Patient-specific interpretation of urinary profiles

Name:	Example report	Diagnosis:	
Participant DOB:		Sample Number:	Example report
Date of analysis:			

Estimation of urinary specific gravity (SG) was carried out by refractometry. Sample analysis of raw urine fractions was conducted using an Agilent 6530 QTOF Mass Spectrometer coupled with an Agilent 1200 series HPLC system with UV-DAD (Ultra Violet - Diode Array Detection) using an Onyx C18 monolithic column (100x3mm). Graph (a) shows UV detection at 250nm, graph (b) shows UV detection at 320nm.

The estimated specific gravity (SG) of this sample was: **1.020 (kg/L).**

Results indicate that levels of urinary *trans*-indolyl-3-acryloylglycine (IAG) are present in this sample as shown by the peak highlighted on graph (a) at **15.505 minutes** and confirmed on graph (b) at **15.506 minutes.** Confirmation of the presence of IAG in the sample is provided on graph (c) and (d). Table (e) shows the relative abundance of IAG detected in the sample by QTOF Mass Spectrometry.

Based on the QTOF integrated data for IAG and estimated SG values, the amount of IAG estimated to be present in this sample is:

IAG abundance (cps*) = 383876 / SG = 376349.01 cps / kg/L

*cps =counts per second

Given the presence of IAG, it would normally be most prudent to attempt a gluten free diet (if it is not already in place) with the purpose of ameliorating some of the symptoms. Preliminary studies have suggested that levels of IAG decrease following the use of a gluten free diet (accompanied by behavioural improvements in many cases of autism spectrum disorders) after several months on dietary intervention. We are currently looking at this relationship more closely. There are a number of caveats that may influence the level of any improvement gained. These include: the chronological age of the person (younger children tend to be best responders) and the level of severity of behaviours (the more severely affected persons show the most positive effects). We always advise that you consult with your medical clinician before implementing any dietary changes.

Sample identification number and participant details are shown.

An estimate of the specific gravity (S/G) of the sample is provided.

The presence of IAG indicated by retention time (in minutes) is indicated on one or both Ultra-Violet (UV) wavelengths measured.

An estimate of the amount of IAG is shown based on the abundance value of IAG derived from the QTOF MS data as a ratio of the sample SG.

Based on the presence of IAG and an estimate of the amount present a recommendation is made on whether a gluten-free diet may be potentially useful or not based on our previous studies.

Analysis of the sample showed one or more specific target gluten-derived peptides listed below to also be present in the sample.

Gluten peptides

- Gluten exorphin A5
- Gluten exorphin B5 * mass = 595.2901
- Gluten exorphin C

The presence of these peptides provides further evidence for the possible introduction of a gluten-free diet.

Analysis of the sample showed one or more specific target casein-derived peptides listed below to be possibly present in the sample.

Casein peptides

- beta-casomorphin 1-3 amide
- beta-casomorphin 1-4 amide
- beta-casomorphin 1-4 acetate
- beta-casomorphin 1-5 amide * mass = 579.2931
- beta-casomorphin 1-5 acetate
- beta-casomorphin 1-6 acetate
- beta-casomorphin 1-7 acetate

The presence of one or more casein-derived peptides would suggest that a casein-free diet may also be useful in ameliorating symptoms. Due to the rapid excretion of casein peptides from the body, we normally suggest an initial trial period of between 4-5 weeks using the casein-free diet. Again, we always advise that you consult with your medical clinician before implementing any dietary changes.

Summary

1. IAG present as largest peak in relevant area.
2. Detection of gluten-derived peptide/s
3. Detection of casein-derived peptide/s

The presence of one or more gluten-derived peptides is indicated based on QTOF MS analysis. Where a particular compound matching the mass of the peptide/s has been detected, the results are highlighted. A recommendation is made for use of a gluten-free diet based on the result.

The presence of one or more casein-derived peptides is indicated based on QTOF MS analysis. Where a particular compound matching the mass of the peptide/s has been detected, the results are highlighted. A recommendation is made for use of a casein-free diet based on the result.

A summary is provided on the main findings. Any decision to implement dietary intervention should be carried out under the guidance of a healthcare practitioner

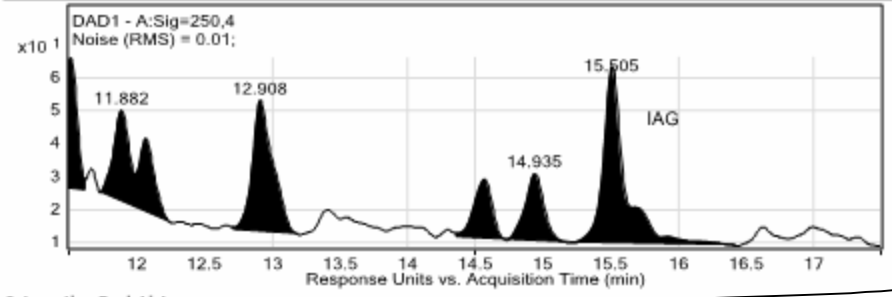
Qualitative Analysis Report

Data Filename	Example report	**Sample Name**	Example report
Sample Type	Example report	**Position**	Example report
Instrument Name	Instrument 1	**User Name**	
Acq Method	urine std.m	**Acquired Time**	Example report
IRM Calibration Status	Success	**DA Method**	urine std.m
Comment			

Sample identification details are provided.

User Chromatograms

(a)



Graph (a) shows truncated results based on UV data at 280nm. Where IAG is present it will be indicated and the appropriate peak highlighted.

Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	1.487	1.663	1.759	1136.57	6561.24	42.6	76676.8
2	1.759	1.805	1.931	103.99	620.56	4.03	7015.5
3	1.934	2.05	2.161	1206.29	6047.12	39.26	81380.2
4	2.161	2.369	2.528	2127.73	15402.1	100	143543.5
5	2.528	2.632	2.821	314.21	2066.71	13.42	21197.3
6	2.821	2.917	2.987	22.29	159.45	1.04	1504
7	2.987	3.331	3.574	169.63	2562.92	16.64	11443.6
8	3.602	4.003	4.038	40.01	477.32	3.1	2699.1
9	4.038	4.166	4.405	141.59	1390.22	9.03	9551.9
10	4.407	4.57	4.82	314.12	2222.64	14.43	21191.6
11	4.841	5.009	5.244	928.81	7611.9	49.42	62660.4
12	5.244	5.35	5.459	486.25	3080.13	20	32804
13	5.459	5.516	5.559	58.56	252.03	1.64	3950.6
14	5.559	5.607	5.714	104.32	531.37	3.45	7037.6
15	5.742	5.828	5.901	76.43	322.27	2.09	5156.3
16	5.901	5.989	6.069	109.9	518.49	3.37	7414
17	6.161	6.311	6.487	88.6	705.89	4.58	5977
18	6.561	6.7	6.756	451.79	2667.64	17.32	30479.3
19	6.756	6.776	6.926	334.74	1509.81	9.8	22582.7
20	6.926	7.003	7.087	90.79	384.25	2.49	6124.9
21	7.154	7.263	7.323	77.75	445.89	2.89	5245.2
22	7.323	7.353	7.441	56.96	240.99	1.56	3842.9
23	7.555	7.6	7.645	38.45	198.26	1.29	2594.1
24	7.645	7.679	7.858	36.41	221.89	1.44	2456.6
25	7.858	7.992	8.033	27.7	184.86	1.2	1868.9
26	8.033	8.126	8.281	50.92	390.16	2.53	3434.9
27	8.474	8.799	9.091	991.26	9347.45	60.69	66873.3
28	9.091	9.193	9.378	55.61	502.18	3.26	3751.7
29	9.378	9.551	9.652	23.01	208.98	1.36	1552.3
30	9.652	9.73	9.92	43.23	233.57	1.52	2916.5

Various data relating to graph (a) is shown. This information provides assistance is ascertaining whether IAG is present as a significant peak in the profile. This information may continue on to the next sheet depending on how many peaks are identified.

Qualitative Analysis Report

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
31	9.934	10.094	10.208	24.8	173.98	1.13	1673.2
32	10.208	10.348	10.606	44.44	432.89	2.81	2997.9
33	10.907	11.02	11.123	26.55	215.36	1.4	1791.5
34	11.123	11.224	11.37	36.17	312.48	2.03	2440.3
35	11.37	11.508	11.616	39.71	330.75	2.15	2678.9
36	11.728	11.882	11.985	27.62	225.31	1.46	1863.3
37	11.985	12.062	12.247	22.28	173.31	1.13	1503.4
38	12.714	12.908	13.194	39.93	423.04	2.75	2693.7
41	15.202	15.505	16.42	53.61	605.21	3.93	3616.9
42	25.334	26.21	28.187	22.18	1245.34	8.09	1496.6

Noise Measurements

Noise Type	Signal Definition	Noise Multiplier	Noise Value
RMS	Height	1	0.01482292

Noise Regions

Start	End
0.65	0.85

(b)

Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	1.601	1.621	1.661	6.59	14.74	1.11	912.1
2	1.534	1.671	1.746	38.16	302.01	22.76	5283.2
3	1.746	1.803	1.931	28.16	235.01	17.71	3899.3
4	1.931	2.027	2.213	23.72	214.61	16.17	3283.7
5	2.214	2.37	2.507	72.59	443	33.39	10051.3
6	2.507	2.579	2.627	4.91	22.52	1.7	679.3
7	2.627	2.694	2.767	11.27	61.55	4.64	1560.2
8	2.767	2.866	3.134	19.97	181.36	13.67	2764.9
12	3.994	4.166	4.285	18.94	159.68	12.03	2622.8
13	4.285	4.353	4.463	9.6	60.15	4.53	1328.6
14	4.463	4.569	4.727	18.86	115.05	8.67	2610.7
16	4.996	5.072	5.253	5.32	39.92	3.01	735.9
17	5.253	5.394	5.534	4.91	32.63	2.46	679.6
18	5.701	5.861	5.893	5.91	30.59	2.31	818
19	5.893	5.972	6.181	10.72	80.05	6.03	1483.8
20	6.201	6.325	6.484	15.77	100.98	7.61	2183.6
21	6.581	6.801	6.951	88.03	576.38	43.44	12189.2
22	6.951	7.007	7.127	3.9	17.97	1.35	540.6
23	7.134	7.254	7.361	3.9	22.46	1.69	540.1
24	7.365	7.568	7.821	5.51	60.44	4.56	763
25	7.822	7.942	8.043	4.66	34.77	2.62	645.7
26	8.043	8.108	8.163	3.32	20.42	1.54	459.6

Graph (b) shows truncated results based on UV data at 320nm. Where IAG is present it will be indicated and the appropriate peak highlighted.

Various data relating to graph (b) is shown. This information provides assistance is ascertaining whether IAG is present as a significant peak in the profile. This information may continue on to the next sheet depending on how many peaks are identified.

Qualitative Analysis Report

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
28	8.461	8.59	8.694	5.25	36.22	2.73	727
29	8.907	9	9.087	7.93	42.76	3.22	1098.4
30	9.087	9.241	9.367	30.34	233.89	17.63	4201.4
31	9.367	9.426	9.527	4.8	28.59	2.15	664.8
33	10.134	10.331	10.634	14.51	123.75	9.33	2009.4
34	10.635	10.808	10.913	6.27	48.22	3.63	868.6
36	11.194	11.498	11.727	65.64	664.28	50.07	9088.3
37	11.728	11.875	11.986	9.66	82.23	6.2	1337.9
38	11.986	12.031	12.207	4.35	29.33	2.21	602.3
39	12.208	12.325	12.72	4.77	50.21	3.78	661
40	12.735	12.99	13.214	12.22	129.58	9.77	1691.8
43	14.228	14.518	14.754	8.69	87.14	6.57	1203
44	15.232	15.506	15.879	162.11	1326.83	100	22445.5
45	15.879	16.03	16.547	3.59	48.77	3.68	496.4
47	19.734	19.899	20.481	4.83	72.27	5.45	668.6
48	20.521	20.71	20.906	4.59	34.85	2.63	635.7
49	23.647	24.078	24.282	8.69	129.36	9.75	1203.3
50	24.282	24.397	24.721	10.97	99.17	7.47	1519.3

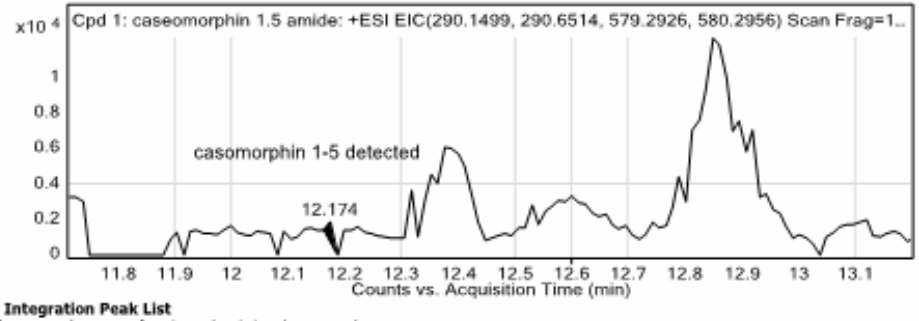
Noise Measurements

Noise Type	Signal Definition	Noise Multiplier	Noise Value
RMS	Height	1	0.007222356

Noise Regions

Start	End
0.65	0.85

Compounds

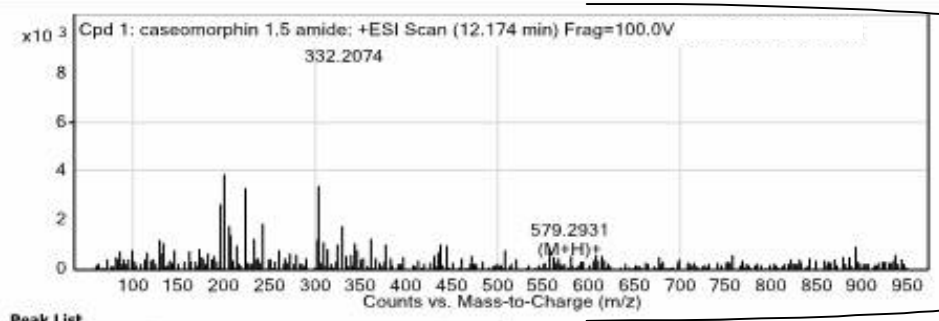


Integration Peak List

Start	RT	End	Height	Area
12.162	12.174	12.186	1149	318

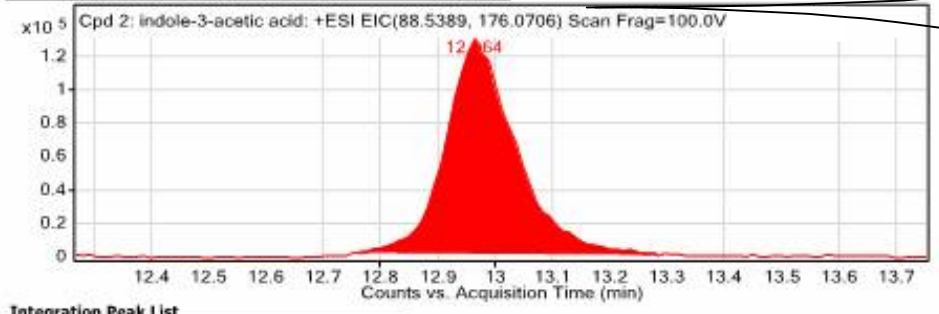
Where compounds that share the same mass as the target peptides have been isolated by QTOF MS in the sample, information is provided on the appearance of the target compound.

Qualitative Analysis Report



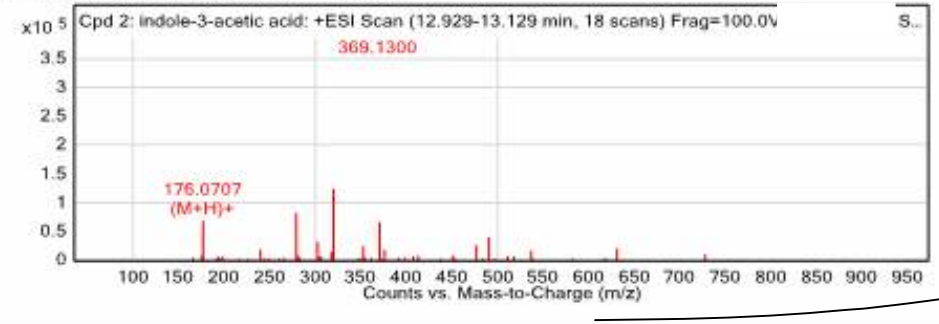
Peak List

m/z	z	Abund	Formula	Ion
329.2133		1755		
329.601		306		
330.2273		1107		
331.2299		331		
331.6274		338		
332.2074		8637		
332.7092		302		
333.2096		557		
334.1809		318		
579.2931	1	318	C30 H39 N6 O6	(M+H)+



Integration Peak List

Start	RT	End	Height	Area
12.764	12.964	13.282	128494	1084488



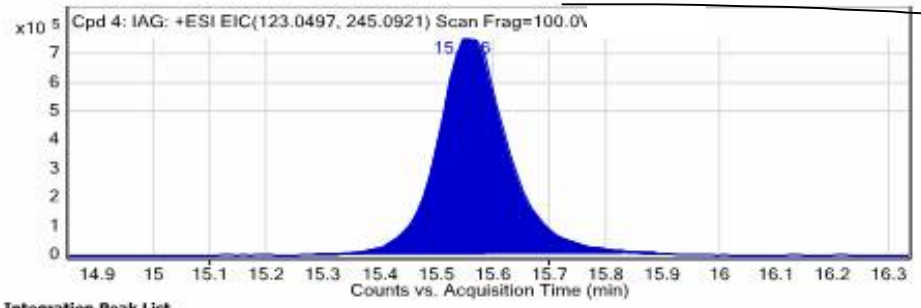
QTOF MS data shows the accurate mass of the compound detected.

The mass and abundance of the compound is provided alongside information about the chemical formula of the compound and the detection.

Details of various other compounds not included in the current analysis are also shown with results. At the present time these compounds are not relevant to the results provided.

Qualitative Analysis Report

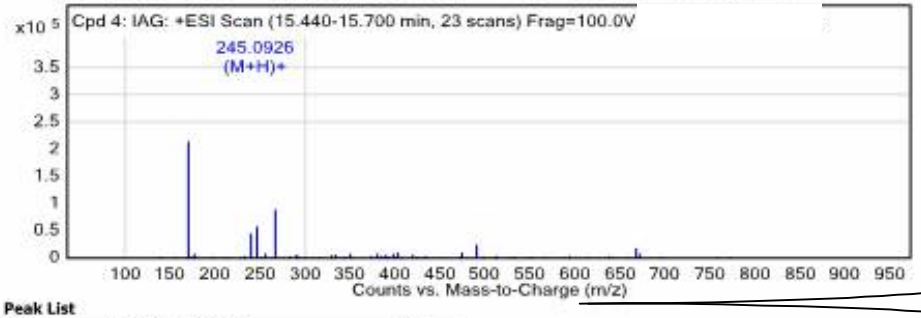
(c)



Integration Peak List

Start	RT	End	Height	Area
15.287	15.546	15.888	748412	6554258

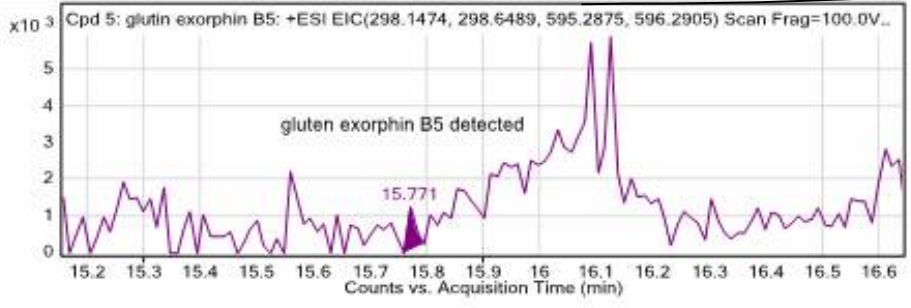
(d)



(e)

Peak List

m/z	Abund	Formula	Ion
240.1426	6871		
241.136	1682		
242.133	461		
244.085	429		
245.0926	383876	C13 H13 N2 O3	(M+H)+
245.232	6921		
245.2866	698		
246.0956	57529	C13 H13 N2 O3	(M+H)+
246.2346	800		
249.1301	848		



Graph (c) shows the isolation of IAG based on QTOF MS analysis.

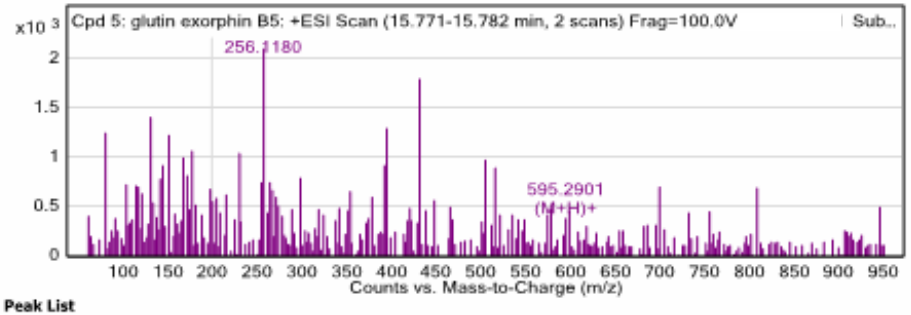
Graph (d) shows the QTOF MS data of the accurate mass of the compound detected.

Graph (e) shows the QTOF MS data on mass and abundance of IAG alongside information about the chemical formula of the compound and the detection.

Qualitative Analysis Report

Integration Peak List

Start	RT	End	Height	Area
15.759	15.771	15.794	1171	1193



Peak List

m/z	z	Abund	Formula	Ion
251.1318		176		
252.1424		357		
252.6297		149		
253.1447		747		
254.1465		170		
256.118		2097		
257.1476		549		
258.1333		185		
260.0242		447		
595.2901	1	363	C30 H39 N6 O7	(M+H)+

--- End Of Report ---