Supporting Information

Aqua-friendly organometallic Ir-Pt complexes: pH responsive AIPE guided imaging of bacterial cells

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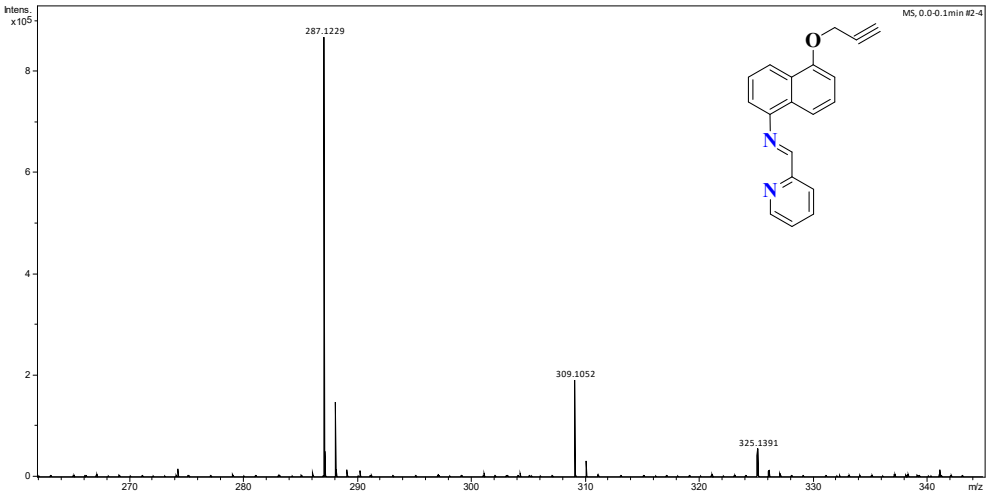
Figure S1: ESI-MS spectra

L:



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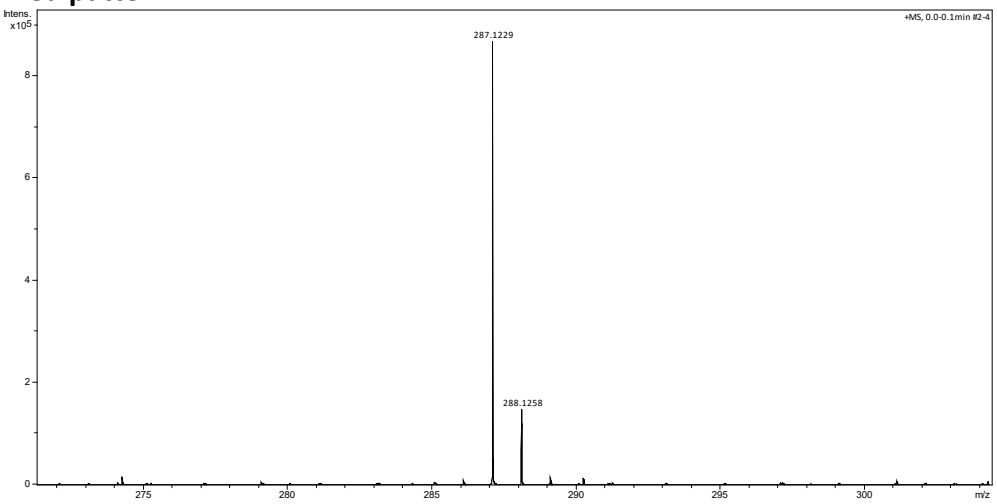

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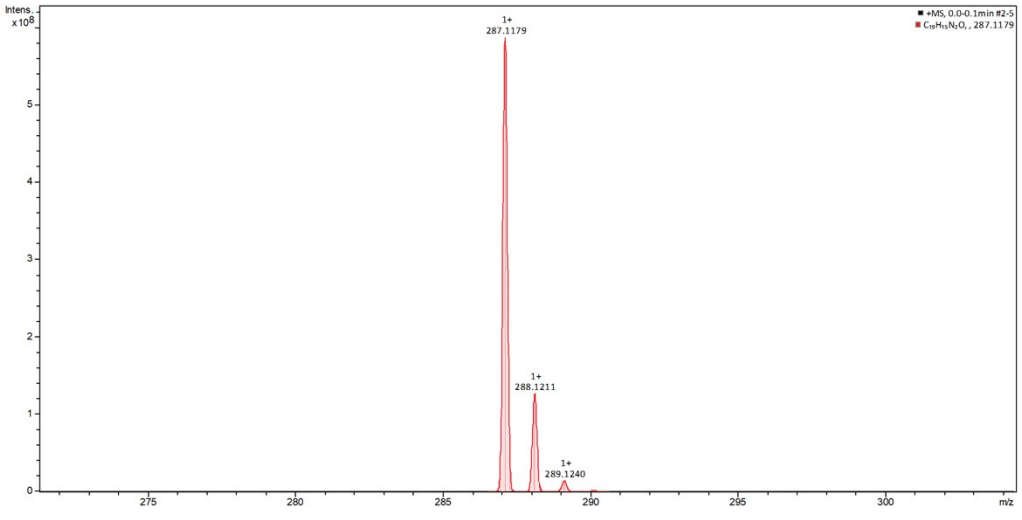

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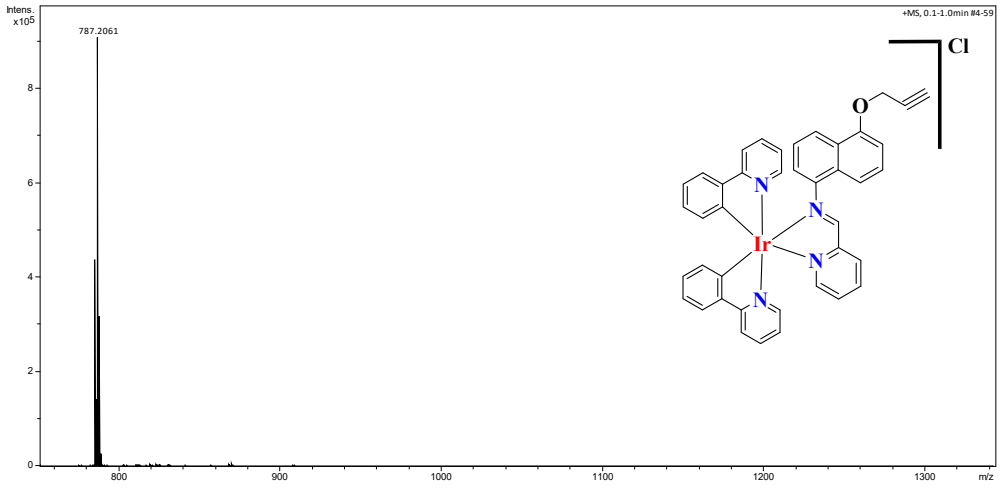

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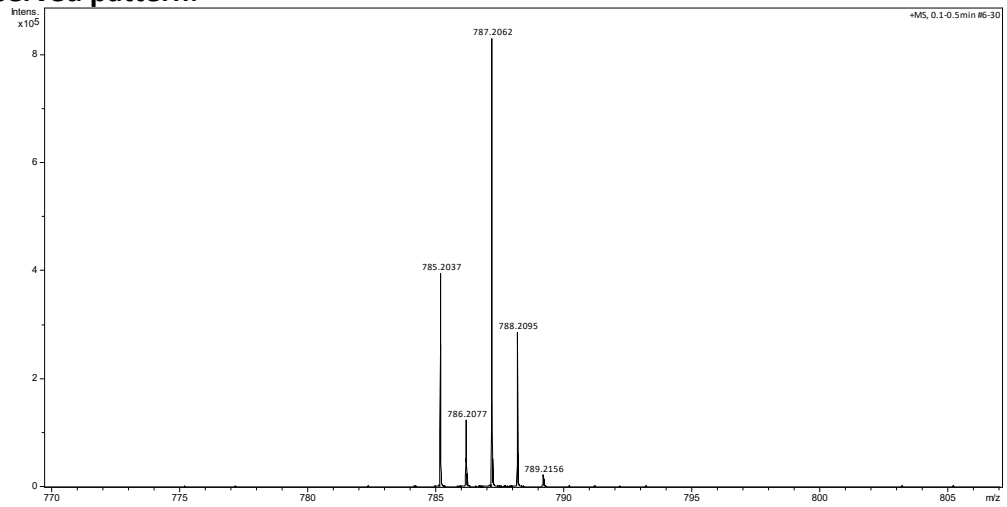

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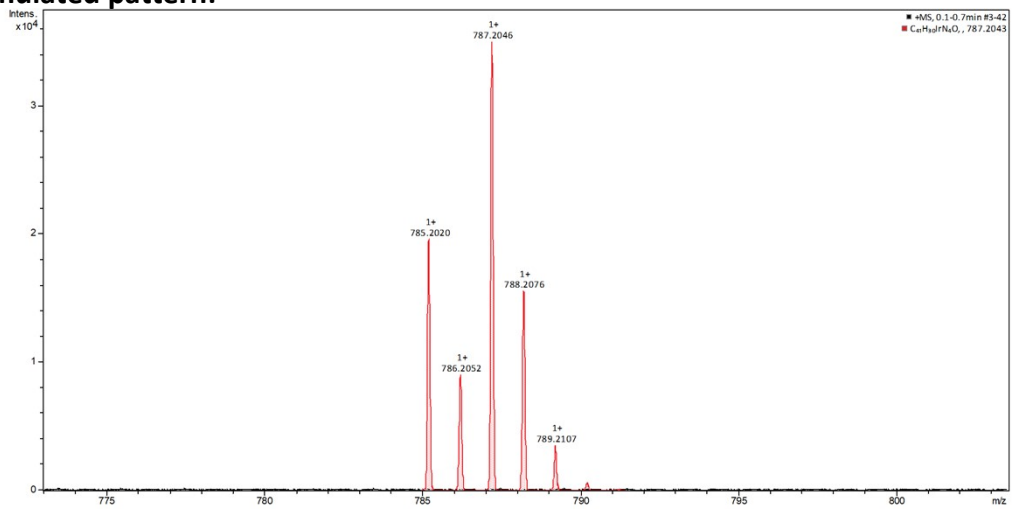

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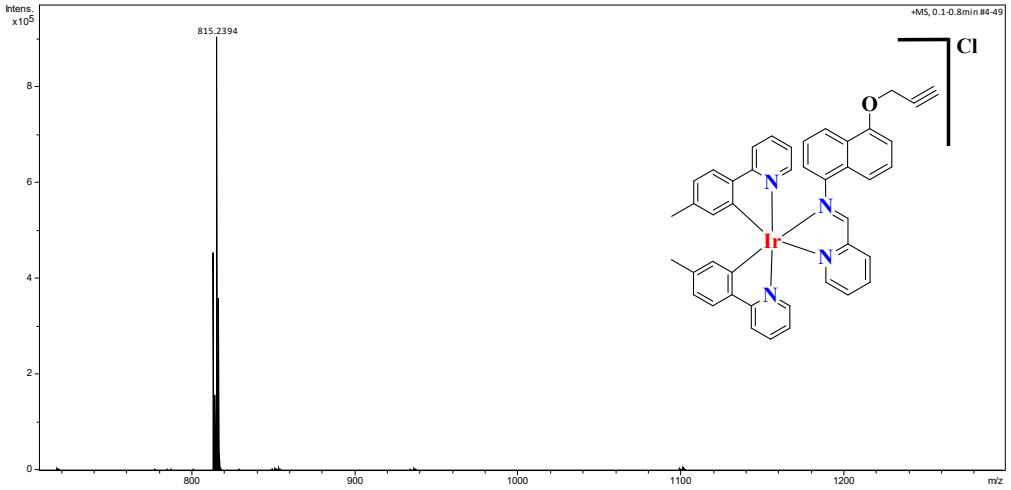

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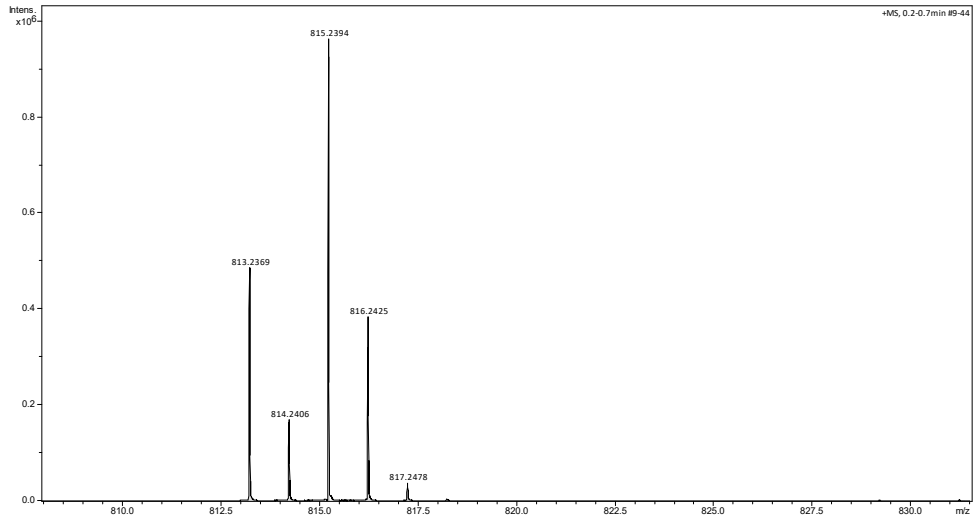

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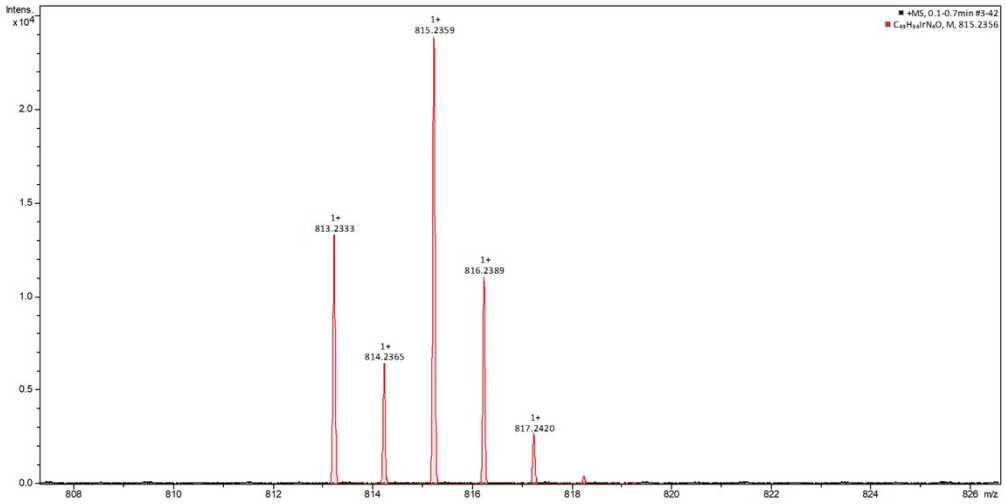

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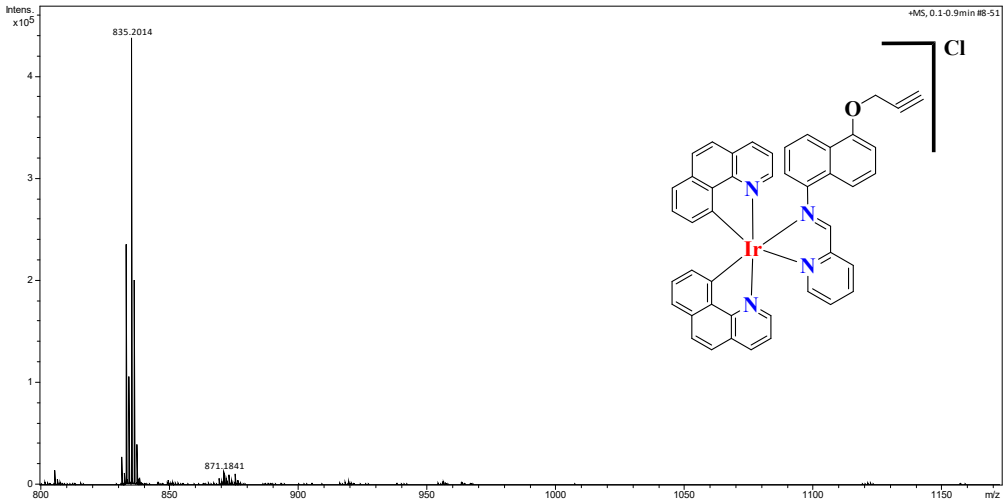

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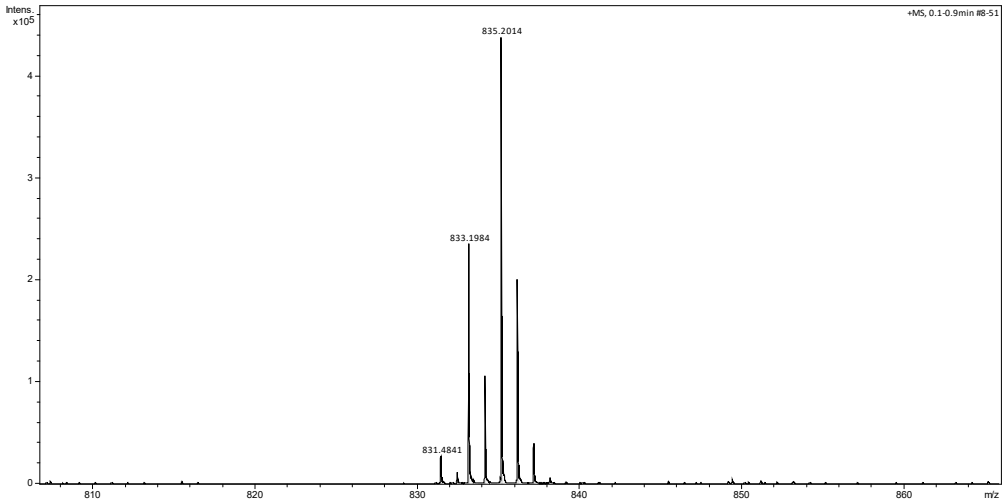

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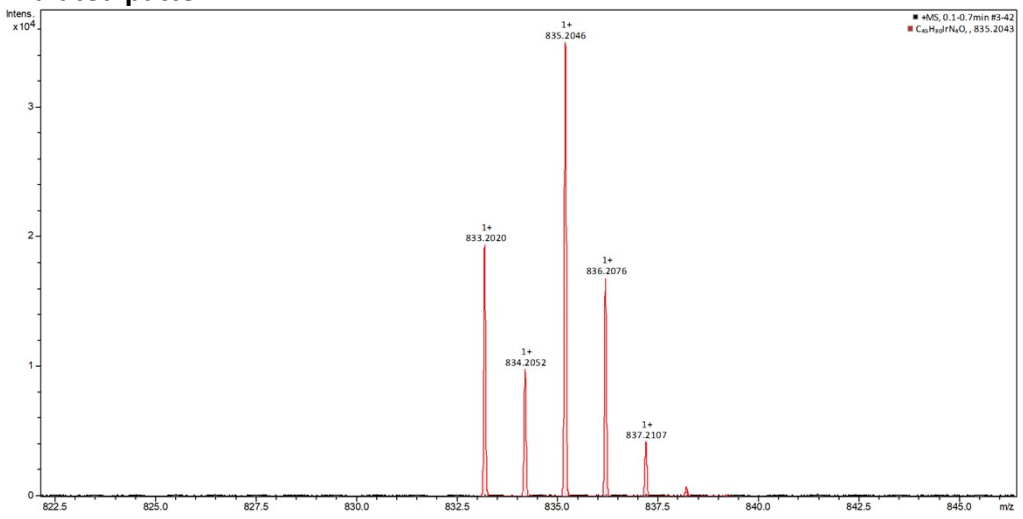

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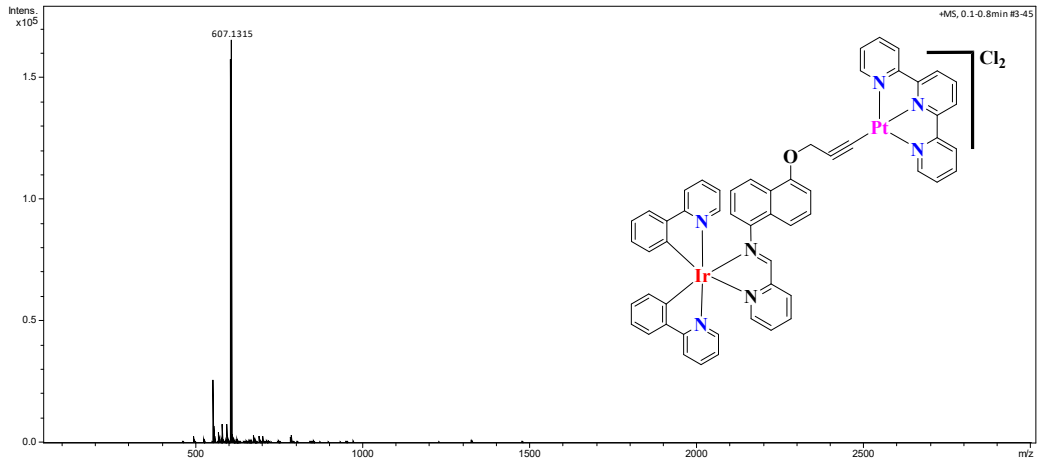

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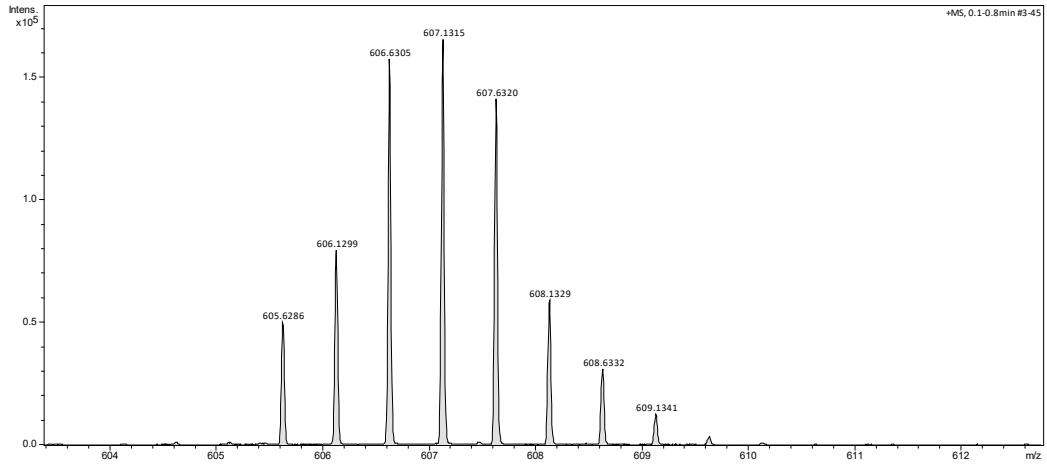

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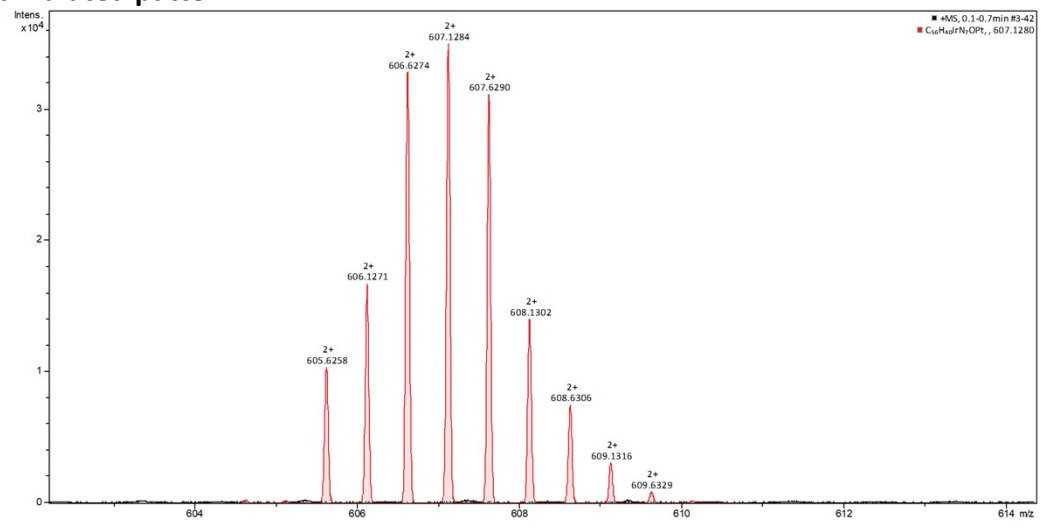

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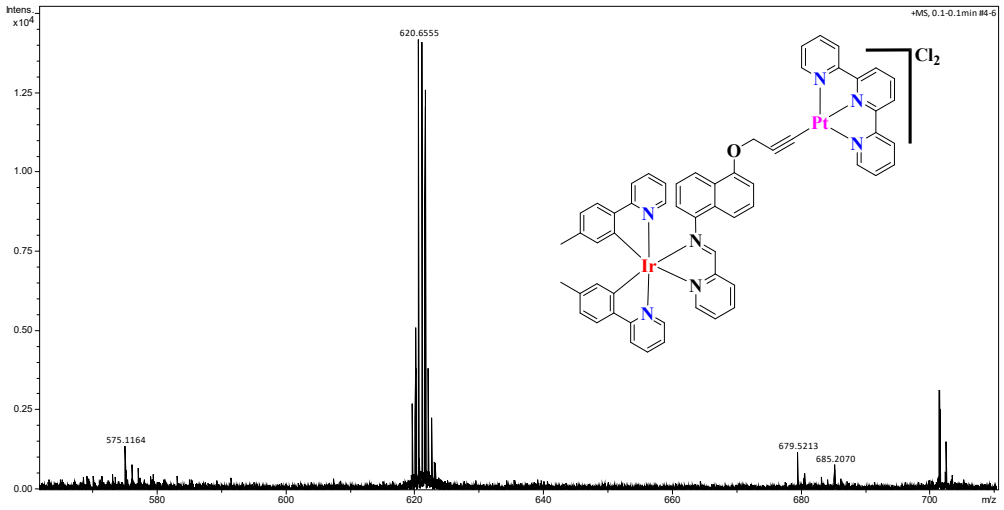

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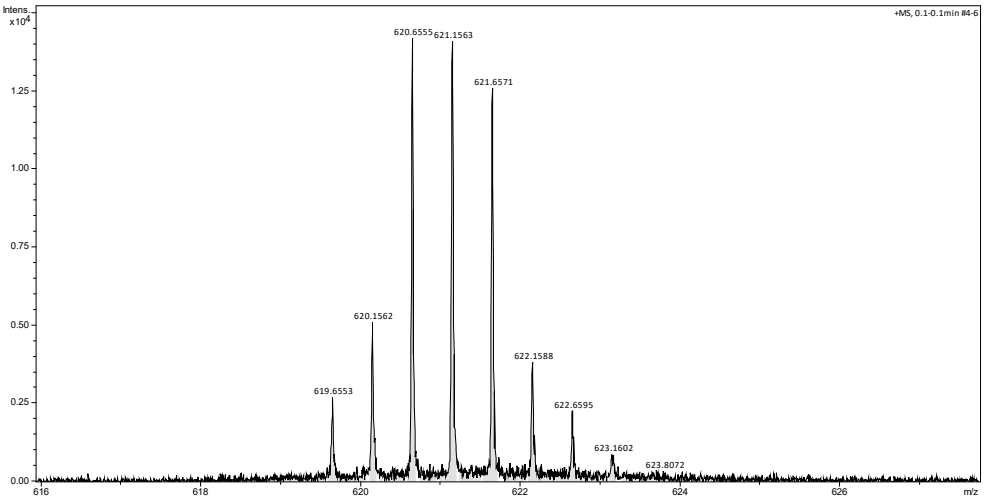

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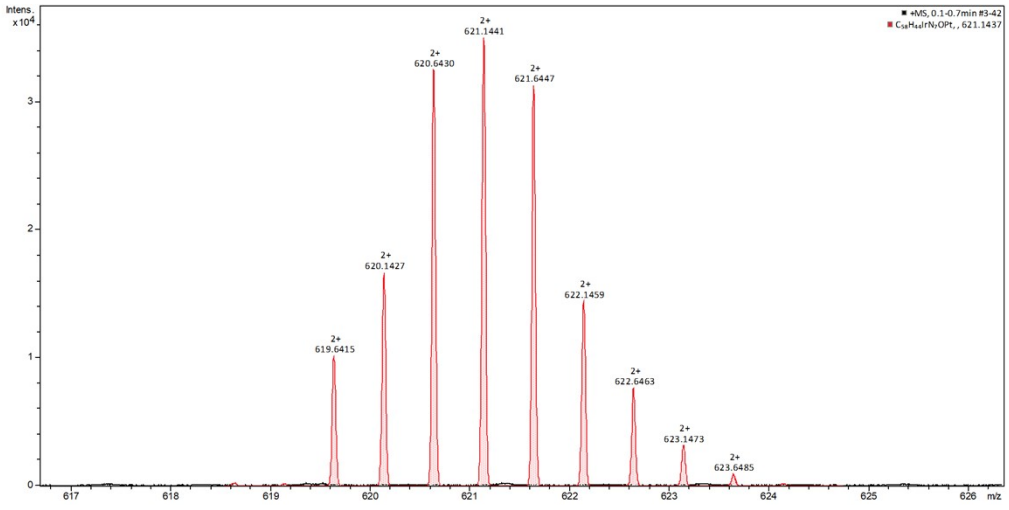

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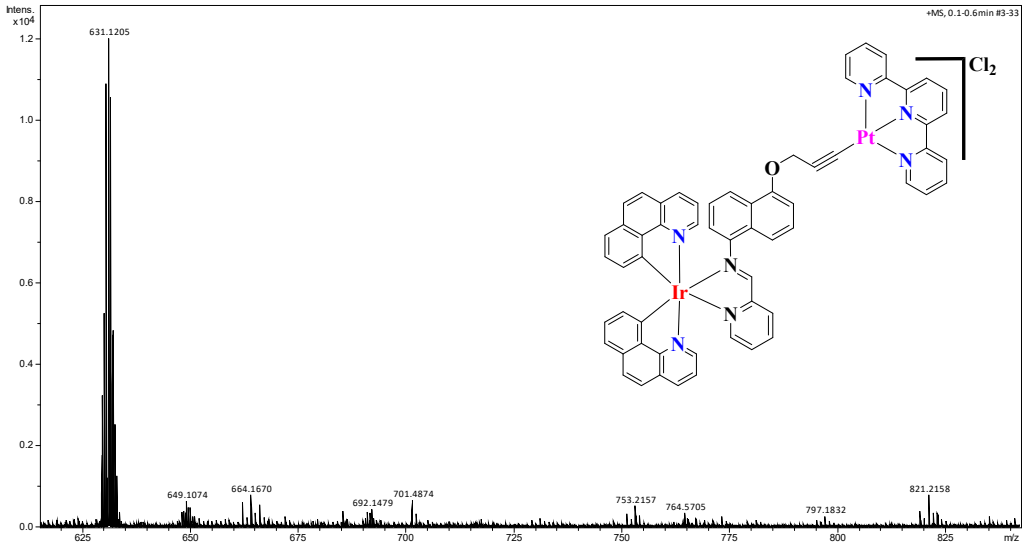

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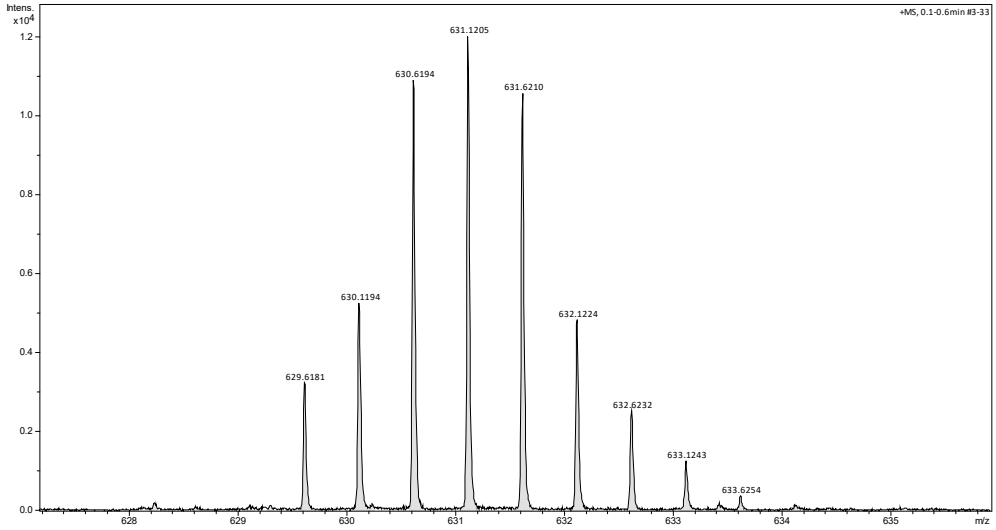

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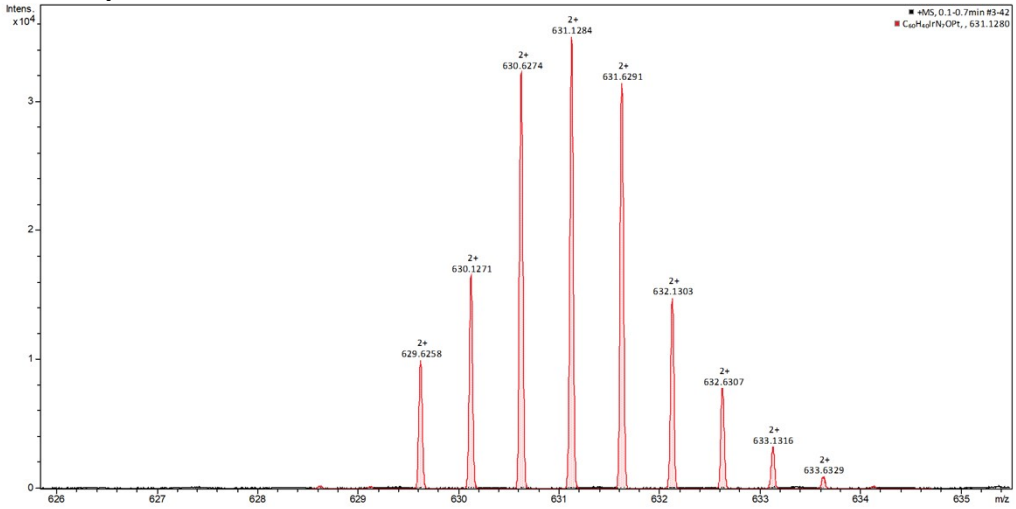
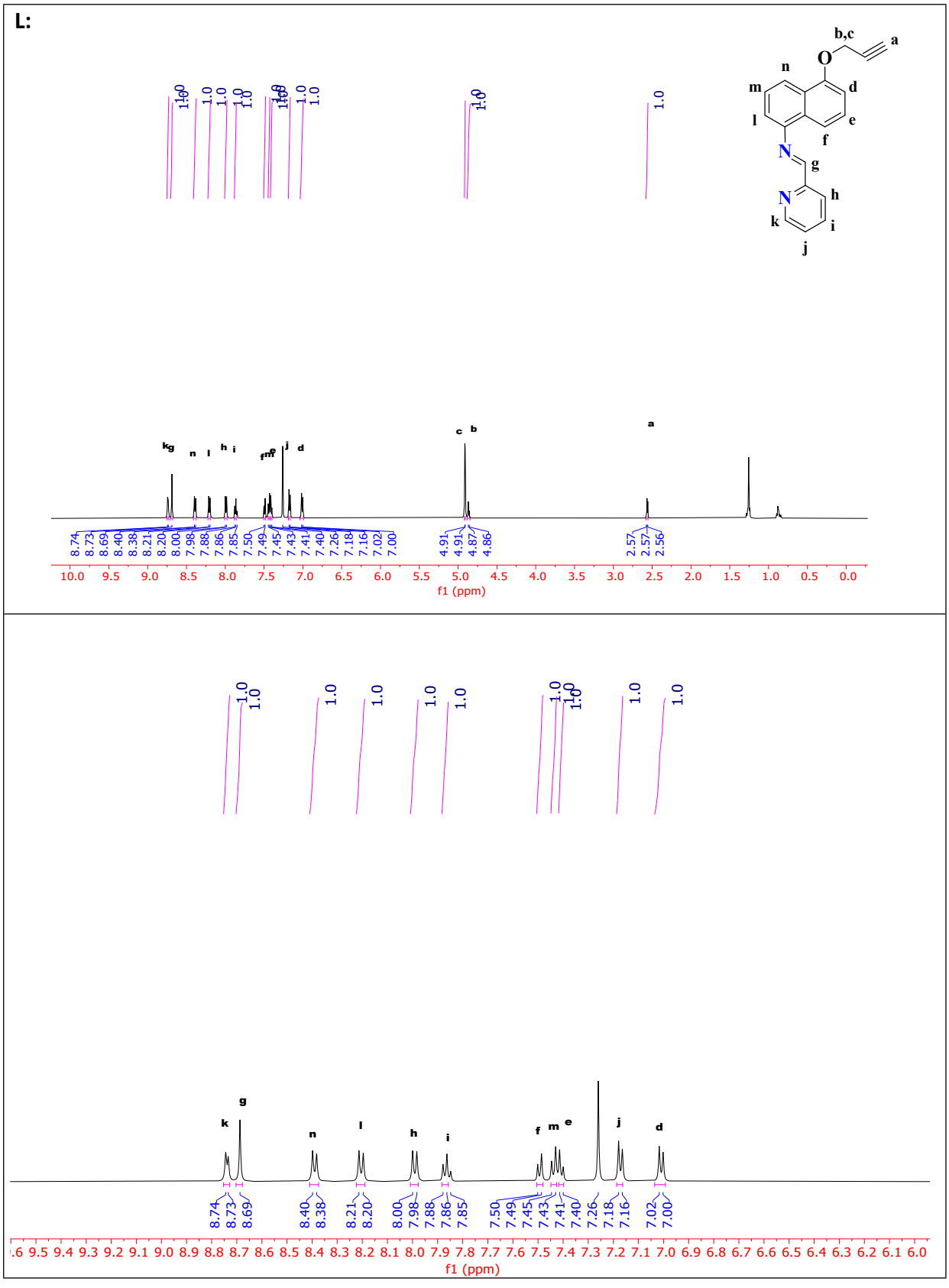


Figure S2: NMR spectra

A. ^{1}H NMR spectra



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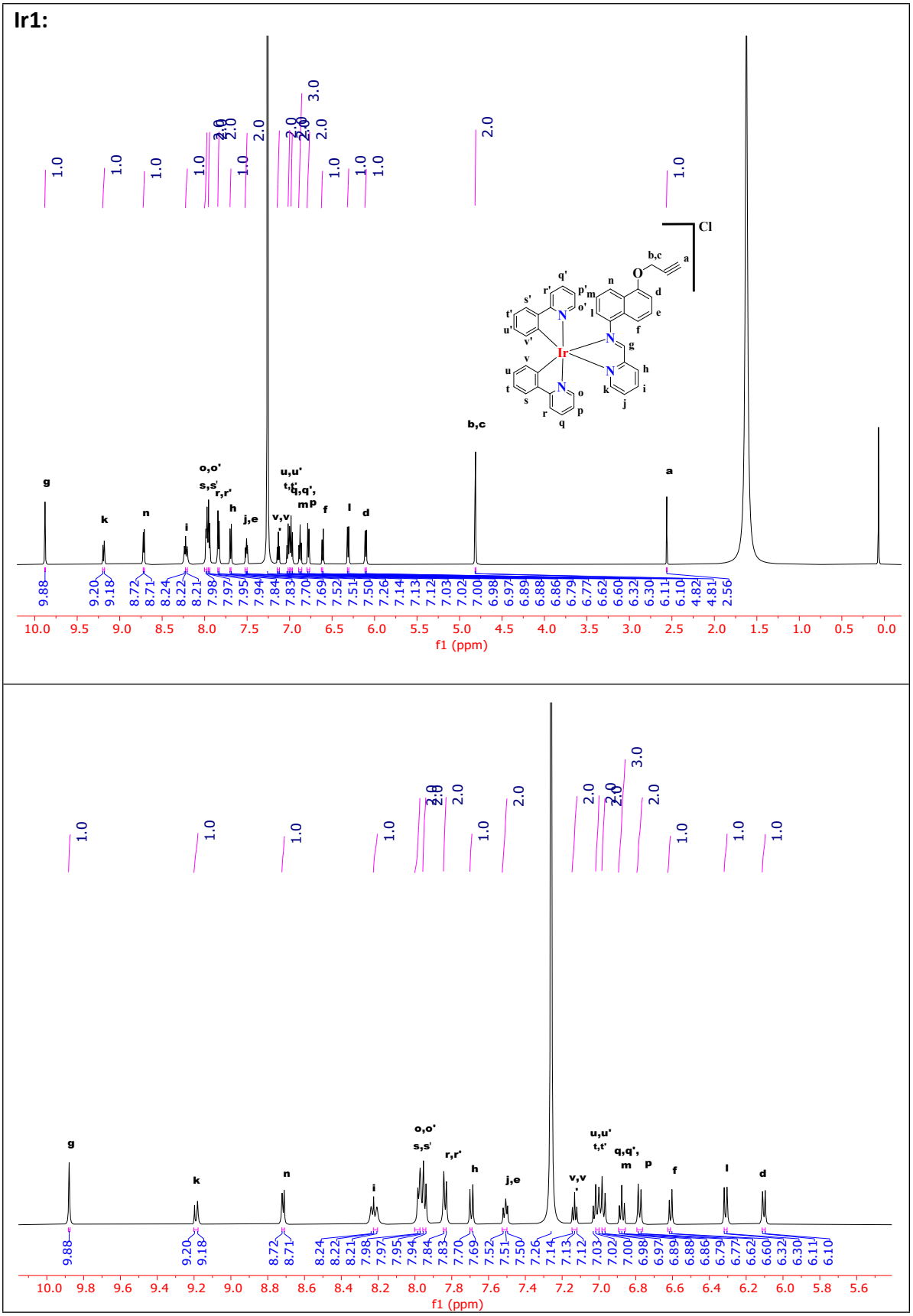

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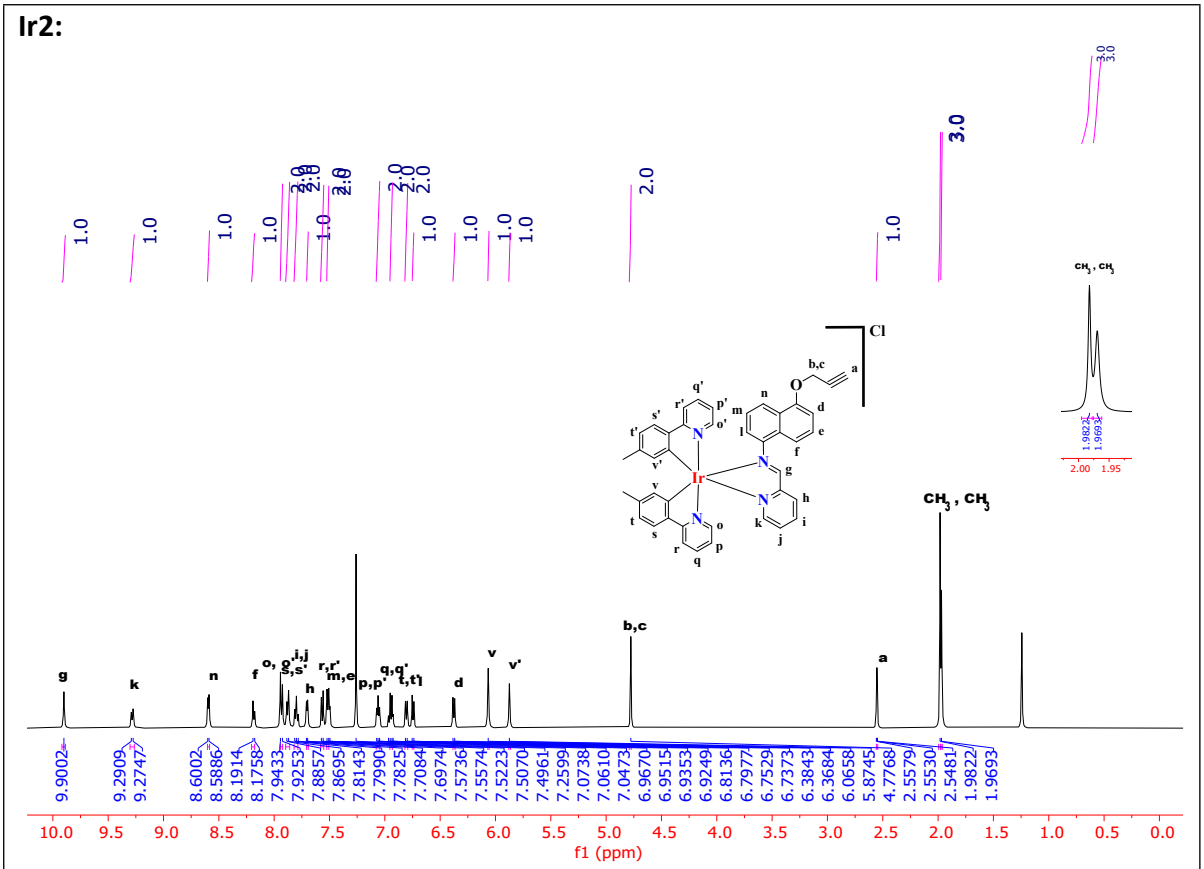

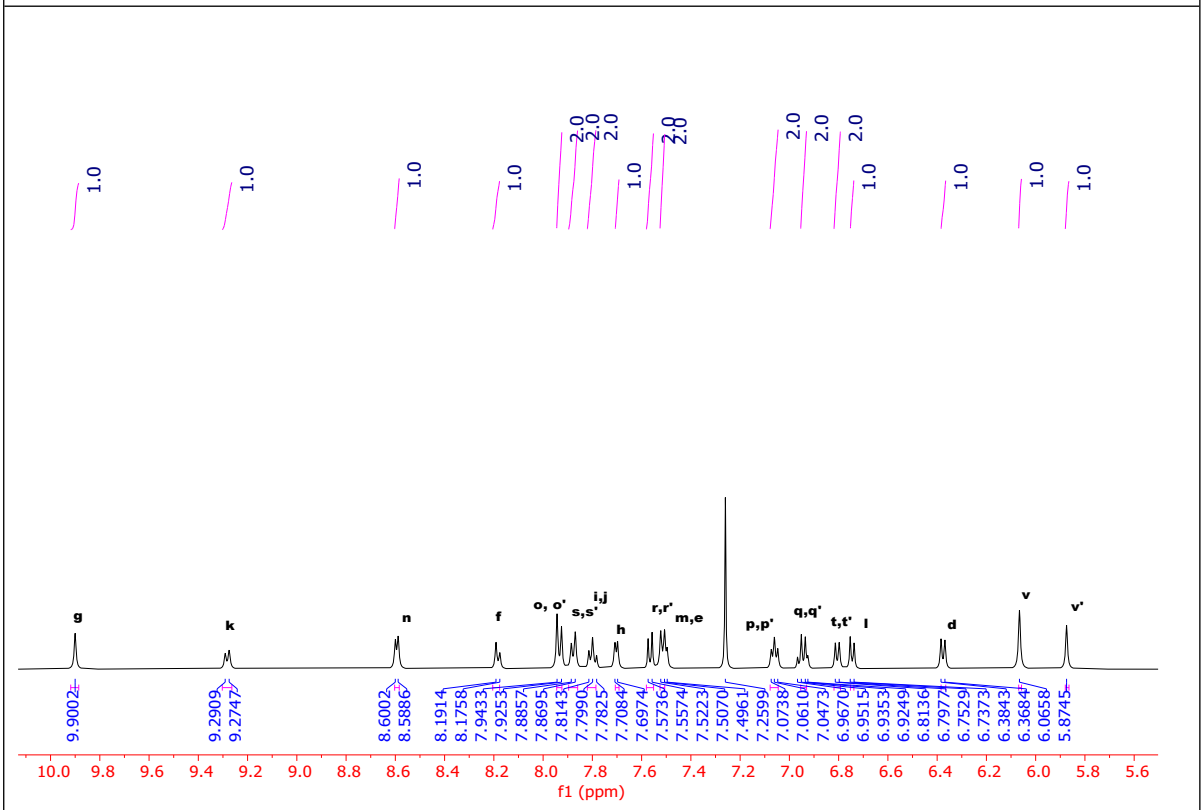

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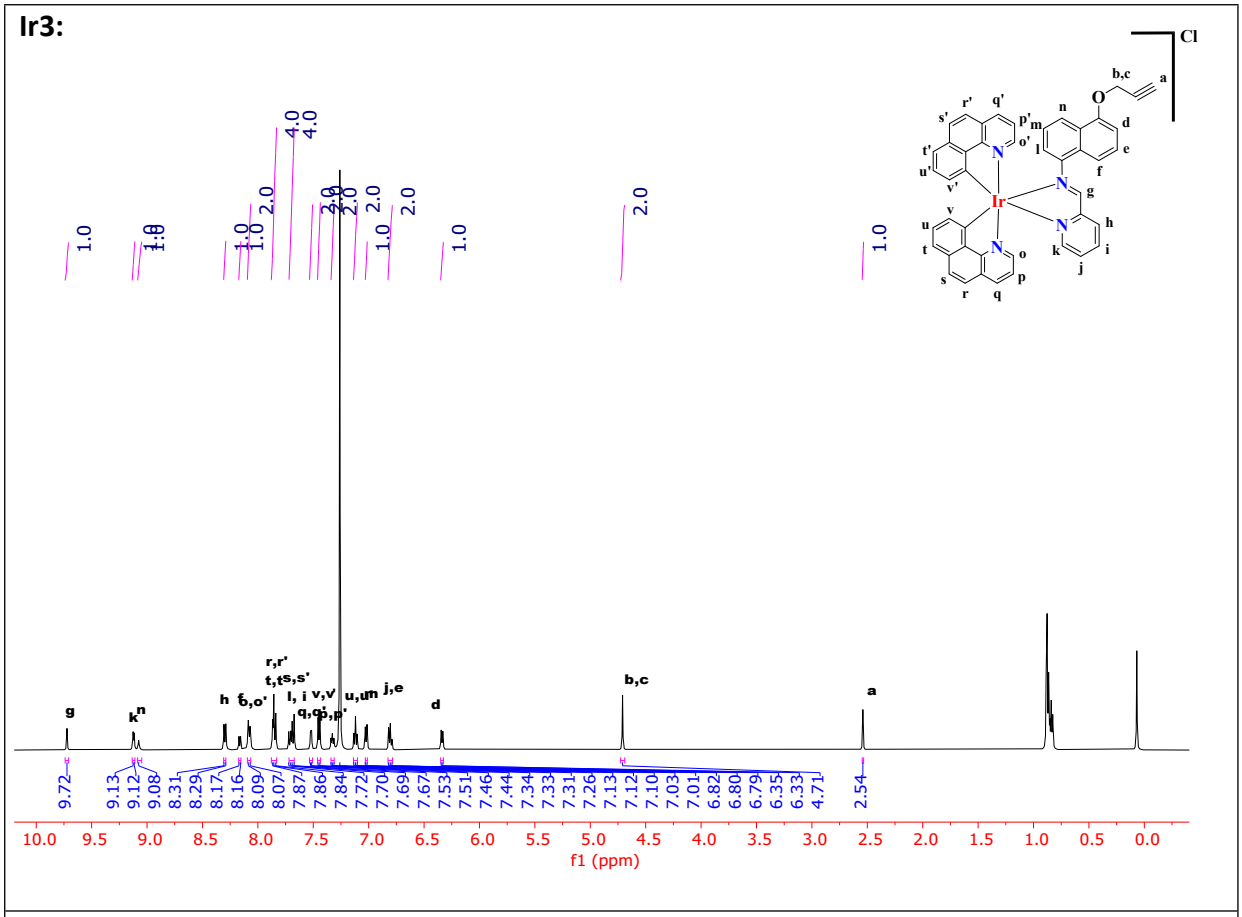

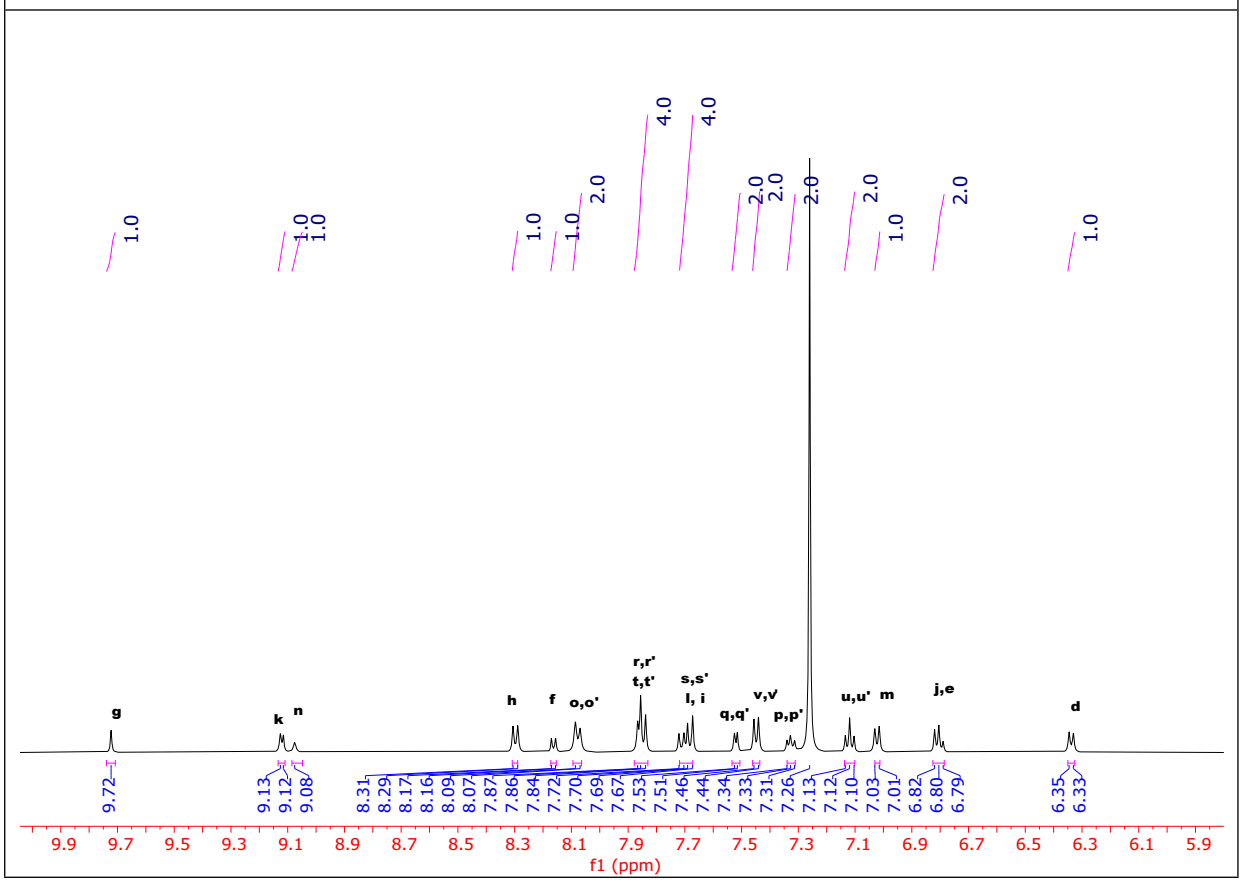

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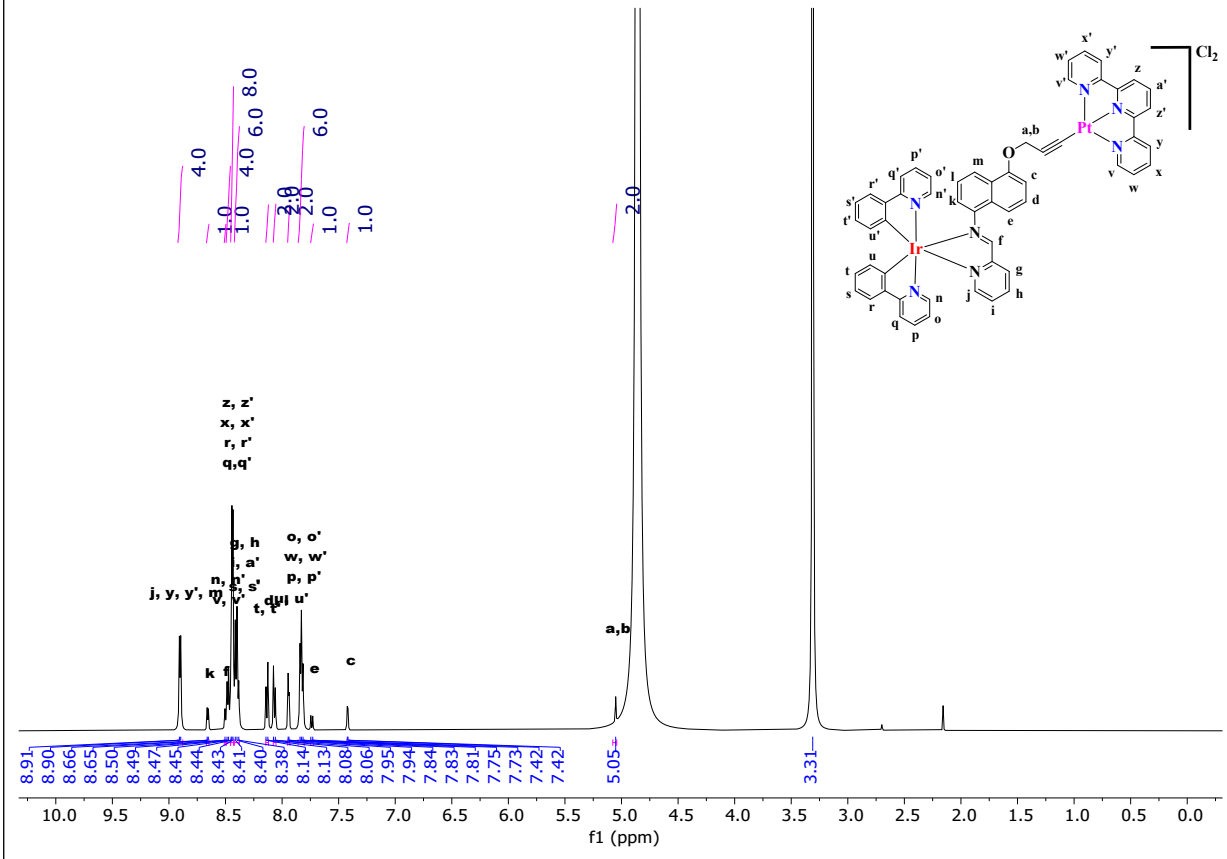
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4.0
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1.0
1.0
2.0
z, z'
x, x'
r, r'
q,q'
g, h
, a'
o, o'
w, w'
p, p'
j, y, y', m
n, n'
v, v'
s, s'
t, t'
d, l
u, u'
a,b
k
f
e
c
8.91
8.90
8.66
8.65
8.50
8.49
8.47
8.45
8.44
8.43
8.41
8.40
8.38
8.14
8.13
8.08
8.06
7.95
7.94
7.84
7.83
7.81
7.75
7.73
7.42
7.42
5.05
3.31
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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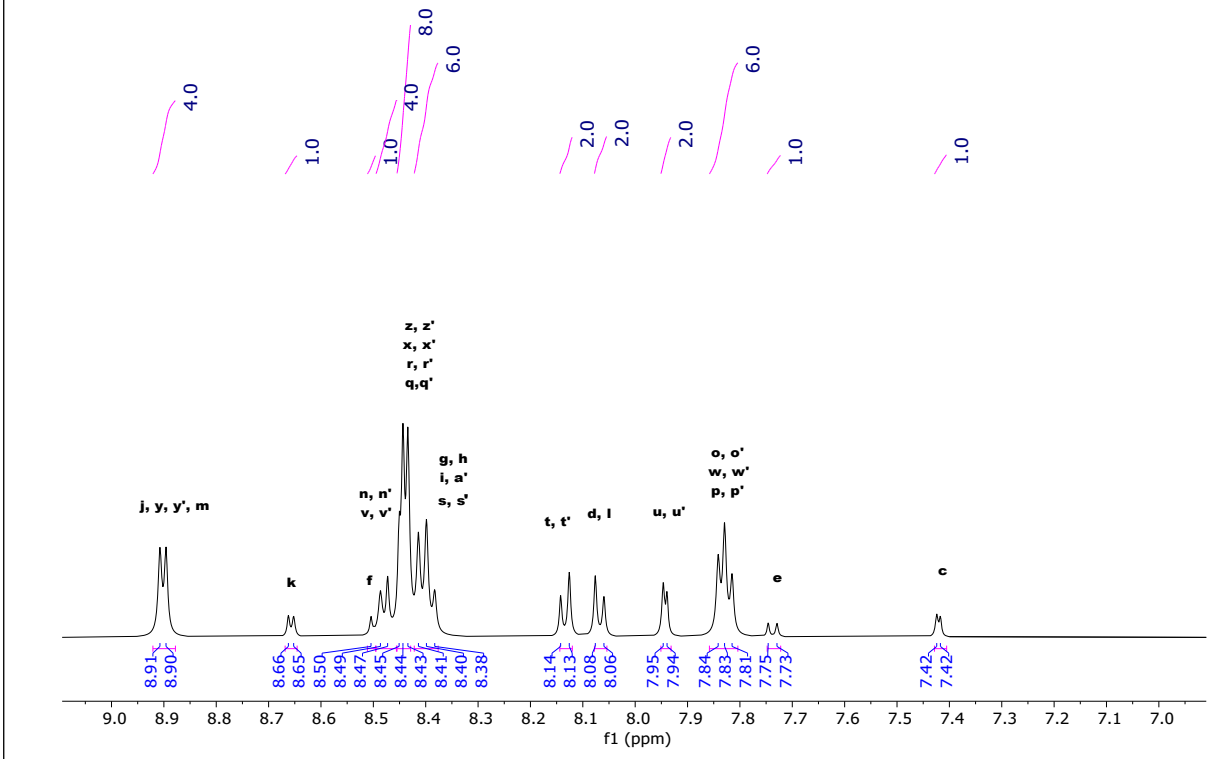
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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1.0
1.0
4.0
8.0
6.0
2.0
2.0
2.0
6.0
1.0
1.0
z, z'
x, x'
r, r'
q,q'
g, h
i, a'
s, s'
o, o'
w, w'
p, p'
j, y, y', m
n, n'
v, v'
t, t'
d, l
u, u'
k
f
e
c
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8.66
8.65
8.50
8.49
8.47
8.45
8.44
8.43
8.41
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8.13
8.08
8.06
7.95
7.94
7.84
7.83
7.81
7.75
7.73
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7.42
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8.8
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
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7.6
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7.4
7.3
7.2
7.1
7.0
f1 (ppm)

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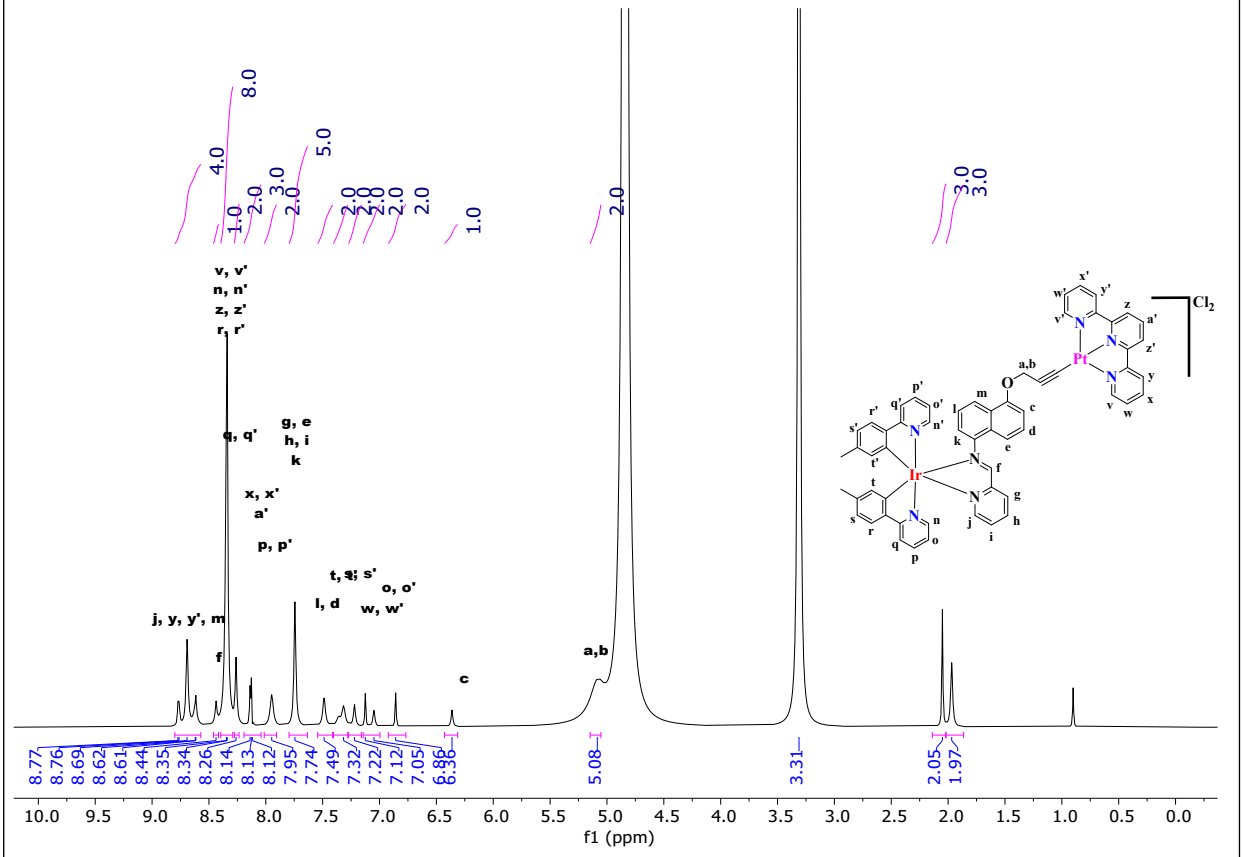
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h, i
k
x, x'
a'
p, p'
t, t'
s, s'
o, o'
l, d
w, w'
j, y, y', m
f
a,b
c
Cl2
Pt
Ir
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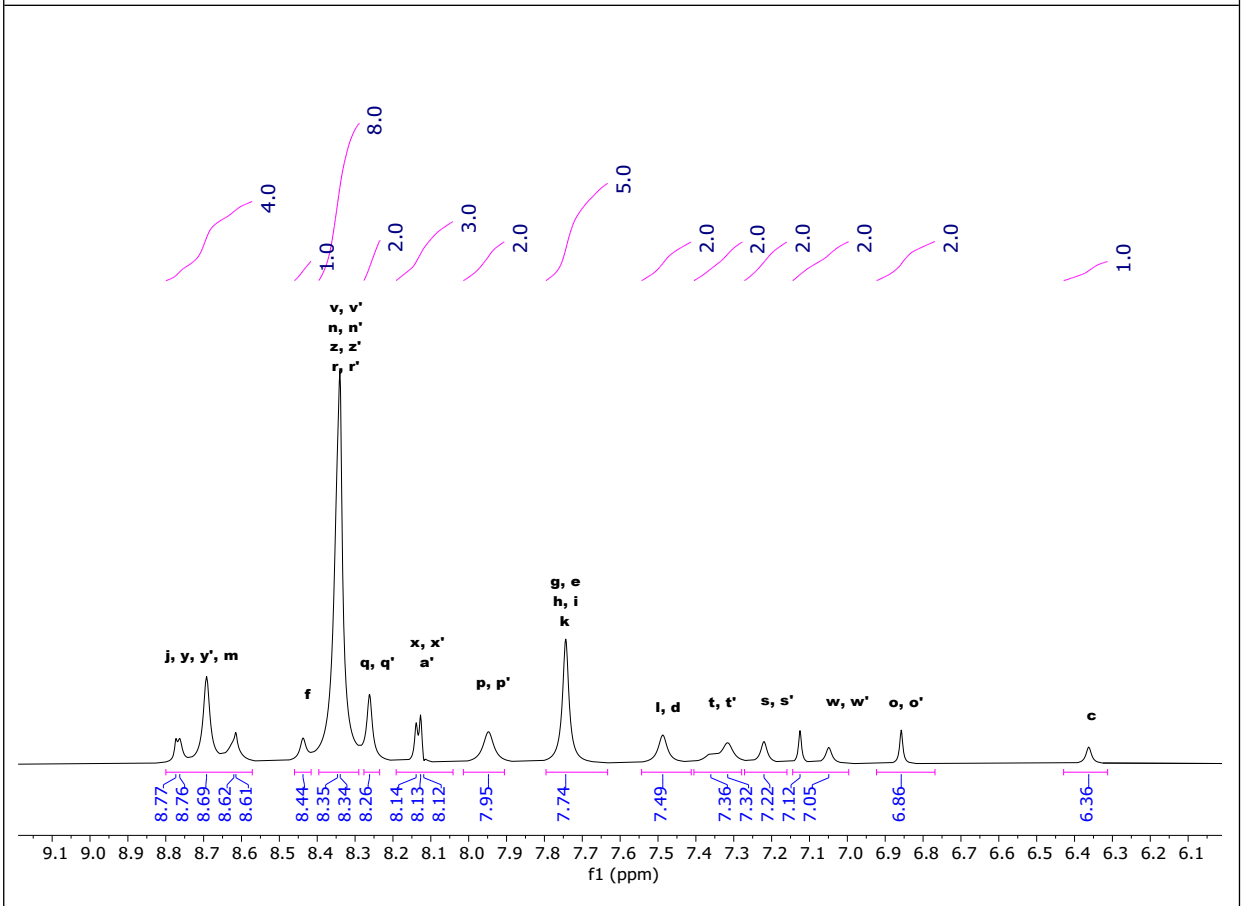
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q, q'
g, e
h, i
k
x, x'
a'
p, p'
t, t'
s, s'
o, o'
l, d
w, w'
j, y, y', m
f
c
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8.61
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8.34
8.26
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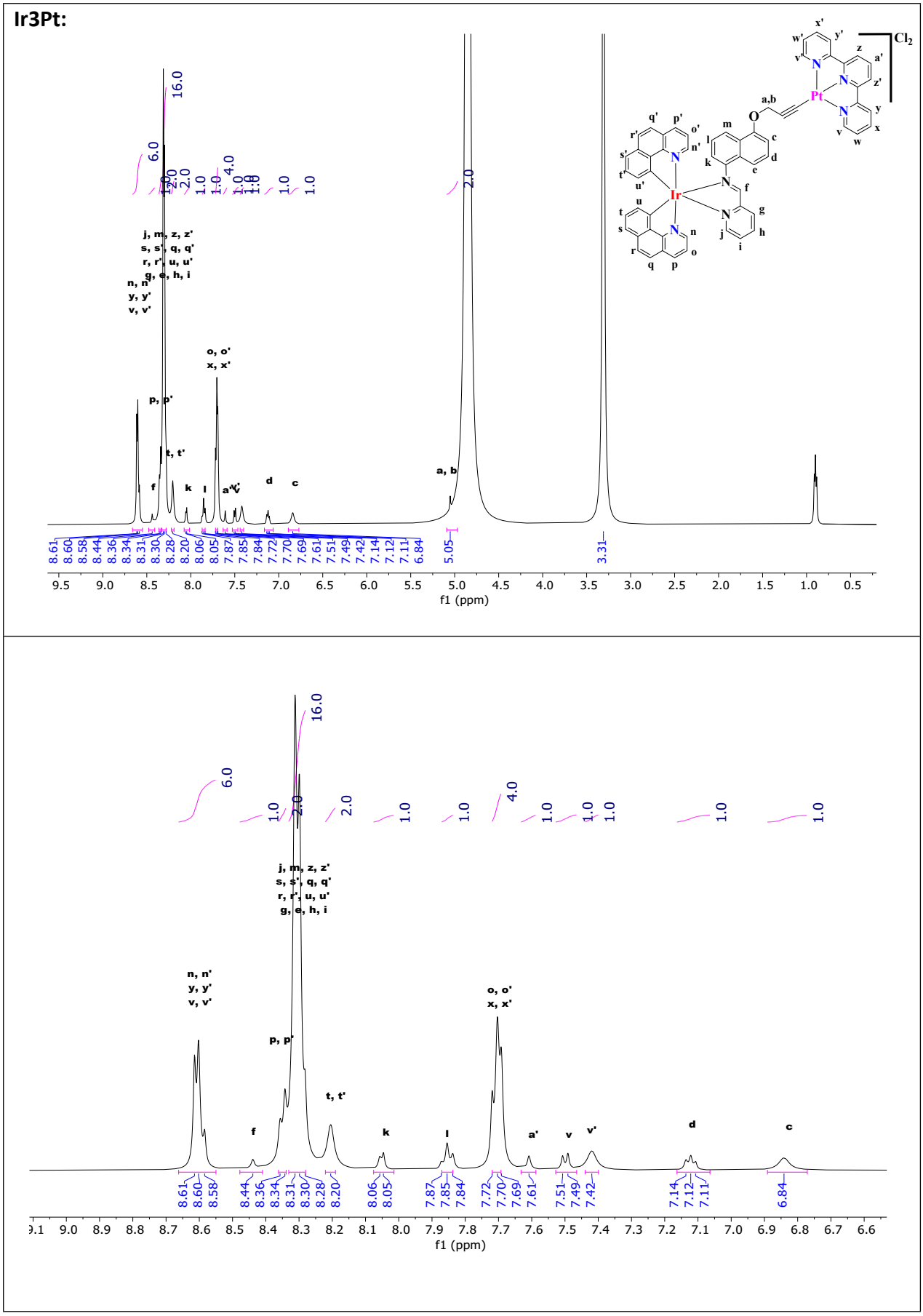
f1 (ppm)

Ir3Pt: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2.0
4.0
1.0
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g, e, h, i
n, n'
y, y'
v, v'
o, o'
x, x'
p, p'
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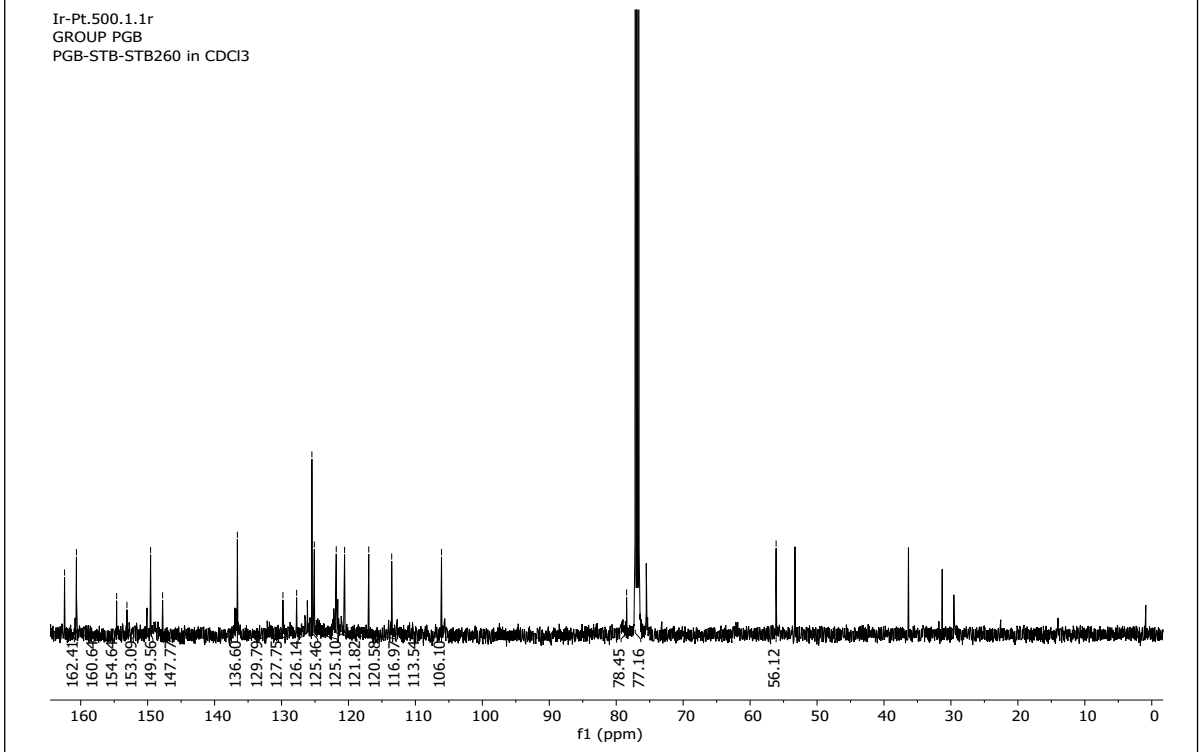
k
l
a'
v
d
c
a, b
3.31
f1 (ppm)

B. ^{13}C NMR spectra

L:



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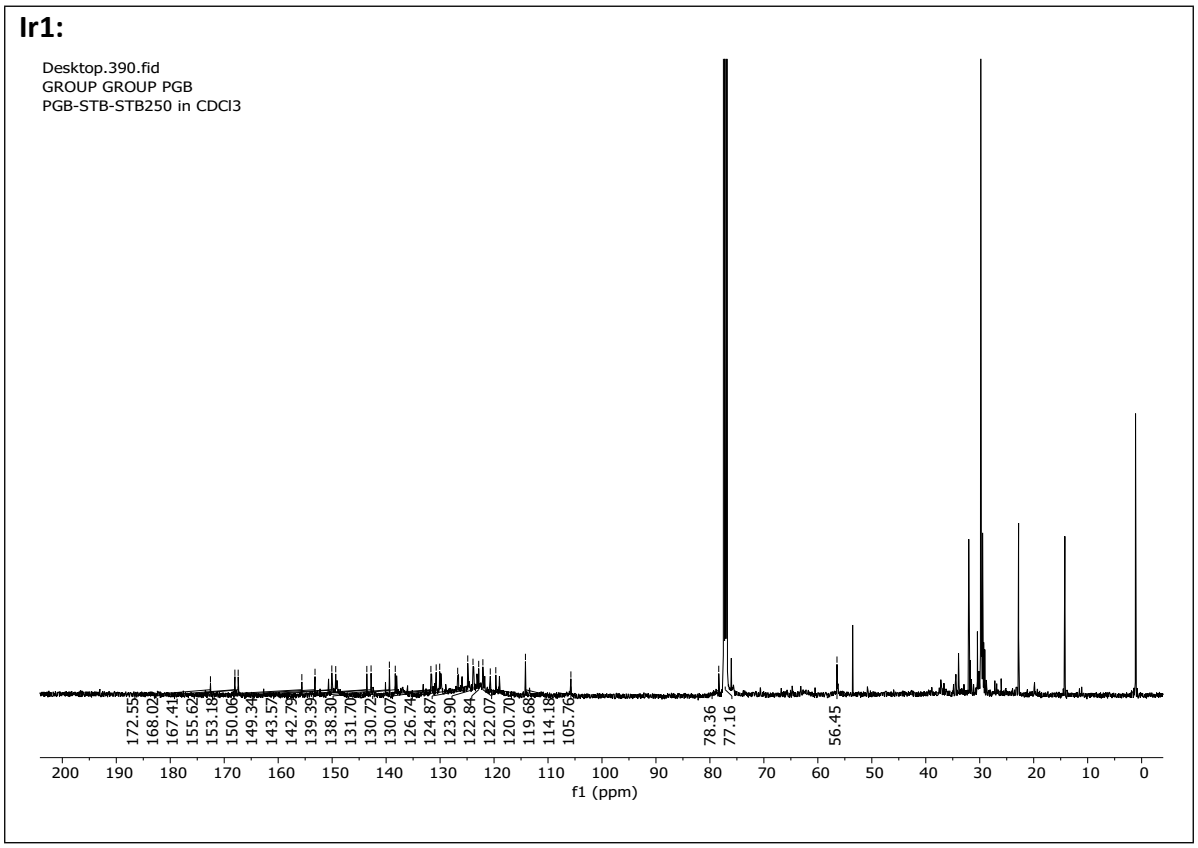

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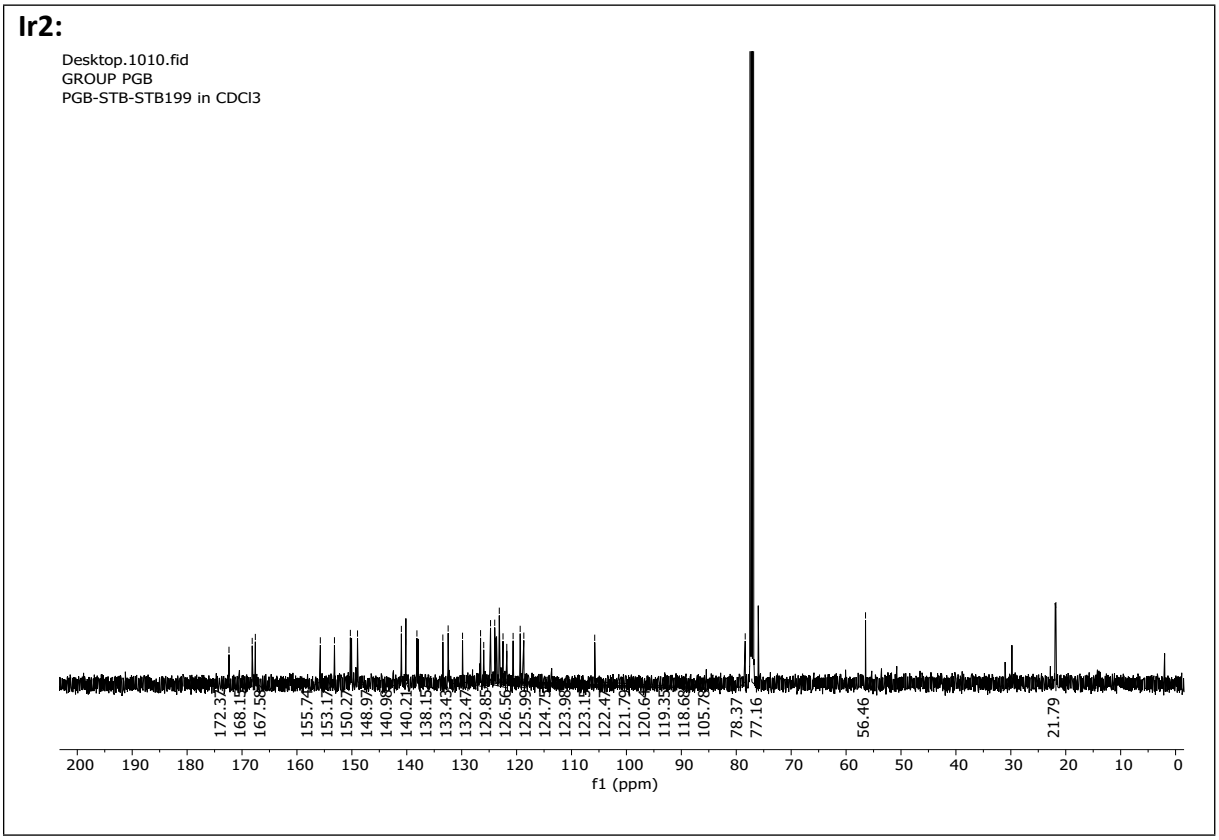
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PGB-STB-STB199 in CDCl3
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155.74
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140.21
138.15
133.43
132.47
129.85
126.56
125.99
124.75
123.96
123.15
122.47
121.79
120.64
119.33
118.69
105.78
78.37
77.16
56.46
21.79
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f1 (ppm)

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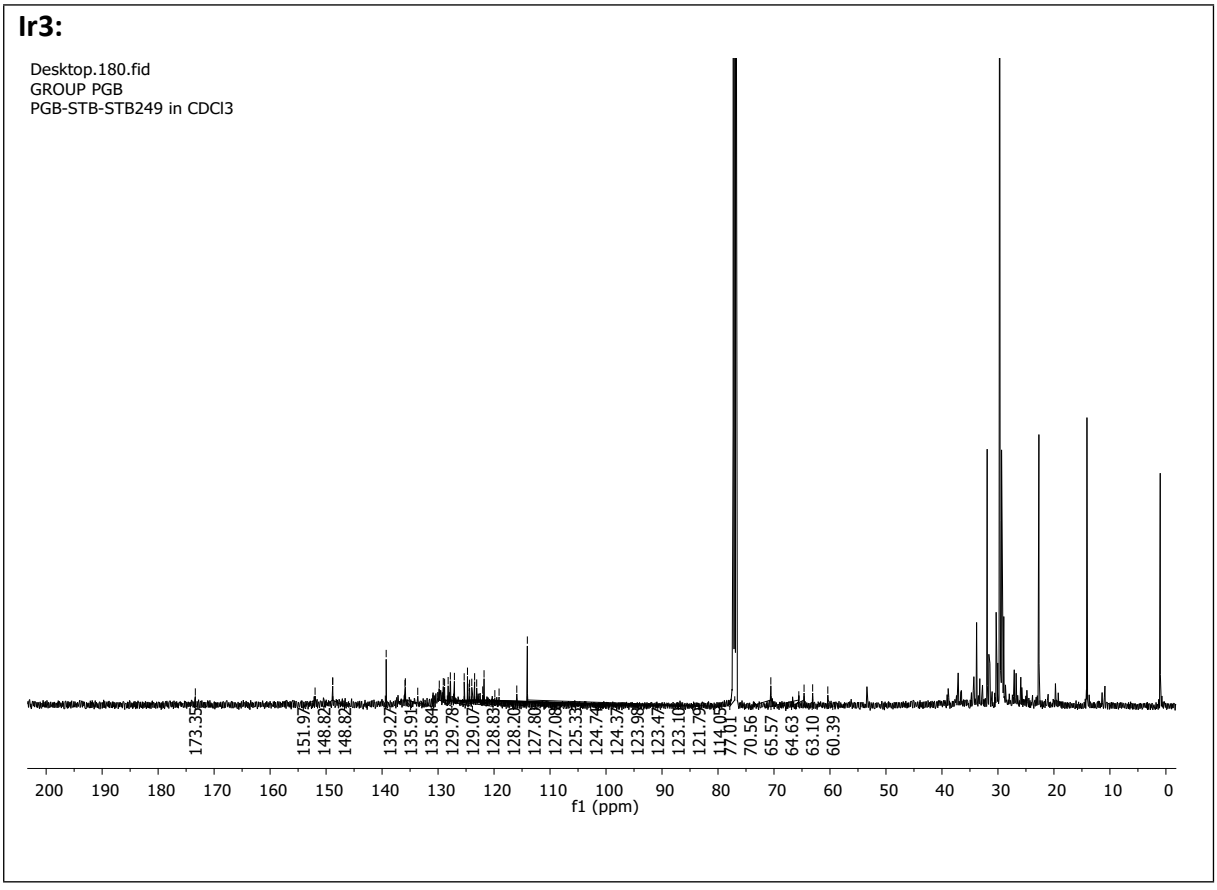
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PGB-STB-STB249 in CDCl3
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128.83
128.20
127.80
127.08
125.33
124.74
124.37
123.98
123.47
123.10
121.79
114.05
77.01
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63.10
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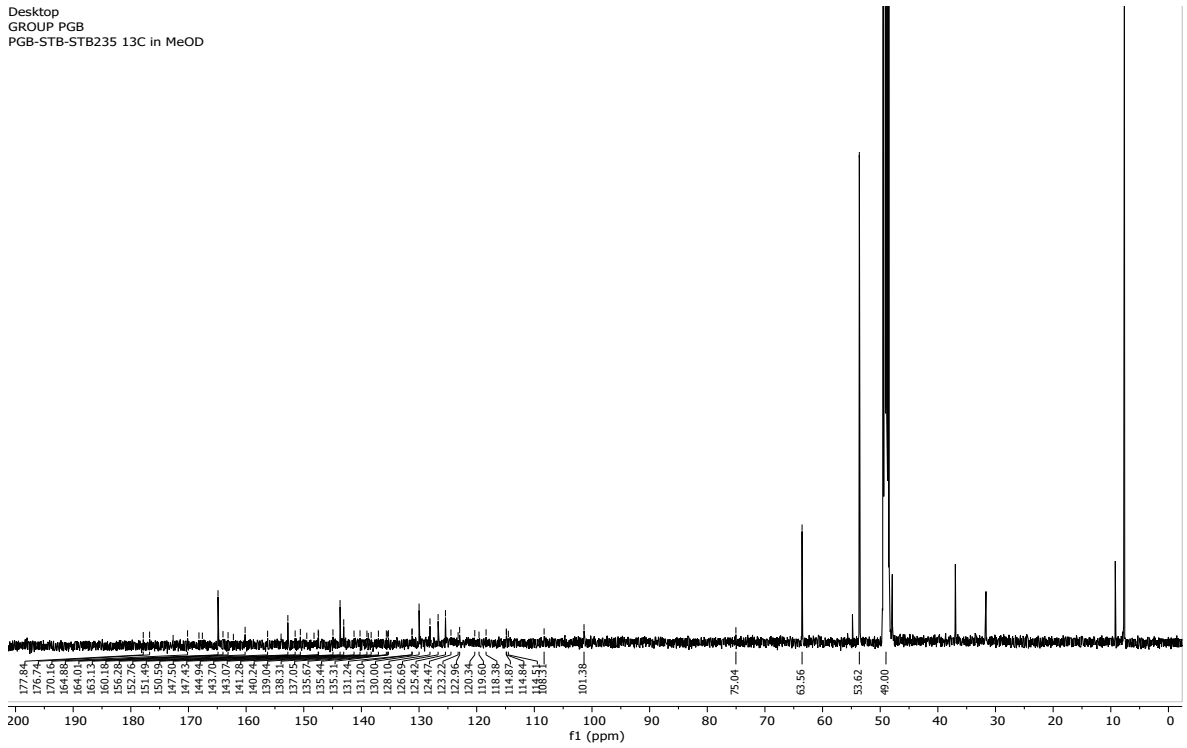
f1 (ppm)

Ir1Pt: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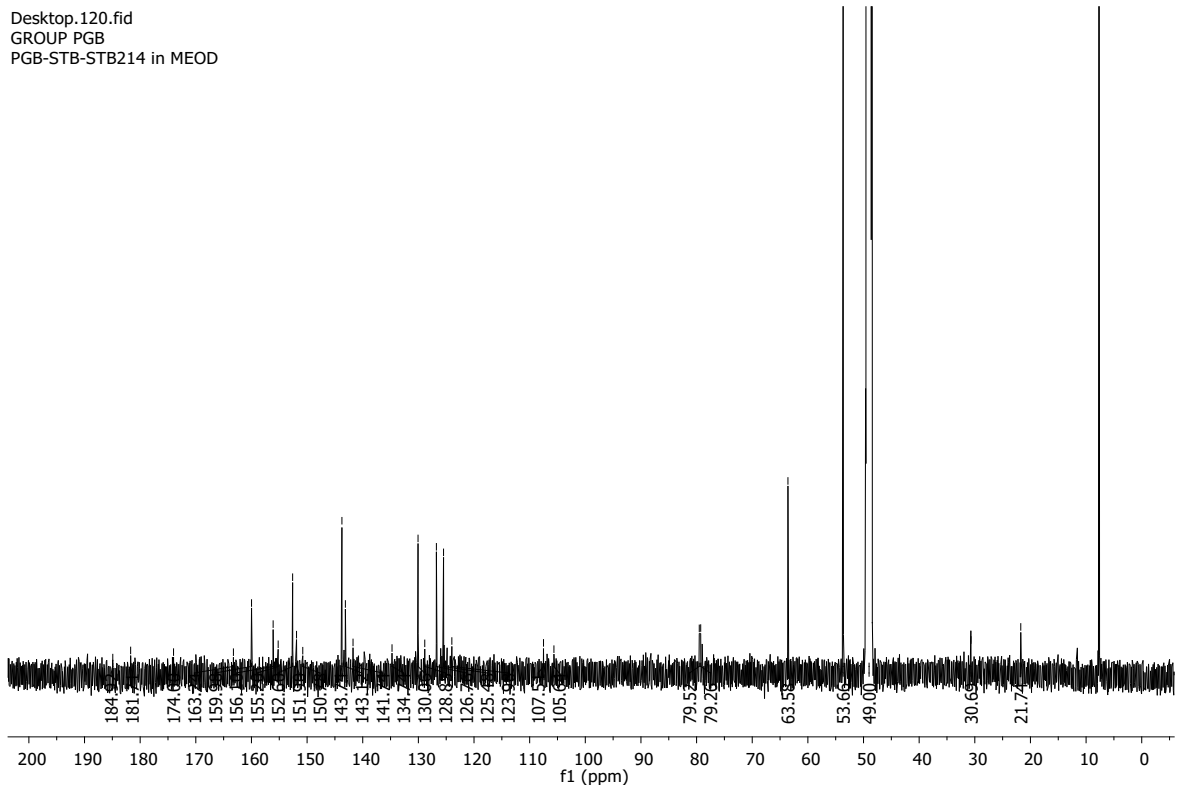
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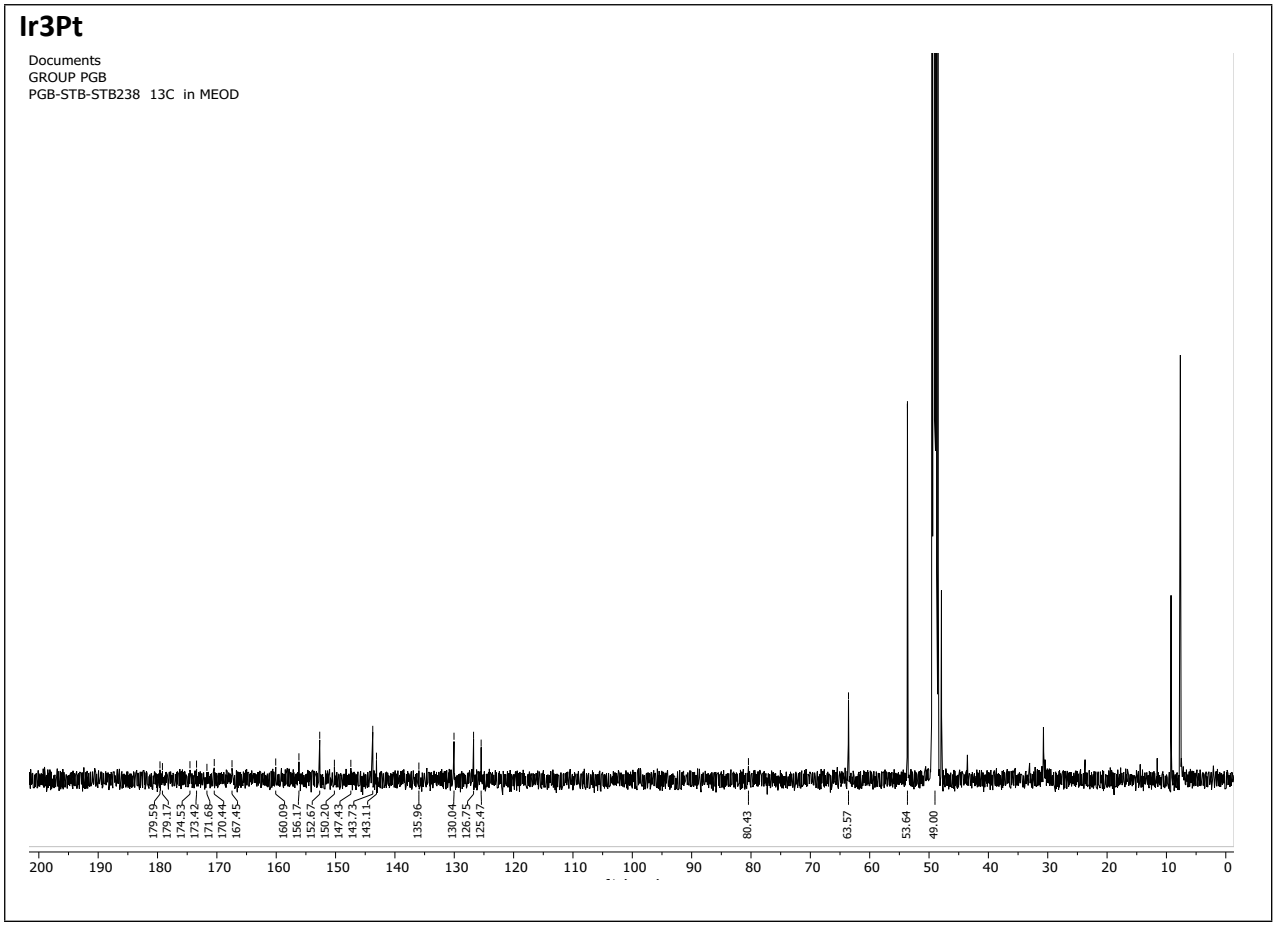
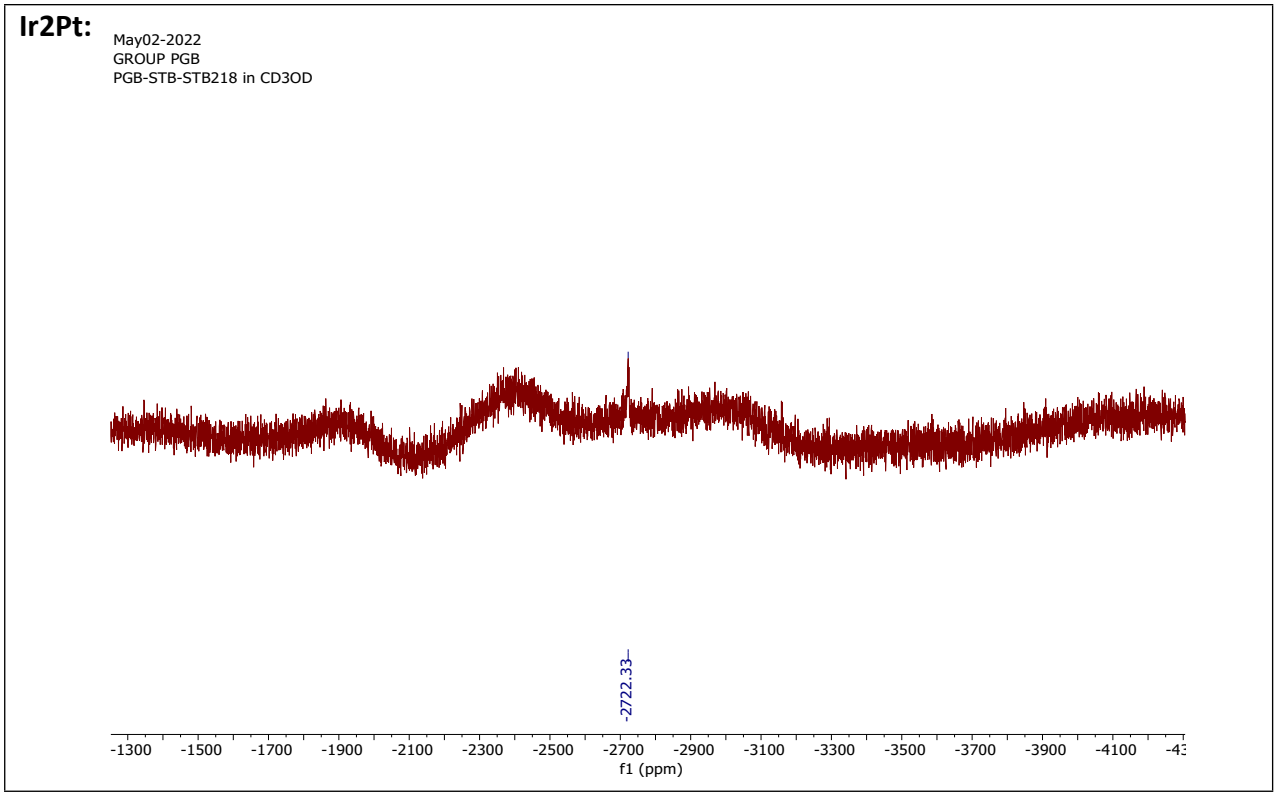


C. ^{195}Pt NMR spectra

Ir2Pt:



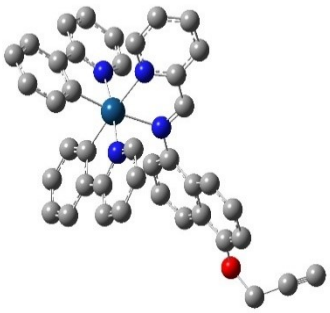
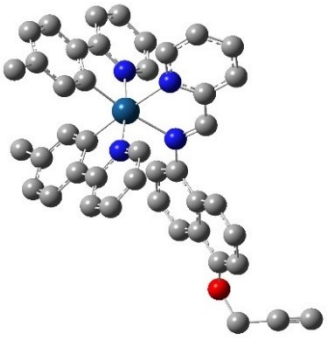
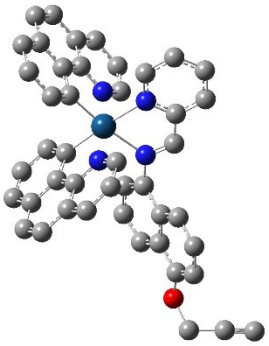
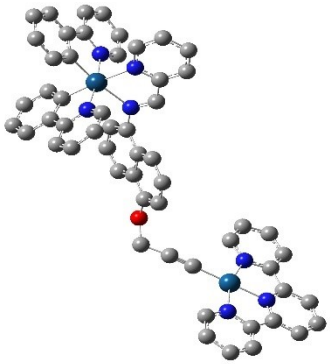
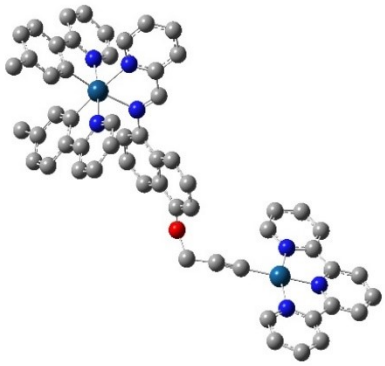
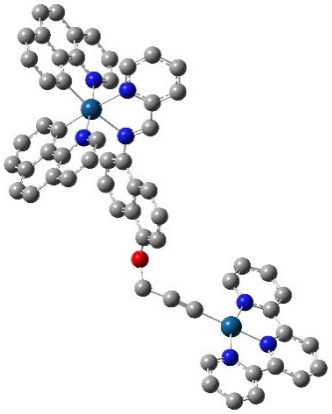
Ir1	Ir2	Ir3
		
Ir1Pt	Ir2Pt	Ir3Pt
		

Figure S3: Geometry optimized structure of Ir1, Ir2, Ir3, Ir1Pt, Ir2Pt and Ir3Pt

Figure S4: The overlaid absorption spectral profile of experimental and theoretical data

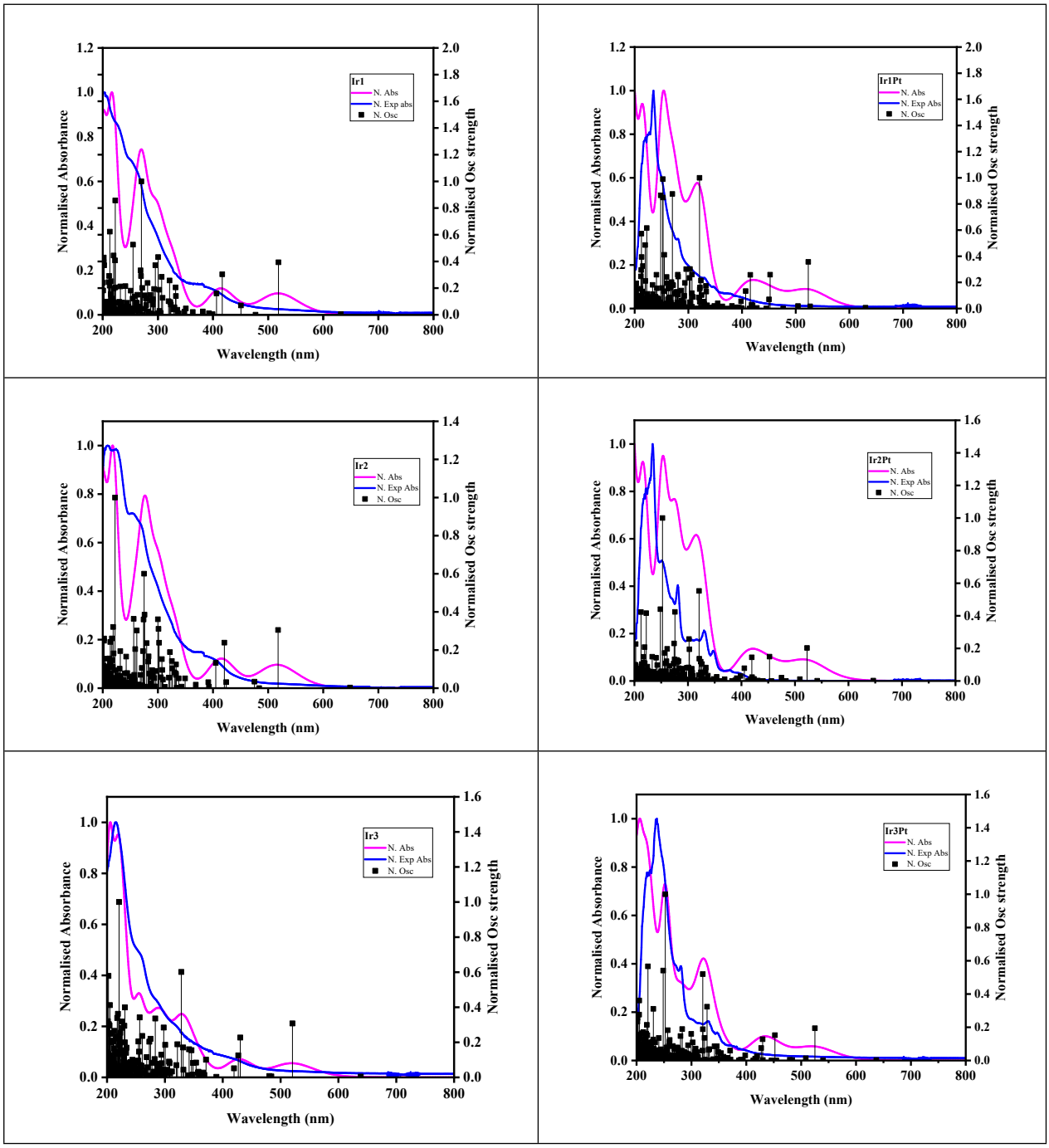
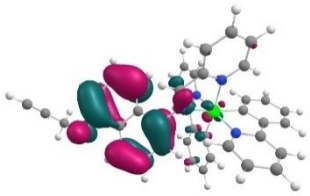
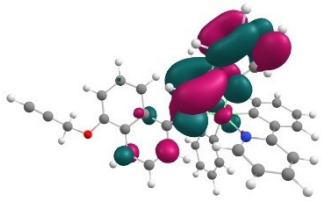
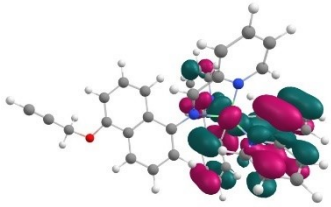
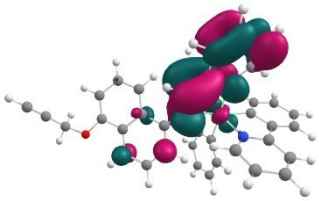
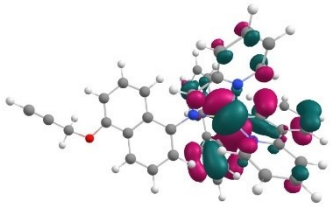
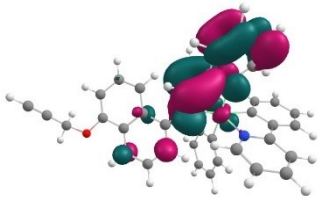
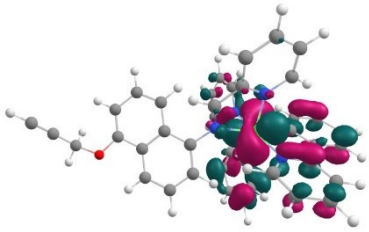
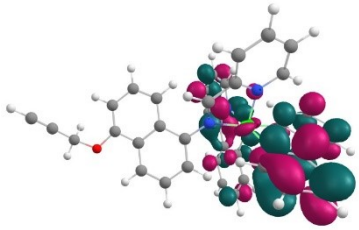
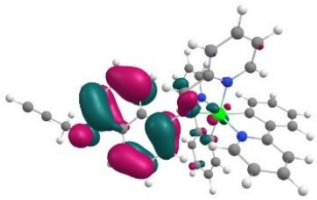
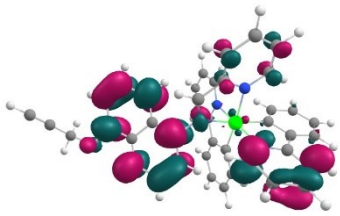
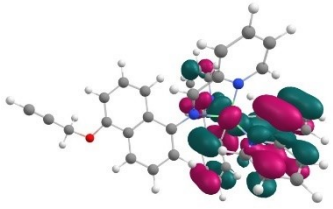
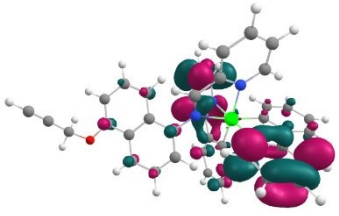
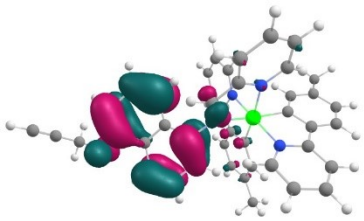
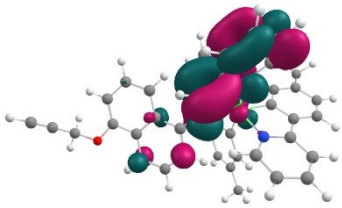
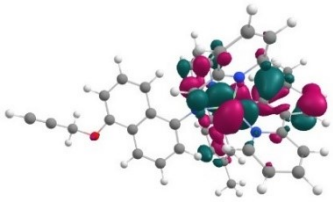
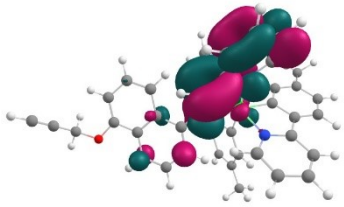
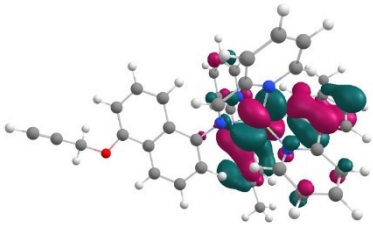
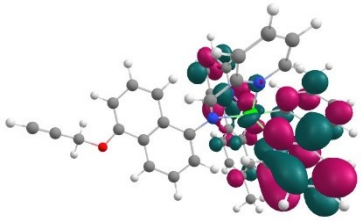
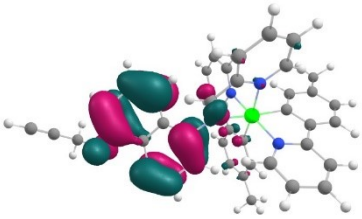
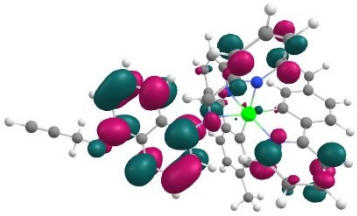
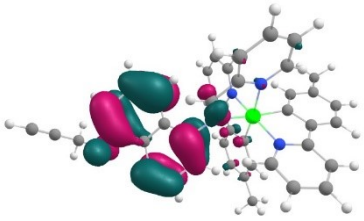
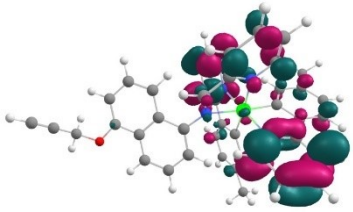
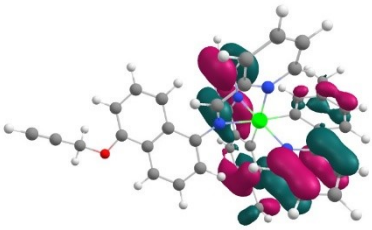
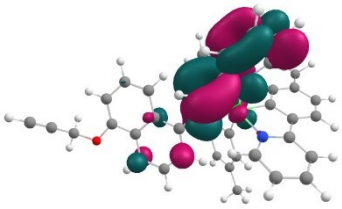
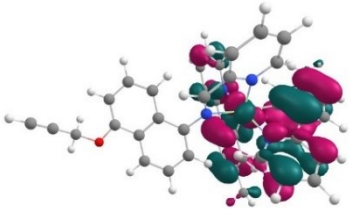
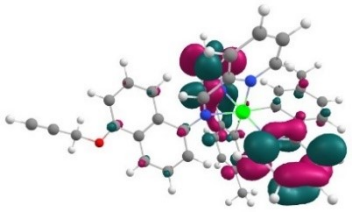
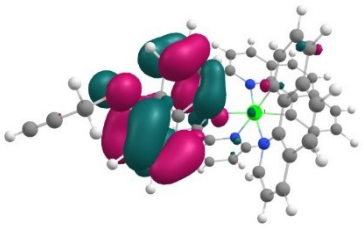
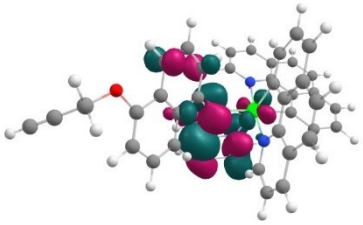
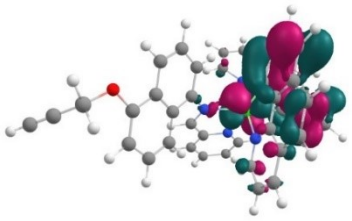
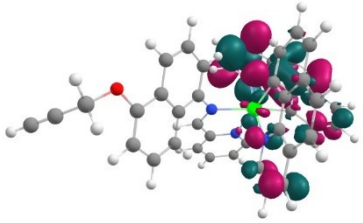
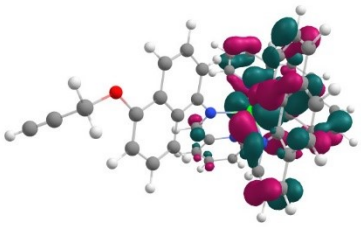
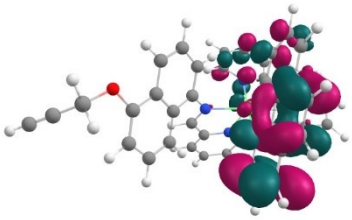
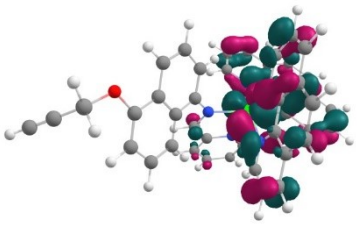
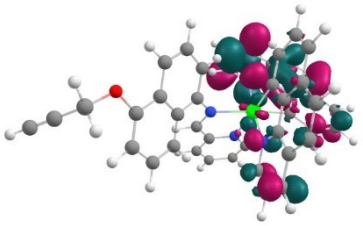
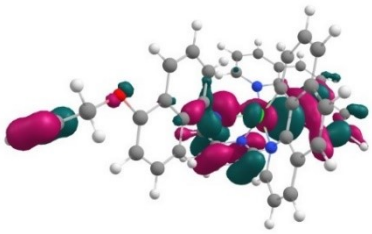
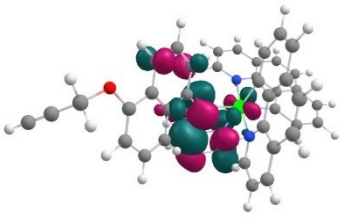
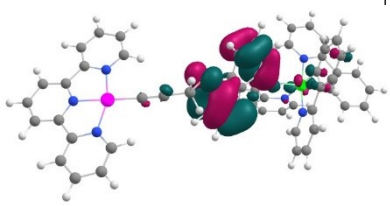
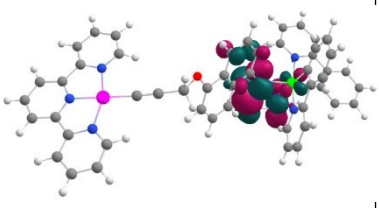
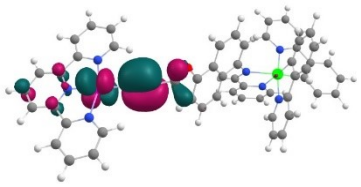
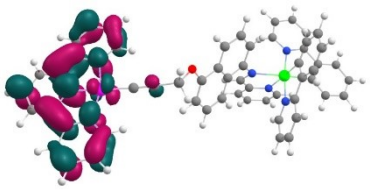
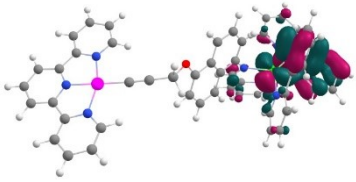
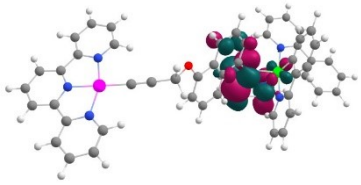
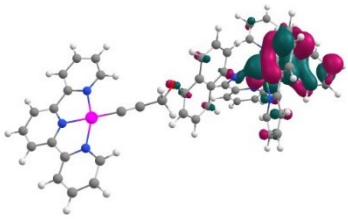
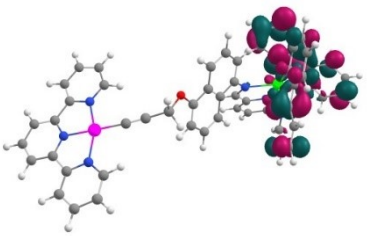
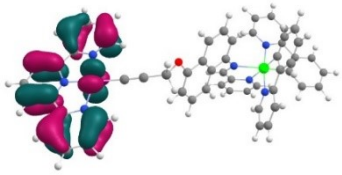
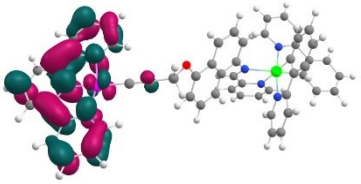
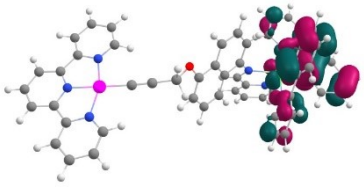
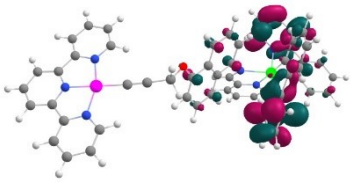
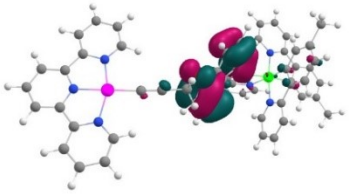
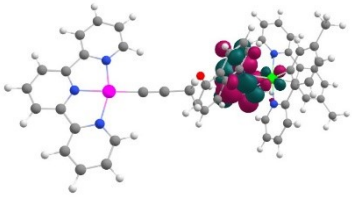
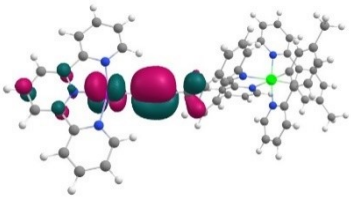
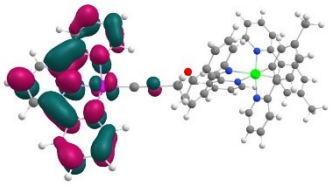


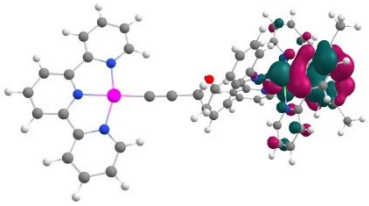
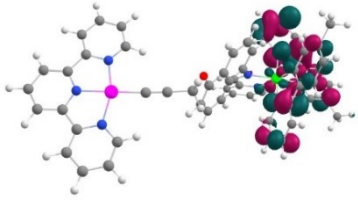
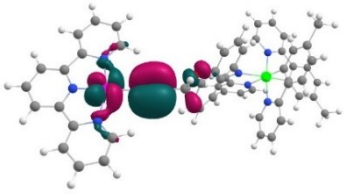
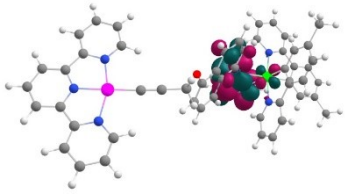
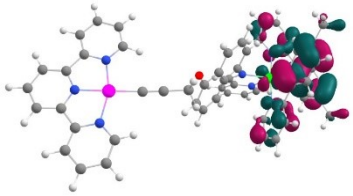
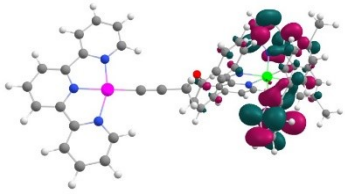
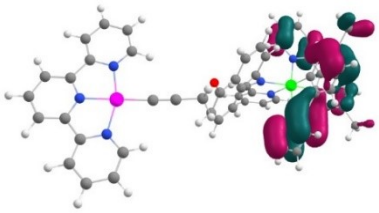
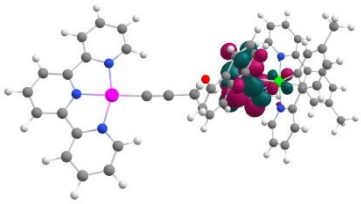
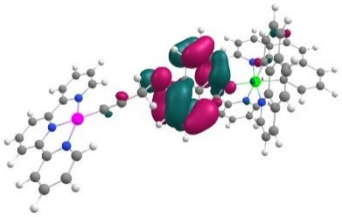
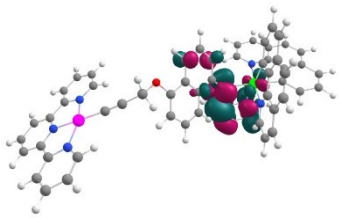
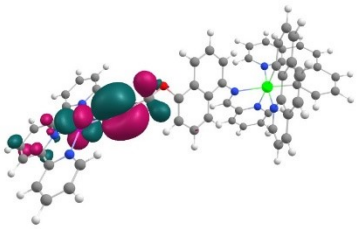
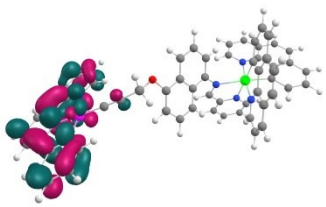
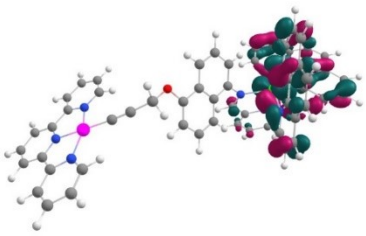
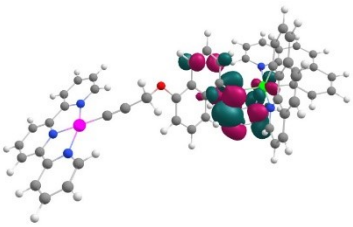
Table S1: Frontier orbital diagram of complexes Ir1, Ir2, Ir3, Ir1Pt, Ir2Pt and Ir3Pt

Absorption			
Ir1	Calculated λ_{Abs}(nm, force constant)		
	518.8492 f = 0.1111 HOMO-1->LUMO		
	450.6713 f = 0.0198 HOMO-2->LUMO		
	416.7816 f = 0.0857 HOMO-4->LUMO		
	332.2103 f = 0.058 HOMO-3->LUMO+1		
	300.4803 f = 0.1221 HOMO-1->LUMO+4		
	270.1946 f = 0.2821 HOMO-2->LUMO+6		

Ir2	Calculated λ_{Abs}(nm, force constant)		
	518.047 f = 0.1099 HOMO-1->LUMO		
	420.6419 f = 0.086 HOMO-5->LUMO		
	405.1109 f = 0.0478 HOMO->LUMO+1		
	300.0295 f = 0.1301 HOMO-1->LUMO+4		
	HOMO-1->LUMO+5		
	275.1108 f = 0.2161 HOMO-13->LUMO		
	HOMO-2->LUMO+6		

Ir3	Calculated λ_{Abs}(nm, force constant)		
	520.5483 f = 0.103 HOMO-1->LUMO		
	426.9722 f = 0.042 HOMO->L+1		
	328.3045 f = 0.2012 H-4->L+2		
	H-4->L+1		
	283.3924 f = 0.1124 HOMO-13->LUMO		
Ir1Pt	Calculated λ_{Abs}(nm, force constant)		
	523.4051 f = 0.1176 HOMO-1->LUMO+1		

	452.398 f = 0.0854 HOMO-4->LUMO		
	415.4409 f = 0.085 HOMO-5->LUMO+1		
	406 f = 0.0441 HOMO>L+3		
	320.8452 f = 0.3298 HOMO-13->LUMO		
	270.3124 f = 0.289 HOMO-2->LUMO+10		
Ir2Pt	Calculated λ_{Abs}(nm, force constant)		
	522.6108 f = 0.1205 HOMO-1->LUMO+1		
	452.5466 f = 0.0888 HOMO-4->LUMO		

	405.5217 f = 0.0465 HOMO->LUMO+3		
	353.7655 f = 0.0151 HOMO-8->LUMO+1		
	275.7288 f = 0.2522 HOMO-2->LUMO+10		
	HOMO-17->LUMO+1		
Ir3Pt	Calculated λ_{Abs}(nm, force constant)		
	525.1342 f = 0.1131 HOMO-1->LUMO+1		
	452.2 f = 0.0889 HOMO-4->LUMO		
	429.7844 f = 0.0747 HOMO-5->LUMO+1		

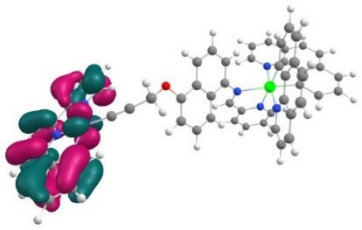
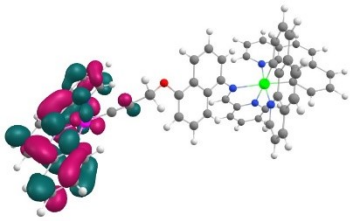
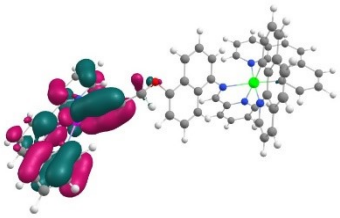
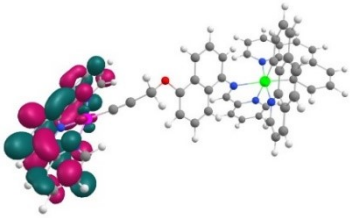
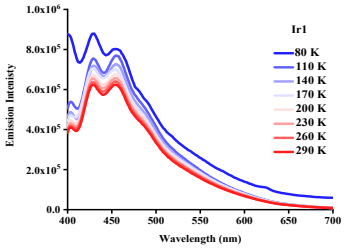
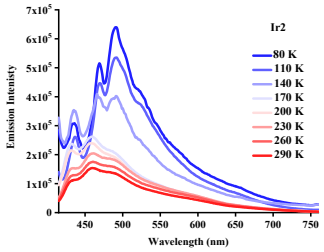
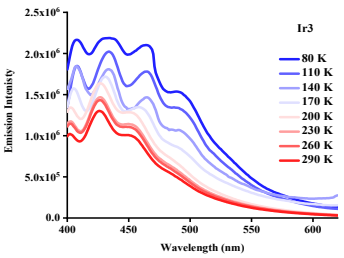
	320.7373 f = 0.303 HOMO-14->LUMO		
	252.3749 f = 0.5829 HOMO-18->LUMO+2		

Figure S5: Temperature dependent (290 – 80 K) emission spectra of

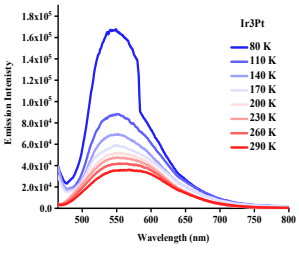
A: Ir1 -Ir3 in Acetonitrile: MeTHF (λ_{ex} = 380 - 400 nm)

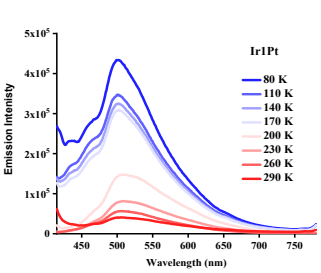


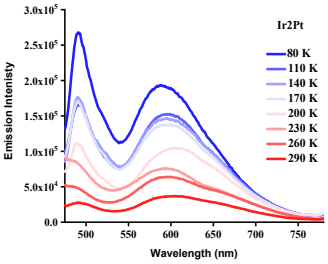




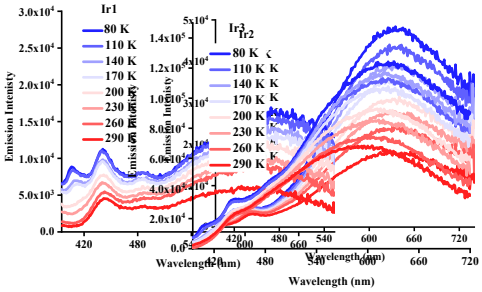
B: Ir1Pt -Ir3Pt in Acetonitrile: MeTHF (λ_{ex} = 380 - 400 nm)



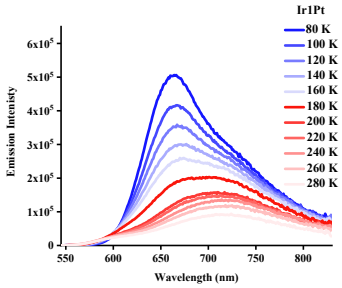


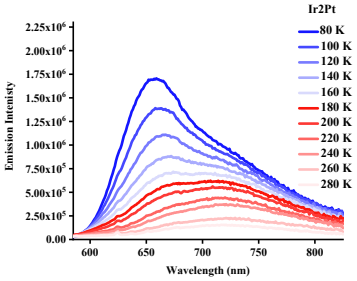


C: Ir1 -Ir3 in solid state (Thin film on glass) (λ_{ex} = 400 nm)



D: Ir1Pt -Ir3Pt in solid state (λ_{ex} = 500 nm, Thin film on glass)





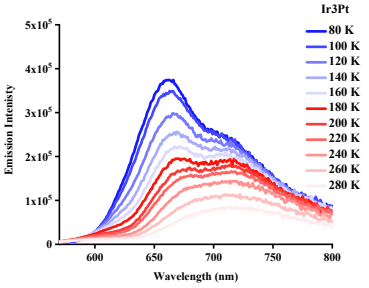


Figure S6: Concentration dependent AIE of Ir1Pt – Ir3Pt

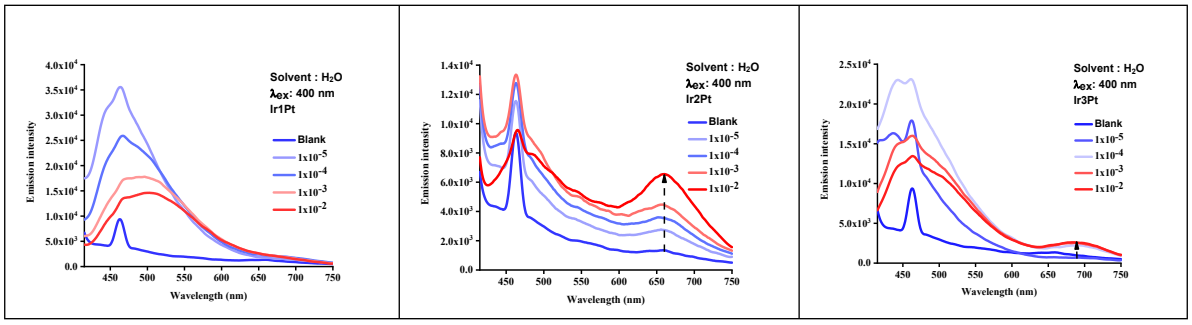
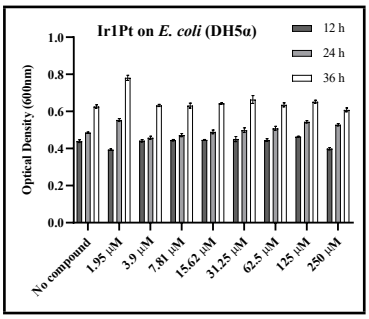
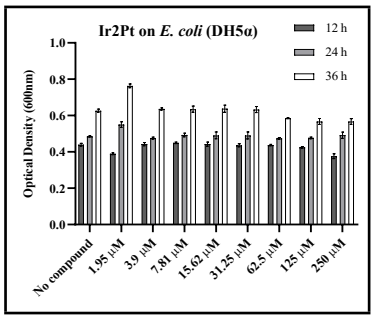


Figure S7: Toxicity of Ir1Pt, Ir2Pt & Ir3Pt on *E. coli* (DH5α)





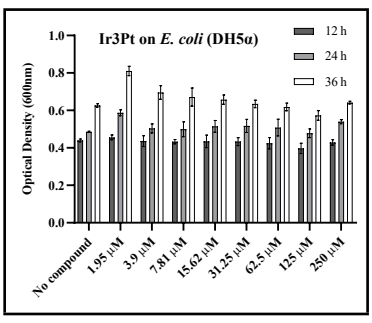
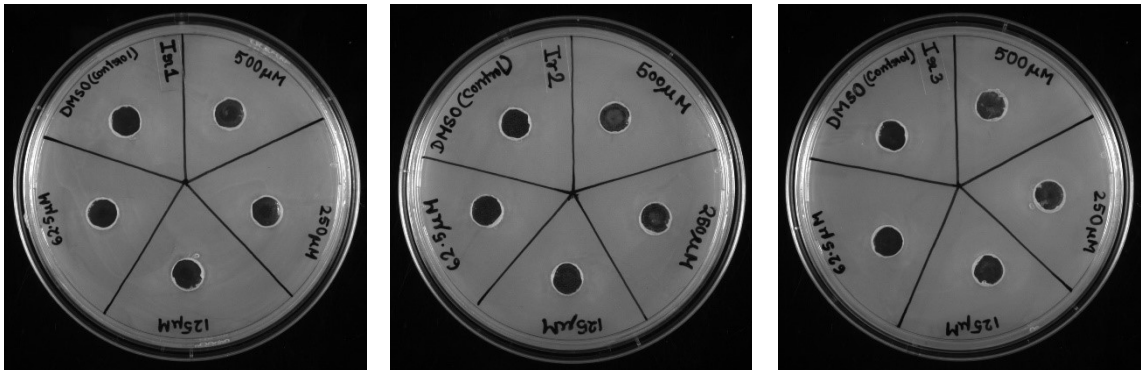
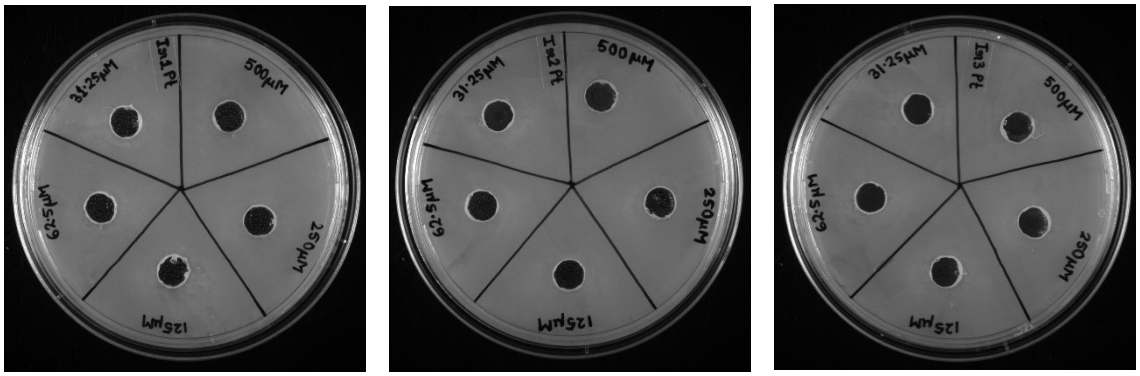


Figure S8: Agar well diffusion assay using A. mononuclear B. dinuclear complexes



A.



B.