The masses of some monosaccharide residues and their derivatized residues

Table I. Monosaccharide residue masses Monosaccharides	Un-derivatized Monoisotopic (Average)	Per-methylated Monoisotopic (Average)	Deutero-methylated Monoisotopic (Average)	Per-acetylated Monoisotopic (Average)	Deutero-acetylated Monoisotopic (Average)
Deoxypentose (DeoxyPent) Deoxyribose (dRib) $C_5H_{10}O_4$	116.04734 (116.1167)	130.06299 (130.1436)	133.08182 (133.1621)	158.05791 (158.1540)	161.07674 (161.1725)
Pentose (Pent) $C_5H_{10}O_5$ Arabinose (Ara), Ribose (Rib), Xylose (Xyl)	132.04226 (132.1161)	160.07356 (160.1699)	166.11122 (166.2069)	216.06339 (216.1907)	222.10105 (222.2277)
Deoxyhexose (DeoxyHex) $C_6H_{12}O_5$ Fucose (Fuc), Rhamnose (Rha)	146.05791 (146.1430)	174.08921 (174.1968)	180.12687 (180.2337)	230.07904 (230.2176)	236.11670 (236.2545)
Hexosamine (HexN) $C_6H_{13}NO_5$ Galactosamine (GalN), Glucosamine (GlcN)	161.06881 (161.1577)	217.13141(a) (217.2652)	229.20673(a) (229.3391)	287.10050 (287.2695)	296.15699 (296.3250)
Hexose (Hex) $C_6H_{12}O_6$ Fructose (Fru),Galactose (Gal), Glucose (Glc), Mannose (Man)	162.05282 (162.1424)	204.09977 (204.2230)	213.15626 (213.2785)	288.08452 (288.2542)	297.14101 (297.3097)
Hexuronic acid (HexA) $C_6H_{10}O_7$ Glucuronic acid (GlcA)	176.03209 (176.1259)	218.07904 (218.2066)	227.13553 (227.2620)	260.05322 (260.2005)	266.09088 (266.2375)
Heptose (Hep) $C_7H_{14}O_7$	192.06339 (192.1687)	248.12599 (248.2762)	260.20131 (260.3501)	360.10565 (360.3178)	372.18097 (372.3917)
N-acetylhexosamine (HexNAc) N-acetylgalactosamine (GalNAc) N-acetylglucosamine (GlcNAc) $C_8H_{15}NO_6$	203.07937 (203.1950)	245.12632 (245.2756)	254.18281 (254.3311)	287.10050 (287.2695)	293.13816 (293.3065)
2-keto-3-deoxyoctonate (KDO) $C_8H_{14}O_8$	220.05830 (220.1791)	276.12090 (276.2866)	288.19622 (288.3605)	346.09000 (346.2909)	355.14649 (355.3464)
Muramic acid (Mur) $C_{11}H_{19}NO_8$	275.10050 (275.2585)	317.14745 (317.3392)	326.20394 (326.3946)	317.11107 (317.2958)	320.12990 (320.3143)
Sialic acids (SA) N-acetylneuraminic acid (NeuAc) $C_{11}H_{19}NO_9$	291.09542 (291.2579)	361.17367 (361.3923)	376.26782 (376.4847)	417.12711 (417.3698)	426.18360 (426.4252)
N-glycolylneuraminic acid (NeuGc) $C_{11}H_{19}NO_{10}$	307.09033 (307.2573)	391.18423 (391.4186)	409.29721 (409.5295)	475.13259 (475.4064)	487.20791 (487.4804)

(a) These masses are for dimethylation of the amino group. Some trimethylation [trideuteromethylation] can also occur to give ions higher in mass by 14.01565 (monoisotopic); 14.0269 (average) [17.03448 (monoisotopic); 17.0454 (average)]

Table II. Terminal group masses	Un-derivatized Monoisotopic (Average)	Per-methylated Monoisotopic (Average)	Deutero-methylated Monoisotopic (Average)	Per-acetylated Monoisotopic (Average)	Deutero-acetylated Monoisotopic (Average)
Free reducing end	18.01056 (18.0153)	46.04186 (46.0690)	52.07953 (52.1060)	102.03169 (102.0898)	108.06935 (108.1268)
Reduced reducing end	20.02621 (20.0312)	62.07316 (62.1118)	71.12966 (71.1673)	146.05791 (146.1430)	155.11440 (155.1985)

Table III. Changes due to modifications	Un-derivatized Monoisotopic (Average)	Per-methylated Monoisotopic (Average)	Deutero-methylated Monoisotopic (Average)	Per-acetylated Monoisotopic (Average)	Deutero-acetylated Monoisotopic (Average)
Acetate	42.01056 (42.0373)	0.00000 (0.0000)	0.00000 (0.0000)	0.00000 (0.0000)	-3.01883 (-3.0185)
Pyruvate	70.00548 (70.0477)	55.98983 (56.0208)	52.97100 (53.0023)	-14.01565 (-14.0269)	-20.05331 (-20.0639)
Phosphate	79.96633 (79.9799)	93.98198 (94.0068)	97.00081 (97.0253)	37.95577(b) (37.9426)	34.93694(b) (34.9241)
Sulfate	79.95682 (80.0642)	65.94117 (66.0373)	62.92234 (63.0188)	37.94625 (38.0269)	34.92742 (35.0084)
Inositol	162.05282 (162.1424)	218.11542 (218.2499)	230.19074 (230.3239)	330.09508 (330.2915)	342.17040 (342.3655)

(b) These masses are for underivatized phosphate. Some acetylation [deuteroacetylation] may occur to give ions higher in mass by 42.01056 (monoisotopic); 42.0373 (average) [45.02940 (monoisotopic); 45.0558 (average)]

Ref. A. Dell, in Methods in Enzymology, **193**, 647-660, J.A. McClosky (ed), Academic Press Inc., (1990).

The monoisotopic masses are based on the following atomic masses of the most abundant isotope of the elements:
C = 12.0000000, H = 1.0078250, D = 2.0141018, N = 14.0030740, O = 15.9949146, P = 30.9737634 and S = 31.9720718.

The average masses are based on the following atomic weights of the elements:
C = 12.011, H = 1.00794, D = 2.01410, N = 14.00674, O = 15.9994, P = 30.97376 and S = 32.066.

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Data for the calculation of the molecular masses of glycopeptides, glycoproteins and oligosaccharides for use in mass spectrometry

Glycopeptides and glycoproteins

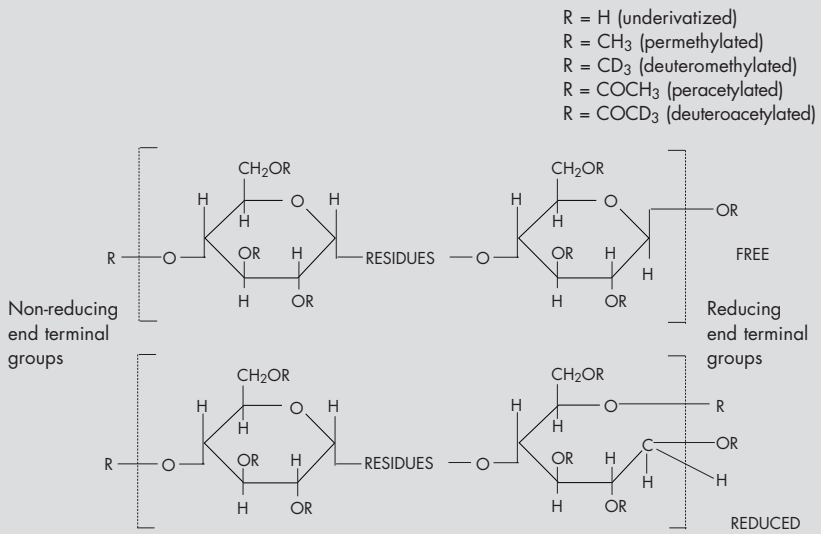
The molecular mass of a glycopeptide or glycoprotein may be calculated by adding the sum of the appropriate monosaccharide residue masses from Table I overleaf directly to the molecular mass of the peptide or protein.

Oligosaccharides

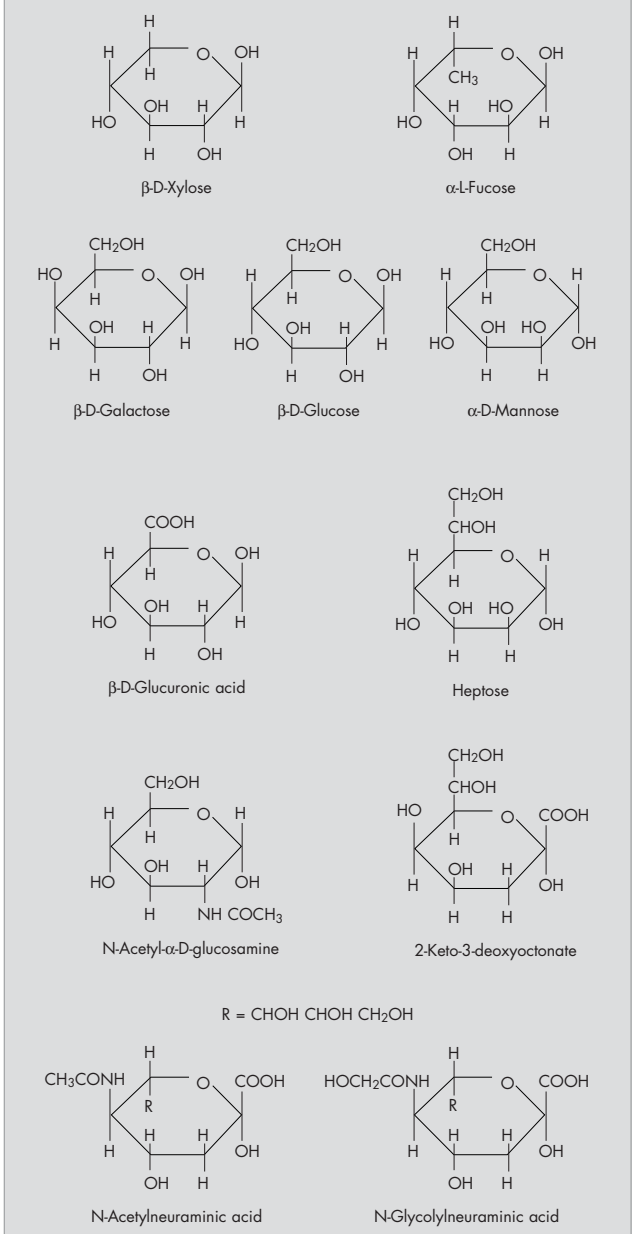
The molecular mass of an unmodified oligosaccharide may be calculated by summing the residue masses of the appropriate monosaccharides or derivatized monosaccharides from Table I overleaf, and adding a mass for the appropriate terminal groups given in Table II. In the case of a cyclic oligosaccharide, the terminal group masses are omitted. The residue mass of an underivatized monosaccharide is defined as the molecular mass minus H_2O.

The mass of an oligosaccharide modified by substituent groups is derived by adding an appropriate mass for each modifying group from Table III, to the mass of the unmodified oligosaccharide obtained above. Table III gives the mass change per modifying group.

Schematic representation of an oligosaccharide showing the two arrangements of the reducing end



Some monosaccharides



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