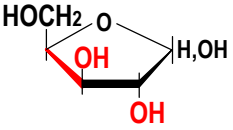
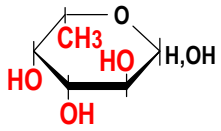
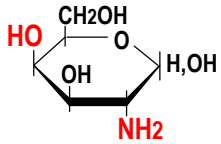
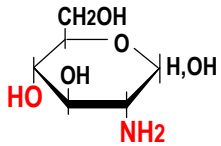
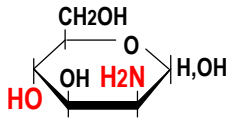
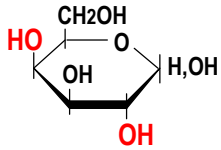
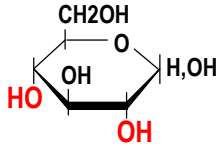
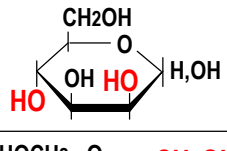
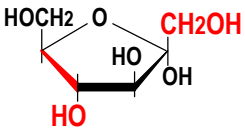
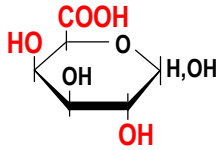
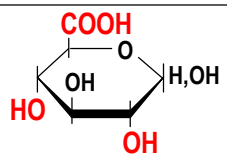
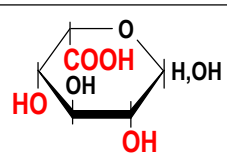
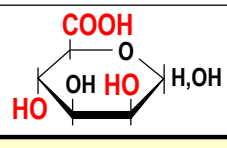
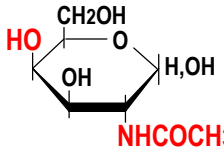
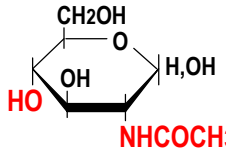
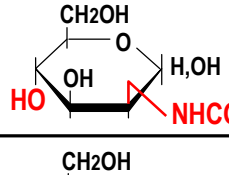
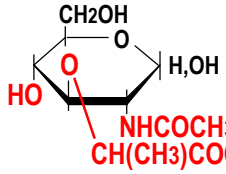
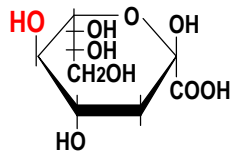
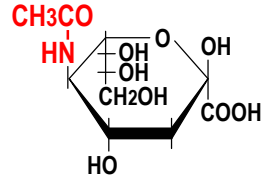
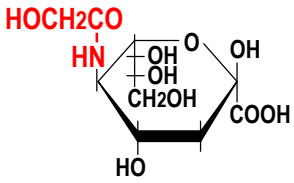
Monosaccharide List for Mass Spectrometry [MS, MS/MS and MS^n] (1/2)

Koichi Tanaka Laboratory of Advanced Science and Technology

	Name	CAS No.[1]	Symbol[2] [R,G,B]	Symbol[2] Grey	Empir. Formula / Residual[3] (Full[3])	Monoiso. Mass[4]	*Average Mass*[4]	Nom. Mass	Structure
	D-Xylose	Xyl 58-86-6	 [250,100,0]		$C_5H_8O_4$ ($C_5H_{10}O_5$)	132.0423 150.0528	*132.114* *150.129*	132 150	
	L-Fucose	Fuc 2438-80-4	 [250,0,0]	 Dark Grey	$C_6H_{10}O_4$ ($C_6H_{12}O_5$)	146.0579 164.0685	*146.141* *164.156*	146 164	
Hexosamines	D-Galactosamine	GalNH2 (7535-00-4)	 [255,255,0]		$C_6H_{11}NO_4$ ($C_6H_{13}NO_5$)	161.0688 179.0794	*161.156* *179.171*	161 179	
	D-Glucosamine	GlcNH2 3416-24-8	 [0,0,250]		$C_6H_{11}NO_4$ ($C_6H_{13}NO_5$)	161.0688 179.0794	*161.156* *179.171*	161 179	
	D-Mannosamine	ManNH2 (2636-92-2)	 [0,200,50]		$C_6H_{11}NO_4$ ($C_6H_{13}NO_5$)	161.0688 179.0794	*161.156* *179.171*	161 179	
Hexoses	D-Galactose	Gal 59-23-4	 [255,255,0]		$C_6H_{10}O_5$ ($C_6H_{12}O_6$)	162.0528 180.0634	*162.140* *180.155*	162 180	
	D-Glucose	Glc 50-99-7	 [0,0,250]		$C_6H_{10}O_5$ ($C_6H_{12}O_6$)	162.0528 180.0634	*162.140* *180.155*	162 180	
	D-Mannose	Man 3458-28-4	 [0,200,50]		$C_6H_{10}O_5$ ($C_6H_{12}O_6$)	162.0528 180.0634	*162.140* *180.155*	162 180	
	D-Fructose	Fru 57-48-7			$C_6H_{10}O_5$ ($C_6H_{12}O_6$)	162.0528 180.0634	*162.140* *180.155*	162 180	
Uronic acids (Acidic Sugars)	D-Galacturonic acid	GalA 685-73-4	 [255,255,0]		$C_6H_8O_6$ ($C_6H_{10}O_7$)	176.0321 194.0427	*176.123* *194.138*	176 194	
	D-Glucuronic Acid	GlcA 6556-12-3	 [0,0,250]		$C_6H_8O_6$ ($C_6H_{10}O_7$)	176.0321 194.0427	*176.123* *364.207*	176 194	
	L-Iduronic Acid	IdoA (3402-98-0)	 [150,100,50]		$C_6H_8O_6$ ($C_6H_{10}O_7$)	176.0321 194.0427	*176.123* *194.138*	176 194	
	D-Mannuronic acid	ManA (1986-14-7)	 [0,200,50]		$C_6H_8O_6$ ($C_6H_{10}O_7$)	176.0321 194.0427	*176.123* *194.138*	176 194	

Monosaccharide List for Mass Spectrometry [MS, MS/MS and MS^n] (2/2)

Koichi Tanaka Laboratory of Advanced Science and Technology

	Name	CAS No. [1]	Symbol [2] [R,G,B]	Grey	Empir. Formula / Residual [3] (Full [3])	Monoiso. Mass [4]	*Average Mass* [4]	Nom. Mass	Structure
N-Acetyl hexosamines	N-Acetyl galactosamine	GalNAc 1811-31-0	[255,255,0]		$C_8H_{13}NO_5$	**203**.0794	*203.193*	**203**	
					(C8H15NO6)	221.0899	*221.208*	221	
	N-Acetyl glucosamine	GlcNAc 7512-17-6	[0,0,250]		$C_8H_{13}NO_5$	**203**.0794	*203.193*	**203**	
					(C8H15NO6)	221.0899	*221.208*	221	
	N-Acetyl mannosamine	ManNAc (7772-94-3)	[0,200,50]		$C_8H_{13}NO_5$	**203**.0794	*203.193*	**203**	
					(C8H15NO6)	221.0899	*221.208*	221	
	N-Acetyl muramic acid	MurNAc (10597-89-4)			$C_{11}H_{17}NO_7$	**275**.1005	*275.255*	**275**	
					(C11H19NO8)	293.1111	*293.270*	293	
Sialic Acids (Acidic Sugars)	2-keto-3-deoxy-D-glycero-D-galacto-nononic acid	KDN (22594-61-2)	[0,200,50] w/ pattern	Light grey w/ pattern	$C_9H_{14}O_8$	**250**.0689	*250.202*	**250**	
					(C9H16O9)	268.0794	*268.216*	268	
	N-Acetyl neuraminic acid	Neu5Ac (NANA) 131-48-6	[125,0,125]	Dark Grey	$C_{11}H_{17}NO_8$	**291**.0954	*291.254*	**291**	
					(C11H19NO9)	309.1060	*309.269*	309	
	N-Glycolyl neuraminic acid	Neu5Gc (1113-83-3)	[200,250,250]		$C_{11}H_{17}NO_9$	**307**.0903	*307.253*	**307**	
					(C11H19NO10)	325.1009	*325.268*	325	

1) http://www.commonchemistry.org/index.aspx

Modification		Monoisotopic	*Average*	Nom.
Methylate	-H+CH_3	**14**.0157	*14.027*	**14**
Acetate	-H+CH_2CHO	**42**.0106	*42.037*	**42**
Phosphate	-H+PO_3H_2	**79**.9663	*79.979*	**80**
Sulfate	-H+SO_3H	**79**.9568	*80.063*	**80**

Free Reducing End [3]	+H+OH	**18**.0106	*18.015*	**18**
Reduced Reducing End [3]	+H+OH+2H	**20**.0262	*20.031*	**20**

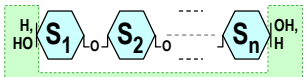
2) Proteomics, Vol.9, pp5398-5399(2009)

4)

Element	Monoisotopic Mass	*Average Mass*
H	1.00782504	*1.0079*
C	**12.0000000**	***12.011***
N	14.0030740	*14.007*
O	15.9949146	*15.999*
P	30.9737615	*30.974*
S	31.9720710	*32.066*

3)

Practical Mass Calculation for Mass Spectrometer



[Oligosaccharide Mass of $S_1S_2 \ldots S_n$] =

[Residual Mass of S_1] +
[Residual Mass of S_2] +
. . . . . +
[Residual Mass of S_n] +
[Mass of Reducing End]

or

[Full Mass of S_1] +
[Full Mass of S_2] +
. . . . . +
[Full Mass of S_n]
- (n-1) x H_2O

ms^{3}d FIRST Program

http://www.first-ms3d.jp/

SHIMADZU

Rev. 1.1 22/November/2010