Supporting Information for:

Statistical correlations between NMR spectroscopy and direct infusion FT-ICR mass spectrometry aid annotation of unknowns in metabolomics

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Figure S1: Numbers of adducts matched of each type, corresponding to categories of ROC curves (Figure 2).

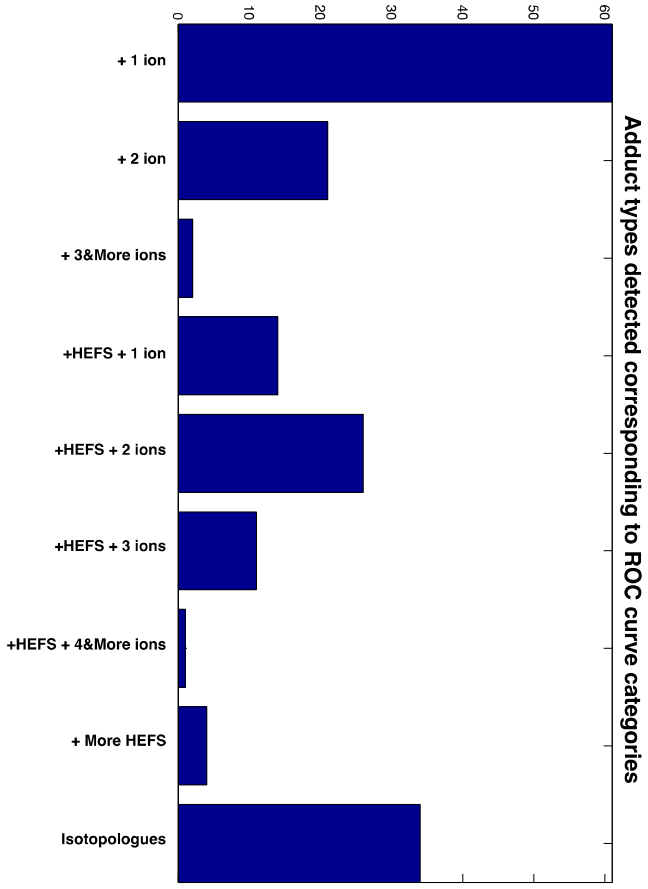

Figure S2: Numbers of adducts matched of each subtype.

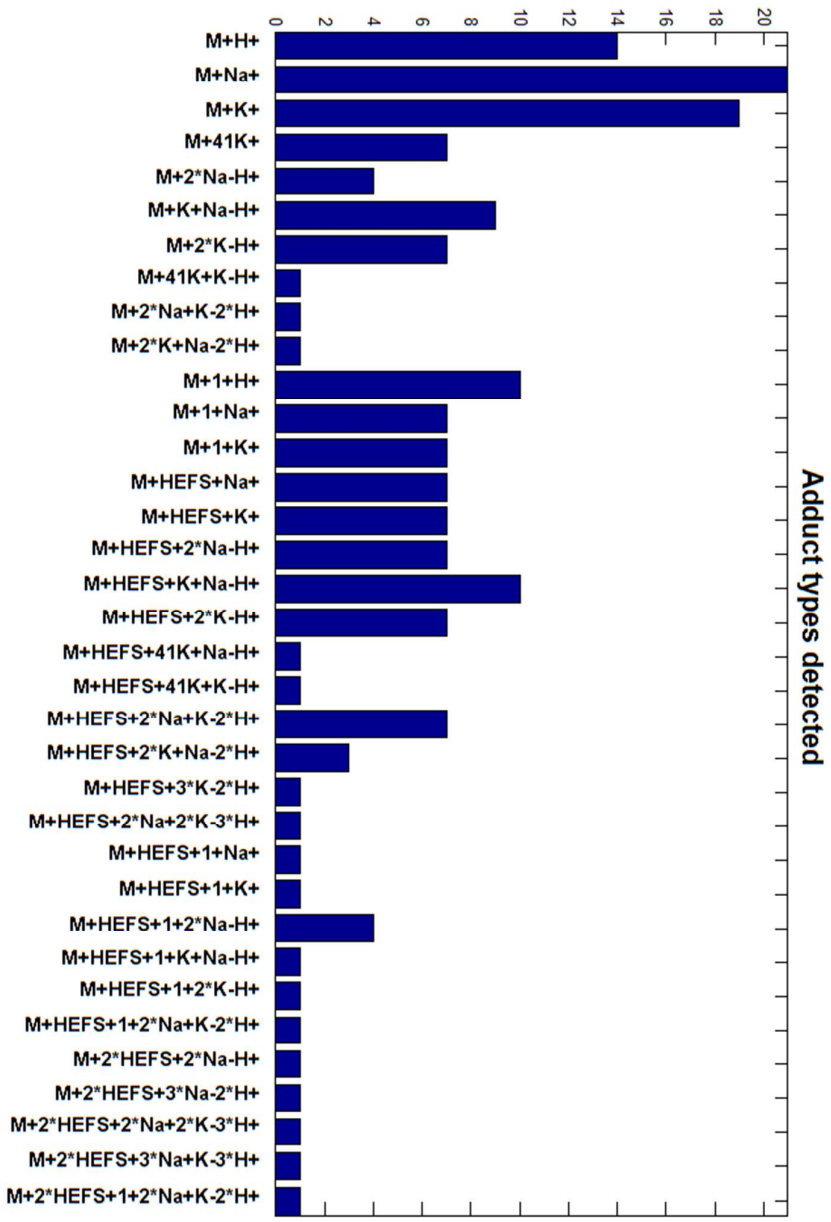

Figure S3: Distribution of NMR-DIMS correlations for the null test.

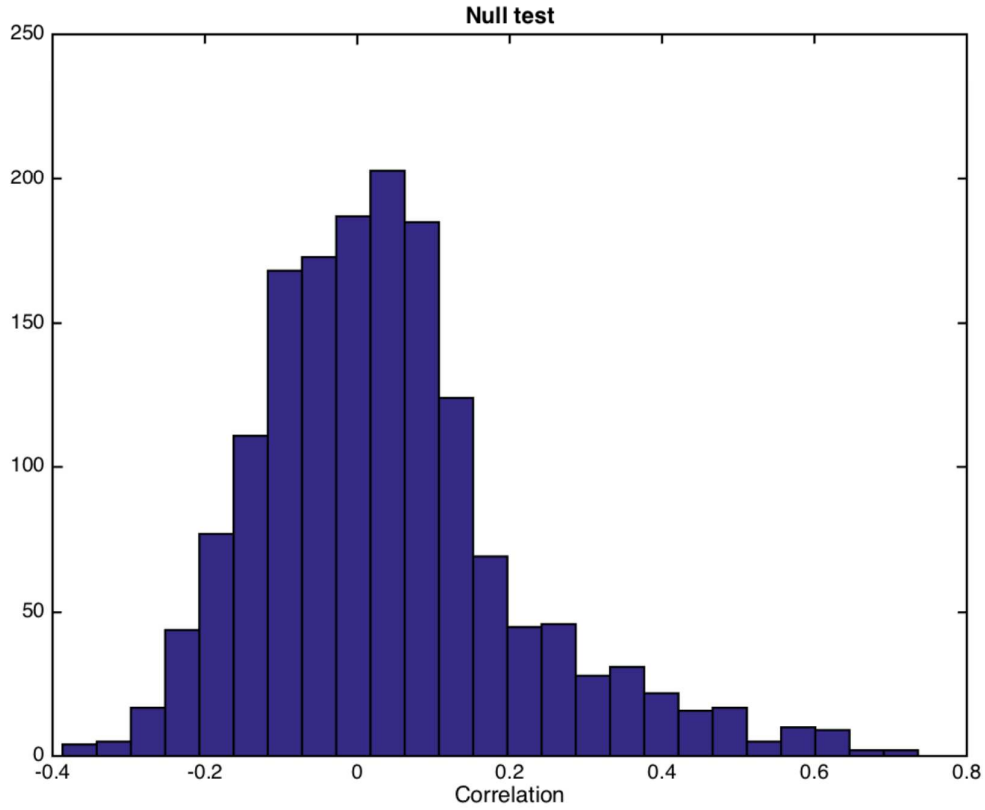

Table S1: Metabolite assignments in NMR and DIMS data. See Excel file SI Table 1.xslx.

Table S2: Top ranked correlations for 2-methyalanine NMR signal. Annotations are from MI-Pack.

2-methylalanine			ppm 1.48~1.49
Rank	Correlation	m/z	Metabolite
1	0.50615	496.3647	
2	0.49451	479.3209	
3	0.4929	478.3177	
4	0.48772	477.2626	
5	0.48769	303.218	Emedastine M+H+
6	0.4861	423.3029	
7	0.47538	422.2995	
8	0.4751	477.8615	
9	0.47051	189.1234	6-Acetamido-3-aminohexanoate,Glycyl-leucine,N6-Acetyl-L-lysine, M+H+
10	0.46411	239.6624	
11	0.46279	440.3101	
12	0.46217	441.3135	
13	0.46099	439.3067	
14	0.45675	104.0706	2-methylalanine M+H+,(R)-3-Amino-2-methylpropanoate,(S)-2-Aminobutanoate,2-Amino-2-methylpropanoate,3-Aminoisobutyric acid,4-Aminobutanoate,D-2-Aminobutyrate,H+D59BA,L-3-Amino-isobutanoate,N,N-Dimethylglycine,N-Ethylglycine,N-Methyl-L-alanine,n-Propyl carbamate
15	0.45606	453.3223	
16	0.45398	700.4189	
17	0.45391	286.1914	Mepyramine M+H+
18	0.45001	495.3157	
19	0.44912	494.3126	
20	0.44883	416.1504	Betaine M+HEFS+K+,Valine
21	0.44873	440.3159	Stellettamide A M+K+, Arachidonoyl dopamine M+H+
22	0.43961	215.1179	Harmaline M+H+
23	0.4396	465.3053	
24	0.43772	464.302	
25	0.43751	216.1213	
26	0.43492	373.7922	
27	0.43423	466.3086	
28	0.4324	511.3641	
29	0.42246	221.1603	
30	0.41244	402.1347	2-methylalanine M+HEFS+K+

Table S3: Correlation coefficients of the NMR and DIMS intensities for the putative novel metabolite with an ABX system at 5.18, 2.81 and 2.60 ppm, and a neutral mass of M=263.0641.

			NMR bin chemical shift (ppm)				
Adduct forms	m/z	Mass Error(ppm)	2.57~2.59	2.60~2.61	2.62~2.63	2.81~2.82	5.16~5.20
M+H+	264.0714	0.018934	0.27543	0.6579	0.52502	0.3357	0.68954
M+1+H+	265.0747	0.037725	0.26903	0.65156	0.51543	0.33261	0.68841
M+Na+	286.0534	0.15032	0.25399	0.50155	0.42666	0.25044	0.54068
M+K+	302.0273	0.14237	0.16539	0.67387	0.56296	0.2685	0.62689
M+Na+K-H+	324.0092	0.027777	0.16179	0.47341	0.45626	0.19343	0.44456
M+HEFS+Na+	546.1617	0.16662	0.23158	0.52457	0.36433	0.31923	0.53777
M+HEFS+K+	562.1355	0.019568	0.27871	0.62174	0.42299	0.40608	0.67471
M+HEFS+Na+K-H+	584.1175	0.015408	0.26906	0.65401	0.45488	0.38587	0.66807
M+HEFS+2*Na+K-2*H+	606.0993	0.13694	0.28477	0.56683	0.3846	0.3054	0.52236