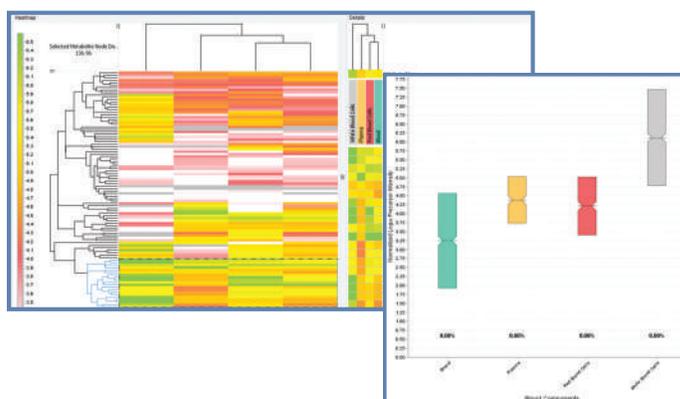


Elements for Metabolomics

Process, Organize and Interpret Large Scale Metabolomics Experiments



#	Metabolite Name	Retention Time	Molecular Weight	Formula	Score	Abundance	Intensity	MS/MS
1	Aspartic acid	133.02	133.02	C ₄ H ₇ O ₄ N	1000	1000	1000	1000
2	Alanine	89.07	89.07	C ₃ H ₇ NO ₂	1000	1000	1000	1000
3	Glutamic acid	146.07	146.07	C ₅ H ₉ NO ₄	1000	1000	1000	1000
4	Proline	97.07	97.07	C ₅ H ₉ NO	1000	1000	1000	1000
5	Valine	89.07	89.07	C ₆ H ₁₁ NO ₂	1000	1000	1000	1000
6	Leucine	133.07	133.07	C ₆ H ₁₃ NO ₂	1000	1000	1000	1000
7	Isoleucine	131.07	131.07	C ₆ H ₁₃ NO ₂	1000	1000	1000	1000
8	Threonine	89.07	89.07	C ₄ H ₉ NO ₃	1000	1000	1000	1000
9	Serine	75.07	75.07	C ₃ H ₇ NO ₃	1000	1000	1000	1000
10	Pyroglutamic acid	146.07	146.07	C ₅ H ₇ NO ₄	1000	1000	1000	1000
11	Glutamine	146.07	146.07	C ₅ H ₁₁ NO ₂	1000	1000	1000	1000
12	Asparagine	133.07	133.07	C ₄ H ₇ NO ₃	1000	1000	1000	1000
13	Protein	100.07	100.07	C ₁₀ H ₁₇ NO ₂	1000	1000	1000	1000
14	Glucose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
15	Fructose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
16	Sucrose	342.04	342.04	C ₁₂ H ₂₂ O ₁₁	1000	1000	1000	1000
17	Galactose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
18	Mannose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
19	Glucose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
20	Fructose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
21	Sucrose	342.04	342.04	C ₁₂ H ₂₂ O ₁₁	1000	1000	1000	1000
22	Galactose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
23	Mannose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
24	Glucose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
25	Fructose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
26	Sucrose	342.04	342.04	C ₁₂ H ₂₂ O ₁₁	1000	1000	1000	1000
27	Galactose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
28	Mannose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
29	Glucose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
30	Fructose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
31	Sucrose	342.04	342.04	C ₁₂ H ₂₂ O ₁₁	1000	1000	1000	1000
32	Galactose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
33	Mannose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
34	Glucose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
35	Fructose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
36	Sucrose	342.04	342.04	C ₁₂ H ₂₂ O ₁₁	1000	1000	1000	1000
37	Galactose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
38	Mannose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
39	Glucose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
40	Fructose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
41	Sucrose	342.04	342.04	C ₁₂ H ₂₂ O ₁₁	1000	1000	1000	1000
42	Galactose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
43	Mannose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
44	Glucose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
45	Fructose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
46	Sucrose	342.04	342.04	C ₁₂ H ₂₂ O ₁₁	1000	1000	1000	1000
47	Galactose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
48	Mannose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
49	Glucose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
50	Fructose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
51	Sucrose	342.04	342.04	C ₁₂ H ₂₂ O ₁₁	1000	1000	1000	1000
52	Galactose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
53	Mannose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
54	Glucose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
55	Fructose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
56	Sucrose	342.04	342.04	C ₁₂ H ₂₂ O ₁₁	1000	1000	1000	1000
57	Galactose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
58	Mannose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
59	Glucose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
60	Fructose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
61	Sucrose	342.04	342.04	C ₁₂ H ₂₂ O ₁₁	1000	1000	1000	1000
62	Galactose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
63	Mannose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
64	Glucose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
65	Fructose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
66	Sucrose	342.04	342.04	C ₁₂ H ₂₂ O ₁₁	1000	1000	1000	1000
67	Galactose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
68	Mannose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
69	Glucose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
70	Fructose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
71	Sucrose	342.04	342.04	C ₁₂ H ₂₂ O ₁₁	1000	1000	1000	1000
72	Galactose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
73	Mannose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
74	Glucose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
75	Fructose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
76	Sucrose	342.04	342.04	C ₁₂ H ₂₂ O ₁₁	1000	1000	1000	1000
77	Galactose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
78	Mannose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
79	Glucose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
80	Fructose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
81	Sucrose	342.04	342.04	C ₁₂ H ₂₂ O ₁₁	1000	1000	1000	1000
82	Galactose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
83	Mannose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
84	Glucose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
85	Fructose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
86	Sucrose	342.04	342.04	C ₁₂ H ₂₂ O ₁₁	1000	1000	1000	1000
87	Galactose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
88	Mannose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
89	Glucose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
90	Fructose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
91	Sucrose	342.04	342.04	C ₁₂ H ₂₂ O ₁₁	1000	1000	1000	1000
92	Galactose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
93	Mannose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
94	Glucose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
95	Fructose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
96	Sucrose	342.04	342.04	C ₁₂ H ₂₂ O ₁₁	1000	1000	1000	1000
97	Galactose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
98	Mannose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
99	Glucose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000
100	Fructose	180.06	180.06	C ₆ H ₁₂ O ₆	1000	1000	1000	1000



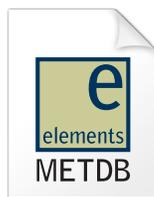
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Change thresholds to focus on highly confident metabolites or view all analytes, including unknowns. Search for metabolites by m/z, retention time, name, molecular formula and more. Search and view the NIST and HMDB spectral libraries or import your own custom databases.

Track Changing Metabolites with Ease

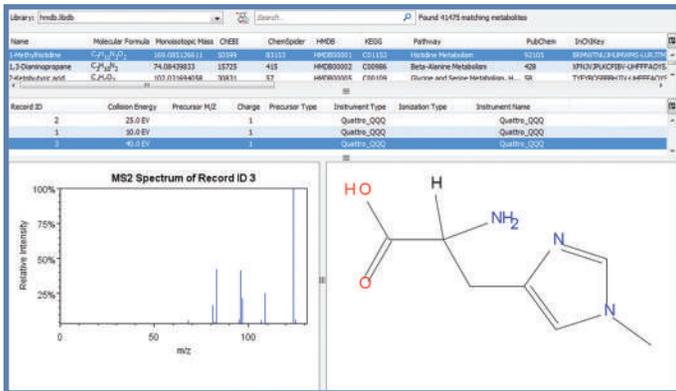
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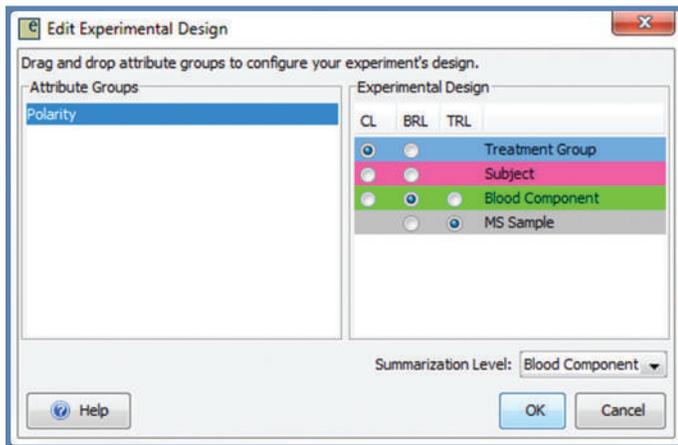
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Elements for LC/MS and LC/MS/MS-based Metabolomics



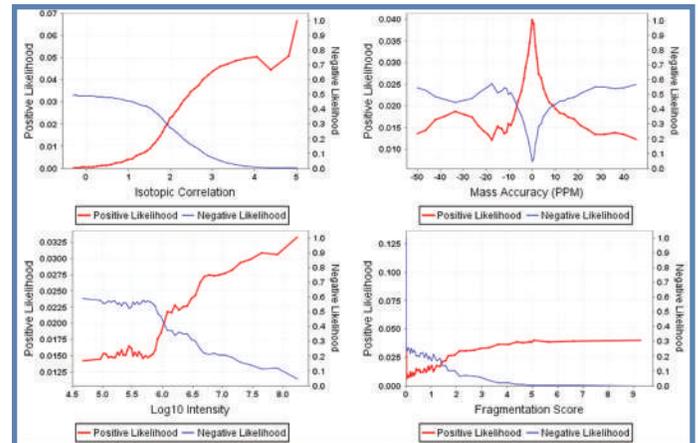
Easily Find Reference Information

View metabolite details, including chemical structure, reference MS2 spectra, and link directly to KEGG pathway charts, PubChem, HMDB and ChemSpider.



Utilize Powerful Statistics

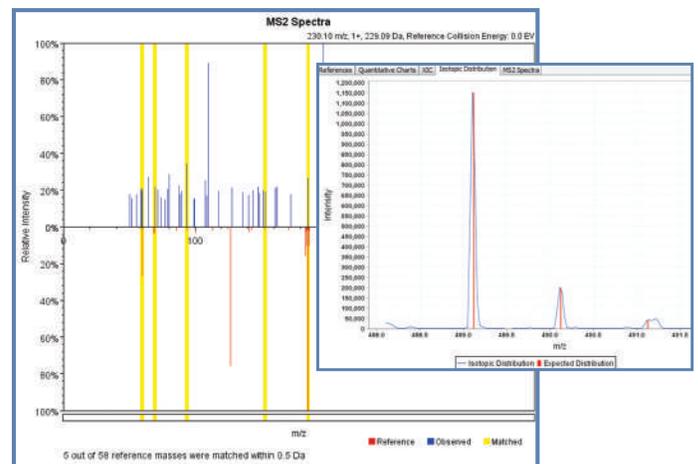
Shape your analysis with experimental metadata. Designate biological and technical replicates for proper statistical interpretation. Compare quantitation between all samples or at any desired level of summarization.



Advanced Scoring

Identifications are made using a combination of mass accuracy, MS2 library matching, isotopic correlation, and peak quality metrics. Elements fills gaps by re-searching samples for missing identifications.

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Interrogate Your Results

Verify identifications by examining matches to the MS2 spectra and expected isotopic distributions.