

Supplementary Material

1 Supplemental File 1

NEGATIVE MODE

Name: fructosyl ile/leu

REF:PUBCHEM_SID_ 129689639

Precursor_type: [M-H]-

Comment:

Int_ref: BEOFIT November 2020 1,57_292.1379m/z

Ext_ref: <https://doi.org/10.1016/j.foodchem.2017.02.007>; doi:10.3390/biomedicines8050104;
doi:10.3390/biomedicines8050104; DOI: 10.1021/acs.jafc.6b02500

Formula: C₁₂H₂₃NO₇

Num Peaks: 28

59.01447567 175

71.01368093 87

73.02932697 522

82.06502121 31

84.08011524 114

98.02410989 30

101.0235604 1214

110.0975574 119

113.0591422 30

115.0761636 206

126.0892647 60

129.6831171 205

130.0864874 47795

130.2168056 30
 130.2447914 35
 130.2820511 35
 130.6466564 31
 130.7836911 44
 130.8608502 36
 130.8887959 33
 130.9132109 30
 130.9673536 30
 131.0845301 30
 152.1059008 30
 172.0961298 406
 202.1062931 274
 214.1061591 215
 226.1078501 58

Name: fructosyl ile/leu -H₂O

REF: PUBCHEM_SID_129689639

Precursor_type: [M-H]-

Comment:

Int_ref: BEOFIT November 2020 1,88_274.1284m/z

Ext_ref: <https://doi.org/10.1016/j.foodchem.2017.02.007>; doi:10.3390/biomedicines8050104;
 doi:10.3390/biomedicines8050104; DOI: 10.1021/acs.jafc.6b02500

Formula: C₁₂H₂₁NO₆

Num Peaks: 8

71.01337621 107

72.02066815 84
73.0293931 747
85.02911546 48
125.0958598 62
134.0993035 67
152.1063626 684
170.1180269 414

Name: fructosyl ile/leu hex

REF: PUBCHEM_SID_129689639

Precursor_type: [M-H]-

Comment:

Int_ref: BEOFIT November 2020 1,81_454,1917m/z

Ext_ref: <https://doi.org/10.1016/j.foodchem.2017.02.007>; doi:10.3390/biomedicines8050104;
doi:10.3390/biomedicines8050104; DOI: 10.1021/acs.jafc.6b02500

Formula: C₁₂H₂₃NO₇C₆O₅H₁₀

Num Peaks: 46

57.03432254 444
59.01339602 699
69.03368887 340
71.01317996 360
72.0213197 757
73.02913476 11071
82.02911518 163
82.06591656 324
84.04494186 819

85.02885323	2151
89.02349893	218
95.03673501	586
96.04460892	174
97.02801062	160
99.03250032	548
100.0378339	141
101.0241307	452
109.0286822	196
110.0966307	565
111.0315067	305
115.0749852	149
119.0341244	154
124.1124308	179
125.0959924	1274
126.092072	258
128.1070958	1786
130.0862564	3010
134.0965405	1237
137.0835025	201
142.1222919	506
151.6336548	241
152.1069521	25209
153.0833304	782
154.085667	164

156.1012574 169
164.1069638 3802
168.1016662 205
170.1170974 10360
172.0972106 195
176.1071247 199
182.1166818 1968
194.1173408 801
212.1262223 656
214.1069207 4170
256.1171782 938
274.1275647 2110

Name: fructosyl ile/leu dihex

REF: PUBCHEM_SID_129689639

Precursor_type: [M-H]-

Comment:

Int_ref: BEOFIT November 2020 2.23_616.2428m/z

Ext_ref: <https://doi.org/10.1016/j.foodchem.2017.02.007>; doi:10.3390/biomedicines8050104;
doi:10.3390/biomedicines8050104; DOI: 10.1021/acs.jafc.6b02500

Formula: C₁₂H₂₃NO₇C₁₂H₂₀O₁₀

Num Peaks: 8

Mass/Charge Height

73.02874853 209
130.086411 914
152.1077909 419

164.1064606 62
 170.1173407 339
 214.1062677 247
 256.1138196 48
 274.1282854 63

Name: fructosyl ile/leu trihex

REF: PUBCHEM_SID_129689639

Precursor_type: [M-H]-

Comment:

Int_ref: BEOFIT November 2020 2.66_778.2939m/z

Ext_ref: <https://doi.org/10.1016/j.foodchem.2017.02.007>; doi:10.3390/biomedicines8050104;
 doi:10.3390/biomedicines8050104; DOI: 10.1021/acs.jafc.6b02500

Formula: C₁₂H₂₃NO₇C₁₂H₂₀O₁₀C₆O₅H₁₀

Num Peaks: 33

59.01357126 12
 73.02947586 279
 82.06844147 12
 84.04261992 12
 85.02953125 12
 89.0227978 18
 101.0233832 24
 110.0970307 18
 111.0301723 12
 113.0270938 12
 119.0337926 40

125.0974983 12
128.1058755 30
130.0863125 104
134.0963595 24
142.1215023 18
152.1061338 752
153.0903937 18
154.0870516 18
161.0433014 12
164.1066535 98
170.1173367 308
172.0939437 12
179.0539855 78
182.1157707 67
194.1143543 30
212.1287885 75
214.1072709 176
221.0665797 24
256.1143778 58
274.1274183 282
383.1147694 201
545.162507 24

Name: fructosyl ile/leu tetrahex

REF: PUBCHEM_SID_129689639

Precursor_type: [M-H]-

Comment:

Int_ref: BEOFIT November 2020 3.18_940.3455m/z

Ext_ref: <https://doi.org/10.1016/j.foodchem.2017.02.007>; doi:10.3390/biomedicines8050104;
doi:10.3390/biomedicines8050104; DOI: 10.1021/acs.jafc.6b02500

Formula: C₁₂H₂₃NO₇C₁₂H₂₀O₁₀C₁₂H₂₀O₁₀

Num Peaks: 29

73.02889449 37

81.02344813 6

89.02422208 12

96.01311656 6

101.0259906 12

101.472288 6

128.1114168 6

130.0876782 12

142.1163321 6

152.1068564 135

161.0424638 18

164.1099919 24

170.1184213 172

176.046889 6

179.0548093 37

182.1164133 6

194.1150321 6

214.1057248 30

214.8447124 6

221.0655205 12

256.1173151 18
274.1276563 33
341.1004162 12
365.1038358 6
383.1161089 30
545.1687291 145
545.7082244 6
707.2208145 12
940.3647399 12

Name: fructosyl Phe

REF: PUBCHEM_SID_85152457

Precursor_type: [M-H]-

Comment: ext_ref in positive

Int_ref: BEOFIT November 2020 2.97_326.1219m/z

Ext_ref: DOI:10.1021/ac048925a

Formula: C₁₅H₂₁NO₇

Num Peaks: 9

72.00882365 1329

73.02895811 275

91.05466403 181

101.0241264 934

103.0539599 2593

144.0800028 277

147.0437101 7558

149.0587938 369

164.0703016 16742

Name: fructosyl Phe -H₂O

REF: PUBCHEM_SID_85152457

Precursor_type: [M-H]⁻

Comment: ext_ref in positive, most likely product of hexoside at 488

Int_ref: BEOFIT November 2020 3.79_308.1117m/z

Ext_ref: DOI:10.1021/ac048925a

Formula: C₁₅H₁₉NO₆

Num Peaks: 14

73.02922712 207

85.02913865 92

94.02915543 82

101.9391657 131

112.0405098 181

118.0675539 30

129.8790586 198

145.9281206 30

159.0809761 30

168.0799549 30

170.0583769 31

173.8694344 507

186.0893884 225

217.8603214 91

Name: fructosyl Phe hex

REF: PUBCHEM_SID_85152457

Precursor_type: [M-H]-

Comment: ext_ref in positive

Int_ref: BEOFIT November 2020 3.79_488.1735

Ext_ref: DOI:10.1021/ac048925a

Formula: C₁₅H₂₁NO₇C₆O₅H₁₀

Num Peaks: 16

73.02903223 3631

85.02901557 1154

91.05396194 252

100.0384382 419

112.039456 1475

118.0647112 555

144.0798066 881

159.0793342 725

168.0802434 1712

170.0595569 324

171.0678363 476

186.0908688 6851

198.0901195 441

204.1014637 309

248.0908882 504

308.1122371 312

Name: fructosyl Phe dihex

REF: PUBCHEM_SID_85152457

Precursor_type: [M-H]-

Comment: ext_ref in positive

Int_ref: BEOFIT November 2020 4.57_650.2256m/z

Ext_ref: DOI:10.1021/ac048925a

Formula: C15H21NO7C6O5H10C6O5H10

Num Peaks: 13

73.02859349 290

85.02913591 81

112.04046 120

118.0647452 30

142.0509164 30

144.0800461 129

159.0811363 83

168.0803686 104

186.0906136 861

198.0914096 30

228.100835 30

248.0915332 101

308.1109422 74

Name: fructosyl Phe trihex

REF: PUBCHEM_SID_85152457

Precursor_type: [M-H]-

Comment: ext_ref in positive

Int_ref: BEOFIT November 2020 5.61_812.2781m/z

Ext_ref: DOI:10.1021/ac048925a

Formula: C₁₅H₂₁NO₇C₆O₅H₁₀C₆O₅H₁₀C₆O₅H₁₀

Num Peaks: 13

73.02932745 42

85.02758042 24

112.0397302 30

144.0825891 18

164.0736548 18

168.0799846 18

186.0903962 399

198.0898524 18

221.0697073 18

228.1008711 24

246.1110221 24

308.1119397 48

383.1167603 37

Name: fructosyl Val hex

REF: PUBCHEM_SID_71777427

Precursor_type: [M-H]-

Comment: ext_ref in positive

Int_ref: BEOFIT November 2020 0.87_440.1735m/z

Ext_ref: DOI:10.1021/ac048925a

Formula: C₁₁H₂₁NO₇C₆O₅H₁₀

Num Peaks: 11

73.02910784 3535

84.04460435 471

85.02927377 676

114.0920434 638

116.0711122 487

138.0911849 7874

150.091334 1188

156.1015653 3653

168.1014163 782

200.0914614 1535

260.111582 803

Name: fructosyl Val dihex

REF: PUBCHEM_SID_71777427

Precursor_type: [M-H]-

Comment: ext_ref in positive

Int_ref: BEOFIT November 2020 1.06_602.2258m/z

Ext_ref: DOI:10.1021/ac048925a

Formula: C₁₁H₂₁NO₇C₁₂O₁₀H₂₀

Num Peaks: 30

59.01416538 101

72.02249625 36

73.02844249 991

78.95964936 114

84.04465346 68

85.02983569	54
89.02365408	89
95.03812299	38
96.07979691	75
96.96132938	103
99.03286389	40
111.0812592	40
114.0917358	168
116.0703416	167
138.0911054	2481
139.0651082	65
146.0587844	166
150.0912534	420
156.1009775	1709
158.0804419	49
161.0430673	33
168.1019182	187
180.1027451	60
198.1131619	78
200.0896541	741
202.084113	37
221.0627557	76
242.1020441	422
259.019579	51
260.111925	645

Name: fructosyl Met hex

REF: PUBCHEM_SID_10859892

Precursor_type: [M-H]-

Comment: ext_ref in positive

Int_ref: BEOFIT November 2020 1.06_472.1453m/z

Ext_ref: DOI:10.1021/ac048925a

Formula: C₁₁H₂₁NO₇SC₆O₅H₁₀

Num Peaks: 21

59.01441911 24

66.0355885 24

68.0505849 31

72.01965269 18

73.0295581 30

80.05088291 24

85.02871402 36

99.03105746 18

122.0606952 62

134.0586394 18

140.0709499 355

148.0418389 52

152.0714773 18

164.0689142 24

170.0636955 193

188.0735426 138

200.0905879 36

221.0637169 18

232.0626901 66

274.0717851 24

292.0836731 42

Name: fructosyl Trp

REF: PUBCHEM_SID_71316984

Precursor_type: [M-H]-

Comment: ext_ref in positive

Int_ref: BEOFIT November 2020 5.18_365.1347m/z

Ext_ref: DOI:10.1021/ac048925a

Formula: C17H22N2O7

Num Peaks: 10

73.02952361 24

74.0243102 89

101.0249671 41

116.0506161 293

130.0670993 30

142.0643893 148

159.0896969 176

183.0917199 24

186.0534136 24

203.0810465 1218

Name: fructosyl Trp - H2O

REF: PUBCHEM_SID_71316984

Precursor_type: [M-H]-

Comment: ext_ref in positive

Int_ref: BEOFIT November 2020 6.47_347.1221m/z

Ext_ref: DOI:10.1021/ac048925a

Formula: C17H20N2O6

Num Peaks: 15

78.95798828 6

85.03220742 6

87.04230704 6

100.9334455 6

114.9593205 6

116.0493572 18

142.0636499 30

156.0705065 6

157.0739865 12

167.0596675 6

169.0767037 31

183.0931824 24

212.8677742 6

225.1015773 18

301.2149929 24

Name: fructosyl Trp hex

REF: PUBCHEM_SID_71316984

Precursor_type: [M-H]-

Comment: ext_ref in positive

Int_ref: BEOFIT November 2020 6.27_527.1836m/z

Ext_ref: DOI:10.1021/ac048925a

Formula: C17H22N2O7C6O5H10

Num Peaks: 44

57.03438073 24

59.01430194 18

72.04346862 12

73.02984846 30

85.02980008 30

87.04418848 18

89.02236078 12

96.0443069 18

97.0225007 12

100.0395399 24

101.0235477 18

108.0466257 24

112.0382401 18

116.049305 237

128.047074 18

130.0654088 12

138.0556377 30

142.0647499 224

154.0558006 12

156.0771314 30

157.0757572 136

158.0604625	12
167.059685	58
168.068235	30
169.0751013	754
171.0912092	24
181.0813073	30
182.08157	18
183.0903954	360
184.0759486	12
198.0884781	18
200.0565987	12
201.1022087	12
207.095766	12
208.0711815	12
225.101127	634
226.0845826	62
237.1035359	48
243.1118109	314
255.1115437	12
267.116826	12
287.1011305	30
329.1108358	30
347.1234403	12

Name: fructosyl Trp dihex

REF: PUBCHEM_SID_71316984

Precursor_type: [M-H]-

Comment: ext_ref in positive

Int_ref: BEOFIT November 2020 6.27_7.36_689.2368m/z

Ext_ref: DOI:10.1021/ac048925a

Formula: C₁₇H₂₂N₂O₇C₁₂O₁₀H₂₀

Num Peaks: 17

73.02857609 24

116.052375 32

138.0542078 12

142.0647852 30

157.0735194 24

168.0695698 12

169.0753925 75

183.092473 30

221.0664741 12

225.0999007 203

226.0802028 18

237.101356 18

243.1118244 74

267.1099072 12

287.1015495 18

329.1167508 12

347.1247462 12

Name: fructosyl p-Glu

REF: PUBCHEM_SID_139292107

Precursor_type: [M-H]-

Comment:

Int_ref: BEOFIT December 2020 0.90_290.0865m/z

Ext-ref: splash10-004i-0960000000-4c1a537a7c06f49b32bd

Formula: C₁₁H₁₇NO₈

Num Peaks: 4

128.0353957 53933

168.0660471 773

170.0449534 1778

200.0560078 9040

Name: fructosyl p-Glu -H₂O

REF: PUBCHEM_SID_139292107

Precursor_type: [M-H]-

Comment:

Int_ref: BEOFIT December 2020 0.94_272.0766m/z

Ext_ref: <http://dx.doi.org/10.1016/j.jcs.2014.07.002>; DOI 10.1007/s00425-014-2061-y

Formula: C₁₁H₁₅NO₇

Num Peaks: 14

69.03473925 33

84.04654334 44

126.0560858 81

128.0346187 30

139.9581857 24

140.0729242 70
150.058978 24
168.066358 288
180.0670264 24
183.9494247 24
192.0664558 68
212.0566459 70
236.0547545 18
272.0748549 24

Name: fructosyl p-Glu hex

REF: PUBCHEM_SID_139292107

Comment: MassBank Record PR309144

Precursor_type: [M-H]-

Int_ref: BEOFIT December 2020 0.98_452.1372m/z

Ext_ref: <http://dx.doi.org/10.1016/j.jcs.2014.07.002>; DOI 10.1007/s00425-014-2061-y

Formula: C₁₁H₁₇NO₈C₆O₅H₁₀

Num Peaks: 24

59.01353449 161
69.03435606 162
84.04423763 245
97.02848919 263
98.05969729 178
101.0233199 246
125.0234868 367
126.054536 528

128.0339	7419
140.0703029	375
150.0553481	194
154.0506959	183
168.0645823	3909
170.0448347	466
180.0639098	228
182.9600949	418
192.064548	1743
200.0545688	1738
212.0544486	1952
236.054169	413
254.0663539	675
272.0757378	470
362.1073515	496
363.0279201	209

Name: fructosyl p-Glu dihex

REF: PUBCHEM_SID_139292107

Precursor_type: [M-H]-

Comment: MassBank Record PR309144

Int_ref: BEOFIT December 2020 1.02_614.1892m/z

Ext_ref: <http://dx.doi.org/10.1016/j.jcs.2014.07.002>; DOI 10.1007/s00425-014-2061-y

Formula: C₁₁H₁₇NO₈C₁₂O₁₀H₂₀

Num Peaks: 20

69.03524806 30
83.01278304 30
97.02944062 80
125.0237106 196
126.0540871 32
128.0342959 556
140.0704019 184
150.0556693 38
154.0504048 60
168.0652549 1443
180.0639806 166
192.0646259 1201
200.0551853 196
210.0757334 62
212.0545544 1175
236.0534181 281
254.0662348 379
272.0750203 437
524.1624053 42
614.1881109 82

Name: fructosyl p-Glu trihex

REF: PUBCHEM_SID_139292107

Precursor_type: [M-H]-

Comment: MassBank Record PR309144

Int_ref: BEOFIT December 2020 1.25_776.2428m/z

Ext_ref: <http://dx.doi.org/10.1016/j.jcs.2014.07.002>; DOI 10.1007/s00425-014-2061-y

Formula: C₁₁H₁₇NO₈C₁₈O₁₅H₃₀

Num Peaks: 27

96.96265519	30
97.02947897	39
101.0244497	30
122.0240735	18
125.023379	70
126.0539262	30
128.03414	930
136.0427563	18
140.0720455	77
150.0565132	18
154.050484	46
168.0645243	848
170.047808	18
179.0513112	24
180.0639702	52
192.0646384	630
200.0548919	504
210.0770511	30
212.0544526	631
221.063864	24
236.0539428	291
254.0647152	445

272.076346 430

383.1162577 47

686.2140999 44

758.2429407 34

776.2423992 94

Name: fructosyl p-Glu tetrahex

REF: PUBCHEM_SID_139292107

Precursor_type: [M-H]-

Comment: in pos.mode DOI:10.1021/ac048925a; look the respective compounds in positive mode

Date: 08062021

Int_ref: BEOFIT December 2020 1.49_938.2952m/z

Ext-ref:

Formula: C₁₁H₁₇NO₈C₂₄O₂₀H₄₀

Num Peaks: 17

125.022476 18

128.0337322 235

168.0645113 87

170.0462124 24

192.0643071 229

200.0561945 224

212.0553904 183

230.0700992 32

236.0561099 39

254.0648364 155

272.0771548 127

383.11795 18
545.1653222 33
707.2238767 24
848.2701989 24
920.2798044 18
938.2961088 65

Name: fructosyl Lys hex

REF: PUBCHEM_SID_9839580

Precursor_type: [M-H]-

Comment: DOI:10.1021/acs.jafc.0c06193

Date: 07062021

Int_ref: BEOFIT december 2020 0.51_469.2005m/z

Ext_ref: CCMSLIB00005720267 splash10-004i-3692000000-8a3352808a87f62f61af

Formula: C₁₂H₂₄N₂O₇C₆H₁₀O₅

Num Peaks: 22

59.01410768 89
73.03067101 53
74.02559811 37
78.95969155 30
82.03113718 79
84.04558447 125
85.02905807 30
102.0549624 49
111.0560131 65

126.0543252 31
126.9014424 30
143.0815675 73
145.0615868 69
145.0980935 89
154.0508153 30
155.0449197 51
167.0813711 79
185.0912529 122
187.1082939 35
229.0795276 68
229.1187605 37
289.102061 48

POSITIVE MODE

Name: fructosyl Val -H₂O

REF: PUBCHEM_SID_71777427

Precursor_type: [M+H]⁺

Comment: DOI:10.1021/ac048925a amadori product (280)

Int_ref: BEOFIT November 2020 0.75_262.1281m/z

Ext_ref: CCMSLIB00005720267 splash10-004i-3692000000-8a3352808a87f62f61af

Formula: C₁₁H₁₉NO₆

Num Peaks: 46

55.0531934 1258

59.03587145 627

67.05329602	166
69.03260343	1049
70.02860362	176
72.07997822	4258
73.02707805	173
81.03224764	253
82.06490184	228
84.04333312	183
84.07939487	2872
85.02687485	792
86.09511879	393
87.03058606	1221
96.07988862	202
97.02734012	1232
98.0941883	231
99.04236363	217
102.0905655	785
110.0585092	177
110.0944138	167
112.0378014	1277
112.0754256	190
114.0900267	610
118.0849625	1055
126.0901345	369
127.0380564	792

130.0851382 1440
138.0535578 270
142.0835065 239
143.0568529 888
145.04931 238
150.0898705 1163
152.1063693 333
154.0844257 647
156.0997482 418
161.0665544 1298
168.1001417 379
180.1002939 529
196.0950639 854
198.1112714 4077
216.121845 11930
226.107008 153
234.1335039 726
244.1165359 5377
262.1279883 3334

Name: fructosyl Val

REF: PUBCHEM_SID_71777427

Precursor_type: [M+H]⁺

Comment: DOI:10.1021/ac048925a amadori product (280)

Int_ref: BEOFIT November 20200.78_280.1217m/z

Ext_ref: CCMSLIB00005720267 splash10-004i-3692000000-8a3352808a87f62f61af

Formula: C₁₁H₂₁NO₇

Num Peaks: 44

55.01746025 900

55.05347354 4284

56.04884557 1097

57.03266913 1367

57.06900986 832

58.02827792 1044

59.03648107 1763

69.03250827 3702

70.0284066 925

72.07986384 25693

73.02728507 974

81.03271665 1074

82.06432788 1046

84.07956701 15205

85.02720945 3564

86.09511425 2148

87.03054074 6132

96.04310162 877

97.02747287 5132

99.04229953 1552

102.0900303 4291

112.0379579 5357

114.0898846 4562

118.0850277 11547
126.0896409 2111
127.0374929 5694
130.084929 9586
138.0533351 872
138.0888005 936
143.0557162 5081
145.047941 1410
150.0896669 4665
152.1048562 917
154.0840708 3293
156.1008508 2147
161.0667623 5169
168.1005676 1913
180.1003871 3297
196.0950106 5215
198.1113637 22608
216.1215499 81313
234.132429 7206
244.1167436 51698
262.1284616 53312

Name: fructosyl Val hex

REF: PUBCHEM_SID_71777427

Precursor_type: [M+H]⁺

Comment: DOI:10.1021/ac048925a amadori product (280)

Int_ref: BEOFIT November 2020 0.9_442.1900m/z

Ext-ref: CCMSLIB00000078880

Formula: C₁₁H₁₉NO₆C₆O₆H₁₂

Num Peaks: 36

55.05354512 444

57.03304876 358

61.02725681 399

69.03220968 1763

72.07997309 4099

73.02727879 528

81.03231998 705

84.0800561 2141

85.02725151 4236

87.03858263 430

97.02728714 2123

99.04249886 656

102.0897722 956

109.0274604 360

112.0381999 438

114.0895713 602

118.0849677 3337

127.0370962 2345

130.0851129 2254

136.0743027 396

143.055914 1565

145.0477505 1029
150.0896083 2919
154.0842922 862
161.065997 961
168.1004402 456
180.0999526 907
196.0955259 5294
198.1118633 5401
216.1219495 17966
226.1062725 492
234.1331715 2669
244.1174105 17636
262.1279847 27865
378.1759285 1691
424.1828463 2026

Name: fructosyl Val dihex

REF: PUBCHEM_SID_71777427

Precursor_type: [M+H]⁺

Comment: DOI:10.1021/ac048925a amadori product (280)

Int_ref: BEOFIT November 2020 0.975_604.2422m/z

Ext-ref: CCMSLIB00000078880

Formula: C₁₁H₁₉NO₆C₆O₆H₁₂C₆O₅H₁₀

Num Peaks: 27

61.02787262 99

69.0318567 286

72.07948308	497
84.07969918	226
85.02730838	1195
97.02739977	442
99.04485428	160
102.0904746	117
109.0283812	253
118.0848878	863
127.037841	559
130.0849969	548
143.05753	430
145.04796	454
150.0899936	396
154.0847703	107
161.0662611	184
180.099722	252
196.0958777	898
198.1105708	934
216.1217835	3482
226.1067978	154
234.1330087	745
244.1179645	4321
262.1287337	7147
378.171973	151
424.1825106	614

Name: fructosyl Ile/Leu

REF: PUBCHEM_SID_ 129689639

Precursor_type: [M+H]⁺

Comment: at RT 0.89 there is a very similar compound but at 294.098

Int_ref: BEOFIT November 2020 1.56_294.1532m/z

Ext-ref: DOI:10.1021/ac048925a amadori product, PR310824 mass bank

Formula: C₁₂H₂₃NO₇

Num Peaks: 32

57.0328762 1433

59.03577939 1557

69.03277238 2582

81.03200571 1244

85.02699449 2302

86.09516594 12119

87.03037168 5529

88.03821076 8455

97.02743795 4148

98.09476184 1974

99.04197543 1264

112.0377101 3354

127.0375723 3195

128.1054449 3457

132.10041 6840

138.0529994 2045

143.0562261 4250

144.0999184 2192
 156.0637337 1441
 161.0666909 5134
 164.1052988 1976
 168.1002507 1271
 170.1161465 1217
 182.1158576 1108
 194.1151299 1378
 210.1107277 3397
 212.1265087 12943
 220.0808519 1267
 230.1373627 40490
 248.1481943 2689
 258.1324952 30153
 276.1430754 25431

Name: fructosyl Ile/Leu -H₂O

REF: PUBCHEM_SID_ 129689639

Precursor_type: [M+H]⁺

Comment: at RT 0.89 there is a very similar compound but at 294.098

Int_ref: BEOFIT November 2020 1.56_276.1431m/z

Ext-ref: DOI:10.1021/ac048925a amadori product, PR310824 mass bank

Formula: C₁₂H₂₁NO₆

Num Peaks: 20

57.0323673 342

59.03564198 437
69.03255266 463
85.02714011 525
86.09518348 2211
87.0299771 1013
88.03833261 1480
97.02737025 739
98.09534879 428
112.0375826 644
127.037869 545
128.1059009 468
132.0995579 726
143.0564936 596
161.0658553 791
210.1109185 366
212.1265152 1983
230.1376449 4594
258.132343 2731
276.1433623 1742

Name: fructosyl Ile/Leu hex

REF: PUBCHEM_SID_ 129689639

Precursor_type: [M+H]⁺

Comment: at RT 0.89 there is a very similar compound but at 294.098

Int_ref: BEOFIT November 2020 1.91_456.2059m/z

Ext-ref: DOI:10.1021/ac048925a amadori product, PR310824 mass bank

Formula: C₁₂H₂₃NO₇C₆O₅H₁₀

Num Peaks: 16

69.03234035 3594

85.0271753 7643

86.09511946 8689

88.03833302 5579

97.02733316 4084

127.037616 3790

132.1004501 8169

144.1004851 4111

164.1051415 4569

210.1111479 9813

212.1270785 9358

230.1377853 39457

248.1473259 4705

258.132861 32141

276.1433977 50009

438.1964969 3133

Name: fructosyl Ile/Leu hex -H₂O

REF: PUBCHEM_SID_ 129689639

Precursor_type: [M+H]⁺

Comment: at RT 0.89 there is a very similar compound but at 294.098

Int_ref: BEOFIT November 2020 1.84_438.1957m/z

Ext-ref: DOI:10.1021/ac048925a amadori product, PR310824 mass bank

Formula: C₁₂H₂₁NO₆C₆O₅H₁₀

Num Peaks: 30

57.03261834	186
69.03239102	501
81.03235282	246
85.02686376	987
86.09584335	1388
87.03192463	249
88.0376557	609
97.02678955	664
98.09427051	218
109.0272679	146
127.0368295	458
128.1042494	236
132.1001699	739
143.0547332	418
144.0992691	351
145.0477682	243
156.0638209	154
161.0673803	469
164.105041	686
168.1011041	213
182.1147297	184
194.1145211	213
210.1107858	1243
212.127609	1307

230.1376587 4514

240.1231707 134

248.1488776 500

258.1324441 3468

276.1435815 3749

392.1916182 229

Name: fructosyl Ile/Leu dihex

REF: PUBCHEM_SID_ 129689639

Precursor_type: [M+H]⁺

Comment: at RT 2.18 the same MS and MS/MS is this the difference between Ile and Leu? these two peaks correspond to the profile in figure 3 DOI:10.1021/ac048925a

Int_ref: BEOFIT November 2020 2.22_618.2589m/z

Ext-ref: DOI:10.1021/ac048925a amadori product, PR310824 mass bank

Formula: C₁₂H₂₃NO₇C₆O₅H₁₀C₆O₅H₁₀

Num Peaks: 19

85.02711137 617

86.09546838 302

88.03893583 175

97.02714346 227

127.035794 293

132.1004859 469

144.1007065 178

145.0480496 319

161.0663971 201

164.1052216 260

210.1108332 610
212.1272361 470
230.1380675 2071
248.1476016 324
258.1328167 2337
276.1428411 2875
392.1921172 148
420.1870502 133
438.1973133 320

Name: fructosyl Ile/Leu dihex -H₂O

REF: PUBCHEM_SID_129689639

Precursor_type: [M+H]⁺

Comment: at RT 2.18 the same MS and MS/MS is this the difference between Ile and Leu? these two peaks correspond to the profile in figure 3 DOI:10.1021/ac048925a

Int_ref: BEOFIT November 2020 2.22_600.2483m/z

Ext-ref: DOI:10.1021/ac048925a amadori product, PR310824 mass bank

Formula: C₁₂H₂₁NO₆C₆O₅H₁₀C₆O₅H₁₀

Num Peaks: 13

85.02721866 59
86.09691399 34
127.0371255 35
132.0989809 34
164.1049894 30
210.108705 70
212.1274782 105

230.1362273 193

248.1464519 30

258.1339841 153

276.1395766 326

392.1968998 24

438.2048169 30

Name: fructosyl Ile/Leu trihex

REF: PUBCHEM_SID_129689639

Precursor_type: [M+H]⁺

Comment: at RT 2.2 the same MS but no MS/MS is this the difference between Ile and Leu? these two peaks correspond to the profile in figure 3 DOI:10.1021/ac048925a

Int_ref: BEOFIT November 2020 2.61_780.3114m/z

Ext-ref: DOI:10.1021/ac048925a amadori product, PR310824 mass bank

Formula: C₁₂H₂₁NO₆C₆O₅H₁₀C₆O₆H₁₂C₆O₅H₁₀

Num Peaks: 13

85.02789966 148

127.0364889 57

132.1003268 69

145.0497981 54

164.1075119 56

210.1098605 329

212.1232763 127

230.1379382 352

240.1199405 52

258.1312435 449

276.1434444 690

420.1882822 49

438.1958597 152

Name: fructosyl Pro

REF: PUBCHEM_SID_ 129681495

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 0.59_278.1210m/z

Ext-ref: DOI:10.1021/ac048925a amadori product (280)

Formula: C₁₁H₁₉NO₇

Num Peaks: 12

70.06441063 5297

84.07970752 1256

100.074197 3616

112.0747803 1778

116.0694013 3714

128.069087 9982

154.0837436 1265

196.0953315 2105

214.1066137 10063

232.117119 7286

242.101484 18254

260.1125916 21161

Name: fructosyl Pro hex

REF: PUBCHEM_SID_129681495

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 0.59_440.1736m/z

Ext-ref: DOI:10.1021/ac048925a amadori product (280)

Formula: C₁₁H₁₇NO₆C₆O₆H₁₂

Num Peaks: 17

70.06434435 2158

85.02742922 1204

97.02726205 865

100.0745754 1840

116.0693375 2122

128.0691802 6261

180.1007047 675

194.0790813 742

196.0948543 1509

214.1062668 3443

232.1165459 3565

242.1016111 11540

260.1120302 11553

376.161813 1769

394.1708097 2443

404.155941 2606

422.1669249 5588

Name: fructosyl Pro hex -H₂O

REF: PUBCHEM_SID_129681495

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 0.59_422.1631m/z

Ext-ref: DOI:10.1021/ac048925a amadori product (280)

Formula: C₁₁H₁₇NO₆C₆O₅H₁₀

Num Peaks: 22

69.03355381 101

70.06469669 303

81.03235052 123

85.02881954 348

97.02633705 125

100.0740001 184

116.0698405 220

127.038345 114

128.0693275 688

154.0844953 70

180.1008084 134

194.0803798 157

196.0954105 231

212.0916389 67

214.1081785 493

232.1178176 514

242.1020784 1105

260.1137705 924

376.160914 171

394.1692056 252

404.152865 271

422.1716486 309

Name: fructosyl Tyr -H2O

REF: PUBCHEM_SID_ 129843880

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 1.01_326.1221m/z

Ext-ref: DOI:10.1021/ac048925a amadori product (344)

Formula: C₁₅H₁₉NO₇

Num Peaks: 31

69.03253328 293

85.0272264 298

87.03139855 177

91.05275845 231

95.04745179 200

97.02634903 231

99.95844789 166

103.0513905 208

107.0473385 545

112.0374034 197

119.0473927 500

121.0632492 712

123.0425201 999
127.0374399 240
127.9541624 171
136.0734694 930
143.9480684 306
144.0629992 233
146.0580194 300
147.0417587 631
148.0735781 1095
160.0746549 183
165.0530083 1016
182.0806849 274
189.9543497 275
214.0856733 163
260.0884505 183
262.1076185 268
280.1173791 1143
308.1128354 895
326.1201271 563

Name: fructosyl Tyr

REF: PUBCHEM_SID_129843880

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 1.01_343.1263m/z

Ext-ref: DOI:10.1021/ac048925a amadori product (344)

Formula: C₁₅H₂₁NO₈

Num Peaks: 51

57.03243203 362

69.03246334 1263

77.03702571 509

85.02739331 785

87.02989553 1152

91.05302379 1005

95.04765828 1439

96.04346936 346

97.02637142 1861

99.04219565 346

103.0522374 358

107.047587 2458

112.0374803 753

119.0475698 3747

121.0631343 1520

123.0425694 6544

127.0375395 1172

131.047569 287

133.0537966 513

135.0655396 626

136.0739686 6787

138.0530726 796

143.0559835 802

144.0636827 1588
145.0586352 303
146.0574546 1953
147.0424759 3445
148.0738904 9328
150.089657 291
156.0642312 697
160.0738337 1846
161.0661583 1237
162.0754232 476
165.0526644 7445
172.0732112 536
178.0842511 791
182.0803209 3354
184.066137 395
187.072395 410
194.0792241 1823
202.0728003 669
214.0842875 1084
218.0778498 310
220.0951037 438
244.0932852 438
260.0903717 1133
262.1064745 1809
280.1170073 11488
298.1276699 474

308.1122038 10058

326.1227149 8383

Name: fructosyl Tyr hex -H20

REF: PUBCHEM_SID_129843880

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 1.21_488.1737m/z

Ext-ref: DOI:10.1021/ac048925a amadori product (344)

Formula: C₁₅H₁₉NO₇C₆O₅H₁₀

Num Peaks: 40

57.0319736 12

69.03223164 24

73.02858132 12

85.0273755 32

86.09495045 24

91.05159756 12

97.02591605 30

107.0488717 18

109.0272728 12

119.0483287 12

121.0605576 18

123.042812 12

127.0368297 30

132.0994282 18

136.0741131 56
143.052465 12
144.0687791 30
145.0507874 18
147.0434685 18
148.0756709 147
152.1101314 12
160.0779147 12
161.067226 12
165.052957 53
174.0879081 12
182.0820134 47
184.0617676 18
194.0805514 31
214.0843113 18
218.0772009 12
227.9745101 12
260.0912859 44
262.1064706 30
280.1168767 76
298.1298981 12
308.1147719 75
325.1338097 12
326.1254424 113
488.1810156 12
488.2895205 12

Name: fructosyl Tyr hex

REF: PUBCHEM_SID_129843880

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 1.21_506.1847m/z

Ext-ref: DOI:10.1021/ac048925a amadori product (344)

Formula: C₁₅H₁₉NO₇C₆O₆H₁₂

Num Peaks: 20

69.03273411 399

85.02702891 637

97.0272991 576

119.0485484 430

123.042817 432

127.0382805 446

136.0739928 1315

144.0651198 416

147.0429802 469

148.0742577 2049

160.0744668 358

165.0530488 1652

182.0797296 1340

194.0807971 628

214.0858098 314

260.0913096 1162

262.1073152 475
280.1174388 2633
308.1123694 3950
326.1242855 4522

Name: fructosyl Tyr dihex

REF: PUBCHEM_SID_129843880

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 1.32_668.2378m/z

Ext-ref: DOI:10.1021/ac048925a amadori product (344)

Formula: C₁₅H₁₉NO₇C₆O₆H₁₂C₆O₅H₁₀

Num Peaks: 19

85.02683517 239
97.02673101 146
123.0413047 88
127.0381994 123
136.073756 287
144.0653281 81
145.047404 81
148.0747561 305
165.0538675 348
182.0806001 434
194.0795984 166
214.0839506 103
260.0890655 275

262.1073559 115
 280.1174902 785
 298.1299355 212
 308.1129985 1101
 326.1236204 1528
 488.1787467 106

Name: fructosyl Phe

REF: PUBCHEM_SID_193670

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 2.883_328.1373m/z

Ext_ref: DOI:10.1021/ac048925a

Formula: C₁₅H₂₁NO₇

Num Peaks: 23

69.03253859 902
 87.02992916 1283
 91.05307105 2079
 97.02693959 1665
 103.0531811 1198
 105.0686867 1196
 112.0383379 1296
 120.0797605 9628
 127.0379137 1090
 130.0634306 2282

132.0797046 8975
143.0567644 1297
144.0789903 1730
161.0658483 1351
162.0898119 1304
166.0854564 2765
178.0852782 1339
198.0897307 1041
244.0968975 1390
246.1116373 2728
264.1222164 9002
292.1175786 9132
310.1284437 6103

Name: fructosyl Phe -H₂O

REF: PUBCHEM_SID_193670

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 2.883_310.1271m/z

Ext_ref: DOI:10.1021/ac048925a

Formula: C₁₅H₁₉NO₆

Num Peaks: 17

87.03022058 188
91.05272831 400
97.02643049 250
103.0523374 283

105.0691395 217
 112.0386038 223
 120.079178 1011
 130.0640421 336
 132.0788639 894
 143.0572759 247
 144.0801762 249
 156.0786429 120
 166.0829172 227
 246.1112915 245
 264.1221657 609
 292.1178195 536
 310.1304098 174

Name: fructosyl Phe -2H₂O

REF: PUBCHEM_SID_193670

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 2.883_292.1174m/z

Ext_ref: DOI:10.1021/ac048925a

Formula: C₁₅H₁₇NO₅

Num Peaks: 9

91.05463842 30

97.02767542 31

112.0371674 24

120.080482 24
130.0635423 24
132.0795512 30
147.0444849 77
246.1072057 24
292.1246464 30

Name: fructosyl Phe hex

REF: PUBCHEM_SID_193670

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 3.622_490.1899m/z

Ext_ref: DOI:10.1021/ac048925a

Formula: C₁₅H₂₁NO₇C₆O₅H₁₀

Num Peaks: 32

57.03281322 287
69.03247782 555
81.03224431 258
85.02724372 1364
91.05247413 299
97.02731953 688
120.0790507 2604
127.0375879 731
130.0633246 627
131.0458193 229
132.0796562 2717

143.0565112	596
143.0846502	230
144.0784338	499
145.050008	257
156.0772214	277
161.066306	386
162.0902278	299
166.0849545	2446
171.0787285	423
178.085199	980
198.0900713	977
202.0857285	343
228.1011539	251
244.0966115	2003
246.1117392	1430
264.1225803	4539
282.1316577	292
292.1182244	5484
310.1291743	7037
426.1725275	315
472.1821595	358

Name: fructosyl Phe hex -H₂O

REF: PUBCHEM_SID_193670

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 3.622_472.1796m/z

Ext_ref: DOI:10.1021/ac048925a

Formula: C₁₅H₁₉NO₆C₆O₅H₁₀

Num Peaks: 11

85.02740236 331

120.080352 281

127.0386686 125

132.0801876 330

166.0844202 185

178.0850875 226

244.0965214 243

246.112786 128

264.1245051 742

292.1177414 448

310.1273596 514

Name: fructosyl Phe dihex

REF: PUBCHEM_SID_193670

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 4.478_652.2424m/z

Ext_ref: DOI:10.1021/ac048925a

Formula: C₁₅H₂₁NO₇C₆O₅H₁₀C₆O₅H₁₀

Num Peaks: 21

85.02686472 304

97.02634082 39
120.0795521 180
127.0357316 80
130.0647251 36
132.0796176 286
145.0511378 58
156.0780661 30
161.0639112 30
166.0850654 245
171.0770052 32
178.0848622 258
198.08921 50
228.097091 48
244.0946659 219
246.1132531 68
264.1228872 307
282.1318109 33
292.1160017 545
310.1272036 689
472.1821229 50

Name: fructosyl Phe dihex -H₂O

REF: PUBCHEM_SID_193670

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 4.478_634.2306m/z

Ext_ref: DOI:10.1021/ac048925a

Formula: C₁₅H₁₉NO₆C₆O₅H₁₀C₆O₅H₁₀

Num Peaks: 14

85.02824592 24

97.03071295 24

120.0823033 18

127.0344592 18

132.0811852 65

178.0836313 24

198.0875051 24

244.1054653 24

246.1220528 12

264.1313312 42

282.1403728 12

292.115348 123

310.1293676 116

472.1822391 12

Name: fructosyl Met -H₂O

REF: PUBCHEM_SID_5487578

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 0.85_294.0987m/z

Ext_ref: CCMSLIB00005467655

Formula: C₁₁H₁₉NO₆S

Num Peaks: 20

56.04858715 102

61.00942309 136

81.03133615 114

84.07949297 176

85.02648237 94

87.02735942 89

88.0389631 100

104.0513717 67

120.0814073 253

127.0353256 127

130.087261 71

133.0302123 292

138.0532552 153

143.0570671 84

147.1110974 187

150.0559948 92

212.0725325 64

230.0822212 177

248.0945372 94

276.0902701 256

Name: fructosyl Met hex

REF: PUBCHEM_SID_5487578

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 0.8596_474.1620m/z

Ext_ref: CCMSLIB00005467655

Formula: C₁₁H₂₁NO₇SC₆O₅H₁₀

Num Peaks: 14

81.03222551 254

85.02680801 292

88.03891079 225

97.02805441 186

127.0386028 169

133.0293205 560

150.0566915 275

212.070727 304

228.06639 415

230.0814075 492

248.0930246 207

258.0783724 230

276.0897726 1313

294.0998973 647

Name: fructosyl Trp

REF: PUBCHEM_SID_71316984

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 5.36_367.1476m/z

Ext_ref: CCMSLIB00005467655

Formula: C₁₇H₂₂N₂O₇

Num Peaks: 29

69.03182116	78
118.0642117	368
129.0671305	123
130.063101	710
132.0793532	283
143.0714852	157
144.0787161	745
146.0579514	1149
154.0587158	74
156.0789837	624
158.0906448	102
167.0720615	76
168.0779857	291
170.0586885	369
172.0612958	131
180.0789368	139
183.0900801	312
184.0775095	147
188.068239	1029
198.0920378	89
202.0816167	195
218.0642885	117
229.0965931	649

230.0802631 148

258.1080577 314

276.1211917 166

303.134389 168

332.111995 447

349.1404183 137

Name: fructosyl Trp -H₂O

REF: PUBCHEM_SID_71316984

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 5.36_349.1371m/z

Ext_ref: CCMSLIB00005467655

Formula: C₁₇H₂₀N₂O₆

Num Peaks: 10

130.0660335 62

144.0790344 31

146.058903 99

156.0786455 47

168.0800644 45

170.0591226 34

188.0669733 55

229.0973091 39

276.1202019 30

332.1090802 30

Name: fructosyl Trp hex

REF: PUBCHEM_SID_71316984

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 6.44_529.2007m/z

Ext_ref: CCMSLIB00005467655

Formula: C₁₇H₂₂N₂O₇C₆O₅H₁₀

Num Peaks: 13

85.02641576 222

130.0625374 173

144.0784288 265

146.0584384 241

156.0790524 387

168.0789925 151

183.0902756 154

188.0681946 278

202.0863222 107

229.0950145 839

276.1224578 262

332.1100677 247

349.1383808 148

Name: fructosyl Trp hex -H₂O

REF: PUBCHEM_SID_71316984

Precursor_type: [M+H]⁺

Comment:

Int_ref: BEOFIT November 2020 6.44_511.1901m/z

Ext_ref: CCMSLIB00005467655

Formula: C₁₇H₂₀N₂O₆C₆O₅H₁₀

Num Peaks: 24

85.02580015 12

118.0600563 12

129.0615848 12

130.0655955 18

132.0817205 12

144.078659 42

146.0547914 18

152.0414901 12

156.0755881 30

168.0831489 12

170.0525156 12

183.0844941 12

186.0842463 12

188.0656855 18

229.0938932 48

240.0955152 12

250.083482 12

254.0777053 12

258.1083366 24

276.1228516 18

296.0949259 18

331.1319318 12

332.1152155 18

349.1435234 12

Name: fructosyl GABA -H₂O

REF: PUBCHEM_SID_131752417

Precursor_type: [M+H]⁺

Comment: compound without the loss of H₂O also observed (266.12080) amadori product of GABA and glucose, found in beer and malt Nachweis von Maillard-Produkten in Malzen, Bieren und Braucouleuren (Wittmann & Eichner)

Date: 01062021

Int_ref: BEOFIT November 2020 0.55_248.1104m/z

Ext_ref: CCMSLIB00005467684

Formula: C₁₀H₁₇NO₆

Num Peaks: 12

70.06508606 165

80.97393573 92

97.02865078 96

98.05953061 97

98.98358803 1664

116.0686034 98

128.0706671 107

173.0221794 122

174.0221221 106

182.0818627 113

230.1029698 248

248.1141245 323

Name: fructosyl GABA

REF: PUBCHEM_SID_131752417

Precursor_type: [M+H]⁺

Comment: compound without the loss of H₂O also observed (266.12080) amadori product of GABA and glucose, found in beer and malt Nachweis von Maillard-Produkten in Malzen, Bieren und Braucouleuren (Wittmann & Eichner)

Date: 01062021

Int_ref: BEOFIT November 2020 0.55_266.1224m/z

Ext_ref: CCMSLIB00005467684

Formula: C₁₀H₁₉NO₇

Num Peaks: 16

69.03401157 333

70.06450047 689

86.05897049 695

87.04408123 775

97.02846954 412

98.05993995 1646

116.0706117 1108

127.0401677 410

128.0695922 362

182.0830882 566

194.0837558 262

202.1071066 252

212.0911393 285

230.1015916 1457

248.1136009 3684

266.1240053 656

Name: fructosyl GABA hex

REF: PUBCHEM_SID_131752417

Precursor_type: [M+H]⁺

Comment: compound without the loss of H₂O also observed (266.12080) amadori product of GABA and glucose, found in beer and malt Nachweis von Maillard-Produkten in Malzen, Bieren und Braucouleuren (Wittmann & Eichner)

Date: 01062021

Int_ref: BEOFIT November 2020 0.55_428.1734m/z

Ext_ref: CCMSLIB00005467684

Formula: C₁₀H₁₉NO₇C₆O₅H₁₀

Num Peaks: 15

69.03378584 368

70.06586181 360

85.02804721 493

86.06023261 330

87.04406207 306

97.02830229 327

98.06004238 869

116.0701078 933

164.0703008 334

182.0811561 1111

194.0818117 515

212.0928201 361

230.1016639 1630

248.1130439 4668

410.1679969 981

Name: fructosyl Lys

REF: PUBCHEM_SID_9839580

Precursor_type: [M+H]⁺

Comment: DOI:10.1021/acs.jafc.0c06193

Date: 07062021

Int_ref: BEOFIT december 2020 0.51_309.1636m/z

Ext_ref: CCMSLIB00005720267 splash10-004i-3692000000-8a3352808a87f62f61af

Formula: C₁₂H₂₄N₂O₇

Num Peaks: 19

81.03179337 117

84.04457917 216

84.08087989 322

85.03054745 249

97.02752629 177

122.0597543 253

126.0563507 85

128.0708357 153

130.0509128 249

134.0597541 121

154.0498134 75

192.067082 96

208.0589631 470

225.0857408 776

238.0775067 221

255.0904442 68

256.0997491 78

273.1092528 272

291.1259507 86

Name: fructosyl Arg

REF: PUBCHEM_SID_129825164

Precursor_type: [M+H]⁺

Comment: +Hex also present but mass used by Progenesis does not correspond with the mass observed in peakview <https://doi.org/10.1021/acsomega.6b00220>, MS/MS below 175 (Arg - H₂O) identical to that of Arg, highly quoted as health promoting

Date: 08062021

Int_ref: BEOFIT december 2020 0.51_337.1729m/z

Ext_ref: <https://doi.org/10.1021/acsomega.6b00220> supplemental fig 1 for Arg
CCMSLIB00003138816

Formula: C₁₂H₂₄N₄O₇

Num Peaks: 16

60.05425294 18

69.03285663 30

70.06539753 111

81.03226891 18

98.98577606 33

112.0860893 18

114.1035804 12

116.0675415 18

129.0540242 24
158.0902759 18
175.116074 73
198.1083347 24
242.1032197 18
319.1440095 12
319.1805314 12
337.1662826 83

Name: fructosyl Gly -H₂O

REF: PUBCHEM_SID_3081391

Precursor_type: [M+H]⁺

Comment: DOI:10.1021/ac048925a

Date: 08062021

Int_ref: BEOFIT december 2020 0.51_220.0808m/z

Ext_ref: DOI:10.1021/ac048925a figure 2

Formula: C₈H₁₃NO₆

Num Peaks: 11

60.04486704 30
69.03205069 53
81.03267919 65
88.03795187 116
97.02757029 167
143.0580013 30
156.0606196 53
174.0769146 30

202.0684659 190

205.1650079 50

220.0811402 37

Name: fructosyl His hex

REF: PUBCHEM_SID_131752243

Precursor_type: [M+H]⁺

Comment:

Date: 09062021

Int_ref: BEOFIT december 2020 0.51_480.1792m/z

Ext_ref: <https://doi.org/10.1021/jf501464g> figure S4

Formula: C₁₂H₁₉N₃O₇C₆O₅H₁₀

Num Peaks: 19

85.03099219 24

95.05868451 117

97.02897837 24

98.98384821 30

110.0714603 18

140.0736898 18

155.0063749 37

156.073908 30

190.0938092 167

198.081676 18

220.1041498 61

236.1070101 18

238.1169677 18
272.1155705 18
318.1241774 24
365.1006436 42
400.1778852 50
462.2032353 18
480.1622583 18

Name: fructosyl Ala -H₂O

REF: PUBCHEM_SID_129636428

Precursor_type: [M+H]⁺

Comment:

Date: 09062021

Int_ref: BEOFIT december 2020 0.55_234.0970m/z

Ext_ref: DOI:10.1021/ac048925 table 2

Formula: C₉H₁₅NO₆

Num Peaks: 17

56.04988494 845
74.06004458 338
87.03084728 539
90.05425706 387
97.02853193 619
102.0546584 684
112.0394984 482
122.059025 302
127.0381283 387

143.0577442	667
152.0726271	250
161.0694398	318
168.0636395	251
170.0809022	789
188.0922098	1028
216.0867972	1903
234.0975977	730