Multi-step fractionation and mass spectrometry reveals zwitterionic and anionic modifications of the N- and O-glycans of a marine snail

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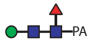
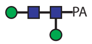
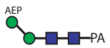
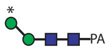
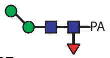
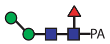
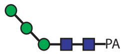
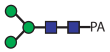
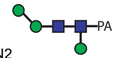
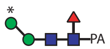
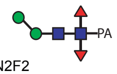
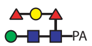
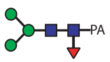
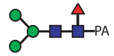
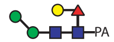
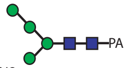
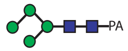
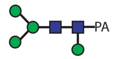
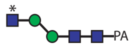
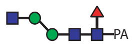
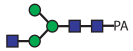
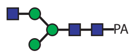
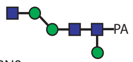
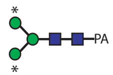
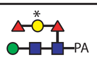
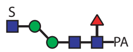
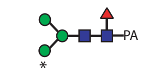
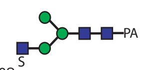
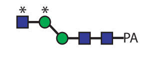
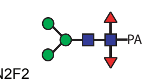
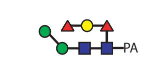
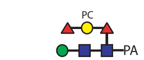
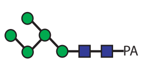
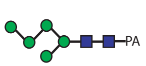
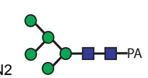
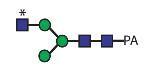
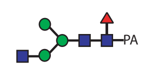
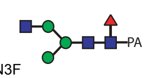
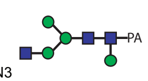
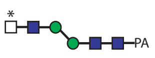
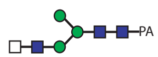
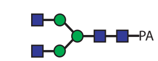
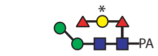
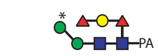
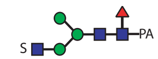
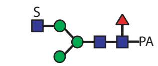
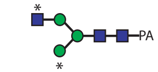
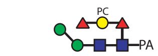
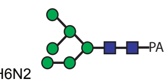
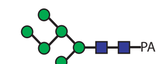
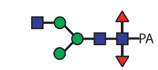
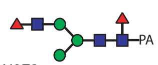
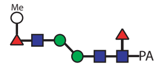
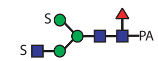
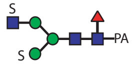
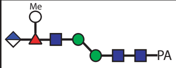
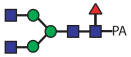
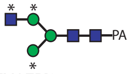
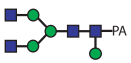
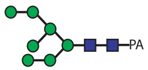
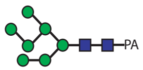
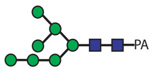
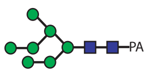
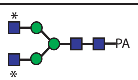
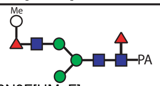
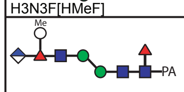
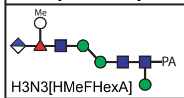
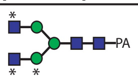
Supplementary Table

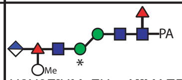
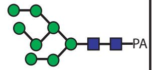
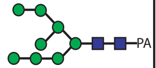
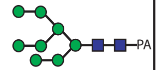
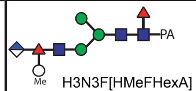
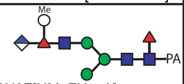
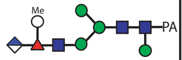
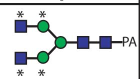
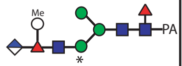
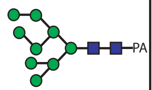
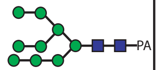
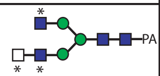
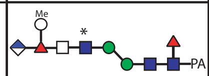
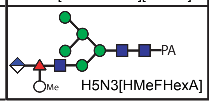
Summary of evidence for the proposed structures of N-glycans from *Volvarina rubella* (C. B. Adams, 1845). For each predicted structure, brief summaries of the evidence referring also to relevant figures are presented: key fragments, digest data and co-elution in terms of glucose units (g.u.) using the same Kinetex XB-C18 column as previously published for *Pristionchus pacificus* (the relative elution position also aids structural prediction). Structures are depicted according to the nomenclature of the Consortium for Functional Glycomics. Semi-quantitation (+++, ++ and +) is according to HPLC fluorescence data and MALDI-TOF MS relative intensity. *m/z* values are calculated with Glycoworkbench generally as $[M+H]^+$, except for glycans well observed in the negative ion mode; the mass accuracy for a representative spectrum for each glycan is given in brackets (Δ *m/z*) and, considering all the glycans listed, is on average +0.03 Da (+ 22 ppm) as compared to the calculated *m/z* values. The minimum criterion for inclusion in the table is an interpretable MALDI-TOF MS/MS spectrum; furthermore, the proposals for 60 of the approximately 100 structures are also supported by MS and MS/MS data obtained after chemical and enzymatic treatments. For about 20 representative glycans there are also LC-MS^n data. Further N-glycans with alternative antennal structures are predicted to be present, but are not included in the Table due to ambiguity in the MS/MS.

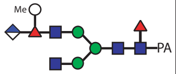
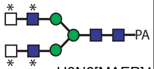
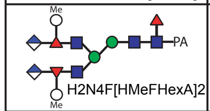
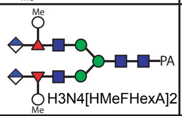
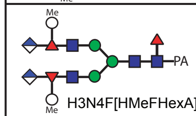
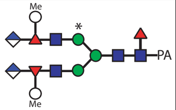
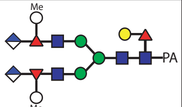
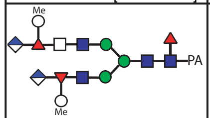
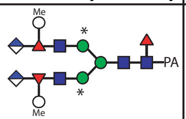
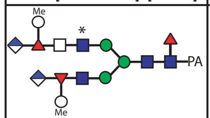
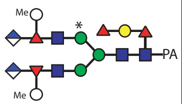
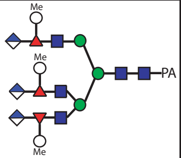
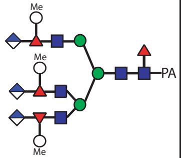
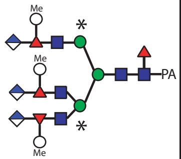
Structure	[M+H]+	[M-H]-	PNGase F			PNGase A	Evidence
			neutral	hydrophobic	anionic		
 H1N2F	811.34 13.5 g.u. [-0.02]		++		+		key fragment [446] co-elution with *Pristionchus*
 H2N2	827.34 8.5 g.u. [-0.01]		+				key fragment [462] insensitive to α1,6- and α1,2/3-mannosidase sensitive to ß-mannosidase (-2Man)
 H2N2	827.34 9.8 g.u. [-0.03]		++				co-elution with *Pristionchus* sensitive to α1,6-mannosidase (-1Man)
 H2N2[AEP]	934.34 6.2 g.u. [0.09]	932.36	+				key fragments [635/827] **see Fig.10A** *m/z* ∆107 instead of 121
 H2N2[MAEP]	948.38 6.8 g.u. [0.08]	946.36	++			+	key fragments [283/649/827], **see Fig.10B/ Fig.12 A+B** JB-mannosidase insensitive, HF sensitive (loss of 121) prior to α1,6-mannosidase (-1Man)
 H2N2F	973.39 5.5 g.u. [0.06]					+	key fragment [446] in PNGase A pool only co-elution with *Pristionchus*
 H2N2F	973.39 16.0 g.u. [-0.03]		+++	+	+	+	key fragment [446] co-elution with *Pristionchus* sensitive to α1,6-mannosidase (-1Man) and bovine fucosidase (-1Fuc)
 H3N2	989.39 8.5 g.u. [-0.03]		+				key fragment [665] sensitive to α1,6-mannosidase (-2Man) insensitive to α1,2/3-mannosidase
 H3N2	989.39 9.3 g.u. [-0.04]		+				key fragment [827] co-elution with *Pristionchus* sensitive to α1,2/3-mannosidase (-1Man)
 H3N2	989.39 11.0 g.u. [0.08]		+				key fragment [462] **see Fig. 8A** sensitive to α1,6-mannosidase, β-mannosidase and JB-mannosidase (each -1Man) **see Fig. 9** insensitive to α1,2/3-mannosidase
 H2N2F[MAEP]	1094.44 11.0 g.u. [0.07]	1092.42	++				key fragments [283/446/948/973] **see Fig. 10C** sensitive to HF (loss of 121, afterwards insensitive to α1,2/3-mannosidase)
 H2N2F2	1119.45 8.4 g.u. [0.11]					++	key fragment [592] in PNGase A pool only insensitive to α1,2/3-mannosidase
 H2N2F2	1119.45 > 20 g.u. [-0.03]			+++			key fragments [665/754] **see Fig. 3C** fragmentation similar to m/z 1281 (< 20 g.u)
 H3N2F	1135.45 5.3 g.u. [0.10]					++	key fragment [446] in PNGase A pool only co-elution with *Pristionchus*
 H3N2F	1135.45 15.5 g.u. [0.08]		++		+	+	key fragment [446] co-elution with *Pristionchus* sensitive to α1,2/3-mannosidase (-1Man) and bovine fucosidase(-1Fuc)
 H3N2F	1135.45 > 20 g.u. [-0.04]		+	++			key fragments [608/827] **see Fig.3B** sensitive to β-galactosidase (-1Gal) prior to bovine fucosidase (-1Fuc) sensitive to α1,6-mannosidase(-1Man)
 H4N2	1151.44 7.4 g.u. [-0.03]		+				key fragment [665] α1,2/3-mannosidase sensitive only after α1,6-mannosidase (each -1Man)
 H4N2	1151.44 8.5 g.u. [0.04]		+				key fragment [827] sensitive to α1,6-mannosidase (-1Man)
 H4N2	1151.44 9.3 g.u. [-0.03]						key fragment [827] co-elution with *Pristionchus*
 H4N2	1151.44 9.8 g.u. [0.01]		++				key fragment [462] **see Fig. 8B** sensitive to JB-mannosidase (-2 Man)
 H2N3[MAEP]	1151.46 14.5 g.u. [0.03]	1149.44	++			+	key fragments [324/486/827/1030] sensitive to HF (loss of 121) afterwards insensitive to FDL **see Fig. 11/ Fig. 12C-D**
 H2N3F	1176.47 >20 g.u. [0.10]		+		+		key fragments [446/1030] late elution indicative of upper arm
 H3N3	1192.47 8.2 g.u. [0.04]		+				key fragment [1030] co-elution with *Pristionchus* sensitive to FDL (-1GlcNAc)
 H3N3	1192.47 16.0 g.u. [-0.12]		++				key fragment [989] co-elution with *Pristionchus* sensitive to α1,2/3-mannosidase (-1Man)
 H3N3	1192.47 17.0 g.u. [0.07]		+				key fragments [462/989] **see Fig. 8C** late elution indicative of upper arm
 H3N2[MAEP]2	1231.48 4.7 g.u. [0.05]	1229.46	++			+	key fragments [283/729/932/948] **see Fig.10D**; sensitive to HF (loss of 2x121),afterwards sensitive to α1,2/3-mannosidase (-1Man)
 H2N2F2[MAEP]	1240.49 11.8 g.u. [-0.06]	1238.48	+	+			key fragments [665/875] HF sensitive (loss of 121), then same fragmentation as 1119 >20 g.u.
 H2N3FS		1254.42 17.0 g.u. [0.09]	+				key fragment [282 negative mode] sensitive to bovine fucosidase sulphation results in earlier elution as m/z 1176 (<20 g.u)

Structure	[M+H]+	[M-H]-	PNGase F			PNGase A	Evidence
			neutral	hydrophobic	anionic		
 H3N2F[MAEP]	**1256.44 10.8 g.u. [0.11]**	**1254.42**	**++**				key fragments [283/446/1135] sensitive to HF (loss of 121), insensitive to α1,2/3-mannosidase, sensitive to JB-mannosidase (-1Man)
 H3N3S		**1270.41 6.8 g.u. [-0.01]**	**++**		**+**		key fragments [282/444 negative mode] **see Fig. 14 A** sulphation results in earlier elution as m/z 1192 (8.2 g.u)
 H2N3[MAEP]2	**1272.50 5.2 g.u. [0.06]**	**1270.49**	**++**			**+**	key fragments [283/324/608/948] **see Fig.10E** sensitive to HF (loss of 2x121), afterwards insensitive to FDL
 H3N2F2	**1281.50 8.4 g.u. [0.11]**					**+++**	key fragments [446/592] **see Fig. 3A** in PNGase A pool only co-elution with *Pristionchus* sensitive to α1,2/3-mannosidase (-1Man)
 H3N2F2	**1281.50 >20 g.u. [0.09]**			**+++**			key fragments [754/827] **see Fig.3D** sensitive to α1,2-fucosidase (-1Fuc) prior to ß-galactosidase (-1Gal), prior to bovine fucosidase (-1Fuc) sensitive to α1,6-mannosidase (-1Man) **see Fig.4**
 H2N2F2PC	**1284.51 11.3 g.u. [-0.04]**		**+**	**+**			key fragments [474/620/919] HF sensitive (loss of 165), then same fragmentation as 1119 >20 g.u.
 H5N2	**1313.49 7.2 g.u. [-0.04]**		**+++**				key fragment [665] sensitive to JB-mannosidase (- 4Man) insensitive to α1,2/3-mannosidase sensitive to α1,6-mannosidase (-1Man) then coeluting with standard B /**see Fig. 7D**
 H5N2	**1313.49 7.8 g.u. [0.02]**		**+**				key fragment [827] sensitive to α1,6-mannosidase and to α1,2/3-mannosidase (each -1Man). Only after α1,6-mannosidase treatment, α1,2/3-mannosidase removes 2Man
 H5N2	**1313.49 8.5 g.u. [0.03]**		**+**				key fragment [827] co-elution with *Pristionchus* sensitive to α1,2/3-mannosidase (-1Man)
 H3N3[MAEP]	**1313.51 14.5 g.u. [-0.08]**	**1311.50**	**+**				key fragments [324/1192] sensitive to α1,2/3-mannosidase (-1Man)
 H3N3F	**1338.53 13.0 g.u. [-0.06]**		**+**		**+**	**+**	key fragments [446/1176] co-elution with *Pristionchus* sensitive to FDL (-1GlcNAc) **see Fig. 11**
 H3N3F	**1338.53 >20 g.u. [0.12]**		**+**	**+**			key fragment [446/1135] co-elution with *Pristionchus*
 H4N3	**1354.52 9.0 g.u. [0.11]**		**+**				key fragments [462/1192] **see Fig. 8D** sensitive to FDL (-1GlcNAc) insensitive to α1,2/3-mannosidase
 H2N4[MAEP]	**1354.54 14.5 g.u. [0.14]**	**1352.52**	**+**				key fragment [324/527/1030] sensitive to HF (loss of 121) late elution indicative of upper arm

Structure	[M+H]+	[M-H]-	PNGase F			PNGase A	Evidence
			neutral	hydrophobic	anionic		
 H3N4	**1395.55 9.0 g.u. [0.06]**		**+**				key fragments [406/827] insensitive to FDL and α1,2/3-mannosidase elution before biantennary *m/z* 1395
 H3N4	**1395.55 11.0 g.u. [0.15]**		**++**				key fragments [1030/1192] co-elution with *Pristionchus*
 H3N2F2[MAEP]	**1402.55 14.2 g.u. [-0.06]**	**1400.53**	**+**	**++**			key fragments [430/576/827/875] **see Fig. 3E** sensitive to α1,2-fucosidase (-1Fuc) and α1,6-mannosidase (-1Man) sensitive to HF (loss of 121), then fragmentation as 1281 > 20 g.u., **see Fig. 5**
 H3N2F2[MAEP]	**1402.55 >20 g.u. [0.09]**	**1400.53**		**+**			key fragments [649/754/948] **see Fig. 3F**
 H3N3FS		**1416.47 9.8 g.u. [-0.03]**	**++**		**++**		key fragment [282 negative mode] insensitive to HF,JB-hexosaminidase and α1,2/3-mannosidase sensitive to JB-mannosidase (-1Man) **see Fig. 14 B/E/F/G/H**
 H3N3FS		**1416.47 15.0 g.u. [0.02]**	**+**		**+**		key fragment [282 negative mode] sulphation results in earlier elution as m/z 1338 (<20 g.u)
 H3N3[MAEP]2	**1434.55 11.0 g.u. [-0.07]**	**1432.54**	**++**		**+**		key fragments [283/324/948/1110] **see Fig. 10F** insensitive to JB-mannosidase sensitive to HF (loss of 2x121), afterwards sensitive to α1,2/3-mannosidase (-1Man)
 H3N2F2PC	**1446.56 13.7 g.u. [-0.05]**		**+**	**++**			key fragments [474/620/919] **see Fig. 3G** sensitive to α1,2-fucosidase (-1Fuc) and α1,6-mannosidase (-1Man), HF sensitive (loss of 165), then fragmentation as 1281 > 20 g.u., **see Fig. 5**
 H6N2	**1475.55 6.8 g.u. [-0.09]**		**++**				key fragment [989] co-elution with *Pristionchus* sensitive to α1,2-mannosidase (-1Man) and α1,2/3-mannosidase (-2Man)
 H6N2	**1475.55 7.2 g.u. [0.15]**		**+++**		**+**	**+**	key fragment [827] sensitive to JB-mannosidase (-5Man), α1,6-mannosidase (-1Man) then coeluting with standard A (Man5), **see Fig. 7D** sensitive to α1,2/3-mannosidase (-1Man)
 H3N3F2	**1484.58 11.0 g.u. [0.13]**					**+**	key fragments [446/592/1281] in PNGase A pool only co-elution with *Pristionchus*
 H3N3F2	**1484.58 >20g.u. [0.00]**			**+**			key fragments [350/446/1135/1338] insensitive to JB-hexosaminidase sensitive to bovine fucosidase (-2 Fuc) late elution indicative of upper arm
 H2N3F[HMeF]	**1498.60 >20 g.u. [0.00]**			**+**			key fragment [446] not observed in negative mode sensitive to bovine fucosidase(-1Fuc) sensitive to HF (loss of 322)
 H3N3FS2		[M-2H+Na]- **1518.48 6.2 g.u. [-0.06]**			**+**		key fragments [241/282/403/444 negative mode] **see Fig. 14 D**

Structure	[M+H]+	[M-H]-	PNGase F neutral	PNGase F hydrophobic	PNGase F anionic	PNGase A	Evidence
 H3N3FS2		[M-2H+Na]- 1518.48 7.9 g.u. [-0.08]			+		key fragments [241/282/403/444 negative mode]
 H2N3[HMeFHexA]	1528.57 13.5 g.u. [-0.01]	1526.56	++		++		key fragments [827/1030] **see Fig. 15A** sensitive to HF (loss of 498)
 H3N4F	1541.60 >20 g.u. [0.13]		+				key fragment [446] co-elution with *Pristionchus* sensitive to bovine fucosidase (-1Fuc)
 H3N3[MAEP]3	1555.60 4.0 g.u. [0.13]	1553.58	++		+		key fragments [283/324/607/932/1231] **see Fig. 10G**, insensitive to JB-mannosidase, sensitive to HF (loss of 3x121) prior to α1,2/3- mannosidase (-1Man)
 H4N4	1557.60 12.5 g.u. [-0.16]		+				key fragments [462/1192/1354] **see Fig. 8E**
 H7N2	1637.60 5.4 g.u. [0.10]		+++		+	+	key fragment [989] co-elution with *Pristionchus* sensitive to α1,2-mannosidase (-2Man)
 H7N2	1637.60 5.8 g.u. [0.16]		++				key fragment [989] sensitive to α1,2-mannosidase and α1,6-mannosidase (each -1Man), then co-elution with H6N2 at 6.8 g.u. **see Fig. 7B+C**
 H7N2	1637.60 6.2. g.u. [0.16]		+				key fragment [1151] co-elution with *Pristionchus* sensitive to α1,2-mannosidase (-2Man)
 H7N2	1637.60 7.4 g.u. [0.15]		+				key fragment [989] sensitive to α1,2/3-mannosidase (-3Man) insensitive to α1,6-mannosidase
 H3N4[MAEP]2	1637.63 9.8 g.u. [0.07]	1635.62	+			+	key fragments [324/486/827/1516] **see Fig.10H** sensitive to HF (loss of 2x121) then fragmentation as m/z 1395 (11.0 g.u)
 H3N3F[HMeF]	1660.65 > 20 g.u. [0.16]			+			key fragments [446/1135/1338] not observed in negative mode sensitive to bovine fucosidase (-1Fuc) sensitive to HF (loss of 322)
 H2N3F[HMeFHexA]	1674.63 >20 g.u. [0.09]	1672.62	++		++		key fragments [446/973/1176] **see Fig. 15B** negative mode [497/700] **see Fig. 17B** sensitive to HF (loss of 498) sensitive to bovine fucosidase (-1Fuc) insensitive to FDL after HF
 H3N3[HMeFHexA]	1690.63 14.0 g.u. [0.02]	1688.61	+		++		key fragments [462/989/1192] **see Fig. 15C** sensitive to HF (loss of 498)
 H3N4[MAEP]3	1758.68 7.9 g.u. [0.13]	1756.66	+				key fragments [324/607/1272/1434] **see Fig. 10I** loss of 324 then 162 sensitive to HF (loss of 3x121) prior to FDL (-1GlcNAc)

Structure	[M+H]+	[M-H]-	PNGase F neutral	PNGase F hydrophobic	PNGase F anionic	PNGase A	Evidence
 H2N3F[HMeFHexA][MAEP]	1795.67 6.5 g.u. [0.00]	1793.66			+		key fragments [446/648/1094/1297] loss of 498 then 203 **see Fig. 15D** sensitive to HF, loss of 498 and 121 resulting in m/z 1176
 H8N2	1799.65 4.7 g.u. [0.11]		++				key fragment [989] sensitive to α1,2-mannosidase (- 2Man), α1,2/3-mannosidase (- 3Man) and α1,6-mannosidase (- 1Man) then coeluting with H7N2 (5,4g.u.) **see Fig.7A**
 H8N2	1799.65 5.0 g.u. [0.15]		+++		+		key fragment [1151], Man8B co-elution with *Pristionchus*
 H8N2	1799.65 5.8 g.u. [0.17]		+				key fragment [989], Man8A co-elution with *Pristionchus* sensitive to α1,2-mannosidase (-3Man)
 H3N3F[HMeFHexA]	1836.68 12.0 g.u. [0.16]	1834.67	+		+		key fragments [446/973/1338] in negative mode [497/700] sensitive to HF (loss of 498), prior to FDL (-1GlcNAc) **see Fig. 16**
 H3N3F[HMeFHexA]	1836.68 >20 g.u. [0.06]	1834.67	+		+		key fragments [446/1135/1338] sensitive to HF (loss of 498) sensitive to bovine fucosidase (-1Fuc) and JB-mannosidase (-1Man)
 H4N3[HMeFHexA]	1852.68 8.0 g.u. [-0.01]	1850.66			+		key fragments [462/989/1151/1354]
 H3N4[MAEP]4	1879.72 3.4 g.u. [0.13]	1877.71	+		+		key fragments [283/324/607/1272/1555]
 H3N3F[HMeFHexA][MAEP]	1957.73 5.7 g.u. [-0.01]	1955.71			+		key fragments [324/446/648/1094/1256/1459] loss of 498 then 203
 H9N2	1961.71 4.4 g.u. [0.11]		++				key fragment [1151] sensitive to α1,2-mannosidase (- 2Man) prior to α1,2/3- mannosidase (-2Man),sensitive to α1,6-mannosidase (- 1Man) **see Fig. 7 F-I**
 H9N2	1961.71 5.4 g.u. [0.17]		+++		+		key fragment [1151] co-elution with *Pristionchus* sensitive to JB-mannosidase (-8Man) sensitive to α1,2-mannosidase (-4Man)
 H3N5[MAEP]3	1961.76 7.9 g.u. [0.14]	1959.74	+				key fragments [324/648/827/1475/1637] **see Fig. 10J** insensitive to JB-mannosidase sensitive to HF (loss of 3x121), key fragment then m/z 406, afterwards insensitive to FDL
 H2N4F[HMeFHexA][MAEP]	1998.75 >20 g.u. [0.02]	1996.74			+		key fragments [324/446/486/527/973/1297/1500] loss of 498 then 203 then 324 **see Fig. 15E**
 H5N3[HMeFHexA]	2014.73 6.8 g.u. [-0.11]	2012.72			+		key fragments [827/1313/1516] loss of 498 then 203

Structure	[M+H]+	[M-H]-	PNGase F			PNGase A	Evidence
			neutral	hydrophobic	anionic		
 H3N4F[HMeFHexA]	**2039.76 17.0 g.u. [-0.02]**	**2037.75**			**+**		key fragments [446/1176/1338/1541] loss of 498 then 203 then 162
 H3N6[MAEP]4	**2285.88 7.8 g.u. [0.17]**	**2283.86**	**+**				key fragments [324/649/1475] loss of 324 then 324 then 162
 H2N4F[HMeFHexA]2	**2375.87 6.5 g.u. [-0.04]**	**2373.85**			**+**		key fragments [446/1176/1674] negative mode [497/700] loss of 498 then 203 **see Fig. 15F**
 H3N4[HMeFHexA]2	**2391.86 9.8 g.u. [0.00]**	**2389.85**	**+**		**++**		key fragments [525/702/989/1192 /1528/1690/1894] negative mode [497/700] loss of 498 then 203 then 162 **see Fig. 15G**
 H3N4F[HMeFHexA]2	**2537.92 13.5 g.u. [-0.06]**	**2535.91**	**+**		**+++**		key fragments [446/1674/1837/2040] negative mode [497/700] loss of 498 then 203 then 162 sensitive to HF (loss of 2x498) sensitive to bovine fucosidase **see Fig. 17A**
 H3N4F[HMeFHexA]2[MAEP]	**2658.97 12.0 g.u. [-0.12]**	**2656.95**			**+**		key fragments [283/446/1256/1459/ 1675/1958] loss of 498 then 203 then 283
 H4N4F[HMeFHexA]2	**2699.97 15.0 g.u. [-0.01]**	**2697.96**			**+**		key fragments [608/1135/1837/1999] loss of 498 then 203 then 162 or loss of 146 then 162 **see Fig. 15H**
 H3N5F[HMeFHexA]2	**2741.00 14.0 g.u. [0.00]**	**2738.99**			**+**		key fragments [407/446/568/701/730/ 1338/1837/2040/2243] loss of 498 then 203 then 203 **see Fig. 15I**
 H3N4F[HMeFHexA]2[MAEP]2	**2780.01 4.5 g.u. [-0.09]**	**2777.99**			**+**		key fragments [283/446/649/932/1796 /2079/2282] negative mode [497] loss of 498 then 203 then 283 **see Fig. 15J**
 H3N5F[HMeFHexA]2[MAEP]	**2862.04 14.0 g.u. [-0.03]**	**2860.03**			**+**		key fragments [324/446/527/1338/1837/2162/2365] loss of 498 then 203 then 324 then 162 **see Fig. 15K**
 H4N4F2[HMeFHexA]2[MAEP]	**2967.08 19.0 g.u. [0.03]**	**2965.06**			**+**		key fragments [754/957/1768/ 2266/2469] negative mode [497/700/983] loss of 498 then 203 or 454
 H3N5[HMeFHexA]3	**3093.10 5.0 g.u. [-0.10]**	**3091.09**			**+**		key fragments [701/1528/2391] negative mode [497/700] loss of 498 then 203; 498 then 203 then 162
 H3N5F[HMeFHexA]3	**3239.16 6.5 g.u. [-0.08]**	**3237.15**			**+**		key fragments [446/1837/2537/2741] negative mode [497/700] **see Fig. 15L** loss of 700 then 700 then 162
 H3N5F[HMeFHexA]3[MAEP]2	**3481.25 4.3 g.u. [-0.16]**	**3479.23**			**+**		key fragments [283/446/1094/ 1377/2080]