< *Arabian Journal of Chemistry* >

Supporting Information

Comparative identification of the metabolites of dehydrocorydaline from rat plasma, bile, urine and feces by both the targeted and untargeted liquid chromatography/mass spectrometry strategies

Contents

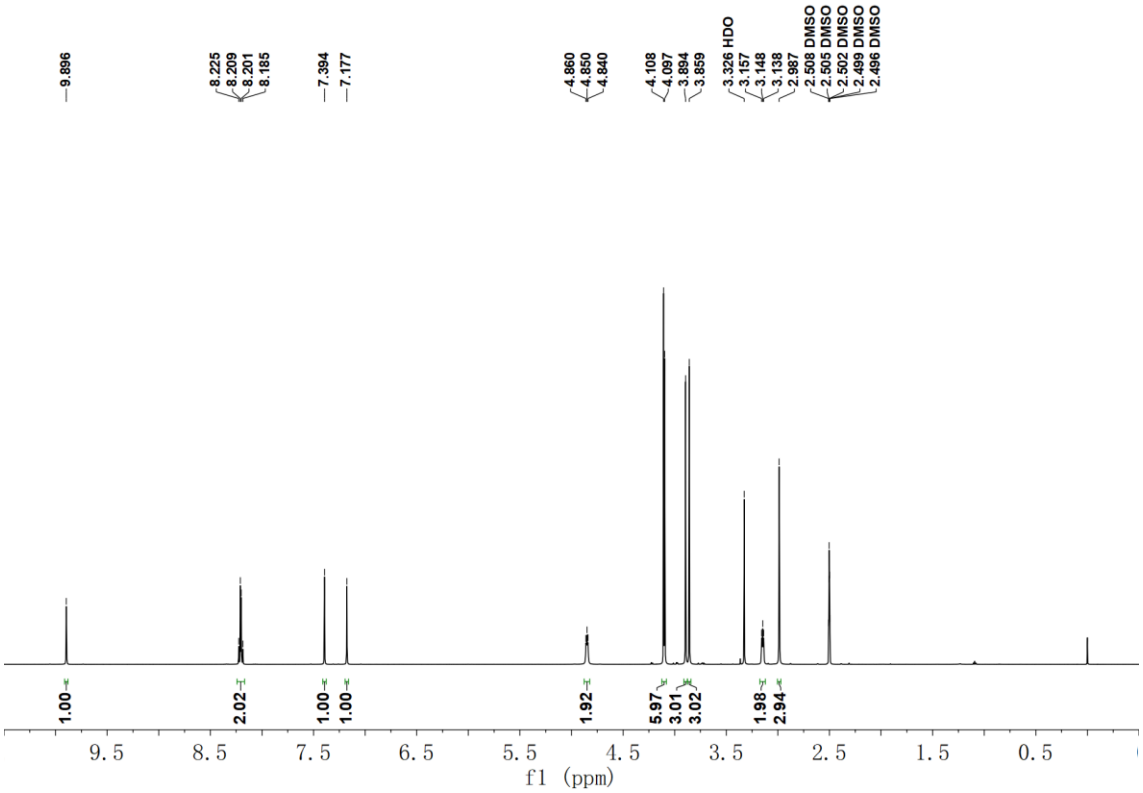

Fig. S1 The ^{1}H NMR spectrum of dehydrocorydaline in DMSO-d_6.

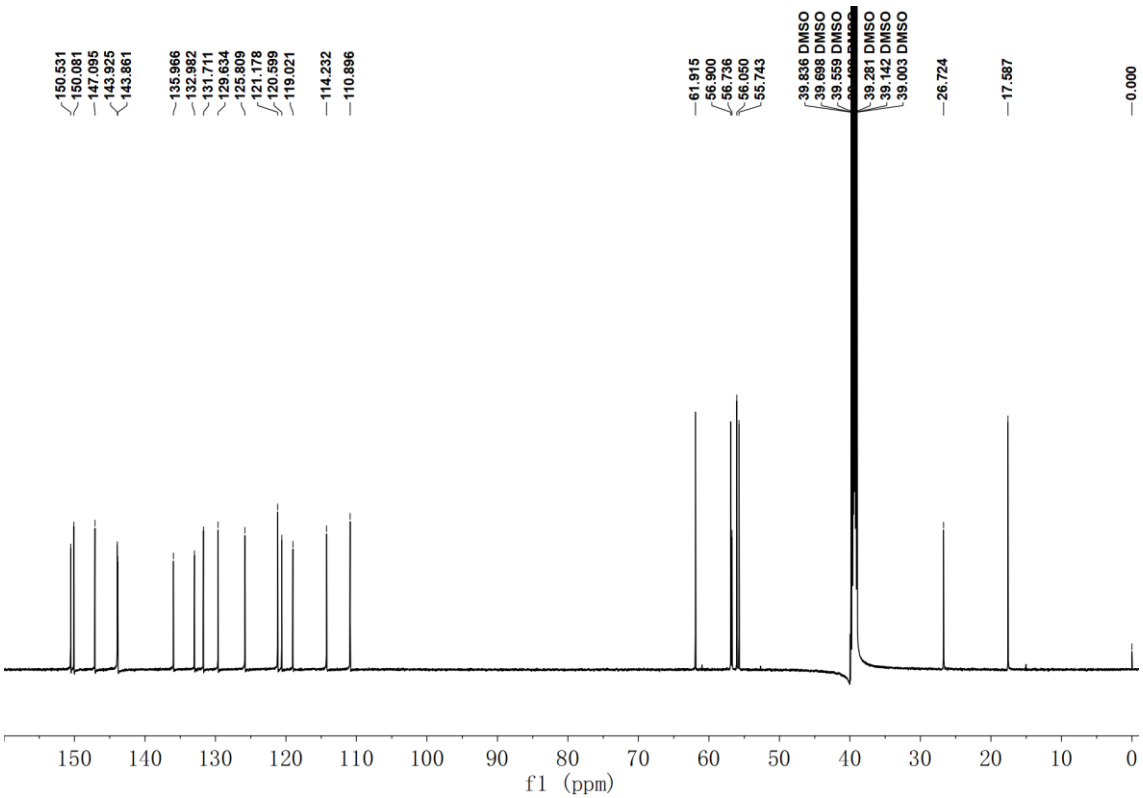

Fig. S2 The ^{13}C NMR spectrum of dehydrocorydaline in DMSO-d_6.

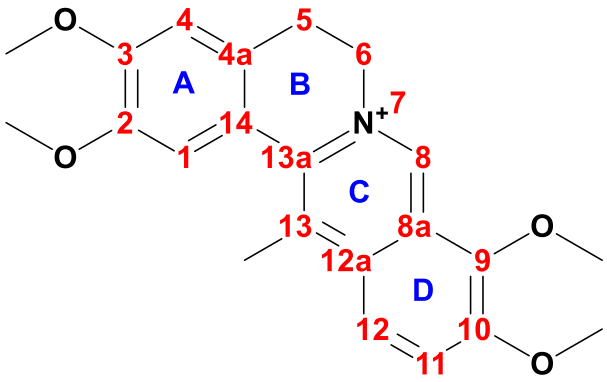

Fig. S3 The structure of dehydrocorydaline identified by the ^{1}H NMR and ^{13}C NMR data analysis.

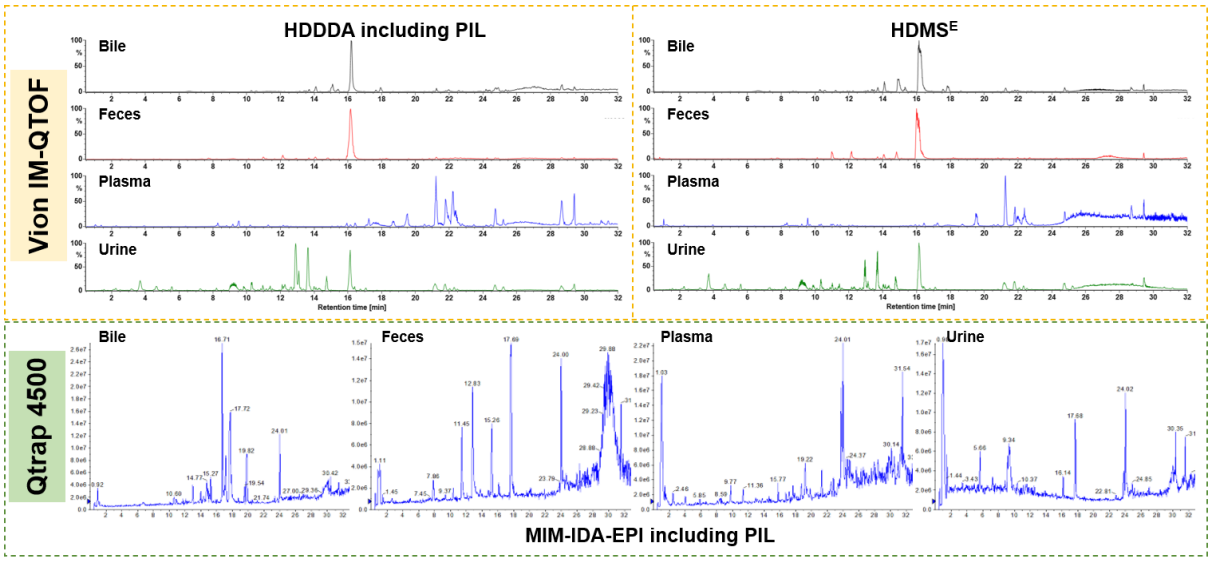

Fig. S4 Total ion chromatograms (TICs) of the plasma, bile, urine, and feces of rats acquired by QTrap 4500 and Vion IM-QTOF using different methods (MIM-IDA-EPI including PIL, HDDDA including PIL, and HDMS^E).

Table S1 The ^{1}H NMR (600 MHz) and ^{13}C NMR (150 MHz) data of dehydrocorydaline in DMSO-d_6.

No.	δ_H	Ref. δ_H*	δ_C	Ref. δ_C*
1	7.39 (1H, s)	7.39 (1H, s)	114.23	114.18
2			147.10	147.07
3			150.53	150.50
4	7.18 (1H, s)	7.17 (1H, s)	110.90	110.86
4a			131.71	131.96
5	3.15 (2H, t, *J*=6.0 Hz)	3.14 (2H, t)	26.72	26.71
6	4.85 (2H, t, *J*=6.0 Hz)	4.84 (2H, t)	56.74	56.72
8	9.90 (1H, s)	9.89 (1H, s)	143.86	143.85
8a			120.60	120.58
9			143.93	143.89
10			150.08	150.07
11	8.23 (1H, d, *J*=6.0 Hz)	8.20 (1H, s)	125.81	125.77
12	8.21 (1H, d, *J*=6.0 Hz)	8.18 (1H, s)	121.18	121.18
12a			132.98	132.96
13			129.63	129.62
13a			119.02	119.00
14			135.97	135.95
13-CH_3	2.99 (3H, s)	2.98 (3H, s)	17.59	17.58
2-OCH_3	4.11 (3H, s)	4.10 (3H, s)	56.05	56.02
3-OCH_3	4.10 (3H, s)	4.09 (3H, s)	55.74	55.72
9-OCH_3	3.89 (3H, s)	3.89 (3H, s)	61.92	61.91
10-OCH_3	3.86 (3H, s)	3.85 (3H, s)	56.90	56.88

*:Xiao, Y.H., Shuai, W., Cao, H., et al, 2012. Structure of dehydrocorydaline. Journal of Wuhan Institute of Technology 34, 26-30.

Table S2 Biotransformation pathways reported in the literature.

Biotransformation reaction	Delta Formula	Formula	Delta Mass	Delta Mass	Metabolic Category
Demethylation × 1	M-CH_2	$C_{21}H_{22}NO_4^+$	-14.0157	352.1543	Phase I
Demethylation × 2	M-C_2H_4	$C_{20}H_{20}NO_4^+$	-28.0313	338.1387	Phase I
Oxidation × 1	M+O	$C_{22}H_{24}NO_5^+$	15.9949	382.1649	Phase I
Oxidation × 2	M+O_2	$C_{22}H_{24}NO_6^+$	31.9898	398.1598	Phase I
Oxidation × 1 + dehydrogenation × 1	M+O-H_2	$C_{22}H_{22}NO_7^+$	45.9691	412.1391	Phase I + Phase I
Oxidation × 2+ dehydrogenation × 1	M+O_2-H_2	$C_{22}H_{22}NO_6^+$	29.9742	396.1442	Phase I + Phase I
Demethylation × 1 - Dehydrogenation × 1	M-CH_2-H_2	$C_{21}H_{20}NO_4^+$	-16.0313	350.1387	Phase I + Phase I
Demethylation × 2 - Dehydrogenation × 2	M-C_2H_4-H_4	$C_{20}H_{16}NO_4^+$	-32.0626	334.1074	Phase I + Phase I
Demethylation × 1 + Sulfation × 1	M-CH_2+SO_3	$C_{21}H_{22}NO_7S^+$	65.9411	432.1111	Phase I + Phase II
Demethylation × 2 + Sulfation × 2	M-C_2H_4+S_2O_6	$C_{20}H_{20}NO_{10}S_2^+$	498.0523	864.2223	Phase I + Phase II
Demethylation × 1 + Glucuronidation × 1	M-CH_2+$C_6H_8O_6$	$C_{27}H_{30}NO_{10}^+$	162.0164	528.1864	Phase I + Phase II
Demethylation × 2 + Glucuronidation × 2	M-C_2H_4+$C_{12}H_{16}O_{12}$	$C_{32}H_{36}NO_{16}^+$	324.0329	690.2029	Phase I + Phase II

Table S3 Prediction of biotransformation pathways based on UNIFI Met ID function.

Biotransformation reaction	Delta Formula	Formula	Delta Mass	Theoretical Mass	Metabolic Category
Oxidation × 1	M+O_2	$C_{22}H_{24}NO_6^+$	31.9898	398.1598	Phase I
Oxidation × 2 + Desaturation	M-H_2+O_2	$C_{22}H_{22}NO_6^+$	29.9742	396.1442	Phase I
Oxidation × 3	M+O_3	$C_{22}H_{24}NO_7^+$	47.9847	414.1547	Phase I
Aromatization	M-H_6	$C_{22}H_{18}NO_4^+$	-6.0470	360.1230	Phase I
Decarbonylation	M-CO	$C_{21}H_{24}NO_3^+$	-27.9949	338.1751	Phase I
Decarboxylation	M-COO	$C_{21}H_{24}NO_2^+$	43.9898	410.1598	Phase I
Dehydration	M-H_2O	$C_{22}H_{22}NO_3^+$	-18.0106	348.1594	Phase I
Desaturation	M-H_2	$C_{22}H_{22}NO_4^+$	-2.0157	364.1543	Phase I

Dihvdrodiol formation	M+H_2O_2	$C_{22}H_{26}NO_6^+$	34.0055	400.1755	Phase I
Ethyl ketone to acid	M-C_3H_6+O	$C_{19}H_{18}NO_5^+$	-26.052	340.1180	Phase I
Hydration	M+H_2O	$C_{22}H_{26}NO_5^+$	18.0106	384.1806	Phase I
Isopropy to alcohol	M-C_3H_6+O	$C_{19}H_{18}NO_5^+$	-26.052	340.1180	Phase I
Nitro reduction	M-O_2+H_2	$C_{22}H_{22}NO_2^+$	29.9742	396.1442	Phase I
Oxidation	M+O	$C_{22}H_{24}NO_5^+$	15.9949	382.1649	Phase I
Oxidation+ desaturation	M+O-H_2	$C_{22}H_{22}NO_5^+$	13.9793	380.1493	Phase I
Propyl ketone to acid	M-C_4H_8+O	$C_{18}H_{16}NO_5^+$	-40.0677	326.1023	Phase I
Reduction	M+H_2	$C_{22}H_{22}NO_4^+$	2.0157	368.1857	Phase I
Tert-butyl to alcohol	M-C_4H_8+O	$C_{18}H_{16}NO_5^+$	-40.0677	326.1023	Phase I
Acetyl cysteine conjugation	M+$C_5H_7NO_3S$	$C_{27}H_{31}N_2O_7S^+$	161.0147	527.1847	Phase II
Acetylation	M+C_2H_2O	$C_{24}H_{26}NO_5^+$	42.0106	408.1806	Phase II
Butyryl conjugation	M+C_4H_6O	$C_{26}H_{30}NO_5^+$	70.0419	436.2119	Phase II
Carnitine conjugation	M+$C_7H_{14}O_2N$	$C_{29}H_{38}N_2O_6^+$	144.1025	510.2725	Phase II
CysGly S adduction	M+$C_5H_8N_2O_3S$	$C_{27}H_{32}N_3O_7S^+$	176.0256	542.1956	Phase II
Cysteine conjugation	M+C_3H_5NOS	$C_{25}H_{29}N_2O_5S^+$	103.0092	469.1792	Phase II
Cysteine S-conjugation	M+$C_3H_5NO_2S$	$C_{25}H_{29}N_2O_6S^+$	119.0041	485.1741	Phase II
Formylation	M+CO	$C_{23}H_{24}NO_5^+$	27.9949	394.1649	Phase II
Glucosylation	M+$C_6H_{10}O_5$	$C_{28}H_{34}NO_9^+$	162.0528	528.2228	Phase II
Glucuronidation	M+$C_6H_8O_6$	$C_{28}H_{32}NO_{10}^+$	176.0321	542.2021	Phase II
Glucuronidation of carbamate	M+$C_7H_8O_8$	$C_{29}H_{32}NO_{12}^+$	220.0219	586.1919	Phase II
Glutamine conjugation	M+$C_5H_7O_3N$	$C_{27}H_{31}N_2O_7^+$	129.0426	495.2126	Phase II
Glutathione conjugation	M+$C_{10}H_{15}N_3O_5S$	$C_{32}H_{39}N_4O_9S^+$	289.0732	655.2432	Phase II
Glulathione S-conjugation	M+$C_{10}H_{15}N_3O_6S$	$C_{32}H_{39}N_4O_{10}S^+$	305.0682	671.2382	Phase II
Glycine conjugation	M+C_2H_3NO	$C_{24}H_{27}N_2O_5^+$	57.0215	423.1915	Phase II
Methylation	M+CH_2	$C_{23}H_{26}NO_4^+$	14.0157	380.1857	Phase II
Phosphorylation	M+HPO_3	$C_{22}H_{25}NO_7P^+$	79.9663	446.1363	Phase II
Propionyl conjugation	M+C_3H_4O	$C_{25}H_{28}NO_5^+$	56.0262	422.1962	Phase II

Sulfation	M+SO_3	$C_{22}H_{24}NO_7S^+$	79.9568	446.1268	Phase II
Taurine conjugation	M+$C_2H_5NO_2S$	$C_{24}H_{29}N_2O_6S^+$	107.0041	473.1741	Phase II

Table S4 Construction of the precursor ions list used in data-dependent acquisition(MIM-IDA-EPI on QTrap 4500 and HDDDA on Vion IM-QTOF).

No.	Biotransformation reaction	Delta Formula	Formula	Delta Mass	Theoretical Mass	Metabolic Category
1	Demethylation × 3 + Dehydrogenation × 3	M-C_4H_8-H_6	$C_{18}H_{10}NO_4^+$	-62.1096	304.0604	Phase I + Phase I
2	Demethylation × 3 + Dehydrogenation × 2	M-C_4H_8-H_4	$C_{18}H_{12}NO_4^+$	-60.0939	306.0761	Phase I + Phase I
3	Demethylation × 3 + Dehydrogenation × 1	M-C_4H_8-H_2	$C_{18}H_{14}NO_4^+$	-58.0783	308.0917	Phase I + Phase I
4	Demethylation × 4	M-C_4H_8	$C_{18}H_{16}NO_4^+$	-56.0626	310.1074	Phase I
5	Demethylation × 3 + Dehydrogenation × 3	M-C_3H_6-H_6	$C_{19}H_{12}NO_4^+$	-48.0939	318.0761	Phase I + Phase I
6	Demethylation × 3 + Dehydrogenation × 2	M-C_3H_6-H_4	$C_{19}H_{14}NO_4^+$	-46.0783	320.0917	Phase I + Phase I
7	Demethylation × 3 + Dehydrogenation × 1	M-C_3H_6-H_2	$C_{19}H_{16}NO_4^+$	-44.0626	322.1074	Phase I + Phase I
8	Demethylation × 4 + Oxidation × 1 + Dehydrogenation × 1	M-C_4H_8+O-H_2	$C_{18}H_{14}NO_5^+$	-42.0834	324.0866	Phase I + Phase I
9	Demethylation × 3	M-C_3H_6	$C_{19}H_{18}NO_4^+$	-42.0470	324.1230	Phase I
10	Demethylation × 4 + Oxidation × 1	M-C_4H_8+O	$C_{18}H_{16}NO_5^+$	-40.0677	326.1023	Phase I + Phase I
11	Demethylation × 2 + Dehydrogenation × 3	M-C_2H_4-H_6	$C_{20}H_{14}NO_4^+$	-34.0783	332.0917	Phase I + Phase I + Phase II
12	Demethylation × 2 + Dehydrogenation × 2	M-C_2H_4-H_4	$C_{20}H_{16}NO_4^+$	-32.0626	334.1074	Phase I + Phase I
13	Demethylation × 2 + Dehydrogenation × 1	M-C_2H_4-H_2	$C_{20}H_{18}NO_4^+$	-30.0470	336.1230	Phase I + Phase I
14	Demethylation × 3 + Oxidation × 1 + Dehydrogenation × 1	M-C_3H_6+O-H_2	$C_{19}H_{16}NO_5^+$	-28.0677	338.1023	Phase I + Phase I
15	Demethylation × 2	M-C_2H_4	$C_{20}H_{20}NO_4^+$	-28.0313	338.1387	Phase I
16	Demethylation × 4 + Oxidation × 2 + Dehydrogenation × 1	M-C_4H_8+O_2-H_2	$C_{18}H_{14}NO_6^+$	-26.0884	340.0816	Phase I + Phase I
17	Demethylation × 3 + Oxidation × 1	M-C_3H_6+O	$C_{19}H_{18}NO_5^+$	-26.0521	340.1179	Phase I + Phase I
18	Demethylation × 4 + Oxidation × 2	M-C_4H_8+O_2	$C_{18}H_{16}NO_6^+$	-24.0728	342.0972	Phase I + Phase I
19	Demethylation × 1 + Dehydrogenation × 1	M-CH_2-H_2	$C_{21}H_{20}NO_4^+$	-16.0313	350.1387	Phase I + Phase I

20	Demethylation × 2 + Oxidation × 1 + Dehydrogenation × 1	M-C_2H_4+O-H_2	$C_{20}H_{18}NO_5^+$	-14.0521	352.1179	Phase I + Phase I
21	Demethylation × 1	M-CH_2	$C_{21}H_{22}NO_4^+$	-14.0157	352.1543	Phase I
22	Demethylation × 3 + Oxidation × 2 + Dehydrogenation × 1	M-C_3H_6+O_2-H_2	$C_{19}H_{16}NO_6^+$	-12.0728	354.0972	Phase I + Phase I
23	Demethylation × 2 + Oxidation × 1	M-C_2H_4+O	$C_{20}H_{20}NO_5^+$	-12.0364	354.1336	Phase I + Phase I
24	Demethylation × 3 + Oxidation × 2	M-C_3H_6+O_2	$C_{19}H_{18}NO_6^+$	-10.0571	356.1129	Phase I + Phase I
25	Demethylation × 4 + Oxidation × 3	M-C_4H_8+O_3	$C_{18}H_{16}NO_7^+$	-8.0779	358.0921	Phase I + Phase I
26	Demethylation × 1 + Oxidation × 1 + Dehydrogenation × 1	M-CH_2+O-H_2	$C_{21}H_{20}NO_5^+$	-0.0364	366.1336	Phase I + Phase I
27	Demethylation × 2 + Oxidation × 2 + Dehydrogenation × 1	M-C_2H_4+O_2-H_2	$C_{20}H_{18}NO_6^+$	1.9429	368.1129	Phase I + Phase I
28	Demethylation × 1 + Oxidation × 1	M-CH_2+O	$C_{21}H_{22}NO_5^+$	1.9792	368.1492	Phase I + Phase I
29	Demethylation × 2 + Oxidation × 2	M-C_2H_4+O_2	$C_{20}H_{20}NO_6^+$	3.9585	370.1285	Phase I + Phase I
30	Demethylation × 3 + Oxidation × 3	M-C_3H_6+O_3	$C_{19}H_{18}NO_7^+$	5.9378	372.1078	Phase I + Phase I
31	Oxidation × 1 + Dehydrogenation × 1	M+O-H_2	$C_{22}H_{22}NO_5^+$	13.9792	380.1492	Phase I
32	Demethylation × 1 + Oxidation × 2 + Dehydrogenation × 1	M-CH_2+O_2-H_2	$C_{21}H_{20}NO_6^+$	15.9585	382.1285	Phase I + Phase I
33	Oxidation × 1	M+O	$C_{22}H_{24}NO_5^+$	15.9949	382.1649	Phase I
34	Demethylation × 3 + Dehydrogenation × 3 + Sulfation × 1	M-C_4H_8-H_6+SO_3	$C_{18}H_{10}NO_7S^+$	17.8472	384.0172	Phase I + Phase I + Phase II
35	Demethylation × 1 + Oxidation × 2	M-CH_2+O_2	$C_{21}H_{22}NO_6^+$	17.9742	384.1442	Phase I + Phase I
36	Demethylation × 3 + Dehydrogenation × 2 + Sulfation × 1	M-C_4H_8-H_4+SO_3	$C_{18}H_{12}NO_7S^+$	19.8629	386.0329	Phase I + Phase I + Phase II
37	Demethylation × 2 + Oxidation × 3	M-C_2H_4+O_3	$C_{20}H_{20}NO_7^+$	19.9534	386.1234	Phase I + Phase I
38	Demethylation × 3 + Dehydrogenation × 1 + Sulfation × 1	M-C_4H_8-H_2+SO_3	$C_{18}H_{14}NO_7S^+$	21.8785	388.0485	Phase I + Phase I + Phase II
39	Demethylation × 4 + Sulfation × 1	M-C_4H_8+SO_3	$C_{18}H_{16}NO_7S^+$	23.8942	390.0642	Phase I + Phase II

40	Oxidation × 2 + Dehydrogenation × 1	M+O_2-H_2	$C_{22}H_{22}NO_6^+$	29.9742	396.1442	Phase I
41	Demethylation × 3 + Dehydrogenation × 3 + Sulfation × 1	M-C_3H_6-H_6+SO_3	$C_{19}H_{12}NO_7S^+$	31.8629	398.0329	Phase I + Phase I + Phase II
42	Oxidation × 2	M+O_2	$C_{22}H_{24}NO_6^+$	31.9898	398.1598	Phase I
43	Demethylation × 3 + Dehydrogenation × 2 + Sulfation × 1	M-C_3H_6-H_4+SO_3	$C_{19}H_{14}NO_7S^+$	33.8785	400.0485	Phase I + Phase I + Phase II
44	Demethylation × 1 + Oxidation × 3	M-CH_2+O_3	$C_{21}H_{22}NO_7^+$	33.9691	400.1391	Phase I + Phase I
45	Demethylation × 3 + Dehydrogenation × 1 + Sulfation × 1	M-C_3H_6-H_2+SO_3	$C_{19}H_{16}NO_7S^+$	35.8942	402.0642	Phase I + Phase I + Phase II
46	Demethylation × 4 + Sulfation × 1 + Oxidation × 1 + Dehydrogenation × 1	M-C_4H_8+SO_3+O-H_2	$C_{18}H_{14}NO_8S^+$	37.8735	404.0435	Phase I + Phase II
47	Demethylation × 3 + Sulfation × 1	M-C_3H_6+SO_3	$C_{19}H_{18}NO_7S^+$	37.9098	404.0798	Phase I + Phase II
48	Demethylation × 4 + Oxidation × 1 + Sulfation × 1	M-C_4H_8+O+SO_3	$C_{18}H_{16}NO_8S^+$	39.8891	406.0591	Phase I + Phase I + Phase II
49	Demethylation × 2 + Dehydrogenation × 3 + Sulfation × 1	M-C_2H_4-H_6+SO_3	$C_{20}H_{14}NO_7S^+$	45.8785	412.0485	Phase I + Phase I + Phase II
50	Demethylation × 2 + Dehydrogenation × 2 + Sulfation × 1	M-C_2H_4-H_4+SO_3	$C_{20}H_{16}NO_7S^+$	47.8942	414.0642	Phase I + Phase I + Phase II
51	Oxidation × 3	M+O_3	$C_{22}H_{24}NO_7^+$	47.9847	414.1547	Phase I
52	Demethylation × 2 + Dehydrogenation × 1 + Sulfation × 1	M-C_2H_4-H_2+SO_3	$C_{20}H_{18}NO_7S^+$	49.9098	416.0798	Phase I + Phase I + Phase II
53	Demethylation × 3 + Sulfation × 1 + Oxidation × 1 + Dehydrogenation × 1	M-C_3H_6+SO_3+O-H_2	$C_{19}H_{16}NO_8S^+$	51.8891	418.0591	Phase I + Phase II
54	Demethylation × 2 + Sulfation × 1	M-C_2H_4+SO_3	$C_{20}H_{20}NO_7S^+$	51.9255	418.0955	Phase I + Phase II
55	Demethylation × 4 + Sulfation × 1 + Oxidation × 2 + Dehydrogenation × 1	M-C_4H_8+SO_3+O_2-H_2	$C_{18}H_{14}NO_9S^+$	53.8684	420.0384	Phase I + Phase II
56	Demethylation × 3 + Oxidation × 1 + Sulfation × 1	M-C_3H_6+O+SO_3	$C_{19}H_{18}NO_8S^+$	53.9048	420.0748	Phase I + Phase I + Phase II

57	Demethylation × 4 + Oxidation × 2 + Sulfation × 1	M-C_4H_8+O_2+SO_3	$C_{18}H_{16}NO_9S^+$	55.884	422.0540	Phase I + Phase I + Phase II
58	Demethylation × 1 + Dehydrogenation × 1 + Sulfation × 1	M-CH_2-H_2+SO_3	$C_{21}H_{20}NO_7S^+$	63.9255	430.0955	Phase I + Phase I + Phase II
59	Oxidation × 4	M+O_4	$C_{22}H_{24}NO_8^+$	63.9796	430.1496	Phase I
60	Demethylation × 2 + Sulfation × 1 + Oxidation × 1 + Dehydrogenation × 1	M-C_2H_4+SO_3+O-H_2	$C_{20}H_{18}NO_8S^+$	65.9048	432.0748	Phase I + Phase II
61	Demethylation × 1 + Sulfation × 1	M-CH_2+SO_3	$C_{21}H_{22}NO_7S^+$	65.9411	432.1111	Phase I + Phase II
62	Demethylation × 3 + Sulfation × 1 + Oxidation × 2 + Dehydrogenation × 1	M-C_3H_6+SO_3+O_2-H_2	$C_{19}H_{16}NO_9S^+$	67.8840	434.0540	Phase I + Phase II
63	Demethylation × 2 + Oxidation × 1 + Sulfation × 1	M-C_2H_4+O+SO_3	$C_{20}H_{20}NO_8S^+$	67.9204	434.0904	Phase I + Phase I + Phase II
64	Demethylation × 3 + Oxidation × 2 + Sulfation × 1	M-C_3H_6+O_2+SO_3	$C_{19}H_{18}NO_9S^+$	69.8997	436.0697	Phase I + Phase I + Phase II
65	Demethylation × 4 + Oxidation × 3 + Sulfation × 1	M-C_4H_8+O_3+SO_3	$C_{18}H_{16}NO_{10}S^+$	71.8789	438.0489	Phase I + Phase I + Phase II
66	Demethylation × 1 + Sulfation × 1 + Oxidation × 1 + Dehydrogenation × 1	M-CH_2+SO_3+O-H_2	$C_{21}H_{20}NO_8S^+$	79.9204	446.0904	Phase I + Phase II
67	Oxidation × 5	M+O_5	$C_{22}H_{24}NO_9^+$	79.9746	446.1446	Phase I
68	Demethylation × 2 + Sulfation × 1 + Oxidation × 2 + Dehydrogenation × 1	M-C_2H_4+SO_3+O_2-H_2	$C_{20}H_{18}NO_9S^+$	81.8997	448.0697	Phase I + Phase II
69	Demethylation × 1 + Oxidation × 2 + Sulfation × 1	M-CH_2+O+SO_3	$C_{21}H_{22}NO_8S^+$	81.9361	448.1061	Phase I + Phase I + Phase II
70	Demethylation × 2 + Oxidation × 2 + Sulfation × 1	M-C_2H_4+O_2+SO_3	$C_{20}H_{20}NO_9S^+$	83.9153	450.0853	Phase I + Phase I + Phase II
71	Demethylation × 3 + Oxidation × 3 + Sulfation × 1	M-C_3H_6+O_3+SO_3	$C_{19}H_{18}NO_{10}S^+$	85.8946	452.0646	Phase I + Phase I + Phase II
72	Demethylation × 1 + Sulfation × 1 + Oxidation × 2 +	M-CH_2+SO_3+O_2-H_2	$C_{21}H_{20}NO_9S^+$	95.9153	462.0853	Phase I + Phase II

	Dehydrogenation × 1					
73	Oxidation × 1 + Sulfation × 1	M+O+SO_3	$C_{22}H_{24}NO_8S^+$	95.9517	462.1217	Phase I + Phase II
74	Demethylation × 3 + Dehydrogenation × 3 + Sulfation × 2	M-C_4H_8-H_6+S_2O_6	$C_{18}H_{10}NO_{10}S_2^+$	97.8041	463.9741	Phase I + Phase I + Phase II
75	Demethylation × 1 + Oxidation × 2 + Sulfation × 1	M-CH_2+O_2+SO_3	$C_{21}H_{22}NO_9S^+$	97.9310	464.1010	Phase I + Phase I + Phase II
76	Demethylation × 3 + Dehydrogenation × 2 + Sulfation × 2	M-C_4H_8-H_4+S_2O_6	$C_{18}H_{12}NO_{10}S_2^+$	99.8197	465.9897	Phase I + Phase I + Phase II
77	Demethylation × 2 + Oxidation × 3 + Sulfation × 1	M-C_2H_4+O_3+SO_3	$C_{20}H_{20}NO_{10}S^+$	99.9102	466.0802	Phase I + Phase I + Phase II
78	Demethylation × 3 + Dehydrogenation × 1 + Sulfation × 2	M-C_4H_8-H_2+S_2O_6	$C_{18}H_{14}NO_{10}S_2^+$	101.8354	468.0054	Phase I + Phase I + Phase II
79	Demethylation × 4 + Sulfation × 2	M-C_4H_8+S_2O_6	$C_{18}H_{16}NO_{10}S_2^+$	103.8510	470.0210	Phase I + Phase II
80	Demethylation × 3 + Dehydrogenation × 3 + Sulfation × 2	M-C_3H_6-H_6+S_2O_6	$C_{19}H_{12}NO_{10}S_2^+$	111.8197	477.9897	Phase I + Phase I + Phase II
81	Oxidation × 2 + Sulfation × 1	M+O_2+SO_3	$C_{22}H_{24}NO_9S^+$	111.9466	478.1166	Phase I + Phase II
82	Demethylation × 3 + Dehydrogenation × 2 + Sulfation × 2	M-C_3H_6-H_4+S_2O_6	$C_{19}H_{14}NO_{10}S_2^+$	113.8354	480.0054	Phase I + Phase I + Phase II
83	Demethylation × 3 + Dehydrogenation × 3 + Glucuronidation × 1	M-C_4H_8-H_6+$C_6H_8O_6$	$C_{24}H_{18}NO_{10}^+$	113.9225	480.0925	Phase I + Phase I + Phase II
84	Demethylation × 1 + Oxidation × 3 + Sulfation × 1	M-CH_2+O_3+SO_3	$C_{21}H_{22}NO_{10}S^+$	113.9259	480.0959	Phase I + Phase I + Phase II
85	Demethylation × 3 + Dehydrogenation × 1 + Sulfation × 2	M-C_3H_6-H_2+S_2O_6	$C_{19}H_{16}NO_{10}S_2^+$	115.8510	482.0210	Phase I + Phase I + Phase II
86	Demethylation × 3 + Dehydrogenation × 2 + Glucuronidation × 1	M-C_4H_8-H_4+$C_6H_8O_6$	$C_{24}H_{20}NO_{10}^+$	115.9382	482.1082	Phase I + Phase I + Phase II
87	Demethylation × 4 + Sulfation × 2 + Oxidation × 1 + Dehydrogenation × 1	M-C_4H_8+S_2O_6+O-H_2	$C_{18}H_{14}NO_{11}S_2^+$	117.8303	484.0003	Phase I + Phase II

88	Demethylation × 3 + Sulfation × 2	M-C_3H_6+S_2O_6	$C_{19}H_{18}NO_{10}S_2^+$	117.8667	484.0367	Phase I + Phase II
89	Demethylation × 3 + Dehydrogenation × 1 + Glucuronidation × 1	M-C_4H_8-H_2+$C_6H_8O_6$	$C_{24}H_{22}NO_{10}^+$	117.9538	484.1238	Phase I + Phase I + Phase II
90	Demethylation × 4 + Oxidation × 1 + Sulfation × 2	M-C_4H_8+O+S_2O_6	$C_{18}H_{16}NO_{11}S_2^+$	119.8459	486.0159	Phase I + Phase I + Phase II
91	Demethylation × 4 + Glucuronidation × 1	M-C_4H_8+$C_6H_8O_6$	$C_{24}H_{24}NO_{10}^+$	119.9695	486.1395	Phase I + Phase II
92	Demethylation × 2 + Dehydrogenation × 3 + Sulfation × 2	M-C_2H_4-H_6+S_2O_6	$C_{20}H_{14}NO_{10}S_2^+$	125.8354	492.0054	Phase I + Phase I + Phase II
93	Demethylation × 2 + Dehydrogenation × 2 + Sulfation × 2	M-C_2H_4-H_4+S_2O_6	$C_{20}H_{16}NO_{10}S_2^+$	127.8510	494.0210	Phase I + Phase I + Phase II
94	Demethylation × 3 + Dehydrogenation × 3 + Glucuronidation × 1	M-C_3H_6-H_6+$C_6H_8O_6$	$C_{25}H_{20}NO_{10}^+$	127.9382	494.1082	Phase I + Phase I + Phase II
95	Oxidation × 3 + Sulfation × 1	M+O_3+SO_3	$C_{22}H_{24}NO_{10}S^+$	127.9415	494.1115	Phase I + Phase II
96	Demethylation × 2 + Dehydrogenation × 1 + Sulfation × 2	M-C_2H_4-H_2+S_2O_6	$C_{20}H_{18}NO_{10}S_2^+$	129.8667	496.0367	Phase I + Phase I + Phase II
97	Demethylation × 3 + Dehydrogenation × 2 + Glucuronidation × 1	M-C_3H_6-H_4+$C_6H_8O_6$	$C_{25}H_{22}NO_{10}^+$	129.9538	496.1238	Phase I + Phase I + Phase II
98	Demethylation × 3 + Sulfation × 2 + Oxidation × 1 + Dehydrogenation × 1	M-C_3H_6+S_2O_6+O-H_2	$C_{19}H_{16}NO_{11}S_2^+$	131.8459	498.0159	Phase I + Phase II
99	Demethylation × 2 + Sulfation × 2	M-C_2H_4+S_2O_6	$C_{20}H_{20}NO_{10}S_2^+$	131.8823	498.0523	Phase I + Phase II
100	Demethylation × 3 + Dehydrogenation × 1 + Glucuronidation × 1	M-C_3H_6-H_2+$C_6H_8O_6$	$C_{25}H_{24}NO_{10}^+$	131.9695	498.1395	Phase I + Phase I + Phase II
101	Demethylation × 4 + Sulfation × 2 + Oxidation × 2 + Dehydrogenation × 1	M-C_4H_8+S_2O_6+O_2-H_2	$C_{18}H_{14}NO_{12}S_2^+$	133.8252	499.9952	Phase I + Phase II
102	Demethylation × 3 + Oxidation × 1 + Sulfation × 2	M-C_3H_6+O+S_2O_6	$C_{19}H_{18}NO_{11}S_2^+$	133.8616	500.0316	Phase I + Phase I + Phase II
103	Demethylation × 4 + Glucuronidation × 1 + Oxidation × 1 + Dehydrogenation × 1	M-C_4H_8+$C_6H_8O_6$+O-H_2	$C_{24}H_{22}NO_{11}^+$	133.9487	500.1187	Phase I + Phase II

104	Demethylation × 3 + Glucuronidation × 1	M-C_3H_6+$C_6H_8O_6$	$C_{25}H_{26}NO_{10}^+$	133.9851	500.1551	Phase I + Phase II
105	Demethylation × 4 + Oxidation × 2 + Sulfation × 2	M-C_4H_8+O_2+S_2O_6	$C_{18}H_{16}NO_{12}S_2^+$	135.8408	502.0108	Phase I + Phase I + Phase II
106	Demethylation × 4 + Oxidation × 1 + Glucuronidation × 1	M-C_4H_8+O+$C_6H_8O_6$	$C_{24}H_{24}NO_{11}^+$	135.9644	502.1344	Phase I + Phase I + Phase II
107	Demethylation × 2 + Dehydrogenation × 3 + Glucuronidation × 1	M-C_2H_4-H_6+$C_6H_8O_6$	$C_{26}H_{22}NO_{10}^+$	141.9538	508.1238	Phase I + Phase I + Phase II
108	Oxidation × 4 + Sulfation × 1	M+O_4+SO_3	$C_{22}H_{24}NO_{11}S^+$	143.9365	510.1065	Phase I + Phase II
109	Demethylation × 2 + Dehydrogenation × 2 + Glucuronidation × 1	M-C_2H_4-H_4+$C_6H_8O_6$	$C_{26}H_{24}NO_{10}^+$	143.9695	510.1395	Phase I + Phase I + Phase II
110	Demethylation × 2 + Sulfation × 2 + Oxidation × 1 + Dehydrogenation × 1	M-C_2H_4+S_2O_6+O-H_2	$C_{20}H_{18}NO_{11}S_2^+$	145.8616	512.0316	Phase I + Phase II
111	Demethylation × 2 + Dehydrogenation × 1 + Glucuronidation × 1	M-C_2H_4-H_2+$C_6H_8O_6$	$C_{26}H_{26}NO_{10}^+$	145.9851	512.1551	Phase I + Phase I + Phase II
112	Demethylation × 3 + Sulfation × 2 + Oxidation × 2 + Dehydrogenation × 1	M-C_3H_6+S_2O_6+O_2-H_2	$C_{19}H_{16}NO_{12}S_2^+$	147.8408	514.0108	Phase I + Phase II
113	Demethylation × 2 + Oxidation × 1 + Sulfation × 2	M-C_2H_4+O+S_2O_6	$C_{20}H_{20}NO_{11}S_2^+$	147.8772	514.0472	Phase I + Phase I + Phase II
114	Demethylation × 3 + Glucuronidation × 1 + Oxidation × 1 + Dehydrogenation × 1	M-C_3H_6+$C_6H_8O_6$+O-H_2	$C_{25}H_{24}NO_{11}^+$	147.9644	514.1344	Phase I + Phase II
115	Demethylation × 2 + Glucuronidation × 1	M-C_2H_4+$C_6H_8O_6$	$C_{26}H_{28}NO_{10}^+$	148.0008	514.1708	Phase I + Phase II
116	Demethylation × 3 + Oxidation × 2 + Sulfation × 2	M-C_3H_6+O_2+S_2O_6	$C_{19}H_{18}NO_{12}S_2^+$	149.8565	516.0265	Phase I + Phase I + Phase II
117	Demethylation × 4 + Glucuronidation × 1 + Oxidation × 2 + Dehydrogenation × 1	M-C_4H_8+$C_6H_8O_6$+O_2-H_2	$C_{24}H_{22}NO_{12}^+$	149.9437	516.1137	Phase I + Phase II
118	Demethylation × 3 + Oxidation × 1 + Glucuronidation × 1	M-C_3H_6+O+$C_6H_8O_6$	$C_{25}H_{26}NO_{11}^+$	149.9800	516.1500	Phase I + Phase I + Phase II
119	Demethylation × 4 + Oxidation × 3 + Sulfation × 2	M-C_4H_8+O_3+S_2O_6	$C_{18}H_{16}NO_{13}S_2^+$	151.8358	518.0058	Phase I + Phase I +

						Phase II
120	Demethylation × 4 + Oxidation × 2 + Glucuronidation × 1	M-C_4H_8+O_2+$C_6H_8O_6$	$C_{24}H_{24}NO_{12}^+$	151.9593	518.1293	Phase I + Phase I + Phase II
121	Oxidation × 5 + Sulfation × 1	M+O_5+SO_3	$C_{22}H_{24}NO_{12}S^+$	159.9314	526.1014	Phase I + Phase II
122	Demethylation × 1 + Dehydrogenation × 1 + Glucuronidation × 1	M-CH_2-H_2+$C_6H_8O_6$	$C_{27}H_{28}NO_{10}^+$	160.0008	526.1708	Phase I + Phase I + Phase II
123	Demethylation × 2 + Sulfation × 2 + Oxidation × 2 + Dehydrogenation × 1	M-C_2H_4+S_2O_6+O_2-H_2	$C_{20}H_{18}NO_{12}S_2^+$	161.8565	528.0265	Phase I + Phase II
124	Demethylation × 1 + Oxidation × 1 + Sulfation × 2	M-CH_2+O+S_2O_6	$C_{21}H_{22}NO_{11}S_2^+$	161.8929	528.0629	Phase I + Phase I + Phase II
125	Demethylation × 2 + Glucuronidation × 1 + Oxidation × 1 + Dehydrogenation × 1	M-C_2H_4+$C_6H_8O_6$+O-H_2	$C_{26}H_{26}NO_{11}^+$	161.9800	528.1500	Phase I + Phase II
126	Demethylation × 1 + Glucuronidation × 1	M-CH_2+$C_6H_8O_6$	$C_{27}H_{30}NO_{10}^+$	162.0164	528.1864	Phase I + Phase II
127	Demethylation × 2 + Oxidation × 2 + Sulfation × 2	M-C_2H_4+O_2+S_2O_6	$C_{20}H_{20}NO_{12}S_2^+$	163.8721	530.0421	Phase I + Phase I + Phase II
128	Demethylation × 3 + Glucuronidation × 1 + Oxidation × 2 + Dehydrogenation × 1	M-C_3H_6+$C_6H_8O_6$+O_2-H_2	$C_{25}H_{24}NO_{12}^+$	163.9593	530.1293	Phase I + Phase II
129	Demethylation × 2 + Oxidation × 1 + Glucuronidation × 1	M-C_2H_4+O+$C_6H_8O_6$	$C_{26}H_{28}NO_{11}^+$	163.9957	530.1657	Phase I + Phase I + Phase II
130	Demethylation × 3 + Oxidation × 3 + Sulfation × 2	M-C_3H_6+O_3+S_2O_6	$C_{19}H_{18}NO_{13}S_2^+$	165.8514	532.0214	Phase I + Phase I + Phase II
131	Demethylation × 3 + Oxidation × 2 + Glucuronidation × 1	M-C_3H_6+O_2+$C_6H_8O_6$	$C_{25}H_{26}NO_{12}^+$	165.9750	532.1450	Phase I + Phase I + Phase II
132	Demethylation × 4 + Oxidation × 3 + Glucuronidation × 1	M-C_4H_8+O_3+$C_6H_8O_6$	$C_{24}H_{24}NO_{13}^+$	167.9542	534.1242	Phase I + Phase I + Phase II
133	Demethylation × 1 + Glucuronidation × 1 + Oxidation × 1 + Dehydrogenation × 1	M-CH_2+$C_6H_8O_6$+O-H_2	$C_{27}H_{28}NO_{11}^+$	175.9957	542.1657	Phase I + Phase II
134	Demethylation × 1 + Oxidation × 2 + Sulfation × 2	M-CH_2+O_2+S_2O_6	$C_{21}H_{22}NO_{12}S_2^+$	177.8878	544.0578	Phase I + Phase I +

						Phase II
135	Demethylation × 2 + Glucuronidation × 1 + Oxidation × 2 + Dehydrogenation × 1	M-C_2H_4+$C_6H_8O_6$+O_2-H_2	$C_{26}H_{26}NO_{12}^+$	177.9750	544.1450	Phase I + Phase II
136	Demethylation × 1 + Oxidation × 1 + Glucuronidation × 1	M-CH_2+O+$C_6H_8O_6$	$C_{27}H_{30}NO_{11}^+$	178.0113	544.1813	Phase I + Phase I + Phase II
137	Demethylation × 2 + Oxidation × 3 + Sulfation × 2	M-C_2H_4+O_3+S_2O_6	$C_{20}H_{20}NO_{13}S_2^+$	179.8671	546.0371	Phase I + Phase I + Phase II
138	Demethylation × 2 + Oxidation × 2 + Glucuronidation × 1	M-C_2H_4+O_2+$C_6H_8O_6$	$C_{26}H_{28}NO_{12}^+$	179.9906	546.1606	Phase I + Phase I + Phase II
139	Demethylation × 3 + Oxidation × 3 + Glucuronidation × 1	M-C_3H_6+O_3+$C_6H_8O_6$	$C_{25}H_{26}NO_{13}^+$	181.9699	548.1399	Phase I + Phase I + Phase II
140	Demethylation × 4 + Sulfation × 3	M-C_4H_8+S_3O_9	$C_{18}H_{16}NO_{13}S_3^+$	183.8078	549.9778	Phase I + Phase II
141	Oxidation × 2 + Sulfation × 2	M+O_2+S_2O_6	$C_{22}H_{24}NO_{12}S_2^+$	191.9034	558.0734	Phase I + Phase II
142	Demethylation × 1 + Glucuronidation × 1 + Oxidation × 2 + Dehydrogenation × 1	M-CH_2+$C_6H_8O_6$+O_2-H_2	$C_{27}H_{28}NO_{12}^+$	191.9906	558.1606	Phase I + Phase II
143	Oxidation × 1 + Glucuronidation × 1	M+O+$C_6H_8O_6$	$C_{28}H_{32}NO_{11}^+$	192.0270	558.1970	Phase I + Phase II
144	Demethylation × 3 + Dehydrogenation × 3 + Glucuronidation × 1 + Sulfation × 1	M-C_4H_8-H_6+$C_6H_8O_6$+SO_3	$C_{24}H_{18}NO_{13}S^+$	193.8793	560.0493	Phase I + Phase I + Phase II
145	Demethylation × 1 + Oxidation × 3 + Sulfation × 2	M-CH_2+O_3+S_2O_6	$C_{21}H_{22}NO_{13}S_2^+$	193.8827	560.0527	Phase I + Phase I + Phase II
146	Demethylation × 1 + Oxidation × 2 + Glucuronidation × 1	M-CH_2+O_2+$C_6H_8O_6$	$C_{27}H_{30}NO_{12}^+$	194.0063	560.1763	Phase I + Phase I + Phase II
147	Demethylation × 3 + Dehydrogenation × 1 + Sulfation × 3	M-C_3H_6-H_2+S_3O_9	$C_{19}H_{16}NO_{13}S_3^+$	195.8078	561.9778	Phase I + Phase I + Phase II
148	Demethylation × 3 + Dehydrogenation × 2 + Glucuronidation × 1 + Sulfation × 1	M-C_4H_8-H_4+$C_6H_8O_6$+SO_3	$C_{24}H_{20}NO_{13}S^+$	195.8950	562.0650	Phase I + Phase I + Phase II
149	Demethylation × 2 + Oxidation × 3 + Glucuronidation × 1	M-C_2H_4+O_3+$C_6H_8O_6$	$C_{26}H_{28}NO_{13}^+$	195.9855	562.1555	Phase I + Phase I + Phase II

150	Demethylation × 4 + Sulfation × 3 + Oxidation × 1 + Dehydrogenation × 1	M-C_4H_8+S_3O_9+O-H_2	$C_{18}H_{14}NO_{14}S_3^+$	197.7871	563.9571	Phase I + Phase II
151	Demethylation × 3 + Sulfation × 3	M-C_3H_6+S_3O_9	$C_{19}H_{18}NO_{13}S_3^+$	197.8235	563.9935	Phase I + Phase II
152	Demethylation × 3 + Dehydrogenation × 1 + Glucuronidation × 1 + Sulfation × 1	M-C_4H_8-H_2+$C_6H_8O_6$+SO_3	$C_{24}H_{22}NO_{13}S^+$	197.9106	564.0806	Phase I + Phase I + Phase II
153	Demethylation × 4 + Oxidation × 1 + Sulfation × 3	M-C_4H_8+O+S_3O_9	$C_{18}H_{16}NO_{14}S_3^+$	199.8027	565.9727	Phase I + Phase I + Phase II
154	Demethylation × 4 + Glucuronidation × 1 + Sulfation × 1	M-C_4H_8+$C_6H_8O_6$+SO_3	$C_{24}H_{24}NO_{13}S^+$	199.9263	566.0963	Phase I + Phase II
155	Demethylation × 3 + Dehydrogenation × 3 + Glucuronidation × 1 + Sulfation × 1	M-C_3H_6-H_6+$C_6H_8O_6$+SO_3	$C_{25}H_{20}NO_{13}S^+$	207.8950	574.0650	Phase I + Phase I + Phase II
156	Oxidation × 3 + Sulfation × 2	M+O_3+S_2O_6	$C_{22}H_{24}NO_{13}S_2^+$	207.8984	574.0684	Phase I + Phase II
157	Oxidation × 2 + Glucuronidation × 1	M+O_2+$C_6H_8O_6$	$C_{28}H_{32}NO_{12}^+$	208.0219	574.1919	Phase I + Phase II
158	Demethylation × 3 + Dehydrogenation × 2 + Glucuronidation × 1 + Sulfation × 1	M-C_3H_6-H_4+$C_6H_8O_6$+SO_3	$C_{25}H_{22}NO_{13}S^+$	209.9106	576.0806	Phase I + Phase I + Phase II
159	Demethylation × 1 + Oxidation × 3 + Glucuronidation × 1	M-CH_2+O_3+$C_6H_8O_6$	$C_{27}H_{30}NO_{13}^+$	210.0012	576.1712	Phase I + Phase I + Phase II
160	Demethylation × 3 + Sulfation × 3 + Oxidation × 1 + Dehydrogenation × 1	M-C_3H_6+S_3O_9+O-H_2	$C_{19}H_{16}NO_{14}S_3^+$	211.8027	577.9727	Phase I + Phase II
161	Demethylation × 3 + Dehydrogenation × 1 + Glucuronidation × 1 + Sulfation × 1	M-C_3H_6-H_2+$C_6H_8O_6$+SO_3	$C_{25}H_{24}NO_{13}S^+$	211.9263	578.0963	Phase I + Phase I + Phase II
162	Demethylation × 4 + Sulfation × 3 + Oxidation × 2 + Dehydrogenation × 1	M-C_4H_8+S_3O_9+O_2-H_2	$C_{18}H_{14}NO_{15}S_3^+$	213.7820	579.9520	Phase I + Phase II
163	Demethylation × 3 + Oxidation × 1 + Sulfation × 3	M-C_3H_6+O+S_3O_9	$C_{19}H_{18}NO_{14}S_3^+$	213.8184	579.9884	Phase I + Phase I + Phase II
164	Demethylation × 4 + Glucuronidation × 1 + Sulfation × 1 + Oxidation × 1 + Dehydrogenation × 1	M-C_4H_8+$C_6H_8O_6$+SO_3+O-H_2	$C_{24}H_{22}NO_{14}S^+$	213.9056	580.0756	Phase I + Phase II
165	Demethylation × 3 + Glucuronidation × 1 + Sulfation ×	M-C_3H_6+$C_6H_8O_6$+SO_3	$C_{25}H_{26}NO_{13}S^+$	213.9419	580.1119	Phase I + Phase II

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166	Demethylation × 4 + Oxidation × 2 + Sulfation × 3	M-C_4H_8+O_2+S_3O_9	$C_{18}H_{16}NO_{15}S_3^+$	215.7977	581.9677	Phase I + Phase I + Phase II
167	Demethylation × 4 + Oxidation × 1 + Glucuronidation × 1 + Sulfation × 1	M-C_4H_8+O+$C_6H_8O_6$+SO_3	$C_{24}H_{24}NO_{14}S^+$	215.9212	582.0912	Phase I + Phase I + Phase II
168	Demethylation × 2 + Dehydrogenation × 3 + Glucuronidation × 1 + Sulfation × 1	M-C_2H_4-H_6+$C_6H_8O_6$+SO_3	$C_{26}H_{22}NO_{13}S^+$	221.9106	588.0806	Phase I + Phase I + Phase II
169	Oxidation × 4 + Sulfation × 2	M+O_4+S_2O_6	$C_{22}H_{24}NO_{14}S_2^+$	223.8933	590.0633	Phase I + Phase II
170	Demethylation × 2 + Dehydrogenation × 2 + Glucuronidation × 1 + Sulfation × 1	M-C_2H_4-H_4+$C_6H_8O_6$+SO_3	$C_{26}H_{24}NO_{13}S^+$	223.9263	590.0963	Phase I + Phase I + Phase II
171	Oxidation × 3 + Glucuronidation × 1	M+O_3+$C_6H_8O_6$	$C_{28}H_{32}NO_{13}^+$	224.0168	590.1868	Phase I + Phase II
172	Demethylation × 2 + Dehydrogenation × 1 + Glucuronidation × 1 + Sulfation × 1	M-C_2H_4-H_2+$C_6H_8O_6$+SO_3	$C_{26}H_{26}NO_{13}S^+$	225.9419	592.1119	Phase I + Phase I + Phase II
173	Demethylation × 3 + Sulfation × 3 + Oxidation × 2 + Dehydrogenation × 1	M-C_3H_6+S_3O_9+O_2-H_2	$C_{19}H_{16}NO_{15}S_3^+$	227.7977	593.9677	Phase I + Phase II
174	Demethylation × 2 + Oxidation × 1 + Sulfation × 3	M-C_2H_4+O+S_3O_9	$C_{20}H_{20}NO_{14}S_3^+$	227.8340	594.0040	Phase I + Phase I + Phase II
175	Demethylation × 3 + Glucuronidation × 1 + Sulfation × 1 + Oxidation × 1 + Dehydrogenation × 1	M-C_3H_6+$C_6H_8O_6$+SO_3+O-H_2	$C_{25}H_{24}NO_{14}S^+$	227.9212	594.0912	Phase I + Phase II
176	Demethylation × 2 + Glucuronidation × 1 + Sulfation × 1	M-C_2H_4+$C_6H_8O_6$+SO_3	$C_{26}H_{28}NO_{13}S^+$	227.9576	594.1276	Phase I + Phase II
177	Demethylation × 3 + Oxidation × 2 + Sulfation × 3	M-C_3H_6+O_2+S_3O_9	$C_{19}H_{18}NO_{15}S_3^+$	229.8133	595.9833	Phase I + Phase I + Phase II
178	Demethylation × 4 + Glucuronidation × 1 + Sulfation × 1 + Oxidation × 2 + Dehydrogenation × 1	M-C_4H_8+$C_6H_8O_6$+SO_3+O_2-H_2	$C_{24}H_{22}NO_{15}S^+$	229.9005	596.0705	Phase I + Phase II
179	Demethylation × 3 + Oxidation × 1 + Glucuronidation × 1 + Sulfation × 1	M-C_3H_6+O+$C_6H_8O_6$+SO_3	$C_{25}H_{26}NO_{14}S^+$	229.9369	596.1069	Phase I + Phase I + Phase II
180	Demethylation × 4 + Oxidation × 3 + Sulfation × 3	M-C_4H_8+O_3+S_3O_9	$C_{18}H_{16}NO_{16}S_3^+$	231.7926	597.9626	Phase I + Phase I +

						Phase II
181	Demethylation × 4 + Oxidation × 2 + Glucuronidation × 1 + Sulfation × 1	M-C_4H_8+O_2+$C_6H_8O_6$+SO_3	$C_{24}H_{24}NO_{15}S^+$	231.9161	598.0861	Phase I + Phase I + Phase II
182	Oxidation × 5 + Sulfation × 2	M+O_5+S_2O_6	$C_{22}H_{24}NO_{15}S_2^+$	239.8882	606.0582	Phase I + Phase II
183	Oxidation × 4 + Glucuronidation × 1	M+O_4+$C_6H_8O_6$	$C_{28}H_{32}NO_{14}^+$	240.0117	606.1817	Phase I + Phase II
184	Demethylation × 2 + Glucuronidation × 1 + Sulfation × 1 + Oxidation × 1 + Dehydrogenation × 1	M-C_2H_4+$C_6H_8O_6$+SO_3+O-H_2	$C_{26}H_{26}NO_{14}S^+$	241.9369	608.1069	Phase I + Phase II
185	Demethylation × 2 + Oxidation × 2 + Sulfation × 3	M-C_2H_4+O_2+S_3O_9	$C_{20}H_{20}NO_{15}S_3^+$	243.8290	609.9990	Phase I + Phase I + Phase II
186	Demethylation × 3 + Glucuronidation × 1 + Sulfation × 1 + Oxidation × 2 + Dehydrogenation × 1	M-C_3H_6+$C_6H_8O_6$+SO_3+O_2-H_2	$C_{25}H_{24}NO_{15}S^+$	243.9161	610.0861	Phase I + Phase II
187	Demethylation × 2 + Oxidation × 1 + Glucuronidation × 1 + Sulfation × 1	M-C_2H_4+O+$C_6H_8O_6$+SO_3	$C_{26}H_{28}NO_{14}S^+$	243.9525	610.1225	Phase I + Phase I + Phase II
188	Demethylation × 3 + Oxidation × 3 + Sulfation × 3	M-C_3H_6+O_3+S_3O_9	$C_{19}H_{18}NO_{16}S_3^+$	245.8082	611.9782	Phase I + Phase I + Phase II
189	Demethylation × 3 + Oxidation × 2 + Glucuronidation × 1 + Sulfation × 1	M-C_3H_6+O_2+$C_6H_8O_6$+SO_3	$C_{25}H_{26}NO_{15}S^+$	245.9318	612.1018	Phase I + Phase I + Phase II
190	Demethylation × 4 + Oxidation × 3 + Glucuronidation × 1 + Sulfation × 1	M-C_4H_8+O_3+$C_6H_8O_6$+SO_3	$C_{24}H_{24}NO_{16}S^+$	247.9110	614.0810	Phase I + Phase I + Phase II
191	Oxidation × 5 + Glucuronidation × 1	M+O_5+$C_6H_8O_6$	$C_{28}H_{32}NO_{15}^+$	256.0066	622.1766	Phase I + Phase II
192	Demethylation × 1 + Oxidation × 2 + Sulfation × 3	M-CH_2+O_2+S_3O_9	$C_{21}H_{22}NO_{15}S_3^+$	257.8446	624.0146	Phase I + Phase I + Phase II
193	Demethylation × 2 + Glucuronidation × 1 + Sulfation × 1 + Oxidation × 2 + Dehydrogenation × 1	M-C_2H_4+$C_6H_8O_6$+SO_3+O_2-H_2	$C_{26}H_{26}NO_{15}S^+$	257.9318	624.1018	Phase I + Phase II
194	Demethylation × 1 + Oxidation × 1 + Glucuronidation × 1 + Sulfation × 1	M-CH_2+O+$C_6H_8O_6$+SO_3	$C_{27}H_{30}NO_{14}S^+$	257.9682	624.1382	Phase I + Phase I + Phase II
195	Demethylation × 2 + Oxidation × 3 + Sulfation × 3	M-C_2H_4+O_3+S_3O_9	$C_{20}H_{20}NO_{16}S_3^+$	259.8239	625.9939	Phase I + Phase I + Phase II

196	Demethylation × 2 + Oxidation × 2 + Glucuronidation × 1 + Sulfation × 1	M-C_2H_4+O_2+$C_6H_8O_6$+SO_3	$C_{26}H_{28}NO_{15}S^+$	259.9474	626.1174	Phase I + Phase I + Phase II
197	Demethylation × 3 + Oxidation × 3 + Glucuronidation × 1 + Sulfation × 1	M-C_3H_6+O_3+$C_6H_8O_6$+SO_3	$C_{25}H_{26}NO_{16}S^+$	261.9267	628.0967	Phase I + Phase I + Phase II
198	Demethylation × 4 + Sulfation × 4	M-C_4H_8+S_4O_{12}	$C_{18}H_{16}NO_{16}S_4^+$	263.7646	629.9346	Phase I + Phase II
199	Demethylation × 1 + Oxidation × 3 + Sulfation × 3	M-CH_2+O_3+S_3O_9	$C_{21}H_{22}NO_{16}S_3^+$	273.8395	640.0095	Phase I + Phase I + Phase II
200	Demethylation × 1 + Oxidation × 2 + Glucuronidation × 1 + Sulfation × 1	M-CH_2+O_2+$C_6H_8O_6$+SO_3	$C_{27}H_{30}NO_{15}S^+$	273.9631	640.1331	Phase I + Phase I + Phase II
201	Demethylation × 2 + Oxidation × 3 + Glucuronidation × 1 + Sulfation × 1	M-C_2H_4+O_3+$C_6H_8O_6$+SO_3	$C_{26}H_{28}NO_{16}S^+$	275.9423	642.1123	Phase I + Phase I + Phase II
202	Demethylation × 4 + Sulfation × 4 + Oxidation × 1 + Dehydrogenation × 1	M-C_4H_8+S_4O_{12}+O-H_2	$C_{18}H_{14}NO_{17}S_4^+$	277.7439	643.9139	Phase I + Phase II
203	Demethylation × 4 + Oxidation × 1 + Sulfation × 4	M-C_4H_8+O+S_4O_{12}	$C_{18}H_{16}NO_{17}S_4^+$	279.7596	645.9296	Phase I + Phase I + Phase II
204	Demethylation × 4 + Glucuronidation × 1 + Sulfation × 2	M-C_4H_8+$C_6H_8O_6$+S_2O_6	$C_{24}H_{24}NO_{16}S_2^+$	279.8831	646.0531	Phase I + Phase II
205	Oxidation × 3 + Sulfation × 3	M+O_3+S_3O_9	$C_{22}H_{24}NO_{16}S_3^+$	287.8552	654.0252	Phase I + Phase II
206	Oxidation × 2 + Glucuronidation × 1 + Sulfation × 1	M+O_2+$C_6H_8O_6$+SO_3	$C_{28}H_{32}NO_{15}S^+$	287.9787	654.1487	Phase I + Phase II
207	Demethylation × 3 + Dehydrogenation × 3 + Glucuronidation × 2	M-C_4H_8-H_6+$C_{12}H_{16}O_{12}$	$C_{30}H_{26}NO_{16}^+$	289.9546	656.1246	Phase I + Phase I + Phase II
208	Demethylation × 1 + Oxidation × 3 + Glucuronidation × 1 + Sulfation × 1	M-CH_2+O_3+$C_6H_8O_6$+SO_3	$C_{27}H_{30}NO_{16}S^+$	289.9580	656.1280	Phase I + Phase I + Phase II
209	Demethylation × 3 + Dehydrogenation × 1 + Glucuronidation × 1 + Sulfation × 2	M-C_3H_6-H_2+$C_6H_8O_6$+S_2O_6	$C_{25}H_{24}NO_{16}S_2^+$	291.8831	658.0531	Phase I + Phase I + Phase II
210	Demethylation × 3 + Dehydrogenation × 2 + Glucuronidation × 2	M-C_4H_8-H_4+$C_{12}H_{16}O_{12}$	$C_{30}H_{28}NO_{16}^+$	291.9703	658.1403	Phase I + Phase I + Phase II
211	Demethylation × 4 + Sulfation × 4 + Oxidation × 2 +	M-C_4H_8+S_4O_{12}+O_2-H_2	$C_{18}H_{14}NO_{18}S_4^+$	293.7388	659.9088	Phase I + Phase II

	Dehydrogenation × 1					
212	Demethylation × 3 + Oxidation × 1 + Sulfation × 4	M-C_3H_6+O+S_4O_{12}	$C_{19}H_{18}NO_{17}S_4^+$	293.7752	659.9452	Phase I + Phase I + Phase II
213	Demethylation × 4 + Glucuronidation × 1 + Sulfation × 2 + Oxidation × 1 + Dehydrogenation × 1	M-C_4H_8+$C_6H_8O_6$+S_2O_6 +O-H_2	$C_{24}H_{22}NO_{17}S_2^+$	293.8624	660.0324	Phase I + Phase II
214	Demethylation × 3 + Glucuronidation × 1 + Sulfation × 2	M-C_3H_6+$C_6H_8O_6$+S_2O_6	$C_{25}H_{26}NO_{16}S_2^+$	293.8988	660.0688	Phase I + Phase II
215	Demethylation × 3 + Dehydrogenation × 1 + Glucuronidation × 2	M-C_4H_8-H_2+$C_{12}H_{16}O_{12}$	$C_{30}H_{30}NO_{16}^+$	293.9859	660.1559	Phase I + Phase I + Phase II
216	Demethylation × 4 + Oxidation × 2 + Sulfation × 4	M-C_4H_8+O_2+S_4O_{12}	$C_{18}H_{16}NO_{18}S_4^+$	295.7545	661.9245	Phase I + Phase I + Phase II
217	Demethylation × 4 + Oxidation × 1 + Glucuronidation × 1 + Sulfation × 2	M-C_4H_8+O+$C_6H_8O_6$+S_2O_6	$C_{24}H_{24}NO_{17}S_2^+$	295.8780	662.0480	Phase I + Phase I + Phase II
218	Demethylation × 4 + Glucuronidation × 2	M-C_4H_8+$C_{12}H_{16}O_{12}$	$C_{30}H_{32}NO_{16}^+$	296.0016	662.1716	Phase I + Phase II
219	Oxidation × 4 + Sulfation × 3	M+O_4+S_3O_9	$C_{22}H_{24}NO_{17}S_3^+$	303.8501	670.0201	Phase I + Phase II
220	Demethylation × 3 + Dehydrogenation × 3 + Glucuronidation × 2	M-C_3H_6-H_6+$C_{12}H_{16}O_{12}$	$C_{31}H_{28}NO_{16}^+$	303.9703	670.1403	Phase I + Phase I + Phase II
221	Oxidation × 3 + Glucuronidation × 1 + Sulfation × 1	M+O_3+$C_6H_8O_6$+SO_3	$C_{28}H_{32}NO_{16}S^+$	303.9736	670.1436	Phase I + Phase II
222	Demethylation × 3 + Dehydrogenation × 2 + Glucuronidation × 2	M-C_3H_6-H_4+$C_{12}H_{16}O_{12}$	$C_{31}H_{30}NO_{16}^+$	305.9859	672.1559	Phase I + Phase I + Phase II
223	Demethylation × 3 + Glucuronidation × 1 + Sulfation × 2 + Oxidation × 1 + Dehydrogenation × 1	M-C_3H_6+$C_6H_8O_6$+S_2O_6 +O-H_2	$C_{25}H_{24}NO_{17}S_2^+$	307.8780	674.0480	Phase I + Phase II
224	Demethylation × 3 + Dehydrogenation × 1 + Glucuronidation × 2	M-C_3H_6-H_2+$C_{12}H_{16}O_{12}$	$C_{31}H_{32}NO_{16}^+$	308.0016	674.1716	Phase I + Phase I + Phase II
225	Demethylation × 3 + Oxidation × 2 + Sulfation × 4	M-C_3H_6+O_2+S_4O_{12}	$C_{19}H_{18}NO_{18}S_4^+$	309.7701	675.9401	Phase I + Phase I + Phase II
226	Demethylation × 4 + Glucuronidation × 1 + Sulfation × 2 + Oxidation × 2 + Dehydrogenation × 1	M-C_4H_8+$C_6H_8O_6$+S_2O_6 +O_2-H_2	$C_{24}H_{22}NO_{18}S_2^+$	309.8573	676.0273	Phase I + Phase II

227	Demethylation × 3 + Oxidation × 1 + Glucuronidation × 1 + Sulfation × 2	M-C_3H_6+O+$C_6H_8O_6$+S_2O_6	$C_{25}H_{26}NO_{17}S_2^+$	309.8937	676.0637	Phase I + Phase I + Phase II
228	Demethylation × 4 + Glucuronidation × 2 + Oxidation × 1 + Dehydrogenation × 1	M-C_4H_8+$C_{12}H_{16}O_{12}$+O-H_2	$C_{30}H_{30}NO_{17}^+$	309.9808	676.1508	Phase I + Phase II
229	Demethylation × 3 + Glucuronidation × 2	M-C_3H_6+$C_{12}H_{16}O_{12}$	$C_{31}H_{34}NO_{16}^+$	310.0172	676.1872	Phase I + Phase II
230	Demethylation × 4 + Oxidation × 3 + Sulfation × 4	M-C_4H_8+O_3+S_4O_{12}	$C_{18}H_{16}NO_{19}S_4^+$	311.7494	677.9194	Phase I + Phase I + Phase II
231	Demethylation × 4 + Oxidation × 2 + Glucuronidation × 1 + Sulfation × 2	M-C_4H_8+O_2+$C_6H_8O_6$+S_2O_6	$C_{24}H_{24}NO_{18}S_2^+$	311.8729	678.0429	Phase I + Phase I + Phase II
232	Demethylation × 4 + Oxidation × 1 + Glucuronidation × 2	M-C_4H_8+O+$C_{12}H_{16}O_{12}$	$C_{30}H_{32}NO_{17}^+$	311.9965	678.1665	Phase I + Phase I + Phase II
233	Demethylation × 2 + Dehydrogenation × 3 + Glucuronidation × 2	M-C_2H_4-H_6+$C_{12}H_{16}O_{12}$	$C_{32}H_{30}NO_{16}^+$	317.9859	684.1559	Phase I + Phase I + Phase II
234	Oxidation × 5 + Sulfation × 3	M+O_5+S_3O_9	$C_{22}H_{24}NO_{18}S_3^+$	319.8450	686.0150	Phase I + Phase II
235	Oxidation × 4 + Glucuronidation × 1 + Sulfation × 1	M+O_4+$C_6H_8O_6$+SO_3	$C_{28}H_{32}NO_{17}S^+$	319.9685	686.1385	Phase I + Phase II
236	Demethylation × 2 + Dehydrogenation × 2 + Glucuronidation × 2	M-C_2H_4-H_4+$C_{12}H_{16}O_{12}$	$C_{32}H_{32}NO_{16}^+$	320.0016	686.1716	Phase I + Phase I + Phase II
237	Demethylation × 2 + Dehydrogenation × 1 + Glucuronidation × 2	M-C_2H_4-H_2+$C_{12}H_{16}O_{12}$	$C_{32}H_{34}NO_{16}^+$	322.0172	688.1872	Phase I + Phase I + Phase II
238	Demethylation × 2 + Oxidation × 2 + Sulfation × 4	M-C_2H_4+O_2+S_4O_{12}	$C_{20}H_{20}NO_{18}S_4^+$	323.7858	689.9558	Phase I + Phase I + Phase II
239	Demethylation × 3 + Glucuronidation × 1 + Sulfation × 2 + Oxidation × 2 + Dehydrogenation × 1	M-C_3H_6+$C_6H_8O_6$+S_2O_6+O_2-H_2	$C_{25}H_{24}NO_{18}S_2^+$	323.8729	690.0429	Phase I + Phase II
240	Demethylation × 2 + Oxidation × 1 + Glucuronidation × 1 + Sulfation × 2	M-C_2H_4+O+$C_6H_8O_6$+S_2O_6	$C_{26}H_{28}NO_{17}S_2^+$	323.9093	690.0793	Phase I + Phase I + Phase II
241	Demethylation × 3 + Glucuronidation × 2 + Oxidation × 1 + Dehydrogenation × 1	M-C_3H_6+$C_{12}H_{16}O_{12}$+O-H_2	$C_{31}H_{32}NO_{17}^+$	323.9965	690.1665	Phase I + Phase II
242	Demethylation × 2 + Glucuronidation × 2	M-C_2H_4+$C_{12}H_{16}O_{12}$	$C_{32}H_{36}NO_{16}^+$	324.0329	690.2029	Phase I + Phase II

243	Demethylation × 3 + Oxidation × 3 + Sulfation × 4	M-C_3H_6+O_3+S_4O_{12}	$C_{19}H_{18}NO_{19}S_4^+$	325.7650	691.9350	Phase I + Phase I + Phase II
244	Demethylation × 3 + Oxidation × 2 + Glucuronidation × 1 + Sulfation × 2	M-C_3H_6+O_2+$C_6H_8O_6$+S_2O_6	$C_{25}H_{26}NO_{18}S_2^+$	325.8886	692.0586	Phase I + Phase I + Phase II
245	Demethylation × 4 + Glucuronidation × 2 + Oxidation × 2 + Dehydrogenation × 1	M-C_4H_8+$C_{12}H_{16}O_{12}$+O_2-H_2	$C_{30}H_{30}NO_{18}^+$	325.9757	692.1457	Phase I + Phase II
246	Demethylation × 3 + Oxidation × 1 + Glucuronidation × 2	M-C_3H_6+O+$C_{12}H_{16}O_{12}$	$C_{31}H_{34}NO_{17}^+$	326.0121	692.1821	Phase I + Phase I + Phase II
247	Demethylation × 4 + Oxidation × 3 + Glucuronidation × 1 + Sulfation × 2	M-C_4H_8+O_3+$C_6H_8O_6$+S_2O_6	$C_{24}H_{24}NO_{19}S_2^+$	327.8678	694.0378	Phase I + Phase I + Phase II
248	Demethylation × 4 + Oxidation × 2 + Glucuronidation × 2	M-C_4H_8+O_2+$C_{12}H_{16}O_{12}$	$C_{30}H_{32}NO_{18}^+$	327.9914	694.1614	Phase I + Phase I + Phase II
249	Oxidation × 5 + Glucuronidation × 1 + Sulfation × 1	M+O_5+$C_6H_8O_6$+SO_3	$C_{28}H_{32}NO_{18}S^+$	335.9635	702.1335	Phase I + Phase II
250	Demethylation × 2 + Glucuronidation × 2 + Oxidation × 1 + Dehydrogenation × 1	M-C_2H_4+$C_{12}H_{16}O_{12}$+O-H_2	$C_{32}H_{34}NO_{17}^+$	338.0121	704.1821	Phase I + Phase II
251	Demethylation × 2 + Oxidation × 3 + Sulfation × 4	M-C_2H_4+O_3+S_4O_{12}	$C_{20}H_{20}NO_{19}S_4^+$	339.7807	705.9507	Phase I + Phase I + Phase II
252	Demethylation × 2 + Oxidation × 2 + Glucuronidation × 1 + Sulfation × 2	M-C_2H_4+O_2+$C_6H_8O_6$+S_2O_6	$C_{26}H_{28}NO_{18}S_2^+$	339.9042	706.0742	Phase I + Phase I + Phase II
253	Demethylation × 3 + Glucuronidation × 2 + Oxidation × 2 + Dehydrogenation × 1	M-C_3H_6+$C_{12}H_8$16O_{12}+O_2-H_2	$C_{31}H_{32}NO_{18}^+$	339.9314	706.1014	Phase I + Phase II
254	Demethylation × 2 + Oxidation × 1 + Glucuronidation × 2	M-C_2H_4+O+$C_{12}H_{16}O_{12}$	$C_{32}H_{36}NO_{17}^+$	340.0278	706.1978	Phase I + Phase I + Phase II
255	Demethylation × 3 + Oxidation × 3 + Glucuronidation × 1 + Sulfation × 2	M-C_3H_6+O_3+$C_6H_8O_6$+S_2O_6	$C_{25}H_{26}NO_{19}S_2^+$	341.8835	708.0535	Phase I + Phase I + Phase II
256	Demethylation × 3 + Oxidation × 2 + Glucuronidation × 2	M-C_3H_6+O_2+$C_{12}H_{16}O_{12}$	$C_{31}H_{34}NO_{18}^+$	342.0070	708.1770	Phase I + Phase I + Phase II
257	Demethylation × 4 + Oxidation × 3 + Glucuronidation	M-C_4H_8+O_3+$C_{12}H_{16}O_{12}$	$C_{30}H_{32}NO_{19}^+$	343.9863	710.1563	Phase I + Phase I +

	× 2					Phase II
258	Demethylation × 1 + Oxidation × 3 + Sulfation × 4	M-CH_2+O_3+S_4O_{12}	$C_{21}H_{22}NO_{19}S_4^+$	353.7963	719.9663	Phase I + Phase I + Phase II
259	Demethylation × 1 + Oxidation × 2 + Glucuronidation × 1 + Sulfation × 2	M-CH_2+O_2+$C_6H_8O_6$+S_2O_6	$C_{27}H_{30}NO_{18}S_2^+$	353.9199	720.0899	Phase I + Phase I + Phase II
260	Demethylation × 2 + Glucuronidation × 2 + Oxidation × 2 + Dehydrogenation × 1	M-C_2H_4+$C_{12}H_{16}O_{12}$+O_2-H_2	$C_{32}H_{34}NO_{18}^+$	354.0070	720.1770	Phase I + Phase II
261	Demethylation × 1 + Oxidation × 1 + Glucuronidation × 2	M-CH_2+O+$C_{12}H_{16}O_{12}$	$C_{33}H_{38}NO_{17}^+$	354.0434	720.2134	Phase I + Phase I + Phase II
262	Demethylation × 2 + Oxidation × 3 + Glucuronidation × 1 + Sulfation × 2	M-C_2H_4+O_3+$C_6H_8O_6$+S_2O_6	$C_{26}H_{28}NO_{19}S_2^+$	355.8991	722.0691	Phase I + Phase I + Phase II
263	Demethylation × 2 + Oxidation × 2 + Glucuronidation × 2	M-C_2H_4+O_2+$C_{12}H_{16}O_{12}$	$C_{32}H_{36}NO_{18}^+$	356.0227	722.1927	Phase I + Phase I + Phase II
264	Demethylation × 3 + Oxidation × 3 + Glucuronidation × 2	M-C_3H_6+O_3+$C_{12}H_{16}O_{12}$	$C_{31}H_{34}NO_{19}^+$	358.0020	724.1720	Phase I + Phase I + Phase II
265	Demethylation × 4 + Oxidation × 1 + Sulfation × 5	M-C_4H_8+O+S_5O_{15}	$C_{18}H_{16}NO_{20}S_5^+$	359.7164	725.8864	Phase I + Phase I + Phase II
266	Demethylation × 4 + Glucuronidation × 1 + Sulfation × 3	M-C_4H_8+$C_6H_8O_6$+S_3O_9	$C_{24}H_{24}NO_{19}S_3^+$	359.8399	726.0099	Phase I + Phase II
267	Demethylation × 1 + Oxidation × 3 + Glucuronidation × 1 + Sulfation × 2	M-CH_2+O_3+$C_6H_8O_6$+S_2O_6	$C_{27}H_{30}NO_{19}S_2^+$	369.9148	736.0848	Phase I + Phase I + Phase II
268	Demethylation × 1 + Oxidation × 2 + Glucuronidation × 2	M-CH_2+O_2+$C_{12}H_{16}O_{12}$	$C_{33}H_{38}NO_{18}^+$	370.0383	736.2083	Phase I + Phase I + Phase II
269	Demethylation × 2 + Oxidation × 3 + Glucuronidation × 2	M-C_2H_4+O_3+$C_{12}H_{16}O_{12}$	$C_{32}H_{36}NO_{19}^+$	372.0176	738.1876	Phase I + Phase I + Phase II
270	Demethylation × 4 + Glucuronidation × 1 + Sulfation × 3 + Oxidation × 1 + Dehydrogenation × 1	M-C_4H_8+$C_6H_8O_6$+S_3O_9+O-H_2	$C_{24}H_{22}NO_{20}S_3^+$	373.8192	739.9892	Phase I + Phase II
271	Demethylation × 4 + Oxidation × 2 + Sulfation × 5	M-C_4H_8+O_2+S_5O_{15}	$C_{18}H_{16}NO_{21}S_5^+$	375.7113	741.8813	Phase I + Phase I +

						Phase II
272	Demethylation × 4 + Oxidation × 1 + Glucuronidation × 1 + Sulfation × 3	M-C_4H_8+O+$C_6H_8O_6$+S_3O_9	$C_{24}H_{24}NO_{20}S_3^+$	375.8348	742.0048	Phase I + Phase I + Phase II
273	Demethylation × 4 + Glucuronidation × 2 + Sulfation × 1	M-C_4H_8+$C_{12}H_{16}O_{12}$+SO_3	$C_{30}H_{32}NO_{19}S^+$	375.9584	742.1284	Phase I + Phase II
274	Oxidation × 4 + Sulfation × 4	M+O_4+S_4O_{12}	$C_{22}H_{24}NO_{20}S_4^+$	383.8069	749.9769	Phase I + Phase II
275	Oxidation × 3 + Glucuronidation × 1 + Sulfation × 2	M+O_3+$C_6H_8O_6$+S_2O_6	$C_{28}H_{32}NO_{19}S_2^+$	383.9304	750.1004	Phase I + Phase II
276	Oxidation × 2 + Glucuronidation × 2	M+O_2+$C_{12}H_{16}O_{12}$	$C_{34}H_{40}NO_{18}^+$	384.0540	750.2240	Phase I + Phase II
277	Demethylation × 1 + Oxidation × 3 + Glucuronidation × 2	M-CH_2+O_3+$C_{12}H_{16}O_{12}$	$C_{33}H_{38}NO_{19}^+$	386.0333	752.2033	Phase I + Phase I + Phase II
278	Demethylation × 3 + Dehydrogenation × 1 + Glucuronidation × 2 + Sulfation × 1	M-C_3H_6-H_2+$C_{12}H_{16}O_{12}$+SO_3	$C_{31}H_{32}NO_{19}S^+$	387.9584	754.1284	Phase I + Phase I + Phase II
279	Demethylation × 3 + Oxidation × 2 + Sulfation × 5	M-C_3H_6+O_2+S_5O_{15}	$C_{19}H_{18}NO_{21}S_5^+$	389.7269	755.8969	Phase I + Phase I + Phase II
280	Demethylation × 4 + Glucuronidation × 1 + Sulfation × 3 + Oxidation × 2 + Dehydrogenation × 1	M-C_4H_8+$C_6H_8O_6$+S_3O_9+O_2-H_2	$C_{24}H_{22}NO_{21}S_3^+$	389.8141	755.9841	Phase I + Phase II
281	Demethylation × 3 + Oxidation × 1 + Glucuronidation × 1 + Sulfation × 3	M-C_3H_6+O+$C_6H_8O_6$+S_3O_9	$C_{25}H_{26}NO_{20}S_3^+$	389.8505	756.0205	Phase I + Phase I + Phase II
282	Demethylation × 4 + Glucuronidation × 2 + Sulfation × 1 + Oxidation × 1 + Dehydrogenation × 1	M-C_4H_8+$C_{12}H_{16}O_{12}$+SO_3+O-H_2	$C_{30}H_{30}NO_{20}S^+$	389.9376	756.1076	Phase I + Phase II
283	Demethylation × 3 + Glucuronidation × 2 + Sulfation × 1	M-C_3H_6+$C_{12}H_{16}O_{12}$+SO_3	$C_{31}H_{34}NO_{19}S^+$	389.9740	756.1440	Phase I + Phase II
284	Demethylation × 4 + Oxidation × 3 + Sulfation × 5	M-C_4H_8+O_3+S_5O_{15}	$C_{18}H_{16}NO_{22}S_5^+$	391.7062	757.8762	Phase I + Phase I + Phase II
285	Demethylation × 4 + Oxidation × 2 + Glucuronidation × 1 + Sulfation × 3	M-C_4H_8+O_2+$C_6H_8O_6$+S_3O_9	$C_{24}H_{24}NO_{21}S_3^+$	391.8297	757.9997	Phase I + Phase I + Phase II
286	Demethylation × 4 + Oxidation × 1 + Glucuronidation × 2 + Sulfation × 1	M-C_4H_8+O+$C_{12}H_{16}O_{12}$+SO_3	$C_{30}H_{32}NO_{20}S^+$	391.9533	758.1233	Phase I + Phase I + Phase II

287	Oxidation × 5 + Sulfation × 4	M+O_5+S_4O_{12}	$C_{22}H_{24}NO_{21}S_4^+$	399.8018	765.9718	Phase I + Phase II
288	Oxidation × 4 + Glucuronidation × 1 + Sulfation × 2	M+O_4+$C_6H_8O_6$+S_2O_6	$C_{28}H_{32}NO_{20}S_2^+$	399.9254	766.0954	Phase I + Phase II
289	Oxidation × 3 + Glucuronidation × 2	M+O_3+$C_{12}H_{16}O_{12}$	$C_{34}H_{40}NO_{19}^+$	400.0489	766.2189	Phase I + Phase II
290	Demethylation × 3 + Glucuronidation × 2 + Sulfation × 1 + Oxidation × 1 + Dehydrogenation × 1	M-C_3H_6+$C_{12}H_{16}O_{12}$+SO_3+O-H_2	$C_{31}H_{32}NO_{20}S^+$	403.9533	770.1233	Phase I + Phase II
291	Demethylation × 3 + Oxidation × 3 + Sulfation × 5	M-C_3H_6+O_3+S_5O_{15}	$C_{19}H_{18}NO_{22}S_5^+$	405.7219	771.8919	Phase I + Phase I + Phase II
292	Demethylation × 3 + Oxidation × 2 + Glucuronidation × 1 + Sulfation × 3	M-C_3H_6+O_2+$C_6H_8O_6$+S_3O_9	$C_{25}H_{26}NO_{21}S_3^+$	405.8454	772.0154	Phase I + Phase I + Phase II
293	Demethylation × 4 + Glucuronidation × 2 + Sulfation × 1 + Oxidation × 2 + Dehydrogenation × 1	M-C_4H_8+$C_{12}H_{16}O_{12}$+SO_3+O_2-H_2	$C_{30}H_{30}NO_{21}S^+$	405.9326	772.1026	Phase I + Phase II
294	Demethylation × 3 + Oxidation × 1 + Glucuronidation × 2 + Sulfation × 1	M-C_3H_6+O+$C_{12}H_{16}O_{12}$+SO_3	$C_{31}H_{34}NO_{20}S^+$	405.9689	772.1389	Phase I + Phase I + Phase II
295	Demethylation × 4 + Oxidation × 3 + Glucuronidation × 1 + Sulfation × 3	M-C_4H_8+O_3+$C_6H_8O_6$+S_3O_9	$C_{24}H_{24}NO_{22}S_3^+$	407.8247	773.9947	Phase I + Phase I + Phase II
296	Demethylation × 4 + Oxidation × 2 + Glucuronidation × 2 + Sulfation × 1	M-C_4H_8+O_2+$C_{12}H_{16}O_{12}$+SO_3	$C_{30}H_{32}NO_{21}S^+$	407.9482	774.1182	Phase I + Phase I + Phase II
297	Oxidation × 5 + Glucuronidation × 1 + Sulfation × 2	M+O_5+$C_6H_8O_6$+S_2O_6	$C_{28}H_{32}NO_{21}S_2^+$	415.9203	782.0903	Phase I + Phase II
298	Oxidation × 4 + Glucuronidation × 2	M+O_4+$C_{12}H_{16}O_{12}$	$C_{34}H_{40}NO_{20}^+$	416.0438	782.2138	Phase I + Phase II
299	Demethylation × 2 + Oxidation × 3 + Sulfation × 5	M-C_2H_4+O_3+S_5O_{15}	$C_{20}H_{20}NO_{22}S_5^+$	419.7375	785.9075	Phase I + Phase I + Phase II
300	Demethylation × 2 + Oxidation × 2 + Glucuronidation × 1 + Sulfation × 3	M-C_2H_4+O_2+$C_6H_8O_6$+S_3O_9	$C_{26}H_{28}NO_{21}S_3^+$	419.8610	786.0310	Phase I + Phase I + Phase II
301	Demethylation × 3 + Glucuronidation × 2 + Sulfation × 1 + Oxidation × 2 + Dehydrogenation × 1	M-C_3H_6+$C_{12}H_{16}O_{12}$+SO_3+O_2-H_2	$C_{31}H_{32}NO_{21}S^+$	419.9482	786.1182	Phase I + Phase II
302	Demethylation × 2 + Oxidation × 1 + Glucuronidation × 2 + Sulfation × 1	M-C_2H_4+O+$C_{12}H_{16}O_{12}$+SO_3	$C_{32}H_{36}NO_{20}S^+$	419.9846	786.1546	Phase I + Phase I + Phase II
303	Demethylation × 3 + Oxidation × 3 + Glucuronidation	M-C_3H_6+O_3+$C_6H_8O_6$+S	$C_{25}H_{26}NO_{22}S_3^+$	421.8403	788.0103	Phase I + Phase I +

	× 1 + Sulfation × 3	$_3O_9$				Phase II
304	Demethylation × 3 + Oxidation × 2 + Glucuronidation × 2 + Sulfation × 1	M-C_3H_6+O_2+$C_{12}H_{16}O_{12}$ +SO_3	$C_{31}H_{34}NO_{21}S^+$	421.9639	788.1339	Phase I + Phase I + Phase II
305	Demethylation × 4 + Oxidation × 3 + Glucuronidation × 2 + Sulfation × 1	M-C_4H_8+O_3+$C_{12}H_{16}O_{12}$ +SO_3	$C_{30}H_{32}NO_{22}S^+$	423.9431	790.1131	Phase I + Phase I + Phase II
306	Oxidation × 5 + Glucuronidation × 2	M+O_5+$C_{12}H_{16}O_{12}$	$C_{34}H_{40}NO_{21}^+$	432.0387	798.2087	Phase I + Phase II
307	Demethylation × 2 + Oxidation × 3 + Glucuronidation × 1 + Sulfation × 3	M-C_2H_4+O_3+$C_6H_8O_6$+S $_3O_9$	$C_{26}H_{28}NO_{22}S_3^+$	435.8560	802.0260	Phase I + Phase I + Phase II
308	Demethylation × 2 + Oxidation × 2 + Glucuronidation × 2 + Sulfation × 1	M-C_2H_4+O_2+$C_{12}H_{16}O_{12}$ +SO_3	$C_{32}H_{36}NO_{21}S^+$	435.9795	802.1495	Phase I + Phase I + Phase II
309	Demethylation × 3 + Oxidation × 3 + Glucuronidation × 2 + Sulfation × 1	M-C_3H_6+O_3+$C_{12}H_{16}O_{12}$ +SO_3	$C_{31}H_{34}NO_{22}S^+$	437.9588	804.1288	Phase I + Phase I + Phase II
310	Demethylation × 1 + Oxidation × 3 + Glucuronidation × 1 + Sulfation × 3	M-CH_2+O_3+$C_6H_8O_6$+S_3 O_9	$C_{27}H_{30}NO_{22}S_3^+$	449.8716	816.0416	Phase I + Phase I + Phase II
311	Demethylation × 1 + Oxidation × 2 + Glucuronidation × 2 + Sulfation × 1	M-CH_2+O_2+$C_{12}H_{16}O_{12}$+ SO_3	$C_{33}H_{38}NO_{21}S^+$	449.9952	816.1652	Phase I + Phase I + Phase II
312	Demethylation × 2 + Oxidation × 3 + Glucuronidation × 2 + Sulfation × 1	M-C_2H_4+O_3+$C_{12}H_{16}O_{12}$ +SO_3	$C_{32}H_{36}NO_{22}S^+$	451.9744	818.1444	Phase I + Phase I + Phase II
313	Demethylation × 3 + Oxidation × 3 + Glucuronidation × 1 + Sulfation × 4	M-C_3H_6+O_3+$C_6H_8O_6$+S $_3O_9$	$C_{25}H_{26}NO_{22}S_4^+$	453.8124	819.9824	Phase I + Phase I + Phase II
314	Demethylation × 4 + Oxidation × 2 + Sulfation × 6	M-C_4H_8+O_2+S_6O_{18}	$C_{18}H_{16}NO_{24}S_6^+$	455.6681	821.8381	Phase I + Phase I + Phase II
315	Demethylation × 4 + Oxidation × 1 + Glucuronidation × 1 + Sulfation × 4	M-C_4H_8+O+$C_6H_8O_6$+S_4 O_{12}	$C_{24}H_{24}NO_{23}S_4^+$	455.7916	821.9616	Phase I + Phase I + Phase II
316	Demethylation × 4 + Glucuronidation × 2 + Sulfation × 2	M-C_4H_8+$C_{12}H_{16}O_{12}$+S_2 O_6	$C_{30}H_{32}NO_{22}S_2^+$	455.9152	822.0852	Phase I + Phase II
317	Demethylation × 1 + Oxidation × 3 + Glucuronidation × 2 + Sulfation × 1	M-CH_2+O_3+$C_{12}H_{16}O_{12}$+ SO_3	$C_{33}H_{38}NO_{22}S^+$	465.9901	832.1601	Phase I + Phase I + Phase II

318	Demethylation × 4 + Glucuronidation × 2 + Sulfation × 2 + Oxidation × 1 + Dehydrogenation × 1	M-C_4H_8+$C_{12}H_{16}O_{12}$+S_2O_6+O-H_2	$C_{30}H_{30}NO_{23}S_2^+$	469.8945	836.0645	Phase I + Phase II
319	Demethylation × 4 + Oxidation × 3 + Sulfation × 6	M-C_4H_8+O_3+S_6O_{18}	$C_{18}H_{16}NO_{25}S_6^+$	471.6630	837.8330	Phase I + Phase I + Phase II
320	Demethylation × 4 + Oxidation × 2 + Glucuronidation × 1 + Sulfation × 4	M-C_4H_8+O_2+$C_6H_8O_6$+S_4O_{12}	$C_{24}H_{24}NO_{24}S_4^+$	471.7866	837.9566	Phase I + Phase I + Phase II
321	Demethylation × 4 + Oxidation × 1 + Glucuronidation × 2 + Sulfation × 2	M-C_4H_8+O+$C_{12}H_{16}O_{12}$+S_2O_6	$C_{30}H_{32}NO_{23}S_2^+$	471.9101	838.0801	Phase I + Phase I + Phase II
322	Demethylation × 4 + Glucuronidation × 3	M-C_4H_8+$C_{18}H_{24}O_{18}$	$C_{36}H_{40}NO_{22}^+$	472.0336	838.2036	Phase I + Phase II
323	Oxidation × 5 + Sulfation × 5	M+O_5+S_5O_{15}	$C_{22}H_{24}NO_{24}S_5^+$	479.7586	845.9286	Phase I + Phase II
324	Oxidation × 4 + Glucuronidation × 1 + Sulfation × 3	M+O_4+$C_6H_8O_6$+S_3O_9	$C_{28}H_{32}NO_{23}S_3^+$	479.8822	846.0522	Phase I + Phase II
325	Oxidation × 3 + Glucuronidation × 2 + Sulfation × 1	M+O_3+$C_{12}H_{16}O_{12}$+SO_3	$C_{34}H_{40}NO_{22}S^+$	480.0057	846.1757	Phase I + Phase II
326	Demethylation × 3 + Dehydrogenation × 1 + Glucuronidation × 3	M-C_3H_6-H_2+$C_{18}H_{24}O_{18}$	$C_{37}H_{40}NO_{22}^+$	484.0336	850.2036	Phase I + Phase I + Phase II
327	Demethylation × 3 + Oxidation × 3 + Sulfation × 6	M-C_3H_6+O_3+S_6O_{18}	$C_{19}H_{18}NO_{25}S_6^+$	485.6787	851.8487	Phase I + Phase I + Phase II
328	Demethylation × 3 + Oxidation × 2 + Glucuronidation × 1 + Sulfation × 4	M-C_3H_6+O_2+$C_6H_8O_6$+S_4O_{12}	$C_{25}H_{26}NO_{24}S_4^+$	485.8022	851.9722	Phase I + Phase I + Phase II
329	Demethylation × 4 + Glucuronidation × 2 + Sulfation × 2 + Oxidation × 2 + Dehydrogenation × 1	M-C_4H_8+$C_{12}H_{16}O_{12}$+S_2O_6+O_2-H_2	$C_{30}H_{30}NO_{24}S_2^+$	485.8894	852.0594	Phase I + Phase II
330	Demethylation × 3 + Oxidation × 1 + Glucuronidation × 2 + Sulfation × 2	M-C_3H_6+O+$C_{12}H_{16}O_{12}$+S_2O_6	$C_{31}H_{34}NO_{23}S_2^+$	485.9258	852.0958	Phase I + Phase I + Phase II
331	Demethylation × 4 + Glucuronidation × 3 + Oxidation × 1 + Dehydrogenation × 1	M-C_4H_8+$C_{18}H_{24}O_{18}$+O-H_2	$C_{36}H_{38}NO_{23}^+$	486.0129	852.1829	Phase I + Phase II
332	Demethylation × 3 + Glucuronidation × 3	M-C_3H_6+$C_{18}H_{24}O_{18}$	$C_{37}H_{42}NO_{22}^+$	486.0493	852.2193	Phase I + Phase II
333	Demethylation × 4 + Oxidation × 3 + Glucuronidation × 1 + Sulfation × 4	M-C_4H_8+O_3+$C_6H_8O_6$+S_4O_{12}	$C_{24}H_{24}NO_{25}S_4^+$	487.7815	853.9515	Phase I + Phase I + Phase II
334	Demethylation × 4 + Oxidation × 2 + Glucuronidation	M-C_4H_8+O_2+$C_{12}H_{16}O_{12}$	$C_{30}H_{32}NO_{24}S_2^+$	487.9050	854.0750	Phase I + Phase I +

	× 2 + Sulfation × 2	+S_2O_6				Phase II
335	Demethylation × 4 + Oxidation × 1 + Glucuronidation × 3	M-C_4H_8+O+$C_{18}H_{24}O_{18}$	$C_{36}H_{40}NO_{23}^+$	488.0286	854.1986	Phase I + Phase I + Phase II
336	Oxidation × 5 + Glucuronidation × 1 + Sulfation × 3	M+O_5+$C_6H_8O_6$+S_3O_9	$C_{28}H_{32}NO_{24}S_3^+$	495.8771	862.0471	Phase I + Phase II
337	Oxidation × 4 + Glucuronidation × 2 + Sulfation × 1	M+O_4+$C_{12}H_{16}O_{12}$+SO_3	$C_{34}H_{40}NO_{23}S^+$	496.0006	862.1706	Phase I + Phase II
338	Demethylation × 3 + Glucuronidation × 3 + Oxidation × 1 + Dehydrogenation × 1	M-C_3H_6+$C_{18}H_{24}O_{18}$+O-H_2	$C_{37}H_{40}NO_{23}^+$	500.0286	866.1986	Phase I + Phase II
339	Demethylation × 3 + Oxidation × 2 + Glucuronidation × 2 + Sulfation × 2	M-C_3H_6+O_2+$C_{12}H_{16}O_{12}$+S_2O_6	$C_{31}H_{34}NO_{24}S_2^+$	501.9207	868.0907	Phase I + Phase I + Phase II
340	Demethylation × 4 + Glucuronidation × 3 + Oxidation × 2 + Dehydrogenation × 1	M-C_4H_8+$C_{18}H_{24}O_{18}$+O_2-H_2	$C_{36}H_{38}NO_{24}^+$	502.0078	868.1778	Phase I + Phase II
341	Demethylation × 3 + Oxidation × 1 + Glucuronidation × 3	M-C_3H_6+O+$C_{18}H_{24}O_{18}$	$C_{37}H_{42}NO_{23}^+$	502.0442	868.2142	Phase I + Phase I + Phase II
342	Demethylation × 4 + Oxidation × 3 + Glucuronidation × 2 + Sulfation × 2	M-C_4H_8+O_3+$C_{12}H_{16}O_{12}$+S_2O_6	$C_{30}H_{32}NO_{25}S_2^+$	503.8999	870.0699	Phase I + Phase I + Phase II
343	Demethylation × 4 + Oxidation × 2 + Glucuronidation × 3	M-C_4H_8+O_2+$C_{18}H_{24}O_{18}$	$C_{36}H_{40}NO_{24}^+$	504.0235	870.1935	Phase I + Phase I + Phase II
344	Oxidation × 5 + Glucuronidation × 2 + Sulfation × 1	M+O_5+$C_{12}H_{16}O_{12}$+SO_3	$C_{34}H_{40}NO_{24}S^+$	511.9955	878.1655	Phase I + Phase II
345	Demethylation × 2 + Oxidation × 3 + Glucuronidation × 1 + Sulfation × 4	M-C_2H_4+O_3+$C_6H_8O_6$+S_4O_{12}	$C_{26}H_{28}NO_{25}S_4^+$	515.8128	881.9828	Phase I + Phase I + Phase II
346	Demethylation × 2 + Oxidation × 2 + Glucuronidation × 2 + Sulfation × 2	M-C_2H_4+O_2+$C_{12}H_{16}O_{12}$+S_2O_6	$C_{32}H_{36}NO_{24}S_2^+$	515.9363	882.1063	Phase I + Phase I + Phase II
347	Demethylation × 3 + Glucuronidation × 3 + Oxidation × 2 + Dehydrogenation × 1	M-C_3H_6+$C_{18}H_{24}O_{18}$+O_2-H_2	$C_{37}H_{40}NO_{24}^+$	516.0235	882.1935	Phase I + Phase II
348	Demethylation × 2 + Oxidation × 1 + Glucuronidation × 3	M-C_2H_4+O+$C_{18}H_{24}O_{18}$	$C_{38}H_{44}NO_{23}^+$	516.0599	882.2299	Phase I + Phase I + Phase II
349	Demethylation × 3 + Oxidation × 3 + Glucuronidation × 2 + Sulfation × 2	M-C_3H_6+O_3+$C_{12}H_{16}O_{12}$+S_2O_6	$C_{31}H_{34}NO_{25}S_2^+$	517.9156	884.0856	Phase I + Phase I + Phase II

350	Demethylation × 3 + Oxidation × 2 + Glucuronidation × 3	M-C_3H_6+O_2+$C_{18}H_{24}O_{18}$	$C_{37}H_{42}NO_{24}^+$	518.0391	884.2091	Phase I + Phase I + Phase II
351	Demethylation × 4 + Oxidation × 3 + Glucuronidation × 3	M-C_4H_8+O_3+$C_{18}H_{24}O_{18}$	$C_{36}H_{40}NO_{25}^+$	520.0184	886.1884	Phase I + Phase I + Phase II
352	Demethylation × 2 + Oxidation × 3 + Glucuronidation × 2 + Sulfation × 2	M-C_2H_4+O_3+$C_{12}H_{16}O_{12}$ +S_2O_6	$C_{32}H_{36}NO_{25}S_2^+$	531.9312	898.1012	Phase I + Phase I + Phase II
353	Demethylation × 2 + Oxidation × 2 + Glucuronidation × 3	M-C_2H_4+O_2+$C_{18}H_{24}O_{18}$	$C_{38}H_{44}NO_{24}^+$	532.0548	898.2248	Phase I + Phase I + Phase II
354	Demethylation × 3 + Oxidation × 3 + Glucuronidation × 3	M-C_3H_6+O_3+$C_{18}H_{24}O_{18}$	$C_{37}H_{42}NO_{25}^+$	534.0340	900.2040	Phase I + Phase I + Phase II
355	Demethylation × 1 + Oxidation × 3 + Glucuronidation × 2 + Sulfation × 2	M-CH_2+O_3+$C_{12}H_{16}O_{12}$+ S_2O_6	$C_{33}H_{38}NO_{25}S_2^+$	545.9469	912.1169	Phase I + Phase I + Phase II
356	Demethylation × 1 + Oxidation × 2 + Glucuronidation × 3	M-CH_2+O_2+$C_{18}H_{24}O_{18}$	$C_{39}H_{46}NO_{24}^+$	546.0704	912.2404	Phase I + Phase I + Phase II
357	Demethylation × 2 + Oxidation × 3 + Glucuronidation × 3	M-C_2H_4+O_3+$C_{18}H_{24}O_{18}$	$C_{38}H_{44}NO_{25}^+$	548.0497	914.2197	Phase I + Phase I + Phase II
358	Demethylation × 3 + Oxidation × 3 + Glucuronidation × 2 + Sulfation × 3	M-C_3H_6+O_3+$C_{12}H_{16}O_{12}$ +S_2O_6	$C_{31}H_{34}NO_{25}S_3^+$	549.8877	916.0577	Phase I + Phase I + Phase II
359	Demethylation × 4 + Oxidation × 3 + Sulfation × 7	M-C_4H_8+O_3+S_7O_{21}	$C_{18}H_{16}NO_{28}S_7^+$	551.6198	917.7898	Phase I + Phase I + Phase II
360	Demethylation × 4 + Oxidation × 1 + Glucuronidation × 2 + Sulfation × 3	M-C_4H_8+O+$C_{12}H_{16}O_{12}$+ S_3O_9	$C_{30}H_{32}NO_{26}S_3^+$	551.8669	918.0369	Phase I + Phase I + Phase II
361	Demethylation × 4 + Glucuronidation × 3 + Sulfation × 1	M-C_4H_8+$C_{18}H_{24}O_{18}$+SO_3	$C_{36}H_{40}NO_{25}S^+$	551.9905	918.1605	Phase I + Phase II
362	Demethylation × 1 + Oxidation × 3 + Glucuronidation × 3	M-CH_2+O_3+$C_{18}H_{24}O_{18}$	$C_{39}H_{46}NO_{25}^+$	562.0653	928.2353	Phase I + Phase I + Phase II
363	Demethylation × 4 + Glucuronidation × 3 + Sulfation × 1 + Oxidation × 1 + Dehydrogenation × 1	M-C_4H_8+$C_{18}H_{24}O_{18}$+SO_3+O-H_2	$C_{36}H_{38}NO_{26}S^+$	565.9697	932.1397	Phase I + Phase II

364	Demethylation × 4 + Oxidation × 2 + Glucuronidation × 2 + Sulfation × 3	M-C_4H_8+O_2+$C_{12}H_{16}O_{12}$+S_3O_9	$C_{30}H_{32}NO_{27}S_3^+$	567.8618	934.0318	Phase I + Phase I + Phase II
365	Demethylation × 4 + Oxidation × 1 + Glucuronidation × 3 + Sulfation × 1	M-C_4H_8+O+$C_{18}H_{24}O_{18}$+SO_3	$C_{36}H_{40}NO_{26}S^+$	567.9854	934.1554	Phase I + Phase I + Phase II
366	Oxidation × 5 + Glucuronidation × 1 + Sulfation × 4	M+O_5+$C_6H_8O_6$+S_4O_{12}	$C_{28}H_{32}NO_{27}S_4^+$	575.8339	942.0039	Phase I + Phase II
367	Oxidation × 4 + Glucuronidation × 2 + Sulfation × 2	M+O_4+$C_{12}H_{16}O_{12}$+S_2O_6	$C_{34}H_{40}NO_{26}S_2^+$	575.9574	942.1274	Phase I + Phase II
368	Oxidation × 3 + Glucuronidation × 3	M+O_3+$C_{18}H_{24}O_{18}$	$C_{40}H_{48}NO_{25}^+$	576.0810	942.2510	Phase I + Phase II
369	Demethylation × 3 + Oxidation × 2 + Glucuronidation × 2 + Sulfation × 3	M-C_3H_6+O_2+$C_{12}H_{16}O_{12}$+S_3O_9	$C_{31}H_{34}NO_{27}S_3^+$	581.8775	948.0475	Phase I + Phase I + Phase II
370	Demethylation × 4 + Glucuronidation × 3 + Sulfation × 1 + Oxidation × 2 + Dehydrogenation × 1	M-C_4H_8+$C_{18}H_{24}O_{18}$+SO_3+O_2-H_2	$C_{36}H_{38}NO_{27}S^+$	581.9646	948.1346	Phase I + Phase II
371	Demethylation × 3 + Oxidation × 1 + Glucuronidation × 3 + Sulfation × 1	M-C_3H_6+O+$C_{18}H_{24}O_{18}$+SO_3	$C_{37}H_{42}NO_{26}S^+$	582.0010	948.1710	Phase I + Phase I + Phase II
372	Demethylation × 4 + Oxidation × 3 + Glucuronidation × 2 + Sulfation × 3	M-C_4H_8+O_3+$C_{12}H_{16}O_{12}$+S_3O_9	$C_{30}H_{32}NO_{28}S_3^+$	583.8567	950.0267	Phase I + Phase I + Phase II
373	Demethylation × 4 + Oxidation × 2 + Glucuronidation × 3 + Sulfation × 1	M-C_4H_8+O_2+$C_{18}H_{24}O_{18}$+SO_3	$C_{36}H_{40}NO_{27}S^+$	583.9803	950.1503	Phase I + Phase I + Phase II
374	Oxidation × 5 + Glucuronidation × 2 + Sulfation × 2	M+O_5+$C_{12}H_{16}O_{12}$+S_2O_6	$C_{34}H_{40}NO_{27}S_2^+$	591.9524	958.1224	Phase I + Phase II
375	Oxidation × 4 + Glucuronidation × 3	M+O_4+$C_{18}H_{24}O_{18}$	$C_{40}H_{48}NO_{26}^+$	592.0759	958.2459	Phase I + Phase II
376	Demethylation × 3 + Oxidation × 2 + Glucuronidation × 3 + Sulfation × 1	M-C_3H_6+O_2+$C_{18}H_{24}O_{18}$+SO_3	$C_{37}H_{42}NO_{27}S^+$	597.9959	964.1659	Phase I + Phase I + Phase II
377	Demethylation × 4 + Oxidation × 3 + Glucuronidation × 3 + Sulfation × 1	M-C_4H_8+O_3+$C_{18}H_{24}O_{18}$+SO_3	$C_{36}H_{40}NO_{28}S^+$	599.9752	966.1452	Phase I + Phase I + Phase II
378	Oxidation × 5 + Glucuronidation × 3	M+O_5+$C_{18}H_{24}O_{18}$	$C_{40}H_{48}NO_{27}^+$	608.0708	974.2408	Phase I + Phase II
379	Demethylation × 2 + Oxidation × 3 + Glucuronidation × 2 + Sulfation × 3	M-C_2H_4+O_3+$C_{12}H_{16}O_{12}$+S_3O_9	$C_{32}H_{36}NO_{28}S_3^+$	611.8880	978.0580	Phase I + Phase I + Phase II
380	Demethylation × 2 + Oxidation × 2 + Glucuronidation × 3 + Sulfation × 1	M-C_2H_4+O_2+$C_{18}H_{24}O_{18}$+SO_3	$C_{38}H_{44}NO_{27}S^+$	612.0116	978.1816	Phase I + Phase I + Phase II

381	Demethylation × 3 + Oxidation × 3 + Glucuronidation × 3 + Sulfation × 1	M-C_3H_6+O_3+$C_{18}H_{24}O_{18}$+SO_3	$C_{37}H_{42}NO_{28}S^+$	613.9909	980.1609	Phase I + Phase I + Phase II
382	Demethylation × 2 + Oxidation × 3 + Glucuronidation × 3 + Sulfation × 1	M-C_2H_4+O_3+$C_{18}H_{24}O_{18}$+SO_3	$C_{38}H_{44}NO_{28}S^+$	628.0065	994.1765	Phase I + Phase I + Phase II
383	Demethylation × 1 + Oxidation × 3 + Glucuronidation × 3 + Sulfation × 1	M-CH_2+O_3+$C_{18}H_{24}O_{18}$+SO_3	$C_{39}H_{46}NO_{28}S^+$	642.0222	1008.1922	Phase I + Phase I + Phase II
384	Demethylation × 3 + Oxidation × 3 + Glucuronidation × 3 + Sulfation × 2	M-C_3H_6+O_3+$C_{18}H_{24}O_{18}$+S_2O_6	$C_{37}H_{42}NO_{28}S_2^+$	645.9629	1012.1329	Phase I + Phase I + Phase II
385	Demethylation × 4 + Oxidation × 1 + Glucuronidation × 3 + Sulfation × 2	M-C_4H_8+O+$C_{18}H_{24}O_{18}$+S_2O_6	$C_{36}H_{40}NO_{29}S_2^+$	647.9422	1014.1122	Phase I + Phase I + Phase II
386	Demethylation × 4 + Glucuronidation × 4	M-C_4H_8+$C_{24}H_{32}O_{24}$	$C_{42}H_{48}NO_{28}^+$	648.0657	1014.2357	Phase I + Phase II
387	Demethylation × 4 + Glucuronidation × 4 + Oxidation × 1 + Dehydrogenation × 1	M-C_4H_8+$C_{24}H_{32}O_{24}$+O-H_2	$C_{42}H_{46}NO_{29}^+$	662.0450	1028.2150	Phase I + Phase II
388	Demethylation × 4 + Oxidation × 2 + Glucuronidation × 3 + Sulfation × 2	M-C_4H_8+O_2+$C_{18}H_{24}O_{18}$+S_2O_6	$C_{36}H_{40}NO_{30}S_2^+$	663.9371	1030.1071	Phase I + Phase I + Phase II
389	Demethylation × 4 + Oxidation × 1 + Glucuronidation × 4	M-C_4H_8+O+$C_{24}H_{32}O_{24}$	$C_{42}H_{48}NO_{29}^+$	664.0607	1030.2307	Phase I + Phase I + Phase II
390	Oxidation × 5 + Glucuronidation × 2 + Sulfation × 3	M+O_5+$C_{12}H_{16}O_{12}$+S_3O_9	$C_{34}H_{40}NO_{30}S_3^+$	671.9092	1038.0792	Phase I + Phase II
391	Oxidation × 4 + Glucuronidation × 3 + Sulfation × 1	M+O_4+$C_{18}H_{24}O_{18}$+SO_3	$C_{40}H_{48}NO_{29}S^+$	672.0327	1038.2027	Phase I + Phase II
392	Demethylation × 3 + Oxidation × 2 + Glucuronidation × 3 + Sulfation × 2	M-C_3H_6+O_2+$C_{18}H_{24}O_{18}$+S_2O_6	$C_{37}H_{42}NO_{30}S_2^+$	677.9528	1044.1228	Phase I + Phase I + Phase II
393	Demethylation × 4 + Glucuronidation × 4 + Oxidation × 2 + Dehydrogenation × 1	M-C_4H_8+$C_{24}H_{32}O_{24}$+O_2-H_2	$C_{42}H_{46}NO_{30}^+$	678.0399	1044.2099	Phase I + Phase II
394	Demethylation × 3 + Oxidation × 1 + Glucuronidation × 4	M-C_3H_6+O+$C_{24}H_{32}O_{24}$	$C_{43}H_{50}NO_{29}^+$	678.0763	1044.2463	Phase I + Phase I + Phase II
395	Demethylation × 4 + Oxidation × 3 + Glucuronidation × 3 + Sulfation × 2	M-C_4H_8+O_3+$C_{18}H_{24}O_{18}$+S_2O_6	$C_{36}H_{40}NO_{31}S_2^+$	679.9320	1046.1020	Phase I + Phase I + Phase II
396	Demethylation × 4 + Oxidation × 2 + Glucuronidation	M-C_4H_8+O_2+$C_{24}H_{32}O_{24}$	$C_{42}H_{48}NO_{30}^+$	680.0556	1046.2256	Phase I + Phase I +

	× 4					Phase II
397	Oxidation × 5 + Glucuronidation × 3 + Sulfation × 1	M+O_5+$C_{18}H_{24}O_{18}$+SO_3	$C_{40}H_{48}NO_{30}S^+$	688.0276	1054.1976	Phase I + Phase II
398	Demethylation × 3 + Oxidation × 2 + Glucuronidation × 4	M-C_3H_6+O_2+$C_{24}H_{32}O_{24}$	$C_{43}H_{50}NO_{30}^+$	694.0712	1060.2412	Phase I + Phase I + Phase II
399	Demethylation × 4 + Oxidation × 3 + Glucuronidation × 4	M-C_4H_8+O_3+$C_{24}H_{32}O_{24}$	$C_{42}H_{48}NO_{31}^+$	696.0505	1062.2205	Phase I + Phase I + Phase II
400	Demethylation × 2 + Oxidation × 3 + Glucuronidation × 3 + Sulfation × 2	M-C_2H_4+O_3+$C_{18}H_{24}O_{18}$ +S_2O_6	$C_{38}H_{44}NO_{31}S_2^+$	707.9633	1074.1333	Phase I + Phase I + Phase II
401	Demethylation × 2 + Oxidation × 2 + Glucuronidation × 4	M-C_2H_4+O_2+$C_{24}H_{32}O_{24}$	$C_{44}H_{52}NO_{30}^+$	708.0869	1074.2569	Phase I + Phase I + Phase II
402	Demethylation × 3 + Oxidation × 3 + Glucuronidation × 4	M-C_3H_6+O_3+$C_{24}H_{32}O_{24}$	$C_{43}H_{50}NO_{31}^+$	710.0661	1076.2361	Phase I + Phase I + Phase II
403	Demethylation × 2 + Oxidation × 3 + Glucuronidation × 4	M-C_2H_4+O_3+$C_{24}H_{32}O_{24}$	$C_{44}H_{52}NO_{31}^+$	724.0818	1090.2518	Phase I + Phase I + Phase II
404	Demethylation × 1 + Oxidation × 3 + Glucuronidation × 4	M-CH_2+O_3+$C_{24}H_{32}O_{24}$	$C_{45}H_{54}NO_{31}^+$	738.0974	1104.2674	Phase I + Phase I + Phase II
405	Demethylation × 4 + Oxidation × 1 + Glucuronidation × 3 + Sulfation × 1	M-C_4H_8+O+$C_{24}H_{32}O_{24}$+ SO_3	$C_{42}H_{48}NO_{32}S^+$	744.0175	1110.1875	Phase I + Phase I + Phase II
406	Demethylation × 4 + Oxidation × 2 + Glucuronidation × 3 + Sulfation × 1	M-C_4H_8+O_2+$C_{24}H_{32}O_{24}$ +SO_3	$C_{42}H_{48}NO_{33}S^+$	760.0124	1126.1824	Phase I + Phase I + Phase II
407	Oxidation × 5 + Glucuronidation × 3 + Sulfation × 2	M+O_5+$C_{18}H_{24}O_{18}$+S_2O_6	$C_{40}H_{48}NO_{33}S_2^+$	767.9845	1134.1545	Phase I + Phase II
408	Demethylation × 3 + Oxidation × 2 + Glucuronidation × 4 + Sulfation × 1	M-C_3H_6+O_2+$C_{24}H_{32}O_{24}$ +SO_3	$C_{43}H_{50}NO_{33}S^+$	774.0280	1140.1980	Phase I + Phase I + Phase II
409	Demethylation × 4 + Oxidation × 3 + Glucuronidation × 3 + Sulfation × 1	M-C_4H_8+O_3+$C_{24}H_{32}O_{24}$ +SO_3	$C_{42}H_{48}NO_{34}S^+$	776.0073	1142.1773	Phase I + Phase I + Phase II
410	Demethylation × 3 + Oxidation × 3 + Glucuronidation × 4 + Sulfation × 1	M-C_3H_6+O_3+$C_{24}H_{32}O_{24}$ +SO_3	$C_{43}H_{50}NO_{34}S^+$	790.0229	1156.1929	Phase I + Phase I + Phase II
411	Demethylation × 2 + Oxidation × 3 + Glucuronidation	M-C_2H_4+O_3+$C_{24}H_{32}O_{24}$	$C_{44}H_{52}NO_{34}S^+$	804.0386	1170.2086	Phase I + Phase I +

	× 4 + Sulfation × 1	+SO_3				Phase II
412	Demethylation × 4 + Oxidation × 1 + Glucuronidation × 5	M-C_4H_8+O+$C_{30}H_{40}O_{30}$	$C_{48}H_{56}NO_{35}^+$	840.0927	1206.2627	Phase I + Phase I + Phase II
413	Demethylation × 4 + Oxidation × 2 + Glucuronidation × 5	M-C_4H_8+O_2+$C_{30}H_{40}O_{30}$	$C_{48}H_{56}NO_{36}^+$	856.0877	1222.2577	Phase I + Phase I + Phase II
414	Oxidation × 5 + Glucuronidation × 4 + Sulfation × 1	M+O_5+$C_{24}H_{32}O_{24}$+SO_3	$C_{46}H_{56}NO_{36}S^+$	864.0597	1230.2297	Phase I + Phase II
415	Demethylation × 4 + Oxidation × 3 + Glucuronidation × 5	M-C_4H_8+O_3+$C_{30}H_{40}O_{30}$	$C_{48}H_{56}NO_{37}^+$	872.0826	1238.2526	Phase I + Phase I + Phase II
416	Demethylation × 2 + Oxidation × 3 + Glucuronidation × 5	M-C_2H_4+O_3+$C_{30}H_{40}O_{30}$	$C_{50}H_{60}NO_{37}^+$	900.1139	1266.2839	Phase I + Phase I + Phase II
417	Demethylation × 4 + Oxidation × 2 + Glucuronidation × 6	M-C_4H_8+O_2+$C_{36}H_{48}O_{36}$	$C_{54}H_{64}NO_{42}^+$	1032.1197	1398.2897	Phase I + Phase I + Phase II
418	Demethylation × 4 + Oxidation × 3 + Glucuronidation × 6	M-C_4H_8+O_3+$C_{36}H_{48}O_{36}$	$C_{54}H_{64}NO_{43}^+$	1048.1147	1414.2847	Phase I + Phase I + Phase II
419	Demethylation × 4 + Oxidation × 3 + Glucuronidation × 7	M-C_4H_8+O_3+$C_{42}H_{56}O_{42}$	$C_{60}H_{72}NO_{49}^+$	1224.1467	1590.3167	Phase I + Phase I + Phase II

Table S5 The metabolites of dehydrocorydaline identified from rat bile, feces, plasma, and urine by QTrap 4500.

Metabolites ID	t_R (min)	m/z	Adducts	Formula	MS^2	Biotransformation reaction	Source
M2	10.32	324.1	$[M-e]^+$	$C_{19}H_{18}NO_4$	324.0,309.1,308.0,280.2,281.2,266.2	DHC-3CH_2	F
M3	11.38	324.1	$[M-e]^+$	$C_{19}H_{18}NO_4$	324.0,309.0,308.0,280.1,266.0	DHC-3CH_2	F
M6	12.54	338.1	$[M-e]^+$	$C_{20}H_{20}NO_4$	338.0,323.0,308.0,295.1,279.1	DHC-2CH_2	B, F
M8	13.82	338.1	$[M-e]^+$	$C_{20}H_{20}NO_4$	338.2,323.0,308.0,294.1,280.1	DHC-2CH_2	F, U
M7	12.76	338.1	$[M-e]^+$	$C_{20}H_{20}NO_4$	338.2,322.1,320.0,308.0,294.1	DHC-2CH_2	B, F
M9	13.08	340.1	$[M-e]^+$	$C_{19}H_{18}NO_5$	310.1,296.0,294.0,282.1	DHC-3CH_2+O	F
M11	13.03	352.1	$[M-e]^+$	$C_{21}H_{22}NO_4$	336.1,321.0,308.3,293.2	DHC-CH_2	B
M12	14.76	352.1	$[M-e]^+$	$C_{21}H_{22}NO_4$	352.0,337.1,321.1,309.0,293.0	DHC-CH_2	B, F, U
M14	16.08	352.1	$[M-e]^+$	$C_{21}H_{22}NO_4$	352.1,336.1,321.0,308.0,293.0	DHC-CH_2	F, U
M13	15.16	352.1	$[M-e]^+$	$C_{21}H_{22}NO_4$	352.1,336.1,321.1,308.2,293.0	DHC-CH_2	B, F, U
M15	9.06	356.1	$[M-e]^+$	$C_{19}H_{18}NO_6$	356.3,338,322.1,308.0	DHC-3CH_2+O_2	U
Parent drug*	17.57	366.1	$[M-e]^+$	$C_{22}H_{24}NO_4$	350.2,334.1,322.1,308.2,306.1	DHC	B, F, P, U
M16	10.84	370.1	$[M-e]^+$	$C_{20}H_{20}NO_6$	370.1,340.1,338.0,322.1,324.1,308.0	DHC-2CH_2+O_2	F
M17	11.57	370.1	$[M-e]^+$	$C_{20}H_{20}NO_6$	370.1,354.0,338.0,326.2,310.0	DHC-2CH_2+O_2	B
M18	13.55	382.1	$[M-e]^+$	$C_{22}H_{24}NO_5$	382.1,366.1,367.0,352.1,350.0	DHC+O	F
M20	10.69	384.1	$[M-e]^+$	$C_{21}H_{22}NO_6$	384.0,368.2,366.0,354.1	DHC-CH_2+2O	B
M21	13.16	384.1	$[M-e]^+$	$C_{21}H_{22}NO_6$	366.1,350.0,334.1,322.1,306.1	DHC-CH_2+2O	P
M24	15.05	398.2	$[M-e]^+$	$C_{22}H_{24}NO_6$	398.2,382.1,368.3,352.1,336.1	DHC+O2	F
M25	11.81	418.1	$[M-e]^+$	$C_{20}H_{20}NO_7S$	338.2,323.0,321.1,308.2	DHC-2CH_2+SO_3	B
M26	12.97	432.1	$[M-e]^+$	$C_{21}H_{22}NO_7S$	352.1,336.0,308.0,293.2	DHC-CH_2+SO_3	B
M27	13.96	432.1	$[M-e]^+$	$C_{21}H_{22}NO_7S$	352.2,350.0,337.1321.1	DHC-CH_2+SO_3	B
M28	13.87	462.1	$[M-e]^+$	$C_{22}H_{24}NO_8S$	382.1,366.1,350.0,338.2	DHC+O+SO_3	B
M32	9.00	514.2	$[M-e]^+$	$C_{26}H_{28}NO_{10}$	338.0,323.0,308.0,295.0	DHC-2CH_2+$C_6H_8O_6$	B
M31	8.73	514.2	$[M-e]^+$	$C_{26}H_{28}NO_{10}$	338.2,323.0,308.0	DHC-2CH_2+$C_6H_8O_6$	B

M35	10.54	528.1	$[M-e]^+$	$C_{26}H_{28}NO_{10}$	352.1,336.1,321.1,308.1	DHC-CH_2+$C_6H_8O_6$	B
M36	10.86	528.1	$[M-e]^+$	$C_{26}H_{28}NO_{10}$	352.1,337.0,322.1308.2	DHC-CH_2+$C_6H_8O_6$	B
M37	11.74	528.1	$[M-e]^+$	$C_{26}H_{28}NO_{10}$	352.1,337.2,324.1,320.9,308.0	DHC-CH_2+$C_6H_8O_6$	B, P
M38	6.67	532.1	$[M-e]^+$	$C_{25}H_{26}NO_{12}$	532.1,356.2,338.0,323.0,322.1,308.2	DHC-3CH_2+O_2+$C_6H_8O_6$	B, P
M39	11.79	544.2	$[M-e]^+$	$C_{27}H_{30}NO_{11}$	368.2,353.0,352.1,324.1	DHC-CH_2+O+$C_6H_8O_6$	B
M40	12.31	558.1	$[M-e]^+$	$C_{28}H_{32}NO_{11}$	382.2,366.2,352.0,338.3	DHC+O+$C_6H_8O_6$	B

Note: **B**: bile; **F**: feces; **U**: urine; **P**: plasma; *: unambiguously identified by comparing with the reference substances.

Table S6 The metabolites of dehydrocorydaline identified from rat bile, feces, plasma, and urine by Vion IM-QTOF.

Metabolites ID	t_R (min)	*m/z*	Adducts	Formula	Error (ppm)	CCS (Å^2)	MS^2	Scan mode	Biotransformation reaction	Source
M1	9.61	324.1225	$[M-e]^+$	$C_{19}H_{18}NO_4$	–1.5	153.26	309.0992,280.0957,266.0803	HDDDA	DHC-3CH_2	B
M2	10.13	324.1220	$[M-e]^+$	$C_{19}H_{18}NO_4$	–2.6	166.56	309.0982,280.0954,265.0712	HDDDA, $HDMS^E$	DHC-3CH_2	F
M3	11.01	324.1222	$[M-e]^+$	$C_{19}H_{18}NO_4$	–2.1	169.48	309.0979,280.0956,266.0791	HDDDA, $HDMS^E$	DHC-3CH_2	F, U
M5	16.15	336.1223	$[M-e]^+$	$C_{19}H_{18}NO_5$	–1.9	173.99	304.0956,291.0969	HDDDA, $HDMS^E$	DHC-2CH_2-H_2	B, F, U
M4	14.09	336.1224	$[M-e]^+$	$C_{20}H_{18}NO_4$	–1.7	172.20	321.0985,305.1035,293.1031	$HDMS^E$	DHC-2CH_2-H_2	B, F, U
M7	12.15	338.1376	$[M-e]^+$	$C_{20}H_{20}NO_4$	–2.8	176.10	322.1059,320.0904,306.1111,294.1111,280.0951	HDDDA, $HDMS^E$	DHC-2CH_2	F, U
M8	12.90	338.1378	$[M-e]^+$	$C_{20}H_{20}NO_4$	–2.2	173.98	323.1129,308.0905,280.0951	HDDDA, $HDMS^E$	DHC-2CH_2	F, U
M6	11.91	338.1378	$[M-e]^+$	$C_{20}H_{20}NO_4$	–2.3	175.24	323.1108,308.0904,280.0951	HDDDA, $HDMS^E$	DHC-2CH_2	B, F, P, U
M9	10.79	340.1172	$[M-e]^+$	$C_{19}H_{18}NO_5$	–1.9	172.80	310.0707,296.0905,294.0761,282.0746	HDDDA, $HDMS^E$	DHC-3CH_2+O	F
M10	16.07	350.1378	$[M-e]^+$	$C_{21}H_{20}NO_4$	–2.4	178.54	334.1419,302.0803	HDDDA, $HDMS^E$	DHC-CH_2-H_2	B, F, U
M12	13.71	352.1536	$[M-e]^+$	$C_{21}H_{22}NO_4$	–1.9	181.45	336.1241,321.0984,293.1028	HDDDA, $HDMS^E$	DHC-CH_2	B, F, U
M13	14.11	352.1538	$[M-e]^+$	$C_{21}H_{22}NO_4$	–1.4	180.82	336.1219,321.0985,305.1035,293.1031	HDDDA, $HDMS^E$	DHC-CH_2	B, F, U
M14	14.80	352.1544	$[M-e]^+$	$C_{21}H_{22}NO_4$	0.3	179.59	321.0985,306.11144,292.0957	HDDDA, $HDMS^E$	DHC-CH_2	B, F, P, U

Parent drug*	16.16	366.1694	$[M-e]^+$	$C_{22}H_{24}NO_4$	–1.5	186.25	350.1377,334.1061,318.1115,308.1269,306.1113	HDDDA, $HDMS^E$	DHC	B, F, P, U
M19	15.47	382.1645	$[M-e]^+$	$C_{22}H_{24}NO_5$	–1.0	187.91	350.1003,322.1068,308.0901	HDDDA, $HDMS^E$	DHC+O	B, F
M18	12.73	382.1647	$[M-e]^+$	$C_{22}H_{24}NO_5$	–0.5	189.24	366.1332,350.1020,334.1074,324.1218	HDDDA, $HDMS^E$	DHC+O	B
M20	10.39	384.1442	$[M-e]^+$	$C_{21}H_{22}NO_6$	–0.6	188.65	368.1125,340.1169,308.0906	HDDDA, $HDMS^E$	DHC-CH_2+2O	B
M21	12.41	384.1442	$[M-e]^+$	$C_{21}H_{22}NO_6$	0.2	190.03	350.1021,334.0705,322.1074,306.0752	HDDDA, $HDMS^E$	DHC-CH_2+2O	P
M22	12.65	398.1595	$[M-e]^+$	$C_{22}H_{24}NO_6$	–0.7	193.38	382.1287,322.1069	HDDDA, $HDMS^E$	DHC+O_2	B
M23	13.20	398.1595	$[M-e]^+$	$C_{22}H_{24}NO_6$	–0.8	197.25	382.1284,322.1062	HDDDA, $HDMS^E$	DHC+O_2	B
M25	11.23	418.0948	$[M-e]^+$	$C_{20}H_{20}NO_7S$	–1.3	241.23	323.1112,308.0904,280.0940	$HDMS^E$	DHC-2CH_2+SO_3	B
M26	12.25	432.1109	$[M-e]^+$	$C_{21}H_{22}NO_7S$	–0.3	200.50	336.1219,321.0984,308.1271,293.1034	HDDDA, $HDMS^E$	DHC-CH_2+SO_3	B
M27	12.99	432.1113	$[M-e]^+$	$C_{21}H_{22}NO_7S$	0.4	199.92	337.1302,321.0987,306.1112,293.1033	HDDDA, $HDMS^E$	DHC-CH_2+SO_3	B
M29	9.87	498.1393	$[M-e]^+$	$C_{25}H_{24}NO_{10}$	–0.1	255.62	322.1062,307.0835,279.0899	$HDMS^E$	DHC-3CH_2-H_2+$C_6H_8O_6$	B
M30	8.85	500.1548	$[M-e]^+$	$C_{25}H_{26}NO_{10}$	–0.3	215.61	324.1227,309.0978,281.1033	HDDDA, $HDMS^E$	DHC-3CH_2+$C_6H_8O_6$	U
M32	8.70	514.1708	[M-e]+	$C_{26}H_{28}NO_{10}$	0.2	224.61	338.1377,322.1141,308.0905,280.0952	HDDDA, $HDMS^E$	DHC-2CH_2+$C_6H_8O_6$	B, U
M33	9.82	514.1711	[M-e]+	$C_{26}H_{28}NO_{10}$	0.9	218.91	338.1062,294.1112	HDDDA, $HDMS^E$	DHC-2CH_2+$C_6H_8O_6$	B, U
M34	11.28	514.1712	[M-e]+	$C_{26}H_{28}NO_{10}$	0.9	218.71	338.1355,322.1058,294.1110	HDDDA,	DHC-2CH_2+$C_6H_8O_6$	U

								HDMS^{E}		
M35	11.22	528.1865	[M-e]+	$C_{27}H_{30}NO_{10}$	0.2	222.02	352.1534,337.1293,308.1269	HDDDA, HDMS^{E}	DHC-CH_2+$C_6H_8O_6$	B, P, U
M36	10.30	528.1867	[M-e]+	$C_{27}H_{30}NO_{10}$	0.6	225.27	352.1536,336.1221,308.1271	HDDDA, HDMS^{E}	DHC-CH_2+$C_6H_8O_6$	B, U
M37	10.58	528.1868	[M-e]+	$C_{27}H_{30}NO_{10}$	0.8	230.39	352.1539,336.1222,308.1273	HDDDA, HDMS^{E}	DHC-CH_2+$C_6H_8O_6$	B, U
M39	11.25	544.1813	[M-e]+	$C_{27}H_{30}NO_{11}$	0.1	228.39	368.1484,352.1165,338.0994,324.1216,310.1059	HDDDA, HDMS^{E}	DHC-CH_2+O+$C_6H_8O_6$	B
M40	11.66	558.1972	[M-e]+	$C_{28}H_{32}NO_{11}$	0.4	231.14	382.1641,366.1328,352.1164,338.1378,321.1352	HDDDA, HDMS^{E}	DHC+O+$C_6H_8O_6$	B

Note: **B**: bile; **F**: feces; **U**: urine; **P**: plasma; *: unambiguously identified by comparing with the reference substances.