

Supplemental Table 2: The relative abundances of fragments upon IRMPD for G3-H/cisplatin cross-links (3-).

Fragment	m/z	Relative abundance (%)	Fragment	m/z	Relative abundance (%)
<i>G4G5</i>			<i>G3G4</i>		
G _n :G _n ⁻	506.4	13.9	G _n :G _n ⁻	506.4	10.6
b ₂ ⁻	554.4	6.1	c ₂ ⁻	616.4	2.7
w ₂ ⁻	634.5	100.0	w ₂ ⁻	634.4	54.7
T ₆ :C ₉ ²⁻	681.5	4.7	a ₃ -BH ⁻	714.4	83.4
a ₃ -BH ⁻	714.5	56.2	C ₈ :C ₉ ⁻	755.3	3.1
a ₇ -BH+◆ ³⁻	744.3	5.5	d ₄ ²⁻	760.4	3.5
C _n :C _{n+1} ⁻	755.4	16.3	T ₆ :T ₇ ⁻	785.4	22.7
T ₆ :T ₇ ⁻	785.4	24.0	G ₅ :T ₆ ⁻	810.3	35.7
T ₂ :G ₃ ⁻	810.7	21.4	T ₆ :C ₁₀ ²⁻	826.7	3.9
z ₃ ⁻	825.8	13.5	a ₈ -BH+◆ ³⁻	846.3	2.4
a ₃ ⁻	865.4	1.8	w ₃ ⁻	923.3	44.1
w ₃ ⁻	923.5	50.0	a ₆ -BH+◆ ²⁻	965.2	2.3
G ₃ :C ₁₀ +◆ ²⁻	954.4	5.8	[G ₄ :A ₁₁ +G+◆] ³⁻	999.3	1.0
d ₃ ⁻	963.2	6.7	a ₄ -BH ⁻	1043.4	43.3
G ₄ :C ₈ +◆ ⁻	980.9	1.5	w ₇ ²⁻	1054.4	11.6
a ₄ -BH ⁻	1043.5	46.4	T ₆ :C ₈ ⁻	1074.3	26.1
T ₇ :C ₉ ⁻	1059.6	8.9	γ ₁₀ +◆ ³⁻	1081.3	4.9
T ₆ :C ₈ ⁻	1074.3	19.2	G ₅ :T ₇ ⁻	1114.3	12.3
T ₂ :T ₇ +◆ ²⁻	1152.4	32.8	T ₂ :T ₇ +◆ ²⁻	1152.2	27.6
a ₁₁ +◆ ³⁻	1179.9	15.1	T ₂ :A ₁₁ +◆ ³⁻	1161.1	30.5
x ₁₁ +◆ ³⁻	1204.3	23.3	[G ₄ :C ₉ +G+◆] ²⁻	1200.0	24.6
w ₄ ⁻	1212.4	100.0	w ₄ ⁻	1212.3	100.0
-GH+◆ ³⁻	1236.3	41.4	-GH+◆ ³⁻	1236.8	24.6
-TH+◆ ³⁻	1244.9	68.5	-TH+◆ ³⁻	1244.3	24.1
a ₈ -BH+◆ ²⁻	1269.3	37.0	a ₈ +◆ ²⁻	1324.8	15.1
a ₈ +◆ ²⁻	1324.3	43.1	b ₈ +◆ ²⁻	1333.2	26.9
b ₈ +◆ ²⁻	1333.3	57.9	[G ₄ :C ₁₀ +G+◆] ²⁻	1344.2	27.2
C ₈ +◆ ²⁻	1364.3	17.5	T ₆ :C ₉ ⁻	1363.3	18.6
a ₅ -BH ⁻	1372.3	75.8	G ₅ :C ₈ ⁻	1404.2	55.0
G ₃ :G ₅ +◆ ⁻	1394.0	9.9	a ₉ -BH+◆ ²⁻	1413.2	32.6
[x ₈ +G+◆] ²⁻	1399.7	32.0	G ₃ :C ₁₀ +◆ ²⁻	1433.2	48.4
[w ₈ +G+◆] ²⁻	1408.2	44.4	b ₄ ⁻	1441.7	16.0
T ₂ :C ₉ +◆ ²⁻	1441.2	73.4	c ₉ +◆ ²⁻	1509.7	7.0
x ₉ +◆ ²⁻	1489.7	63.6	a ₁₀ -BH+◆ ²⁻	1558.2	14.4
w ₉ +◆ ²⁻	1498.2	57.1	[x ₉ +G+◆] ²⁻	1564.7	7.4
c ₉ +◆ ²⁻	1509.7	37.7	T ₂ :C ₁₀ +◆ ²⁻	1586.1	13.2
a ₁₀ -BH+◆ ²⁻	1558.2	31.3	T ₆ :C ₁₀ ⁻	1653.2	13.2
T ₂ :C ₁₀ +◆ ²⁻	1586.1	64.4	a ₁₁ -BH+◆ ²⁻	1702.8	12.5
a ₁₀ +◆ ²⁻	1614.2	15.0	z ₁₁ +◆ ²⁻	1766.1	4.1
a ₁₁ -BH+◆ ²	1703.2	27.9	-CH+◆ ^{3•}	1876.7	2.3
z ₁₁ +◆ ²⁻	1766.3	16.1			
[G ₅ :C ₈ +G+◆] ⁻	1783.1	9.0			
-CH+◆ ^{3•}	1877.2	3.7			

◆ stands for Pt(NH₃)₂ modification