

Supporting Information

IDENTIFICATION AND QUANTIFICATION OF ALKALOID COMPOUNDS FROM DIFFERENT PARTS AND PRODUCTION AREAS OF *DATURA METEL L.*

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Table S2. Information of *D. metel* L. materials

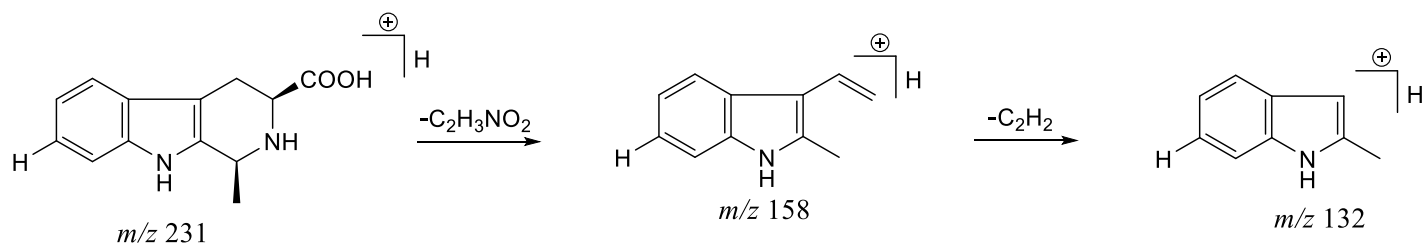
Table S3. ^{13}C -NMR data of 22 quantitative alkaloids (400 MHz in ^{13}C -NMR)

Table S4. Quantitative method validation data of 22 quantitative alkaloids, the concentration levels used to estimate stability, repeatability and recovery

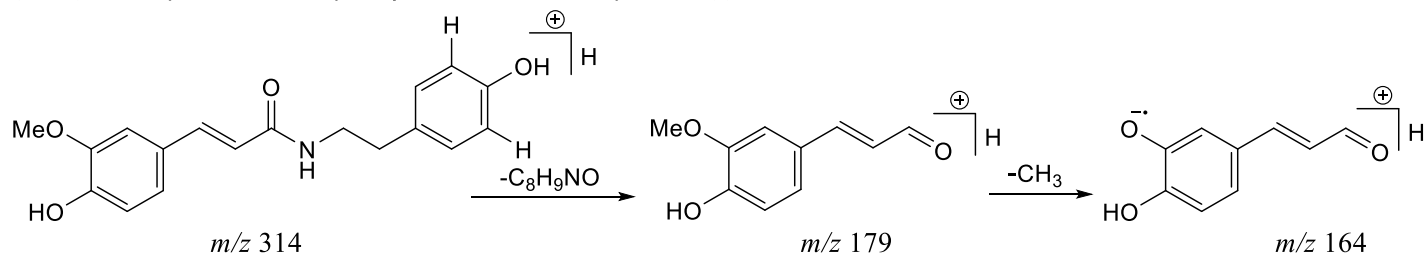
Table S5. The total alkaloid contents of different extraction conditions for *D. metel* L.

Experimental

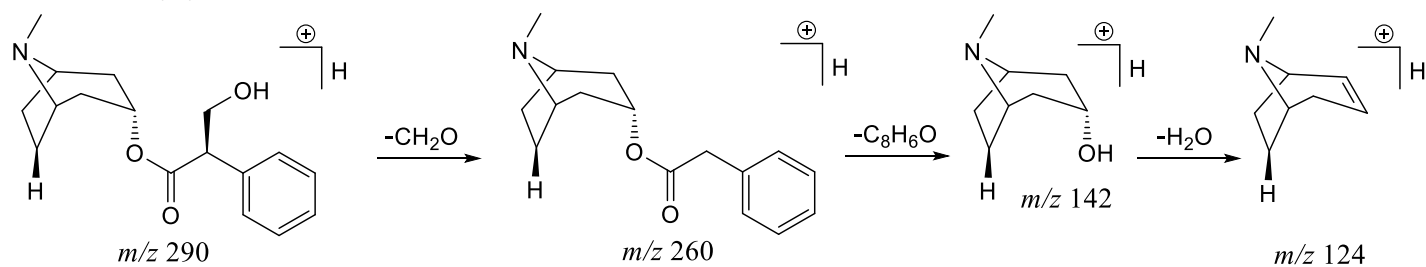
For optimizing the extraction procedure, ultra-sonication at room temperature, cold soaking and heat-reflux were considered for extracting samples, and the total content of alkaloids obtained was compared by using ultraviolet and visible spectrophotometry. Heat-reflux performed the top extraction efficiency for total alkaloids. In addition, different extraction solvents (MeOH : water = 70 : 30, MeOH : water = 100 : 0, EtOH : water = 70 : 30 and EtOH : water = 100 : 0) were compared and the results indicated that 70% ethanol could extract more alkaloids. Next, to determine extraction duration, 30 min, 60 min, 90 min, 120 min, 150 min and 180 min were examined and 120 min were sufficient to extract all alkaloids. Although the total of three extractions cycles was more than that of two extractions, it could be seen from Figure S27 and Table S5 that there was not much increase. For the sake of experimental efficiency, two extraction cycles are selected as the final extraction times. Finally, the optimized extraction procedure was obtained using 70% ethanol (EtOH : water = 70 : 30) for 120 min in heat-reflux with two times.



(1S,3S)-1-methyl-1,2,3,4-tetrahydro- β -carboline-3-carboxylic acid (7)



N-trans-feruloyltyramine (31)



atropine (18)

Figure S1. The possible fragment pathways of three types of alkaloid from *Datura metel* L (*D. metel* L.) by using UPLC-Q-TOF-MS/MS

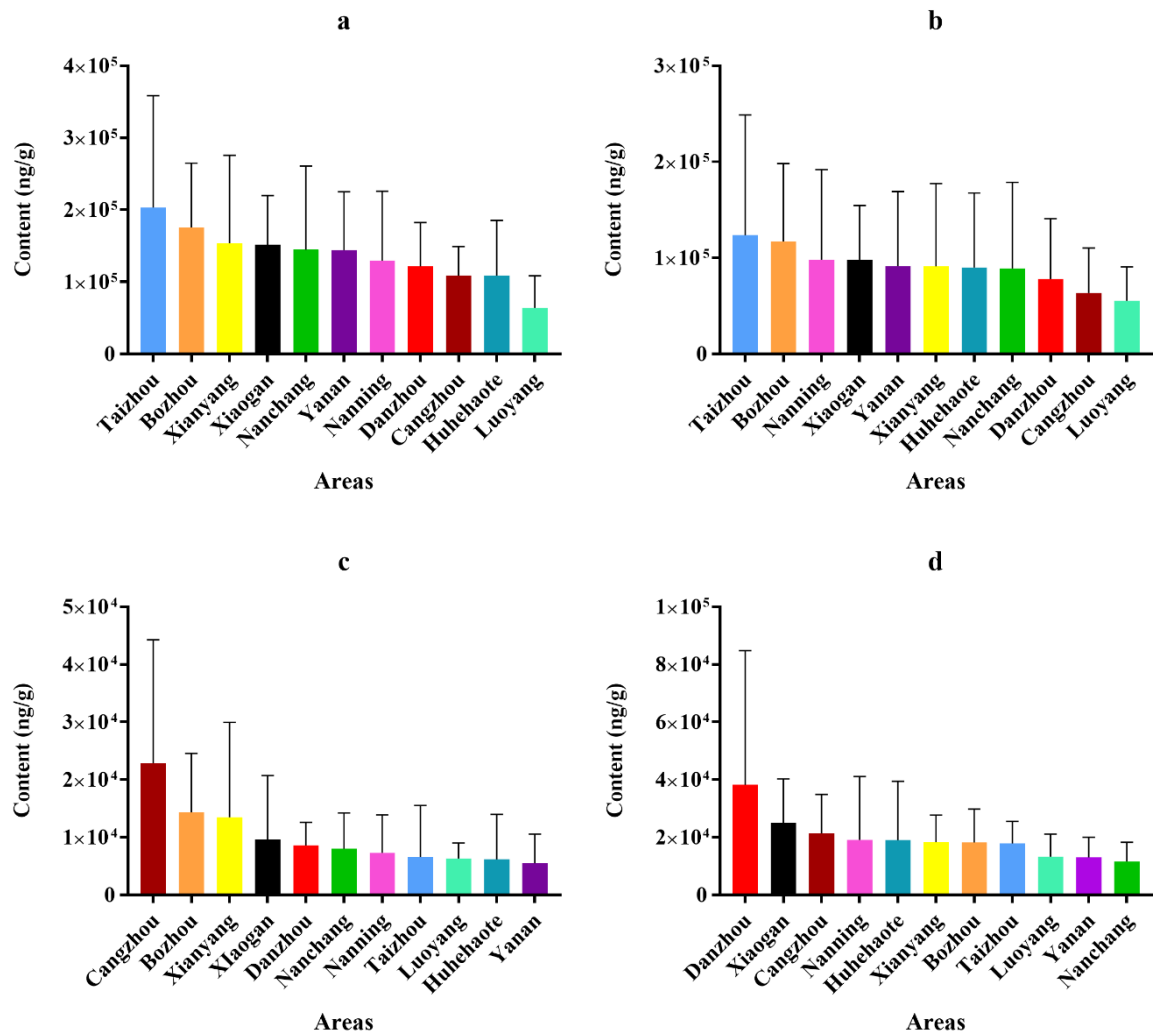


Figure S2. The contents of accumulation tropine alkaloids (a), amide alkaloids (b), tropine alkaloids (c) and indole alkaloids (d) in 11 production areas

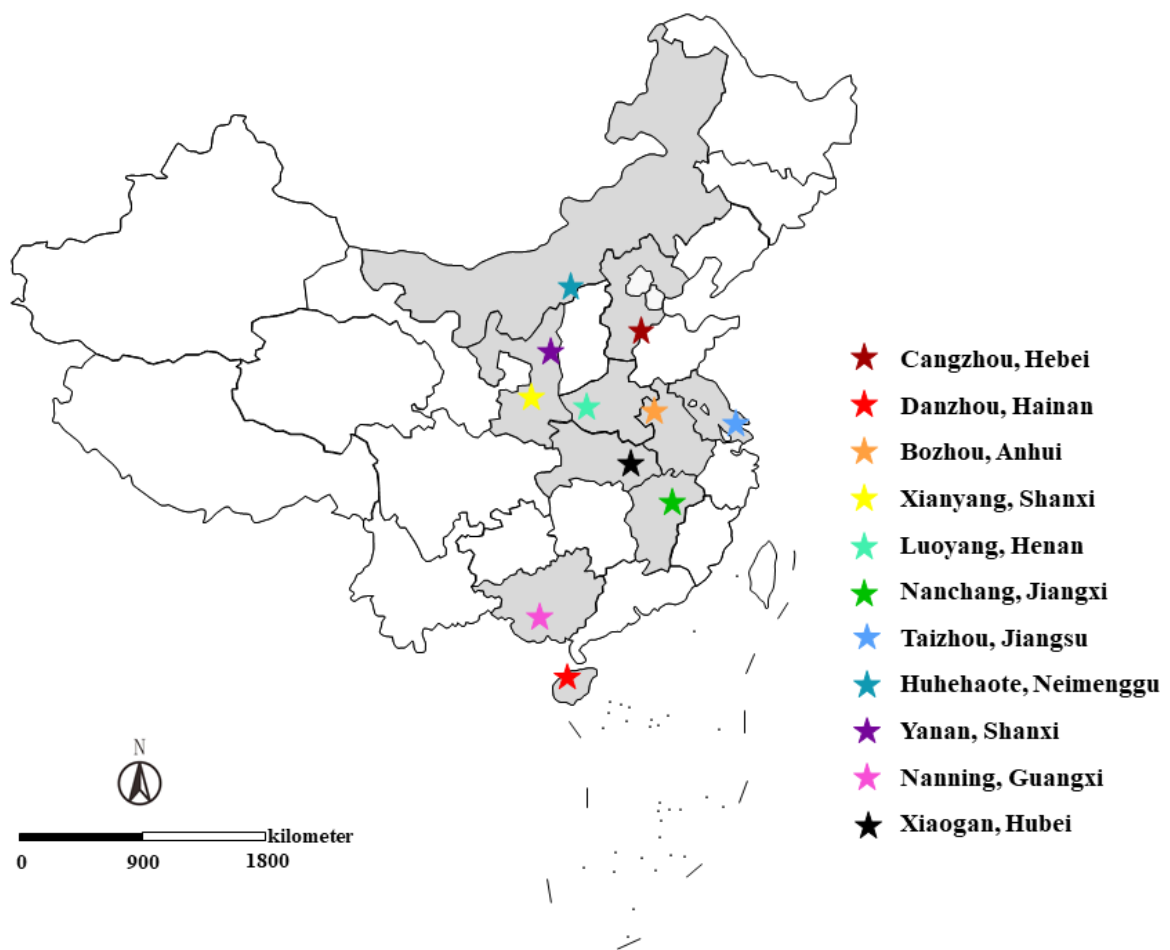


Figure S3. Sample collection, origins of *D. metel* L.

1H-pyrido-[3,4-*b*]indol-1-1,2,3,4,9-tetrahydro-7-hydroxy (3)
400 MHz

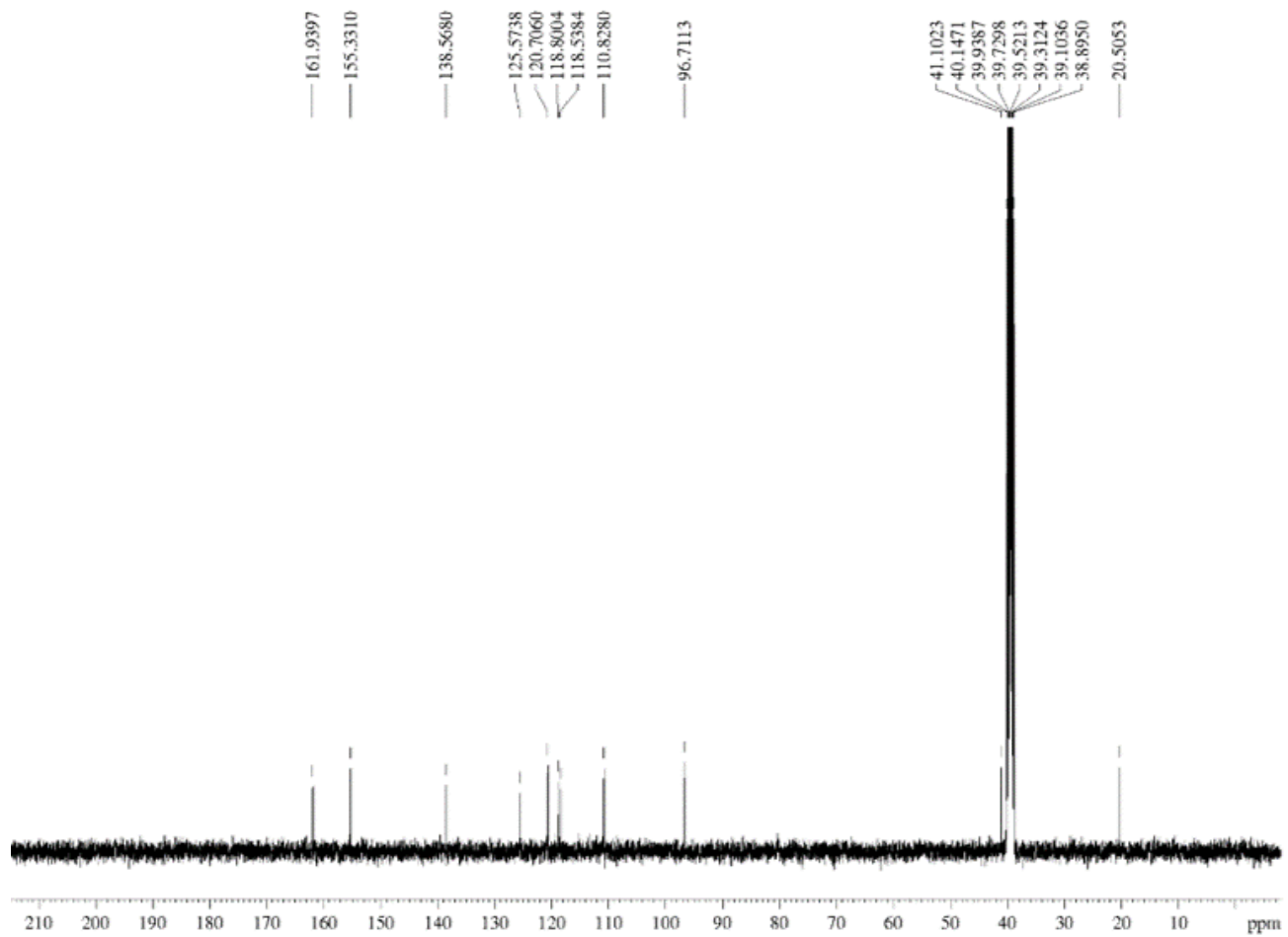


Figure S4. ^{13}C NMR spectrum of **3**

(S)-methyl-2-amino-2-phenylacetate (5)
400 MHz

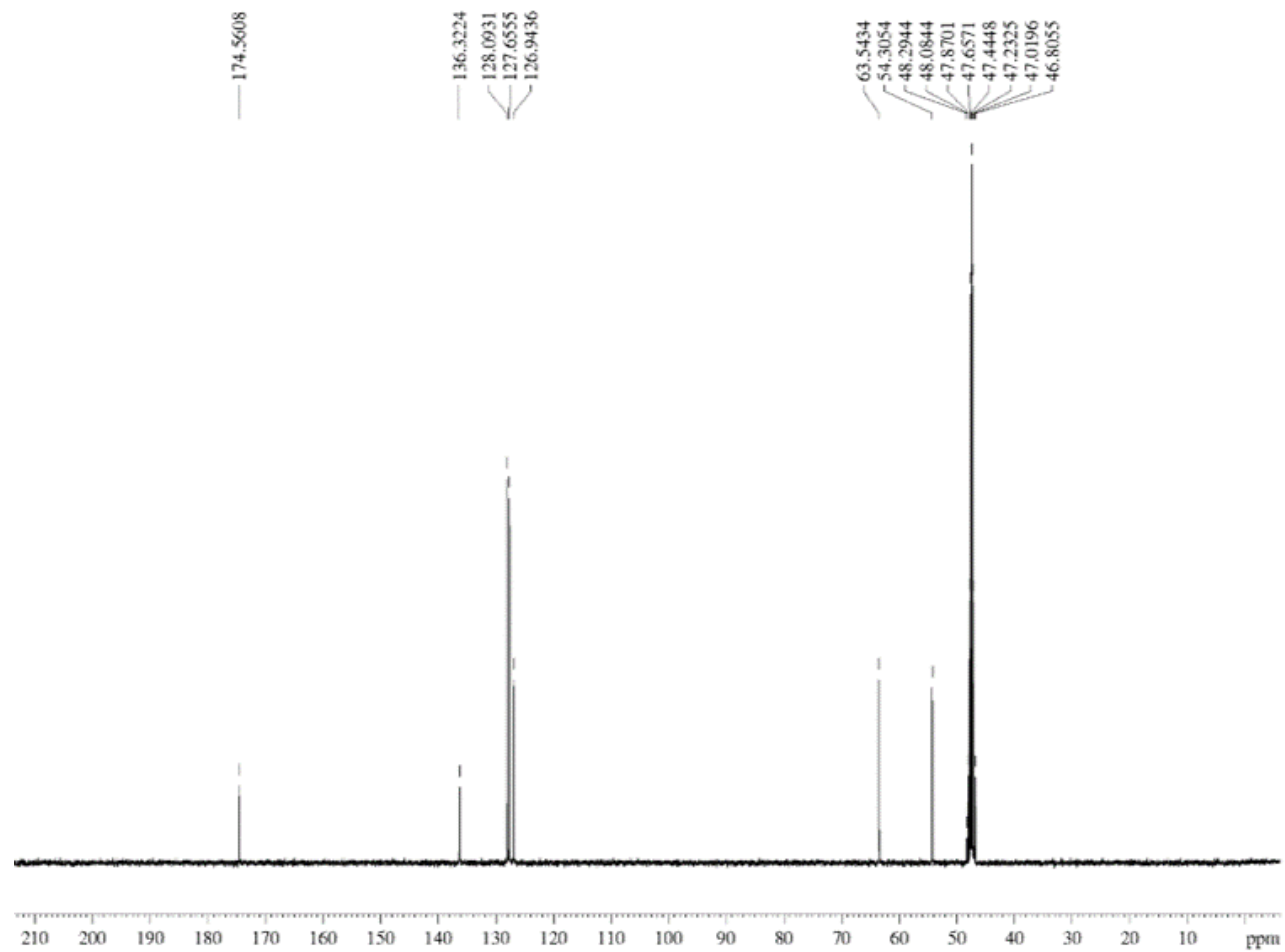


Figure S5. ¹³C NMR spectrum of **5**

(1*S*,3*S*)-1-methyl-1,2,3,4-tetrahydro- β -carboline-3-carboxylic acid (7)

400 MHz

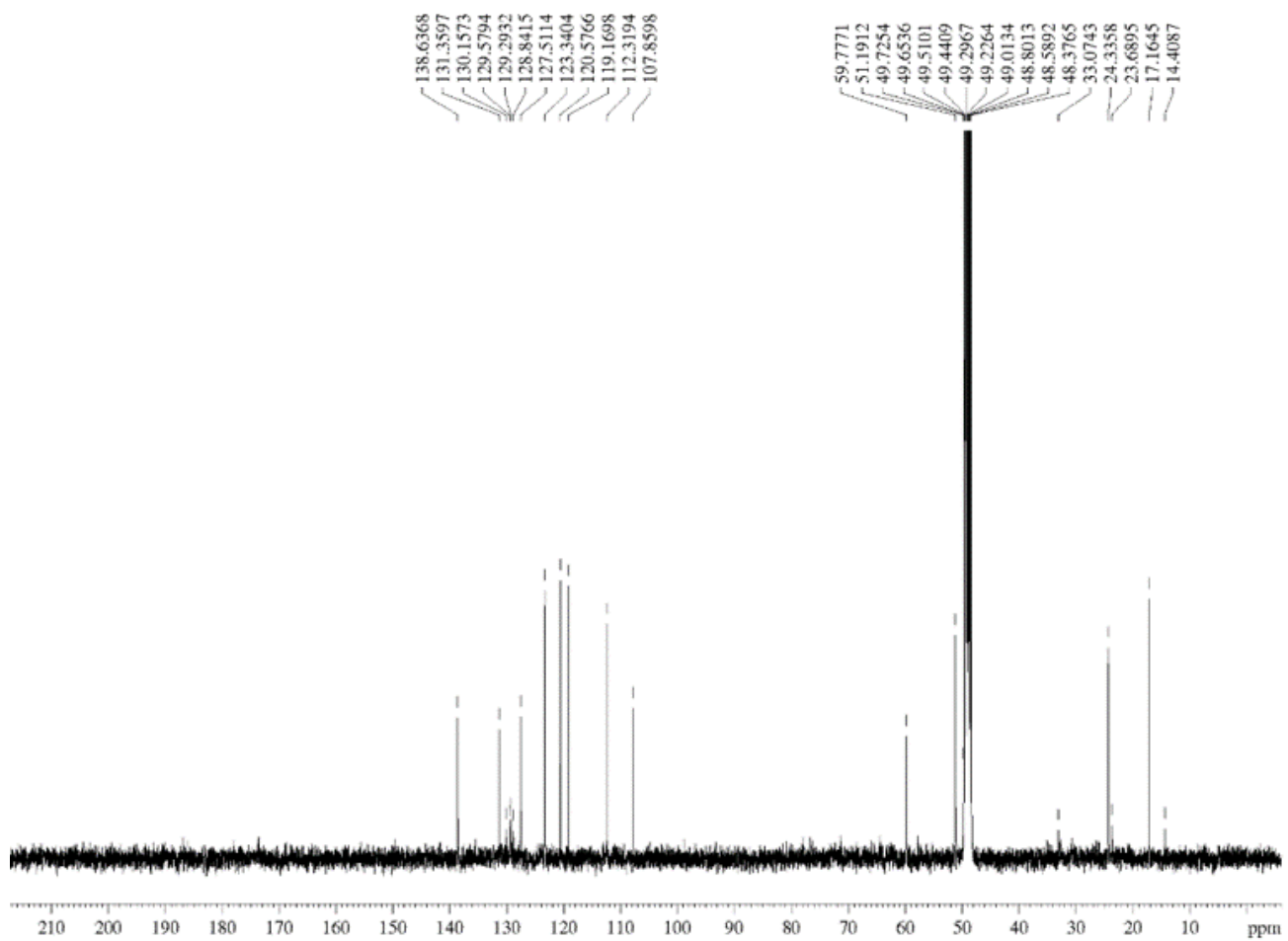


Figure S6. ^{13}C NMR spectrum of **7**

cyclo (PheTyr) (9)

400 MHz

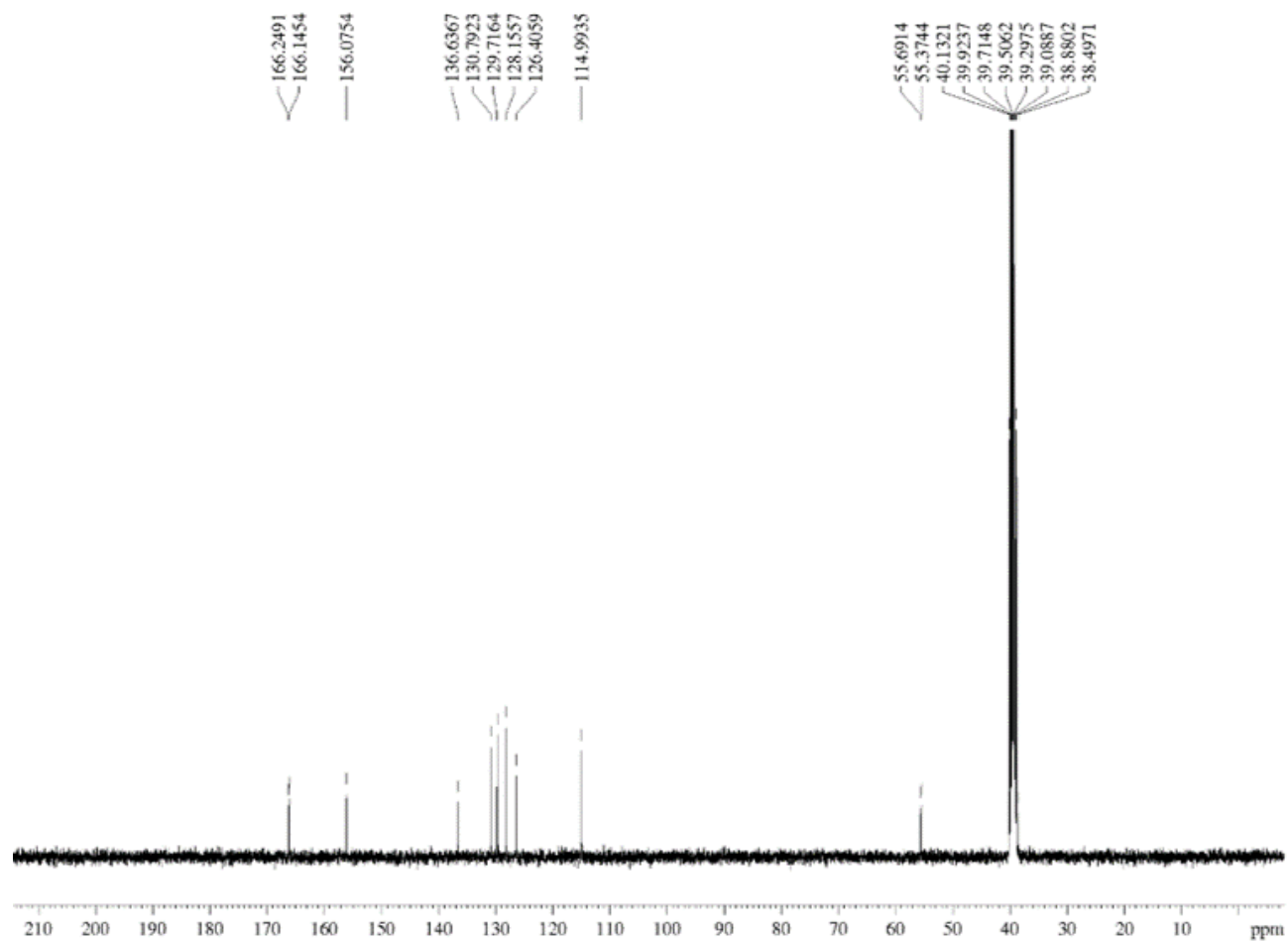


Figure S7. ^{13}C NMR spectrum of 9

anisodamine (14)
400 MHz

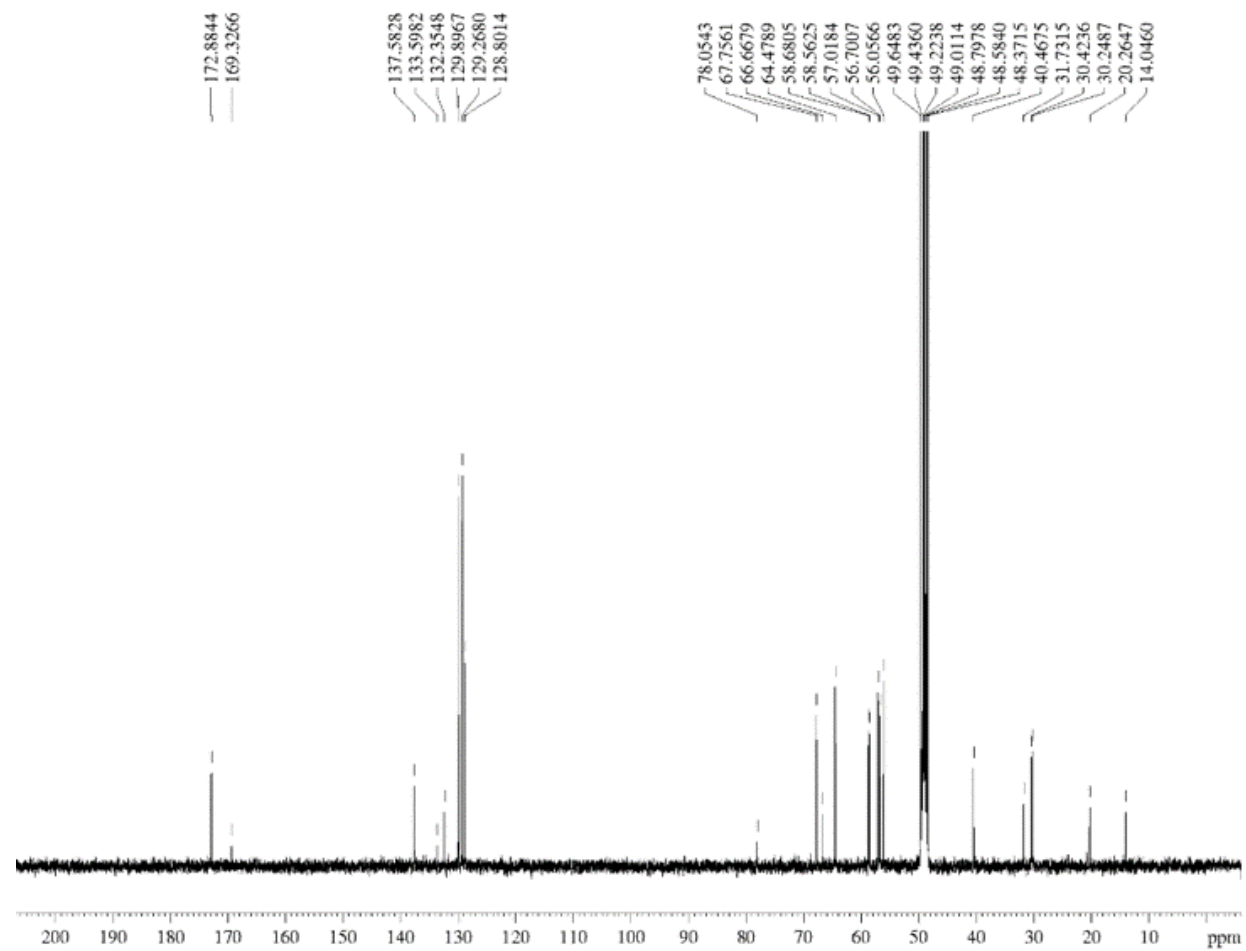


Figure S8. ^{13}C NMR spectrum of **14**

atropine (18)
400 MHz

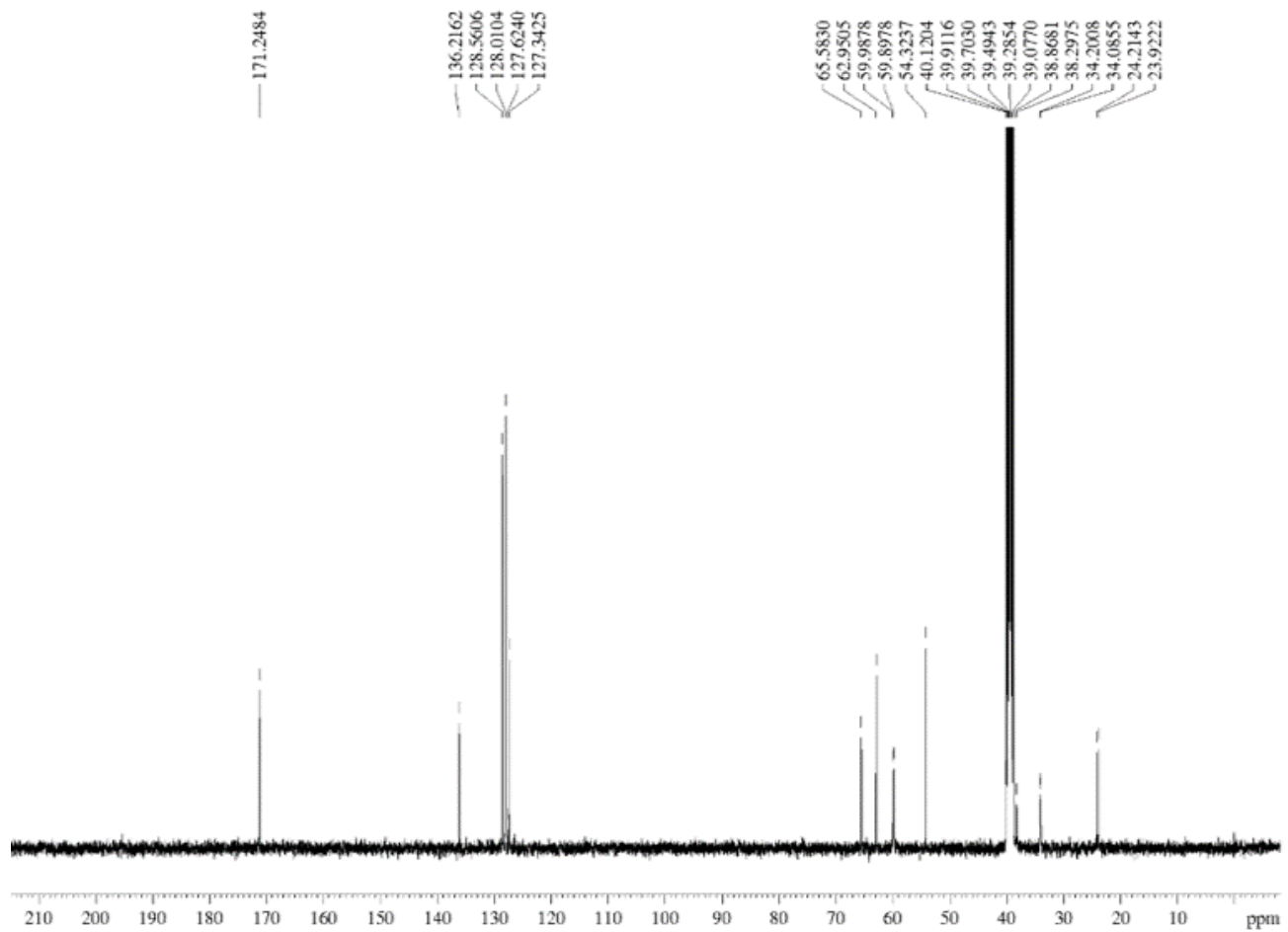


Figure S9. ^{13}C NMR spectrum of **18**

N-trans-p-coumaroyloctopamine (**20**)

400 MHz

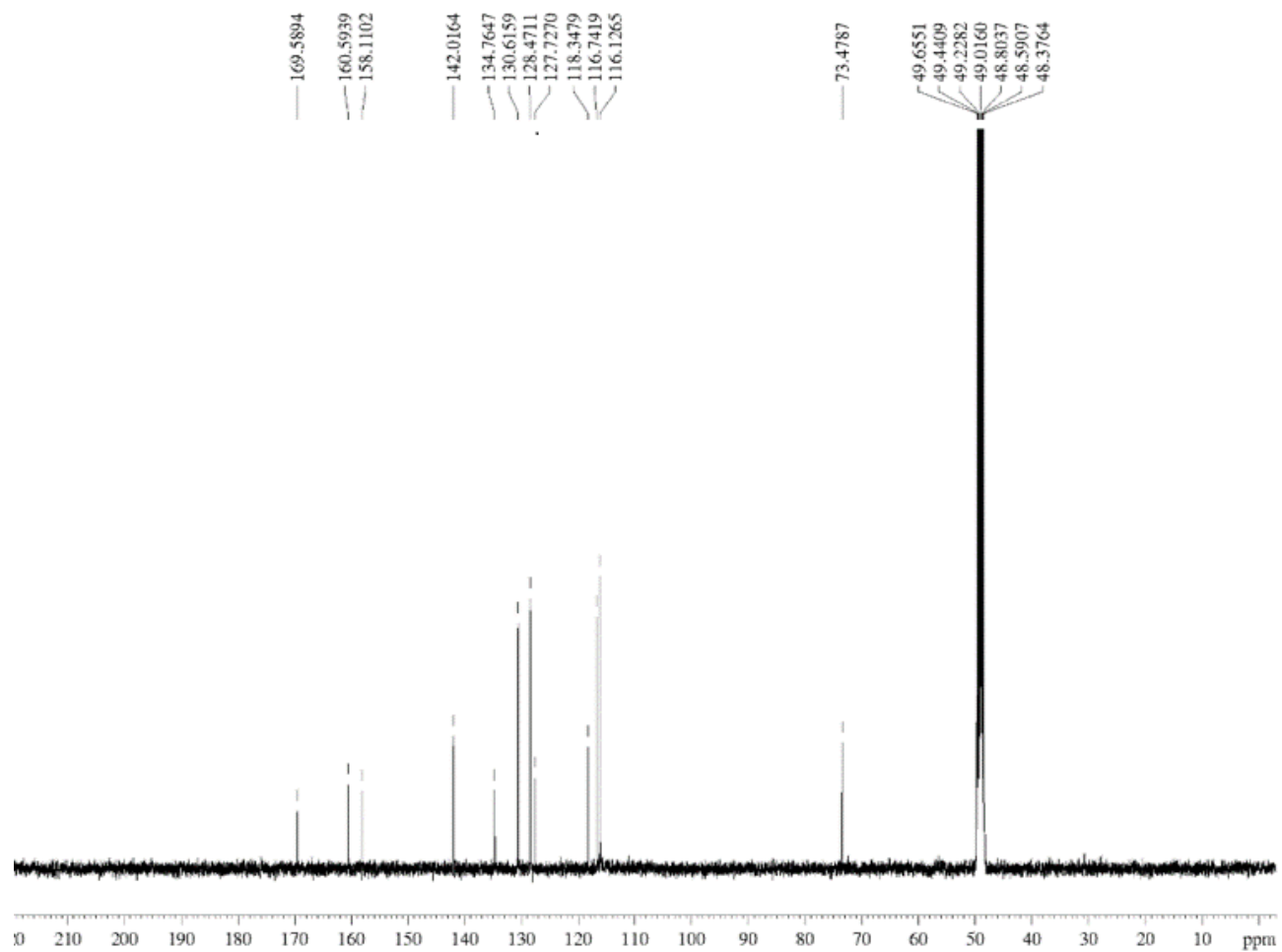


Figure S10. ¹³C NMR spectrum of **20**

N-trans-feruloyloctopamine (**23**)

400 MHz

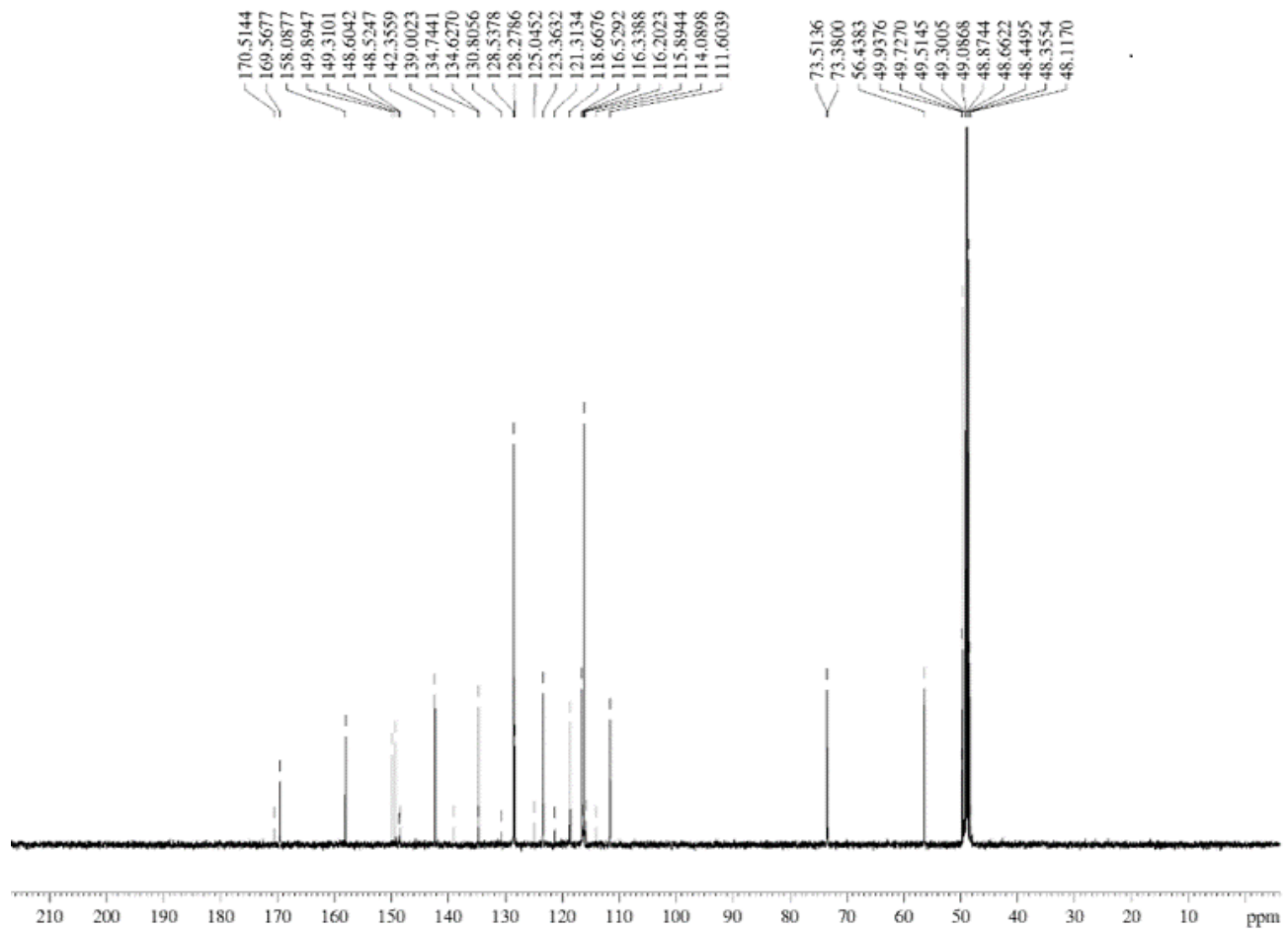


Figure S11. ¹³C NMR spectrum of **23**

***N-trans*-feruloyl-3',4'-dihydroxyphenylethylamine (25)**
400 MHz

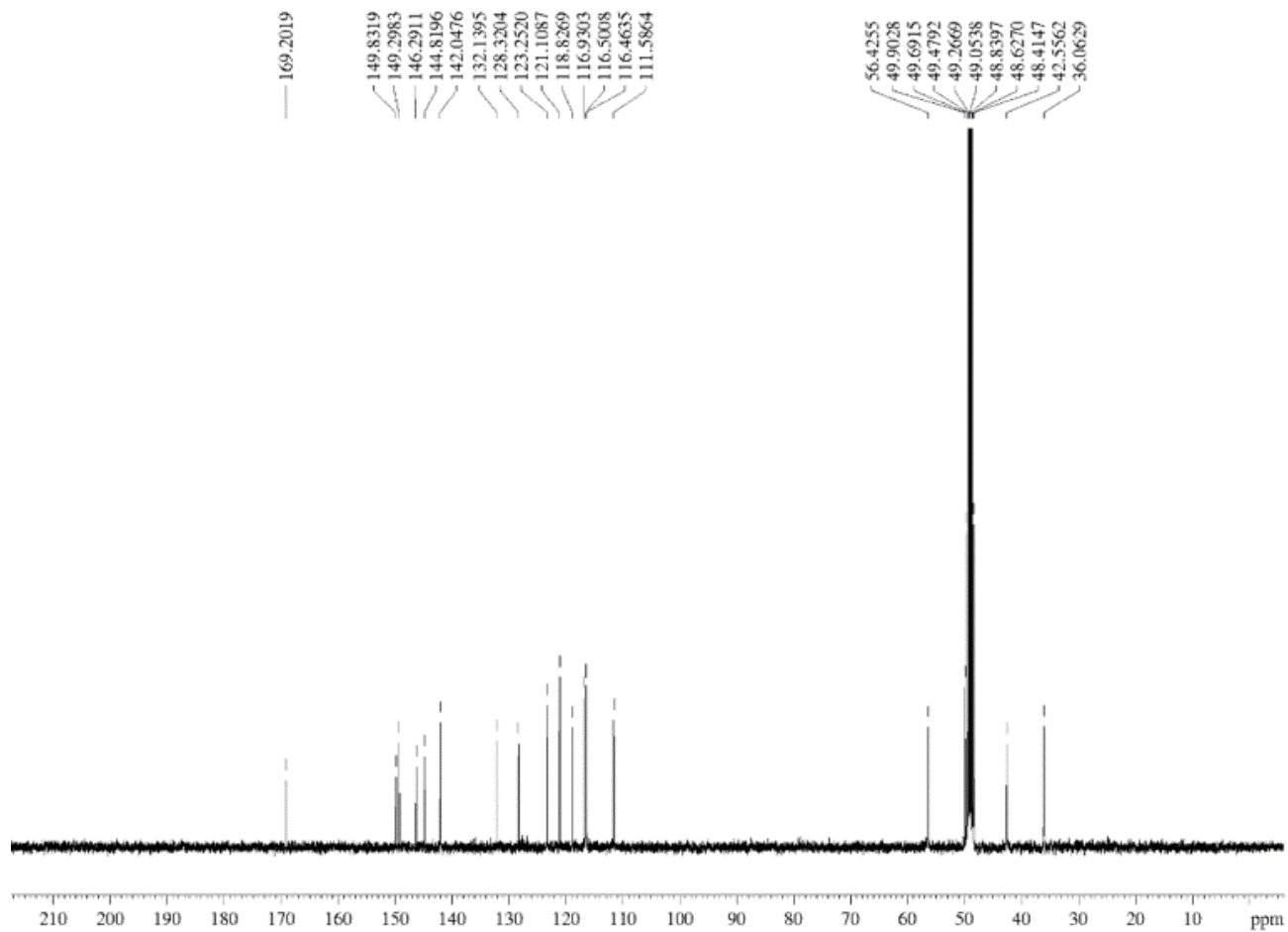


Figure S12. ¹³C NMR spectrum of **25**

N-cis-coumaroyltyramine (**26**)

400 MHz

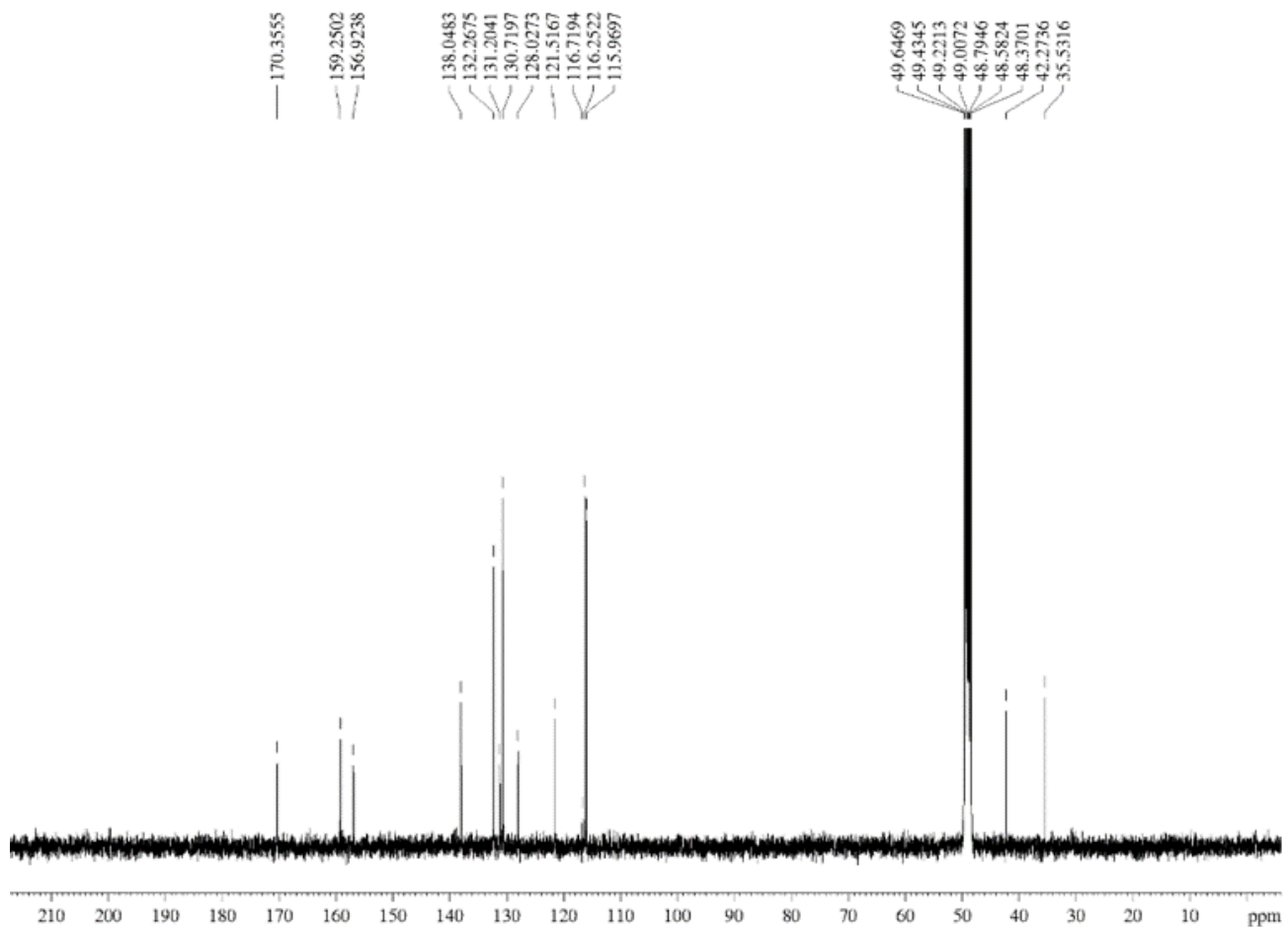


Figure S13. ¹³C NMR spectrum of **26**

N-cis-feruloyltyramine (**30**)

400 MHz

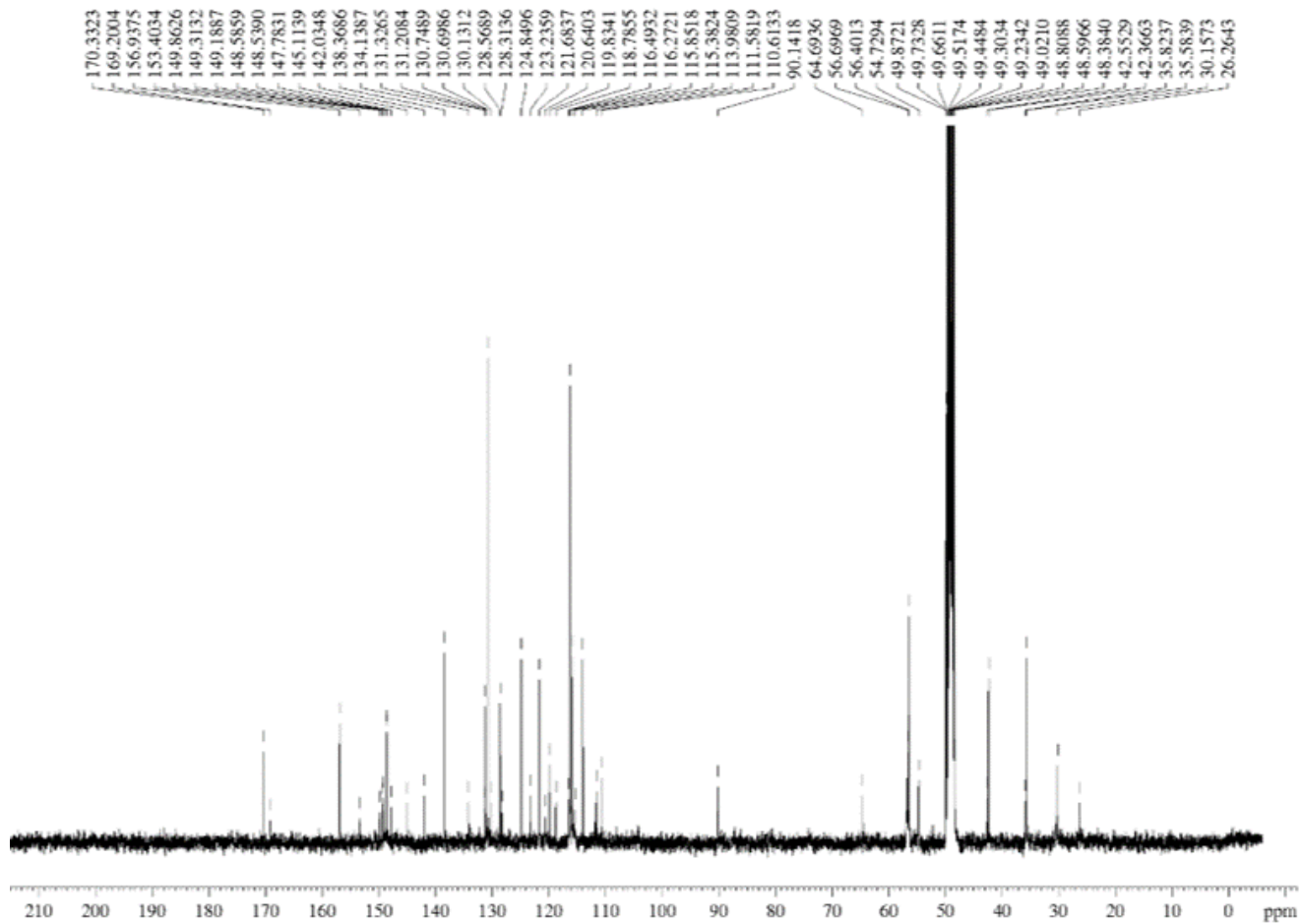


Figure S14. ^{13}C NMR spectrum of **30**

N-trans-feruloyltyramine (31)

400 MHz

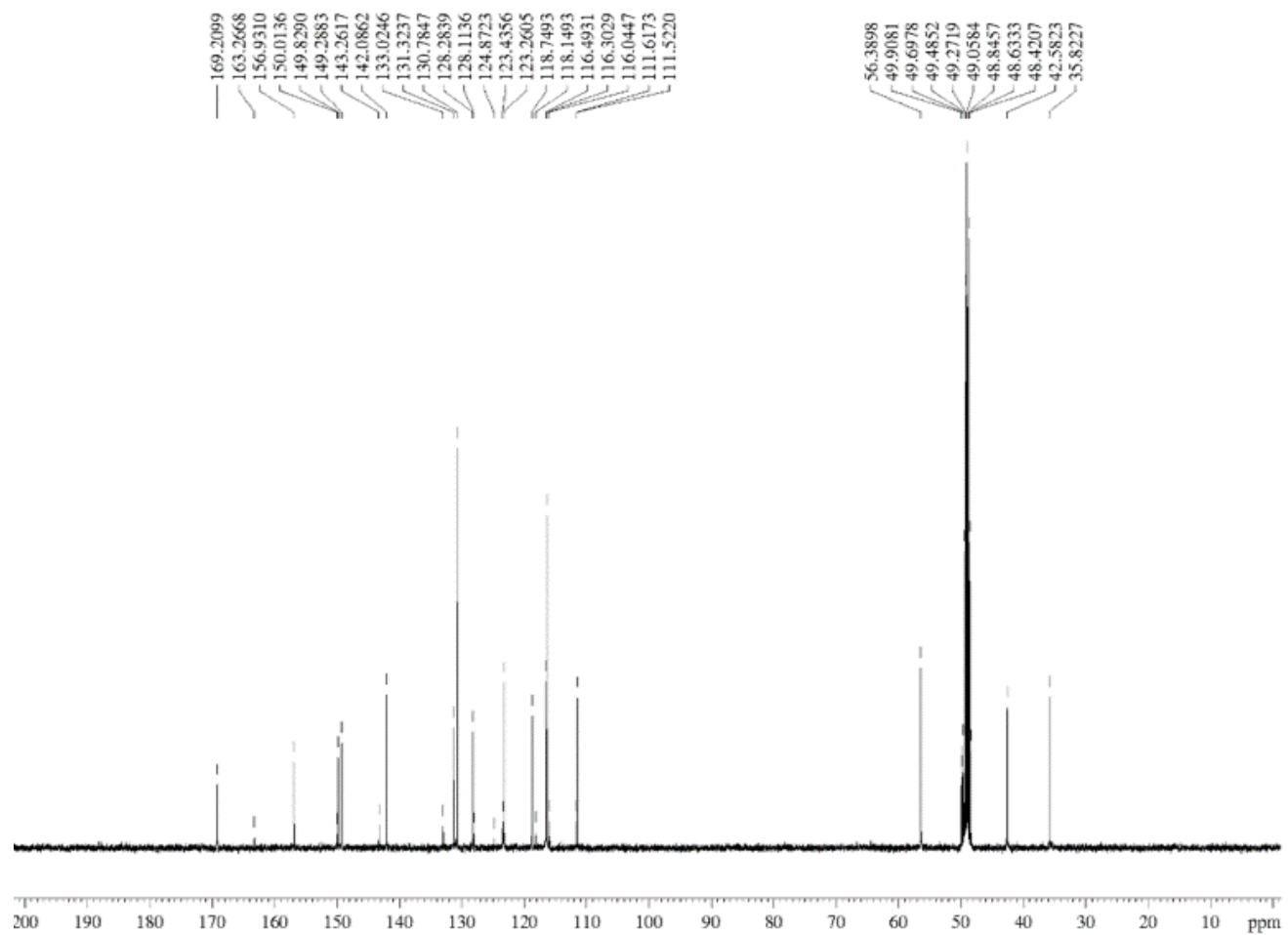


Figure S15. ¹³C NMR spectrum of **31**

3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)-2-methoxyethyl]acrylamide (36)
400 MHz

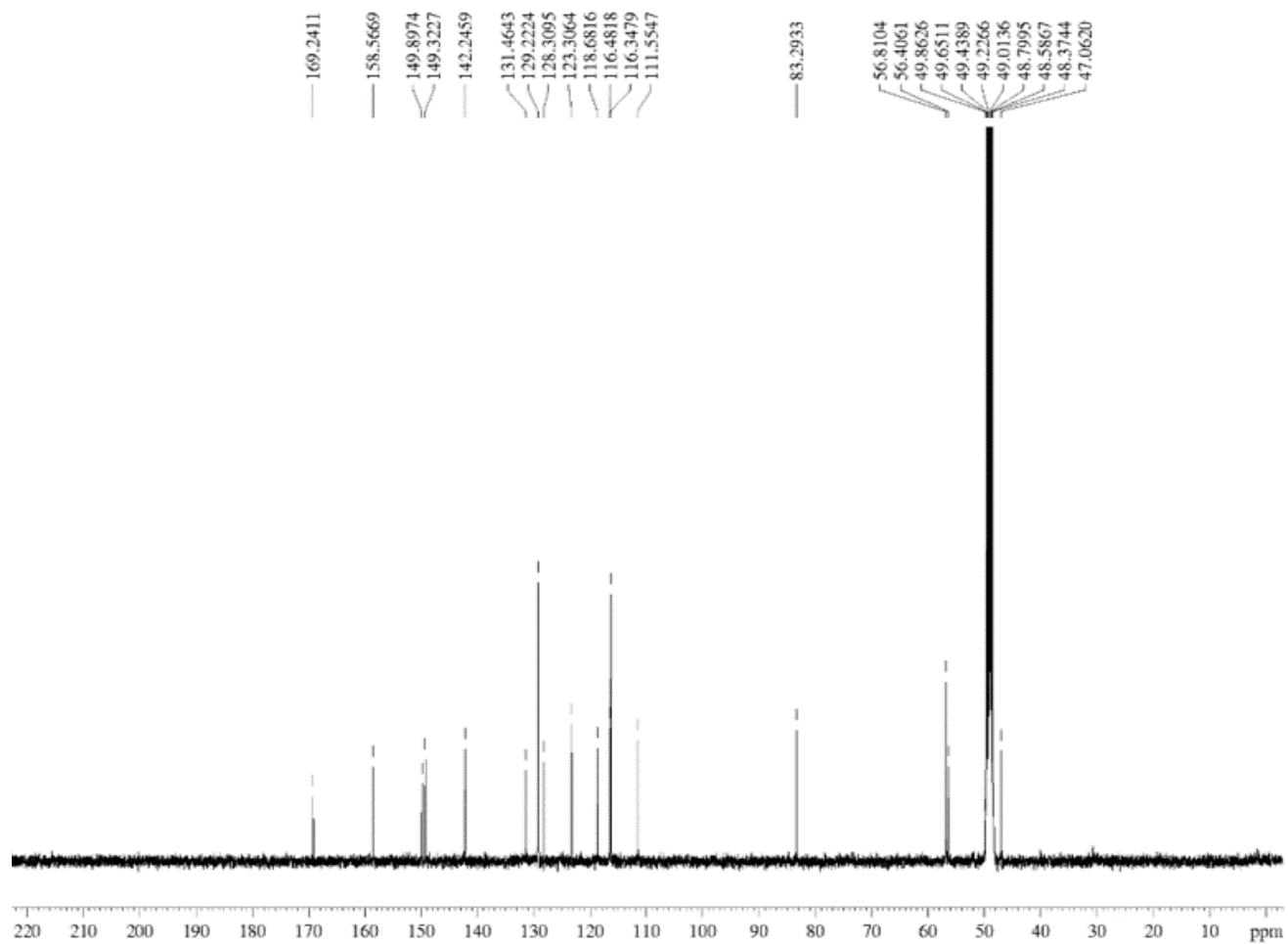


Figure S16. ¹³C NMR spectrum of **36**

cannabinin E (38)

400 MHz

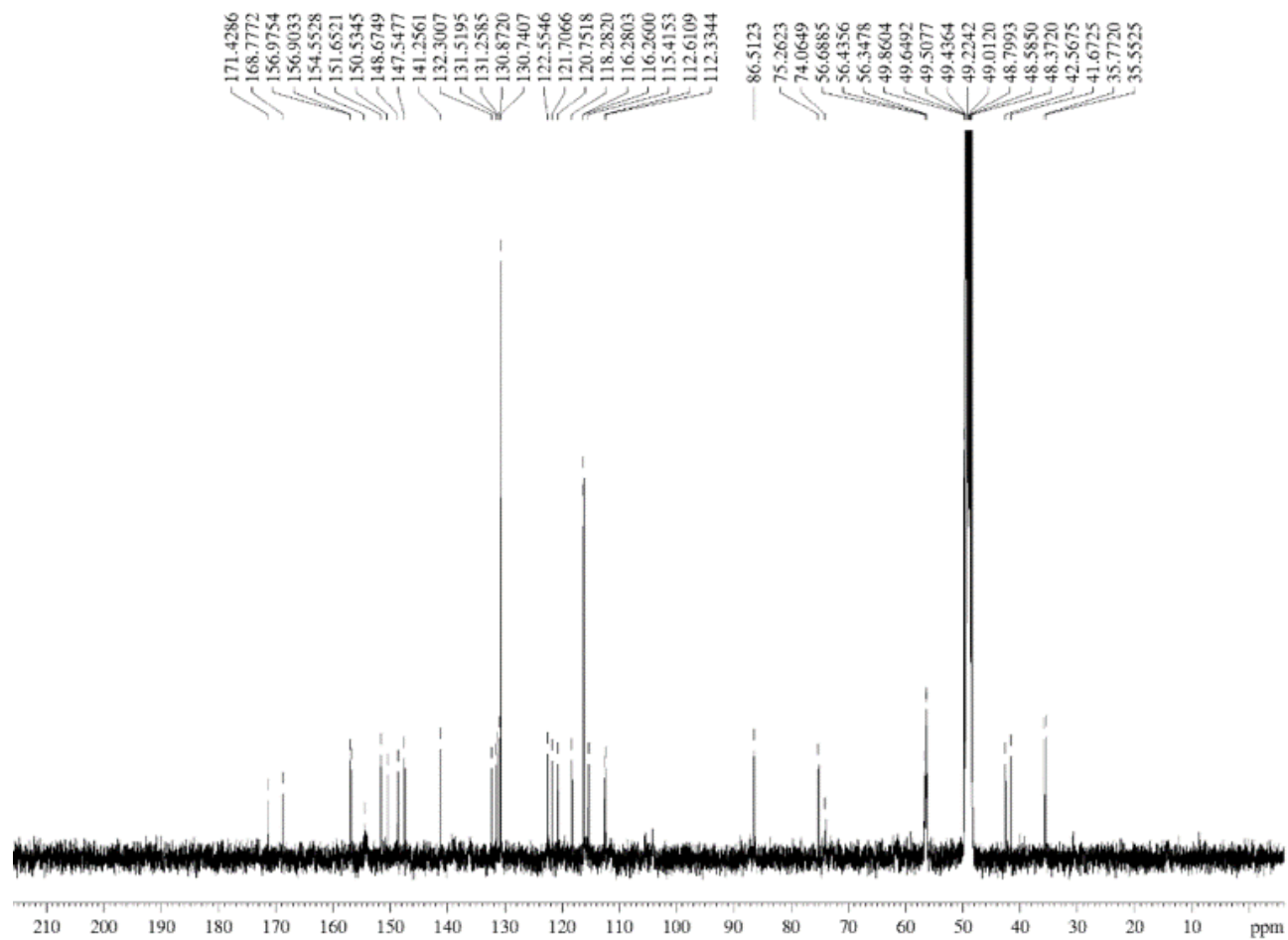


Figure S17. ¹³C NMR spectrum of **38**

lyciumamide B (47)

400 MHz

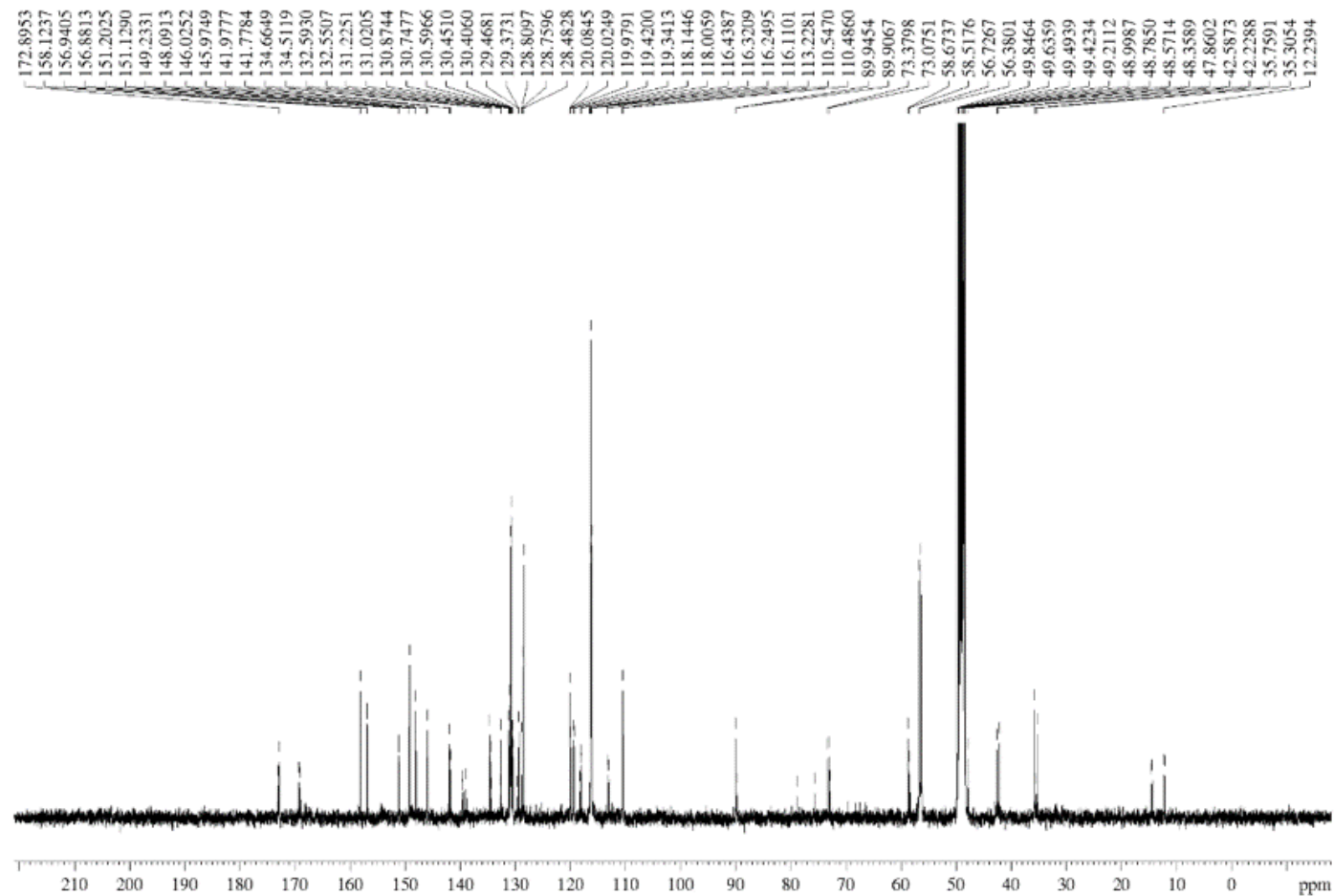


Figure S18. ¹³C NMR spectrum of 47

grossamide (49)

400 MHz

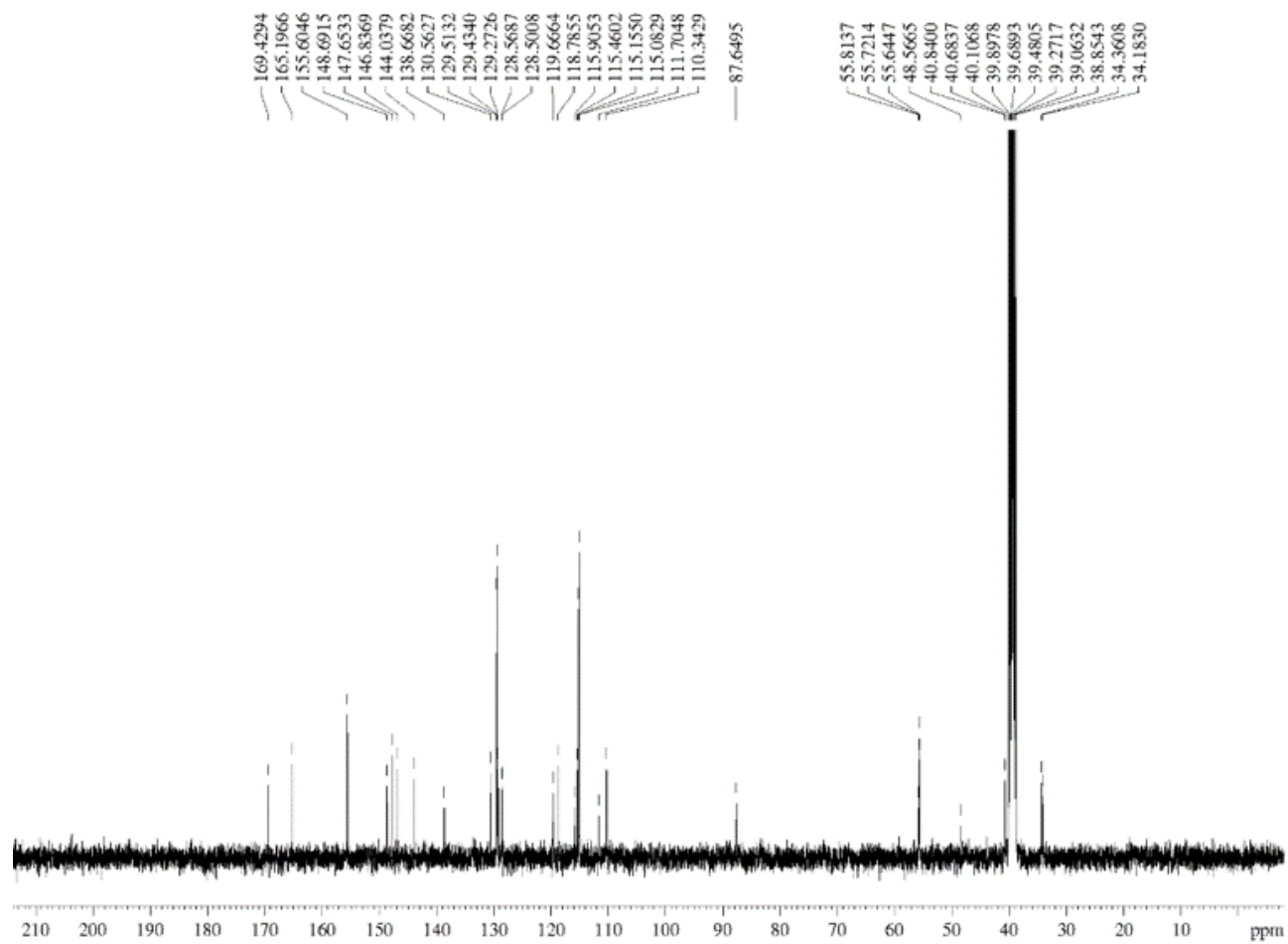


Figure S19. ^{13}C NMR spectrum of **49**

cannabinin D (52)

400 MHz

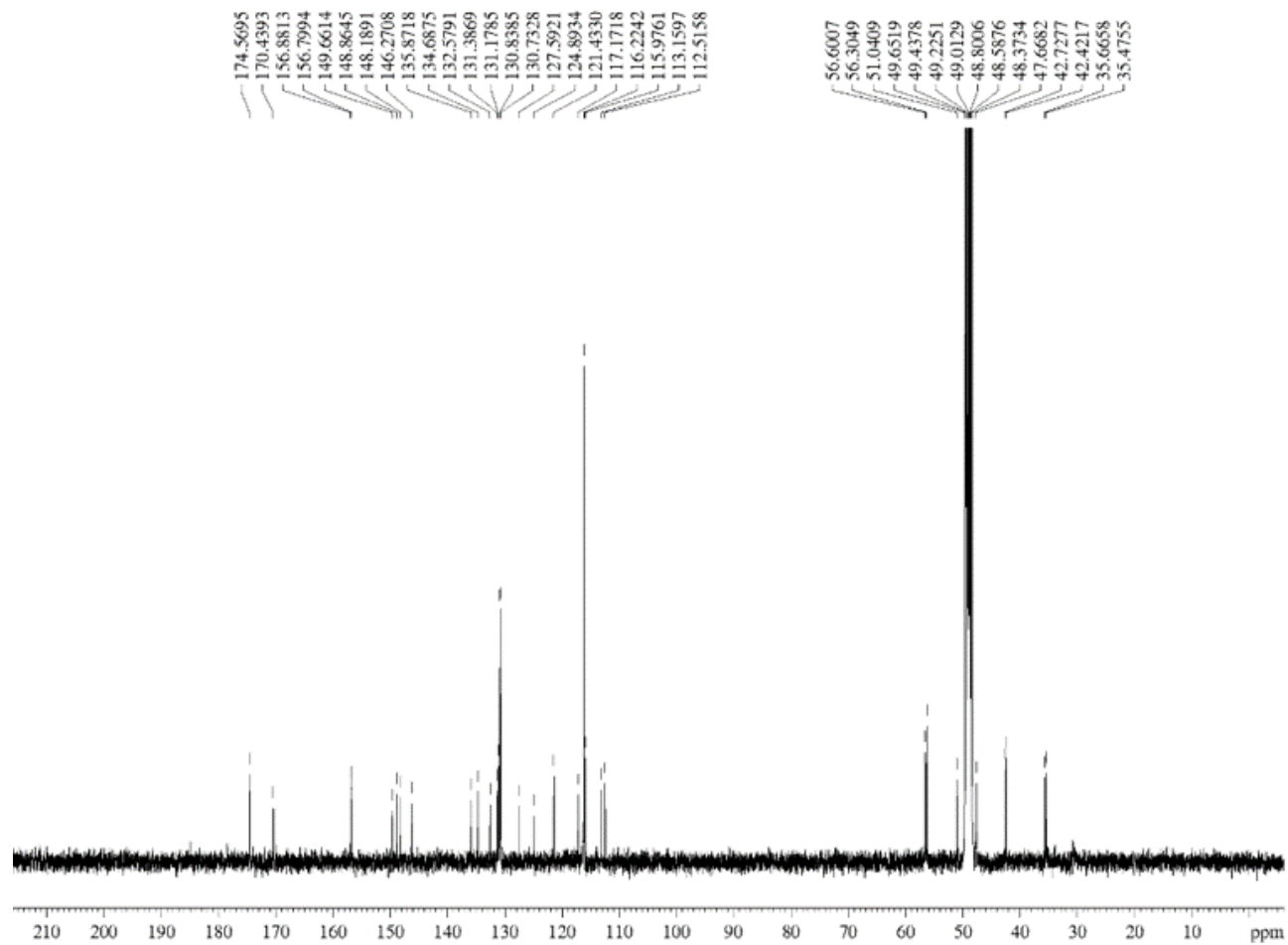


Figure S20. ^{13}C NMR spectrum of **52**

thoreliamide C (55)

400 MHz

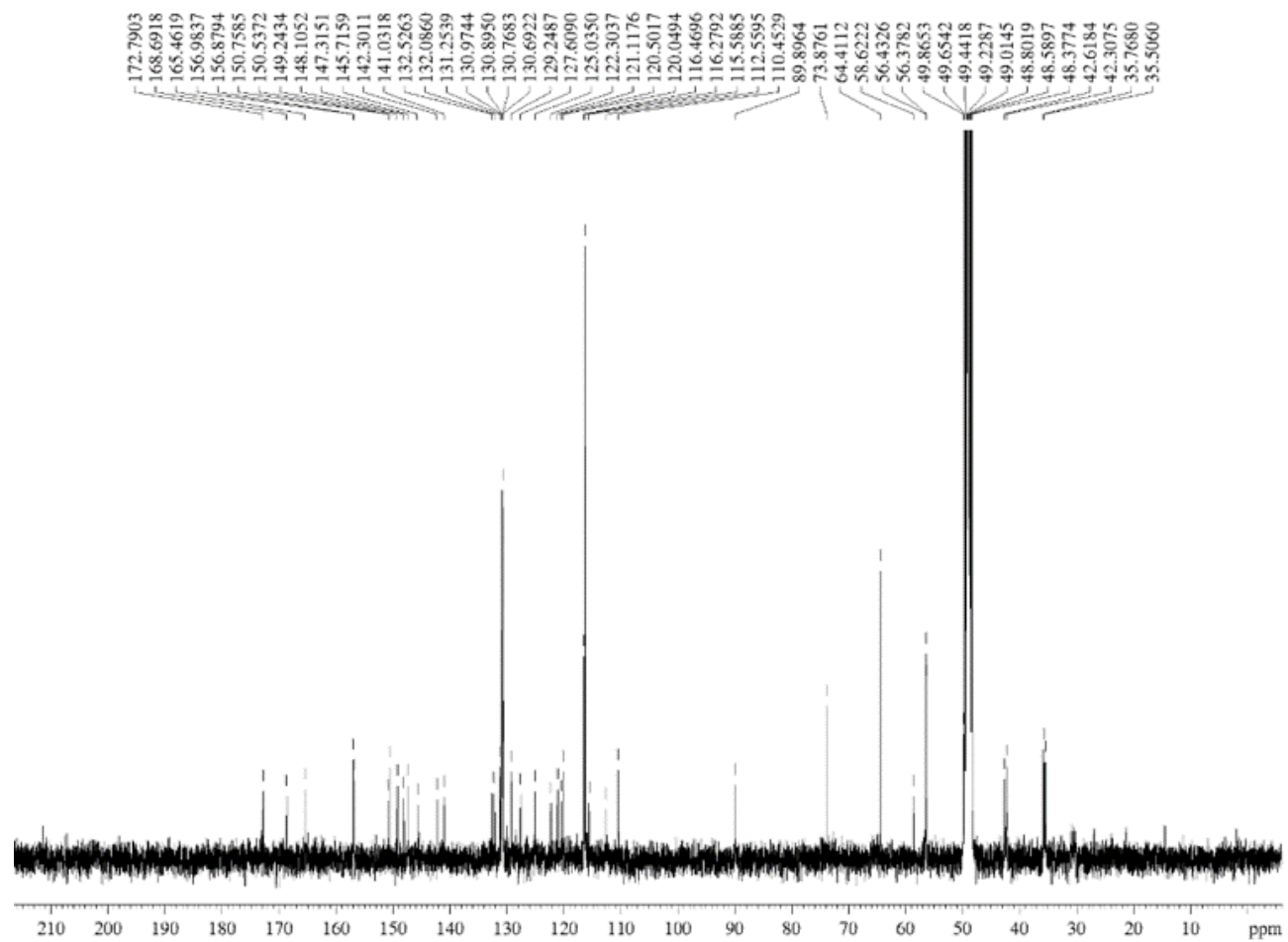


Figure S21. ^{13}C NMR spectrum of **55**

melongenamine B (56)

400 MHz

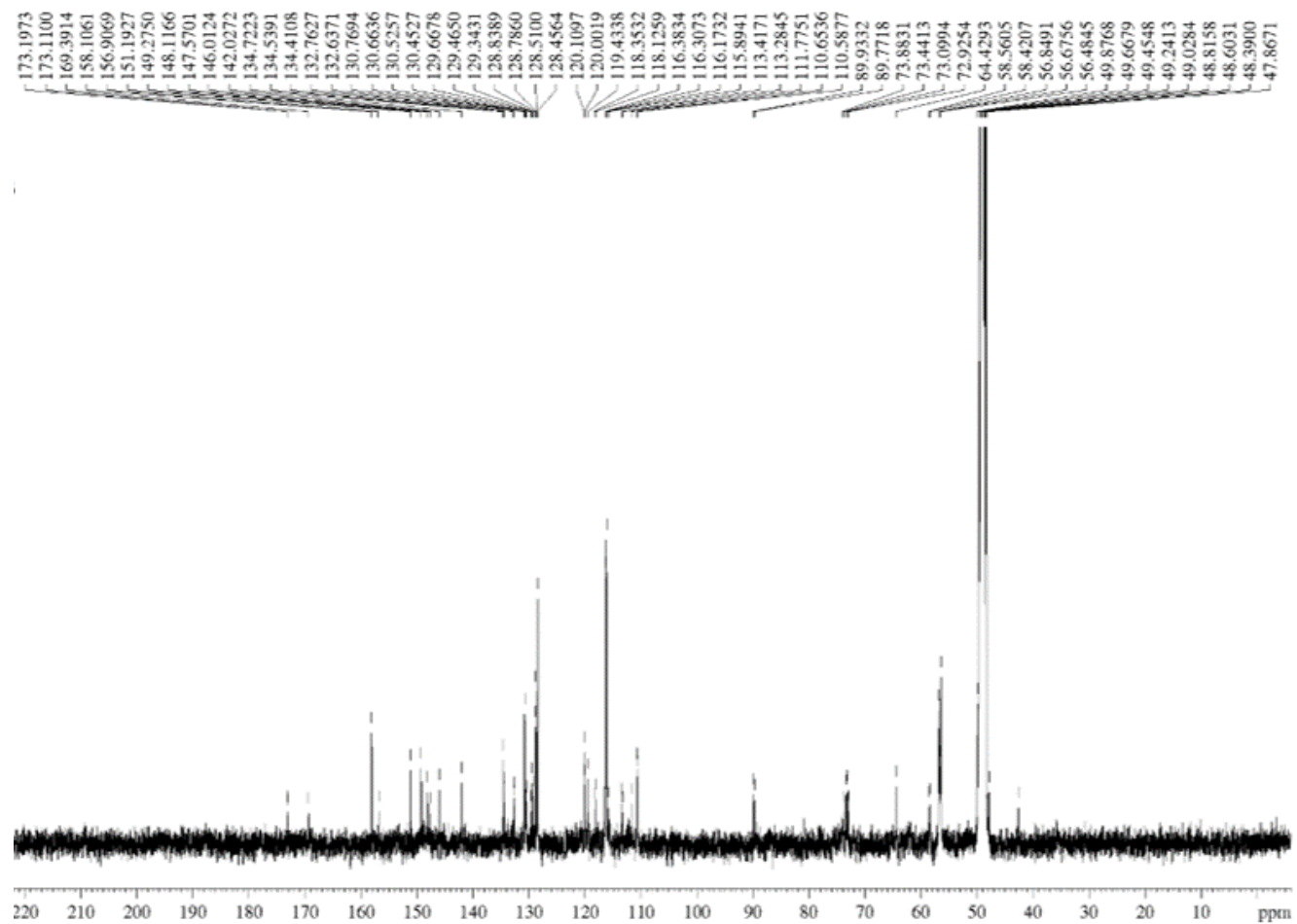


Figure S22. ^{13}C NMR spectrum of **56**

cannabinin L (61)
400 MHz

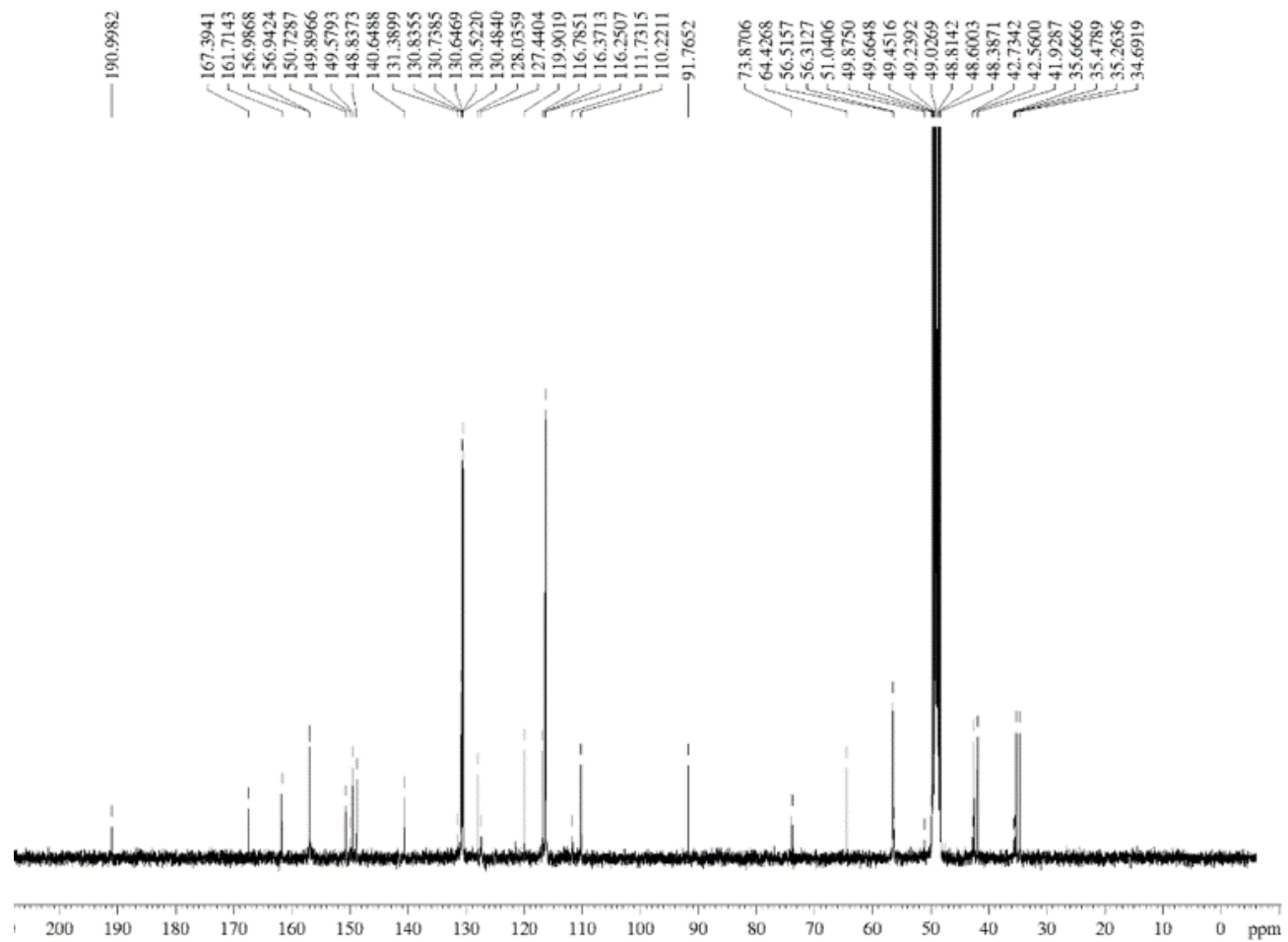


Figure S23. ^{13}C NMR spectrum of **61**

***N*-[2-(3,4-dihydroxyphenyl)-2-hydroxyethyl]-3-(4-methoxyphenyl)prop-2-enamide (62)**
400 MHz

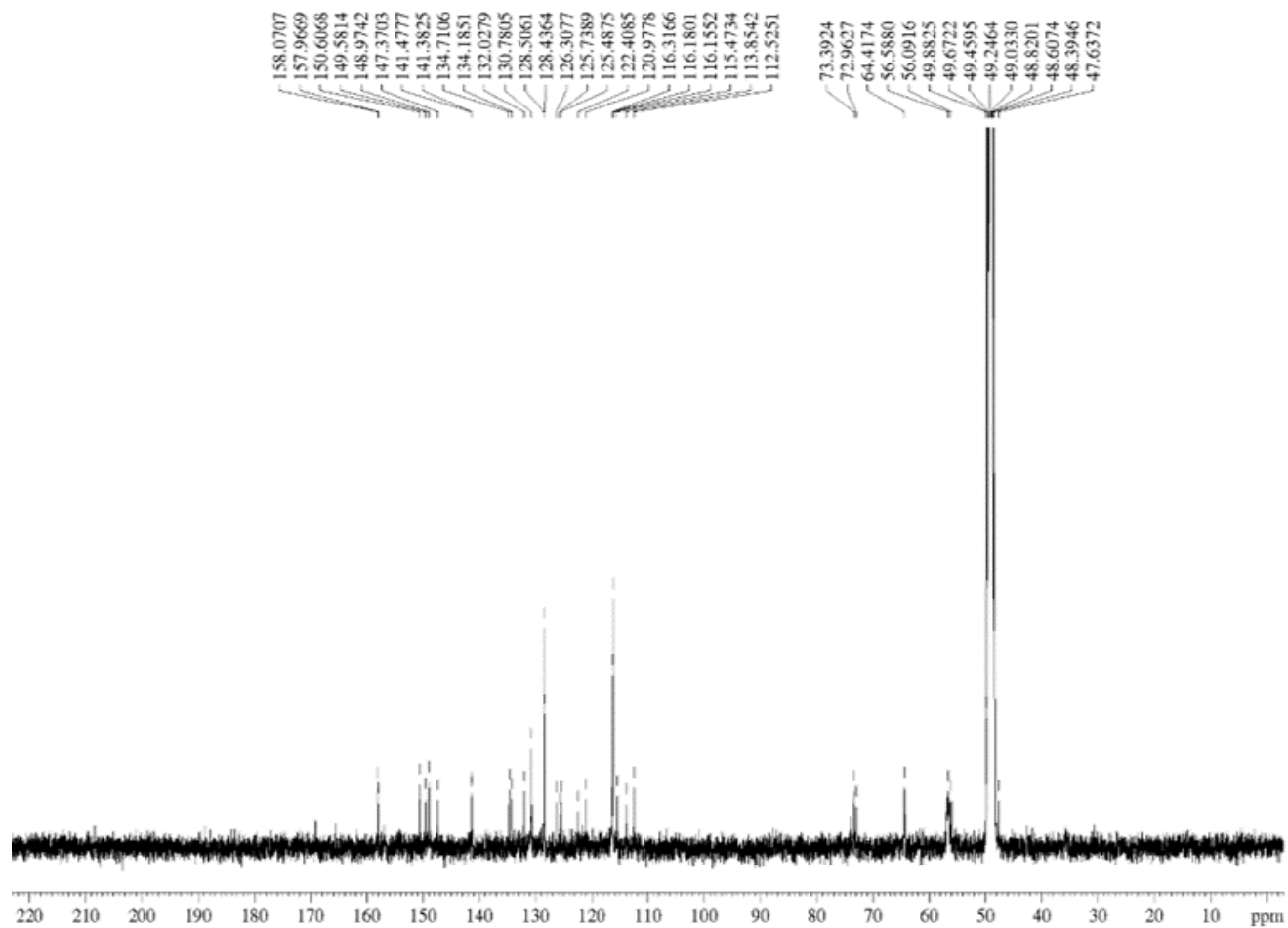


Figure S24. ¹³C NMR spectrum of **62**

chenoalbicin (65)
400 MHz

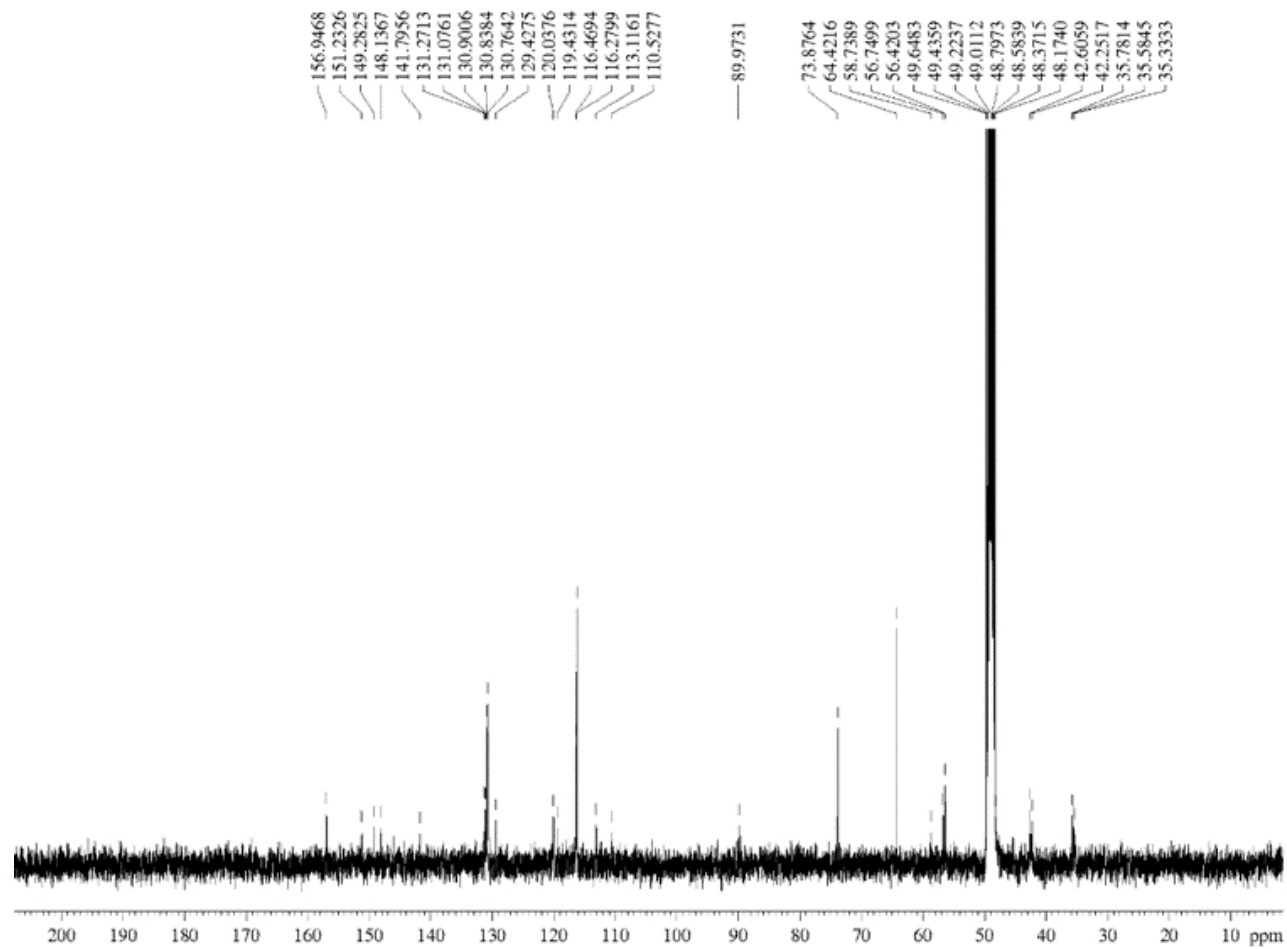
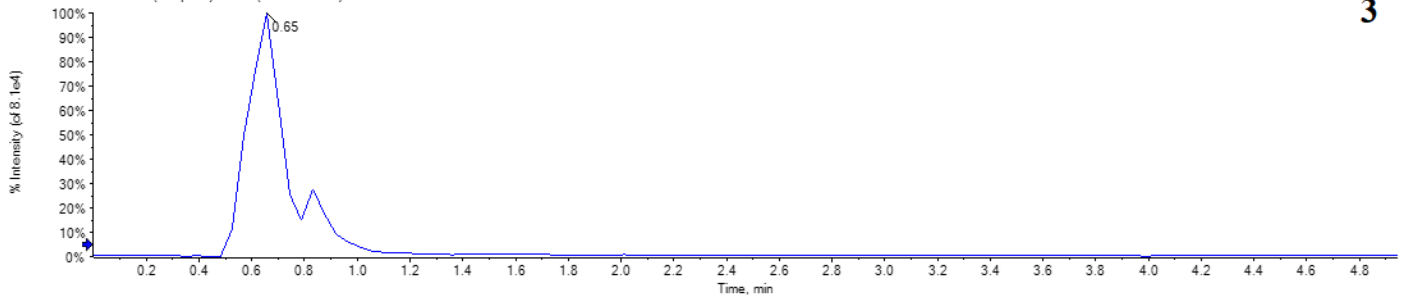


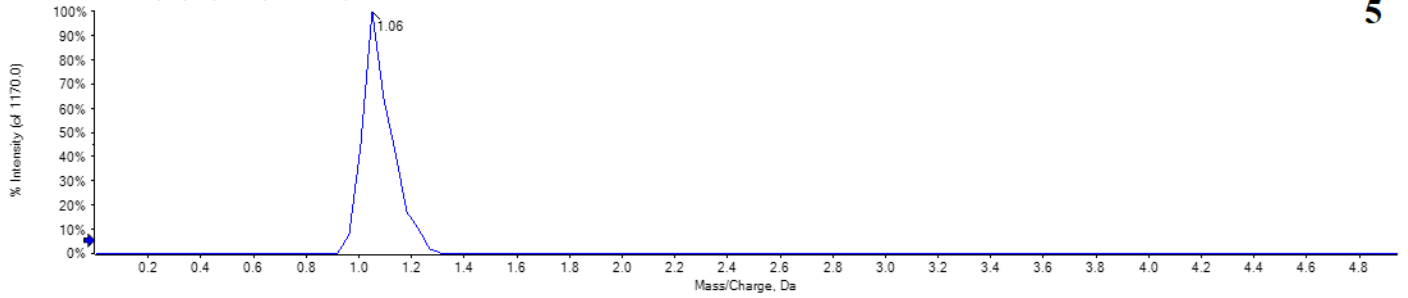
Figure S25. ^{13}C NMR spectrum of **65**

XIC from Datura metel L (sample 1) - MRM (25 transitions): 203.0 / 143.0 Da



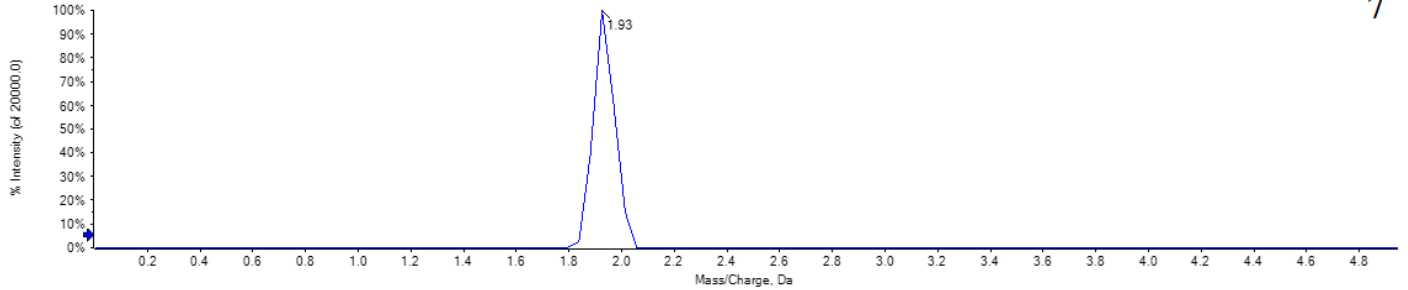
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XIC from Datura metel L (sample 1) - MRM (25 transitions): 166.0 / 124.0 Da



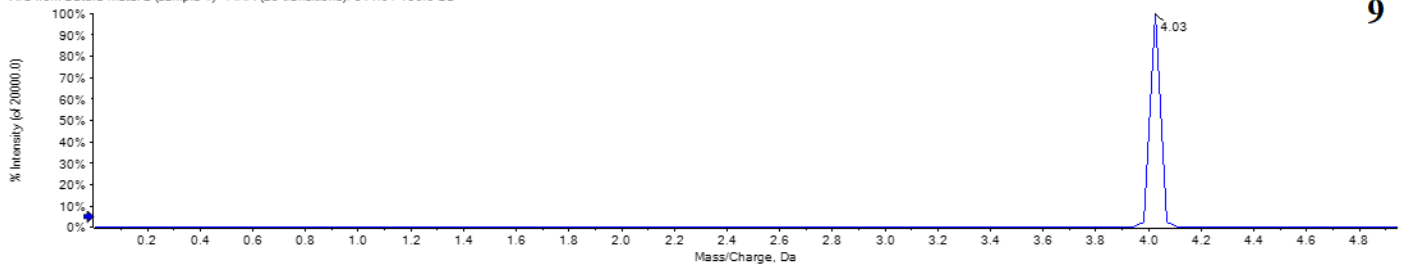
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XIC from Datura metel L (sample 1) - MRM (25 transitions): 231.0 / 158.0 Da



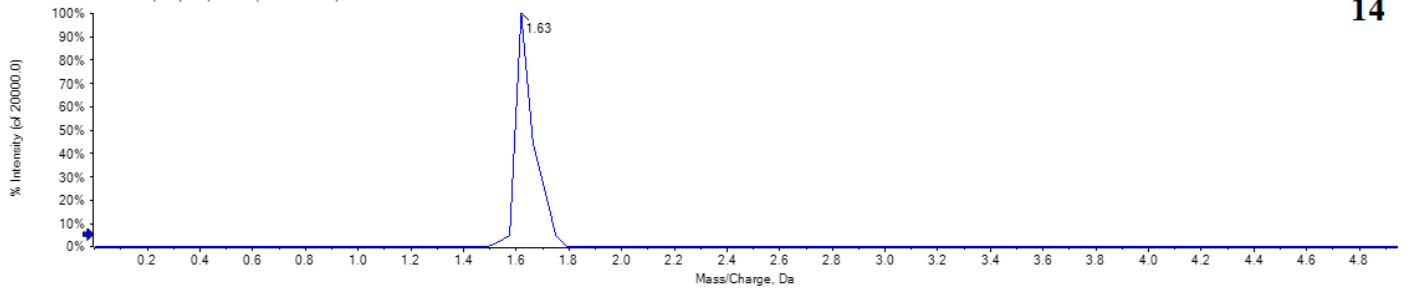
7

XIC from Datura metel L (sample 1) - MRM (25 transitions): 311.0 / 136.0 Da



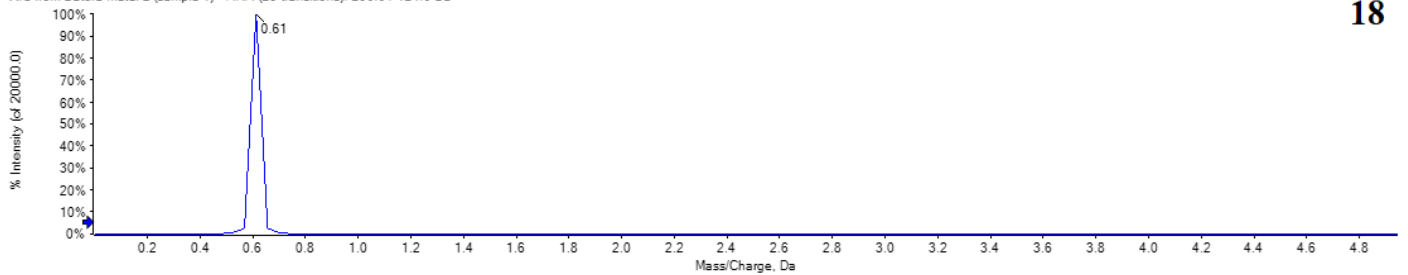
9

XIC from Datura metel L (sample 1) - MRM (25 transitions): 306.0 / 140.0 Da



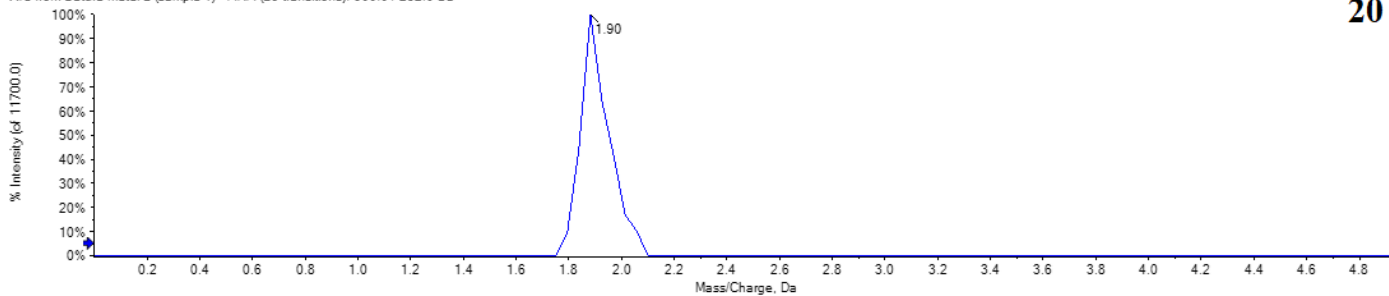
14

XIC from Datura metel L (sample 1) - MRM (25 transitions): 290.0 / 124.0 Da



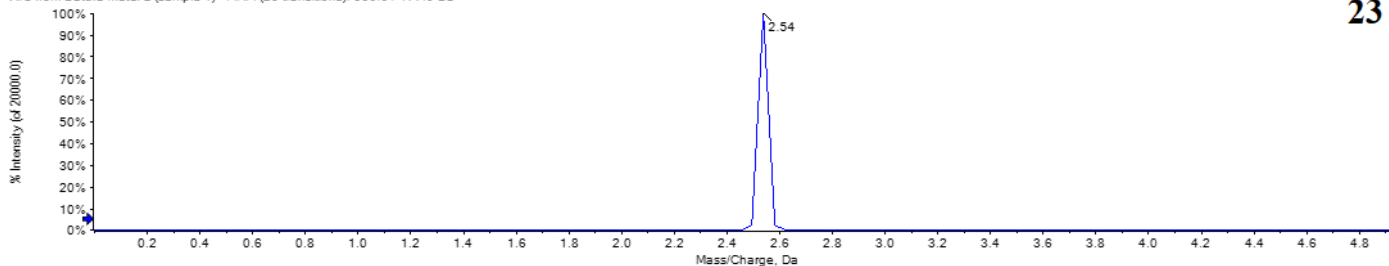
18

XIC from Datura metel L (sample 1) - MRM (25 transitions): 300.0 / 282.0 Da



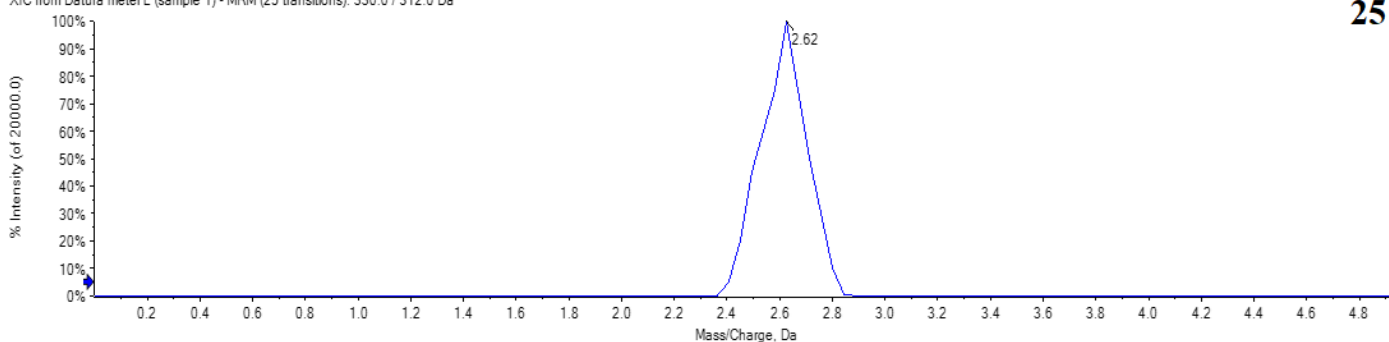
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XIC from Datura metel L (sample 1) - MRM (25 transitions): 330.0 / 177.0 Da



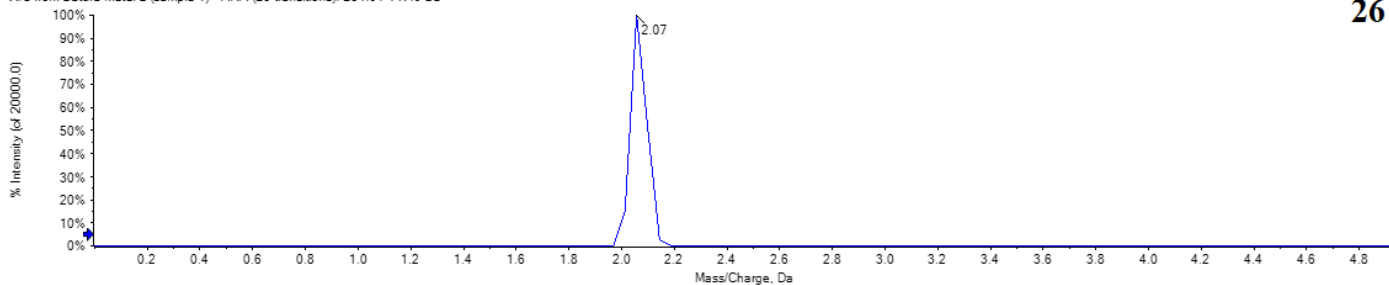
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XIC from Datura metel L (sample 1) - MRM (25 transitions): 330.0 / 312.0 Da



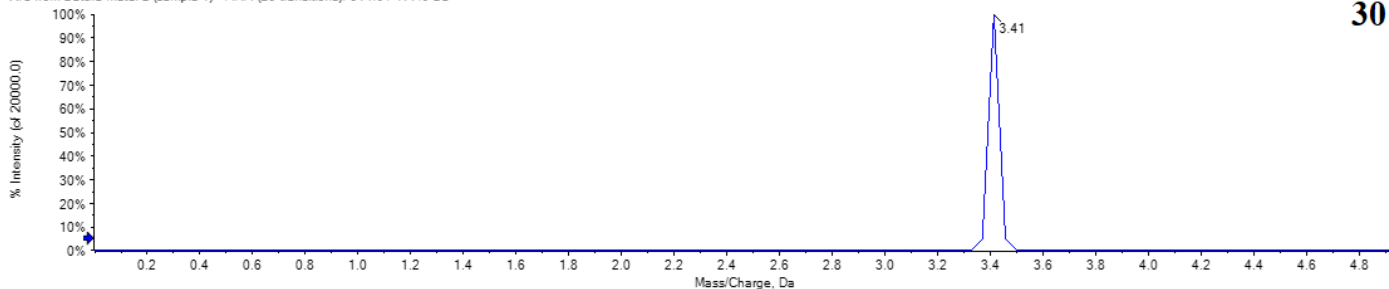
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XIC from Datura metel L (sample 1) - MRM (25 transitions): 284.0 / 147.0 Da



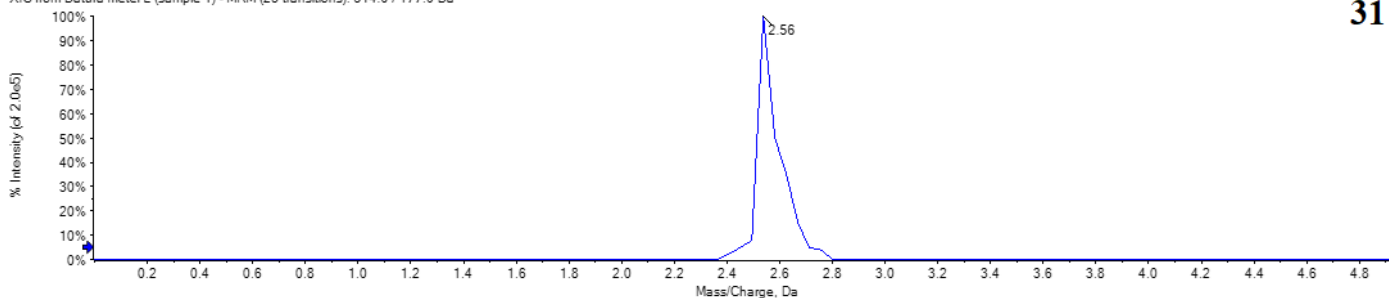
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XIC from Datura metel L (sample 1) - MRM (25 transitions): 314.0 / 177.0 Da



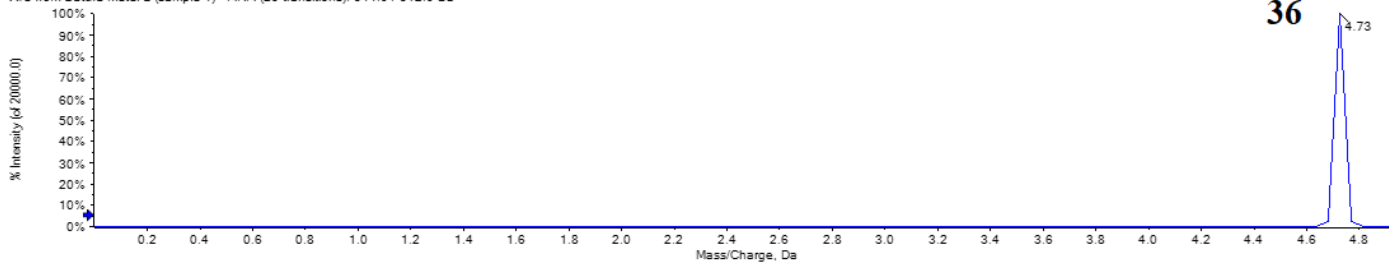
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XIC from Datura metel L (sample 1) - MRM (25 transitions): 314.0 / 177.0 Da



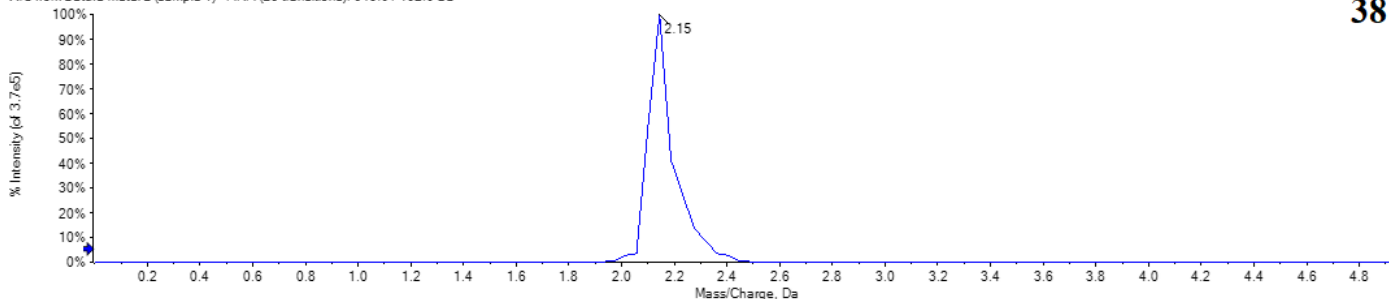
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XIC from Datura metel L (sample 1) - MRM (25 transitions): 344.0 / 312.0 Da



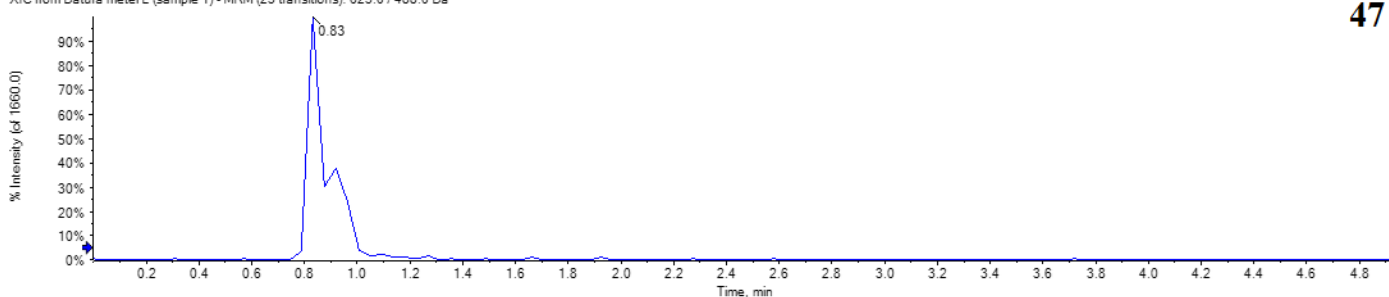
36

XIC from Datura metel L (sample 1) - MRM (25 transitions): 643.0 / 462.0 Da



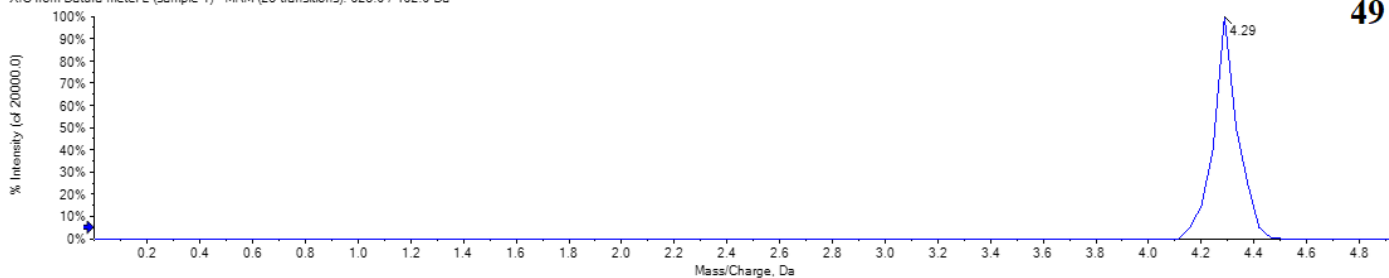
38

XIC from Datura metel L (sample 1) - MRM (25 transitions): 625.0 / 488.0 Da



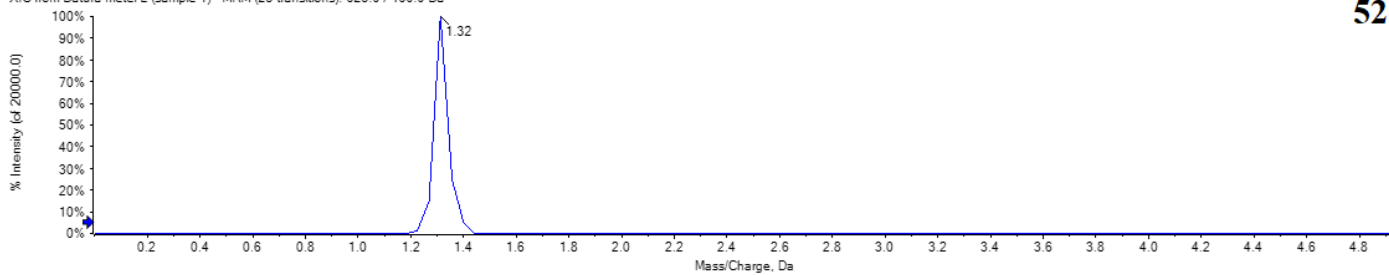
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XIC from Datura metel L (sample 1) - MRM (25 transitions): 625.0 / 462.0 Da



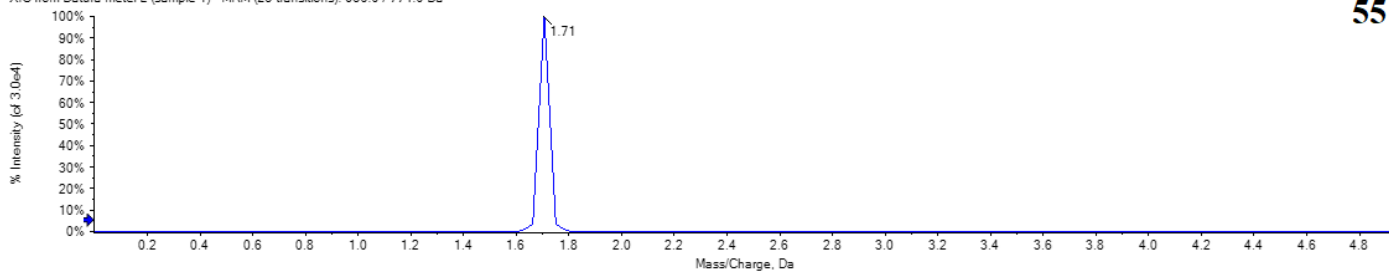
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XIC from Datura metel L (sample 1) - MRM (25 transitions): 625.0 / 460.0 Da



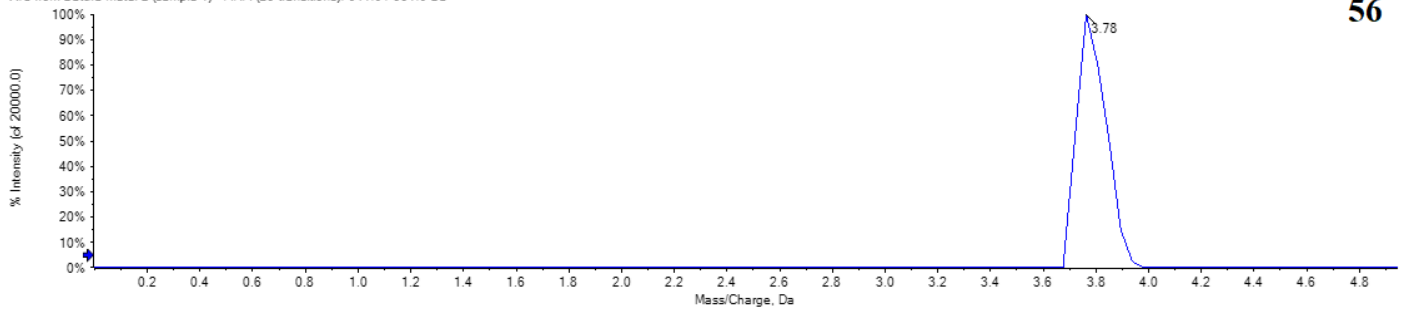
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XIC from Datura metel L (sample 1) - MRM (25 transitions): 936.0 / 774.0 Da



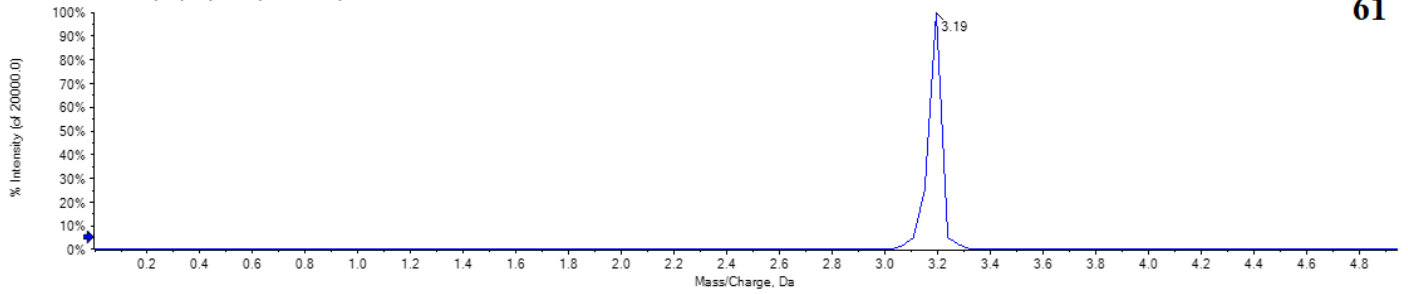
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XIC from Datura metel L (sample 1) - MRM (25 transitions): 641.0 / 351.0 Da



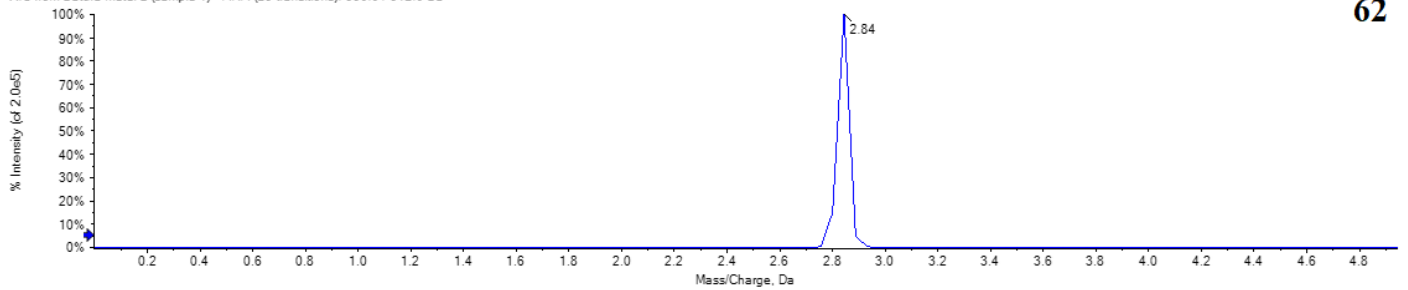
56

XIC from Datura metel L (sample 1) - MRM (25 transitions): 655.0 / 637.0 Da



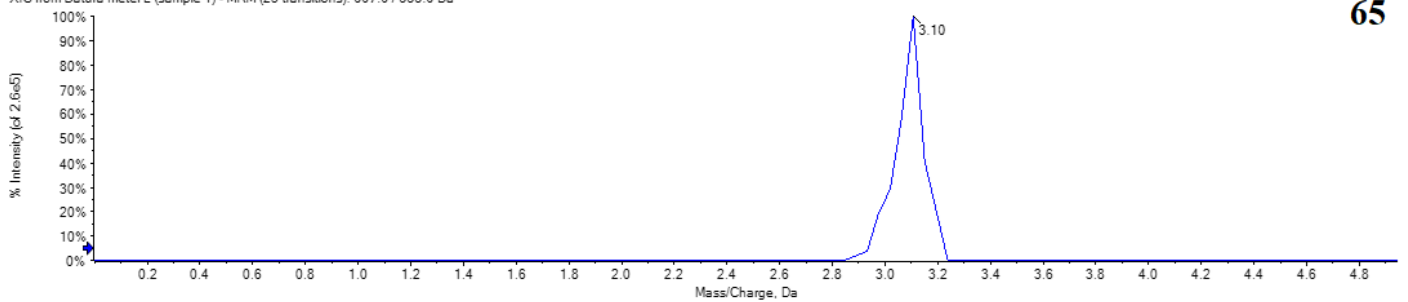
61

XIC from Datura metel L (sample 1) - MRM (25 transitions): 330.0 / 312.0 Da



62

XIC from Datura metel L (sample 1) - MRM (25 transitions): 607.0 / 353.0 Da



65

Figure S26. The MRM chromatograms of 22 quantitative alkaloids

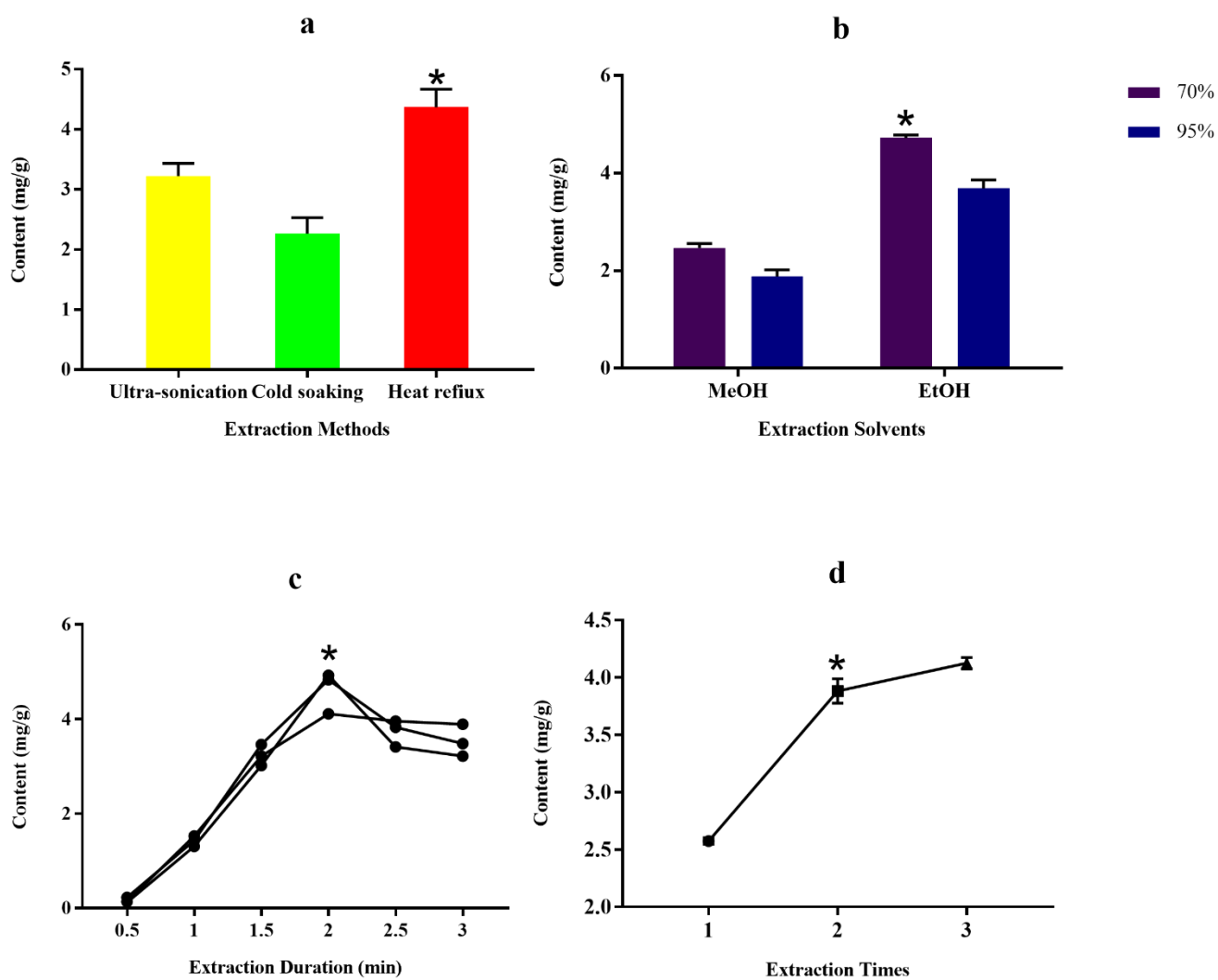


Figure S27. The total alkaloid contents of different extraction conditions: extraction methods (**a**), extraction solvents (**b**), extraction duration (**c**) and extraction times (**d**)

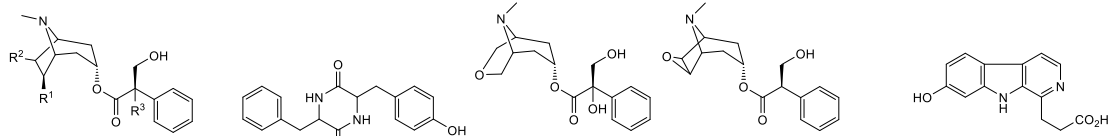
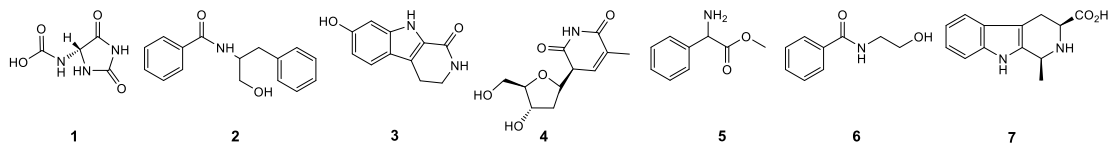
^a (extraction solvent: EtOH; extraction time: 120 min; extraction times: 2)

^b (extraction method: heat reflux; extraction time: 120 min; extraction times: 2)

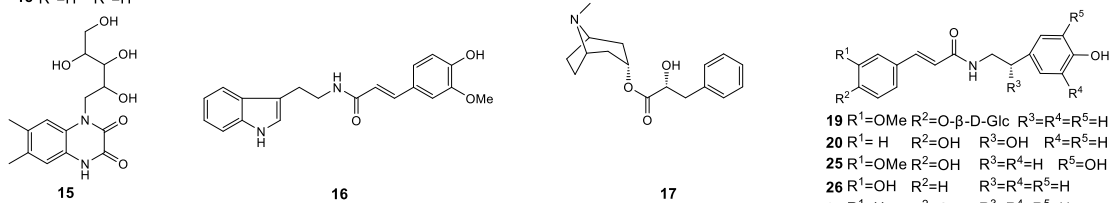
^c (extraction method: heat reflux; extraction solvent: 70% EtOH; extraction times: 2)

^d (extraction method: heat reflux; extraction solvent: 70% EtOH; extraction time: 120 min)

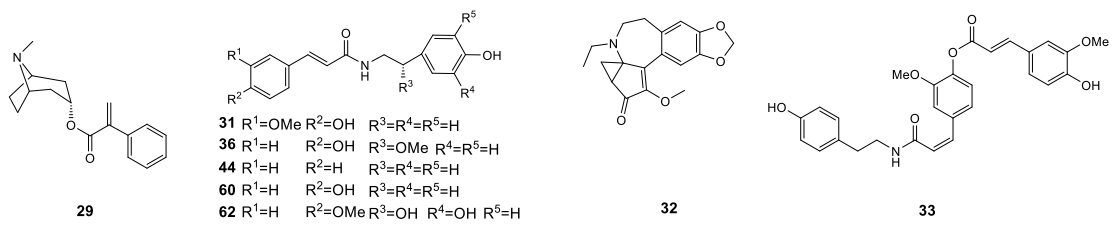
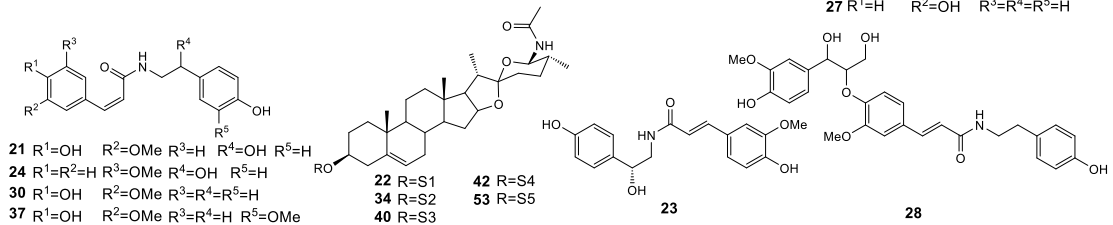
** The best choice of each extraction condition.*



8 R¹=H R²=OH R³=OH
 11 R¹=H R²=H R³=OH
 14 R¹=OH R²=H
 18 R¹=H R²=H



19 R¹=OMe R²=O-β-D-Glc R³=R⁴=R⁵=H
 20 R¹=H R²=OH R³=OH R⁴=R⁵=H
 25 R¹=OMe R²=OH R³=R⁴=H R⁵=OH
 26 R¹=OH R²=H R³=R⁴=R⁵=H
 27 R¹=H R²=OH R³=R⁴=R⁵=H



31 R¹=OMe R²=OH R³=R⁴=R⁵=H
 36 R¹=H R²=OH R³=OMe R⁴=R⁵=H
 44 R¹=H R²=H R³=R⁴=R⁵=H
 60 R¹=H R²=OH R³=R⁴=R⁵=H
 62 R¹=H R²=OMe R³=OH R⁴=OH R⁵=H

49 R¹=OH R²=R³=H
 56 R¹=OH R²=H R³=OH

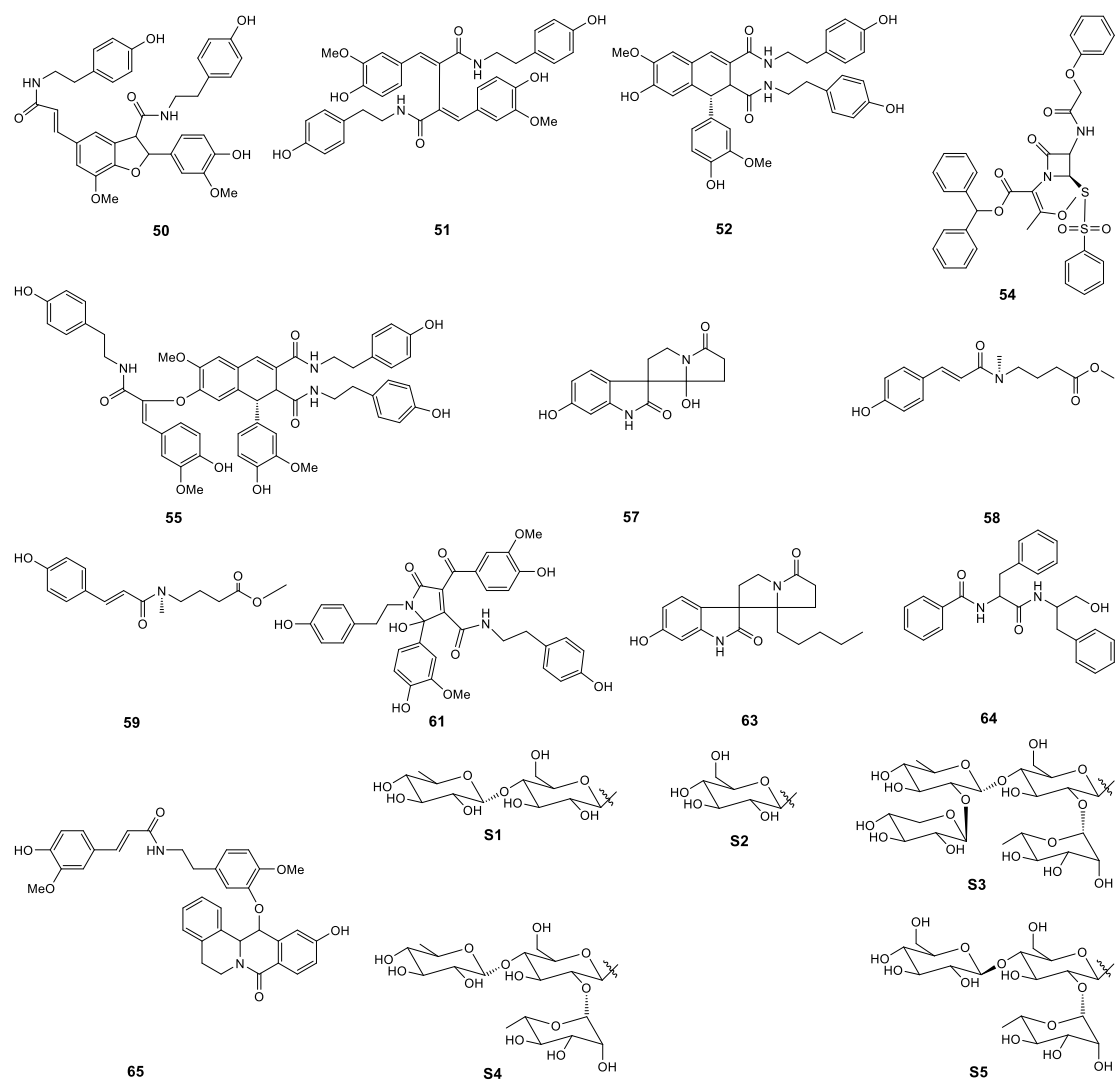


Figure S28. Chemical structures of 65 preliminary identified alkaloids

Table S1. The contents of 22 quantitative alkaloids in *Datura metel* L (*D. metel* L.)

Source (ng/g)	S1-Flower	S1-Seed	S1-Root	S1-Peel	S1-Leaf	S1-Stem	S2-Flower	S2-Seed	S2-Root	S2-Peel	S2-Leaf	S2-Stem
3	30624.77	-	24287.759	19460.115	14631.667	39074.943	13123.161	22778.851	38469.253	5578.851	18856.207	13122.989
5	15956.961	7941.328	2445.266	10477.006	30983.313	4177.19	23517.807	10690.188	5005.697	7023.462	75351.762	5598.105
7	-	-	-	-	82.073	-	-	-	-	-	-	-
9	144.13	38.23	50.648	24.956	92.964	98.144	134.846	62.571	66.407	52.158	135.713	79.578
14	1747.453	2615	41283.402	2912.839	3428.407	54383.469	2120.216	2415.23	5612.558	3847.116	3322.872	3711.717
18	2028.311	4895.037	248.846	22659.328	1249.809	-	9145.957	4975.618	971.742	8909.791	5072.854	9826.921
20	7385.741	961.981	999.484	497.843	23354.361	1291.345	117518.831	1676.667	4207.665	10564.158	12206.304	1544.768
23	38.87	127.537	40.925	18.022	37.673	24.657	30.736	26.415	82.538	37.758	55.566	140.035
25	100.466	938.154	69.181	75.809	90.322	58.646	73.821	126.514	424.213	221.759	89.916	158.33
26	344.416	205.471	681.405	368.245	217.643	627.028	180.654	100.454	681.602	163.582	193.853	276.169
30	1270.267	6028.68	907.246	6083.27	1487.257	385.547	274.565	2472.169	1364.543	10511.306	1044.59	2868.932
31	4256.268	22598.183	3046.609	22373.717	5060.575	1060.475	659.869	8631.836	4837.119	37907.959	3351.001	9731.617
36	43.188	57.189	34.817	31.961	38.439	40.269	49.948	38.689	77.549	37.282	67.284	410.78
38	2785.461	20278.118	4719.146	38966.049	957.038	1914.894	330.537	9782.478	5390.785	53463.525	1655.842	2270.317
47	4501.846	11628.705	4508.412	36741.756	2767.171	2809.569	2260.001	8013.541	5093.192	38974.39	2958.205	3268.413
49	187.46	1095.789	265.034	2896.96	85.253	162.264	42.974	677.852	332.941	2958.447	118.491	191.305
52	793.828	3568.012	879.832	11112.491	275.986	357.301	102.954	2047.447	1057.964	11817.67	349.738	458.093
55	166.912	515.29	217.279	1496.654	232.393	141.725	192.097	504.386	126.618	1426.138	287.804	40.987
56	145.761	2419.28	151.424	604.528	-	-	100.45	423.285	666.813	479.926	151.422	293.012
61	986.422	8317.949	1420.542	10003.192	606.55	660.808	276.624	2919.913	1448.654	15256.036	897.417	1023.356
62	244.331	3225.631	109.194	106.273	425.743	100.064	275.945	298.658	1022.268	141.432	490.138	1176.977
65	-	-	4335.873	-	-	3919.524	-	585.873	21420.556	5586.349	-	3086.111

Source (ng/g)	S3-Flower	S3-Seed	S3-Root	S3-Peel	S3-Leaf	S3-Stem	S4-Flower	S4-Seed	S4-Root	S4-Peel	S4-Leaf	S4-Stem
3	24891.724	3617.414	31830.92	15235.287	27004.54	6484.023	29418.046	4673.678	27305.805	17648.621	11915.805	19459.598
5	28887.618	3905.028	5551.324	9351.288	91038.385	3529.65	12768.71	8301.368	5627.121	8489.678	10680.121	4128.928
7	-	-	-	-	144.433	-	-	-	-	-	-	-
9	141.109	-	50.215	45.466	116.713	62.307	174.143	35.535	59.284	63.386	108.725	61.227
14	2589.171	4975.514	4605.435	2893.467	2875.306	3036.736	2216.872	5934.208	3344.463	2252.387	2225.751	2077.841
18	16645.03	27678.125	1082.947	3196.037	8089.563	8437.458	2431.377	40245.242	1569.529	4989.515	11912.703	1597.355
20	187550.296	1073.725	2800.402	2179.091	9129.512	1871.497	26165.824	1610.633	56400.708	2606.933	4224.333	5306.483
23	37.758	23.331	106.898	58.821	50.429	158.827	43.71	32.533	41.267	25.942	51.672	124.275
25	75.715	96.949	104.116	124.567	109.581	184.161	76.62	93.311	82.693	88.536	67.044	133.764
26	229.261	179.765	234.537	203.416	650.383	357.022	495.71	217.663	252.853	162.752	-	408.02
30	334.203	13912.915	1336.928	3415.384	1512.677	3514.232	614.973	16131.277	1038.83	4017.249	340.732	2261.397
31	881.272	49016.827	4537.271	11900.219	5285.041	12685.681	1952.919	59402.154	3412.923	14116.608	900.017	7842.336
36	52.079	35.325	71.989	67.31	78.03	328.297	72.813	45.554	47.615	41.676	57.707	63.714
38	607.651	56836.631	4457.1	17496.108	2303.359	2692.07	836.568	75138.605	4234.061	25111.069	1071.522	3866.691
47	2442.871	44744.099	4621.109	12720.708	3717.762	3657.811	2806.304	54689.792	4444.344	17596.12	2726.174	4273.258
49	56.497	3466.065	288.453	1062.172	142.901	232.583	75.857	3835.473	257.351	1424.314	96.358	250.807
52	178.024	13849.652	897.192	3571.83	570.994	583.477	285.631	16691.977	840.648	5122.215	265.448	702.896
55	237.429	1740.928	202.16	600.084	40.987	40.987	121.578	1869.39	182.024	982.898	217.281	197.132
56	26.822	451.609	819.737	655.493	219.392	355.317	140.098	474.256	276.027	298.68	-	219.383
61	267.941	17429.108	1926.23	4244.493	1887.369	819.299	1005.948	19628.473	1062.376	5633.731	1196.988	821.437
62	302.918	119.721	1411.887	394.712	540.004	1374.129	255.945	126.156	227.38	152.203	192.407	346.932
65	-	-	20170.556	7253.492	-	-	585.873	-	13503.651	-	4336.27	5169.762

Source (ng/g)	S5-Flower	S5-Seed	S5-Root	S5-Peel	S5-Leaf	S5-Stem	S6-Flower	S6-Seed	S6-Root	S6-Peel	S6-Leaf	S6-Stem
3	17045.862	2561.207	22175.172	6635	20365.805	10708.966	21119.885	4371.782	6785.805	7992.989	18252.931	11010.402
5	30234.216	3471.262	4231.61	4015.764	48313.804	4540.191	9494.001	10585.373	4228.531	3936.827	38213.727	6353.716
7	-	-	-	-	110.974	-	-	-	-	-	100.325	-
9	163.345	17.832	63.169	31.865	143.539	30.785	108.077	-	64.897	64.465	124.269	34.455
14	1996.036	4100.36	6341.416	1982.274	3509.122	3990.789	1273.191	8202.303	5924.522	7272.667	2998.195	3479.863
18	3821.345	6074.207	2507.76	1013.452	2083.794	415.669	485.2	10911.379	1221.965	3460.217	1805.891	1034.302
20	62025.166	251.818	7224.163	767.33	28319.069	4402.069	24097.621	2312.521	20108.337	613.941	20991.915	6345.091
23	69.61	15.154	89.13	39.64	16.738	72.219	66.697	13.367	45.592	51.456	22.039	83.008
25	97.003	56.603	102.209	75.173	61.675	118.833	83.044	116.288	74.551	68.816	67.302	358.827
26	441.887	-	1397.133	253.11	114.904	775.003	18.156	110.802	1110.273	30.66	186.997	863.701
30	830.335	431.35	2269.627	1463.025	344.645	1997.224	1513.409	15001.064	1851.65	1047.516	539.177	2329.064
31	2631.129	1256.638	7962.14	5082.45	941.444	6749.958	4974.087	55145.045	6610.298	3364.799	1601.346	7927.814
36	90.596	36.08	116.29	54.723	45.128	61.62	41.846	36.808	49.503	47.032	60.9	66.152
38	1776.338	1198.013	11270.317	8830.665	1101.634	3559.44	3336.631	74305.654	9595.695	5776.283	902.836	3583.534
47	3216.803	2787.669	7215.792	6702.534	2620.168	3570.44	3899.141	64220.193	6407.571	5064.796	2618.074	3925.052
49	121.408	109.306	631.439	456.505	84.543	200.983	236.14	4180.916	456.923	260.485	81.268	240.413
52	424.434	293.569	1734.403	1439.221	222.467	518.232	655.709	19816.662	1419.125	1067.4	253.102	612.023
55	187.059	146.759	207.199	166.908	252.546	171.946	232.395	1552.075	187.058	192.09	297.875	166.908
56	202.398	-	661.161	366.639	145.757	242.046	168.413	372.313	372.309	632.845	117.442	242.045
61	1123.177	1164.425	2538.414	1954.508	1915.482	615.215	982.069	19777.302	1691.907	1843.878	2184.697	680.336
62	705.99	91.986	900.9	362.784	235.048	686.954	334.735	135.104	414.241	414.443	285.699	704.488
65	1002.778	-	11420.238	9753.73	-	-	10586.429	1418.968	5586.667	4752.857	6002.778	5169.444

Source (ng/g)	S7-Flower	S7-Seed	S7-Root	S7-Peel	S7-Leaf	S7-Stem	S8-Flower	S8-Seed	S8-Root	S8-Peel	S8-Leaf	S8-Stem
3	19158.218	5579.023	26400.057	13726.494	24590.345	17800.115	58085.805	-	20667.126	9200.057	14631.839	11311.494
5	40639.853	9703.038	5789.376	5620.015	87858.424	6041.049	30691.964	2947.309	15174.702	6377.403	13665.257	1094.286
7	-	-	-	-	132.266	-	301.085	-	-	-	-	-
9	102.896	32.081	57.556	57.341	192.054	52.16	136.612	32.081	126.643	29.49	81.954	23.661
14	789.889	7853.009	2129.095	-	3010.908	4175.223	648.719	1894.779	16147.094	3650.172	2024.367	792.351
18	276.669	16709.102	151.551	1861.506	2014.395	596.41	485.195	930.082	5044.53	4391.681	1013.466	-
20	75022.02	1807.716	654.352	1190.997	6953.051	1202.477	5813.754	594.288	32579.635	2124.154	1277.484	653.264
23	46.792	33.391	66.697	46.486	22.26	47.989	51.075	30.054	258.583	18.792	61.43	30.394
25	78.717	138.065	90.43	142.216	61.54	112.733	172.529	118.936	207.726	122.51	110.744	103.94
26	139.152	411.873	111.608	375.181	116.07	524.183	198.496	103.565	339.318	223.531	136.949	109.014
30	374.089	20254.356	1326.138	3648.559	321.693	1444.371	562.952	4687.421	3734.605	12653.771	730.993	1006.551
31	1012.014	78675.248	4516.406	12983.173	864.513	5110.718	1654.047	16891.637	13074.037	45772.674	2332.829	3298.368
36	69.277	48.452	40.131	57.019	47.79	61.209	70.067	51.494	245.761	31.617	53.939	30.965
38	511.264	103176.696	8683.121	17619.789	312.466	3493.355	860.667	27511.253	8884.819	81643.883	3167.976	4854.759
47	2318.94	86184.485	6242.164	13061.46	2155.397	3751.482	2651.138	21445.196	8609.147	45839.119	5010.666	4527.047
49	38.846	6023.024	529.097	1165.68	45.394	259.347	65.465	1810.423	728.603	4282.906	270.879	305.895
52	125.831	27935.944	1414.227	3464.504	71.182	580.639	233.056	6525.874	2216.431	17821.416	992.128	823.072
55	161.877	2280.008	197.136	680.678	166.909	131.652	40.987	887.181	454.024	1723.32	343.205	182.02
56	123.107	655.496	695.156	530.902	89.123	219.392	145.762	445.938	1765.576	377.974	185.406	151.426
61	550.126	28030.708	1893.653	4648.317	593.518	1401.029	1199.172	6235.332	2078.201	15859.621	1535.636	845.324
62	609.219	201.53	638.613	555.542	237.201	318.21	330.811	331.506	3128.322	160.414	176.513	147.082
65	-	4335.873	7252.778	7253.254	-	11003.095	3502.937	4336.032	-	2252.46	11836.349	4752.698

Source (ng/g)	S9-Flower	S9-Seed	S9-Root	S9-Peel	S9-Leaf	S9-Stem	S10-Flower	S10-Seed	S10-Root	S10-Peel	S10-Leaf	S10-Stem
3	18252.816	6031.437	3466.379	15234.828	13424.885	21723.506	-	52805.575	6182.414	-	38470.92	16894.31
5	19724.356	4967.324	1145.568	6258.968	5465.873	43946.539	1744.075	14209.463	4077.646	6671.12	166445.502	20976.799
7	-	-	-	-	-	-	-	-	-	-	202.225	-
9	118.871	21.286	51.512	46.571	80.009	129.667	135.082	218.402	48.272	-	190.985	90.806
14	1583.158	3312.379	2230.392	1740.431	3632.414	333.627	164.454	3038.351	1898.048	4820.743	4566.087	9967.14
18	1631.999	3501.978	360.064	3057.048	11259.275	360.077	276.677	2765.054	304.467	13622.526	1110.776	1221.941
20	51083.76	5409.213	3962.491	2427.326	6814.859	88723.865	512.606	17599.62	1050.849	2656.768	3131.893	3433.109
23	38.785	25.086	81.896	30.994	88.36	26.8	43.837	44.01	66.7	26.37	64.985	140.631
25	262.262	125.688	136.44	137.779	63.172	83.869	57.455	68.638	156.383	93.757	354.644	527.352
26	321.002	201.539	39.14	157.568	4.489	160.401	-	395.77	555.619	209.107	136.56	8.275
30	751.814	11478.753	956.386	2154.777	389.268	310.693	753.177	503.881	1498.413	16433.032	1255.454	2084.276
31	2344.876	43211.678	3191.856	7135.958	1081.911	795.76	2465.152	1605.485	5157.833	58395.928	4128.723	7048.46
36	73.636	35.668	31.055	49.673	52.765	40.543	23.584	70.297	63.063	44.971	61.345	173.087
38	1661.861	67841.68	5315.521	12851.547	920.901	390.779	2324.47	917.879	6005.287	68344.204	1288.359	2583.534
47	3036.24	50712.579	4835.499	9785.096	2698.683	2409.931	3876.602	2810.492	7133.443	53564.601	2976.378	3703.706
49	105.749	3451.533	258.349	815.194	85.676	51.8	178.064	77.283	421.338	3585.514	105.966	205.538
52	365.246	16037.939	945.236	2622.467	288.195	143.803	595.96	285.436	1670.44	15957.265	338.011	595.009
55	161.871	1547.015	202.17	489.274	277.733	277.719	131.651	40.987	312.98	1703.173	182.018	116.541
56	213.723	496.917	264.698	304.35	117.442	60.804	-	157.091	372.309	394.964	208.066	394.959
61	1218.679	15627.282	1203.446	3326.217	1698.356	259.245	610.891	1359.687	2405.956	18851.253	738.971	671.683
62	583.748	160.797	250.497	232.874	203.708	233.77	43.304	230.43	320.004	142.019	787.941	1306.169
65	-	3502.619	4753.095	3086.19	3502.46	-	-	-	28505.476	-	-	-

Source (ng/g)	S11-Flower	S11-Seed	S11-Root	S11-Peel	S11-Leaf	S11-Stem
3	26098.621	-	45108.103	18253.046	33642.931	27003.966
5	17152.555	5969.397	4526.867	7890.993	47625.7	9450.773
7	-	-	-	-	177.891	-
9	128.586	-	67.702	39.365	96.419	155.141
14	925.753	4296.498	5399.269	2000.556	2502.806	1650.353
18	1006.55	27566.926	791.001	3564.591	5976.775	2042.205
20	70408.532	1717.402	3342.71	3860.696	6031.034	6364.736
23	20.825	18.536	106.213	51.46	46.747	97.176
25	67.626	118.426	621.98	105.334	106.444	95.718
26	153.6	291.403	155.025	184.29	307.783	77.58
30	278.762	12821.108	1180.563	6093.054	1478.936	1221.712
31	686.084	47354.366	3838.97	21794.885	5150.766	4119.637
36	36.286	36.492	67.25	37.49	72.881	73.155
38	493.191	58791.657	5902.717	28080.321	2047.439	4198.036
47	2278.405	43787.509	5846.75	20298.708	3578.834	4101.285
49	51.942	867.03	384.608	1581.935	155.432	271.443
52	1273.767	13092.611	5864.85	114.486	543.003	711.691
55	171.947	1647.761	161.868	796.517	257.576	328.088
56	-	462.93	978.323	332.661	185.409	247.708
61	265.773	16417.069	2662.108	7135.749	836.648	1058.029
62	192.261	103.317	1471.349	245.497	562.806	355.452
65	2252.381	-	33922.063	8086.508	1002.46	7253.175
- Not detected						

Table S2. Information of *D. metel* L. materials

Production areas No.	Locality	Coordinate	Parts (Harvest time)
S1	Cangzhou, Hebei	116°51'31"N 38°22'48"E	Flower, Root, Leaf and Stem (2019, 07); Peel and Seed (2019, 08)
S2	Danzhou, Hainan	109°39'60"N 19°29'38"E	Flower, Root, Leaf and Stem (2019, 06); Peel and Seed (2019, 07)
S3	Bozhou, Anhui	115°41'39"N 33°51'60"E	Flower, Root, Leaf and Stem (2019, 07); Peel and Seed (2019, 08)
S4	Xianyang, Shanxi	108°37'30"N 34°20'56"E	Flower, Root, Leaf and Stem (2019, 07); Peel and Seed (2019, 08)
S5	Luoyang, Henan	112°30'39"N 34°52'35"E	Flower, Root, Leaf and Stem (2019, 07); Peel and Seed (2019, 08)
S6	Nanchang, Jiangxi	115°57'10"N 28°45'44"E	Flower, Root, Leaf and Stem (2019, 07); Peel and Seed (2019, 08)
S7	Taizhou, Jiangsu	119°59'44"N 32°28'47"E	Flower, Root, Leaf and Stem (2019, 07); Peel and Seed (2019, 08)
S8	Huhehaote, Neimenggu	111°46'35"N 40°57'13"E	Flower, Root, Leaf and Stem (2019, 07); Peel and Seed (2019, 08)
S9	Yanan, Shanxi	109°33'20"N 36°36'17"E	Flower, Root, Leaf and Stem (2019, 07); Peel and Seed (2019, 08)
S10	Nanning, Guangxi	108°26'24"N 22°47'92"E	Flower, Root, Leaf and Stem (2019, 06); Peel and Seed (2019, 07)
S11	Xiaogan, Hubei	113°52'13"N 30°54'38"E	Flower, Root, Leaf and Stem (2019, 07); Peel and Seed (2019, 08)

Table S3. ^{13}C -NMR data of 22 quantitative alkaloids (400 MHz in ^{13}C -NMR)

No	3 ^a	5 ^a	7 ^a	9 ^b	14 ^c	18 ^b	20 ^a	23 ^a	25 ^a	26 ^a	30 ^a	31 ^a	36 ^a	38 ^a	47 ^a	49 ^b	52 ^a	55 ^a	56 ^a	61 ^a	62 ^a	65 ^a
1	138.6	136.3	138.6	136.6	64.2	59.9	127.7	134.7	128.3	127.9	128.6	128.3	128.3	132.3	133.4	129.2	124.9	128.0	130.5	129.6	128.4	131.4
2	96.7	127.6	112.3	129.7	36.5	34.1	130.6	128.5	111.6	132.3	114.0	111.6	111.6	112.3	111.7	129.5	113.2	113.6	113.3	110.2	128.5	113.4
3	155.3	128.1	123.3	128.2	67.7	65.6	116.7	116.2	149.8	116.2	148.5	149.3	149.3	148.7	148.9	115.1	148.2	149.3	146.0	149.5	116.3	151.4
4	110.8	126.9	120.6	126.4	36.5	34.2	158.1	158.1	149.3	159.3	148.6	149.8	149.9	147.5	147.3	155.6	148.9	146.9	151.2	148.8	158.0	146.2
5	118.8	128.1	119.2	128.2	70	60.0	116.7	116.2	116.5	116.2	115.8	116.5	116.5	115.4	115.9	115.1	117.2	116.2	129.3	116.0	116.3	116.8
6	120.7	127.6	127.5	129.7	73.6	23.9	130.6	128.5	123.2	132.3	124.8	123.2	123.3	121.7	120.6	129.5	132.6	132.2	118.1	116.8	128.5	130.6
7	118.5	54.3	107.9	38.5	36.9	24.2	142.0	73.5	118.8	138.0	138.4	142.0	142.2	75.3	75.1	34.3	134.7	133.3	142.0	91.7	141.5	141.8
8	125.6	174.6	131.4	55.4	42.3	38.3	118.3	48.3	142.0	121.5	121.7	118.8	118.7	86.5	87.3	40.8	127.6	130.1	120.0	140.6	121.0	119.4
9	161.9	63.5	51.2	166.2	172.8	171.2	169.6	169.6	169.2	170.3	170.3	169.2	169.2	171.4	171.6	165.2	170.4	172.8	169.4	161.7	169.1	169.4
1'	41.1		59.8	126.4	137.5	136.2	134.8	128.3	132.1	131.2	131.2	131.3	131.5	130.9	131.5	130.5	131.4	131.3	132.8	128.0	134.2	130.8
2'	20.5		24.3	130.8	129.2	128.6	128.5	111.6	117.0	130.7	130.7	130.8	129.2	130.7	112.2	110.3	130.8	130.7	110.6	111.9	112.5	116.3
3'				115.0	129.8	128.0	116.1	149.9	146.3	116.0	116.2	116.3	116.3	116.3	151.4	147.6	116.2	116.3	149.3	149.6	149.6	156.9
4'				156.1	128.8	127.3	160.6	149.3	144.8	156.9	156.9	156.9	158.6	157.0	150.2	146.8	156.9	157.0	148.1	154.9	149.0	149.3
5'				115.0	129.8	128.0	116.1	116.5	116.5	116.0	116.2	116.3	116.3	116.3	117.8	115.4	116.2	116.3	119.4	119.9	116.5	116.4
6'				130.8	129.2	128.6	128.5	123.4	121.1	130.7	130.7	130.8	129.2	130.7	122.4	118.8	130.8	130.7	120.1	127.0	122.4	130.9
7'				38.5	54.6	54.3	73.5	142.4	42.6	35.5	35.6	35.8	83.3	35.6	35.8	87.6	35.7	35.6	89.9	191.2	73.5	35.8
8'				55.7	64.4	63.0	47.8	118.7	36.1	42.3	42.4	42.6	47.1	41.7	42.6	55.8	42.7	42.5	58.6	150.8	47.7	42.3
9'				166.1												169.4			173.1	167.3		
1''														131.5	131.0	129.2	135.9	135.7	134.7	130.8		130.6
2''														112.6	130.7	129.5	112.5	112.1	128.5	130.6		116.5
3''														151.6	116.2	115.1	149.6	148.6	116.4	116.4		120.0
4''														150.5	156.9	155.6	146.3	146.2	156.9	157.0		118.3
5''														118.3	116.2	115.1	116.0	116.1	116.4	116.4		130.8
6''														122.6	130.7	129.5	121.4	121.0	128.5	130.6		131.3
7''														141.5	141.2	34.3	47.7	47.6	73.4	35.2		35.6
8''														120.8	120.8	40.8	51.0	50.4	48.4	41.9		42.6
9''														168.8	168.7		174.6	168.7				172.9
1'''														131.3	131.2	129.2	131.2	131.0	130.7	130.5		132.9

7'-OMe		56.8
9-Me	17.2	
1'-CO ₂ H	173.6	

^a Measured in CD₃OD

^b Measured in CD₃SOCD₃

^c Measured in CD₃Cl₃

Table S4. Quantitative method validation data of 22 quantitative alkaloids, the concentration levels used to estimate stability, repeatability and recovery

No.	Compound	Calibration curve	r ²	Linear range ^a	LOQ ^a	LOD ^a	Precision ^b		Stability ^c	Repeat-ability ^b	Recovery ^d		
							Intraday	Interday			50%	100%	150%
3	1H-pyrido-[3,4- <i>b</i>]indol-1-1,2,3,4,9-tetrahydro-7-hydroxy	Y = 0.087 x + 197.22	0.996	2000-100000	2000	600	1.63	1.17	1.82	3.96	49.66	100.55	150.45
5	(S)-methyl-2-amino-2-phenylacetate	Y = 16.887 x + 6934.8	0.996	125-200000	125	41.25	1.30	1.25	1.04	1.48	50.02	103.71	151.71
7	(1 <i>S</i> ,3 <i>S</i>)-1-methyl-1,2,3,4-tetrahydro-β-carboline-3-carboxylic acid	Y = 198.41 x - 1652.5	0.998	6.25-1000	6.25	1.88	1.24	2.53	1.11	4.52	50.90	101.66	150.25
9	cyclo (PheTyr)	Y = 60.801 x - 349.09	0.998	18.75-3000	18.75	6.19	2.31	2.28	3.08	4.04	50.95	99.48	151.20
14	anisodamine	Y = 95.57 x + 9184.5	0.998	1.25-2000	1.25	0.41	1.04	1.61	1.95	1.49	49.73	102.59	151.22
18	atropine	Y = 1.8885 x + 133.86	0.998	81.25-65000	81.25	24.38	2.02	2.80	0.02	4.90	50.25	100.11	150.06
20	<i>N-trans-p</i> -coumaroyloctopamine	Y = 114.64 x + 79294.3	0.992	138.75-222000	138.75	41.63	3.44	4.39	1.30	1.42	50.59	100.98	149.22
23	<i>N-trans</i> -feruloyloctopamine	Y = 306.61 x + 1812	0.998	6.25-1000	6.25	1.88	1.39	2.34	2.08	2.65	50.70	100.39	150.12
25	<i>N-trans</i> -feruloyl-3',4'-dihydroxyphenylethylamine	Y = 970.54 x - 51746	0.994	2.5-4000	2.5	0.75	2.56	2.97	1.63	3.31	50.68	100.52	150.25
26	<i>N-cis</i> -coumaroyltyramine	Y = 506.1 x + 19781	0.996	3.75-3000	3.75	1.24	1.54	1.98	1.34	2.21	49.68	100.42	150.27
30	<i>N-cis</i> -feruloyltyramine	Y = 1093.6 x - 88164	0.996	56.25-22500	56.25	16.88	2.17	2.93	0.88	0.63	49.83	101.56	150.86
31	<i>N-trans</i> -feruloyltyramine	Y = 297.15 x + 306647	0.996	56.25-22500	56.25	16.88	2.04	2.44	0.38	1.46	50.69	105.04	149.43
36	3-(4-hydroxy-3-methoxyphenyl)- <i>N</i> -[2-(4-hydroxyphenyl)-2-methoxyethyl]acrylamide	Y = 382.38 x - 5684.1	0.998	2.5-2000	2.5	0.75	2.95	2.44	1.61	3.18	50.25	100.37	151.33
38	cannabisin E	Y = 4.358 x + 265.96	0.998	187.5-150000	187.5	61.88	2.17	2.86	1.76	3.25	51.39	101.04	152.35
47	lyciumamide B	Y = 56.346 x - 108951	0.996	312.5-100000	312.5	103.13	1.76	1.76	3.04	0.80	50.30	102.16	151.35
49	grossamide	Y = 184.43 x - 3326.3	0.996	31.25-5000	31.25	10.31	2.62	1.89	2.29	3.52	51.36	101.87	150.15
52	cannabisin D	Y = 138.83 x - 247.12	0.998	37.5-60000	37.5	12.36	0.85	2.30	1.06	4.30	53.83	101.83	151.55
55	thoreliamide C	Y = 5.2121 x - 213.63	0.994	50-4000	50	16.50	0.96	1.97	0.63	2.38	53.53	102.75	149.49
56	melongenamide B	Y = 4.6354 x - 124.33	0.994	12.5-10000	12.5	4.13	1.06	3.96	2.73	1.35	50.43	102.93	151.44
61	cannabisin L	Y = 6.0472 x + 2422.7	0.998	50-40000	50	16.50	0.48	1.04	2.72	0.82	49.52	101.72	155.54
62	<i>N</i> -[2-(3,4-dihydroxyphenyl)-2-hydroxyethyl]-3-(4-methoxyphenyl)prop-2-enamide	Y = 446 x - 831.59	0.998	50-4000	50	16.50	2.21	2.48	2.03	4.21	49.84	100.07	150.23
65	chenoalbicin	Y = 0.063 x + 251.88	0.996	312.5-50000	312.5	93.75	2.41	3.06	2.55	4.74	51.25	100.15	151.93

^a ng/mL; ^b n=6, RSD, %; ^c 48h, RSD, %; ^d n=6, %

Table S5. The total alkaloid contents of different extraction conditions for *D. metel* L

Extraction methods (mg/g)	Content (mg/g)			$\bar{x}\pm s$ (mg/g)
	1	2	3	
ultra-sonication	3.227	3.429	3.011	3.22±0.21
cold soaking	2.549	2.206	2.028	2.26±0.26
heat reflux	4.462	4.029	4.608	4.37±0.3
Extraction solvents (mg/g)	Content (mg/g)			$\bar{x}\pm s$ (mg/g)
	1	2	3	
70% MeOH	2.569	2.403	2.425	2.47±0.09
95% MeOH	1.802	2.039	1.800	1.88±0.14
70% EtOH	4.791	4.698	4.681	4.72±0.06
95% EtOH	3.705	3.854	3.502	3.69±0.18
Extraction duration (mg/g)	Content (mg/g)			$\bar{x}\pm s$ (mg/g)
	1	2	3	
30 min	0.137	0.124	0.225	0.16±0.05
60 min	1.525	1.305	1.432	1.42±0.11
90 min	3.216	3.016	3.461	3.23±0.22
120 min	4.112	4.928	4.833	4.62±0.45
150 min	3.956	3.411	3.829	3.73±0.29
180 min	3.892	3.219	3.484	3.53±0.34
Extraction times (mg/g)	Content (mg/g)			$\bar{x}\pm s$ (mg/g)
	1	2	3	
1	2.589	2.542	2.592	2.57±0.03
2	3.830	4.004	3.813	3.88±0.11
3	4.163	4.070	4.142	4.13±0.05