.20
132.70
129.18
127.91
126.19
126.02
125.90
125.24
125.19
124.59
123.85
97.94
80.92
71.57
22.96
14.70
10.33
6.05

129.18
127.91
126.19
126.02
125.90
125.24
125.19
124.59
123.85

129 128 127 126 125 124
ppm

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

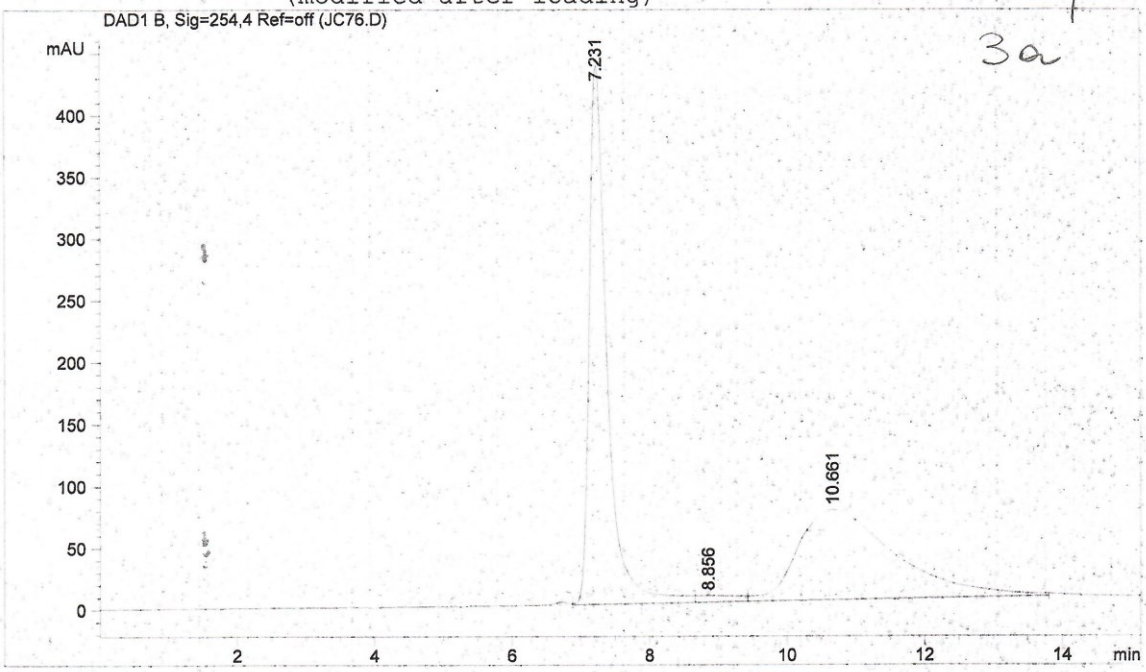
Data File C:\HPCHEM\1\DATA\JC76.D Sample Name: jc76 10ipa dea

amy 2

==========

Injection Date : 04/06/18 9.41.31
Sample Name : jc76 10ipa dea Vial : 1
Acq. Operator : 1
Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed : 04/06/18 9.34.42 by 1
(modified after loading)

TABLE 3 Entry 1
3a



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Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %	
1	7.231	VV	0.2714	7893.33594	435.56964	51.4545	52%
2	8.856	VV	0.5236	227.53470	5.40026	1.4832	
3	10.661	VB	1.4147	7219.55859	72.94357	47.0623	48%
Totals :				1.53404e4	513.91347		

98.51

Results obtained with enhanced integrator!

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*** End of Report ***

Instrument 1 04/06/18 9.57.24 1 Page 1 of 1

Data File C:\HPCHEM\1\DATA\JC78.D Sample Name: 78

amy2 10ipa dea

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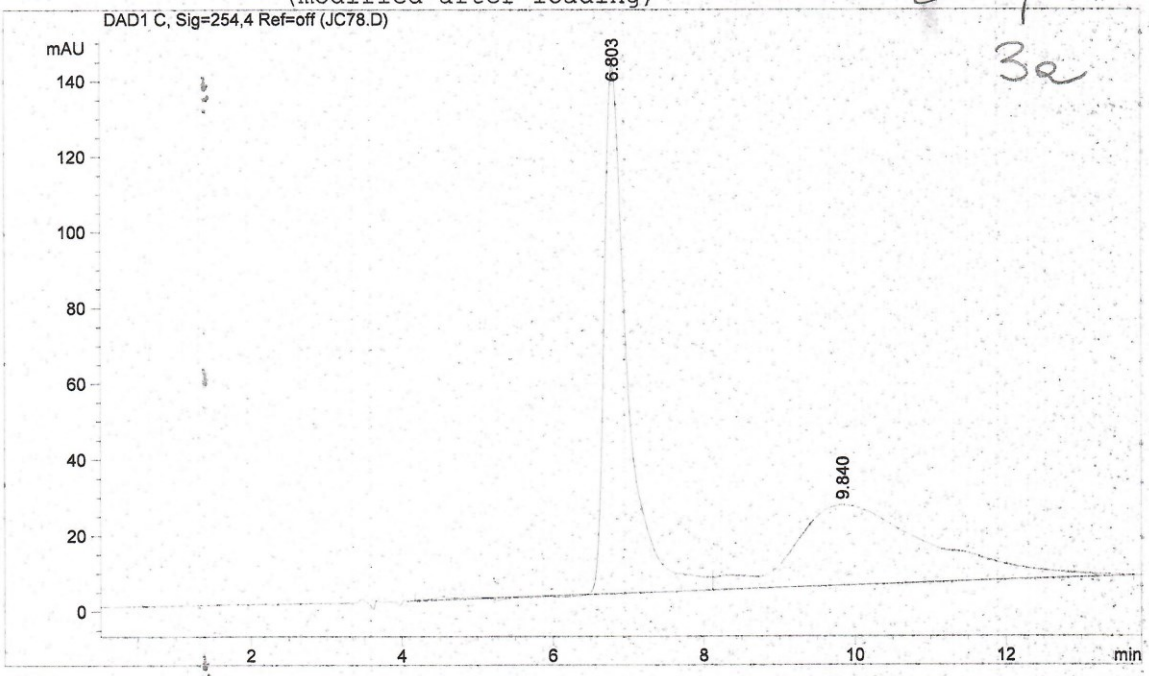
Injection Date : 15/06/18 14.18.07
Sample Name : 78 Vial : 1
Acq. Operator : 1
Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed : 15/06/18 14.14.57 by 1
(modified after loading)

TABLE 3 Entry 2
3a



==========

Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 C, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.803	PB	0.3159	2983.44092	138.19337	52.3626
2	9.840	BB	1.8506	2714.21069	21.35872	47.6374
Totals :				5697.65161	159.55210	

Results obtained with enhanced integrator!

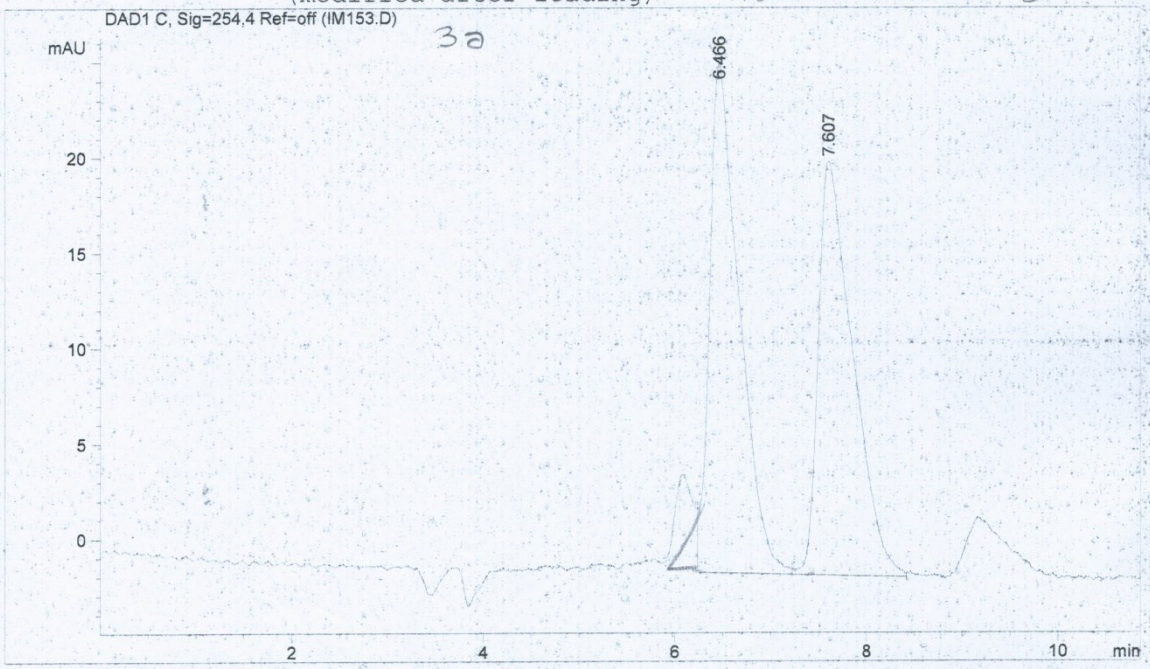
==========

*** End of Report ***

Instrument 1 15/06/18 14.32.55 1 Page 1 of 1

Data File C:\HPCHEM\1\DATA\IM153.D Sample Name: im153 ad 25ipade

Injection Date : 09/10/19 14.30.04
Sample Name : im153 ad 25ipade Vial : 1
Acq. Operator : 1
Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed : 09/10/19 14.28.26 by 1
(modified after loading) TABLE 3 ENTRY 3



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 C, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.466	VV	0.3078	576.03357	26.69318	51.3411 52
2	7.607	VV	0.3575	545.94073	21.69959	48.6589 48
Totals :				1121.97430	48.39278	

Results obtained with enhanced integrator!

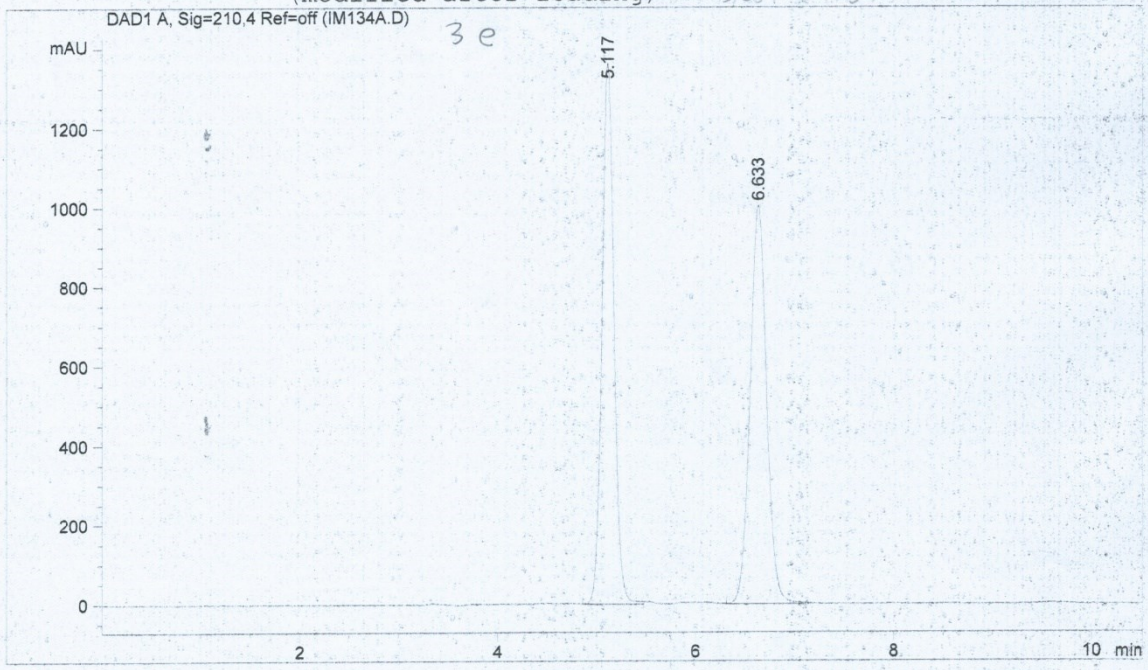
*** End of Report ***

Instrument 1 09/10/19 14.41.52 1 Page 1 of 1

Data File C:\HPCHEM\1\DATA\IM134A.D Sample Name: im134a kr10ipa

fr3-6 0'8 ml-m

```
==========================================================================
Injection Date  : 27/06/19 11.46.32
Sample Name     : im134a kr10ipa                          Vial :   1
Acq. Operator   : 1
Acq. Method     : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 27/06/19 11.43.45  by 1
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 27/06/19 11.58.30  by 1
                  (modified after loading) TABLE 4 ENTRY 1
```



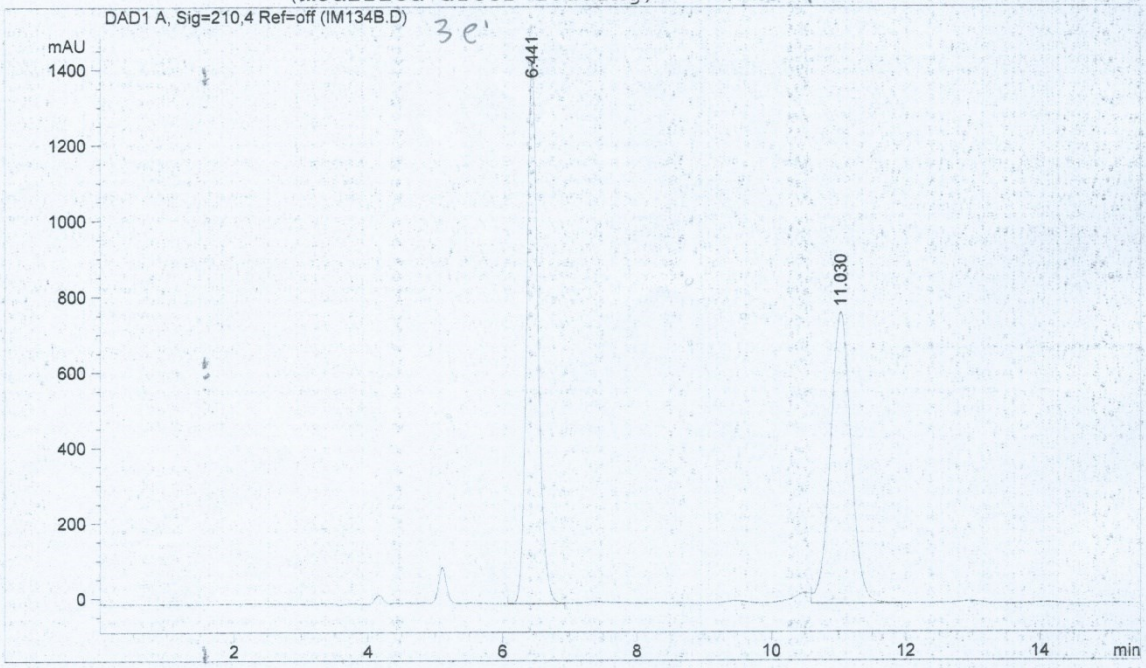

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.117 VV    0.1287 1.15327e4  1363.24573  49.6710
   2   6.633 VV    0.1757 1.16854e4  1004.92108  50.3290

Totals :                  2.32181e4  2368.16681

 Results obtained with enhanced integrator!
==========================================================================
                     *** End of Report ***

Instrument 1 27/06/19 11.58.36  1                        Page 1 of 1
```

Data File C:\HPCHEM\1\DATA\IM134B.D Sample Name: im134b kr10ipa

fr7-17 0'8 ml-m

==========

Injection Date : 27/06/19 14.09.38
Sample Name : im134b kr10ipa Vial : 1
Acq. Operator : 1
Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed : 27/06/19 12.18.47 by 1
(modified after loading) TABLE 4 ENTRY 1



==========

Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.441	VV	0.1709	1.68148e4	1433.14026	50.4507
2	11.030	VV	0.3176	1.65144e4	771.86340	49.5493

Totals : 3.33292e4 2205.00366

Results obtained with enhanced integrator!

==========

*** End of Report ***

Instrument 1 27/06/19 14.25.57 1 Page 1 of 1

Data File C:\HPCHEM\1\DATA\IM10912N.D Sample Name: im109 12kr10ipa

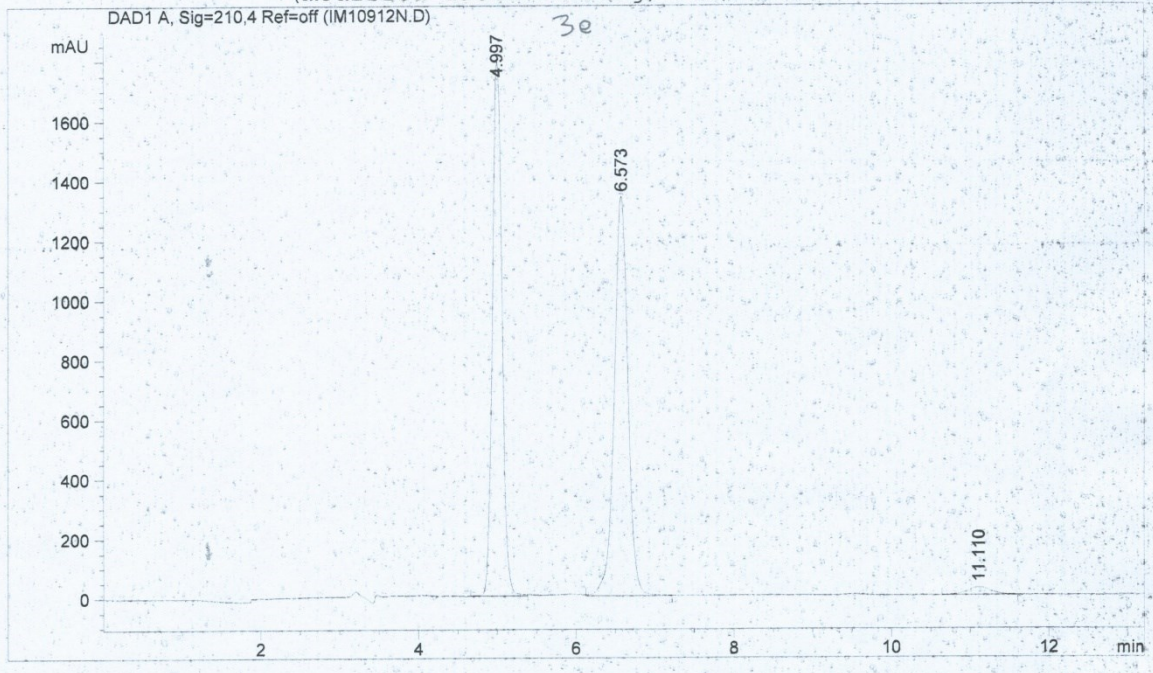
t0

SCIOLTO IN ESANO

==========

Injection Date : 11/04/19 10.52.01
Sample Name : im109 12kr10ipa Vial : 1
Acq. Operator : 1
Acq. Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed : 11/04/19 9.52.21 by 1
(modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed : 11/04/19 11.07.07 by 1
(modified after loading) TABLE 4 ENTRY 1

3e



==========

Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

47.42 : 97.97 = x : 100

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.997	VV	0.1306	1.51359e4	1791.01379	47.4201
2	6.573	VV	0.1812	1.62078e4	1339.61487	50.7784
3	11.110	VV	0.2807	575.02222	26.76270	1.8015

Totals : 3.19187e4 3157.39137

Results obtained with enhanced integrator!

==========

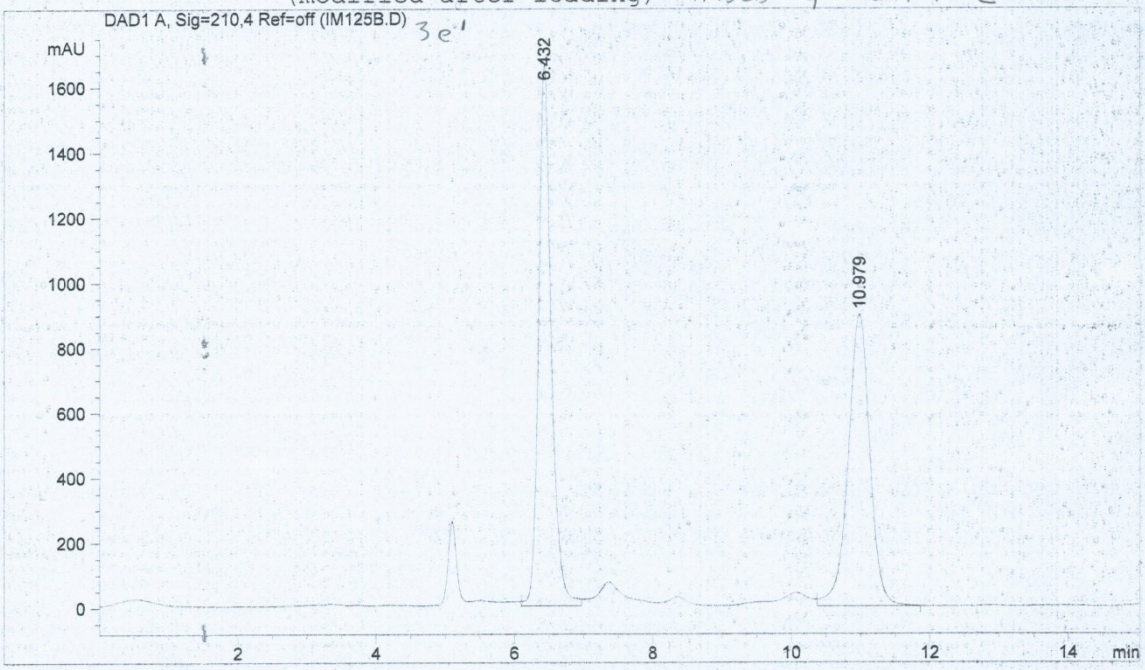
Instrument 1 11/04/19 11.07.10 1 Page 1 of 1

Data File C:\HPCHEM\1\DATA\IM125B.D Sample Name: im125b kr10ipa

fr32-45 0'8 ml-m

```
==========================================================================
Injection Date  : 27/06/19 14.47.46
Sample Name     : im125b kr10ipa                        Vial :   1
Acq. Operator   : 1
Acq. Method     : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 27/06/19 14.45.55  by 1
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 27/06/19 15.03.51  by 1
                  (modified after loading)
```

TABLE 4 ENTRY 2



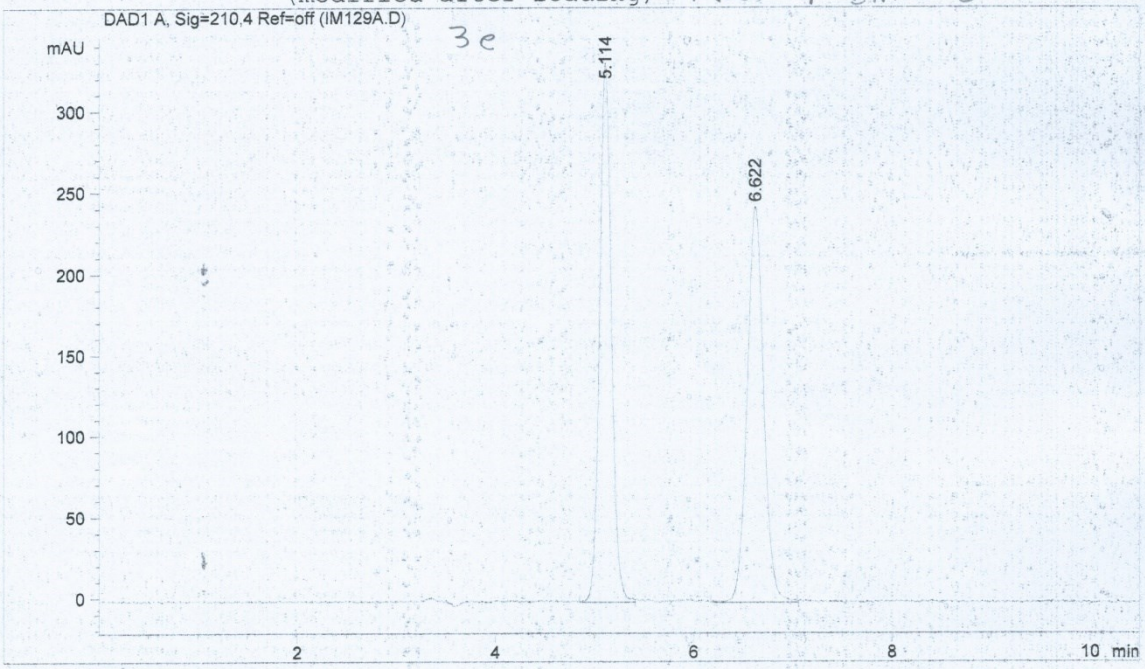

```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.432 VV    0.1857 2.13672e4  1665.37781  52.0321
   2  10.979 VV    0.3261 1.96982e4   897.27808  47.9679

Totals :                  4.10655e4  2562.65588

 Results obtained with enhanced integrator!
==========================================================================
                          *** End of Report ***

Instrument 1 27/06/19 15.04.00  1                          Page 1 of 1
```

Data File C:\HPCHEM\1\DATA\IM129A.D Sample Name: im129a kr10ipa

fr3-6 0'8 ml-m

```
==========================================================================
Injection Date  : 27/06/19 11.30.46
Sample Name     : im129a kr10ipa                        Vial :   1
Acq. Operator   : 1
Acq. Method     : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 27/06/19 11.27.35  by 1
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 27/06/19 11.43.45  by 1
                  (modified after loading)
```

TABLE 4 ENTRY 3



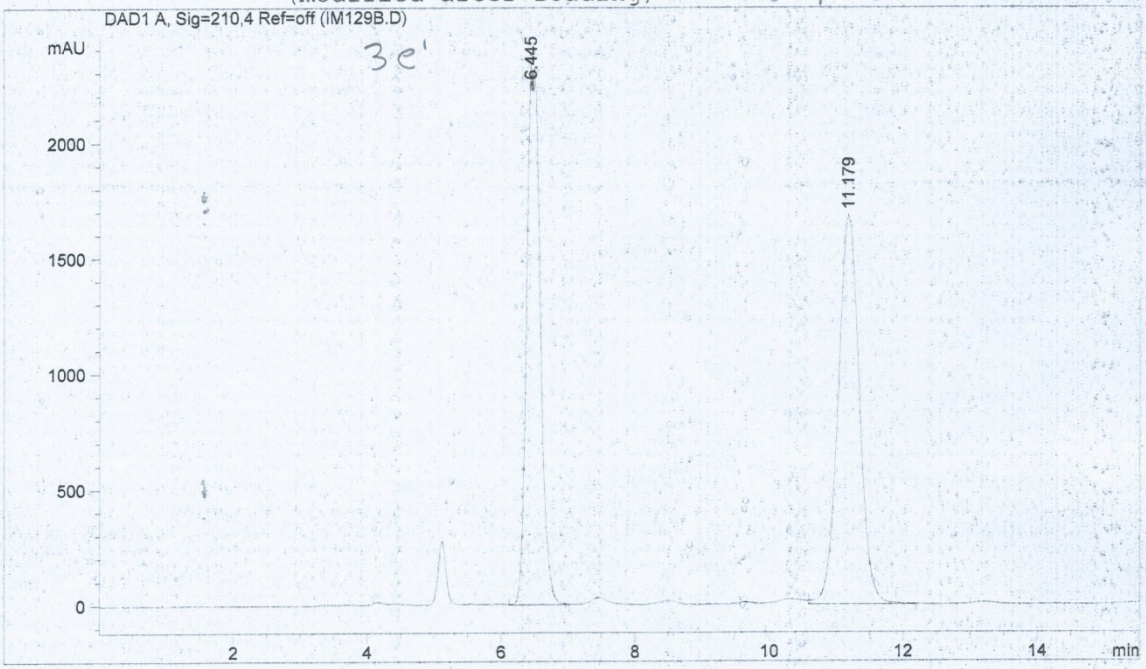

```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.114 VV    0.1295 2778.87964  332.38516  49.5765
   2   6.622 VV    0.1754 2826.35474  243.45102  50.4235

Totals :                  5605.23438  575.83618

 Results obtained with enhanced integrator!
==========================================================================
                          *** End of Report ***

Instrument 1 27/06/19 11.43.48  1                        Page 1 of 1
```

Data File C:\HPCHEM\1\DATA\IM129B.D Sample Name: im129b kr10ipa

fr8-31 0'8 ml-m

```
==========================================================================
Injection Date  : 27/06/19 12.00.46
Sample Name     : im129b kr10ipa                        Vial :   1
Acq. Operator   : 1
Acq. Method     : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 27/06/19 11.58.30  by 1
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 27/06/19 12.18.47  by 1
                  (modified after loading)
```

TABLE 4 ENTRY 3




```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000


Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.445 VV    0.1716 3.31915e4  2338.24268  47.1060
   2  11.179 VV    0.2657 3.72698e4  1686.96448  52.8940

Totals :                  7.04613e4  4025.20715

 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***

Instrument 1 27/06/19 12.18.51  1                        Page 1 of 1
```

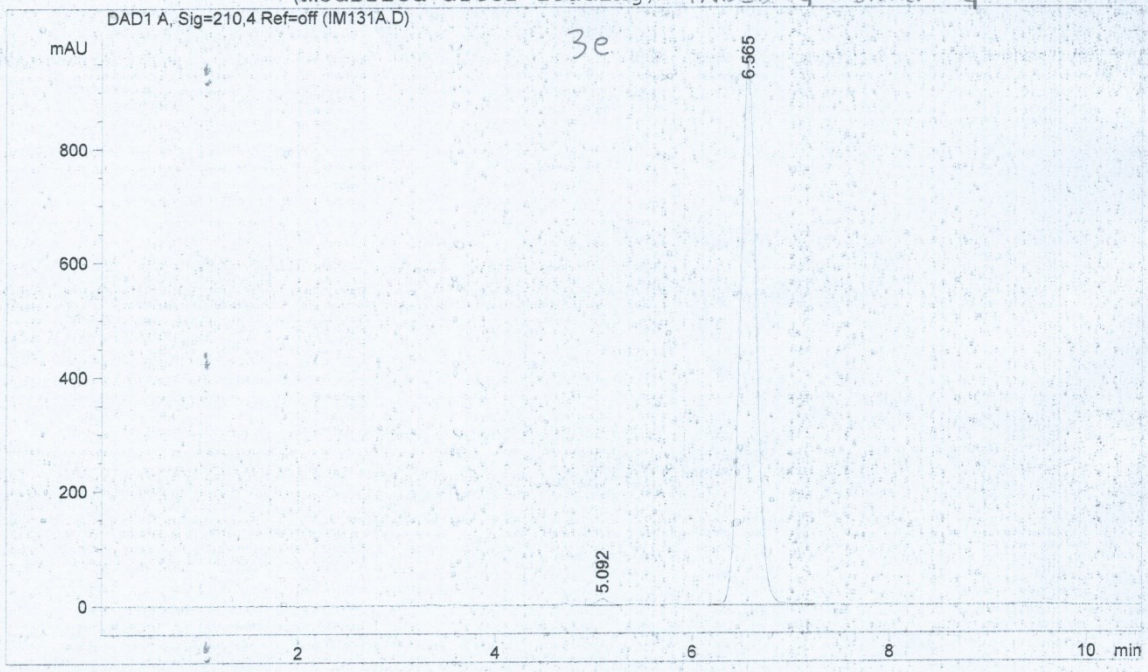
Data File C:\HPCHEM\1\DATA\IM131A.D Sample Name: im131a kr10ipa

fr4-8 0'8 ml-m

```
==========================================================================
Injection Date  : 27/06/19 11.14.14
Sample Name     : im131a kr10ipa                    Vial :   1
Acq. Operator   : 1
Acq. Method     : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 27/06/19 11.09.08  by 1
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 27/06/19 11.25.52  by 1
                  (modified after loading)
```

TABLE 4 ENTRY 4

3e



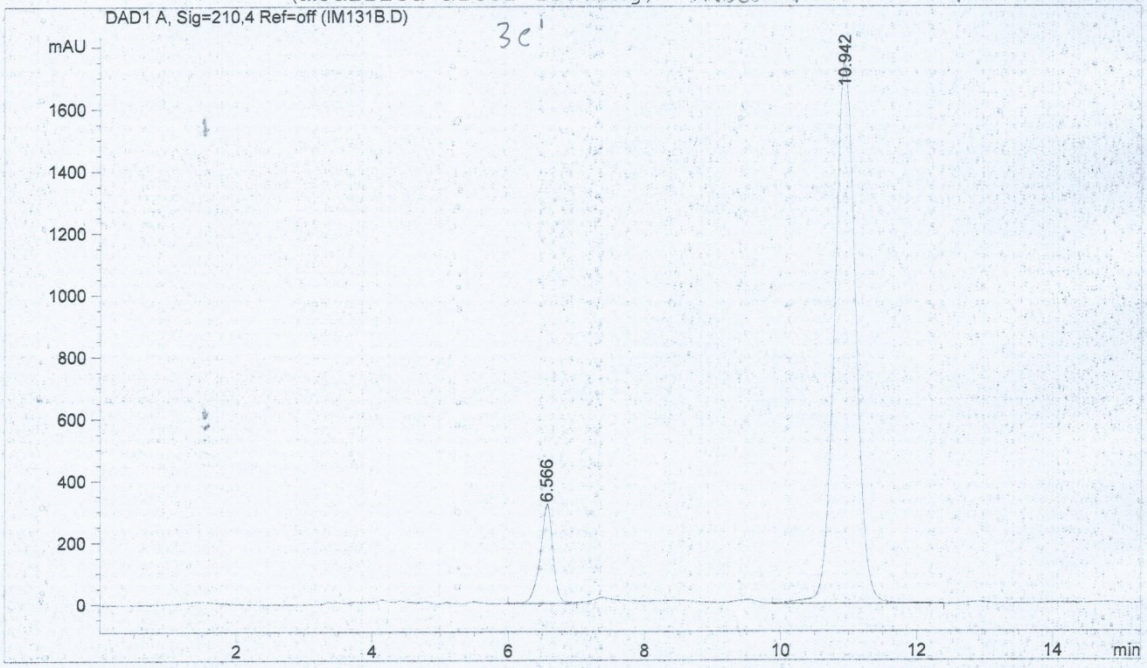

```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.092 VV    0.1381  105.77605   12.08538   0.9626
   2   6.565 VB    0.1778 1.08832e4   949.27765  99.0374

Totals :                   1.09890e4   961.36303

 Results obtained with enhanced integrator!
==========================================================================
                          *** End of Report ***

Instrument 1 27/06/19 11.25.55  1                          Page 1 of 1
```

Data File C:\HPCHEM\1\DATA\IM131B.D Sample Name: im131b kr10ipa

fr11-23 0'8 ml-m

```
==========================================================================
Injection Date  : 27/06/19 15.05.59
Sample Name     : im131b kr10ipa                        Vial :   1
Acq. Operator   : 1
Acq. Method     : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 27/06/19 15.03.51  by 1
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 27/06/19 15.25.35  by 1
                  (modified after loading)
```

TABLE 4 ENTRY 4




```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000


Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.566 BV    0.2361 4198.35449  313.80237   9.9705
   2  10.942 VP    0.3533 3.79094e4  1719.00916  90.0295

Totals :                  4.21078e4  2032.81152

 Results obtained with enhanced integrator!
==========================================================================
                          *** End of Report ***

Instrument 1 27/06/19 15.25.46  1                          Page 1 of 1
```

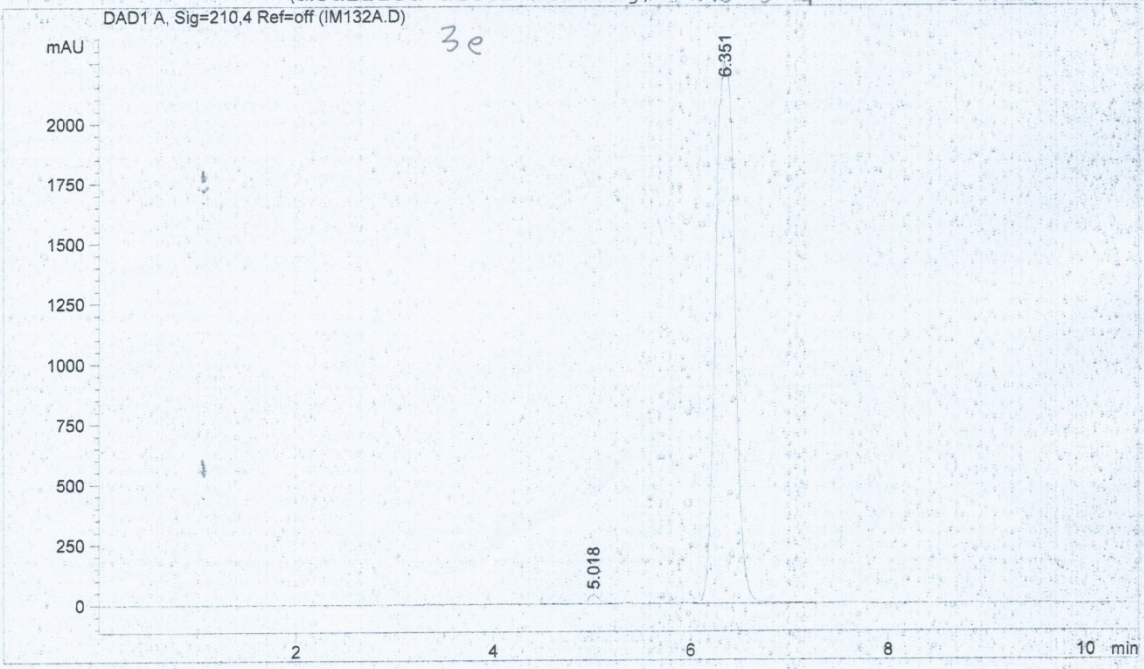
Data File C:\HPCHEM\1\DATA\IM132A.D Sample Name: im132a kr10ipa

fr4-7 0'8 ml-m

```
==========================================================================
Injection Date  : 27/06/19 10.53.35
Sample Name     : im132a kr10ipa                        Vial :   1
Acq. Operator   : 1
Acq. Method     : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 27/06/19 10.52.21  by 1
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 27/06/19 11.09.08  by 1
                  (modified after loading)
```

TABLE 4 ENTRY 5

3e




```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]      [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.018 VV    0.1312  328.00766   38.57288   1.0621
   2   6.351 VV    0.2242 3.05557e4  2225.55713  98.9379

Totals :                  3.08837e4  2264.13000

 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***

Instrument 1 27/06/19 11.10.42  1                          Page 1 of 1
```

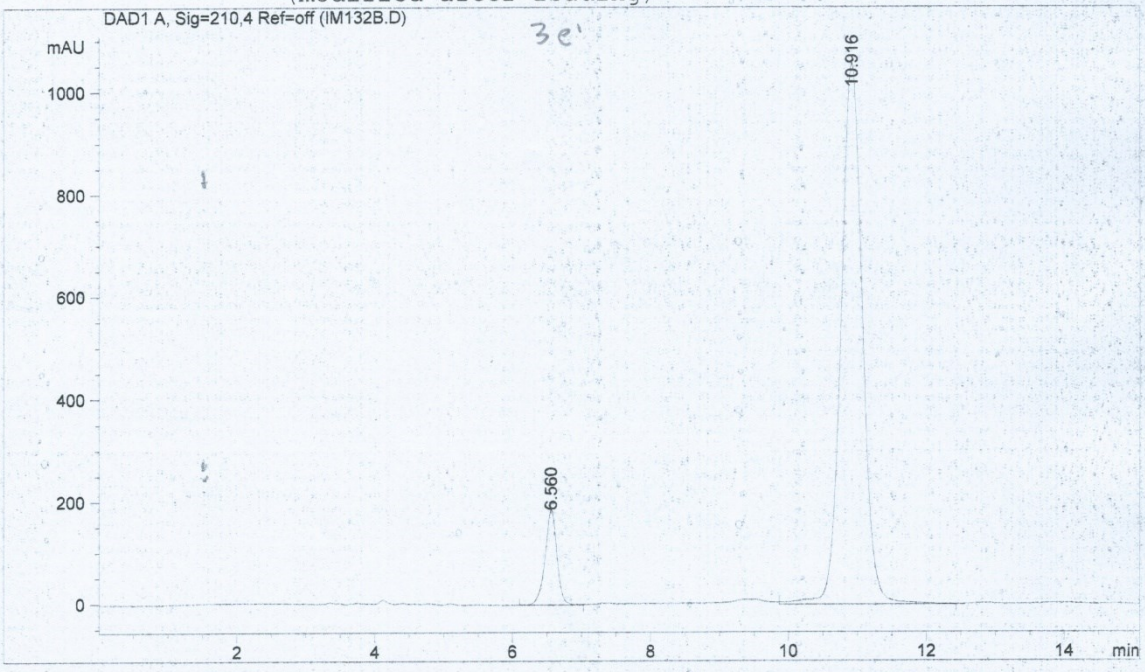
Data File C:\HPCHEM\1\DATA\IM132B.D Sample Name: im132b kr10ipa

fr8-19 0'8 ml-m

```
==========================================================================
Injection Date  : 27/06/19 15.27.50
Sample Name     : im132b kr10ipa                        Vial :   1
Acq. Operator   : 1
Acq. Method     : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 27/06/19 15.25.35  by 1
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 27/06/19 15.45.07  by 1
                  (modified after loading)
```

TABLE 4 ENTRY 5

3e'



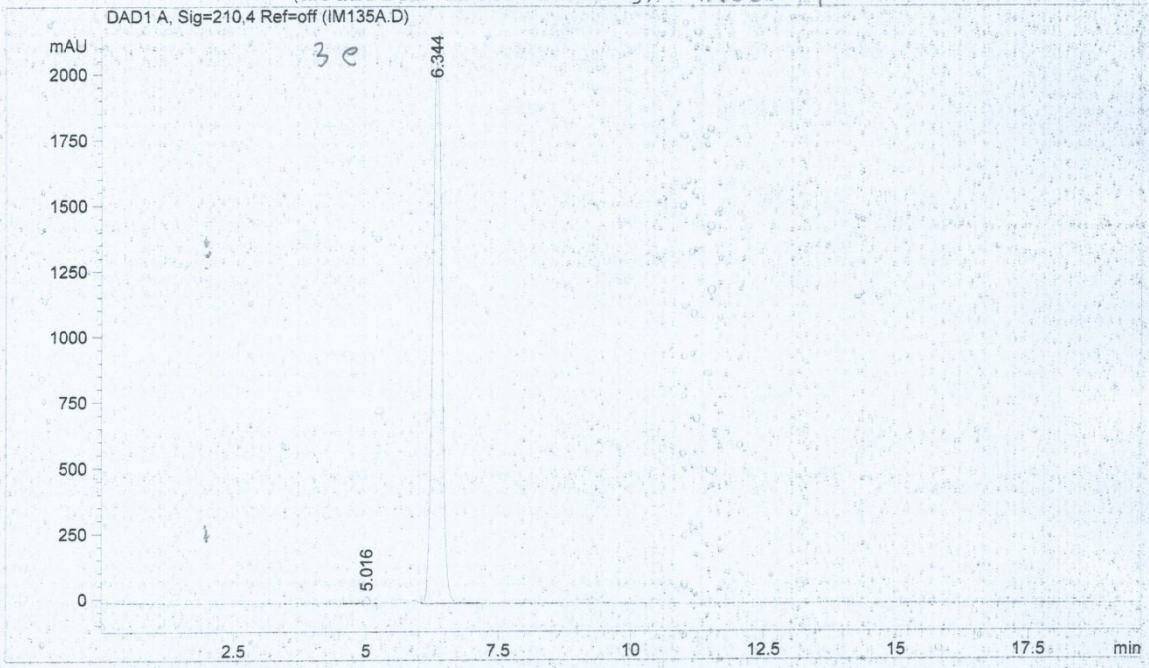

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]      [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.560 BV    0.2118 2242.47217  176.98854   8.9123
   2  10.916 VV    0.3509 2.29191e4  1048.93250  91.0877

Totals :                  2.51616e4  1225.92104

 Results obtained with enhanced integrator!
==========================================================================
                          *** End of Report ***

Instrument 1 27/06/19 15.45.11  1                        Page 1 of 1
```

Data File C:\HPCHEM\1\DATA\IM135A.D Sample Name: im135a kr10ipa

fr5-11 0'8 ml-m

```
==========================================================================
Injection Date  : 27/06/19 10.28.00
Sample Name     : im135a kr10ipa                    Vial :   1
Acq. Operator   : 1
Acq. Method     : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 27/06/19 10.10.15  by 1
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 27/06/19 10.49.56  by 1
                  (modified after loading)
```

3e TABLE 4 ENTRY 6




```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.016 BV    0.1426  251.93456   27.56786   1.0032
   2   6.344 VV    0.1888 2.48621e4  2060.62988  98.9968

Totals :                  2.51140e4  2088.19774

 Results obtained with enhanced integrator!
==========================================================================
                          *** End of Report ***

Instrument 1 27/06/19 10.50.27  1                        Page 1 of 1
```

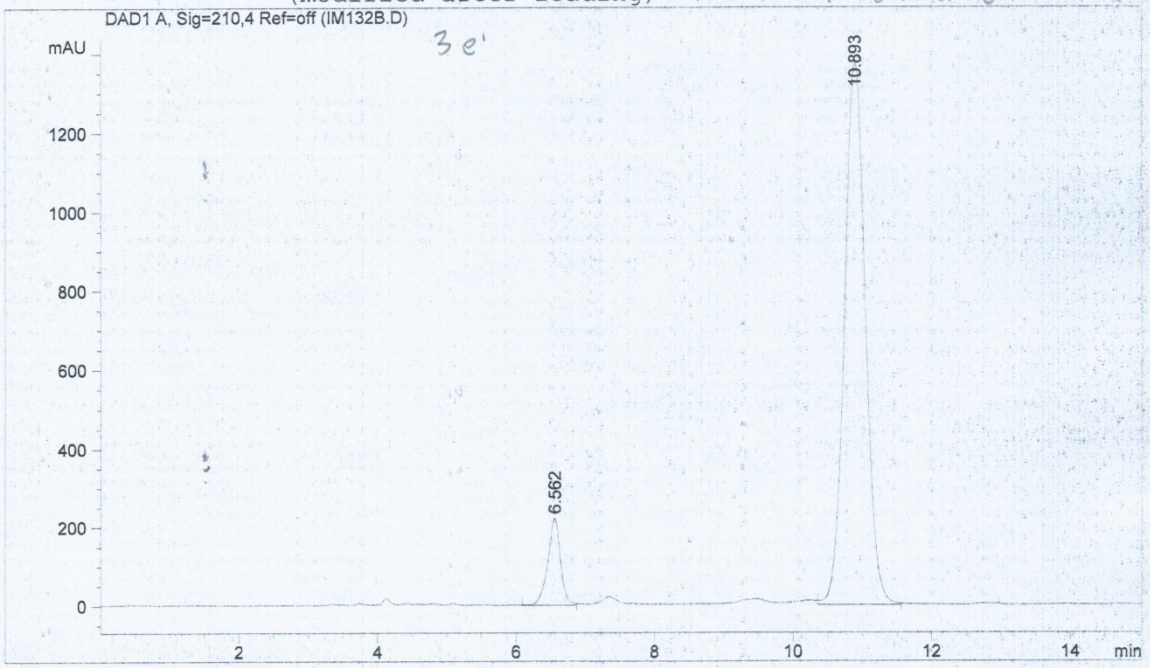
Data File C:\HPCHEM\1\DATA\IM132B.D Sample Name: im132b kr10ipa

135

fr8-19 0'8 ml-m

==========

Injection Date : 27/06/19 15.46.56
Sample Name : im132b kr10ipa Vial : 1
Acq. Operator : 1
Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed : 27/06/19 15.45.53 by 1
(modified after loading) TABLE 4 ENTRY 6



==========

Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.562	VV	0.1861	2848.50171	221.42374	8.9817
2	10.893	VV	0.2669	2.88660e4	1374.85510	91.0183
Totals :				3.17145e4	1596.27884	

Results obtained with enhanced integrator!

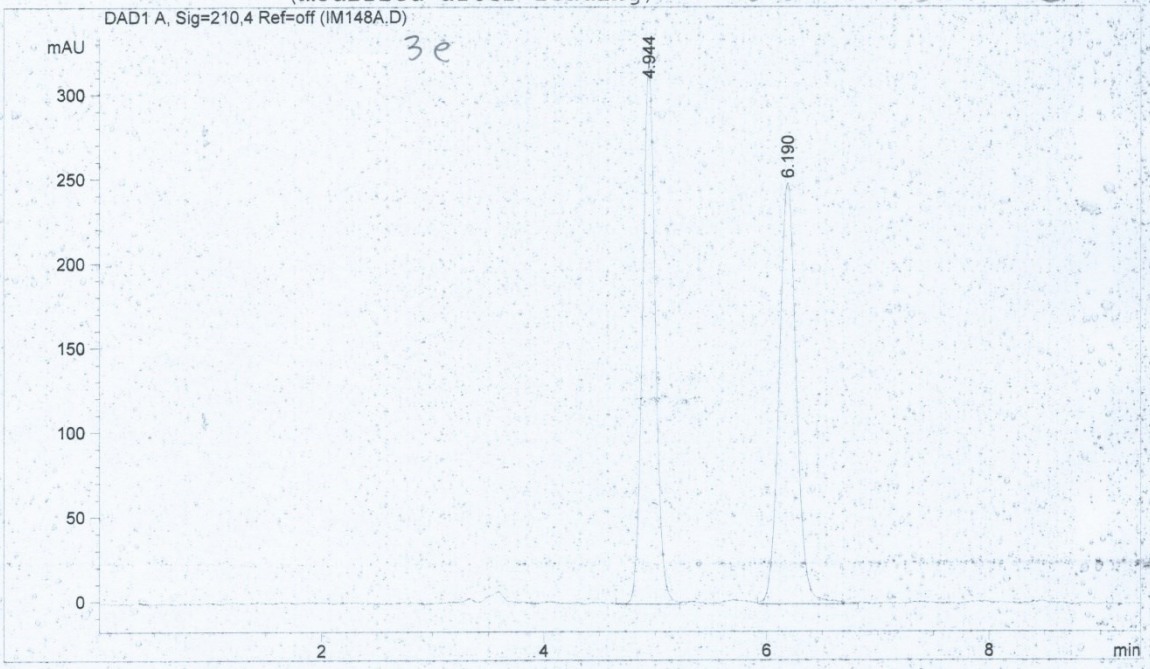
==========

*** End of Report ***

Instrument 1 27/06/19 16.02.50 1 Page 1 of 1

Data File C:\HPCHEM\1\DATA\IM148A.D Sample Name: im148a kr10ipa

Injection Date : 20/09/19 14.36.22
Sample Name : im148a kr10ipa Vial : 1
Acq. Operator : 1
Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed : 20/09/19 10.44.33 by 1
(modified after loading) TABLE 5 ENTRY 1



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.944	VV	0.1195	2564.90039	320.19781	48.8509
2	6.190	VV	0.1639	2685.57178	248.83321	51.1491

Totals : 5250.47217 569.03102

Results obtained with enhanced integrator!

*** End of Report ***

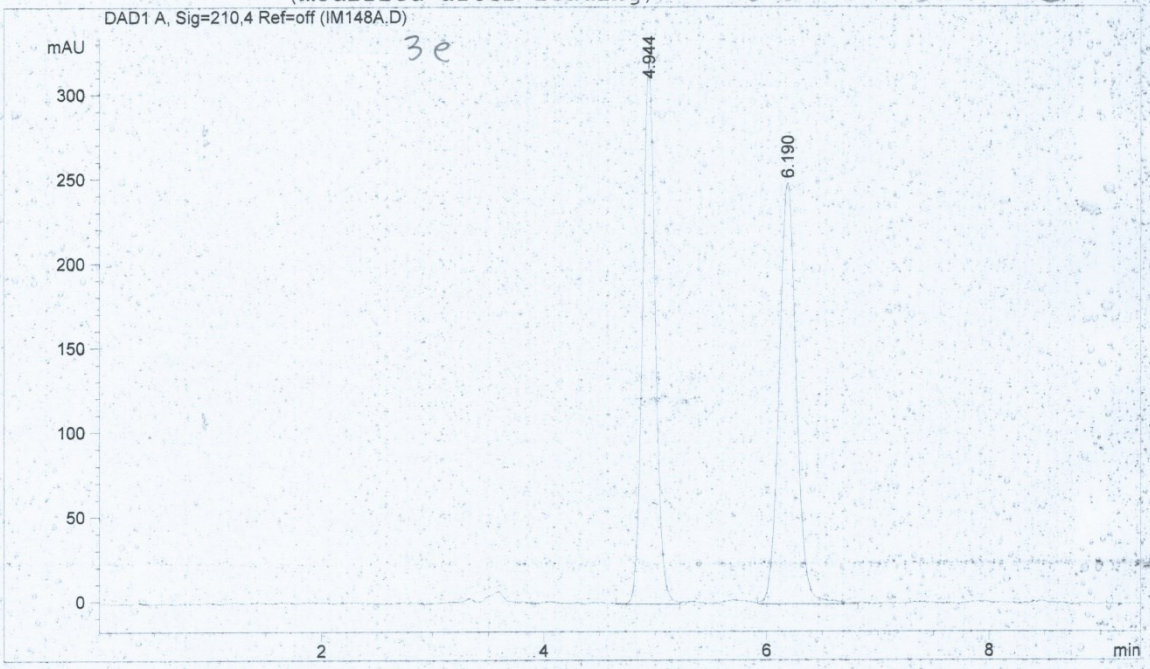
Instrument 1 20/09/19 14.48.54 1 Page 1 of 1

Data File C:\HPCHEM\1\DATA\IM148A.D Sample Name: im148a kr10ipa

```
Injection Date  : 20/09/19 14.36.22
Sample Name     : im148a kr10ipa                    Vial :  1
Acq. Operator   : 1
Method          : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 20/09/19 10.44.33  by 1
                  (modified after loading)
```

TABLE 5 ENTRY 1

3e



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.944 VV    0.1195 2564.90039  320.19781  48.8509
   2   6.190 VV    0.1639 2685.57178  248.83321  51.1491

Totals :                   5250.47217  569.03102

 Results obtained with enhanced integrator!
```

*** End of Report ***

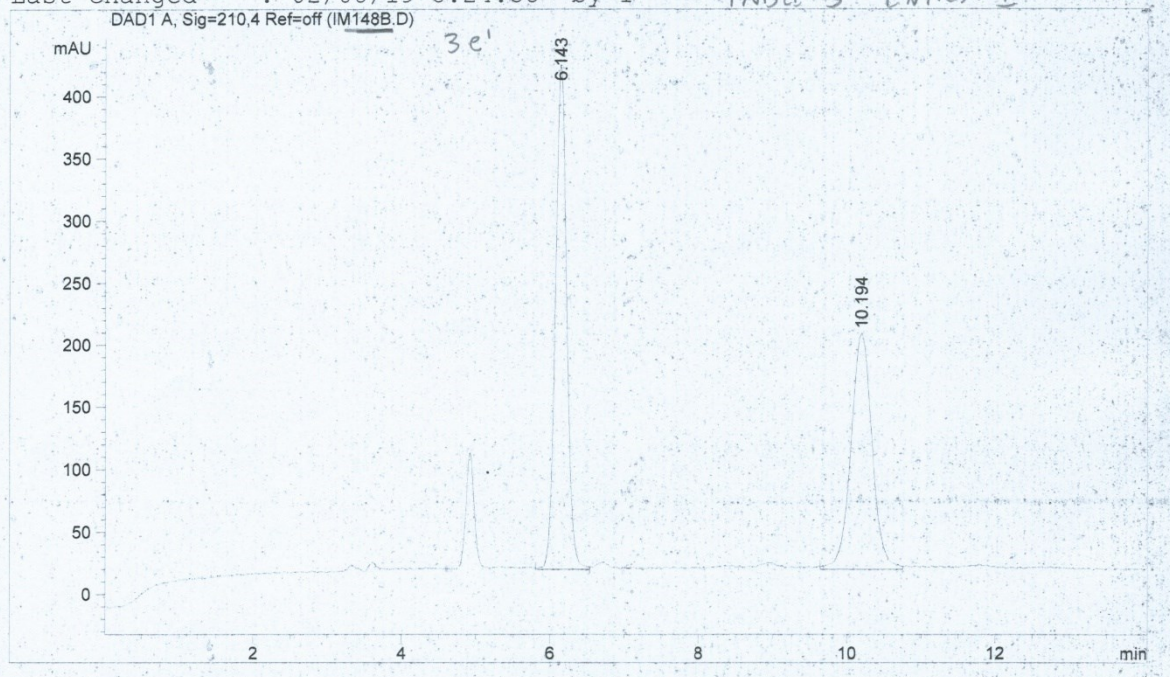
Instrument 1 20/09/19 14.48.54 1 Page 1 of 1

Data File C:\HPCHEM\1\DATA\IM148B.D Sample Name: im150a kr10ipa

148B

```
Injection Date  : 03/10/19 10.51.12
Sample Name     : im150a kr10ipa                    Vial :   1
Acq. Operator   : 1
Method          : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 02/08/19 8.24.58  by 1
```

TABLE 5 ENTRY 1




```
                        Area Percent Report

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.143 VV    0.1614 4290.62256  405.53687  53.2600
   2  10.194 VV    0.2965 3765.37646  188.91107  46.7400

Totals :                  8055.99902  594.44794

 Results obtained with enhanced integrator!

                        *** End of Report ***
```

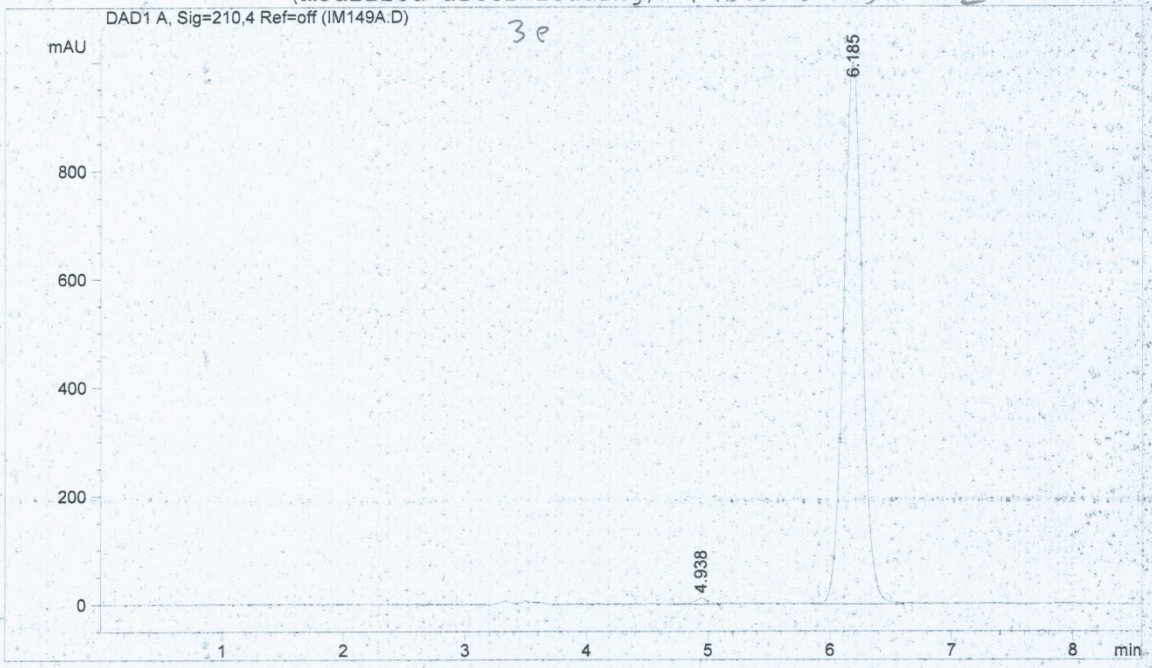
Instrument 1 03/10/19 11.06.33 1 Page 1 of 1

Data File C:\HPCHEM\1\DATA\IM149A.D Sample Name: im149a kr10ipa

```
==========================================================================
Injection Date  : 20/09/19 14.53.46
Sample Name     : im149a kr10ipa                    Vial :   1
Acq. Operator   : 1
Acq. Method     : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 20/09/19 14.52.45  by 1
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 20/09/19 15.04.30  by 1
                  (modified after loading)
```

TABLE 5 ENTRY 2

3e




```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000


Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.938 VV    0.1227  101.26032   11.50448   0.9384
   2   6.185 VV    0.1648 1.06896e4   999.59778  99.0616

Totals :                  1.07908e4  1011.10226

 Results obtained with enhanced integrator!
==========================================================================
                          *** End of Report ***
```

Instrument 1 20/09/19 15.04.35 1 Page 1 of 1

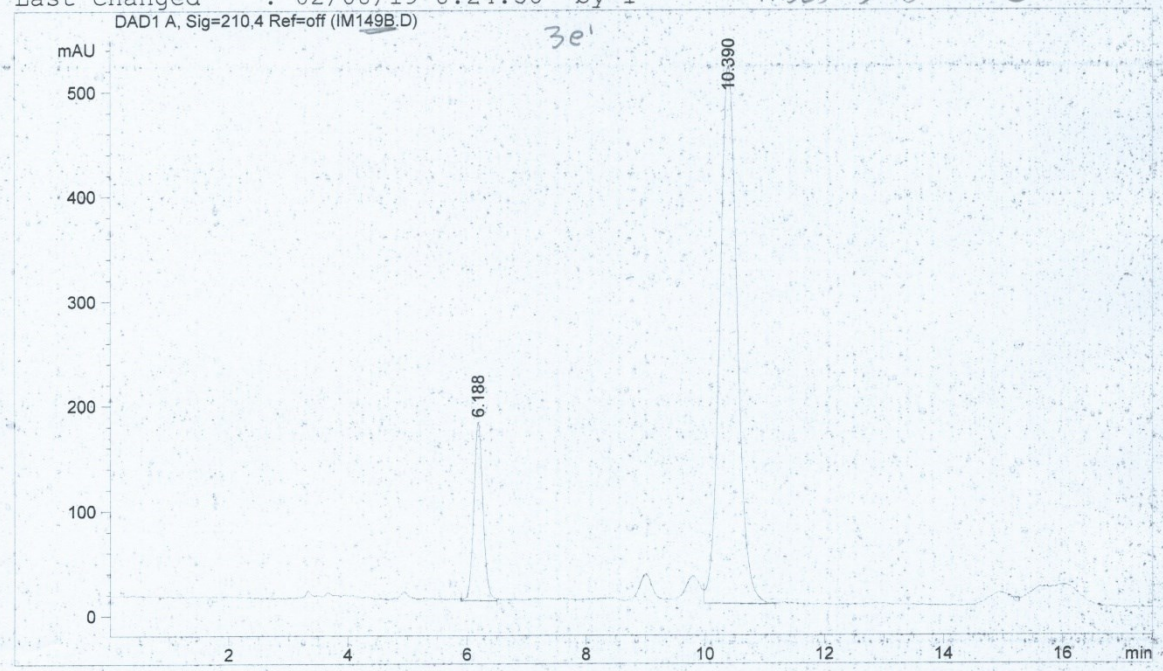
Data File C:\HPCHEM\1\DATA\IM149B.D Sample Name: im150a kr10ipa

149B

Injection Date : 03/10/19 11.08.55
Sample Name : im150a kr10ipa Vial : 1
Acq. Operator : 1
Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed : 02/08/19 8.24.58 by 1

TABLE 5 ENTRY 2

3e'



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.188	VV	0.1670	1816.95398	169.59091	14.8409
2	10.390	VV	0.3092	1.04259e4	512.76941	85.1591
Totals :				1.22429e4	682.36032	

Results obtained with enhanced integrator!

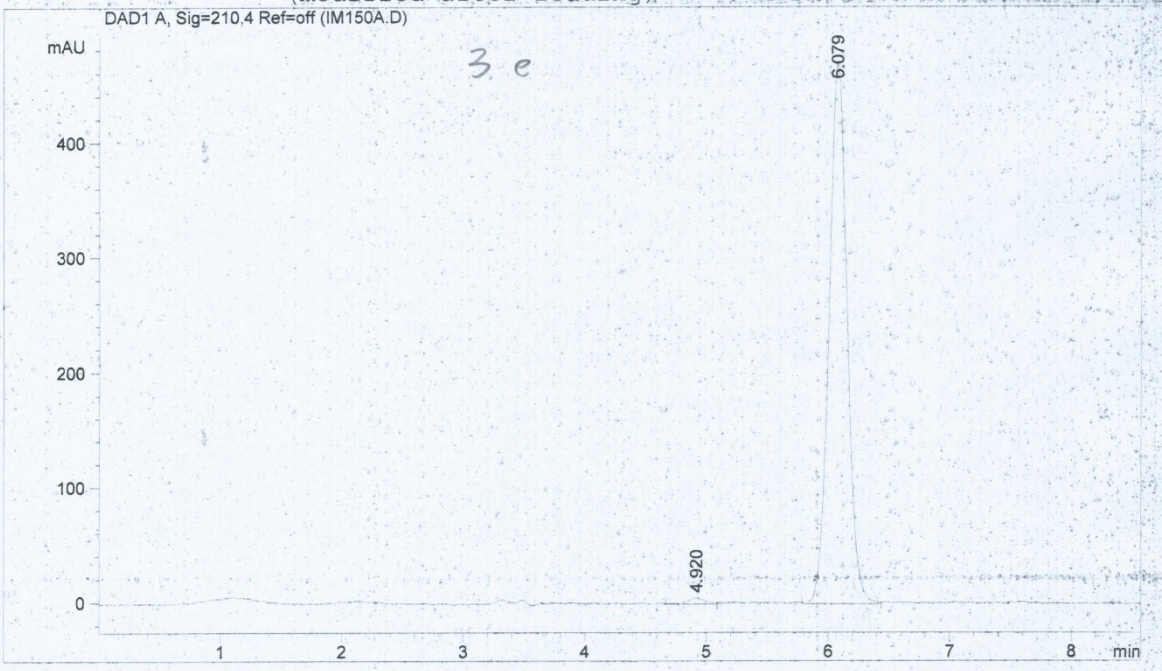
*** End of Report ***

Instrument 1 03/10/19 11.27.40 1 Page 1 of 1

Data File C:\HPCHEM\1\DATA\IM150A.D Sample Name: im150a kr10ipa

```
==========================================================================
Injection Date  : 20/09/19 15.17.32
Sample Name     : im150a kr10ipa                        Vial :   1
Acq. Operator   : 1
Acq. Method     : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 20/09/19 15.04.30  by 1
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 20/09/19 15.27.54  by 1
                  (modified after loading)
```

TABLE 5 ENTRY 3

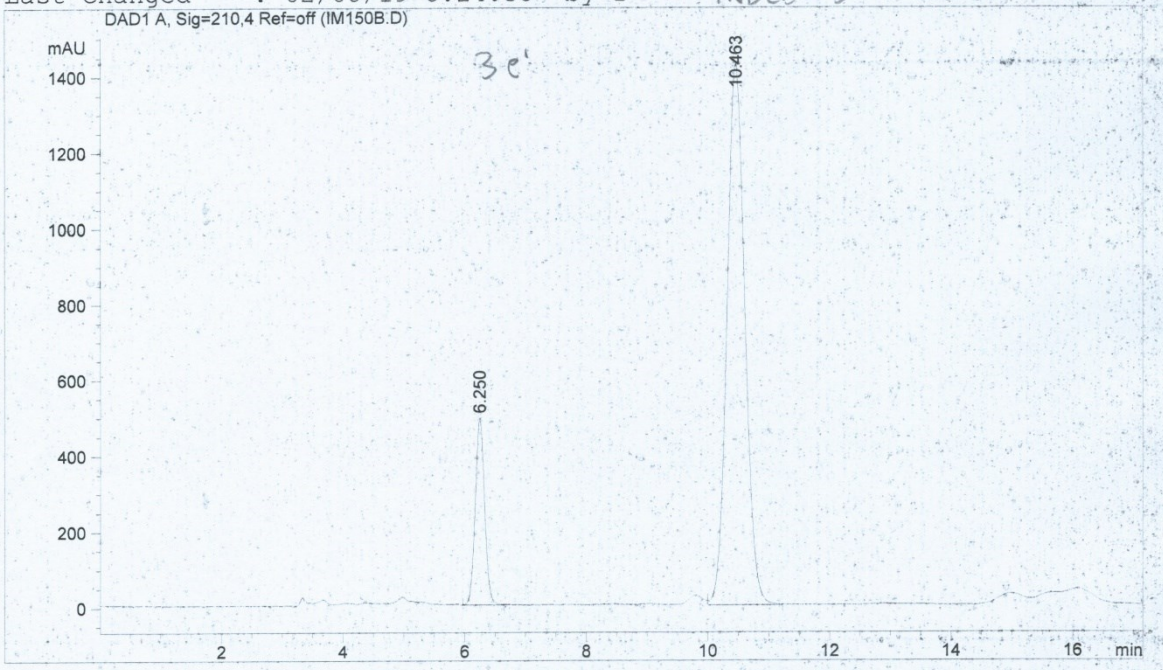



```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.920 VV    0.1376   55.83516    5.35870   1.1355
   2   6.079 VV    0.1587 4861.47998  469.95435  98.8645

Totals :                   4917.31514  475.31304

 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***

Instrument 1 20/09/19 15.27.57  1                      Page 1 of 1
```

Data File C:\HPCHEM\1\DATA\IM150B.D Sample Name: im150b kr10ipa

```
Injection Date  : 03/10/19 11.30.16
Sample Name     : im150b kr10ipa                    Vial :   1
Acq. Operator   : 1
Method          : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 02/08/19 8.24.58  by 1
```

TABLE 5 ENTRY 3



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.250 VV    0.1634 5282.56885  491.66080  15.3890
   2  10.463 VV    0.2713 2.90444e4  1428.02686  84.6110

Totals :                  3.43269e4  1919.68765

 Results obtained with enhanced integrator!
```

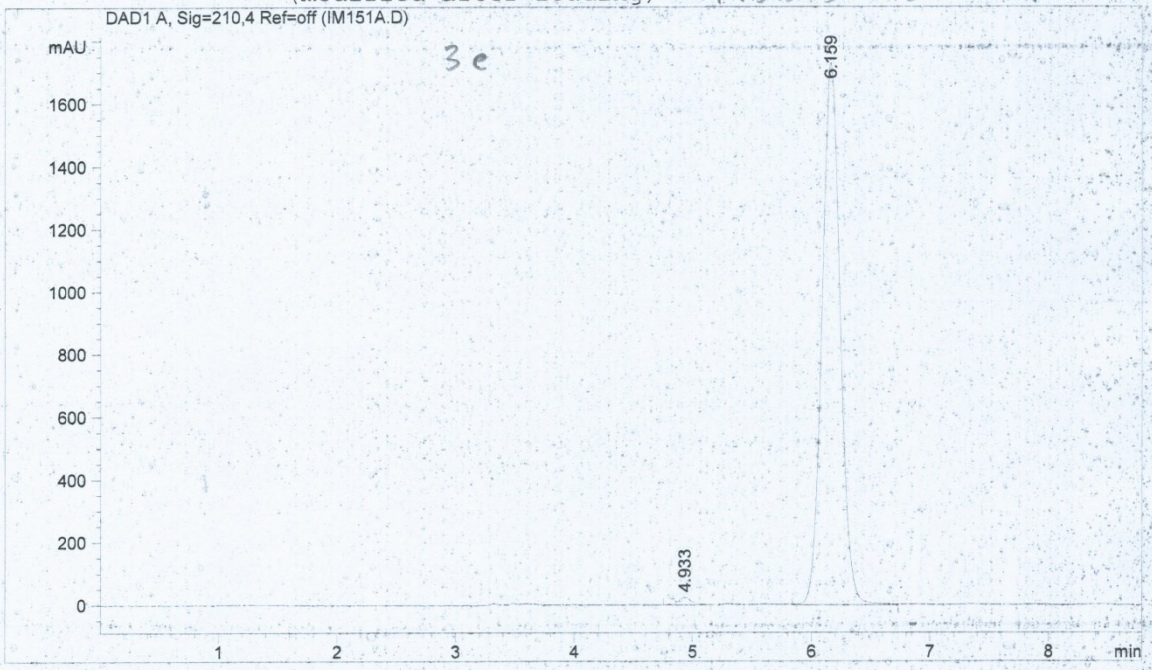
*** End of Report ***

Instrument 1 03/10/19 11.48.12 1 Page 1 of 1

Data File C:\HPCHEM\1\DATA\IM151A.D Sample Name: im151a kr10ipa

```
==========================================================================
Injection Date  : 20/09/19 15.05.40
Sample Name     : im151a kr10ipa                    Vial :   1
Acq. Operator   : 1
Method          : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 20/09/19 15.04.30  by 1
                  (modified after loading)
```

TABLE 5 ENTRY 4



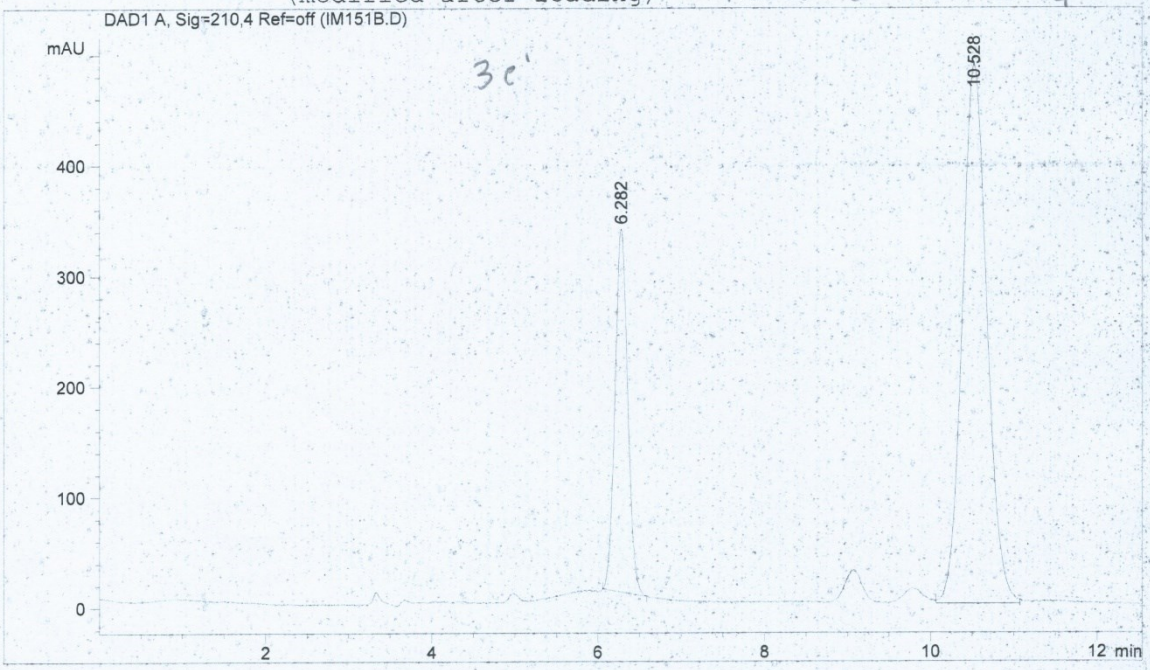

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.933 VV    0.1188  201.15071   25.28632   1.0770
   2   6.159 VV    0.1666 1.84751e4  1730.34595  98.9230

Totals :                   1.86762e4  1755.63227

 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Instrument 1 20/09/19 15.16.00 1 Page 1 of 1

Data File C:\HPCHEM\1\DATA\IM151B.D Sample Name: im151b kr10ipa

```
Injection Date  : 03/10/19 11.50.37
Sample Name     : im151b kr10ipa                    Vial :  1
Acq. Operator   : 1
Acq. Method     : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 02/08/19 8.24.58  by 1
Analysis Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 03/10/19 12.09.05  by 1
                  (modified after loading)
```

TABLE 5 ENTRY 4



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.282 BBA   0.1598 3479.49243  327.91263  25.7601
   2  10.528 VV    0.2875 1.00278e4   488.52579  74.2399

Totals :                  1.35073e4   816.43842

 Results obtained with enhanced integrator!
```

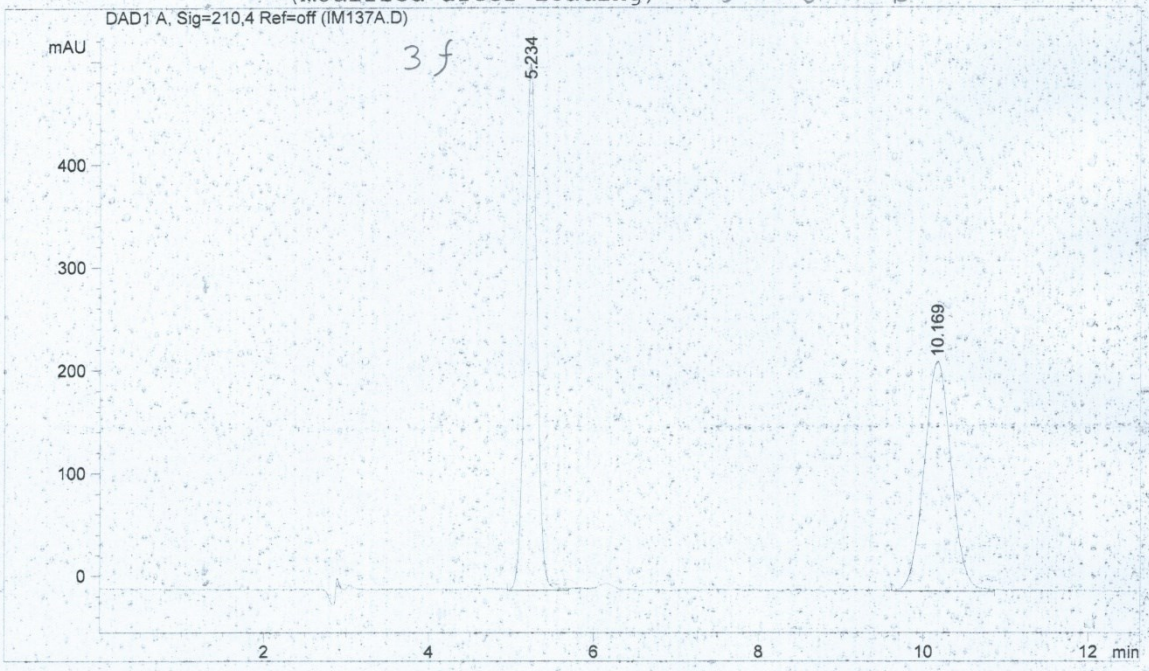
*** End of Report ***

Instrument 1 03/10/19 12.09.09 1 Page 1 of 1

Data File C:\HPCHEM\1\DATA\IM137A.D Sample Name: im137A kr 10ipa

```
Injection Date  : 09/10/19 10.31.46
Sample Name     : im137A kr 10ipa                    Vial :   1
Acq. Operator   : 1
Acq. Method     : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 09/10/19 10.24.05  by 1
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 09/10/19 10.46.22  by 1
                  (modified after loading)
```

TABLE 6 ENTRY 1

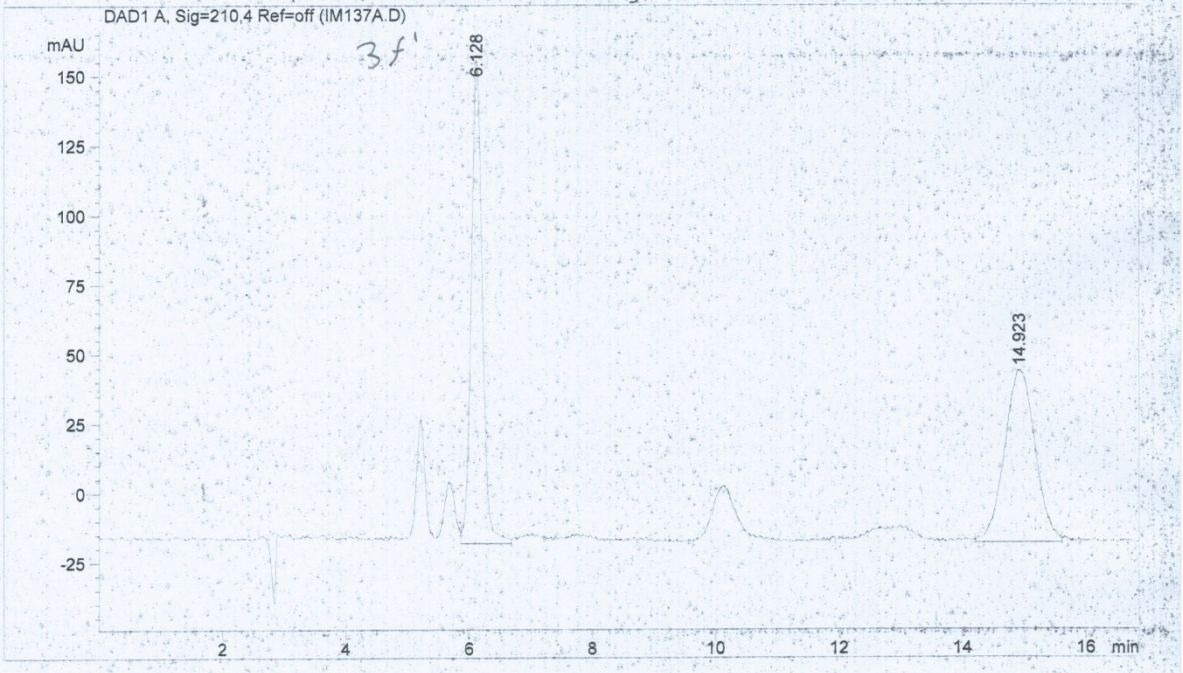



```
                          Area Percent Report

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.234 VV    0.1520 5087.54736  511.58527  49.9008
   2  10.169 VV    0.3358 5107.77490  222.55507  50.0992

Totals :                  1.01953e4   734.14034

 Results obtained with enhanced integrator!

                          *** End of Report ***
```

Instrument 1 09/10/19 10.46.25 1 Page 1 of 1

Data File C:\HPCHEM\1\DATA\IM137A.D Sample Name: im137A kr 10ipa
B

Injection Date : 09/10/19 10.50.10
Sample Name : im137A kr 10ipa Vial : 1
Acq. Operator : 1
Acq. Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed : 09/10/19 10.46.22 by 1
(modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed : 09/10/19 11.08.14 by 1
(modified after loading) TABLE 6 ENTRY 1



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.128	VV	0.1973	2160.35645	173.43279	50.3545
2	14.923	VV	0.4329	2129.94067	61.36561	49.6455
Totals :				4290.29712	234.79839	

Results obtained with enhanced integrator!

*** End of Report ***

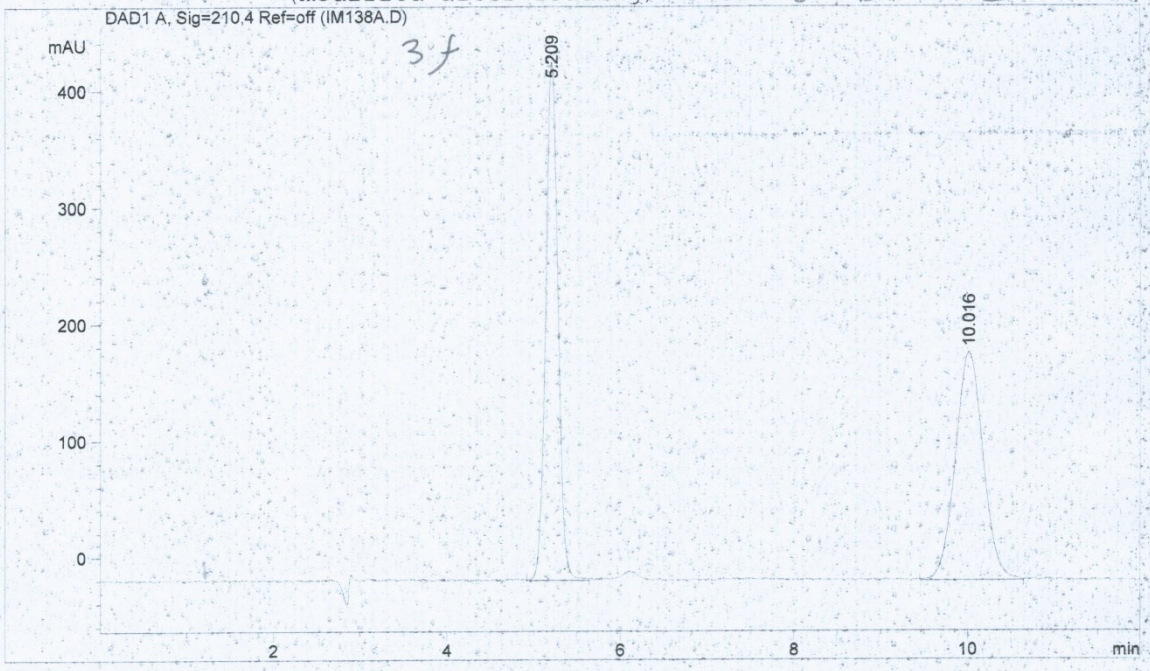
Instrument 1 09/10/19 11.08.18 1 Page 1 of 1

Data File C:\HPCHEM\1\DATA\IM138A.D Sample Name: im138A kr 10ipa

```
Injection Date  : 09/10/19 11.11.15
Sample Name     : im138A kr 10ipa                    Vial :   1
Acq. Operator   : 1
Acq. Method     : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 09/10/19 11.08.14  by 1
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 09/10/19 11.24.14  by 1
                  (modified after loading)
```

TABLE 6 ENTRY 2

3f

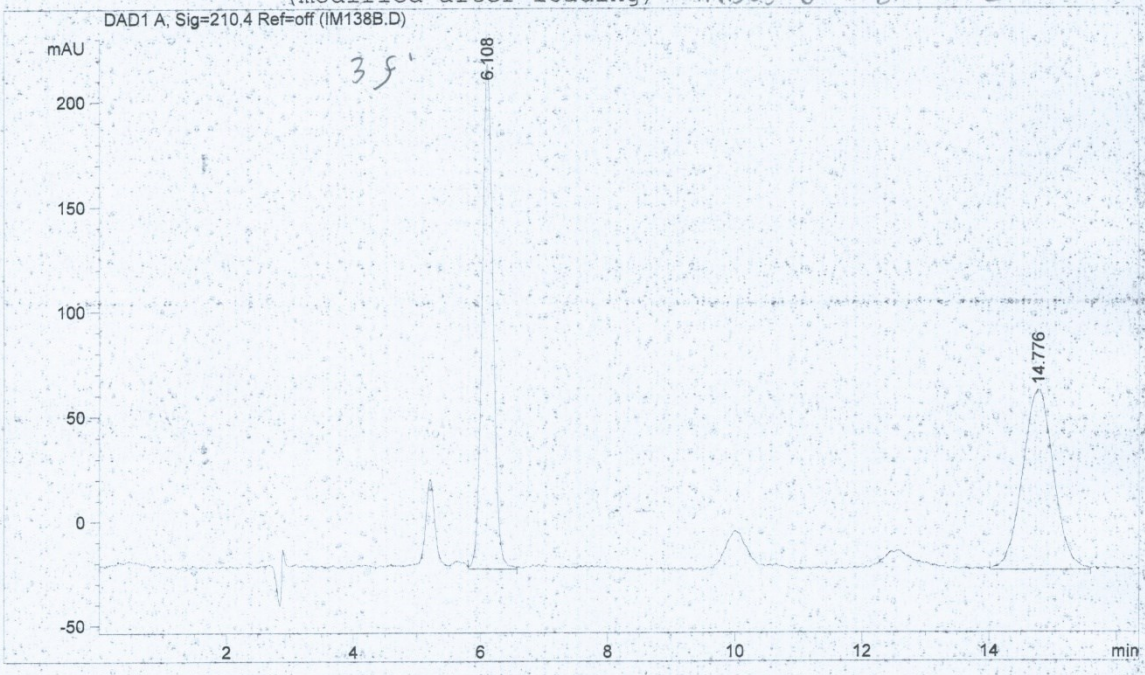



```
                          Area Percent Report

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.209 VV    0.1530 4374.18848  443.88419  50.0081
   2  10.016 VV    0.2966 4372.76660  195.79478  49.9919

Totals :                  8746.95508  639.67897

 Results obtained with enhanced integrator!

                          *** End of Report ***
```

Instrument 1 09/10/19 11.24.17 1 Page 1 of 1

Data File C:\HPCHEM\1\DATA\IM138B.D Sample Name: im138B kr 10ipa

Injection Date : 09/10/19 11.25.36
Sample Name : im138B kr 10ipa Vial : 1
Acq. Operator : 1
Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed : 09/10/19 11.24.14 by 1
(modified after loading) TABLE 6 ENTRY 2



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.108	VV	0.1795	2877.52539	240.62816	49.5786
2	14.776	VV	0.4112	2926.43872	85.52875	50.4214
Totals :				5803.96411	326.15691	

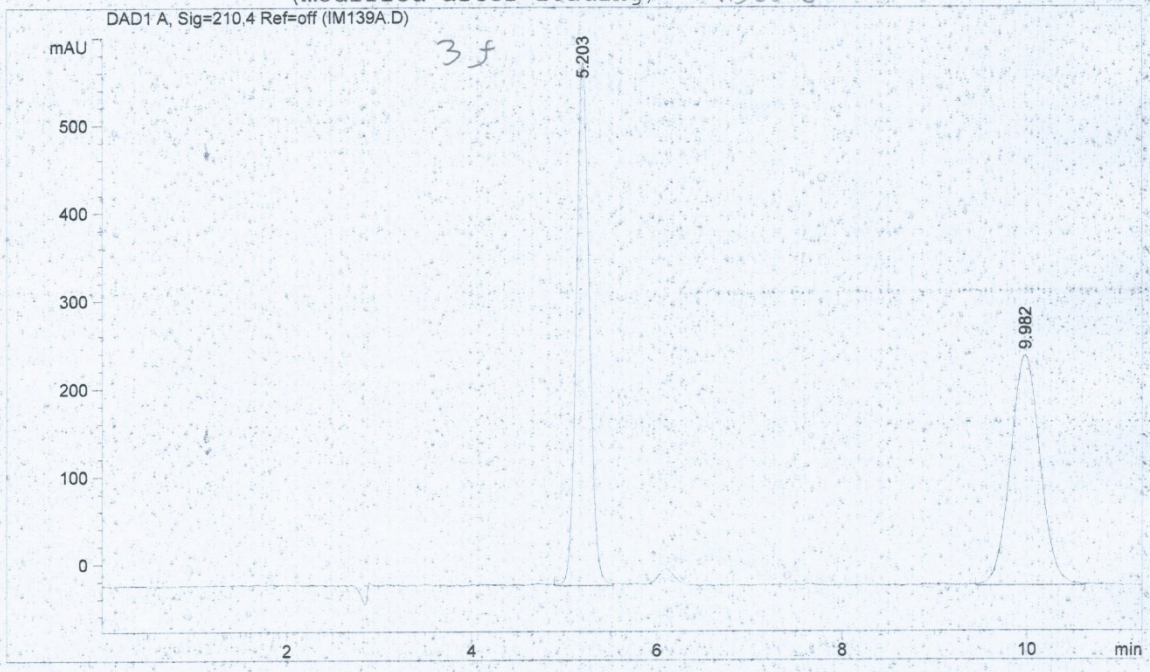
Results obtained with enhanced integrator!

*** End of Report ***

Instrument 1 09/10/19 11.42.45 1 Page 1 of 1

Data File C:\HPCHEM\1\DATA\IM139A.D Sample Name: im139A kr 10ipa

Injection Date : 09/10/19 11.44.02
Sample Name : im139A kr 10ipa Vial : 1
Acq. Operator : 1
Method : C:\HPCHEM\1\METHODS\CECE.M
Last changed : 09/10/19 11.24.14 by 1
(modified after loading) TABLE 6 ENTRY 3



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.203	VV	0.1504	5839.23828	595.65338	49.8522
2	9.982	VV	0.3209	5873.85596	262.67551	50.1478

Totals : 1.17131e4 858.32889

Results obtained with enhanced integrator!

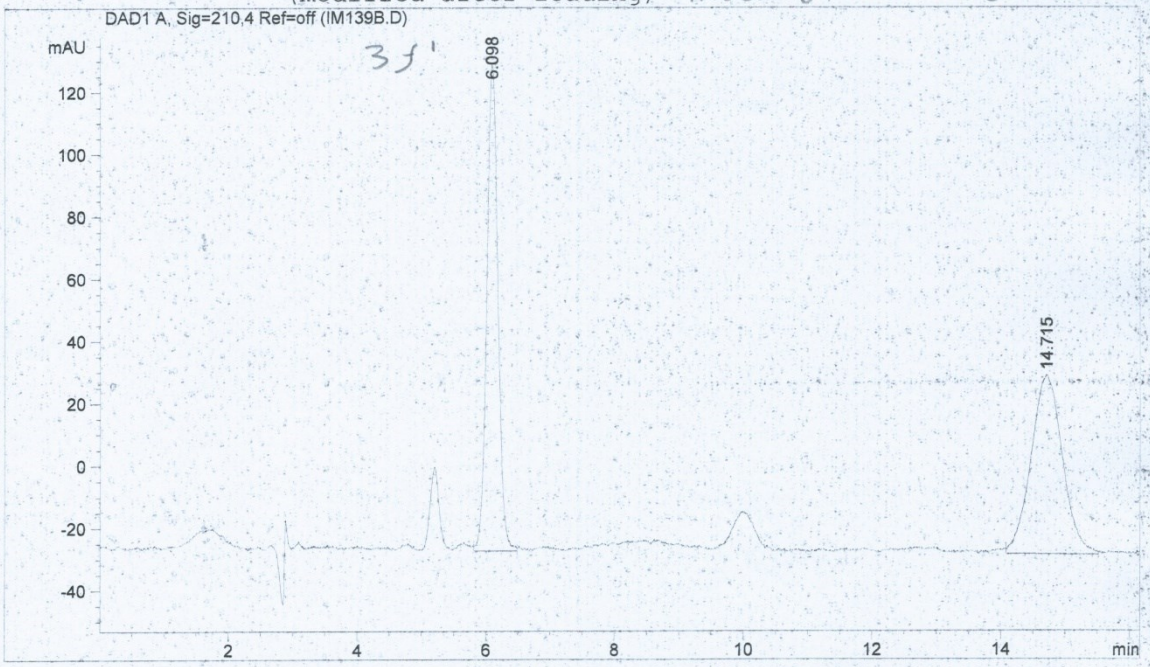
*** End of Report ***

Instrument 1 09/10/19 11.56.02 1 Page 1 of 1

Data File C:\HPCHEM\1\DATA\IM139B.D Sample Name: im139B kr 10ipa

```
Injection Date  : 09/10/19 11.57.06
Sample Name     : im139B kr 10ipa                    Vial :   1
Acq. Operator   : 1
Method          : C:\HPCHEM\1\METHODS\CECE.M
Last changed    : 09/10/19 11.24.14  by 1
                  (modified after loading)
```

TABLE 6 ENTRY 3




```
                          Area Percent Report

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.098 VV    0.1817 1874.77197  156.57124  49.0483
   2  14.715 VV    0.4084 1947.52405   57.32010  50.9517

Totals :                  3822.29602  213.89135

 Results obtained with enhanced integrator!

                          *** End of Report ***
```

Instrument 1 09/10/19 12.14.05 1 Page 1 of 1