

Supplemental Table 3: The relative abundances of fragments upon IRMPD for unmodified G3-D and G3-H (3-).

| Fragment                                      | m/z    | Relative abundance (%) | Fragment                                      | m/z    | Relative abundance (%) |
|---|--------|------------------------|---|--------|------------------------|
| <i>G3-D</i>                                   |        |                        |   |        |                        |
| G <sub>n</sub> :G <sub>n</sub> <sup>-</sup>   | 506.2  | 7.7                    | G <sub>n</sub> :G <sub>n</sub> <sup>-</sup>   | 506.1  | 11.4                   |
| w <sub>2</sub> <sup>-</sup>                   | 634.2  | 20.0                   | b <sub>4</sub> <sup>2-</sup>                  | 605.2  | 0.7                    |
| a <sub>3</sub> -BH <sup>-</sup>               | 714.3  | 38.5                   | w <sub>2</sub> <sup>-</sup>                   | 634.0  | 39.0                   |
| w <sub>5</sub> <sup>2-</sup>                  | 750.7  | 2.5                    | a <sub>3</sub> -BH <sup>-</sup>               | 714.1  | 17.8                   |
| C <sub>n</sub> :C <sub>n+1</sub> <sup>-</sup> | 755.1  | 2.2                    | C <sub>n</sub> :C <sub>n+1</sub> <sup>-</sup> | 755.1  | 11.4                   |
| T <sub>6</sub> :A <sub>7</sub> <sup>-</sup>   | 794.3  | 17.4                   | T <sub>6</sub> :T <sub>7</sub> <sup>-</sup>   | 785.1  | 10.0                   |
| d <sub>5</sub> <sup>2-</sup>                  | 810.2  | 23.5                   | d <sub>5</sub> <sup>2-</sup>                  | 810.1  | 16.1                   |
| a <sub>3</sub> <sup>-</sup>                   | 865.4  | 1.7                    | z <sub>3</sub> <sup>-</sup>                   | 825.6  | 6.0                    |
| T <sub>2</sub> :T <sub>6</sub> <sup>2-</sup>  | 885.7  | 10.0                   | a <sub>3</sub> <sup>-</sup>                   | 864.9  | 3.5                    |
| y <sub>9</sub> <sup>3-</sup>                  | 898.6  | 1.7                    | b <sub>9</sub> <sup>3-</sup>                  | 909.0  | 4.4                    |
| w <sub>3</sub> <sup>-</sup>                   | 923.3  | 18.5                   | w <sub>3</sub> <sup>-</sup>                   | 923.1  | 17.7                   |
| d <sub>3</sub> <sup>-</sup>                   | 964.1  | 1.1                    | d <sub>3</sub> <sup>-</sup>                   | 963.2  | 5.2                    |
| G <sub>5</sub> :C <sub>10</sub> <sup>2-</sup> | 995.2  | 8.9                    | T <sub>2</sub> :C <sub>10</sub> <sup>3-</sup> | 981.1  | 2.0                    |
| a <sub>7</sub> -BH <sup>2-</sup>              | 1002.8 | 15.0                   | G <sub>5</sub> :C <sub>10</sub> <sup>2-</sup> | 990.1  | 18.1                   |
| d <sub>10</sub> <sup>3-</sup>                 | 1035.1 | 1.7                    | a <sub>10</sub> <sup>3-</sup>                 | 999.6  | 6.0                    |
| a <sub>4</sub> -BH <sup>-</sup>               | 1043.3 | 50.9                   | a <sub>4</sub> -BH <sup>-</sup>               | 1043.1 | 52.7                   |
| w <sub>7</sub> <sup>2-</sup>                  | 1059.2 | 100                    | w <sub>7</sub> <sup>2-</sup>                  | 1054.2 | 100.0                  |
| A <sub>7</sub> :C <sub>9</sub> <sup>-</sup>   | 1068.1 | 3.4                    | T <sub>7</sub> :C <sub>9</sub> <sup>-</sup>   | 1059.6 | 13.6                   |
| b <sub>7</sub> <sup>2-</sup>                  | 1078.6 | 2.8                    | T <sub>6</sub> :C <sub>8</sub> <sup>-</sup>   | 1074.1 | 7.8                    |
| G <sub>5</sub> :A <sub>7</sub> <sup>-</sup>   | 1123.2 | 7.9                    | T <sub>2</sub> :A <sub>11</sub> <sup>3-</sup> | 1086.1 | 1.8                    |
| d <sub>11</sub> <sup>3-</sup>                 | 1139.2 | 35.7                   | d <sub>7</sub> <sup>2-</sup>                  | 1114.1 | 20.3                   |
| G <sub>3</sub> :C <sub>9</sub> <sup>2-</sup>  | 1179.6 | 1.1                    | x <sub>11</sub> <sup>3-</sup>                 | 1127.6 | 2.7                    |
| T <sub>2</sub> :C <sub>8</sub> <sup>2-</sup>  | 1186.7 | 2.2                    | T <sub>2</sub> :G <sub>4</sub> <sup>-</sup>   | 1139.1 | 33.5                   |
| a <sub>4</sub> <sup>-</sup>                   | 1194.2 | 1.4                    | G <sub>4</sub> :C <sub>10</sub> <sup>2-</sup> | 1155.6 | 10.5                   |
| w <sub>4</sub> <sup>-</sup>                   | 1212.3 | 38.6                   | z <sub>8</sub> <sup>2-</sup>                  | 1170.2 | 1.8                    |
| w <sub>8</sub> <sup>2-</sup>                  | 1224.3 | 26.8                   | w <sub>4</sub> <sup>-</sup>                   | 1212.1 | 31.7                   |
| a <sub>9</sub> -BH <sup>2-</sup>              | 1304.3 | 2.7                    | w <sub>8</sub> <sup>2-</sup>                  | 1219.1 | 46.5                   |
| T <sub>6</sub> :C <sub>9</sub> <sup>-</sup>   | 1372.2 | 77.1                   | d <sub>8</sub> <sup>2-</sup>                  | 1259.6 | 1.6                    |
| w <sub>9</sub> <sup>2-</sup>                  | 1388.3 | 8.7                    | d <sub>4</sub> <sup>-</sup>                   | 1292.1 | 2.4                    |
| G <sub>5</sub> :C <sub>8</sub> <sup>-</sup>   | 1412.2 | 5.7                    | a <sub>9</sub> -BH <sup>2-</sup>              | 1300.2 | 6.2                    |
| y <sub>5</sub> <sup>-</sup>                   | 1421.3 | 4.5                    | T <sub>2</sub> :C <sub>9</sub> <sup>2-</sup>  | 1327.6 | 2.8                    |
| G <sub>4</sub> :A <sub>7</sub> <sup>-</sup>   | 1453.3 | 3.8                    | b <sub>9</sub> <sup>2-</sup>                  | 1364.1 | 9.2                    |
| T <sub>2</sub> :C <sub>10</sub> <sup>2-</sup> | 1476.2 | 0.5                    | a <sub>5</sub> -BH <sup>-</sup>               | 1372.2 | 63.8                   |
| x <sub>5</sub> <sup>-</sup>                   | 1483.4 | 0.6                    | w <sub>9</sub> <sup>2-</sup>                  | 1383.6 | 10.8                   |
| w <sub>5</sub> <sup>-</sup>                   | 1501.3 | 51.0                   | G <sub>5</sub> :C <sub>8</sub> <sup>-</sup>   | 1404.3 | 10.7                   |
| a <sub>11</sub> -BH <sup>2</sup>              | 1593.7 | 1.1                    | T <sub>2</sub> :C <sub>10</sub> <sup>2-</sup> | 1572.1 | 4.7                    |
| a <sub>11</sub> <sup>2-</sup>                 | 1661.2 | 15.7                   | x <sub>5</sub> <sup>-</sup>                   | 1483.2 | 3.9                    |
| a <sub>6</sub> -BH <sup>-</sup>               | 1702.3 | 6.2                    | w <sub>5</sub> <sup>-</sup>                   | 1502.0 | 3.1                    |
| -GH <sup>3-•</sup>                            | 1746.2 | 1.6                    | a <sub>5</sub> <sup>-</sup>                   | 1524.2 | 1.5                    |
| -TH <sup>3-•</sup>                            | 1759.3 | 2.6                    | a <sub>11</sub> -BH <sup>2</sup>              | 1588.7 | 3.4                    |
| G <sub>5</sub> :C <sub>10</sub> <sup>2-</sup> | 1991.3 | 7.0                    | z <sub>11</sub> <sup>2-</sup>                 | 1652.2 | 30.4                   |

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