

Supplementary Materials

H₂O-Induced Hydrophobic Interactions in MS-Guided Counter-Current Chromatography Separation of Anti-Cancer Mollugin from *Rubia cordifolia*

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Table S1. The *K* values and phase volume ratio of mollugin in several solvent systems^a

Solvent system (v%)			Phase volume ratio	<i>K</i> ^b
<i>n</i> -Hexane	Methanol	Water	V _U /V _L	A _U /A _L
40.00	40.00	20.00	0.68	43.16
40.00	45.00	15.00	0.68	15.18
40.00	50.00	10.00	0.63	8.22
40.00	52.00	8.00	0.60	4.31
40.00	53.33	6.67	0.57	3.26
40.00	54.44	5.56	0.55	2.37
40.00	55.00	5.00	0.52	2.05
40.00	56.00	4.00	0.48	1.71
50.00	30.00	20.00	1.04	68.45
50.00	35.00	15.00	1.03	24.71
50.00	40.00	10.00	0.99	8.95
50.00	42.00	8.00	0.97	5.09
50.00	42.86	7.14	0.91	3.94
50.00	45.00	5.00	0.87	2.00
50.00	46.15	3.85	0.82	1.95
50.00	47.06	2.94	0.75	1.40
50.00	47.62	2.38	0.73	1.10
60.00	20.00	20.00	1.55	172.11
60.00	25.00	15.00	1.55	64.76
60.00	30.00	10.00	1.55	15.78
60.00	32.00	8.00	1.55	8.74
60.00	33.33	6.67	1.43	5.89
60.00	34.44	5.56	1.43	4.32
60.00	35.00	5.00	1.45	3.62
60.00	36.00	4.00	1.36	2.82

^a *n*-Hexane-methanol-water.^b *K* value was expressed as the peak area of the compound in the upper phase divided by the peak area of the compound in the lower phase.

Table S2. The *K* values and phase volume ratio of mollugin in several solvent systems^a

Solvent system (v%)			Phase volume ratio	<i>K</i> ^b
<i>n</i> -Hexane	Methanol	Water	V _U /V _L	A _U /A _L
40.00	40.00	20.00	0.68	43.16
45.00	40.00	15.00	0.81	20.31
50.00	40.00	10.00	0.97	8.95
52.00	40.00	8.00	1.02	5.85
55.00	40.00	5.00	1.12	2.97
30.00	50.00	20.00	0.43	23.20
35.00	50.00	15.00	0.53	9.52
40.00	50.00	10.00	0.63	6.08
42.00	50.00	8.00	0.66	3.69
45.00	50.00	5.00	0.70	2.00
20.00	60.00	20.00	0.23	15.11
25.00	60.00	15.00	0.31	7.39
30.00	60.00	10.00	0.35	4.16
32.00	60.00	8.00	0.37	3.07
35.00	60.00	5.00	0.38	1.88

^a *n*-Hexane-methanol-water.^b *K* value was expressed as the peak area of the compound in the upper phase divided by the peak area of the compound in the lower phase.

Table S3. The *K* values and phase volume ratio of mollugin in several solvent systems^a

Solvent system (v%)			Phase volume ratio	<i>K</i> ^b
<i>n</i> -Hexane	Methanol	Water	V _U /V _L	A _U /A _L
50.00	30.00	20.00	1.04	68.45
40.00	40.00	20.00	0.68	42.29
30.00	50.00	20.00	0.43	23.20
20.00	60.00	20.00	0.23	15.10
10.00	70.00	20.00	0.08	11.54
60.00	30.00	10.00	1.55	15.78
50.00	40.00	10.00	0.99	8.95
40.00	50.00	10.00	0.63	6.08
30.00	60.00	10.00	0.35	4.26
20.00	70.00	10.00	0.18	3.55
65.00	30.00	5.00	1.44	5.19
55.00	40.00	5.00	1.13	2.78
45.00	50.00	5.00	0.68	2.30
35.00	60.00	5.00	0.38	1.88
25.00	70.00	5.00	0.17	1.67
68.00	30.00	2.00	1.86	1.77
58.00	40.00	2.00	1.06	1.34
48.00	50.00	2.00	0.60	1.23
38.00	60.00	2.00	0.27	1.04
28.00	70.00	2.00	0.06	1.01

^a *n*-Hexane-methanol-water.^b *K* value was expressed as the peak area of the compound in the upper phase divided by the peak area of the compound in the lower phase.

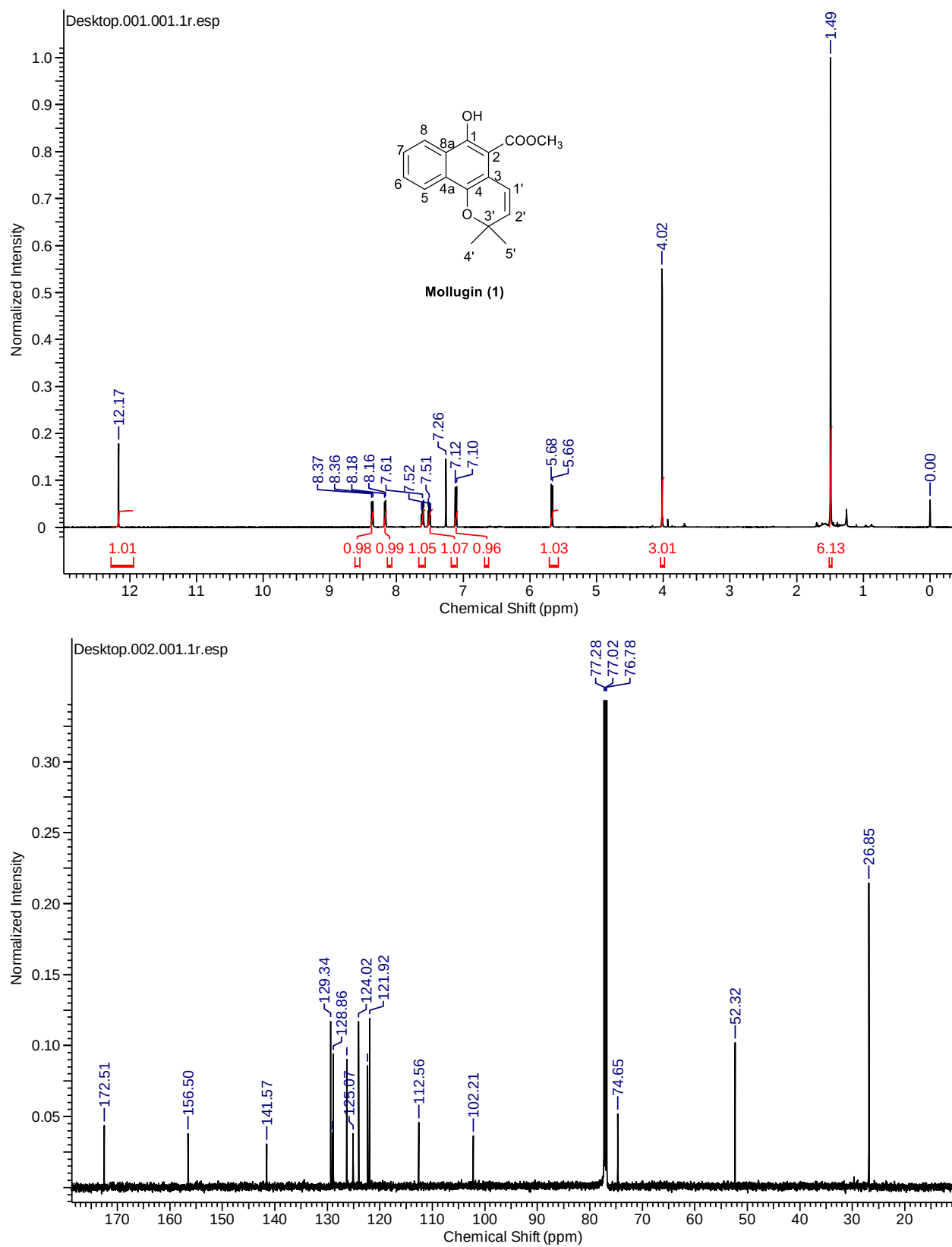


Figure S1. the representative ¹H, ¹³C NMR spectra of mullugin isolated by CCC with the two-phase solvents of *n*-hexane-methanol-water