Electronic Supplementary Material (ESI) for Dalton Transactions.

Cyclometalated Trinuclear Ir(III)/Pt(II) Complex as a Luminescent probe for Histidine-rich Proteins and Its Application as a Protein Staining Agent

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Figure S1: A) ESI-MS B) ^{1}HNMR spectrum C) ^{13}C NMR spectrum of complex **2**

Figure S2:A) ESI-MS B) ^{1}HNMR spectrum C) ^{13}C NMR spectrum of complex **3**

Figure S3: ESI-MS of complex **3** + L-histidine-methyl ester

Figure S4: Plot of concentration of histidine added to Complex 3 solution (10^{-5}M) against emission intensity

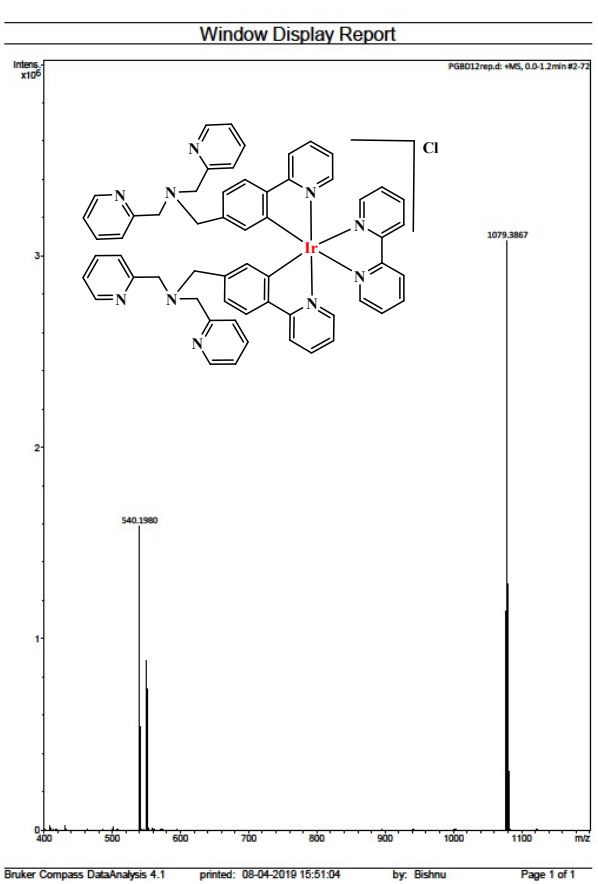
Figure S5: Titration of complex 3 with a) N-Boc-L-Histidine b) L-Histidine Methyl ester

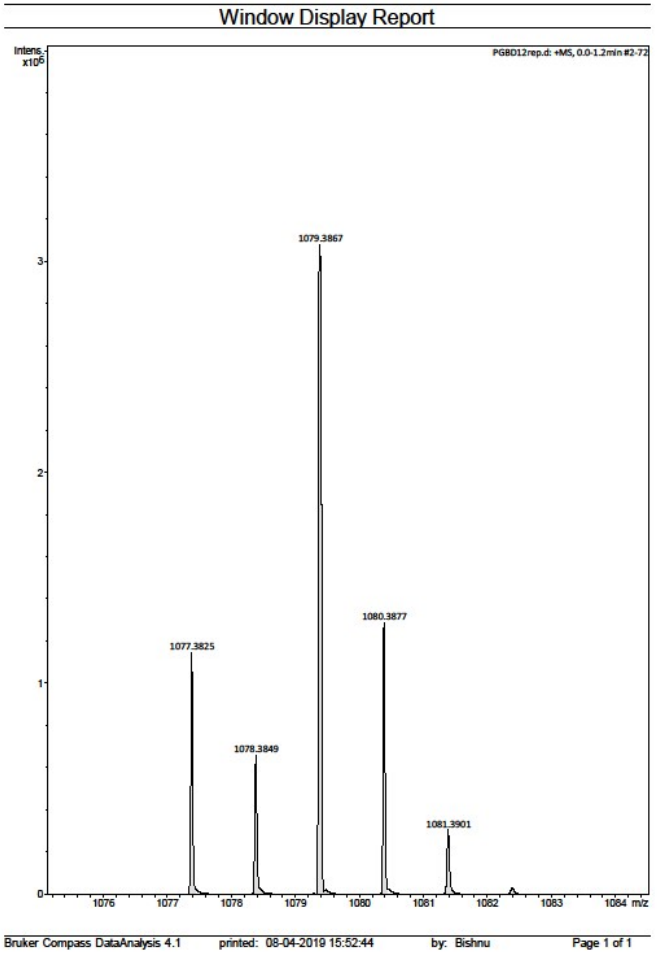
Figure S6: A)**3**+ histidinewith increasing cysteine concentrationB) **3** + cysteine with increasing histidine concentration

Table S1: Frontier orbital diagram of complexes **1**, **2** and **3**

Figure S1: a) ESI-MS b) ^{1}HNMR spectrum c) ^{13}C NMR spectrum of **complex 2**

a)





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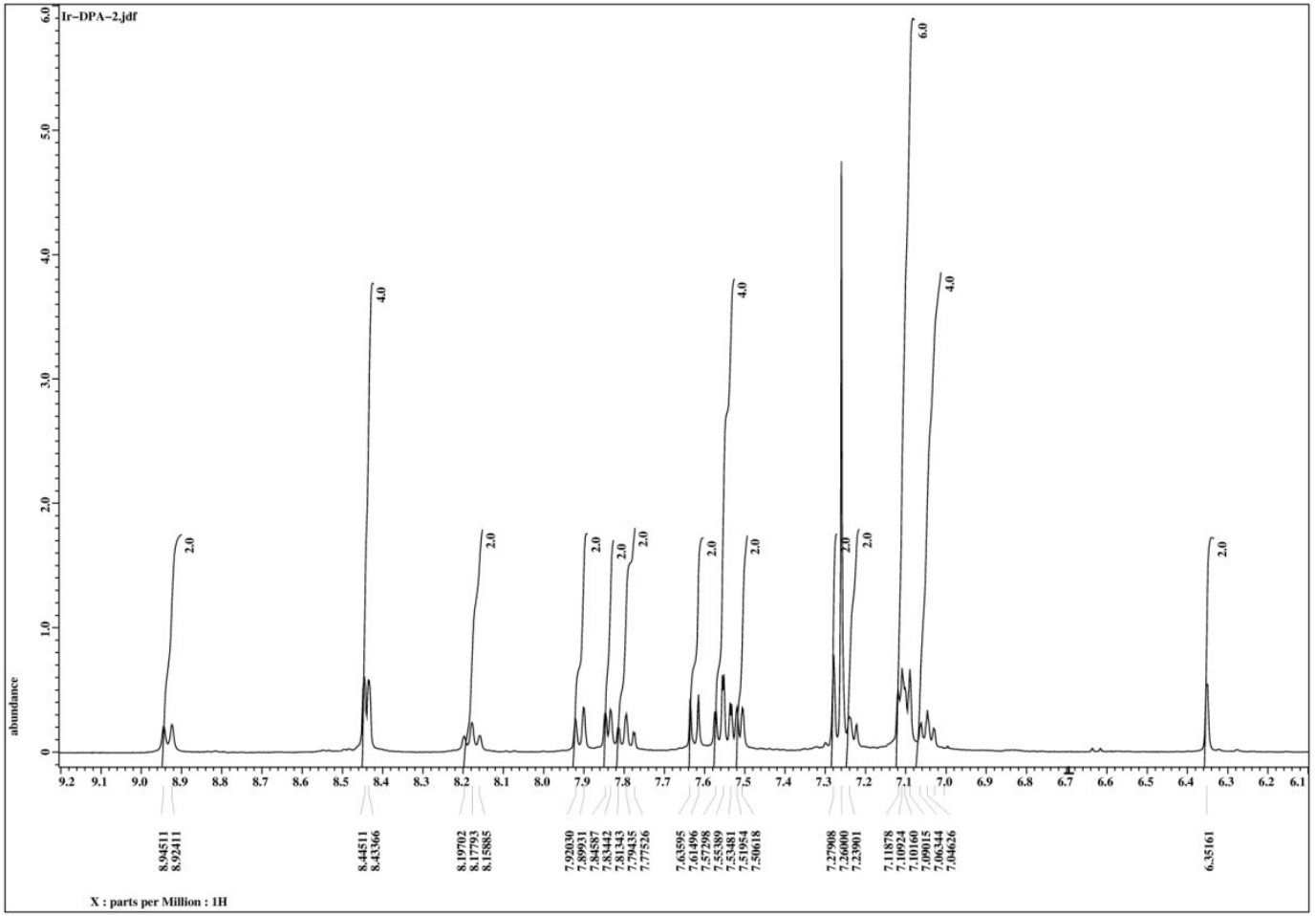
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abundance
X : parts per Million : 1H
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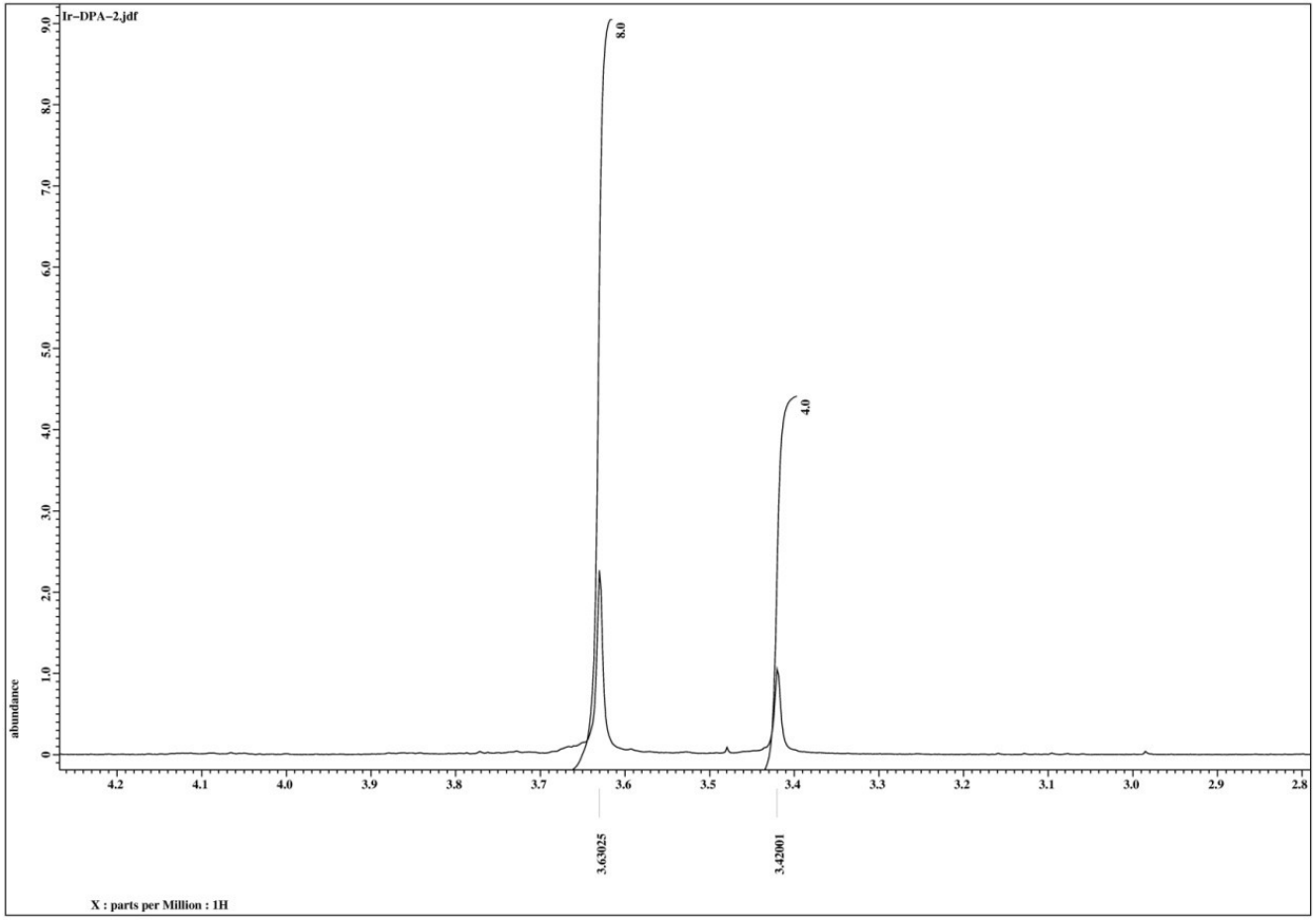
8.92411
8.44511
8.43366
8.19702
8.17793
8.15885
7.92030
7.89931
7.84587
7.83442
7.81343
7.79435
7.77526
7.63595
7.61496
7.57298
7.55389
7.53481
7.51954
7.50618
7.27908
7.26000
7.23901
7.11878
7.10924
7.10160
7.09015
7.06114
7.04626
6.35161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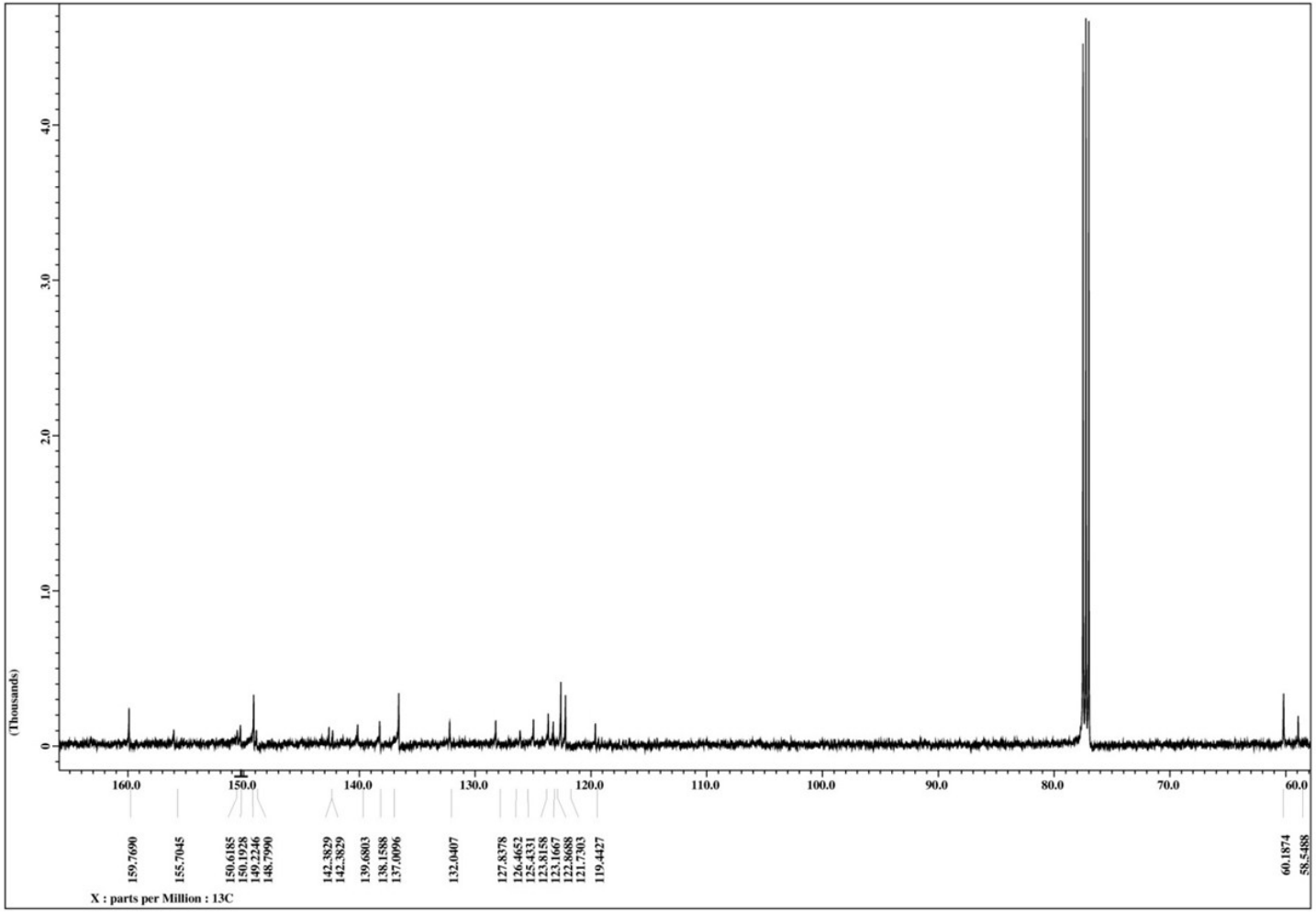
8.0
4.0
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
4.2
4.1
4.0
3.9
3.8
3.7
3.6
3.5
3.4
3.3
3.2
3.1
3.0
2.9
2.8
3.63025
3.42001
X : parts per Million : 1H

C)


(Thousands)
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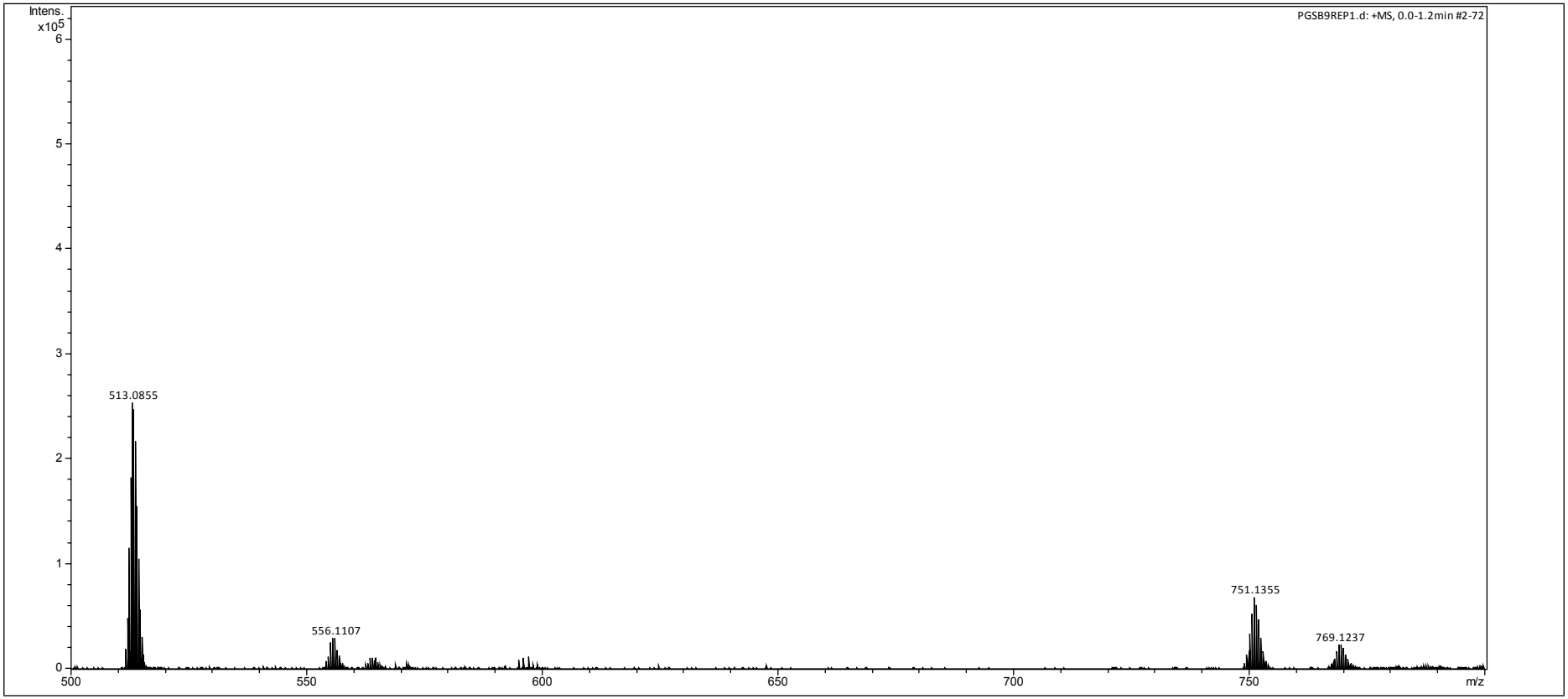
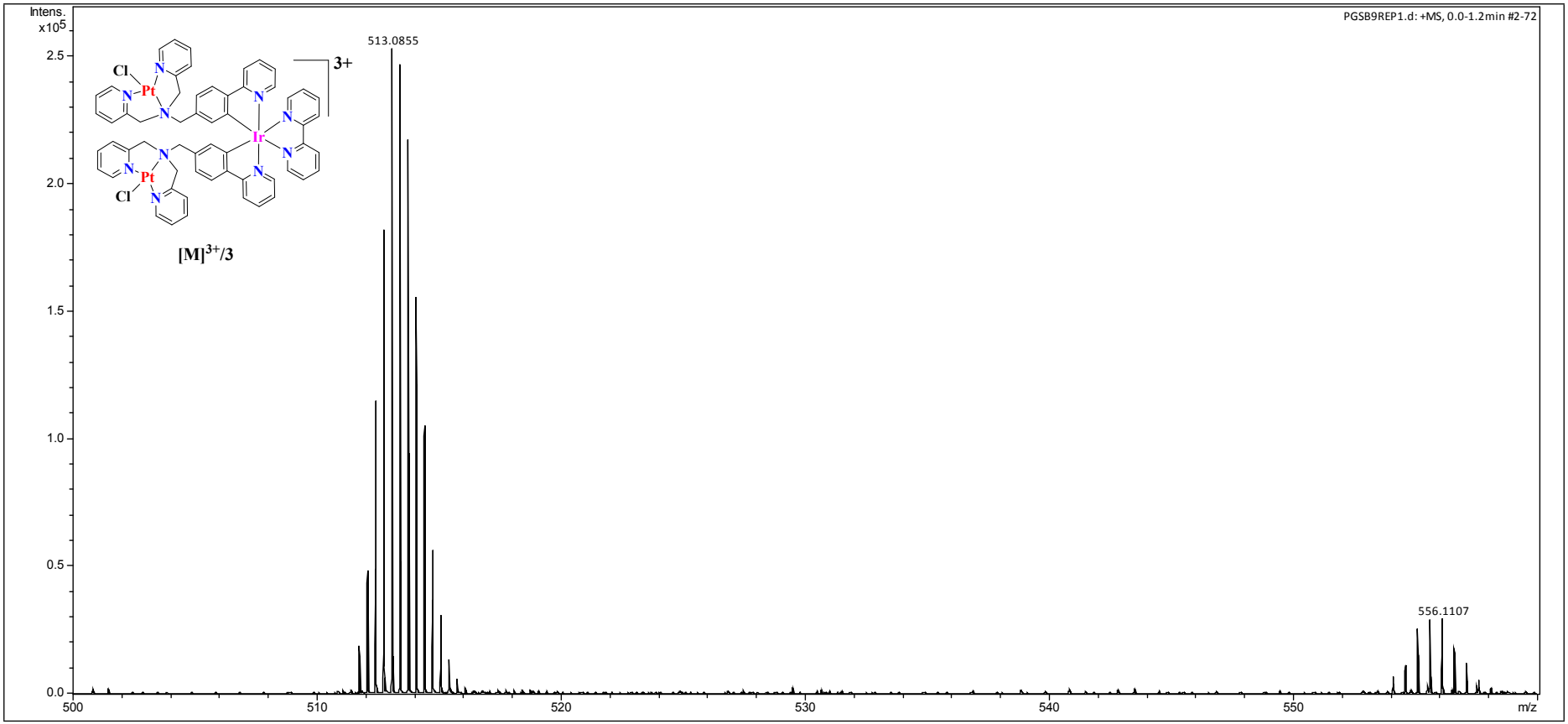
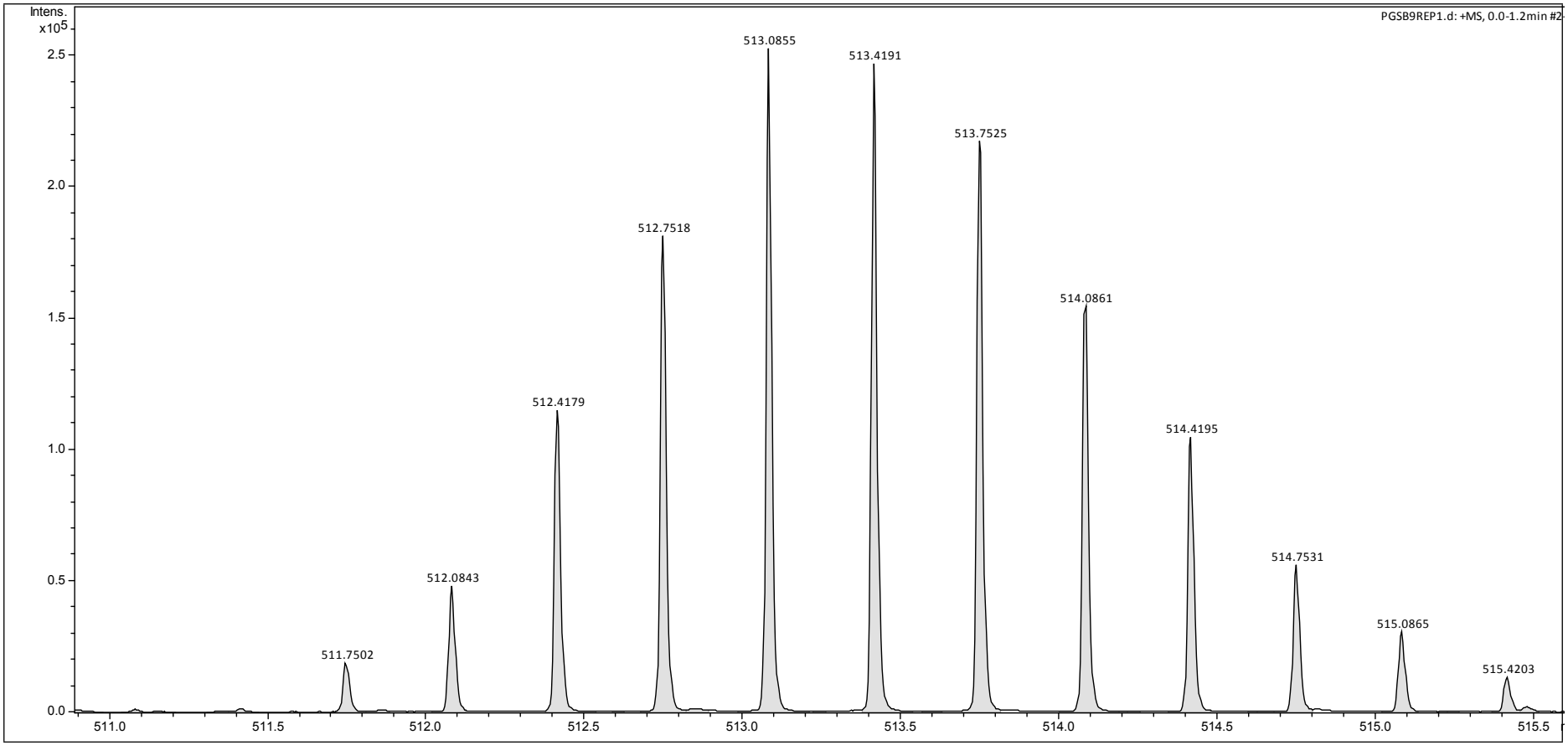
3.0
2.0
1.0
0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
159.7690
155.7045
150.6185
150.1928
149.2246
148.7990
142.3829
142.3829
139.6803
138.1588
137.0096
132.0407
127.8378
126.4652
125.4331
123.8158
123.1667
122.8688
121.7303
119.4427
60.1874
58.5488
X : parts per Million : 13C

Figure S2: a) ESI-MS b) ^{1}HNMR spectrum c) ^{13}C NMR spectrum of complex 3

a) ESI-MS




Intens.
x10^5
2.5
2.0
1.5
1.0
0.5
0.0
500
510
520
530
540
550
m/z
PGSB9REP1.d: +MS, 0.0-1.2min #2-72
513.0855
556.1107
3+
[M]3+/3


Intens.
x10^5
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2.0
1.5
1.0
0.5
0.0
511.7502
512.0843
512.4179
512.7518
513.0855
513.4191
513.7525
514.0861
514.4195
514.7531
515.0865
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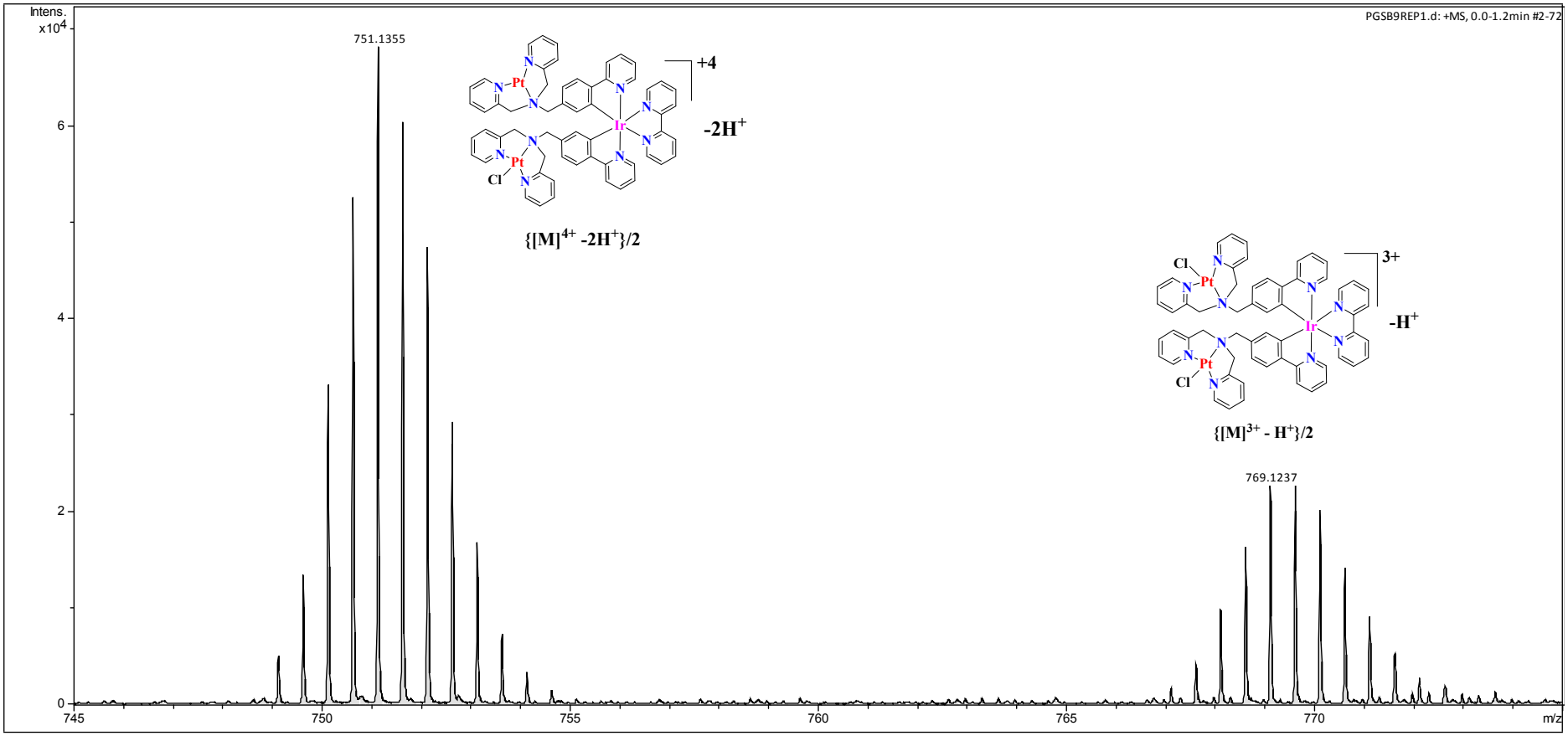
513.0
513.5
514.0
514.5
515.0
515.5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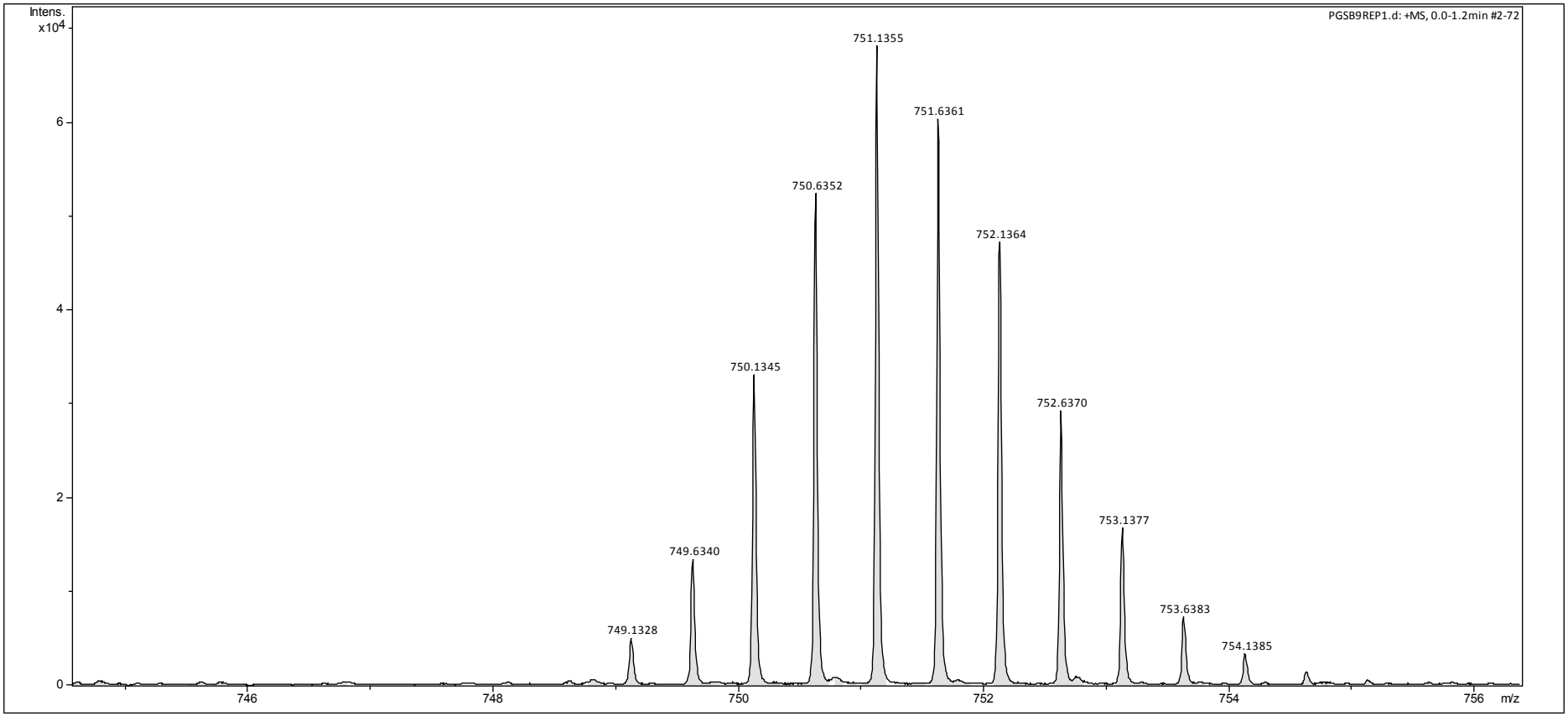
x10^4
PGSB9REP1.d: +MS, 0.0-1.2min #2-72
751.1355
+4
-2H+
{[M]4+ -2H+}/2
3+
-H+
{[M]3+ - H+}/2
769.1237
0
2
4
6
745
750
755
760
765
770
m/z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x10^4
PGSB9REP1.d: +MS, 0.0-1.2min #2-72
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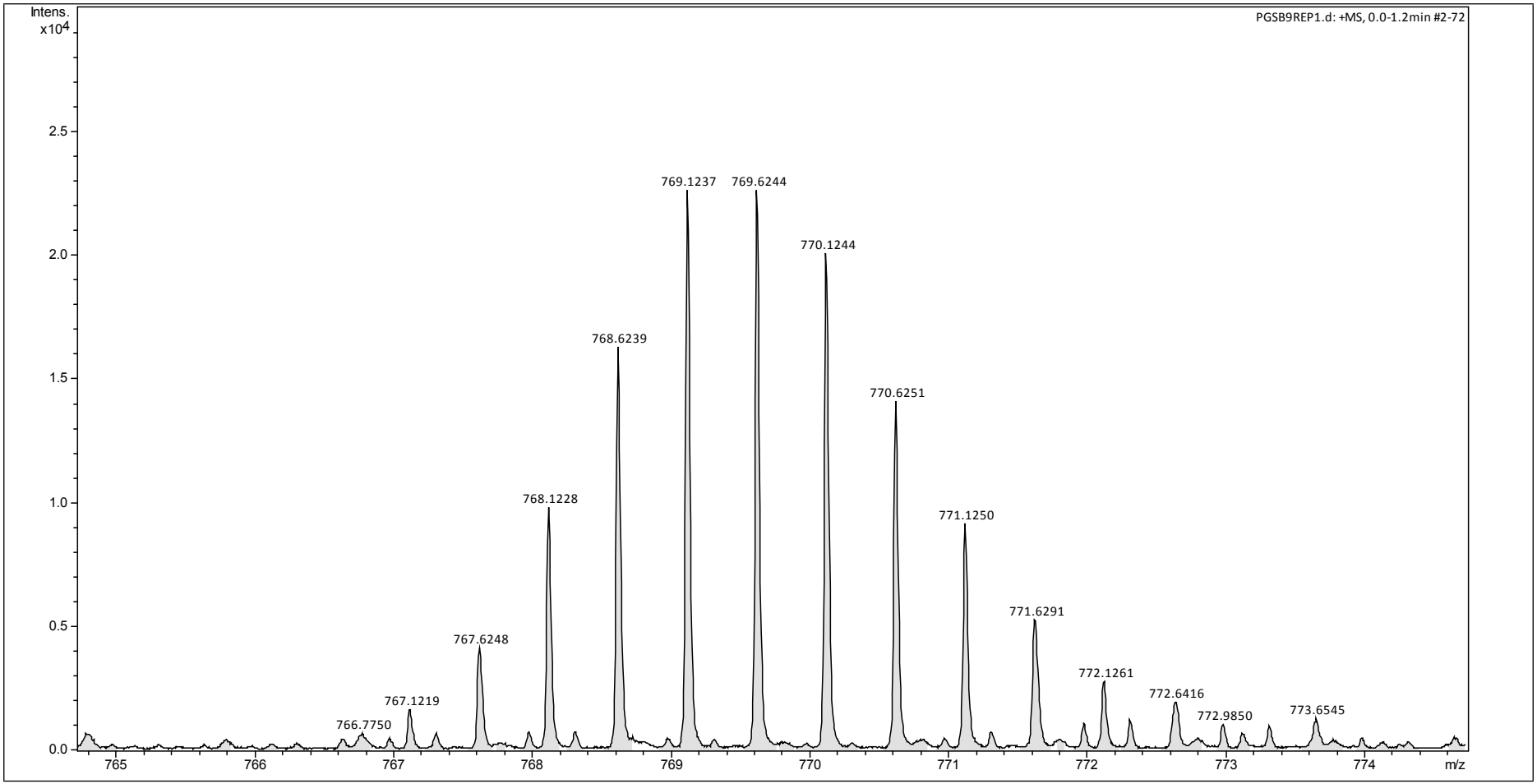
751.6361
750.6352
752.1364
750.1345
752.6370
753.1377
749.6340
753.6383
749.1328
754.1385
0
2
4
6
746
748
750
752
754
756
m/z


Intens.
x10^4
PGSB9REP1.d: +MS, 0.0-1.2min #2-72
2.5
2.0
1.5
1.0
0.5
0.0
765
766
767
768
769
770
771
772
773
774
m/z
766.7750
767.1219
767.6248
768.1228
768.6239
769.1237
769.6244
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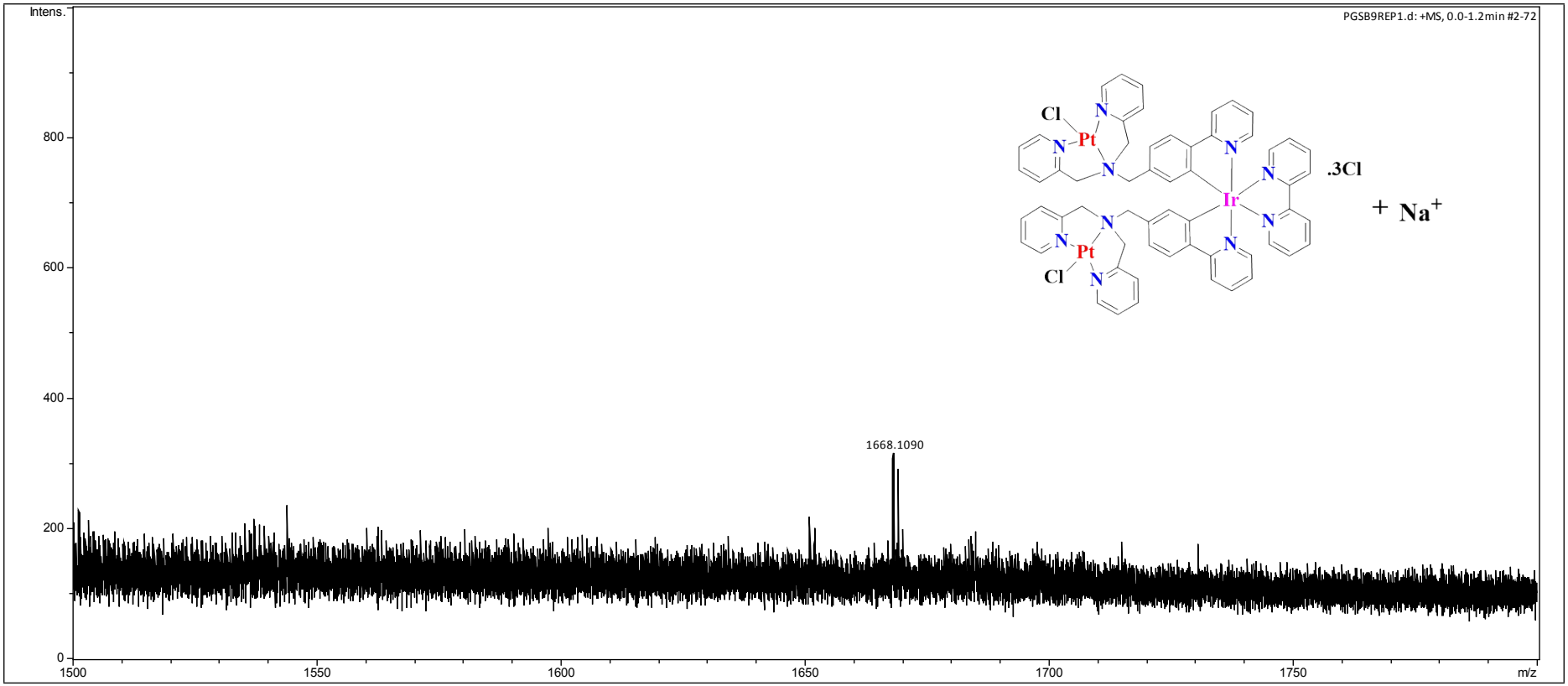
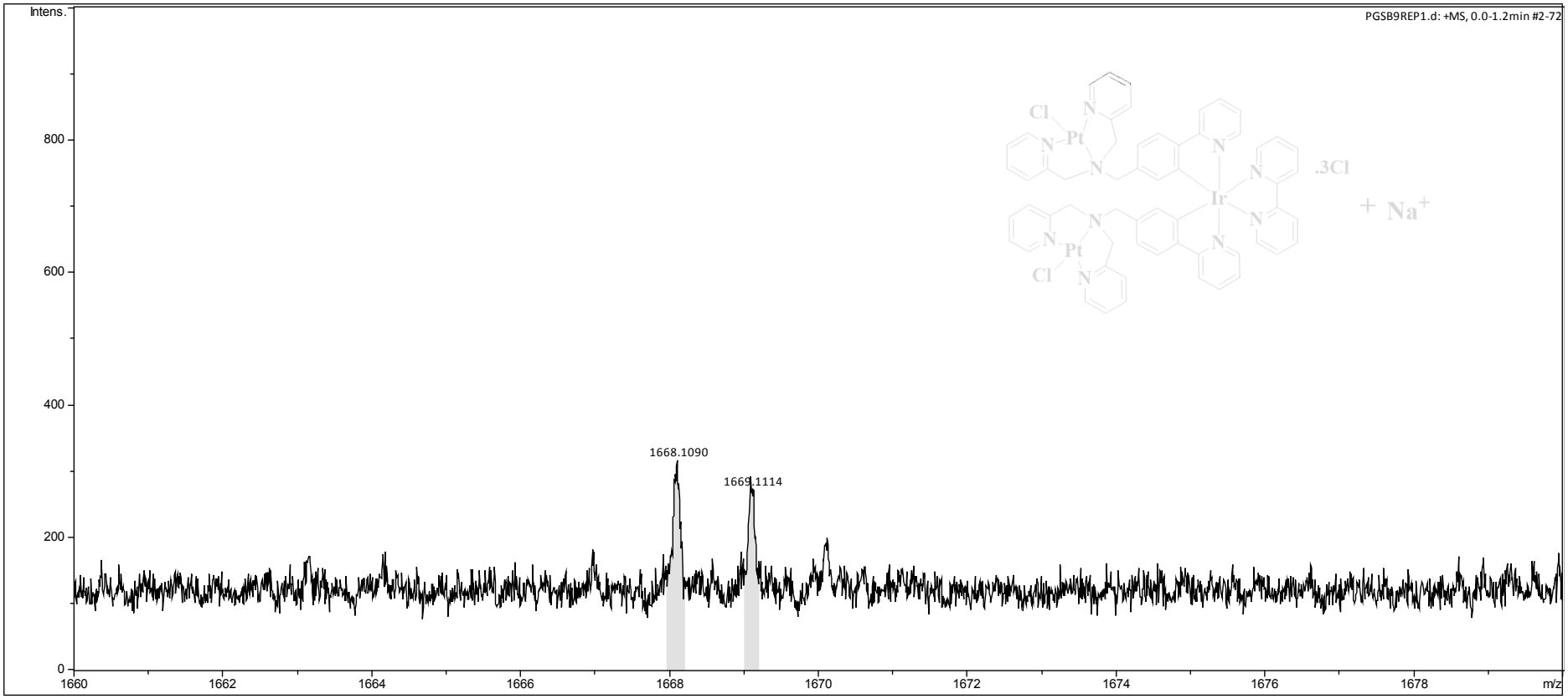
771.1250
771.6291
772.1261
772.6416
772.9850
773.6545


Intens.
PGSB9REP1.d: +MS, 0.0-1.2min #2-72
800
600
400
200
0
1668.1090
1500
1550
1600
1650
1700
1750
m/z
Cl
Pt
N
Ir
.3Cl
+ Na+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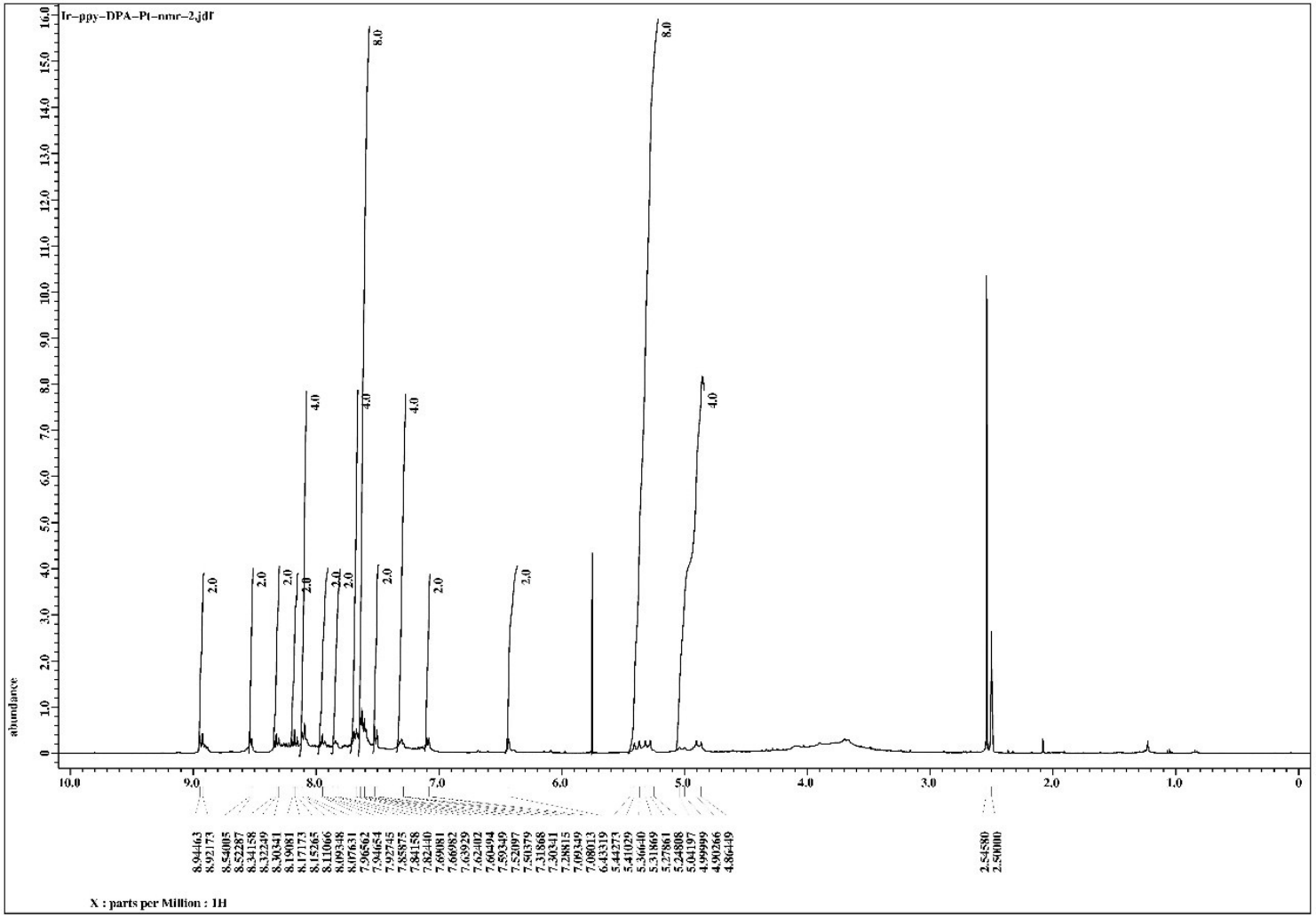
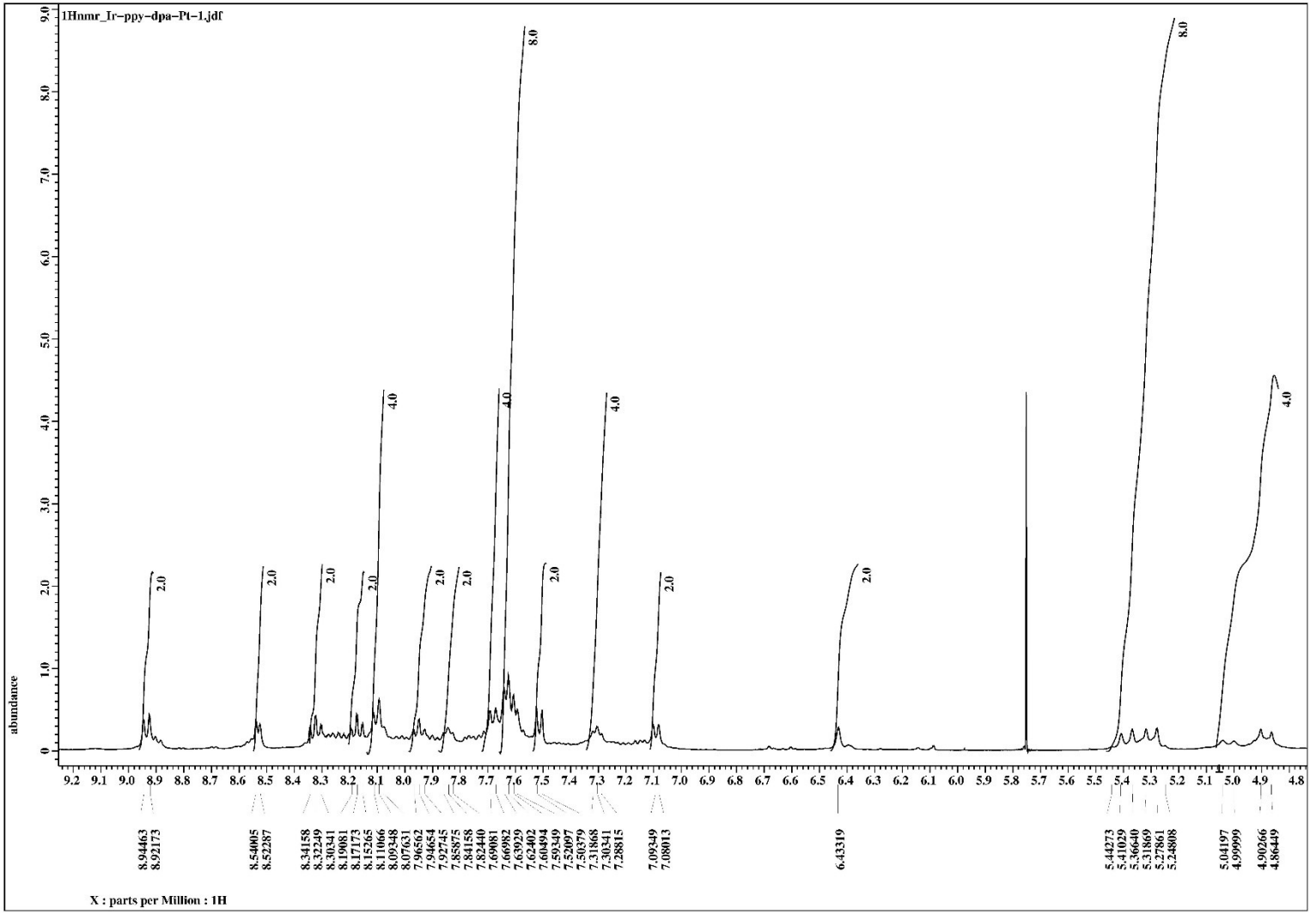
PGSB9REP1.d: +MS, 0.0-1.2min #2-72
800
600
400
200
0
1668.1090
1669.1114
1660
1662
1664
1666
1668
1670
1672
1674
1676
1678
m/z
Cl
Pt
N
Ir
.3Cl
+ Na+

b) ^{1}HNMR spectrum



B)


1Hnmr_Ir-ppy-dpa-Pt-1.jdf
abundance
X : parts per Million : 1H
8.94463
8.92173
8.54005
8.52287
8.34158
8.32349
8.30341
8.19081
8.17173
8.15265
8.11066
8.09348
8.07631
7.96562
7.94654
7.92745
7.85875
7.84158
7.82440
7.69081
7.66982
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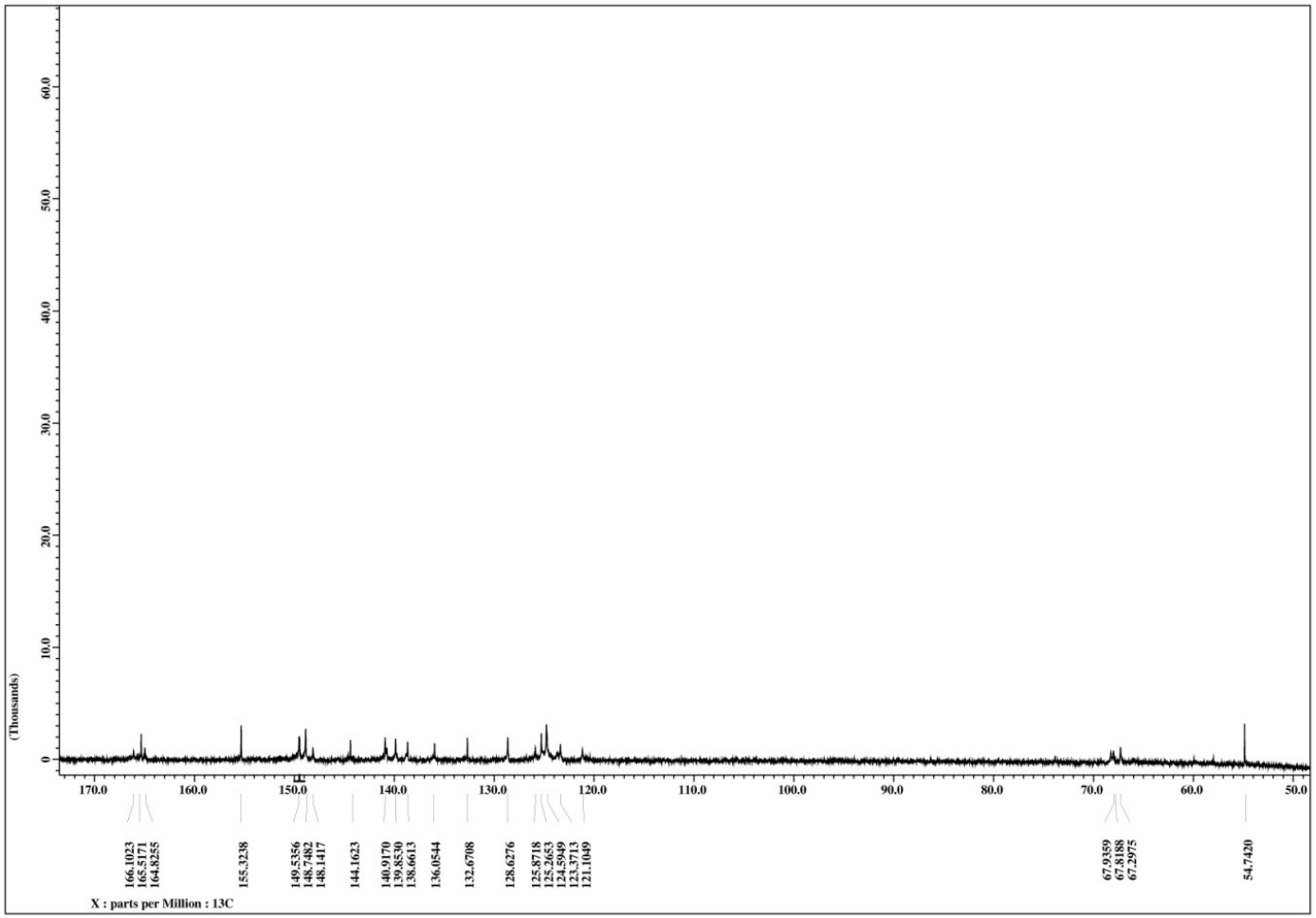
7.52097
7.50379
7.31868
7.30341
7.28815
7.09349
7.08013
6.43319
5.44273
5.41029
5.36640
5.31869
5.27861
5.24808
5.04197
4.99999
4.90266
4.86449

c) ^{13}C NMR of **3**


(Thousands)
60.0
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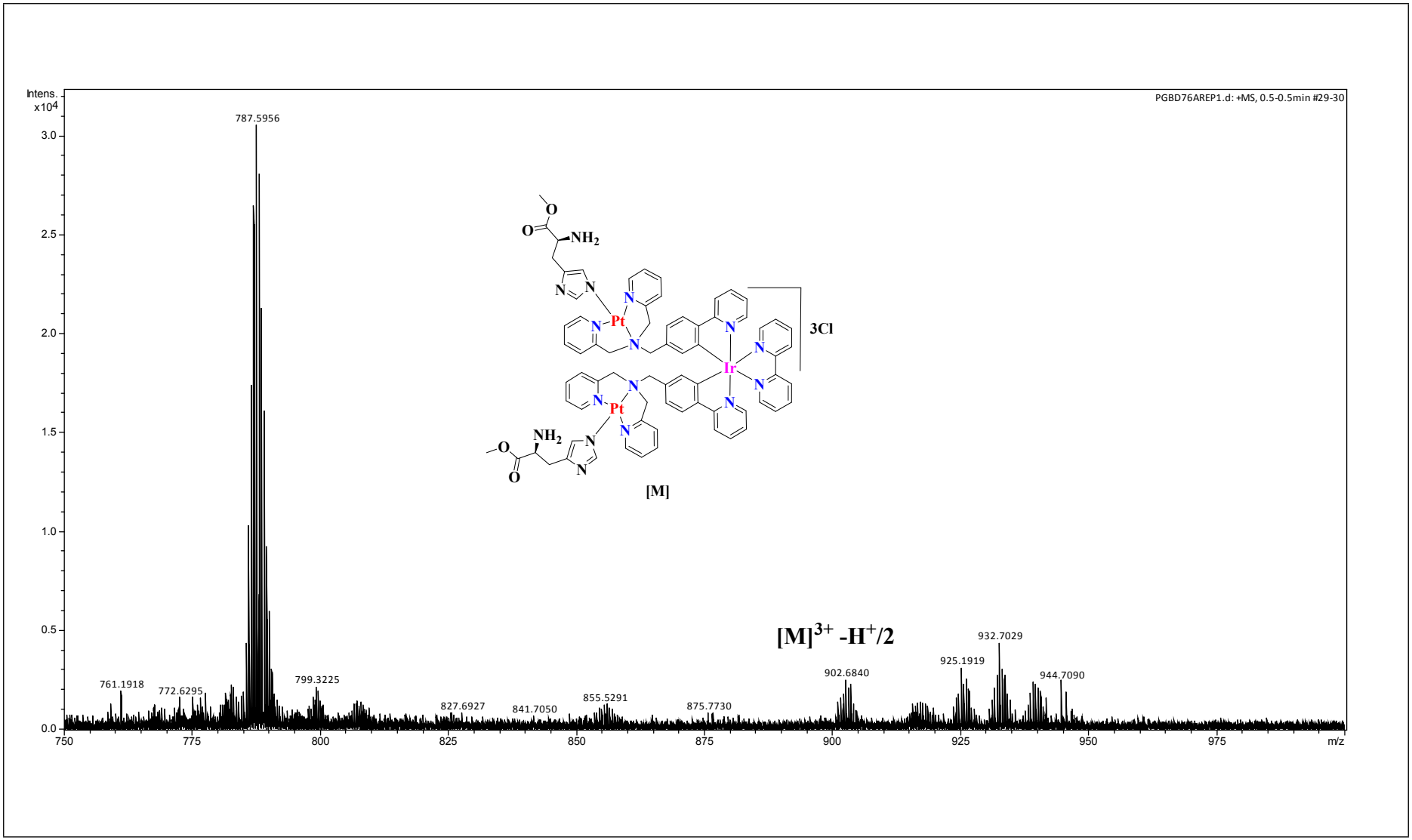
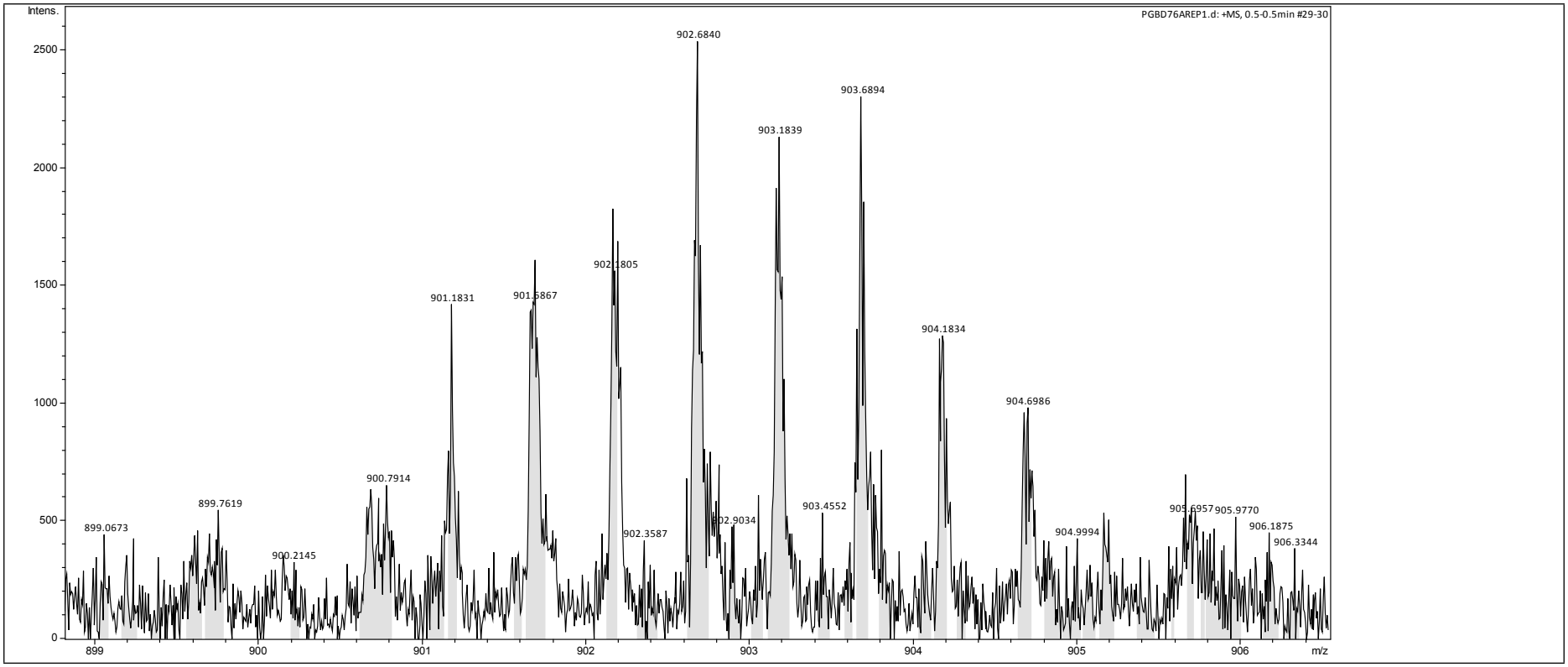
40.0
30.0
20.0
10.0
0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
166.1023
165.5171
164.8255
155.3238
149.5356
148.7482
148.1417
144.1623
140.9170
139.8530
138.6613
136.0544
132.6708
128.6276
125.8718
125.2653
124.5949
123.3713
121.1049
67.9359
67.8188
67.2975
54.7420
X : parts per Million : 13C

Figure S3: ESI-MS of complex **3** + L-histidine-methyl ester

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2000
1500
1000
500
0
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899.7619
900.2145
900.7914
901.1831
901.5867
902.1805
902.3587
902.6840
902.9034
903.1839
903.4552
903.6894
904.1834
904.6986
904.9994
905.6957
905.9770
906.1875
906.3344
899
900
901
902
903
904
905
906
m/z

Figure S4: Plot of concentration of histidine added to complex **3** solution (10^{-5}M) against emission intensity

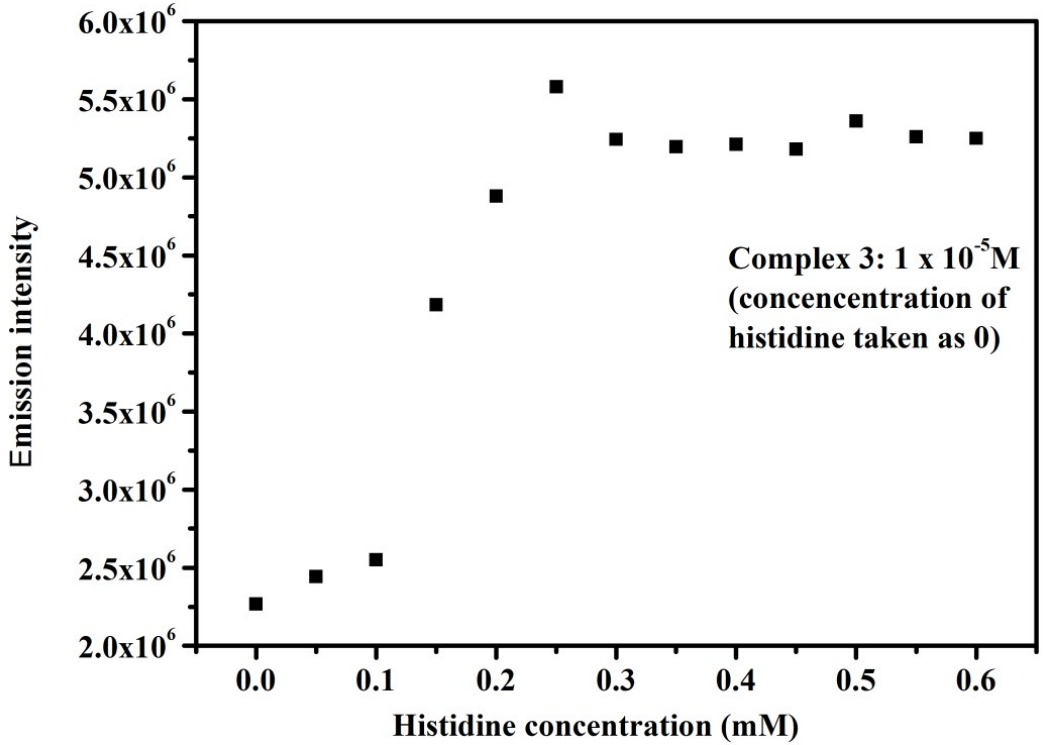


Figure S5: Titration of complex **3** with a) N-Boc-L-Histidine b) L-Histidine Methyl ester

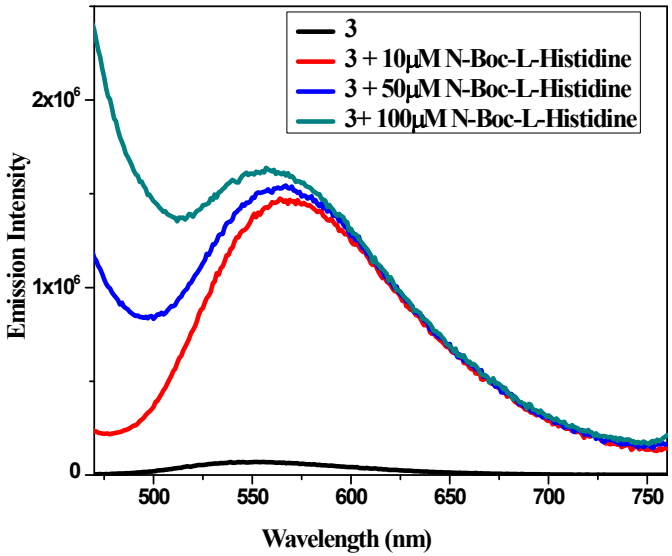
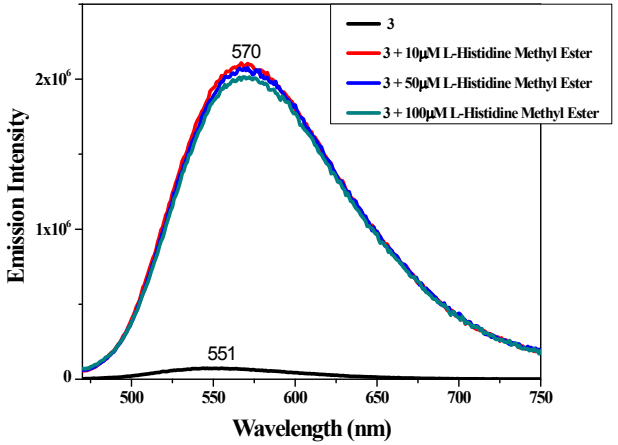
a	b
	

Figure S6: a) **3** (10 μM) + histidine(5 x 10^{-5}M) with increasing cysteine concentration

b) **3** (10 μM) + cysteine (5 x 10^{-5}M) with increasing histidine concentration

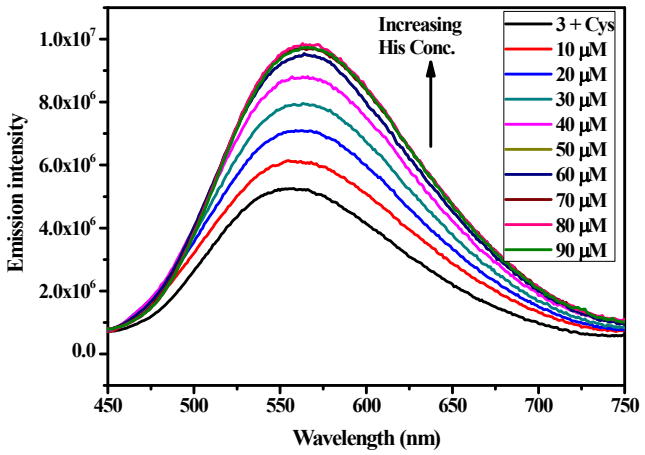
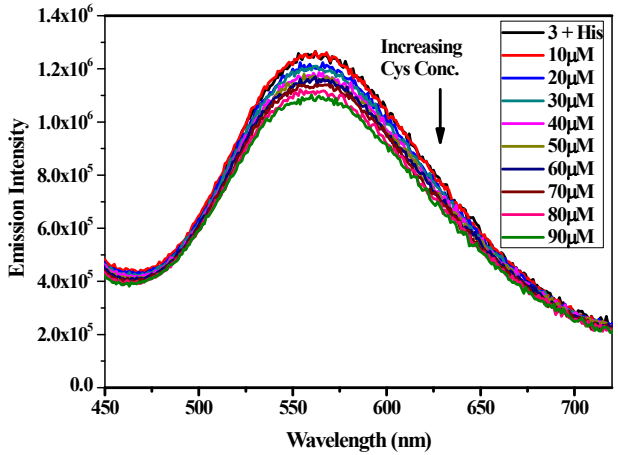
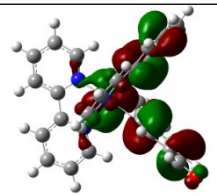
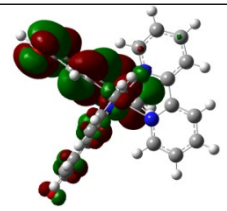
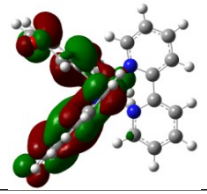
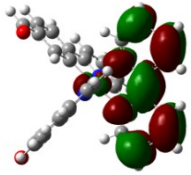
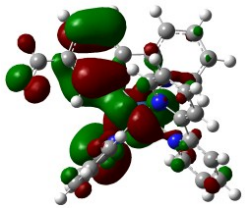
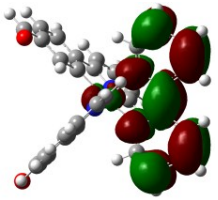
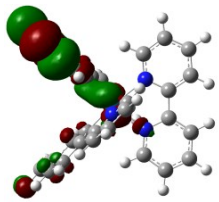
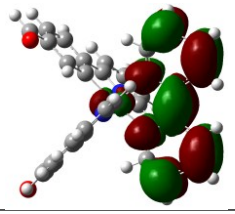
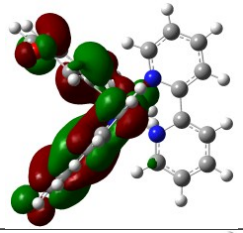
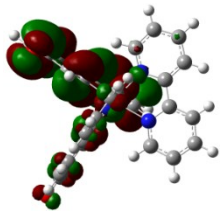
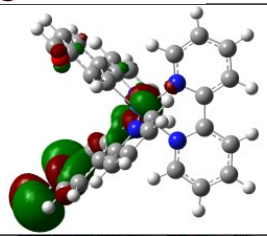
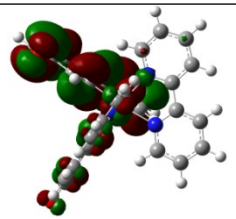
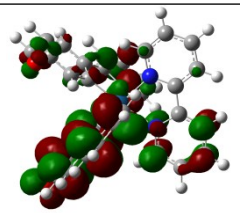
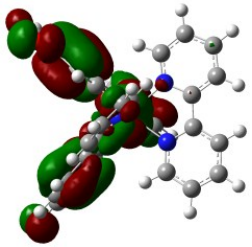
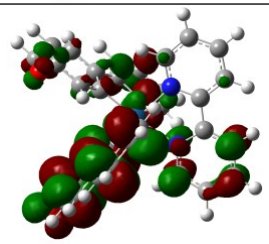
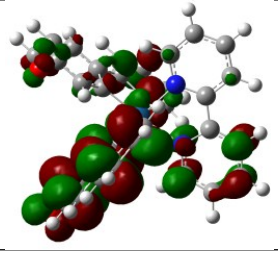
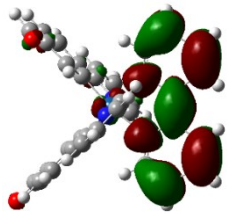
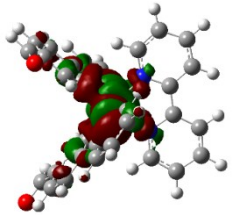
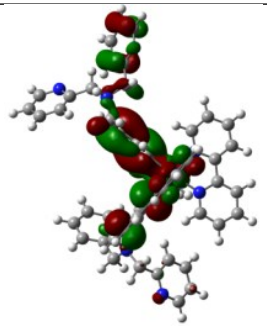
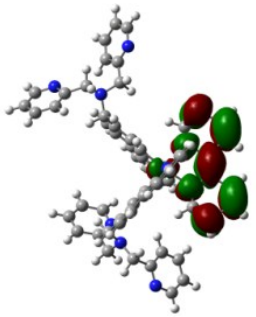
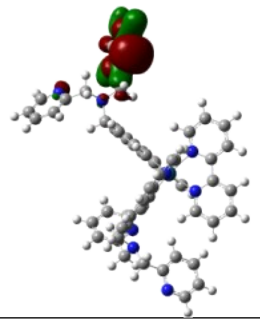
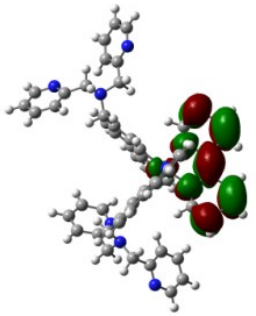
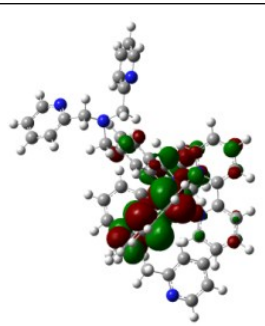
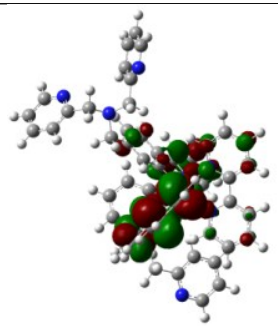
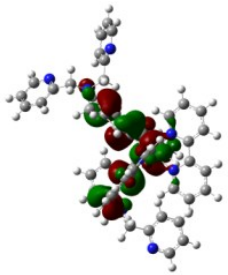
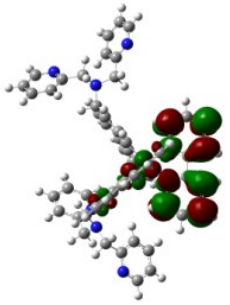
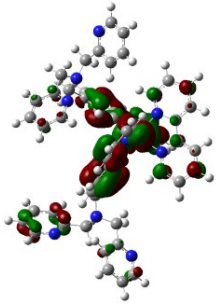
a)	b)
	

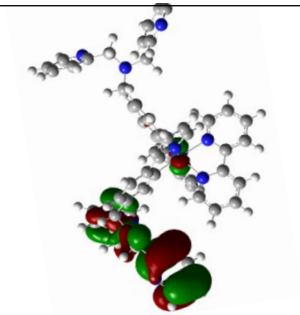
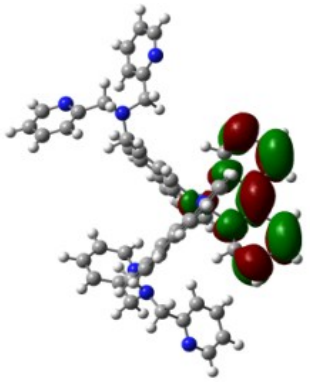
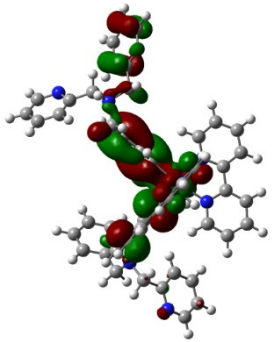
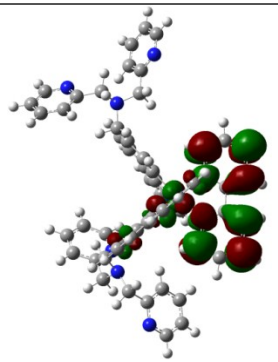
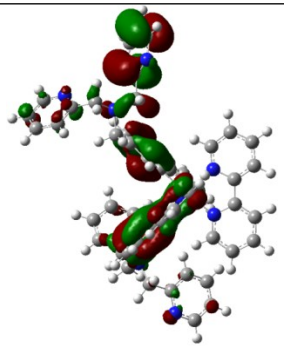
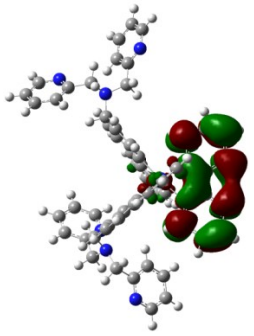
Table S1: Frontier orbital diagram of complexes **1**, **2** and **3**

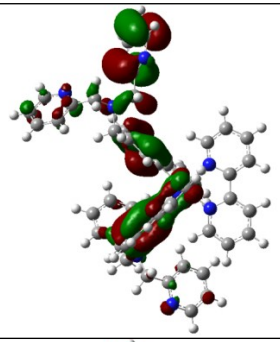
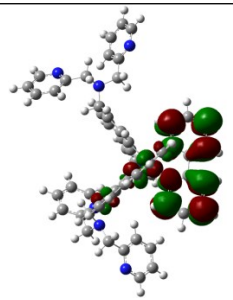
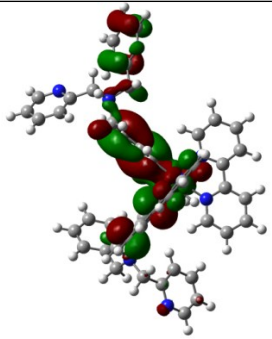
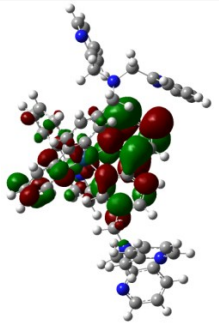
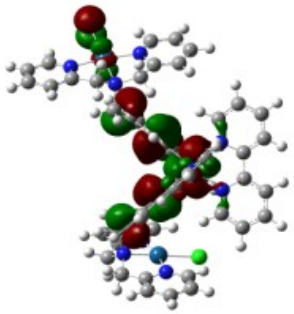
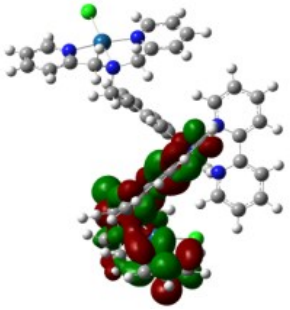
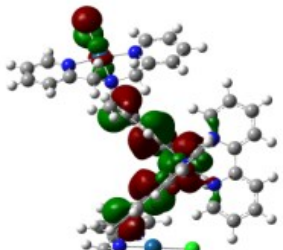
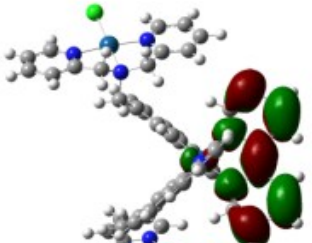
	Absorption			
	Calculated λ_{Abs}(nm, force constant)			
1	442.38 (f=0.0370)	HOMO → LUMO + 1		
	431.12 (f=0.0236)	HOMO - 2 → LUMO		
	389.94 (f=0.0178)	HOMO - 5 → LUMO		
		HOMO - 3 → LUMO		

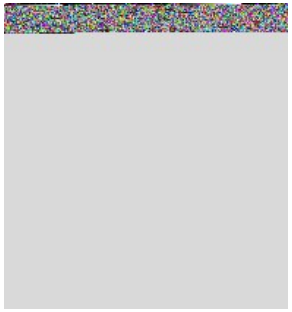
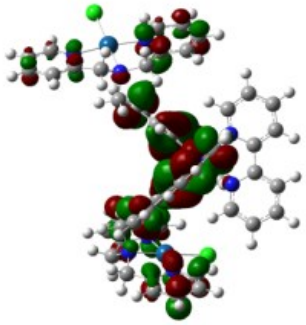
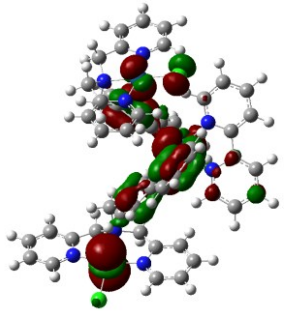
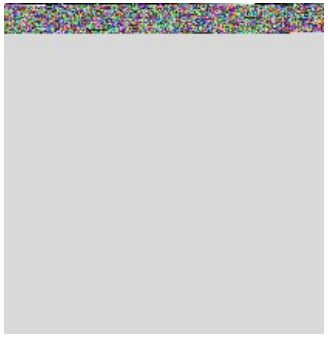
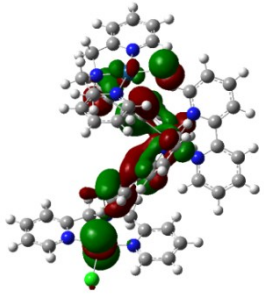
	350.74 (f=0.0207)	HOMO – 2 → LUMO + 1		
		HOMO – 1 → LUMO + 1		
	325.69 (f=0.0273)	HOMO – 5 → LUMO + 2		
		HOMO – 4 → LUMO + 2		
		HOMO – 3 → LUMO + 2		

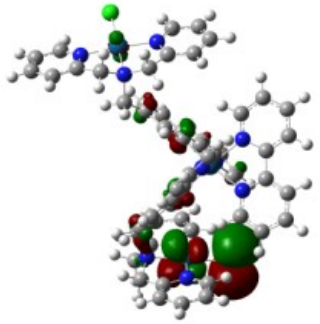
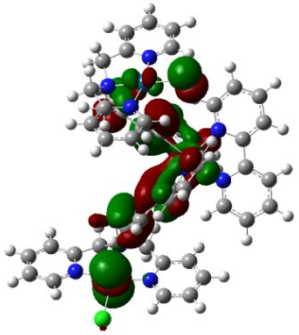
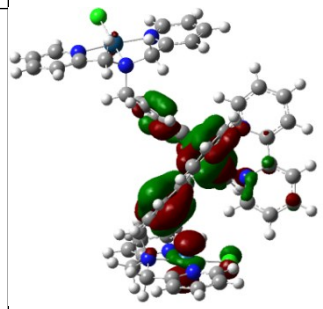
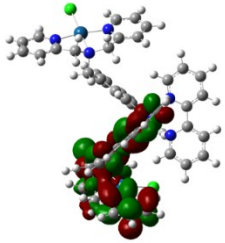
Emission				
	566.46	HOMO → LUMO+11		
2	483.31 (f=0.0048)	HOMO – 5 → LUMO		
		HOMO - 3 → LUMO		

	414.70 (f=0.0215)	HOMO – 2 → LUMO + 3		
		HOMO – 2 → LUMO + 2		
	402(f=0.0285)	HOMO – 10 → LUMO		

	394 (f=0.0151)	HOMO – 11 → LUMO		
	343 (f=0.029)	HOMO – 5 → LUMO +2		
		HOMO – 7 → LUMO +1		

		HOMO – 7 → LUMO +2		
		HOMO – 5 → LUMO +4		
	Absorption			
3	501 (f = 0.0003)	HOMO →LUMO		
	409.(f=0.0297)	HOMO →LUMO +1		

		HOMO →LUMO +2		
	378 (f=0.0332)	HOMO -7 →LUMO		
		HOMO-4 →LUMO		

		HOMO – 3 → LUMO		
	370.11 (f=0.0253)	HOMO-4 →LUMO		
	338.84 (f=0.0119)	HOMO-5 →LUMO +1		

		HOMO-5 →LUMO +2