**Supporting Information**

# Investigation of the Experimental Parameters of Ultraviolet Photodissociation for the Structural Characterization of Chondroitin Sulfate Glycosaminoglycan Isomers

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Table of Contents


| Content | Figure Number |
|---|---|
| UVPD Orbitrap schematic | S1 |
| HCD spectrum of $[M-H]^-$ of DS dp4 | S2 |
| Zoom in of $^{1,4}A_4$ fragment ion | S3 |
| Zoom in of $^{2,4}X_2$ fragment ion | S4 |
| 193 nm UVPD full spectrum of $[M-H]^-$ precursor ion of CS-A dp4 | S5 |
| 193 nm UVPD of $[M-4H+Na]^{3-}$ precursor ion of CS-A dp4 and DS dp4 | S6 |
| $MS^3$ of DS dp4 | S7 |
| $MS^3$ of CS-A dp4 | S8 |
| DS dp4 annotated structures | S9 |
| 193 nm UVPD of $[M-2H]^{2-}$ precursor ion using 4 laser pulses in the high-pressure cell | S10 |
| 193 nm UVPD of $[M-3H]^{3-}$ precursor ion with 4 laser pulses in the high-pressure cell | S11 |
| 193 nm UVPD of $[M-2H]^{2-}$ precursor ion using 8 laser pulses in the high-pressure cell | S12 |
| 193 nm UVPD of $[M-3H]^{3-}$ precursor ion with 8 laser pulses in the high-pressure cell | S13 |
| 213 nm UVPD spectra of $[M-3H]^{3-}$ precursor ion of DS dp4 using 750 laser pulses | S14 |

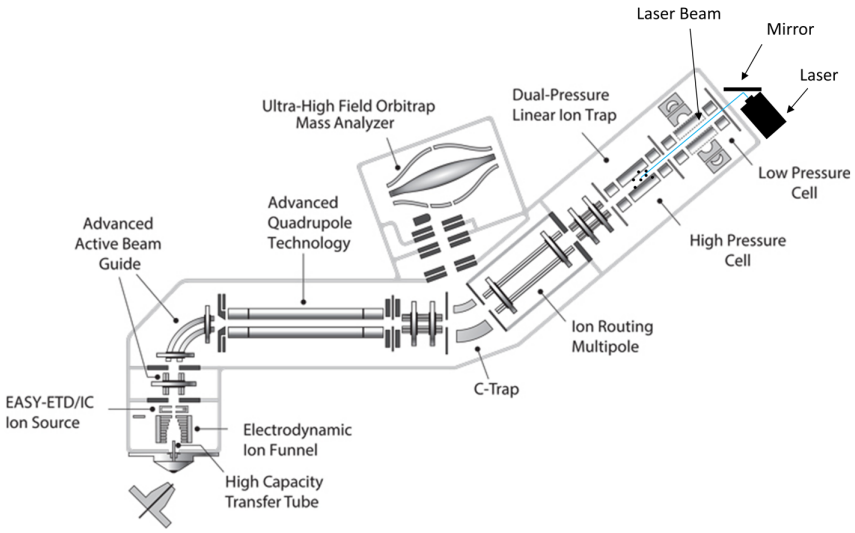


Figure S1. UVPD schematic on a Thermo Fisher Orbitrap Fusion Lumos modified with a Coherent Excistar 193 nm excimer laser or a 213 nm CryLas solid state laser. The position of the laser and mirror are shown in black at the right of the figure, and the path of the laser beam is shown in blue.

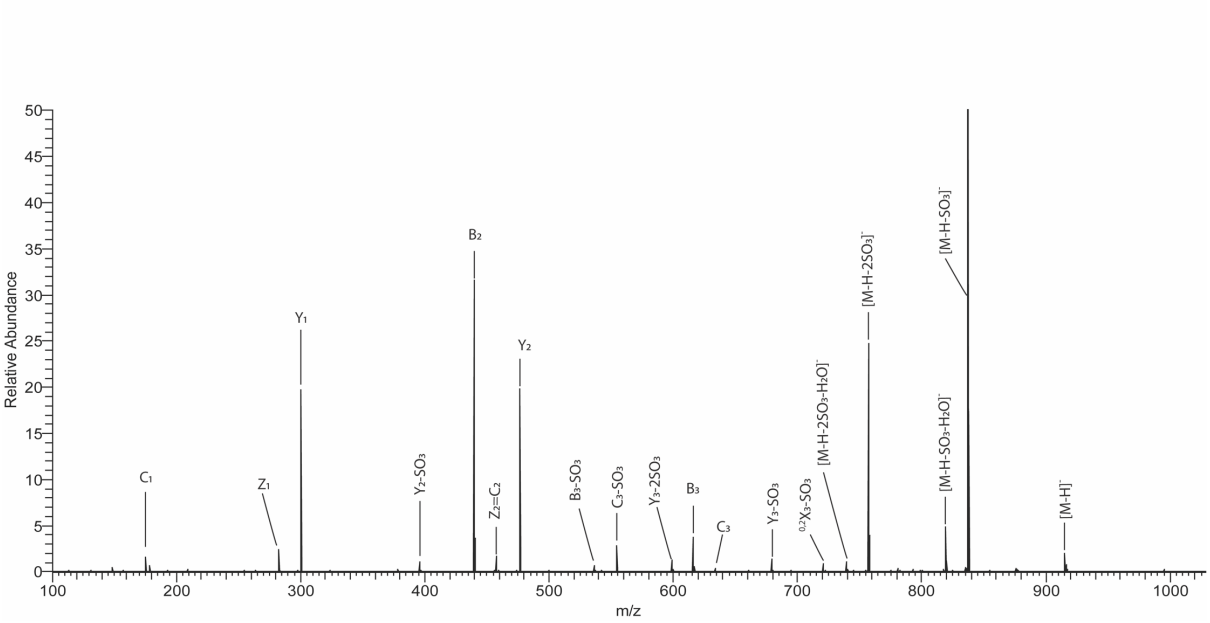


Figure S1. HCD (NCE 25) spectrum of the [M-H]- precursor ion of CS-A dp4.

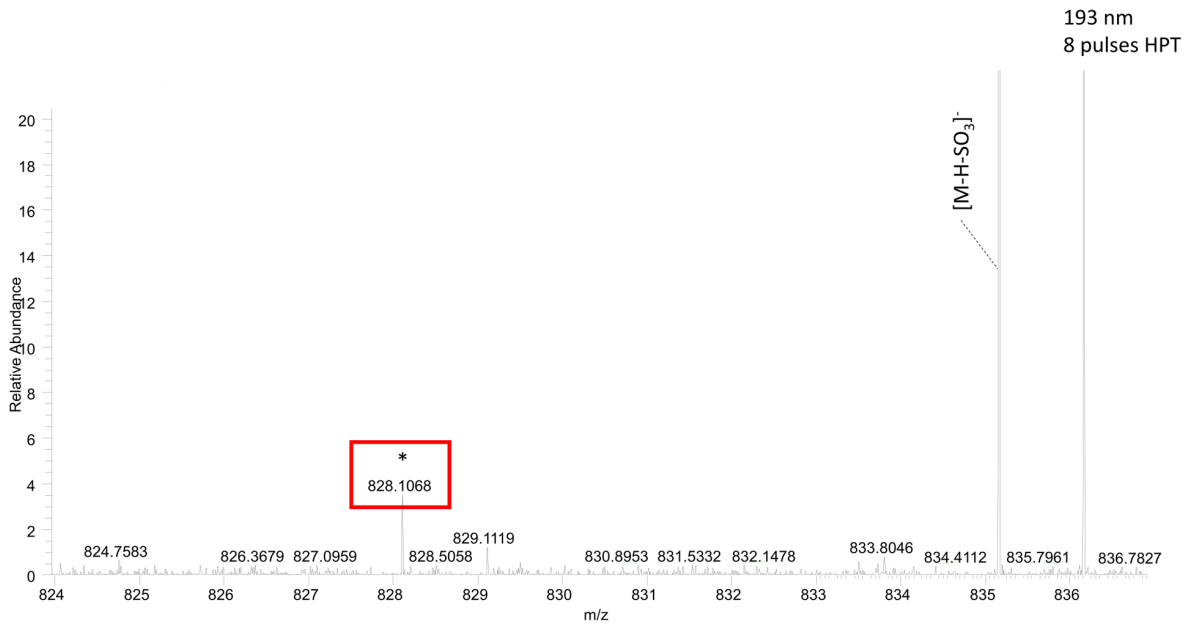


Figure S2. Mass scale expansion focusing on the $^{1,4}A_4$ fragment ion (828.1068 m/z) produced upon UVPD of the [M-H]- precursor ion of DS dp4.

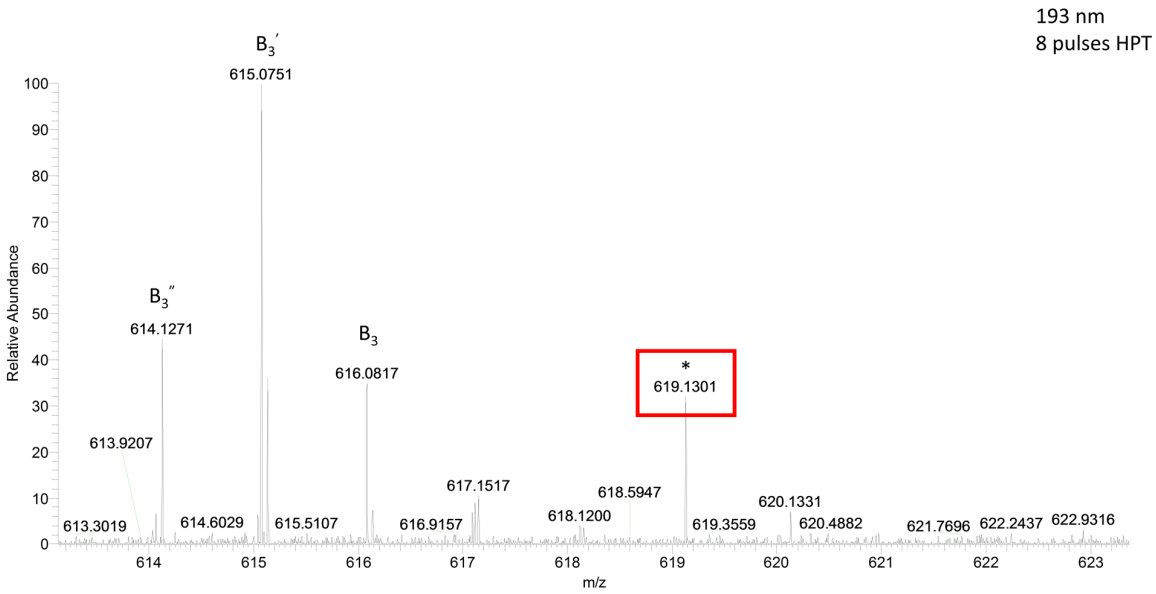


Figure S3. Mass scale expansion focusing on the $^{2,4}X_2$ fragment ion (619.1301 m/z) produce upon UVPD of the [M-H]- precursor ion of DS dp4.

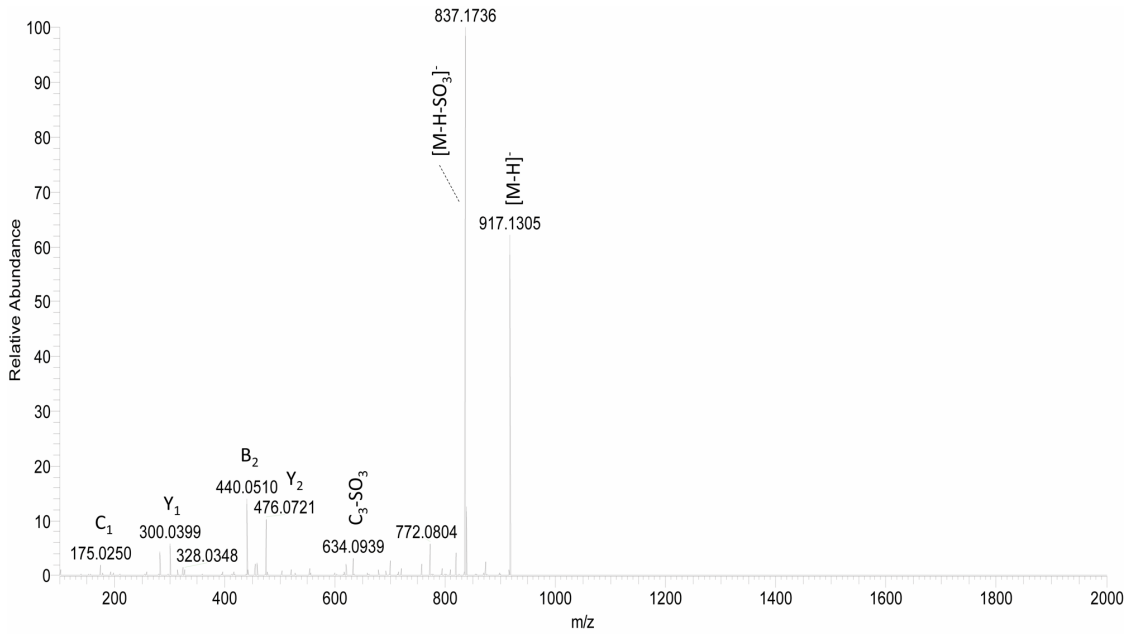


Figure S5. Full scan UVPD spectrum of $[M-H]^-$ precursor ion of CS-A dp4.

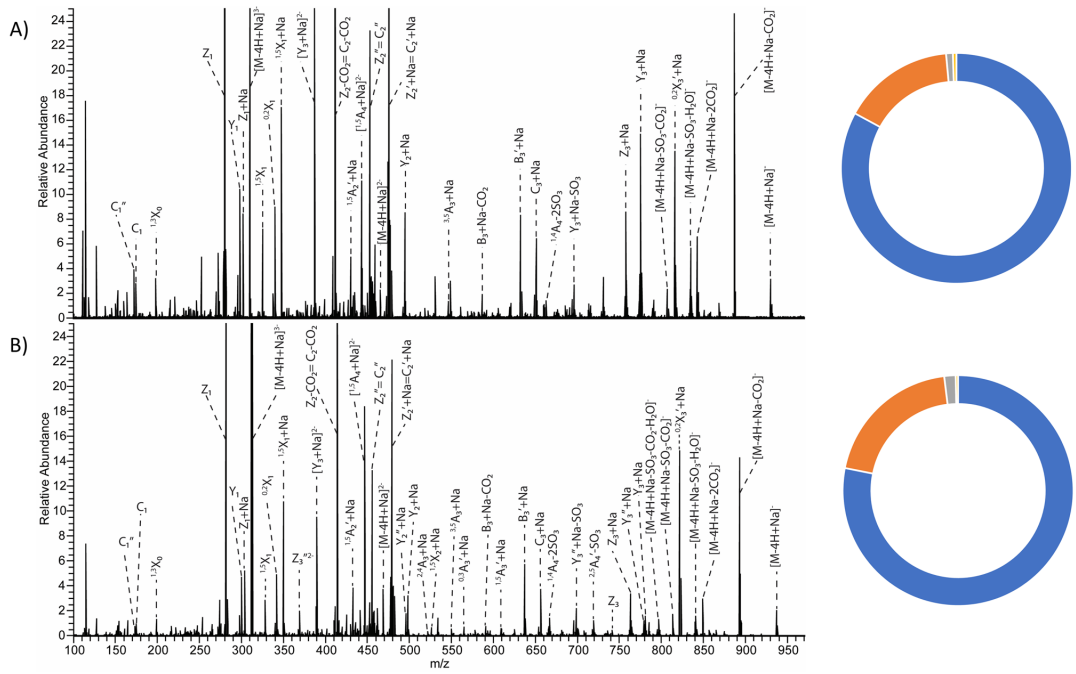


Figure S6. 193 nm UVPD with 8 laser pulses (4 mJ per pulse) in the high-pressure cell of the $[M-4H+Na]^{3-}$ precursor of DS dp4 (A) and CS-A dp4 (B). Donut plots depict intensity distributions if glycosidic fragments (blue), cross-ring fragments (orange), glycosidic fragments with -$SO_3$ loss (grey) and cross-ring fragments with -$SO_3$ loss (yellow). Fragment ion lists are shown in Tables S15 and S16.

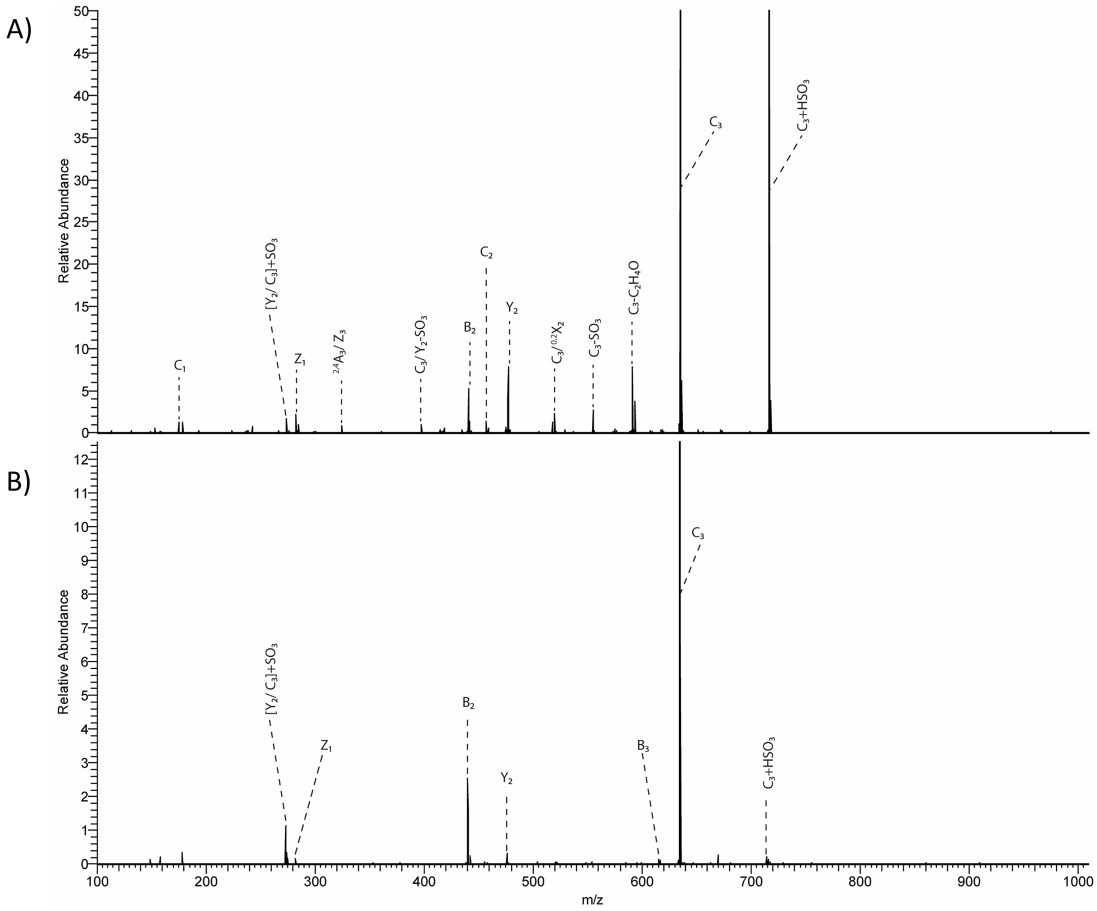


Figure S7. $MS^3$ activation of the fragment ion m/z 715.05 of DS dp4 using (A) 193 nm UVPD (8 pulses, 4 mJ)/ 193 nm UVPD (8 pulses, 4 mJ) and (B) 193 nm UVPD (8 pulses, 4 mJ)/ HCD (NCE 20). Fragment ion lists are shown in Tables S23 and S24.

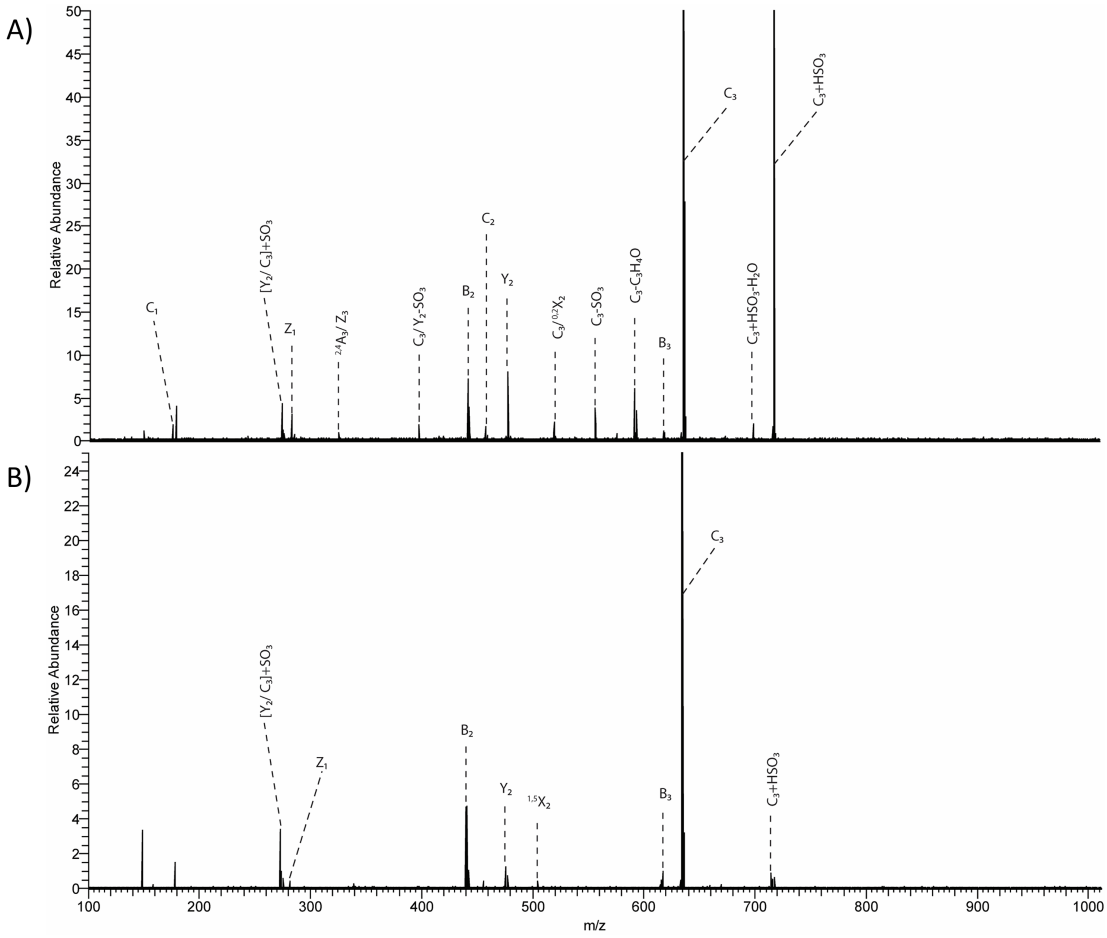


Figure S8. $MS^3$ activation of the fragment ion m/z 715.05 of CS-A dp4 using (A) 193 nm UVPD (8 pulses, 4 mJ)/ 193 nm UVPD (8 pulses, 4 mJ) and (B) 193 nm UVPD (8 pulses, 4 mJ)/ HCD (NCE 20). Fragment ion lists are shown in Tables S25 and S26.

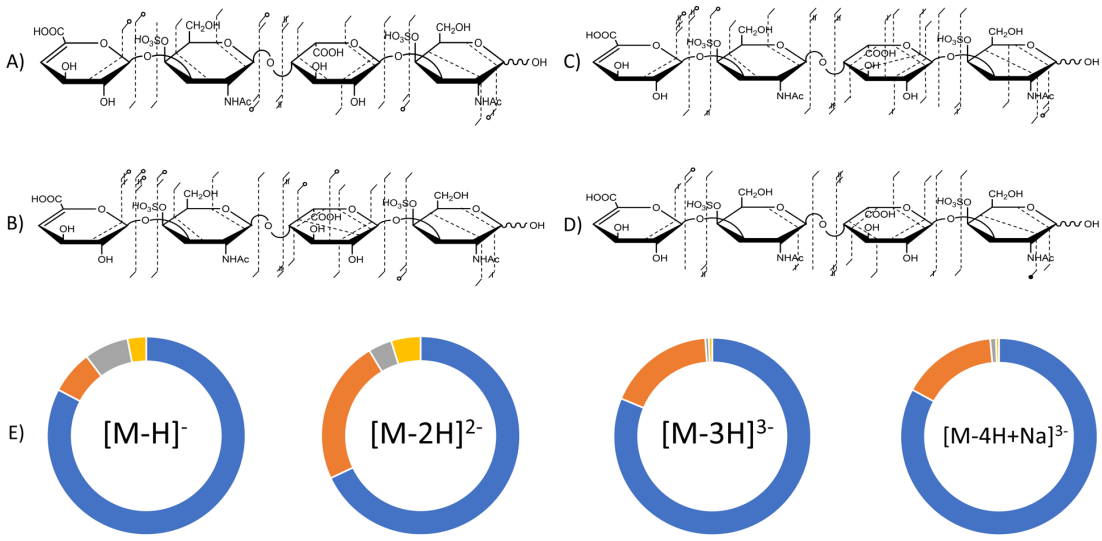


Figure S9. Annotated fragment maps depicting 193 nm UVPD fragment ion diversity using 8 laser pulses (4 mJ per pulse) in the high-pressure cell for (A) DS dp4 $[M-H]^-$ precursor, (B) DS dp4 $[M-2H]^{2-}$ precursor, (C) DS dp4 $[M-3H]^{3-}$ precursor and (D) DS dp4 $[M-4H+Na]^{3-}$ precursor. (E) Donut plots depicting the intensity distribution of glycosidic fragments (blue), cross-ring fragments (orange), glycosidic fragments with $-SO_3$ loss (grey) and cross-ring fragments with $-SO_3$ loss (yellow) of each precursor.

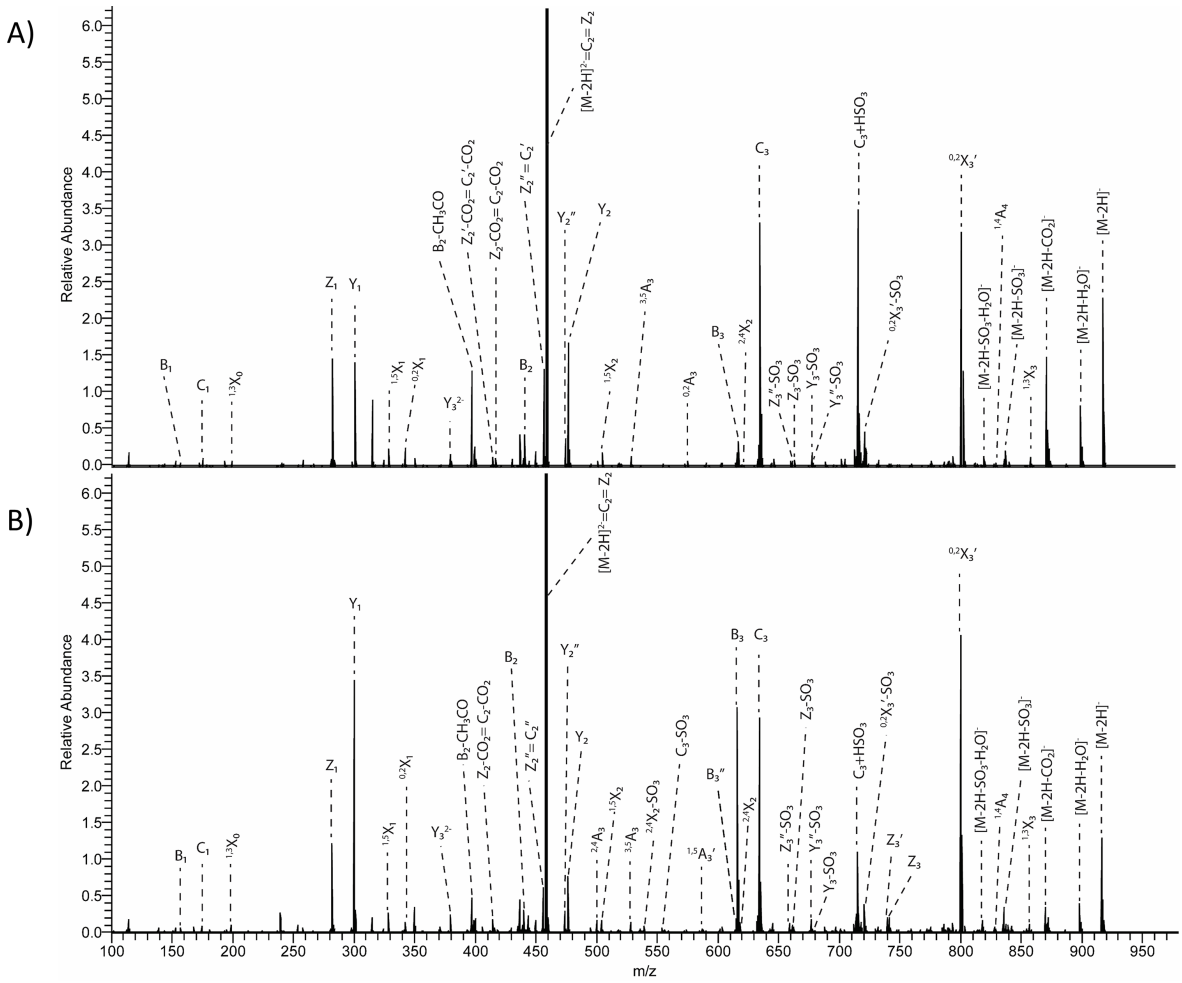


Figure S10. 193 nm UVPD spectra of the $[M-2H]^{2-}$ precursor ion using 4 laser pulses (4 mJ per pulse) in the high-pressure cell of (A) DS dp4 and (B) CS-A dp4.

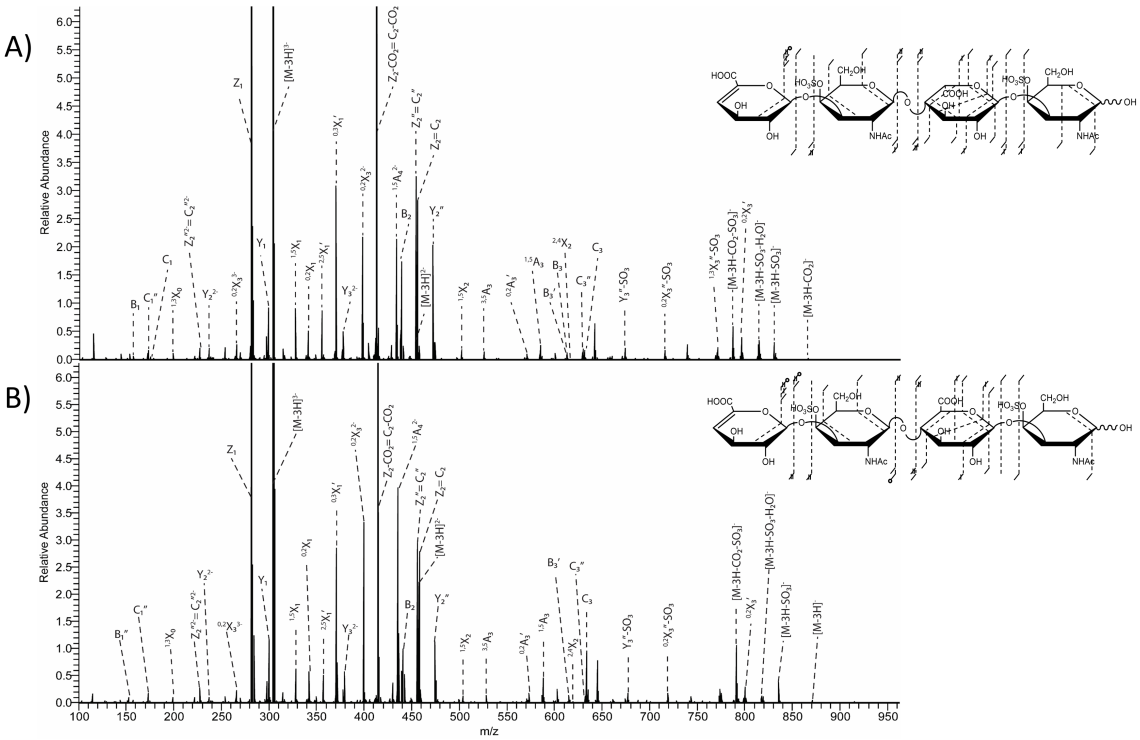


Figure S11. 193 nm UVPD with 4 laser pulses (4 mJ per pulse) in the high-pressure cell spectra and annotated fragment map insets of (A) DS dp4 and (B) CS- A dp4 using the $[M-3H]^{3-}$ precursor ion.

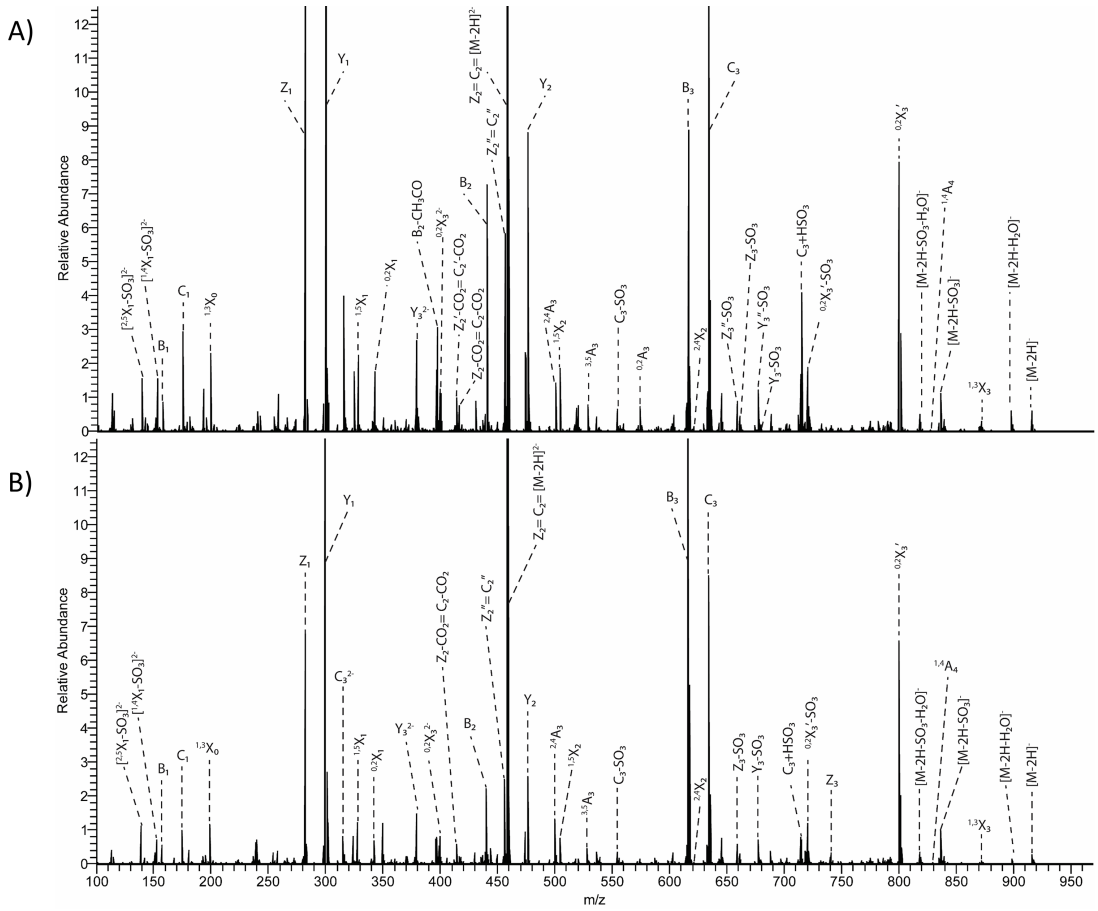


Figure S12. 193 nm UVPD spectra of the $[M-2H]^{2-}$ precursor ion using 8 laser pulses (4 mJ per pulse) in the low-pressure cell of (A) DS dp4 and (B) CS-A dp4.

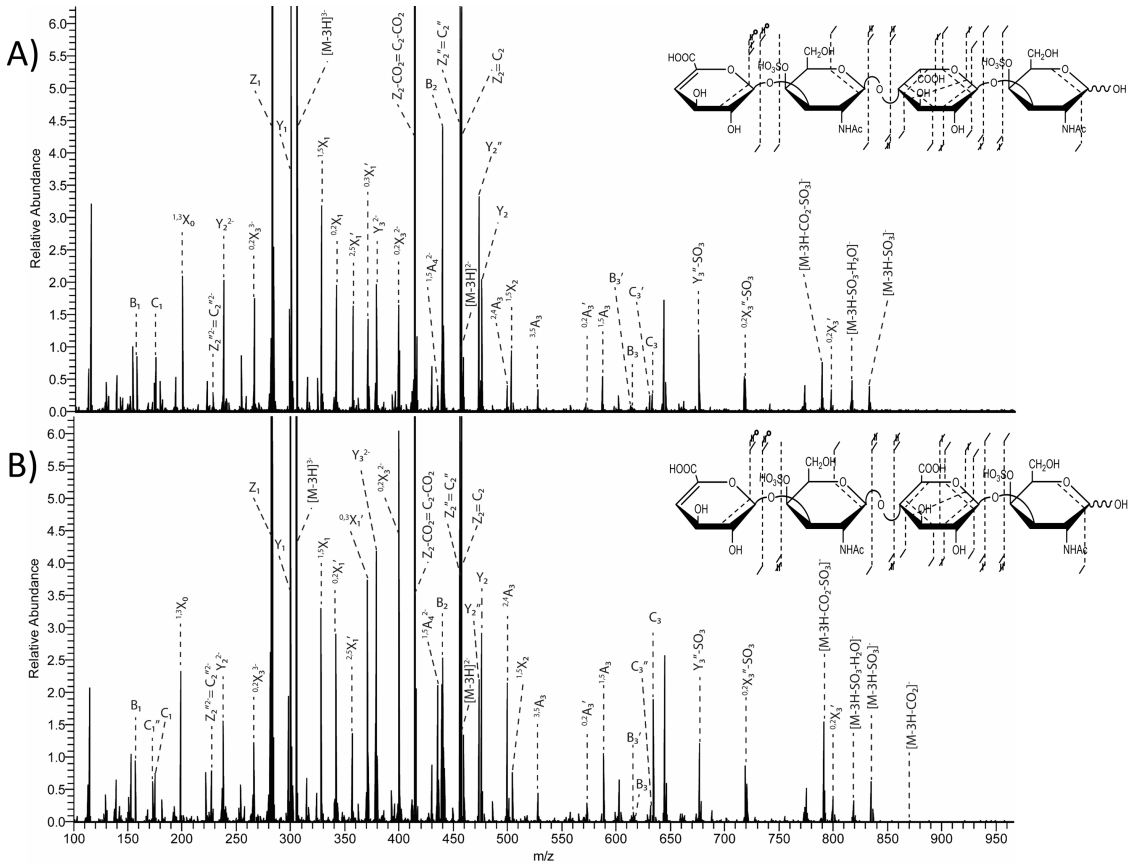


Figure S13. 193 nm UVPD using 8 laser pulses (4 mJ per pulse) in the low-pressure cell spectra and fragment map insets of the $[M-3H]^{3-}$ precursor of (A) DS dp4 and (B) CS- A dp4.

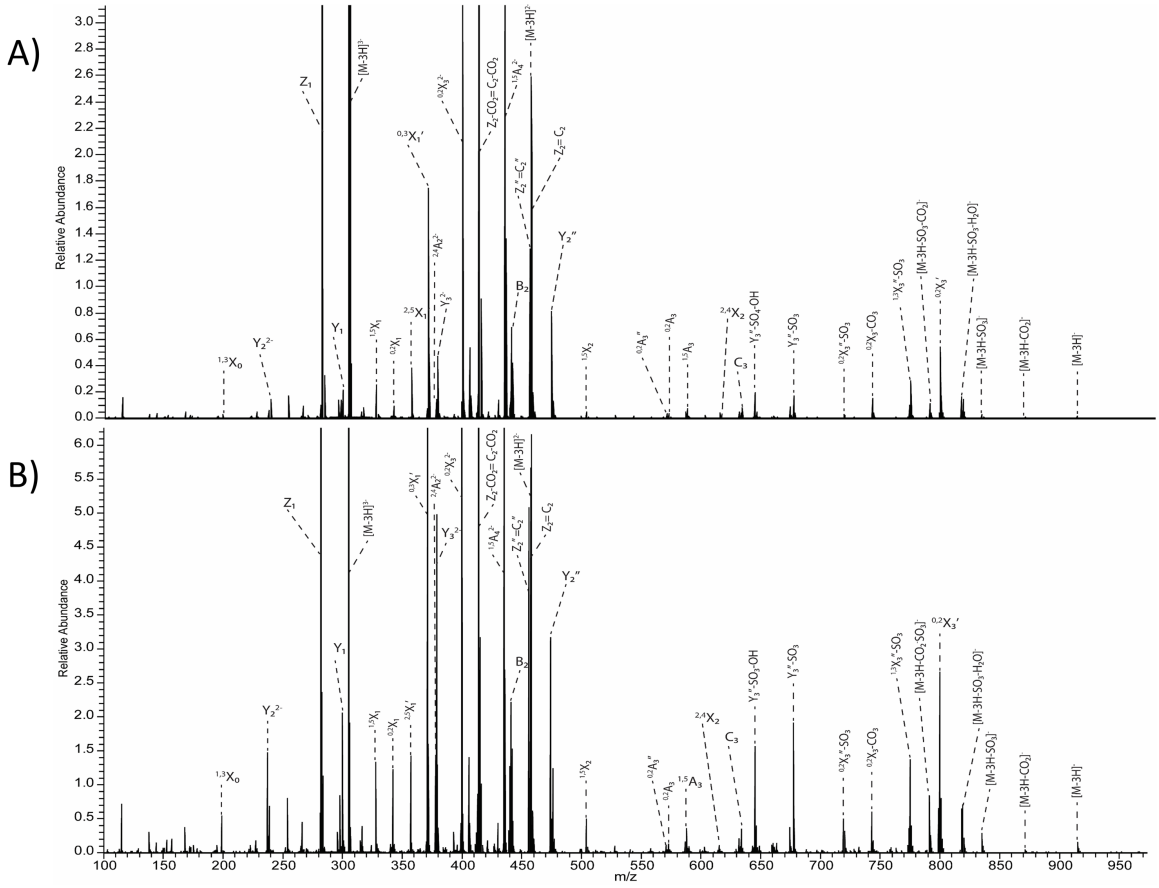


Figure S14. 213 nm UVPD spectra of the $[M-3H]^{3-}$ precursor ion of DS dp4 using 750 laser pulses (3 μJ/ pulse) in the (A) low-pressure cell and (B) high-pressure cell.

Table of Contents


| Content | Table Number |
|---|---|
| 193 nm UVPD activation of the $[M-H]^-$ precursor of CS-A dp4 (8 pulses, 4 mJ) | S1 |
| 193 nm UVPD activation of the $[M-H]^-$ precursor of DS dp4 (8 pulses, 4 mJ) | S2 |
| 193 nm UVPD activation of the $[M-2H]^{2-}$ precursor of DS dp4 in the high-pressure cell (8 pulses, 4 mJ) | S3 |
| 193 nm UVPD activation of the $[M-2H]^{2-}$ precursor of DS dp4 in the low-pressure cell (8 pulses, 4 mJ) | S4 |
| 193 nm UVPD activation of the $[M-2H]^{2-}$ precursor of DS dp4 in the high-pressure cell (4 pulses, 4 mJ) | S5 |
| 193 nm UVPD activation of the $[M-2H]^{2-}$ precursor of CS-A dp4 in the high-pressure cell (8 pulses, 4 mJ) | S6 |
| 193 nm UVPD activation of the $[M-2H]^{2-}$ precursor of CS-A dp4 in the low-pressure cell (8 pulses, 4 mJ) | S7 |
| 193 nm UVPD activation of the $[M-2H]^{2-}$ precursor of CS-A dp4 in the high-pressure cell (4 pulses, 4 mJ) | S8 |
| 193 nm UVPD activation of the $[M-3H]^{3-}$ precursor of DS dp4 in the high-pressure cell (8 pulses, 4 mJ) | S9 |
| 193 nm UVPD activation of the $[M-3H]^{3-}$ precursor of DS dp4 in the low-pressure cell (8 pulses, 4 mJ) | S10 |
| 193 nm UVPD activation of the $[M-3H]^{3-}$ precursor of DS dp4 in the high-pressure cell (4 pulses, 4 mJ) | S11 |
| 193 nm UVPD activation of the $[M-3H]^{3-}$ precursor of CS-A dp4 in the high-pressure cell (8 pulses, 4 mJ) | S12 |
| 193 nm UVPD activation of the $[M-3H]^{3-}$ precursor of CS-A dp4 in the low-pressure cell (8 pulses, 4 mJ) | S13 |
| 193 nm UVPD activation of the $[M-3H]^{3-}$ precursor of CS-A dp4 in the high-pressure cell (4 pulses, 4 mJ) | S14 |
| 193 nm UVPD activation of the $[M-4H+Na]^{3-}$ precursor of CS-A dp4 in the high-pressure cell (8 pulses, 4 mJ) | S15 |
| 193 nm UVPD activation of the $[M-4H+Na]^{3-}$ precursor of DS dp4 in the high-pressure cell (8 pulses, 4 mJ) | S16 |
| 213 nm UVPD activation of the $[M-3H]^{3-}$ precursor of DS dp4 in the high-pressure cell (50 ms) | S17 |
| 213 nm UVPD activation of the $[M-3H]^{3-}$ precursor of DS dp4 in the low-pressure cell (50 ms) | S18 |
| 213 nm UVPD activation of the $[M-3H]^{3-}$ precursor of DS dp4 in the high-pressure cell (150 ms) | S19 |
| 213 nm UVPD activation of the $[M-3H]^{3-}$ precursor of DS dp4 in the high-pressure cell (300 ms) | S20 |
| 213 nm UVPD activation of the $[M-3H]^{3-}$ precursor of DS dp4 in the high-pressure cell (400 ms) | S21 |
| 213 nm UVPD activation of the $[M-3H]^{3-}$ precursor of DS dp4 in the low-pressure cell (400 ms) | S22 |
| $MS^3$ activation of the fragment ion m/z 715.05 of DS dp4 using 193 nm UVPD (8 pulses, 4 mJ)/ 193 nm UVPD (8 pulses, 4 mJ) | S23 |
| $MS^3$ activation of the fragment ion m/z 715.05 of DS dp4 using 193 nm UVPD (8 pulses, 4 mJ)/ HCD (NCE 20) | S24 |
| $MS^3$ activation of the fragment ion m/z 715.05 of CS-A dp4 using 193 nm UVPD (8 pulses, 4 mJ)/ 193 nm UVPD (8 pulses, 4 mJ) | S25 |
| $MS^3$ activation of the fragment ion m/z 715.05 of CS-A dp4 using 193 nm UVPD (8 pulses, 4 mJ)/ HCD (NCE 20) | S26 |

Table S1: Fragment ion list for 193 nm UVPD activation of the $[M-H]^-$ precursor of CS-A dp4 (8 pulses, 4 mJ).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 157.0144 | 157.0142 | 0.97 | 4754.8 | $B_1$ |
| 175.025 | 175.0248 | 1.1 | 27347.4 | $C_1$ |
| 198.9921 | 198.9917 | 1.5 | 6025.7 | $^{1,3}X_0$ |
| 282.0293 | 282.0289 | 1.4 | 63313.8 | $Z_1$ |
| 300.0399 | 300.0394 | 1.4 | 83608.1 | $Y_1$ |
| 328.0348 | 328.0343 | 1.2 | 16121.5 | $^{1,5}X_1$ |
| 360.0941 | 360.0936 | 1.3 | 4561.8 | $B_2$-$SO_3$ |
| 396.1153 | 396.1147 | 1.4 | 8744.8 | $Y_2$-$SO_3$ |
| 416.051 | 416.0504 | 1.4 | 10277.6 | $^{2,4}X_1$ |
| 440.051 | 440.0504 | 1.3 | 206886.1 | $B_2$ |
| 456.0459 | 456.0458 | 0 | 29959.4 | $Z_2$" |
| 456.0459 | 456.0458 | 0 | 29959.4 | $C_2$" |
| 458.0616 | 458.0609 | 1.3 | 33634.5 | $Z_2$ |
| 458.0616 | 458.0609 | 1.3 | 33634.5 | $C_2$ |
| 476.0721 | 476.0715 | 1.1 | 145963.3 | $Y_2$ |
| 504.0672 | 504.0664 | 1.4 | 12921.9 | $^{1,5}X_2$ |
| 554.137 | 554.1362 | 1.3 | 17647.9 | $C_3$-$SO_3$ |
| 599.195 | 599.1941 | 1.5 | 6341.5 | $Y_3$-$2SO_3$ |
| 616.0833 | 616.0825 | 1.3 | 10504 | $B_3$ |
| 619.1306 | 619.1298 | 1.3 | 6574.7 | $^{2,4}X_2$ |
| 634.0939 | 634.0930 | 1.3 | 45667.9 | $C_3$-$SO_3$ |
| 659.1258 | 659.1253 | 0.65 | 7025.5 | $Z_3$"-$SO_3$ |
| 661.1414 | 661.1403 | 1.6 | 4845.1 | $Z_3$-$SO_3$ |
| 679.152 | 679.1509 | 1.6 | 15239.8 | $Y_3$-$SO_3$ |
| 715.059 | 715.0564 | 3.6 | 11169.5 | $C_3$+$HSO_3$ |
| 721.1627 | 721.1615 | 1.7 | 17917.1 | $^{0,2}X_3$-$SO_3$ |
| 757.2169 | 757.2156 | 1.7 | 29523.8 | $[M-H-2SO_3]^-$ |
| 793.1836 | 793.1832 | 0.5 | 2483.7 | $[M-H-SO_3-CO_2]^-$ |
| 819.1631 | 819.1624 | 0.78 | 61997.5 | $[M-H-SO_3-H_2O]^-$ |
| 827.0969 | 827.0975 | -0.82 | 187.8 | $^{1,4}A_4$ |
| 837.1736 | 837.1724 | 1.4 | 1448867.4 | $[M-H-SO_3]^-$ |
| 873.1342 | 873.1399 | -6.6 | 1528 | $[M-H-CO_2]^-$ |
| 899.1179 | 899.1192 | -1.5 | 1730.4 | $[M-H-H_2O]^-$ |
| 917.1305 | 917.1292 | 1.3 | 872408.2 | $[M-H]^-$ |

Table S2: Fragment ion list for 193 nm UVPD activation of the $[M-H]^-$ precursor of DS dp4 (8 pulses, 4 mJ).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 157.0139 | 157.0142 | -2.2 | 1766.1 | $B_1$ |
| 175.0246 | 175.0248 | -1.2 | 13065.1 | $C_1$ |
| 198.9913 | 198.9917 | -2.5 | 1559.4 | $^{1,3}X_0$ |
| 282.0282 | 282.0289 | -2.5 | 26137.3 | $Z_1$ |
| 300.0388 | 300.0394 | -2.3 | 19226.8 | $Y_1$ |
| 328.0339 | 328.0343 | -1.5 | 3473.2 | $^{1,5}X_1$ |
| 360.0932 | 360.0936 | -1.2 | 1391.2 | $B_2$-$SO_3$ |
| 396.1143 | 396.1147 | -1.1 | 3578.2 | $Y_2$-$SO_3$ |
| 416.0499 | 416.0504 | -1.3 | 3842.2 | $^{2,4}X_1$ |
| 440.0498 | 440.0504 | -1.4 | 48973.7 | $B_2$ |
| 456.0447 | 456.0458 | -2.6 | 14909.7 | $Z_2$" |
| 456.0447 | 456.0458 | -2.6 | 14909.7 | $C_2$" |
| 458.0604 | 458.0609 | -1.3 | 6574.3 | $Z_2$ |
| 458.0604 | 458.0609 | -1.3 | 6574.3 | $C_2$ |
| 476.0708 | 476.0715 | -1.6 | 40616.8 | $Y_2$ |
| 504.0657 | 504.0664 | -1.5 | 7956.5 | $^{1,5}X_2$ |
| 554.1354 | 554.1362 | -1.6 | 6185.4 | $C_3$-$SO_3$ |
| 574.0715 | 574.0719 | -0.79 | 424.7 | $^{0,2}A_3$ |
| 616.0817 | 616.0825 | -1.3 | 3080.5 | $B_3$ |
| 619.129 | 619.1298 | -1.3 | 2409.7 | $^{2,4}X_2$ |
| 634.092 | 634.0930 | -1.7 | 20116.8 | $C_3$ |
| 679.15 | 679.1509 | -1.4 | 4901 | $Y_3$-$SO_3$ |
| 715.0565 | 715.0564 | 0.13 | 6828.5 | $C_3$+$HSO_3$ |
| 721.1603 | 721.1615 | -1.7 | 4935.5 | $^{0,2}X_3$-$SO_3$ |
| 757.2144 | 757.2156 | -1.6 | 3623.9 | $[M-H-2SO_3]^-$ |
| 793.1798 | 793.1832 | -4.3 | 6211.2 | $[M-H-SO_3-CO_2]^-$ |
| 819.1605 | 819.1624 | -2.4 | 18817 | $[M-H-SO_3-H_2O]^-$ |
| 828.1042 | 828.1049 | -0.84 | 397 | $^{1,4}A_4$ |
| 837.1713 | 837.1724 | -1.4 | 475284.8 | $[M-H-SO_3]^-$ |
| 873.1326 | 873.1399 | -8.5 | 9581.9 | $[M-H-CO_2]^-$ |
| 899.1152 | 899.1192 | -4.5 | 1583.4 | $[M-H-H_2O]^-$ |
| 917.1278 | 917.1292 | -1.6 | 216655.7 | $[M-H]^-$ |

Table S3: Fragment ion list for 193 nm UVPD activation of the $[M-2H]^{2-}$ precursor of DS dp4 in the high-pressure cell (8 pulses, 4 mJ).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 157.0142 | 157.0142 | -0.29 | 386771 | $B_1$ |
| 175.0247 | 175.0248 | -0.63 | 660087.6 | $C_1$ |
| 198.9917 | 198.9917 | -0.48 | 950130.3 | $^{1,3}X_0$ |
| 282.0289 | 282.0289 | -0.03 | 7631718.5 | $Z_1$ |
| 300.0394 | 300.0394 | -0.25 | 1.80E+07 | $Y_1$ |
| 328.0343 | 328.0343 | -0.27 | 1600171.8 | $^{1,5}X_1$ |
| 342.05 | 342.0500 | -0.11 | 833672 | $^{0,2}X_1$ |
| 379.0501 | 379.0502 | -0.36 | 1109182.6 | $Y_3^{2-}$ |
| 414.071 | 414.0717 | -1.7 | 939309.6 | $Z_2$-$CO_2$ |
| 414.071 | 414.0717 | -1.7 | 939309.6 | $C_2$-$CO_2$ |
| 440.0505 | 440.0504 | 0.15 | 2134325.8 | $B_2$ |
| 456.0463 | 456.0459 | 0.67 | 3582480 | $Z_2$" |
| 456.0463 | 456.0459 | 0.67 | 3582480 | $C_2$" |
| 458.0615 | 458.0609 | 1.1 | 2.47E+08 | $Z_2$ |
| 458.0615 | 458.0609 | 1.1 | 2.47E+08 | $[M-2H]^{2-}$ |
| 458.0615 | 458.0609 | 1.1 | 2.47E+08 | $C_2$ |
| 476.0714 | 476.0715 | -0.34 | 4630654.5 | $Y_2$ |
| 500.0718 | 500.0715 | 0.47 | 1065457.4 | $^{2,4}A_3$ |
| 504.0664 | 504.0664 | -0.15 | 1073665.1 | $^{1,5}X_2$ |
| 528.0667 | 528.0664 | 0.42 | 894172.8 | $^{3,5}A_3$ |
| 554.1364 | 554.1362 | 0.23 | 701168.8 | $C_3$-$SO_3$ |
| 616.0828 | 616.0825 | 0.45 | 1.56E+07 | $B_3$ |
| 619.1304 | 619.1298 | 0.95 | 102350.4 | $^{2,4}X_2$ |
| 634.0933 | 634.0930 | 0.33 | 1.71E+07 | $C_3$ |
| 659.125 | 659.1253 | -0.56 | 7.65E+05 | $Z_3$"-$SO_3$ |
| 661.1411 | 661.1403 | 1.1 | 715256 | $Z_3$-$SO_3$ |
| 677.1356 | 677.1359 | -0.49 | 1.75E+06 | $Y_3$"-$SO_3$ |
| 679.1539 | 679.1509 | 4.4 | 169428.4 | $Y_3$-$SO_3$ |
| 715.0581 | 715.0563 | 2.4 | 5721797 | $C_3$+$HSO_3$ |
| 720.154 | 720.1545 | -0.69 | 4002868.8 | $^{0,2}X_3$'-$SO_3$ |
| 740.0898 | 740.0901 | -0.4 | 1088177.6 | $Z_3$' |
| 741.0971 | 741.0971 | -0.11 | 1063499.8 | $Z_3$ |
| 801.1146 | 801.1183 | -4.6 | 6340332 | $^{0,2}X_3$' |
| 818.1544 | 818.1554 | -1.3 | 876701.9 | $[M-2H-SO_3-H_2O]^-$ |
| 827.0975 | 827.0975 | -0.09 | 99521.7 | $^{1,4}A_4$ |
| 836.1647 | 836.1654 | -0.83 | 2034560.1 | $[M-2H-SO_3]^-$ |
| 857.108 | 857.1081 | -0.16 | 516611.3 | $^{1,3}X_3$ |
| 872.1333 | 872.1332 | 0.03 | 898920.7 | $[M-2H-CO_2]^-$ |
| 898.1113 | 898.1122 | -1.1 | 2054511.9 | $[M-2H-H_2O]^-$ |
| 916.1216 | 916.1222 | -0.73 | 6796009 | $[M-2H]^-$ |

Table S4: Fragment ion list for 193 nm UVPD activation of the $[M-2H]^{2-}$ precursor of DS dp4 in the low-pressure cell (8 pulses, 4 mJ).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 157.0141 | 157.0142 | -0.93 | 17872.5 | $B_1$ |
| 175.0248 | 175.0248 | -0.06 | 58180.2 | $C_1$ |
| 198.9917 | 198.9917 | -0.48 | 45844.3 | $^{1,3}X_0$ |
| 282.0285 | 282.0289 | -1.5 | 339557.2 | $Z_1$ |
| 300.0391 | 300.0394 | -1.3 | 704381.8 | $Y_1$ |
| 328.0342 | 328.0343 | -0.57 | 44679.4 | $^{1,5}X_1$ |
| 342.05 | 342.0500 | -0.11 | 35065 | $^{0,2}X_1$ |
| 379.05 | 379.0502 | -0.62 | 54292.4 | $Y_3^{2-}$ |
| 397.0319 | 397.0315 | 1 | 60756.7 | $B_2$-$CH_3CO$ |
| 400.0556 | 400.0555 | 0.2 | 22921.3 | $^{0,2}X_3^{2}$- |
| 413.0633 | 413.0647 | -3.4 | 3320.1 | $Z_2'$-$CO_2$ |
| 413.0633 | 413.0647 | -3.4 | 3320.1 | $C_2'$-$CO_2$ |
| 414.071 | 414.0717 | -1.7 | 19815.1 | $Z_2$-$CO_2$ |
| 414.071 | 414.0717 | -1.7 | 19815.1 | $C_2$-$CO_2$ |
| 440.0502 | 440.0504 | -0.53 | 148273.9 | $B_2$ |
| 456.0453 | 456.0459 | -1.5 | 117860 | $Z_2''$ |
| 456.0453 | 456.0459 | -1.5 | 117860 | $C_2''$ |
| 458.0608 | 458.0609 | -0.43 | 2006954.3 | $Z_2$ |
| 458.0608 | 458.0609 | -0.43 | 2006954.3 | $[M-2H]^{2-}$ |
| 458.0608 | 458.0609 | -0.43 | 2006954.3 | $C_2$ |
| 476.0712 | 476.0715 | -0.76 | 177077.2 | $Y_2$ |
| 500.0713 | 500.0715 | -0.52 | 29257.2 | $^{2,4}A_3$ |
| 504.0662 | 504.0664 | -0.55 | 37637.9 | $^{1,5}X_2$ |
| 554.1359 | 554.1362 | -0.67 | 13126.2 | $C_3$-$SO_3$ |
| 574.0715 | 574.0719 | -0.79 | 15225.3 | $^{0,2}A_3$ |
| 616.082 | 616.0825 | -0.84 | 182301.3 | $B_3$ |
| 619.1295 | 619.1298 | -0.49 | 1388.3 | $^{2,4}X_2$ |
| 634.0926 | 634.0930 | -0.76 | 359430.4 | $C_3$ |
| 659.1243 | 659.1253 | -1.6 | 17811.9 | $Z_3''$-$SO_3$ |
| 661.1404 | 661.1403 | 0.04 | 9227.2 | $Z_3$-$SO_3$ |
| 677.1348 | 677.1359 | -1.7 | 24949.8 | $Y_3''$-$SO_3$ |
| 679.152 | 679.1509 | 1.6 | 3678.1 | $Y_3$-$SO_3$ |
| 715.0571 | 715.0563 | 1 | 81697 | $C_3$+$HSO_3$ |
| 720.153 | 720.1545 | -2.1 | 37093.3 | $^{0,2}X_3'$-$SO_3$ |
| 800.11 | 800.1113 | -1.6 | 166729.6 | $^{0,2}X_3'$ |
| 818.1535 | 818.1554 | -2.4 | 9743.9 | $[M-2H-SO_3-H_2O]^-$ |
| 827.0982 | 827.0975 | 0.75 | 693.7 | $^{1,4}A_4$ |
| 836.1641 | 836.1654 | -1.6 | 23056.5 | $[M-2H-SO_3]^-$ |
| 857.1071 | 857.1081 | -1.2 | 1212.1 | $^{1,3}X_3$ |
| 898.1103 | 898.1122 | -2.2 | 11987.5 | $[M-2H-H_2O]^-$ |
| 916.1208 | 916.1222 | -1.6 | 11957 | $[M-2H]^-$ |

Table S5: Fragment ion list for 193 nm UVPD activation of the $[M-2H]^{2-}$ precursor of DS dp4 in the high-pressure cell (4 pulses, 4 mJ).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 157.014 | 157.0142 | -1.6 | 6953.8 | $B_1$ |
| 175.0249 | 175.0248 | 0.5 | 16848.2 | $C_1$ |
| 198.9918 | 198.9917 | 0.01 | 10000 | $^{1,3}X_0$ |
| 282.0286 | 282.0289 | -1.1 | 199780 | $Z_1$ |
| 300.0392 | 300.0394 | -0.91 | 189802.1 | $Y_1$ |
| 328.0343 | 328.0343 | -0.27 | 31623.4 | $^{1,5}X_1$ |
| 342.0501 | 342.0500 | 0.17 | 34777.3 | $^{0,2}X_1$ |
| 379.0503 | 379.0502 | 0.16 | 22734.6 | $Y_3^{2-}$ |
| 397.032 | 397.0315 | 1.3 | 170944.9 | $B_2$-$CH_3CO$ |
| 413.0632 | 413.0647 | -3.6 | 3858.2 | $Z_2'$-$CO_2$ |
| 413.0632 | 413.0647 | -3.6 | 3858.2 | $C_2'$-$CO_2$ |
| 414.0709 | 414.0717 | -2 | 17390.1 | $Z_2$-$CO_2$ |
| 414.0709 | 414.0717 | -2 | 17390.1 | $C_2$-$CO_2$ |
| 440.0505 | 440.0504 | 0.15 | 60421.8 | $B_2$ |
| 456.0465 | 456.0459 | 1.1 | 172432.4 | $Z_2''$ |
| 456.0465 | 456.0459 | 1.1 | 172432.4 | $C_2''$ |
| 458.0617 | 458.0609 | 1.5 | 1.28E+07 | $Z_2$ |
| 458.0617 | 458.0609 | 1.5 | 1.28E+07 | $[M-2H]^{2-}$ |
| 458.0617 | 458.0609 | 1.5 | 1.28E+07 | $C_2$ |
| 474.0558 | 474.0566 | -1.7 | 5.23E+04 | $Y_2''$ |
| 476.0714 | 476.0715 | -0.34 | 218874.9 | $Y_2$ |
| 504.0662 | 504.0664 | -0.55 | 26911.2 | $^{1,5}X_2$ |
| 528.0667 | 528.0664 | 0.42 | 19263.5 | $^{3,5}A_3$ |
| 574.0716 | 574.0719 | -0.62 | 11317.6 | $^{0,2}A_3$ |
| 616.0824 | 616.0825 | -0.19 | 47829.5 | $B_3$ |
| 619.1302 | 619.1298 | 0.63 | 3900.4 | $^{2,4}X_2$ |
| 634.093 | 634.0930 | -0.13 | 441769.4 | $C_3$ |
| 659.1245 | 659.1253 | -1.3 | 11566 | $Z_3''$-$SO_3$ |
| 661.1411 | 661.1403 | 1.1 | 10554.9 | $Z_3$-$SO_3$ |
| 677.1351 | 677.1359 | -1.2 | 26784.8 | $Y_3''$-$SO_3$ |
| 679.1534 | 679.1509 | 3.6 | 2733.1 | $Y_3$-$SO_3$ |
| 715.0577 | 715.0563 | 1.9 | 448555.6 | $C_3$+$HSO_3$ |
| 720.1536 | 720.1545 | -1.2 | 62417 | $^{0,2}X_3'$-$SO_3$ |
| 800.1106 | 800.1113 | -0.87 | 424307 | $^{0,2}X_3'$ |
| 818.1541 | 818.1554 | -1.7 | 19694.3 | $[M-2H-SO_3-H_2O]^-$ |
| 827.098 | 827.0975 | 0.5 | 5531.3 | $^{1,4}A_4$ |
| 836.1641 | 836.1654 | -1.6 | 41388.1 | $[M-2H-SO_3]^-$ |
| 857.108 | 857.1081 | -0.16 | 17270.3 | $^{1,3}X_3$ |
| 872.1346 | 872.1332 | 1.5 | 32983.9 | $[M-2H-CO_2]^-$ |
| 898.111 | 898.1122 | -1.4 | 108724 | $[M-2H-H_2O]^-$ |
| 916.1217 | 916.1222 | -0.62 | 295978.7 | $[M-2H]^-$ |

Table S6: Fragment ion list for 193 nm UVPD activation of the $[M-2H]^{2-}$ precursor of CS-A dp4 in the high-pressure cell (8 pulses, 4 mJ).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 157.0142 | 157.0142 | -0.29 | 386771 | $B_1$ |
| 175.0247 | 175.0248 | -0.63 | 660087.6 | $C_1$ |
| 198.9917 | 198.9917 | -0.48 | 950130.3 | $^{1,3}X_0$ |
| 282.0289 | 282.0289 | -0.03 | 7631718.5 | $Z_1$ |
| 300.0394 | 300.0394 | -0.25 | 1.80E+07 | $Y_1$ |
| 328.0343 | 328.0343 | -0.27 | 1600171.8 | $^{1,5}X_1$ |
| 342.05 | 342.0500 | -0.11 | 833672 | $^{0,2}X_1$ |
| 379.0501 | 379.0502 | -0.36 | 1109182.6 | $Y_3^{2-}$ |
| 414.071 | 414.0717 | -1.7 | 939309.6 | $Z_2$-$CO_2$ |
| 414.071 | 414.0717 | -1.7 | 939309.6 | $C_2$-$CO_2$ |
| 440.0505 | 440.0504 | 0.15 | 2134325.8 | $B_2$ |
| 456.0463 | 456.0459 | 0.67 | 3582480 | $Z_2$" |
| 456.0463 | 456.0459 | 0.67 | 3582480 | $C_2$" |
| 458.0615 | 458.0609 | 1.1 | 2.47E+08 | $Z_2$ |
| 458.0615 | 458.0609 | 1.1 | 2.47E+08 | $[M-2H]^{2-}$ |
| 458.0615 | 458.0609 | 1.1 | 2.47E+08 | $C_2$ |
| 476.0714 | 476.0715 | -0.34 | 4630654.5 | $Y_2$ |
| 500.0718 | 500.0715 | 0.47 | 1065457.4 | $^{2,4}A_3$ |
| 504.0664 | 504.0664 | -0.15 | 1073665.1 | $^{1,5}X_2$ |
| 528.0667 | 528.0664 | 0.42 | 894172.8 | $^{3,5}A_3$ |
| 554.1364 | 554.1362 | 0.23 | 701168.8 | $C_3$-$SO_3$ |
| 616.0828 | 616.0825 | 0.45 | 1.56E+07 | $B_3$ |
| 619.1304 | 619.1298 | 0.95 | 102350.4 | $^{2,4}X_2$ |
| 634.0933 | 634.0930 | 0.33 | 1.71E+07 | $C_3$ |
| 659.125 | 659.1253 | -0.56 | 7.65E+05 | $Z_3$"-$SO_3$ |
| 661.1411 | 661.1403 | 1.1 | 715256 | $Z_3$-$SO_3$ |
| 677.1356 | 677.1359 | -0.49 | 1.75E+06 | $Y_3$"-$SO_3$ |
| 679.1539 | 679.1509 | 4.4 | 169428.4 | $Y_3$-$SO_3$ |
| 715.0581 | 715.0563 | 2.4 | 5721797 | $C_3$+$HSO_3$ |
| 720.154 | 720.1545 | -0.69 | 4002868.8 | $^{0,2}X_3$'-$SO_3$ |
| 740.0898 | 740.0901 | -0.4 | 1088177.6 | $Z_3$' |
| 741.0971 | 741.0971 | -0.11 | 1063499.8 | $Z_3$ |
| 801.1146 | 801.1183 | -4.6 | 6340332 | $^{0,2}X_3$' |
| 818.1544 | 818.1554 | -1.3 | 876701.9 | $[M-2H-SO_3-H_2O]^-$ |
| 827.0975 | 827.0975 | -0.09 | 99521.7 | $^{1,4}A_4$ |
| 836.1647 | 836.1654 | -0.83 | 2034560.1 | $[M-2H-SO_3]^-$ |
| 857.108 | 857.1081 | -0.16 | 516611.3 | $^{1,3}X_3$ |
| 872.1333 | 872.1332 | 0.03 | 898920.7 | $[M-2H-CO_2]^-$ |
| 898.1113 | 898.1122 | -1.1 | 2054511.9 | $[M-2H-H_2O]^-$ |
| 916.1216 | 916.1222 | -0.73 | 6796009 | $[M-2H]^-$ |

Table S7: Fragment ion list for 193 nm UVPD activation of the $[M-2H]^{2-}$ precursor of CS-A dp4 in the low-pressure cell (8 pulses, 4 mJ).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 157.0141 | 157.0142 | -0.93 | 667880.4 | $B_1$ |
| 175.0246 | 175.0248 | -1.2 | 1189419 | $C_1$ |
| 198.9916 | 198.9917 | -0.98 | 1433519 | $^{1,3}X_0$ |
| 282.0287 | 282.0289 | -0.74 | 8009461 | $Z_1$ |
| 300.0392 | 300.0394 | -0.91 | 3.72E+07 | $Y_1$ |
| 316.5426 | 316.5429 | -0.96 | 314679.3 | $C_3^{2-}$ |
| 328.0341 | 328.0343 | -0.88 | 1437117 | $^{1,5}X_1$ |
| 342.0497 | 342.0500 | -0.99 | 801432.8 | $^{0,2}X_1$ |
| 379.0499 | 379.0502 | -0.88 | 1757168 | $Y_3^{2-}$ |
| 400.0553 | 400.0555 | -0.54 | 970361.3 | $^{0,2}X_3^{2-}$ |
| 414.0708 | 414.0717 | -2.2 | 702227.4 | $Z_2$-$CO_2$ |
| 414.0708 | 414.0717 | -2.2 | 702227.4 | $C_2$-$CO_2$ |
| 440.0502 | 440.0504 | -0.53 | 2661253 | $B_2$ |
| 456.0455 | 456.0459 | -1.1 | 2974363 | $Z_2$" |
| 456.0455 | 456.0459 | -1.1 | 2974363 | $C_2$" |
| 458.0608 | 458.0609 | -0.43 | 1.23E+08 | $Z_2$ |
| 458.0608 | 458.0609 | -0.43 | 1.23E+08 | $[M-2H]^{2-}$ |
| 458.0608 | 458.0609 | -0.43 | 1.23E+08 | $C_2$ |
| 476.0711 | 476.0715 | -0.97 | 3012829 | $Y_2$ |
| 500.0714 | 500.0715 | -0.32 | 1600320 | $^{2,4}A_3$ |
| 504.0661 | 504.0664 | -0.74 | 940149.9 | $^{1,5}X_2$ |
| 528.0663 | 528.0664 | -0.33 | 530744.2 | $^{3,5}A_3$ |
| 554.1359 | 554.1362 | -0.67 | 415093.5 | $C_3$-$SO_3$ |
| 616.0823 | 616.0825 | -0.36 | 2.59E+07 | $B_3$ |
| 619.1299 | 619.1298 | 0.15 | 41896 | $^{2,4}X_2$ |
| 634.0928 | 634.0930 | -0.45 | 1.02E+07 | $C_3$ |
| 661.1408 | 661.1403 | 0.64 | 364385.8 | $Z_3$-$SO_3$ |
| 679.1525 | 679.1509 | 2.3 | 141212.1 | $Y_3$-$SO_3$ |
| 715.0571 | 715.0563 | 1 | 850519.6 | $C_3$+$HSO_3$ |
| 720.1534 | 720.1545 | -1.5 | 1401252 | $^{0,2}X_3$'-$SO_3$ |
| 741.0969 | 741.0971 | -0.38 | 385652 | $Z_3$ |
| 801.1146 | 801.1183 | -4.6 | 8021901 | $^{0,2}X_3$' |
| 818.1537 | 818.1554 | -2.1 | 418205.8 | $[M-2H-SO_3-H_2O]^-$ |
| 828.1041 | 828.1049 | -0.96 | 30484 | $^{1,4}A_4$ |
| 836.1643 | 836.1654 | -1.3 | 12194995 | $[M-2H-SO_3]^-$ |
| 857.1077 | 857.1081 | -0.51 | 29294.8 | $^{1,3}X_3$ |
| 898.1104 | 898.1122 | -2.1 | 189617.8 | $[M-2H-H_2O]^-$ |
| 916.121 | 916.1222 | -1.4 | 340443.9 | $[M-2H]^-$ |

Table S8: Fragment ion list for 193 nm UVPD activation of the $[M-2H]^{2-}$ precursor of CS-A dp4 in the high-pressure cell (4 pulses, 4 mJ).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 157.0142 | 157.0142 | -0.29 | 230344.6 | $B_1$ |
| 175.0248 | 175.0248 | -0.06 | 316772.8 | $C_1$ |
| 198.9918 | 198.9917 | 0.01 | 370501.2 | $^{1,3}X_0$ |
| 282.029 | 282.0289 | 0.31 | 4713021.5 | $Z_1$ |
| 300.0395 | 300.0394 | 0.08 | 1.33E+07 | $Y_1$ |
| 328.0344 | 328.0343 | 0.03 | 1025935.8 | $^{1,5}X_1$ |
| 342.0501 | 342.0500 | 0.17 | 505210.3 | $^{0,2}X_1$ |
| 379.0503 | 379.0502 | 0.16 | 937570.5 | $Y_3^{2-}$ |
| 414.0711 | 414.0717 | -1.5 | 647141.5 | $Z_2$-$CO_2$ |
| 414.0711 | 414.0717 | -1.5 | 647141.5 | $C_2$-$CO_2$ |
| 440.0508 | 440.0504 | 0.83 | 1144941.4 | $B_2$ |
| 456.0469 | 456.0459 | 2 | 2330769.3 | $Z_2$'' |
| 456.0469 | 456.0459 | 2 | 2330769.3 | $C_2$'' |
| 458.0619 | 458.0609 | 2 | 4.08E+08 | $Z_2$ |
| 458.0619 | 458.0609 | 2 | 4.08E+08 | $[M-2H]^{2-}$ |
| 458.0619 | 458.0609 | 2 | 4.08E+08 | $C_2$ |
| 474.0559 | 474.0566 | -1.5 | 1.13E+06 | $Y_2$'' |
| 476.0715 | 476.0715 | -0.13 | 2979715 | $Y_2$ |
| 500.0721 | 500.0715 | 1.1 | 604170.8 | $^{2,4}A_4$ |
| 504.0666 | 504.0664 | 0.24 | 621596 | $^{1,5}X_2$ |
| 528.067 | 528.0664 | 0.98 | 530658.8 | $^{3,5}A_3$ |
| 539.1733 | 539.173 | 0.55 | 7734.6 | $^{2,4}X_2$-$SO_3$ |
| 554.1367 | 554.1362 | 0.77 | 240976 | $C_3$-$SO_3$ |
| 587.0799 | 587.0806 | -1.2 | 194752.9 | $^{1,5}A_3$' |
| 614.0679 | 614.0675 | 0.65 | 23024.5 | $B_3$'' |
| 616.0831 | 616.0825 | 0.93 | 1.19E+07 | $B_3$ |
| 619.1314 | 619.1298 | 2.6 | 47981.4 | $^{2,4}X_2$ |
| 634.0936 | 634.0930 | 0.8 | 1.16E+07 | $C_3$ |
| 659.1252 | 659.1253 | -0.25 | 5.11E+05 | $Z_3$''-$SO_3$ |
| 661.1415 | 661.1403 | 1.7 | 376637.7 | $Z_3$-$SO_3$ |
| 677.1358 | 677.1359 | -0.19 | 6.53E+05 | $Y_3$''-$SO_3$ |
| 679.154 | 679.1509 | 4.5 | 86170.9 | $Y_3$-$SO_3$ |
| 715.0584 | 715.0563 | 2.9 | 4254010 | $C_3$+$HSO_3$ |
| 720.1542 | 720.1545 | -0.41 | 1496160.4 | $^{0,2}X_3$'-$SO_3$ |
| 740.0901 | 740.0901 | 0 | 821365.9 | $Z_3$' |
| 741.0974 | 741.0971 | 0.28 | 796138.7 | $Z_3$ |
| 800.1113 | 800.1113 | 0 | 15970153 | $^{0,2}X_3$' |
| 818.1545 | 818.1554 | -1.2 | 655793.9 | $[M-2H-SO_3-H_2O]^-$ |
| 827.097 | 827.0975 | -0.7 | 64767 | $^{1,4}A_4$ |
| 836.1651 | 836.1654 | -0.35 | 1351615.3 | $[M-2H-SO_3]^-$ |
| 857.1083 | 857.1081 | 0.18 | 399077.3 | $^{1,3}X_3$ |
| 872.1334 | 872.1332 | 0.14 | 747082.9 | $[M-2H-CO_2]^-$ |
| 898.1116 | 898.1122 | -0.74 | 1520385.9 | $[M-2H-H_2O]^-$ |
| 916.122 | 916.1222 | -0.29 | 4964973 | $[M-2H]^-$ |

Table S9: Fragment ion list for 193 nm UVPD activation of the $[M-3H]^{3-}$ precursor of DS dp4 in the high-pressure cell (8 pulses, 4 mJ).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 173.0092 | 173.0098 | -3.5 | 381285.4 | $C_1$" |
| 198.9918 | 198.9917 | 0.01 | 779947.4 | $^{1,3}X_0$ |
| 227.5187 | 227.5198 | -5.1 | 326737.8 | $Z_2$"$^{2-}$ |
| 227.5187 | 227.5198 | -5.1 | 326737.8 | $C_2$"$^{2-}$ |
| 266.3678 | 266.3679 | -0.45 | 7675.3 | $^{0,2}X_3^{3-}$ |
| 282.0287 | 282.0289 | -0.74 | 9.23E+07 | $Z_1$ |
| 300.0392 | 300.0394 | -0.91 | 4664430 | $Y_1$ |
| 305.0382 | 305.0382 | -0.13 | 6.44E+07 | $[M-3H]^{3-}$ |
| 328.0345 | 328.0343 | 0.33 | 2638980.5 | $^{1,5}X_1$ |
| 342.0502 | 342.0500 | 0.46 | 3176481.5 | $^{0,2}X_1$ |
| 357.0374 | 357.0379 | -1.5 | 1947957.5 | $^{2,5}X_1$' |
| 371.0528 | 371.0536 | -2.2 | 5988777.5 | $^{0,3}X_1$' |
| 379.0504 | 379.0502 | 0.43 | 1156924.5 | $Y_3^{2-}$ |
| 400.0536 | 400.0555 | -4.8 | 1049798.8 | $^{0,2}X_3^{2-}$ |
| 414.073 | 414.0717 | 2.9 | 38247732 | $Z_2$-$CO_2$ |
| 414.073 | 414.0717 | 2.9 | 38247732 | $C_2$-$CO_2$ |
| 435.0583 | 435.0582 | 0.09 | 274987.8 | $^{1,5}A_4^{2-}$ |
| 440.0507 | 440.0504 | 0.6 | 1500656.8 | $B_2$ |
| 456.0455 | 456.0469 | -3.3 | 8195103.5 | $Z_2$" |
| 456.0455 | 456.0469 | -3.3 | 8195103.5 | $C_2$" |
| 457.5572 | 457.5576 | -1.1 | 2972730 | $[M-3H]^{2-}$ |
| 458.0609 | 458.0609 | -0.21 | 6815683.5 | $Z_2$ |
| 458.0609 | 458.0609 | -0.21 | 6815683.5 | $[M-2H]^{2-}$ |
| 458.0609 | 458.0609 | -0.21 | 6815683.5 | $C_2$ |
| 474.056 | 474.0565 | -1.2 | 5208735 | $Y_2$" |
| 476.0717 | 476.0715 | 0.28 | 997905.3 | $Y_2$ |
| 504.0667 | 504.0664 | 0.44 | 624601.4 | $^{1,5}X_2$ |
| 528.0666 | 528.0664 | 0.23 | 348820.6 | $^{3,5}A_3$ |
| 573.0613 | 573.0649 | -6.3 | 7014 | $^{0,2}A_3$' |
| 588.0879 | 588.0876 | 0.49 | 684368 | $^{1,5}A_3$ |
| 616.0817 | 616.0825 | -1.3 | 73377.5 | $B_3$ |
| 619.1301 | 619.1298 | 0.47 | 66204.4 | $^{2,4}X_2$ |
| 633.0854 | 633.0861 | -1.1 | 474579.1 | $C_3$' |
| 634.0934 | 634.0930 | 0.49 | 450427.7 | $C_3$ |
| 677.1357 | 677.1359 | -0.29 | 678578.2 | $Y_3$"-$SO_3$ |
| 719.1464 | 719.1465 | -0.13 | 805124.3 | $^{0,2}X_3$"-$SO_3$ |
| 791.1675 | 791.1682 | -0.88 | 2156252 | $[M-3H-SO_3-CO_2]^-$ |
| 800.111 | 800.1113 | -0.37 | 1065954.3 | $^{0,2}X_3$' |
| 817.1469 | 817.148 | -1.3 | 205586.5 | $[M-3H-SO_3-H_2O]^-$ |
| 828.1068 | 828.1049 | 2.3 | 37981 | $^{1,4}A_4$ |
| 835.1575 | 835.1580 | -0.63 | 1022026.5 | $[M-3H-SO_3]^-$ |
| 871.1244 | 871.1251 | -0.8 | 134517.5 | $[M-3H-CO_2]^-$ |
| 915.1144 | 915.1143 | 0.1 | 106567.8 | $[M-3H]^-$ |

Table S10: Fragment ion list for 193 nm UVPD activation of the $[M-3H]^{3-}$ precursor of DS dp4 in the low-pressure cell (8 pulses, 4 mJ).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 157.0141 | 157.0142 | -0.93 | 227634.4 | $B_1$ |
| 175.0248 | 175.0248 | -0.06 | 218615.2 | $C_1$ |
| 198.9917 | 198.9917 | -0.48 | 541126.6 | $^{1,3}X_0$ |
| 227.5187 | 227.5198 | -5.1 | 63811.5 | $C_2"^{2-}$ |
| 227.5187 | 227.5198 | -5.1 | 63811.5 | $Z_2"^{2-}$ |
| 237.5321 | 237.5321 | -0.18 | 525358.5 | $Y_2^{2-}$ |
| 266.3678 | 266.3679 | -0.45 | 464912 | $^{0,2}X_3^{3-}$ |
| 282.0285 | 282.0289 | -1.5 | 2.63E+07 | $Z_1$ |
| 300.0391 | 300.0394 | -1.3 | 1661497.8 | $Y_1$ |
| 305.0377 | 305.0382 | -1.8 | 4184672.3 | $[M-3H]^{3-}$ |
| 328.0341 | 328.0343 | -0.88 | 821421.7 | $^{1,5}X_1$ |
| 342.05 | 342.0500 | -0.11 | 506899.2 | $^{0,2}X_1$ |
| 357.0371 | 357.0379 | -2.4 | 428356.6 | $^{2,5}X_1'$ |
| 371.0526 | 371.0536 | -2.7 | 378142.3 | $^{0,3}X_1'$ |
| 379.05 | 379.0502 | -0.62 | 517511.9 | $Y_3^{2-}$ |
| 400.0548 | 400.0555 | -1.8 | 245070.9 | $^{0,2}X_3^{2-}$ |
| 414.0709 | 414.0717 | -2.1 | 9353081 | $Z_2$-$CO_2$ |
| 414.0709 | 414.0717 | -2.1 | 9353081 | $C_2$-$CO_2$ |
| 440.0502 | 440.0504 | -0.53 | 1163178.1 | $B_2$ |
| 456.0451 | 456.0469 | -4.1 | 1724189.4 | $Z_2"$ |
| 456.0451 | 456.0469 | -4.1 | 1724189.4 | $C_2"$ |
| 457.5567 | 457.5576 | -2.2 | 64861.9 | $[M-3H]^{2-}$ |
| 458.0607 | 458.0609 | -0.65 | 1622287.1 | $C_2$ |
| 458.0607 | 458.0609 | -0.65 | 1622287.1 | $[M-2H]^{2-}$ |
| 458.0607 | 458.0609 | -0.65 | 1622287.1 | $Z_2$ |
| 474.0556 | 474.0565 | -2 | 876162.2 | $Y_2"$ |
| 476.0712 | 476.0715 | -0.76 | 533658.4 | $Y_2$ |
| 500.0714 | 500.0715 | -0.32 | 106240.6 | $^{2,4}A_3$ |
| 504.0662 | 504.0664 | -0.55 | 246322.6 | $^{1,5}X_2$ |
| 528.0662 | 528.0664 | -0.52 | 88348 | $^{3,5}A_3$ |
| 588.0872 | 588.0876 | -0.69 | 145997.2 | $^{1,5}A_3$ |
| 633.0811 | 633.0861 | -7.9 | 14447.8 | $C_3'$ |
| 634.0929 | 634.0930 | -0.29 | 70532.3 | $C_3$ |
| 677.1348 | 677.1359 | -1.6 | 321440.4 | $Y_3"$-$SO_3$ |
| 719.1453 | 719.1465 | -1.7 | 138785.3 | $^{0,2}X_3"$-$SO_3$ |
| 791.1664 | 791.1682 | -2.3 | 196611.8 | $[M-3H-SO_3-CO_2]^-$ |
| 800.1136 | 800.1113 | 2.9 | 26510.4 | $^{0,2}X_3'$ |
| 817.1457 | 817.148 | -2.8 | 16450.2 | $[M-3H-SO_3-H_2O]^-$ |
| 835.1558 | 835.1580 | -2.7 | 101698 | $[M-3H-SO_3]^-$ |

Table S11: Fragment ion list for 193 nm UVPD activation of the $[M-3H]^{3-}$ precursor of DS dp4 in the high-pressure cell (4 pulses, 4 mJ).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 157.0143 | 157.0142 | 0.33 | 112723 | $B_1$ |
| 173.0094 | 173.0098 | -2.3 | 325398 | $C_1$" |
| 175.0247 | 175.0248 | -0.63 | 93456.5 | $C_1$ |
| 198.9917 | 198.9917 | -0.48 | 247650.4 | $^{1,3}X_0$ |
| 227.5192 | 227.5198 | -2.9 | 416323.8 | $Z_2"^{2-}$ |
| 227.5192 | 227.5198 | -2.9 | 416323.8 | $C_2"^{2-}$ |
| 237.5322 | 237.5321 | 0.23 | 430151.8 | $Y_2^{2-}$ |
| 266.3676 | 266.3679 | -1.2 | 15420.1 | $^{0,2}X_3^{3-}$ |
| 282.0288 | 282.0289 | -0.39 | 7.44E+07 | $Z_1$ |
| 300.0394 | 300.0394 | -0.25 | 1976159.1 | $Y_1$ |
| 305.0387 | 305.0382 | 1.5 | 2.24E+08 | $[M-3H]^{3-}$ |
| 328.0346 | 328.0343 | 0.64 | 1982057.5 | $^{1,5}X_1$ |
| 342.0503 | 342.0500 | 0.76 | 1089795.6 | $^{0,2}X_1$ |
| 357.0375 | 357.0379 | -1.3 | 1835419.3 | $^{2,5}X_1$' |
| 371.053 | 371.0536 | -1.6 | 6579420.5 | $^{0,3}X_1$' |
| 379.0506 | 379.0502 | 0.95 | 1039833.5 | $Y_3^{2-}$ |
| 400.0539 | 400.0555 | -4 | 1381661.6 | $^{0,2}X_3^{2-}$ |
| 414.0715 | 414.0717 | -0.7 | 37404120 | $Z_2$-$CO_2$ |
| 414.0715 | 414.0717 | -0.7 | 37404120 | $C_2$-$CO_2$ |
| 435.0586 | 435.0582 | 0.78 | 262323.9 | $^{1,5}A_4^{2-}$ |
| 440.051 | 440.0504 | 1.3 | 1094002.9 | $B_2$ |
| 456.0458 | 456.0469 | -2.6 | 6997210 | $Z_2$" |
| 456.0458 | 456.0469 | -2.6 | 6997210 | $C_2$" |
| 457.5575 | 457.5576 | -0.41 | 3677603.3 | $[M-3H]^{2-}$ |
| 458.0611 | 458.0609 | 0.22 | 6162838.5 | $Z_2$ |
| 458.0611 | 458.0609 | 0.22 | 6162838.5 | $[M-2H]^{2-}$ |
| 458.0611 | 458.0609 | 0.22 | 6162838.5 | $C_2$ |
| 474.0563 | 474.0565 | -0.54 | 4324970 | $Y_2$" |
| 504.067 | 504.0664 | 1 | 363802.8 | $^{1,5}X_2$ |
| 528.067 | 528.0664 | 0.98 | 292350.1 | $^{3,5}A_3$ |
| 573.0597 | 573.0649 | -9.1 | 205772.9 | $^{0,2}A_3$' |
| 588.0883 | 588.0876 | 1.2 | 532729.5 | $^{1,5}A_3$ |
| 615.0756 | 615.0755 | 0.16 | 186421.2 | $B_3$' |
| 616.0819 | 616.0825 | -1 | 61322 | $B_3$ |
| 619.1323 | 619.1298 | 4 | 20744.1 | $^{2,4}X_2$ |
| 632.0782 | 632.0780 | 0.18 | 246210.8 | $C_3$" |
| 634.094 | 634.0930 | 1.4 | 347995.8 | $C_3$ |
| 677.1363 | 677.1359 | 0.59 | 428713.9 | $Y_3$"-$SO_3$ |
| 719.1467 | 719.1465 | 0.27 | 335221 | $^{0,2}X_3$"-$SO_3$ |
| 775.137 | 775.1363 | 0.9 | 450231.7 | $^{1,3}X_3$"-$SO_3$ |
| 791.1682 | 791.1682 | 0 | 1263949 | $[M-3H-SO_3-CO_2]^-$ |
| 800.1117 | 800.1113 | 0.49 | 833865.9 | $^{0,2}X_3$' |
| 817.1481 | 817.148 | 0.12 | 114732.1 | $[M-3H-SO_3-H_2O]^-$ |
| 835.1581 | 835.1580 | 0.08 | 642817.6 | $[M-3H-SO_3]^-$ |
| 871.1254 | 871.1251 | 0.34 | 41361.7 | $[M-3H-CO_2]^-$ |

Table S12: Fragment ion list for 193 nm UVPD activation of the $[M-3H]^{3-}$ precursor of CS-A dp4 in the high-pressure cell (8 pulses, 4 mJ).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 173.009 | 173.0098 | -4.6 | 1428054.1 | $C_1$" |
| 198.9916 | 198.9917 | -0.98 | 2410980.5 | $^{1,3}X_0$ |
| 227.5188 | 227.5198 | -4.7 | 1909038.5 | $Z_2$"$^{2-}$ |
| 227.5188 | 227.5198 | -4.7 | 1909038.5 | $C_2$"$^{2-}$ |
| 266.3676 | 266.3679 | -1.2 | 55167.8 | $^{0,2}X_3^{3-}$ |
| 282.0286 | 282.0289 | -1.1 | 2.77E+08 | $Z_1$ |
| 300.0393 | 300.0394 | -0.58 | 1.74E+07 | $Y_1$ |
| 305.0381 | 305.0382 | -0.45 | 2.63E+08 | $[M-3H]^{3-}$ |
| 328.0341 | 328.0343 | -0.88 | 6353023.5 | $^{1,5}X_1$ |
| 342.0497 | 342.0500 | -0.99 | 1.24E+07 | $^{0,2}X_1$ |
| 357.0368 | 357.0379 | -3.2 | 4.24E+06 | $^{2,5}X_1$' |
| 371.0524 | 371.0536 | -3.2 | 2.10E+07 | $^{0,3}X_1$' |
| 379.0499 | 379.0502 | -0.88 | 4756848 | $Y_3^{2-}$ |
| 400.0532 | 400.0555 | -5.8 | 6957444 | $^{0,2}X_3^{2-}$ |
| 414.0708 | 414.0717 | -2.4 | 173417392 | $Z_2$-$CO_2$ |
| 414.0708 | 414.0717 | -2.4 | 173417392 | $C_2$-$CO_2$ |
| 435.0579 | 435.0582 | -0.82 | 2015001.1 | $^{1,5}A_4^{2-}$ |
| 440.0505 | 440.0504 | 0.15 | 4174323.3 | $B_2$ |
| 456.0451 | 456.0469 | -4.1 | 26351570 | $Z_2$" |
| 456.0451 | 456.0469 | -4.1 | 26351570 | $C_2$" |
| 457.5568 | 457.5576 | -1.9 | 16107254 | $[M-3H]^{2-}$ |
| 458.0602 | 458.0609 | -1.7 | 2.41E+07 | $Z_2$ |
| 458.0602 | 458.0609 | -1.7 | 2.41E+07 | $[M-2H]^{2-}$ |
| 458.0602 | 458.0609 | -1.7 | 2.41E+07 | $C_2$ |
| 474.0556 | 474.0565 | -2 | 1.04E+07 | $Y_2$" |
| 476.0712 | 476.0715 | -0.76 | 4496472 | $Y_2$ |
| 500.0717 | 500.0715 | 0.27 | 501382.8 | $^{2,4}A_3$ |
| 504.0662 | 504.0664 | -0.55 | 1589974.6 | $^{1,5}X_2$ |
| 528.0662 | 528.0664 | -0.52 | 1369161.5 | $^{3,5}A_3$ |
| 573.0597 | 573.0649 | -9.1 | 24935.5 | $^{0,2}A_3$' |
| 588.0874 | 588.0876 | -0.35 | 4527201 | $^{1,5}A_3$ |
| 615.0745 | 615.0755 | -1.6 | 1289869.4 | $B_3$' |
| 616.0814 | 616.0825 | -1.8 | 507767.9 | $B_3$ |
| 619.1296 | 619.1298 | -0.33 | 358531.8 | $^{2,4}X_2$ |
| 632.0773 | 632.0780 | -1.2 | 1338071.6 | $C_3$" |
| 634.0929 | 634.0930 | -0.29 | 9563548 | $C_3$ |
| 677.1351 | 677.1359 | -1.2 | 2473670.5 | $Y_3$"-$SO_3$ |
| 719.1458 | 719.1465 | -0.97 | 3517010.5 | $^{0,2}X_3$"-$SO_3$ |
| 791.1668 | 791.1682 | -1.8 | 14645490 | $[M-3H-CO_2-SO_3]^-$ |
| 800.11 | 800.1113 | -1.6 | 3338681 | $^{0,2}X_3$' |
| 817.146 | 817.148 | -2.4 | 971407.4 | $[M-3H-SO_3-H_2O]^-$ |
| 828.105 | 828.1049 | 0.12 | 132965.6 | $^{1,4}A_4$ |
| 835.1566 | 835.1580 | -1.7 | 5283968.5 | $[M-3H-SO_3]^-$ |
| 871.1234 | 871.1251 | -2 | 1028001.1 | $[M-3H-CO_2]^-$ |
| 915.1132 | 915.1143 | -1.2 | 708207.2 | $[M-3H]^-$ |

Table S13: Fragment ion list for 193 nm UVPD activation of the $[M-3H]^{3-}$ precursor of CS-A dp4 in the low-pressure cell (8 pulses, 4 mJ).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 157.0139 | 157.0142 | -2.2 | 764433.8 | $B_1$ |
| 173.0088 | 173.0098 | -5.8 | 509262.8 | $C_1$" |
| 175.0245 | 175.0248 | -1.8 | 616644 | $C_1$ |
| 198.9914 | 198.9917 | -2 | 1931929.1 | $^{1,3}X_0$ |
| 227.5186 | 227.5198 | -5.5 | 630660.4 | $Z_2"^{2-}$ |
| 227.5186 | 227.5198 | -5.5 | 630660.4 | $C_2"^{2-}$ |
| 237.5317 | 237.5321 | -1.9 | 1307501.1 | $Y_2^{2-}$ |
| 266.3674 | 266.3679 | -2 | 102129.3 | $^{0,2}X_3^{3-}$ |
| 282.0284 | 282.0289 | -1.8 | 7.74E+07 | $Z_1$ |
| 300.0389 | 300.0394 | -1.9 | 1.13E+07 | $Y_1$ |
| 305.0377 | 305.0382 | -1.8 | 8.02E+07 | $[M-3H]^{3-}$ |
| 328.0338 | 328.0343 | -1.8 | 2645442 | $^{1,5}X_1$ |
| 341.0416 | 341.043 | -4.1 | 3.03E+05 | $^{0,2}X_1$' |
| 357.0364 | 357.0379 | -4.3 | 1.16E+06 | $^{2,5}X_1$' |
| 371.052 | 371.0536 | -4.3 | 3.12E+06 | $^{0,3}X_1$' |
| 379.0495 | 379.0502 | -1.9 | 3390571.5 | $Y_3^{2-}$ |
| 400.0537 | 400.0555 | -4.5 | 1971418.6 | $^{0,2}X_3^{2-}$ |
| 414.0704 | 414.0717 | -3.4 | 4.16E+07 | $Z_2$-$CO_2$ |
| 414.0704 | 414.0717 | -3.4 | 4.16E+07 | $C_2$-$CO_2$ |
| 435.0573 | 435.0582 | -2.2 | 233480.2 | $^{1,5}A_4^{2-}$ |
| 440.0499 | 440.0504 | -1.2 | 2026331.4 | $B_2$ |
| 456.0444 | 456.0469 | -5.7 | 6713159 | $Z_2$" |
| 456.0444 | 456.0469 | -5.7 | 6713159 | $C_2$" |
| 457.5562 | 457.5576 | -3.3 | 887101.1 | $[M-3H]^{2-}$ |
| 458.0601 | 458.0609 | -2 | 8004435.5 | $Z_2$ |
| 458.0601 | 458.0609 | -2 | 8004435.5 | $[M-2H]^{2-}$ |
| 458.0601 | 458.0609 | -2 | 8004435.5 | $C_2$ |
| 474.055 | 474.0565 | -3.3 | 1762344 | $Y_2$" |
| 476.0706 | 476.0715 | -2 | 2468611.5 | $Y_2$ |
| 500.0707 | 500.0715 | -1.7 | 1716128 | $^{2,4}A_3$ |
| 504.0656 | 504.0664 | -1.7 | 610999.5 | $^{1,5}X_2$ |
| 528.0655 | 528.0664 | -1.9 | 368275.9 | $^{3,5}A_3$ |
| 588.0865 | 588.0876 | -1.9 | 862843.8 | $^{1,5}A_3$ |
| 615.0734 | 615.0755 | -3.4 | 49127.7 | $B_3$' |
| 616.0815 | 616.0825 | -1.7 | 120361.8 | $B_3$ |
| 619.1285 | 619.1298 | -2.1 | 19601 | $^{2,4}X_2$ |
| 632.0765 | 632.0780 | -2.5 | 200389.6 | $C_3$" |
| 634.092 | 634.0930 | -1.7 | 1529364.6 | $C_3$ |
| 677.1342 | 677.1359 | -2.5 | 969444.1 | $Y_3$"-$SO_3$ |
| 719.1447 | 719.1465 | -2.5 | 710339.9 | $^{0,2}X_3$"-$SO_3$ |
| 791.1657 | 791.1682 | -3.2 | 1261714.9 | $[M-3H-SO_3-CO_2]^-$ |
| 800.1089 | 800.1113 | -3 | 282980.8 | $^{0,2}X_3$' |
| 817.1447 | 817.148 | -4 | 56492.6 | $[M-3H-SO_3-H_2O]^-$ |
| 835.1555 | 835.1580 | -3 | 503955.9 | $[M-3H-SO_3]^-$ |

Table S14: Fragment ion list for 193 nm UVPD activation of the $[M-3H]^{3-}$ precursor of CS-A dp4 in the high-pressure cell (4 pulses, 4 mJ).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 173.0091 | 173.0098 | -4 | 1211537.6 | $C_1$" |
| 198.9917 | 198.9917 | -0.48 | 7.56E+05 | $^{1,3}X_0$ |
| 227.5189 | 227.5198 | -4.2 | 1958871.6 | $Z_2$"$^{2-}$ |
| 227.5189 | 227.5198 | -4.2 | 1958871.6 | $C_2$"$^{2-}$ |
| 266.3672 | 266.3679 | -2.7 | 108060 | $^{0,2}X_3^{3-}$ |
| 282.0288 | 282.0289 | -0.39 | 2.12E+08 | $Z_1$ |
| 300.0396 | 300.0394 | 0.41 | 8292346.5 | $Y_1$ |
| 305.0386 | 305.0382 | 1.2 | 7.54E+08 | $[M-3H]^{3-}$ |
| 328.0343 | 328.0343 | -0.27 | 4495393.5 | $^{1,5}X_1$ |
| 342.0499 | 342.0500 | -0.4 | 4077744.8 | $^{0,2}X_1$ |
| 357.037 | 357.0379 | -2.7 | 3750311.8 | $^{2,5}X_1$' |
| 371.0527 | 371.0536 | -2.4 | 21302490 | $^{0,3}X_1$' |
| 379.0502 | 379.0502 | -0.09 | 4104255.3 | $Y_3^{2-}$ |
| 400.0535 | 400.0555 | -5 | 7853565 | $^{0,2}X_3^{2-}$ |
| 414.0711 | 414.0717 | -1.7 | 157626288 | $Z_2$-$CO_2$ |
| 414.0711 | 414.0717 | -1.7 | 157626288 | $C_2$-$CO_2$ |
| 435.0583 | 435.0582 | 0.09 | 1531235.5 | $^{1,5}A_4^{2-}$ |
| 440.051 | 440.0504 | 1.3 | 2608724 | $B_2$ |
| 456.0454 | 456.0469 | -3.5 | 21768876 | $Z_2$" |
| 456.0454 | 456.0469 | -3.5 | 21768876 | $C_2$" |
| 457.5572 | 457.5576 | -1.1 | 16673176 | $[M-3H]^{2-}$ |
| 458.0605 | 458.0609 | -1.1 | 2.03E+07 | $Z_2$ |
| 458.0605 | 458.0609 | -1.1 | 2.03E+07 | $[M-2H]^{2-}$ |
| 458.0605 | 458.0609 | -1.1 | 2.03E+07 | $C_2$ |
| 474.056 | 474.0565 | -1.2 | 8.20E+06 | $Y_2$" |
| 504.0665 | 504.0664 | 0.04 | 850755.9 | $^{1,5}X_2$ |
| 528.0667 | 528.0664 | 0.42 | 977573.4 | $^{3,5}A_3$ |
| 573.0659 | 573.0649 | 1.7 | 4.27E+04 | $^{0,2}A_3$' |
| 588.0879 | 588.0876 | 0.49 | 3291947.8 | $^{1,5}A_3$ |
| 615.075 | 615.0755 | -0.81 | 967091.1 | $B_3$' |
| 616.0808 | 616.0825 | -2.8 | 313427.3 | $B_3$ |
| 619.1295 | 619.1298 | -0.49 | 106927.9 | $^{2,4}X_2$ |
| 632.0778 | 632.0780 | -0.44 | 864503.6 | $C_3$" |
| 634.0934 | 634.0930 | 0.49 | 7280671 | $C_3$ |
| 677.1356 | 677.1359 | -0.44 | 1257629.9 | $Y_3$"-$SO_3$ |
| 719.1462 | 719.1465 | -0.41 | 1309795.9 | $^{0,2}X_3$"-$SO_3$ |
| 791.1674 | 791.1682 | -1 | 7875305.5 | $[M-3H-CO_2-SO_3]^-$ |
| 800.1107 | 800.1113 | -0.74 | 2201241.3 | $^{0,2}X_3$' |
| 817.1465 | 817.148 | -1.8 | 509871.3 | $[M-3H-SO_3-H_2O]^-$ |
| 835.157 | 835.1580 | -1.2 | 2740336.5 | $[M-3H-SO_3]^-$ |
| 871.1241 | 871.1251 | -1.1 | 299677.5 | $[M-3H-CO_2]^-$ |
| 915.1143 | 915.1143 | 0 | 170128 | $[M-3H]^-$ |

Table S15: Fragment ion list for 193 nm UVPD activation of the $[M-4H+Na]^{3-}$ precursor of CS-A dp4 in the high-pressure cell (8 pulses, 4 mJ).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 173.009 | 173.0098 | -4.6 | 256207.8 | $C_1$" |
| 175.0246 | 175.0248 | -1.2 | 321594.2 | $C_1$" |
| 198.9916 | 198.9917 | -0.98 | 440792 | $^{1,3}X_0$ |
| 282.0286 | 282.0289 | -1.1 | 1.20E+07 | $Z_1$ |
| 300.0392 | 300.0394 | -0.91 | 1607087.6 | $Y_1$ |
| 304.0105 | 304.0108 | -1.2 | 1736888.6 | $Z_1$+Na |
| 312.3652 | 312.3655 | -1.1 | 3.36E+07 | $[M-4H+Na]^{3-}$ |
| 328.034 | 328.0343 | -1.2 | 1000586.1 | $^{1,5}X_1$ |
| 342.0497 | 342.0500 | -0.99 | 1696293.6 | $^{0,2}X_1$ |
| 350.0159 | 350.0163 | -1.2 | 3717047.5 | $^{1,5}X_1$+Na |
| 369.0355 | 369.038 | -6.8 | 661124.3 | $Z_3"^{2-}$ |
| 390.0408 | 390.0412 | -1 | 3203229 | $[Y_3+Na]^{2-}$ |
| 414.0707 | 414.0717 | -2.6 | 14669782 | $Z_2$-$CO_2$ |
| 414.0707 | 414.0717 | -2.6 | 14669782 | $C_2$-$CO_2$ |
| 434.0314 | 434.0374 | -14 | 142960 | $^{1,5}A_2$'+Na |
| 446.0487 | 446.0492 | -1.2 | 276977.2 | $[^{1,5}A_4+Na]^{2-}$ |
| 456.0448 | 456.0469 | -4.8 | 4493237 | $Z_2$" |
| 456.0448 | 456.0469 | -4.8 | 4493237 | $C_2$" |
| 469.0493 | 469.0519 | -5.7 | 450568.3 | $[M-4H+Na]^{2-}$ |
| 479.0346 | 479.0359 | -2.7 | 7654003.5 | $Z_2$'+Na |
| 479.0346 | 479.0359 | -2.7 | 7654003.5 | $C_2$'+Na |
| 496.0374 | 496.0395 | -4.2 | 613693.5 | $Y_2$"+Na |
| 498.053 | 498.0535 | -1 | 1105643 | $Y_2$+Na |
| 522.053 | 522.0535 | -0.97 | 120183.5 | $^{2,4}A_3$+Na |
| 526.0479 | 526.0484 | -0.99 | 218115.1 | $^{1,5}X_2$+Na |
| 528.0659 | 528.0664 | -1.1 | 28116.8 | $^{3,5}A_3$+Na |
| 565.0331 | 565.0363 | -5.7 | 4081 | $^{0,3}A_3$'+Na |
| 609.0611 | 609.0626 | -2.5 | 200538.7 | $^{1,5}A_3$'+Na |
| 637.056 | 637.0575 | -2.4 | 1934383.6 | $B_3$'+Na |
| 656.0745 | 656.0750 | -0.8 | 1324433.8 | $C_3$+Na |
| 699.1167 | 699.1179 | -1.7 | 748532.2 | $Y_3$"+Na-$SO_3$ |
| 719.1248 | 719.1229 | 2.6 | 407274.6 | $^{2,5}A_4$'-$SO_3$ |
| 741.0984 | 741.0971 | 1.6 | 21590.1 | $Z_3$ |
| 763.0785 | 763.0791 | -0.82 | 1177829.3 | $Z_3$+Na |
| 779.0733 | 779.0747 | -1.8 | 406034.2 | $Y_3$"+Na |
| 781.089 | 781.0896 | -0.88 | 530058.4 | $Y_3$+Na |
| 795.1592 | 795.1517 | 9.4 | 8380.3 | $[M-4H+Na-SO_3-CO_2-H_2O]^-$ |
| 813.1481 | 813.1517 | -4.4 | 579796.9 | $[M-4H+Na-SO_3-CO_2]^-$ |
| 823.0952 | 823.1002 | -6.1 | 1539003.9 | $^{0,2}X_3$'+Na |
| 839.1268 | 839.1309 | -4.9 | 59953 | $[M-4H+Na-SO_3-H_2O]^-$ |
| 849.1151 | 849.1186 | -4.1 | 1044659.8 | $[M-4H+Na-2CO_2]^-$ |
| 893.1048 | 893.1079 | -3.4 | 77258 | $[M-4H+Na-CO_2]^-$ |
| 937.0945 | 937.0972 | -2.9 | 705435.6 | $[M-4H+Na]^-$ |

Table S16: Fragment ion list for 193 nm UVPD activation of the $[M-4H+Na]^{3-}$ precursor of DS dp4 in the high-pressure cell (8 pulses, 4 mJ).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 173.0089 | 173.0098 | -5.2 | 199847.3 | $C_1$" |
| 175.0249 | 175.0248 | 0.5 | 138870.5 | $C_1$ |
| 198.9916 | 198.9917 | -0.98 | 160745.4 | $^{1,3}X_0$ |
| 282.0284 | 282.0289 | -1.8 | 4998976.5 | $Z_1$ |
| 300.0391 | 300.0394 | -1.3 | 518889.6 | $Y_1$ |
| 304.0104 | 304.0108 | -1.5 | 418420.8 | $Z_1$+Na |
| 312.3649 | 312.3655 | -2.1 | 1477232.5 | $[M-4H+Na]^{3-}$ |
| 328.0341 | 328.0343 | -0.88 | 356449.3 | $^{1,5}X_1$ |
| 342.0499 | 342.0500 | -0.4 | 445879.2 | $^{0,2}X_1$ |
| 350.0162 | 350.0163 | -0.38 | 857283.6 | $^{1,5}X_1$+Na |
| 390.041 | 390.0412 | -0.53 | 1308640.3 | $[Y_3+Na]^{2-}$ |
| 414.0709 | 414.0717 | -2.1 | 3926893 | $Z_2$-$CO_2$ |
| 414.0709 | 414.0717 | -2.1 | 3926893 | $C_2$-$CO_2$ |
| 434.0379 | 434.0374 | 1 | 9910.1 | $^{1,5}A_2$'+Na |
| 456.045 | 456.0469 | -4.4 | 1151781.3 | $Z_2$" |
| 456.045 | 456.0469 | -4.4 | 1151781.3 | $C_2$" |
| 469.0496 | 469.0519 | -5.1 | 46750 | $[M-4H+Na]^{2-}$ |
| 479.0348 | 479.0359 | -2.3 | 2121329.3 | $Z_2$'+Na |
| 479.0348 | 479.0359 | -2.3 | 2121329.3 | $C_2$'+Na |
| 498.0531 | 498.0535 | -0.81 | 437572.4 | $Y_2$+Na |
| 550.048 | 550.0484 | -0.76 | 67685.5 | $^{3,5}A_3$+Na |
| 637.0561 | 637.0575 | -2.2 | 420323.8 | $B_3$'+Na |
| 656.0743 | 656.0750 | -1.1 | 334548.3 | $C_3$+Na |
| 701.1324 | 701.1328 | -0.68 | 134599 | $Y_3$+Na-$SO_3$ |
| 763.0783 | 763.0791 | -1.1 | 435433.5 | $Z_3$+Na |
| 781.0889 | 781.0896 | -1 | 766180.5 | $Y_3$+Na |
| 813.1483 | 813.1517 | -4.2 | 115379.3 | $[M-4H+Na-SO_3-CO_2]^-$ |
| 823.0953 | 823.1002 | -6 | 221509.7 | $^{0,2}X_3$'+Na |
| 839.1274 | 839.1309 | -4.2 | 20041.1 | $[M-4H+Na-SO_3-H_2O]^-$ |
| 849.1151 | 849.1186 | -4.1 | 328856.4 | $[M-4H+Na-2CO_2]^-$ |
| 893.1049 | 893.1079 | -3.4 | 1227829.5 | $[M-4H+Na-CO_2]^-$ |
| 937.0947 | 937.0972 | -2.7 | 158982 | $[M-4H+Na]^-$ |

Table S17: Fragment ion list for 213 nm UVPD activation of the $[M-3H]^{3-}$ precursor of DS dp4 in the high-pressure cell (50 ms).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 237.5332 | 237.5321 | 4.4 | 6723.1 | $Y_2^{2-}$ |
| 282.0301 | 282.0289 | 4.2 | 423403.3 | $Z_1$ |
| 305.0403 | 305.0382 | 6.8 | 3.50E+07 | $[M-3H]^{3-}$ |
| 316.5452 | 316.5429 | 7.2 | 7486.9 | $C_3^{2-}$ |
| 357.0385 | 357.0379 | 1.5 | 20369.2 | $^{2,5}X_1'$ |
| 371.0544 | 371.0536 | 2.2 | 74936.7 | $^{0,3}X_1'$ |
| 379.0522 | 379.0502 | 5.2 | 25672.9 | $Y_3^{2-}$ |
| 400.0553 | 400.0555 | -0.54 | 49641.2 | $^{0,2}X_3^{2-}$ |
| 414.0731 | 414.0717 | 3.2 | 317054.1 | $Z_2$-$CO_2$ |
| 414.0731 | 414.0717 | 3.2 | 317054.1 | $C_2$-$CO_2$ |
| 435.0578 | 435.0582 | -1.1 | 992.9 | $^{1,5}A_4^{2-}$ |
| 440.053 | 440.0504 | 5.8 | 9500.1 | $B_2$ |
| 456.0475 | 456.0469 | 1.1 | 57571.7 | $Z_2''$ |
| 456.0475 | 456.0469 | 1.1 | 57571.7 | $C_2''$ |
| 457.5592 | 457.5576 | 3.3 | 115132 | $[M-3H]^{2-}$ |
| 458.0625 | 458.0609 | 3.3 | 80651.5 | $Z_2$ |
| 458.0625 | 458.0609 | 3.3 | 80651.5 | $C_2$ |
| 458.0625 | 458.0609 | 3.3 | 80651.5 | $[M-2H]^{2-}$ |
| 474.0582 | 474.0565 | 3.5 | 35859.6 | $Y_2''$ |
| 588.0893 | 588.0876 | 2.9 | 3066.1 | $^{1,5}A_3$ |
| 677.1381 | 677.1359 | 3.2 | 5116 | $Y_3''$-$SO_3$ |
| 775.1725 | 775.1739 | -1.8 | 3332.4 | $[M-3H-SO_4-CO_2]^-$ |
| 800.1141 | 800.1113 | 3.5 | 23743.4 | $^{0,2}X_3'$ |

Table S18: Fragment ion list for 213 nm UVPD activation of the $[M-3H]^{3-}$ precursor of DS dp4 in the low-pressure cell (50 ms).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 237.5322 | 237.5321 | 0.23 | 25591.9 | $Y_2^{2-}$ |
| 282.029 | 282.0289 | 0.31 | 376801.5 | $Z_1$ |
| 305.0385 | 305.0382 | 0.85 | 1.34E+07 | $[M-3H]^{3-}$ |
| 357.0372 | 357.0379 | -2.1 | 15926.8 | $^{2,5}X_1'$ |
| 379.0504 | 379.0502 | 0.43 | 57966.1 | $Y_3^{2-}$ |
| 435.0593 | 435.0582 | 2.4 | 1136.4 | $^{1,5}A_4^{2-}$ |
| 440.0507 | 440.0504 | 0.6 | 18277.4 | $B_2$ |
| 458.0608 | 458.0609 | -0.43 | 62375.6 | $Z_2$ |
| 458.0608 | 458.0609 | -0.43 | 62375.6 | $[M-2H]^{2-}$ |
| 458.0608 | 458.0609 | -0.43 | 62375.6 | $C_2$ |
| 474.0561 | 474.0565 | -0.97 | 29513.2 | $Y_2''$ |
| 775.1706 | 775.1739 | -4.3 | 3723.3 | $[M-3H-SO_4-CO_2]^-$ |
| 800.111 | 800.1113 | -0.37 | 21056 | $^{0,2}X_3'$ |

Table S19: Fragment ion list for 213 nm UVPD activation of the $[M-3H]^{3-}$ precursor of DS dp4 in the high-pressure cell (150 ms).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 237.5329 | 237.5321 | 3.2 | 76668.1 | $Y_2^{2-}$ |
| 282.0298 | 282.0289 | 3.2 | 7391485.5 | $Z_1$ |
| 300.0408 | 300.0394 | 4.4 | 125171.5 | $Y_1$ |
| 305.0401 | 305.0382 | 6.1 | 2.20E+08 | $[M-3H]^{3-}$ |
| 316.5446 | 316.5429 | 5.4 | 94324.7 | $C_3^{2-}$ |
| 328.0354 | 328.0343 | 3.1 | 233104.1 | $^{1,5}X_1$ |
| 342.051 | 342.0500 | 2.8 | 44843.4 | $^{0,2}X_1$ |
| 357.0383 | 357.0379 | 0.98 | 335265.5 | $^{2,5}X_1'$ |
| 372.058 | 372.0606 | -7 | 65620 | $^{0,3}X_1'$ |
| 379.0516 | 379.0502 | 3.6 | 458945.8 | $Y_3^{2-}$ |
| 400.055 | 400.0555 | -1.3 | 1026168.4 | $^{0,2}X_3^{2-}$ |
| 414.0726 | 414.0717 | 2 | 5869078 | $Z_2$-$CO_2$ |
| 414.0726 | 414.0717 | 2 | 5869078 | $C_2$-$CO_2$ |
| 435.0593 | 435.0582 | 2.4 | 3672126 | $^{1,5}A_4^{2-}$ |
| 440.0523 | 440.0504 | 4.2 | 138030.9 | $B_2$ |
| 456.0471 | 456.0469 | 0.24 | 1099505.1 | $Z_2''$ |
| 456.0471 | 456.0469 | 0.24 | 1099505.1 | $C_2''$ |
| 457.5588 | 457.5576 | 2.4 | 2260667.8 | $[M-3H]^{2-}$ |
| 458.0618 | 458.0609 | 1.7 | 1614808.9 | $Z_2$ |
| 458.0618 | 458.0609 | 1.7 | 1614808.9 | $[M-2H]^{2-}$ |
| 458.0618 | 458.0609 | 1.7 | 1614808.9 | $C_2$ |
| 474.0577 | 474.0565 | 2.4 | 681351 | $Y_2''$ |
| 504.0676 | 504.0664 | 2.2 | 31038.9 | $^{1,5}X_2$ |
| 588.0897 | 588.0876 | 3.6 | 63162.5 | $^{1,5}A_3$ |
| 677.1378 | 677.1359 | 2.8 | 117259.2 | $Y_3''$-$SO_3$ |
| 775.172 | 775.1739 | -2.5 | 228915.2 | $[M-3H-SO_4-CO_2]^-$ |
| 800.1134 | 800.1113 | 2.6 | 452784.7 | $^{0,2}X_3'$ |

Table S20: Fragment ion list for 213 nm UVPD activation of the $[M-3H]^{3-}$ precursor of DS dp4 in the high-pressure cell (300 ms).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 198.9921 | 198.9917 | 1.5 | 40082.5 | $^{1,3}X_0$ |
| 237.5327 | 237.5321 | 2.3 | 72358.8 | $Y_2^{2-}$ |
| 282.0295 | 282.0289 | 2.1 | 9184308 | $Z_1$ |
| 300.0404 | 300.0394 | 3.1 | 263792.7 | $Y_1$ |
| 305.0396 | 305.0382 | 4.5 | 1.25E+08 | $[M-3H]^{3-}$ |
| 328.0351 | 328.0343 | 2.2 | 327671.6 | $^{1,5}X_1$ |
| 342.0506 | 342.0500 | 1.6 | 124282.4 | $^{0,2}X_1$ |
| 358.0414 | 358.0449 | -9.9 | 46280.9 | $^{2,5}X_1'$ |
| 372.0565 | 372.0606 | -11 | 92391.4 | $^{0,3}X_1'$ |
| 377.5278 | 377.5265 | 3.2 | 20384.1 | $^{2,4}A_4^{2-}$ |
| 379.0511 | 379.0502 | 2.3 | 607442.9 | $Y_3^{2-}$ |
| 400.0545 | 400.0555 | -2.5 | 1429674.9 | $^{0,2}X_3^{2-}$ |
| 414.0722 | 414.0717 | 0.99 | 8176075.5 | $Z_2$-$CO_2$ |
| 414.0722 | 414.0717 | 0.99 | 8176075.5 | $C_2$-$CO_2$ |
| 435.0596 | 435.0582 | 3.1 | 23605.7 | $^{1,5}A_4^{2-}$ |
| 440.0518 | 440.0504 | 3.1 | 163650.5 | $B_2$ |
| 456.0466 | 456.0469 | -0.85 | 1577052.9 | $Z_2''$ |
| 456.0466 | 456.0469 | -0.85 | 1577052.9 | $C_2''$ |
| 457.5583 | 457.5576 | 1.3 | 3198577.5 | $[M-3H]^{2-}$ |
| 458.0611 | 458.0609 | 0.22 | 2480923.3 | $Z_2$ |
| 458.0611 | 458.0609 | 0.22 | 2480923.3 | $[M-2H]^{2-}$ |
| 458.0611 | 458.0609 | 0.22 | 2480923.3 | $C_2$ |
| 474.0572 | 474.0565 | 1.4 | 998110.1 | $Y_2''$ |
| 504.0675 | 504.0664 | 2 | 55947.7 | $^{1,5}X_2$ |
| 573.0823 | 573.0886 | -11 | 2330.8 | $^{2,5}X_2''$ |
| 575.1074 | 575.1036 | -6.6 | 10056.4 | $^{2,5}X_2$ |
| 588.0892 | 588.0876 | 2.7 | 93418.8 | $^{1,5}A_3$ |
| 619.131 | 619.1298 | 1.9 | 1550 | $^{2,4}X_2$ |
| 634.0949 | 634.0930 | 2.9 | 100005.6 | $C_3$ |
| 677.1371 | 677.1359 | 1.8 | 211551.5 | $Y_3''$-$SO_3$ |
| 719.1479 | 719.1465 | 1.9 | 37529.5 | $^{0,2}X_3''$-$SO_3$ |
| 775.1714 | 775.1739 | -3.2 | 348810.4 | $[M-3H-SO_4-CO_2]^-$ |
| 791.1692 | 791.1682 | 1.3 | 142279.2 | $[M-3H-SO_3-CO_2]^-$ |
| 800.1126 | 800.1113 | 1.6 | 687008.6 | $^{0,2}X_3'$ |
| 817.1465 | 817.148 | -1.8 | 2505.6 | $[M-3H-SO_3-H_2O]^-$ |
| 835.1588 | 835.1580 | 0.92 | 33927.3 | $[M-3H-SO_3]^-$ |

Table S21: Fragment ion list for 213 nm UVPD activation of the $[M-3H]^{3-}$ precursor of DS dp4 in the high-pressure cell (400 ms).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 198.9917 | 198.9917 | -0.48 | 937290.9 | $^{1,3}X_0$ |
| 237.5321 | 237.5321 | -0.18 | 1475916.5 | $Y_2^{2-}$ |
| 266.0339 | 266.0326 | 4.9 | 529746.9 | $^{0,2}X_3'^{3-}$ |
| 282.0289 | 282.0289 | -0.03 | 2.65E+07 | $Z_1$ |
| 300.0394 | 300.0394 | -0.25 | 3660405 | $Y_1$ |
| 305.0382 | 305.0382 | -0.13 | 5.87E+07 | $[M-3H]^{3-}$ |
| 316.5428 | 316.5429 | -0.33 | 342631.5 | $C_3^{2-}$ |
| 328.0343 | 328.0343 | -0.27 | 1862910.3 | $^{1,5}X_1$ |
| 342.0499 | 342.0500 | -0.4 | 2212737 | $0,2X_1$ |
| 357.037 | 357.0379 | -2.7 | 1601530.4 | $2,5X_1'$ |
| 371.0526 | 371.0536 | -2.7 | 7530043.5 | $0,3X_1'$ |
| 377.5264 | 377.5265 | -0.51 | 42948 | $^{2,4}A_4^{2-}$ |
| 378.0423 | 378.0435 | -3.2 | 1696612.1 | $Y_3''^{2-}$ |
| 379.0501 | 379.0502 | -0.36 | 6254056 | $Y_3^{2-}$ |
| 400.0538 | 400.0555 | -4.3 | 3270166.8 | $^{0,2}X_3^{2-}$ |
| 414.071 | 414.0717 | -1.9 | 26811848 | $Z_2\text{-}CO_2$ |
| 414.071 | 414.0717 | -1.9 | 26811848 | $C_2\text{-}CO_2$ |
| 435.0581 | 435.0582 | -0.36 | 202104.9 | $^{1,5}A_4^{2-}$ |
| 440.0504 | 440.0504 | -0.07 | 1519904.6 | $B_2$ |
| 456.0452 | 456.0469 | -3.9 | 6185014 | $Z_2''$ |
| 456.0452 | 456.0469 | -3.9 | 6185014 | $C_2''$ |
| 457.5569 | 457.5576 | -1.7 | 6338524.5 | $[M-3H]^{2-}$ |
| 458.0604 | 458.0609 | -1.3 | 7186134 | $Z_2$ |
| 458.0604 | 458.0609 | -1.3 | 7186134 | $[M-2H]^{2-}$ |
| 458.0604 | 458.0609 | -1.3 | 7186134 | $C_2$ |
| 474.0558 | 474.0565 | -1.6 | 4013836 | $Y_2''$ |
| 476.0714 | 476.0715 | -0.34 | 1698655.8 | $Y_2$ |
| 504.0664 | 504.0664 | -0.15 | 660264.5 | $^{1,5}X_2$ |
| 588.0876 | 588.0876 | -0.01 | 426564 | $^{1,5}A_3$ |
| 619.1296 | 619.1298 | -0.33 | 13311.4 | $^{2,4}X_2$ |
| 634.0931 | 634.0930 | 0.02 | 430736.5 | $C_3$ |
| 677.1353 | 677.1359 | -0.88 | 2404114 | $Y_3''\text{-}SO_3$ |
| 719.1458 | 719.1465 | -0.97 | 955455.3 | $^{0,2}X_3''\text{-}SO_3$ |
| 775.1707 | 775.1739 | -4.1 | 461205.3 | $[M-3H-SO_4-CO_2]^-$ |
| 791.1671 | 791.1682 | -1.4 | 1145811.9 | $[M-3H-SO_3-CO_2]^-$ |
| 800.1103 | 800.1113 | -1.2 | 3441741.3 | $^{0,2}X_3'$ |
| 817.1457 | 817.148 | -2.8 | 66057.8 | $[M-3H-SO_3-H_2O]^-$ |
| 835.1567 | 835.1580 | -1.6 | 460815.9 | $[M-3H-SO_3]^-$ |
| 915.1133 | 915.1143 | -1.1 | 305314.3 | $[M-3H]^-$ |

Table S22: Fragment ion list for 213 nm UVPD activation of the $[M-3H]^{3-}$ precursor of DS dp4 in the low-pressure cell (400 ms).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 198.992 | 198.9917 | 1 | 54469.5 | $^{1,3}X_0$ |
| 237.5326 | 237.5321 | 1.9 | 70144 | $Y_2^{2-}$ |
| 266.0344 | 266.0326 | 6.8 | 125775.3 | $^{0,2}X_3'^{3-}$ |
| 282.0294 | 282.0289 | 1.7 | 9037220 | $Z_1$ |
| 300.0401 | 300.0394 | 2.1 | 414498.3 | $Y_1$ |
| 305.0394 | 305.0382 | 3.8 | 7.73E+07 | $[M-3H]^{3-}$ |
| 316.5437 | 316.5429 | 2.5 | 89387.4 | $C_3^{2-}$ |
| 328.0349 | 328.0343 | 1.6 | 372294.6 | $^{1,5}X_1$ |
| 342.0504 | 342.0500 | 1.1 | 221333.5 | $^{0,2}X_1$ |
| 358.0411 | 358.0449 | -11 | 51533.2 | $^{2,5}X_1'$ |
| 372.0562 | 372.0606 | -12 | 114927.5 | $^{0,3}X_1'$ |
| 377.5275 | 377.5265 | 2.4 | 23318 | $^{2,4}A_4^{2-}$ |
| 379.0509 | 379.0502 | 1.7 | 713679.8 | $Y_3^{2-}$ |
| 400.0543 | 400.0555 | -3 | 1561209.5 | $^{0,2}X_3^{2-}$ |
| 414.0719 | 414.0717 | 0.26 | 8909531 | $Z_2\text{-}CO_2$ |
| 414.0719 | 414.0717 | 0.26 | 8909531 | $C_2\text{-}CO_2$ |
| 435.0592 | 435.0582 | 2.2 | 32272.3 | $^{1,5}A_4^{2-}$ |
| 440.0515 | 440.0504 | 2.4 | 171774.2 | $B_2$ |
| 456.0463 | 456.0469 | -1.5 | 1751302.5 | $Z_2''$ |
| 456.0463 | 456.0469 | -1.5 | 1751302.5 | $C_2''$ |
| 457.5581 | 457.5576 | 0.89 | 3460587.5 | $[M-3H]^{2-}$ |
| 458.0608 | 458.0609 | -0.43 | 2780777.3 | $Z_2$ |
| 458.0608 | 458.0609 | -0.43 | 2780777.3 | $[M-2H]^{2-}$ |
| 458.0608 | 458.0609 | -0.43 | 2780777.3 | $C_2$ |
| 476.0724 | 476.0715 | 1.8 | 210474.1 | $Y_2^{2-}$ |
| 504.0673 | 504.0664 | 1.6 | 85287.7 | $^{1,5}X_2$ |
| 573.0821 | 573.0886 | -11 | 51388.5 | $^{2,5}X_2''$ |
| 588.089 | 588.0876 | 2.4 | 110024.5 | $^{1,5}A_3$ |
| 619.1309 | 619.1298 | 1.8 | 2101.3 | $^{2,4}X_2$ |
| 634.0947 | 634.0930 | 2.5 | 120173.9 | $C_3$ |
| 677.1367 | 677.1359 | 1.2 | 313029.1 | $Y_3''\text{-}SO_3$ |
| 719.1473 | 719.1465 | 1.1 | 73862.1 | $^{0,2}X_3''\text{-}SO_3$ |
| 775.171 | 775.1739 | -3.7 | 112104.8 | $[M-3H\text{-}SO_4\text{-}CO_2]^-$ |
| 791.1686 | 791.1682 | 0.5 | 222651.9 | $[M-3H\text{-}SO_3\text{-}CO_2]^-$ |
| 800.1122 | 800.1113 | 1.1 | 807399.1 | $^{0,2}X_3'$ |
| 817.1459 | 817.148 | -2.6 | 4722.2 | $[M-3H\text{-}SO_3\text{-}H_2O]^-$ |
| 835.1584 | 835.1580 | 0.44 | 47343.2 | $[M-3H\text{-}SO_3]^-$ |
| 915.1148 | 915.1143 | 0.54 | 41853.7 | $[M-3H]^-$ |

Table S23: $MS^3$ activation of the fragment ion m/z 715.05 of DS dp4 using 193 nm UVPD (8 pulses, 4 mJ)/ 193 nm UVPD (8 pulses, 4 mJ).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 175.0246 | 175.0248 | -1.1 | 77009.5 | $C_1$ |
| 272.992 | 272.9916 | 1.5 | 101466.1 | $[Y_2/C_3]+SO_3$ |
| 282.0287 | 282.0289 | -0.74 | 132838.8 | $Z_1$ |
| 325.032 | 325.0291 | 8.9 | 2086.7 | $[^{1,4}A_3'/Z_3']^{2-}$ |
| 396.1143 | 396.1147 | -1.1 | 55170.3 | $C_3/Y_2-SO_3$ |
| 440.0499 | 440.0504 | -1.2 | 322608.3 | $B_2$ |
| 456.0603 | 456.0609 | -1.5 | 31145.2 | $Z_2''$ |
| 456.0603 | 456.0609 | -1.5 | 31145.2 | $C_2''$ |
| 476.071 | 476.0715 | -1.2 | 456067.5 | $Y_2$ |
| 518.0816 | 518.0821 | -1 | 134232.8 | $C_3/^{0,2}X_2$ |
| 554.1356 | 554.1363 | -1.3 | 158272.3 | $C_3-SO_3$ |
| 590.0663 | 590.0674 | -1.9 | 459146.9 | $C_3-C_2H_4O$ |
| 634.0924 | 634.0931 | -1.1 | 5880742 | $C_3$ |
| 715.0571 | 715.0571 | -0.12 | 5776643 | $C_3+HSO_3$ |

Table S24: $MS^3$ activation of the fragment ion m/z 715.05 of DS dp4 using 193 nm UVPD (8 pulses, 4 mJ)/ HCD (NCE 20).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 272.9922 | 272.9916 | 2.2 | 218682.5 | $[Y_2/C_3]+SO_3$ |
| 282.0289 | 282.0289 | -0.03 | 31981 | $Z_1$ |
| 440.0503 | 440.0504 | -0.3 | 490020.3 | $B_2$ |
| 476.0714 | 476.0715 | -0.34 | 60841.8 | $Y_2$ |
| 616.0821 | 616.0825 | -0.64 | 11841 | $B_3$ |
| 634.093 | 634.0931 | -0.15 | 20435110 | $C_3$ |

Table S25: $MS^3$ activation of the fragment ion m/z 715.05 of CS-A dp4 using 193 nm UVPD (8 pulses, 4 mJ)/ 193 nm UVPD (8 pulses, 4 mJ).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 175.0246 | 175.0248 | -1.1 | 25957.2 | $C_1$ |
| 272.9918 | 272.9916 | 0.73 | 58237.1 | $[Y_2/C_3]+SO_3$ |
| 282.0285 | 282.0289 | -1.5 | 42349.1 | $Z_1$ |
| 396.1145 | 396.1147 | -0.62 | 25369.6 | $C_3/Y_2-SO_3$ |
| 440.0498 | 440.0504 | -1.4 | 99417.8 | $B_2$ |
| 456.0445 | 456.0469 | -5.3 | 23296.5 | $C_2"$ |
| 456.0445 | 456.0469 | -5.3 | 23296.5 | $Z_2"$ |
| 476.0709 | 476.0715 | -1.4 | 109280.8 | $Y_2$ |
| 518.0809 | 518.0821 | -2.3 | 29465.8 | $C_3/^{0,2}X_2$ |
| 554.1354 | 554.1363 | -1.6 | 53173.5 | $C_3-SO_3$ |
| 590.066 | 590.0674 | -2.4 | 81207.7 | $C_3-C_3H_4O$ |
| 616.082 | 616.0825 | -0.81 | 15116.6 | $B_3$ |
| 634.0922 | 634.0931 | -1.4 | 1258890.4 | $C_3$ |
| 697.0464 | 697.0472 | -1.1 | 26059.2 | $C_3+HSO_3-H_2O$ |
| 715.056 | 715.0571 | -1.7 | 1330775.6 | $C_3+HSO_3$ |

Table S26: $MS^3$ activation of the fragment ion m/z 715.05 of CS-A dp4 using 193 nm UVPD (8 pulses, 4 mJ)/ HCD (NCE 20).

| Measured m/z | Calculated m/z | Accuracy (PPM) | Intensity | Assigned Fragment |
|---|---|---|---|---|
| 272.9919 | 272.9916 | 1.1 | 168492.5 | $[Y_2/C_3]+SO_3$ |
| 282.0284 | 282.0289 | -1.8 | 21308.3 | $Z_1$ |
| 440.0497 | 440.0504 | -1.7 | 234610.4 | $B_2$ |
| 476.0708 | 476.0715 | -1.6 | 62210.2 | $Y_2$ |
| 504.0658 | 504.0665 | -1.4 | 20400.4 | $^{1,5}X_2$ |
| 616.0815 | 616.0825 | -1.6 | 23458.2 | $B_3$ |
| 634.0922 | 634.0931 | -1.4 | 4795857 | $C_3$ |