

Supplemental table 2.

Characterization of liver metabolites that were influenced by PPAR α activation in mice treated with bezafibrate.

RT (min)	Detected mass	Actual mass	Change in (% of Cont)	P-value	Estimate molecular formula	Estimate metabolite
4.062	154.06154	155.06882	141	7.83 $\times 10^{-3}$	C ₆ H ₉ N ₃ O ₂	L-Histidine
4.068	133.09701	132.08973	185	1.22 $\times 10^{-4}$	C ₉ H ₁₂ N ₂ O ₂	L-Ornithine
4.099	156.07658	155.06931	162	1.30 $\times 10^{-3}$	C ₆ H ₉ N ₃ O ₂	L-Histidine
4.391	206.10247	207.10975	576	2.63 $\times 10^{-11}$	C ₈ H ₁₇ N ₁ O ₅	N-Ethylglycocyamine
4.394	145.06126	146.06854	118	2.39 $\times 10^{-2}$	C ₉ H ₁₀ N ₂ O ₃	L-Glutamine
4.411	346.05395	347.06122	207	7.74 $\times 10^{-5}$	C ₁₀ H ₁₄ N ₅ O ₇ P ₁	AMP
4.501	162.11228	161.105	368	1.21 $\times 10^{-10}$	C ₇ H ₁₅ N ₁ O ₃	L-Carnitine
4.508	146.04529	147.05257	64	4.84 $\times 10^{-3}$	C ₅ H ₉ N ₁ O ₄	L-Glutamate
4.532	132.02971	133.03699	65	3.32 $\times 10^{-2}$	C ₄ H ₇ N ₁ O ₄	L-Aspartate
4.537	119.03454	120.04182	39	1.08 $\times 10^{-6}$	C ₄ H ₈ O ₄	D-Erythrose
4.537	179.05537	134.05717	50	3.66 $\times 10^{-7}$	C ₅ H ₁₀ O ₄	Deoxyribose
4.541	101.02408	102.03136	42	2.60 $\times 10^{-6}$	C ₄ H ₆ O ₃	Acetoacetate
4.542	161.04488	162.05216	40	3.70 $\times 10^{-8}$	C ₆ H ₁₀ O ₅	3-Ethylmalate
4.543	113.02402	114.03129	36	1.50 $\times 10^{-6}$	C ₅ H ₆ O ₃	2-Hydroxy-2,4-pentadienoate
4.621	160.13304	159.12577	344	2.80 $\times 10^{-5}$	C ₈ H ₁₇ N ₁ O ₂	3-amino-octanoic acid
4.645	195.05029	196.05756	206	4.27 $\times 10^{-6}$	C ₆ H ₁₂ O ₇	L-Gulonate
4.872	371.08144	372.08871	376	1.61 $\times 10^{-7}$	C ₁₉ H ₁₇ N ₂ O ₄ Cl ₁	Quizalofop-ethyl
4.993	325.04286	324.03559	191	2.56 $\times 10^{-4}$	C ₉ H ₁₃ N ₂ O ₉ P ₁	UMP
5.012	285.08248	284.07521	42	4.86 $\times 10^{-4}$	C ₁₀ H ₁₂ N ₄ O ₆	Xanthosine
5.063	273.00072	274.008	149	1.25 $\times 10^{-2}$	C ₆ H ₁₁ O ₁₀ P ₁	6-Phospho-2-dehydro-D-gluconate
6.218	250.09302	249.08574	55	3.52 $\times 10^{-3}$	C ₁₀ H ₁₉ N ₁ O ₂ S ₂	S-Acetyldihydroliipoamide
7.297	359.10321	358.09594	786	1.00 $\times 10^{-3}$	C ₁₁ H ₂₃ N ₂ O ₇ P ₁ S ₁	Pantetheine 4'-phosphate
7.318	161.0085	162.01578	35	2.21 $\times 10^{-3}$	C ₅ H ₆ O ₆	4-Hydroxy-2-oxoglutarate
7.319	115.00324	70.005034	38	8.30 $\times 10^{-4}$	C ₃ H ₂ O ₂	Propynoate
7.32	218.10243	219.10971	274	2.20 $\times 10^{-4}$	C ₉ H ₁₇ N ₁ O ₅	Pantothenate
7.353	166.08608	165.07881	146	9.26 $\times 10^{-3}$	C ₉ H ₁₁ N ₁ O ₂	L-Phenylalanine
7.364	232.15423	231.14696	740	8.44 $\times 10^{-5}$	C ₁₁ H ₂₁ N ₁ O ₄	O-Butanoylcarnitine
7.377	220.11787	219.11059	272	1.08 $\times 10^{-3}$	C ₉ H ₁₇ N ₁ O ₅	Pantothenate
10.47	212.11807	211.1108	733	4.22 $\times 10^{-2}$	C ₁₃ H ₁₃ N ₃	Trp-P-1
10.88	260.18546	259.17818	1816	3.24 $\times 10^{-5}$	C ₁₃ H ₂₅ N ₁ O ₄	O-hexanoyl-R-carnitine
25.32	362.09634	363.10362	12024	1.23 $\times 10^{-7}$	C ₁₇ H ₁₈ N ₃ O ₃ S ₁ F ₁	Rufloxacin
25.32	360.09932	315.10111	10261	7.25 $\times 10^{-8}$	C ₁₆ H ₁₅ N ₃ F ₂ Si ₁	Flusilazole

Supplemental table 2 (continue)

28.72	502.29194	501.28466	179	8.60×10^{-4}	$C_{25}H_{44}N_1O_7P_1$	LPE(20:4)
28.75	520.3388	519.33152	185	3.18×10^{-6}	$C_{26}H_{50}N_1O_7P_1$	LPC(18:2)
28.91	544.33876	543.33148	78	4.14×10^{-2}	$C_{28}H_{50}N_1O_7P_1$	LPC(20:4)
30.41	496.33883	495.33156	309	2.53×10^{-3}	$C_{24}H_{50}N_1O_7P_1$	LPC(16:0)
30.96	276.12281	275.11553	197	2.70×10^{-3}	$C_{15}H_{17}N_1O_4$	Dubininidene
31	454.29204	453.28477	188	3.46×10^{-3}	$C_{21}H_{44}N_1O_7P_1$	LPE(16:0)
31.18	330.33606	329.32879	52	6.32×10^{-3}	$C_{20}H_{43}N_1O_2$	N,N-dimethyl-Safingol
31.25	496.33886	495.33158	164	1.65×10^{-3}	$C_{24}H_{50}N_1O_7P_1$	PC(O-14:0/2:0)
31.76	522.35444	521.34716	341	1.93×10^{-8}	$C_{26}H_{52}N_1O_7P_1$	PC(P-16:0/2:0)
32.29	480.30755	479.30028	623	2.37×10^{-7}	$C_{23}H_{46}N_1O_7P_1$	LPE(18:1)
32.52	522.35443	521.34715	418	3.87×10^{-6}	$C_{26}H_{52}N_1O_7P_1$	LPC(18:1)
36.31	290.13838	289.1311	166	1.49×10^{-3}	$C_{16}H_{19}N_1O_4$	Balfourodine
37.5	550.38592	549.37865	576	2.32×10^{-5}	$C_{28}H_{56}N_1O_7P_1$	LPC(20:1)
46.44	209.15323	208.14595	63	8.32×10^{-3}	$C_{13}H_{20}O_2$	4-Heptyloxyphenol