

Figure S1: ¹H NMR spectrum of VR1

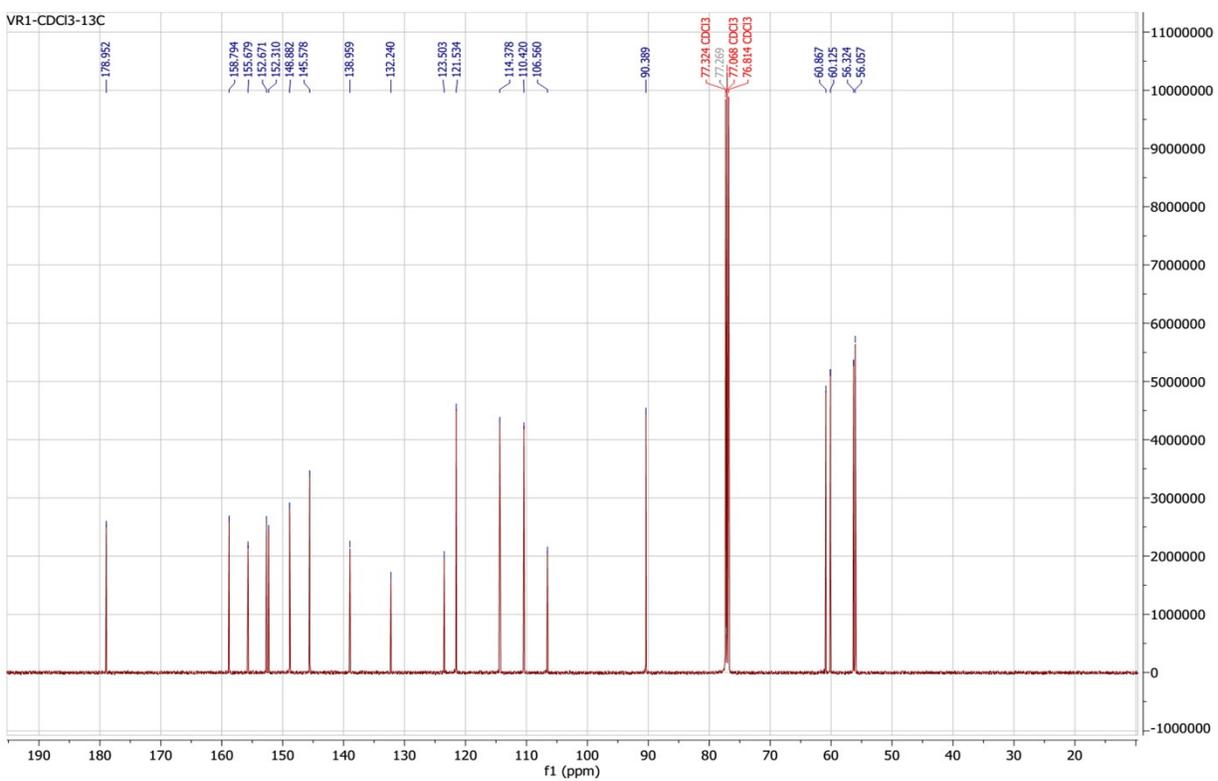


Figure S2: ¹³C NMR spectrum of VR1

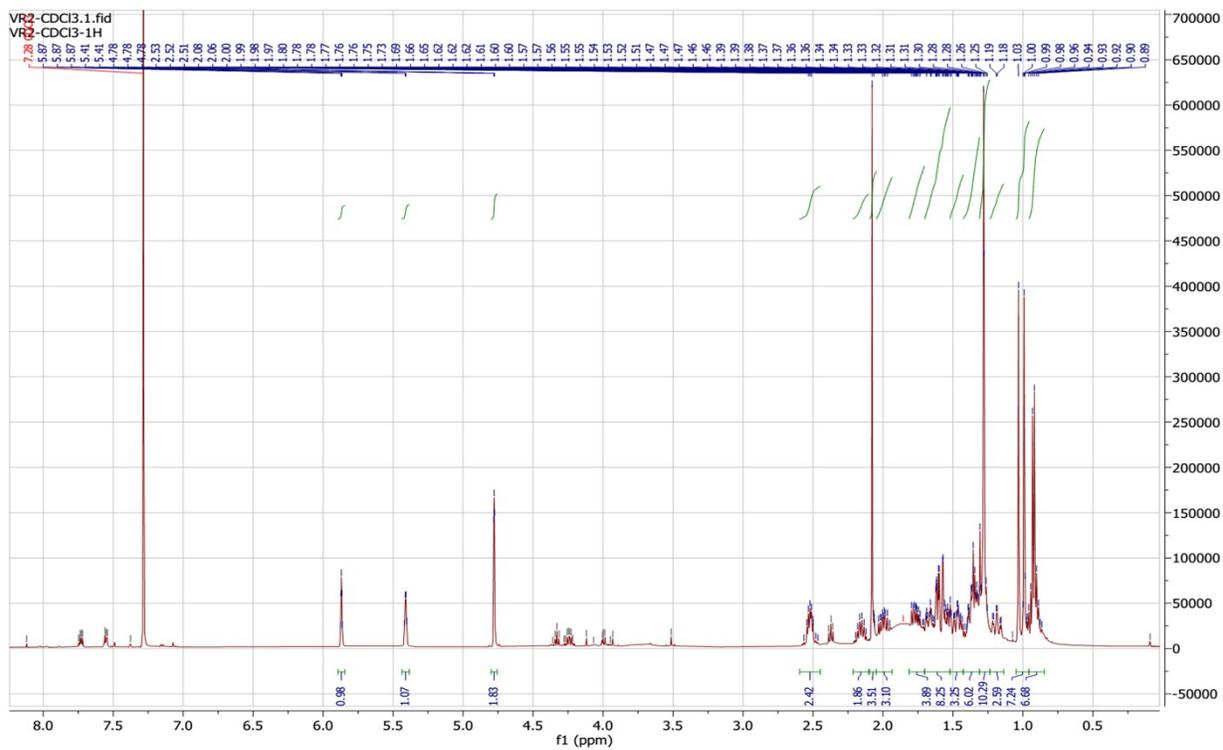


Figure S3: ¹H NMR spectrum of VR2

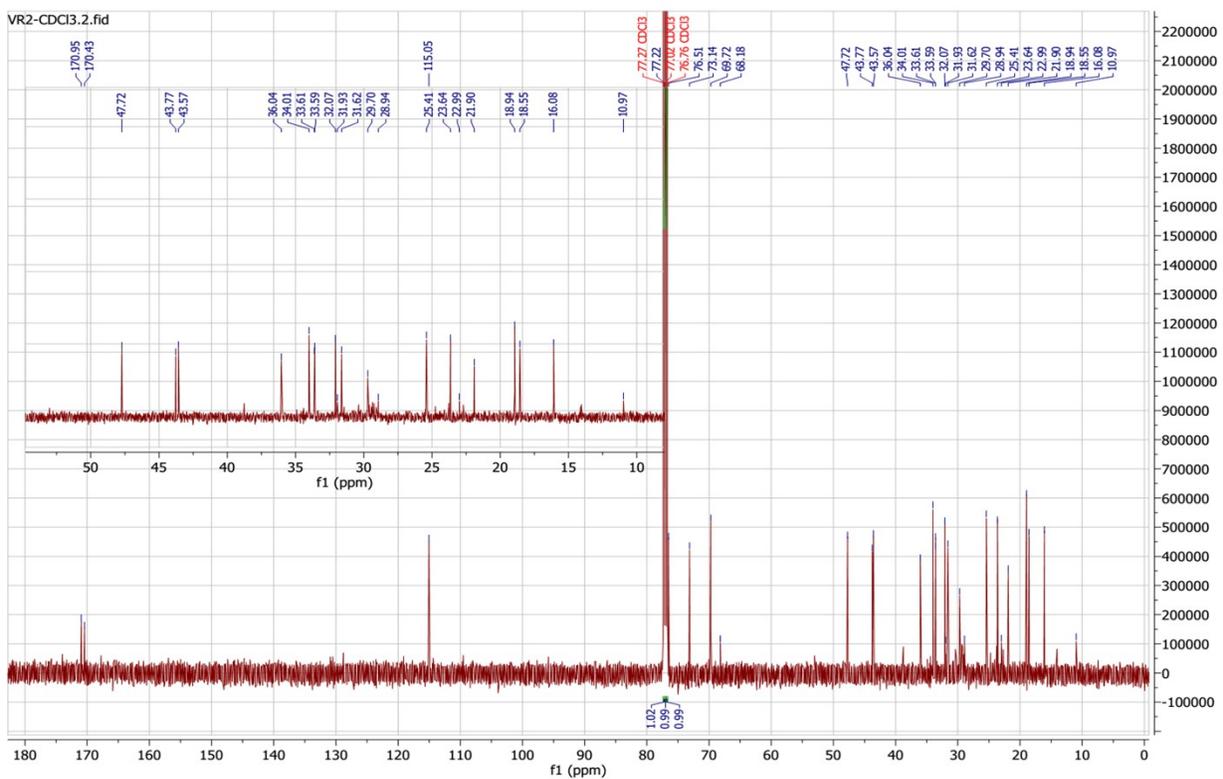


Figure S4: ¹³C NMR spectrum of VR2

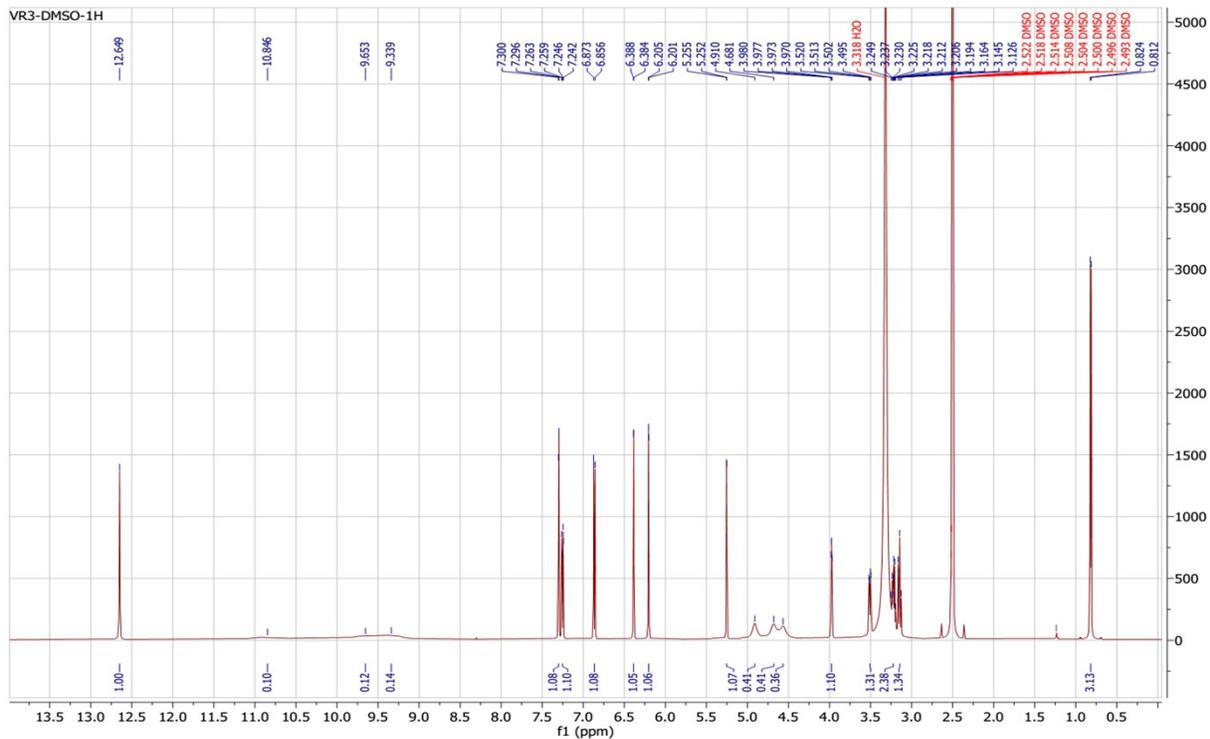


Figure S5: ¹H NMR spectrum of VR3

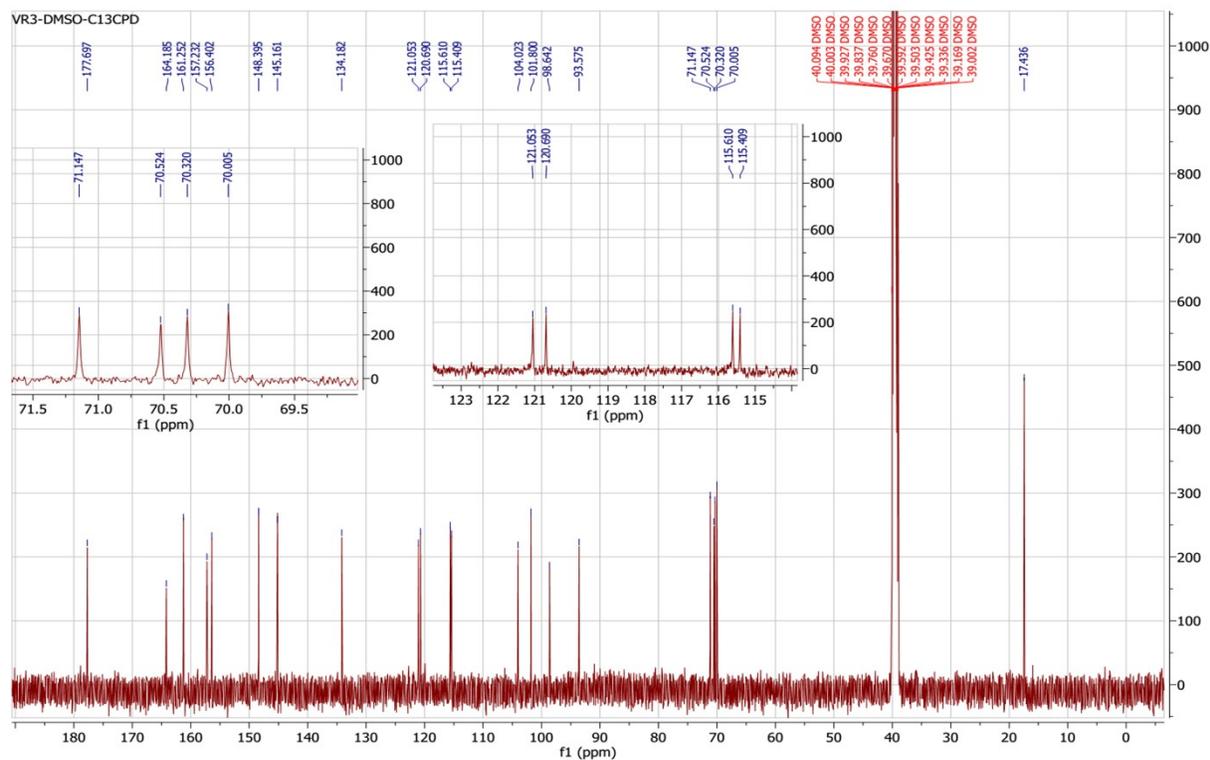


Figure S6: ¹³C NMR spectrum of VR3

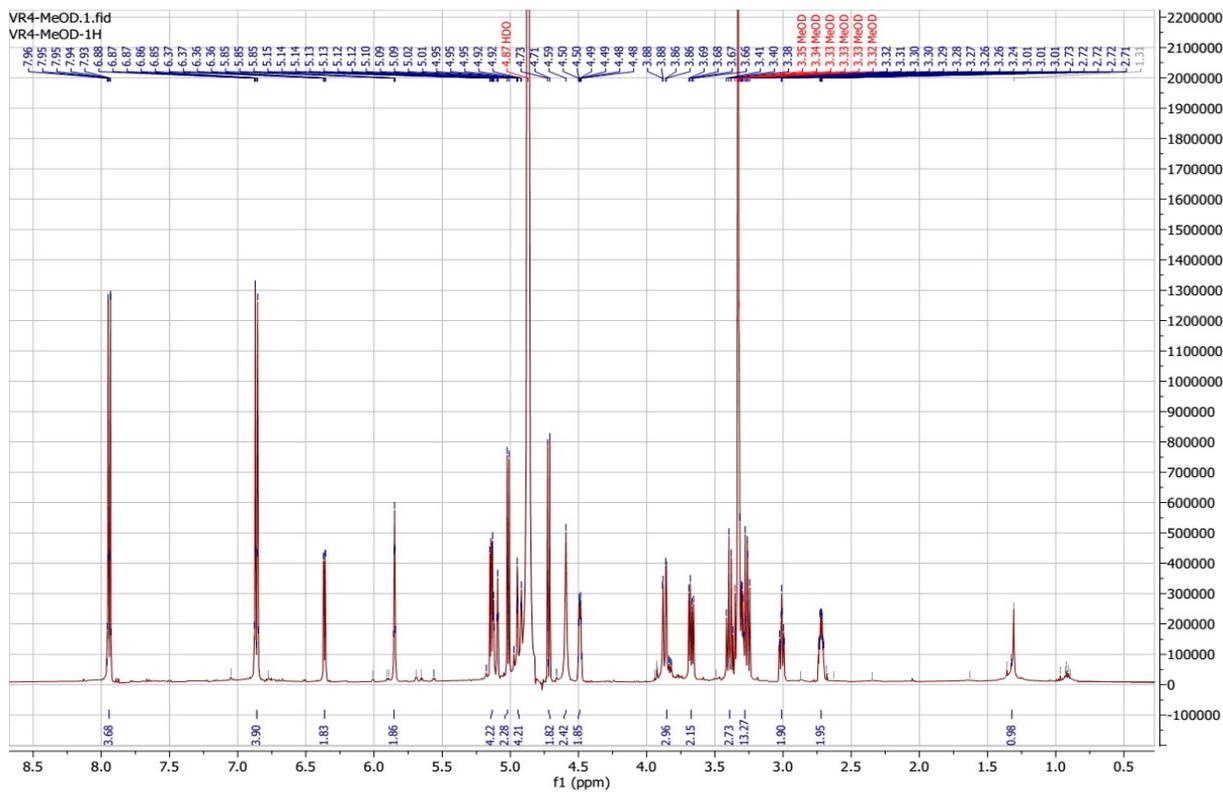


Figure S7: ¹H NMR spectrum of VR4

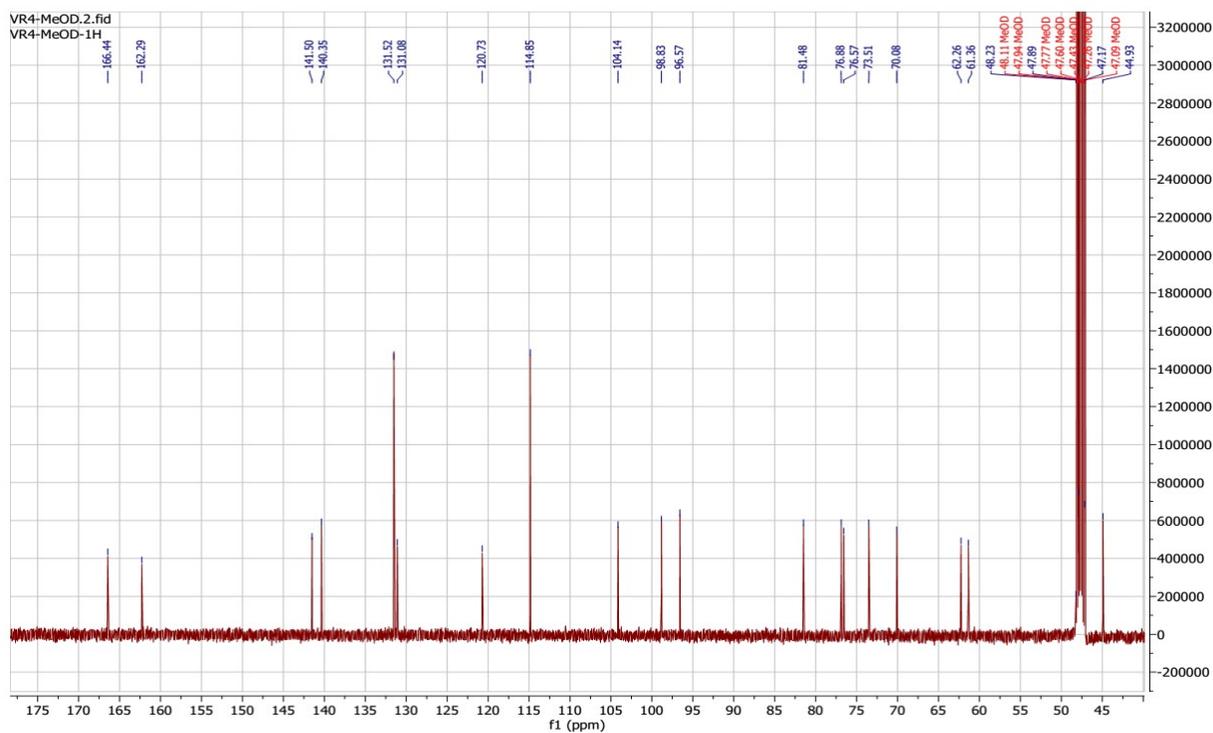


Figure S8: ¹³C NMR spectrum of VR4

Table S1: Major volatile constituents of *V. rotundifolia* essential oil at 3, 4, and 5 hours

RT (min)	Compound	Content (%)		
		EO3	EO4	EO5
7.339	α -Thujene	0	0	0.26
7.633	α -Pinene	0	0	5.69
9.556	Sabinene	0	0	0.53
9.744	β -Pinene	0	0	1.06
12.016	α -Terpinene	0	0	0.38
12.461	o-Cymene	0	0	0.2
12.751	Bornylene	0	0	0.4
12.86	1,8-Cineole	0	0	3
14.59	γ -Terpinene	0	0	0.6
16.327	4-Carene	0	0	0.19
22.091	4-Terpineol	0.3	0.2	0.43
22.854	α -Terpinol	0.18	0.18	0.22
26.586	a-Fenchyl acetate	0.2	0.06	0.19
27.652	d-Terpineol acetate	0.4	0.18	0.32
28.792	α -Terpinenyl acetate	12.2	5.9	8.56
29.699	α -Copaene	0.1	0.06	0
30.15	β -Eelemene	0.08	0.04	0
31.019	trans-Caryophyllene	1.24	0.67	1.13
31.343	Bicyclosquiphellandrene	0.07	0.06	0.09
32.07	α -Humulene	0.6	0.27	0.63
32.657	γ -Muurolene	0.3	0.2	0.28
32.81	Germacrene-D	0.38	0.16	0.28
33.028	Eudesma-4(14),11-diene	0.08	0	0.07
33.234	α -Selinene	0.12	0.06	0.09
33.315	β -Selinene	0.25	0.14	0.18
33.668	β -Humulen	0.96	0.59	0.91
33.81	δ -Cadinene	1.42	0.81	1.39
34.13	α -Muurolene	0	0	0.05
34.225	Muurola-4,9-diene	0.11	0.06	0.09
34.656	α -Cadinene	0.23	0	0.24
34.66	Valencane	0	0.17	0
34.746	d-Nerolidol	0.23	0.13	0.23
35.185	(-)-Caryophyllene oxide	0.41	0.25	0.25
35.609	β -Oplopenone	0.06	0.05	0.06
35.725	Humulene oxide	0.09	0.05	0.05
35.833	Epicubenol	0.15	0.14	0.14
36.33	Muurolol	0	0	0.49
36.533	α -Cadinol	0.63	0.55	0.51
36.621	Ar-tumerone	0.21	0.13	0.12

37.995	Driminol	0.42	0.34	0.57
38.332	4'-Hydroxypalmitophenone	0.04	0	0.12
39.016	Isopimaral	0.34	0.3	0.36
39.05	Hexahydrofarnesylacetone	0.16	0.17	0.15
39.482	β -iso methyl ionone	1.96	2.08	1.87
39.717	Abietal	0	0	0.18
39.807	Cupressene	1.97	0	1.74
39.808	Phyllocladene	0	1.85	0.14
39.882	Isopimaridienne	0.5	0.48	0.45
40.001	Widdrol	6.7	6.49	0
40.146	Biformene	3.97	3.98	3.74
40.319	Sclareol	21.35	21.74	18.44
40.428	7a-Isopropenyl-4,5-dimethyloctahydro-1H-inden-4-yl)methanol	0	8.69	6.71
40.503	Pogostole	1.27	1.33	0
40.559	Manoyl oxide	1.23	1.27	1.03
40.648	Kolavenol	0.61	0.7	0.67
40.784	Isophyllocladene	9.33	8.89	16.5
40.99	Dehydroabietane	18.94	18.93	10.29
41.123	Kolavelool	1.03	1.13	0.86
41.188	δ -4,16-Androstadien-3-one	1.65	1.58	2.79
41.3	Dromostanolone Propionate	0	0.21	0.13
41.35	1-(4-tert-Butylphenyl)adamantane	4.6	4.74	2.64
41.6	Pyracarbolid	0.19	0.23	0
42.067	Caryophyllenyl alcohol	0	0.21	0
42.491	Totara-7 β ,13-diol	0.11	0.29	0
42.541	Epidehydroabietol	0.07	0.29	0
42.915	Spathulenol	0.22	0.13	0.13
43.023	4-epi-Dehydroabietinol acetate	0.58	0.83	0.14
	Oxygenated compounds	53.34	56.04	49.08
	Non-oxygenated compounds	44.67	41.95	49.64

Table S2: PCA loadings of each variable for PC1 and PC2

Variable	PC1	PC2
Yield (%)	0.27584	0.36180
TPC	-0.43218	-0.22255
TFC	-0.45502	0.00808
DPPH	0.41221	-0.36194
ABTS	0.41689	-0.25973
NO	0.40310	-0.13594
XO	0.15454	0.77625

Table S3. Pearson correlation coefficients (r) and corresponding p-values among total phenolic content (TPC), total flavonoid content (TFC), and IC₅₀-based biological activities (DPPH, ABTS, NO, XO)

		TPC	TFC	DPPH	ABTS	NO	XO
TPC	Pearson Corr.	1.000	0.956	-0.759	-0.773	-0.756	-0.535
TPC	p-value	--	0.000	0.029	0.024	0.030	0.172
TFC	Pearson Corr.	0.956	1.000	-0.901	-0.897	-0.877	-0.344
TFC	p-value	0.000	--	0.002	0.002	0.004	0.404
DPPH	Pearson Corr.	-0.759	-0.901	1.000	0.958	0.790	-0.035
DPPH	p-value	0.029	0.002	--	0.000	0.020	0.935
ABTS	Pearson Corr.	-0.773	-0.897	0.958	1.000	0.777	0.118
ABTS	p-value	0.024	0.002	0.000	--	0.023	0.781
NO	Pearson Corr.	-0.756	-0.877	0.790	0.777	1.000	0.183
NO	p-value	0.030	0.004	0.020	0.023	--	0.664
XO	Pearson Corr.	-0.535	-0.344	-0.035	0.118	0.183	1.000
XO	p-value	0.172	0.404	0.935	0.781	0.664	--

Table S4: Summary of annotated metabolites by chemical class in the R70 extract

Note: Table S4 entries are supported by MS/MS spectra and reported as putative MSI level 2 annotations based on precursor mass accuracy (≤ 10 ppm) and direct MS/MS library comparison against MoNA and MassBank. An internal confidence tier is assigned using Δ ppm and matched fragments (n_frag): High ($|\Delta$ ppm ≤ 5 ; n_frag ≥ 8), Medium ($|\Delta$ ppm ≤ 10 ; n_frag = 4–7), and Low ($|\Delta$ ppm ≤ 10 ; n_frag < 4). No authentic standards were used; annotations provide dereplication-level context and are not intended as definitive identification or quantification.

No.	Compound	RT (min)	mz_exp	mz_calc	error (ppm)	Fragments	Class	n_frag	Confidence
1.	Emodic acid	10.5	299.0185	299.0197	-4.0345	91.9780; 167.0500; 183.0440; 199.0400; 211.0400; 227.0350; 255.0310; 271.0250; 299.0210	Anthraquinone	9	High
2.	Emodin	13.4	269.0455	269.0455	-0.1741	105.0330; 117.0350; 143.0500; 157.0690; 182.0360; 197.0600; 210.0310; 225.0550; 241.0490; 269.0440	Anthraquinone	10	High
3.	Aesculetin	6.1	177.0196	177.0193	1.4382	89.0400; 105.0350; 133.0290; 149.0240; 177.0200	Coumarin	5	Medium
4.	Isofraxidin	7.4	221.0450	221.0455	-2.4798	51.0211; 64.9971; 79.0171; 91.0178; 107.0123; 119.0125; 135.0073; 147.0110; 163.0015; 177.0180; 190.9969; 206.0219	Coumarin	12	High
5.	Aurapten	15.4	297.1516	297.1496	6.7174	61.9870; 79.9560; 96.9590; 149.0080; 170.0030; 183.0110; 197.0270; 211.0430; 230.0250; 244.8610; 297.1530	Coumarin	11	High
6.	Rutamarin	19.6	355.1552	355.1551	0.4033	35.7510; 59.0130; 79.6040	Coumarin	3	Low
7.	1,3-Dideacetyl-7-Deacetoxy-7-Oxokhivorin	20.1	457.2251	457.2232	4.2659	59.0130; 71.0490; 97.0650; 147.0810; 159.0810; 175.0760; 203.0710; 247.1700; 295.1340; 323.1290; 353.1760; 457.2240	Diterpenoid	12	High
8.	Forskolin	12.6	409.2237	409.2232	1.3631	59.0140; 275.1660; 313.1810; 331.1920; 349.2020; 367.2130;	Diterpenoid	7	Medium

						409.2230			
9.	dehydroAbietic acid	14.8	299.2011	299.2017	-1.7723	79.9560; 119.0490; 183.0110; 219.9640; 299.2010	Diterpenoid	5	Medium
10.	1,2-dihydroxyHeptadec-16-en-4-yl acetate	15.1	327.2533	327.2541	-2.3939	61.9870; 79.9560; 119.0490; 133.0650; 170.0030; 183.0110; 197.0270; 211.0430; 230.0250; 326.1880	Fatty acid derivative	10	High
11.	Tridecanedioic acid	11.7	243.1593	243.1602	-3.5673	57.0350; 83.0500; 153.1290; 181.1600; 199.1700; 225.1500; 243.1600	Fatty acid derivative	7	Medium
12.	Undecanedioic acid	11.3	215.1281	215.1289	-3.4135	57.0340; 71.0500; 83.0500; 97.0660; 125.0970; 153.1280; 171.1390; 197.1180; 215.1290	Fatty acid derivative	9	High
13.	Vaccenic acid	19.7	281.2476	281.2486	-3.4164	281.2450	Fatty acid derivative	1	Low
14.	methyl (2E,4E,8E)-7,13-dihydroxy-4,8,12-trimethyltetradeca-2,4,8-trienoate	14.1	309.2061	309.2071	-3.3495	59.0120; 71.0490; 89.0410; 111.0440; 123.0440; 149.0080; 183.0110; 197.0270; 221.0490; 279.0360; 311.1690	Fatty acid derivative	11	High
15.	3,4',5,6,7-Pentamethoxyflavone	9.7	371.1129	371.1136	-1.8389	59.0120; 78.9850; 94.9800; 115.9190; 130.9420; 142.9430; 174.9330; 188.9480; 279.8970; 327.0510; 357.0620; 372.0850	Flavonoid	12	High
16.	3-hydroxyflavone	12.4	283.0608	283.0612	-1.3023	107.0140; 130.0380; 151.0030; 171.0420; 183.0420; 196.0540; 211.0400; 239.0360; 268.0370	Flavonoid	9	High
17.	4',5,7-trihydroxy-3,6-dimethoxyflavone	11.4	329.0659	329.0667	-2.4635	65.0040; 82.0060; 105.0340; 133.0290; 145.0300; 165.9910; 199.0400; 215.0350; 227.0350; 243.0300; 271.0240; 299.0180	Flavonoid	12	High
18.	5,7-Dihydroxyflavanone	12.1	255.0656	255.0663	-2.8690	65.0020; 83.0130; 95.0130; 107.0130; 119.0490; 136.0150; 151.0030; 171.0440; 185.0600; 213.0550; 227.0710; 255.0660	Flavonoid	12	High

19.	7-O-beta-glucopyranosyl-4'-hydroxy-5-methoxyisoflavone	10.2	445.1126	445.1140	-3.1364	29.7440; 44.5880; 65.0040; 78.9570; 102.9460; 116.7330; 135.0050; 149.9940; 165.0200; 177.3800	Flavonoid	10	High
20.	Abrquinone B	7.3	389.1238	389.1242	-1.0177	59.0120; 124.9860; 141.0180; 165.0180; 180.0420; 195.0650; 227.0710; 316.0590; 329.0300; 344.0540; 359.0770; 375.1080	Flavonoid	12	High
21.	Cyanidin	8.1	285.0394	285.0399	-1.7695	63.0224; 77.0372; 105.0299; 117.0322; 130.0383; 143.0498; 156.0635; 183.0476; 201.0487; 215.0294; 255.0404; 285.0447	Flavonoid	12	High
22.	Dihydrokaempferol	7.1	287.0556	287.0561	-1.8109	107.0150; 125.0260; 137.0260; 151.0060; 165.0210; 177.0580; 201.0580; 215.0740; 241.0530; 259.0650	Flavonoid	10	High
23.	Epigallocatechin	6.4	305.0678	305.0667	3.6805	111.0450; 125.0240; 139.0370; 160.8400; 174.9560; 188.8530; 203.0260; 219.0640; 242.9050; 261.0760; 288.8670; 305.0670	Flavonoid	12	High
24.	Genistein	10.0	269.0447	269.0455	-3.0192	63.0230; 91.0180; 107.0130; 133.0280; 159.0440; 171.0440; 183.0440; 201.0550; 224.0470; 240.0420; 269.0460	Flavonoid	11	High
25.	Hesperetin	10.1	301.0710	301.0718	-2.6581	65.0017; 83.0123; 108.0199; 124.0140; 136.0149; 151.0016; 164.0107; 185.0537; 199.0416; 215.0299; 240.0417; 285.0410	Flavonoid	12	High
26.	Irigenin	10.4	359.0748	359.0772	-6.8105	136.9870; 174.0310; 186.0320; 202.0270; 214.0270; 230.0220; 242.0220; 258.0170; 270.0170; 286.0120; 298.0120; 314.0070	Flavonoid	12	High
27.	Isovitexin	7.1	431.0969	431.0984	-3.5211	269.0420; 283.0580; 311.0500; 323.0520; 341.0610; 383.0720; 413.0850; 431.0890	Flavonoid	8	High

28.	Kaempferol	9.1	285.0381	285.0405	-8.3453	63.0240; 93.0350; 117.0340; 143.0500; 159.0450; 171.0450; 187.0400; 211.0400; 227.0350; 239.0350; 255.0300; 285.0400	Flavonoid	12	High
29.	Kaempferol 3-glucuronide	8.1	461.0704	461.0725	-4.6475	57.0330; 71.0140; 85.0290; 99.0070; 135.0070; 150.9990; 163.0030; 187.0390; 211.0380; 229.0500; 257.0450; 285.0400	Flavonoid	12	High
30.	Kaempferol-3-O-glucoside-2"-p-coumaroyl	12.5	593.1273	593.1301	-4.6494	65.0031; 119.0453; 151.0006; 163.0363; 213.0540; 227.0274; 241.0539; 257.0511; 285.0392; 307.0816; 447.0909; 593.1303	Flavonoid	12	High
31.	Kaempferol-4'-methyl ether	10.1	299.0549	299.0561	-3.9058	65.0014; 83.0125; 107.0128; 120.0194; 132.0205; 151.0022; 164.0091; 199.0354; 211.0421; 227.0356; 255.0294; 284.0316	Flavonoid	12	High
32.	Limocitrin	8.7	345.0607	345.0616	-2.5323	110.0010; 149.0260; 164.9860; 187.0370; 203.0320; 215.0320; 231.0270; 243.0300; 258.0150; 271.0240; 315.0080; 330.0400	Flavonoid	12	High
33.	Luteolin-6-C-glucoside	6.6	447.0891	447.0933	-9.4181	133.0314; 175.0406; 203.0290; 243.0297; 269.0443; 284.0313; 297.0390; 311.0551; 327.0502; 339.0522; 357.0593; 381.0615	Flavonoid	12	High
34.	Pelargonidin-3-O-glucoside	7.8	431.0974	431.0978	-0.9567	147.0089; 167.0401; 180.0578; 196.0507; 211.0424; 225.0573; 240.0358; 269.0457; 311.0616; 341.0428; 431.0953	Flavonoid	11	High
35.	Peonidin-3-O-beta-galactoside	7.2	461.1075	461.1089	-3.0244	147.0118; 190.9911; 211.0393; 239.0312; 255.0271; 268.0455; 283.0271; 298.0468; 313.0663; 341.0729; 383.0638; 461.1107	Flavonoid	12	High
36.	Quercetin	9.2	301.0348	301.0354	-1.9870	65.0010; 93.0337; 107.0120; 121.0274; 133.0285; 151.0014; 164.0116; 183.0400; 199.0352; 211.0417; 227.0329; 243.0298	Flavonoid	12	High

37.	Quercetin 3,7-dimethyl ether	10.5	329.0650	329.0667	-5.2277	199.0360; 227.0280; 243.0270; 257.0400; 271.0200; 285.0350; 299.0150; 314.0390; 329.0620	Flavonoid	9	High
38.	Quercetin-3-(6"-malonyl)-Glucoside	6.8	549.0896	549.0886	1.8803	101.0141; 181.1069; 225.0899; 255.0084; 271.0041; 300.0042; 387.1231; 505.0595; 549.1680	Flavonoid	9	High
39.	Quercetin-3-O-glucoside	6.3	463.0864	463.0882	-3.9099	151.0000; 163.0027; 178.9955; 192.0058; 215.0304; 227.0349; 242.0161; 255.0267; 271.0233; 300.0260; 343.0456; 463.0856	Flavonoid	12	High
40.	Rotenone	18.7	393.1374	393.1344	7.7058	26.0970; 39.2920; 54.6100; 69.6680; 86.5870; 108.5120; 126.6860; 146.9820; 161.0260	Flavonoid	9	High
41.	Villol	8.6	441.1162	441.1191	-6.6454	65.0020; 79.0540; 107.0490; 137.0230; 149.0600; 173.0600; 189.0190; 217.0500; 293.0820; 309.0770; 337.0720; 365.0660	Flavonoid	12	High
42.	Xanthohumol	18.4	353.1398	353.1394	1.1266	119.0500; 145.0290; 165.0920; 189.0920; 218.0580; 233.0820; 251.0920; 295.0610; 338.1150; 353.1390	Flavonoid	10	High
43.	isorhamnetin	9.5	315.0499	315.0510	-3.6676	83.0133; 107.0117; 120.0231; 136.0125; 151.0024; 164.0075; 227.0323; 243.0280; 255.0316; 271.0228; 283.0230; 300.0254	Flavonoid	12	High
44.	Kaempferol	9.2	285.0386	285.0405	-6.5123	41.0020; 63.0240; 93.0350; 117.0340; 133.0300; 159.0450; 187.0400; 211.0390; 227.0340; 239.0350; 255.0280; 285.0400	Flavonoid	12	High
45.	Luteolin-7-glucoside	7.3	447.0905	447.0933	-6.2920	94.9790; 135.0440; 151.0020; 285.0400; 297.0400; 311.0560; 327.0510; 339.0510; 357.0610; 447.0930; 461.0720	Flavonoid	11	High
46.	Santin	11.7	343.0804	343.0823	-5.7465	126.0280; 186.0300; 242.0210; 255.1810; 270.0160; 285.0410; 298.0100; 313.0350; 328.0580;	Flavonoid	10	High

						343.0800			
47.	Skullcapflavone II	11.5	373.0892	373.0929	-9.7663	79.9910; 133.0290; 151.9750; 179.9700; 194.9930; 213.0190; 257.0080; 269.0090; 285.0040; 300.0270; 328.0220; 343.0450	Flavonoid	12	High
48.	Taxifolin	7.5	303.0501	303.0510	-3.2211	41.0040; 57.0350; 83.0140; 107.0130; 125.0240; 150.0310; 175.0380; 188.0470; 201.0180	Flavonoid	9	High
49.	5,7-dihydroxy-3,6-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one	11.6	403.1022	403.1035	-3.0613	315.0130; 330.0370; 345.0600; 358.0300; 373.0540; 388.0780; 403.1010	Flavonoid	7	Medium
50.	Catechol	4.8	109.0294	109.0295	-0.8306	109.0284	Flavonoid	1	Low
51.	Aceroside VII	12.8	461.2135	461.2181	-9.8855	59.0110; 71.0120; 85.0280; 101.0230; 121.0640; 149.0600; 177.0900; 191.1050; 281.1550; 299.1640; 461.2150	Glycoside	11	High
52.	Apigenin-8-C-glucoside	7.1	431.0960	431.0984	-5.4768	117.0332; 149.0230; 163.0377; 179.0362; 197.0582; 239.0693; 268.0301; 283.0598; 296.0600; 311.0545; 341.0657; 431.0969	Glycoside	12	High
53.	Agnuside	6.8	465.1362	465.1402	-8.7641	59.0120; 71.0130; 89.0230; 101.0230; 121.0280; 137.0230; 165.0550; 183.0650; 241.0870; 285.0770; 303.0870; 465.1400	Glycoside	12	High
54.	Catalposide	6.3	481.1334	481.1351	-3.5613	59.0150; 93.0340; 111.0080; 137.0240; 151.0390; 163.0400; 177.0560; 205.0510; 235.0590; 301.0740; 319.0800; 481.1330	Glycoside	12	High
55.	Fragransin D3	12.3	327.1598	327.1602	-1.1494	59.0120; 79.9560; 93.0330; 108.0200; 133.0650; 145.0650; 159.0810; 183.0110; 197.0270; 211.0430; 237.0550; 325.1840	Lignan	12	High
56.	Nortrachelogenin	8.2	373.1286	373.1293	-1.8478	99.0070; 122.0360; 136.0520; 149.0600; 164.0470; 179.0700;	Lignan	12	High

						193.0860; 207.0660; 221.0450; 237.0770; 312.1000; 327.1240			
57.	3-O-methylfunicone	8.9	387.1082	387.1085	-0.9325	59.0120; 96.9590; 123.0080; 138.0310; 166.0260; 191.1070; 263.0560; 282.0280; 297.0520; 310.0720; 325.0470; 345.1710	Other	12	High
58.	(9Z,12R)-12-Hydroxyoctadec-9-enoic acid	15.3	297.2430	297.2435	-1.6430	59.0140; 93.0350; 113.0970; 127.1120; 149.0970; 165.1280; 183.1390; 279.2330; 297.2440	Oxylipin	9	High
59.	(Z)-5,8,11-trihydroxyoctadec-9-enoic acid	10.3	329.2316	329.2333	-5.3313	57.0330; 99.0800; 125.0950; 139.1110; 157.1220; 171.1010; 183.1370; 211.1320; 229.1430; 293.2110; 311.2220	Oxylipin	11	High
60.	12-Hydroxyoctadecanoic acid	16.1	299.2580	299.2592	-3.9487	57.0350; 113.0970; 127.1130; 139.1130; 169.1600; 183.1760; 213.1500; 253.2540; 281.2490; 299.2590	Oxylipin	10	High
61.	13-hydroxy-octadecatrienoic acid	12.9	293.2116	293.2122	-2.0749	179.1840; 195.1710; 221.1480; 236.1050; 249.2840; 275.2120; 293.1540	Oxylipin	7	Medium
62.	5,12-dihydroxy-eicosatetraenoic acid	14.7	335.2220	335.2228	-2.3241	59.0130; 71.0140; 129.0560; 151.1130; 181.0870; 195.1030; 273.2220; 317.2120; 335.2230	Oxylipin	9	High
63.	9,10-dihydroxy-octadecenoic acid	11.8	313.2374	313.2384	-3.2452	127.1050; 155.0900; 171.0750; 183.1050; 201.0710; 233.1870; 277.1670; 295.1650; 313.1640	Oxylipin	9	High
64.	9-hydroxy-octadecatrienoic acid	15.4	293.2112	293.2122	-3.3962	59.0130; 121.1020; 171.1030; 185.1180; 231.2110; 275.2010; 293.2130	Oxylipin	7	Medium
65.	9-hydroxy-10,12-octadecadienoic acid	14.8	295.2254	295.2279	-8.2330	59.0130; 80.9640; 94.9800; 113.0960; 134.8940; 171.1020; 183.1020; 195.1380; 215.3750; 259.2070; 277.2170; 295.2280	Oxylipin	12	High
66.	Demethoxycurcumin	9.5	337.1071	337.1081	-3.2414	119.0500; 134.0380; 149.0610; 161.0610; 173.0610; 187.0410; 202.0280; 217.0510; 322.0840;	Phenolic acid	10	High

						337.1080			
67.	3,4-dihydroxybenzoic acid	4.9	153.0194	153.0193	0.1208	65.0090; 91.0190; 109.0290; 153.0190	Phenolic acid	4	Medium
68.	Salicylic acid	5.8	137.0244	137.0244	-0.4465	65.0400; 93.0350	Phenolic acid	2	Low
69.	Gentisaldehyde	5.6	137.0243	137.0244	-0.9116	55.1000; 81.0330; 95.0130; 109.0280; 137.0230	Phenolic aldehyde	5	Medium
70.	4-hydroxybenzaldehyde	6.5	121.0304	121.0295	7.1005	65.0420; 92.0290; 121.0300	Phenolic aldehyde	3	Low
71.	3-O-Feruloylquinic acid	8.4	367.1028	367.1035	-1.6671	67.0180; 81.0330; 93.0330; 111.0440; 134.0360; 160.0160; 173.0450; 191.0550	Phenyl propanoid	8	High
72.	Caffeic acid	6.3	179.0352	179.0350	1.4320	58.2300; 89.0360; 107.0530; 135.0450; 179.0290	Phenyl propanoid	5	Medium
73.	Cynarin	7.9	515.1179	515.1195	-3.1244	93.0349; 111.0403; 135.0443; 161.0199; 179.0341; 191.0554; 227.0711; 285.3592; 308.0903; 335.0744; 353.0860; 515.1185	Phenyl propanoid	12	High
74.	Dimethylcaffeic acid	9.5	207.0657	207.0663	-2.7794	103.0540; 118.9910; 133.0640; 162.9790; 178.8200; 207.0640	Phenyl propanoid	6	Medium
75.	Dicaffeoyl quinic acid	8.0	515.1166	515.1195	-5.6488	93.0350; 135.0460; 155.0330; 173.0430; 191.0550; 255.0650; 300.0600; 353.0850; 515.1150	Phenyl propanoid	9	High
76.	Scutellarioside II	8.5	507.1489	507.1508	-3.7796	59.0120; 71.0130; 85.0280; 97.0280; 119.0490; 145.0280; 163.0390; 181.0500; 199.0610; 307.0830	Phenyl propanoid	10	High
77.	Curcumenol	14.8	233.1541	233.1547	-2.4173	59.0120; 89.0230; 102.9320; 121.0280; 149.0080; 163.0060; 184.0010; 214.9140; 233.1540	Sesquiterpenoid	9	High
78.	Carapin	8.1	467.2111	467.2075	7.5640	104.1770; 189.0100; 215.8940; 229.2410; 251.4180; 364.3060; 393.1690; 408.9270; 467.2140	Steroid	9	High
79.	18alpha-glycyrrhetic acid	14.5	469.3308	469.3323	-3.1883	61.9870; 78.9850; 94.9800; 255.2330; 283.2640; 311.1690; 325.1840; 339.2000; 395.2950;	Triterpenoid	12	High

						423.3270; 469.3320; 485.3280			
80.	Asiatic acid	19.6	487.3401	487.3429	-5.8294	131.7710; 198.6040; 296.9120; 428.2980; 487.3400	Triterpenoid	5	Medium
81.	Corosolic acid	15.1	471.3443	471.3480	-7.8674	196.1357; 407.3213; 471.3460	Triterpenoid	3	Low
82.	Hederagenin	14.6	471.3463	471.3480	-3.5143	59.0120; 83.0490; 99.9240; 163.8610; 183.0110; 221.0120; 268.2650; 375.2700; 393.3160; 405.3160; 428.2170; 471.3470	Triterpenoid	12	High
83.	Madecassic acid	9.5	503.3369	503.3378	-1.7450	61.9870; 79.9560; 96.9590; 119.0490; 133.4160; 183.0110; 221.1580; 264.3680; 331.4400; 484.2660; 503.3380; 528.7780	Triterpenoid	12	High
84.	Pygenic acid A	15.3	471.3454	471.3480	-5.4668	423.3260; 471.3480	Triterpenoid	2	Low
85.	Pygenic acid B	13.7	487.3404	487.3429	-5.0491	487.3430	Triterpenoid	1	Low
86.	Ursolic Acid	17.5	455.3520	455.3531	-2.3077	59.0120; 74.9890; 99.9240; 115.9190; 183.0110; 221.0400; 407.3320; 455.3530	Triterpenoid	8	High
87.	Irisxanthone	7.0	435.0919	435.0933	-3.1587	108.0200; 137.0230; 199.0390; 215.0340; 227.0340; 243.0290; 258.0170; 272.0320; 285.0040; 299.0190	Xanthone	10	High
88.	Norlichexanthone	10.3	257.0456	257.0455	0.2970	105.0350; 127.0520; 149.0250; 166.8660; 185.0590; 199.0210; 213.0580; 228.0420; 257.0440	Xanthone	9	High

Table S5. Distribution of identified metabolites by chemical class and their median MS¹ signal intensities.

Class	Number of compounds	Median peak area (a.u.)
Flavonoid	36	147.47
Glycoside	4	323.47
Coumarin	4	1777.88
Triterpenoid	8	381.32

Oxylipin	8	509.37
Fatty acid derivative	5	74.66
Phenyl propanoid	6	81.38
Diterpenoid	3	197.64
Phenolic acid	3	144.63
Phenolic aldehyde	2	164.25
Lignan	2	83.11
Sesquiterpenoid	1	114.63
Anthraquinone	2	52.25
Xanthone	2	32.79
Steroid	1	42.61
Other	1	25.00

Note: MS¹ peak areas are reported as relative signal intensities in arbitrary units (a.u.). Median values were used to reduce the influence of extreme ionization responses. Arbitrary units (a.u.)

Table S6. Cell viability (%) of ethanol extracts (E30–E96) and residue extracts (R30–R96) in RAW264.7 macrophages under the same treatment conditions used for NO inhibition (mean ± SD, n = 3).

Concentration (µg/mL)	E96	E70	E50	E30	R96	R70	R50	R30	DMSO 0.5%	Dexamethasone
400	64.19 ± 1.84	89.03 ± 4.56	72.16 ± 5.14	52.46 ± 1.97	88.90 ± 2.62	73.51 ± 3.50	88.85 ± 1.73	89.31 ± 2.26	92.19 ± 4.28	96.10 ± 2.79

200	82.39 ± 2.32	88.90 ± 2.62	81.85 ± 2.59	83.44 ± 5.11	89.74 ± 3.23	82.93 ± 3.99	83.73 ± 2.81	95.59 ± 3.26	–	–
100	88.19 ± 2.70	89.78 ± 2.84	86.45 ± 3.14	87.64 ± 1.45	93.44 ± 5.86	85.45 ± 3.88	91.59 ± 7.52	101.68 ± 1.08	–	–
50	95.11 ± 3.17	92.23 ± 1.60	90.62 ± 0.48	97.64 ± 2.68	93.56 ± 2.26	90.62 ± 0.48	88.92 ± 2.48	100.79 ± 1.79	–	–

Note: Values are expressed as percentage of untreated control (100%). DMSO was maintained at 0.5% (v/v) in all wells. Concentrations maintaining $\geq 80\%$ viability were considered non-cytotoxic for interpretation of NO inhibition.

Table S7A. Process-level energy breakdown (kWh) used for screening-level environmental assessment

Route	Milling	Extraction	Evaporation	Partition	Total
Raw material route (batch 2.9 kg)	0.25	0.00	41.76	14.28	56.29
PDR route (per 100 g PDR)	—	0.25	0.87	0.435	1.56

Note: Electricity values are screening-level estimates compiled from the internal worksheet. Total for the raw-material route includes a milling step ($1000 \text{ W} \times 0.25 \text{ h}$).

Table S7B. Material input breakdown (per 100 g feedstock)

Route	Electricity (kWh)	Water (L)	Ethanol (L)
Raw material route	1.94	1.58	2.16
PDR route	1.56	2.60	1.40

Note: Raw-material values are normalized from batch-scale inputs (2.9 kg) by dividing by 29 to obtain per-100 g feedstock values.

Table S7C. Sensitivity check (screening-level) for electricity and solvent recovery assumptions

Scenario	Parameter change	Expected direction of change	Ranking change
Electricity +20%	All step electricity $\times 1.2$	Climate/energy-driven indicators increase proportionally	No
Electricity -20%	All step electricity $\times 0.8$	Climate/energy-driven indicators decrease proportionally	No
Solvent recovery $\pm 20\%$	Assumed solvent loss/recovery $\pm 20\%$	PMI/E-factor shift proportionally (mass-balance driven)	No

Note: This sensitivity check is intended to demonstrate robustness of qualitative trends only. No stochastic uncertainty analysis was conducted.