**Table S1: Literature containing carbohydrate CCSs.** CCSs from bold references are implemented in Table S2 if not noted otherwise. References in green contain large CCS collections.

| reference label | instru-ment type† | CCS drift gas # | investigated carbohydrates | comment | reference |
|---|---|---|---|---|---|
| **Both2014** | TW | He | mono-, disaccharides, glycopeptide | fragment CCSs available | P. Both et al., Nat. Chem. 2014, 6, 65-74. |
| **Clowers2005** | DT | $N_2$ | di-, trisaccharides | | B. H. Clowers et al., J. Am. Soc. Mass Spectrom. 2005, 16, 660-669. |
| Dwivedi2007 | DT | $N_2$, He, $CO_2$, $SF_6$ | methyl-monosaccharides | different adducts, different drift gases | P. Dwivedi et al., J. Am. Soc. Mass Spectrom. 2007, 18, 1163-1175. |
| **Fenn2011** | DT | He | milk oligosaccharides of different sizes | underivatized and Sp derivatized carbohydrates, CCSs of intact ions and their fragments, adducts | L. S. Fenn, J. A. McLean, Phys. Chem. Chem. Phys. 2011, 13, 2196-2205. |
| **Gaye2015** | DT | He | mono-, di- and trisaccharides | fragment CCS available | M. M. Gaye et al., Analyst 2015, 140, 6922-6932. |
| **Gelb2014** | DT | He | milk oligosaccharides | | A. S. Gelb et al., Anal. Chem. 2014, 86, 11396-11402. |
| **Guttman2016** | TW | $N_2$ | glycopeptides, trisaccharides | sialic acid linkage identification, further fragment CCSs available | M. Guttman, K. K. Lee, Anal. Chem. 2016, 88, 5212-5217. |
| Harvey2014 | TW | $N_2$, He | N-glycans | | D. J. Harvey et al., Rapid Commun. Mass Spectrom. 2014, 28, 2008-2018. |
| Harvey2016 | TW | $N_2$ | reduced N-glycans | | D. J. Harvey, J. L. Abrahams, Rapid Commun. Mass Spectrom. 2016, 30, 627-634. |
| Harvey2016 | TW | $N_2$, He | N-glycans | CCSs of intact and fragment ions | D. J. Harvey et al., J. Mass Spectrom. 2016, 51, 1064-1079. |
| **Hinneburg2016** | TW | $N_2$ | glycopeptides | sialic acid linkage identification | H. Hinneburg et al., Chem. Commun. 2016, 52, 4381-4384. |
| Hofmann2014 | DT | $N_2$, He | large number of N-glycans, dextran | CCSs of intact and fragment ions available | J. Hofmann et al., Anal. Chem. 2014, 86, 10789-10795. |
| Hofmann2015 | TW | $N_2$ | trisaccharides | data in pos+neg ion mode | J. Hofmann et al., Nature 2015, 526, 241-244. |
| **Hofmann2017** | TW | $N_2$ | Lewis and blood group tri- and tetrasaccharides, milk oligosaccharides, N-glycans | CCSs of intact and fragment ions available | J. Hofmann et al., Anal. Chem. 2017, 89, 2318-2325. |
| **Huang2013** | TW | He | di-, trisaccharides, LNFP, LNDFH | different adducts | Y. Huang, E. D. Dodds, Anal. Chem. 2013, 85, 9728-9735. |
| **Huang2015** | TW | He | trisaccharides and milk oligosaccharides | different adducts and additional CCSs, ETD product ions | Y. T. Huang, E. D. Dodds, Analyst 2015, 14, 6912-6921. |
| **Lee1997** | DT | He | tetra- and hexasaccharides | theoretical CCS calculations | S. Lee et al., Int. J. Mass Spectrom. Ion Process. 1997, 167, 605-614. |
| **Li2012** | DT | $N_2$ | methyl-monosaccharides | | H. Li et al., Anal. Chem. 2012, 84, 3231-3239. |
| **May2014** | DT | $N_2$ | large number of different saccharides | different adducts | J. C. May et al., Anal. Chem. 2014, 86, 2107-2116. |
| Pagel2013 | DT | $N_2$, He | large number of N-glycans | CCSs of intact and fragment ions available | K. Pagel, D. J. Harvey, Anal. Chem. 2013, 85, 5138-5145. |
| **Paglia2014** | TW | $N_2$ | mono-, di- and trisaccharides | data in pos+neg ion mode,validation of CCS on 3 instruments in different labs, theoretical calculations available | G. Paglia et al., Anal. Chem. 2014, 86, 3985-3993. |

| reference label | instru-ment type† | CCS drift gas # | investigated carbohydrates | comment | reference |
|---|---|---|---|---|---|
| Plasencia2008 | DT | He | N-glycans | | M. D. Plasencia et al., J. Am. Soc. Mass Spectrom. 2008, 19, 1706-1715. |
| **Pu2016** | TIMS, DT | $N_2$ | permetylated LNnT/LNT | | Y. Pu et al., Anal. Chem. 2016, 88, 3440-3443. |
| Rashid2014 | TW | He | dextran, pullulan, maltooligosaccharide | neg ion mode | A. M. Rashid et al., Rapid Commun. Mass Spectrom. 2014, 28, 191-199. |
| Seo2011 | TW | $N_2$ | heparin octasaccharides | different adducts | Y. Seo et al., Int. J. Mass Spectrom. 2011, 303, 191-198. |
| Seo2012 | TW | $N_2$ | heparin octasaccharides | different adducts | Y. Seo et al., Anal. Chem. 2012, 84, 2416-2423. |
| Struwe2015 | DT | $N_2$ | high-mannose glycans | data in pos+neg ion mode | W. B. Struwe et al., Analyst 2015, 140, 6799-6803. |
| **Struwe2016** | TW | He | milk oligosaccharides (syntetic and biol. source) | data in pos+neg ion mode, theoretical calculations available | W. B. Struwe et al., Chem. Commun. 2016, 52, 12353-12356. |
| **Wiliams2010** | DT | He | N-glycans and milk oligosaccharides | further CCSs available | J. P. Williams et al., Int. J. Mass Spectrom. 2010, 298, 119-127. |
| **Yang2016** | TW | He | mono-, disaccharides | underivatized, and labeled with phenylhydrazine (PHN), and 1-phenyl-3-methyl-5-pyrazolone (PMP) | H. M. Yang et al., Sci. Rep. 2016, 6, 28079. |
| Zheng2017 | DT | $N_2$ | mono- to hexasaccharides | data in pos+neg ion mode; several isomer separations, but no CCS reported | X. Zheng et al., Anal. Bioanal. Chem. 2017, 409, 467-476. |

† TW and TIMS CCSs were obtained from calibrations with reference substances with known CCSs.

# Drift gas for which the CCS was calculated or estimated. This is not necessarily the drift gas used during the measurement. Often He calibrant values are used to estimate He CCS from N2 measurements.

The CCS values of Table S2 are collected from references listed in Table S1. Please cite the appropriate publication(s), if you use any of these values for your research.

**Table S2: CCS values in Å² of carbohydrates reported in the references of Table S1.** CCS errors correspond to the standard deviations of replicate measurements. Blue values result from measurements in the negative ion mode.

**Monosaccharides**

| molecule | MW in Da | type | *m/z* | $^{TW}CCS_{He}$ Both14 | $^{TW}CCS_{He}$ Yang16 | $^{DT}CCS_{N2}$ May14 | $^{DT}CCS_{N2}$ Li12 | $^{TW}CCS_{N2}$ Paglia14 |
|---|---|---|---|---|---|---|---|---|
| α-Me-All | 178.18 | $[M + Na]^+$ | 201.07 | | | | 133.04 | |
| α-Me-Alt | 178.18 | $[M + Na]^+$ | 201.07 | | | | 138.74 | |
| α-Me-Gal | 178.18 | $[M + Na]^+$ | 201.07 | | | | 140.8 | |
| α-Me-Glc | 178.18 | $[M + Na]^+$ | 201.07 | | | | 141.77 | |
| α-Me-Gul | 178.18 | $[M + Na]^+$ | 201.07 | | | | 131.34 | |
| α-Me-Ido | 178.18 | $[M + Na]^+$ | 201.07 | | | | 133.04 | |
| α-Me-Man | 178.18 | $[M + Na]^+$ | 201.07 | | | | 136.8 | |
| α-Me-Tal | 178.18 | $[M + Na]^+$ | 201.07 | | | | 126.98 | |
| β-Me-All | 178.18 | $[M + Na]^+$ | 201.07 | | | | 139.83 | |
| β-Me-Alt | 178.18 | $[M + Na]^+$ | 201.07 | | | | 131.34 | |
| β-Me-Gal | 178.18 | $[M + Na]^+$ | 201.07 | | | | 135.83 | |
| β-Me-Glc | 178.18 | $[M + Na]^+$ | 201.07 | | | | 139.83 | |
| β-Me-Gul | 178.18 | $[M + Na]^+$ | 201.07 | | | | 131.34 | |
| β-Me-Ido | 178.18 | $[M + Na]^+$ | 201.07 | | | | 132.19 | |
| β-Me-Man | 178.18 | $[M + Na]^+$ | 201.07 | | | | 134.01 | |
| β-Me-Tal | 178.18 | $[M + Na]^+$ | 201.07 | | | | 131.34 | |
| Glucosamine | 179.17 | $[M + H]^+$ | 180.09 | | | | | 135 |
| Fructose | 180.16 | $[M - H]^-$ | 179.06 | | | | | 135 |
| Fructose | 180.16 | $[M + Na]^+$ | 203.05 | | 83.7 ± 0.4 | | | 135 |
| Galactose | 180.16 | $[M - H]^-$ | 179.06 | | | | | 130 |
| Galactose | 180.16 | $[M + Na]^+$ | 203.05 | 75 | 83.5 ± 0.3 | | | 136 |
| Glucose | 180.16 | $[M - H]^-$ | 179.06 | | | | | 135 |
| Glucose | 180.16 | $[M + Na]^+$ | 203.05 | 78 | | | | 138 |
| Mannose | 180.16 | $[M - H]^-$ | 179.06 | | | | | 130 |
| Mannose | 180.16 | $[M + Na]^+$ | 203.05 | 76 | 83.4 ± 0.5 | | | 138 |
| Mannitol | 182.17 | $[M - H]^-$ | 181.07 | | | | | 131 |
| Mannitol | 182.17 | $[M + Li]^+$ | 189.10 | | | 144.5 | | |
| Mannitol | 182.17 | $[M + Na]^+$ | 205.07 | | | 140.6 | | 137 |
| Sorbitol | 182.17 | $[M + H]^+$ | 183.09 | | | 147.2 | | |

| molecule | MW in Da | type | *m/z* | $^{TW}CCS_{He}$ Both14 | $^{TW}CCS_{He}$ Yang16 | $^{DT}CCS_{N2}$ May14 | $^{DT}CCS_{N2}$ Li12 | $^{TW}CCS_{N2}$ Paglia14 |
|---|---|---|---|---|---|---|---|---|
| Sorbitol | 182.17 | $[M + Na]^+$ | 205.07 | | | 139.4 | | |
| Glucuronic acid | 194.14 | $[M - H]^-$ | 193.03 | | | | | 130 |
| Glucuronic acid | 194.14 | $[M + Na]^+$ | 217.03 | | | | | 140 |
| Gluconic acid | 196.16 | $[M - H]^-$ | 195.05 | | | | | 132 |
| Gluconic acid | 196.16 | $[M + Na]^+$ | 219.05 | | | | | 148 |
| α-Me-GalNAc | 219.24 | $[M + Na]^+$ | 242.10 | | | | 145.05 | |
| α-Me-GlcNAc | 219.24 | $[M + Na]^+$ | 242.10 | | | | 151.84 | |
| β-Me-GalNAc | 219.24 | $[M + Na]^+$ | 242.10 | | | | 146.14 | |
| β-Me-GlcNAc | 219.24 | $[M + Na]^+$ | 242.10 | | | | 151.84 | |
| N-Acetylgalactosamine | 221.21 | $[M + Na]^+$ | 244.08 | 85 | | | | |
| N-Acetylglucosamine | 221.21 | $[M - H]^-$ | 220.08 | | | | | 143 |
| N-Acetylglucosamine | 221.21 | $[M + Na]^+$ | 244.08 | 90 | | | | 153 |
| N-Acetylmannosamine | 221.21 | $[M + Na]^+$ | 244.08 | 84 | | | | |
| Ribose 5-phosphate | 230.11 | $[M - H]^-$ | 229.01 | | | | | 137 |
| Ribose 5-phosphate | 230.11 | $[M + Na]^+$ | 253.01 | | | | | 146 |
| Glucosamine 1-phosphate | 259.15 | $[M - H]^-$ | 258.04 | | | | | 146 |
| Glucosamine 1-phosphate | 259.15 | $[M + H]^+$ | 260.05 | | | | | 153 |
| Glucosamine 6-phosphate | 259.15 | $[M - H]^-$ | 258.04 | | | | | 146 |
| Glucosamine 6-phosphate | 259.15 | $[M + H]^+$ | 260.05 | | | | | 150 |
| Fructose 6-phosphate | 260.14 | $[M + Na]^+$ | 259.02 | | | | | 150 |
| Fructose 6-phosphate | 260.14 | $[M - H]^-$ | 259.02 | | | | | 143 |
| Glucose 6-phosphate | 260.14 | $[M - H]^-$ | 259.02 | | | | | 143 |
| Glucose 6-phosphate | 260.14 | $[M + Na]^+$ | 283.02 | | | | | 154 |
| Fructose (PHN label) | 270.29 | $[M + Na]^+$ | 293.11 | | 100.3 ± 0.5 | | | |
| Galactose (PHN label) | 270.29 | $[M + Na]^+$ | 293.11 | | 98.2 ± 0.4 | | | |
| Mannose (PHN label) | 270.29 | $[M + Na]^+$ | 293.11 | | 98.0 ± 0.5 | | | |
| 6-Phosphogluconate | 276.14 | $[M - H]^-$ | 275.02 | | | | | 142 |
| 6-Phosphogluconate | 276.14 | $[M + Na]^+$ | 299.01 | | | | | 159 |
| Fructose 1,6-diphosphate | 340.12 | $[M - H]^-$ | 338.99 | | | | | 150 |
| Fructose (PMP lable) | 510.55 | $[M + H]^+$ | 511.22 | | 154.4 ± 0.2 | | | |
| Galactose (PMP label) | 510.55 | $[M + H]^+$ | 511.22 | | 152.8 ± 0.1 | | | |
| Mannose (PMP label) | 510.55 | $[M + H]^+$ | 511.22 | | 153.7 ± 0.2 | | | |

## Milk oligosaccharides

| molecule | MW in Da | type | *m/z* | $^{DT}CCS_{He}$ Fenn11 | $^{DT}CCS_{He}$ Williams10 | $^{TW}CCS_{He}$ Huang13 | $^{TW}CCS_{He}$ Gelb14 ‡ | $^{TW}CCS_{He}$ Huang15 | $^{DT}CCS_{N2}$ May14 | $^{TIMS|DT}CCS_{N2}$ Pu16 § | $^{TW}CCS_{N2}$ Hofmann17 | $^{TW}CCS_{N2}$ Struwe16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| blood group A trisaccharide | 529.49 | $[M + Na]^+$ | 552.19 | | | | | | | | 225 ± 1 | |
| blood group H type 1 trisaccharide | 529.49 | $[M + Na]^+$ | 552.19 | | | | | | | | 224 ± 1 | |
| blood group H type 2 trisaccharide | 529.49 | $[M + Na]^+$ | 552.19 | | | | | | | | 229 ± 2 | |
| Lewis a trisaccharide | 529.49 | $[M + Na]^+$ | 552.19 | | | | | | | | 223 ± 2 | |
| Lewis x trisaccharide | 529.49 | $[M + Na]^+$ | 552.19 | | | | | | | | 215 ± 2 | |
| Lewis b tetrasaccharide | 675.63 | $[M + Na]^+$ | 698.25 | | | | | | | | 252 ± 1 | |
| Lewis y tetrasaccharide | 675.63 | $[M + Na]^+$ | 698.25 | | | | | | | | 248 ± 1 | |
| Lacto-N-neotetraose (LNnT) | 707.63 | $[M - H]^-$ | 706.24 | | | | | | | | | 186.3 ± 0.8 |
| Lacto-N-neotetraose (LNnT) | 707.63 | $[M + H]^+$ | 708.26 | | | | | | | | | 189.1 ± 0.4 |
| Lacto-N-neotetraose (LNnT) | 707.63 | $[M + Na]^+$ | 730.24 | | | | | | | | | 169.6 ± 1.0 |
| Lacto-N-neotetraose (LNnT) | 707.63 | $[M + Cl]^-$ | 742.22 | | | | | | | | | 180.4 ± 0.8 |
| Lacto-N-neotetraose (LNnT) - permethylated | 707.63 | $[M + Na]^+$ | 926.46 | | | | | | | 300 \| 299 | | |
| Lacto-N-tetraose (LNT) | 707.63 | $[M - H]^-$ | 706.24 | | | | | | | | | 172.2 ± 1.0 |
| Lacto-N-tetraose (LNT) | 707.63 | $[M + H]^+$ | 708.26 | | | | | | | | | 177.9 ± 0.8 |
| Lacto-N-tetraose (LNT) | 707.63 | $[M + Na]^+$ | 730.24 | | | | | | | | | 170.5 ± 1.0 |
| Lacto-N-tetraose (LNT) | 707.63 | $[M + Cl]^-$ | 742.22 | | | | | | | | | 182.1 ± 1.2 |
| Lacto-N-tetraose (LNT) - permethylated | 707.63 | $[M + Na]^+$ | 926.46 | | | | | | | 291 \| 293 | | |
| Lacto-N-fucopentaose I | 853.77 | $[M + Be]^{2+}$ | 431.16 | | | | | 204.0 ± 0.3 | | | | |
| Lacto-N-fucopentaose I | 853.77 | $[M + Mg]^{2+}$ | 438.65 | | | | | 201.1 ± 0.4 | | | | |
| Lacto-N-fucopentaose I | 853.77 | $[M + Ca]^{2+}$ | 446.63 | | | | | 198.2 ± 0.8 | | | | |
| Lacto-N-fucopentaose I | 853.77 | $[M + Sr]^{2+}$ | 470.61 | | | | | 200.8 ± 1.0 | | | | |
| Lacto-N-fucopentaose I | 853.77 | $[M + Ba]^{2+}$ | 495.61 | | | | | 193.5 ± 0.9 | | | | |
| Lacto-N-fucopentaose I | 853.77 | $[M + Li]^+$ | 860.32 | 203.1 ± 1.2 | | 198.1 ± 0.2 | 200.2 ± 0.3 | | 269.6 | | | |
| Lacto-N-fucopentaose I | 853.77 | $[M + Na]^+$ | 876.30 | 204.4 ± 1.4 | 196 | 201.5 ± 0.3 | 203.8 ± 0.3 | | 276.1 | | | |
| Lacto-N-fucopentaose I | 853.77 | $[M + K]^+$ | 892.27 | 205.0 ± 0.7 | | 201.1 ± 0.3 | 203.4 ± 0.3 | | 274.7 | | | |
| Lacto-N-fucopentaose I | 853.77 | $[M + Rb]^+$ | 938.22 | 198.4 ± 1.5 | | 200.8 ± 0.2 | 203.1 ± 0.2 | | 275.2 | | | |
| Lacto-N-fucopentaose I | 853.77 | $[M + Cs]^+$ | 986.21 | 204.0 ± 2.1 | | 202.0 ± 0.6 | 204.3 ± 0.6 | | 275.6 | | | |
| Lacto-N-fucopentaose I (peak 1) | 853.77 | $[M + H]^+$ | 854.31 | | 185 | | | | | | | |

| molecule | MW in Da | type | *m/z* | $^{DT}CCS_{He}$ Fenn11 | $^{DT}CCS_{He}$ Williams10 | $^{TW}CCS_{He}$ Huang13 | $^{TW}CCS_{He}$ Gelb14 ‡ | $^{TW}CCS_{He}$ Huang15 | $^{DT}CCS_{N2}$ May14 | $^{TIMS\|DT}CCS_{N2}$ Pu16 § | $^{TW}CCS_{N2}$ Hofmann17 | $^{TW}CCS_{N2}$ Struwe16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Lacto-N-fucopentaose I (peak2) | 853.77 | $[M + H]^+$ | 854.31 | | 201 | | | | | | | |
| Lacto-N-fucopentaose II | 853.77 | $[M + Be]^{2+}$ | 431.16 | | | | | 201.2 ± 0.4 | | | | |
| Lacto-N-fucopentaose II | 853.77 | $[M + Mg]^{2+}$ | 438.65 | | | | | 203.2 ± 1.2 | | | | |
| Lacto-N-fucopentaose II | 853.77 | $[M + Ca]^{2+}$ | 446.63 | | | | | 201.7 ± 0.5 | | | | |
| Lacto-N-fucopentaose II | 853.77 | $[M + Sr]^{2+}$ | 470.61 | | | | | 201.5 ± 0.5 | | | | |
| Lacto-N-fucopentaose II | 853.77 | $[M + Ba]^{2+}$ | 495.61 | | | | | 205.5 ± 0.5 | | | | |
| Lacto-N-fucopentaose II | 853.77 | $[M + Li]^+$ | 860.32 | 198.7 ± 1.3 | | | | 194.1 ± 0.5 | | | | |
| Lacto-N-fucopentaose II | 853.77 | $[M + Na]^+$ | 876.30 | 201.3 ± 1.2 | | | | 195.6 ± 0.6 | 271.1 | | | |
| Lacto-N-fucopentaose II | 853.77 | $[M + K]^+$ | 892.27 | 202.6 ± 1.6 | | | | 198.5 ± 0.4 | 267.2 | | | |
| Lacto-N-fucopentaose II | 853.77 | $[M + Rb]^+$ | 938.22 | 197.5 ± 1.7 | | | | 200.0 ± 0.4 | 278.4 | | | |
| Lacto-N-fucopentaose II | 853.77 | $[M + Cs]^+$ | 986.21 | | | | | 200.9 ± 0.4 | | | | |
| Lacto-N-fucopentaose III | 853.77 | $[M + Be]^{2+}$ | 431.16 | | | | | 201.3 ± 0.7 | | | | |
| Lacto-N-fucopentaose III | 853.77 | $[M + Mg]^{2+}$ | 438.65 | | | | | 199.8 ± 0.8 | | | | |
| Lacto-N-fucopentaose III | 853.77 | $[M + Ca]^{2+}$ | 446.63 | | | | | 195.9 ± 0.9 | | | | |
| Lacto-N-fucopentaose III | 853.77 | $[M + Sr]^{2+}$ | 470.61 | | | | | 196.2 ± 1.0 | | | | |
| Lacto-N-fucopentaose III | 853.77 | $[M + Ba]^{2+}$ | 495.61 | | | | | 197.4 ± 1.1 | | | | |
| Lacto-N-fucopentaose III | 853.77 | $[M + Li]^+$ | 860.32 | | | | | 192.9 ± 0.2 | | | | |
| Lacto-N-fucopentaose III | 853.77 | $[M + Na]^+$ | 876.30 | | | | | 196.6 ± 0.4 | | | | |
| Lacto-N-fucopentaose III | 853.77 | $[M + Na]^+$ | 876.30 | 199.2 ± 1.0 | | | | | | | | |
| Lacto-N-fucopentaose III | 853.77 | $[M + K]^+$ | 892.27 | | | | | 194.5 ± 0.4 | | | | |
| Lacto-N-fucopentaose III | 853.77 | $[M + Rb]^+$ | 938.22 | | | | | 195.3 ± 0.5 | | | | |
| Lacto-N-fucopentaose III | 853.77 | $[M + Cs]^+$ | 986.21 | | | | | 195.7 ± 0.3 | | | | |
| Lacto-N-fucopentaose V | 853.77 | $[M + Be]^{2+}$ | 431.16 | | | | | 197.3 ± 0.3 | | | | |
| Lacto-N-fucopentaose V | 853.77 | $[M + Mg]^{2+}$ | 438.65 | | | | | 197.4 ± 0.5 | | | | |
| Lacto-N-fucopentaose V | 853.77 | $[M + Ca]^{2+}$ | 446.63 | | | | | 196.7 ± 0.2 | | | | |
| Lacto-N-fucopentaose V | 853.77 | $[M + Sr]^{2+}$ | 470.61 | | | | | 197.8 ± 1.1 | | | | |
| Lacto-N-fucopentaose V | 853.77 | $[M + Ba]^{2+}$ | 495.61 | | | | | 197.6 ± 0.9 | | | | |
| Lacto-N-fucopentaose V | 853.77 | $[M + H]^+$ | 854.31 | | 195 | | | | | | | |
| Lacto-N-fucopentaose V | 853.77 | $[M + Li]^+$ | 860.32 | | | 198.0 ± 0.3 | | | | | | |
| Lacto-N-fucopentaose V | 853.77 | $[M + Na]^+$ | 876.30 | 201.8 ± 0.7 | 194 | 198.4 ± 0.3 | | | | | | |

| molecule | MW in Da | type | *m/z* | $^{DT}CCS_{He}$ Fenn11 | $^{DT}CCS_{He}$ Williams10 | $^{TW}CCS_{He}$ Huang13 | $^{TW}CCS_{He}$ Gelb14 ‡ | $^{TW}CCS_{He}$ Huang15 | $^{DT}CCS_{N2}$ May14 | $^{TIMS\|DT}CCS_{N2}$ Pu16 § | $^{TW}CCS_{N2}$ Hofmann17 | $^{TW}CCS_{N2}$ Struwe16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Lacto-N-fucopentaose V | 853.77 | $[M + K]^+$ | 892.27 | | | 199.4 ± 0.3 | | | | | | |
| Lacto-N-fucopentaose V | 853.77 | $[M + Rb]^+$ | 938.22 | | | 199.9 ± 0.4 | | | | | | |
| Lacto-N-fucopentaose V | 853.77 | $[M + Cs]^+$ | 986.21 | | | 201.7 ± 1.0 | | | | | | |
| Lacto-N-difucohexaose I | 999.91 | $[M + Be]^{2+}$ | 504.19 | | | | | 226.5 ± 0.5 | | | | |
| Lacto-N-difucohexaose I | 999.91 | $[M + Mg]^{2+}$ | 511.67 | | | | | 226.0 ± 0.5 | | | | |
| Lacto-N-difucohexaose I | 999.91 | $[M + Ca]^{2+}$ | 519.66 | | | | | 22.1 ± 0.6 | | | | |
| Lacto-N-difucohexaose I | 999.91 | $[M + Sr]^{2+}$ | 543.63 | | | | | 223.1 ± 0.5 | | | | |
| Lacto-N-difucohexaose I | 999.91 | $[M + Ba]^{2+}$ | 568.63 | | | | | 220.2 ± 1.1 | | | | |
| Lacto-N-difucohexaose I | 999.91 | $[M + Li]^+$ | 1006.38 | | | 221.5 ± 0.8 | | | 301.4 | | | |
| Lacto-N-difucohexaose I | 999.91 | $[M + K]^+$ | 1038.33 | | | 223.7 ± 0.6 | | | 303.5 | | | |
| Lacto-N-difucohexaose I | 999.91 | $[M + Rb]^+$ | 1084.28 | | | 223.7 ± 0.7 | | | 303.2 | | | |
| Lacto-N-difucohexaose I | 999.91 | $[M + Cs]^+$ | 1132.27 | | | 223.7 ± 0.6 | | | 301.2 | | | |
| Lacto-N-difucohexaose I (peak 1) | 999.91 | $[M + Na]^+$ | 1022.35 | 225.6 ± 1.1 | **217** | 223.5 ± 0.7 | | | 290.6 | | | |
| Lacto-N-difucohexaose I (peak 2) | 999.91 | $[M + Na]^+$ | 1022.35 | | | | | | 304.2 | | | |
| Lacto-N-difucohexaose II | 999.91 | $[M + Be]^{2+}$ | 504.19 | | | | | 226.5 ± 0.4 | | | | |
| Lacto-N-difucohexaose II | 999.91 | $[M + Mg]^{2+}$ | 511.67 | | | | | 227.2 ± 0.8 | | | | |
| Lacto-N-difucohexaose II | 999.91 | $[M + Ca]^{2+}$ | 519.66 | | | | | 225.5 ± 0.5 | | | | |
| Lacto-N-difucohexaose II | 999.91 | $[M + Sr]^{2+}$ | 543.63 | | | | | 225.7 ± 1.4 | | | | |
| Lacto-N-difucohexaose II | 999.91 | $[M + Ba]^{2+}$ | 568.63 | | | | | 225.5 ± 0.9 | | | | |
| Lacto-N-difucohexaose II | 999.91 | $[M + Li]^+$ | 1006.38 | | | 217.7 ± 0.3 | 220.6±0.4 | | | | | |
| Lacto-N-difucohexaose II | 999.91 | $[M + K]^+$ | 1038.33 | | | 219.9 ± 0.3 | 222.9±0.4 | | 305.8 | | | |
| Lacto-N-difucohexaose II | 999.91 | $[M + Rb]^+$ | 1084.28 | | | 219.8 ± 0.2 | 222.8±0.4 | | | | | |
| Lacto-N-difucohexaose II | 999.91 | $[M + Cs]^+$ | 1132.27 | | | 220.4 ± 0.2 | 223.5±0.3 | | | | | |
| Lacto-N-difucohexaose II (peak 1) | 999.91 | $[M + Na]^+$ | 1022.35 | 220.6 ± 1.0 | 214 | 218.7 ± 0.3 | 221.6±0.5 | | 291.2 | | | |
| Lacto-N-difucohexaose II (peak 2) | 999.91 | $[M + Na]^+$ | 1022.35 | | | | | | 306.3 | | | |
| Lacto-N-hexaose (LNH) | 1072.96 | $[M - H]^-$ | 1071.37 | | | | | | | | | 255.2 ± 1.6 |
| Lacto-N-hexaose (LNH) | 1072.96 | $[M + H]^+$ | 1073.39 | | | | | | | | | 225.5 ± 0.4 |
| Lacto-N-hexaose (LNH) | 1072.96 | $[M + Na]^+$ | 1095.37 | | | | | | | | | 232.6 ± 0.2 |
| Lacto-N-hexaose (LNH) | 1072.96 | $[M + Cl]^-$ | 1107.35 | | | | | | | | | 244.5 ± 2.4 |
| Lacto-N-neohexaose (LNnH) | 1072.96 | $[M - H]^-$ | 1071.37 | | | | | | | | | 227.6 ± 1.6 |

| molecule | MW in Da | type | *m/z* | $^{DT}CCS_{He}$ Fenn11 | $^{DT}CCS_{He}$ Williams10 | $^{TW}CCS_{He}$ Huang13 | $^{TW}CCS_{He}$ Gelb14 ‡ | $^{TW}CCS_{He}$ Huang15 | $^{DT}CCS_{N2}$ May14 | $^{TIMS|DT}CCS_{N2}$ Pu16 § | $^{TW}CCS_{N2}$ Hofmann17 | $^{TW}CCS_{N2}$ Struwe16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Lacto-N-neohexaose (LNnH) | 1072.96 | $[M + H]^+$ | 1073.39 | | | | | | | | | 228.6 ± 1.0 |
| Lacto-N-neohexaose (LNnH) | 1072.96 | $[M + Na]^+$ | 1095.37 | | | | | | | | | 224.9 ± 0.2 |
| Lacto-N-neohexaose (LNnH) | 1072.96 | $[M + Cl]^-$ | 1107.35 | | | | | | | | | 244.3 ± 1.2 |

‡ Values before and after the vertical bar | are derived from a calibration with carbohydrates and peptides, respectively.

§ Values separated by the vertical bar | are values from the same reference but different instruments.

## Oligosaccharides

| molecule | MW in Da | type | *m/z* | $^{DT}CCS_{He}$ Gaye15 | $^{DT}CCS_{He}$ Lee97 | $^{DT}CCS_{He}$ Fenn11 | $^{TW}CCS_{He}$ Gelb14 ‡ | $^{TW}CCS_{He}$ Huang13 | $^{TW}CCS_{He}$ Huang15 | $^{TW}CCS_{He}$ Yang16 | $^{DT}CCS_{N2\ 200°C}$ Clowers05 | $^{DT}CCS_{N2}$ May14 | $^{TW}CCS_{N2}$ Paglia14 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Cellobiose | 342.30 | $[M + Li]^+$ | 349.13 | 108.6 | | | | 110.3 ± 0.4 | | | | | |
| Cellobiose | 342.30 | $[M + Na]^+$ | 365.11 | | | | | 112.4 ± 0.4 | | | | | |
| Cellobiose | 342.30 | $[M + K]^+$ | 381.08 | | | | | 114.4 ± 0.4 | | | | | |
| Cellobiose | 342.30 | $[M + Rb]^+$ | 427.03 | | | | | 115.1 ± 0.4 | | | | | |
| Cellobiose | 342.30 | $[M + Cs]^+$ | 475.02 | | | | | 116.9 ± 0.4 | | | | | |
| Gentiobiose | 342.30 | $[M + Li]^+$ | 349.13 | 108.1 | | | | | | | | | |
| Gentiobiose | 342.30 | $[M + Na]^+$ | 365.11 | | | | | | | 114.7 ± 0.9 | | | |
| Isomaltose | 342.30 | $[M + Li]^+$ | 349.13 | 108.6 | | | | | | | | | |
| Isomaltose | 342.30 | $[M + Na]^+$ | 365.11 | | | | | | | 113.3 ± 0.4 | | | |
| Kojibiose | 342.30 | $[M + Na]^+$ | 365.11 | | | | | | | 114.3 ± 0.4 | | | |
| Lactose | 342.30 | $[M - H]^-$ | 341.11 | | | | | | | | | | 167 |
| Lactose | 342.30 | $[M + Li]^+$ | 349.13 | 103 | | | | | | | | 186.3 | |
| Lactose | 342.30 | $[M + Na]^+$ | 365.11 | | | 121.1 ± 6.4 | | | | | | 178.1 | 173 |
| Laminaribiose | 342.30 | $[M + Na]^+$ | 365.11 | | | | | | | 113.9 ± 0.5 | | | |
| Leucrose | 342.30 | $[M + Li]^+$ | 349.13 | 104.6 | | | | | | | | | |
| Maltose | 342.30 | $[M + Li]^+$ | 349.13 | 110.6 | | | | 110.2 ± 0.4 | | | | | |
| Maltose | 342.30 | $[M + Na]^+$ | 365.11 | | | 124.6 ± 2.0 | | 112.6 ± 0.4 | | | | | |
| Maltose | 342.30 | $[M + K]^+$ | 381.08 | | | | | 115.5 ± 0.4 | | | | | |
| Maltose | 342.30 | $[M + Rb]^+$ | 427.03 | | | | | 116.3 ± 0.4 | | | | | |
| Maltose | 342.30 | $[M + Cs]^+$ | 475.02 | | | | | 118.2 ± 0.2 | | | | | |
| Melibiose | 342.30 | $[M + Li]^+$ | 349.13 | 107.4 | | | | 110.1 ± 0.2 | | | | | |
| Melibiose | 342.30 | $[M + Na]^+$ | 365.11 | | | | | 112.2 ± 0.2 | | | | | |
| Melibiose | 342.30 | $[M + K]^+$ | 381.08 | | | | | 114.5 ± 0.2 | | | | | |
| Melibiose | 342.30 | $[M + Rb]^+$ | 427.03 | | | | | 115.1 ± 0.2 | | | | | |
| Melibiose | 342.30 | $[M + Cs]^+$ | 475.02 | | | | | 116.3 ± 0.2 | | | | | |
| Nigerose | 342.30 | $[M + Na]^+$ | 365.11 | | | | | | | 112.9 ± 0.5 | | | |
| Palatinose (Isomaltulose) | 342.30 | $[M + Li]^+$ | 349.13 | 106.4 | | | | | | | | | |
| Sophorose | 342.30 | $[M + Na]^+$ | 365.11 | | | | | | | 114.6 ± 0.6 | | | |
| Sucrose | 342.30 | $[M - H]^-$ | 341.11 | | | | | | | | | | 165 |

| molecule | MW in Da | type | *m/z* | $^{DT}CCS_{He}$ Gaye15 | $^{DT}CCS_{He}$ Lee97 | $^{DT}CCS_{He}$ Fenn11 | $^{TW}CCS_{He}$ Gelb14 ‡ | $^{TW}CCS_{He}$ Huang13 | $^{TW}CCS_{He}$ Huang15 | $^{TW}CCS_{He}$ Yang16 | $^{DT}CCS_{N2\ 200°C}$ Clowers05 | $^{DT}CCS_{N2}$ May14 | $^{TW}CCS_{N2}$ Paglia14 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Sucrose | 342.3 | $[M + Li]^+$ | 349.13 | 104.5 | | | | 107.1 ± 0.3 | | | | | |
| Sucrose | 342.3 | $[M + Na]^+$ | 365.11 | | | | | 108.9 ± 0.3 | | | | | 170 |
| Sucrose | 342.3 | $[M + K]^+$ | 381.08 | | | | | 110.3 ± 0.3 | | | | | |
| Sucrose | 342.3 | $[M + Rb]^+$ | 427.03 | | | | | 111.3 ± 0.2 | | | | | |
| Sucrose | 342.3 | $[M + Cs]^+$ | 475.02 | | | | | 112.9 ± 0.3 | | | | | |
| Trehalose | 342.30 | $[M - H]^-$ | 341.11 | | | | | | | | | | 166 |
| Trehalose | 342.3 | $[M + Li]^+$ | 349.13 | 105.1 | | | | 107.9 ± 0.3 | | | | | |
| Trehalose | 342.3 | $[M + Na]^+$ | 365.11 | | | | | 110.6 ± 0.4 | | | | | 173 |
| Trehalose | 342.3 | $[M + K]^+$ | 381.08 | | | | | 114.0 ± 0.4 | | | | | |
| Trehalose | 342.3 | $[M + Rb]^+$ | 427.03 | | | | | 115.0 ± 0.4 | | | | | |
| Trehalose | 342.3 | $[M + Cs]^+$ | 475.02 | | | | | 116.5 ± 0.4 | | | | | |
| Cellobiitol | 344.31 | $[M + Na]^+$ | 367.12 | | | | | | | | 146.09 | | |
| Melibiitol | 344.31 | $[M + Na]^+$ | 367.12 | | | | | | | | 146.52 | | |
| N-acetyl-lactoseamine | 383.35 | $[M + Na]^+$ | 406.13 | | | 129.2 ± 2.1 | | | | | | | |
| Cellobiose (PHN label) | 432.43 | $[M + Na]^+$ | 455.16 | | | | | | | 139.4 ± 0.3 | | | |
| Gentiobiose (PHN label) | 432.43 | $[M + Na]^+$ | 455.16 | | | | | | | 134.3 ± 0.2 | | | |
| Isomaltose (PHN label) | 432.43 | $[M + Na]^+$ | 455.16 | | | | | | | 134.7 ± 0.3 | | | |
| Kojibiose (PHN label) | 432.43 | $[M + Na]^+$ | 455.16 | | | | | | | 134.0 ± 0.2 | | | |
| Lactose (PHN label) | 432.43 | $[M + Na]^+$ | 455.16 | | | | | | | 137.3 ± 0.3 | | | |
| Laminaribiose (PHN label) | 432.43 | $[M + Na]^+$ | 455.16 | | | | | | | 128.6 ± 0.5 | | | |
| Maltose (PHN label) | 432.43 | $[M + Na]^+$ | 455.16 | | | | | | | 138.1 ± 0.2 | | | |
| Nigerose (PHN label) | 432.43 | $[M + Na]^+$ | 455.16 | | | | | | | 126.5 ± 0.6 | | | |
| Sophorose (PHN label) | 432.43 | $[M + Na]^+$ | 455.16 | | | | | | | 133.4 ± 0.7 | | | |
| Isomaltotriose | 504.44 | $[M + Mg]^{2+}$ | 264.08 | | | | | | 138.3 ± 0.3 | | | | |
| Isomaltotriose | 504.44 | $[M + Ca]^{2+}$ | 272.07 | | | | | | 136.0 ± 1.0 | | | | |
| Isomaltotriose | 504.44 | $[M + Sr]^{2+}$ | 296.04 | | | | | | 142.2 ± 0.3 | | | | |
| Isomaltotriose | 504.44 | $[M + Ba]^{2+}$ | 321.04 | | | | | | 145.5 ± 0.4 | | | | |
| Isomaltotriose | 504.44 | $[M + Li]^+$ | 511.19 | | | | | 140.8 ± 0.1 | | | | | |
| Isomaltotriose | 504.44 | $[M + Na]^+$ | 527.16 | | | | | 142.3 ± 0.1 | | | 184.14 | | |
| Isomaltotriose | 504.44 | $[M + K]^+$ | 543.13 | | | | | 143.4 ± 0.1 | | | | | |
| Isomaltotriose | 504.44 | $[M + Rb]^+$ | 589.08 | | | | | 143.4 ± 0.1 | | | | | |

| molecule | MW in Da | type | *m/z* | $^{DT}CCS_{He}$ Gaye15 | $^{DT}CCS_{He}$ Lee97 | $^{DT}CCS_{He}$ Fenn11 | $^{TW}CCS_{He}$ Gelb14 ‡ | $^{TW}CCS_{He}$ Huang13 | $^{TW}CCS_{He}$ Huang15 | $^{TW}CCS_{He}$ Yang16 | $^{DT}CCS_{N2\ 200°C}$ Clowers05 | $^{DT}CCS_{N2}$ May14 | $^{TW}CCS_{N2}$ Paglia14 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Isomaltotriose | 504.44 | $[M + Cs]^+$ | 637.07 | | | | | 144.2 ± 0.1 | | | | | |
| Maltotriose | 504.44 | $[M + Mg]^{2+}$ | 264.08 | | | | | | 136.5 ± 0.7 | | | | |
| Maltotriose | 504.44 | $[M + Ca]^{2+}$ | 272.07 | | | | | | 136.0 ± 0.6 | | | | |
| Maltotriose | 504.44 | $[M + Sr]^{2+}$ | 296.04 | | | | | | 139.4 ± 0.7 | | | | |
| Maltotriose | 504.44 | $[M + Ba]^{2+}$ | 321.04 | | | | | | 142.8 ± 1.1 | | | | |
| Maltotriose | 504.44 | $[M + H]^+$ | 505.18 | | | | | | | | | 216.3 | |
| Maltotriose | 504.44 | $[M + Li]^+$ | 511.19 | 138 | | | | 138.6 ± 0.2 | | | | | |
| Maltotriose | 504.44 | $[M + Na]^+$ | 527.16 | | | | 140.6 ± 0.9 \| 145.3 ± 1.5 ‡ | 142.9 ± 0.2 | | | | 212.8 | |
| Maltotriose | 504.44 | $[M + K]^+$ | 543.13 | | | | | 144.4 ± 0.2 | | | | 216.8 | |
| Maltotriose | 504.44 | $[M + Rb]^+$ | 589.08 | | | | | 147.0 ± 0.3 | | | | | |
| Maltotriose | 504.44 | $[M + Cs]^+$ | 637.07 | | | | | 150.8 ± 0.2 | | | | | |
| Melezitose | 504.44 | $[M + Mg]^{2+}$ | 264.08 | | | | | | 137.9 ± 0.5 | | | | |
| Melezitose | 504.44 | $[M + Ca]^{2+}$ | 272.07 | | | | | | 137.7 ± 0.6 | | | | |
| Melezitose | 504.44 | $[M + Sr]^{2+}$ | 296.04 | | | | | | 142.6 ± 0.4 | | | | |
| Melezitose | 504.44 | $[M + Ba]^{2+}$ | 321.04 | | | | | | 146.5 ± 0.3 | | | | |
| Melezitose | 504.44 | $[M + H]^+$ | 505.18 | | | | | | | | | 202.6 | |
| Melezitose | 504.44 | $[M + Li]^+$ | 511.19 | 132.6 | | | | 134.1 ± 0.2 | | | | 202.9 | |
| Melezitose | 504.44 | $[M + Na]^+$ | 527.16 | | | | | 133.5 ± 0.2 | | | 173.57 | 202.7 | |
| Melezitose | 504.44 | $[M + K]^+$ | 543.13 | | | | | 134.2 ± 0.2 | | | | 221.9 | |
| Melezitose | 504.44 | $[M + Cs]^+$ | 637.07 | | | | | 136.9 ± 0.2 | | | | 205.8 | |
| Melezitose (peak 1) | 504.44 | $[M + Rb]^+$ | 294.54 | | | | | 134.7 ± 0.3 | | | | 204.1 | |
| Melezitose (peak2) | 504.44 | $[M + Rb]^+$ | 294.54 | | | | | | | | | 219.2 | |
| Raffinose | 504.44 | $[M + Mg]^{2+}$ | 264.08 | | | | | | 136.2 ± 0.3 | | | | |
| Raffinose | 504.44 | $[M + Ca]^{2+}$ | 272.07 | | | | | | 133.6 ± 0.4 | | | | |
| Raffinose | 504.44 | $[M + Sr]^{2+}$ | 296.04 | | | | | | 138.4 ± 0.6 | | | | |
| Raffinose | 504.44 | $[M + Ba]^{2+}$ | 321.04 | | | | | | 141.3 ± 1.1 | | | | |
| Raffinose | 504.44 | $[M - H]^-$ | 503.16 | | | | | | | | | | 201 |
| Raffinose | 504.44 | $[M + Li]^+$ | 511.19 | 137.4 | | | | 137.3 ± 0.4 | | | | | |
| Raffinose | 504.44 | $[M + Na]^+$ | 527.16 | | | | | 138.8 ± 0.4 | | | 180.91 | 210.7 | 210 |
| Raffinose | 504.44 | $[M + K]^+$ | 543.13 | | | | | 140.0 ± 0.4 | | | | 212.7 | |

| molecule | MW in Da | type | *m/z* | $^{DT}CCS_{He}$ Gaye15 | $^{DT}CCS_{He}$ Lee97 | $^{DT}CCS_{He}$ Fenn11 | $^{TW}CCS_{He}$ Gelb14 ‡ | $^{TW}CCS_{He}$ Huang13 | $^{TW}CCS_{He}$ Huang15 | $^{TW}CCS_{He}$ Yang16 | $^{DT}CCS_{N2\ 200°C}$ Clowers05 | $^{DT}CCS_{N2}$ May14 | $^{TW}CCS_{N2}$ Paglia14 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Raffinose | 504.44 | $[M + Cs]^+$ | 637.07 | | | | | 141.8 ± 0.4 | | | | | |
| Raffinose (peak1) | 504.44 | $[M + Rb]^+$ | 589.08 | | | | | 140.5 ± 0.4* | | | | 218.7 | |
| Raffinose (peak2) | 504.44 | $[M + Rb]^+$ | 589.08 | | | | | | | | | 229.7 | |
| Cellotetraose | 666.58 | $[M + Na]^+$ | 689.21 | | 160 | | | | | | | | |
| Isomaltotetraose | 666.58 | $[M + Na]^+$ | 689.21 | | 163 | | | | | | | | |
| Maltotetraose | 666.58 | $[M + H]^+$ | 665.21 | | | | | | | | | 238.3 | |
| Maltotetraose | 666.58 | $[M + Na]^+$ | 689.21 | | 159 | | | | | | | 235.3 | |
| Cellobiose (PMP label) | 672.69 | $[M + H]^+$ | 673.27 | | | | | | | 177.1 ± 0.2 | | | |
| Gentiobiose (PMP label) | 672.69 | $[M + H]^+$ | 673.27 | | | | | | | 176.2 ± 0.3 | | | |
| Isomaltose (PMP label) | 672.69 | $[M + H]^+$ | 673.27 | | | | | | | 174.7 ± 0.2 | | | |
| Kojibiose (PMP label) | 672.69 | $[M + H]^+$ | 673.27 | | | | | | | 180.0 ± 0.5 | | | |
| Lactose (PMP label) | 672.69 | $[M + H]^+$ | 673.27 | | | | | | | 177.9 ± 0.6 | | | |
| Laminaribiose (PMP label) | 672.69 | $[M + H]^+$ | 673.27 | | | | | | | 184.4 ± 0.3 | | | |
| Maltose (PMP label) | 672.69 | $[M + H]^+$ | 673.27 | | | | | | | 182.5 ± 0.3 | | | |
| Nigerose (PMP label) | 672.69 | $[M + H]^+$ | 673.27 | | | | | | | 180.1 ± 0.4 | | | |
| Sophorose (PMP label) | 672.69 | $[M + H]^+$ | 673.27 | | | | | | | 179.2 ± 0.2 | | | |
| Maltohexaose | 990.86 | $[M + Na]^+$ | 1013.32 | | 206 | | | | | | | 286.4 | |
| Maltohexaose | 990.86 | $[M + K]^+$ | 1029.29 | | | | | | | | | 293.3 | |
| Maltoheptaose | 1153.00 | $[M + H]^+$ | 1153.40 | | | | | | | | | 303.3 | |
| Maltoheptaose | 1153.00 | $[M + Na]^+$ | 1175.37 | | | | | | | | | 303.1 | |
| Maltoheptaose | 1153.00 | $[M + K]^+$ | 1191.34 | | | | | | | | | 303.4 | |

‡ Values before and after the vertical bar | are derived from a calibration with carbohydrates and peptides, respectively.

*Peak 2 is not reported here.

| molecule | MW in Da | type | *m/z* | $^{DT}CCS_{N2}$ Clowers05 | $^{TW}CCS_{N2}$ Hinneburg16 | $^{TW}CCS_{N2}$ Guttman16 |
|---|---|---|---|---|---|---|
| α-D-GalNAc-(1–3)-D-GalNAc-ol | 426.42 | $[M + Na]^+$ | 449.17 | 160.98 | | |
| α-D-GalNAc-(1–6)-D-GalNAc-ol | 426.42 | $[M + Na]^+$ | 449.17 | 164.28 | | |
| β-D-GlcNAc-(1–3)-D-GalNAc-ol | 426.42 | $[M + Na]^+$ | 449.17 | 163.49 | | |
| β-D-GlcNAc-(1–4)-D-GlcNAc-ol | 426.42 | $[M + Na]^+$ | 449.17 | 165.44 | | |
| β-D-GlcNAc-(1–6)-D-GalNAc-ol | 426.42 | $[M + Na]^+$ | 449.17 | 169.70 | | |
| αNeuAc-2,3-β-Gal-1,4-GlcNAc | fragment | $[M - H_2O + H]^+$ | 657.23 | | 246 | 247.2 ± 0.6 |
| αNeuAc-2,6-β-Gal-1,4-GlcNAc | fragment | $[M - H_2O + H]^+$ | 657.23 | | 236 | 236.9 ± 0.4 |
| βGal-1,3-(αNeuAc-2,6-)GlcNAc | fragment | $[M - H_2O + H]^+$ | 657.23 | | | 231 ± 0.6 |

## Cyclodextrin

| molecule | MW in Da | type | *m/z* | $^{DT}CCS_{He}$ Lee97 | $^{DT}CCS_{He}$ Fenn11 | $^{DT}CCS_{N2}$ May14 |
|---|---|---|---|---|---|---|
| Alpha-Cyclodextrin | 972.84 | $[M + H]^+$ | 973.32 | | | 285.2 |
| Alpha-Cyclodextrin | 972.84 | $[M + K]^+$ | 1011.28 | | | 287.7 |
| Alpha-Cyclodextrin | 972.84 | $[M + Na]^+$ | 995.31 | 204 | 200.7 ± 0.5 | 285.5 |
| Beta-Cyclodextrin | 1134.98 | $[M + K]^+$ | 1173.33 | | | 320.3 |
| Beta-Cyclodextrin | 1134.98 | $[M + Na]^+$ | 1157.36 | | 231.4 ± 0.6 | 319.7 |
| Beta-Cyclodextrin (peak 1) | 1134.98 | $[M + H]^+$ | 1135.38 | | | 301.3 |
| Beta-Cyclodextrin (peak 2) | 1134.98 | $[M + H]^+$ | 1135.38 | | | 319.6 |
| Gamma-Cyclodextrin | 1297.12 | $[M + Cs]^+$ | 1429.33 | | | 338.2 |
| Gamma-Cyclodextrin | 1297.12 | $[M + H]^+$ | 1297.43 | | | 322.6 |
| Gamma-Cyclodextrin | 1297.12 | $[M + K]^+$ | 1335.39 | | | 324.8 |
| Gamma-Cyclodextrin | 1297.12 | $[M + Li]^+$ | 1303.44 | | | 317.7 |
| Gamma-Cyclodextrin | 1297.12 | $[M + Na]^+$ | 1319.41 | | | 322.1 |
| Gamma-Cyclodextrin | 1297.12 | $[M + Rb]^+$ | 1381.33 | | | 327.3 |