Supplementary Material For Dalton Trans. Manuscript (Version: 25 July 2008)

"Gas Phase Supramolecular Cluster Ions of Deoxyguanosine Induced by Binding to (2,2':6'2''-terpyridine)- platinum(II) and (diethylenetriamine)- platinum(II)."

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Table S1:
The calculated m/z (of the most intense peak) of the various clusters.

$[Pt(terpy)(dG)_x - yH]^{n+}$

x	y=1; n=1	y=0; n=2
1	693.2	
2	960.3	480.6
3	1227.4	614.2
4	1494.5	747.7
5	1761.6	881.3
6	2028.7	1014.8
7	2295.8	1148.4
8	2562.9	1281.9
9	2830.0	1415.5
10	3097.1	1549.0

$[Pt(dien)(dG)_x - yH]^{n+}$

x	y=1; n=1	y=0; n=2
1	563.2	
2	830.3	415.6
3	1097.4	549.2
4	1364.5	682.7
5	1631.6	816.3
6	1898.7	949.8
7	2165.8	1083.4
8	2432.9	1216.9
9	2700.0	1350.5
10	2967.1	1484.0

Table S2 :

Distribution of P values for L = dien, where n = parent cluster size (before collision), n-x = collided cluster size, P = arbitrary value approximating a normal distribution curve and Run temp = the simulated temperature for CID, for all cluster sizes.

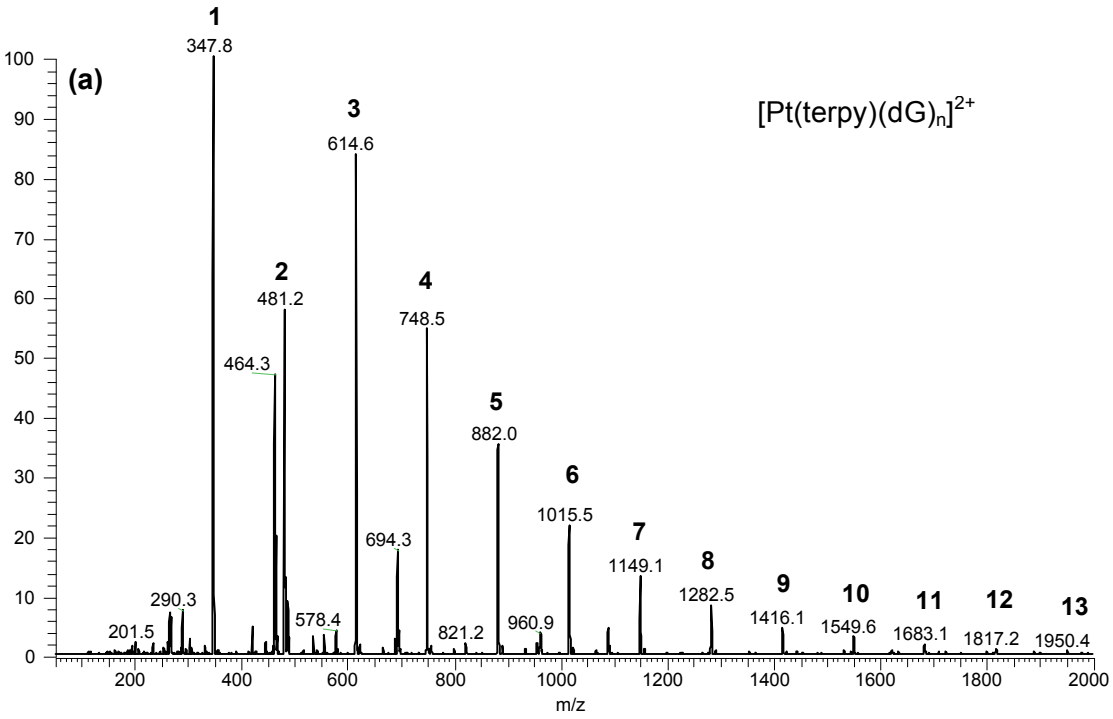
n = 3			**n = 4**			**n = 5**			**n = 6**			**n = 7**			**n = 8**			**n = 9**			**n = 10**		
Run Temp	n-x	P	Run Temp	n-x	P	Run Temp	n-x	P	Run Temp	n-x	P	Run Temp	n-x	P	Run Temp	n-x	P	Run Temp	n-x	P	Run Temp	n-x	P
900	3	0	900	3	0.25	800	5	0	900	6	0	1000	7	0	1000	8	0	1000	9	0	1050	8	0
950	3	0	950	3	0.50	850	5	0.2	1000	5	0	1050	6	0	1100	6	0	1100	6	0	1100	8	0
1000	3	0	1000	4	0.75	900	4	0.4	1050	5	0	1100	5	0	1200	5	0	1200	4	0	1150	7	0
1050	3	0	1050	4	1.00	950	4	0.6	1100	4	0	1150	6	0.2	1300	5	0.167	1300	5	0.125	1200	8	0.111
1100	3	0	1100	4	0.75	1000	5	0.8	1150	5	0	1200	6	0.4	1350	5	0.333	1350	7	0.250	1250	6	0.222
1150	3	0	1150	3	0.50	1050	5	1.0	1200	5	0	1250	5	0.6	1400	6	0.500	1400	6	0.375	1300	5	0.333
1200	3	0	1200	2	0.25	1100	4	0.8	1250	4	0.2	1300	4	0.8	1450	3	0.667	1450	5	0.500	1350	7	0.444
1250	2	0.25	1250	2	0	1150	3	0.6	1300	4	0.4	1350	4	1.0	1500	3	0.833	1500	7	0.625	1400	5	0.555
1300	3	0.50	1300	2	0	1200	3	0.4	1350	4	0.6	1400	4	0.8	1550	4	1.000	1550	4	0.750	1450	6	0.666
1350	3	0.75	1350	2	0	1250	3	0.2	1400	4	0.8	1450	3	0.6	1600	4	0.833	1600	5	0.875	1500	5	0.777
1400	3	1.00	1400	2	0	1300	3	0	1450	5	1.0	1500	3	0.4	1650	4	0.667	1650	4	1.000	1550	4	0.888
1450	1	0.75	1450	2	0	1350	3	0	1500	3	0.8	1550	2	0.2	1700	2	0.500	1700	4	0.875	1600	4	1.000
1500	1	0.50	1500	2	0	1400	3	0	1550	4	0.6	1600	2	0	1750	2	0.333	1750	4	0.750	1650	5	0.888
1550	1	0.25				1450	3	0	1600	3	0.4	1650	2	0	1800	3	0.167	1800	3	0.625	1700	6	0.777
						1500	3	0	1650	4	0.2	1700	2	0	1850	2	0	1850	2	0.500	1750	6	0.666
						1550	3	0	1700	3	0				1900	3	0	1900	3	0.375	1800	3	0.555
						1600	2	0	1750	4	0				1950	3	0	1950	2	0.250	1850	4	0.444
						1650	3	0	1800	3	0							2000	3	0.125	1900	4	0.333
						1700	1	0										2050	3	0	1950	3	0.222
																		2100	2	0	2000	3	0.111
																					2050	3	0
Sum(P)	1	1.25	Sum(P)	1	0	Sum(P)	1	0	Sum(P)	1	0	Sum(P)	1	0	Sum(P)	1	0	Sum(P)	1	0	Sum(P)	1	0
	2	0.25		2	0.25		2	0		2	0		2	0.2		2	0.833		2	0.75		2	0
				3	1.25		3	1.2		3	0.8		3	1		3	1.667		3	1.125		3	0.888
							4	1.8		4	2.8		4	2.6		4	2.5		4	3.375		4	2.665
										5	1.0		5	0.6		5	0.5		5	1.5		5	2.553
													6	0.6		6	0.5		6	0.375		6	2.109
																7	0		7	0.875		7	0.444
																			8	0		8	0
																						9	0

Table S3 :

Distribution of P values for L = terpy, where n = parent cluster size (before collision), n-x = collided cluster size, P = arbitrary value approximating a normal distribution curve and Run temp = the simulated temperature for CID, for all cluster sizes.

n = 3			**n = 4**			**n = 5**			**n = 6**			**n = 7**			**n = 8**			**n = 9**			**n = 10**		
Run Temp	n-x	P	Run Temp	n-x	P	Run Temp	n-x	P	Run Temp	n-x	P	Run Temp	n-x	P	Run Temp	n-x	P	Run Temp	n-x	P	Run Temp	n-x	P
1000	3	0.2	950	4	0	900	5	0	1050	5	0.167	1100	7	0.167	950	8	0	1000	8	0	950	10	0.125
1050	3	0.4	1000	4	0	950	5	0	1100	6	0.333	1150	7	0.333	1050	8	0	1050	9	0.125	1000	9	0.250
1100	3	0.6	1050	3	0	1000	5	0.167	1150	5	0.500	1200	6	0.500	1100	6	0	1100	8	0.250	1050	9	0.375
1150	3	0.8	1100	4	0	1050	5	0.333	1200	6	0.667	1250	7	0.667	1150	8	0.167	1150	7	0.375	1100	8	0.500
1200	2	1	1150	2	0	1100	5	0.500	1250	5	0.833	1300	5	0.833	1200	8	0.333	1200	6	0.500	1150	7	0.625
1250	3	0.8	1200	3	0.2	1150	4	0.667	1300	5	1.000	1350	5	1.000	1250	6	0.500	1250	5	0.625	1200	5	0.750
1300	2	0.6	1250	4	0.4	1200	4	0.833	1350	5	0.833	1400	5	0.833	1300	6	0.667	1300	5	0.750	1250	6	0.875
1350	3	0.4	1300	2	0.6	1250	4	1.000	1400	4	0.667	1450	4	0.667	1350	7	0.833	1350	5	0.875	1300	4	1.000
1400	1	0.2	1350	3	0.8	1300	5	0.833	1450	4	0.500	1500	5	0.500	1400	5	1.000	1400	6	1.000	1350	5	0.875
1450	3	0	1400	3	1.0	1350	5	0.667	1500	3	0.333	1550	4	0.333	1450	4	0.833	1450	5	0.875	1400	5	0.750
1500	3	0	1450	3	0.8	1400	3	0.500	1550	3	0.167	1600	4	0.167	1500	5	0.667	1500	5	0.750	1450	4	0.625
1550	3	0	1500	3	0.6	1450	3	0.333	1600	2	0	1650	4	0	1550	3	0.500	1550	5	0.625	1500	4	0.500
1600	3	0	1550	3	0.4	1500	3	0.167				1700	4	0	1600	3	0.333	1600	5	0.500	1550	**3**	0.375
			1600	3	0.2	1550	3	0				1750	3	0	1650	3	0.167	1650	5	0.375	1600	4	0.250
						1600	3	0							1700	3	0	1700	3	0.250	1650	4	0.125
						1650	3	0										1750	4	0.125	1700	3	0
						1700	2	0															
Sum(P)	1	0.2	Sum(P)	1	0	Sum(P)	1	0	Sum(P)	1	0	Sum(P)	1	0	Sum(P)	1	0	Sum(P)	1	0	Sum(P)	1	0
	2	1.6		2	0.6		2	0		2	0		2	0		2	0		2	0		2	0
				3	4.0		3	1.0		3	0.5		3	0		3	1		3	0.25		3	0.625
							4	2.5		4	1.167		4	1.167		4	0.833		4	0.125		4	2.875
										5	3.333		5	3.166		5	1.667		5	5.375		5	2.5
													6	0.5		6	1.167		6	1.5		6	0.75
																7	0.833		7	0.375		7	0.5
																			8	0.25		8	0.375
																						9	0.375

Figure S1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2
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3
614.6
4
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5
882.0
6
1015.5
7
1149.1
8
1282.5
9
1416.1
10
1549.6
11
1683.1
12
1817.2
13
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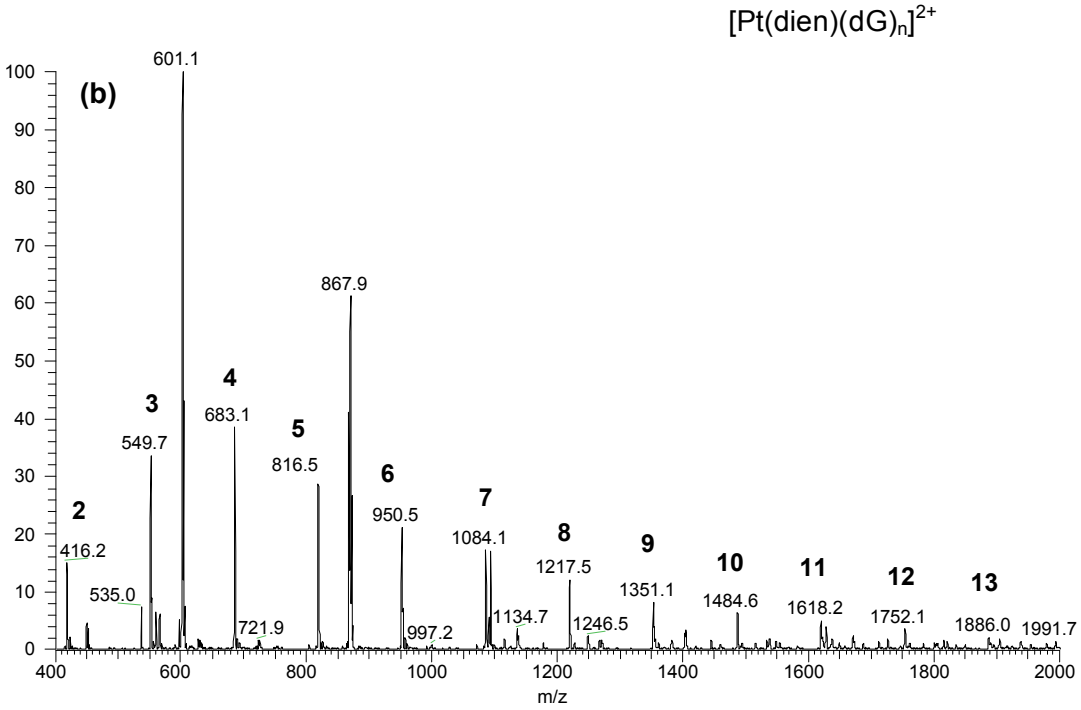
201.5
464.3
578.4
694.3
821.2
960.9
m/z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2
416.2
3
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4
683.1
5
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6
867.9
7
950.5
8
1084.1
9
1217.5
10
1351.1
11
1484.6
12
1618.2
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997.2
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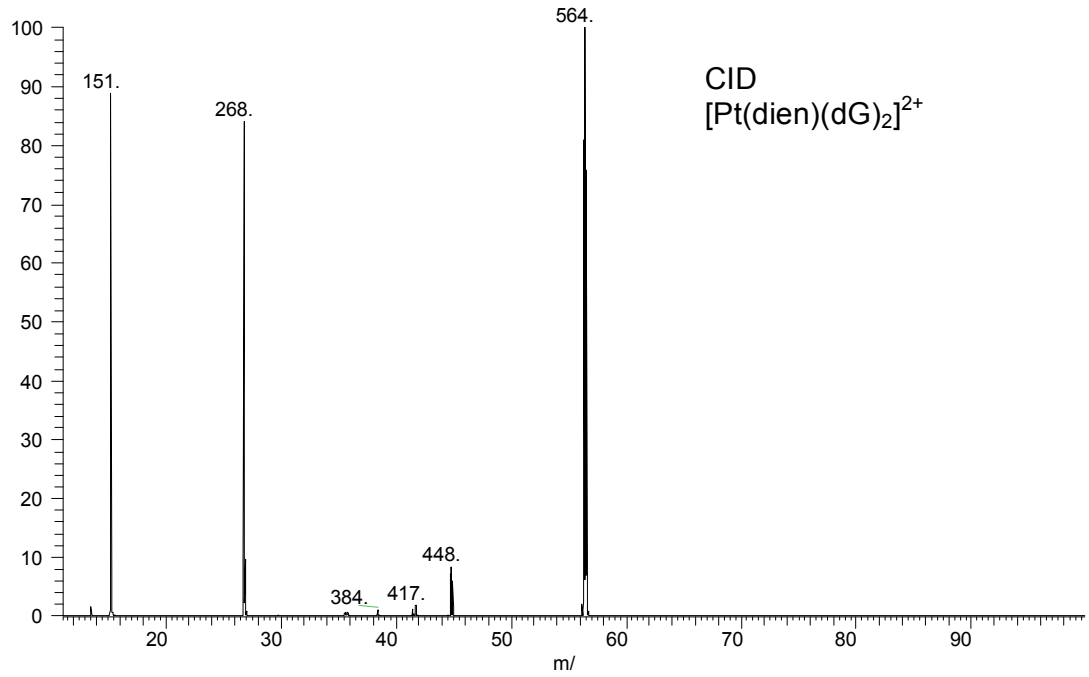
Figure S2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268.
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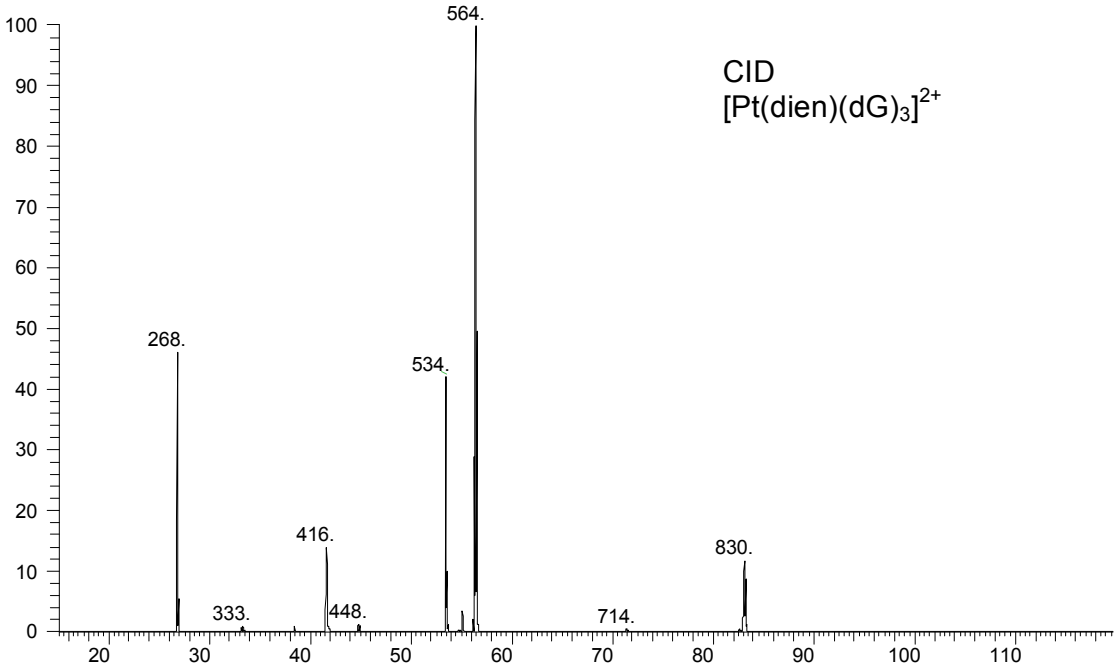
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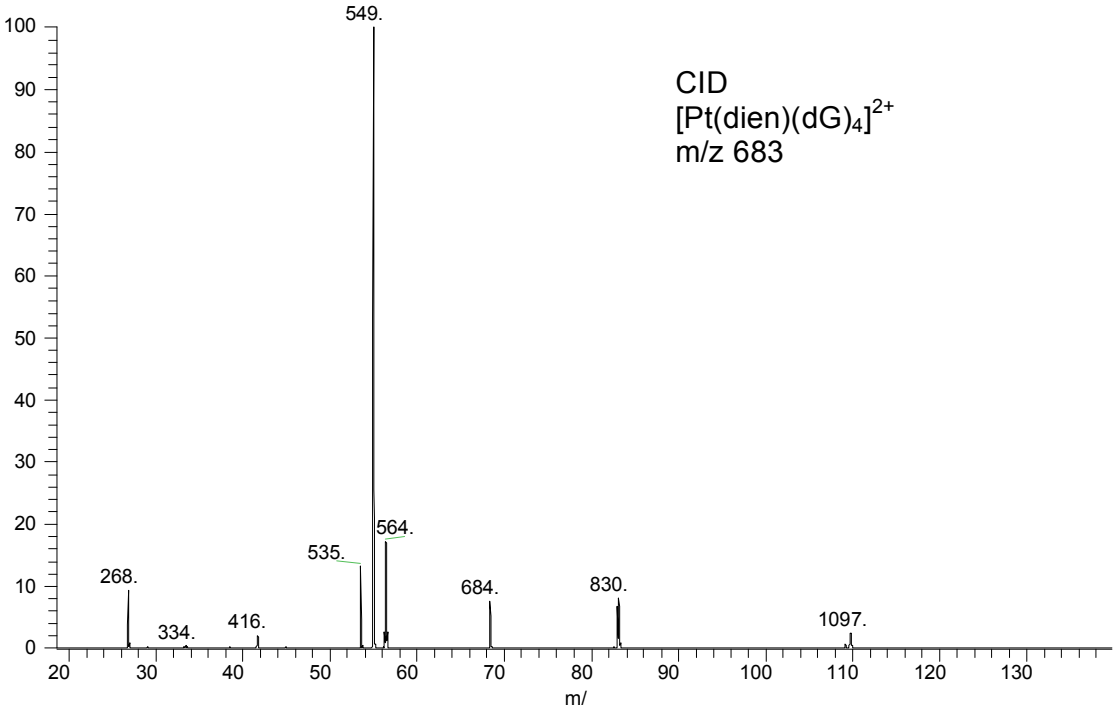
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535.
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684.
830.
1097.
m/
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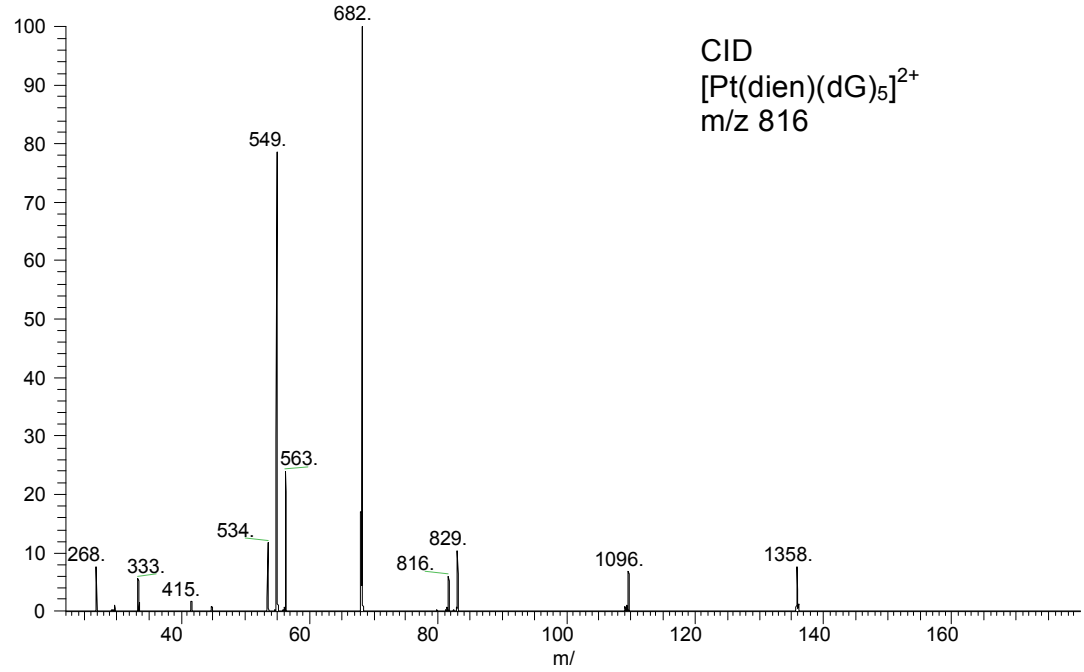
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549.
563.
534.
268.
333.
415.
816.
829.
1096.
1358.
m/
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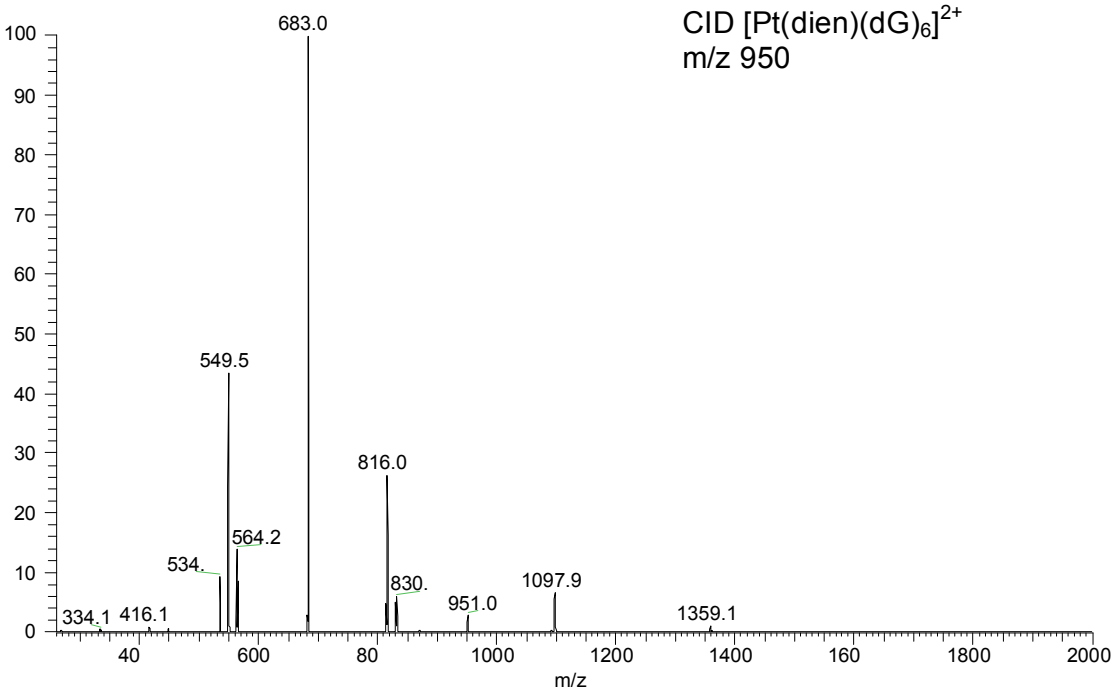
m/z 816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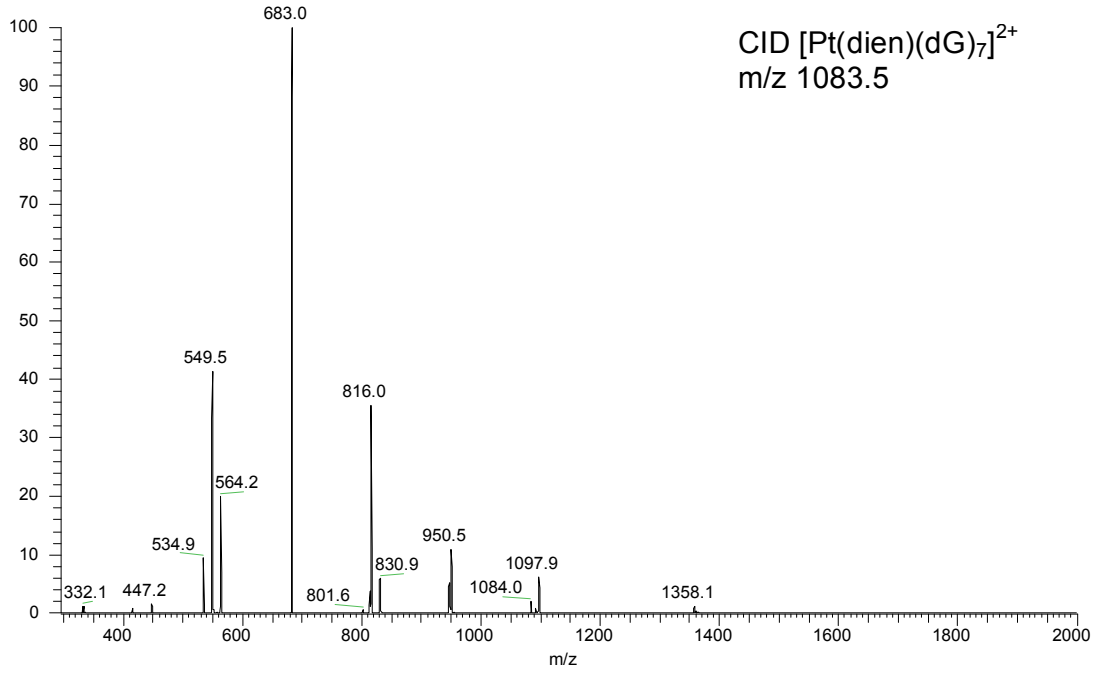
830.
1097.9
951.0
334.1
416.1
1359.1
m/z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447.2
801.6
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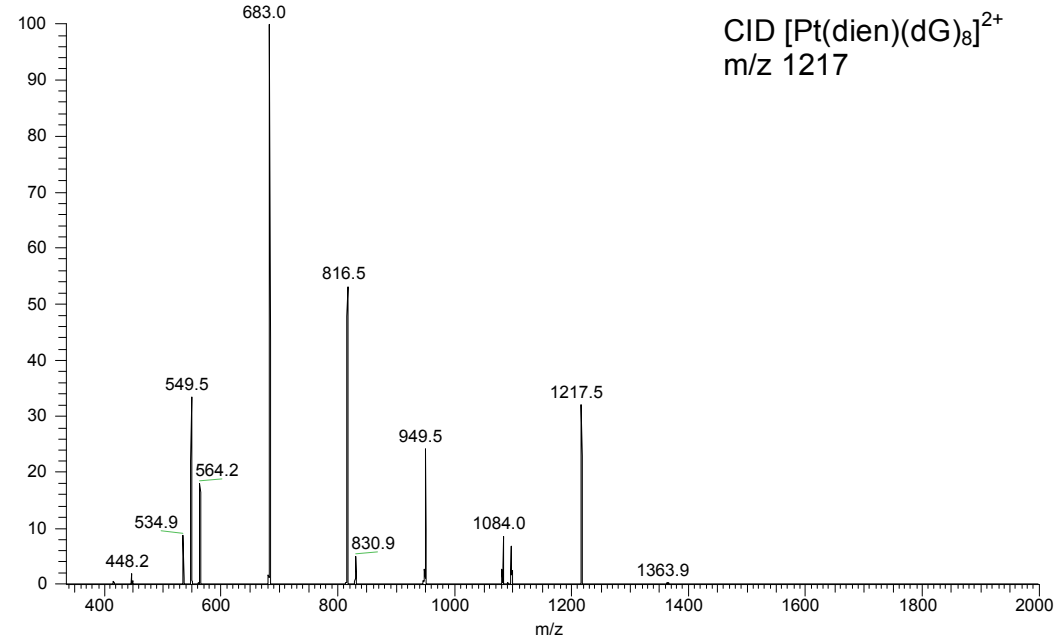
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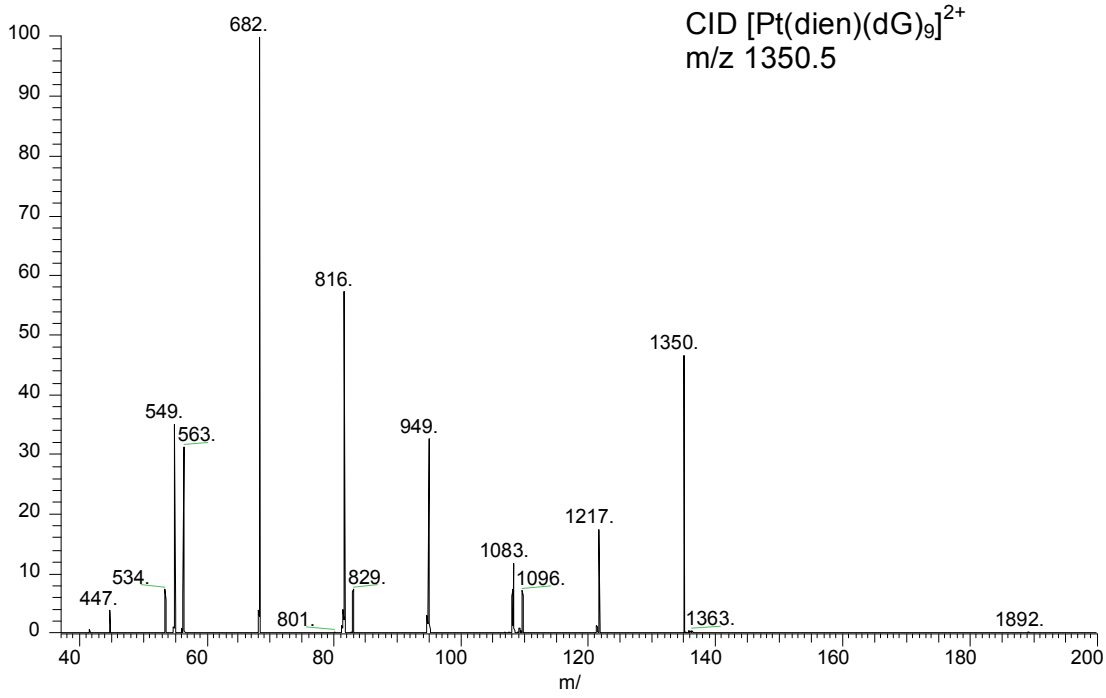
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816.
1350.
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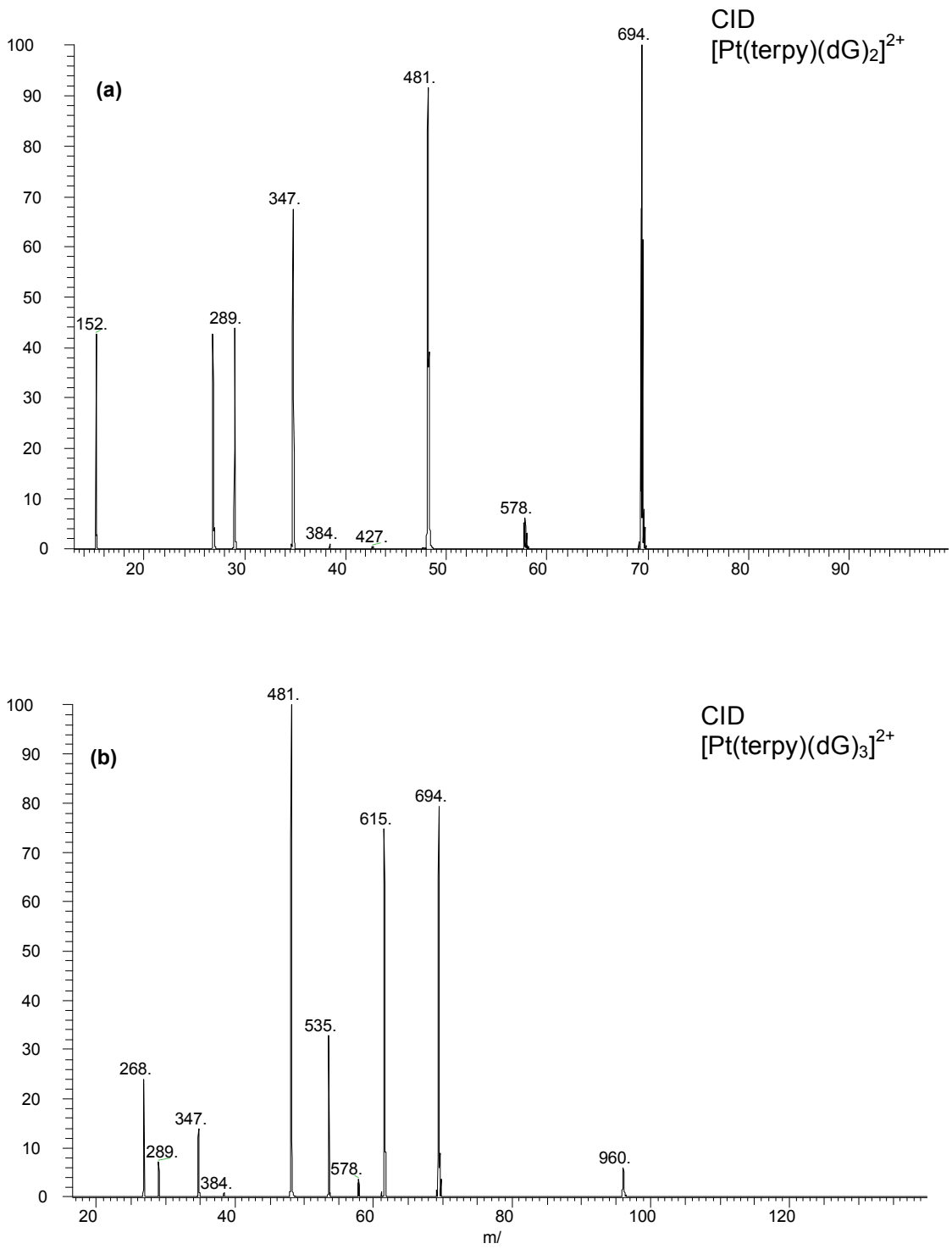
447.
801.
1363.
1892.
m/

Figure S3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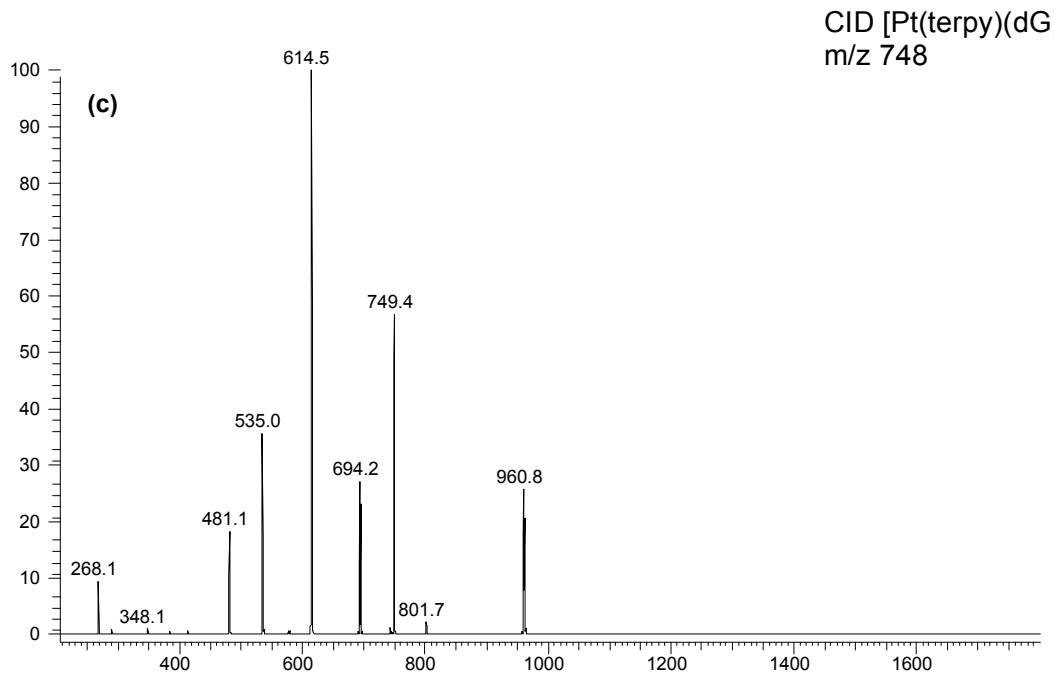
481.
347.
289.
152.
578.
384.
427.
(b)
CID
[Pt(terpy)(dG)3]2+
481.
694.
615.
535.
268.
347.
289.
384.
578.
960.
m/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(c)
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749.4
535.0
694.2
960.8
481.1
268.1
348.1
801.7
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90
80
70
60
50
40
30
20
10
0
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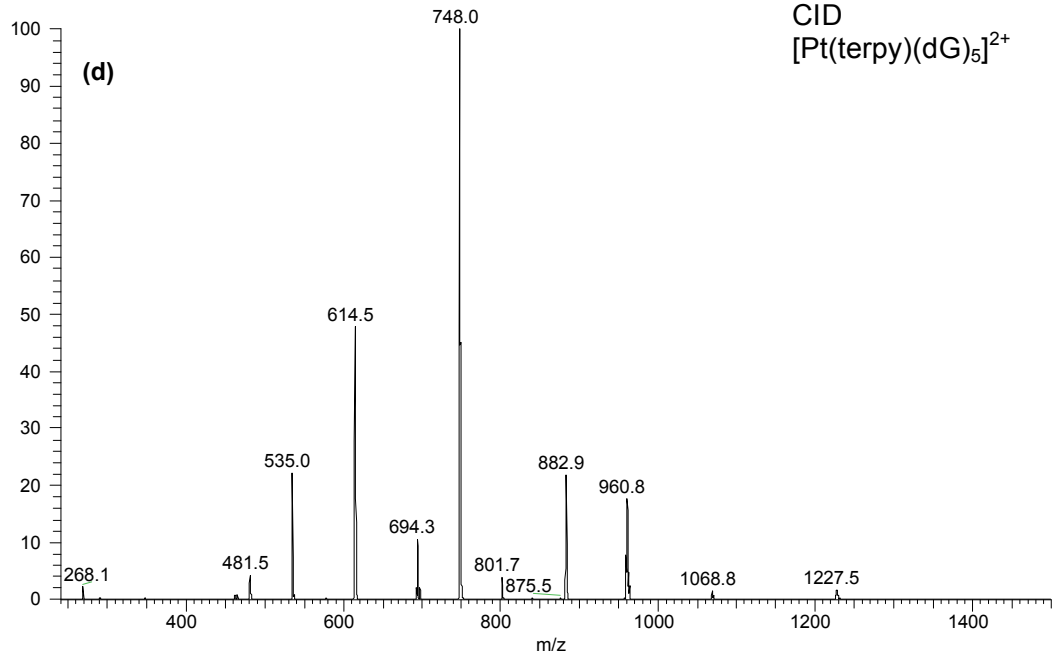
800
1000
1200
1400
1600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(d)
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614.5
535.0
882.9
960.8
694.3
481.5
801.7
875.5
268.1
1068.8
1227.5
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60
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1200
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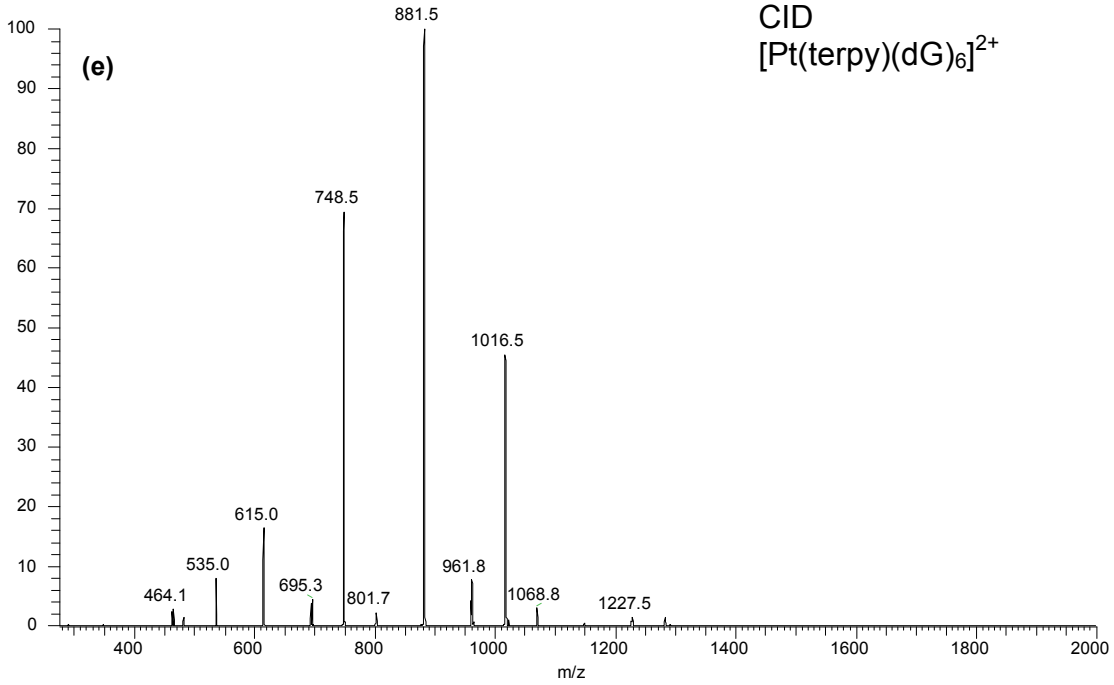
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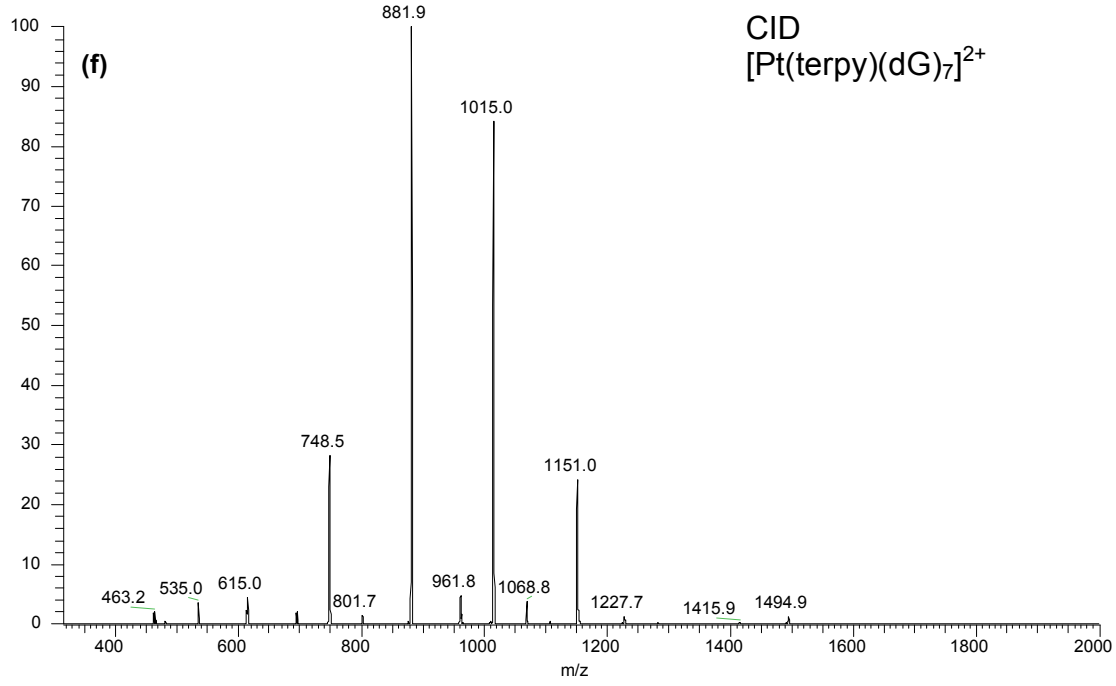
1227.5
m/z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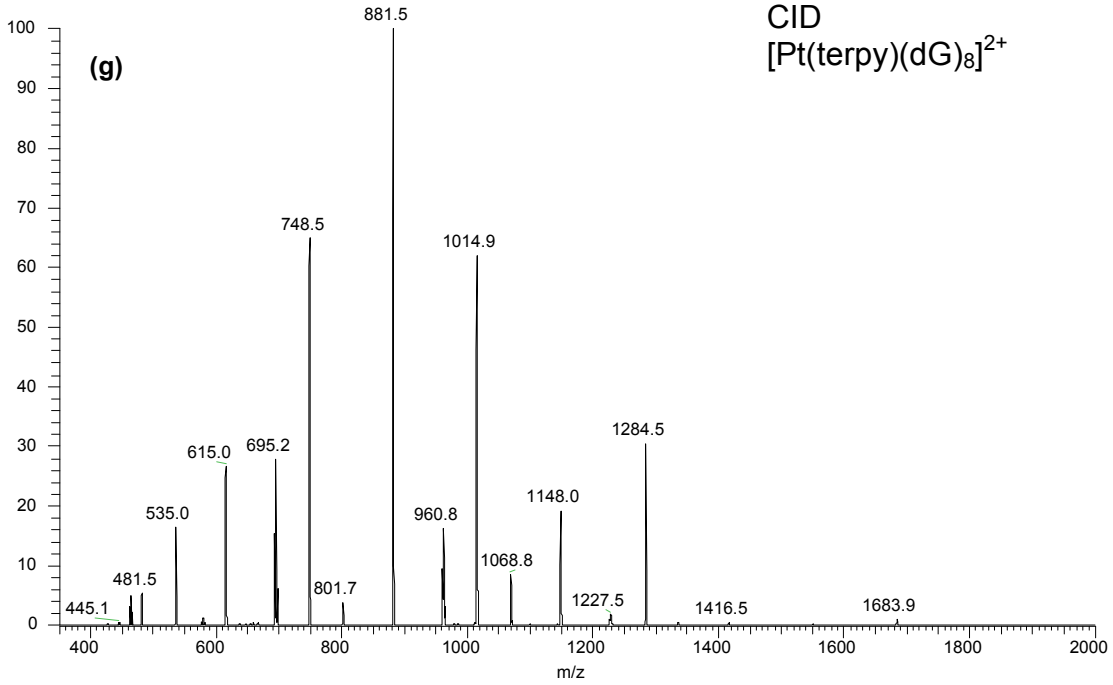
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615.0
695.2
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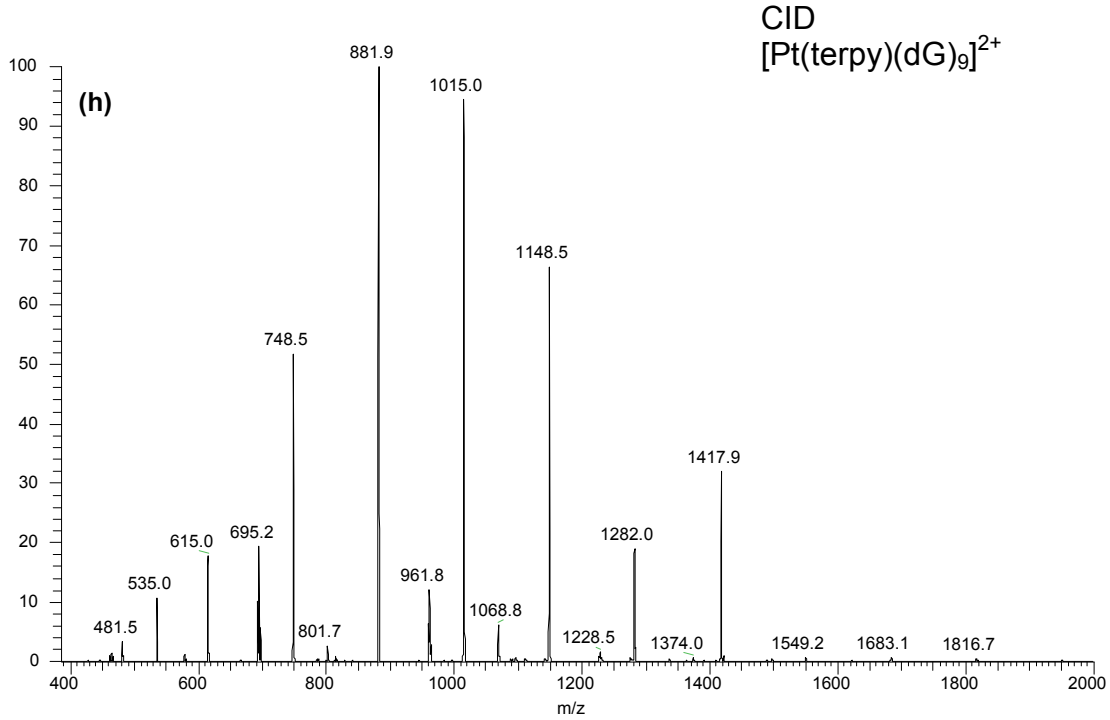
481.5
801.7
445.1
1227.5
1416.5
1683.9
m/z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CID
[Pt(terpy)(dG)9]2+
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1015.0
1148.5
748.5
1417.9
1282.0
615.0
695.2
961.8
535.0
1068.8
481.5
801.7
1228.5
1374.0
1549.2
1683.1
1816.7
m/z

Figures S4 and S5:
CID mass spectra at various collision energies for $[Pt(L)dG_{10}]^{2+}$ for L= dien and terpy respectively

Fig. S4_1

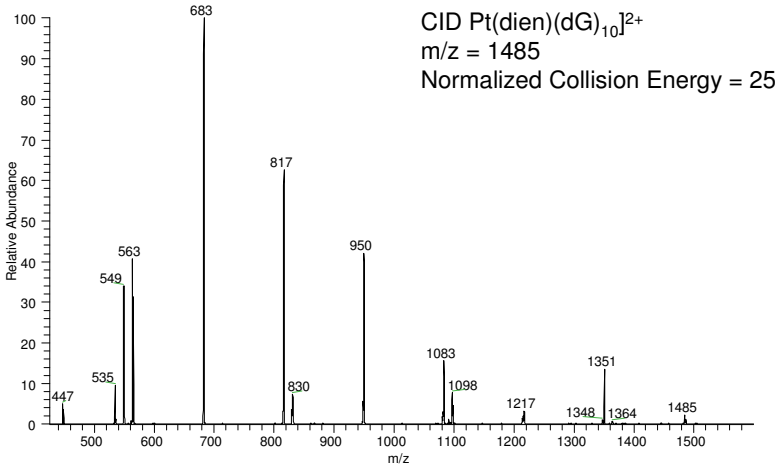


Fig. S4_2

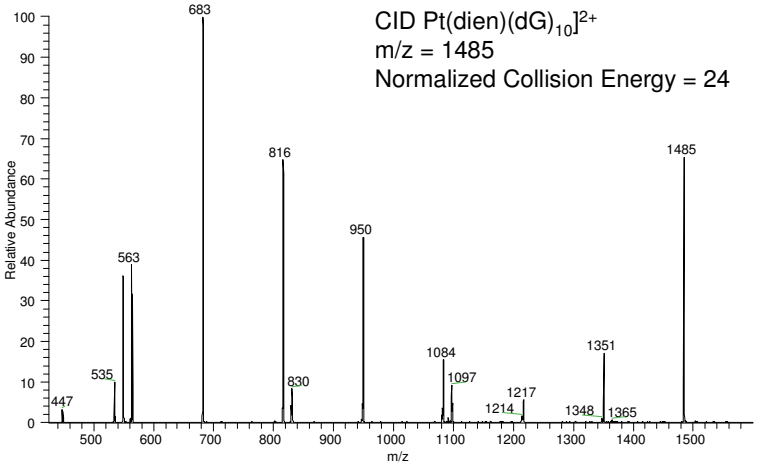


Fig. S4_3

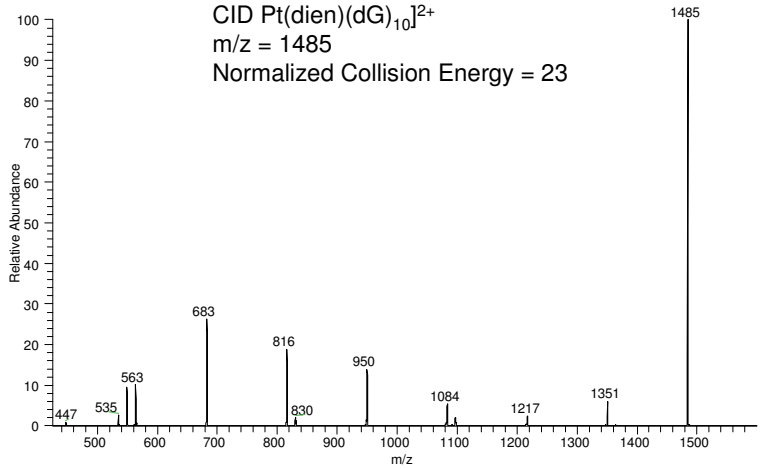


Fig. S4_4

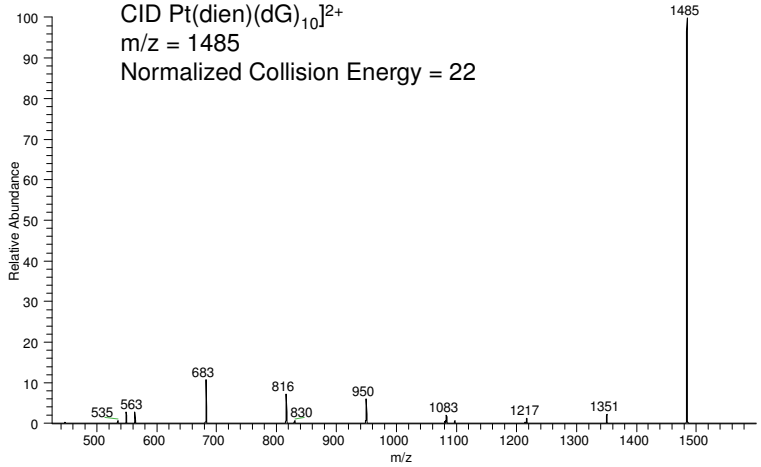


Fig. S5_1

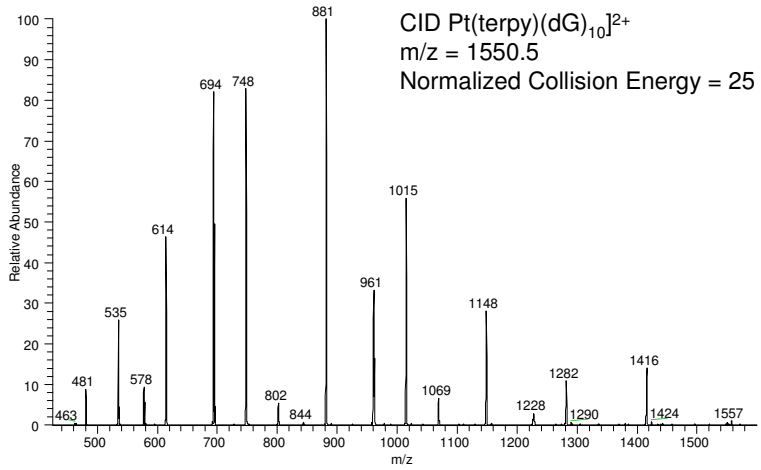


Fig. S5_2

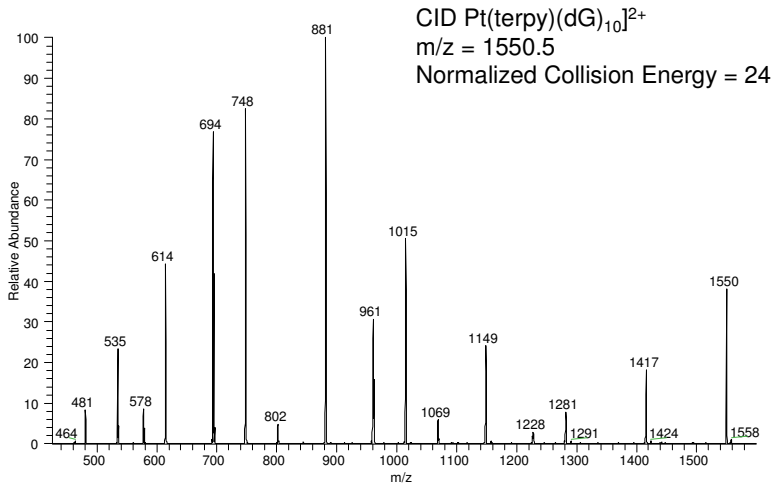


Fig. S5_3

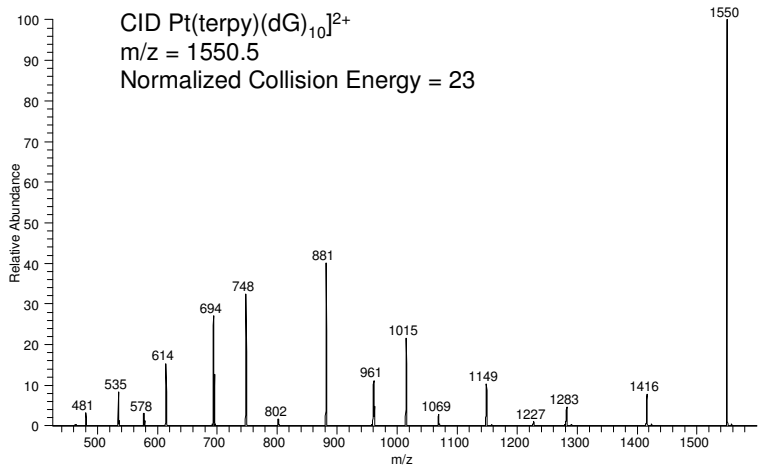
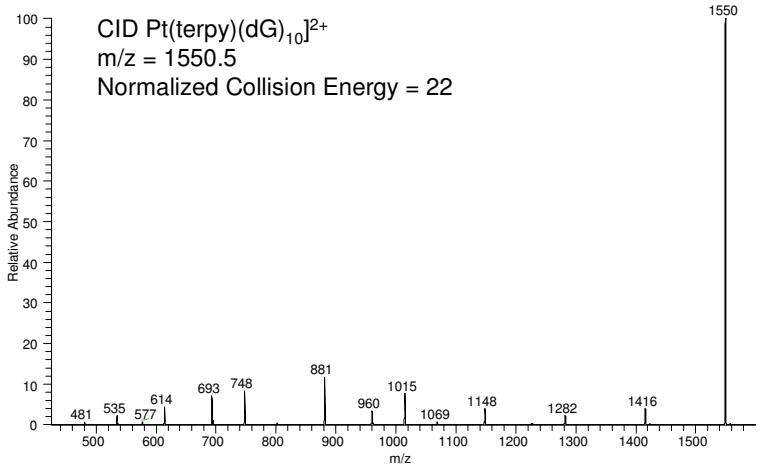
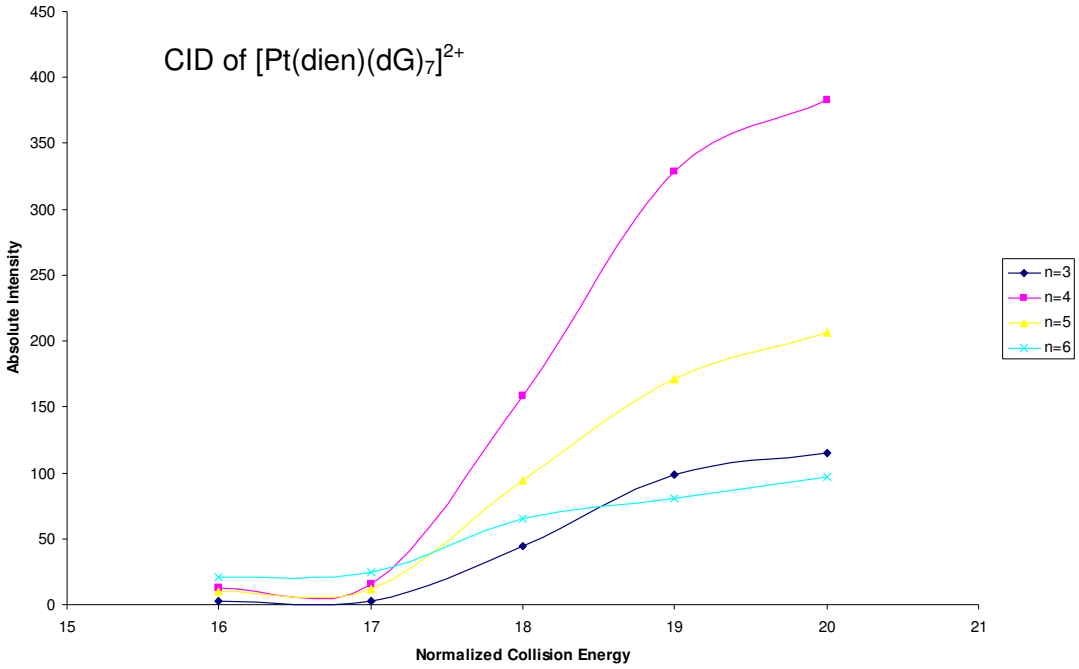


Fig. S5_4

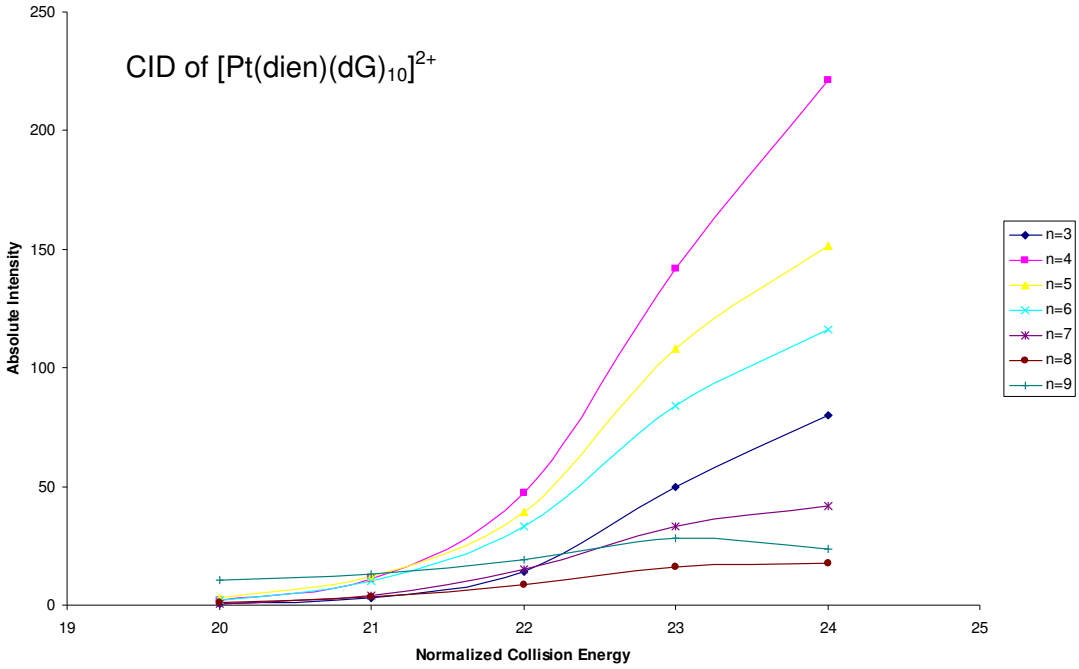


In order to prove that the n=4 and n=5 are "preferred clusters", we have collected spectra at a wide range of collision energies where the results showed that the abundances of the clusters in question are persistently the highest amongst the products. **Graphs 1 and 2** are a representation of the relative abundance ratios of the CID product ions versus the collision energies. The absolute intensities of the desired peaks were generated by integration of the ion count within a mass selected window.
Graph 1: CID of $[Pt(dien)dG_n]^{2+}$ for n =7 and n=10.
Graph 2: CID of $[Pt(terpy)dG_n]^{2+}$ for n =7 and n=10.

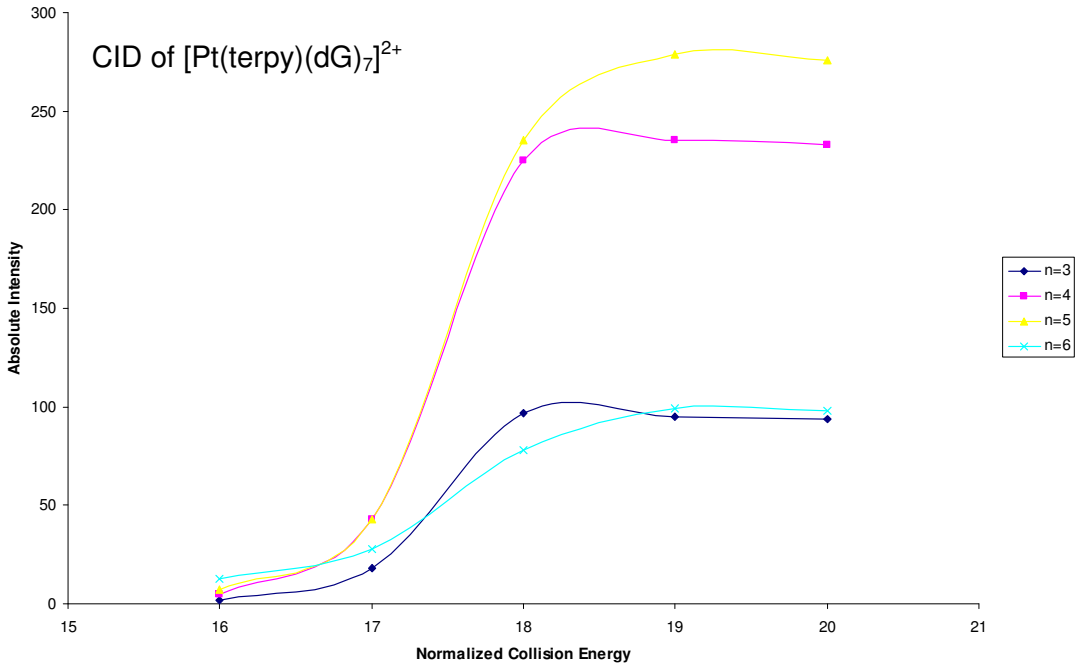
Graph 1a



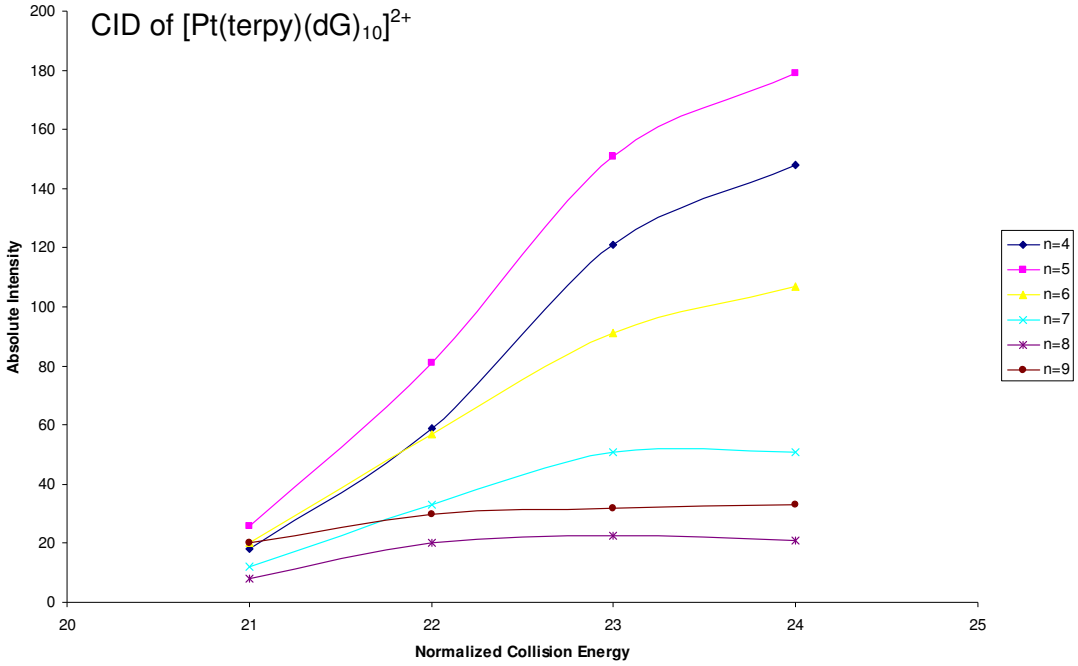
Graph 1b



Graph 2a



Graph 2b


CID of [Pt(terpy)(dG)10]2+
Absolute Intensity
Normalized Collision Energy
0
20
40
60
80
100
120
140
160
180
200
20
21
22
23
24
25
n=4
n=5
n=6
n=7
n=8
n=9