

Supplemental Table 1: The relative abundances of fragments upon IRMPD for G3-D/cisplatin cross-links (3-)

Fragment	m/z	Relative abundance (%)	Fragment	m/z	Relative abundance (%)
<i>G4G5</i>			<i>G3G4</i>		
G <sub>n</sub> :G <sub>n</sub> <sup>-</sup>	506.5	6.1	G <sub>n</sub> :G <sub>n</sub> <sup>-</sup>	506.4	2.4
b <sub>2</sub> <sup>-</sup>	554.7	13.7	a <sub>5</sub> -BH+◆ <sup>3-</sup>	533.4	1.0
w <sub>2</sub> <sup>-</sup>	634.4	68.3	b <sub>2</sub> <sup>-</sup>	554.4	1.8
a <sub>6</sub> -BH+◆ <sup>3-</sup>	642.9	3.1	c <sub>2</sub> <sup>-</sup>	616.3	1.6
a <sub>3</sub> -BH <sup>-</sup>	714.6	25.4	w <sub>2</sub> <sup>-</sup>	634.4	31.0
C <sub>n</sub> :C <sub>n+1</sub> <sup>-</sup>	755.3	11.8	G <sub>3</sub> :A <sub>7</sub> +◆ <sup>3-</sup>	669.1	1.8
T <sub>6</sub> :A <sub>7</sub> <sup>-</sup>	794.5	12.9	T <sub>2</sub> :G <sub>4</sub> +◆ <sup>2-</sup>	684.4	1.5
T <sub>2</sub> :G <sub>3</sub> <sup>-</sup>	810.4	57.5	G <sub>3</sub> :G <sub>5</sub> +◆ <sup>2-</sup>	696.4	1.1
b <sub>8</sub> +◆ <sup>3-</sup>	812.3	5.4	a <sub>3</sub> -BH <sup>-</sup>	714.4	16.7
z <sub>3</sub> <sup>-</sup>	825.4	6.6	C <sub>n</sub> :C <sub>n+1</sub> <sup>-</sup>	755.4	15.5
a <sub>8</sub> +◆ <sup>3-</sup>	885.8	1.9	T <sub>6</sub> :A <sub>7</sub> <sup>-</sup>	794.3	8.5
w <sub>6</sub> <sup>2-</sup>	907.1	13.9	G <sub>5</sub> :T <sub>6</sub> <sup>-</sup>	810.4	29.1
w <sub>3</sub> <sup>-</sup>	923.4	32.5	w <sub>3</sub> <sup>-</sup>	923.4	13.9
T <sub>2</sub> :T <sub>6</sub> +◆ <sup>2-</sup>	1000.4	3.9	a <sub>9</sub> -BH+◆ <sup>3-</sup>	945.3	7.1
d <sub>9</sub> +◆ <sup>3-</sup>	1014.6	2.8	a <sub>9</sub> +◆ <sup>3-</sup>	982.0	1.4
a <sub>4</sub> -BH <sup>-</sup>	1043.4	24.8	C <sub>8</sub> :C <sub>10</sub> <sup>-</sup>	1044.4	13.5
w <sub>7</sub> <sup>2-</sup>	1059.7	4.9	w <sub>7</sub> <sup>2-</sup>	1059.4	4.1
T <sub>6</sub> :C <sub>8</sub> <sup>-</sup>	1083.3	27.3	T <sub>6</sub> :C <sub>8</sub> <sup>-</sup>	1083.4	5.5
a <sub>7</sub> -BH+◆ <sup>2-</sup>	1117.0	7.0	a <sub>7</sub> -BH+◆ <sup>2-</sup>	1117.1	4.0
T <sub>2</sub> :A <sub>7</sub> +◆ <sup>2-</sup>	1156.5	10.0	G <sub>5</sub> :A <sub>7</sub> <sup>-</sup>	1123.4	4.0
T <sub>2</sub> :A <sub>11</sub> +◆ <sup>3-</sup>	1164.4	21.5	T <sub>2</sub> :A <sub>7</sub> +◆ <sup>2-</sup>	1157.3	8.9
a <sub>7</sub> +◆ <sup>2-</sup>	1185.1	7.6	T <sub>2</sub> :A <sub>11</sub> +◆ <sup>3-</sup>	1164.3	6.9
[G <sub>5</sub> :T <sub>6</sub> +G+◆] <sup>-</sup>	1189.3	6.9	[G <sub>4</sub> :C <sub>9</sub> +G+◆] <sup>2-</sup>	1204.7	5.0
w <sub>4</sub> <sup>-</sup>	1212.3	100.0	w <sub>4</sub> <sup>-</sup>	1212.3	100.0
c <sub>7</sub> +◆ <sup>2-</sup>	1224.8	6.6	d <sub>7</sub> +◆ <sup>2-</sup>	1233.5	3.5
-GH+◆ <sup>3-</sup>	1239.7	26.2	-GH+◆ <sup>3-</sup>	1239.2	4.6
-AH+◆ <sup>3-</sup>	1244.1	10.4	a <sub>4</sub> -BH+◆ <sup>-</sup>	1272.7	21.5
-TH+◆ <sup>3-</sup>	1247.8	9.1	[G <sub>4</sub> :C <sub>10</sub> +G+◆] <sup>2-</sup>	1349.1	7.7
a <sub>8</sub> +◆ <sup>2-</sup>	1329.1	16.7	T <sub>6</sub> :C <sub>9</sub> <sup>-</sup>	1373.2	9.1
[G <sub>5</sub> :A <sub>11</sub> +G+◆] <sup>-</sup>	1341.7	9.5	a <sub>9</sub> -BH+◆ <sup>2-</sup>	1418.1	7.1
T <sub>6</sub> :C <sub>9</sub> <sup>-</sup>	1372.2	36.5	γ <sub>5</sub> <sup>-</sup>	1422.1	4.6
[x <sub>8</sub> +G+◆] <sup>2-</sup>	1404.3	8.3	w <sub>5</sub> <sup>-</sup>	1501.1	20.6
a <sub>9</sub> -BH+◆ <sup>2-</sup>	1418.4	8.1	c <sub>9</sub> +◆ <sup>2-</sup>	1514.6	1.6
T <sub>2</sub> :C <sub>9</sub> +◆ <sup>2-</sup>	1446.1	6.6	d <sub>4</sub> +◆ <sup>-</sup>	1522.1	2.8
a <sub>9</sub> +◆ <sup>2-</sup>	1474.6	6.2	T <sub>2</sub> :C <sub>10</sub> +◆ <sup>2-</sup>	1591.1	1.4
w <sub>5</sub> <sup>-</sup>	1501.1	28.1	T <sub>6</sub> :C <sub>10</sub> <sup>-</sup>	1662.1	3.4
a <sub>10</sub> -BH+◆ <sup>2-</sup>	1563.2	5.8	γ <sub>6</sub> <sup>-</sup>	1735.2	3.8
a <sub>10</sub> +◆ <sup>2-</sup>	1618.1	5.5	a <sub>11</sub> +◆ <sup>2-</sup>	1775.1	2.4
T <sub>6</sub> :C <sub>10</sub> <sup>-</sup>	1662.1	6.3	-TH+◆ <sup>3•</sup>	1871.1	1.7
T <sub>2</sub> :G <sub>5</sub> +◆ <sup>-</sup>	1698.0	5.4	-CH+◆ <sup>3•</sup>	1878.3	5.6
a <sub>11</sub> +◆ <sup>2-</sup>	1775.1	6.3			
-TH+◆ <sup>3•</sup>	1871.1	6.5			
-CH+◆ <sup>3•</sup>	1879.1	12.4			

◆ stands for Pt(NH<sub>3</sub>)<sub>2</sub> modification