

Optimization of Extraction Conditions and Cytotoxic Activity of Rapanone in Comparison to Its Homologue, Embelin

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Content:

Table S1. Significant differences between pairs of medians of rapanone content in dried plant material. The medians are encoded according to the codes of extracts that they refer to (Table 1).

Figure S1. Representative HPLC chromatograms showing content of rapanone in extracts from leaves of white-berried *A. crenata* Sims, obtained by different methods (HRE, SE, UAE). Details are provided in “Materials and methods” section in the main manuscript.

Figures S2-S5. ¹H NMR and ¹³C NMR data for rapanone and embelin. NMR spectra were recorded by means of the JEOL spectrometer at 500 MHz (JNM-ECZR500 RS1, JOEL Ltd., Tokyo, Japan) in CDCl₃.

¹H NMR (CDCl₃, 500.13 MHz) δ ppm: 7.6 (2H, bs, 2xOH), 5.9 (1H, s, H of the ring), 2.45 (2H, t, CH₂), 1.48 (2H, t, CH₂), 1.26 (24H, bs, CH₂ x12), 0.87 (3H, t, CH₃)

¹³C NMR (CDCl₃, 125.77 MHz) δ ppm: 169.0 – not visible, which is characteristic for 1,4-dihydroxybenzoquinones, 117.1 (C-3 of the ring), 102.2 (C-6 of the ring), 31.9 – 14.0 (signals from carbons of the side chain)

Table S1. Significant differences between pairs of medians of rapanone content in dried plant material.

Significantly different pairs of medians	Level of significance
18H <i>vs</i> 19S	*
8H <i>vs</i> 21S	*
18H <i>vs</i> 26S	*
18H <i>vs</i> 22U	*
18H <i>vs</i> 26U	*
11S <i>vs</i> 19S	*
11S <i>vs</i> 21S	*
11S <i>vs</i> 22S	*
11S <i>vs</i> 26S	**
11S <i>vs</i> 22U	*
11S <i>vs</i> 26U	*
12S <i>vs</i> 19S	*
12S <i>vs</i> 21S	*
12S <i>vs</i> 22S	*
12S <i>vs</i> 26S	*
12S <i>vs</i> 22U	*
12S <i>vs</i> 26U	*
19S <i>vs</i> 1U	*
19S <i>vs</i> 3U	**
19S <i>vs</i> 4U	**
19S <i>vs</i> 5U	**
19S <i>vs</i> 6U	*
19S <i>vs</i> 7U	**
19S <i>vs</i> 8U	*
19S <i>vs</i> 13U	**
19S <i>vs</i> 14U	**
19S <i>vs</i> 16U	*
19S <i>vs</i> 17U	**
20S <i>vs</i> 3U	*
20S <i>vs</i> 4U	*
20S <i>vs</i> 5U	*
20S <i>vs</i> 7U	*
20S <i>vs</i> 13U	*
20S <i>vs</i> 14U	*

20S vs 17U	*
21S vs 1U	*
21S vs 3U	**
21S vs 4U	**
21S vs 5U	**
21S vs 6U	*
21S vs 7U	**
21S vs 8U	*
21S vs 13U	**
21S vs 14U	**
21S vs 16U	*
21S vs 17U	**
22S vs 3U	*
22S vs 4U	**
22S vs 5U	*
22S vs 6U	*
22S vs 7U	**
22S vs 8U	*
22S vs 13U	**
22S vs 14U	**
22S vs 16U	*
22S vs 17U	*
23S vs 3U	*
23S vs 4U	*
23S vs 5U	*
23S vs 7U	*
23S vs 13U	*
23S vs 14U	*
23S vs 17U	*
25S vs 3U	*
25S vs 4U	*
25S vs 5U	*
25S vs 7U	*
25S vs 13U	*
25S vs 14U	*
25S vs 17U	*
26S vs 1U	*
26S vs 2U	*
26S vs 3U	**
26S vs 4U	**
26S vs 5U	**
26S vs 6U	**
26S vs 7U	**
26S vs 8U	**
26S vs 9U	*

26S vs 13U	**
26S vs 14U	**
26S vs 15U	*
26S vs 16U	**
26S vs 17U	**
1U vs 22U	*
1U vs 26U	*
2U vs 22U	*
2U vs 26U	*
3U vs 22U	**
3U vs 23U	*
3U vs 25U	*
3U vs 26U	**
3U vs 27U	*
4U vs 22U	**
4U vs 23U	*
4U vs 25U	*
4U vs 26U	**
4U vs 27U	*
5U vs 22U	**
5U vs 23U	*
5U vs 25U	*
5U vs 26U	**
5U vs 27U	*
6U vs 22U	**
6U vs 26U	*
7U vs 22U	**
7U vs 23U	*
7U vs 25U	*
7U vs 26U	**
7U vs 27U	*
8U vs 22U	*
8U vs 26U	*
9U vs 22U	*
9U vs 26U	*
13U vs 22U	**
13U vs 23U	**
13U vs 25U	*
13U vs 26U	**
13U vs 27U	**
14U vs 22U	**
14U vs 23U	*
14U vs 25U	*
14U vs 26U	**
14U vs 27U	*

16U vs 22U	*
16U vs 26U	*
17U vs 22U	**
17U vs 23U	*
17U vs 25U	*
17U vs 26U	**
17U vs 27U	*

* $p < 0.05$, ** $p < 0.01$

To compare the results obtained for all combination of parameters a Kruskal-Wallis test with a Dunn's post-hoc test were performed. 78 combinations were compared, and the medians varied significantly at level $p < 0.0001$, while Kruskal-Wallis statistic for the whole set of combinations was 377.3.

The medians are encoded according to the codes of extracts that they refer to. Codes are presented in Materials and Methods in the main body of manuscript (Table 5).

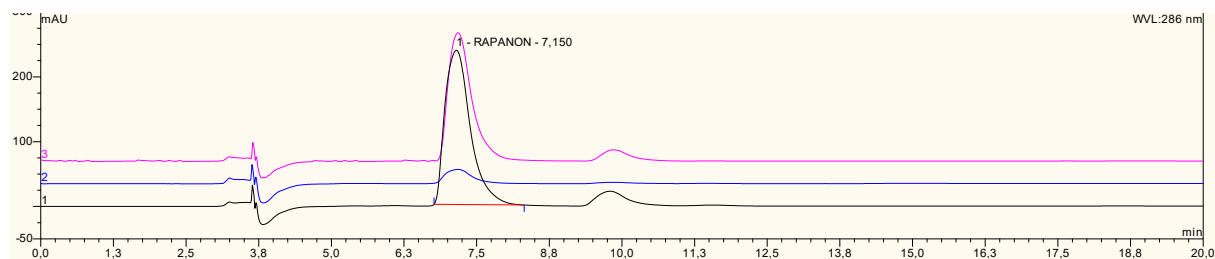


Figure S1. Representative HPLC chromatograms showing content of rapanone in extracts from leaves of white-berried *A. crenata* Sims, obtained by different methods (HRE, SE, UAE).

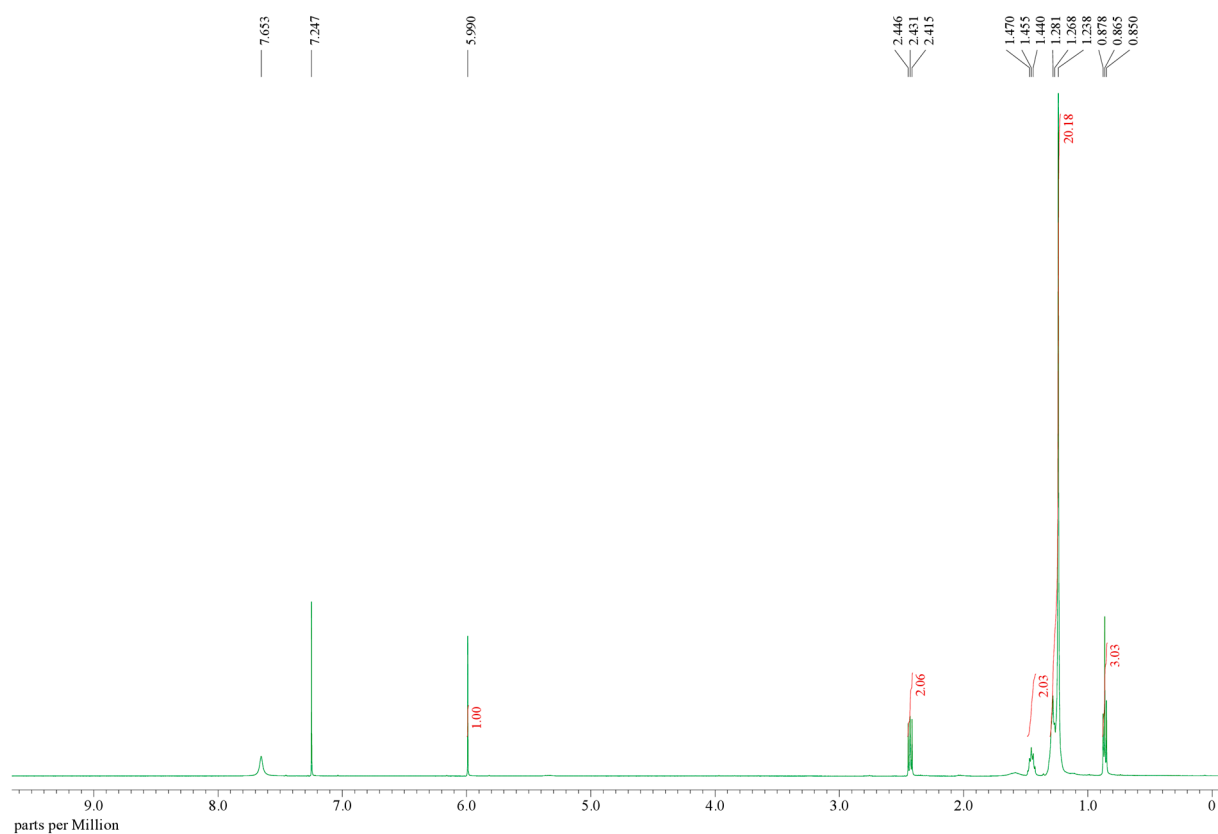


Figure S2. ¹H NMR data for rapanone.

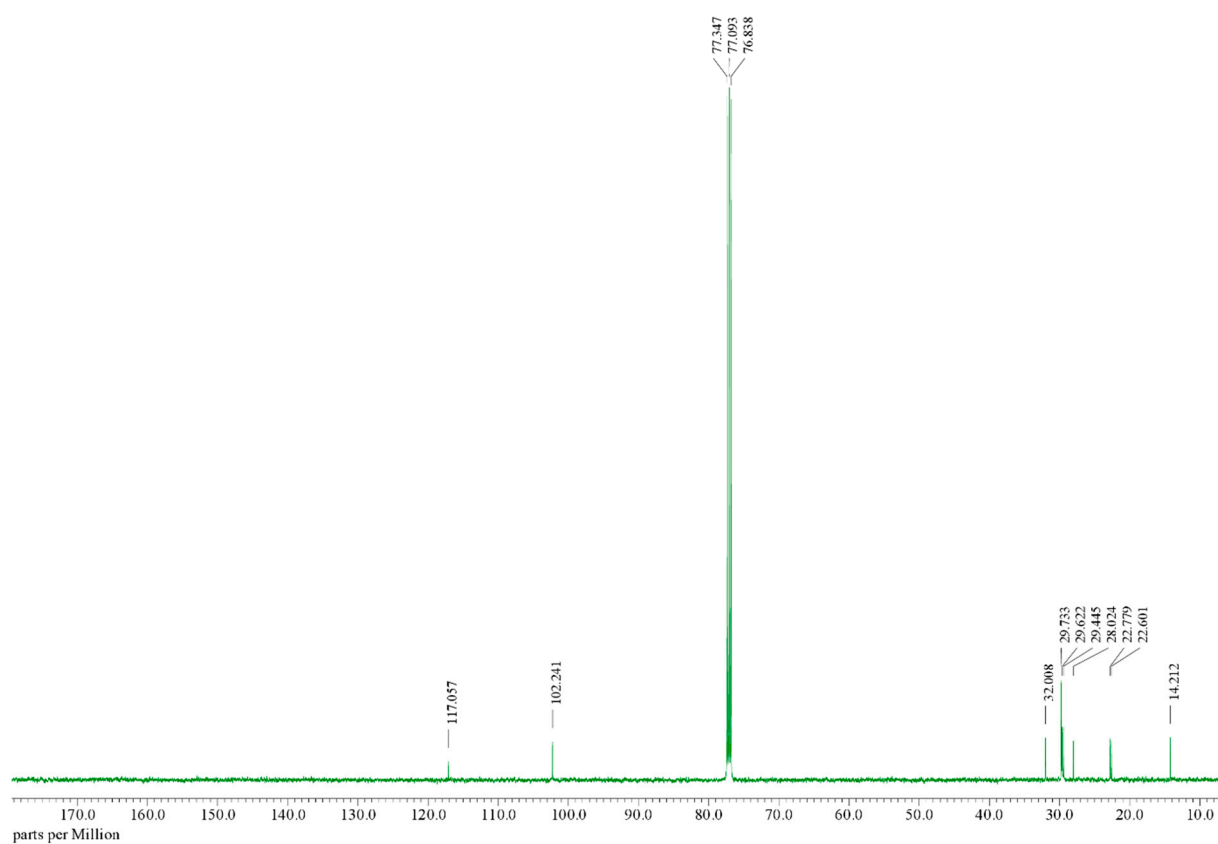


Figure S3. ¹³C NMR data for rapanone.

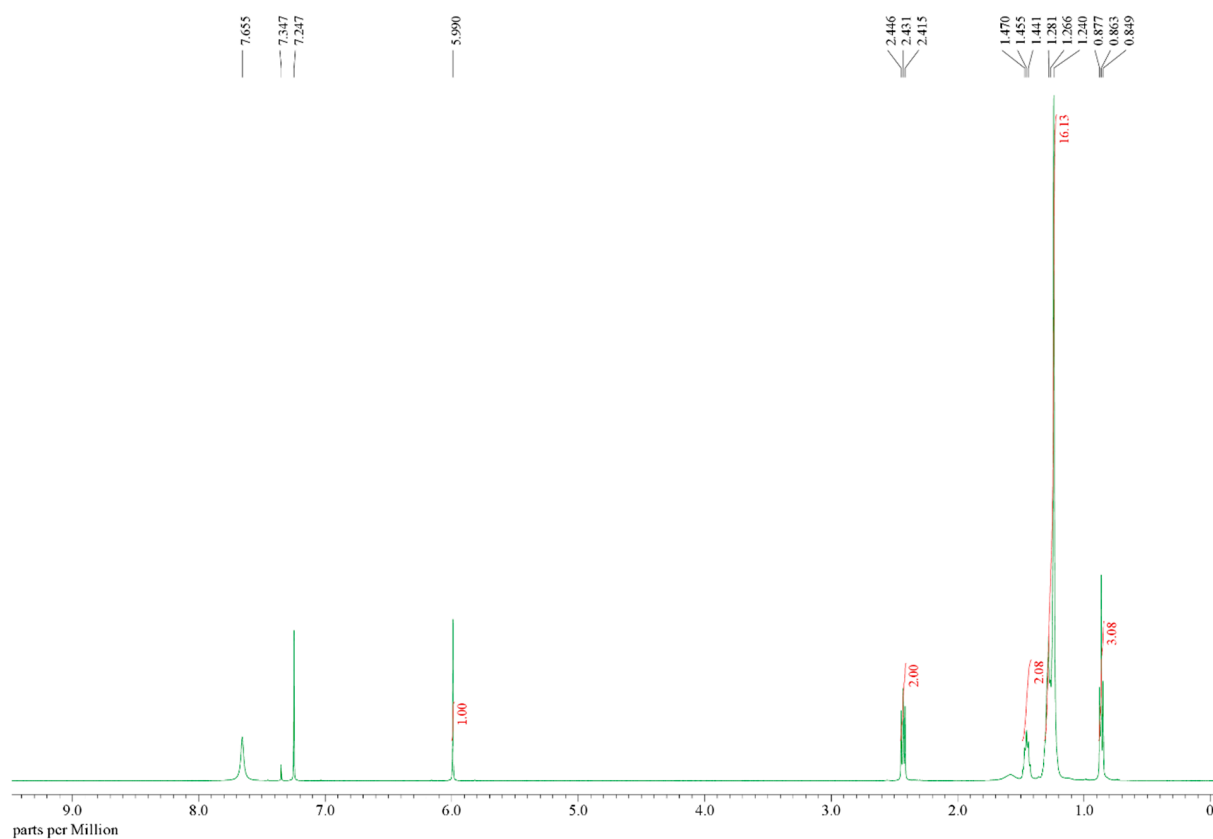


Figure S4. ¹H NMR data for embelin.

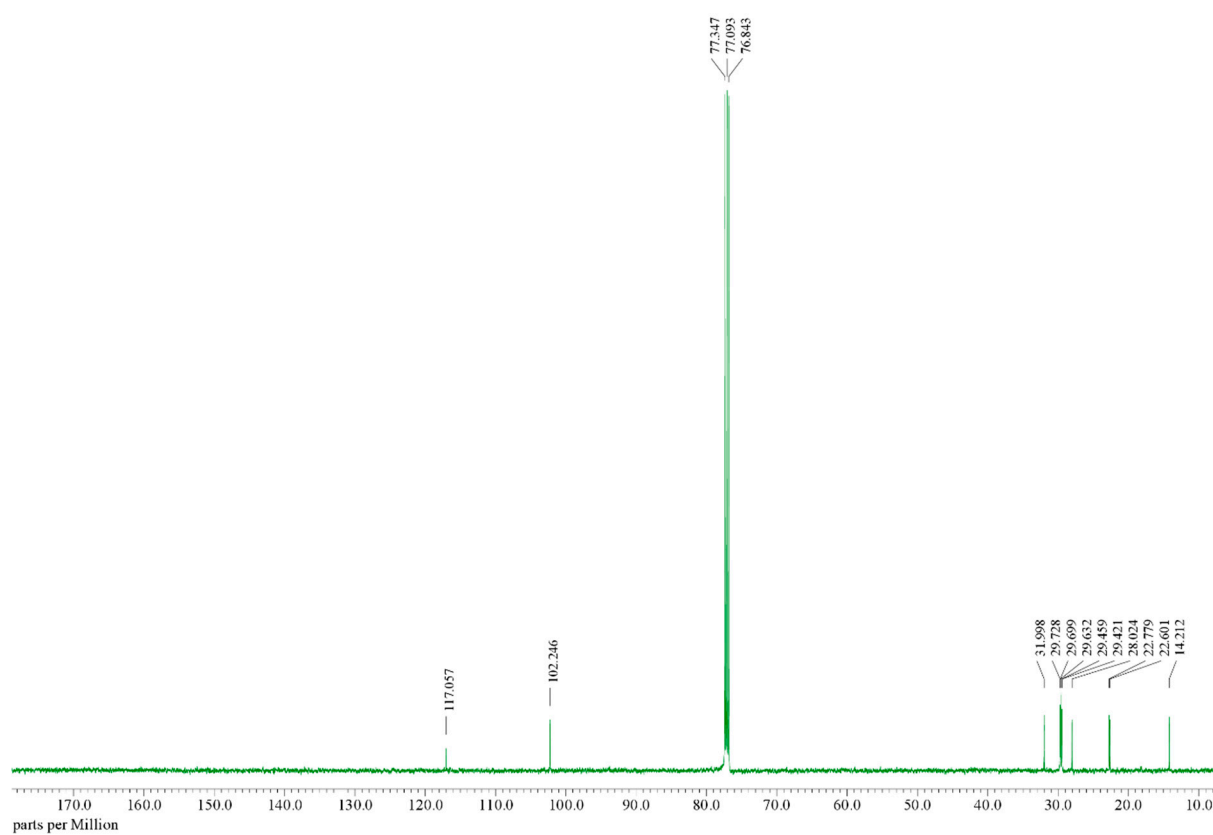


Figure S5. ¹³C NMR data for embelin.