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Microwave-Assisted Reactivity of a Fischer Alkynyl Carbene Complex with Benzylidene Anilines

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Supplementary Information

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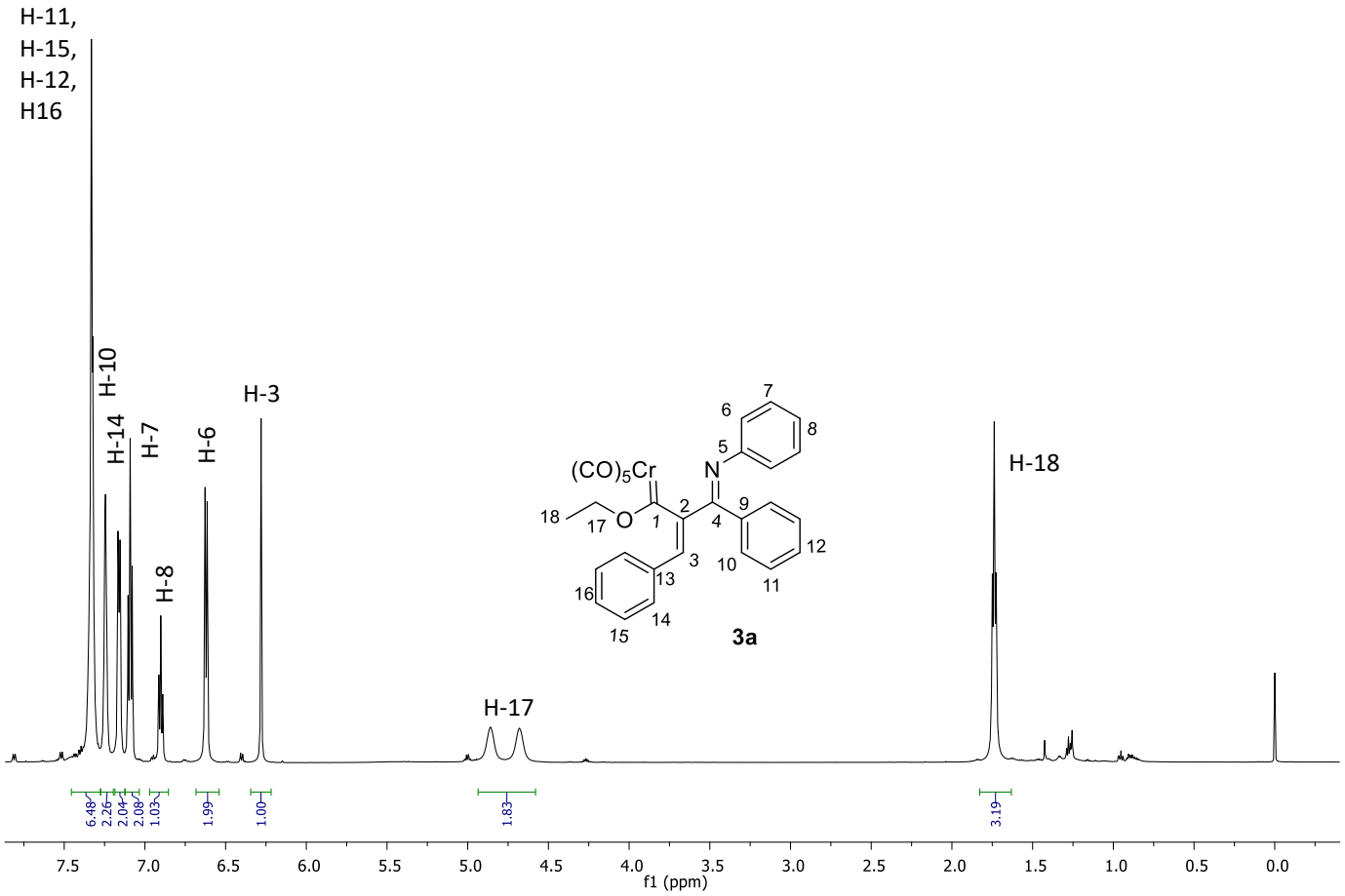

^{1}H NMR for **3a**

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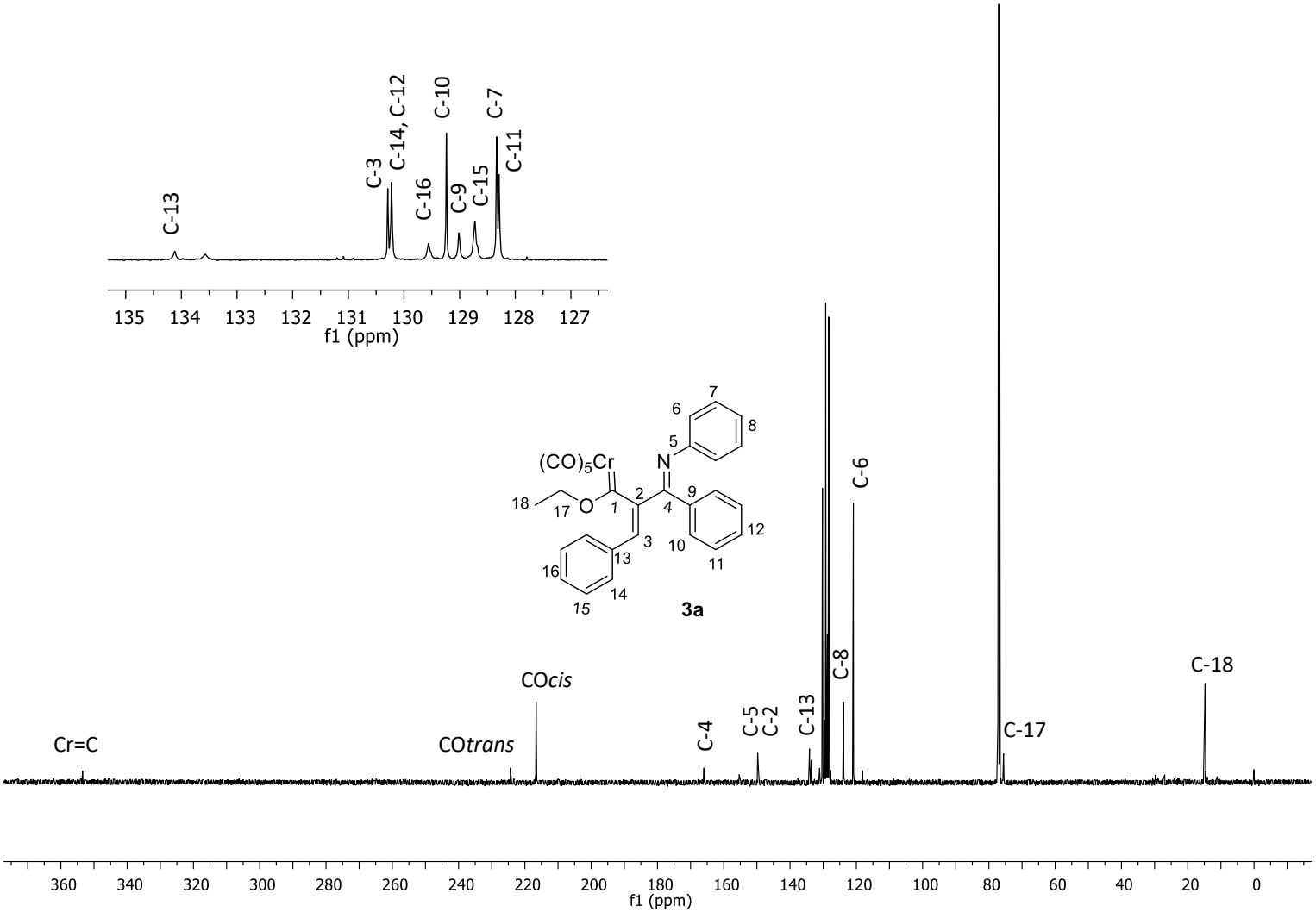

^{13}C NMR for **3a**

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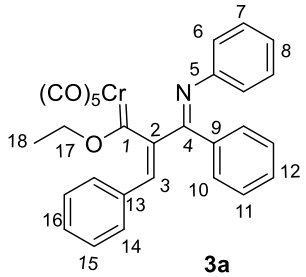
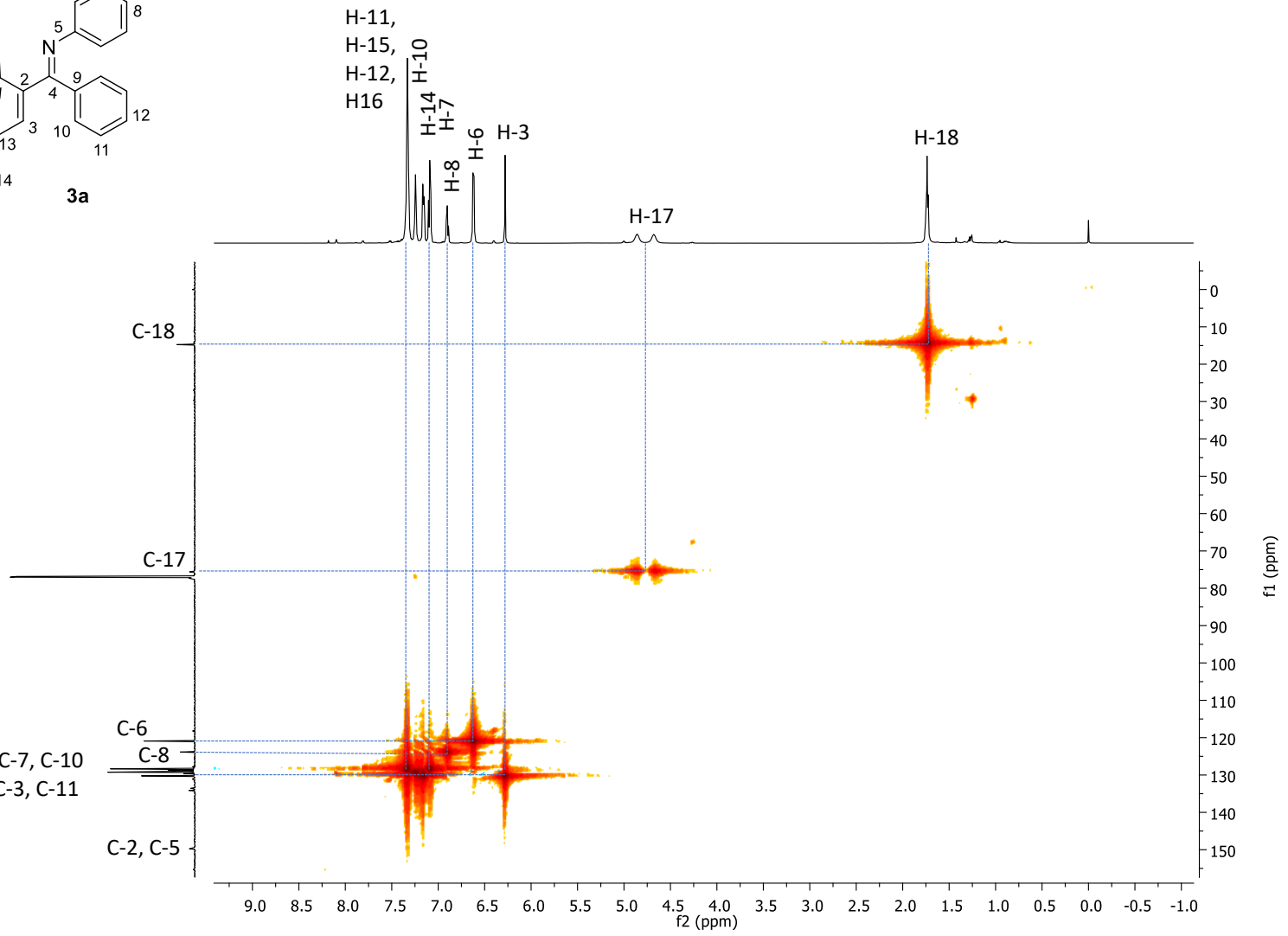


3a



gHMQC experiment for **3a**

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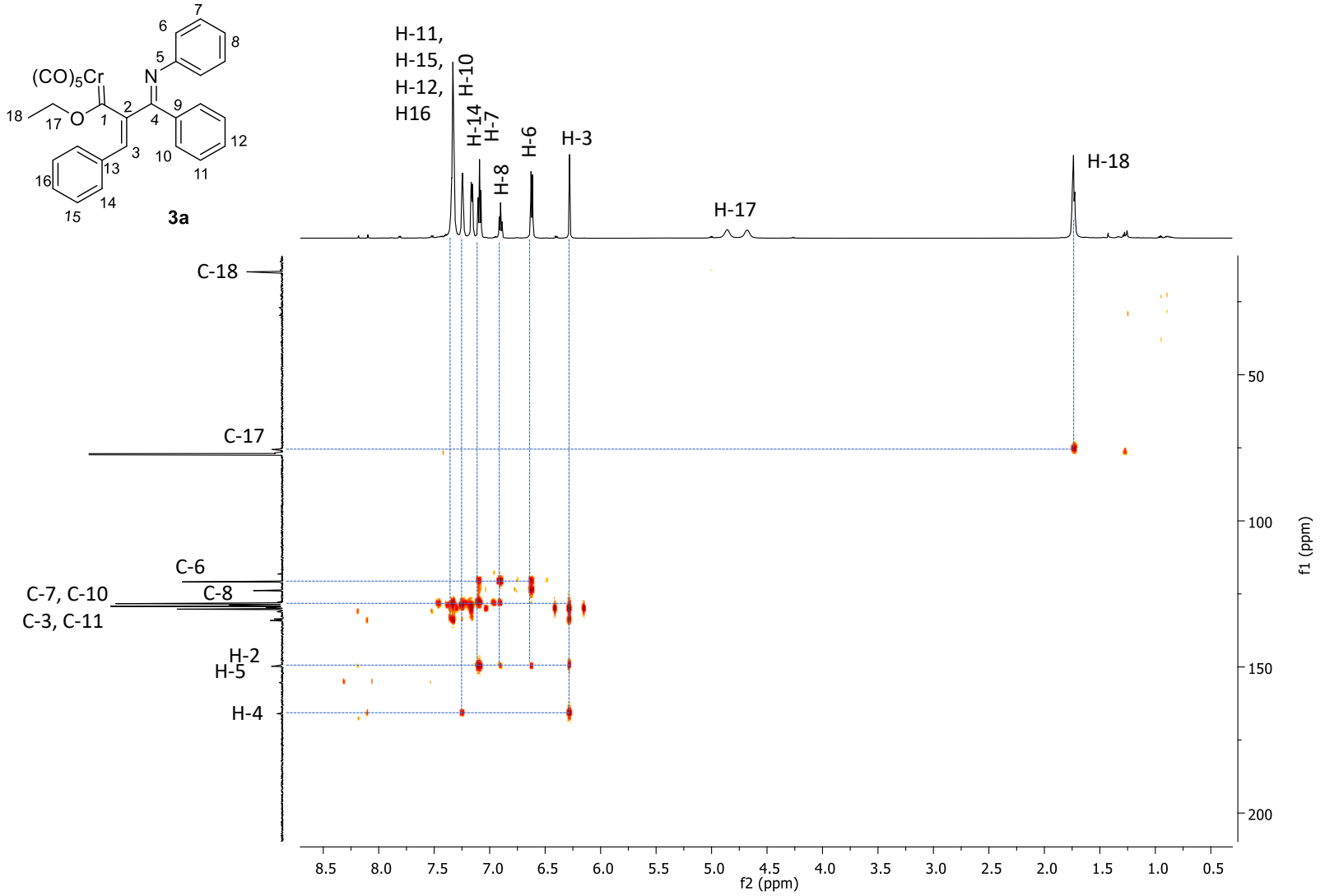

gHMBC experiment for **3a**

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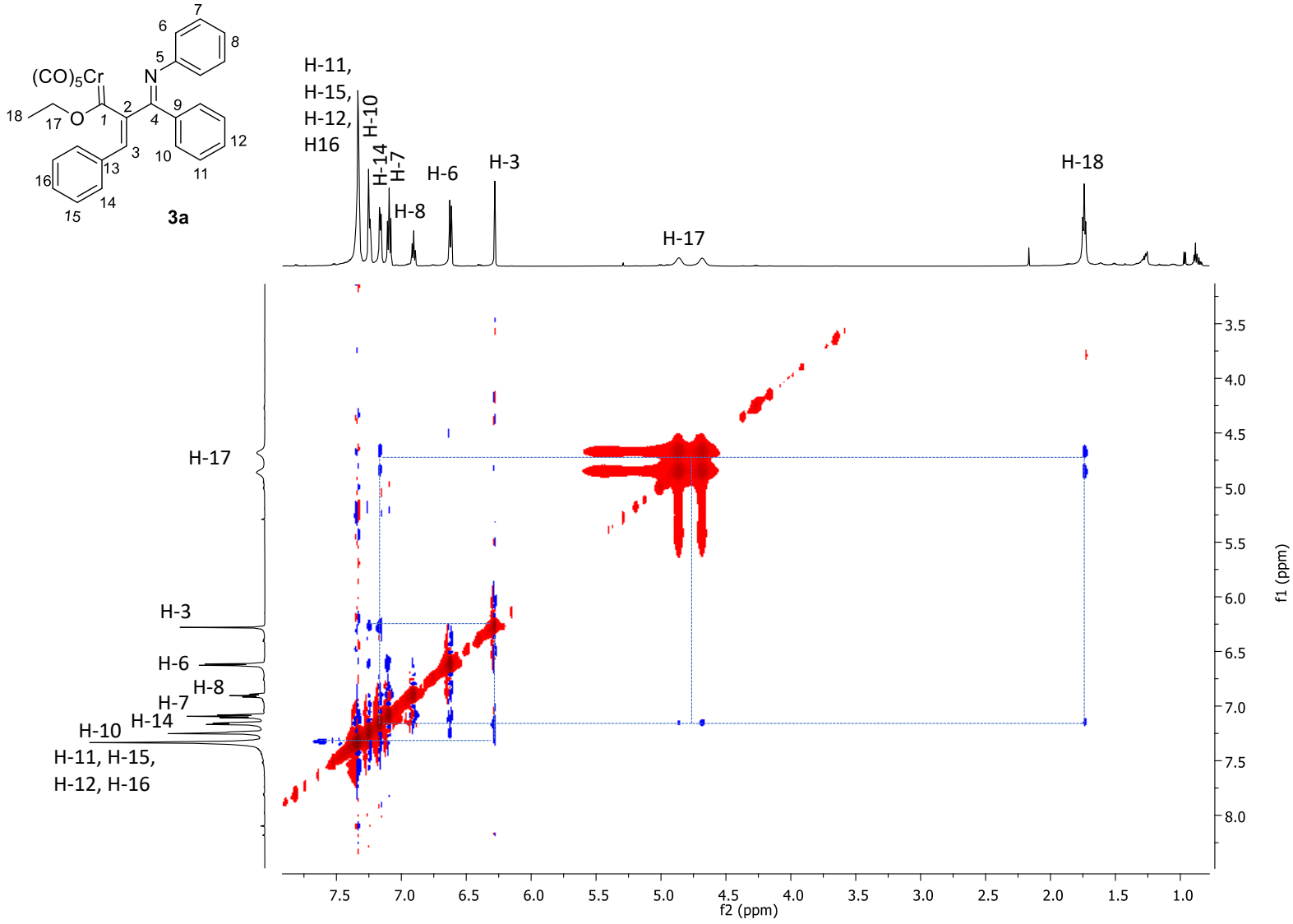

NOESY experiment for **3a**

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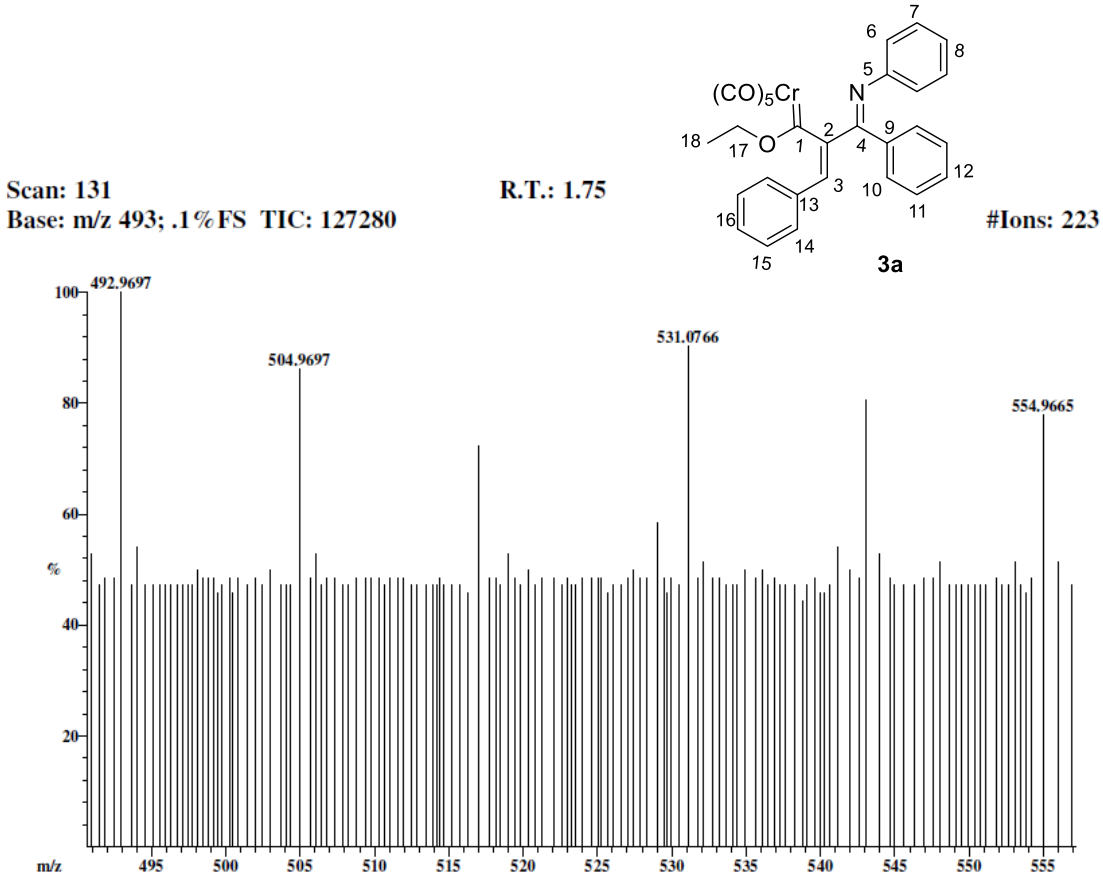

HRMS (EI) $[M]^+$ for **3a**

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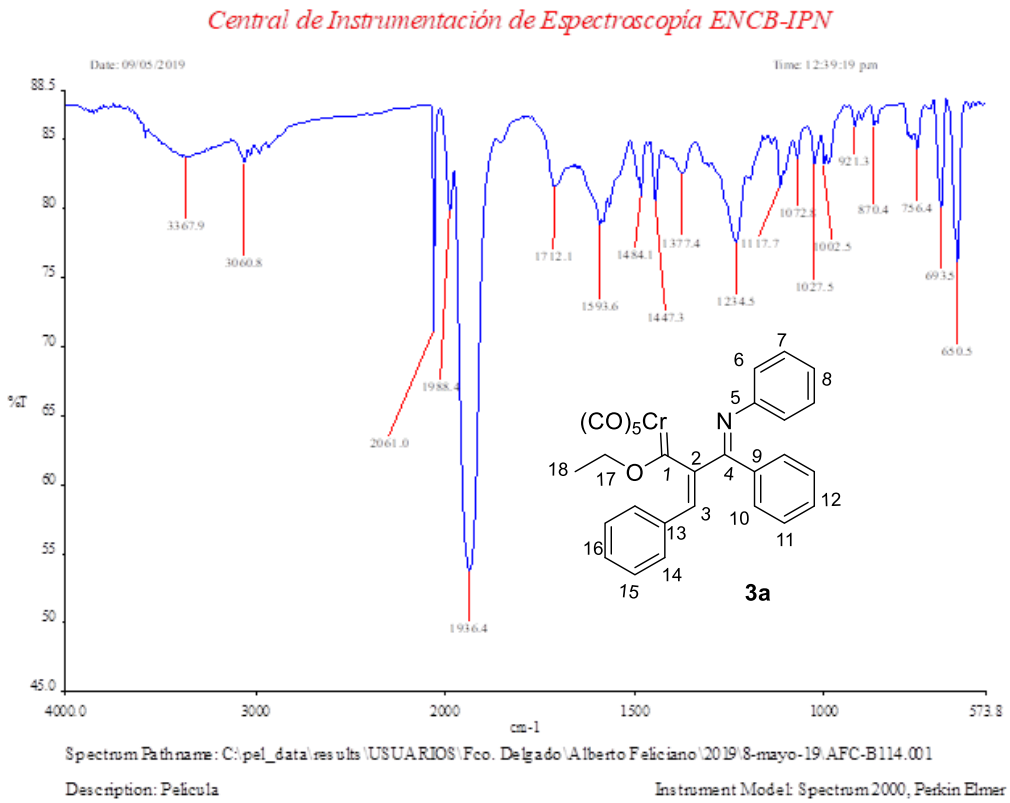

FT-IR for **3a**

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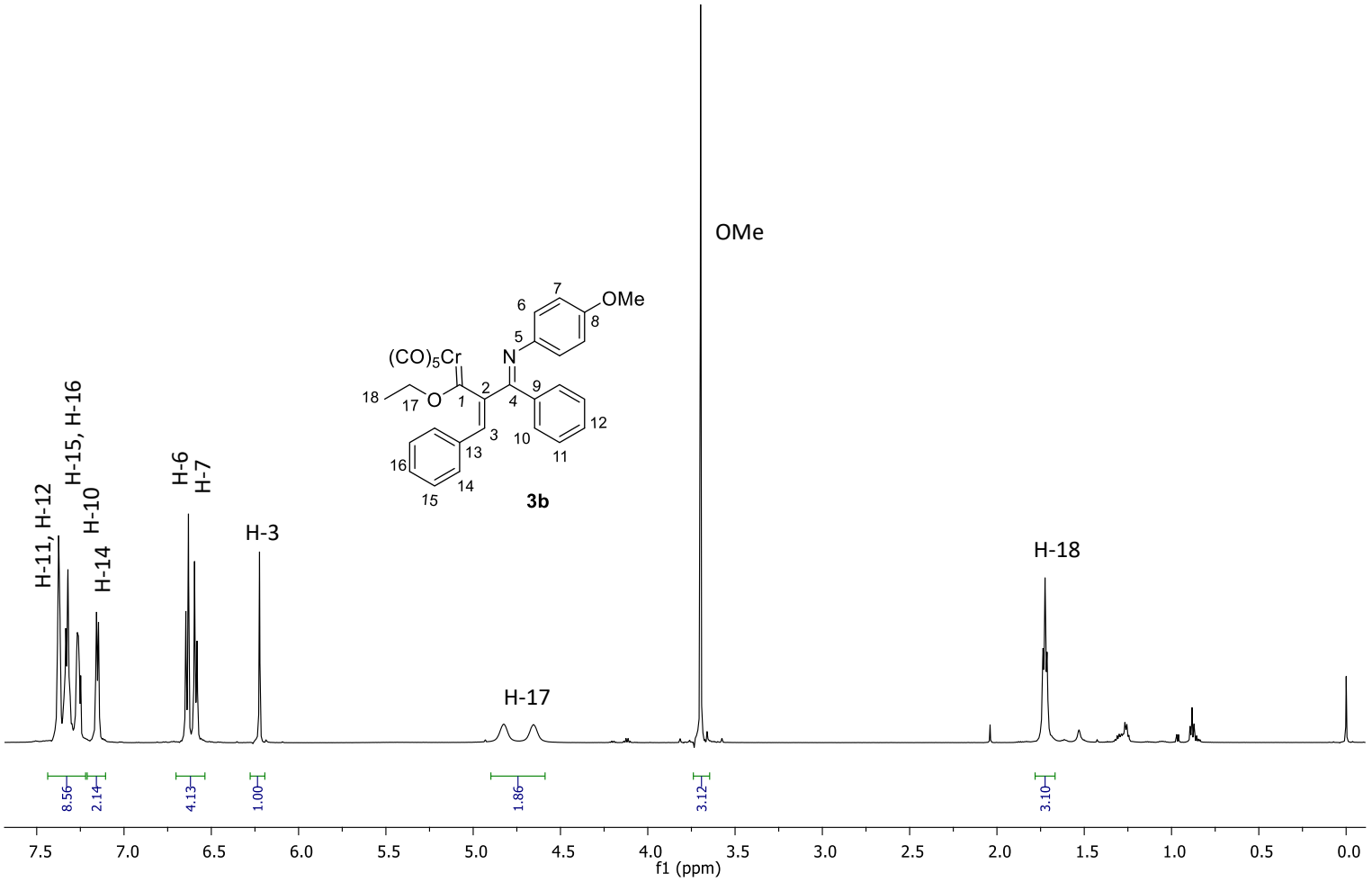

^{1}H NMR for **3b**

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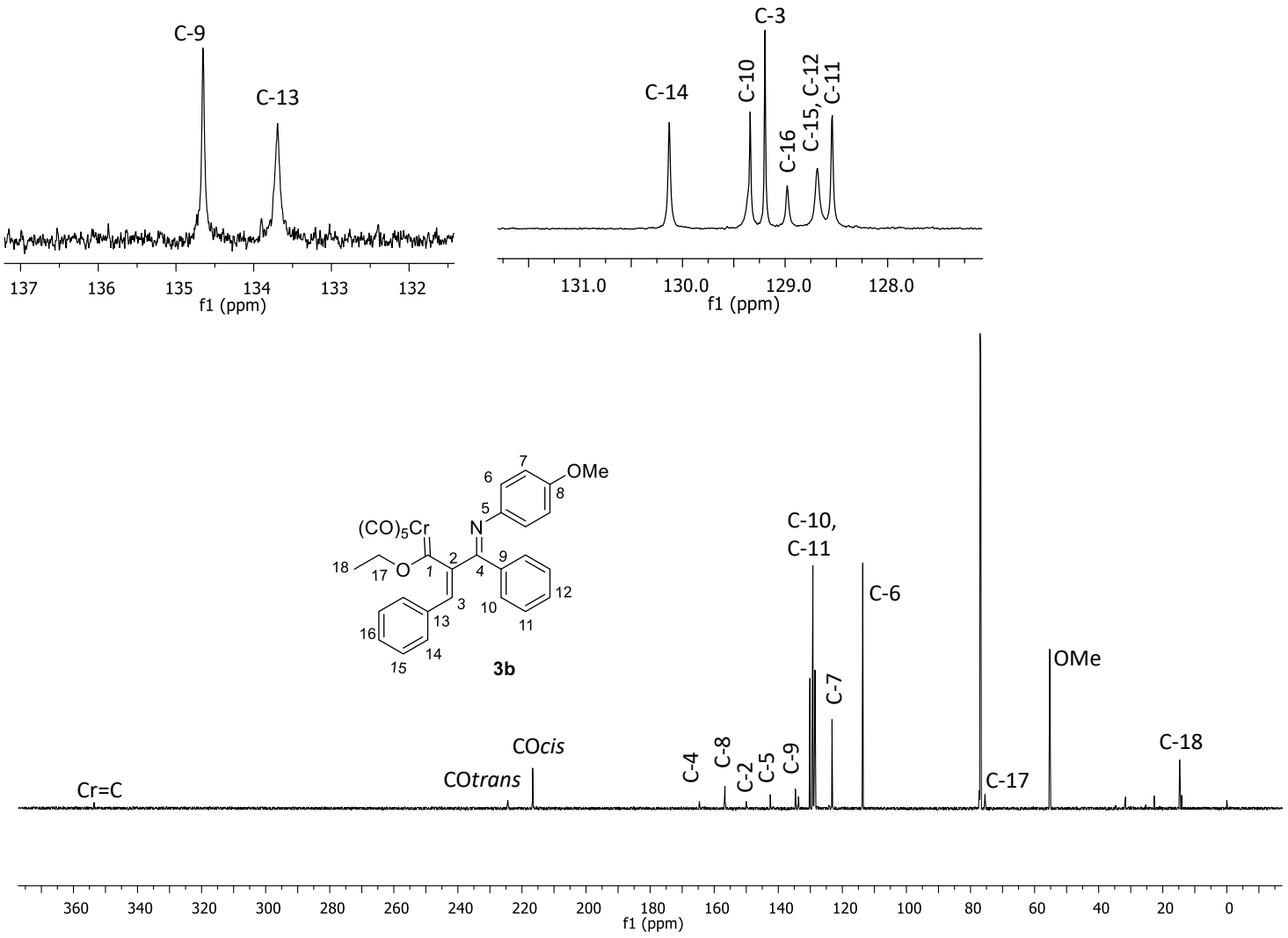

^{13}C NMR for **3b**

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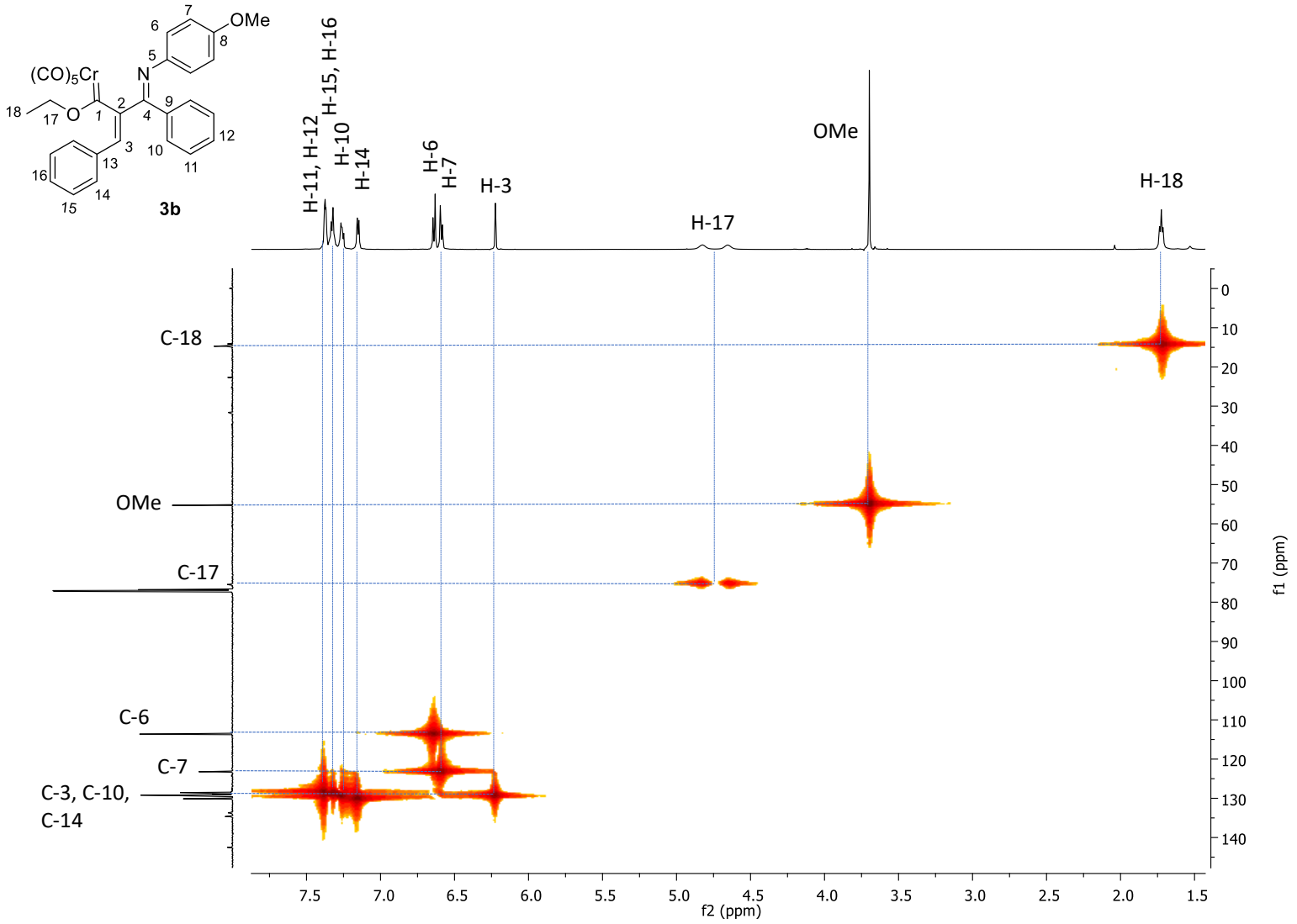

gHMQC experiment for **3b**

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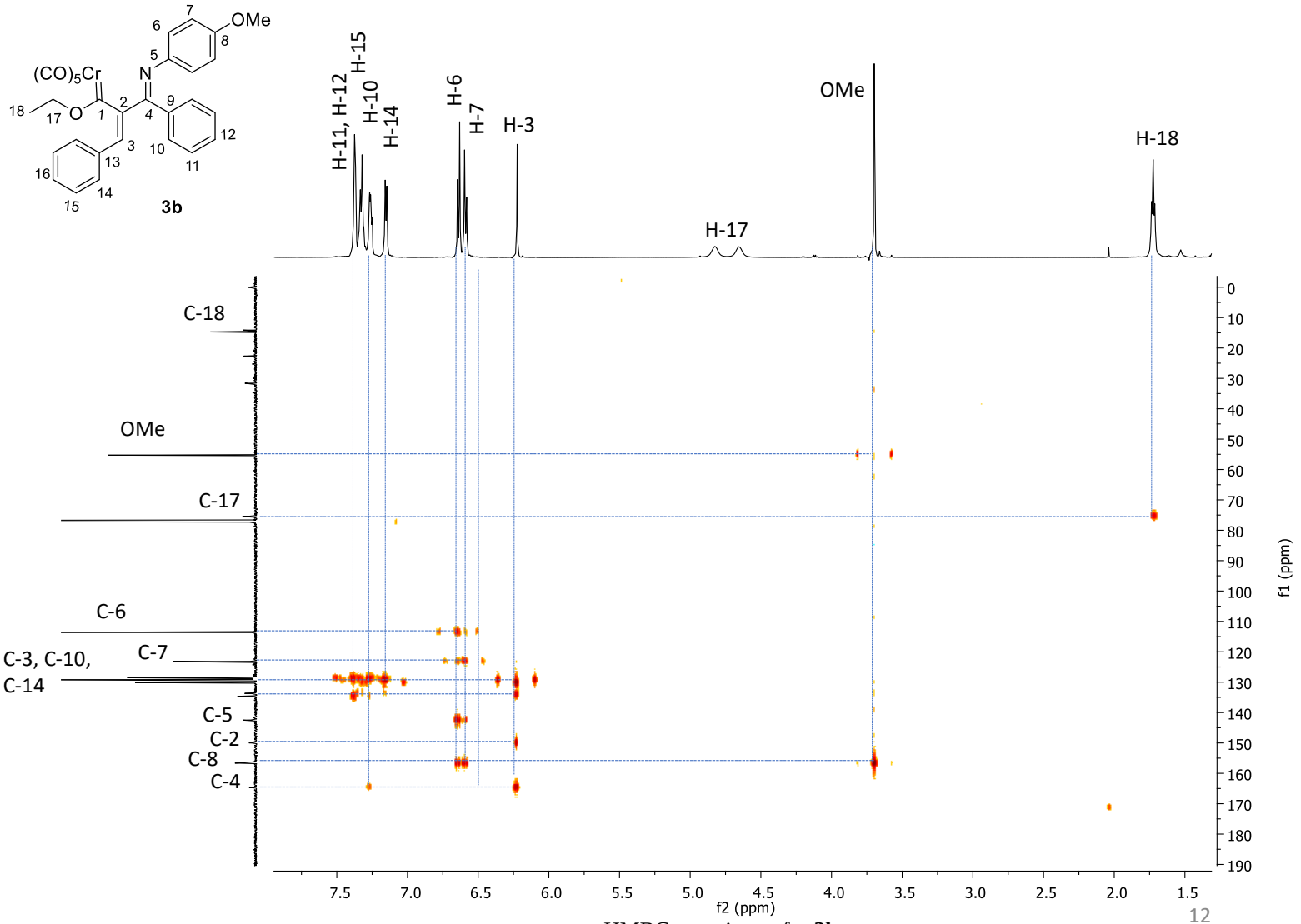
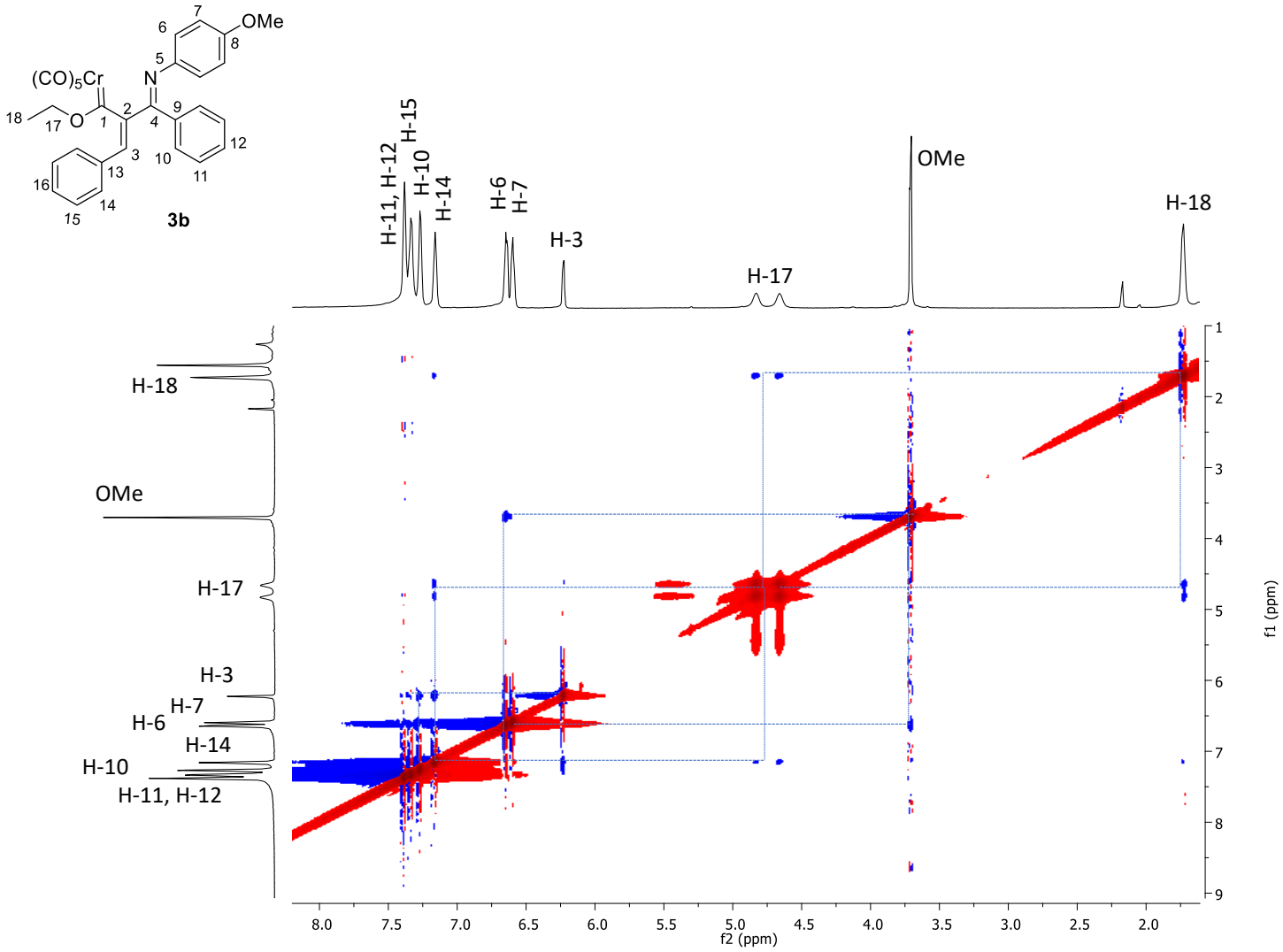


gHMBC experiment for **3b**



NOESY experiment for **3b**

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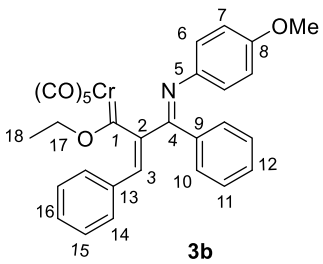
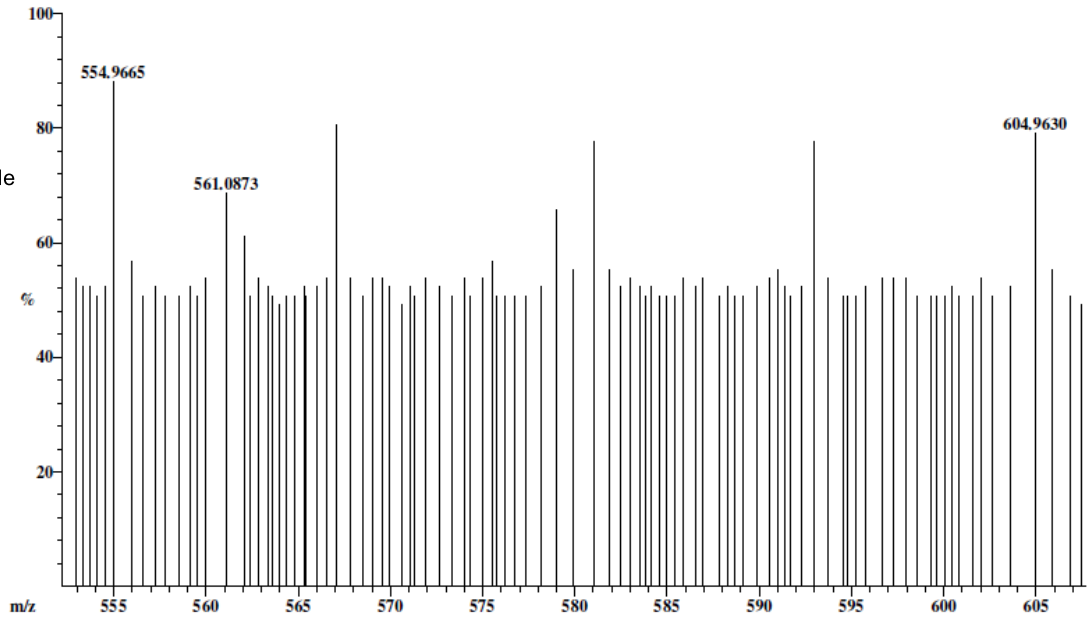
Scan: 182 **R.T.: 2.43**
Base: m/z 531; .1% FS TIC: 82896 **#Ions: 143**



3b



Selected Isotopes : $H_{0-23}C_{0-30}N_{0-1}O_{0-7}Cr_{0-1}$ Error Limit : 5 ppm

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*
561.0873	68.7%	$C_{30}H_{23}NO_7Cr$	561.0880	-1.2

HRMS (EI) $[M]^+$ for **3b**

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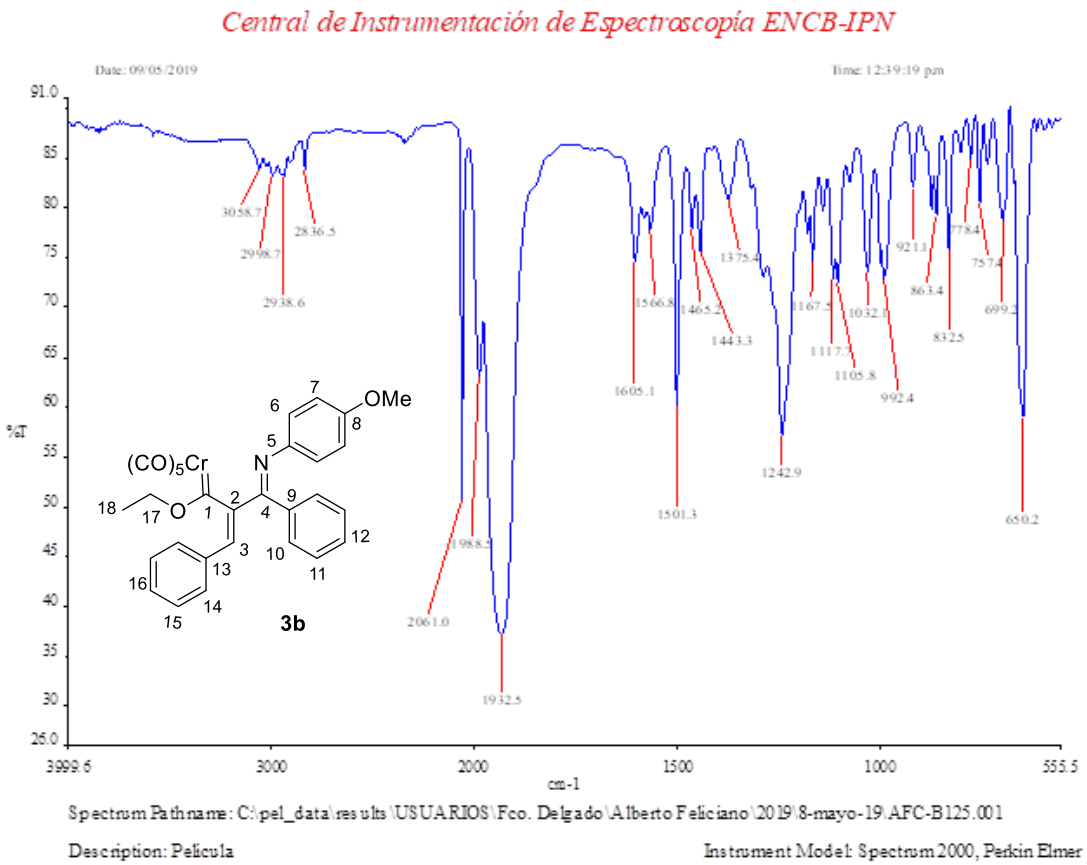

FT-IR for **3b**

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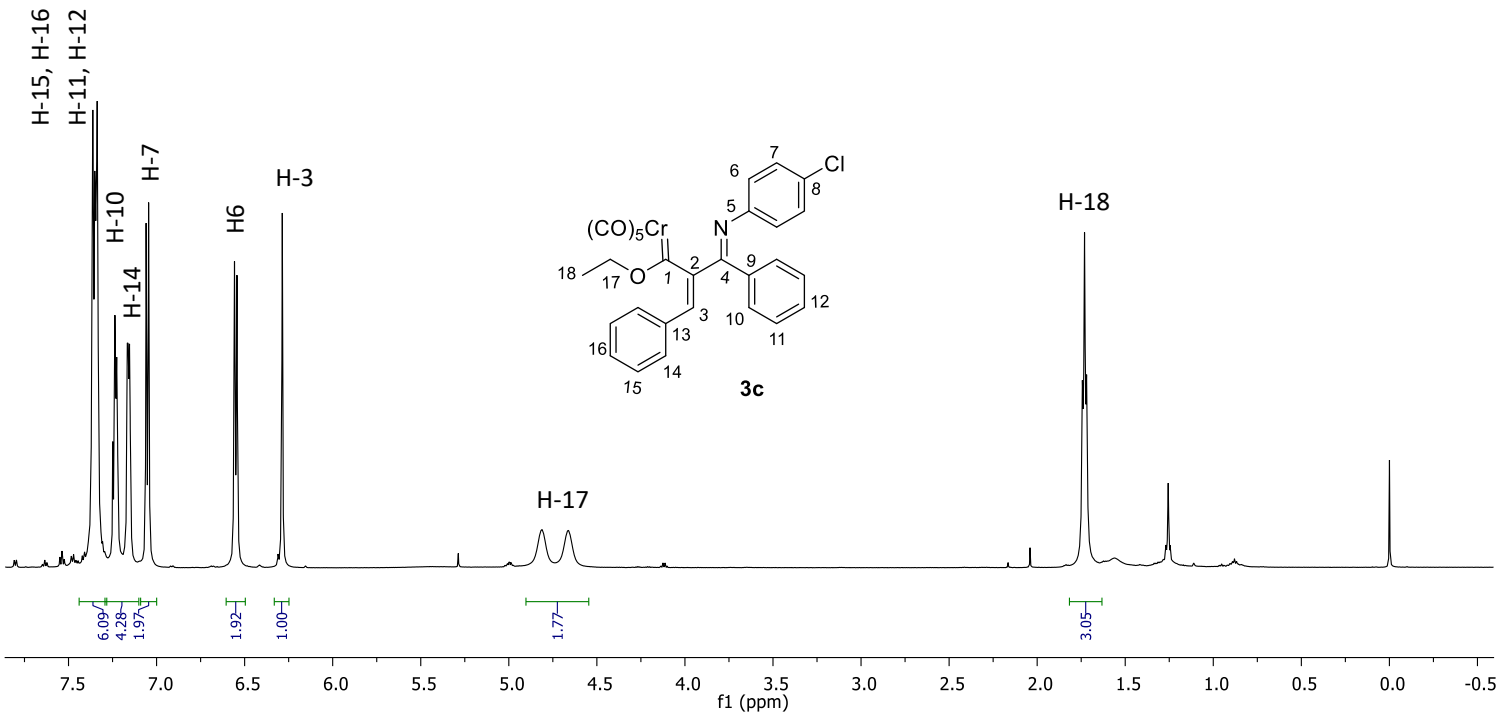

^{1}H NMR for **3c**

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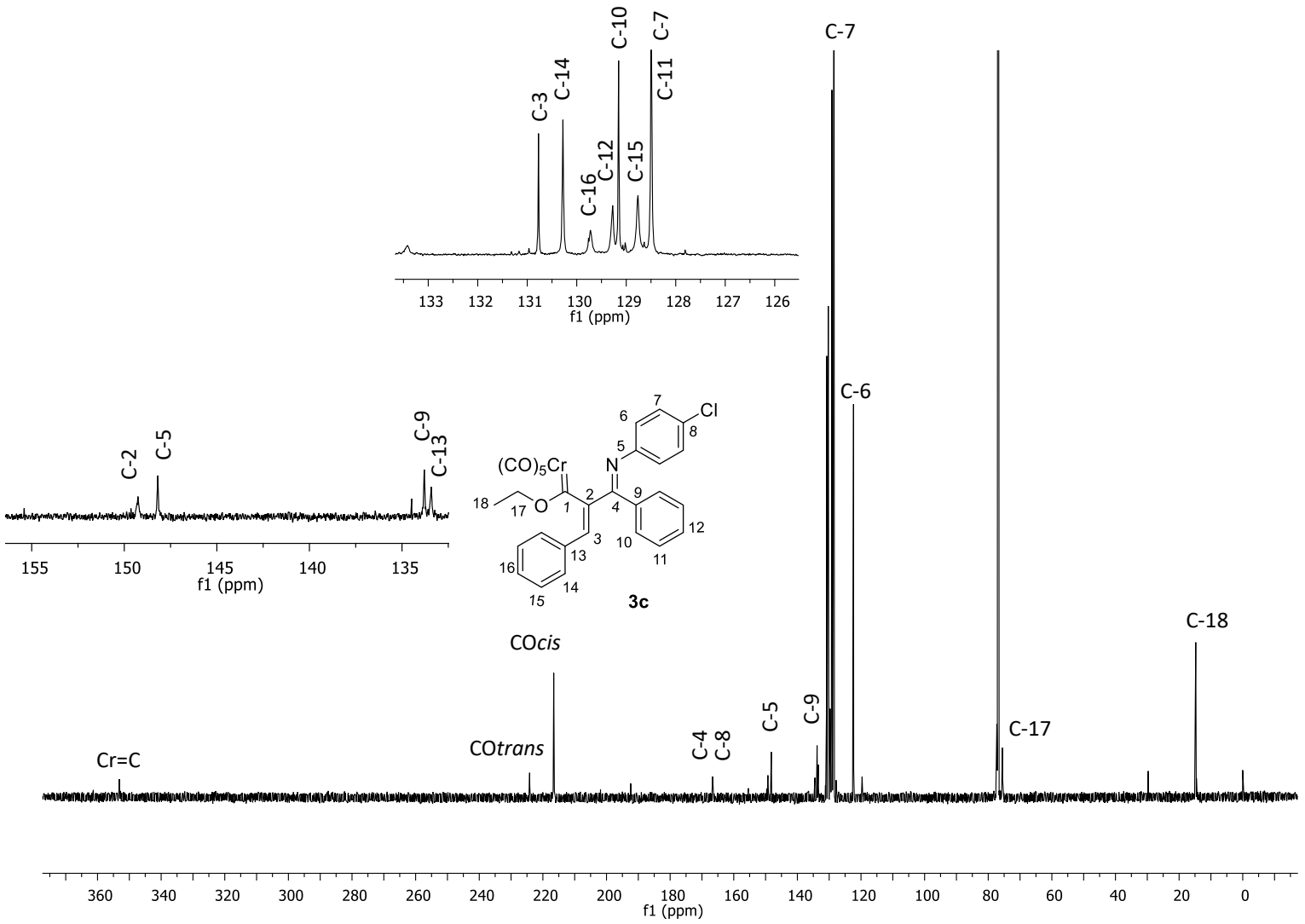
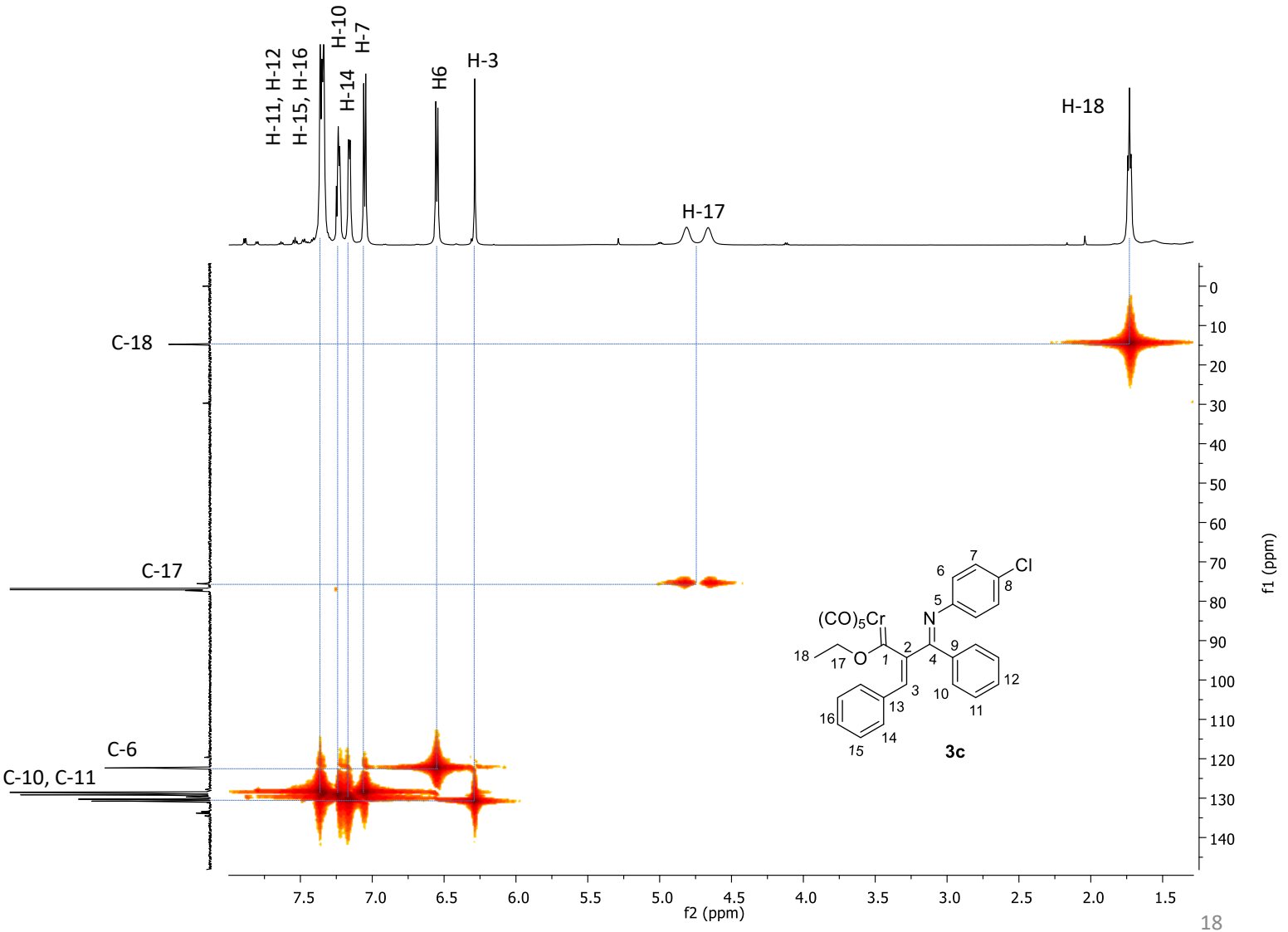


^{13}C NMR for **3c**

ISSN-e 2594-0317



gHMQC experiment for **3c**

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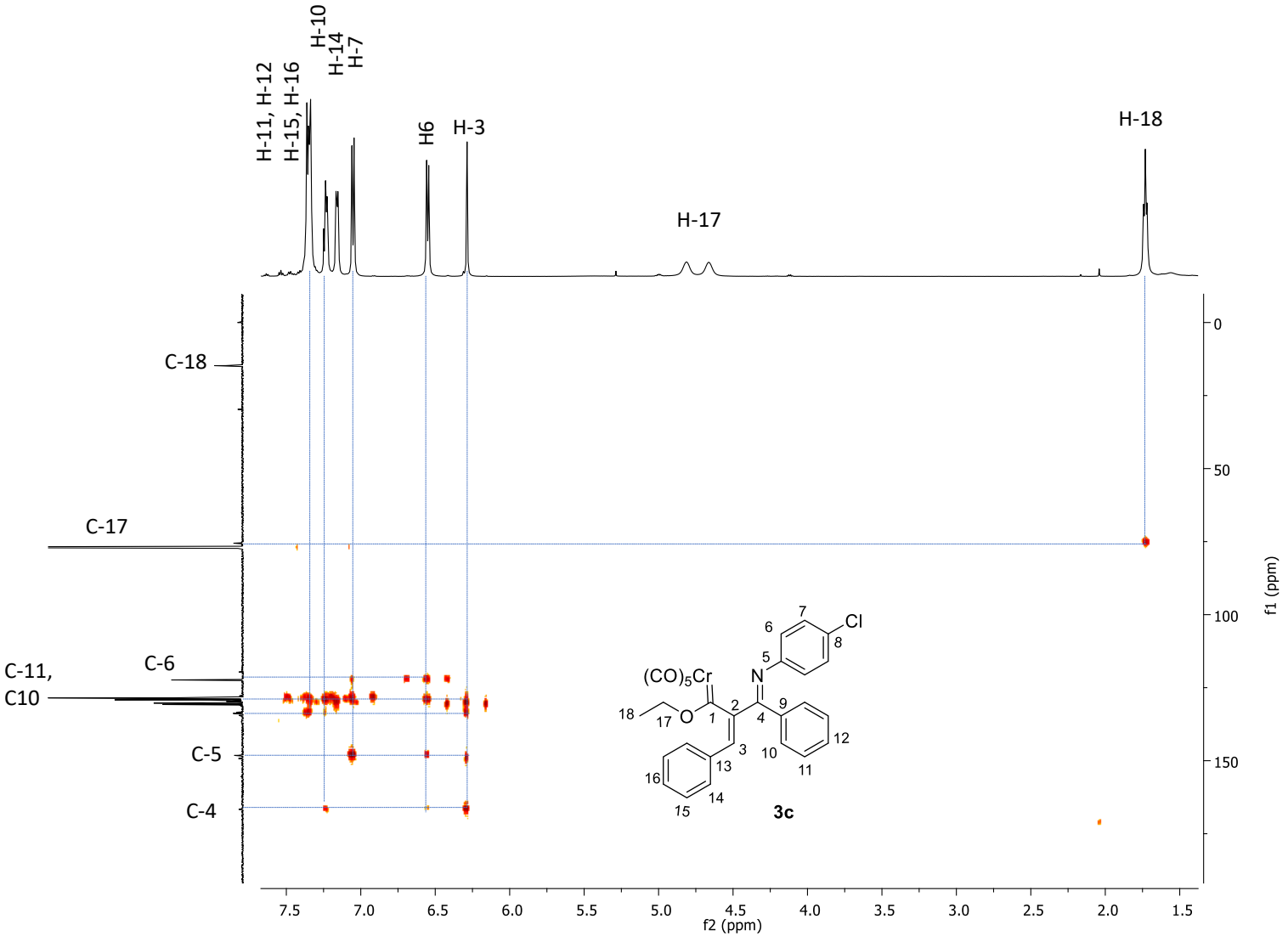

gHMBC experiment for **3c**

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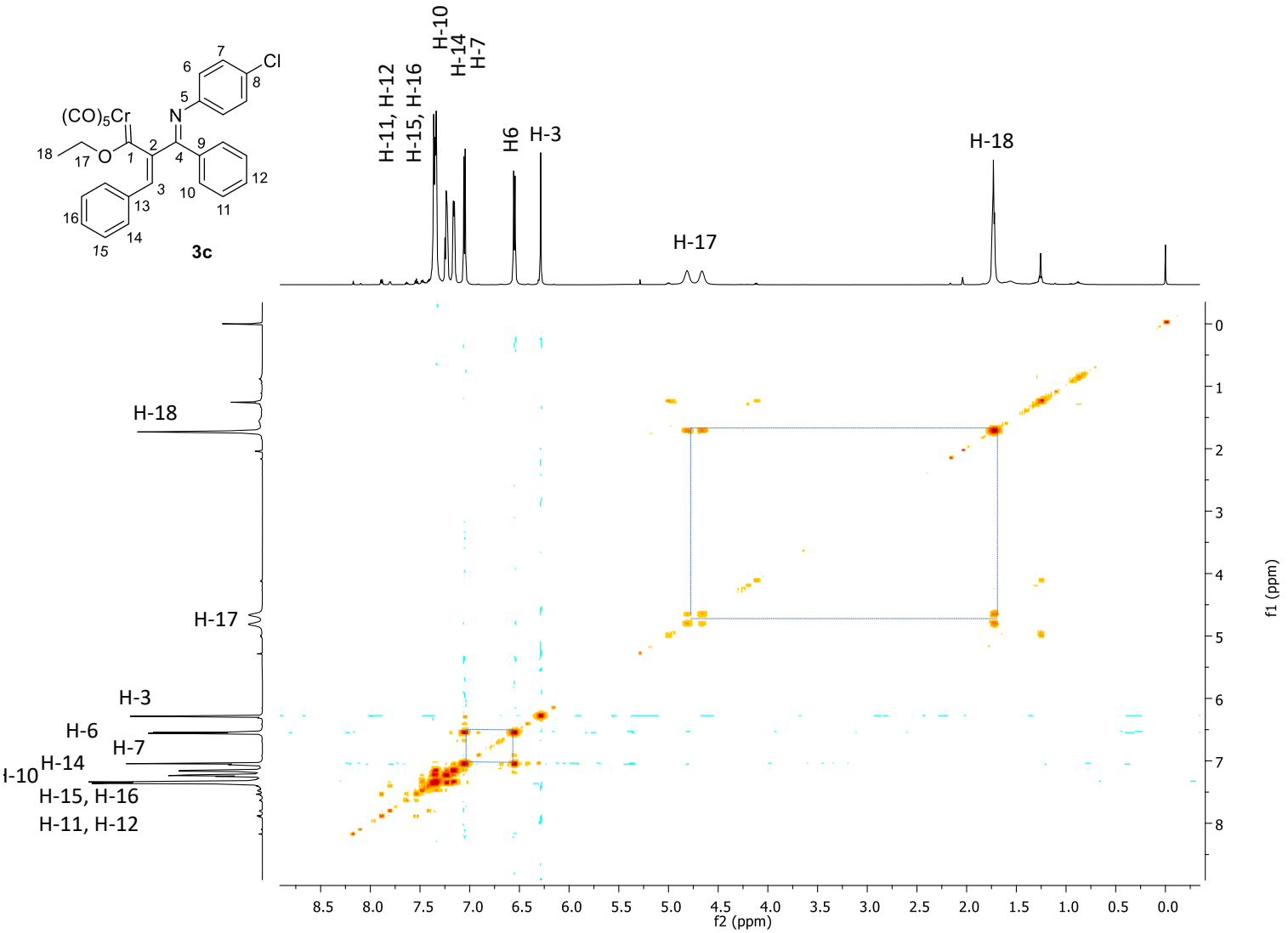

COSY experiment for **3c**

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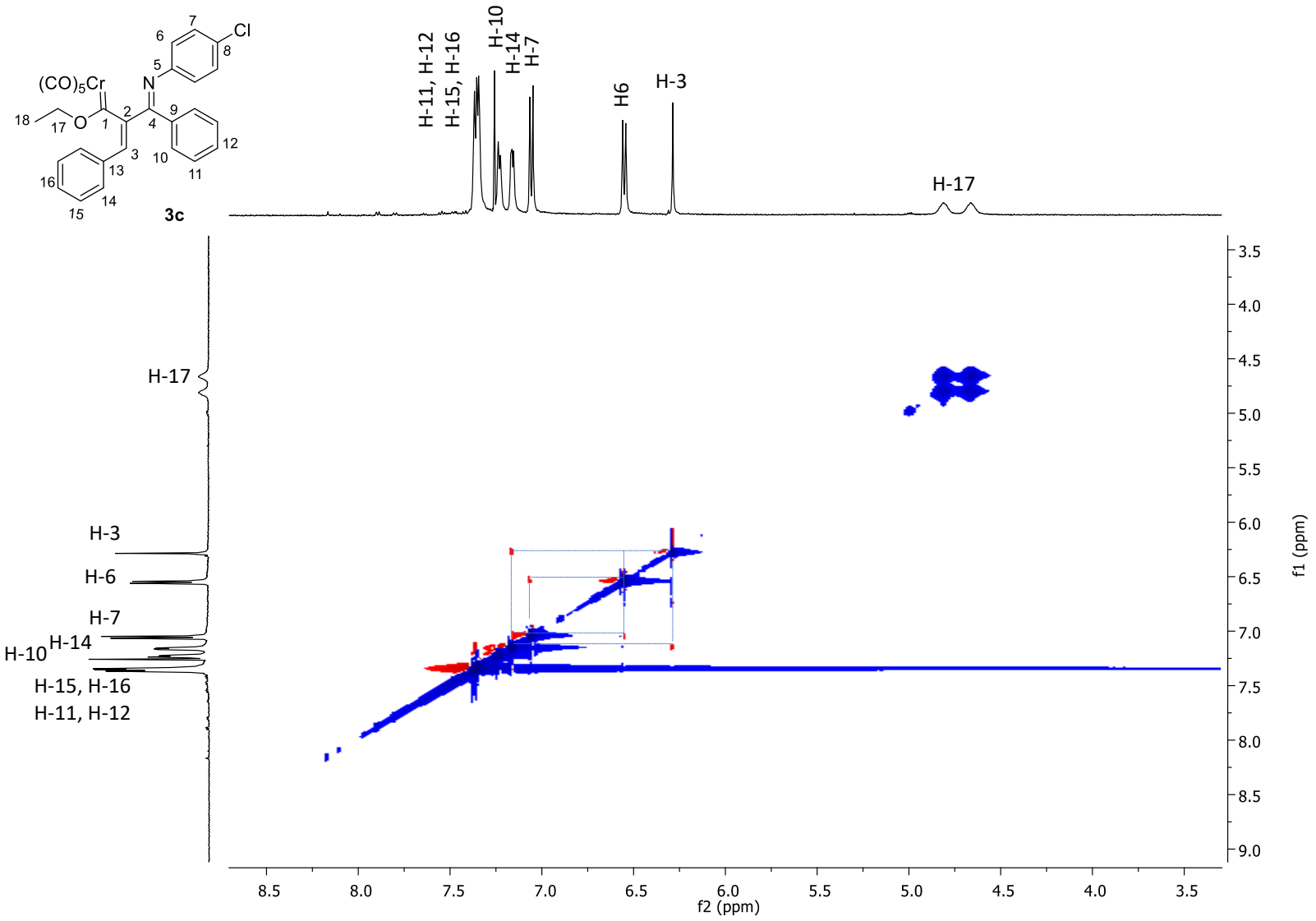

NOESY experiment for **3c**

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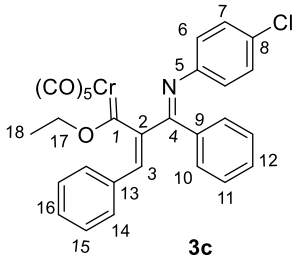
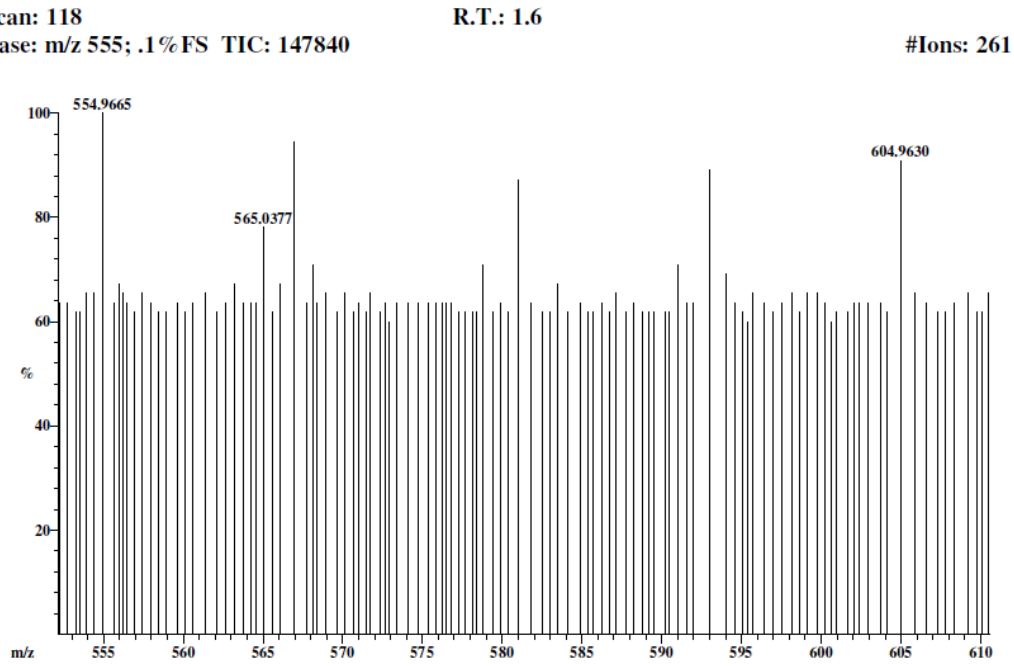


3c



Selected Isotopes : $H_{0-20}C_{0-29}N_{0-1}O_{0-6}Cl_{0-1}Cr_{0-1}$ Error Limit : 5 ppm

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*
565.0377	78.2%	$C_{29}H_{20}NO_6ClCr$	565.0384	-1.3

HRMS (EI) $[M]^+$ for **3c**

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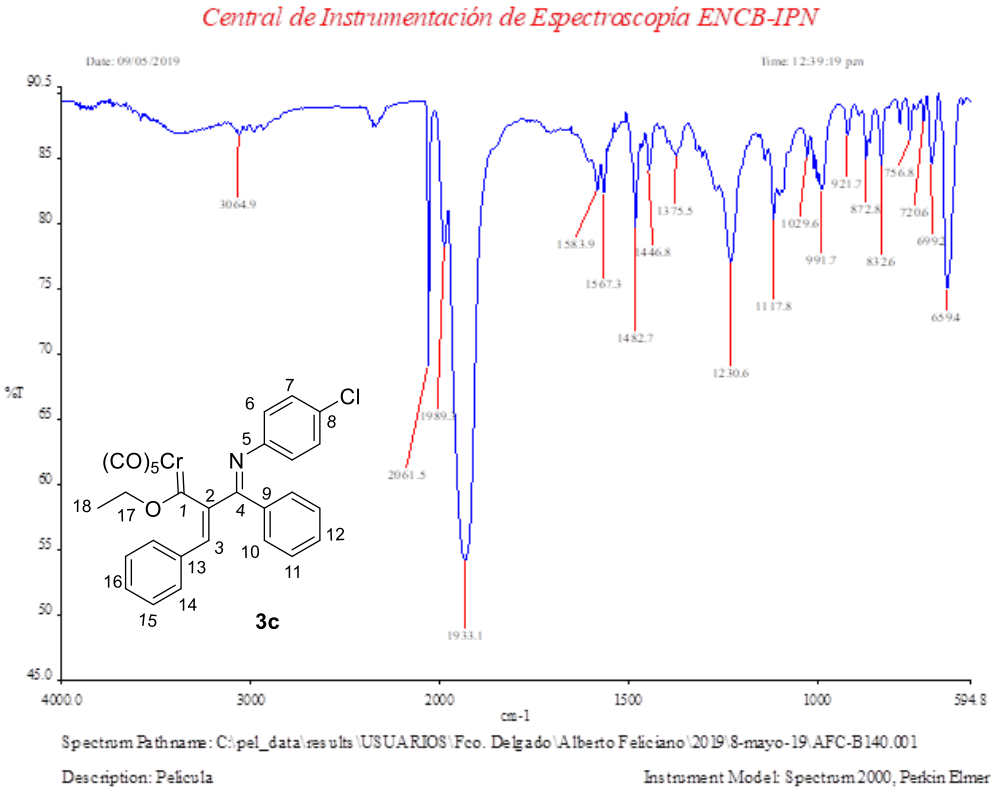

FT-IR for **3c**

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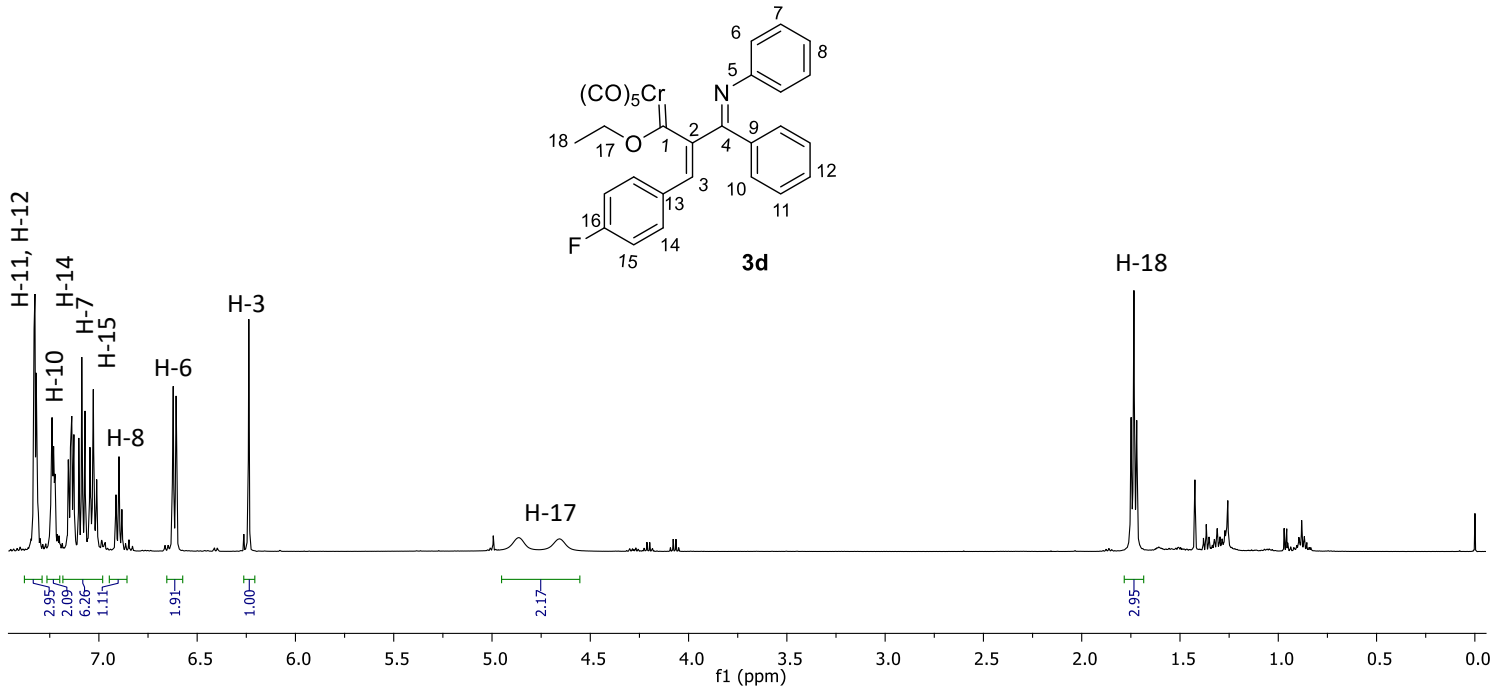

^{1}H NMR for **3d**

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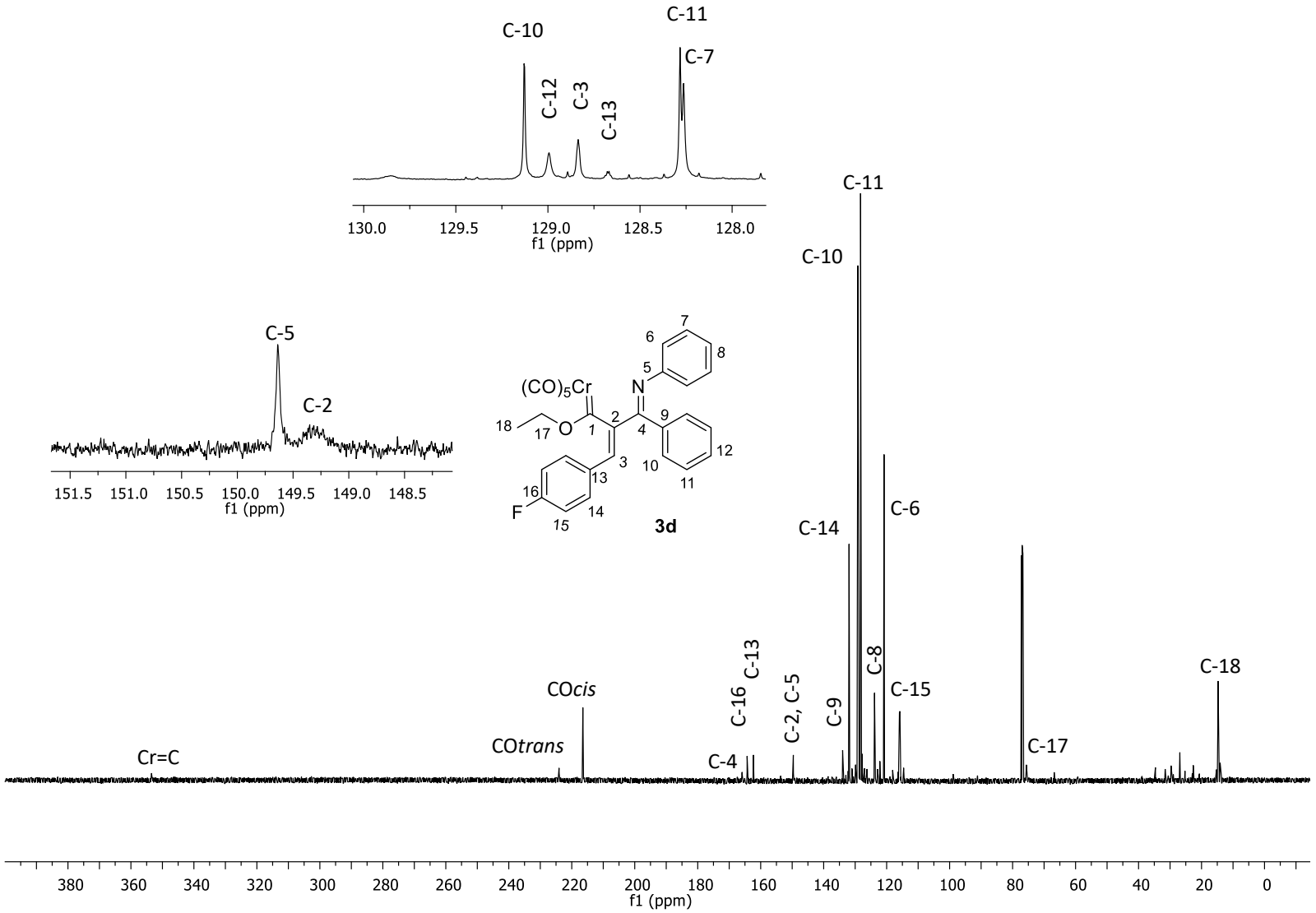

^{13}C NMR for **3d**

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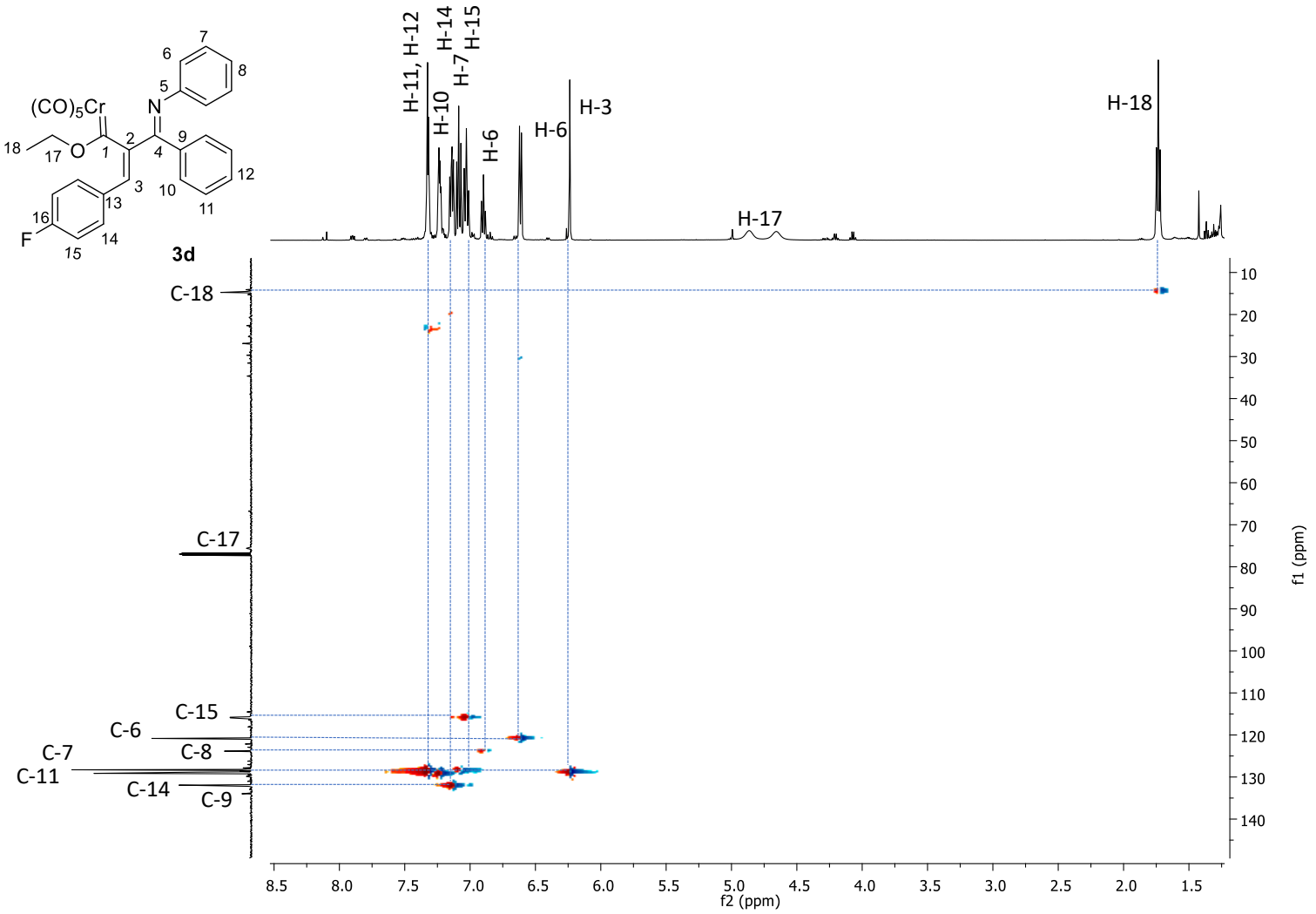
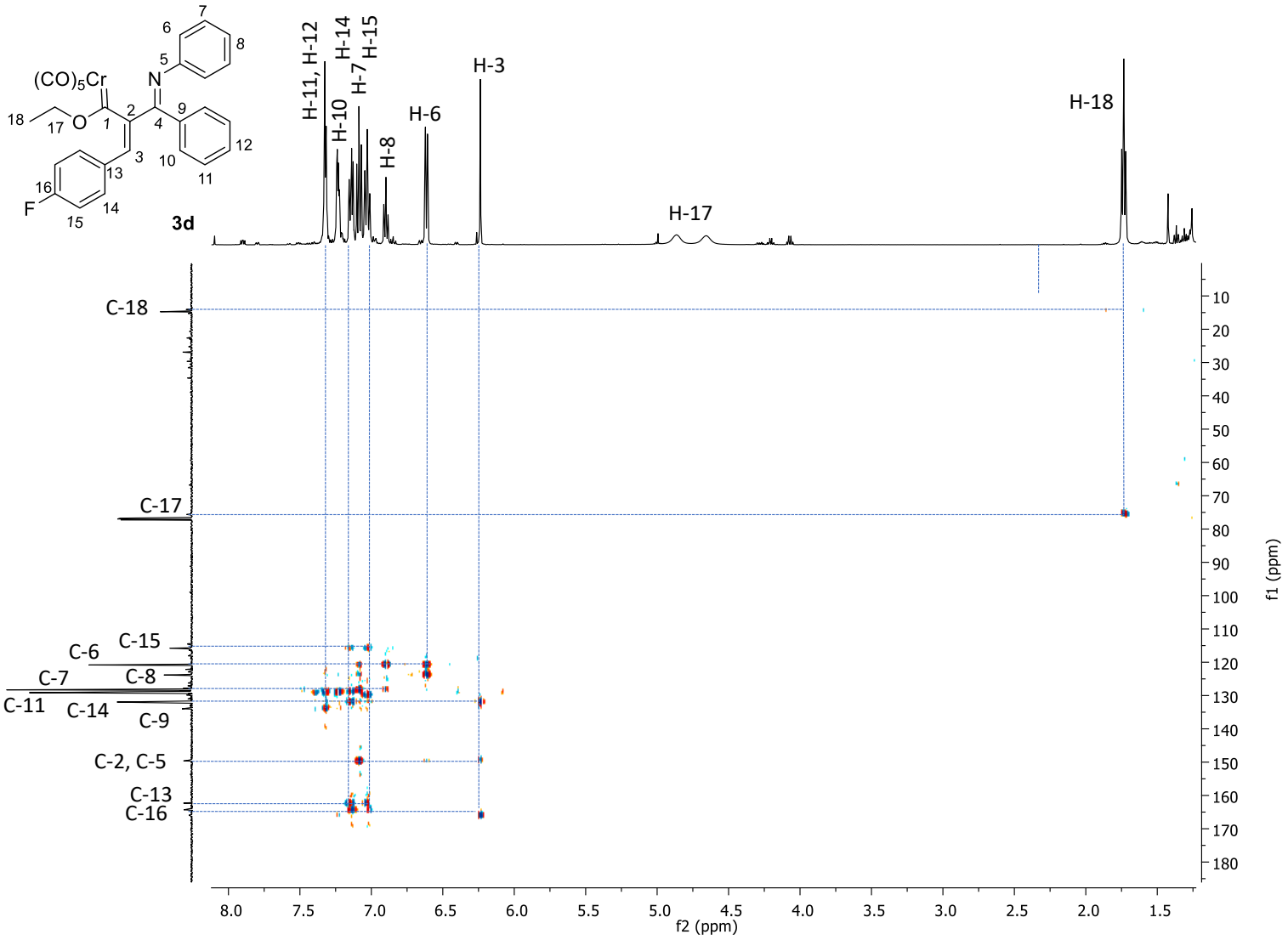


gHMQC experiment for **3d**

ISSN-e 2594-0317



gHMBC experiment for **3d**

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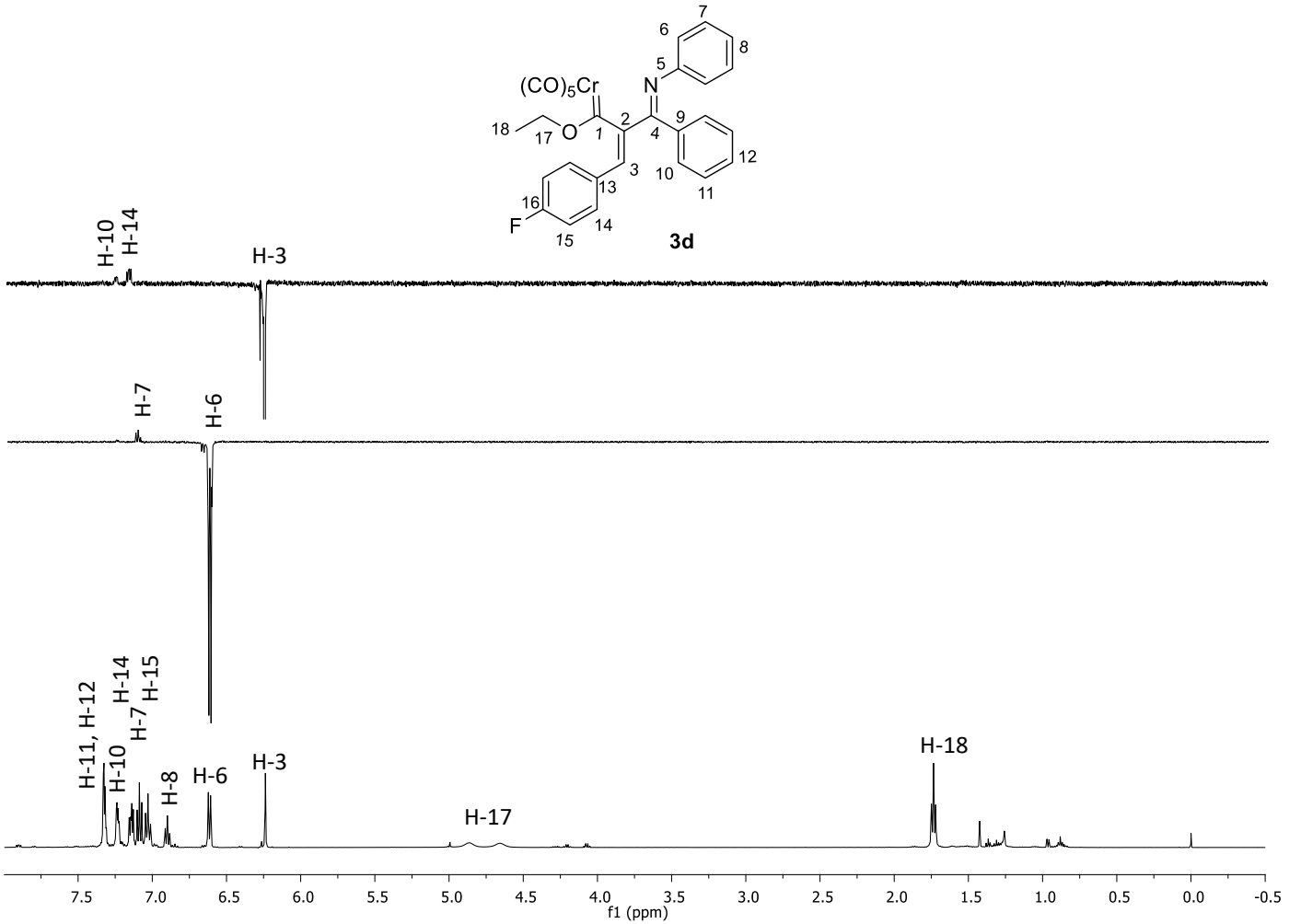

nOe experiment for **3d**

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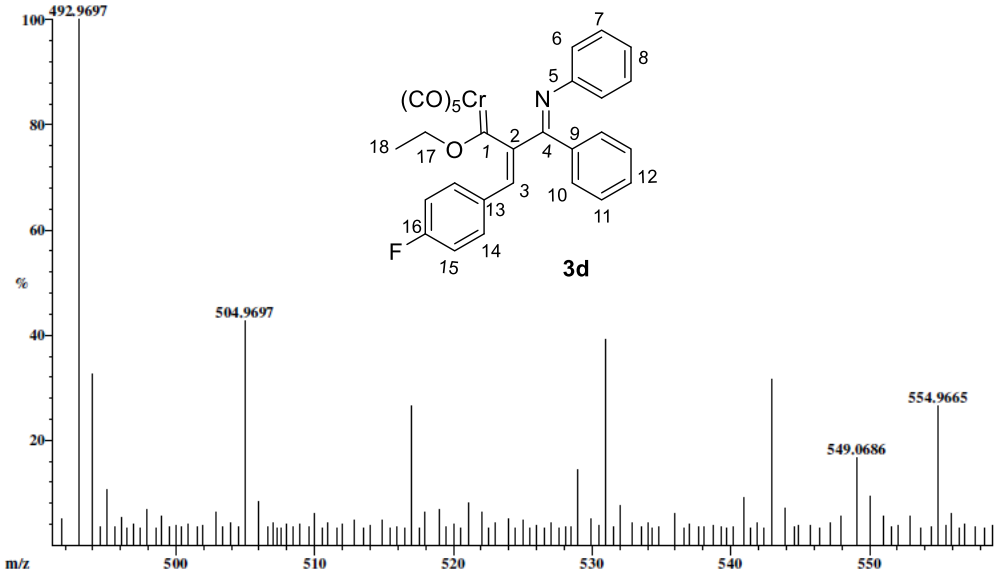
Sample: FDR-AFC-B122
Instrument: JEOL GCmate
Inlet: Direct Probe **Ionization mode: EI+**

Scan: 320 **R.T.: 4.26**
Base: m/z 493; 1.6%FS TIC: 183392 **#Ions: 175**



Selected Isotopes : $H_{0-20}C_{0-29}Cr_{0-1}F_{0-1}N_{0-1}O_{0-6}$ **Error Limit : 5 ppm**

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*
549.0686	16.7%	$C_{29}H_{20}CrFNO_6$	549.0680	1.1

HRMS (EI) $[M]^+$ for **3d**

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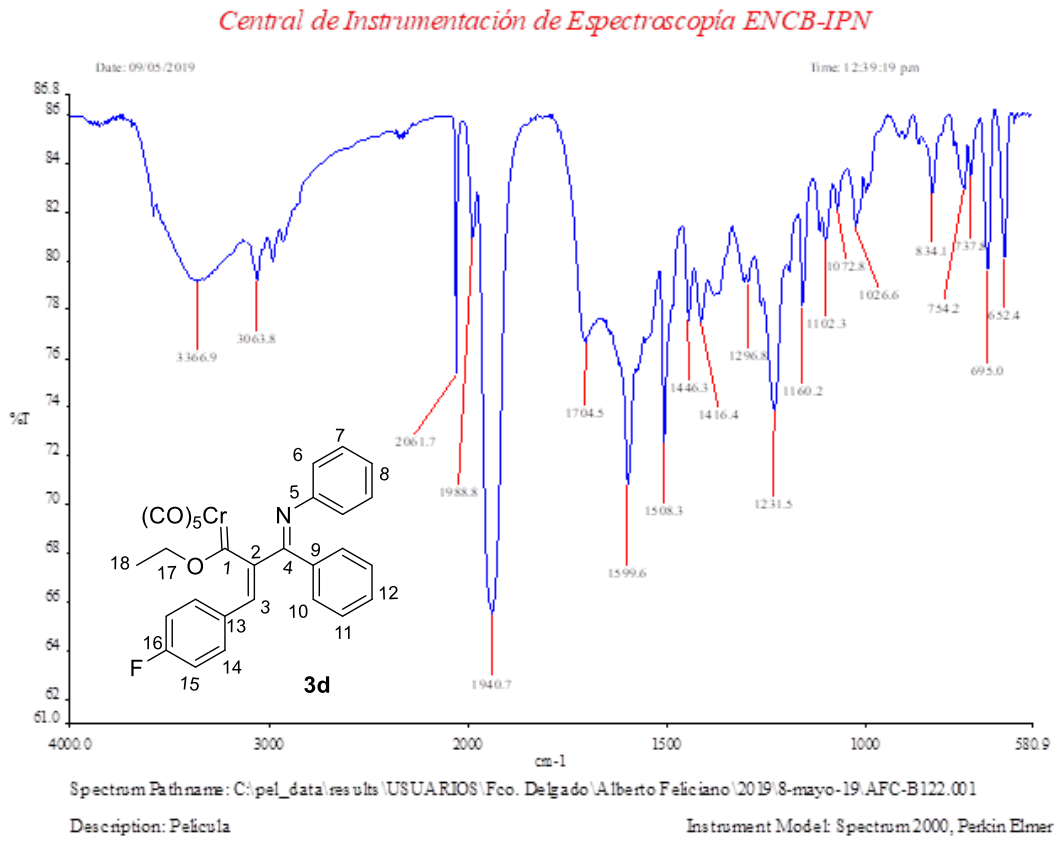

FT-IR for **3d**

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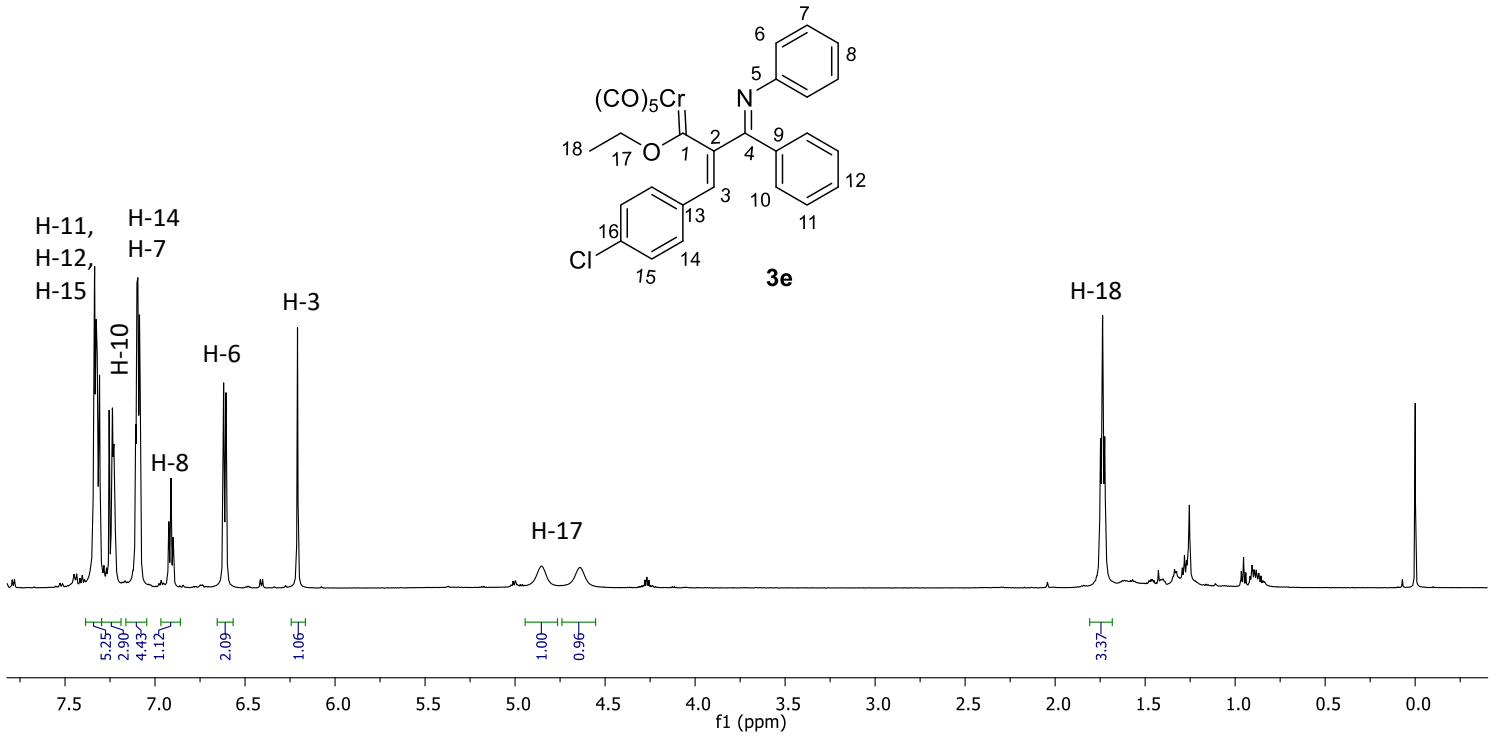

^{1}H NMR for **3e**

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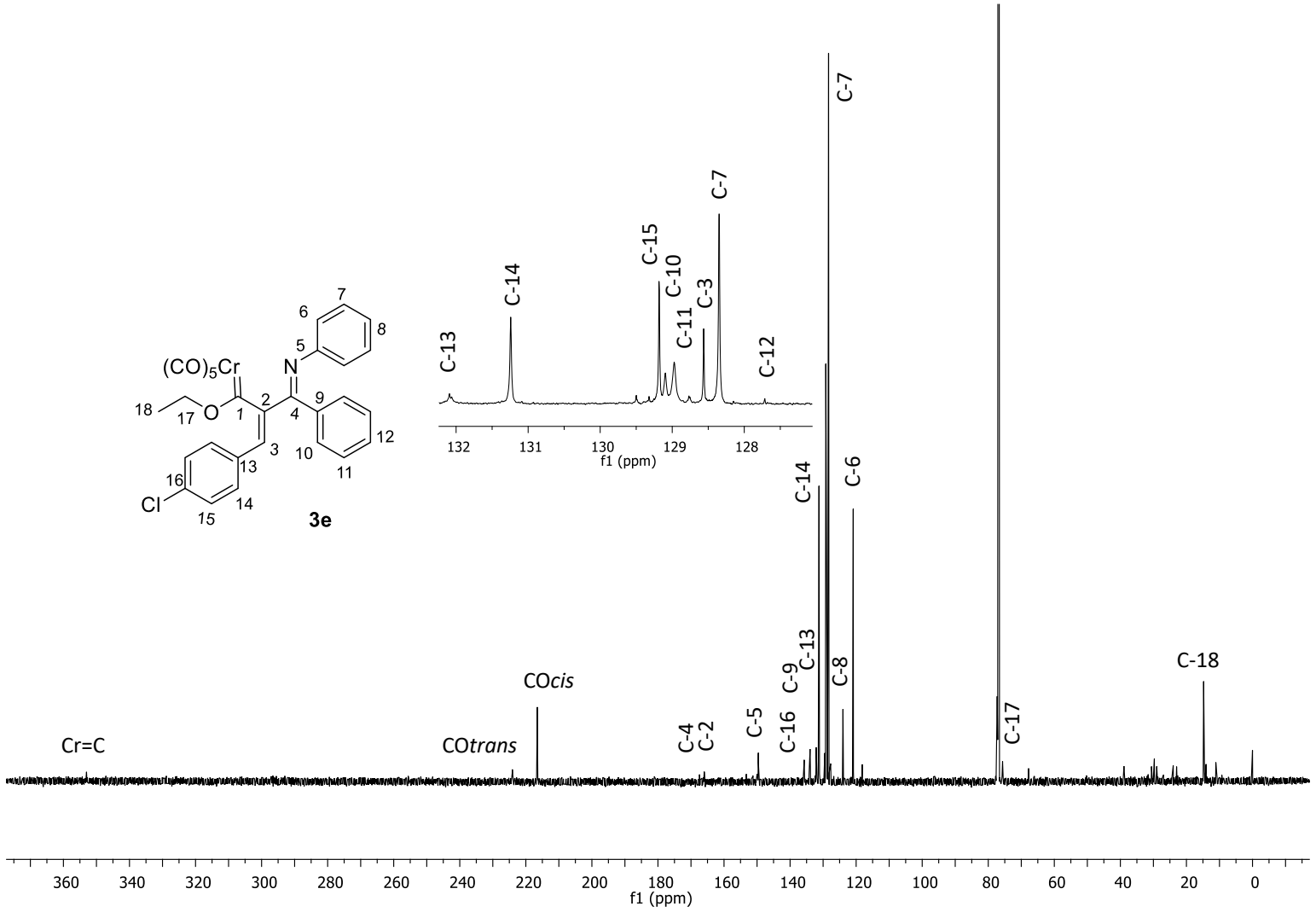

^{13}C NMR for **3e**

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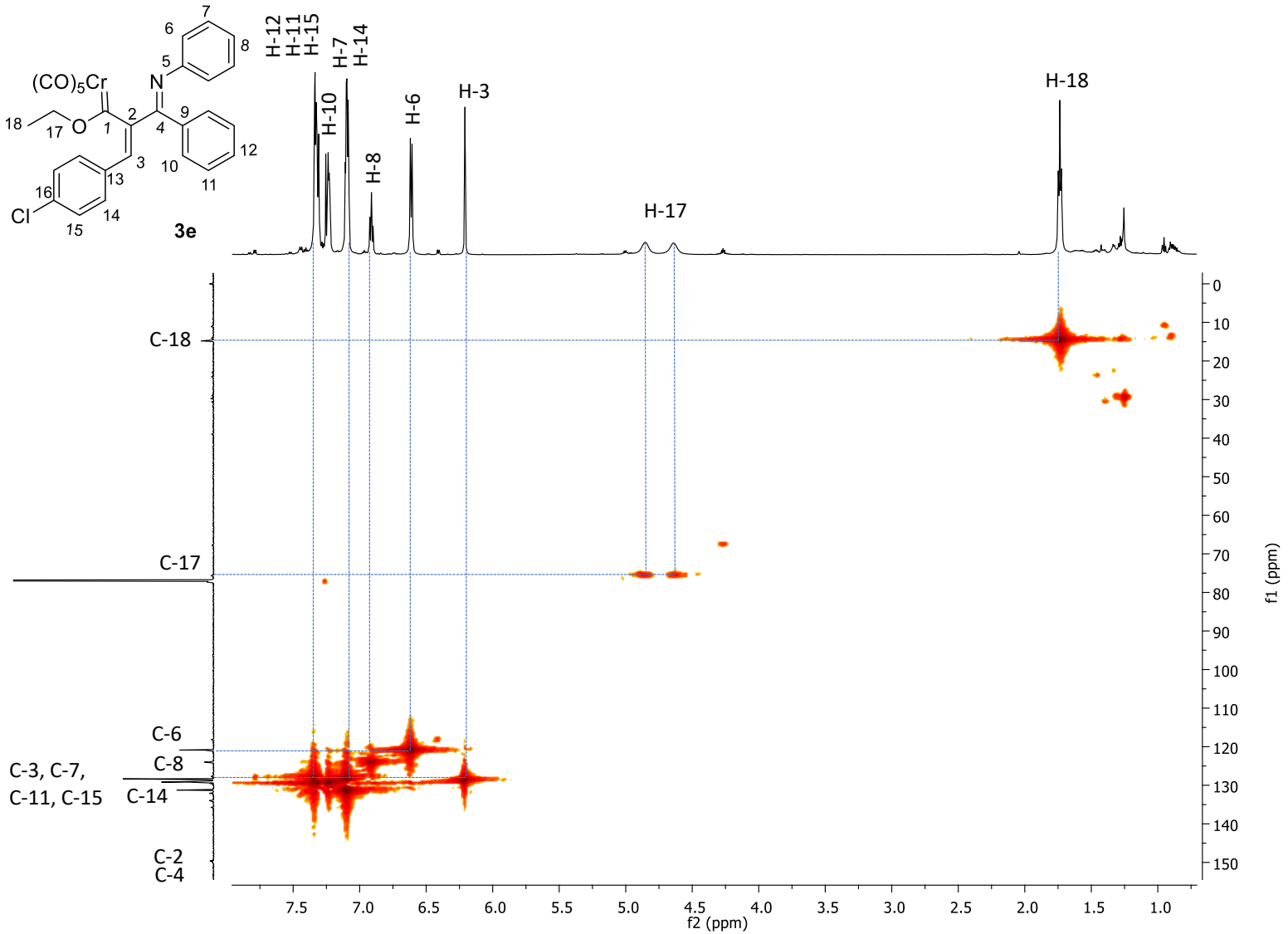
ISSN-e 2594-0317



gHMQC experiment for **3e**

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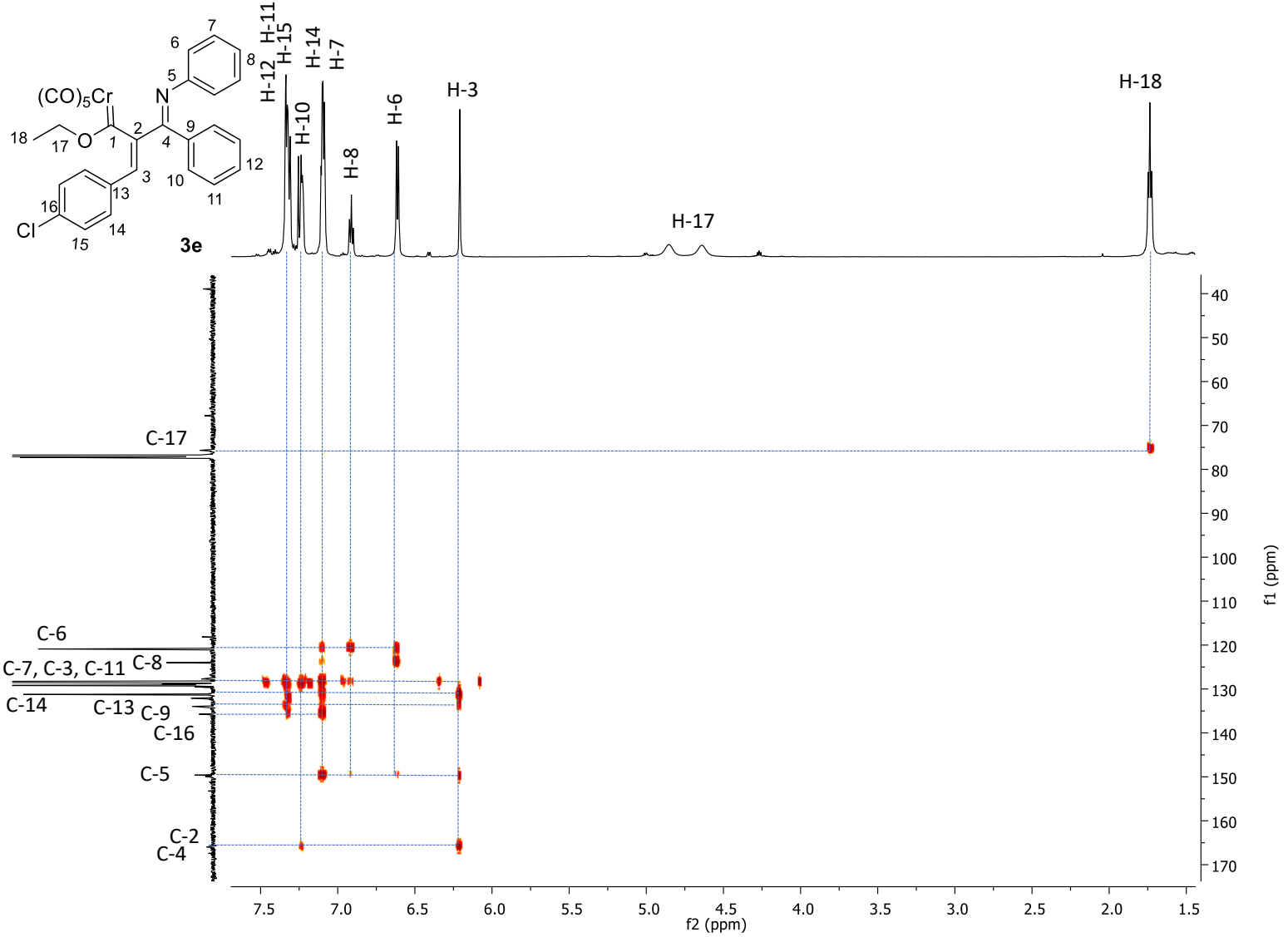

gHMBC experiment for **3e**

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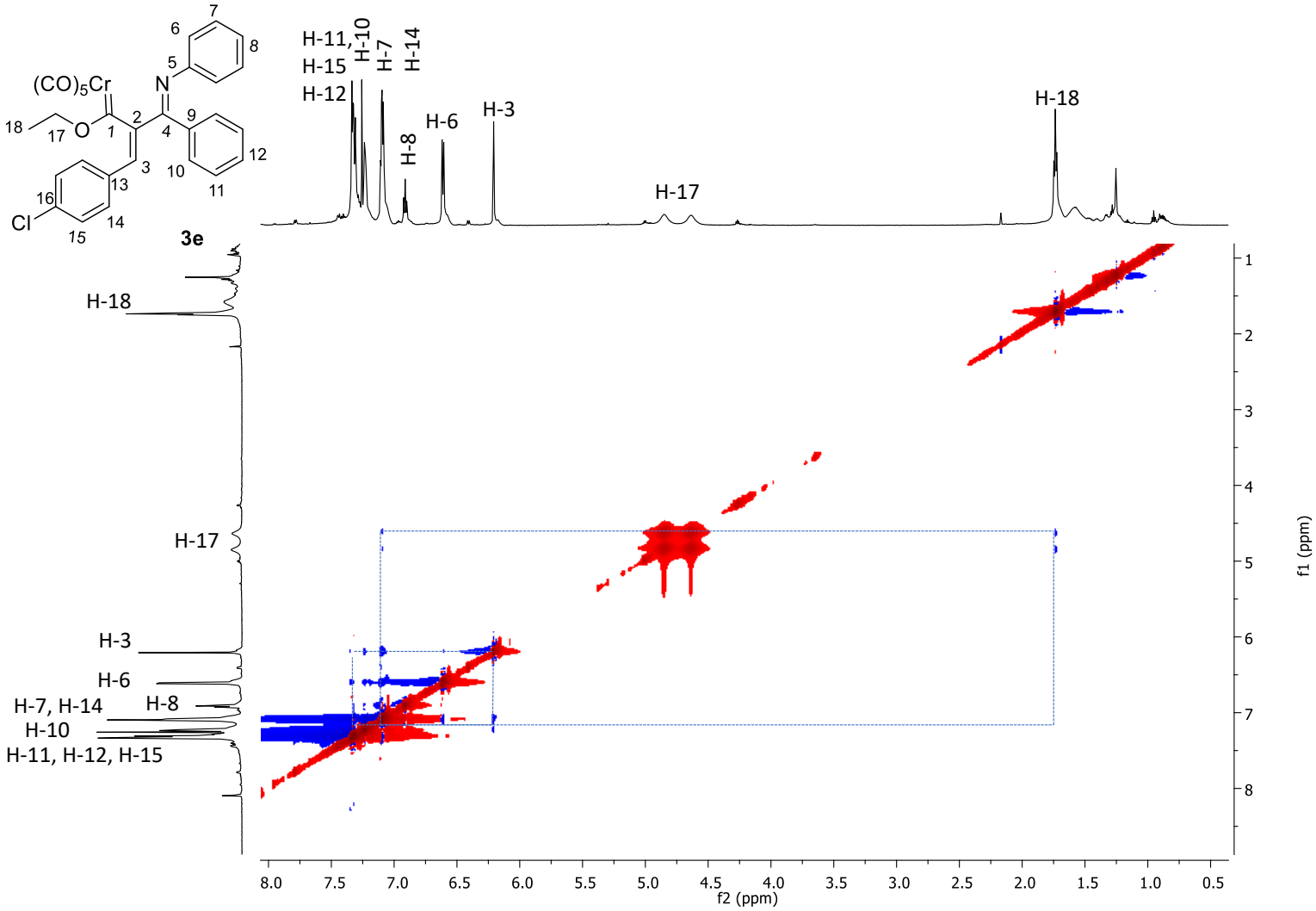

ROESY experiment for **3e**

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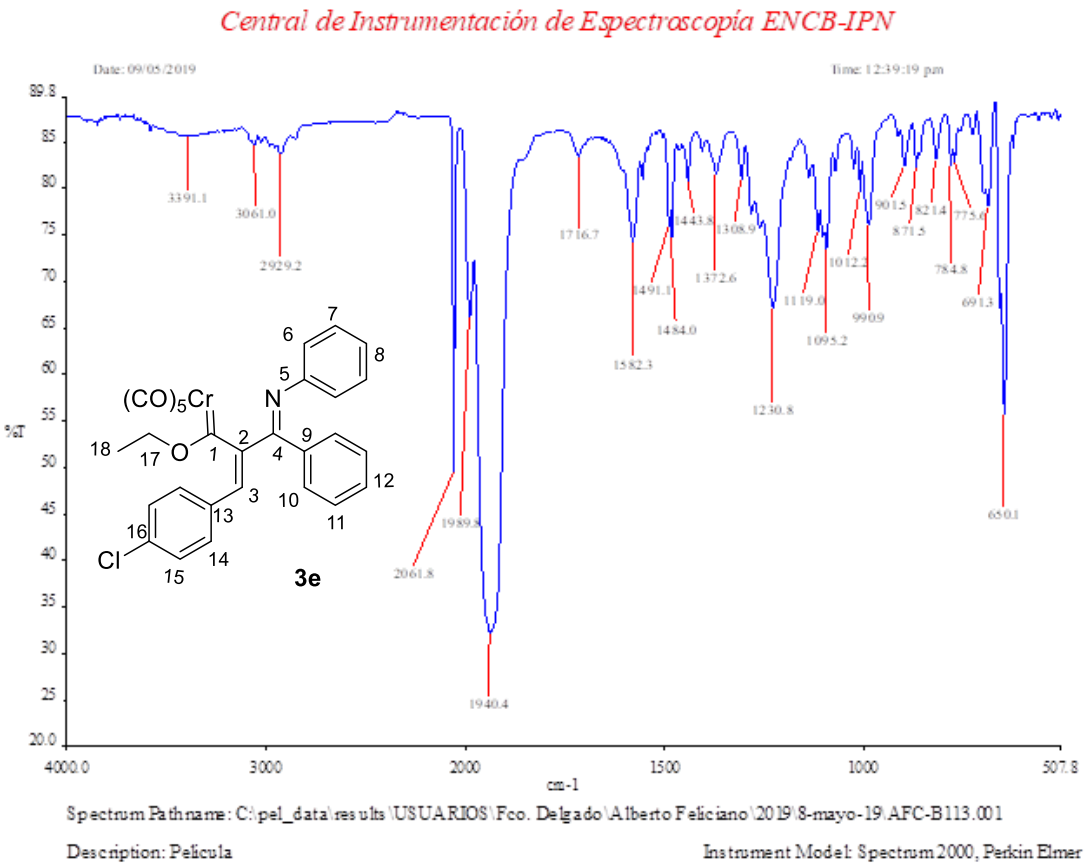

FT-IR for **3e**

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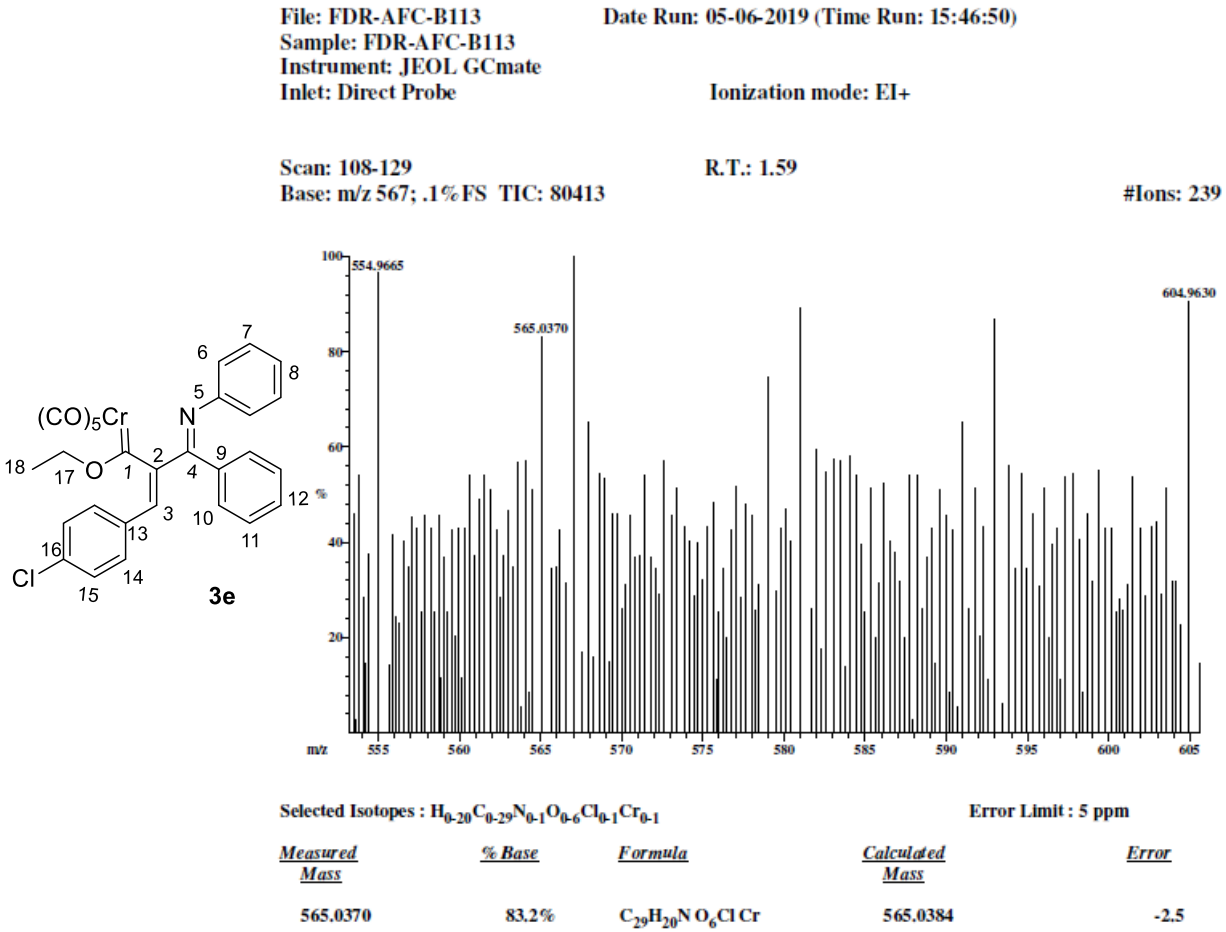

HRMS (EI) $[M]^+$ for **3e**

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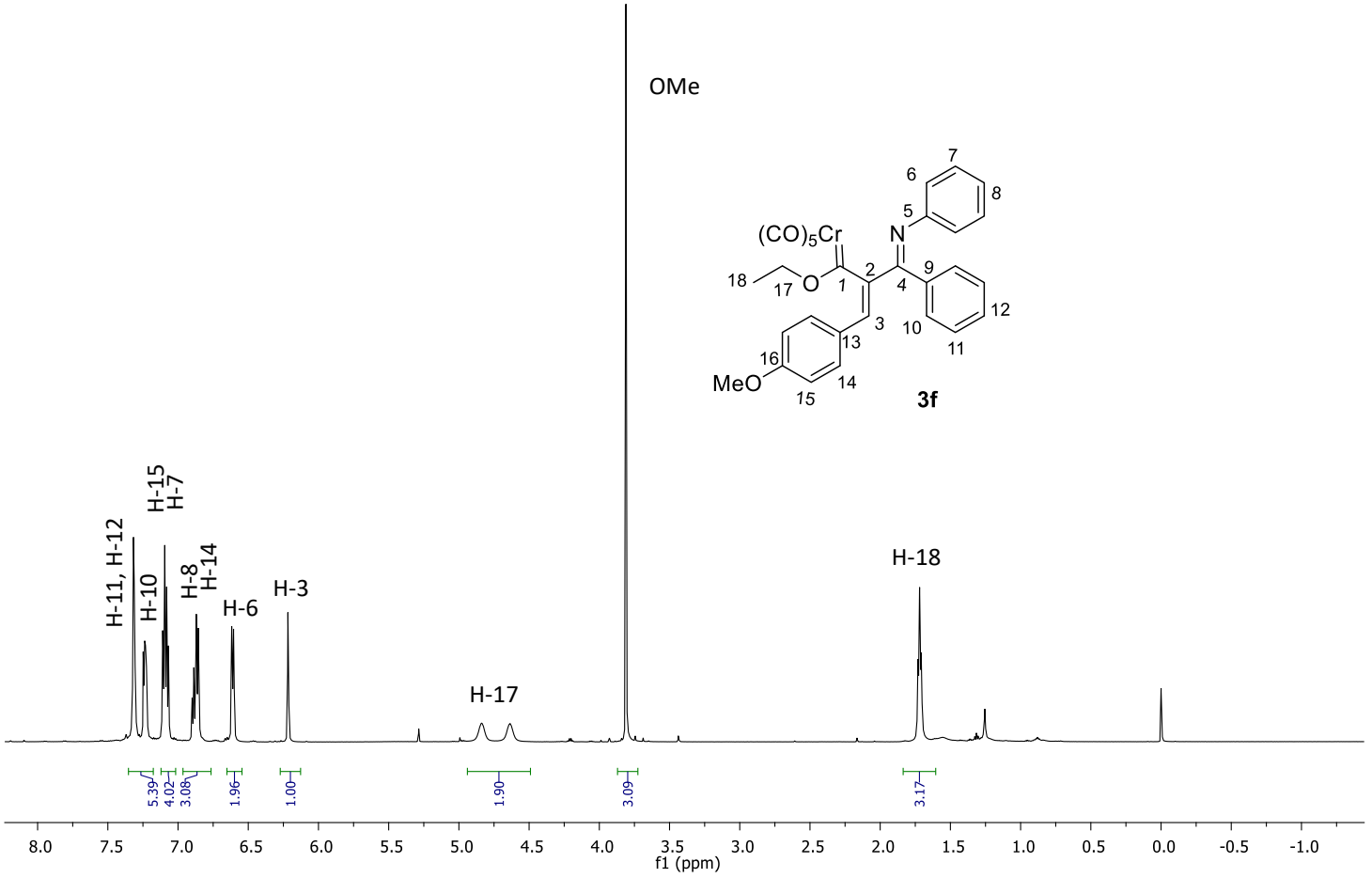
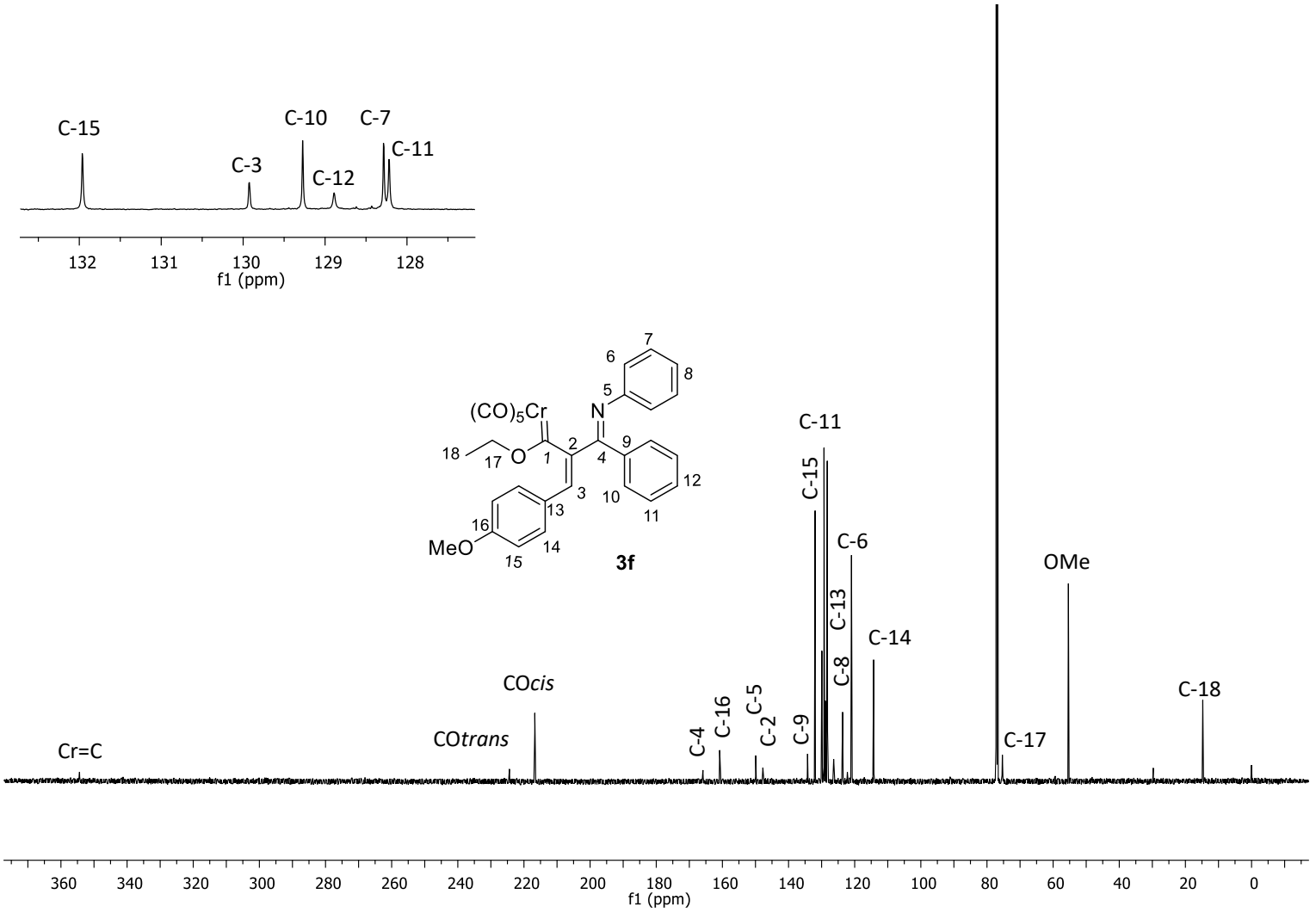
AFC-B126



^{1}H NMR for **3f**

ISSN-e 2594-0317



^{13}C NMR for **3f**

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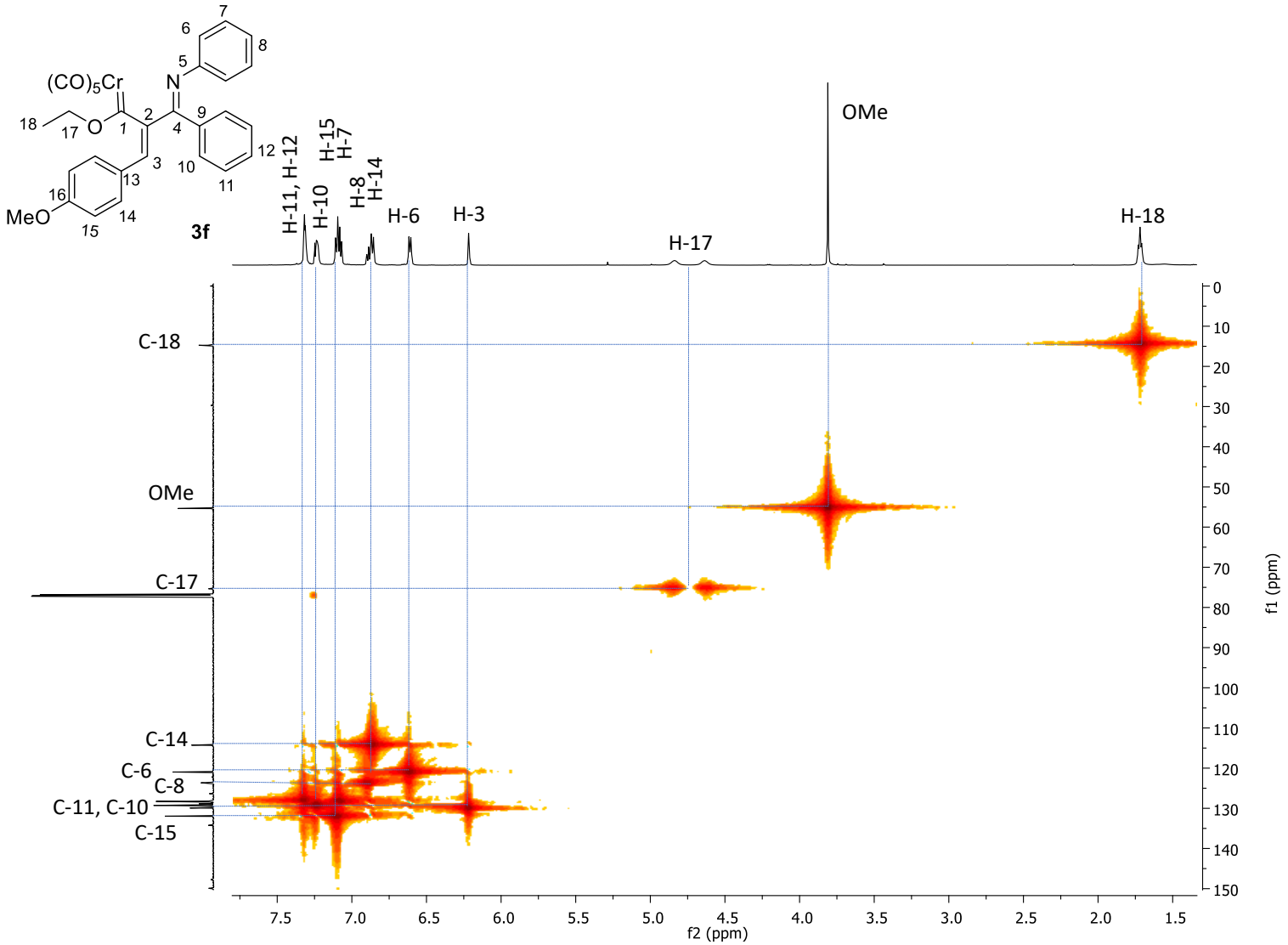
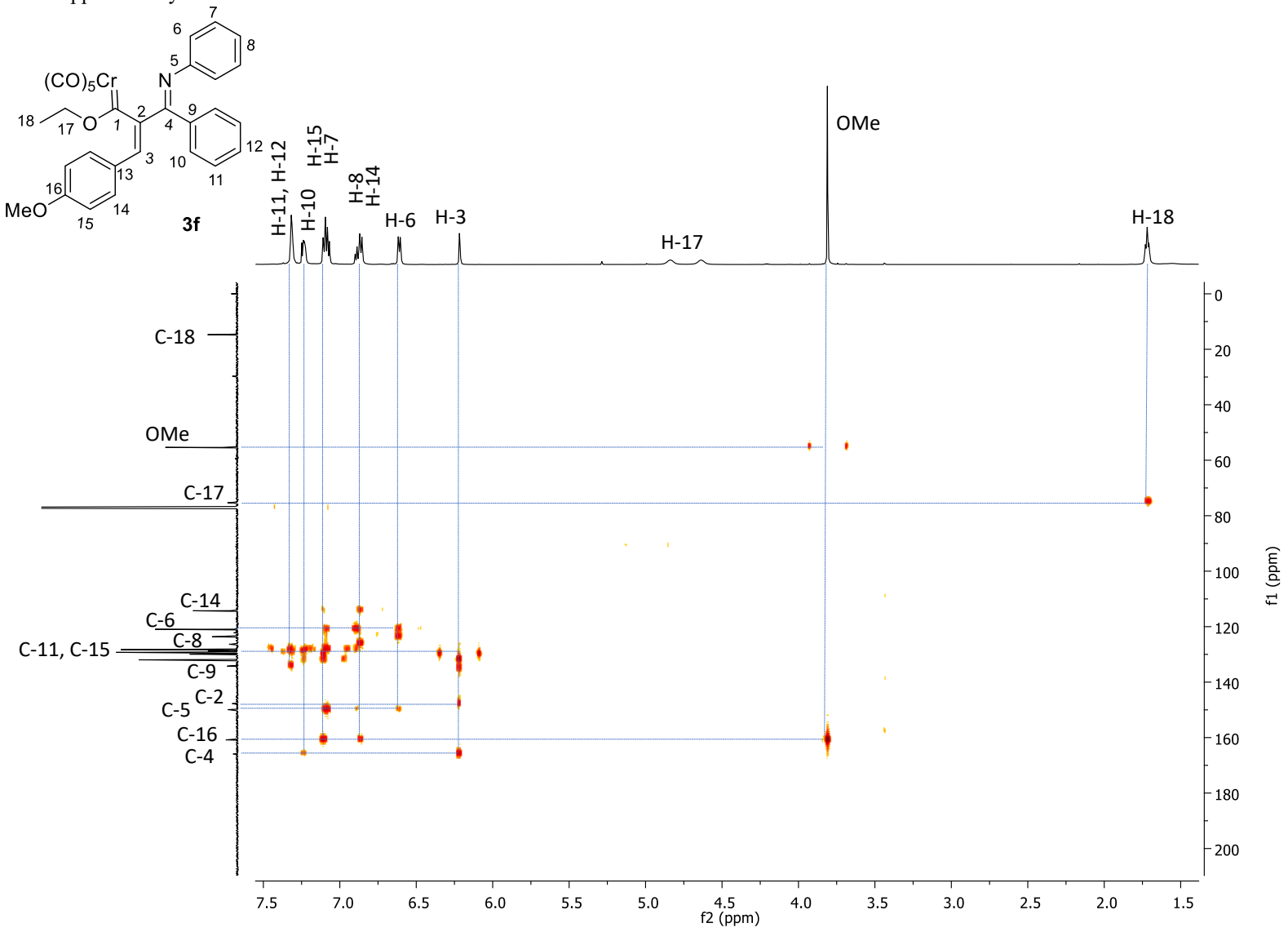


gHMQC experiment for **3f**



gHMBC experiment for **3f**

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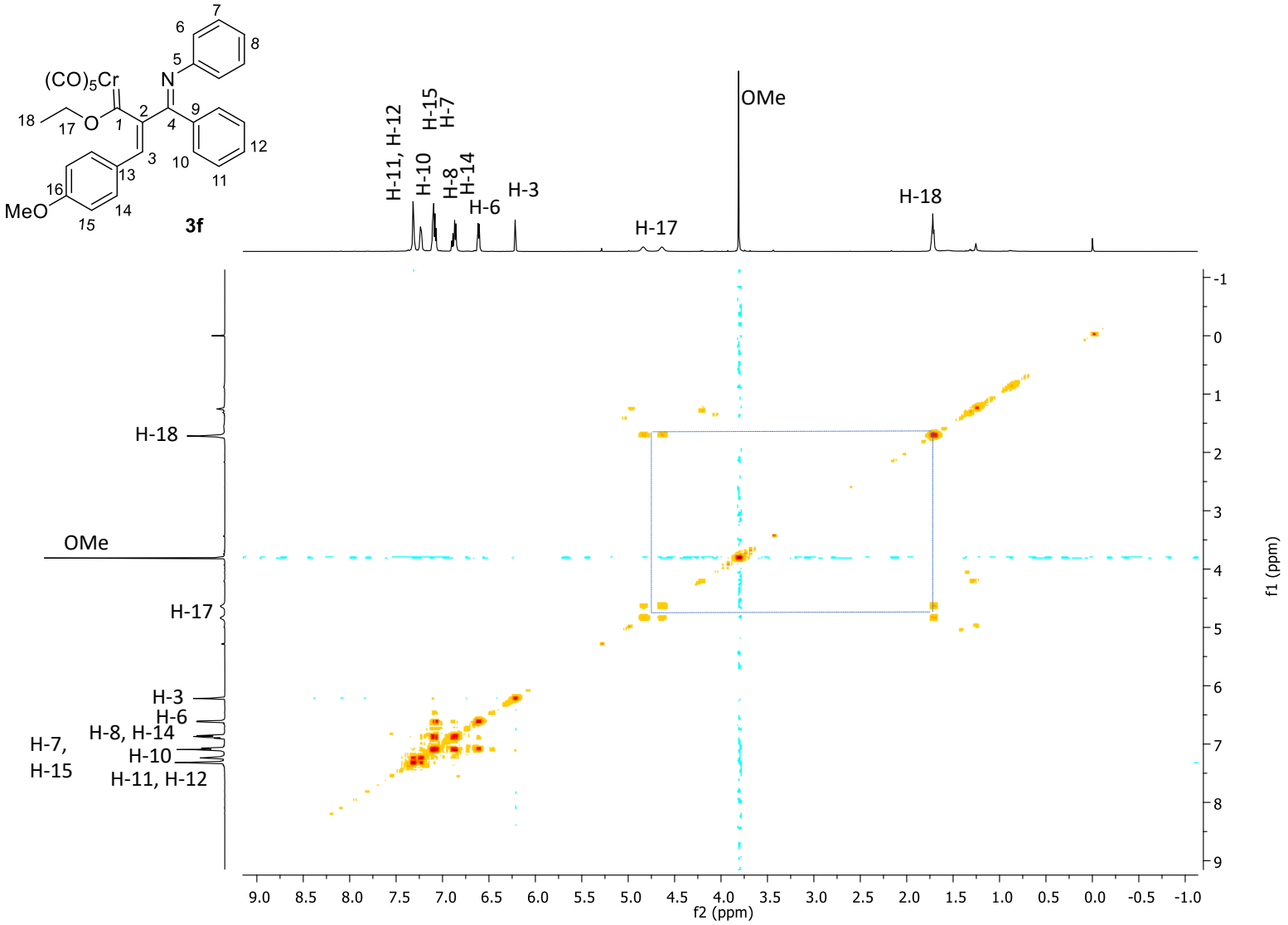

COSY experiment for **3f**

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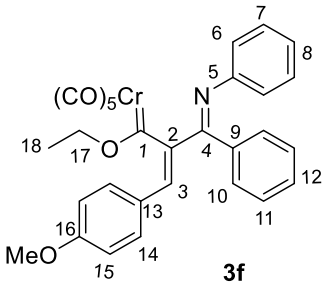

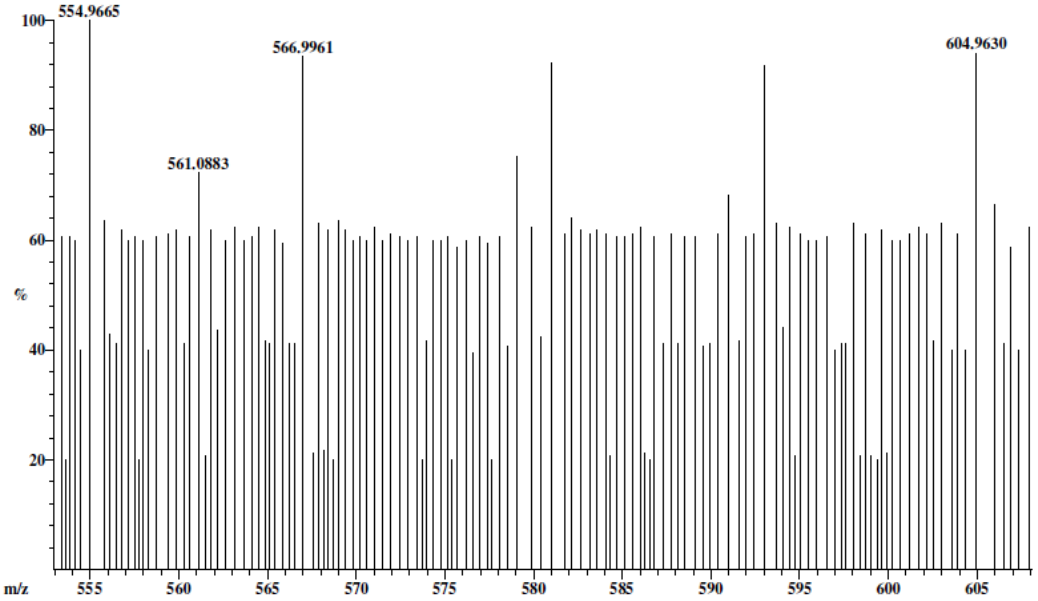

Selected Isotopes : $H_{0-23}C_{0-30}N_{0-1}O_{0-7}Cr_{0-1}$ Error Limit : 5 ppm

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*
561.0883	72.3%	$C_{30}H_{23}NO_7Cr$	561.0880	0.6

HRMS (EI) $[M]^+$ for **3f**

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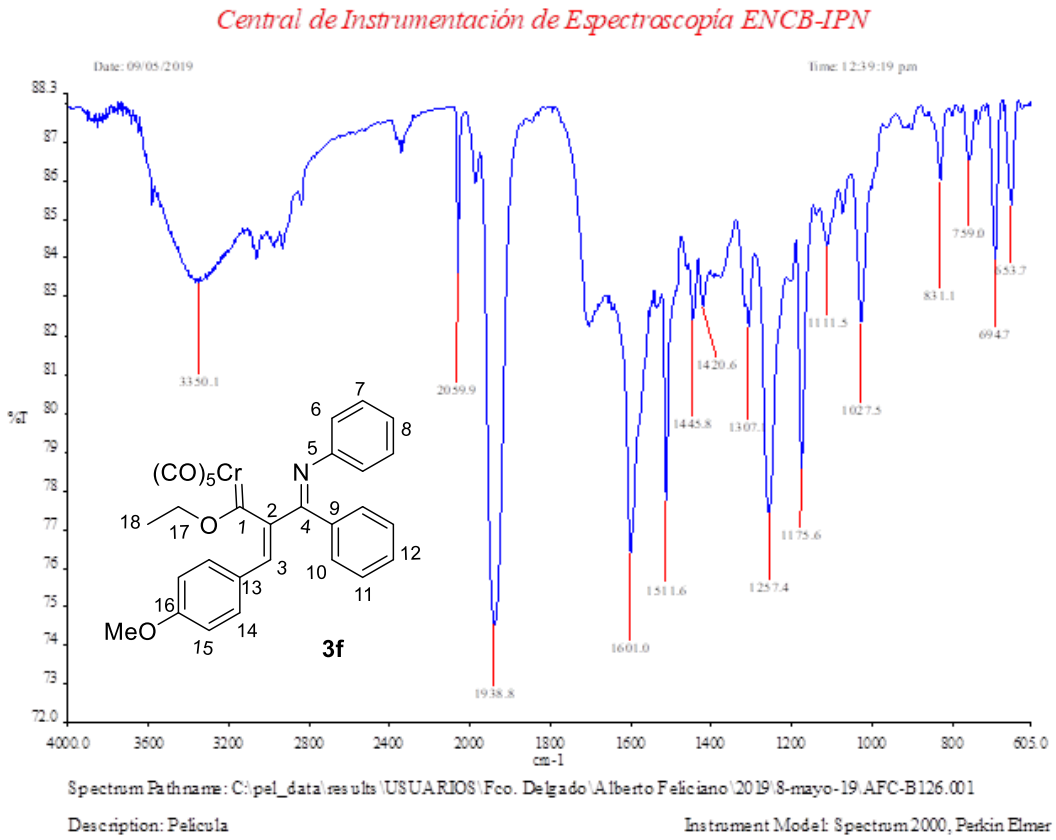

FT-IR for **3f**

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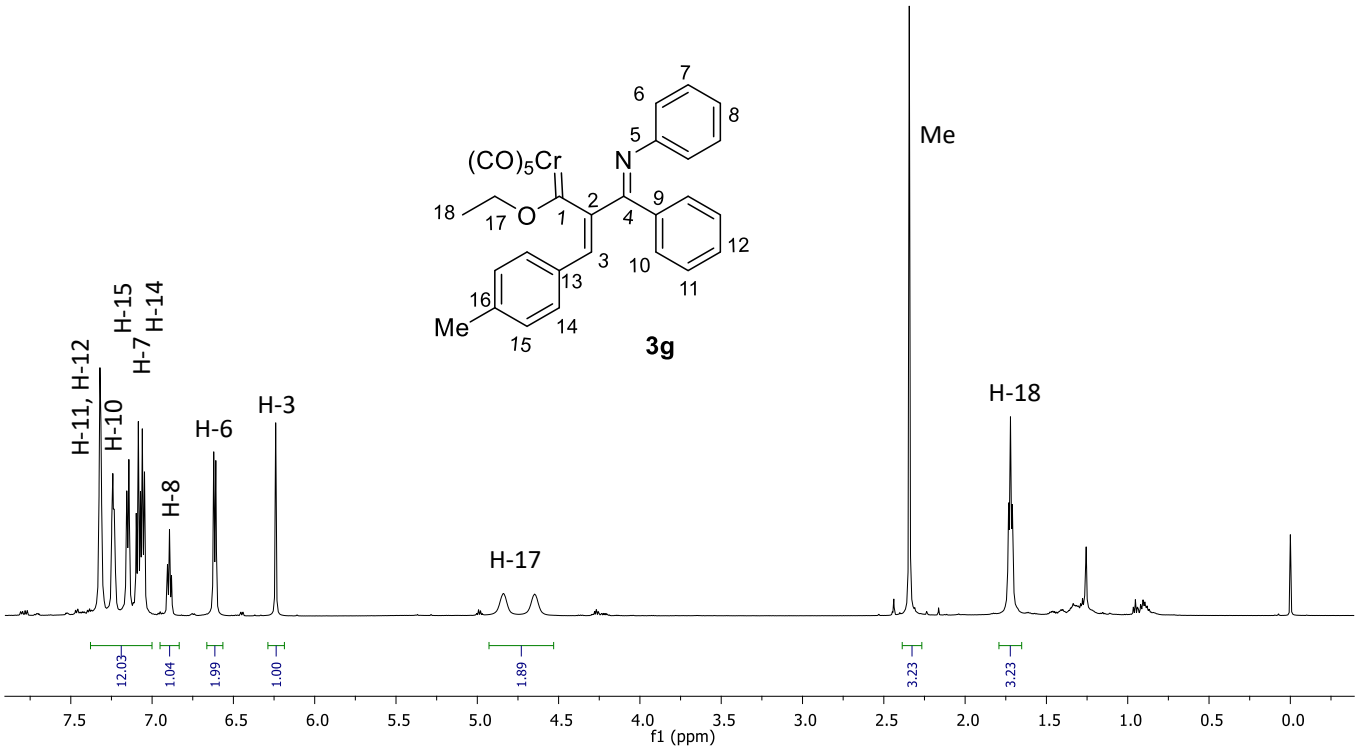

^{1}H NMR for **3g**

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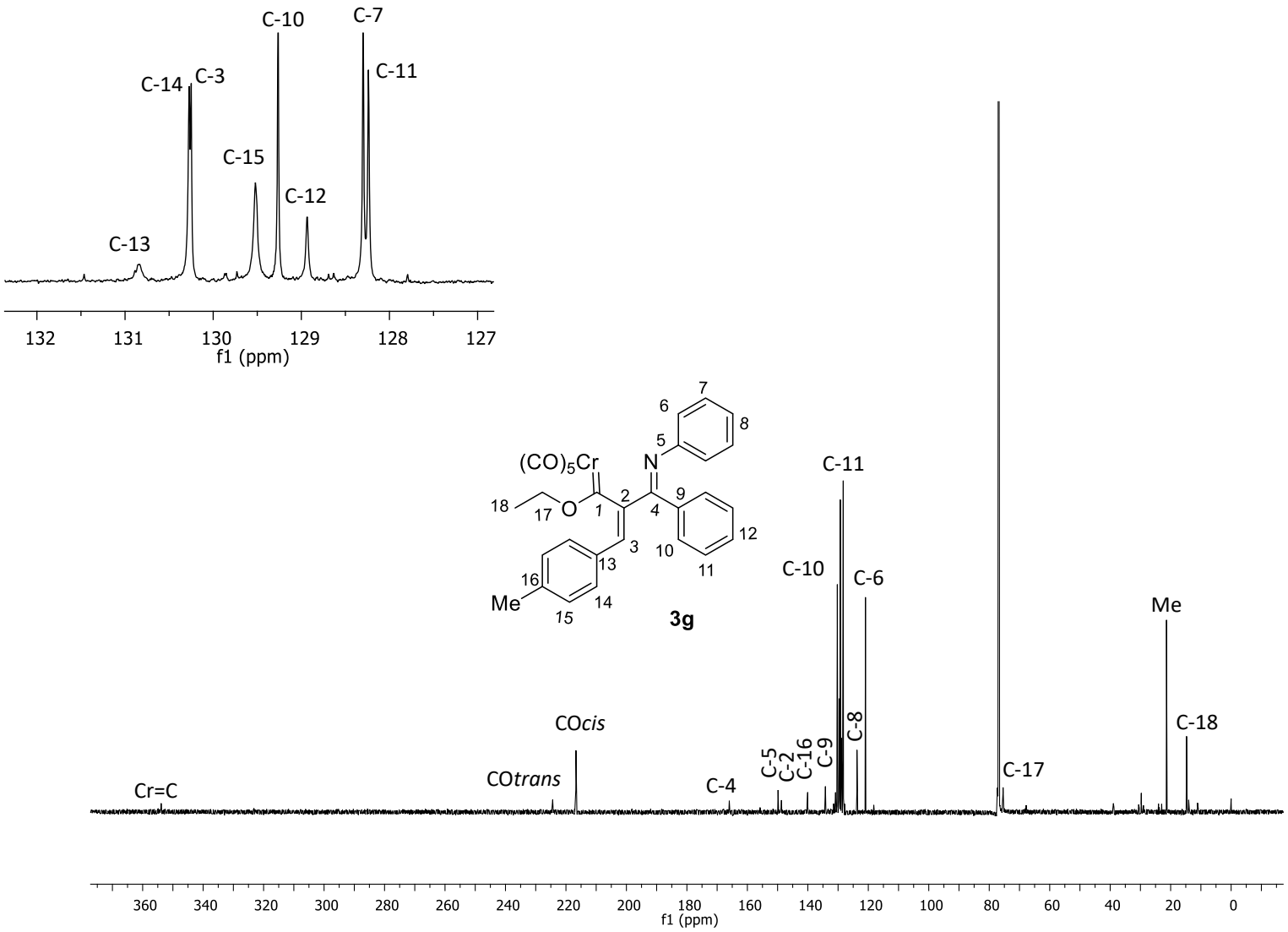
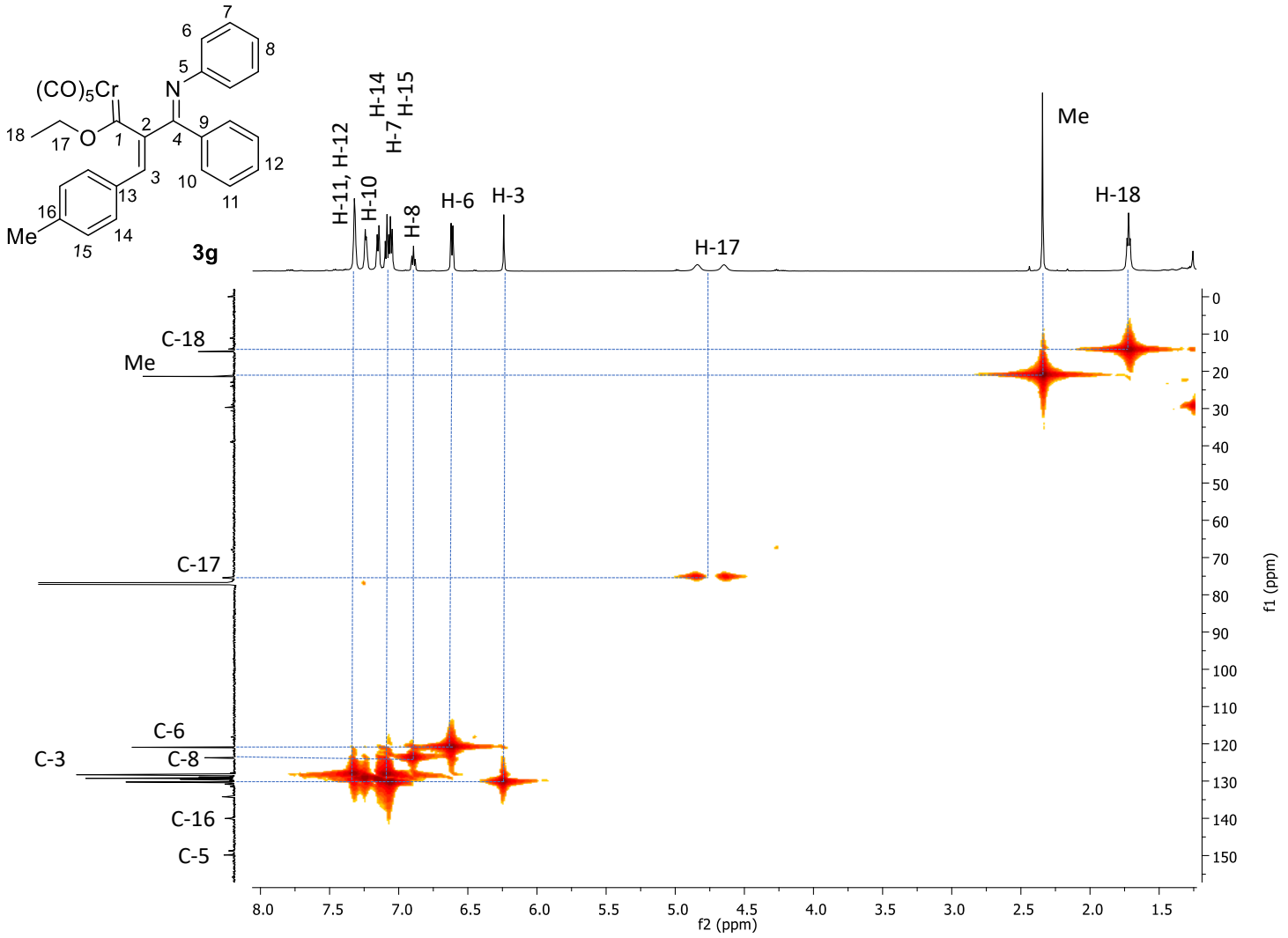


^{13}C NMR for **3g**



gHMQC experiment for **3g**

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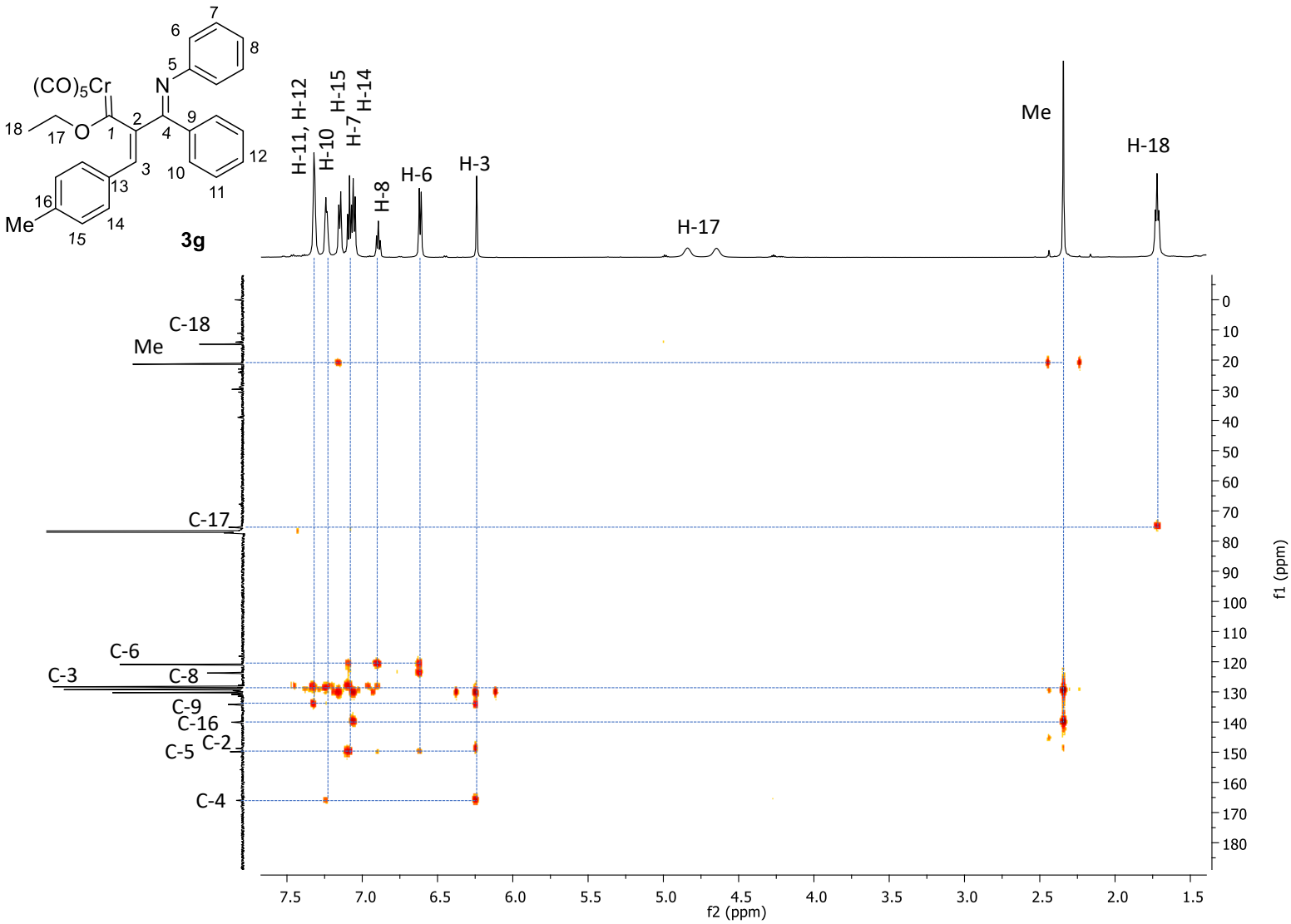
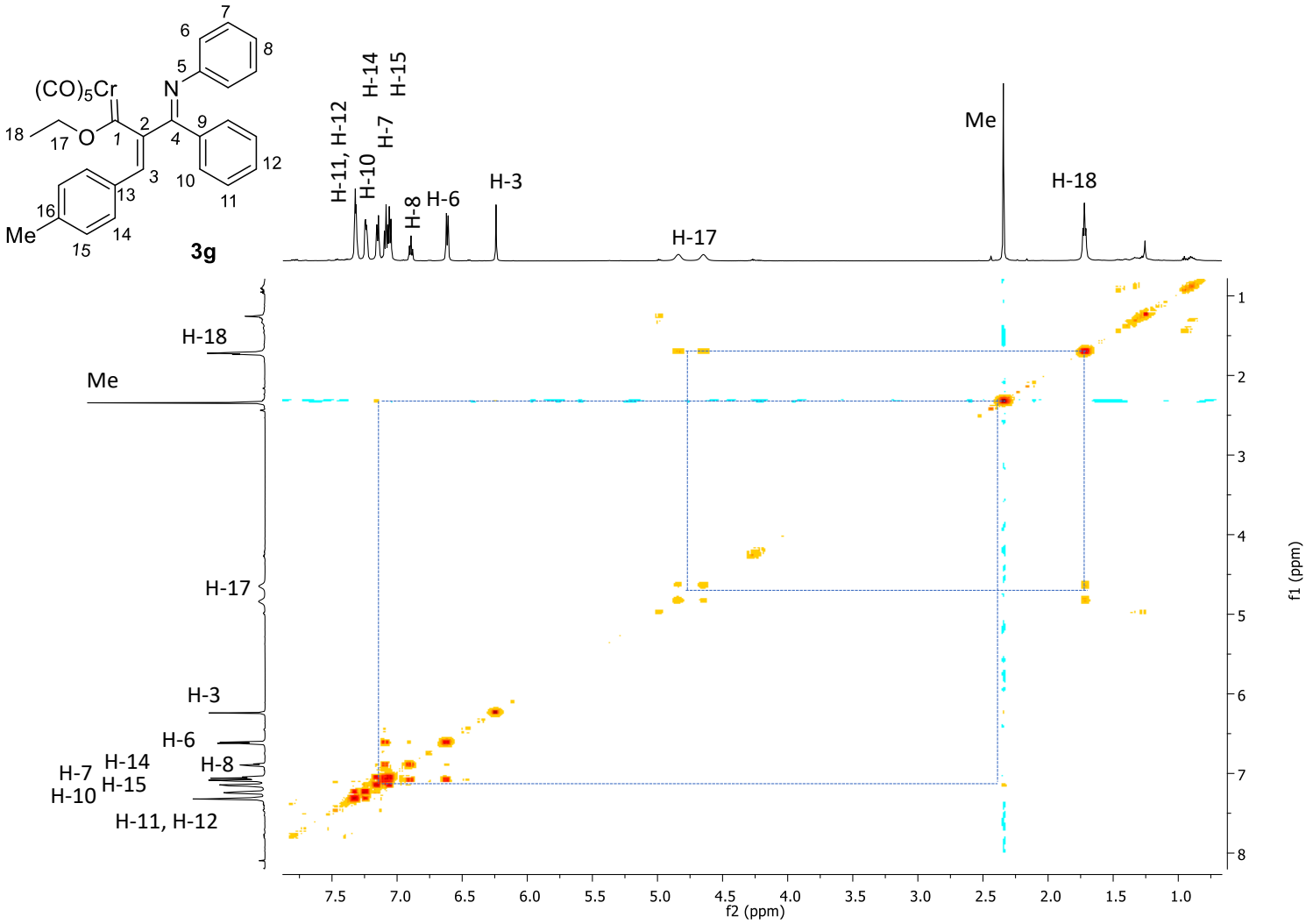
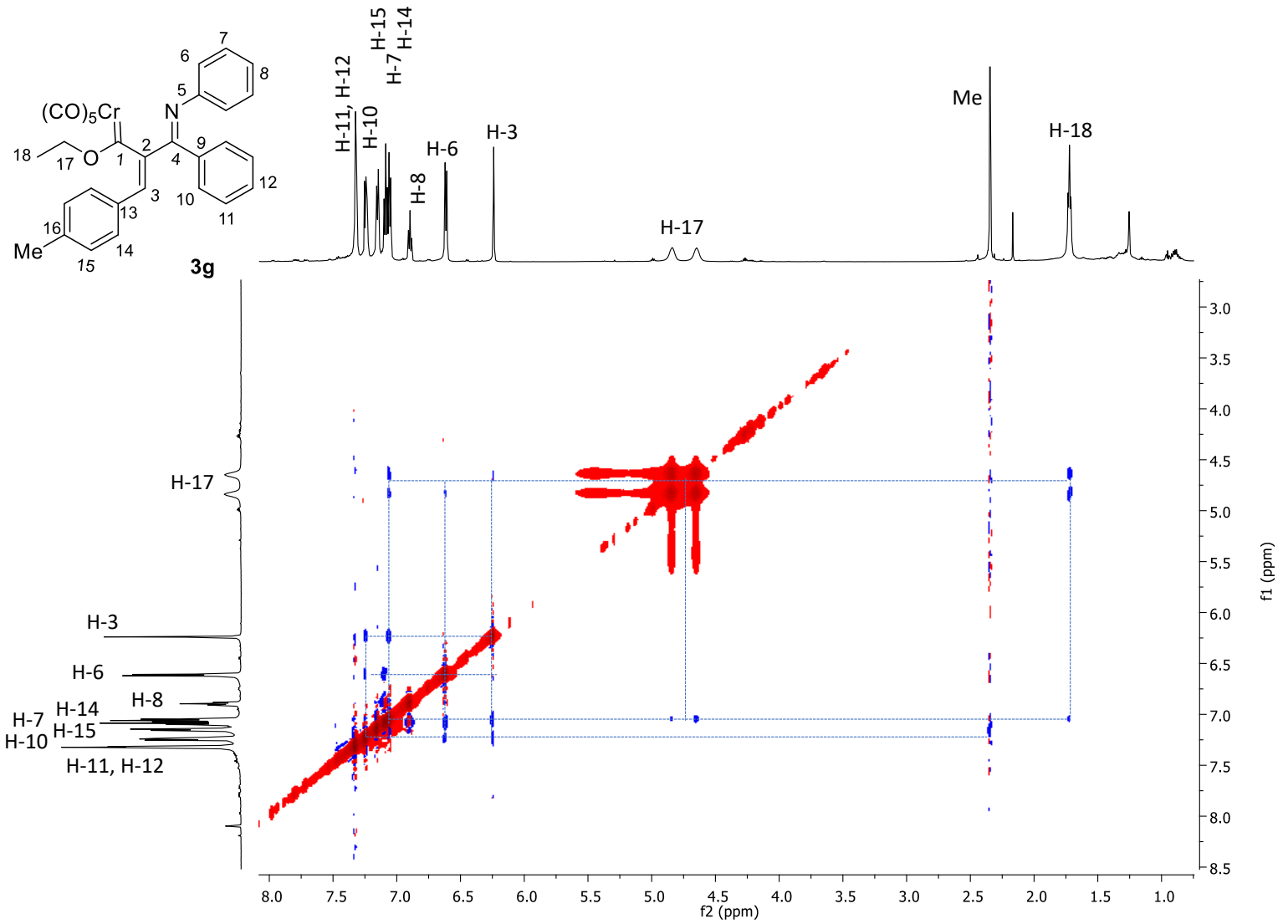


gHMBC experiment for **3g**



COSY experiment for **3g**



ROESY experiment for **3g**

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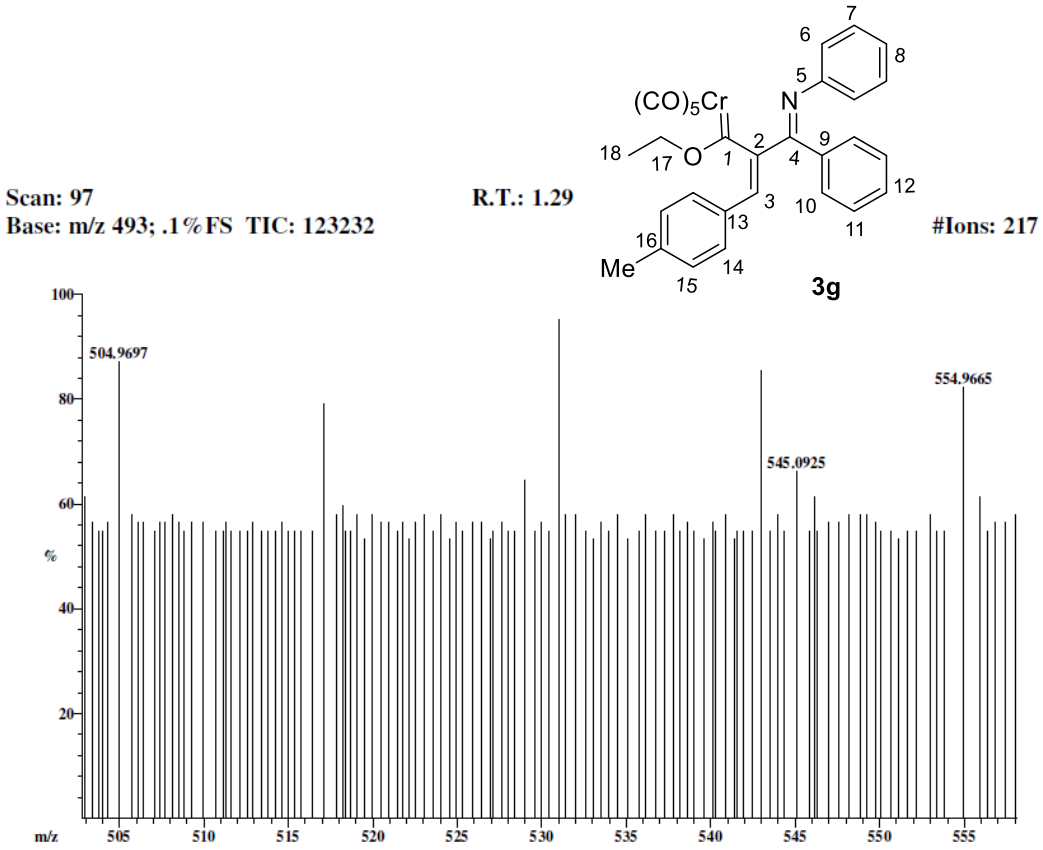

Selected Isotopes : $H_{0-23}C_{0-30}N_{0-1}O_{0-6}Cr_{0-1}$ Error Limit : 5 ppm

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*
545.0925	66.1%	$C_{30}H_{23}NO_6Cr$	545.0930	-1.0

HRMS (EI) $[M]^+$ for **3g**

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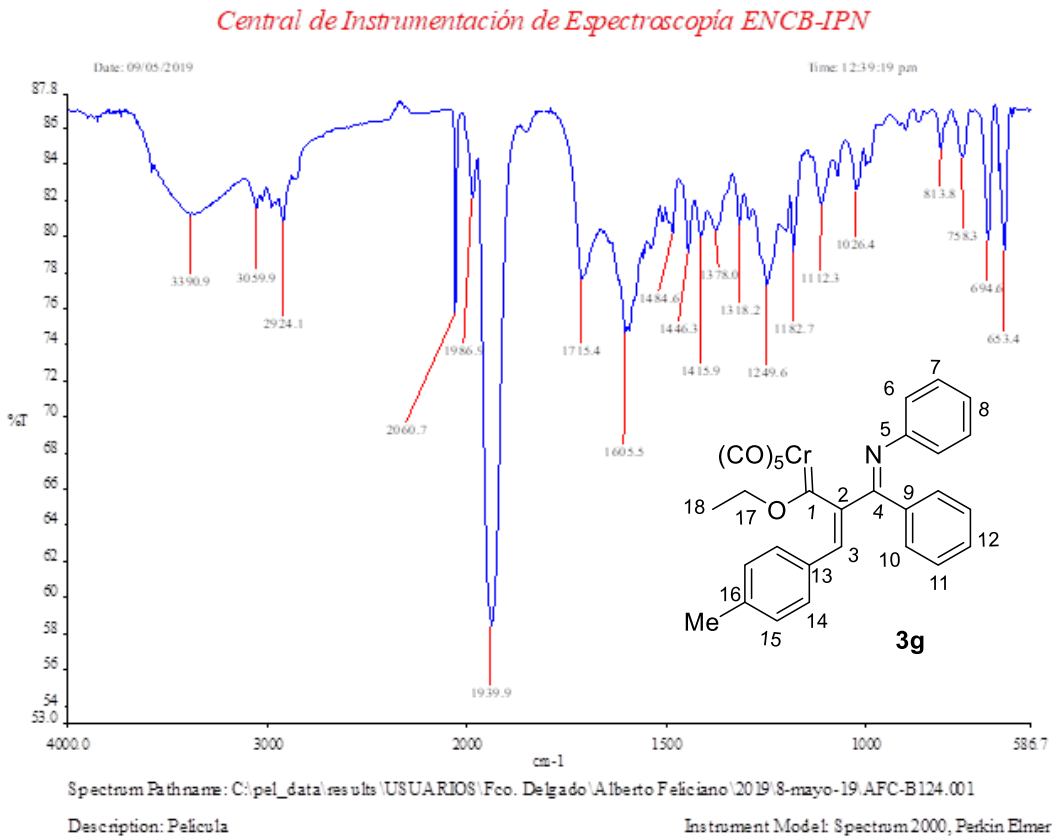

FT-IR for **3g**

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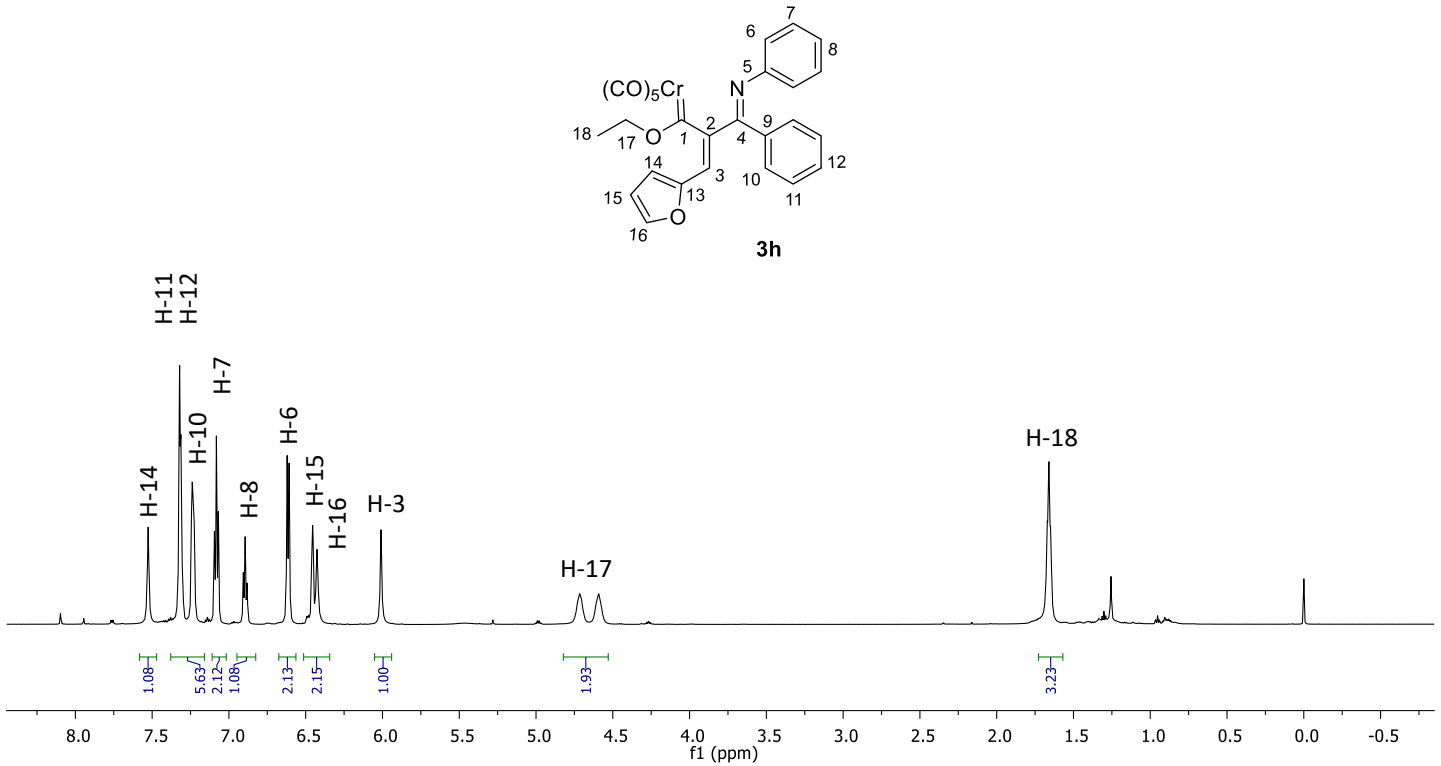

^{1}H NMR for **3h**

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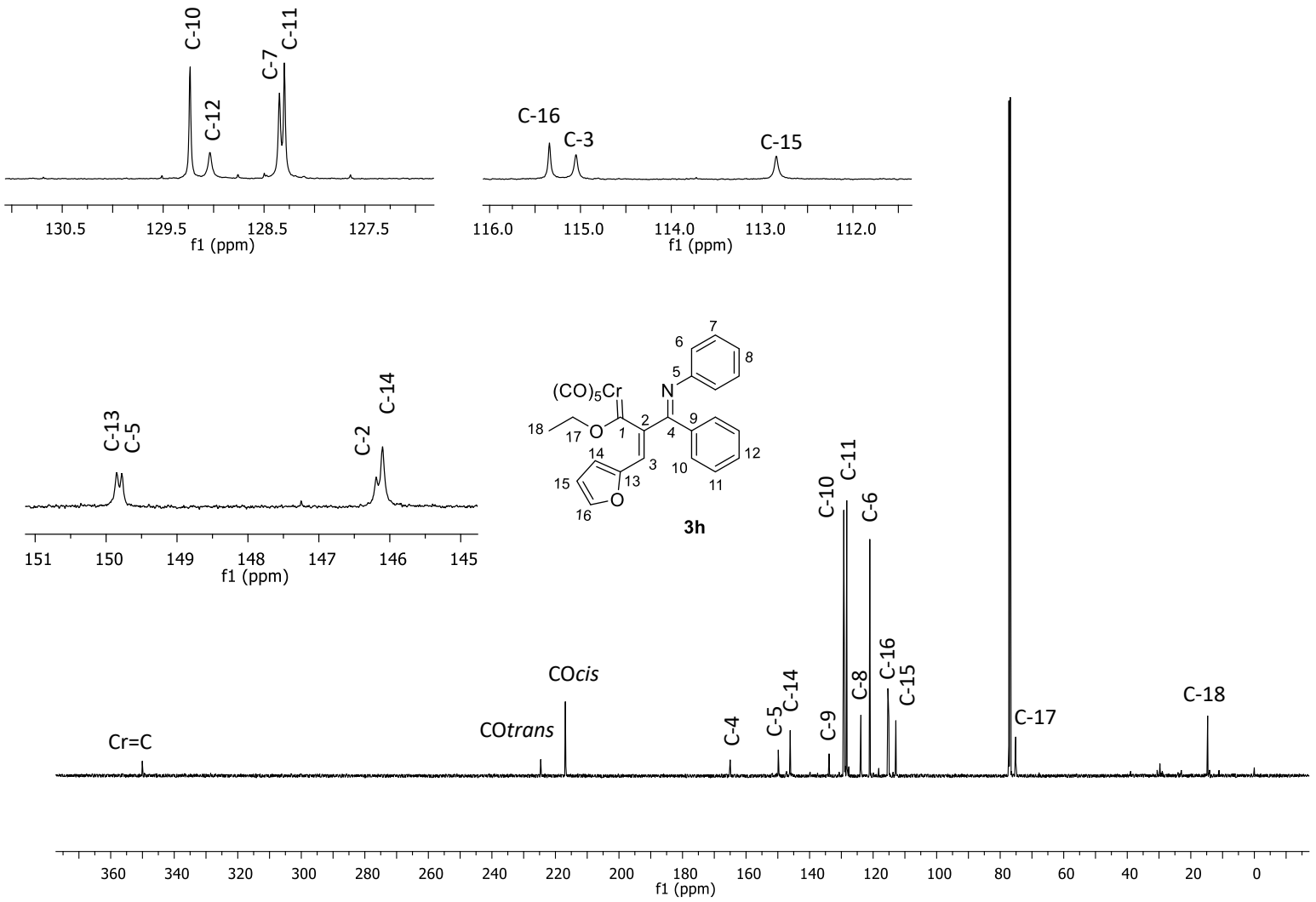
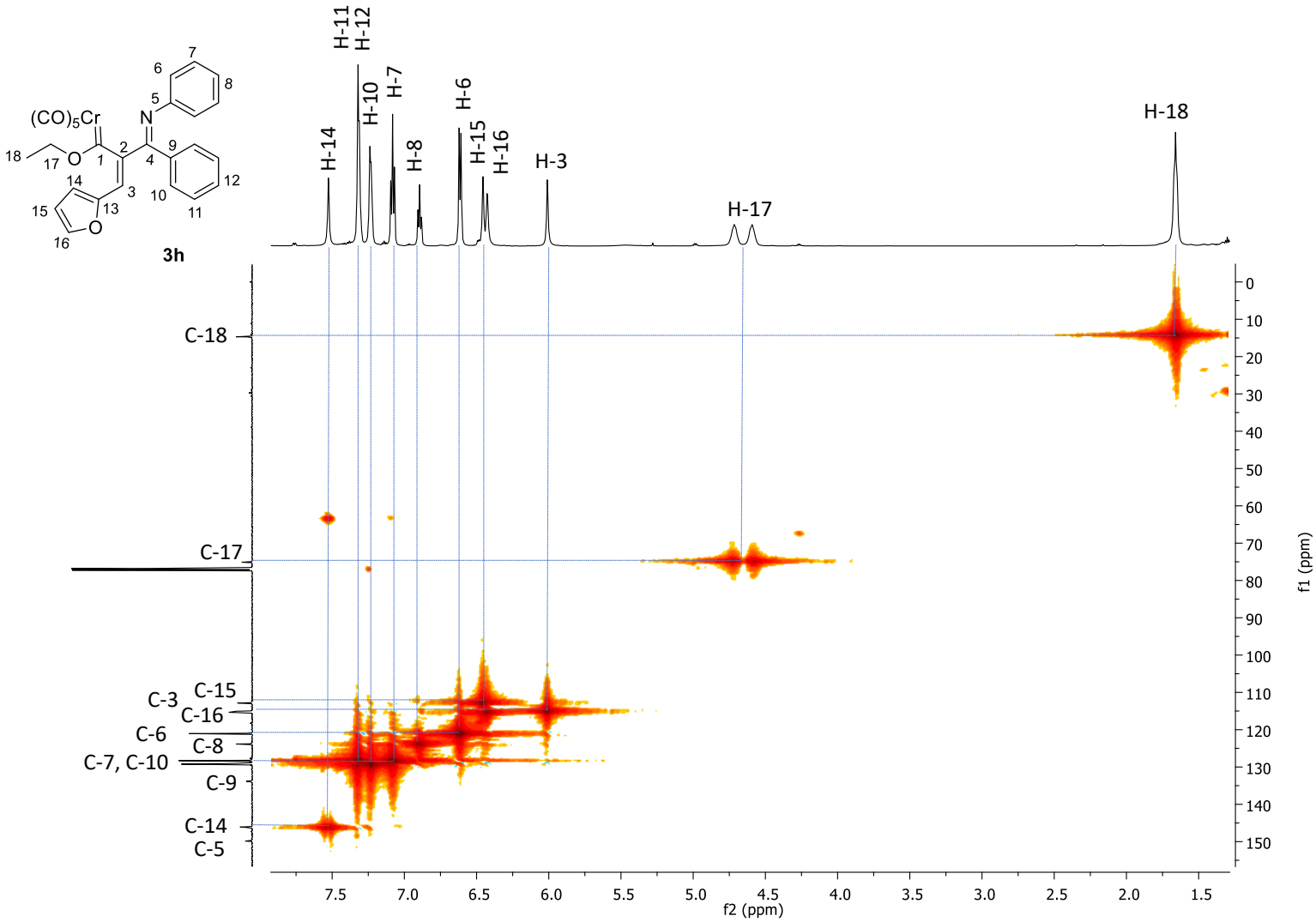
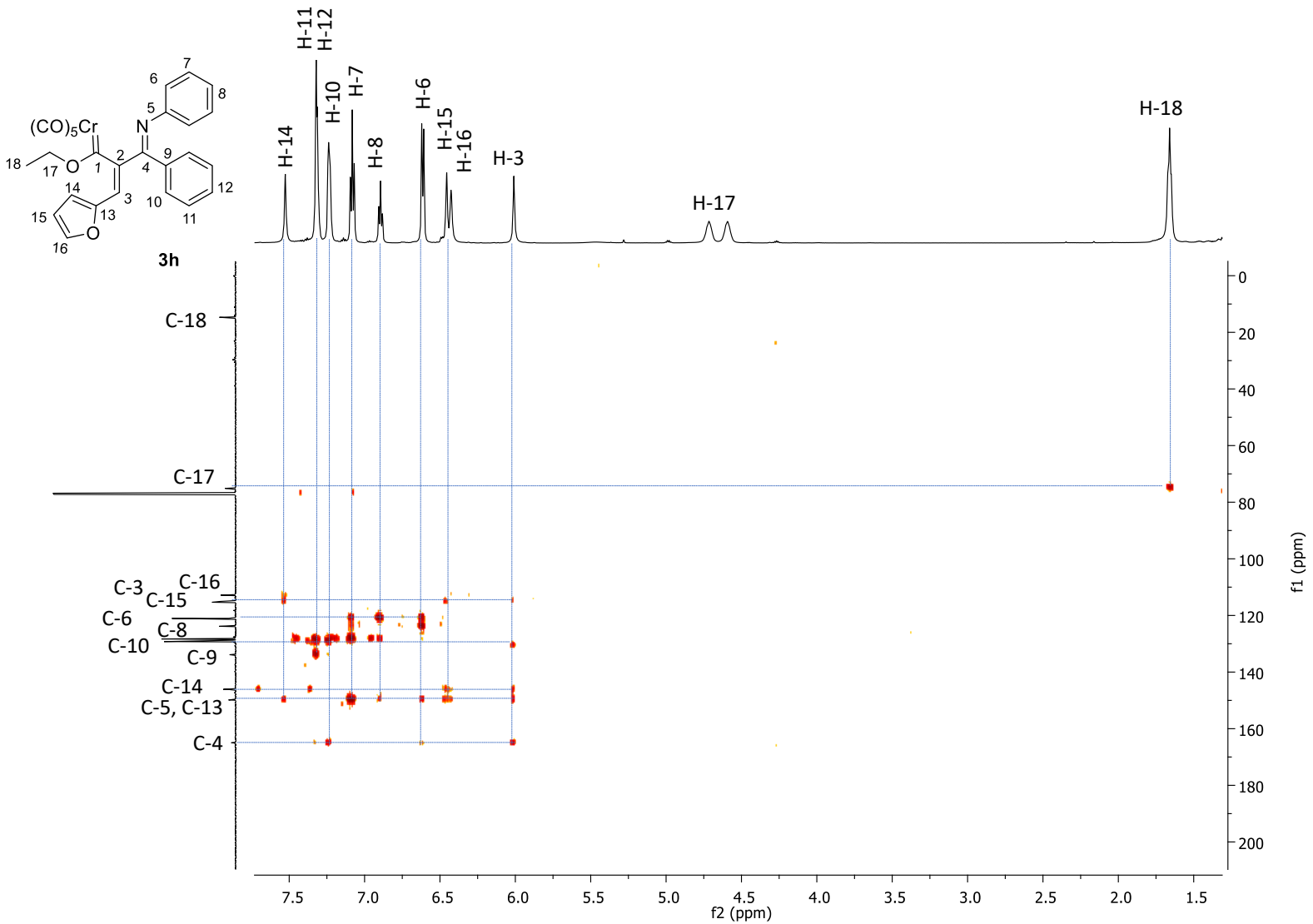


^{13}C NMR for **3h**



gHMQC experiment for **3h**



gHMBC experiment for **3h**

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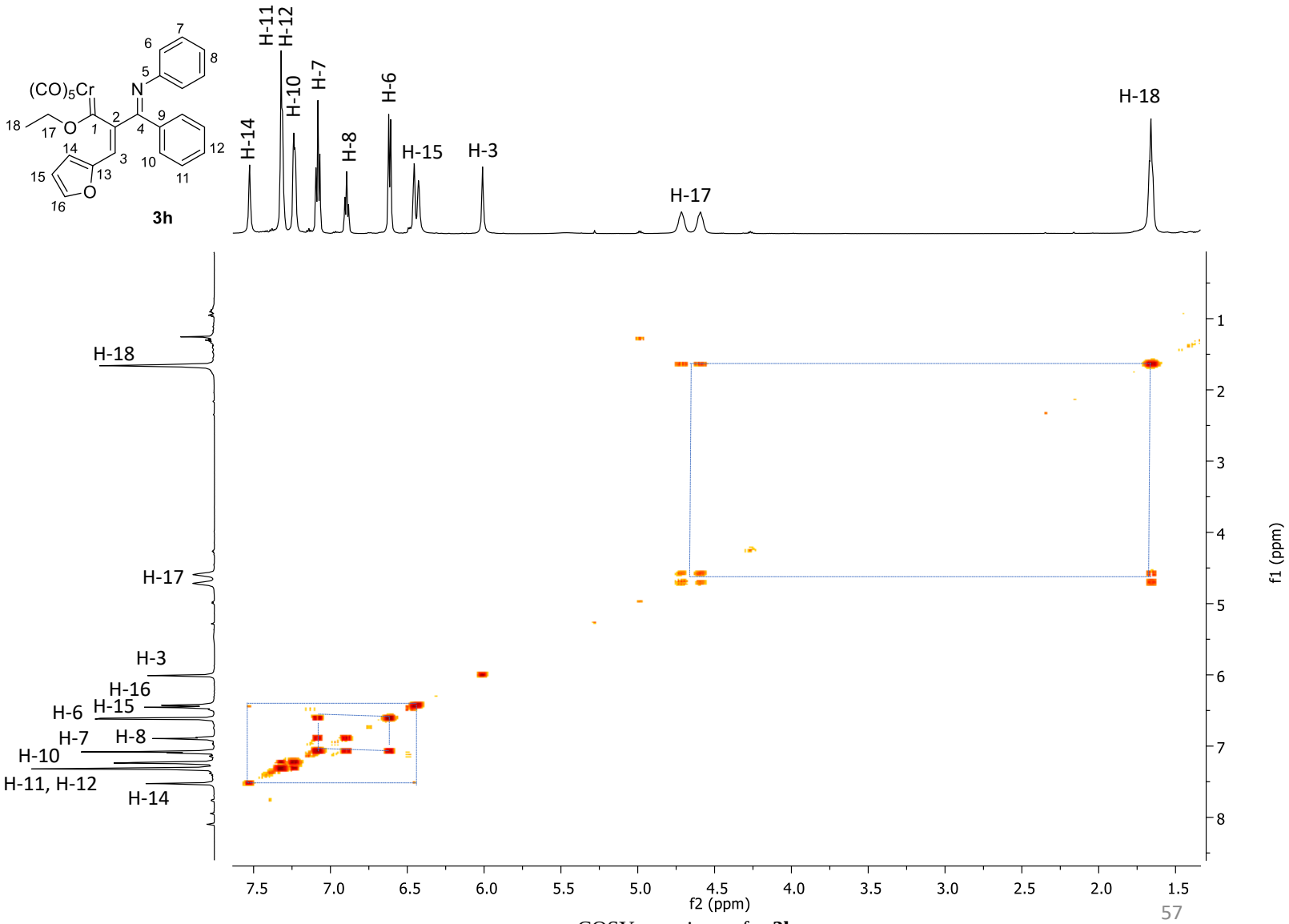

COSY experiment for **3h**

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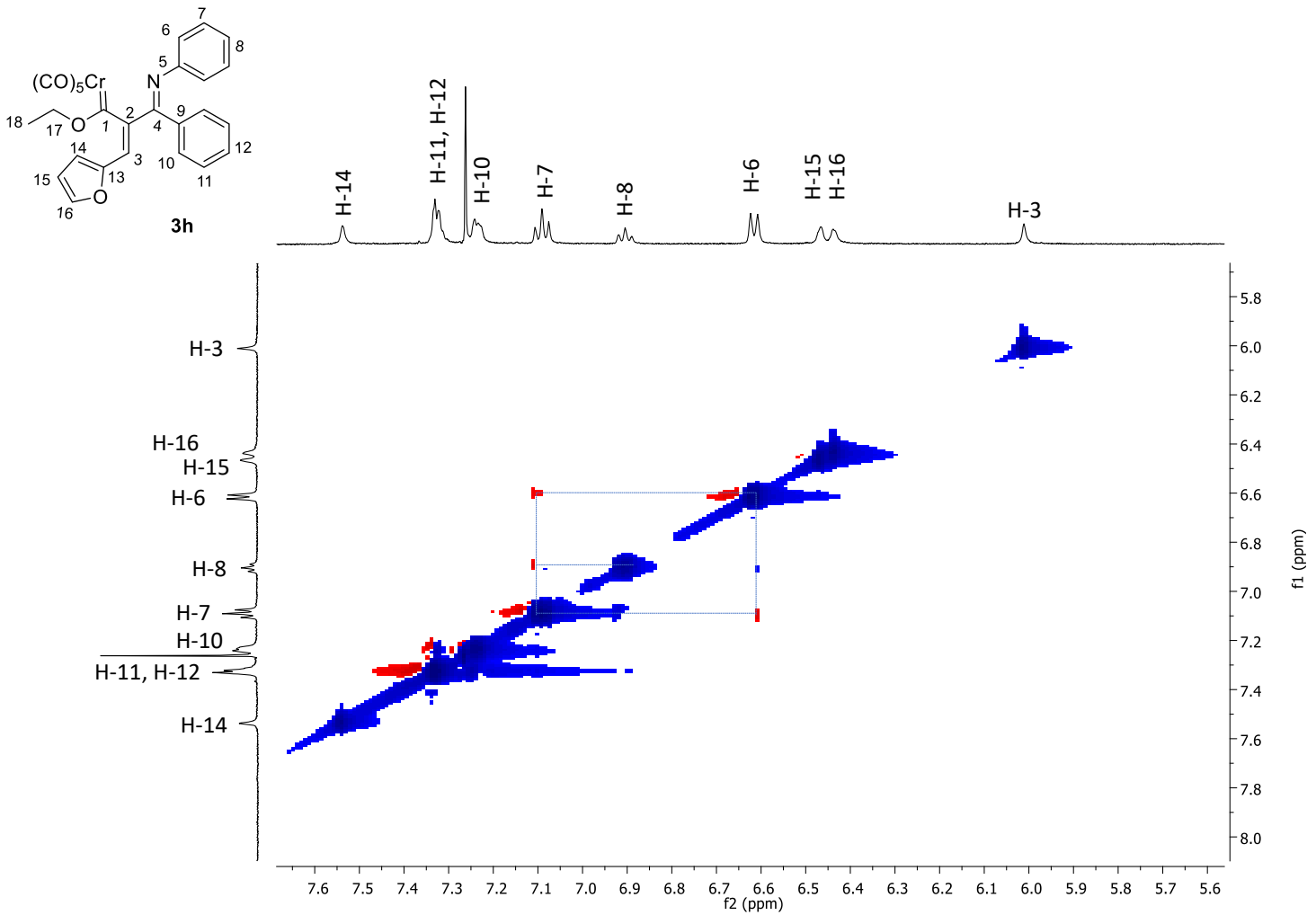

NOESY experiment for **3h**

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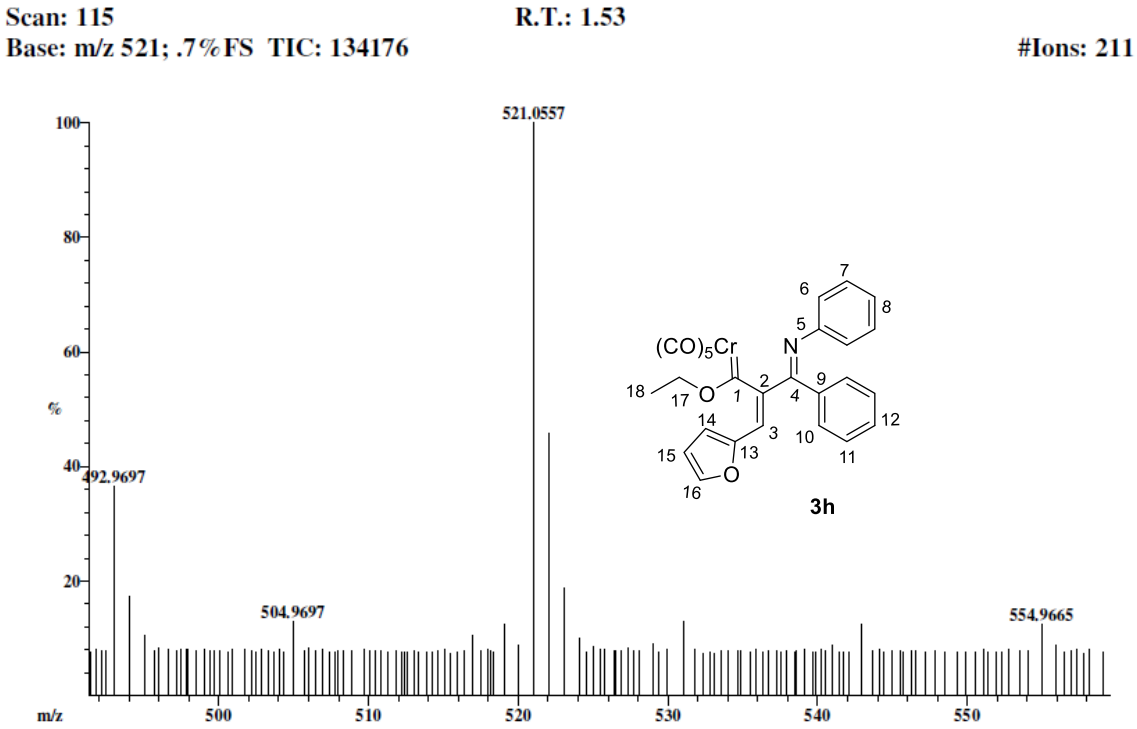

Selected Isotopes : $H_{0-19}C_{0-27}Cr_{0-1}N_{0-1}O_{0-7}$ Error Limit : 5 ppm

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*
521.0557	100.0%	$C_{27}H_{19}CrNO_7$	521.0567	-1.8

HRMS (EI) $[M]^+$ for **3h**

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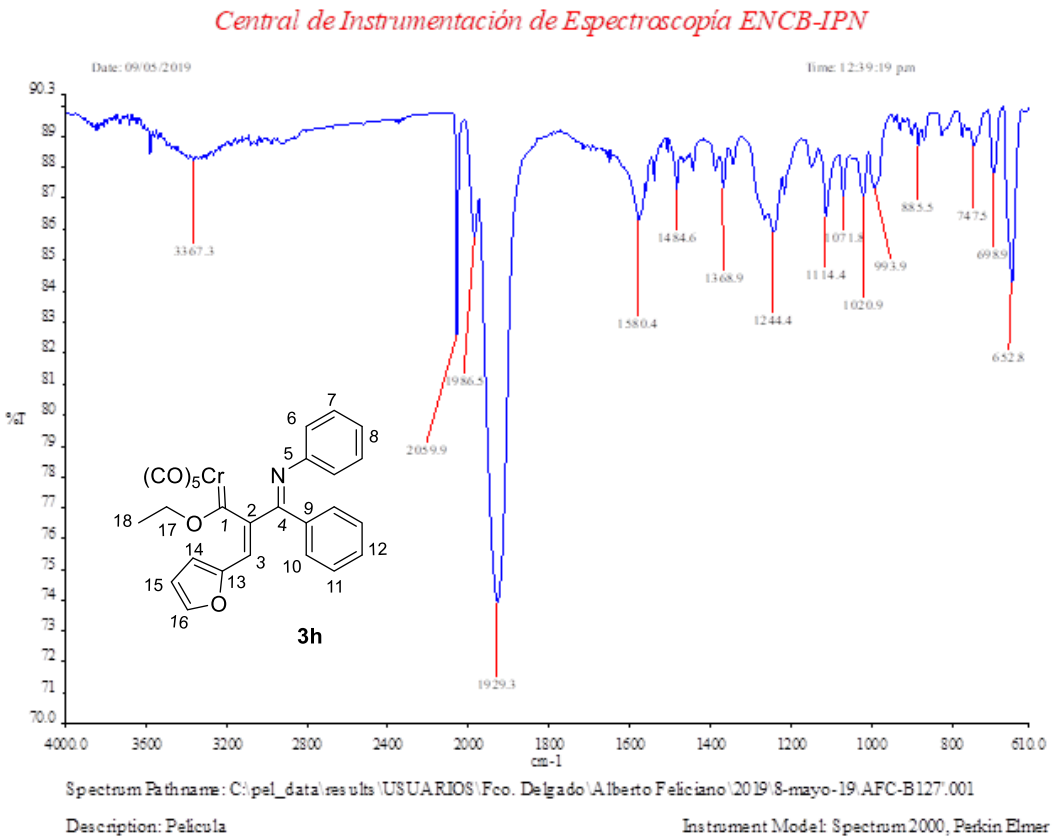

FT-IR for **3h**

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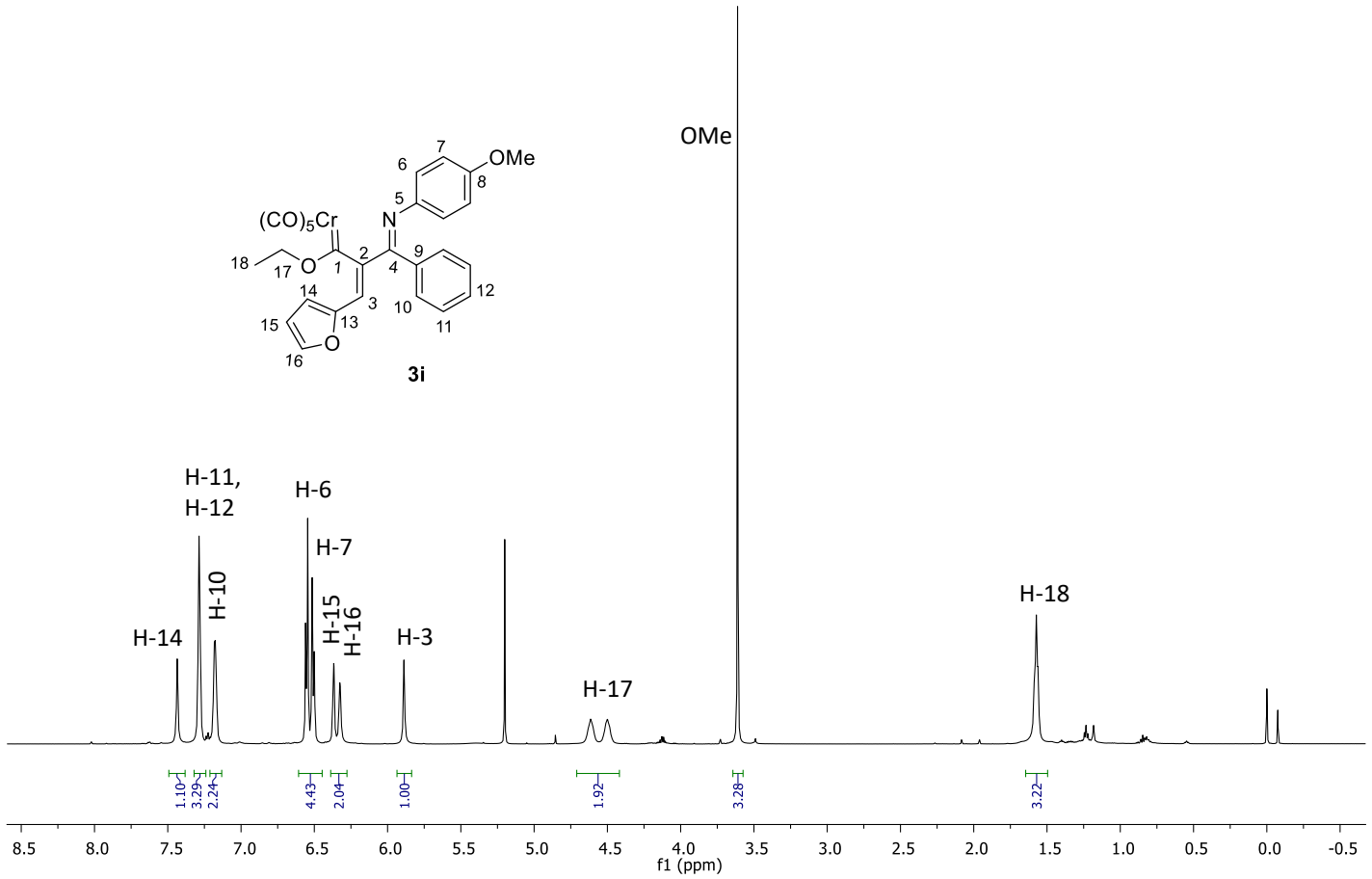

3i

^{1}H NMR for **3i**

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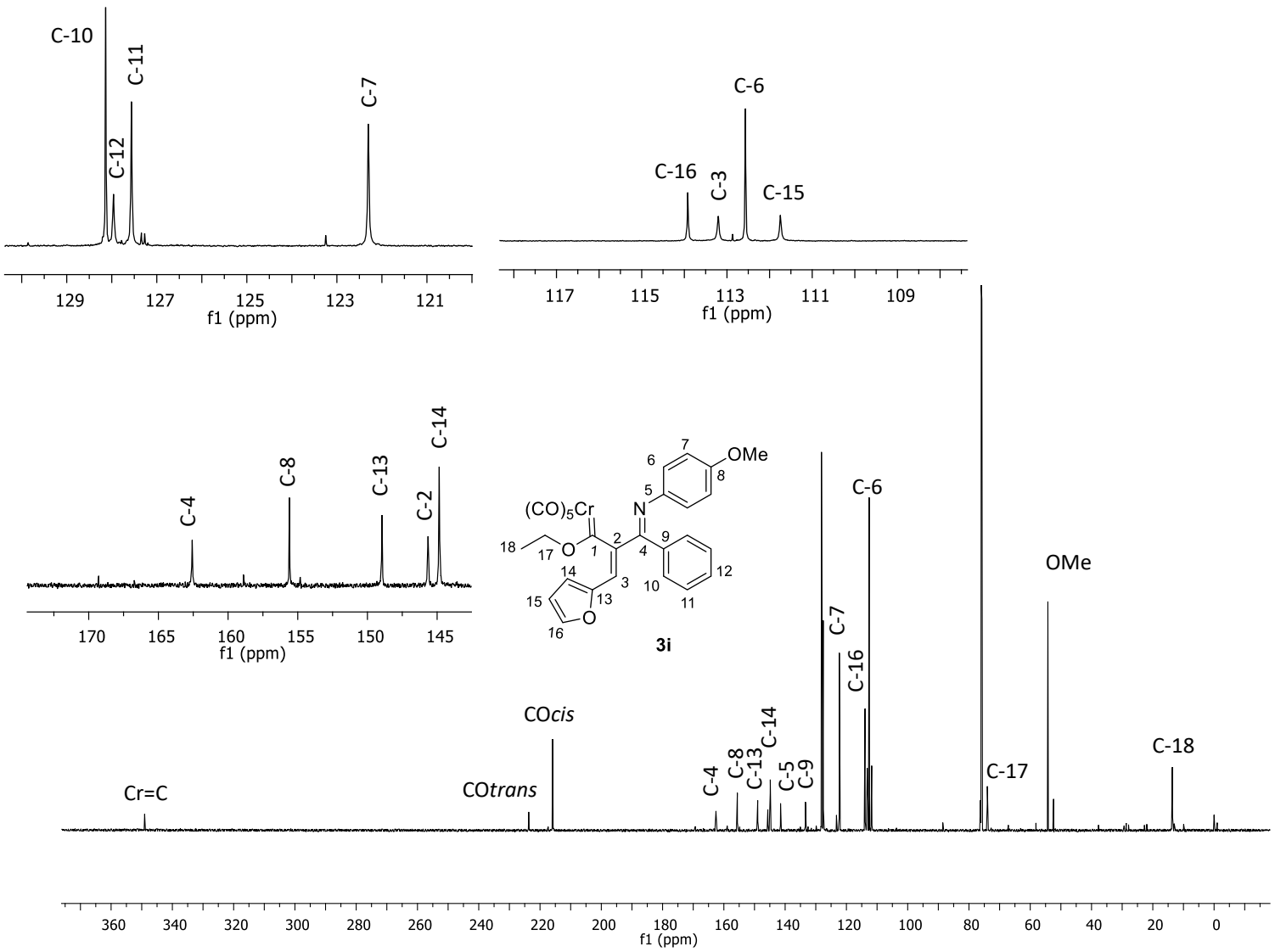

^{13}C NMR for **3i**

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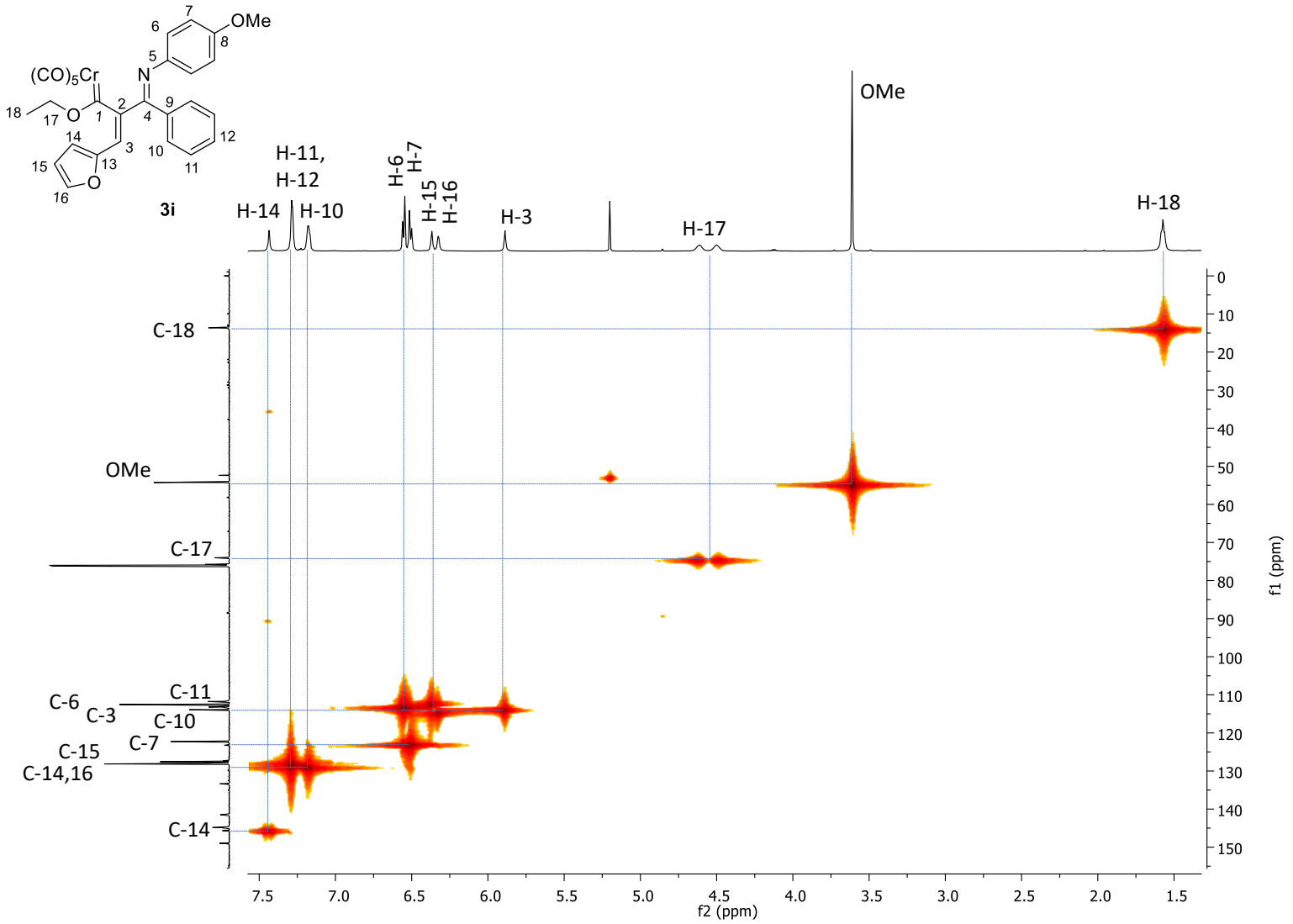

gHMQC experiment for **3i**

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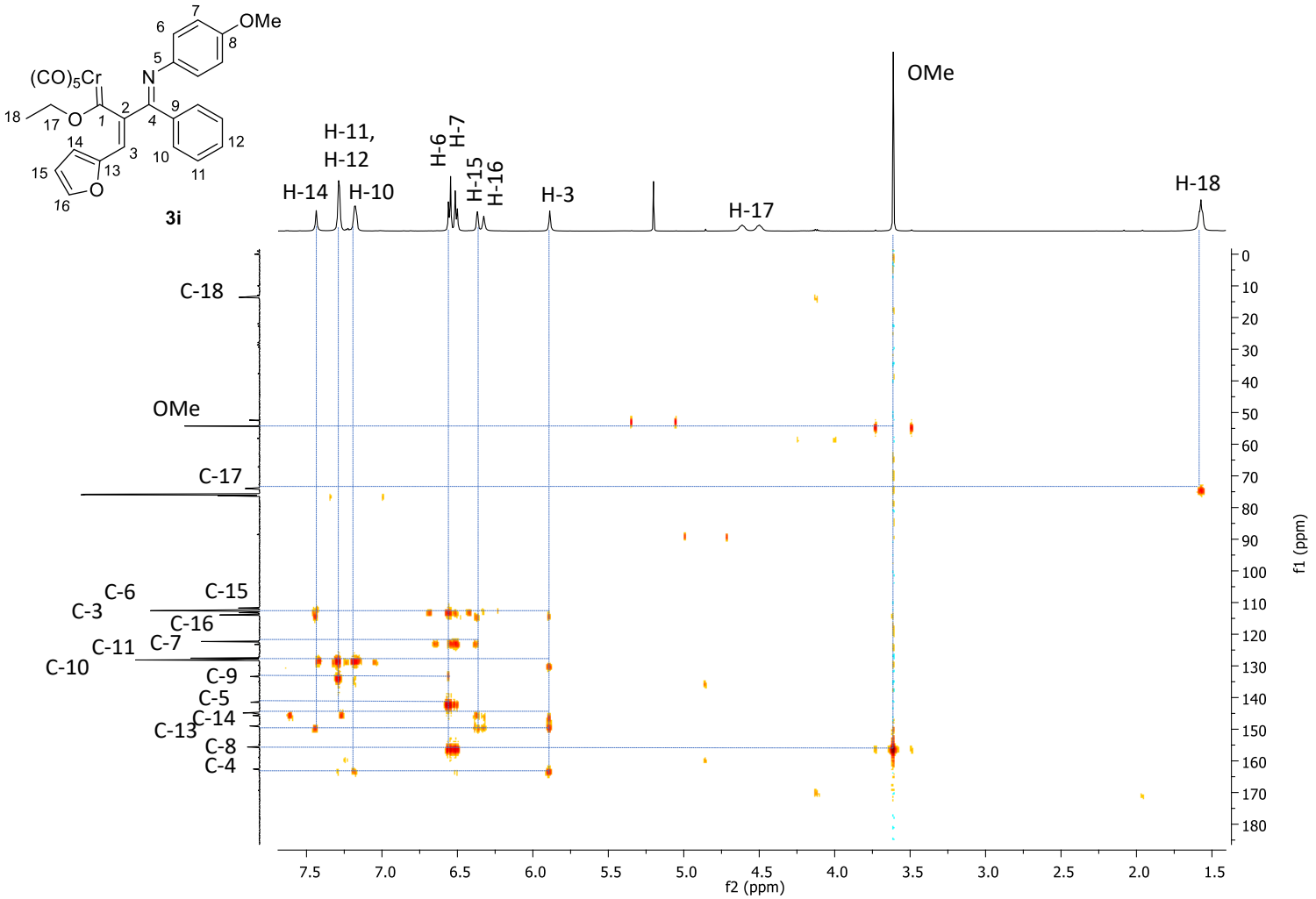

gHMBC experiment for **3i**

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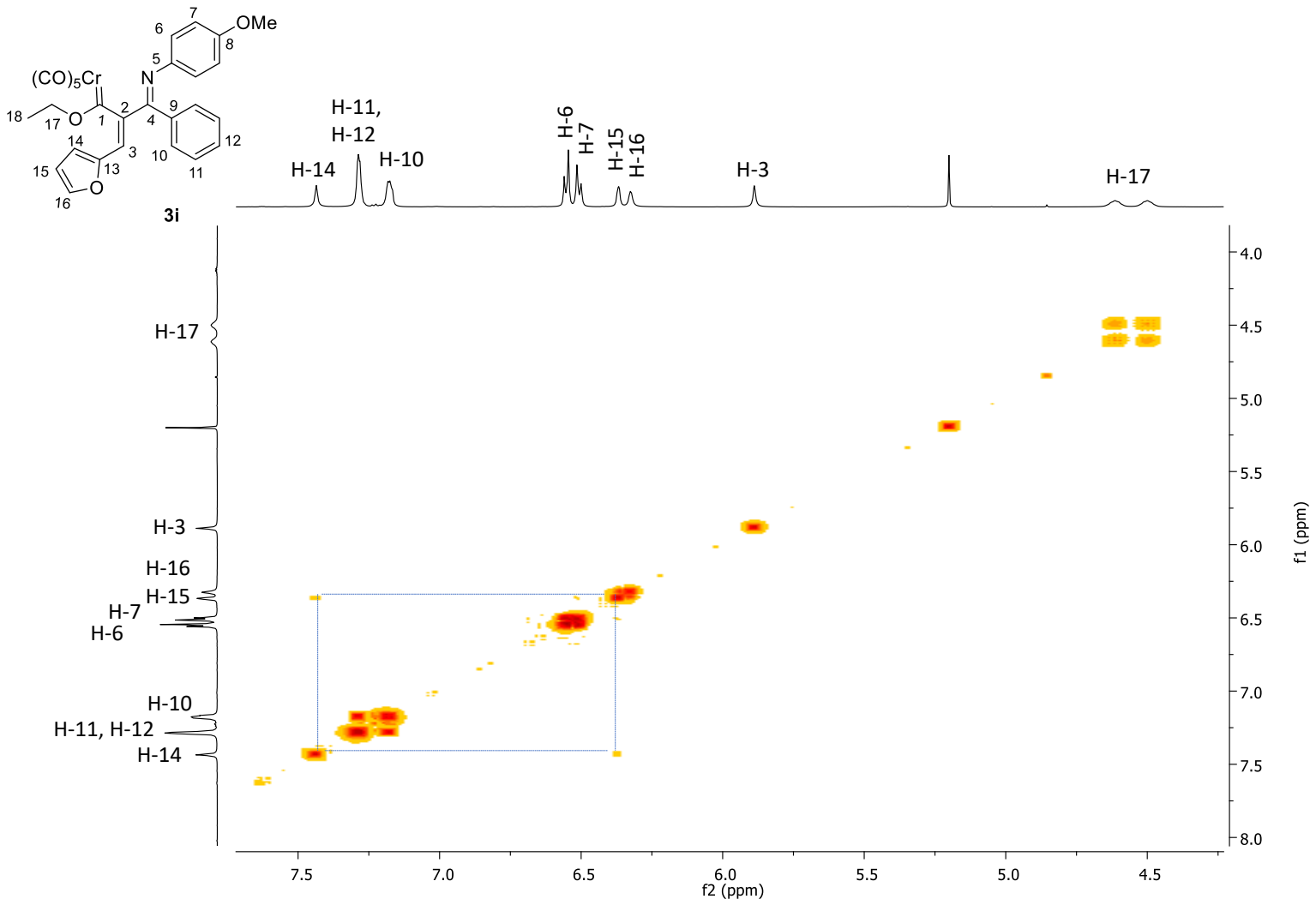

COSY experiment for **3i**

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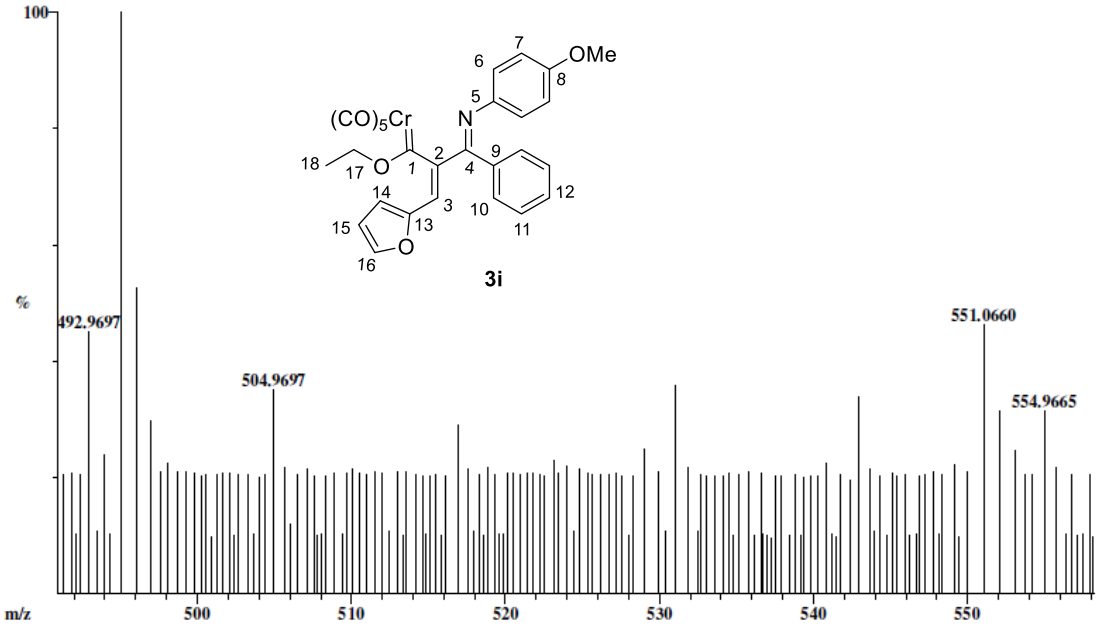
Scan: 180-181 **R.T.: 2.4**
Base: m/z 495; .3%FS TIC: 119488 **#Ions: 231**



3i

Selected Isotopes : $H_{0-21}C_{0-28}Cr_{0-1}N_{0-1}O_{0-8}$ **Error Limit : 5 ppm**

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*
551.0660	46.3%	$C_{28}H_{21}Cr\,N\,O_8$	551.0672	-2.2

HRMS (EI) $[M]^+$ for **3i**

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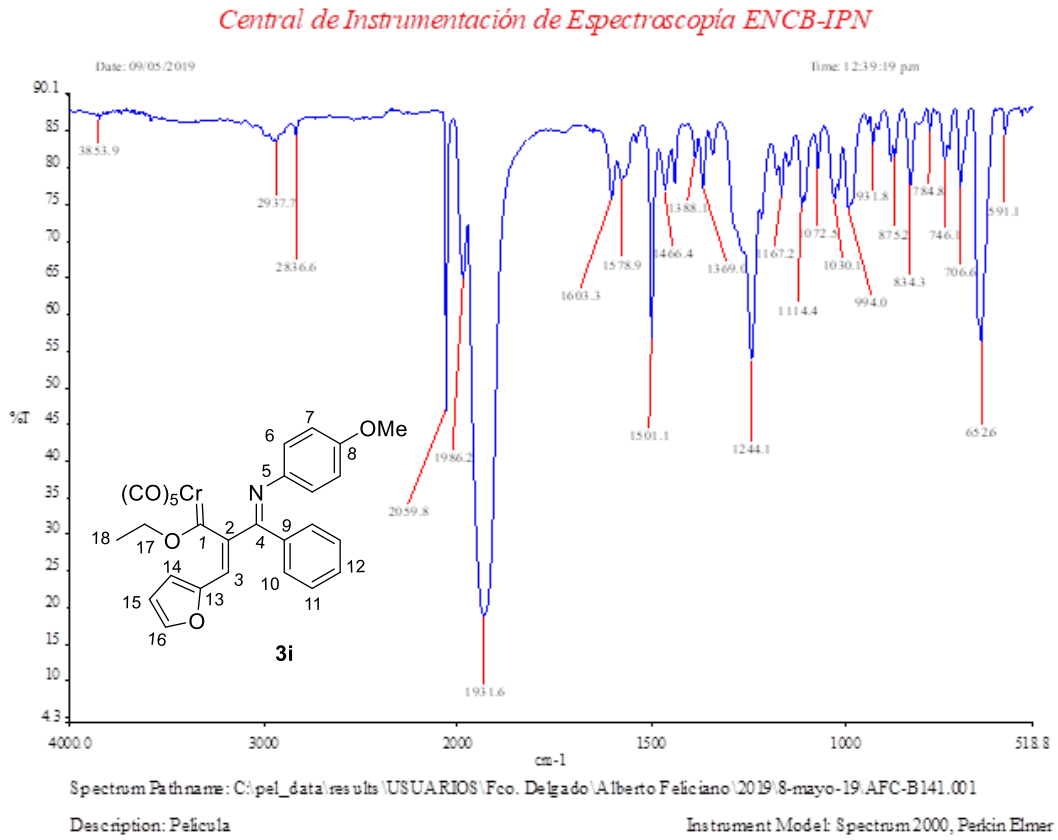

FT-IR for **3i**

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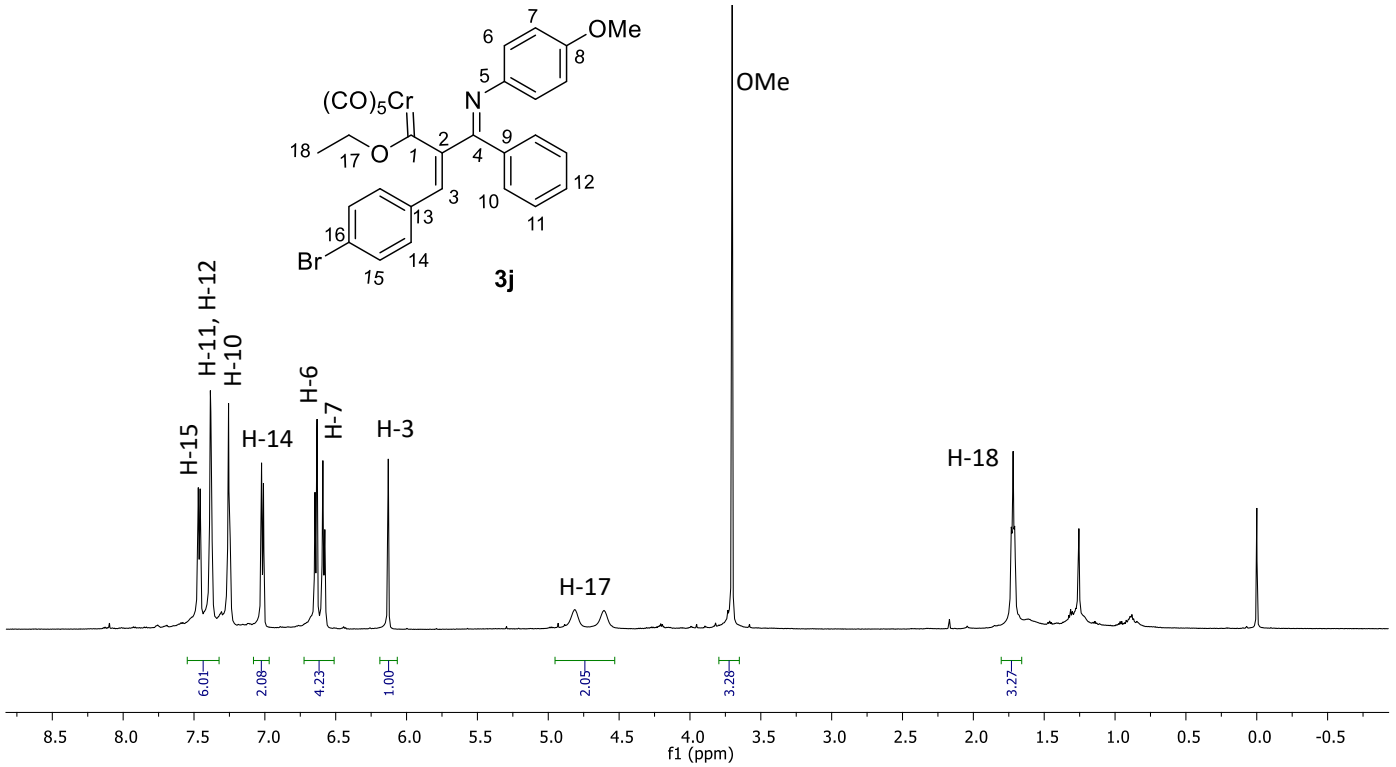
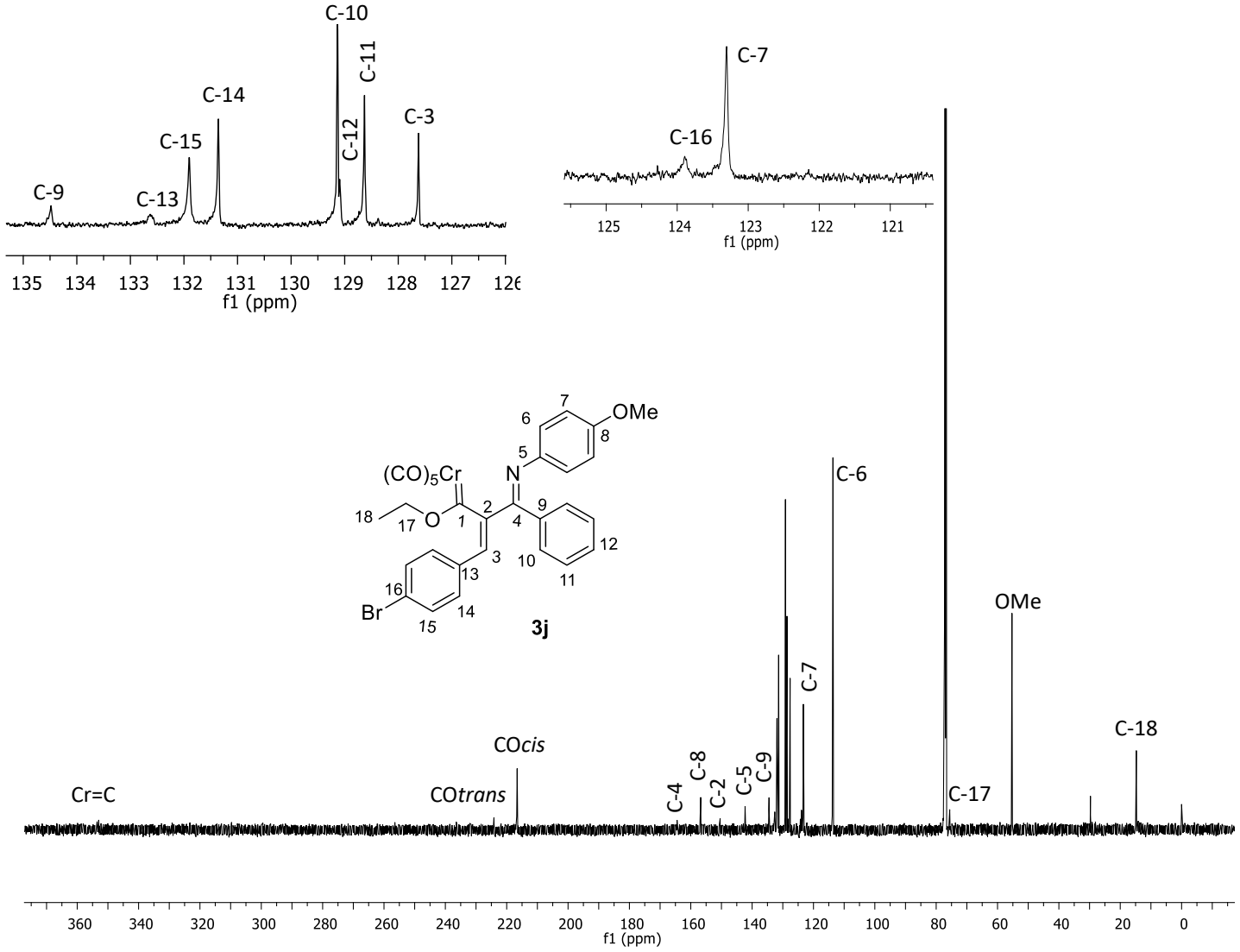
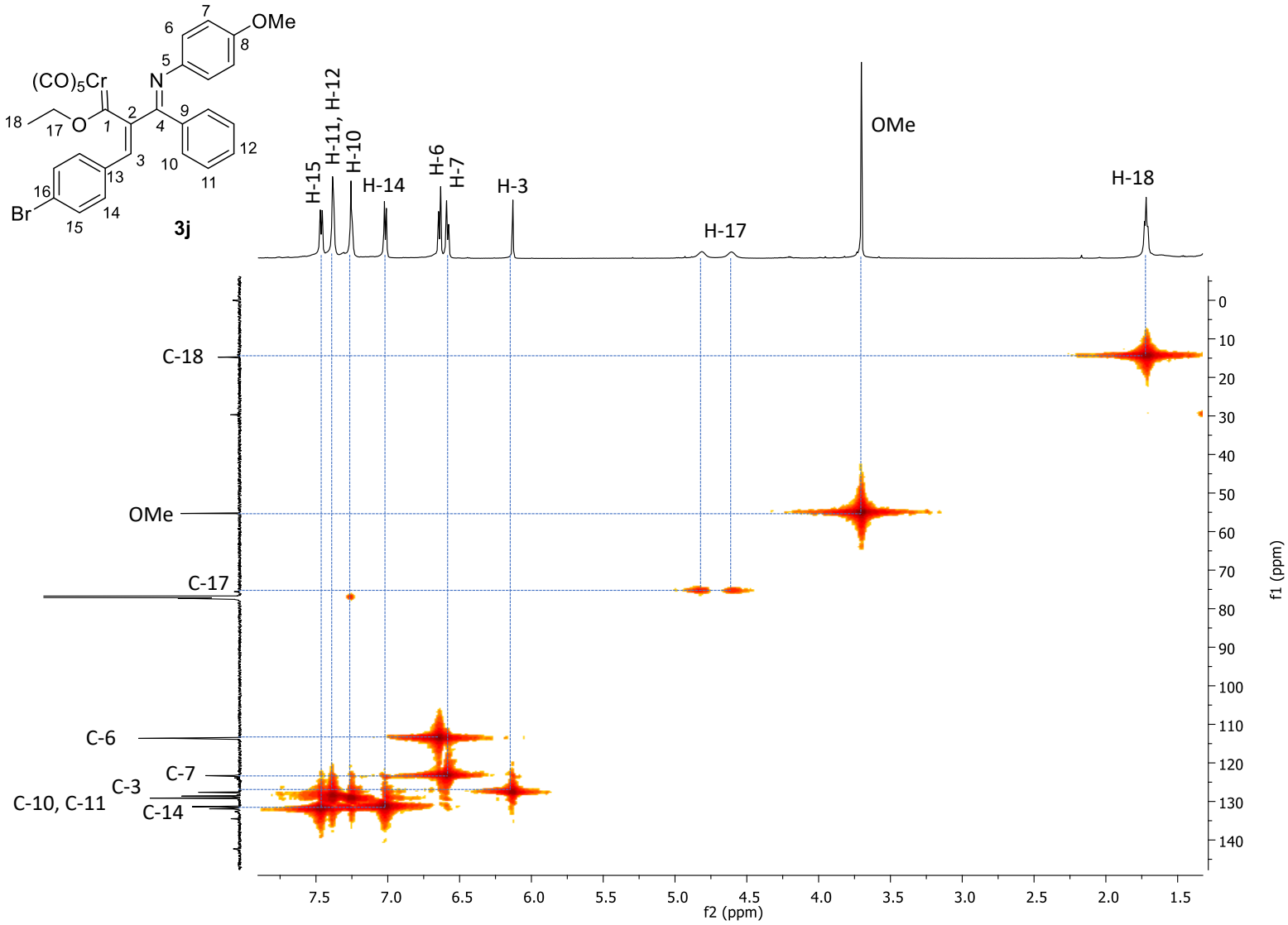


^{1}H NMR for **3j**

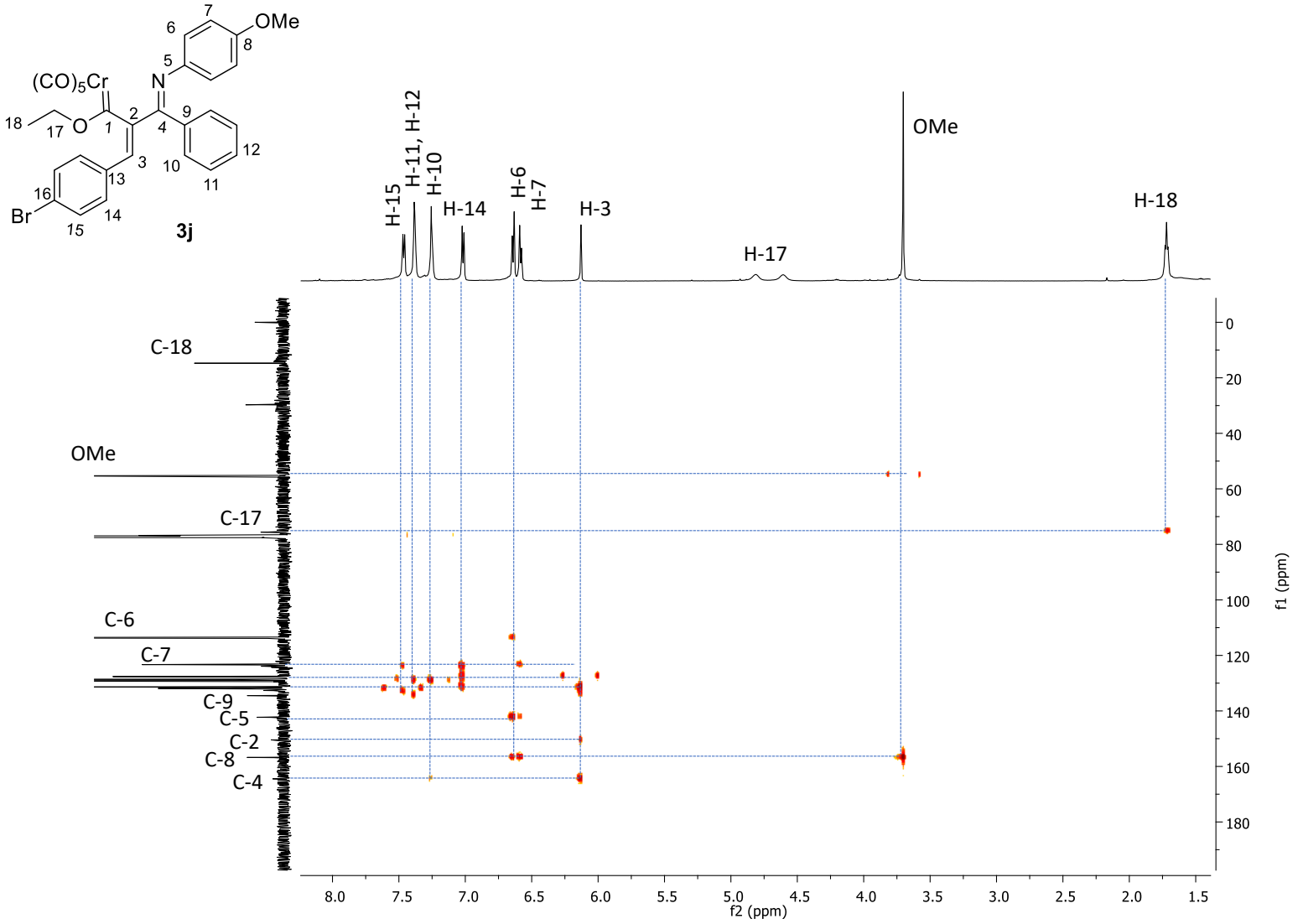


^{13}C NMR for **3j**



gHMQC experiment for **3j**

Supplementary Information



gHMBC experiment for **3j**

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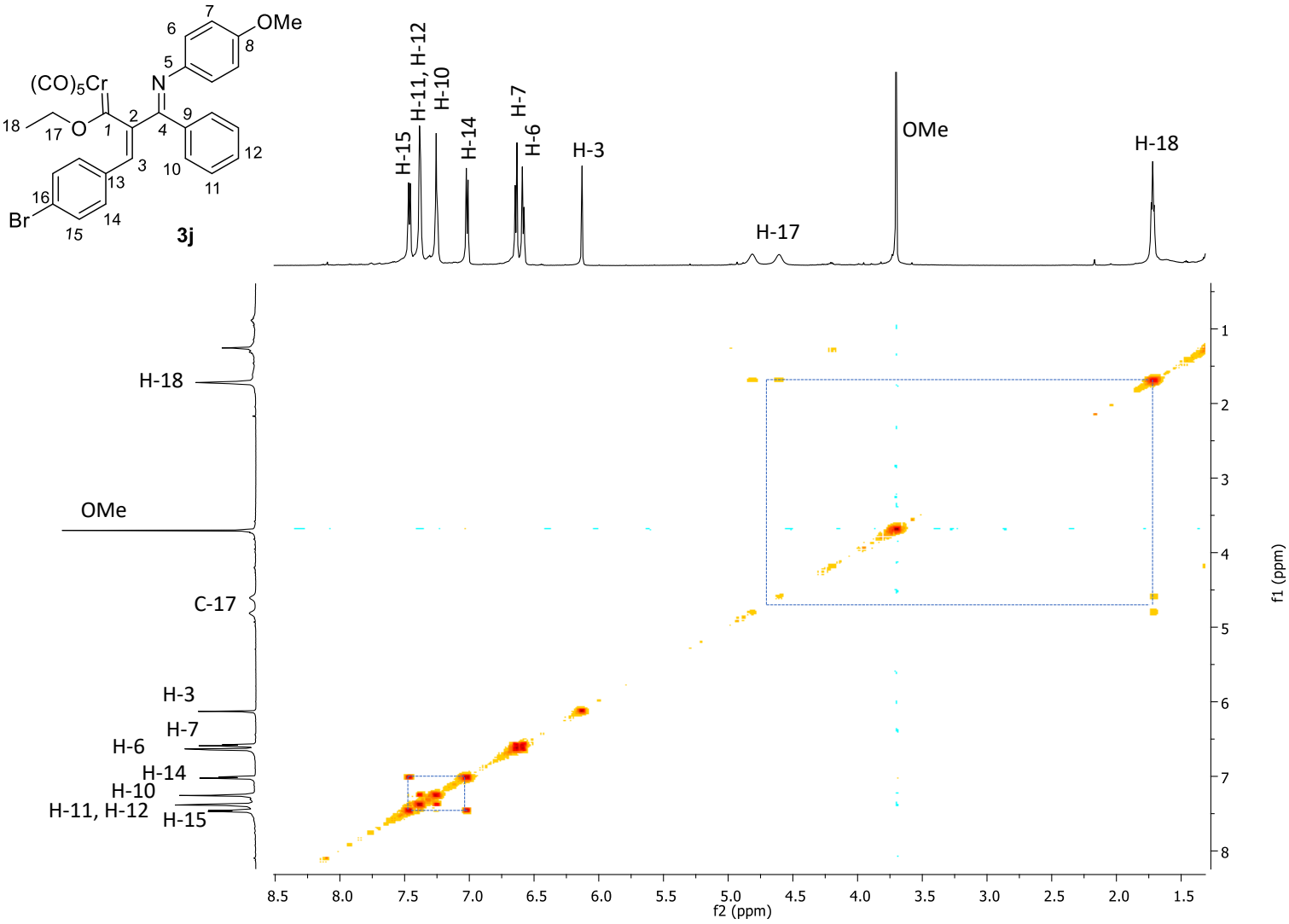

COSY experiment for **3j**

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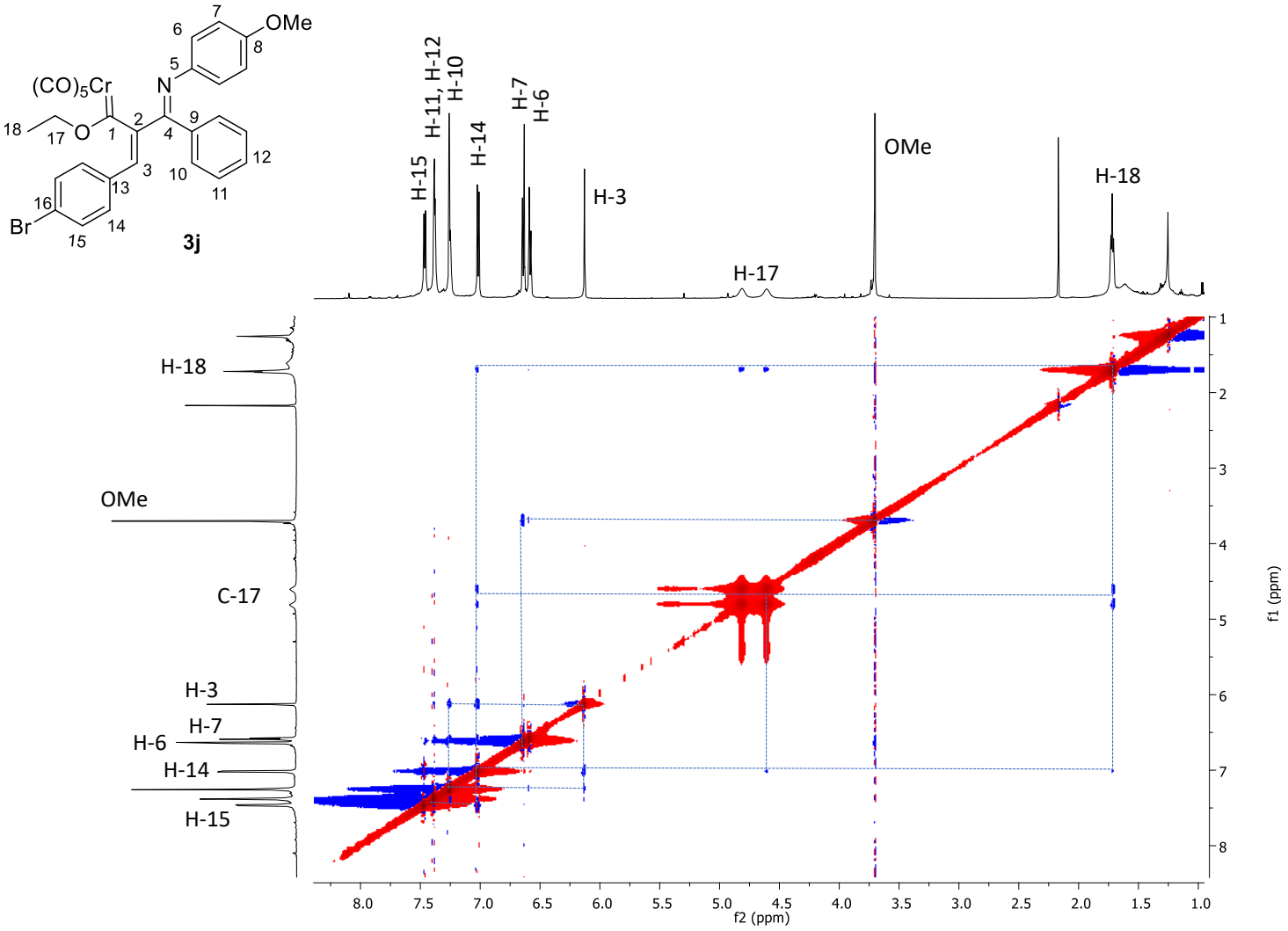

NOESY experiment for **3j**

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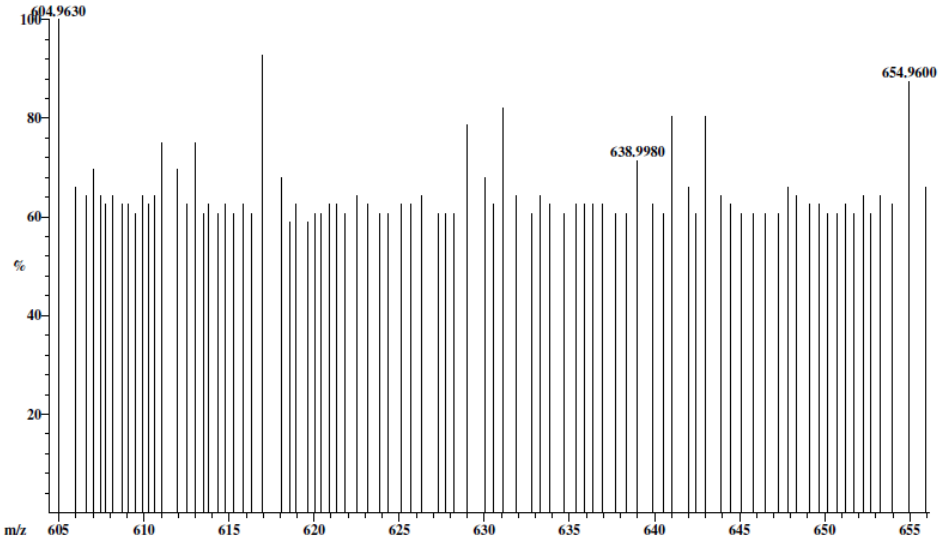
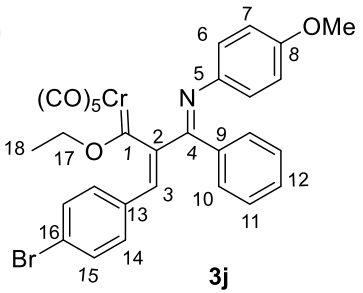
File: FDR-AFC-B118 **Date Run: 05-06-2019 (Time Run: 12:35:37)**
Sample: FDR-AFC-B118
Instrument: JEOL GCmate
Inlet: Direct Probe **Ionization mode: EI+**

Scan: 125 **R.T.: 1.67**
Base: m/z 605; .1%FS TIC: 78048 **#Ions: 136**





3j

Selected Isotopes : $H_{0-22}C_{0-30}Br_{0-1}Cr_{0-1}N_{0-1}O_{0-7}$ Error Limit : 5 ppm

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*
638.9980	71.4%	$C_{30}H_{22}BrCrNO_7$	638.9985	-0.7

HRMS (EI) $[M]^+$ for **3j**

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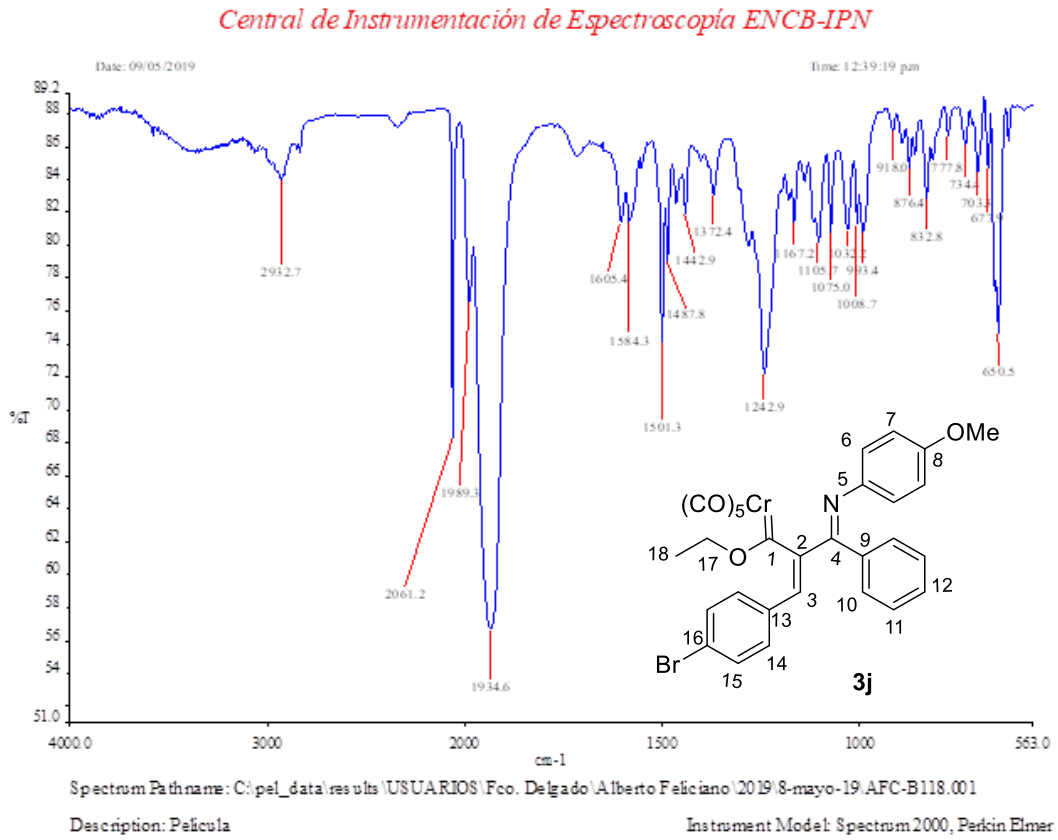

FT-IR for **3j**

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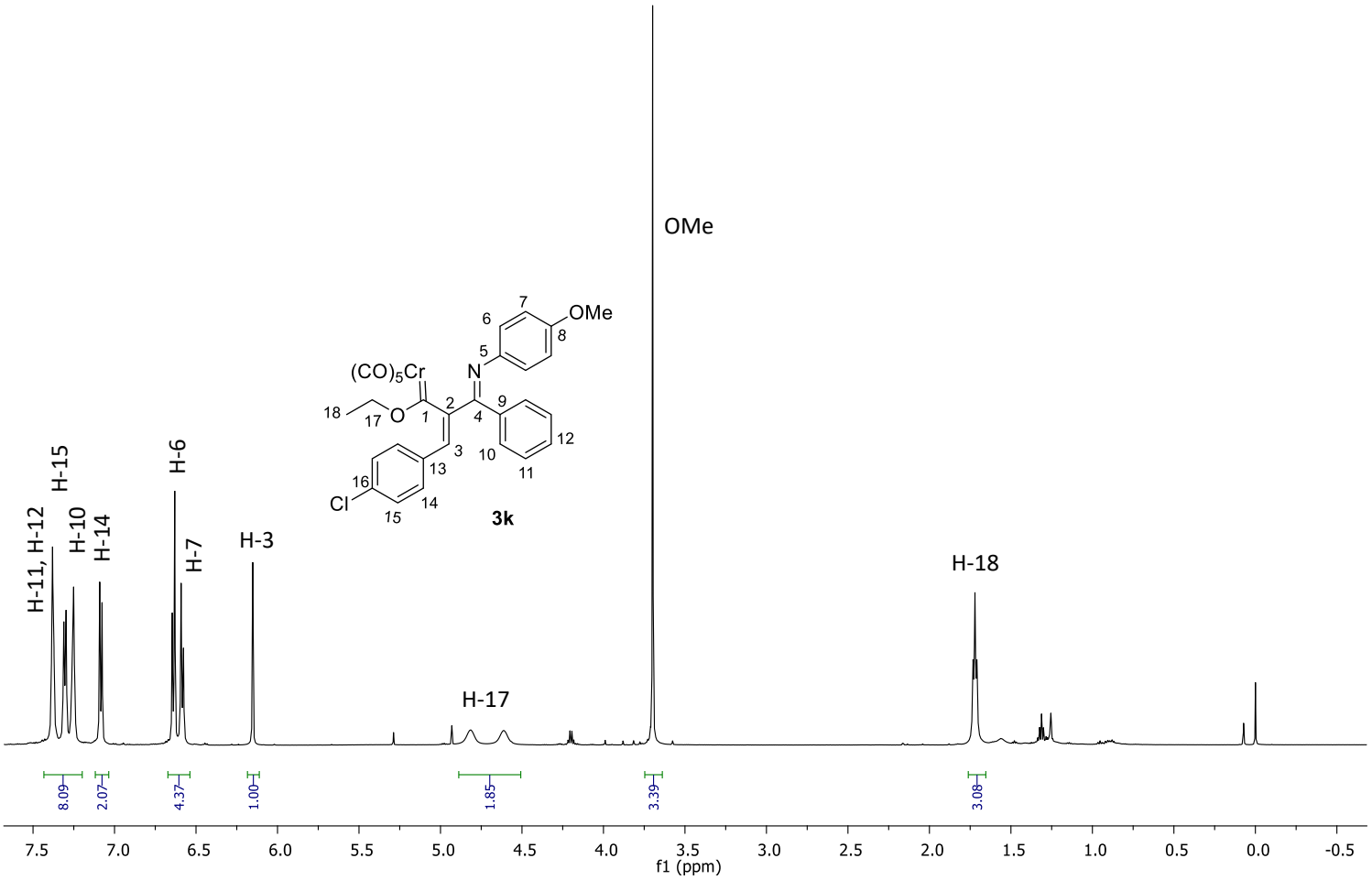

^{1}H NMR for **3k**

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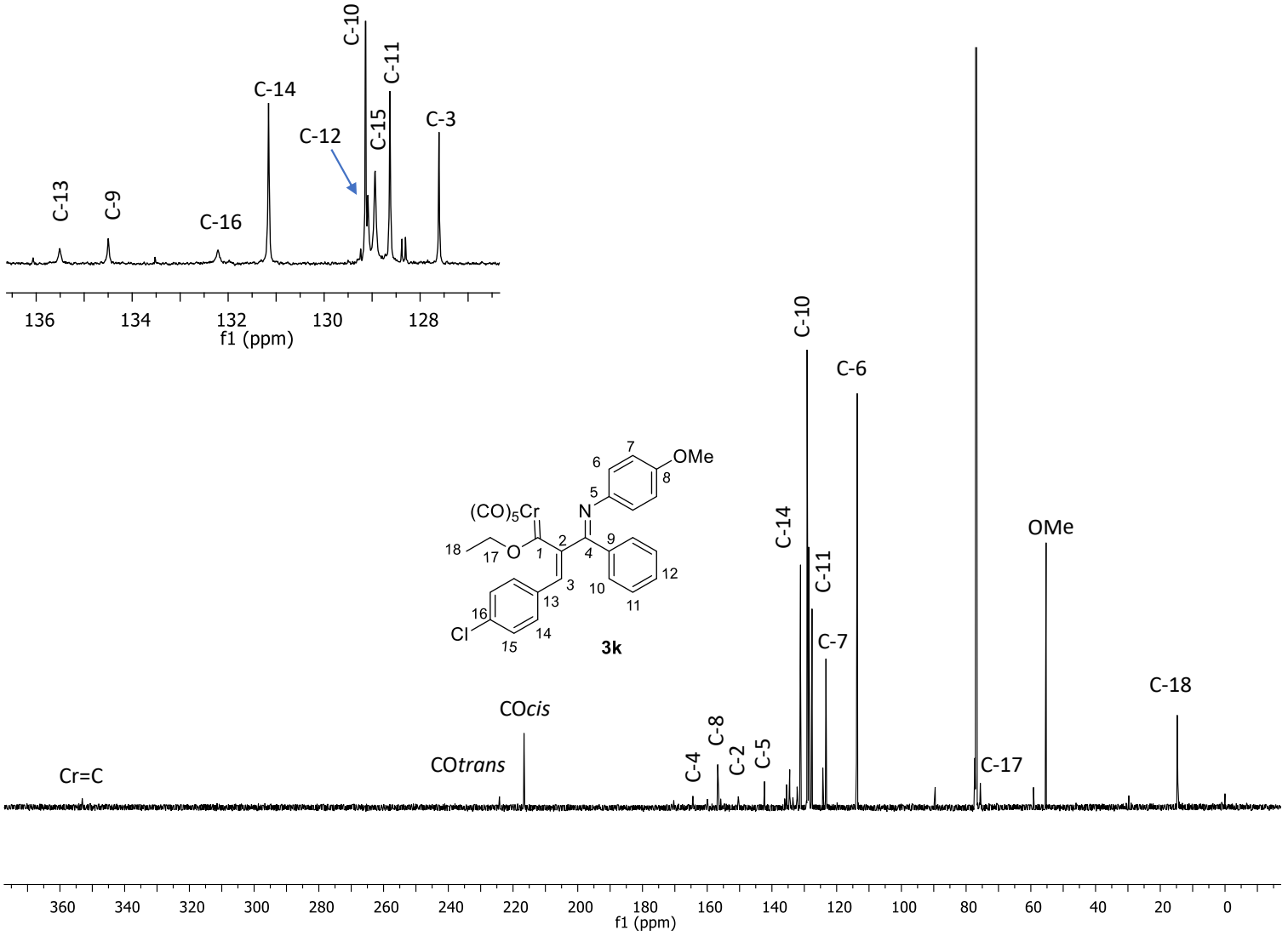

^{13}C NMR for **3k**

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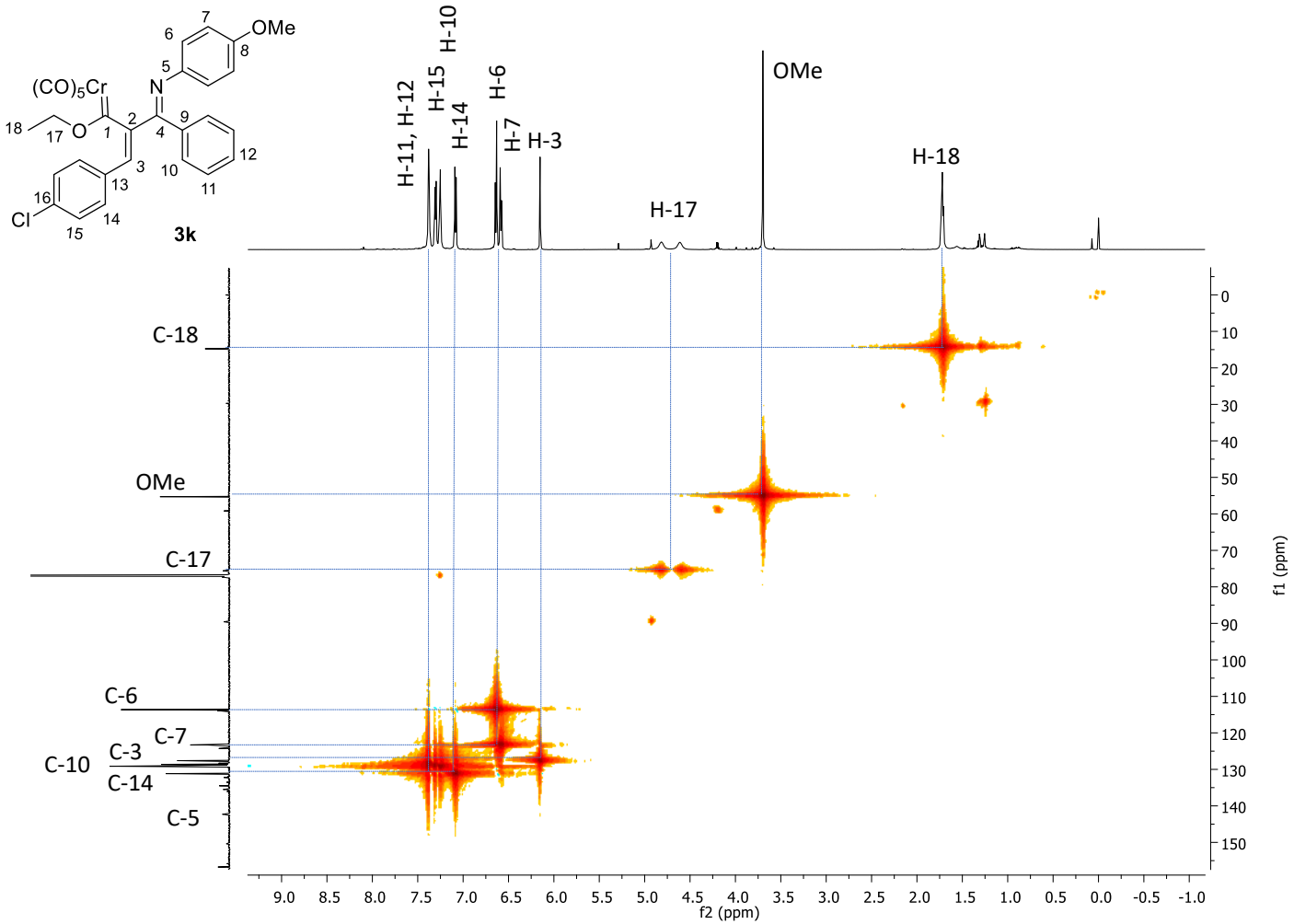
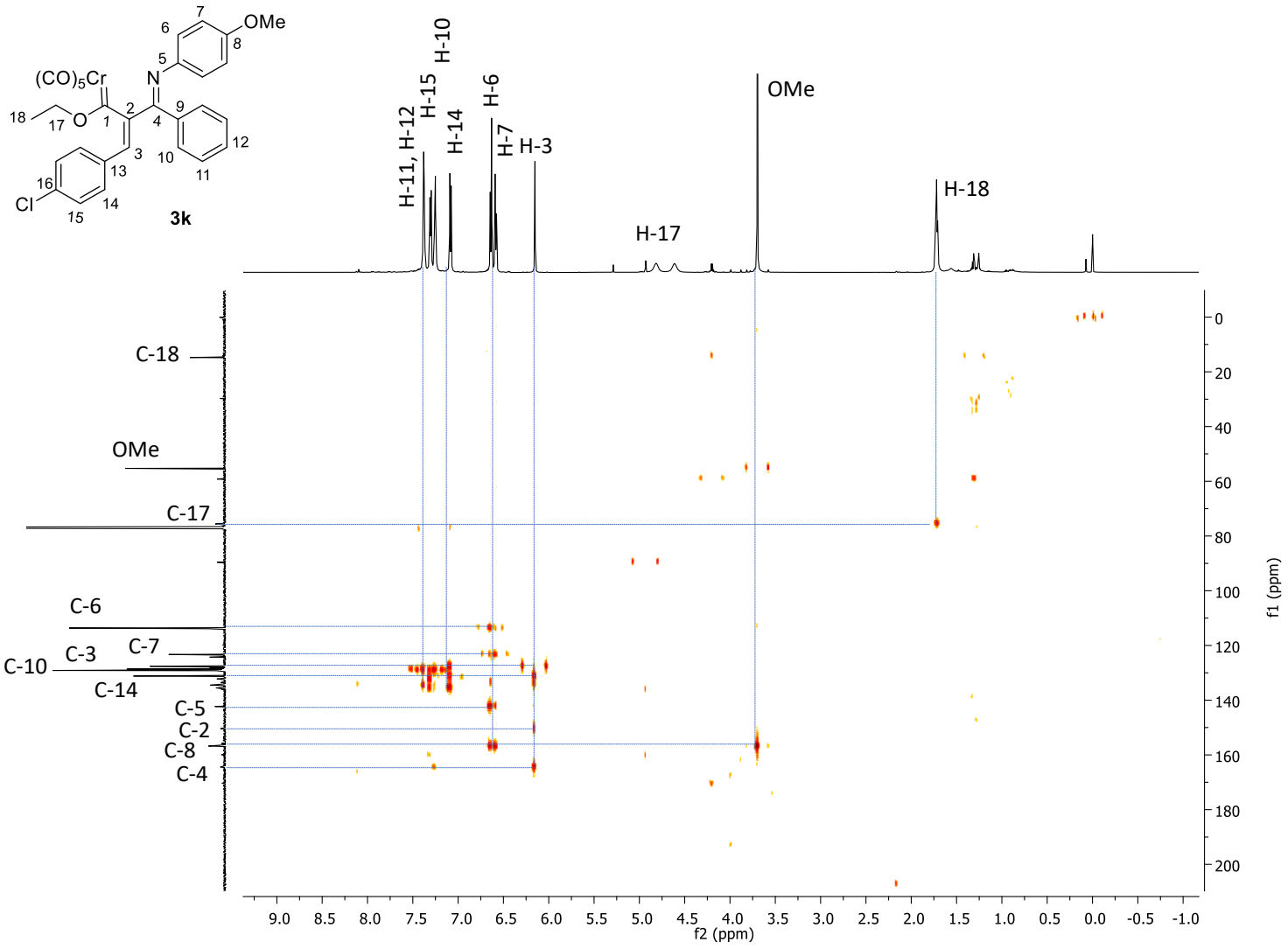


gHMQC experiment for **3k**



gHMBC experiment for **3k**

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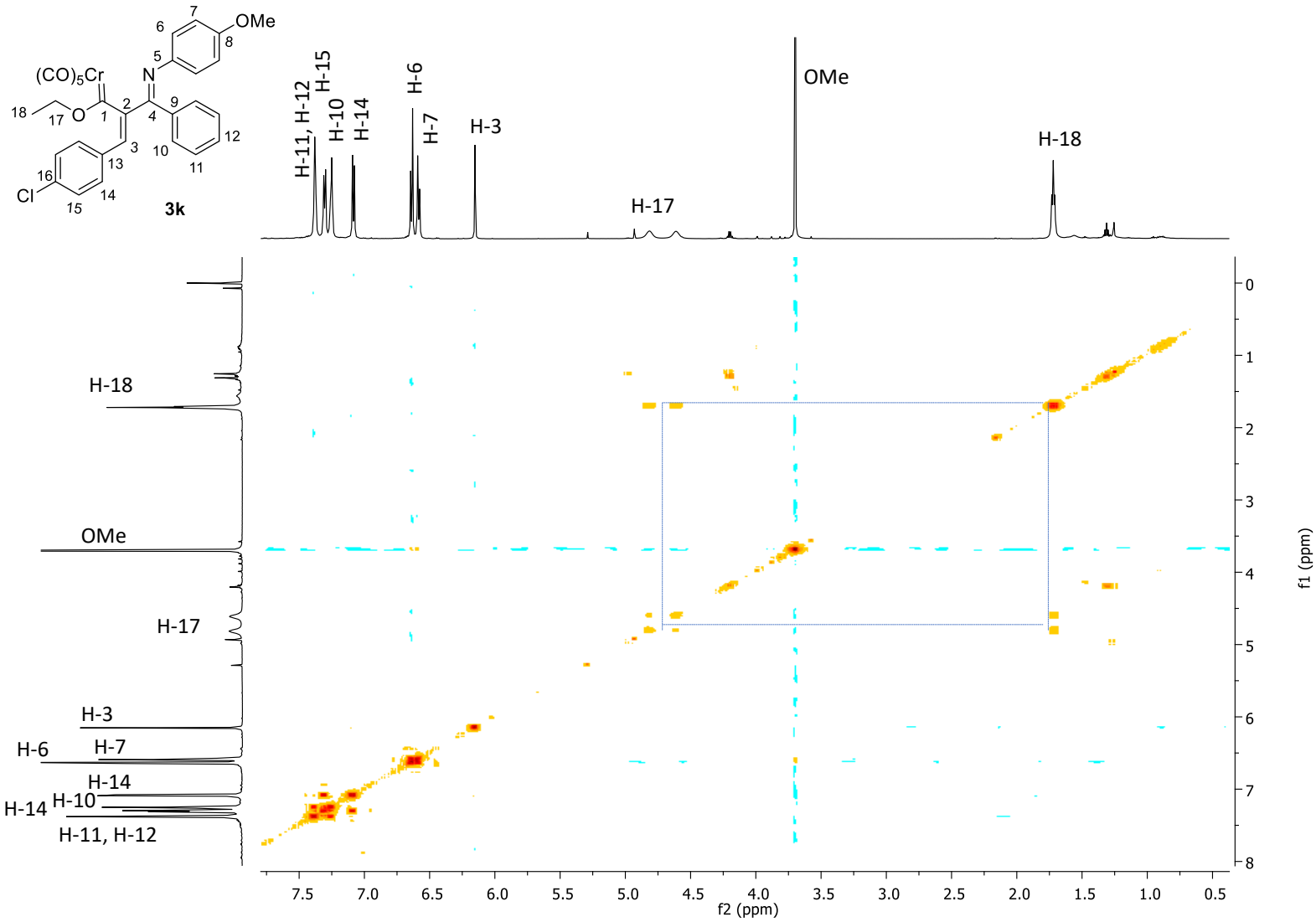
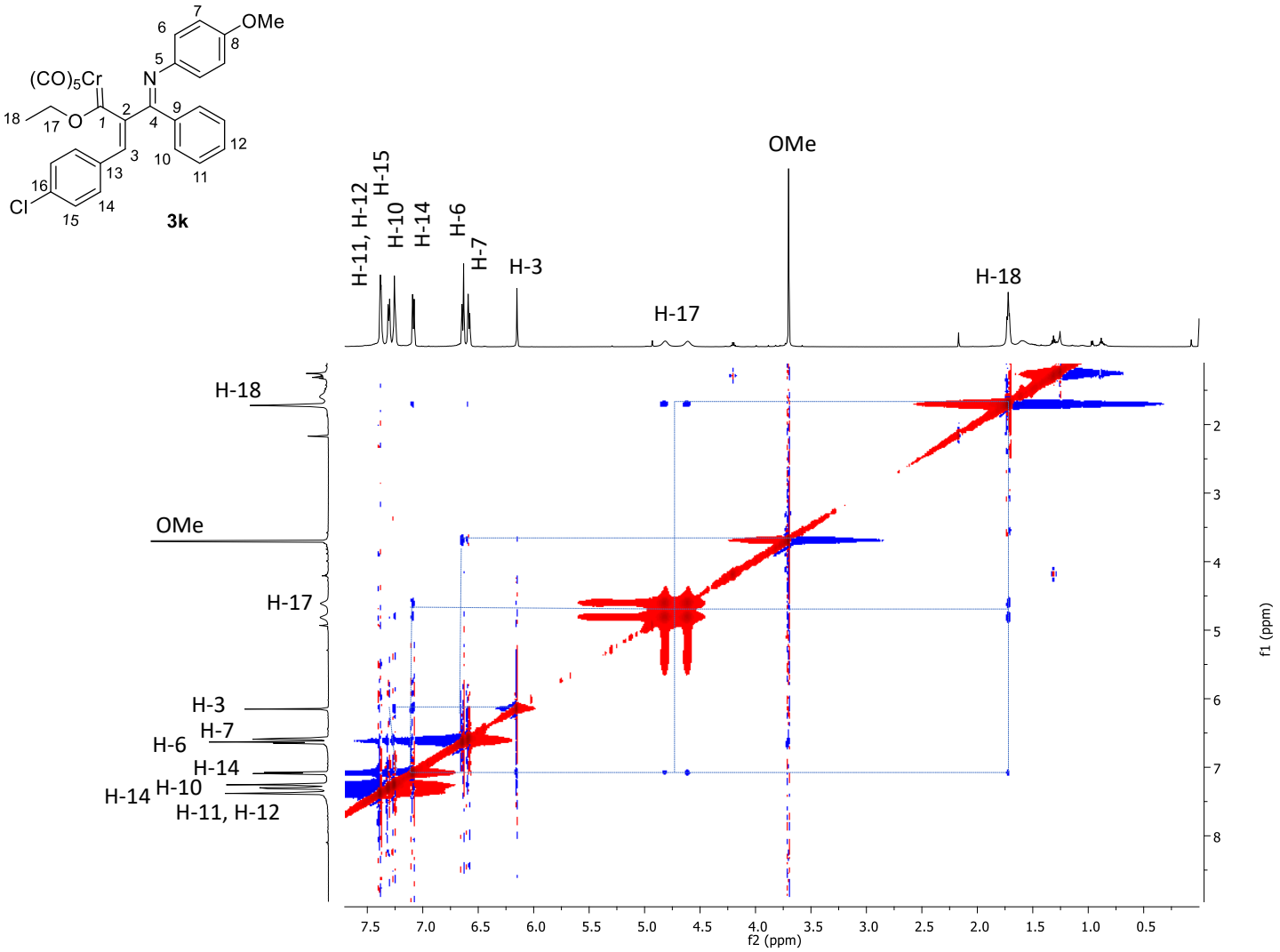


COSY experiment for **3k**



NOESY experiment for **3k**

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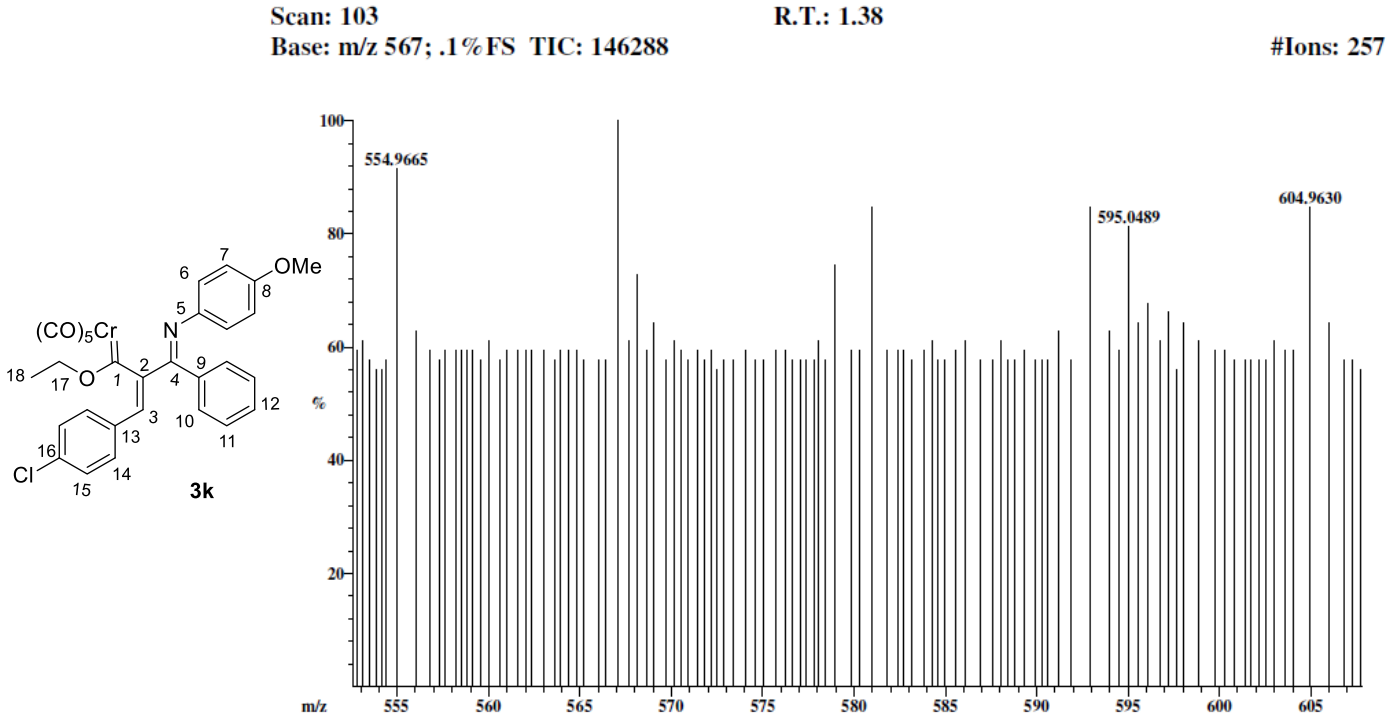

Selected Isotopes : $H_{0-22}C_{0-30}N_{0-1}O_{0-7}Cl_{0-1}Cr_{0-1}$ Error Limit : 5 ppm

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*
595.0489	81.4%	$C_{30}H_{22}NO_7ClCr$	595.0490	-0.1

HRMS (EI) $[M]^+$ for **3k**

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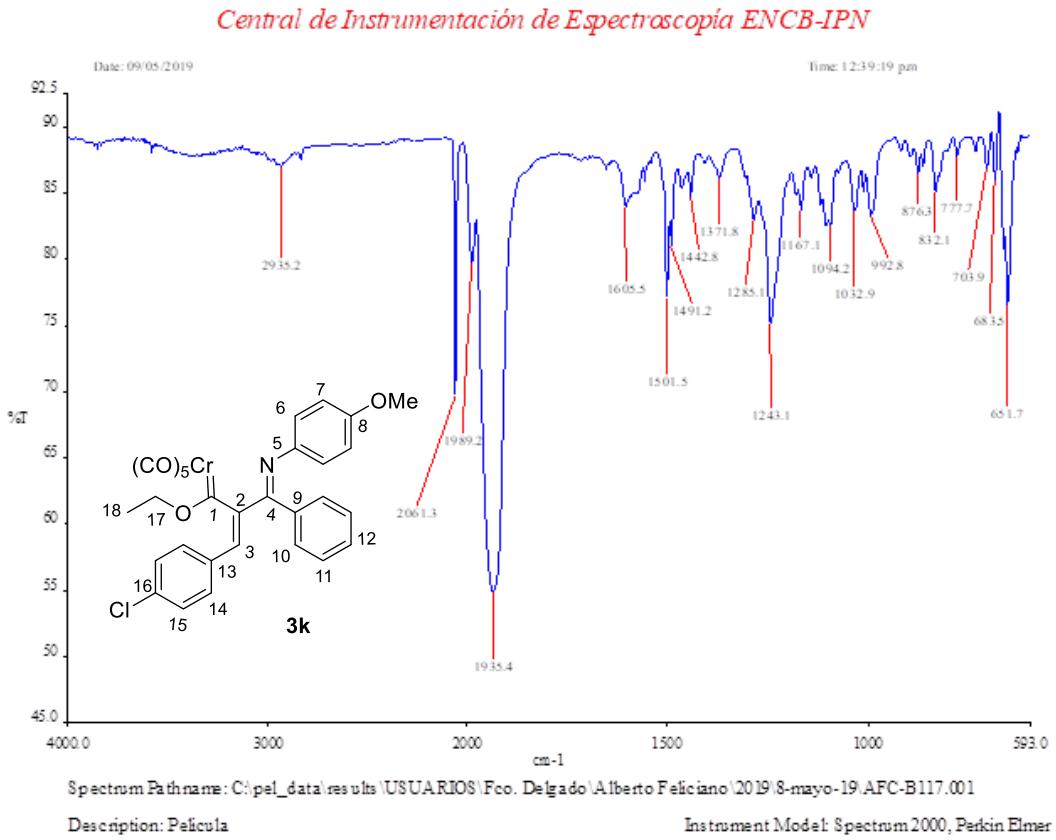

FT-IR for **3k**

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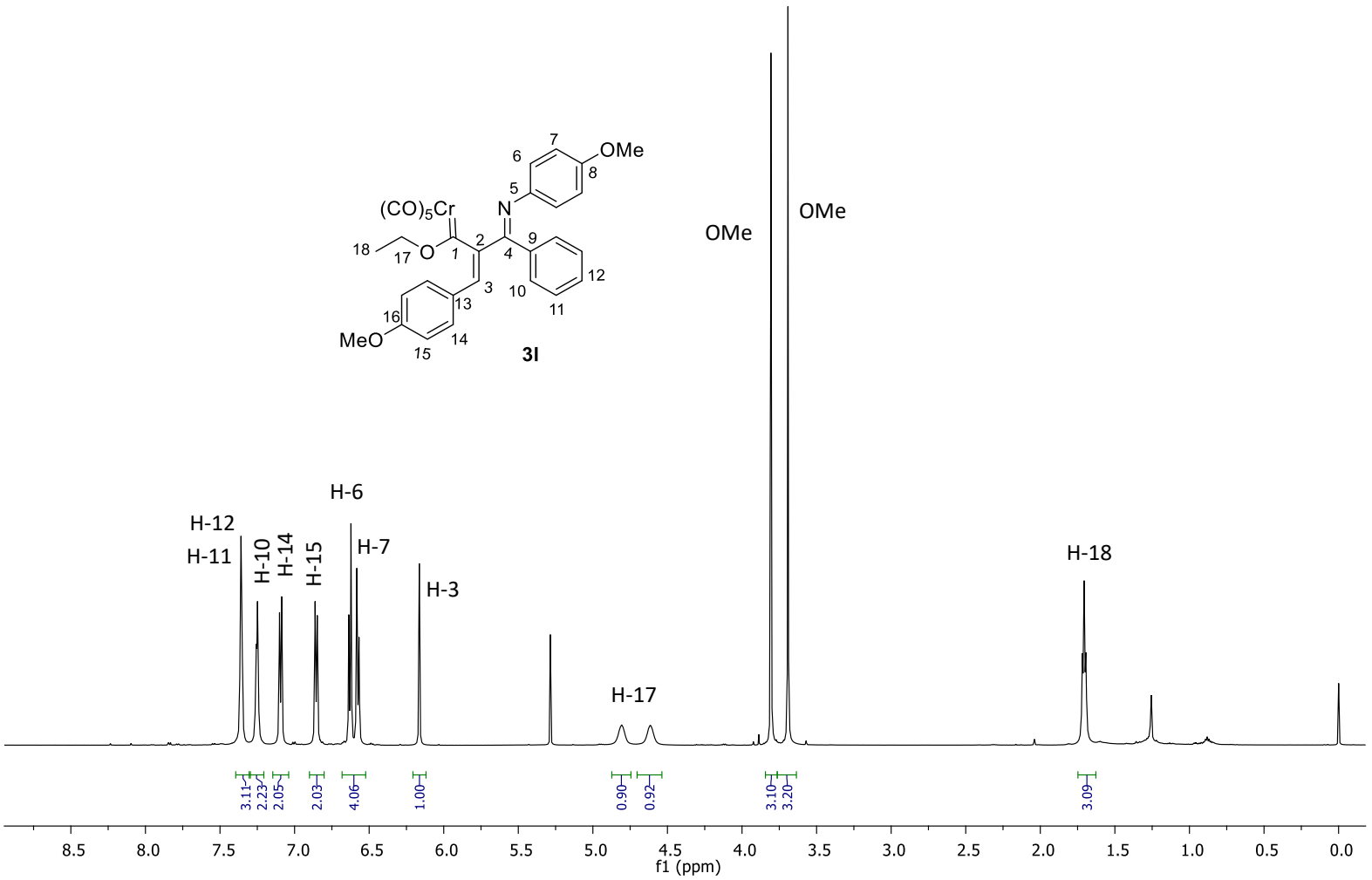

^{1}H NMR for **3l**

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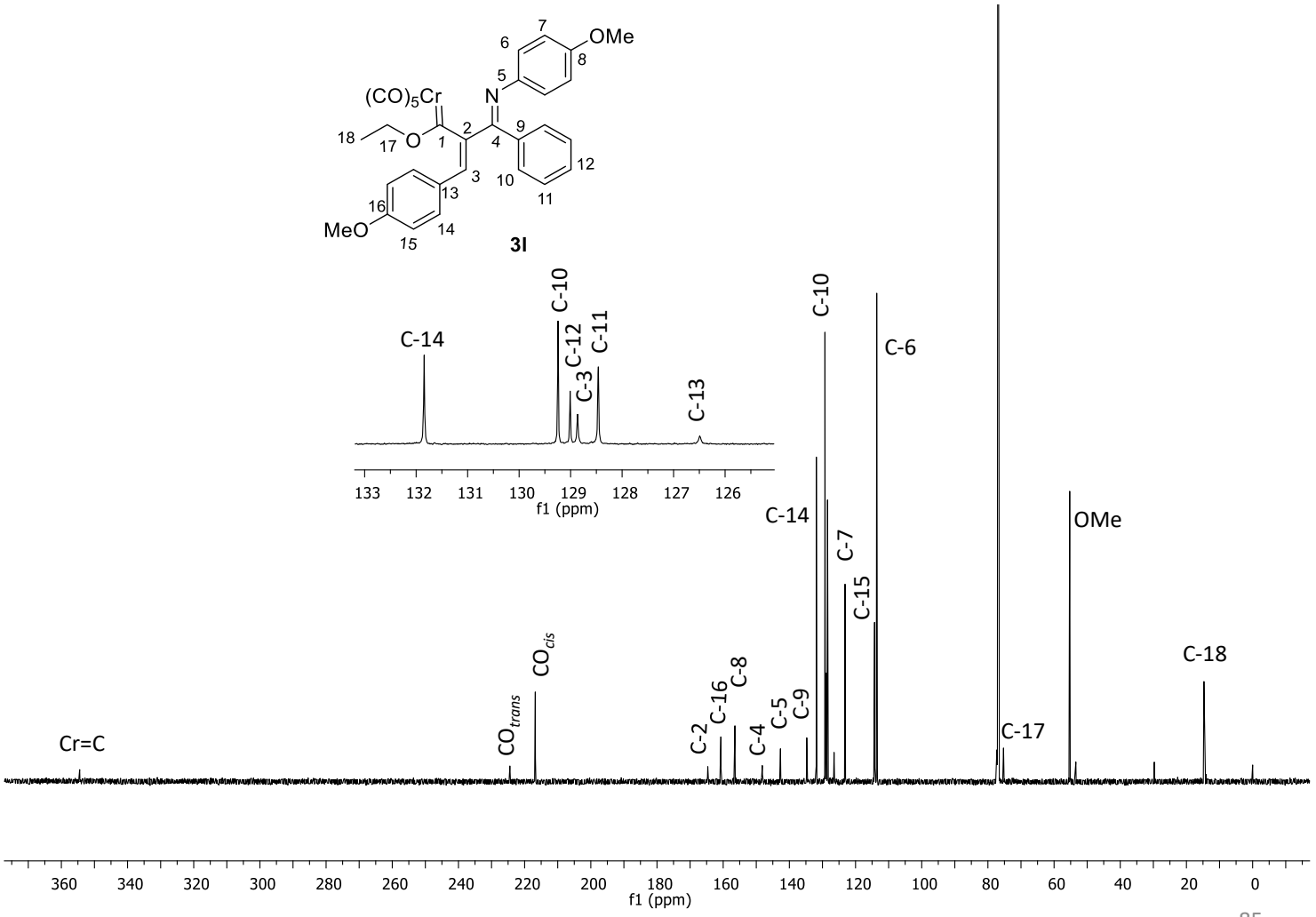

^{13}C NMR for **3l**

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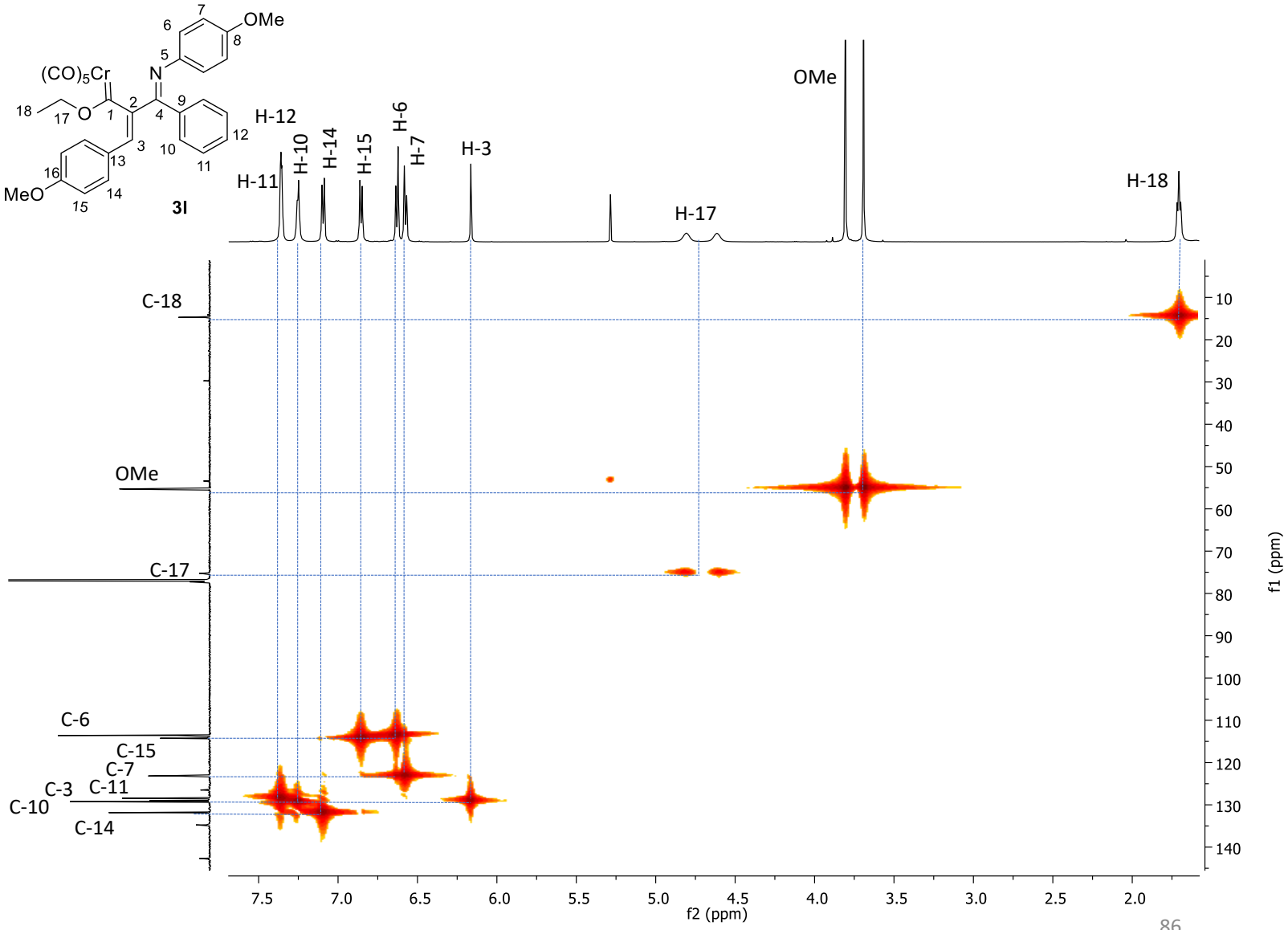

gHMQC experiment for **3l**

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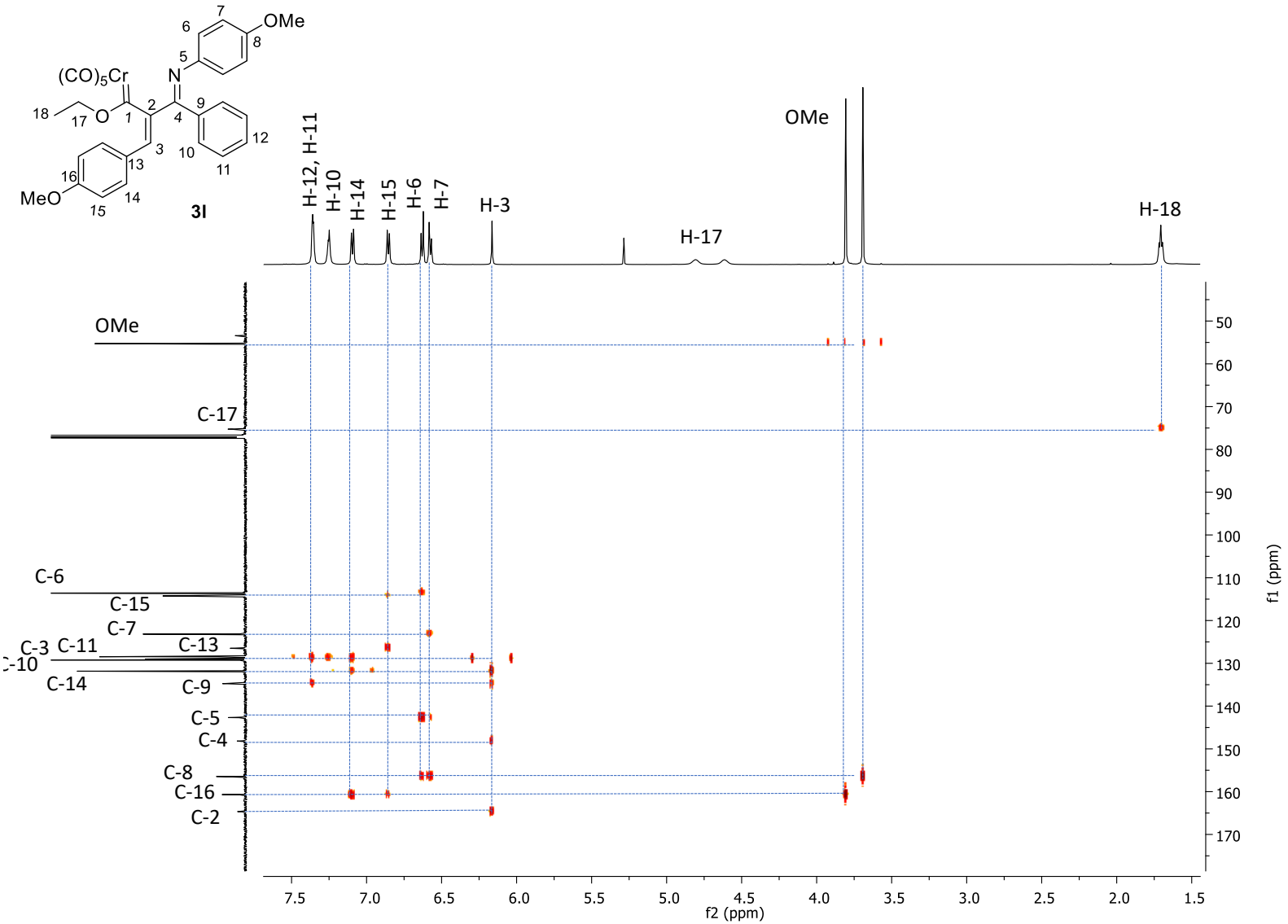
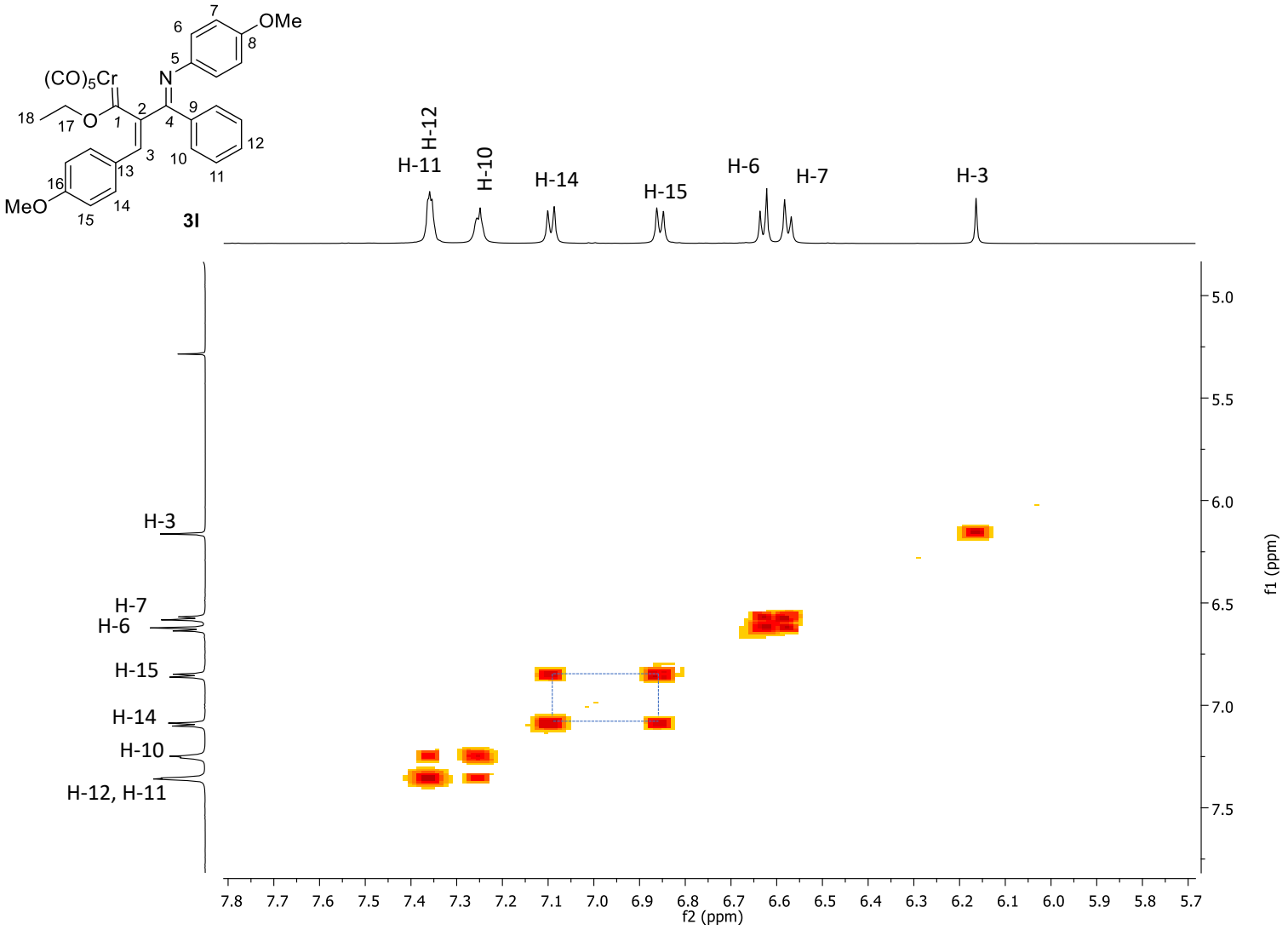


gHMBC experiment for **3l**



gCOSY experiment for **3l**

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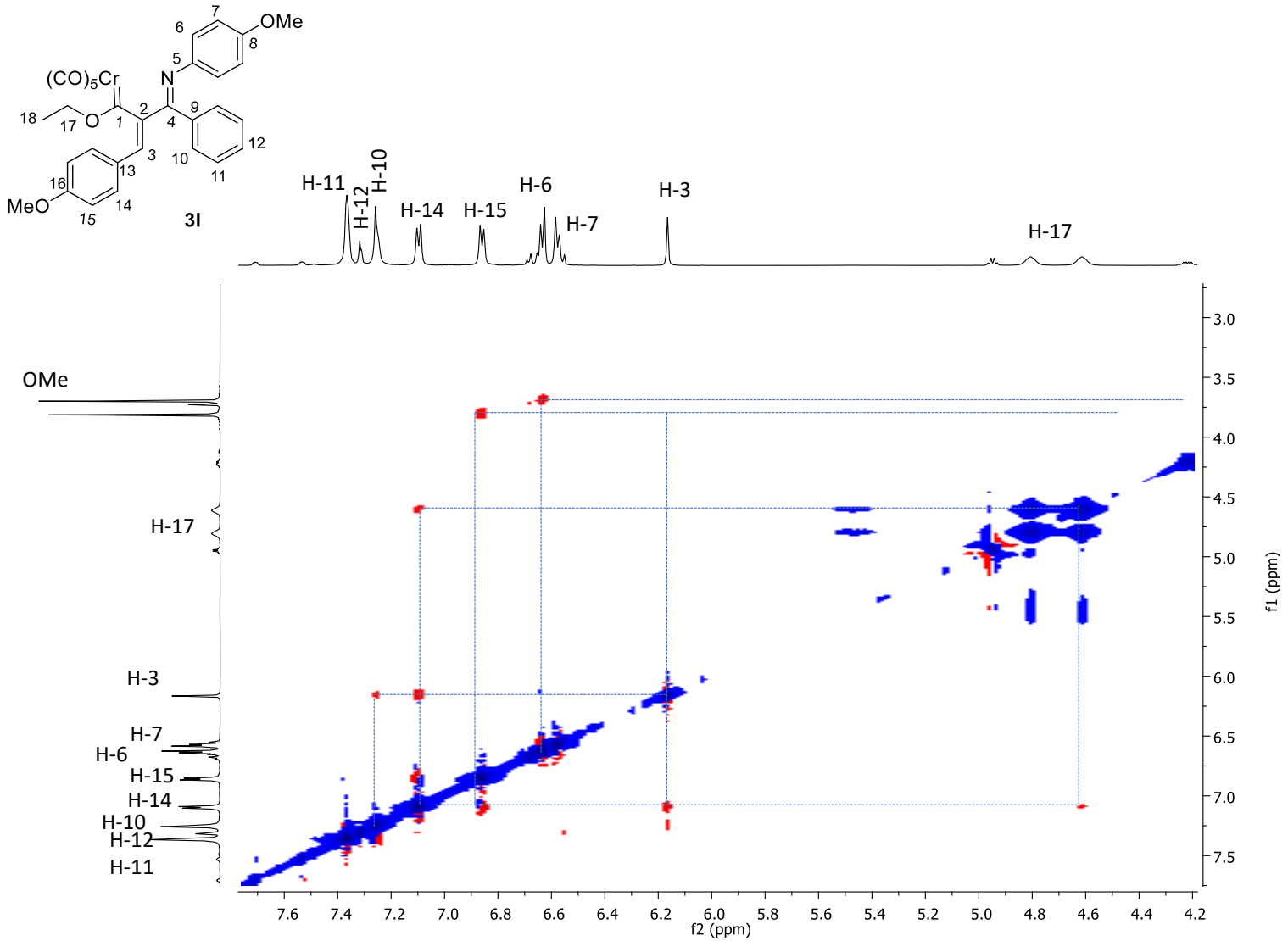

ROESY experiment for **3l**

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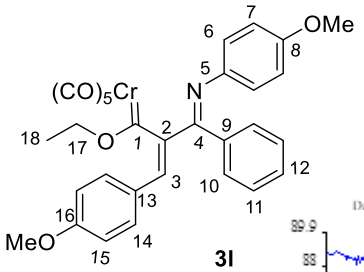
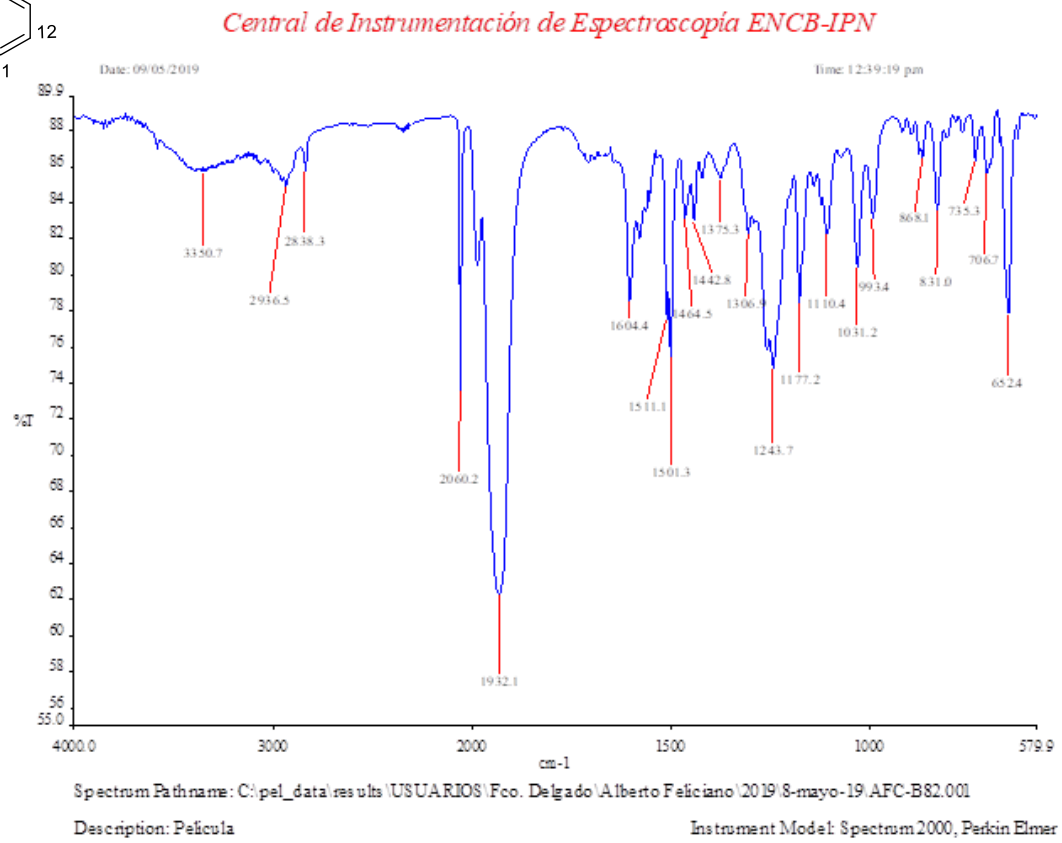


3l



FT-IR for **3l**

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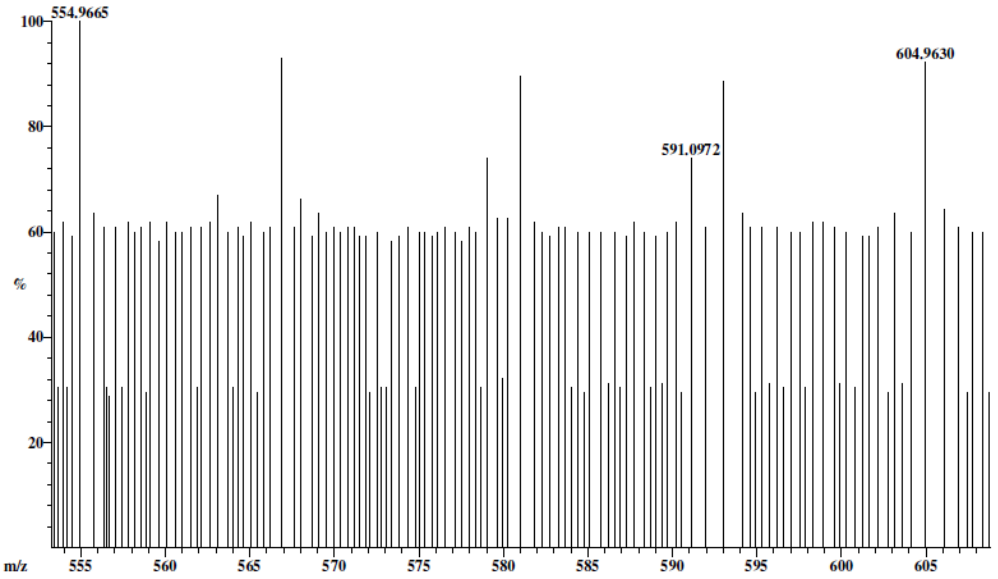
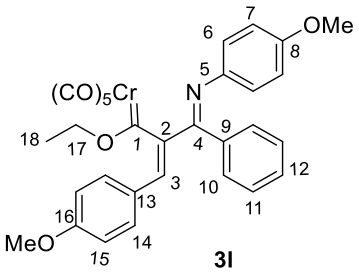
File: FDR-AFC-B82 **Date Run: 05-06-2019 (Time Run: 16:08:01)**
Sample: FDR-AFC-B82
Instrument: JEOL GCmate
Inlet: Direct Probe **Ionization mode: EI+**

Scan: 119-120 **R.T.: 1.61**
Base: m/z 555; .1%FS TIC: 147848 **#Ions: 298**





3l

Selected Isotopes : $H_{0-25}C_{0-31}N_{0-1}O_{0-8}Cr_{0-1}$ Error Limit : 5 ppm

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*
591.0972	73.9%	$C_{31}H_{25}NO_8Cr$	591.0985	-2.2

HRMS (EI) $[M]^+$ for **3l**

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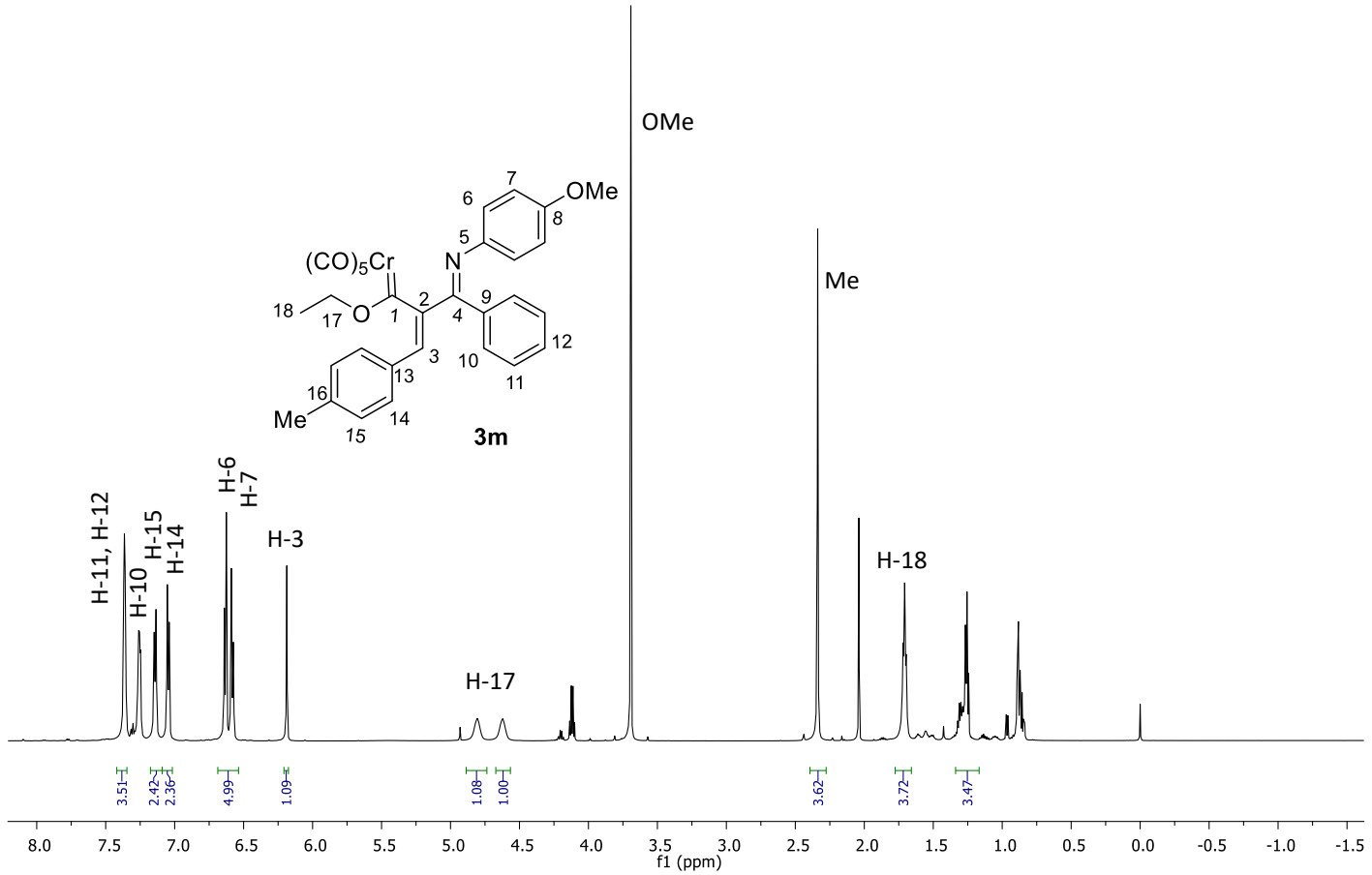

^{1}H NMR for **3m**

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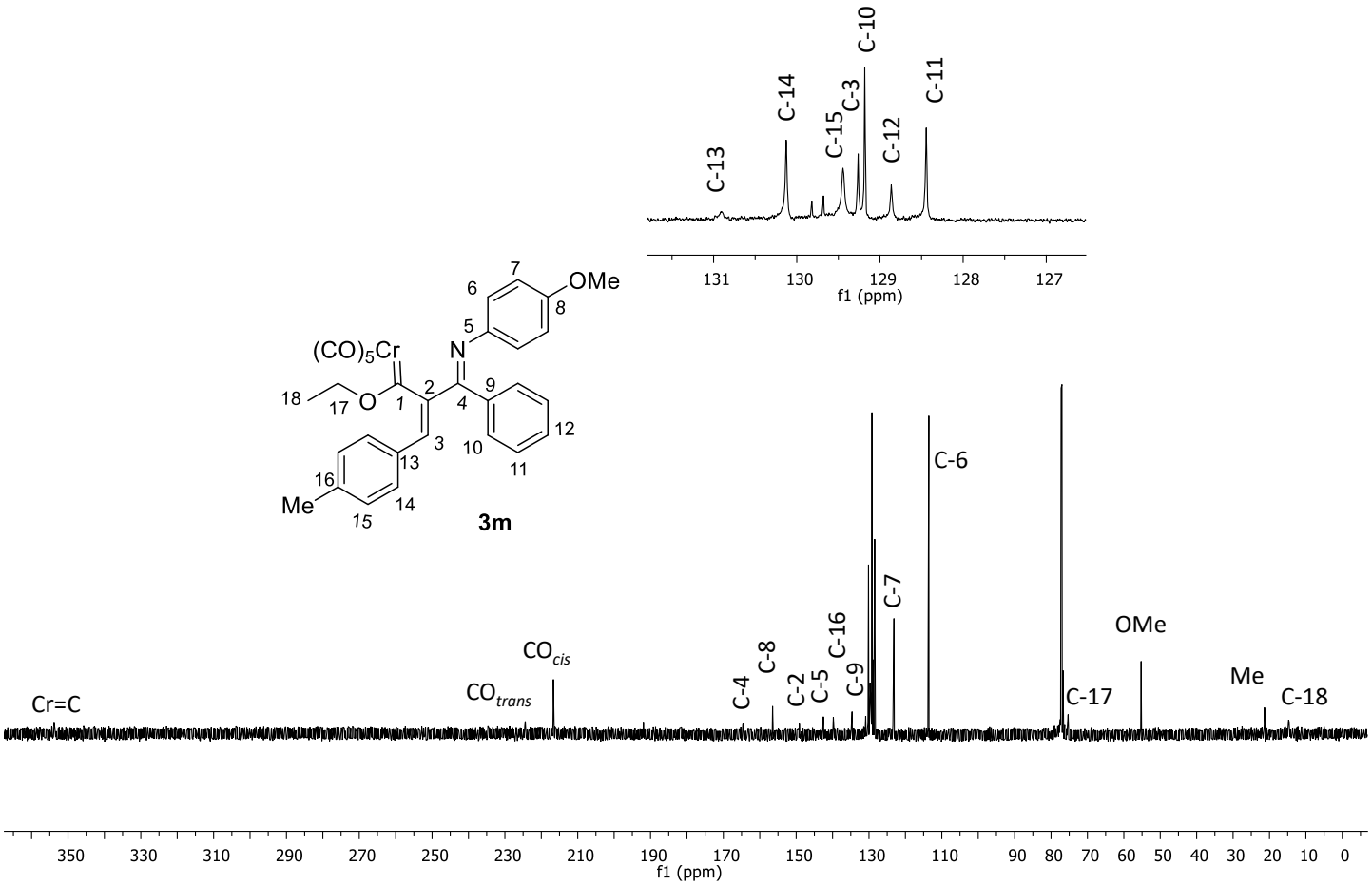

^{13}C NMR for **3m**

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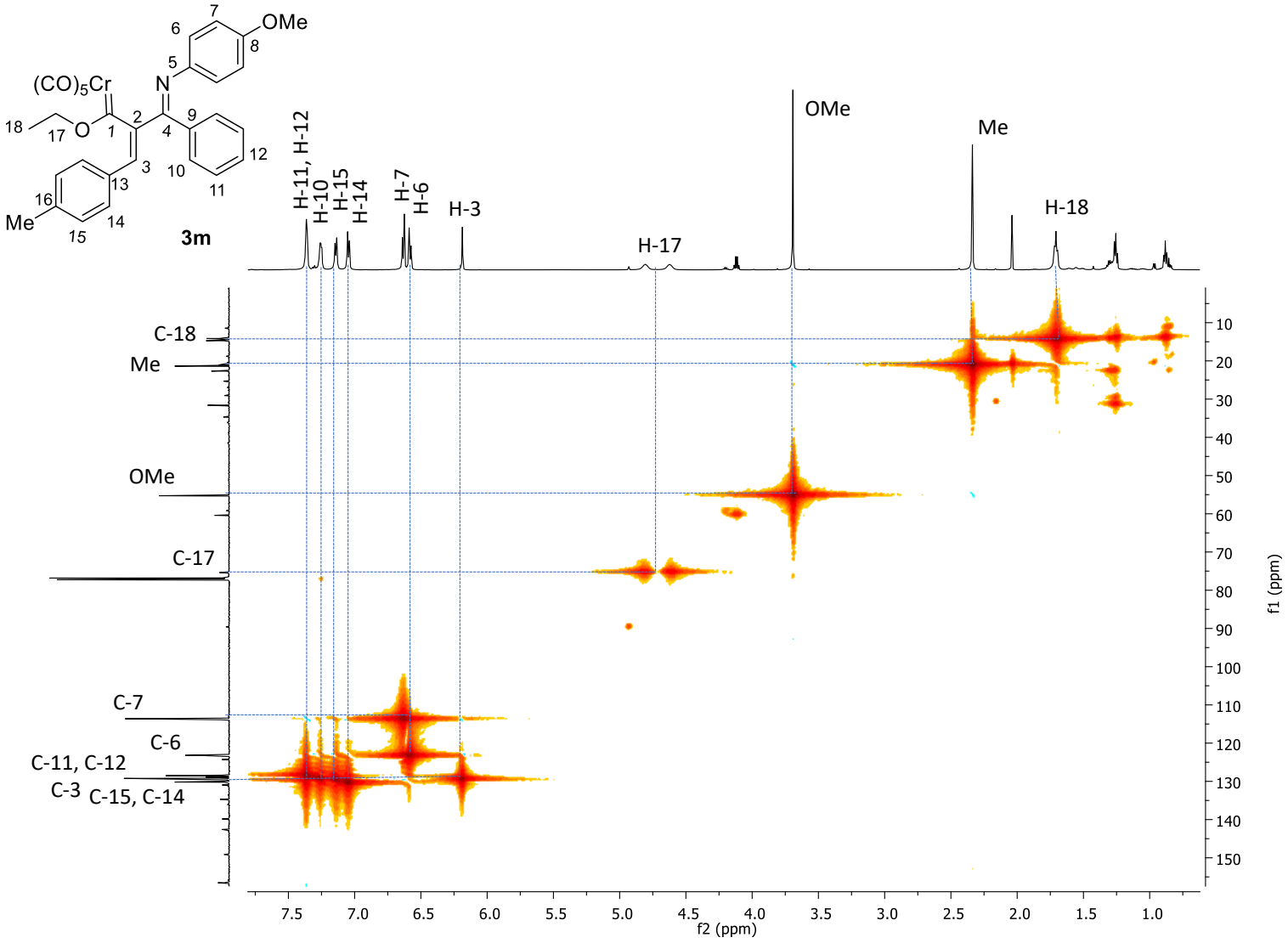

gHMQC experiment for **3m**

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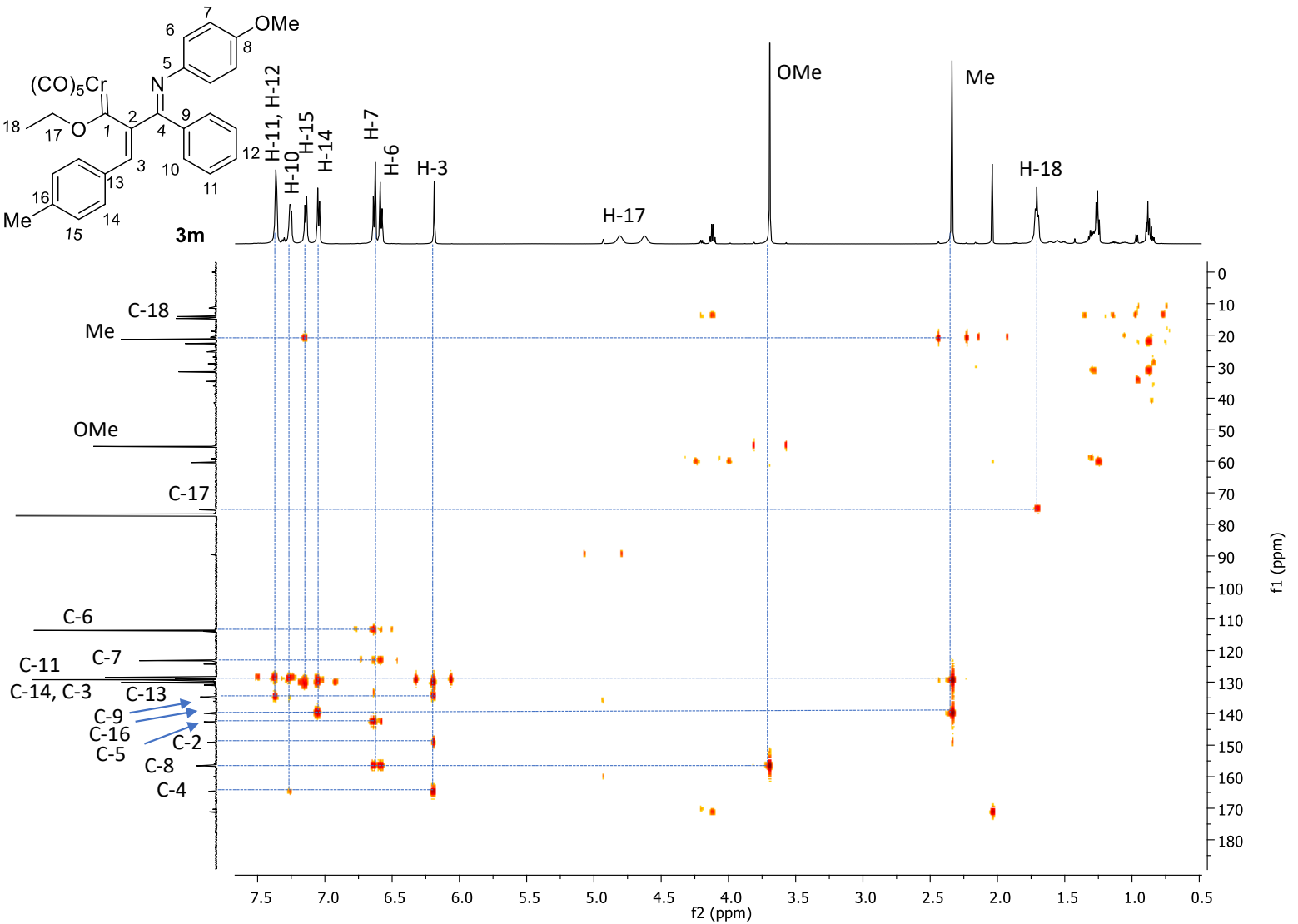
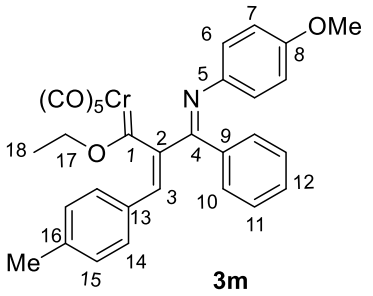
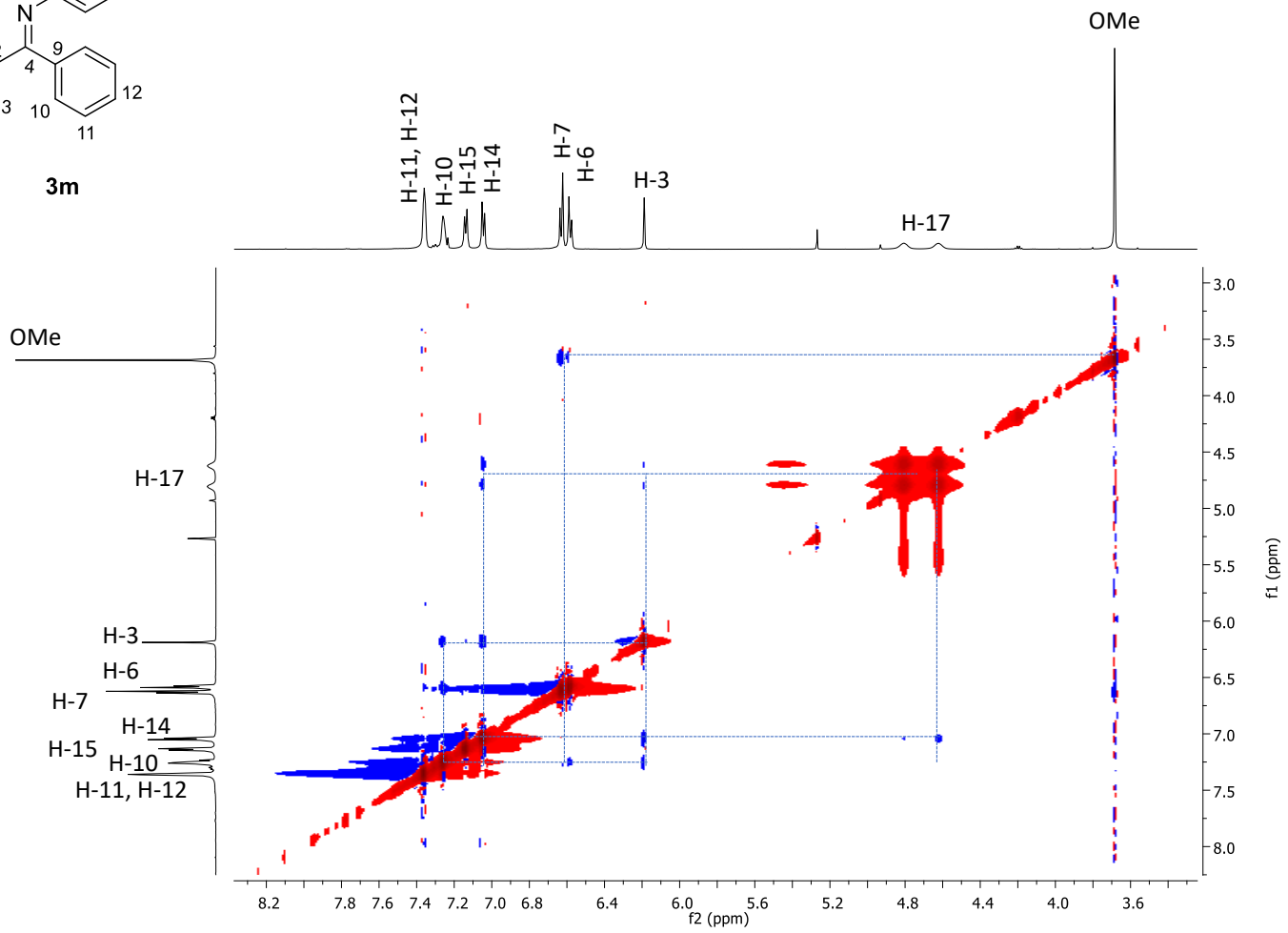


gHMBC experiment for **3m**



3m



NOESY experiment for **3m**

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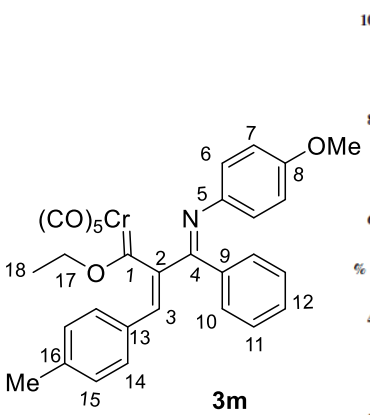
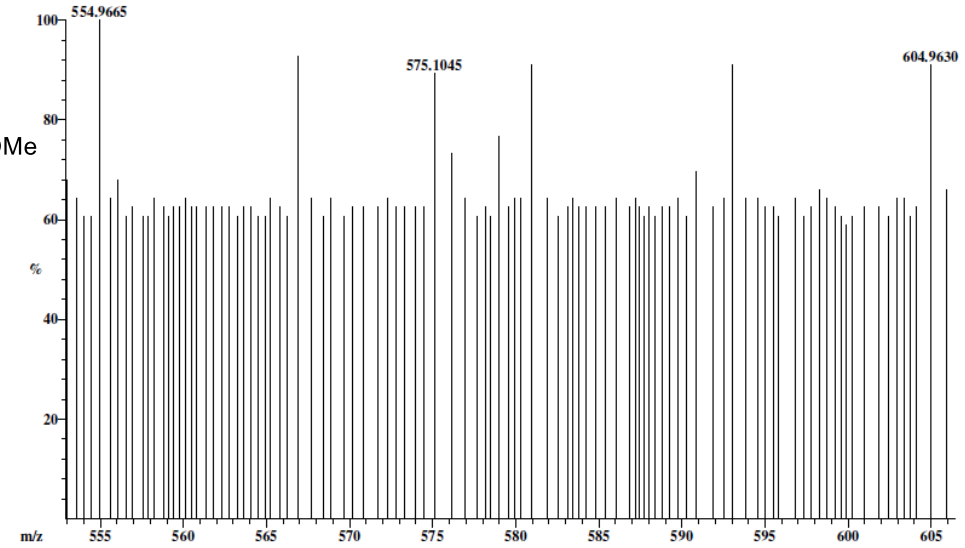


3m

File: FDR-AFC-B115 **Date Run: 05-06-2019 (Time Run: 15:57:18)**
Sample: FDR-AFC-B115
Instrument: JEOL GCmate
Inlet: Direct Probe **Ionization mode: EI+**

Scan: 143 **R.T.: 1.93**
Base: m/z 555; .1%FS TIC: 144336 **#Ions: 252**



Selected Isotopes : $H_{0-25}C_{0-31}N_{0-1}O_{0-7}Cr_{0-1}$ **Error Limit : 5 ppm**

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*
575.1045	89.3%	$C_{31}H_{25}NO_7Cr$	575.1036	1.6

HRMS (EI) $[M]^+$ for **3m**

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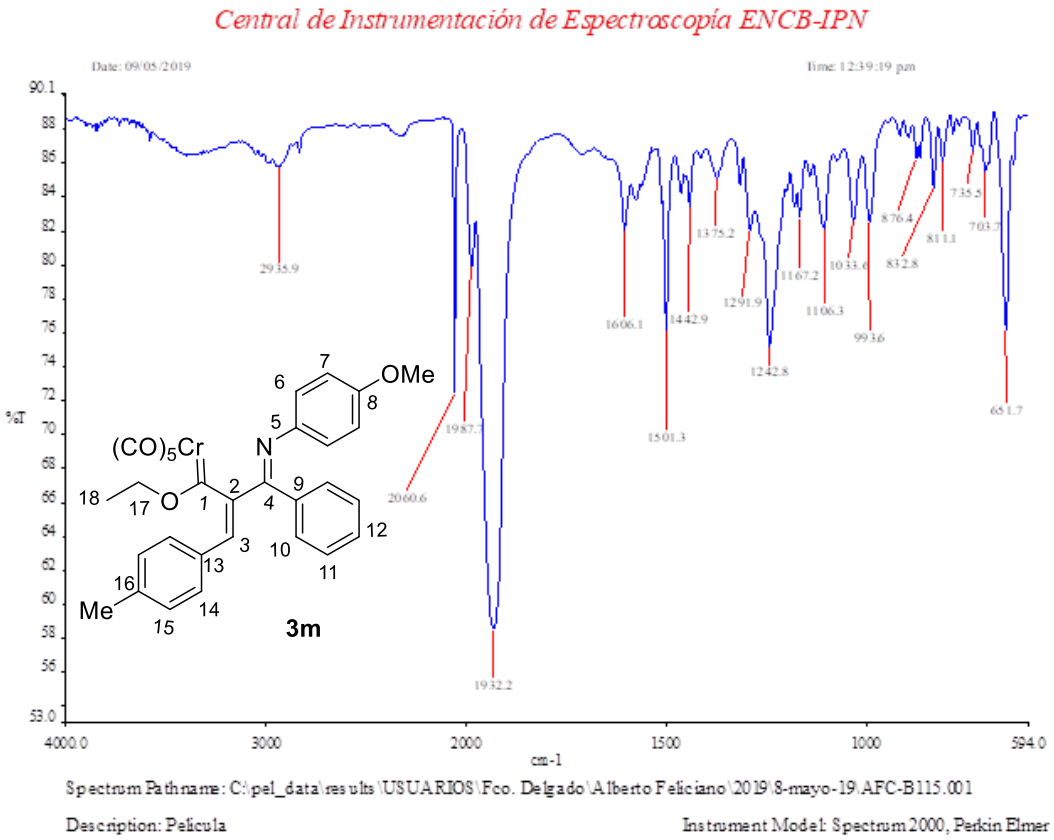

FT-IR for **3m**

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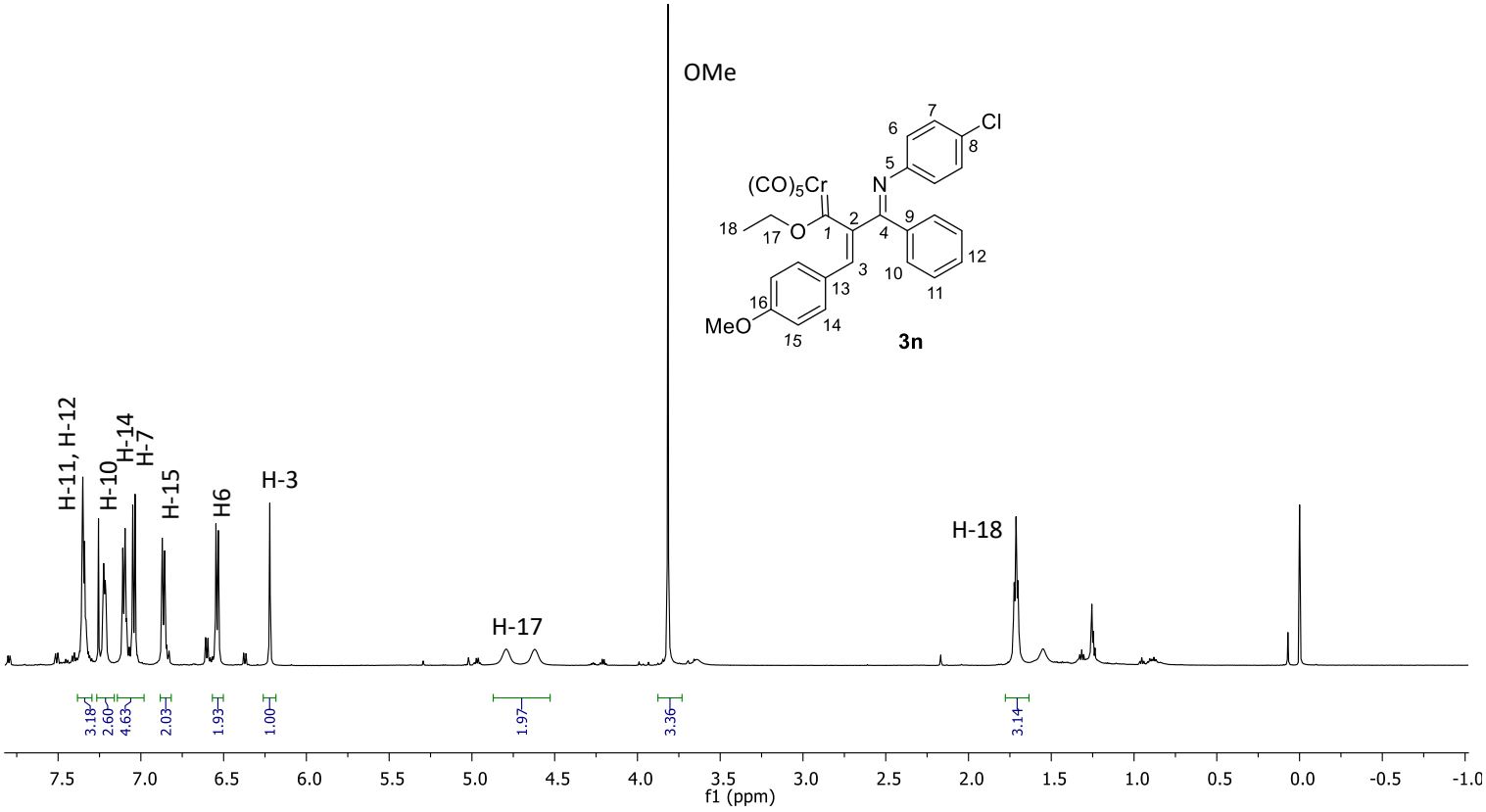

^{1}H NMR for **3n**

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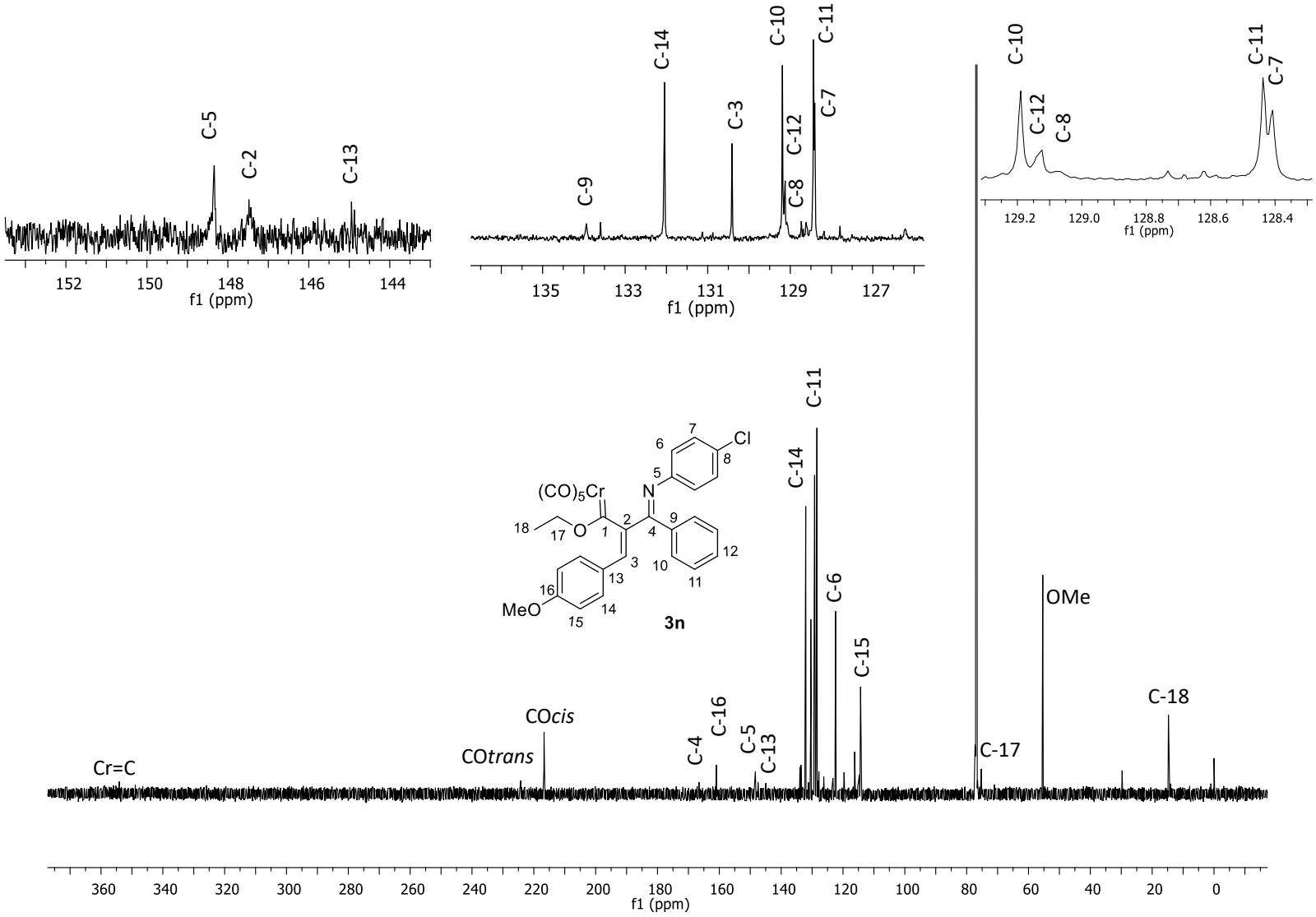

^{13}C NMR for **3n**

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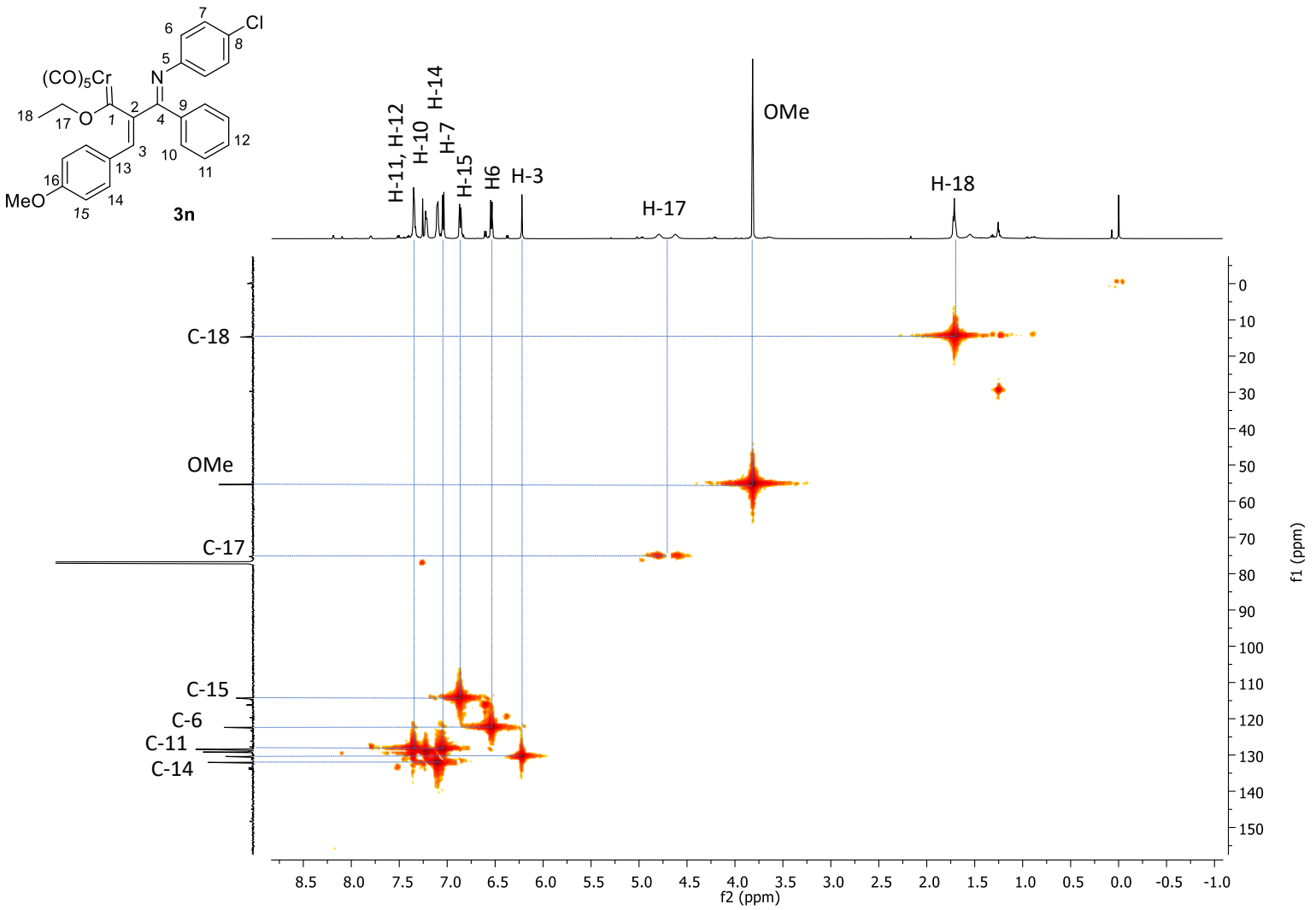

gHMQC experiment for **3n**

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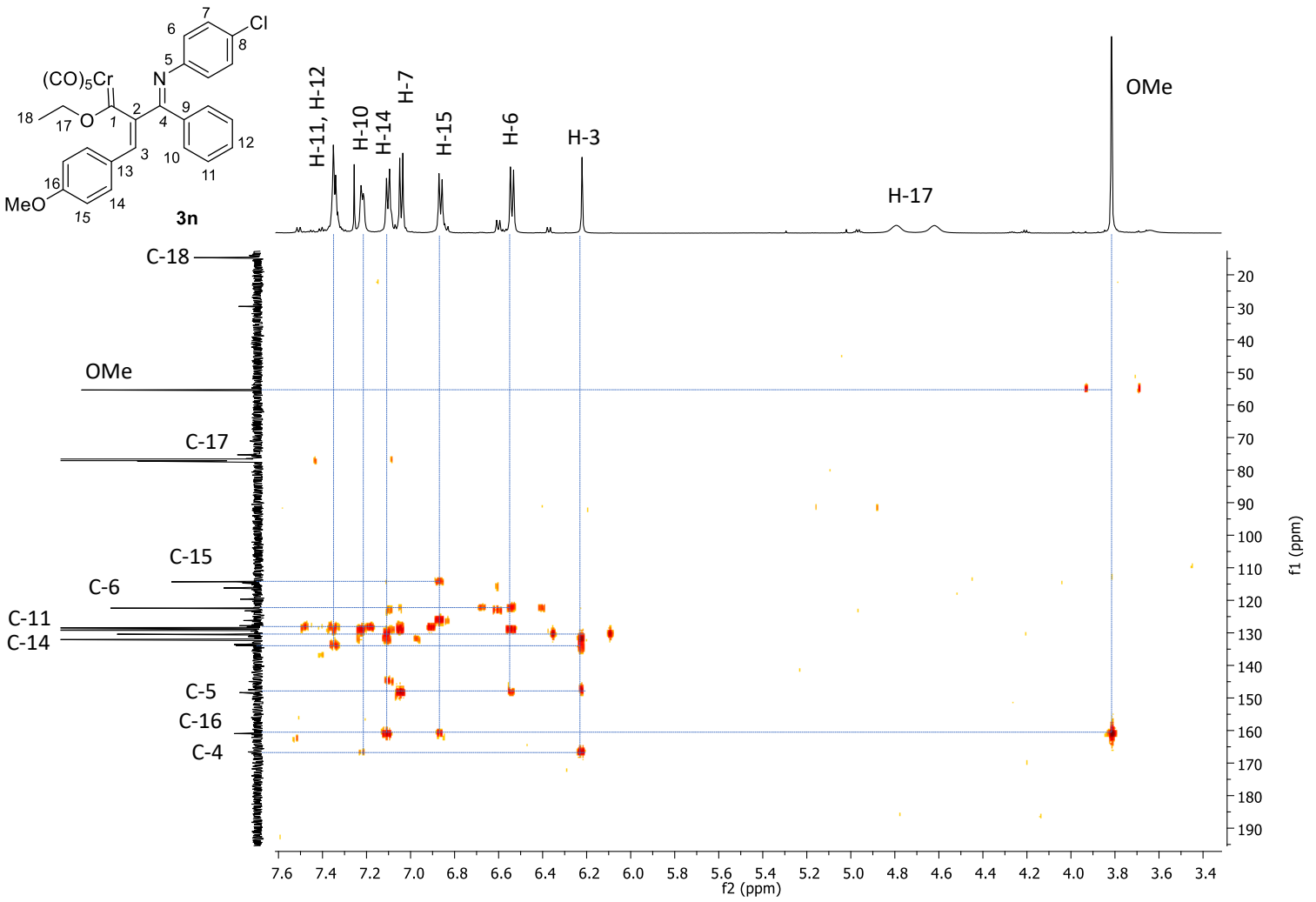

gHMBC experiment for **3n**

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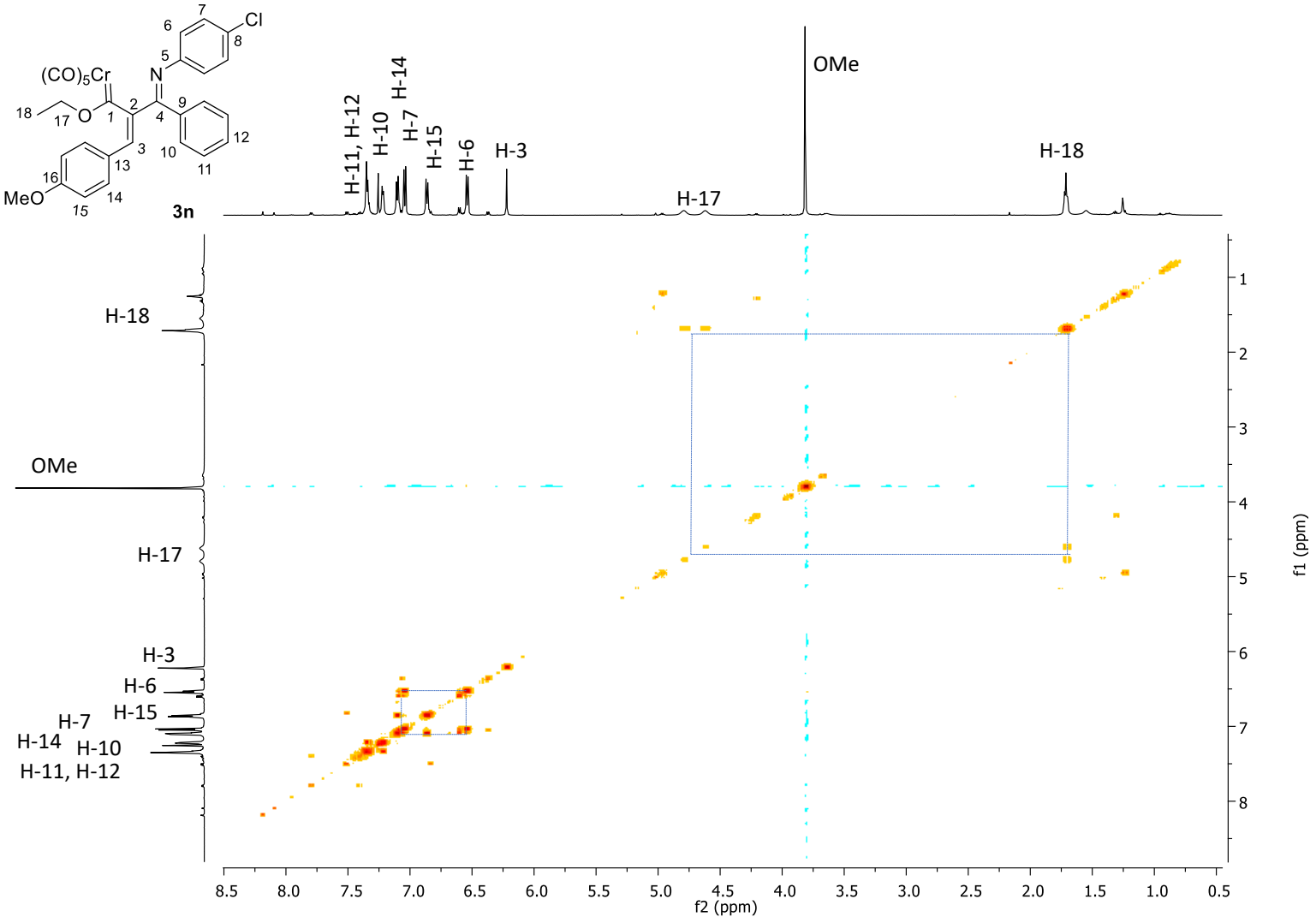

COSY experiment for **3n**

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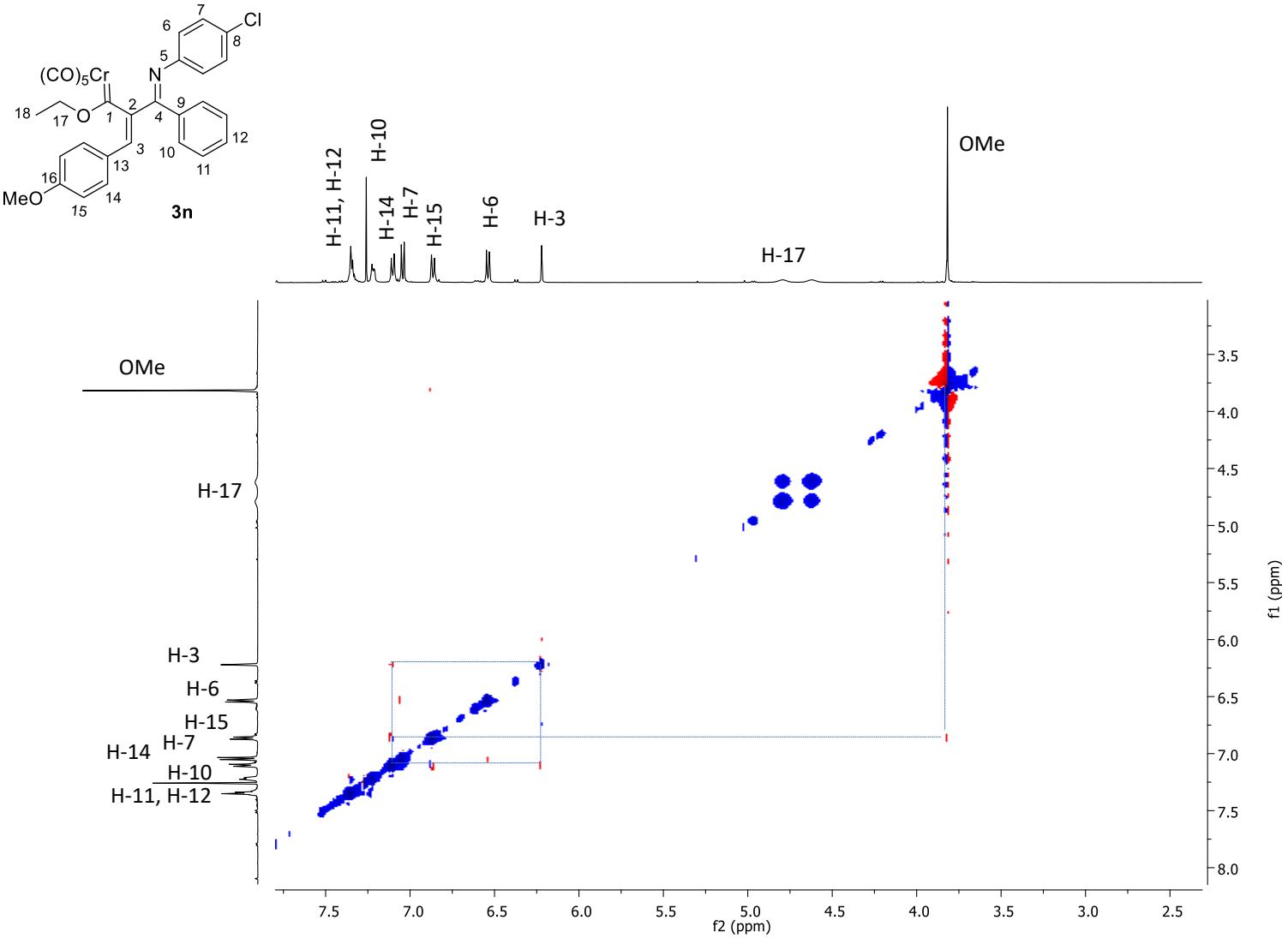

NOESY experiment for **3n**

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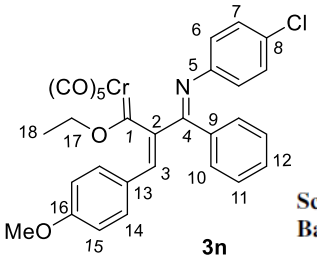
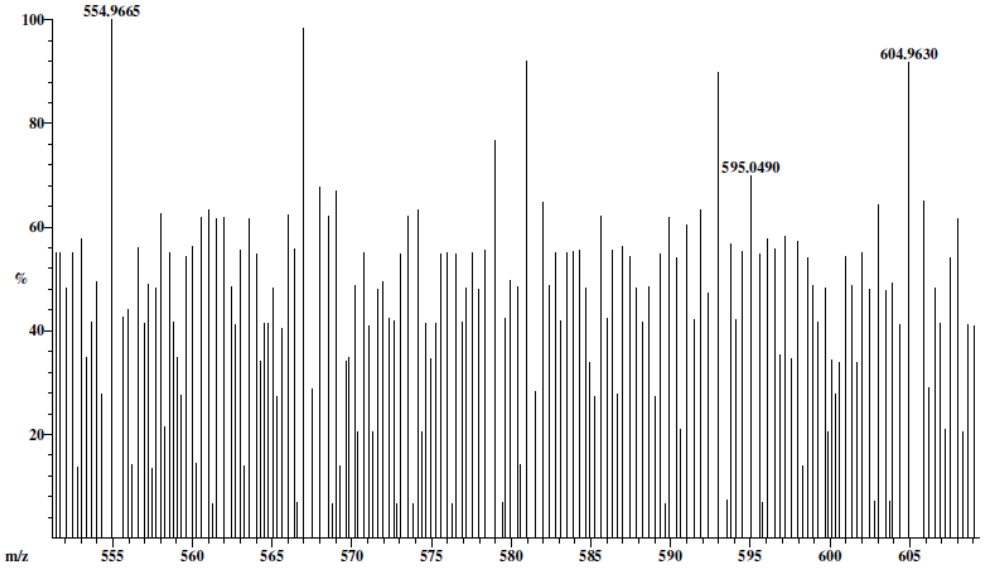


3n

Scan: 123-131 **R.T.: 1.71**

Base: m/z 555; .1%FS TIC: 149702 **#Ions: 384**



Selected Isotopes : $H_{0-22}C_{0-30}N_{0-1}O_{0-7}Cl_{0-1}Cr_{0-1}$ **Error Limit : 5 ppm**

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*
595.0490	69.8%	$C_{30}H_{22}NO_7ClCr$	595.0490	0.0

HRMS (EI) $[M]^+$ for **3n**

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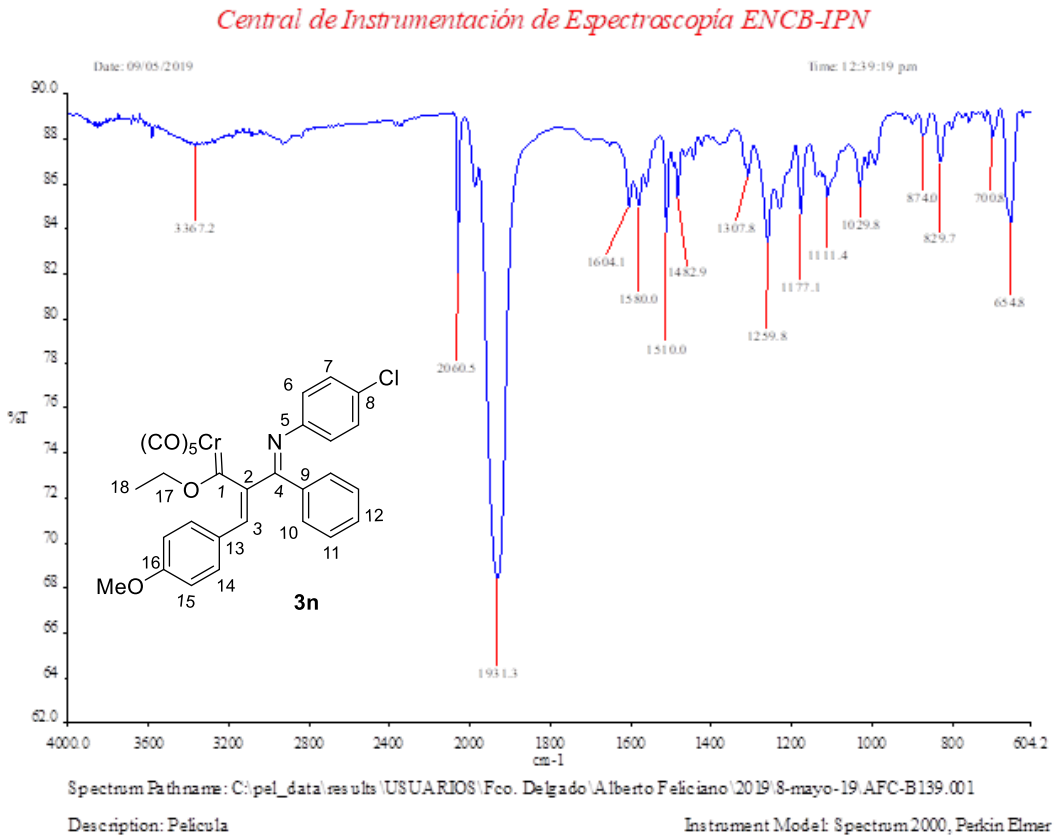

FT-IR for **3n**

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Table SD1. Select signal of complexes **3a-n.**

entry	complex	H-3*	H-10*	H-14*	C-3*	C-10*	C-14*
1	**3a**	6.28	7.22-7.26	7.14-7.17	130.3	129.2	130.2
2	**3b**	6.22	7.24-7.29	7.15	129.2	129.3	130.1
3	**3c**	6.29	7.21-7.26	7.14-7.19	130.7	129.1	130.2
4	**3d**	6.24	7.21-7.25	7.12-7.16	128.8	129.1	132.0
5	**3e**	6.21	7.21-7.25	7.07-7.12	128.5	129.1	131.2
6	**3f**	6.22	7.20-7.25	6.82-6.93	129.9	129.2	114.2
7	**3g**	6.24	7.22-7.26	7.02-7.11	130.2	129.2	130.3
8	**3h**	6.01	7.20-7.26	7.53	115.0	129.2	146.1
9	**3i**	5.88	7.14-7.22	7.43	114.2	129.1	145.8
10	**3j**	6.13	7.22-7.28	7.02	127.6	129.1	131.3
11	**3k**	6.15	7.23-7.27	7.08	127.6	129.1	131.1
12	**3l**	6.16	7.23-7.27	7.09	128.8	129.2	131.8
13	**3m**	6.19	7.24-7.28	7.05	129.3	129.2	130.1
14	**3n**	6.22	7.20-7.24	7.10	130.4	129.2	132.0

*The main signals are in δ ppm.

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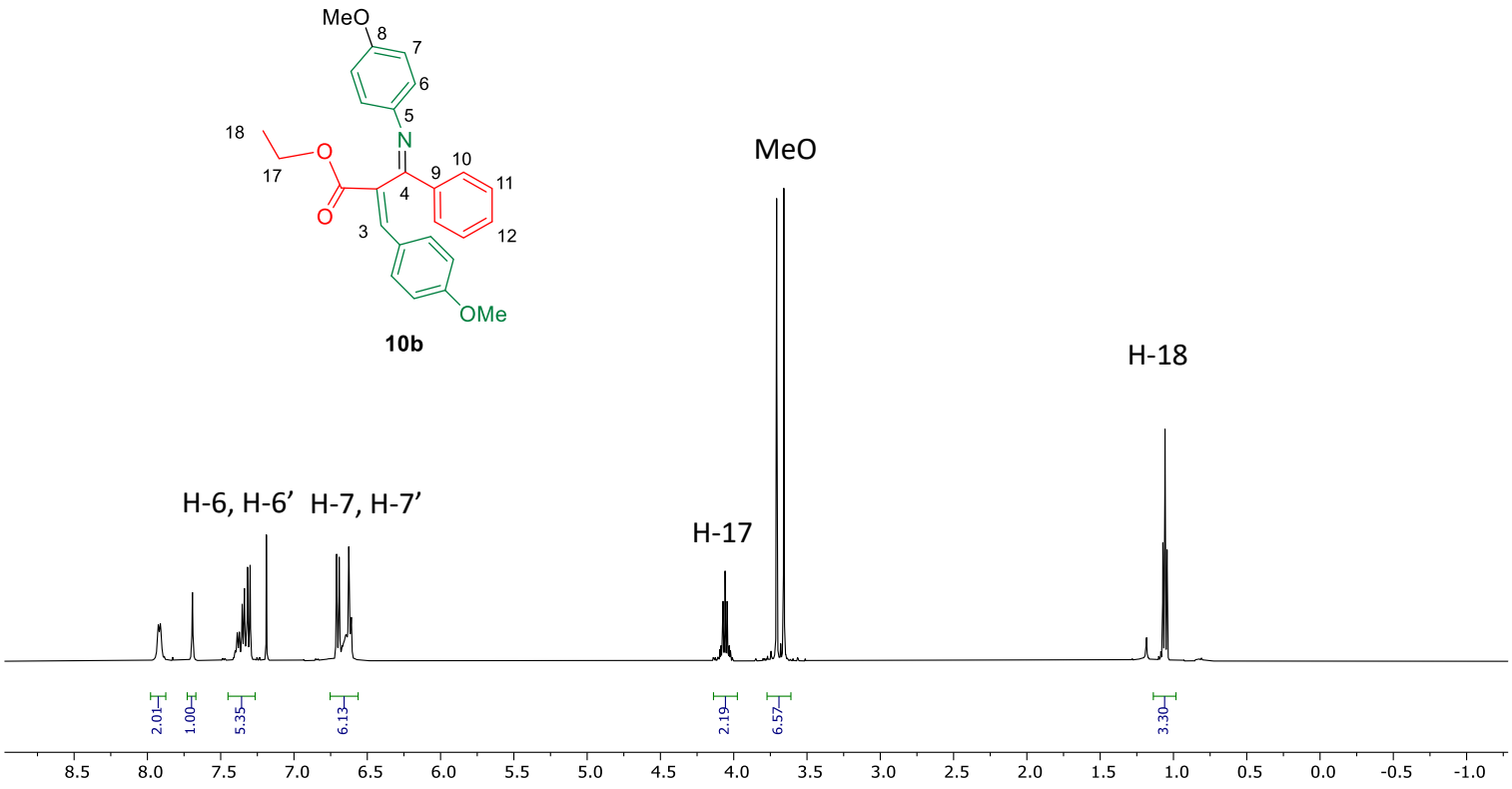

^{1}H NMR for **10b**

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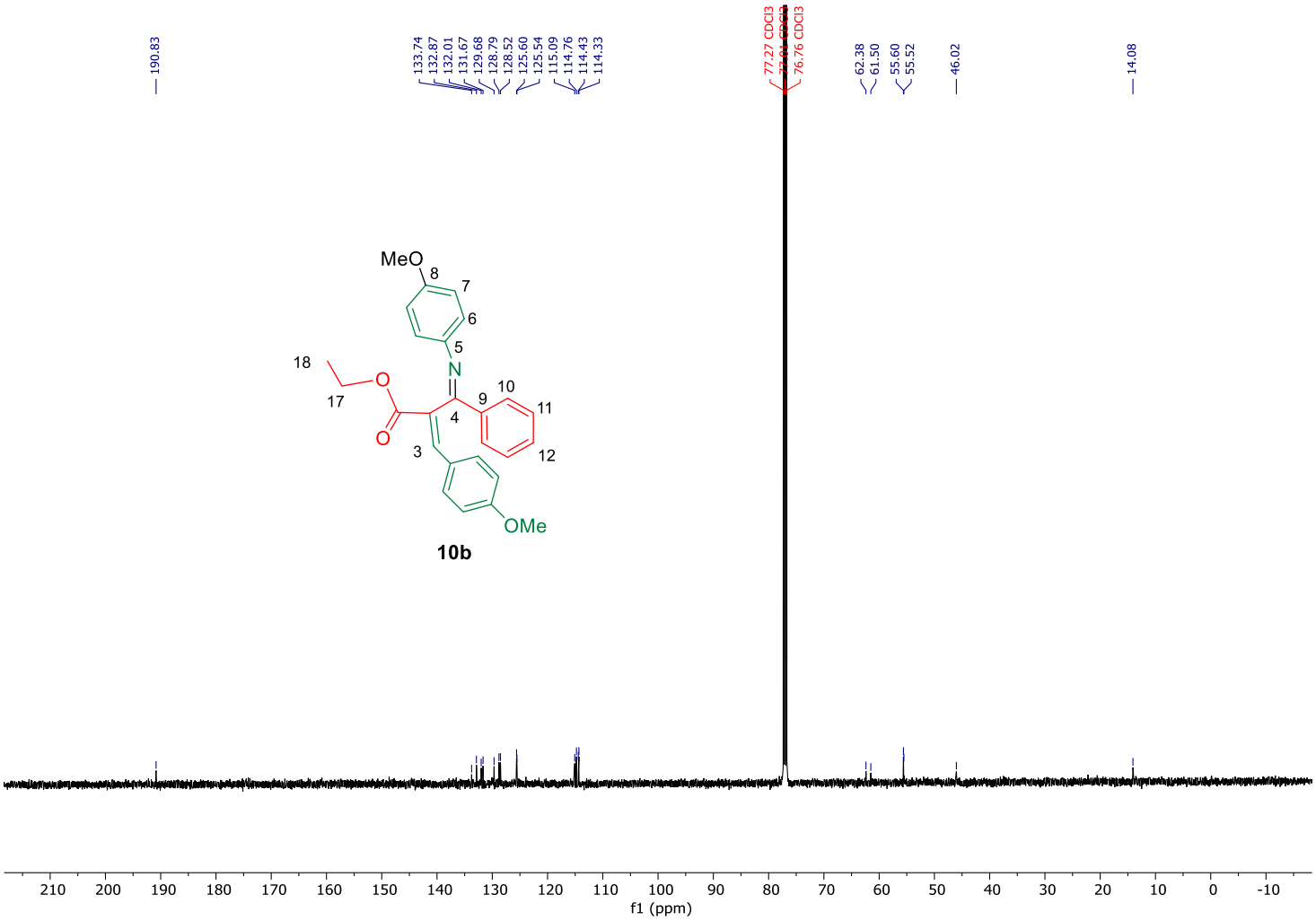

10b

^{13}C NMR for **10b**

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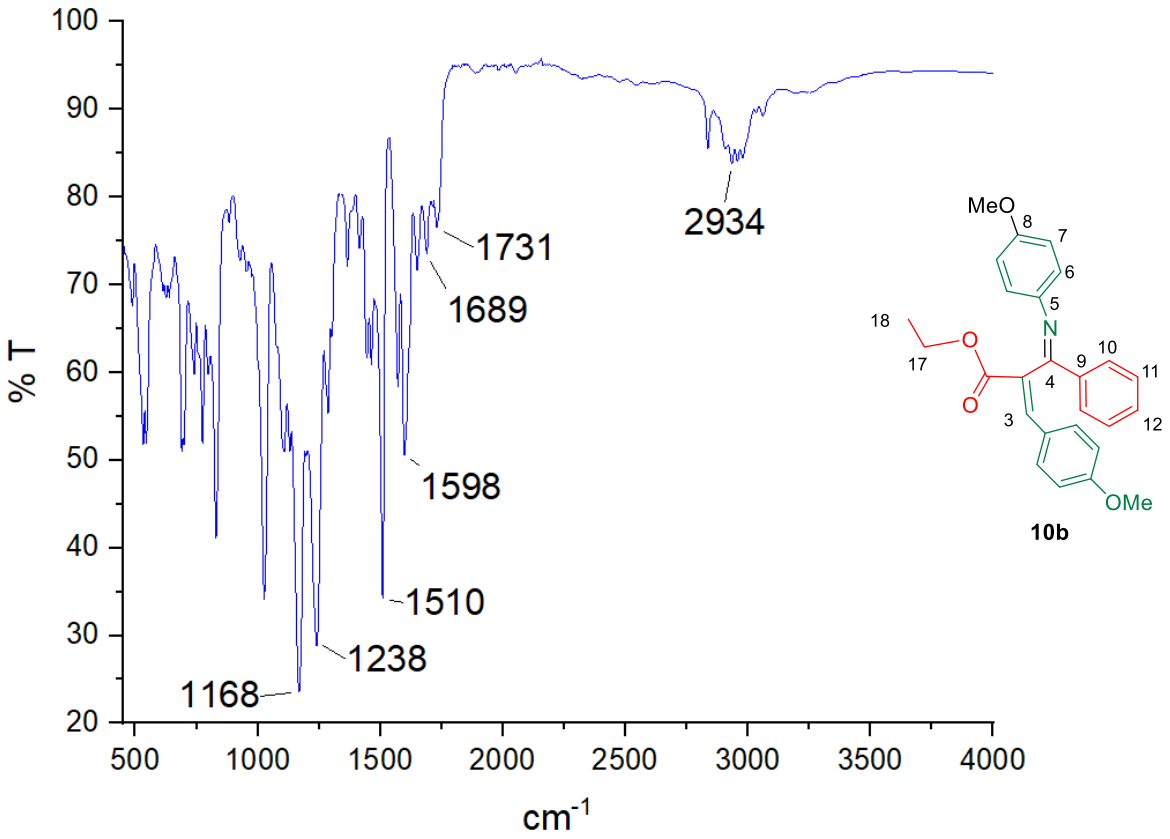

FT-IR for **10b**

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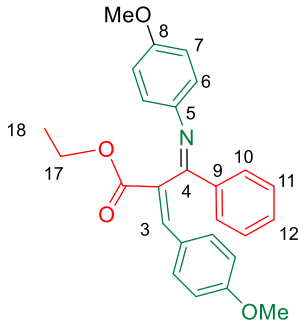
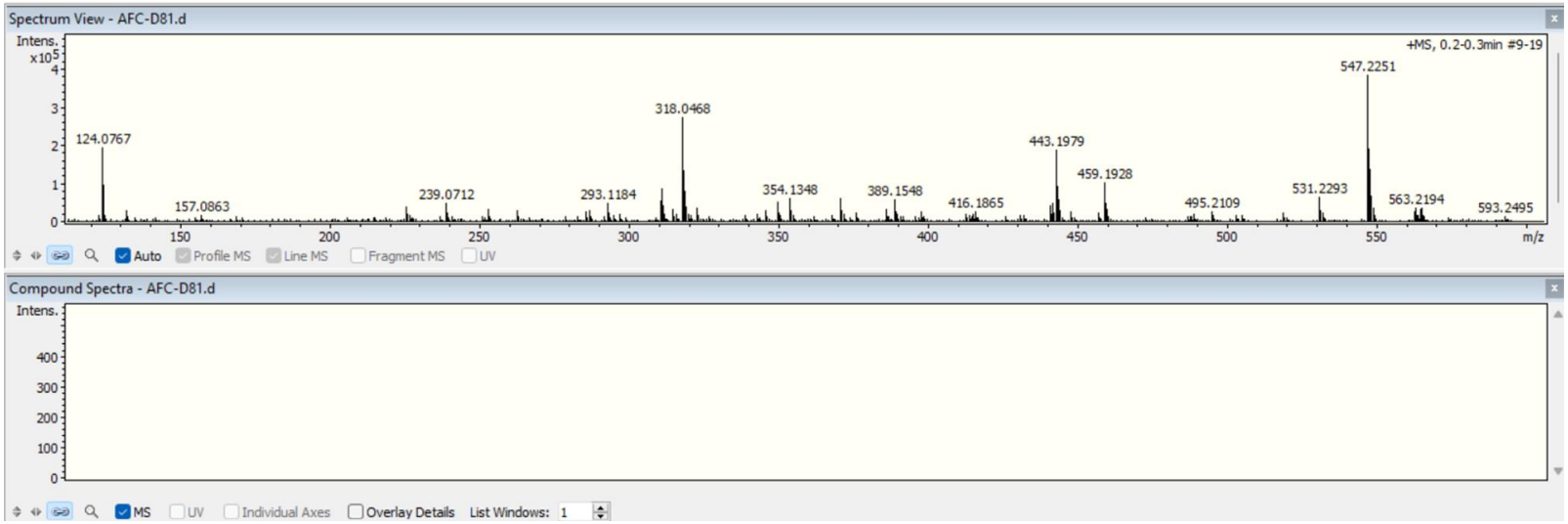


10b



HRMS (ESI) $[M+H]^+$ for **10b**

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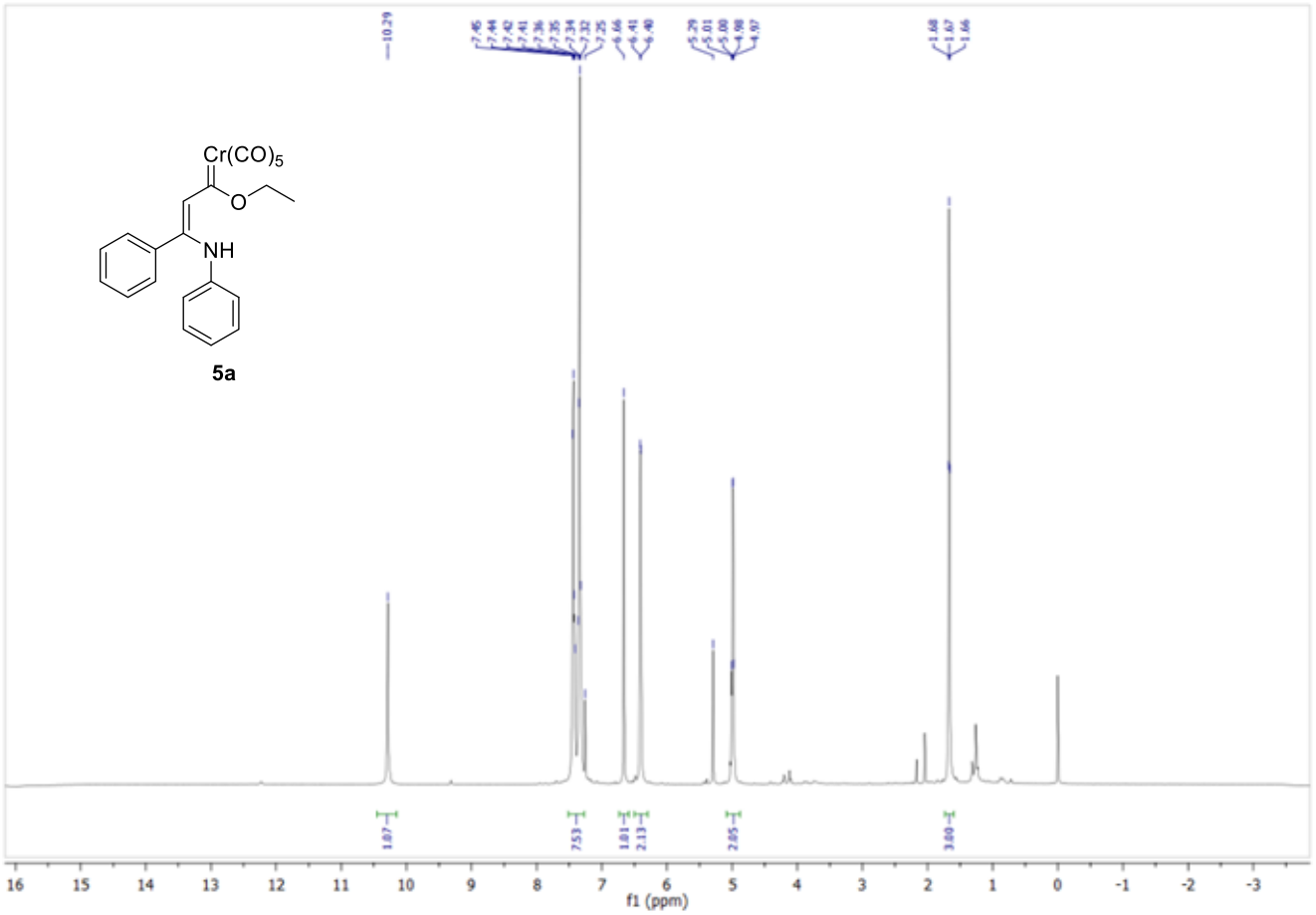

^{1}H NMR for **5a**

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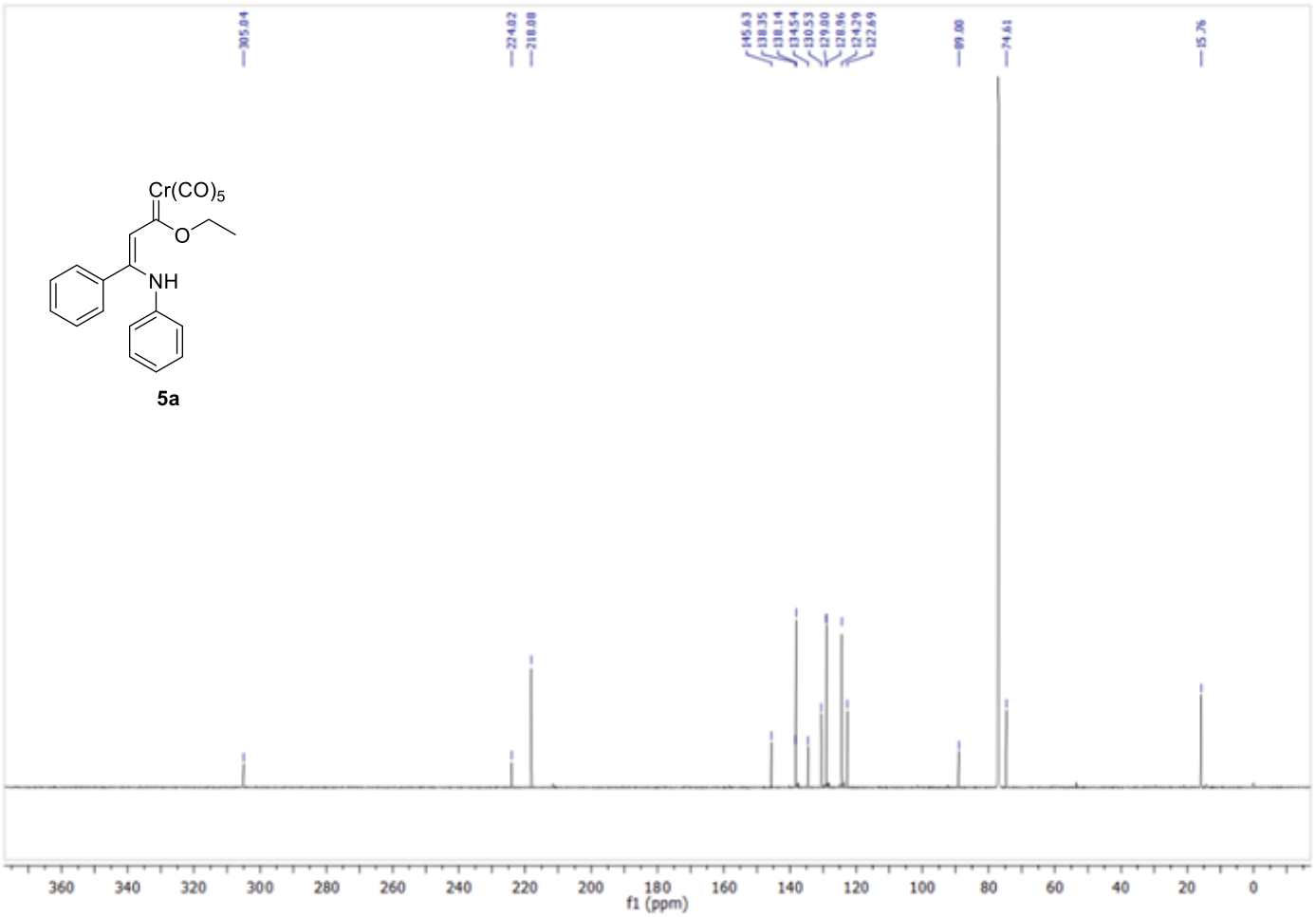

^{13}C NMR for **5a**

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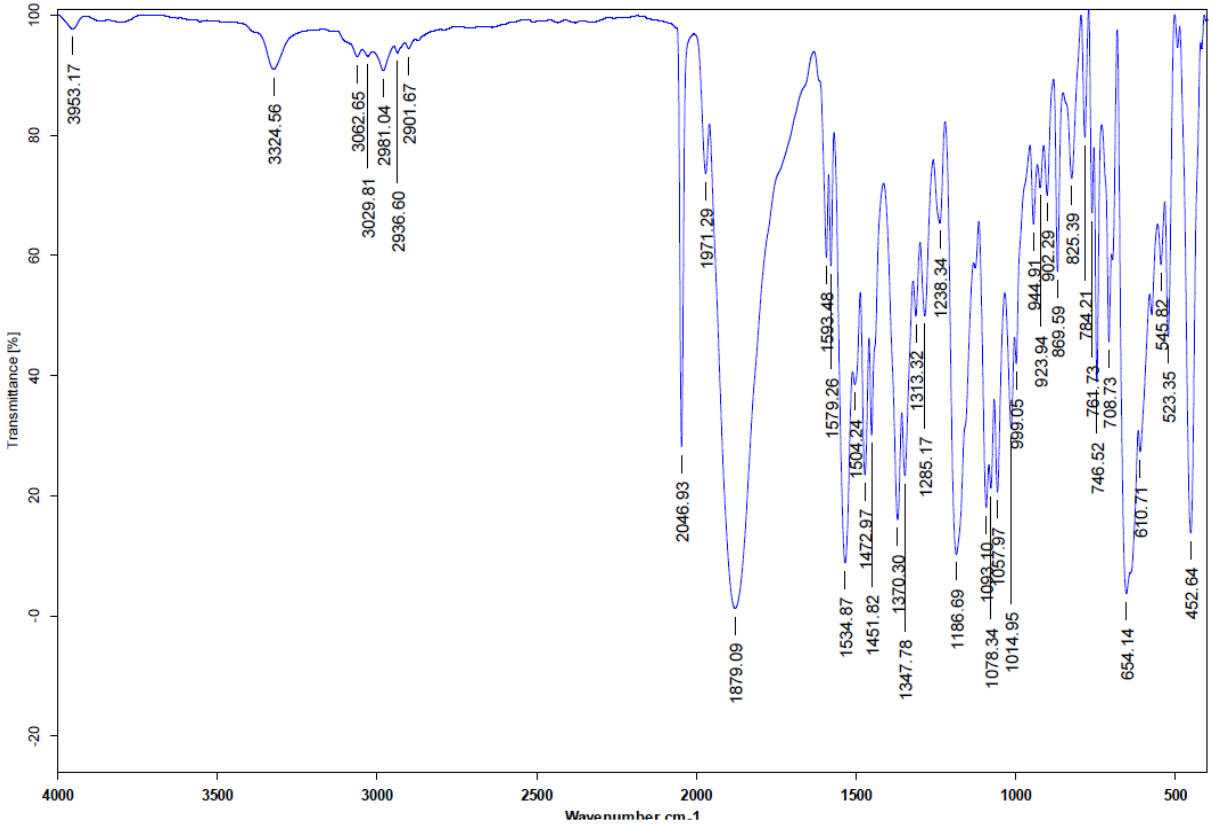

FT-IR for **5a**

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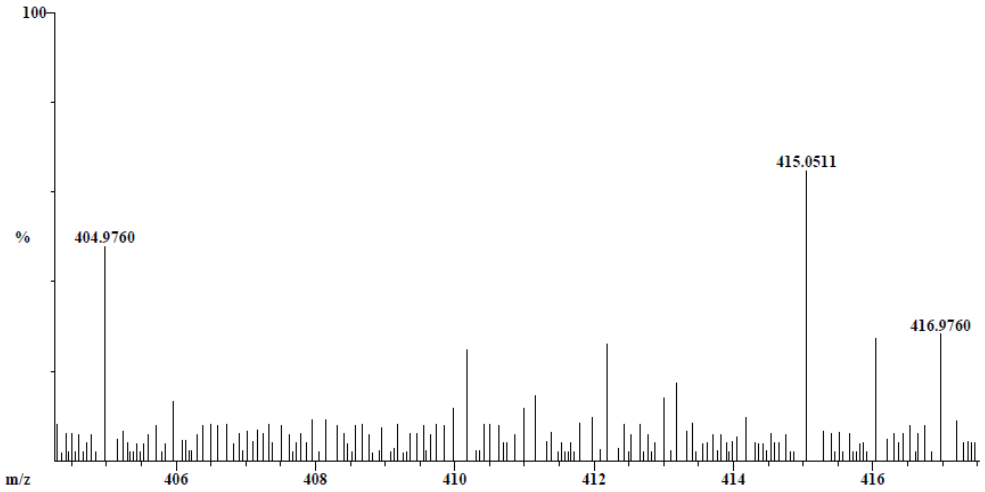
File: FDR_JLAD14 **Date Run: 12-22-2022 (Time Run: 12:32:42)**
Sample: FDR_JLAd14
Instrument: JEOL GCmate
Inlet: Direct Probe **Ionization mode: EI+**

Scan: 120-123 **R.T.: 4.07**
Base: m/z 431; .9%FS TIC: 372892 **#Ions: 762**



Selected Isotopes : $H_{0-17}C_{0-21}N_{0-1}O_{0-5}Cr_{0-1}$ **Error Limit : 5 ppm** **Unsaturation Limits : 0 to 50**

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*	*Unsaturation*
415.0511	64.7%	$C_{21}H_{17}N O_5Cr$	415.0512	-0.2	16.0

HRMS (EI) $[M]^+$ for **5a**

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X-ray diffraction

Table 1 Crystal data and structure refinement for 10b.

Identification code	exp_979
Empirical formula	$C_{26}H_{25}NO_4$
Formula weight	415.47
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	17.0269(12)
b/Å	9.6109(5)
c/Å	14.1952(8)
α/°	90
β/°	104.895(7)
γ/°	90
Volume/Å^3	2244.9(2)
Z	4
ρ_{calc}g/cm^3	1.229
μ/mm^{-1}	0.083
F(000)	880.0
Crystal size/mm^3	0.371 × 0.219 × 0.173
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	6.614 to 59.254
Index ranges	$-14 \leq h \leq 23$, $-12 \leq k \leq 12$, $-16 \leq l \leq 19$
Reflections collected	11393
Independent reflections	5267 [R_{int} = 0.0228, R_{sigma} = 0.0391]
Data/restraints/parameters	5267/0/283
Goodness-of-fit on F^2	1.138
Final R indexes [I>=2σ (I)]	R_1 = 0.0602, wR_2 = 0.1748
Final R indexes [all data]	R_1 = 0.1010, wR_2 = 0.2041
Largest diff. peak/hole / e Å^{-3}	0.18/-0.18

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

Atom	*x*	*y*	*z*	U(eq)
O2	8345.4(10)	916.6(15)	4532.3(10)	52.9(4)

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

Atom	*x*	*y*	*z*	U(eq)
O1	7038.5(11)	1054.8(16)	3682.9(11)	64.1(5)
N1	8347.9(10)	2546.5(17)	6468.4(11)	43.1(4)
O3	6910.1(11)	7211.8(15)	4372.8(12)	69.9(5)
O4	5282.7(10)	-85.1(18)	8670.5(13)	72.6(5)
C7	7964.8(12)	3693.2(19)	5889.6(14)	41.3(5)
C6	8083.7(11)	1305.5(19)	6272.9(14)	38.3(5)
C21	8518.5(11)	147(2)	6887.4(14)	41.2(5)
C3	7545.7(14)	993.0(19)	4452.2(15)	46.7(5)
C2	7380.1(12)	949.0(19)	5429.2(14)	40.7(5)
C10	7289.7(14)	6057(2)	4848.3(17)	50.4(5)
C15	6588.7(12)	1076(2)	7201.1(16)	46.6(5)
C14	6307.9(12)	354(2)	6320.1(16)	48.5(5)
C1	6643.8(13)	521(2)	5482.1(15)	48.0(5)
C8	8257.4(13)	4197(2)	5139.8(16)	47.4(5)
C26	8335.1(14)	-1234(2)	6650.3(18)	55.4(6)
C9	7925.9(14)	5364(2)	4618.9(16)	52.6(6)
C12	7332.9(13)	4411(2)	6135.1(17)	54.6(6)
C16	6230.8(13)	918(2)	7953.4(17)	50.4(5)
C17	5586.2(13)	-1(2)	7875.3(18)	54.8(6)
C22	9149.0(13)	435(2)	7704.9(16)	53.0(6)
C11	7001.6(14)	5577(2)	5614.2(18)	57.3(6)
C19	5653.3(14)	-547(3)	6256.5(19)	62.1(6)
C18	5301.4(15)	-740(3)	7017(2)	68.7(7)
C24	9391.7(16)	-1981(3)	8021(2)	69.9(7)
C4	8589.2(18)	1019(3)	3632.2(18)	66.5(7)
C23	9574.9(15)	-623(3)	8262.7(18)	67.4(7)
C25	8772.6(17)	-2289(3)	7212(2)	70.9(7)
C13	7126(2)	7639(3)	3518(2)	80.8(8)
C5	9488(2)	1004(3)	3877(2)	93.4(10)
C20	4751(2)	-1227(3)	8712(3)	95.5(10)

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

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O2	66.4(10)	61.8(9)	33.3(8)	3.8(7)	17.6(7)	4.8(8)
O1	82.2(12)	63.3(10)	36.2(9)	4.7(7)	-4.0(8)	-0.1(8)
N1	42.3(9)	47.0(10)	37.7(9)	1.1(8)	6.3(8)	-1.6(8)
O3	89.3(13)	49.8(9)	70.7(12)	14.0(8)	20.6(10)	12.1(8)
O4	65.4(11)	85.6(12)	74.5(12)	-6.6(10)	32.0(10)	-21.6(9)
C7	41.8(11)	43.3(10)	35.2(10)	-4.1(9)	3.2(9)	-5.1(8)
C6	38.6(10)	46.3(11)	31.3(10)	-2.2(8)	11.1(8)	0.0(8)
C21	39.5(10)	50.4(11)	35.2(10)	3.0(9)	12.5(9)	5.0(9)
C3	63.0(14)	38.2(10)	35.8(11)	1.2(9)	7.0(10)	1.2(10)
C2	46.8(11)	39.9(10)	32.2(10)	-0.3(8)	4.4(9)	3.2(9)
C10	58.6(13)	40.7(11)	48.3(13)	-0.3(10)	6.9(11)	-1.6(10)
C15	38.7(10)	48.0(11)	50.9(13)	-2.5(10)	7.7(10)	-4.5(9)
C14	38.0(11)	53.8(12)	48.8(12)	0.9(10)	1.8(9)	-2.1(9)
C1	46.2(12)	50.4(12)	40.3(11)	-2.9(10)	-1.7(10)	-1.6(9)
C8	50.2(12)	46.9(11)	45.7(12)	-3.2(10)	13.2(10)	-0.2(9)
C26	55.9(13)	50.7(13)	56.5(14)	6.9(11)	9.1(11)	-1.2(10)
C9	62.4(14)	50.4(12)	47.0(13)	2.1(10)	17.2(11)	-5.9(11)
C12	51.5(13)	62.3(13)	52.9(13)	7.7(11)	18.6(11)	1.0(11)
C16	47.2(12)	49.2(12)	54.0(13)	-5.2(10)	11.7(10)	-4.0(10)
C17	42.8(12)	62.6(14)	60.3(15)	-0.2(12)	15.6(11)	-5.2(10)
C22	50.1(12)	62.1(13)	44.3(12)	0.4(11)	7.9(10)	11.6(10)
C11	54.7(14)	56.8(13)	62.7(15)	6.1(12)	19.4(12)	12.3(11)
C19	50.3(13)	74.3(15)	56.6(15)	-12.3(12)	4.8(12)	-17.0(12)
C18	49.8(14)	82.7(18)	71.2(17)	-7.1(14)	11.1(13)	-23.1(13)
C24	65.7(16)	73.9(17)	70.7(18)	31.4(14)	18.8(14)	22.4(14)
C4	99(2)	69.9(15)	38.3(12)	4.5(11)	31.4(14)	-1.5(14)
C23	57.5(14)	89.3(19)	48.5(14)	10.4(13)	1.0(12)	19.8(14)
C25	72.2(17)	52.0(14)	88(2)	17.9(14)	20.3(16)	7.9(12)
C13	117(2)	54.3(14)	70.4(18)	19.9(13)	22.3(17)	-2.1(15)
C5	104(2)	112(2)	81(2)	33.3(18)	54(2)	36.0(19)
C20	78(2)	110(2)	112(3)	-8(2)	49(2)	-36.4(17)

Table 4 Bond Lengths for 10b.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O2	C3	1.339(3)	C10	C9	1.380(3)

Table 4 Bond Lengths for 10b.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O2	C4	1.445(2)	C10	C11	1.382(3)
O1	C3	1.207(3)	C15	C14	1.402(3)
N1	C7	1.428(2)	C15	C16	1.367(3)
N1	C6	1.280(2)	C14	C1	1.455(3)
O3	C10	1.371(3)	C14	C19	1.396(3)
O3	C13	1.416(3)	C8	C9	1.381(3)
O4	C17	1.359(3)	C26	C25	1.383(3)
O4	C20	1.434(3)	C12	C11	1.380(3)
C7	C8	1.374(3)	C16	C17	1.391(3)
C7	C12	1.396(3)	C17	C18	1.385(3)
C6	C21	1.489(3)	C22	C23	1.376(3)
C6	C2	1.500(3)	C19	C18	1.376(3)
C21	C26	1.385(3)	C24	C23	1.364(4)
C21	C22	1.391(3)	C24	C25	1.377(4)
C3	C2	1.485(3)	C4	C5	1.480(4)
C2	C1	1.340(3)			

Table 5 Bond Angles for 10b.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C3	O2	C4	115.99(18)	C16	C15	C14	121.54(19)
C6	N1	C7	120.75(16)	C15	C14	C1	123.97(19)
C10	O3	C13	117.60(19)	C19	C14	C15	116.6(2)
C17	O4	C20	117.3(2)	C19	C14	C1	119.4(2)
C8	C7	N1	120.99(18)	C2	C1	C14	130.5(2)
C8	C7	C12	118.36(19)	C7	C8	C9	121.42(19)
C12	C7	N1	120.36(18)	C25	C26	C21	120.5(2)
N1	C6	C21	118.42(17)	C10	C9	C8	120.2(2)
N1	C6	C2	123.38(17)	C11	C12	C7	120.2(2)
C21	C6	C2	118.15(16)	C15	C16	C17	120.6(2)
C26	C21	C6	121.82(19)	O4	C17	C16	115.6(2)
C26	C21	C22	118.10(19)	O4	C17	C18	125.3(2)
C22	C21	C6	120.04(18)	C18	C17	C16	119.1(2)
O2	C3	C2	110.62(18)	C23	C22	C21	120.8(2)
O1	C3	O2	123.7(2)	C12	C11	C10	120.9(2)
O1	C3	C2	125.7(2)	C18	C19	C14	122.3(2)
C3	C2	C6	115.77(17)	C19	C18	C17	119.8(2)

Table 5 Bond Angles for 10b.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C1	C2	C6	126.32(19)	C23	C24	C25	119.4(2)
C1	C2	C3	117.78(19)	O2	C4	C5	107.9(2)
O3	C10	C9	125.0(2)	C24	C23	C22	120.7(2)
O3	C10	C11	116.10(19)	C24	C25	C26	120.5(2)
C9	C10	C11	118.9(2)				

Table 6 Torsion Angles for 10b.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
O2	C3	C2	C6	19.5(2)	C2	C6	C21	C26	5.6(3)
O2	C3	C2	C1	−156.62(18)	C2	C6	C21	C22	−176.87(17)
O1	C3	C2	C6	−162.2(2)	C15	C14	C1	C2	24.3(3)
O1	C3	C2	C1	21.7(3)	C15	C14	C19	C18	−0.7(3)
N1	C7	C8	C9	−175.54(18)	C15	C16	C17	O4	179.37(18)
N1	C7	C12	C11	175.6(2)	C15	C16	C17	C18	−1.1(3)
N1	C6	C21	C26	−171.76(18)	C14	C15	C16	C17	1.8(3)
N1	C6	C21	C22	5.7(3)	C14	C19	C18	C17	1.4(4)
N1	C6	C2	C3	74.3(2)	C1	C14	C19	C18	−179.2(2)
N1	C6	C2	C1	−110.0(2)	C8	C7	C12	C11	1.7(3)
O3	C10	C9	C8	−179.2(2)	C26	C21	C22	C23	−0.3(3)
O3	C10	C11	C12	179.2(2)	C9	C10	C11	C12	−1.0(4)
O4	C17	C18	C19	179.0(2)	C12	C7	C8	C9	−1.7(3)
C7	N1	C6	C21	178.64(16)	C16	C15	C14	C1	177.53(19)
C7	N1	C6	C2	1.4(3)	C16	C15	C14	C19	−0.9(3)
C7	C8	C9	C10	0.4(3)	C16	C17	C18	C19	−0.5(4)
C7	C12	C11	C10	−0.4(4)	C22	C21	C26	C25	−0.3(3)
C6	N1	C7	C8	−95.8(2)	C11	C10	C9	C8	1.0(3)
C6	N1	C7	C12	90.5(2)	C19	C14	C1	C2	−157.3(2)
C6	C21	C26	C25	177.2(2)	C4	O2	C3	O1	4.6(3)
C6	C21	C22	C23	−177.85(19)	C4	O2	C3	C2	−177.04(15)
C6	C2	C1	C14	3.6(3)	C23	C24	C25	C26	−0.5(4)
C21	C6	C2	C3	−102.96(19)	C25	C24	C23	C22	−0.1(4)
C21	C6	C2	C1	72.8(2)	C13	O3	C10	C9	7.2(3)
C21	C26	C25	C24	0.7(4)	C13	O3	C10	C11	−173.0(2)

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Table 6 Torsion Angles for 10b.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C21	C22	C23	C24	0.5(3)	C20	O4	C17	C16	-166.3(2)
C3	O2	C4	C5	176.4(2)	C20	O4	C17	C18	14.2(4)
C3	C2	C1	C14	179.26(19)					

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 10b.

Atom	*x*	*y*	*z*	U(eq)
H15	7028.72	1676.62	7275.31	56
H1	6289.61	293.29	4886.13	58
H8	8688.02	3743.73	4979.83	57
H26	7914.36	-1453.64	6109.17	66
H9	8131.86	5682.61	4111.82	63
H12	7134.59	4103.98	6651.02	66
H16	6420.19	1429.52	8522.72	60
H22	9284.27	1354.97	7876.4	64
H11	6578.55	6044.95	5780.84	69
H19	5447.94	-1034.63	5679.62	74
H18	4873.7	-1364.08	6955.73	82
H24	9682.49	-2691.86	8400.49	84
H4A	8383.74	1874.56	3295.59	80
H4B	8372.06	241.56	3209.51	80
H23	9991.74	-411.6	8809.77	81
H25	8647.94	-3212.16	7041.72	85
H13A	7047.88	6879.49	3063.92	121
H13B	7685.57	7919.27	3681.98	121
H13C	6789.61	8407.76	3227.91	121
H5A	9665.55	1050.26	3288.02	140
H5B	9685.38	161.12	4219.72	140
H5C	9696.37	1789.89	4281.18	140
H20A	4268.64	-1151.54	8186	143
H20B	4605.51	-1205.95	9322.24	143
H20C	5021.72	-2086.82	8656.1	143

Theoretical calculations

Effect of the R^1 substituent on the aromatic system of benzylidene anilines 2a-p

Computational analysis was performed in relation to the electronic effect of the substituent in the benzylidene anilines **2a**-**p** on the reactivity of the latter with complex **1**. Such reactivity leads to the series of complexes **3a**-**n**. Firstly, the energetic profile for the mechanism of reaction of **1** with imines **2a** (R^1 = C_6H_5), **2b** (R^1 = *p*-$OMeC_6H_4$), and **2o** (R^1 = *p*-$NO_2C_6H_5$) was calculated (M06L/6311++g**/Cr = LANL2TZ / SCRF = THF), focusing on the change of the electronic demand (Scheme SD1). The activation energy for all three transition states was greater for **2o** than **2a**, being 2.68 kcal/mol greater in **TS-1**. This is probably due to the electron withdrawing group (R^1 = *p*-$NO_2C_6H_5$), since it reduces the nucleophilic character of the nitrogen atom in **2o**. In contrast, the cyclic intermediate **Int-2** showed enhanced stability. Although the first step is not the rate-determining step, a comparable effect was detected in the later steps, indicating the low reactivity of **2o**, in agreement with the observed experimental behavior.

Interestingly, the activation energy is similar for imines **2a** and **2b** in **TS-1** and **TS-2** despite the presence of an electron donating group in **2b**. Hence, there was no relevant effect for the 1,4-addition (**TS-1**) and a lower activation energy for **2a** during the intramolecular nucleophilic attack (**TS-2**), which is contrary to the expected reactivity considering the electron donating group in **2b**.

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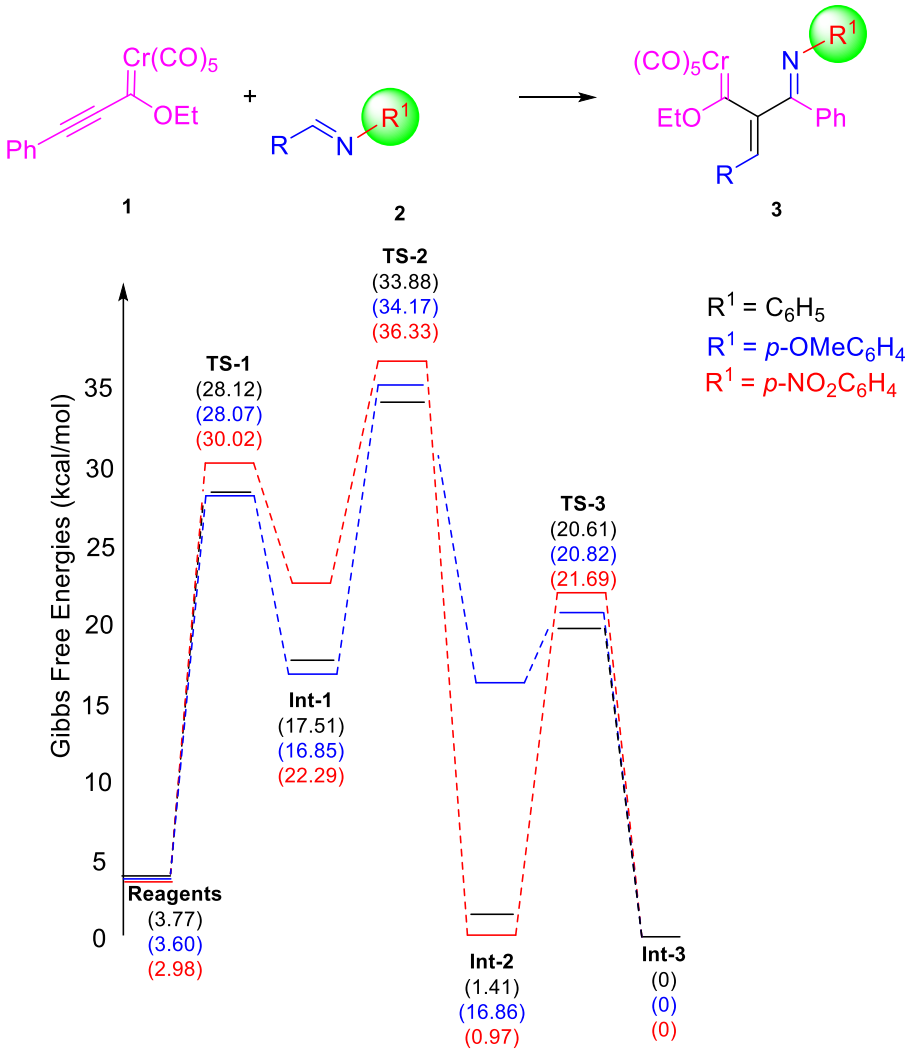

Scheme SD1. Energy profiles for the effect of the substituents in imines **2a** ($R^1 = C_6H_5$, in black), **2b** ($R^1 = p\text{-}OMeC_6H_4$, in blue), and **2o** ($R^1 = p\text{-}NO_2C_6H_5$, in red), calculated at the M06L/6311++g**/Cr=LANL2TZ/SCRF=THF level of theory.

Effect of the R substituent on the aromatic system of benzylidene anilines

The energetic profile of each of the R substituents of imines **2f** (R = p-$OMeC_6H_4$) and **2p** (R = p-$NO_2C_6H_5$) is shown in Scheme SD2, as is their plausible electronic effect compared to the unsubstituted imine **2a** (R = C_6H_5) as the reference. The electron withdrawing group of **2p** increases the activation energy by 2.68 kcal/mol for the 1,4-addition of the imine to **1** (**TS-1**). For **TS-2**, however, the activation energy is 1.04 kcal/mol more stable for **2p** than **2a**, and not significantly different for **2p** than **2f**. Considering that **TS-2** is the rate-determining step, the electronic effect of the R substituent appears not to be relevant in the reactivity of the entire process. Moreover, the perturbation caused by R substituents on the electrocyclic opening (**TS-3**) seems to be negligible.

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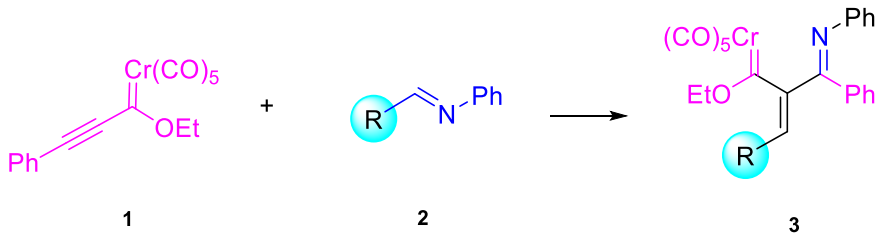

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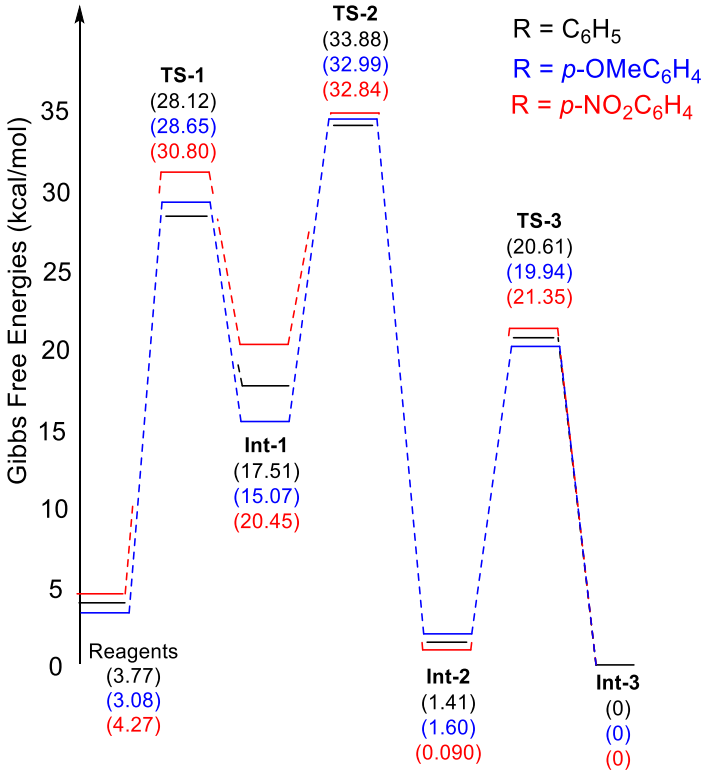

Scheme SD2. Energy profiles for the effect of the substituents in imines **2a** (R = C_6H_5, in black), **2f** (R = *p*-$OMeC_6H_4$, in blue), and **2p** (R = *p*-$NO_2C_6H_5$, in red), calculated at the M06L/6311++g**/Cr=LANL2TZ/SCRF= THF level of theory.

1a

Zero-point correction=	0.219025 (Hartree/Particle)
Thermal correction to Energy=	0.243403
Thermal correction to Enthalpy=	0.244348

Thermal correction to Gibbs Free Energy= 0.161973
Sum of electronic and zero-point Energies= -1153.400807
Sum of electronic and thermal Energies= -1153.376428
Sum of electronic and thermal Enthalpies= -1153.375484
Sum of electronic and thermal Free Energies= -1153.457859

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.018253	-1.686472	-0.000740
2	6	0	-3.687547	-1.300403	-0.000604
3	6	0	-3.350571	0.067292	0.000158
4	6	0	-4.376929	1.031151	0.000739
5	6	0	-5.703412	0.632906	0.000635
6	6	0	-6.026163	-0.723390	-0.000081
7	1	0	-5.273747	-2.740390	-0.001324
8	1	0	-2.893039	-2.040267	-0.001120
9	1	0	-4.114273	2.083372	0.001298
10	1	0	-6.490832	1.378954	0.001115
11	1	0	-7.066520	-1.030864	-0.000158
12	6	0	-1.998412	0.458544	0.000384
13	6	0	-0.821704	0.788369	0.000526
14	6	0	0.565246	0.965583	0.000041
15	24	0	1.836206	-0.648414	0.000048
16	6	0	0.733288	-1.465200	-1.324005
17	8	0	0.038327	-1.957623	-2.099864
18	6	0	2.864198	0.247952	-1.331979
19	8	0	3.478729	0.811959	-2.125422
20	6	0	2.862322	0.246919	1.334178
21	8	0	3.475649	0.810552	2.128821
22	6	0	3.018485	-2.124726	-0.000056
23	8	0	3.746738	-3.021794	-0.000173
24	6	0	0.732268	-1.467048	1.322054
25	8	0	0.036952	-1.960875	2.096708
26	8	0	1.031635	2.201564	-0.000511
27	6	0	0.105523	3.336918	-0.000367
28	1	0	-0.528872	3.248325	-0.886931
29	1	0	-0.528863	3.248150	0.886184
30	6	0	0.929153	4.590266	-0.000234
31	1	0	0.270497	5.460517	-0.000108
32	1	0	1.563773	4.645834	0.885800
33	1	0	1.563743	4.646063	-0.886274

Rotational constants (GHZ): 0.3442186 0.1498786 0.1234654

2a

Zero-point correction= 0.202353 (Hartree/Particle)

Thermal correction to Energy= 0.213295
Thermal correction to Enthalpy= 0.214239
Thermal correction to Gibbs Free Energy= 0.164381
Sum of electronic and zero-point Energies= -556.611141
Sum of electronic and thermal Energies= -556.600199
Sum of electronic and thermal Enthalpies= -556.599255
Sum of electronic and thermal Free Energies= -556.649114

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.343341	-0.996696	0.480805
2	6	0	-1.824939	0.236717	0.058434
3	6	0	-2.711246	1.231663	-0.375735
4	6	0	-4.075357	0.982091	-0.431313
5	6	0	-4.583006	-0.249905	-0.023284
6	6	0	-3.711721	-1.232210	0.440520
7	1	0	-1.669710	-1.754240	0.869819
8	1	0	-2.306338	2.191375	-0.680980
9	1	0	-4.748747	1.756722	-0.784680
10	1	0	-5.651319	-0.437326	-0.051540
11	1	0	-4.101606	-2.185885	0.782775
12	7	0	-0.459495	0.544521	0.103469
13	6	0	0.396098	-0.367937	-0.173471
14	1	0	0.083293	-1.369619	-0.509541
15	6	0	1.836201	-0.159986	-0.085965
16	6	0	2.695068	-1.213482	-0.422691
17	6	0	2.385805	1.061765	0.330212
18	6	0	4.073256	-1.055096	-0.345175
19	1	0	2.270418	-2.160332	-0.745930
20	6	0	3.760440	1.218344	0.404516
21	1	0	1.715621	1.874759	0.589587
22	6	0	4.607902	0.160950	0.069050
23	1	0	4.729784	-1.878227	-0.607114
24	1	0	4.180151	2.165788	0.727251
25	1	0	5.683957	0.288025	0.130643

Rotational constants (GHZ): 2.7200514 0.2781152 0.2577586

1a+2a Int 1

Zero-point correction= 0.424936 (Hartree/Particle)
Thermal correction to Energy= 0.460684
Thermal correction to Enthalpy= 0.461628
Thermal correction to Gibbs Free Energy= 0.353557

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Sum of electronic and zero-point Energies= -1710.015383
Sum of electronic and thermal Energies= -1709.979635
Sum of electronic and thermal Enthalpies= -1709.978691
Sum of electronic and thermal Free Energies= -1710.086762

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.461839	-1.453632	1.987675
2	6	0	-1.286013	-0.754222	1.677670
3	6	0	-0.360179	-0.517120	2.707029
4	6	0	-0.599957	-0.970631	3.994187
5	6	0	-1.768306	-1.672479	4.288706
6	6	0	-2.696059	-1.909853	3.280126
7	1	0	-3.205277	-1.640025	1.217505
8	1	0	0.554949	0.021081	2.473254
9	1	0	0.131003	-0.781315	4.773819
10	1	0	-1.953334	-2.028984	5.296673
11	1	0	-3.611219	-2.451025	3.498714
12	6	0	-1.010874	-0.239231	0.333958
13	6	0	-0.056773	0.605679	-0.021707
14	6	0	1.080026	1.261512	-0.086180
15	24	0	2.963168	0.176661	-0.305969
16	6	0	2.278881	-0.521876	-1.931246
17	8	0	1.819771	-0.930621	-2.910646
18	6	0	3.619690	1.701021	-1.240681
19	8	0	4.053256	2.605937	-1.810070
20	6	0	4.642795	-0.592160	-0.471755
21	8	0	5.700571	-1.065809	-0.575477
22	6	0	3.295208	1.026927	1.356943
23	8	0	3.421037	1.565858	2.370999
24	6	0	2.421093	-1.380414	0.627252
25	8	0	2.171496	-2.364135	1.185669
26	8	0	1.208883	2.608914	-0.032825
27	6	0	0.016155	3.369054	0.259423
28	1	0	0.277018	4.396506	-0.003332
29	1	0	-0.784627	3.031119	-0.412284
30	6	0	-0.385657	3.258157	1.709979
31	1	0	0.446724	3.533039	2.363140
32	1	0	-1.218893	3.932197	1.922843
33	1	0	-0.701884	2.243220	1.966882
34	6	0	-2.885083	-2.872420	-1.478004
35	6	0	-1.761238	-2.154948	-1.071133
36	6	0	-0.518431	-2.771306	-0.957288
37	6	0	-0.398256	-4.116352	-1.275049
38	6	0	-1.510644	-4.840640	-1.695773
39	6	0	-2.751466	-4.217298	-1.795793

40	1	0	-3.857886	-2.391651	-1.506627
41	1	0	0.338433	-2.190974	-0.640641
42	1	0	0.570786	-4.597325	-1.195596
43	1	0	-1.413402	-5.893780	-1.936390
44	1	0	-3.623998	-4.783426	-2.102134
45	7	0	-1.885129	-0.762619	-0.739714
46	6	0	-2.669691	0.005132	-1.454315
47	1	0	-3.019787	-0.436042	-2.386001
48	6	0	-3.111327	1.343003	-1.161234
49	6	0	-3.522739	2.126314	-2.254391
50	6	0	-3.234791	1.864274	0.140781
51	6	0	-3.990850	3.416479	-2.059475
52	1	0	-3.454639	1.715829	-3.257109
53	6	0	-3.741289	3.137419	0.327987
54	1	0	-2.959946	1.262914	0.999877
55	6	0	-4.101622	3.923345	-0.768393
56	1	0	-4.282587	4.020178	-2.911168
57	1	0	-3.854414	3.526164	1.334032
58	1	0	-4.481836	4.927228	-0.611190

Rotational constants (GHZ): 0.1204661 0.0904952 0.0765535

1a+2a TS1

Zero-point correction= 0.422714 (Hartree/Particle)
Thermal correction to Energy= 0.458338
Thermal correction to Enthalpy= 0.459283
Thermal correction to Gibbs Free Energy= 0.352821
Sum of electronic and zero-point Energies= -1710.001265
Sum of electronic and thermal Energies= -1709.965641
Sum of electronic and thermal Enthalpies= -1709.964697
Sum of electronic and thermal Free Energies= -1710.071158

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.760857	1.996336	1.536492
2	6	0	1.615031	1.199548	1.657108
3	6	0	0.982090	1.116046	2.911952
4	6	0	1.487764	1.805819	4.002213
5	6	0	2.627226	2.597697	3.869912
6	6	0	3.257982	2.689754	2.633618
7	1	0	3.259120	2.071900	0.575292
8	1	0	0.089186	0.505520	3.010548
9	1	0	0.984701	1.731854	4.960988
10	1	0	3.017008	3.141676	4.723959
11	1	0	4.145115	3.304353	2.519521

12	6	0	1.046368	0.420653	0.586582
13	6	0	0.187982	-0.485110	0.365380
14	6	0	-0.842132	-1.328180	0.157724
15	24	0	-2.841645	-0.605906	0.176581
16	6	0	-2.743679	-0.422867	-1.712156
17	8	0	-2.680599	-0.344505	-2.863047
18	6	0	-3.473437	-2.380044	-0.065380
19	8	0	-3.892122	-3.445585	-0.213031
20	6	0	-4.609011	-0.014436	0.278882
21	8	0	-5.709643	0.349147	0.349407
22	6	0	-2.676441	-0.921523	2.041887
23	8	0	-2.510665	-1.134274	3.165156
24	6	0	-2.256648	1.190244	0.436040
25	8	0	-1.948389	2.286297	0.623830
26	8	0	-0.655575	-2.649372	0.044965
27	6	0	0.693543	-3.176374	0.185205
28	1	0	0.644299	-4.163633	-0.277579
29	1	0	1.373130	-2.547262	-0.401247
30	6	0	1.105388	-3.258312	1.633228
31	1	0	0.397705	-3.862186	2.205653
32	1	0	2.089816	-3.725556	1.712084
33	1	0	1.167091	-2.268060	2.092046
34	6	0	0.855153	3.337171	-1.082558
35	6	0	0.866979	2.045705	-1.610693
36	6	0	-0.013443	1.692956	-2.634580
37	6	0	-0.888613	2.642711	-3.147593
38	6	0	-0.883748	3.939743	-2.645156
39	6	0	-0.012328	4.282205	-1.614119
40	1	0	1.526909	3.592562	-0.270278
41	1	0	-0.027800	0.669993	-2.998532
42	1	0	-1.581812	2.362020	-3.933890
43	1	0	-1.567079	4.680156	-3.046856
44	1	0	-0.013021	5.290595	-1.213775
45	7	0	1.734524	1.067150	-1.056241
46	6	0	2.443451	0.329353	-1.843339
47	1	0	2.390037	0.543247	-2.915895
48	6	0	3.282519	-0.787940	-1.466404
49	6	0	3.657585	-1.671744	-2.491608
50	6	0	3.721581	-1.037762	-0.155003
51	6	0	4.413192	-2.800140	-2.209640
52	1	0	3.333050	-1.471658	-3.508632
53	6	0	4.494841	-2.154761	0.116263
54	1	0	3.474660	-0.348300	0.643485
55	6	0	4.830462	-3.044278	-0.904345
56	1	0	4.682563	-3.484850	-3.006363
57	1	0	4.837267	-2.337522	1.129337
58	1	0	5.428752	-3.921640	-0.681848

Rotational constants (GHZ): 0.1233370 0.0869310 0.0795347

1a+2a INT 2

Zero-point correction= 0.427305 (Hartree/Particle)
Thermal correction to Energy= 0.462328
Thermal correction to Enthalpy= 0.463273
Thermal correction to Gibbs Free Energy= 0.357500
Sum of electronic and zero-point Energies= -1710.040619
Sum of electronic and thermal Energies= -1710.005596
Sum of electronic and thermal Enthalpies= -1710.004652
Sum of electronic and thermal Free Energies= -1710.110424

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.481642	-1.964066	0.967090
2	6	0	-2.339490	-1.919646	0.157957
3	6	0	-1.973091	-3.046910	-0.586341
4	6	0	-2.747690	-4.198758	-0.530847
5	6	0	-3.879209	-4.239312	0.278852
6	6	0	-4.240277	-3.123823	1.032217
7	1	0	-3.764678	-1.089769	1.545552
8	1	0	-1.089212	-3.007056	-1.216855
9	1	0	-2.467104	-5.064935	-1.119933
10	1	0	-4.481127	-5.140708	0.324345
11	1	0	-5.117940	-3.158137	1.668556
12	6	0	-1.542152	-0.705218	0.078497
13	6	0	-0.180937	-0.359404	0.041037
14	6	0	1.091307	-0.927762	0.176446
15	24	0	2.889076	-0.207340	-0.673844
16	6	0	2.978641	1.079547	0.732136
17	8	0	3.070968	1.831810	1.601439
18	6	0	3.851287	-1.428864	0.432760
19	8	0	4.470237	-2.153067	1.081842
20	6	0	4.525405	0.325115	-1.409418
21	8	0	5.539106	0.651693	-1.869478
22	6	0	2.588574	-1.597811	-1.929868
23	8	0	2.358408	-2.459314	-2.663509
24	6	0	2.096687	1.035937	-1.857039
25	8	0	1.720130	1.805045	-2.637839
26	8	0	1.254273	-2.078297	0.837183
27	6	0	0.299057	-2.617115	1.790736
28	1	0	-0.324355	-1.799577	2.168501

29	1	0	-0.346870	-3.328921	1.271120
30	6	0	1.096237	-3.281390	2.879477
31	1	0	1.731642	-2.561270	3.399177
32	1	0	0.423185	-3.735155	3.609796
33	1	0	1.733859	-4.068250	2.471075
34	6	0	-4.171140	0.386881	-1.222053
35	6	0	-3.191303	1.141488	-0.567408
36	6	0	-3.385420	2.514230	-0.372326
37	6	0	-4.551924	3.118137	-0.820596
38	6	0	-5.537659	2.367317	-1.455147
39	6	0	-5.338621	1.004203	-1.652995
40	1	0	-4.015290	-0.668222	-1.411056
41	1	0	-2.623827	3.096207	0.135332
42	1	0	-4.692214	4.182872	-0.665800
43	1	0	-6.450294	2.841804	-1.799243
44	1	0	-6.091827	0.412903	-2.163536
45	7	0	-1.995170	0.568863	-0.105370
46	6	0	-0.592284	1.075117	-0.268002
47	1	0	-0.455413	1.356919	-1.316000
48	6	0	-0.187196	2.181720	0.656407
49	6	0	0.300170	3.383870	0.146360
50	6	0	-0.324657	2.030455	2.038915
51	6	0	0.647715	4.423335	1.004487
52	1	0	0.400447	3.506145	-0.928631
53	6	0	0.013771	3.068723	2.894739
54	1	0	-0.706170	1.093538	2.438891
55	6	0	0.502509	4.268010	2.378389
56	1	0	1.027975	5.355015	0.598567
57	1	0	-0.097995	2.945481	3.967237
58	1	0	0.770579	5.078260	3.048858

Rotational constants (GHZ): 0.1312041 0.0871406 0.0674669

1a+2a TS 2

Zero-point correction= 0.422986 (Hartree/Particle)
Thermal correction to Energy= 0.458280
Thermal correction to Enthalpy= 0.459224
Thermal correction to Gibbs Free Energy= 0.353478
Sum of electronic and zero-point Energies= -1709.993175
Sum of electronic and thermal Energies= -1709.957881
Sum of electronic and thermal Enthalpies= -1709.956937
Sum of electronic and thermal Free Energies= -1710.062683

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.284106	1.816563	2.412488
2	6	0	0.607700	0.739748	1.816597
3	6	0	-0.291125	-0.005186	2.597839
4	6	0	-0.555925	0.354625	3.910023
5	6	0	0.090342	1.449668	4.477259
6	6	0	1.019979	2.168933	3.727747
7	1	0	2.010410	2.384157	1.839460
8	1	0	-0.775959	-0.871807	2.161605
9	1	0	-1.260660	-0.227243	4.495507
10	1	0	-0.113228	1.731137	5.505158
11	1	0	1.543331	3.008546	4.173205
12	6	0	0.810865	0.378522	0.421059
13	6	0	0.181666	-0.613218	-0.283351
14	6	0	-0.937111	-1.337541	-0.429936
15	24	0	-2.816306	-0.216888	-0.465795
16	6	0	-2.081672	0.673726	-1.980213
17	8	0	-1.595171	1.218625	-2.873062
18	6	0	-3.491636	-1.624817	-1.562021
19	8	0	-3.950825	-2.444830	-2.228467
20	6	0	-4.493242	0.566820	-0.632429
21	8	0	-5.545267	1.045289	-0.741336
22	6	0	-3.243736	-1.193738	1.106753
23	8	0	-3.462506	-1.790814	2.070434
24	6	0	-2.344536	1.300474	0.577336
25	8	0	-2.171305	2.285536	1.158564
26	8	0	-1.016297	-2.623955	-0.758246
27	6	0	0.225873	-3.380013	-0.832983
28	1	0	-0.052118	-4.298608	-1.352177
29	1	0	0.913425	-2.812569	-1.467066
30	6	0	0.803382	-3.656806	0.529785
31	1	0	0.117002	-4.254443	1.133669
32	1	0	1.743246	-4.206575	0.429994
33	1	0	1.024936	-2.731828	1.068625
34	6	0	1.028433	3.136186	-0.635714
35	6	0	2.026452	2.178029	-0.834295
36	6	0	3.179959	2.498069	-1.554872
37	6	0	3.323056	3.771985	-2.090700
38	6	0	2.338124	4.733596	-1.887168
39	6	0	1.196564	4.411557	-1.154272
40	1	0	0.125755	2.871829	-0.093880
41	1	0	3.960547	1.752911	-1.676122
42	1	0	4.216516	4.017366	-2.654832
43	1	0	2.457825	5.730610	-2.296752

44	1	0	0.420964	5.154559	-1.002216
45	7	0	1.880734	0.863516	-0.352377
46	6	0	2.220437	-0.233918	-1.139102
47	1	0	2.230549	-0.067837	-2.218502
48	6	0	3.045745	-1.308470	-0.628731
49	6	0	3.467883	-2.315689	-1.513560
50	6	0	3.481585	-1.358229	0.708082
51	6	0	4.277883	-3.351805	-1.071587
52	1	0	3.151722	-2.275879	-2.552444
53	6	0	4.292871	-2.391597	1.141357
54	1	0	3.182571	-0.575795	1.399482
55	6	0	4.688921	-3.397830	0.257809
56	1	0	4.593562	-4.122453	-1.767009
57	1	0	4.625978	-2.415456	2.173614
58	1	0	5.323741	-4.206615	0.604095

Rotational constants (GHZ): 0.1229238 0.0914307 0.0782148

1a+2a Int 3

Zero-point correction= 0.425553 (Hartree/Particle)
Thermal correction to Energy= 0.460801
Thermal correction to Enthalpy= 0.461745
Thermal correction to Gibbs Free Energy= 0.356643
Sum of electronic and zero-point Energies= -1710.043609
Sum of electronic and thermal Energies= -1710.008361
Sum of electronic and thermal Enthalpies= -1710.007417
Sum of electronic and thermal Free Energies= -1710.112519

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.832497	1.603928	-0.257166
2	6	0	1.903898	0.688884	-0.764941
3	6	0	1.322532	0.926278	-2.014879
4	6	0	1.686336	2.042202	-2.758452
5	6	0	2.611537	2.946533	-2.246984
6	6	0	3.174365	2.731280	-0.991119
7	1	0	3.285080	1.428907	0.714388
8	1	0	0.605108	0.215393	-2.413168
9	1	0	1.243121	2.207569	-3.735043
10	1	0	2.889134	3.823628	-2.822303
11	1	0	3.884768	3.443303	-0.584589
12	6	0	1.575526	-0.564309	-0.040186
13	6	0	0.125491	-0.953475	0.054241
14	6	0	-0.750139	-0.089623	0.895012

15	24	0	-2.080427	1.345956	0.235179
16	6	0	-3.577760	0.295388	0.766847
17	8	0	-4.514866	-0.260249	1.140947
18	6	0	-2.123386	2.070061	1.994116
19	8	0	-2.165172	2.522172	3.052779
20	6	0	-3.294577	2.645290	-0.391624
21	8	0	-4.038782	3.440923	-0.778440
22	6	0	-0.678274	2.603068	-0.119156
23	8	0	0.080268	3.455931	-0.267063
24	6	0	-2.039450	0.587381	-1.516876
25	8	0	-2.055133	0.157081	-2.586220
26	8	0	-0.599168	-0.197601	2.191606
27	6	0	0.278992	-1.178053	2.857556
28	1	0	-0.389239	-1.705565	3.541479
29	1	0	0.672685	-1.876724	2.117802
30	6	0	1.358766	-0.428026	3.583595
31	1	0	0.937477	0.284528	4.294933
32	1	0	1.982145	-1.133176	4.137723
33	1	0	2.000099	0.113771	2.884477
34	6	0	4.402327	-1.167534	-0.960197
35	6	0	3.809893	-1.239488	0.307051
36	6	0	4.626011	-1.275426	1.442726
37	6	0	6.006166	-1.183905	1.314614
38	6	0	6.592669	-1.097133	0.054304
39	6	0	5.784271	-1.103570	-1.080034
40	1	0	3.771502	-1.169406	-1.843821
41	1	0	4.163513	-1.362443	2.420863
42	1	0	6.627799	-1.193354	2.204206
43	1	0	7.671461	-1.039156	-0.043769
44	1	0	6.232750	-1.053456	-2.067477
45	7	0	2.420973	-1.382508	0.472283
46	6	0	-0.276255	-2.010290	-0.682153
47	1	0	0.478525	-2.453341	-1.331862
48	6	0	-1.589900	-2.635971	-0.744222
49	6	0	-1.975251	-3.276369	-1.933676
50	6	0	-2.475379	-2.661475	0.341171
51	6	0	-3.217608	-3.881654	-2.046922
52	1	0	-1.290631	-3.274969	-2.777446
53	6	0	-3.716198	-3.277064	0.230383
54	1	0	-2.179776	-2.229700	1.292423
55	6	0	-4.094657	-3.881457	-0.963849
56	1	0	-3.503114	-4.359269	-2.978708
57	1	0	-4.386807	-3.288890	1.083077
58	1	0	-5.064007	-4.361926	-1.047394

Rotational constants (GHZ): 0.1458531 0.0828558 0.0717475

1a+2a TS 3

Zero-point correction= 0.423623 (Hartree/Particle)
Thermal correction to Energy= 0.458642
Thermal correction to Enthalpy= 0.459586
Thermal correction to Gibbs Free Energy= 0.354241
Sum of electronic and zero-point Energies= -1710.012814
Sum of electronic and thermal Energies= -1709.977795
Sum of electronic and thermal Enthalpies= -1709.976851
Sum of electronic and thermal Free Energies= -1710.082196

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.439414	-1.679058	1.139418
2	6	0	-2.237798	-1.514373	0.438761
3	6	0	-1.703177	-2.599611	-0.266950
4	6	0	-2.363599	-3.820867	-0.279464
5	6	0	-3.553417	-3.978272	0.426581
6	6	0	-4.086971	-2.906699	1.139314
7	1	0	-3.853204	-0.839906	1.691426
8	1	0	-0.777020	-2.474023	-0.821303
9	1	0	-1.948738	-4.652104	-0.840104
10	1	0	-4.065241	-4.935190	0.421135
11	1	0	-5.011587	-3.028543	1.693831
12	6	0	-1.550237	-0.220883	0.438161
13	6	0	-0.182115	0.060913	0.357824
14	6	0	0.981497	-0.732798	0.468986
15	24	0	2.670042	-0.585429	-0.768565
16	6	0	3.589429	-0.549547	0.895888
17	8	0	4.062075	-0.516986	1.947435
18	6	0	2.695838	-2.492544	-0.774970
19	8	0	2.728803	-3.644338	-0.793237
20	6	0	4.189953	-0.640801	-1.872485
21	8	0	5.128657	-0.685518	-2.550174
22	6	0	1.421166	-0.546323	-2.196413
23	8	0	0.602584	-0.508656	-3.010826
24	6	0	2.843000	1.305655	-0.874337
25	8	0	3.075830	2.429180	-1.014439
26	8	0	0.984658	-1.782647	1.299155
27	6	0	0.218740	-1.839619	2.542635
28	1	0	0.881185	-1.410444	3.303044
29	1	0	-0.673744	-1.218373	2.482874
30	6	0	-0.100995	-3.276742	2.839266
31	1	0	0.808027	-3.880209	2.878242
32	1	0	-0.596343	-3.349094	3.809969

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33	1	0	-0.766247	-3.699276	2.084353
34	6	0	-3.634884	0.554240	-1.525433
35	6	0	-3.319949	1.247369	-0.344707
36	6	0	-4.154357	2.291331	0.079127
37	6	0	-5.297740	2.608253	-0.640846
38	6	0	-5.617974	1.899898	-1.797324
39	6	0	-4.779861	0.877211	-2.238697
40	1	0	-2.967504	-0.226042	-1.881292
41	1	0	-3.890462	2.835726	0.980305
42	1	0	-5.942512	3.412034	-0.300157
43	1	0	-6.510898	2.151273	-2.359883
44	1	0	-5.016727	0.335661	-3.149013
45	7	0	-2.161518	0.989795	0.393589
46	6	0	-0.253035	1.464831	-0.096218
47	1	0	-0.562568	1.654375	-1.124104
48	6	0	0.361302	2.563844	0.600010
49	6	0	0.371117	3.844168	0.019603
50	6	0	0.966295	2.379247	1.856256
51	6	0	0.985723	4.903348	0.666710
52	1	0	-0.094794	3.987098	-0.951344
53	6	0	1.593673	3.437032	2.492819
54	1	0	0.943059	1.396675	2.319338
55	6	0	1.603892	4.699483	1.899971
56	1	0	0.995134	5.887610	0.210599
57	1	0	2.070320	3.286197	3.455425
58	1	0	2.092005	5.527884	2.402868

Rotational constants (GHZ): 0.1286296 0.0902786 0.0697105

3a s-trans

Zero-point correction= 0.424825 (Hartree/Particle)
Thermal correction to Energy= 0.459748
Thermal correction to Enthalpy= 0.460692
Thermal correction to Gibbs Free Energy= 0.356360
Sum of electronic and zero-point Energies= -1710.057725
Sum of electronic and thermal Energies= -1710.022803
Sum of electronic and thermal Enthalpies= -1710.021859
Sum of electronic and thermal Free Energies= -1710.126191

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.867945	1.653637	-1.567751
2	6	0	-2.140961	1.798204	-0.381975
3	6	0	-2.254255	2.984562	0.348572

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4	6	0	-3.089743	4.004034	-0.093121
5	6	0	-3.805401	3.854901	-1.277180
6	6	0	-3.689417	2.679893	-2.015235
7	1	0	-2.784323	0.732488	-2.136419
8	1	0	-1.699101	3.098709	1.275819
9	1	0	-3.181061	4.915992	0.487796
10	1	0	-4.453378	4.653081	-1.624552
11	1	0	-4.243755	2.561407	-2.940539
12	6	0	-1.304552	0.668355	0.102278
13	6	0	0.135047	0.853953	0.336154
14	6	0	0.823984	-0.396468	0.759591
15	24	0	1.709531	-1.684070	-0.579887
16	6	0	3.058750	-1.943588	0.737472
17	8	0	3.863912	-2.046107	1.555522
18	6	0	0.561310	-2.974600	0.233946
19	8	0	-0.158943	-3.712852	0.744171
20	6	0	2.443602	-3.004505	-1.711815
21	8	0	2.891753	-3.826386	-2.390555
22	6	0	0.359003	-1.276106	-1.858162
23	8	0	-0.433938	-1.016974	-2.654739
24	6	0	2.781183	-0.361808	-1.441787
25	8	0	3.422993	0.392022	-2.032908
26	8	0	0.764627	-0.740983	2.016755
27	6	0	0.005749	-0.011990	3.043991
28	1	0	0.757449	0.316370	3.765708
29	1	0	-0.460004	0.869326	2.598695
30	6	0	-0.988385	-0.968260	3.639545
31	1	0	-0.485958	-1.824831	4.092775
32	1	0	-1.564024	-0.461794	4.417128
33	1	0	-1.680069	-1.332324	2.877401
34	6	0	-4.069825	-0.182489	1.011188
35	6	0	-3.098731	-0.867642	0.266492
36	6	0	-3.474846	-2.000950	-0.465654
37	6	0	-4.802827	-2.406103	-0.493440
38	6	0	-5.766751	-1.716268	0.238617
39	6	0	-5.390130	-0.612097	0.999812
40	1	0	-3.773536	0.675159	1.608432
41	1	0	-2.713714	-2.544629	-1.016746
42	1	0	-5.084773	-3.274140	-1.080838
43	1	0	-6.800956	-2.043419	0.225874
44	1	0	-6.130890	-0.079129	1.588035
45	7	0	-1.743836	-0.529169	0.318976
46	6	0	0.776848	2.022033	0.074830
47	1	0	0.182222	2.807547	-0.386778
48	6	0	2.170360	2.358097	0.290170
49	6	0	2.698187	3.460726	-0.405789
50	6	0	3.032200	1.639069	1.138315
51	6	0	4.039201	3.796692	-0.304291

52	1	0	2.040665	4.037746	-1.049828
53	6	0	4.374146	1.975592	1.237422
54	1	0	2.652982	0.824771	1.743756
55	6	0	4.885922	3.047508	0.509852
56	1	0	4.427982	4.642158	-0.862376
57	1	0	5.022375	1.403657	1.893651
58	1	0	5.936384	3.307655	0.589221

Rotational constants (GHZ): 0.1386771 0.0908259 0.0713361

3a s-cis

Zero-point correction= 0.425883 (Hartree/Particle)
Thermal correction to Energy= 0.461144
Thermal correction to Enthalpy= 0.462088
Thermal correction to Gibbs Free Energy= 0.357168
Sum of electronic and zero-point Energies= -1710.049563
Sum of electronic and thermal Energies= -1710.014302
Sum of electronic and thermal Enthalpies= -1710.013357
Sum of electronic and thermal Free Energies= -1710.118278

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.567163	-0.536805	2.274697
2	6	0	-1.904215	-0.294624	0.939432
3	6	0	-2.904214	-1.075719	0.346843
4	6	0	-3.539457	-2.073979	1.070765
5	6	0	-3.202636	-2.298082	2.403957
6	6	0	-2.217323	-1.524826	3.006224
7	1	0	-0.818681	0.083090	2.758106
8	1	0	-3.179694	-0.899440	-0.686884
9	1	0	-4.303409	-2.679495	0.594162
10	1	0	-3.705103	-3.076316	2.968890
11	1	0	-1.952337	-1.688746	4.045974
12	6	0	-1.231270	0.795165	0.178729
13	6	0	0.247088	0.936376	0.331714
14	6	0	1.022248	-0.303252	0.536744
15	24	0	1.174579	-1.762322	-0.907328
16	6	0	2.821372	-2.280962	-0.096370
17	8	0	3.825145	-2.593997	0.373086
18	6	0	0.214170	-2.907234	0.289245
19	8	0	-0.338886	-3.595357	1.026168
20	6	0	1.395073	-3.162323	-2.156819
21	8	0	1.535568	-4.027427	-2.909625
22	6	0	-0.410628	-1.285223	-1.852962
23	8	0	-1.317479	-1.056820	-2.529374

24	6	0	2.091742	-0.550012	-2.061080
25	8	0	2.618626	0.170726	-2.789076
26	8	0	1.710170	-0.452341	1.642220
27	6	0	1.782147	0.529320	2.733748
28	1	0	2.682378	1.119133	2.540533
29	1	0	0.920612	1.197644	2.677112
30	6	0	1.863180	-0.238714	4.020850
31	1	0	2.726694	-0.905679	4.026942
32	1	0	1.966321	0.457989	4.854808
33	1	0	0.964444	-0.837326	4.185770
34	6	0	-3.821994	1.767869	-1.938587
35	6	0	-3.218413	1.748786	-0.674433
36	6	0	-4.011879	1.957942	0.463122
37	6	0	-5.378939	2.162377	0.334112
38	6	0	-5.980207	2.145824	-0.922497
39	6	0	-5.194222	1.944388	-2.055333
40	1	0	-3.199599	1.622357	-2.816163
41	1	0	-3.541967	1.966153	1.442345
42	1	0	-5.980166	2.332948	1.222051
43	1	0	-7.050050	2.298155	-1.018807
44	1	0	-5.652260	1.937162	-3.039758
45	7	0	-1.827995	1.630078	-0.598484
46	6	0	0.795663	2.163134	0.118955
47	1	0	0.060212	2.933514	-0.107931
48	6	0	2.168550	2.627835	0.078163
49	6	0	2.361427	4.020499	-0.005040
50	6	0	3.313595	1.809130	0.078605
51	6	0	3.631512	4.572848	-0.065086
52	1	0	1.488582	4.666469	-0.025848
53	6	0	4.583184	2.362413	0.008929
54	1	0	3.217884	0.729567	0.103150
55	6	0	4.750048	3.744385	-0.057708
56	1	0	3.749635	5.649567	-0.126527
57	1	0	5.450339	1.710530	-0.000417
58	1	0	5.746436	4.170430	-0.112947

Rotational constants (GHZ): 0.1274577 0.0898999 0.0748289

2b

Zero-point correction= 0.234525 (Hartree/Particle)
Thermal correction to Energy= 0.248089
Thermal correction to Enthalpy= 0.249033
Thermal correction to Gibbs Free Energy= 0.193144
Sum of electronic and zero-point Energies= -671.121450
Sum of electronic and thermal Energies= -671.107886

Sum of electronic and thermal Enthalpies= -671.106942
Sum of electronic and thermal Free Energies= -671.162831

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.418929	-1.063104	-0.421331
2	6	0	0.895771	0.202000	-0.096727
3	6	0	1.796127	1.227132	0.208013
4	6	0	3.167106	1.004196	0.244648
5	6	0	3.667049	-0.263084	-0.062828
6	6	0	2.781422	-1.290864	-0.408400
7	1	0	0.749853	-1.864608	-0.718816
8	1	0	1.400225	2.211801	0.436367
9	1	0	3.833772	1.818541	0.500781
10	1	0	3.188189	-2.260159	-0.677624
11	7	0	-0.468260	0.513583	-0.107880
12	6	0	-1.335148	-0.398473	0.139455
13	1	0	-1.041336	-1.421065	0.424216
14	6	0	-2.771899	-0.161299	0.081416
15	6	0	-3.646289	-1.214866	0.377569
16	6	0	-3.307540	1.088294	-0.266548
17	6	0	-5.022288	-1.029913	0.327656
18	1	0	-3.234353	-2.184238	0.646643
19	6	0	-4.680102	1.271322	-0.313040
20	1	0	-2.626980	1.901684	-0.495919
21	6	0	-5.542218	0.213622	-0.018055
22	1	0	-5.689217	-1.854418	0.557533
23	1	0	-5.087250	2.240987	-0.582251
24	1	0	-6.616638	0.361598	-0.058305
25	8	0	4.986190	-0.588685	-0.072608
26	6	0	5.913549	0.433277	0.256039
27	1	0	5.748203	0.811048	1.270568
28	1	0	6.899917	-0.022733	0.197914
29	1	0	5.857088	1.266525	-0.452298

Rotational constants (GHZ): 2.5482433 0.1750183 0.1655626

2b+1a TS1

Zero-point correction= 0.455592 (Hartree/Particle)
Thermal correction to Energy= 0.493702
Thermal correction to Enthalpy= 0.494646
Thermal correction to Gibbs Free Energy= 0.382476
Sum of electronic and zero-point Energies= -1824.511607

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Sum of electronic and thermal Energies= -1824.473497
Sum of electronic and thermal Enthalpies= -1824.472553
Sum of electronic and thermal Free Energies= -1824.584723

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.302489	2.249164	1.938617
2	6	0	1.578755	1.049636	1.933512
3	6	0	1.270686	0.445459	3.167639
4	6	0	1.679656	1.026412	4.357592
5	6	0	2.397017	2.221429	4.349838
6	6	0	2.703796	2.827800	3.136393
7	1	0	2.544126	2.726861	0.994865
8	1	0	0.706681	-0.482436	3.171855
9	1	0	1.430382	0.546722	5.298715
10	1	0	2.711700	2.676036	5.283392
11	1	0	3.262829	3.757762	3.118499
12	6	0	1.146269	0.357753	0.749074
13	6	0	0.650490	-0.719460	0.323080
14	6	0	-0.026909	-1.811581	-0.104933
15	24	0	-2.120948	-1.966437	0.169383
16	6	0	-2.369099	-1.310669	-1.599377
17	8	0	-2.514381	-0.954241	-2.688004
18	6	0	-2.075668	-3.724763	-0.544950
19	8	0	-2.086646	-4.795367	-0.975925
20	6	0	-3.954612	-2.153251	0.475437
21	8	0	-5.092411	-2.275574	0.669683
22	6	0	-1.637074	-2.664788	1.868773
23	8	0	-1.297127	-3.093281	2.885849
24	6	0	-2.197559	-0.211061	0.912780
25	8	0	-2.277988	0.831006	1.401181
26	8	0	0.618486	-2.866996	-0.611108
27	6	0	2.074559	-2.843301	-0.663806
28	1	0	2.325880	-3.610785	-1.397755
29	1	0	2.388820	-1.868434	-1.050964
30	6	0	2.677613	-3.137115	0.685719
31	1	0	2.323633	-4.095249	1.072315
32	1	0	3.765532	-3.186795	0.600531
33	1	0	2.434144	-2.357347	1.411924
34	6	0	-0.414685	3.232106	-0.026425
35	6	0	0.024874	2.269503	-0.933142
36	6	0	-0.810847	1.894329	-1.992091
37	6	0	-2.046384	2.491053	-2.155270
38	6	0	-2.470299	3.480643	-1.261956
39	6	0	-1.646589	3.850195	-0.194782
40	1	0	0.216368	3.509161	0.810931

41	1	0	-0.496712	1.103507	-2.666663
42	1	0	-2.709251	2.188869	-2.958652
43	1	0	-1.959883	4.605103	0.515644
44	7	0	1.273103	1.631691	-0.739124
45	6	0	2.035875	1.408982	-1.755966
46	1	0	1.715195	1.789485	-2.732223
47	6	0	3.276582	0.660669	-1.752538
48	6	0	3.763743	0.219422	-2.993584
49	6	0	3.998542	0.346967	-0.588720
50	6	0	4.916404	-0.549332	-3.068497
51	1	0	3.216352	0.472126	-3.897171
52	6	0	5.159633	-0.404659	-0.671363
53	1	0	3.659533	0.706843	0.375136
54	6	0	5.614926	-0.865228	-1.906659
55	1	0	5.273134	-0.897783	-4.031557
56	1	0	5.714946	-0.636202	0.231449
57	1	0	6.519929	-1.461176	-1.962875
58	8	0	-3.695360	4.009318	-1.500806
59	6	0	-4.177544	4.985619	-0.589412
60	1	0	-3.532975	5.870495	-0.575116
61	1	0	-5.166926	5.266797	-0.944171
62	1	0	-4.256832	4.578593	0.423690

Rotational constants (GHZ): 0.0984826 0.0829751 0.0676416

2b+1a Int 1

Zero-point correction= 0.457609 (Hartree/Particle)
Thermal correction to Energy= 0.495745
Thermal correction to Enthalpy= 0.496689
Thermal correction to Gibbs Free Energy= 0.383802
Sum of electronic and zero-point Energies= -1824.527408
Sum of electronic and thermal Energies= -1824.489272
Sum of electronic and thermal Enthalpies= -1824.488328
Sum of electronic and thermal Free Energies= -1824.601215

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.167804	1.291523	2.255011
2	6	0	-0.896541	0.841281	1.869280
3	6	0	0.015217	0.478391	2.873865
4	6	0	-0.338219	0.553321	4.211903
5	6	0	-1.607772	0.994942	4.583152
6	6	0	-2.517694	1.364788	3.598676
7	1	0	-2.890219	1.594277	1.501817
8	1	0	1.003760	0.132824	2.581681

9	1	0	0.379527	0.262558	4.972611
10	1	0	-1.882642	1.051055	5.631178
11	1	0	-3.506535	1.716739	3.875507
12	6	0	-0.480625	0.784990	0.465463
13	6	0	0.745775	0.626423	-0.002063
14	6	0	1.986695	0.264231	-0.228791
15	24	0	2.512208	-1.853904	-0.302091
16	6	0	1.255590	-2.009251	-1.715144
17	8	0	0.476395	-2.053434	-2.568279
18	6	0	3.861105	-1.377419	-1.558545
19	8	0	4.689408	-1.125703	-2.321565
20	6	0	3.111955	-3.606764	-0.388902
21	8	0	3.498322	-4.703009	-0.445886
22	6	0	3.633785	-1.327437	1.134412
23	8	0	4.278179	-0.939205	2.011122
24	6	0	1.218322	-2.426956	0.956465
25	8	0	0.456352	-2.851381	1.719208
26	8	0	3.019312	1.115458	-0.447747
27	6	0	2.742117	2.526178	-0.312077
28	1	0	3.602805	3.017432	-0.771821
29	1	0	1.849573	2.762503	-0.906728
30	6	0	2.580194	2.943046	1.129539
31	1	0	3.447082	2.635738	1.720080
32	1	0	2.494042	4.030221	1.197738
33	1	0	1.684682	2.508661	1.582910
34	6	0	-3.831283	0.046098	-0.953265
35	6	0	-2.508879	-0.190300	-0.585783
36	6	0	-2.097690	-1.479849	-0.239874
37	6	0	-2.995005	-2.523847	-0.290275
38	6	0	-4.323101	-2.296001	-0.679736
39	6	0	-4.739030	-1.001277	-1.008939
40	1	0	-4.166902	1.057708	-1.158801
41	1	0	-1.068083	-1.653493	0.045933
42	1	0	-2.688670	-3.532158	-0.035968
43	1	0	-5.766591	-0.796664	-1.280454
44	7	0	-1.573518	0.888885	-0.529612
45	6	0	-1.643714	1.865643	-1.402433
46	1	0	-2.277980	1.668323	-2.264428
47	6	0	-0.991983	3.148370	-1.344246
48	6	0	-0.803406	3.828483	-2.560651
49	6	0	-0.624124	3.782305	-0.141900
50	6	0	-0.213744	5.083245	-2.580838
51	1	0	-1.110465	3.354539	-3.488137
52	6	0	-0.071296	5.049361	-0.169379
53	1	0	-0.796762	3.291067	0.809471
54	6	0	0.151745	5.696155	-1.386231
55	1	0	-0.053079	5.589222	-3.526262
56	1	0	0.191926	5.539177	0.761995

57	1	0	0.598066	6.685091	-1.399045
58	8	0	-5.125147	-3.379581	-0.693265
59	6	0	-6.479975	-3.200263	-1.088670
60	1	0	-6.935900	-4.186835	-1.048592
61	1	0	-7.006238	-2.528710	-0.403552
62	1	0	-6.546008	-2.809409	-2.108511

Rotational constants (GHZ): 0.0960863 0.0830211 0.0630918

2b+1a TS 2

Zero-point correction= 0.456013 (Hartree/Particle)
Thermal correction to Energy= 0.493659
Thermal correction to Enthalpy= 0.494603
Thermal correction to Gibbs Free Energy= 0.383616
Sum of electronic and zero-point Energies= -1824.503342
Sum of electronic and thermal Energies= -1824.465696
Sum of electronic and thermal Enthalpies= -1824.464751
Sum of electronic and thermal Free Energies= -1824.575739

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.271183	-0.074532	2.911697
2	6	0	-0.231476	0.261089	2.029293
3	6	0	1.060933	0.435562	2.550636
4	6	0	1.319366	0.221435	3.895290
5	6	0	0.287659	-0.149719	4.753088
6	6	0	-1.008410	-0.284016	4.257627
7	1	0	-2.285469	-0.179119	2.540778
8	1	0	1.859251	0.746447	1.886396
9	1	0	2.327043	0.354183	4.276139
10	1	0	0.486372	-0.315198	5.806911
11	1	0	-1.819959	-0.551462	4.926377
12	6	0	-0.451005	0.434811	0.598697
13	6	0	0.492103	0.714151	-0.356330
14	6	0	1.774786	0.596034	-0.729939
15	24	0	2.672682	-1.393349	-0.566673
16	6	0	1.365229	-1.908770	-1.850856
17	8	0	0.542727	-2.197213	-2.606416
18	6	0	3.869012	-0.837660	-1.945210
19	8	0	4.615172	-0.556304	-2.776803
20	6	0	3.556608	-3.027730	-0.601311
21	8	0	4.115250	-4.044918	-0.630249
22	6	0	3.813700	-0.637258	0.752282

23	8	0	4.486967	-0.159095	1.559260
24	6	0	1.567326	-2.144814	0.785134
25	8	0	0.942464	-2.719667	1.570380
26	8	0	2.502079	1.506637	-1.372230
27	6	0	1.917082	2.825107	-1.567596
28	1	0	2.564057	3.296953	-2.308916
29	1	0	0.926644	2.679217	-2.008454
30	6	0	1.862121	3.613197	-0.285678
31	1	0	2.864583	3.787143	0.111753
32	1	0	1.388268	4.582289	-0.464321
33	1	0	1.270694	3.098815	0.476692
34	6	0	-2.491659	-1.720566	0.291881
35	6	0	-2.731385	-0.390448	-0.065225
36	6	0	-3.979241	-0.005333	-0.562697
37	6	0	-4.980720	-0.955778	-0.715628
38	6	0	-4.752004	-2.279049	-0.351869
39	6	0	-3.508261	-2.654119	0.155487
40	1	0	-1.514336	-2.012466	0.662168
41	1	0	-4.158452	1.037263	-0.808458
42	1	0	-5.948380	-0.656030	-1.103553
43	1	0	-3.322796	-3.687157	0.430170
44	7	0	-1.723395	0.585769	0.028063
45	6	0	-1.515450	1.510613	-0.992193
46	1	0	-1.831869	1.202476	-1.990845
47	6	0	-1.461307	2.932344	-0.728324
48	6	0	-1.401031	3.818808	-1.817659
49	6	0	-1.521882	3.464404	0.572781
50	6	0	-1.380020	5.190619	-1.612790
51	1	0	-1.372033	3.417245	-2.826834
52	6	0	-1.504457	4.833580	0.770008
53	1	0	-1.589482	2.792849	1.423819
54	6	0	-1.425801	5.703923	-0.319196
55	1	0	-1.332746	5.861723	-2.463942
56	1	0	-1.557292	5.231449	1.777877
57	1	0	-1.412207	6.776784	-0.158046
58	8	0	-5.789242	-3.252811	-0.496175
59	6	0	-5.837093	-3.701757	-1.853031
60	1	0	-6.540017	-4.503913	-1.938724
61	1	0	-6.139387	-2.893511	-2.485689
62	1	0	-4.867677	-4.043772	-2.149948

Rotational constants (GHZ): 0.1005349 0.0796178 0.0634839

2b+1a INT 2

Zero-point correction= 0.457611 (Hartree/Particle)
Thermal correction to Energy= 0.495745
Thermal correction to Enthalpy= 0.496689

Thermal correction to Gibbs Free Energy= 0.383814
Sum of electronic and zero-point Energies= -1824.527406
Sum of electronic and thermal Energies= -1824.489272
Sum of electronic and thermal Enthalpies= -1824.488328
Sum of electronic and thermal Free Energies= -1824.601203

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.167804	1.291523	2.255011
2	6	0	-0.896541	0.841281	1.869280
3	6	0	0.015217	0.478391	2.873865
4	6	0	-0.338219	0.553321	4.211903
5	6	0	-1.607772	0.994942	4.583152
6	6	0	-2.517694	1.364788	3.598676
7	1	0	-2.890219	1.594277	1.501817
8	1	0	1.003760	0.132824	2.581681
9	1	0	0.379527	0.262558	4.972611
10	1	0	-1.882642	1.051055	5.631178
11	1	0	-3.506535	1.716739	3.875507
12	6	0	-0.480625	0.784990	0.465463
13	6	0	0.745775	0.626423	-0.002063
14	6	0	1.986695	0.264231	-0.228791
15	24	0	2.512208	-1.853904	-0.302091
16	6	0	1.255590	-2.009251	-1.715144
17	8	0	0.476395	-2.053434	-2.568279
18	6	0	3.861105	-1.377419	-1.558545
19	8	0	4.689408	-1.125703	-2.321565
20	6	0	3.111955	-3.606764	-0.388902
21	8	0	3.498322	-4.703009	-0.445886
22	6	0	3.633785	-1.327437	1.134412
23	8	0	4.278179	-0.939205	2.011122
24	6	0	1.218322	-2.426956	0.956465
25	8	0	0.456352	-2.851381	1.719208
26	8	0	3.019312	1.115458	-0.447747
27	6	0	2.742117	2.526178	-0.312077
28	1	0	3.602805	3.017432	-0.771821
29	1	0	1.849573	2.762503	-0.906728
30	6	0	2.580194	2.943046	1.129539
31	1	0	3.447082	2.635738	1.720080
32	1	0	2.494042	4.030221	1.197738
33	1	0	1.684682	2.508661	1.582910
34	6	0	-3.831283	0.046098	-0.953265
35	6	0	-2.508879	-0.190300	-0.585783
36	6	0	-2.097690	-1.479849	-0.239874
37	6	0	-2.995005	-2.523847	-0.290275
38	6	0	-4.323101	-2.296001	-0.679736

39	6	0	-4.739030	-1.001277	-1.008939
40	1	0	-4.166902	1.057708	-1.158801
41	1	0	-1.068083	-1.653493	0.045933
42	1	0	-2.688670	-3.532158	-0.035968
43	1	0	-5.766591	-0.796664	-1.280454
44	7	0	-1.573518	0.888885	-0.529612
45	6	0	-1.643714	1.865643	-1.402433
46	1	0	-2.277980	1.668323	-2.264428
47	6	0	-0.991983	3.148370	-1.344246
48	6	0	-0.803406	3.828483	-2.560651
49	6	0	-0.624124	3.782305	-0.141900
50	6	0	-0.213744	5.083245	-2.580838
51	1	0	-1.110465	3.354539	-3.488137
52	6	0	-0.071296	5.049360	-0.169379
53	1	0	-0.796762	3.291067	0.809471
54	6	0	0.151745	5.696155	-1.386231
55	1	0	-0.053079	5.589222	-3.526262
56	1	0	0.191926	5.539177	0.761995
57	1	0	0.598066	6.685091	-1.399045
58	8	0	-5.125147	-3.379581	-0.693265
59	6	0	-6.479975	-3.200263	-1.088670
60	1	0	-6.935900	-4.186835	-1.048592
61	1	0	-7.006238	-2.528710	-0.403552
62	1	0	-6.546008	-2.809409	-2.108511

Rotational constants (GHZ): 0.0960863 0.0830211 0.0630918

2b+1a TS 3

Zero-point correction= 0.457021 (Hartree/Particle)
Thermal correction to Energy= 0.494288
Thermal correction to Enthalpy= 0.495232
Thermal correction to Gibbs Free Energy= 0.385285
Sum of electronic and zero-point Energies= -1824.523644
Sum of electronic and thermal Energies= -1824.486377
Sum of electronic and thermal Enthalpies= -1824.485433
Sum of electronic and thermal Free Energies= -1824.595380

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.448587	-2.498779	-1.360935
2	6	0	1.405102	-1.987655	-0.578305
3	6	0	0.718369	-2.847424	0.288313
4	6	0	1.074960	-4.186161	0.378671
5	6	0	2.111065	-4.686035	-0.406036

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6	6	0	2.793673	-3.840595	-1.278398
7	1	0	2.978339	-1.836558	-2.039871
8	1	0	-0.084918	-2.454413	0.905656
9	1	0	0.544032	-4.840847	1.061874
10	1	0	2.386641	-5.733534	-0.338816
11	1	0	3.597462	-4.229431	-1.894948
12	6	0	1.024234	-0.573810	-0.665800
13	6	0	-0.245182	-0.004609	-0.478717
14	6	0	-1.547280	-0.568198	-0.447779
15	24	0	-3.037004	-0.134321	0.968984
16	6	0	-4.162382	-0.066410	-0.563944
17	8	0	-4.769603	-0.021716	-1.543090
18	6	0	-3.268120	-2.023095	1.101388
19	8	0	-3.408182	-3.163557	1.190898
20	6	0	-4.398314	0.059464	2.250579
21	8	0	-5.239751	0.167836	3.039413
22	6	0	-1.636644	-0.166520	2.247928
23	8	0	-0.740291	-0.180451	2.976986
24	6	0	-2.951445	1.765850	0.953893
25	8	0	-3.004695	2.917312	1.031935
26	8	0	-1.824714	-1.609660	-1.237734
27	6	0	-1.179121	-1.870009	-2.523294
28	1	0	-1.821915	-1.380808	-3.263762
29	1	0	-0.195284	-1.404550	-2.568099
30	6	0	-1.125031	-3.356009	-2.736025
31	1	0	-2.121921	-3.796738	-2.669890
32	1	0	-0.726062	-3.570333	-3.729948
33	1	0	-0.482671	-3.839993	-1.998106
34	6	0	3.459366	-0.134453	0.951885
35	6	0	3.160560	0.471726	-0.280336
36	6	0	4.165646	1.182061	-0.952706
37	6	0	5.448018	1.246314	-0.426335
38	6	0	5.742134	0.623802	0.785232
39	6	0	4.741511	-0.059725	1.474771
40	1	0	2.671747	-0.648604	1.496318
41	1	0	3.921404	1.666954	-1.892669
42	1	0	6.222341	1.787058	-0.960688
43	1	0	4.962760	-0.529842	2.427821
44	7	0	1.871994	0.465415	-0.822772
45	6	0	0.128293	1.368189	-0.142940
46	1	0	0.683249	1.544252	0.776971
47	6	0	-0.422667	2.526226	-0.785881
48	6	0	-0.173323	3.809624	-0.265120
49	6	0	-1.225488	2.403048	-1.936831
50	6	0	-0.729667	4.929057	-0.859941
51	1	0	0.446976	3.907455	0.621256
52	6	0	-1.790489	3.523522	-2.520465
53	1	0	-1.395391	1.418914	-2.363666

54	6	0	-1.543529	4.787240	-1.983801
55	1	0	-0.539966	5.914551	-0.448405
56	1	0	-2.415803	3.421226	-3.400830
57	1	0	-1.981401	5.665515	-2.447131
58	8	0	7.062837	0.699193	1.328332
59	6	0	7.352854	2.051365	1.692230
60	1	0	8.250909	2.079575	2.273264
61	1	0	7.481915	2.639005	0.807402
62	1	0	6.542742	2.447279	2.268313

Rotational constants (GHZ): 0.1223161 0.0689139 0.0561643

2b+1a Int 3

Zero-point correction= 0.457571 (Hartree/Particle)
Thermal correction to Energy= 0.495476
Thermal correction to Enthalpy= 0.496420
Thermal correction to Gibbs Free Energy= 0.385006
Sum of electronic and zero-point Energies= -1824.553432
Sum of electronic and thermal Energies= -1824.515527
Sum of electronic and thermal Enthalpies= -1824.514583
Sum of electronic and thermal Free Energies= -1824.625997

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.241258	-1.811220	-0.277619
2	6	0	-1.365456	-0.858073	-0.809030
3	6	0	-0.755656	-1.104362	-2.043472
4	6	0	-1.042065	-2.266925	-2.748936
5	6	0	-1.917994	-3.206754	-2.215468
6	6	0	-2.506757	-2.982155	-0.973128
7	1	0	-2.717334	-1.627958	0.681171
8	1	0	-0.080985	-0.364708	-2.463704
9	1	0	-0.578089	-2.439873	-3.714626
10	1	0	-2.135754	-4.118533	-2.762316
11	1	0	-3.177951	-3.721030	-0.547860
12	6	0	-1.128758	0.435211	-0.118716
13	6	0	0.292760	0.911809	-0.000515
14	6	0	1.191454	0.119476	0.883276
15	24	0	2.615116	-1.257258	0.293721
16	6	0	4.040681	-0.104653	0.810670
17	8	0	4.939801	0.514935	1.177876
18	6	0	2.668268	-1.916824	2.077087
19	8	0	2.719765	-2.328374	3.151945
20	6	0	3.916208	-2.502184	-0.265657

21	8	0	4.716258	-3.263074	-0.608489
22	6	0	1.297390	-2.606654	-0.045186
23	8	0	0.594383	-3.507640	-0.180859
24	6	0	2.563542	-0.553885	-1.481136
25	8	0	2.576898	-0.149266	-2.560537
26	8	0	1.003854	0.254698	2.172729
27	6	0	0.062519	1.208451	2.789880
28	1	0	0.689097	1.793164	3.466729
29	1	0	-0.354176	1.859940	2.020305
30	6	0	-0.989742	0.427376	3.523685
31	1	0	-0.544807	-0.237360	4.266415
32	1	0	-1.658620	1.117262	4.042899
33	1	0	-1.589665	-0.170808	2.834155
34	6	0	-3.969220	0.759382	-1.100190
35	6	0	-3.406606	0.995618	0.164160
36	6	0	-4.261538	1.120168	1.259623
37	6	0	-5.635973	0.948933	1.125564
38	6	0	-6.180557	0.698594	-0.135072
39	6	0	-5.336571	0.623800	-1.249063
40	1	0	-3.323103	0.694196	-1.970214
41	1	0	-3.837337	1.335916	2.235454
42	1	0	-6.267989	1.028871	2.001526
43	1	0	-5.775900	0.455057	-2.226442
44	7	0	-2.030895	1.216067	0.357267
45	6	0	0.651753	1.976028	-0.748536
46	1	0	-0.109690	2.359366	-1.427557
47	6	0	1.927439	2.677816	-0.788419
48	6	0	2.306091	3.322915	-1.977616
49	6	0	2.781934	2.770342	0.317922
50	6	0	3.514209	3.997317	-2.068937
51	1	0	1.645200	3.269126	-2.838340
52	6	0	3.987686	3.454947	0.228945
53	1	0	2.488487	2.333709	1.267642
54	6	0	4.361659	4.063407	-0.964508
55	1	0	3.795861	4.477211	-3.000773
56	1	0	4.634720	3.516466	1.097591
57	1	0	5.303128	4.598952	-1.031190
58	8	0	-7.507341	0.528789	-0.382244
59	6	0	-8.391003	0.607166	0.723678
60	1	0	-9.389815	0.437791	0.326293
61	1	0	-8.164571	-0.159873	1.472042
62	1	0	-8.352789	1.593890	1.197543

Rotational constants (GHZ): 0.1442533 0.0618098 0.0552551

2o (G=NO2)

Zero-point correction= 0.204272 (Hartree/Particle)
Thermal correction to Energy= 0.217876
Thermal correction to Enthalpy= 0.218820
Thermal correction to Gibbs Free Energy= 0.161724
Sum of electronic and zero-point Energies= -761.165160
Sum of electronic and thermal Energies= -761.151556
Sum of electronic and thermal Enthalpies= -761.150612
Sum of electronic and thermal Free Energies= -761.207708

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.174511	-0.881095	0.442323
2	6	0	-0.609632	0.353009	0.071177
3	6	0	-1.458084	1.409494	-0.302671
4	6	0	-2.826298	1.231811	-0.346282
5	6	0	-3.357403	-0.005803	0.013393
6	6	0	-2.544086	-1.062579	0.413305
7	1	0	-0.529454	-1.685213	0.779960
8	1	0	-1.016615	2.364146	-0.566223
9	1	0	-3.490904	2.033359	-0.642879
10	1	0	-2.993702	-2.004511	0.701434
11	7	0	0.756405	0.598380	0.124542
12	6	0	1.582326	-0.316889	-0.231487
13	1	0	1.233338	-1.268293	-0.662461
14	6	0	3.024047	-0.167388	-0.118160
15	6	0	3.849340	-1.223358	-0.525810
16	6	0	3.607101	1.000948	0.395810
17	6	0	5.230133	-1.119708	-0.418290
18	1	0	3.396978	-2.126873	-0.925745
19	6	0	4.984333	1.102468	0.498661
20	1	0	2.961218	1.815744	0.705829
21	6	0	5.798371	0.042701	0.094051
22	1	0	5.862742	-1.942494	-0.733703
23	1	0	5.432312	2.007588	0.895560
24	1	0	6.877042	0.127260	0.177249
25	7	0	-4.803291	-0.195057	-0.014556
26	8	0	-5.250353	-1.291279	0.317502
27	8	0	-5.504469	0.750574	-0.369382

Rotational constants (GHZ): 2.1959095 0.1532349 0.1454849

2o + 1a TS 1

Zero-point correction= 0.424900 (Hartree/Particle)
Thermal correction to Energy= 0.463101
Thermal correction to Enthalpy= 0.464045

Thermal correction to Gibbs Free Energy= 0.350764
Sum of electronic and zero-point Energies= -1914.551672
Sum of electronic and thermal Energies= -1914.513471
Sum of electronic and thermal Enthalpies= -1914.512527
Sum of electronic and thermal Free Energies= -1914.625808

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.078755	-2.490040	1.957583
2	6	0	-1.493249	-1.217633	1.936363
3	6	0	-1.208175	-0.585658	3.161866
4	6	0	-1.508218	-1.211814	4.361464
5	6	0	-2.090926	-2.477514	4.370235
6	6	0	-2.371208	-3.112333	3.164734
7	1	0	-2.295898	-2.992447	1.020362
8	1	0	-0.747628	0.397947	3.152053
9	1	0	-1.278239	-0.711313	5.296482
10	1	0	-2.319477	-2.966800	5.311203
11	1	0	-2.821811	-4.099553	3.161239
12	6	0	-1.188556	-0.474892	0.743103
13	6	0	-0.870502	0.657628	0.297361
14	6	0	-0.382787	1.854565	-0.115763
15	24	0	1.645561	2.349071	0.192175
16	6	0	2.009421	1.760110	-1.578001
17	8	0	2.208150	1.411333	-2.661065
18	6	0	1.299725	4.093912	-0.483077
19	8	0	1.123996	5.160495	-0.884866
20	6	0	3.417955	2.854253	0.521361
21	8	0	4.513331	3.175073	0.725105
22	6	0	1.020159	2.888071	1.905426
23	8	0	0.581525	3.190085	2.929438
24	6	0	2.036820	0.622459	0.894875
25	8	0	2.309428	-0.401982	1.351832
26	8	0	-1.192610	2.784254	-0.625012
27	6	0	-2.623217	2.510965	-0.700776
28	1	0	-2.992109	3.235147	-1.428629
29	1	0	-2.758816	1.503164	-1.106954
30	6	0	-3.286490	2.676921	0.642291
31	1	0	-3.103568	3.674596	1.047061
32	1	0	-4.366054	2.546946	0.536694
33	1	0	-2.929628	1.937374	1.363636
34	6	0	0.736615	-3.146611	0.088144
35	6	0	0.243666	-2.210455	-0.827346
36	6	0	1.092561	-1.644453	-1.785182
37	6	0	2.423904	-2.019618	-1.839922

38	6	0	2.888514	-2.964226	-0.932661
39	6	0	2.061976	-3.535661	0.028851
40	1	0	0.075515	-3.567621	0.836009
41	1	0	0.708402	-0.889948	-2.463342
42	1	0	3.102195	-1.584242	-2.562687
43	1	0	2.466485	-4.264772	0.718549
44	7	0	-1.092920	-1.774866	-0.712264
45	6	0	-1.830125	-1.685683	-1.768807
46	1	0	-1.408307	-2.012007	-2.726082
47	6	0	-3.174788	-1.155329	-1.817868
48	6	0	-3.688287	-0.814328	-3.080209
49	6	0	-3.971729	-0.952281	-0.678137
50	6	0	-4.948024	-0.245355	-3.198421
51	1	0	-3.080182	-0.985320	-3.963822
52	6	0	-5.236395	-0.402644	-0.804905
53	1	0	-3.607418	-1.241672	0.300478
54	6	0	-5.722285	-0.037007	-2.060658
55	1	0	-5.329298	0.028439	-4.176023
56	1	0	-5.849801	-0.255601	0.077685
57	1	0	-6.711541	0.399261	-2.151396
58	7	0	4.298796	-3.363263	-0.984177
59	8	0	4.688098	-4.201943	-0.177471
60	8	0	5.013951	-2.839125	-1.831859

Rotational constants (GHZ): 0.0942605 0.0795202 0.0638251

2o + 1a Int 1

Zero-point correction= 0.426909 (Hartree/Particle)
Thermal correction to Energy= 0.465137
Thermal correction to Enthalpy= 0.466081
Thermal correction to Gibbs Free Energy= 0.352121
Sum of electronic and zero-point Energies= -1914.562387
Sum of electronic and thermal Energies= -1914.524159
Sum of electronic and thermal Enthalpies= -1914.523215
Sum of electronic and thermal Free Energies= -1914.637175

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.484070	1.973150	2.310402
2	6	0	-0.415560	1.161155	1.901763
3	6	0	0.365494	0.537756	2.889012
4	6	0	0.078158	0.712147	4.233022
5	6	0	-0.993747	1.512639	4.627382
6	6	0	-1.769742	2.142552	3.660765

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7	1	0	-2.093753	2.488592	1.572841
8	1	0	1.196401	-0.090922	2.578912
9	1	0	0.689758	0.216931	4.980512
10	1	0	-1.218571	1.645286	5.680469
11	1	0	-2.601505	2.773891	3.956270
12	6	0	-0.068982	0.973845	0.491442
13	6	0	1.028147	0.433385	-0.008888
14	6	0	2.078410	-0.310397	-0.269312
15	24	0	1.878647	-2.482453	-0.308506
16	6	0	0.595824	-2.259647	-1.688574
17	8	0	-0.183806	-2.075388	-2.522602
18	6	0	3.271128	-2.490600	-1.609776
19	8	0	4.112611	-2.533376	-2.397331
20	6	0	1.873351	-4.338127	-0.359450
21	8	0	1.879437	-5.500450	-0.392433
22	6	0	3.156305	-2.334171	1.088478
23	8	0	3.916058	-2.169056	1.942238
24	6	0	0.513886	-2.572415	1.000003
25	8	0	-0.317830	-2.697622	1.796871
26	8	0	3.321932	0.156293	-0.529235
27	6	0	3.530310	1.579729	-0.395039
28	1	0	4.494128	1.758152	-0.876663
29	1	0	2.753922	2.099785	-0.972416
30	6	0	3.549287	2.022152	1.047667
31	1	0	4.276117	1.440580	1.620761
32	1	0	3.833312	3.075314	1.112448
33	1	0	2.570817	1.910451	1.522877
34	6	0	-3.508303	1.316219	-0.895920
35	6	0	-2.321454	0.674766	-0.534896
36	6	0	-2.308525	-0.678758	-0.201904
37	6	0	-3.483563	-1.406425	-0.254821
38	6	0	-4.653329	-0.760865	-0.636401
39	6	0	-4.684953	0.590430	-0.956194
40	1	0	-3.518001	2.382226	-1.093183
41	1	0	-1.378515	-1.155518	0.076873
42	1	0	-3.499911	-2.460761	-0.010830
43	1	0	-5.622273	1.059386	-1.225931
44	7	0	-1.100501	1.420798	-0.480366
45	6	0	-0.884990	2.374649	-1.357820
46	1	0	-1.564361	2.382642	-2.208358
47	6	0	0.134648	3.383696	-1.335307
48	6	0	0.440754	3.996162	-2.565543
49	6	0	0.761980	3.849356	-0.161577
50	6	0	1.386039	5.006956	-2.632054
51	1	0	-0.061804	3.657576	-3.466368
52	6	0	1.672665	4.886038	-0.233596
53	1	0	0.513164	3.417693	0.801459
54	6	0	2.000904	5.454506	-1.466470

55	1	0	1.631198	5.456819	-3.587454
56	1	0	2.135879	5.255889	0.674544
57	1	0	2.728813	6.257674	-1.512924
58	7	0	-5.907349	-1.530648	-0.688126
59	8	0	-6.926422	-0.936785	-1.020275
60	8	0	-5.859209	-2.719013	-0.397056

Rotational constants (GHZ): 0.0908800 0.0787216 0.0587289

2o + 1a TS 2

Zero-point correction= 0.425863 (Hartree/Particle)
Thermal correction to Energy= 0.463483
Thermal correction to Enthalpy= 0.464427
Thermal correction to Gibbs Free Energy= 0.353462
Sum of electronic and zero-point Energies= -1914.544127
Sum of electronic and thermal Energies= -1914.506507
Sum of electronic and thermal Enthalpies= -1914.505563
Sum of electronic and thermal Free Energies= -1914.616528

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.121551	0.436806	2.884447
2	6	0	-0.013633	0.459264	2.021555
3	6	0	1.270540	0.306325	2.569889
4	6	0	1.436582	0.071918	3.925585
5	6	0	0.326697	0.010736	4.764887
6	6	0	-0.949983	0.206028	4.240869
7	1	0	-2.119959	0.595904	2.489964
8	1	0	2.133825	0.374248	1.916517
9	1	0	2.435334	-0.053224	4.330924
10	1	0	0.455977	-0.168572	5.827076
11	1	0	-1.815044	0.181891	4.894848
12	6	0	-0.168615	0.630109	0.585585
13	6	0	0.812678	0.633054	-0.364691
14	6	0	2.027744	0.194090	-0.720601
15	24	0	2.317590	-1.956450	-0.557197
16	6	0	0.821616	-2.111979	-1.726353
17	8	0	-0.115841	-2.169303	-2.395673
18	6	0	3.523502	-1.764238	-2.025623
19	8	0	4.258935	-1.699525	-2.909137
20	6	0	2.724877	-3.773525	-0.605813
21	8	0	2.988219	-4.901892	-0.647870
22	6	0	3.695021	-1.507617	0.676181

23	8	0	4.506461	-1.197582	1.435449
24	6	0	1.142671	-2.372791	0.880197
25	8	0	0.437167	-2.753496	1.713648
26	8	0	2.984724	0.891084	-1.321262
27	6	0	2.762294	2.319920	-1.506802
28	1	0	3.526553	2.617090	-2.226329
29	1	0	1.778555	2.435018	-1.971618
30	6	0	2.878426	3.082076	-0.213861
31	1	0	3.880084	2.986127	0.210687
32	1	0	2.679147	4.142847	-0.389093
33	1	0	2.153832	2.733068	0.526413
34	6	0	-2.591311	-1.030464	0.307243
35	6	0	-2.538671	0.297558	-0.140381
36	6	0	-3.648523	0.878303	-0.769168
37	6	0	-4.798593	0.137468	-0.961760
38	6	0	-4.836647	-1.176467	-0.505552
39	6	0	-3.744860	-1.766398	0.128675
40	1	0	-1.719037	-1.481288	0.768208
41	1	0	-3.607791	1.916300	-1.081687
42	1	0	-5.669062	0.565283	-1.442209
43	1	0	-3.807579	-2.796943	0.453549
44	7	0	-1.381108	1.065177	0.001233
45	6	0	-0.957843	1.922428	-1.014673
46	1	0	-1.299559	1.680212	-2.022455
47	6	0	-0.550884	3.280526	-0.759316
48	6	0	-0.241212	4.099447	-1.860444
49	6	0	-0.495690	3.833557	0.534565
50	6	0	0.130806	5.421918	-1.674999
51	1	0	-0.296499	3.682248	-2.862130
52	6	0	-0.129312	5.155493	0.710910
53	1	0	-0.750012	3.220300	1.393809
54	6	0	0.193351	5.953266	-0.389292
55	1	0	0.367582	6.041212	-2.533263
56	1	0	-0.096443	5.574706	1.711035
57	1	0	0.481938	6.988689	-0.241795
58	7	0	-6.052825	-1.960715	-0.699922
59	8	0	-6.055912	-3.126373	-0.311934
60	8	0	-7.010418	-1.414464	-1.242780

Rotational constants (GHZ): 0.0956201 0.0751958 0.0585668

2o + 1a INT 2

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Zero-point correction= 0.428839 (Hartree/Particle)
Thermal correction to Energy= 0.466558
Thermal correction to Enthalpy= 0.467503
Thermal correction to Gibbs Free Energy= 0.355171
Sum of electronic and zero-point Energies= -1914.594848
Sum of electronic and thermal Energies= -1914.557129
Sum of electronic and thermal Enthalpies= -1914.556184
Sum of electronic and thermal Free Energies= -1914.668516

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.902572	3.128476	1.182970
2	6	0	1.078452	2.610716	0.176685
3	6	0	0.541166	3.468233	-0.789670
4	6	0	0.842424	4.824242	-0.759798
5	6	0	1.660481	5.334772	0.243279
6	6	0	2.184549	4.486818	1.216798
7	1	0	2.304109	2.465372	1.944090
8	1	0	-0.107656	3.064233	-1.561581
9	1	0	0.432742	5.482944	-1.517724
10	1	0	1.889763	6.394701	0.269335
11	1	0	2.813712	4.885835	2.005202
12	6	0	0.709532	1.201033	0.159939
13	6	0	-0.480289	0.479827	0.086306
14	6	0	-1.876456	0.687531	0.074865
15	24	0	-3.307378	-0.538030	-0.846034
16	6	0	-3.182724	-1.735873	0.636597
17	8	0	-3.155090	-2.444927	1.544689
18	6	0	-4.665725	0.417535	0.096968
19	8	0	-5.513806	0.968008	0.648864
20	6	0	-4.661661	-1.548251	-1.665940
21	8	0	-5.494835	-2.169528	-2.177220
22	6	0	-3.308395	0.813136	-2.186854
23	8	0	-3.277773	1.662123	-2.966831
24	6	0	-2.097641	-1.571561	-1.868142
25	8	0	-1.451962	-2.248856	-2.550825
26	8	0	-2.394719	1.775913	0.638182
27	6	0	-1.705133	2.633362	1.593665
28	1	0	-0.908296	2.058022	2.075622
29	1	0	-1.251126	3.460336	1.042587
30	6	0	-2.740062	3.112500	2.573030
31	1	0	-3.178546	2.278098	3.123833
32	1	0	-2.280947	3.794094	3.291832

33	1	0	-3.542864	3.647804	2.062499
34	6	0	3.813071	0.829518	-0.307662
35	6	0	2.847832	-0.184717	-0.164877
36	6	0	3.237732	-1.532539	-0.288557
37	6	0	4.555590	-1.858918	-0.527369
38	6	0	5.497914	-0.840544	-0.653791
39	6	0	5.129765	0.499062	-0.553965
40	1	0	3.530473	1.870697	-0.241197
41	1	0	2.500157	-2.319991	-0.192333
42	1	0	4.866866	-2.891832	-0.617836
43	1	0	5.881687	1.268245	-0.674398
44	7	0	1.520740	0.088172	0.099924
45	6	0	0.325941	-0.804295	-0.055421
46	1	0	0.331472	-1.216530	-1.068181
47	6	0	0.166526	-1.876124	0.980405
48	6	0	0.042052	-3.211341	0.599395
49	6	0	0.148635	-1.546694	2.337692
50	6	0	-0.099659	-4.207208	1.561269
51	1	0	0.058033	-3.470686	-0.456170
52	6	0	0.010317	-2.539604	3.297734
53	1	0	0.244416	-0.506059	2.639747
54	6	0	-0.115304	-3.872285	2.910452
55	1	0	-0.197336	-5.243608	1.255124
56	1	0	-0.002845	-2.276298	4.350207
57	1	0	-0.226399	-4.647316	3.661583
58	7	0	6.887915	-1.180436	-0.902167
59	8	0	7.697622	-0.261114	-1.023965
60	8	0	7.189322	-2.371660	-0.976360

Rotational constants (GHZ): 0.1195860 0.0610790 0.0499738

2o + 1a TS 3

Zero-point correction= 0.426099 (Hartree/Particle)
Thermal correction to Energy= 0.463678
Thermal correction to Enthalpy= 0.464622
Thermal correction to Gibbs Free Energy= 0.352892
Sum of electronic and zero-point Energies= -1914.564854
Sum of electronic and thermal Energies= -1914.527275
Sum of electronic and thermal Enthalpies= -1914.526331
Sum of electronic and thermal Free Energies= -1914.638061

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

ISSN-e 2594-0317

1	6	0	2.319022	-2.370481	-1.499511
2	6	0	1.279358	-1.908203	-0.682187
3	6	0	0.635277	-2.808088	0.176416
4	6	0	1.029963	-4.138281	0.224887
5	6	0	2.061900	-4.589469	-0.594069
6	6	0	2.702123	-3.703873	-1.458692
7	1	0	2.815672	-1.677053	-2.172283
8	1	0	-0.164731	-2.453052	0.820447
9	1	0	0.532025	-4.824318	0.902142
10	1	0	2.367209	-5.630290	-0.559549
11	1	0	3.502537	-4.054743	-2.101835
12	6	0	0.858433	-0.503699	-0.725360
13	6	0	-0.421585	0.025270	-0.496996
14	6	0	-1.706919	-0.574754	-0.453033
15	24	0	-3.176627	-0.217905	1.005516
16	6	0	-4.336590	-0.142819	-0.501071
17	8	0	-4.966005	-0.090452	-1.465714
18	6	0	-3.353444	-2.115077	1.094319
19	8	0	-3.460511	-3.260864	1.157509
20	6	0	-4.514428	-0.094040	2.320106
21	8	0	-5.341097	-0.028794	3.129044
22	6	0	-1.748356	-0.243330	2.253369
23	8	0	-0.836273	-0.250688	2.962747
24	6	0	-3.143031	1.683688	1.037325
25	8	0	-3.225805	2.830919	1.145958
26	8	0	-1.973138	-1.603392	-1.263387
27	6	0	-1.348899	-1.813493	-2.568538
28	1	0	-2.020729	-1.323891	-3.282492
29	1	0	-0.379271	-1.319996	-2.622157
30	6	0	-1.259142	-3.291633	-2.820376
31	1	0	-2.242021	-3.761315	-2.744530
32	1	0	-0.876268	-3.469874	-3.827667
33	1	0	-0.587943	-3.775971	-2.108828
34	6	0	3.315435	-0.037727	0.851291
35	6	0	2.973487	0.590610	-0.358408
36	6	0	3.944021	1.345116	-1.033419
37	6	0	5.235349	1.431653	-0.532761
38	6	0	5.572601	0.787381	0.655975
39	6	0	4.606175	0.059358	1.348739
40	1	0	2.554120	-0.586960	1.398873
41	1	0	3.666269	1.846444	-1.955282
42	1	0	5.982872	2.006840	-1.069307
43	1	0	4.860831	-0.428169	2.284545
44	7	0	1.674047	0.562206	-0.873507
45	6	0	-0.078281	1.399046	-0.134105
46	1	0	0.491618	1.567318	0.778096
47	6	0	-0.674361	2.557119	-0.735383
48	6	0	-0.448653	3.833486	-0.187281

49	6	0	-1.498446	2.440616	-1.871909
50	6	0	-1.048017	4.951628	-0.741342
51	1	0	0.187941	3.926230	0.688020
52	6	0	-2.106247	3.559279	-2.414578
53	1	0	-1.650838	1.463151	-2.320144
54	6	0	-1.882040	4.815516	-1.851037
55	1	0	-0.876209	5.931383	-0.308781
56	1	0	-2.747600	3.461783	-3.283880
57	1	0	-2.353590	5.692655	-2.282360
58	7	0	6.939493	0.888441	1.187287
59	8	0	7.196159	0.321752	2.212668
60	8	0	7.743438	1.533546	0.574163

Rotational constants (GHZ): 0.1221349 0.0606465 0.0509974

2o + 1a INT 3

Zero-point correction= 0.427911 (Hartree/Particle)
Thermal correction to Energy= 0.465654
Thermal correction to Enthalpy= 0.466598
Thermal correction to Gibbs Free Energy= 0.355544
Sum of electronic and zero-point Energies= -1914.597589
Sum of electronic and thermal Energies= -1914.559847
Sum of electronic and thermal Enthalpies= -1914.558902
Sum of electronic and thermal Free Energies= -1914.669956

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.102963	1.838337	-0.120514
2	6	0	1.233482	0.892255	-0.674170
3	6	0	0.668172	1.132141	-1.931193
4	6	0	0.986414	2.287585	-2.632856
5	6	0	1.848671	3.225658	-2.073944
6	6	0	2.398191	3.003932	-0.813661
7	1	0	2.542423	1.660172	0.856539
8	1	0	0.009074	0.391255	-2.371676
9	1	0	0.559304	2.456000	-3.615893
10	1	0	2.089333	4.133369	-2.617583
11	1	0	3.060520	3.740441	-0.371327
12	6	0	0.967183	-0.402129	-0.003962
13	6	0	-0.447881	-0.893673	0.065781
14	6	0	-1.400128	-0.081604	0.876885
15	24	0	-2.800350	1.258245	0.175084
16	6	0	-4.260251	0.092568	0.556984
17	8	0	-5.189127	-0.532319	0.826438
18	6	0	-3.024546	1.910325	1.950235

19	8	0	-3.187092	2.313199	3.016715
20	6	0	-4.056648	2.497398	-0.494610
21	8	0	-4.824371	3.255212	-0.908720
22	6	0	-1.466164	2.616362	-0.044809
23	8	0	-0.747106	3.512012	-0.114680
24	6	0	-2.618224	0.547389	-1.585556
25	8	0	-2.566731	0.131204	-2.659665
26	8	0	-1.268459	-0.173429	2.177700
27	6	0	-0.342692	-1.091182	2.868972
28	1	0	-0.989528	-1.653634	3.545341
29	1	0	0.104855	-1.773163	2.144463
30	6	0	0.674799	-0.270579	3.608540
31	1	0	0.196670	0.414117	4.311096
32	1	0	1.334251	-0.932330	4.174160
33	1	0	1.289160	0.313189	2.919126
34	6	0	3.819965	-0.874995	-0.943391
35	6	0	3.233924	-0.959835	0.331494
36	6	0	4.052996	-0.940647	1.471518
37	6	0	5.419929	-0.786197	1.347236
38	6	0	5.975518	-0.684008	0.073693
39	6	0	5.187796	-0.738936	-1.074046
40	1	0	3.187180	-0.915453	-1.823546
41	1	0	3.596644	-1.034486	2.450628
42	1	0	6.065184	-0.750473	2.215848
43	1	0	5.656040	-0.666675	-2.047577
44	7	0	1.867390	-1.175332	0.489391
45	6	0	-0.751019	-2.001403	-0.644237
46	1	0	0.049825	-2.401379	-1.266139
47	6	0	-2.007508	-2.733345	-0.706079
48	6	0	-2.299812	-3.476625	-1.862256
49	6	0	-2.923060	-2.767413	0.354751
50	6	0	-3.482871	-4.191722	-1.969042
51	1	0	-1.589285	-3.473271	-2.684317
52	6	0	-4.102145	-3.493949	0.251226
53	1	0	-2.702048	-2.247496	1.281754
54	6	0	-4.389998	-4.201307	-0.911302
55	1	0	-3.696810	-4.749695	-2.874738
56	1	0	-4.796601	-3.510608	1.084498
57	1	0	-5.311126	-4.769572	-0.989010
58	7	0	7.416734	-0.522464	-0.061710
59	8	0	7.884525	-0.420194	-1.194466
60	8	0	8.096124	-0.494437	0.963230

Rotational constants (GHZ): 0.1427344 0.0555334 0.0498814

2f

Zero-point correction= 0.235090 (Hartree/Particle)
Thermal correction to Energy= 0.248483
Thermal correction to Enthalpy= 0.249427
Thermal correction to Gibbs Free Energy= 0.194118
Sum of electronic and zero-point Energies= -671.123483
Sum of electronic and thermal Energies= -671.110090
Sum of electronic and thermal Enthalpies= -671.109146
Sum of electronic and thermal Free Energies= -671.164455

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.251736	-1.001906	-0.502705
2	6	0	2.758832	0.231623	-0.049562
3	6	0	3.668828	1.194082	0.409819
4	6	0	5.027187	0.913014	0.457463
5	6	0	5.508166	-0.319506	0.019108
6	6	0	4.614521	-1.269833	-0.468176
7	1	0	2.561659	-1.734369	-0.910483
8	1	0	3.286097	2.154481	0.740528
9	1	0	5.717520	1.663339	0.830135
10	1	0	6.571994	-0.531480	0.042477
11	1	0	4.982492	-2.223594	-0.833893
12	7	0	1.401235	0.569397	-0.087939
13	6	0	0.527208	-0.335033	0.169974
14	1	0	0.825803	-1.346975	0.488860
15	6	0	-0.903368	-0.109874	0.084169
16	6	0	-1.782675	-1.147704	0.407257
17	6	0	-1.446716	1.122966	-0.322403
18	6	0	-3.160006	-0.985429	0.332251
19	1	0	-1.377091	-2.105344	0.723467
20	6	0	-2.809927	1.300676	-0.400263
21	1	0	-0.771301	1.933969	-0.574483
22	6	0	-3.679127	0.245953	-0.075498
23	1	0	-3.813431	-1.809879	0.587816
24	1	0	-3.238371	2.246620	-0.713837
25	8	0	-4.998702	0.518935	-0.189806
26	6	0	-5.917765	-0.517414	0.128098
27	1	0	-6.909284	-0.100116	-0.033149
28	1	0	-5.777473	-1.385395	-0.523554
29	1	0	-5.819011	-0.828218	1.172945

Rotational constants (GHZ): 2.5424564 0.1748008 0.1661907

2f +1a INT 1

Zero-point correction= 0.458054 (Hartree/Particle)
Thermal correction to Energy= 0.496087
Thermal correction to Enthalpy= 0.497031
Thermal correction to Gibbs Free Energy= 0.384600
Sum of electronic and zero-point Energies= -1824.531206
Sum of electronic and thermal Energies= -1824.493173
Sum of electronic and thermal Enthalpies= -1824.492229
Sum of electronic and thermal Free Energies= -1824.604660

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.936910	2.789021	1.931322
2	6	0	0.291987	1.563523	1.703966
3	6	0	-0.405599	0.970450	2.769499
4	6	0	-0.462537	1.585807	4.009602
5	6	0	0.174200	2.808659	4.220996
6	6	0	0.873566	3.404248	3.176859
7	1	0	1.496396	3.265602	1.130974
8	1	0	-0.909879	0.021821	2.602341
9	1	0	-1.011347	1.112783	4.817711
10	1	0	0.125750	3.290450	5.192045
11	1	0	1.376916	4.353635	3.330391
12	6	0	0.348070	0.876902	0.410988
13	6	0	-0.069882	-0.347810	0.138426
14	6	0	-0.723745	-1.483468	0.060556
15	24	0	-2.871344	-1.489883	-0.335650
16	6	0	-2.466225	-0.573240	-1.946508
17	8	0	-2.170048	-0.017028	-2.916057
18	6	0	-2.616079	-3.153119	-1.224105
19	8	0	-2.503972	-4.163766	-1.770449
20	6	0	-4.689739	-1.647173	-0.662445
21	8	0	-5.830076	-1.755756	-0.868699
22	6	0	-2.888326	-2.366236	1.346476
23	8	0	-2.827235	-2.877123	2.380948
24	6	0	-3.237746	0.142491	0.552992
25	8	0	-3.537931	1.127127	1.084188
26	8	0	-0.169689	-2.714831	0.198639
27	6	0	1.218366	-2.764808	0.590887
28	1	0	1.513833	-3.801430	0.413999
29	1	0	1.793737	-2.119688	-0.087172
30	6	0	1.416627	-2.377896	2.036577
31	1	0	0.778071	-2.981226	2.687291
32	1	0	2.455357	-2.544043	2.332686
33	1	0	1.182863	-1.324190	2.211083

34	6	0	0.757245	3.879204	-1.754040
35	6	0	0.120449	2.775082	-1.186401
36	6	0	-1.265289	2.745230	-1.052508
37	6	0	-2.017371	3.815199	-1.515170
38	6	0	-1.393409	4.911311	-2.104845
39	6	0	-0.006726	4.940452	-2.221094
40	1	0	1.840707	3.921956	-1.795990
41	1	0	-1.740551	1.881194	-0.606743
42	1	0	-3.097467	3.786644	-1.419068
43	1	0	-1.985438	5.747021	-2.461915
44	1	0	0.487189	5.801673	-2.657874
45	7	0	0.898458	1.668101	-0.712435
46	6	0	1.989578	1.314471	-1.359190
47	1	0	2.097825	1.757819	-2.347456
48	6	0	3.024341	0.428397	-0.937814
49	6	0	3.862061	-0.092676	-1.942609
50	6	0	3.316010	0.102883	0.408722
51	6	0	4.906405	-0.947472	-1.647754
52	1	0	3.668047	0.169938	-2.978023
53	6	0	4.376897	-0.710721	0.714699
54	1	0	2.721092	0.517606	1.214397
55	6	0	5.169572	-1.265346	-0.308867
56	1	0	5.515675	-1.349231	-2.446985
57	1	0	4.621810	-0.947320	1.743719
58	8	0	6.156702	-2.073383	0.098148
59	6	0	6.984123	-2.681634	-0.893106
60	1	0	7.690333	-3.303085	-0.348427
61	1	0	6.390769	-3.303814	-1.568005
62	1	0	7.526966	-1.925929	-1.466751

Rotational constants (GHZ): 0.1063423 0.0751477 0.0617060

2f +1a TS 2

Zero-point correction= 0.455986 (Hartree/Particle)
Thermal correction to Energy= 0.493656
Thermal correction to Enthalpy= 0.494600
Thermal correction to Gibbs Free Energy= 0.383669
Sum of electronic and zero-point Energies= -1824.505992
Sum of electronic and thermal Energies= -1824.468322
Sum of electronic and thermal Enthalpies= -1824.467378
Sum of electronic and thermal Free Energies= -1824.578309

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.080155	2.319083	2.445099

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2	6	0	-0.134277	1.063182	1.854183
3	6	0	-0.683025	0.035166	2.638388
4	6	0	-1.065585	0.273162	3.948914
5	6	0	-0.884630	1.534611	4.512067
6	6	0	-0.298682	2.550776	3.759180
7	1	0	0.536579	3.115610	1.865825
8	1	0	-0.804706	-0.951045	2.203385
9	1	0	-1.498030	-0.529801	4.537457
10	1	0	-1.181476	1.721089	5.538985
11	1	0	-0.136149	3.528640	4.200302
12	6	0	0.184669	0.809930	0.457277
13	6	0	0.019193	-0.348314	-0.244052
14	6	0	-0.704296	-1.475345	-0.378060
15	24	0	-2.869206	-1.265647	-0.472257
16	6	0	-2.528725	-0.168835	-1.991701
17	8	0	-2.277083	0.519910	-2.882638
18	6	0	-2.868035	-2.841013	-1.544057
19	8	0	-2.922142	-3.790547	-2.195485
20	6	0	-4.718063	-1.249322	-0.674684
21	8	0	-5.871670	-1.252301	-0.806495
22	6	0	-2.879771	-2.310576	1.113242
23	8	0	-2.844542	-2.932123	2.086153
24	6	0	-3.075859	0.321991	0.553494
25	8	0	-3.319804	1.296136	1.128058
26	8	0	-0.223999	-2.684361	-0.666037
27	6	0	1.220368	-2.855668	-0.698577
28	1	0	1.360995	-3.827100	-1.175515
29	1	0	1.627725	-2.082534	-1.355905
30	6	0	1.834361	-2.816363	0.676090
31	1	0	1.416735	-3.598447	1.314398
32	1	0	2.913713	-2.975211	0.602038
33	1	0	1.681182	-1.850615	1.164285
34	6	0	-0.801333	3.383057	-0.569149
35	6	0	0.487850	2.920042	-0.848713
36	6	0	1.335149	3.660828	-1.677987
37	6	0	0.884237	4.850707	-2.236619
38	6	0	-0.394456	5.320803	-1.953626
39	6	0	-1.229498	4.584521	-1.115097
40	1	0	-1.460603	2.800694	0.065879
41	1	0	2.344690	3.307422	-1.867187
42	1	0	1.543856	5.419817	-2.883304
43	1	0	-0.739214	6.255600	-2.382083
44	1	0	-2.231061	4.940297	-0.896567
45	7	0	0.955289	1.698542	-0.326824
46	6	0	1.680443	0.814569	-1.134954
47	1	0	1.544387	0.923100	-2.213326
48	6	0	2.908482	0.217708	-0.682897
49	6	0	3.674183	-0.537949	-1.585087

50	6	0	3.394999	0.373269	0.633044
51	6	0	4.860841	-1.142419	-1.202495
52	1	0	3.325213	-0.654167	-2.607695
53	6	0	4.572872	-0.217213	1.023140
54	1	0	2.834765	0.973022	1.344291
55	6	0	5.313550	-0.991726	0.112761
56	1	0	5.427881	-1.716865	-1.924149
57	1	0	4.955053	-0.095455	2.030480
58	8	0	6.447051	-1.536027	0.597274
59	6	0	7.229158	-2.337023	-0.281516
60	1	0	8.074721	-2.687205	0.305746
61	1	0	6.656923	-3.195056	-0.646646
62	1	0	7.592584	-1.751380	-1.131047

Rotational constants (GHZ): 0.1120090 0.0738574 0.0624346

2f +1a INT 2

Zero-point correction= 0.458683 (Hartree/Particle)
Thermal correction to Energy= 0.495570
Thermal correction to Enthalpy= 0.496514
Thermal correction to Gibbs Free Energy= 0.386996
Sum of electronic and zero-point Energies= -1824.552779
Sum of electronic and thermal Energies= -1824.515892
Sum of electronic and thermal Enthalpies= -1824.514948
Sum of electronic and thermal Free Energies= -1824.624466

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.003837	-0.964434	1.284307
2	6	0	-2.947243	-1.401892	0.475577
3	6	0	-2.940967	-2.717721	-0.002164
4	6	0	-3.982261	-3.579183	0.318347
5	6	0	-5.025789	-3.141027	1.128399
6	6	0	-5.032113	-1.835141	1.614457
7	1	0	-4.007832	0.056036	1.655842
8	1	0	-2.124472	-3.053340	-0.635601
9	1	0	-3.977657	-4.594463	-0.063394
10	1	0	-5.835602	-3.817160	1.381884
11	1	0	-5.842330	-1.495486	2.250761
12	6	0	-1.857609	-0.500804	0.135122
13	6	0	-0.462504	-0.580698	-0.002695
14	6	0	0.602710	-1.462490	0.217993
15	24	0	2.456543	-1.477705	-0.799357
16	6	0	3.030682	-0.044436	0.321242

17	8	0	3.413296	0.788831	1.021059
18	6	0	3.121256	-2.700749	0.504818
19	8	0	3.563769	-3.438702	1.272290
20	6	0	4.107732	-1.591543	-1.672375
21	8	0	5.128900	-1.662999	-2.218719
22	6	0	1.681262	-2.930666	-1.744005
23	8	0	1.169844	-3.815003	-2.282432
24	6	0	1.951253	-0.289950	-2.181656
25	8	0	1.744805	0.404588	-3.085859
26	8	0	0.486292	-2.459539	1.101194
27	6	0	-0.480599	-2.485799	2.186108
28	1	0	-0.829183	-1.465580	2.377829
29	1	0	-1.336725	-3.087307	1.871877
30	6	0	0.217828	-3.086029	3.375347
31	1	0	1.073963	-2.478299	3.675599
32	1	0	-0.471579	-3.150619	4.219687
33	1	0	0.575789	-4.093093	3.151496
34	6	0	-4.159194	1.061204	-1.298618
35	6	0	-2.958636	1.600511	-0.823569
36	6	0	-2.734374	2.979984	-0.908979
37	6	0	-3.705136	3.805809	-1.458446
38	6	0	-4.908282	3.275193	-1.916421
39	6	0	-5.126229	1.903211	-1.833522
40	1	0	-4.327492	-0.008428	-1.271473
41	1	0	-1.803023	3.394685	-0.538455
42	1	0	-3.521459	4.873446	-1.520856
43	1	0	-5.666452	3.924484	-2.340602
44	1	0	-6.052601	1.476158	-2.203702
45	7	0	-1.945510	0.798924	-0.274257
46	6	0	-0.471306	0.836425	-0.565133
47	1	0	-0.343049	0.882818	-1.650600
48	6	0	0.311340	1.903451	0.127591
49	6	0	1.117897	2.779967	-0.589364
50	6	0	0.239665	2.045588	1.519270
51	6	0	1.853151	3.775593	0.050082
52	1	0	1.179259	2.687725	-1.670332
53	6	0	0.952866	3.032225	2.169559
54	1	0	-0.387813	1.368772	2.095067
55	6	0	1.772646	3.901535	1.436601
56	1	0	2.478755	4.437280	-0.535774
57	1	0	0.902806	3.146665	3.246975
58	8	0	2.444976	4.829755	2.163351
59	6	0	3.300114	5.716835	1.458772
60	1	0	2.738214	6.330741	0.746928
61	1	0	3.753942	6.360053	2.209961
62	1	0	4.085082	5.172099	0.924317

Rotational constants (GHZ): 0.0999435 0.0834231 0.0589938

2f +1a INT 3

Zero-point correction= 0.457698 (Hartree/Particle)
Thermal correction to Energy= 0.494807
Thermal correction to Enthalpy= 0.495751
Thermal correction to Gibbs Free Energy= 0.386437
Sum of electronic and zero-point Energies= -1824.555564
Sum of electronic and thermal Energies= -1824.518455
Sum of electronic and thermal Enthalpies= -1824.517510
Sum of electronic and thermal Free Energies= -1824.626824

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.537476	0.920840	-0.207934
2	6	0	2.391491	0.314363	-0.731385
3	6	0	1.931493	0.697721	-1.995122
4	6	0	2.622847	1.649614	-2.734598
5	6	0	3.760182	2.250714	-2.204765
6	6	0	4.208488	1.893806	-0.935859
7	1	0	3.906600	0.625110	0.769731
8	1	0	1.048297	0.218579	-2.407554
9	1	0	2.269209	1.925956	-3.722778
10	1	0	4.293450	3.002881	-2.777113
11	1	0	5.088690	2.369952	-0.516181
12	6	0	1.710571	-0.794541	-0.014013
13	6	0	0.222976	-0.731909	0.147032
14	6	0	-0.325831	0.429755	0.898376
15	24	0	-1.265425	2.096602	0.113451
16	6	0	-3.004916	1.526943	0.643589
17	8	0	-4.074890	1.288198	0.997421
18	6	0	-1.166641	2.934287	1.817525
19	8	0	-1.130206	3.463431	2.840401
20	6	0	-2.075500	3.617358	-0.649369
21	8	0	-2.570254	4.549539	-1.122197
22	6	0	0.426424	2.920204	-0.249866
23	8	0	1.388289	3.534983	-0.396457
24	6	0	-1.419601	1.212757	-1.572262
25	8	0	-1.562066	0.709209	-2.599666
26	8	0	-0.097020	0.439553	2.189692
27	6	0	0.523804	-0.669658	2.939638
28	1	0	-0.202799	-0.888978	3.724768
29	1	0	0.628129	-1.538132	2.287306
30	6	0	1.834968	-0.196965	3.499575
31	1	0	1.703508	0.690627	4.121188
32	1	0	2.271755	-0.983913	4.118301
33	1	0	2.546025	0.038974	2.704481

34	6	0	4.211403	-2.192357	-1.040179
35	6	0	3.655057	-2.108942	0.242571
36	6	0	4.453943	-2.397134	1.354445
37	6	0	5.797061	-2.709688	1.188672
38	6	0	6.351385	-2.780456	-0.087081
39	6	0	5.548868	-2.532402	-1.197987
40	1	0	3.587505	-1.992461	-1.906133
41	1	0	4.009300	-2.356569	2.344278
42	1	0	6.411217	-2.912266	2.060495
43	1	0	7.397410	-3.038451	-0.215345
44	1	0	5.968350	-2.599120	-2.197100
45	7	0	2.291300	-1.841554	0.453849
46	6	0	-0.504373	-1.723210	-0.416948
47	1	0	0.058820	-2.428522	-1.027860
48	6	0	-1.925967	-1.992910	-0.316473
49	6	0	-2.556461	-2.715795	-1.340003
50	6	0	-2.708184	-1.620847	0.791283
51	6	0	-3.908351	-3.020992	-1.296693
52	1	0	-1.970299	-3.034981	-2.197315
53	6	0	-4.051767	-1.930503	0.857781
54	1	0	-2.249535	-1.110271	1.632330
55	6	0	-4.667113	-2.623728	-0.190662
56	1	0	-4.359467	-3.569532	-2.114158
57	1	0	-4.648342	-1.646089	1.717219
58	8	0	-5.988569	-2.876124	-0.038444
59	6	0	-6.647756	-3.587109	-1.076654
60	1	0	-7.686920	-3.676315	-0.767179
61	1	0	-6.597103	-3.043264	-2.025188
62	1	0	-6.220825	-4.586394	-1.207766

Rotational constants (GHZ): 0.1232631 0.0713833 0.0573705

2p (G2=NO2)

Zero-point correction= 0.203990 (Hartree/Particle)
Thermal correction to Energy= 0.216833
Thermal correction to Enthalpy= 0.217778
Thermal correction to Gibbs Free Energy= 0.162993
Sum of electronic and zero-point Energies= -761.161011
Sum of electronic and thermal Energies= -761.148168
Sum of electronic and thermal Enthalpies= -761.147224
Sum of electronic and thermal Free Energies= -761.202008

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

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1	6	0	-3.646457	1.081826	-0.000054
2	6	0	-3.021717	-0.177271	-0.000002
3	6	0	-3.825387	-1.325754	0.000047
4	6	0	-5.210001	-1.227139	0.000050
5	6	0	-5.817954	0.024504	-0.000001
6	6	0	-5.029078	1.175151	-0.000053
7	1	0	-3.056376	1.991577	-0.000099
8	1	0	-3.333274	-2.293279	0.000085
9	1	0	-5.815653	-2.127191	0.000089
10	1	0	-6.899711	0.107273	-0.000001
11	1	0	-5.499630	2.153513	-0.000095
12	7	0	-1.637378	-0.402116	-0.000001
13	6	0	-0.800411	0.568652	0.000022
14	1	0	-1.099503	1.625668	0.000053
15	6	0	0.639145	0.340830	0.000010
16	6	0	1.498718	1.449004	0.000039
17	6	0	1.186420	-0.953274	-0.000032
18	6	0	2.872666	1.282248	0.000026
19	1	0	1.077519	2.449784	0.000072
20	6	0	2.554988	-1.134152	-0.000045
21	1	0	0.515719	-1.804708	-0.000054
22	6	0	3.381149	-0.011185	-0.000018
23	1	0	3.549863	2.126366	0.000047
24	1	0	2.998214	-2.122036	-0.000078
25	7	0	4.835137	-0.202258	-0.000032
26	8	0	5.263446	-1.352332	-0.000014
27	8	0	5.547308	0.797708	0.000047

Rotational constants (GHZ): 2.2109258 0.1527929 0.1429162

2p + 1a TS 1

Zero-point correction= 0.425721 (Hartree/Particle)
Thermal correction to Energy= 0.463695
Thermal correction to Enthalpy= 0.464640
Thermal correction to Gibbs Free Energy= 0.352528
Sum of electronic and zero-point Energies= -1914.547661
Sum of electronic and thermal Energies= -1914.509686
Sum of electronic and thermal Enthalpies= -1914.508742
Sum of electronic and thermal Free Energies= -1914.620853

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.237775	3.157457	1.365065
2	6	0	0.456689	2.012981	1.572207

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3	6	0	-0.153193	1.831924	2.827873
4	6	0	0.021876	2.769140	3.834712
5	6	0	0.799670	3.904570	3.616144
6	6	0	1.404516	4.093551	2.378038
7	1	0	1.705591	3.316986	0.398886
8	1	0	-0.765744	0.950619	2.995503
9	1	0	-0.459316	2.615616	4.795078
10	1	0	0.929370	4.637549	4.405133
11	1	0	2.011136	4.974764	2.196715
12	6	0	0.256933	0.979548	0.589376
13	6	0	-0.171171	-0.198445	0.434853
14	6	0	-0.783020	-1.393528	0.267674
15	24	0	-2.894136	-1.521508	0.207726
16	6	0	-2.813320	-1.466590	-1.691983
17	8	0	-2.753265	-1.453874	-2.845128
18	6	0	-2.760659	-3.416208	0.131769
19	8	0	-2.722370	-4.568165	0.083423
20	6	0	-4.756445	-1.686895	0.243610
21	8	0	-5.911011	-1.798293	0.269185
22	6	0	-2.701215	-1.577942	2.097810
23	8	0	-2.514982	-1.598954	3.237038
24	6	0	-3.092802	0.370948	0.303196
25	8	0	-3.269319	1.507487	0.396313
26	8	0	-0.085639	-2.533388	0.253271
27	6	0	1.357636	-2.482839	0.440937
28	1	0	1.709084	-3.438658	0.048972
29	1	0	1.757094	-1.679253	-0.187136
30	6	0	1.723298	-2.305433	1.892256
31	1	0	1.272896	-3.089210	2.505094
32	1	0	2.808041	-2.369245	2.009670
33	1	0	1.399784	-1.334770	2.277211
34	6	0	-1.005631	3.465455	-1.232033
35	6	0	-0.481585	2.268542	-1.723938
36	6	0	-1.132876	1.581081	-2.750178
37	6	0	-2.296097	2.106253	-3.299032
38	6	0	-2.805287	3.314176	-2.832189
39	6	0	-2.157656	3.989492	-1.800532
40	1	0	-0.503876	3.980386	-0.420825
41	1	0	-0.742576	0.624895	-3.085278
42	1	0	-2.810275	1.560558	-4.083186
43	1	0	-3.714148	3.721877	-3.261707
44	1	0	-2.558023	4.926452	-1.428652
45	7	0	0.684635	1.727458	-1.124117
46	6	0	1.623586	1.256779	-1.871643
47	1	0	1.508916	1.334275	-2.957283
48	6	0	2.819205	0.579868	-1.404245
49	6	0	3.524016	-0.193367	-2.341332
50	6	0	3.285242	0.648393	-0.080251

51	6	0	4.637106	-0.924962	-1.964146
52	1	0	3.179961	-0.230360	-3.369695
53	6	0	4.401026	-0.070630	0.304822
54	1	0	2.785376	1.276464	0.645932
55	6	0	5.049445	-0.859590	-0.639510
56	1	0	5.180689	-1.537913	-2.671210
57	1	0	4.773891	-0.032614	1.320365
58	7	0	6.221987	-1.645721	-0.218992
59	8	0	6.498507	-1.659756	0.974628
60	8	0	6.848411	-2.243402	-1.085383

Rotational constants (GHZ): 0.1095368 0.0663780 0.0583485

2p + 1a INT 1

Zero-point correction= 0.427252 (Hartree/Particle)
Thermal correction to Energy= 0.465410
Thermal correction to Enthalpy= 0.466354
Thermal correction to Gibbs Free Energy= 0.352811
Sum of electronic and zero-point Energies= -1914.561627
Sum of electronic and thermal Energies= -1914.523469
Sum of electronic and thermal Enthalpies= -1914.522525
Sum of electronic and thermal Free Energies= -1914.636068

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.408572	2.965701	1.841871
2	6	0	-0.091653	1.672652	1.625317
3	6	0	-0.721251	1.011436	2.692198
4	6	0	-0.861392	1.631229	3.924019
5	6	0	-0.371851	2.921246	4.123815
6	6	0	0.265803	3.582632	3.079033
7	1	0	0.921939	3.492438	1.042416
8	1	0	-1.100379	0.004809	2.535068
9	1	0	-1.356866	1.106817	4.734429
10	1	0	-0.481622	3.403906	5.089188
11	1	0	0.660327	4.582593	3.227788
12	6	0	0.072458	0.980707	0.345589
13	6	0	-0.070710	-0.324944	0.126440
14	6	0	-0.501096	-1.558033	0.129259
15	24	0	-2.633723	-1.849160	-0.286094
16	6	0	-2.396797	-0.891565	-1.912395
17	8	0	-2.217529	-0.298508	-2.887635
18	6	0	-2.097481	-3.460605	-1.154349

19	8	0	-1.810829	-4.443485	-1.683839
20	6	0	-4.397248	-2.316070	-0.625652
21	8	0	-5.498903	-2.621538	-0.834558
22	6	0	-2.562555	-2.704633	1.409109
23	8	0	-2.470345	-3.192685	2.450813
24	6	0	-3.291361	-0.292100	0.573416
25	8	0	-3.783235	0.627616	1.076175
26	8	0	0.224218	-2.679968	0.309446
27	6	0	1.623639	-2.505509	0.630444
28	1	0	2.054524	-3.500498	0.501753
29	1	0	2.063799	-1.838705	-0.122687
30	6	0	1.838958	-1.993627	2.032959
31	1	0	1.327364	-2.630666	2.758986
32	1	0	2.905981	-2.001093	2.270459
33	1	0	1.477482	-0.969357	2.160628
34	6	0	0.032385	4.043438	-1.732213
35	6	0	-0.470430	2.860767	-1.192725
36	6	0	-1.838016	2.673730	-1.011702
37	6	0	-2.712595	3.681167	-1.389397
38	6	0	-2.224078	4.864208	-1.938918
39	6	0	-0.853715	5.042616	-2.110482
40	1	0	1.104646	4.190775	-1.814795
41	1	0	-2.199964	1.740358	-0.600083
42	1	0	-3.779711	3.538234	-1.258847
43	1	0	-2.911969	5.651698	-2.227163
44	1	0	-0.470817	5.970226	-2.520786
45	7	0	0.434072	1.816747	-0.802141
46	6	0	1.489428	1.563699	-1.540920
47	1	0	1.483050	1.995910	-2.539075
48	6	0	2.639617	0.783866	-1.147333
49	6	0	3.362554	0.124818	-2.155320
50	6	0	3.117091	0.755021	0.177929
51	6	0	4.505463	-0.593906	-1.848050
52	1	0	3.010755	0.163177	-3.180413
53	6	0	4.271363	0.066835	0.485757
54	1	0	2.591204	1.290024	0.961373
55	6	0	4.939814	-0.615337	-0.529848
56	1	0	5.061194	-1.126190	-2.608802
57	1	0	4.662275	0.044268	1.494891
58	7	0	6.150751	-1.375636	-0.192598
59	8	0	6.466981	-1.447260	0.990234
60	8	0	6.772504	-1.898335	-1.110886

Rotational constants (GHZ): 0.1019892 0.0725890 0.0583488

2p + 1a TS 2

Zero-point correction= 0.425371 (Hartree/Particle)
Thermal correction to Energy= 0.463183
Thermal correction to Enthalpy= 0.464127
Thermal correction to Gibbs Free Energy= 0.351816
Sum of electronic and zero-point Energies= -1914.544302
Sum of electronic and thermal Energies= -1914.506490
Sum of electronic and thermal Enthalpies= -1914.505546
Sum of electronic and thermal Free Energies= -1914.617857

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.160805	2.298109	2.377587
2	6	0	-0.287060	1.038491	1.767785
3	6	0	-0.694350	-0.052176	2.554492
4	6	0	-1.027960	0.121450	3.887910
5	6	0	-0.938593	1.383293	4.470051
6	6	0	-0.490844	2.465180	3.713653
7	1	0	0.186205	3.149756	1.802530
8	1	0	-0.738311	-1.038091	2.104899
9	1	0	-1.346830	-0.730929	4.478522
10	1	0	-1.198346	1.521550	5.514435
11	1	0	-0.398609	3.445170	4.169512
12	6	0	0.005312	0.822209	0.357783
13	6	0	-0.116970	-0.358335	-0.340674
14	6	0	-0.766461	-1.517446	-0.471767
15	24	0	-2.945992	-1.316060	-0.401782
16	6	0	-2.735496	-0.140184	-1.888011
17	8	0	-2.565640	0.595300	-2.759279
18	6	0	-2.958353	-2.844459	-1.547406
19	8	0	-3.024604	-3.760143	-2.241537
20	6	0	-4.802355	-1.371395	-0.526269
21	8	0	-5.957530	-1.419050	-0.609849
22	6	0	-2.846545	-2.434098	1.135253
23	8	0	-2.748127	-3.098766	2.072627
24	6	0	-3.195622	0.217854	0.700685
25	8	0	-3.482948	1.151417	1.318542
26	8	0	-0.289507	-2.696844	-0.841818
27	6	0	1.155968	-2.835017	-0.970202
28	1	0	1.284652	-3.785327	-1.490082
29	1	0	1.503917	-2.029465	-1.623132
30	6	0	1.841488	-2.829873	0.369855
31	1	0	1.481963	-3.649076	0.996377
32	1	0	2.919264	-2.953346	0.235555
33	1	0	1.683078	-1.889812	0.905134
34	6	0	-1.046023	3.449340	-0.559472

35	6	0	0.255156	3.018114	-0.834191
36	6	0	1.138109	3.836446	-1.542740
37	6	0	0.711620	5.083345	-1.983634
38	6	0	-0.576190	5.525217	-1.698652
39	6	0	-1.448895	4.706128	-0.982745
40	1	0	-1.734338	2.796027	-0.031979
41	1	0	2.152785	3.496606	-1.728415
42	1	0	1.396227	5.717305	-2.536868
43	1	0	-0.902147	6.503714	-2.034004
44	1	0	-2.458773	5.041099	-0.771284
45	7	0	0.688513	1.735264	-0.448478
46	6	0	1.440497	0.926491	-1.298664
47	1	0	1.317243	1.101266	-2.368435
48	6	0	2.683148	0.335180	-0.860601
49	6	0	3.457782	-0.380076	-1.795620
50	6	0	3.172157	0.478478	0.454898
51	6	0	4.655952	-0.961226	-1.429888
52	1	0	3.103260	-0.477129	-2.817230
53	6	0	4.368681	-0.094240	0.827026
54	1	0	2.602854	1.050121	1.180868
55	6	0	5.096667	-0.819983	-0.116770
56	1	0	5.255211	-1.517129	-2.139691
57	1	0	4.755624	0.010626	1.832508
58	7	0	6.358146	-1.434526	0.280495
59	8	0	6.730130	-1.288981	1.443357
60	8	0	6.984747	-2.068381	-0.566870

Rotational constants (GHZ): 0.1095097 0.0682131 0.0573895

2p + 1a INT 2

Zero-point correction= 0.428677 (Hartree/Particle)
Thermal correction to Energy= 0.465577
Thermal correction to Enthalpy= 0.466522
Thermal correction to Gibbs Free Energy= 0.356088
Sum of electronic and zero-point Energies= -1914.592235
Sum of electronic and thermal Energies= -1914.555334
Sum of electronic and thermal Enthalpies= -1914.554390
Sum of electronic and thermal Free Energies= -1914.664823

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.147417	-0.234709	1.398707
2	6	0	-3.207261	-0.878753	0.584421
3	6	0	-3.436557	-2.196502	0.169842
4	6	0	-4.594013	-2.857409	0.558640

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5	6	0	-5.520552	-2.215971	1.375435
6	6	0	-5.293287	-0.907586	1.797916
7	1	0	-3.969940	0.786895	1.721450
8	1	0	-2.708254	-2.690516	-0.467421
9	1	0	-4.771620	-3.874176	0.225444
10	1	0	-6.421992	-2.735088	1.683682
11	1	0	-6.013584	-0.410319	2.438645
12	6	0	-1.989168	-0.204774	0.167635
13	6	0	-0.642047	-0.555964	-0.010973
14	6	0	0.249154	-1.610696	0.233656
15	24	0	2.029561	-2.027319	-0.819004
16	6	0	2.891032	-0.664102	0.194049
17	8	0	3.434427	0.125001	0.837431
18	6	0	2.500382	-3.269680	0.553712
19	8	0	2.822380	-4.025494	1.361275
20	6	0	3.610878	-2.495545	-1.709084
21	8	0	4.587876	-2.785055	-2.261751
22	6	0	0.981274	-3.375053	-1.656387
23	8	0	0.309606	-4.182740	-2.133569
24	6	0	1.697913	-0.867167	-2.274505
25	8	0	1.578841	-0.213275	-3.223759
26	8	0	-0.022061	-2.512671	1.181242
27	6	0	-0.928241	-2.288062	2.297255
28	1	0	-1.060758	-1.209921	2.434531
29	1	0	-1.898088	-2.724684	2.048184
30	6	0	-0.311521	-2.947646	3.500042
31	1	0	0.667035	-2.518659	3.725807
32	1	0	-0.956673	-2.809074	4.370123
33	1	0	-0.187124	-4.020271	3.339099
34	6	0	-4.023727	1.679553	-1.271516
35	6	0	-2.716281	2.008425	-0.898206
36	6	0	-2.238065	3.306809	-1.106018
37	6	0	-3.065232	4.265464	-1.674510
38	6	0	-4.373713	3.947685	-2.029530
39	6	0	-4.843551	2.653934	-1.826386
40	1	0	-4.391563	0.668691	-1.147660
41	1	0	-1.224340	3.559912	-0.813719
42	1	0	-2.685169	5.269183	-1.832986
43	1	0	-5.019160	4.700768	-2.468204
44	1	0	-5.855426	2.390765	-2.116592
45	7	0	-1.847229	1.064824	-0.322232
46	6	0	-0.419747	0.795100	-0.678251
47	1	0	-0.340254	0.745001	-1.767372
48	6	0	0.593959	1.729756	-0.091772
49	6	0	1.548696	2.334471	-0.909657
50	6	0	0.593754	1.992020	1.282187
51	6	0	2.505541	3.181787	-0.369763
52	1	0	1.543463	2.138817	-1.976980

53	6	0	1.533715	2.842466	1.835642
54	1	0	-0.150720	1.520945	1.918167
55	6	0	2.481352	3.420970	0.996641
56	1	0	3.258355	3.654221	-0.987317
57	1	0	1.552247	3.059398	2.895850
58	7	0	3.489203	4.318006	1.579190
59	8	0	4.339462	4.789290	0.831748
60	8	0	3.425303	4.547574	2.782300

Rotational constants (GHZ): 0.0915667 0.0804173 0.0559460

2p + 1aTS 3

Zero-point correction= 0.425782 (Hartree/Particle)
Thermal correction to Energy= 0.463378
Thermal correction to Enthalpy= 0.464322
Thermal correction to Gibbs Free Energy= 0.352120
Sum of electronic and zero-point Energies= -1914.561091
Sum of electronic and thermal Energies= -1914.523495
Sum of electronic and thermal Enthalpies= -1914.522551
Sum of electronic and thermal Free Energies= -1914.634753

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.016346	0.650016	1.413602
2	6	0	-3.030281	0.014055	0.648193
3	6	0	-3.298667	-1.247760	0.102643
4	6	0	-4.530128	-1.854966	0.308417
5	6	0	-5.502759	-1.216796	1.073847
6	6	0	-5.241478	0.034345	1.628930
7	1	0	-3.808881	1.625320	1.844723
8	1	0	-2.541593	-1.741288	-0.500772
9	1	0	-4.731756	-2.827421	-0.128550
10	1	0	-6.463623	-1.693573	1.238584
11	1	0	-5.995914	0.530685	2.230493
12	6	0	-1.727762	0.650234	0.423709
13	6	0	-0.480680	0.032046	0.241949
14	6	0	-0.025388	-1.288089	0.494928
15	24	0	1.131569	-2.456996	-0.812685
16	6	0	2.107909	-2.862145	0.769582
17	8	0	2.657734	-3.038154	1.767658
18	6	0	-0.114515	-3.853979	-0.446455
19	8	0	-0.867649	-4.700227	-0.234470
20	6	0	2.041525	-3.650125	-1.944774
21	8	0	2.595981	-4.394001	-2.638493

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22	6	0	0.025799	-1.764699	-2.189544
23	8	0	-0.667006	-1.295245	-2.986288
24	6	0	2.470328	-1.188619	-1.278670
25	8	0	3.342184	-0.518686	-1.633422
26	8	0	-0.514843	-1.955613	1.543970
27	6	0	-0.993702	-1.329108	2.774994
28	1	0	-0.120723	-1.308975	3.437036
29	1	0	-1.306222	-0.301295	2.594651
30	6	0	-2.096448	-2.176787	3.342239
31	1	0	-1.759437	-3.203806	3.497355
32	1	0	-2.409134	-1.774201	4.308234
33	1	0	-2.965021	-2.193311	2.681406
34	6	0	-3.218877	2.316976	-1.509776
35	6	0	-2.435160	2.784982	-0.441194
36	6	0	-2.511580	4.138104	-0.080534
37	6	0	-3.382812	4.990441	-0.743972
38	6	0	-4.173046	4.513756	-1.788108
39	6	0	-4.081877	3.176631	-2.172431
40	1	0	-3.129784	1.279172	-1.819820
41	1	0	-1.886318	4.497359	0.730817
42	1	0	-3.444616	6.032816	-0.448762
43	1	0	-4.848826	5.184055	-2.309015
44	1	0	-4.682364	2.806611	-2.997517
45	7	0	-1.515451	1.968709	0.224022
46	6	0	0.238697	1.091702	-0.462630
47	1	0	-0.107450	1.383577	-1.452682
48	6	0	1.529977	1.578232	-0.070374
49	6	0	2.246090	2.444565	-0.917206
50	6	0	2.106996	1.194816	1.156174
51	6	0	3.507232	2.890854	-0.561104
52	1	0	1.802533	2.743209	-1.862761
53	6	0	3.373443	1.632647	1.502200
54	1	0	1.546694	0.552920	1.829676
55	6	0	4.074922	2.480859	0.645202
56	1	0	4.056990	3.551922	-1.222393
57	1	0	3.816407	1.326014	2.443626
58	7	0	5.415905	2.952646	1.019477
59	8	0	5.995836	3.681028	0.263462
60	8	0	5.876478	2.590337	2.065905

Rotational constants (GHZ): 0.0980206 0.0760618 0.0542368

2p + 1a INT 3

Zero-point correction= 0.428513 (Hartree/Particle)
Thermal correction to Energy= 0.466149
Thermal correction to Enthalpy= 0.467093
Thermal correction to Gibbs Free Energy= 0.356251
Sum of electronic and zero-point Energies= -1914.593890
Sum of electronic and thermal Energies= -1914.556254
Sum of electronic and thermal Enthalpies= -1914.555310
Sum of electronic and thermal Free Energies= -1914.666152

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.656170	0.888439	-0.463414
2	6	0	2.482484	0.239501	-0.860486
3	6	0	1.933993	0.520394	-2.116366
4	6	0	2.564604	1.413190	-2.973550
5	6	0	3.731917	2.054283	-2.572008
6	6	0	4.268911	1.799394	-1.312216
7	1	0	4.086239	0.675428	0.510830
8	1	0	1.028378	0.009955	-2.429616
9	1	0	2.142326	1.610199	-3.953533
10	1	0	4.220250	2.759535	-3.236624
11	1	0	5.170950	2.310681	-0.992585
12	6	0	1.847774	-0.799402	-0.012740
13	6	0	0.354165	-0.732113	0.169921
14	6	0	-0.171174	0.415399	0.961495
15	24	0	-1.040312	2.123880	0.206469
16	6	0	-2.752598	1.604782	0.857822
17	8	0	-3.793561	1.367365	1.289671
18	6	0	-0.778583	2.959951	1.899183
19	8	0	-0.634041	3.484204	2.913639
20	6	0	-1.855692	3.678466	-0.493964
21	8	0	-2.357829	4.624440	-0.925636
22	6	0	0.648505	2.882590	-0.304514
23	8	0	1.613105	3.454428	-0.558960
24	6	0	-1.320303	1.266383	-1.473274
25	8	0	-1.527036	0.779285	-2.497759
26	8	0	0.006695	0.358608	2.256929

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27	6	0	0.578301	-0.794270	2.980074
28	1	0	-0.182475	-1.037457	3.724703
29	1	0	0.698671	-1.632689	2.291815
30	6	0	1.871852	-0.364431	3.610146
31	1	0	1.724782	0.490787	4.272223
32	1	0	2.277051	-1.187351	4.203013
33	1	0	2.612358	-0.096600	2.852755
34	6	0	4.341994	-2.243525	-0.939441
35	6	0	3.798752	-2.080935	0.341078
36	6	0	4.603200	-2.315104	1.461187
37	6	0	5.942245	-2.648489	1.301834
38	6	0	6.484699	-2.794716	0.027692
39	6	0	5.674597	-2.604208	-1.089084
40	1	0	3.711905	-2.090956	-1.810481
41	1	0	4.167674	-2.219518	2.450727
42	1	0	6.561719	-2.809328	2.178583
43	1	0	7.527284	-3.069106	-0.094220
44	1	0	6.083910	-2.733388	-2.086028
45	7	0	2.437760	-1.790565	0.547082
46	6	0	-0.382949	-1.670331	-0.459990
47	1	0	0.161059	-2.359952	-1.104075
48	6	0	-1.823041	-1.871243	-0.414960
49	6	0	-2.456117	-2.448622	-1.530782
50	6	0	-2.602754	-1.549199	0.706301
51	6	0	-3.821181	-2.657783	-1.548654
52	1	0	-1.860254	-2.716347	-2.397268
53	6	0	-3.970584	-1.760882	0.707284
54	1	0	-2.132707	-1.157711	1.601924
55	6	0	-4.563642	-2.305141	-0.425087
56	1	0	-4.318826	-3.088508	-2.408033
57	1	0	-4.577946	-1.515430	1.568530
58	7	0	-6.012063	-2.530806	-0.430580
59	8	0	-6.647692	-2.220959	0.572659
60	8	0	-6.513143	-3.017375	-1.439837

Rotational constants (GHZ): 0.1223757 0.0645613 0.0542267