

Metabolite ID	Biological Pathway	Mono isotopic M/Z	RT	Exp.	q-value (2-way ANOVA)	Fold change (FC) (HCC vs. Cirrhosis)			Quality control (QC) values		
						FC	Lower	Upper	Average	STD	RSD (%)
							Bound of FC	Bound of FC			
Verified Metabolites											
Phe-Phe	Peptide	(-) 311.1	174.5	B1R&B2F	0.0859	1.161	1.033	1.304	4.744	0.495	10.436
3beta, 6beta -dihydroxy-5beta -cholan-24-oic acid	Cholesterol	(-) 391.3	286.7	B1F&B2F	0.0001	0.587	0.469	0.734	5.922	0.334	5.644
				B1F&B2R	0.0002	0.600	0.480	0.750	5.888	0.353	5.987
				B1R&B2F	0.0001	0.565	0.446	0.717	5.559	0.470	8.456
				B1R&B2R	0.0002	0.579	0.457	0.733	5.528	0.499	9.021
Fragment of GDCA [-2H2O]	Cholesterol	(+) 414.3	256.7	B1F&B2F	0.0013	0.790	0.705	0.885	8.643	0.353	4.085
				B1F&B2R	0.0027	0.781	0.692	0.881	8.551	0.339	3.969
				B1R&B2F	0.0021	0.782	0.692	0.883	8.587	0.257	2.992
				B1R&B2R	0.0030	0.773	0.680	0.879	8.495	0.244	2.872
Fragment of GDCA [-H2O]	Cholesterol	(+) 432.3	256.7	B1F&B2F	0.0010	0.802	0.723	0.889	8.149	0.334	4.096
				B1F&B2R	0.0019	0.791	0.709	0.882	8.099	0.321	3.966
				B1R&B2F	0.0018	0.799	0.718	0.889	8.204	0.261	3.183
				B1R&B2R	0.0023	0.788	0.703	0.882	8.154	0.249	3.055
Fragment of GCDCA [-2H2O]	Cholesterol	(+) 414.3	287.7	B1F&B2F	0.0147	0.882	0.816	0.954	7.354	0.338	4.595
				B1F&B2R	0.0286	0.875	0.806	0.949	7.244	0.343	4.732
				B1R&B2F	0.0201	0.885	0.818	0.957	7.306	0.291	3.989
				B1R&B2R	0.0246	0.878	0.809	0.953	7.194	0.297	4.123
Fragment of GCDCA [- H2O]	Cholesterol	(+) 432.3	287.7	B1F&B2F	0.0194	0.890	0.824	0.961	7.310	0.320	4.378
				B1F&B2R	0.0350	0.885	0.817	0.957	7.282	0.317	4.354
				B1R&B2F	0.0189	0.887	0.823	0.957	7.384	0.290	3.923
				B1R&B2R	0.0246	0.883	0.817	0.954	7.356	0.287	3.904
Oleoylcarnitine	Carnitine	(+) 426.3	374.6	B1R&B2F	0.0019	0.906	0.864	0.950	6.241	0.120	1.927
				B1R&B2R	0.0031	0.907	0.864	0.951	6.439	0.062	0.958

GDCA	Cholesterol	(-) 448.3	256.6	B1F&B2F	0.0011	0.792	0.710	0.884	9.497	0.267	2.808
				B1F&B2R	0.0022	0.793	0.706	0.890	9.469	0.333	3.512
				B1R&B2F	0.0013	0.787	0.702	0.883	8.854	0.782	8.836
				B1R&B2R	0.0039	0.788	0.698	0.890	8.829	0.855	9.683
[Na ⁺ +GDCA]	Cholesterol	(+) 472.3	256.6	B1F&B2F	0.0008	0.717	0.616	0.834	6.553	0.339	5.172
				B1F&B2R	0.0014	0.711	0.607	0.832	6.488	0.310	4.778
				B1R&B2F	0.0013	0.702	0.598	0.825	6.586	0.235	3.564
				B1R&B2R	0.0016	0.696	0.589	0.823	6.520	0.206	3.163
Fragment of GCA [- 2H ₂ O]	Cholesterol	(+) 430.3	257.8	B1F&B2F	0.0658	0.919	0.853	0.991	6.579	0.152	2.317
				B1R&B2F	0.0902	0.910	0.839	0.987	6.490	0.108	1.662
Fragment of GCA [- H ₂ O]	Cholesterol	(+) 448.3	257.8	B1F&B2F	0.0658	0.915	0.847	0.990	6.367	0.148	2.321
				B1R&B2F	0.0896	0.912	0.842	0.987	6.376	0.126	1.970
GCA	Cholesterol	(+) 466.3	257.8	B1F&B2F	0.0658	0.918	0.851	0.991	6.824	0.164	2.405
				B1R&B2F	0.0938	0.919	0.853	0.990	6.940	0.130	1.867
GDCA	Cholesterol	(+) 450.3	256.8	B1F&B2F	0.0021	0.812	0.732	0.900	6.558	0.368	5.611
				B1F&B2R	0.0052	0.792	0.703	0.893	6.586	0.409	6.207
				B1R&B2F	0.0018	0.798	0.716	0.890	6.781	0.243	3.587
				B1R&B2R	0.0030	0.779	0.689	0.882	6.808	0.285	4.180
[Na ⁺ +GCDCA]	Cholesterol	(+) 472.3	287.7	B1F&B2F	0.0081	0.835	0.752	0.927	5.752	0.314	5.453
				B1F&B2R	0.0230	0.834	0.749	0.929	5.690	0.305	5.365
				B1R&B2F	0.0166	0.849	0.767	0.940	5.805	0.278	4.785
				B1R&B2R	0.0252	0.848	0.764	0.942	5.743	0.270	4.698
GCDCA	Cholesterol	(+) 450.3	287.7	B1F&B2F	0.0147	0.849	0.766	0.942	6.185	0.300	4.851
				B1F&B2R	0.0334	0.845	0.760	0.940	6.246	0.297	4.753
				B1R&B2F	0.0219	0.866	0.788	0.952	6.404	0.293	4.568
				B1R&B2R	0.0267	0.862	0.782	0.949	6.466	0.290	4.478

Unidentified Metabolites

3-ganidinopropionicacid	Carboxylic acic (+)	132.1	53	B1F&B2F	0.0599	1.028	1.004	1.053	8.917	0.545	6.107
				B1R&B2F	0.0938	1.027	1.004	1.052	9.066	0.523	5.769
10-hydroxy-2E;8E-decadiene-4,6-diynoic acid	Fatty acid	(+) 181.1	262.7	B1F&B2F	0.0346	1.122	1.031	1.222	5.269	0.365	6.931
				B1F&B2R	0.0835	1.126	1.031	1.228	5.184	0.357	6.895
				B1R&B2F	0.0689	1.119	1.024	1.223	5.250	0.370	7.053
				B1R&B2R	0.0900	1.122	1.025	1.229	5.164	0.363	7.020
Phenylmethyl methyl ketone	Ketone	(+) 135.1	198.8	B1F&B2F	0.0200	0.964	0.941	0.988	4.735	0.207	4.369
				B1F&B2R	0.0924	0.958	0.927	0.990	4.678	0.433	9.251
				B1R&B2F	0.0333	0.957	0.928	0.986	4.455	0.108	2.432
				B1R&B2R	0.0642	0.950	0.915	0.987	4.399	0.239	5.429
L-N2-(2-arboxyethyl) arginine	Peptide	(+) 247.1	256.6	B1R&B2F	0.0018	0.730	0.625	0.853	4.986	0.112	2.241
				B1R&B2R	0.0023	0.681	0.563	0.823	4.912	0.207	4.224
Octadecadienal	Aldehyde	(+) 265.3	428.7	B1F&B2F	0.0419	0.952	0.916	0.989	6.264	0.250	3.990
				B1R&B2F	0.0457	0.943	0.904	0.985	6.230	0.104	1.672
				B1R&B2R	0.0751	0.940	0.897	0.985	6.241	0.255	4.085
Linoelaidic Acid/ otadecadienoic acid	Fatty acid	(+) 281.3	446.3	B1F&B2F	0.0658	0.941	0.892	0.993	6.017	0.068	1.132
Oleamide	Fatty acid	(+) 282.3	429.4	B1F&B2F	0.0503	0.963	0.934	0.993	8.675	0.267	3.073
				B1R&B2F	0.0743	0.962	0.932	0.992	8.719	0.140	1.609
O-octanoyl-R-carnitine	Fatty acid	(+) 288.2	307.3	B1R&B2F	0.0051	0.983	0.974	0.992	7.384	0.228	3.088

n-tosyl-L-lysiny methyl ketone	Ketone	(+)	299.1	445.3	B1F&B2F	0.0490	0.950	0.911	0.990	7.571	0.065	0.855
					B1R&B2F	0.0817	0.950	0.909	0.992	7.588	0.035	0.461
Decanoyl-L-carnitine	Carnitine	(+)	316.3	342.6	B1R&B2F	0.0599	0.985	0.974	0.997	6.755	0.088	1.308
Tetracosahexaenoic acid	Fatty acid	(+)	357.3	296.8	B1F&B2F	0.0004	0.629	0.516	0.767	5.084	0.293	5.770
					B1F&B2R	0.0002	0.560	0.438	0.715	5.047	0.486	9.629
					B1R&B2F	0.0002	0.605	0.491	0.745	4.937	0.360	7.289
					B1R&B2R	0.0001	0.535	0.413	0.692	4.899	0.553	11.290
Palmitoyl carnitine	Carnitine	(+)	400.3	368.9	B1R&B2F	0.0074	0.918	0.876	0.963	5.918	0.154	2.594
					B1R&B2R	0.0167	0.918	0.874	0.965	6.172	0.135	2.183
Linoelaidyl carnitine	Carnitine	(+)	424.3	358.7	B1R&B2F	0.0034	0.883	0.829	0.941	5.791	0.189	3.266
					B1R&B2R	0.0081	0.887	0.831	0.946	5.884	0.115	1.963
PC(O-16:0/0:0)	Phospholipids	(+)	482.4	385.2	B1F&B2F	0.0346	0.943	0.903	0.985	6.378	0.445	6.970
					B1R&B2F	0.0938	0.951	0.910	0.994	6.640	0.161	2.418
LysoPC(20:1)	Phospholipids	(+)	550.4	412.8	B1F&B2F	0.0679	0.957	0.920	0.996	5.499	0.135	2.463
					B1R&B2F	0.0473	0.945	0.907	0.986	5.661	0.098	1.729
					B1R&B2R	0.0822	0.949	0.911	0.988	5.754	0.079	1.377
CerP(d18:1/12:0)	Phospholipids	(+)	562.4	442.2	B1F&B2F	0.0683	0.929	0.869	0.994	5.961	0.113	1.891
LysoPC(20:4)	Phospholipids	(+)	544.3	464.2	B1F&B2R	0.0350	0.840	0.751	0.941	4.673	0.236	5.046
					B1R&B2R	0.0434	0.841	0.743	0.950	5.027	0.401	7.982
4E;15Z-Bilirubin IXa	Porphyrins	(+)	585.3	457	B1F&B2F	0.0597	0.959	0.925	0.994	7.981	0.095	1.188
					B1R&B2F	0.0942	0.960	0.926	0.995	8.059	0.078	0.964
PE(20:4/18:1)	Phospholipids	(+)	766.5	395.5	B1F&B2F	0.0980	0.981	0.961	1.001	9.871	0.082	0.828

				B1R&B2F	0.0305	0.969	0.948	0.990	9.530	0.204	2.143
				B1R&B2R	0.0275	0.963	0.940	0.987	9.464	0.103	1.084
L-alanine/Beta-leucine/T-butyl glycine	Peptide	(-) 131.1	154.5	B1F&B2F	0.0317	0.942	0.905	0.982	5.620	0.131	2.324
				B1F&B2R	0.0334	0.943	0.905	0.982	5.536	0.080	1.448
				B1R&B2F	0.0315	0.941	0.904	0.980	5.216	0.525	10.072
				B1R&B2R	0.0506	0.941	0.904	0.980	5.129	0.465	9.061
Hydroxypalmiticacid	Fatty acid	(-) 271.2	406.1	B1F&B2F	0.0410	0.941	0.900	0.983	5.550	0.153	2.757
				B1F&B2R	0.0813	0.945	0.903	0.990	5.847	0.244	4.166
3-hydroxy-eicosanoic acid	Fatty acid	(-) 327.3	443.4	B1F&B2F	0.0032	0.887	0.832	0.944	5.213	0.158	3.040
				B1F&B2R	0.0084	0.890	0.834	0.951	5.316	0.122	2.294
3 alpha,7beta-dihydroxy-5 beta-cholest-24-en-26-oic acid	Cholesterol	(-) 431.3	411.9	B1F&B2F	0.0806	0.920	0.856	0.988	5.076	0.255	5.022
TCDCa	Cholesterol	(-) 498.3	233.5	B1F&B2F	0.0027	0.737	0.628	0.865	7.686	0.429	5.586
				B1F&B2R	0.0023	0.742	0.637	0.864	7.668	0.399	5.200
				B1R&B2F	0.0036	0.728	0.614	0.864	6.523	1.516	23.238
				B1R&B2R	0.0044	0.733	0.623	0.863	6.503	1.486	22.856
15,16-dihydrobiliverdin	Porphyrins	(-) 581.2	445.3	B1F&B2F	0.0595	0.905	0.837	0.979	5.675	0.121	2.129
				B1F&B2R	0.0916	0.909	0.839	0.985	5.625	0.120	2.138
