

Supporting Information

# Common Liver Metabolites Identification of Natural Bioactive Compound Erinacine A, Purified from *Hericium erinaceus* Mycelium

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Table S1. Identify of erinacine A metabolites in rat and human liver S9 with an UPLC-QTOF/MS.

ID	Metabolic reaction	Formula	RT	Exact mass	Mass error(ppm)	Accurate mass	Fragment	Polarity	Rat	Human
Parent	Erinacine A	C <sub>25</sub> H <sub>36</sub> O <sub>6</sub>	8.782	432.2515	0.73	432.2512	119.0859, 199.1492, 240.1464, 283.2055, 301.2162*	Positive	v	v
M1*	Alcohols Dehydration	C <sub>25</sub> H <sub>34</sub> O <sub>5</sub>	8.799	414.2399	-1.63	414.2406	69.0327, 105.0709, 119.0856*, 135.0817, 181.1249, 235.1701, 283.2036	Positive	v	v
M2*	Demethylation	C <sub>24</sub> H <sub>34</sub> O <sub>6</sub>	4.916	418.2354	-0.25	418.2355	97.0289, 123.0551*, 179.0486, 231.0436, 368.9803	Positive	v	v
M3*	Demethylation + Hydrogenation	C <sub>24</sub> H <sub>36</sub> O <sub>6</sub>	13.28	420.2488	-4.72	420.2512	55.0539, 77.0054*, 95.0854, 147.1172, 277.2183, 353.2141	Positive	v	v
M4*	2x Hydroxylation	C <sub>25</sub> H <sub>36</sub> O <sub>8</sub>	4.071	464.2405	-1.41	464.241	89.0597*, 133.0860, 177.1115, 297.1842	Positive	v	v
M5*	Demethylation and two Hydroxylations	C <sub>24</sub> H <sub>34</sub> O <sub>8</sub>	8.777	450.2265	2.44	450.2254	59.0601*, 101.0705, 178.1225, 321.1516	Positive	v	v
M6	Gluthation conjugation + Demethylation	C <sub>34</sub> H <sub>49</sub> N <sub>3</sub> O <sub>12</sub> S	12.213	723.303	-0.92	723.3037	59.0487*, 133.0856, 211.1383, 459.2802	Positive	v	
M7	Ethyl Ether to Acid	C <sub>23</sub> H <sub>30</sub> O <sub>7</sub>	3.383	418.1998	1.55	418.1992	136.0615, 161.0463, 169.0982, 188.0338, 348.0094, 381.1361	Positive	v	
M8	Gluthation Conjugation + Hydroxylation	C <sub>35</sub> H <sub>51</sub> N <sub>3</sub> O <sub>13</sub> S	11.158	753.314	-0.39	753.3143	59.0489*, 73.0648, 89.0596, 99.0803, 117.0909, 221.1387, 265.1651, 397.2426, 502.3237	Positive	v	
M9	Hydroxylation and Methylation	C <sub>26</sub> H <sub>38</sub> O <sub>7</sub>	16.296	462.2605	-2.68	462.2618	81.0695, 105.0691, 132.0012, 148.0881, 185.0403, 240.1748*, 284.2353, 329.9974	Positive	v	

M10	Alcohols Dehydration	C <sub>25</sub> H <sub>34</sub> O <sub>5</sub>	9.227	414.2399	-1.8	414.2406	69.0327, 105.0709, 119.0856*, 138.0817, 181.1249, 235.1701, 283.2036 67.0539, 91.0535, 119.0852*, 130.0782, 149.0073, 188.1020, 209.0453, 264.0988, 324.1374, 367.0251 73.0284, 115.0389, 149.0960, 183.1165, 227.1430, 271.1691, 313.1797* 112.9368, 255.2009*, 299.2018, 355.2285 89.0611, 103.0768, 157.1003*, 262.8575 61.9885, 77.0065*, 163.1142, 337.2168 127.0724*, 177.1117, 268.1284, 387.1819 171.0843, 203.9762, 212.1586, 250.9992, 283.2429*, 396.1933, 463.0576 59.0135*, 89.0238, 194.0152 57.0696*, 149.0243, 302.186, 376.2594 57.0699, 164.9294*, 226.2190, 279.1032	Positive v
M11	Deethylation	C <sub>23</sub> H <sub>32</sub> O <sub>6</sub>	15.427	404.2194	-1.32	404.2199	130.0782, 149.0073, 188.1020, 209.0453, 264.0988, 324.1374, 367.0251 73.0284, 115.0389, 149.0960, 183.1165, 227.1430, 271.1691, 313.1797* 112.9368, 255.2009*, 299.2018, 355.2285 89.0611, 103.0768, 157.1003*, 262.8575 61.9885, 77.0065*, 163.1142, 337.2168 127.0724*, 177.1117, 268.1284, 387.1819 171.0843, 203.9762, 212.1586, 250.9992, 283.2429*, 396.1933, 463.0576 59.0135*, 89.0238, 194.0152 57.0696*, 149.0243, 302.186, 376.2594 57.0699, 164.9294*, 226.2190, 279.1032	Positive v
M12	Oxidation + 2x Desaturation	C <sub>25</sub> H <sub>32</sub> O <sub>7</sub>	4.89	444.2142	-1.41	444.2148	149.0960, 183.1165, 227.1430, 271.1691, 313.1797* 112.9368, 255.2009*, 299.2018, 355.2285 89.0611, 103.0768, 157.1003*, 262.8575 61.9885, 77.0065*, 163.1142, 337.2168 127.0724*, 177.1117, 268.1284, 387.1819 171.0843, 203.9762, 212.1586, 250.9992, 283.2429*, 396.1933, 463.0576 59.0135*, 89.0238, 194.0152 57.0696*, 149.0243, 302.186, 376.2594 57.0699, 164.9294*, 226.2190, 279.1032	Positive v
M13	Hydration, Hydrolysis (Internal)	C <sub>25</sub> H <sub>38</sub> O <sub>7</sub>	8.453	450.2616	-0.35	450.2618	255.2009*, 299.2018, 355.2285 89.0611, 103.0768, 157.1003*, 262.8575 61.9885, 77.0065*, 163.1142, 337.2168 127.0724*, 177.1117, 268.1284, 387.1819 171.0843, 203.9762, 212.1586, 250.9992, 283.2429*, 396.1933, 463.0576 59.0135*, 89.0238, 194.0152 57.0696*, 149.0243, 302.186, 376.2594 57.0699, 164.9294*, 226.2190, 279.1032	Negative
M14	Alkenes to Dihydrodiol	C <sub>25</sub> H <sub>38</sub> O <sub>8</sub>	5.837	466.2566	-0.18	466.2567	157.1003*, 262.8575 61.9885, 77.0065*, 163.1142, 337.2168 127.0724*, 177.1117, 268.1284, 387.1819 171.0843, 203.9762, 212.1586, 250.9992, 283.2429*, 396.1933, 463.0576 59.0135*, 89.0238, 194.0152 57.0696*, 149.0243, 302.186, 376.2594 57.0699, 164.9294*, 226.2190, 279.1032	Positive
M15	Demethylation + Dehydrogenation	C <sub>24</sub> H <sub>32</sub> O <sub>6</sub>	12.815	416.2204	1.32	416.2199	61.9885, 77.0065*, 163.1142, 337.2168 127.0724*, 177.1117, 268.1284, 387.1819 171.0843, 203.9762, 212.1586, 250.9992, 283.2429*, 396.1933, 463.0576 59.0135*, 89.0238, 194.0152 57.0696*, 149.0243, 302.186, 376.2594 57.0699, 164.9294*, 226.2190, 279.1032	Positive
M16	Acetylation + Oxidation	C <sub>27</sub> H <sub>38</sub> O <sub>8</sub>	7.546	490.2563	-0.76	490.2567	177.1117, 268.1284, 387.1819 171.0843, 203.9762, 212.1586, 250.9992, 283.2429*, 396.1933, 463.0576 59.0135*, 89.0238, 194.0152 57.0696*, 149.0243, 302.186, 376.2594 57.0699, 164.9294*, 226.2190, 279.1032	Positive v
M17	Demethylation + Oxidation + Glucuronidation	C <sub>30</sub> H <sub>42</sub> O <sub>13</sub>	9.173	610.2609	-2.72	610.2625	171.0843, 203.9762, 212.1586, 250.9992, 283.2429*, 396.1933, 463.0576 59.0135*, 89.0238, 194.0152 57.0696*, 149.0243, 302.186, 376.2594 57.0699, 164.9294*, 226.2190, 279.1032	Negative v
M18	Demethylation and Hydroxylation	C <sub>24</sub> H <sub>34</sub> O <sub>7</sub>	5.496	434.2291	-3.16	434.2305	59.0135*, 89.0238, 194.0152 57.0696*, 149.0243, 302.186, 376.2594 57.0699, 164.9294*, 226.2190, 279.1032	Negative v
M19	Decarbonylation	C <sub>24</sub> H <sub>36</sub> O <sub>4</sub>	11.341	404.2545	-4.51	404.2563	57.0696*, 149.0243, 302.186, 376.2594 57.0699, 164.9294*, 226.2190, 279.1032	Positive
M20	Hetero oxide reduction + Hydrogenation	C <sub>25</sub> H <sub>38</sub> O <sub>5</sub>	15.416	418.2717	-0.42	418.2719	57.0699, 164.9294*, 226.2190, 279.1032	Positive

M21	Decarboxylation	C <sub>24</sub> H <sub>36</sub> O <sub>4</sub>	14.928	388.2608	-1.48	388.2614	89.0597*, 133.0862, 211.1443, 279.1310, Positive 328.2057
M22	Hydroxymethylene Loss	C <sub>24</sub> H <sub>34</sub> O <sub>5</sub>	3.312	402.2416	2.49	402.2406	55.0537, 72.0807*, 120.0800, 188.0722, Positive 227.1433, 260.1524
M23	Hydrolysis + 2x Oxidation	C <sub>24</sub> H <sub>36</sub> O <sub>4</sub>	3.282	482.2529	2.67	482.2516	72.0814, 86.0962*, 155.0828, 345.1186 Positive 84.0807*,
M24	Isopropyl Dealkylation	C <sub>35</sub> H <sub>53</sub> N <sub>3</sub> O <sub>12</sub> S	2.62	390.204	-0.6	390.2042	172.1137 ,257.1384, Positive 302.1868

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\*Common liver metabolites of erinacine A detected in Rat and Human Liver S9.