

filename	FC	Feature specificity	MF prediction ratio	LC	Reported compounds in Species	Reported compounds in Genus	SC	CC	New CC in sp	New CC in genus
LQ-01-61-78_pos.mzX ML	0.82	0.84	0.32	1.00	2	8	1	1	{'Agarofuran sesquiterpenoids', 'Primary amides', 'Pyridine alkaloids'}	{'Agarofuran sesquiterpenoids', 'Primary amides', 'Pyridine alkaloids'}
LQ-01-61-37_pos.mzX ML	0.81	0.84	0.54	1.00	1	440	1	1	{'Chromones', 'Simple coumarins', , 'Isoquinoline alkaloids', 'Agarofuran sesquiterpenoids', 'Pyranocoumarins', 'Simple phenolic acids', 'Isocoumarins', 'Furocoumarins'}	{'Chromones', 'Simple coumarins', , 'Isoquinoline alkaloids', 'Pyranocoumarins', 'Simple phenolic acids', 'Isocoumarins', 'Furocoumarins'}
LQ-01-61-06_pos.mzX ML	0.84	0.86	0.48	0.89	212	732	1	1	{'Tetracyclic diterpenoids', 'Paraliane diterpenoids', 'Open-chain	{'Tetracyclic diterpenoids', 'Paraliane diterpenoids', 'Open-chain

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									polyketides '}	polyketides '}
LQ-01-61- 07_pos.mzX ML	0.70	0.71	0.50	0.96	71	732	1	1	{'Paraliane diterpenoid s', 'Labdane diterpenoid s', 'Neutral glycosphin golipids', 'Daucane sesquiterpe noids', 'Tetracyclic diterpenoid s', 'Tetracyclic diterpenoid s', 'Dicarboxyl ic acids', 'Trichothec ane sesquiterpe noids', 'Monoacylg lycerols', 'Diacylglyc erols'}	{'Paraliane diterpenoid s', 'Neutral glycosphin golipids', 'Daucane sesquiterpe noids', 'Tetracyclic diterpenoid s', 'Dicarboxyl ic acids', 'Trichothec ane sesquiterpe noids', 'Monoacylg lycerols', 'Diacylglyc erols'}
LQ-01-61- 05_pos.mzX ML	0.74	0.76	0.39	0.89	212	732	1	1	{'Pyridine alkaloids'}	{'Pyridine alkaloids'}
LQ-01-61- 56_pos.mzX ML	0.64	0.66	0.37	0.99	14	338	1	1	{'Paraliane diterpenoid s', 'Agarofura n sesquiterpe	{'Paraliane diterpenoid s', 'Agarofura n sesquiterpe

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									noids', 'Drimane sesquiterpe noids', 'Daucane sesquiterpe noids'}	noids', 'Drimane sesquiterpe noids', 'Daucane sesquiterpe noids'}
LQ-01-61- 54_pos.mzX ML	0.51	0.57	0.29	0.99	14	338	1	1	{'Agarofuran sesquiterpe noids', 'Trichothecane sesquiterpe noids', 'Lanostane , Tirucallane and Euphane triterpenoids'}	{'Agarofuran sesquiterpe noids', 'Trichothecane sesquiterpe noids', 'Lanostane, Tirucallane and Euphane triterpenoids'}
LQ-01-61- 55_pos.mzX ML	0.50	0.52	0.33	0.99	14	338	1	1	{'Agarofuran sesquiterpe noids', 'Trichothecane sesquiterpe noids', 'Drimane sesquiterpe noids', 'Daucane sesquiterpe noids'}	{'Agarofuran sesquiterpe noids', 'Trichothecane sesquiterpe noids', 'Drimane sesquiterpe noids', 'Daucane sesquiterpe noids'}

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LQ-01-61-03_pos.mzX ML	0.50	0.51	0.27	0.94	126	126	1	1	{'Ursane and Taraxastane triterpenoids', 'Tetraketide meroterpenoids', 'Triketide meroterpenoids', 'Daucane sesquiterpenoids'}	{'Ursane and Taraxastane triterpenoids', 'Daucane sesquiterpenoids', 'Tetraketide meroterpenoids', 'Triketide meroterpenoids'}
LQ-01-61-02_pos.mzX ML	0.49	0.50	0.29	0.94	126	126	1	1	{'Oleanane triterpenoids'}	{'Oleanane triterpenoids'}
LQ-01-61-75_pos.mzX ML	0.38	0.41	0.23	0.49	1011	1353	1	1	{'Vitamin D2 and derivatives'}	{'Vitamin D2 and derivatives'}
LQ-01-61-60_pos.mzX ML	0.81	0.82	0.53	1.00	0	0	1	0		
LQ-01-61-47_pos.mzX ML	0.78	0.81	0.57	1.00	0	0	1	0		
LQ-01-61-23_pos.mzX ML	0.78	0.81	0.50	1.00	0	0	1	0		

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LQ-01-61-62_pos.mzX ML	0.71	0.74	0.44	1.00	3	50	0	1	{'Dipeptide s'}	{'Dipeptide s'}
LQ-01-61-41_pos.mzX ML	0.68	0.78	0.39	1.00	0	0	1	0		
LQ-01-61-19_pos.mzX ML	0.64	0.65	0.40	1.00	0	0	1	0		
LQ-01-61-58_pos.mzX ML	0.61	0.65	0.36	0.99	14	211	0	1	{'Ursane and Taraxastan e triterpenoi ds', 'Agarofura n sesquiterpe noids'}	{'Ursane and Taraxastan e triterpenoi ds', 'Agarofura n sesquiterpe noids'}
LQ-01-61-31_pos.mzX ML	0.58	0.60	0.39	1.00	0	0	1	0		
LQ-01-61-43_pos.mzX ML	0.58	0.63	0.33	0.99	15	329	0	1	{'Flavones' , 'Flavonols' }	{'Flavones' , 'Flavonols' }
LQ-01-61-22_pos.mzX ML	0.55	0.58	0.29	1.00	0	0	1	0		
LQ-01-61-44_pos.mzX ML	0.56	0.59	0.23	0.99	15	329	0	1	{'Lanostan e, Tirucallane	{'Lupane triterpenoi ds',

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									and Euphane triterpenoi ds', 'Pregnane steroids', 'Lupane triterpenoi ds'}	'Pregnane steroids', 'Lanostane, Tirucallane and Euphane triterpenoi ds'}
LQ-01-61- 73_pos.mzX ML	0.61	0.61	0.21	0.92	162	1353	1	0		
LQ-01-61- 72_pos.mzX ML	0.49	0.50	0.41	1.00	0	0	1	0		
LQ-01-61- 53_pos.mzX ML	0.45	0.49	0.28	0.98	43	329	0	1	{'Cholestan e steroids'}	{'Cholestan e steroids'}
LQ-01-61- 52_pos.mzX ML	0.43	0.45	0.32	0.98	43	329	0	1	{'Cholestan e steroids'}	{'Cholestan e steroids'}
LQ-01-61- 01_pos.mzX ML	0.46	0.49	0.27	0.94	126	126	1	0		
LQ-01-61- 16_pos.mzX ML	0.44	0.50	0.29	0.95	92	440	0	1	{'Open- chain polyketides '}	{'Open- chain polyketides '}
LQ-01-61- 04_pos.mzX ML	0.45	0.46	0.31	0.94	126	126	1	0		

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LQ-01-61- 67_pos.mzX ML	0.51	0.57	0.37	0.84	313	514	0	1	{'Straight chain fatty acids', 'Lanostane , Tirucallane and Euphane triterpenoi ds'}	{'Straight chain fatty acids', 'Lanostane, Tirucallane and Euphane triterpenoi ds'}
LQ-01-61- 66_pos.mzX ML	0.50	0.52	0.33	0.84	313	514	0	1	{'Cholestan e steroids', 'Lanostane , Tirucallane and Euphane triterpenoi ds'}	{'Cholestan e steroids', 'Lanostane, Tirucallane and Euphane triterpenoi ds'}
LQ-01-61- 30_pos.mzX ML	0.35	0.37	0.25	0.95	92	440	0	1	{'Zearaleno nes', 'Dicarboxyl ic acids'}	{'Zearaleno nes', 'Dicarboxyl ic acids'}
LQ-01-61- 71_pos.mzX ML	0.42	0.49	0.25	0.84	313	514	0	1	{'Lanostan e, Tirucallane and Euphane triterpenoi ds'}	{'Lanostan e, Tirucallane and Euphane triterpenoi ds'}
LQ-01-61- 74_pos.mzX ML	0.51	0.53	0.29	0.49	1011	1353	1	0		

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LQ-01-61- 27_pos.mzX ML	0.83	0.90	0.51	0.99	11	440	0	0		
LQ-01-61- 28_pos.mzX ML	0.76	0.81	0.63	1.00	1	440	0	0		
LQ-01-61- 42_pos.mzX ML	0.71	0.71	0.41	1.00	0	0	0	0		
LQ-01-61- 57_pos.mzX ML	0.71	0.82	0.38	0.99	14	211	0	0		
LQ-01-61- 70_pos.mzX ML	0.67	0.68	0.28	1.00	0	0	0	0		
LQ-01-61- 09_pos.mzX ML	0.70	0.70	0.19	0.96	71	732	0	0		
LQ-01-61- 08_pos.mzX ML	0.70	0.70	0.48	0.96	71	732	0	0		
LQ-01-61- 68_pos.mzX ML	0.66	0.66	0.34	1.00	0	0	0	0		
LQ-01-61- 33_pos.mzX ML	0.65	0.68	0.50	1.00	0	0	0	0		
LQ-01-61- 40_pos.mzX ML	0.64	0.65	0.42	1.00	0	0	0	0		

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LQ-01-61- 69_pos.mzX ML	0.63	0.74	0.37	1.00	0	0	0	0		
LQ-01-61- 51_pos.mzX ML	0.62	0.65	0.50	1.00	0	0	0	0		
LQ-01-61- 14_pos.mzX ML	0.61	0.62	0.35	1.00	0	0	0	0		
LQ-01-61- 15_pos.mzX ML	0.65	0.71	0.32	0.95	92	440	0	0		
LQ-01-61- 63_pos.mzX ML	0.59	0.63	0.43	1.00	0	0	0	0		
LQ-01-61- 12_pos.mzX ML	0.57	0.61	0.40	1.00	0	0	0	0		
LQ-01-61- 32_pos.mzX ML	0.56	0.59	0.37	1.00	0	0	0	0		
LQ-01-61- 46_pos.mzX ML	0.55	0.57	0.43	1.00	0	0	0	0		
LQ-01-61- 59_pos.mzX ML	0.55	0.56	0.37	0.99	14	211	0	0		
LQ-01-61- 29_pos.mzX ML	0.58	0.62	0.33	0.95	92	440	0	0		

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LQ-01-61- 64_pos.mzX ML	0.53	0.57	0.43	1.00	0	0	0	0		
LQ-01-61- 61_pos.mzX ML	0.48	0.52	0.33	1.00	0	0	0	0		
LQ-01-61- 20_pos.mzX ML	0.46	0.46	0.28	1.00	2	440	0	0		
LQ-01-61- 35_pos.mzX ML	0.45	0.51	0.29	1.00	0	0	0	0		
LQ-01-61- 45_pos.mzX ML	0.45	0.49	0.32	1.00	0	0	0	0		
LQ-01-61- 11_pos.mzXML	0.45	0.49	0.29	1.00	0	0	0	0		
LQ-01-61- 10_pos.mzX ML	0.44	0.50	0.35	1.00	0	0	0	0		
LQ-01-61- 18_pos.mzX ML	0.44	0.44	0.28	1.00	0	0	0	0		
LQ-01-61- 21_pos.mzX ML	0.43	0.46	0.24	1.00	0	0	0	0		
LQ-01-61- 38_pos.mzX ML	0.42	0.43	0.28	1.00	1	440	0	0		

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LQ-01-61-34_pos.mzX ML	0.42	0.42	0.22	1.00	0	0	0	0		
LQ-01-61-36_pos.mzX ML	0.40	0.41	0.26	1.00	0	0	0	0		
LQ-01-61-26_pos.mzX ML	0.39	0.42	0.24	1.00	0	0	0	0		
LQ-01-61-17_pos.mzX ML	0.38	0.40	0.15	1.00	0	0	0	0		
LQ-01-61-39_pos.mzX ML	0.38	0.38	0.28	1.00	1	440	0	0		
LQ-01-61-50_pos.mzX ML	0.38	0.41	0.22	1.00	0	0	0	0		
LQ-01-61-13_pos.mzX ML	0.37	0.42	0.29	1.00	0	0	0	0		
LQ-01-61-24_pos.mzX ML	0.37	0.40	0.27	1.00	0	0	0	0		
LQ-01-61-48_pos.mzX ML	0.36	0.44	0.18	1.00	0	0	0	0		
LQ-01-61-49_pos.mzX ML	0.33	0.33	0.15	1.00	0	0	0	0		

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LQ-01-61- 25_pos.mzX ML	0.30	0.31	0.22	1.00	0	0	0	0		
LQ-01-61- 65_pos.mzX ML	0.29	0.30	0.24	0.84	313	514	0	0		