

Supplementary Material: Toxicity of Carlina Oxide – a Natural Polyacetylene from the *Carlina acaulis* Roots – *in vitro* and *in vivo* study

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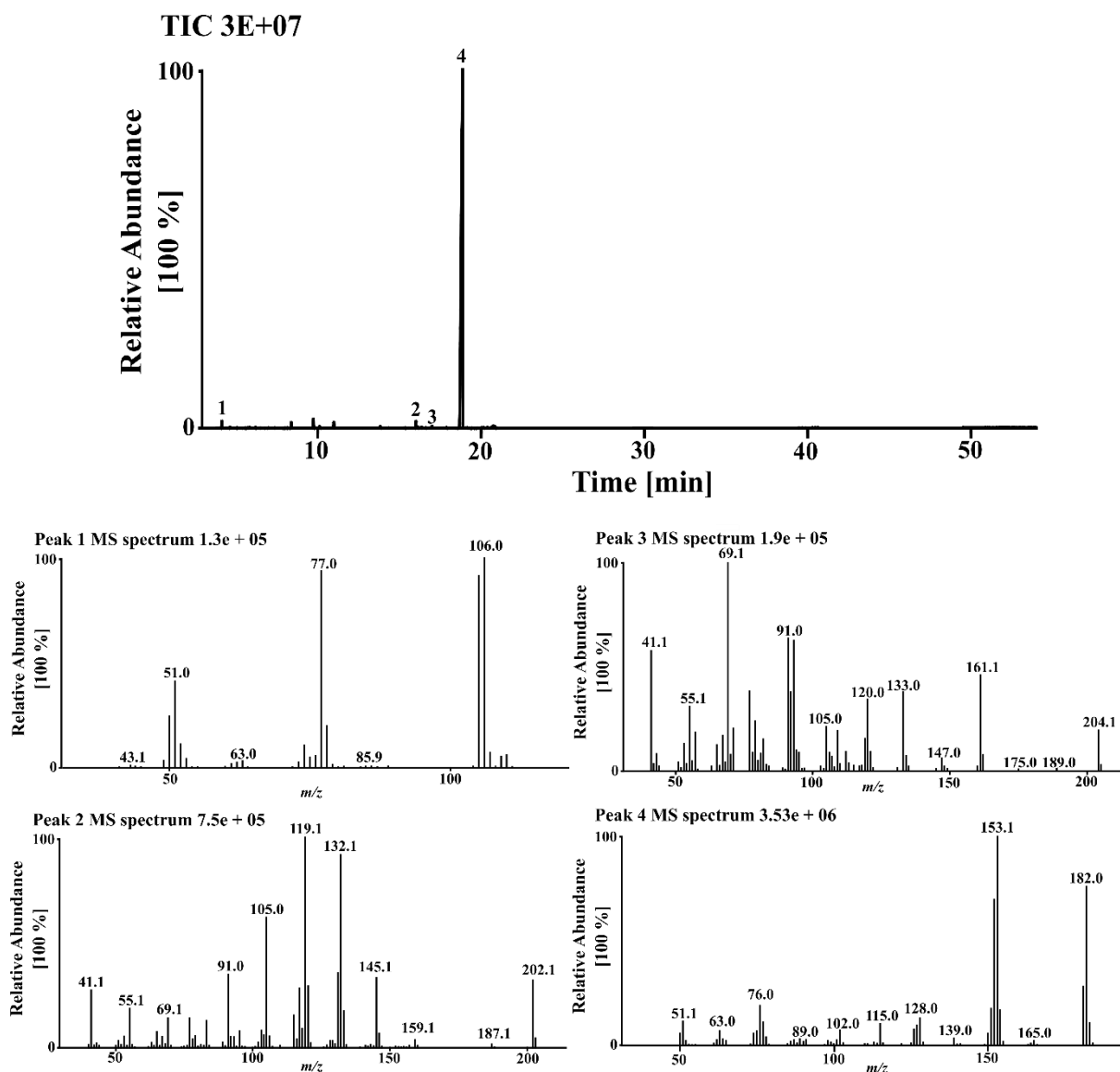


Figure S1. The total ion chromatogram and MS spectra obtained for the tested oil. 1: benzaldehyde, 2: *ar*-curcumene, 3: β -sesquiphellandrene, 4: carlina oxide.

Table S1. Chemical composition (% ± SD) of *Carlina acaulis* L. root essential oil.

Peak no.	Compound	RT (min)	RI	RI*	Mass data	Content %
1	benzaldehyde	4.11	960	952	106.0 (M+), 85.9, 77.0, 63.0, 51.0, 43.1	0.57 ± 0.002
2	ar-curcumene	16.01	1485	1481	202.1 (M+), 187.1, 159.1, 145.1, 132.1, 119.1, 105.0, 91.0, 69.1, 55.1, 41.1	0.56 ± 0.031
3	β-sesquiphellandrene	16.98	1526	1523	204.1 (M+), 189.0, 175.0, 161.1, 147.0, 133.0, 120.0, 105.0, 91.0, 69.1, 55.1, 41.1	0.16 ± 0.012
4	carlina oxide	18.87	1608	1613.1	182.0 (M+), 165.0, 153.1, 139.0, 128.0, 115.0, 102.0, 89.0, 76.0, 63.0, 51.1	96.2 ± 0.566
Total						97.49

RT – retention times; RI - retention indices relative to C8-C20 alkanes on the DB-5MS column; RI* - literature retention indices [1]; M+ - molecular ion.

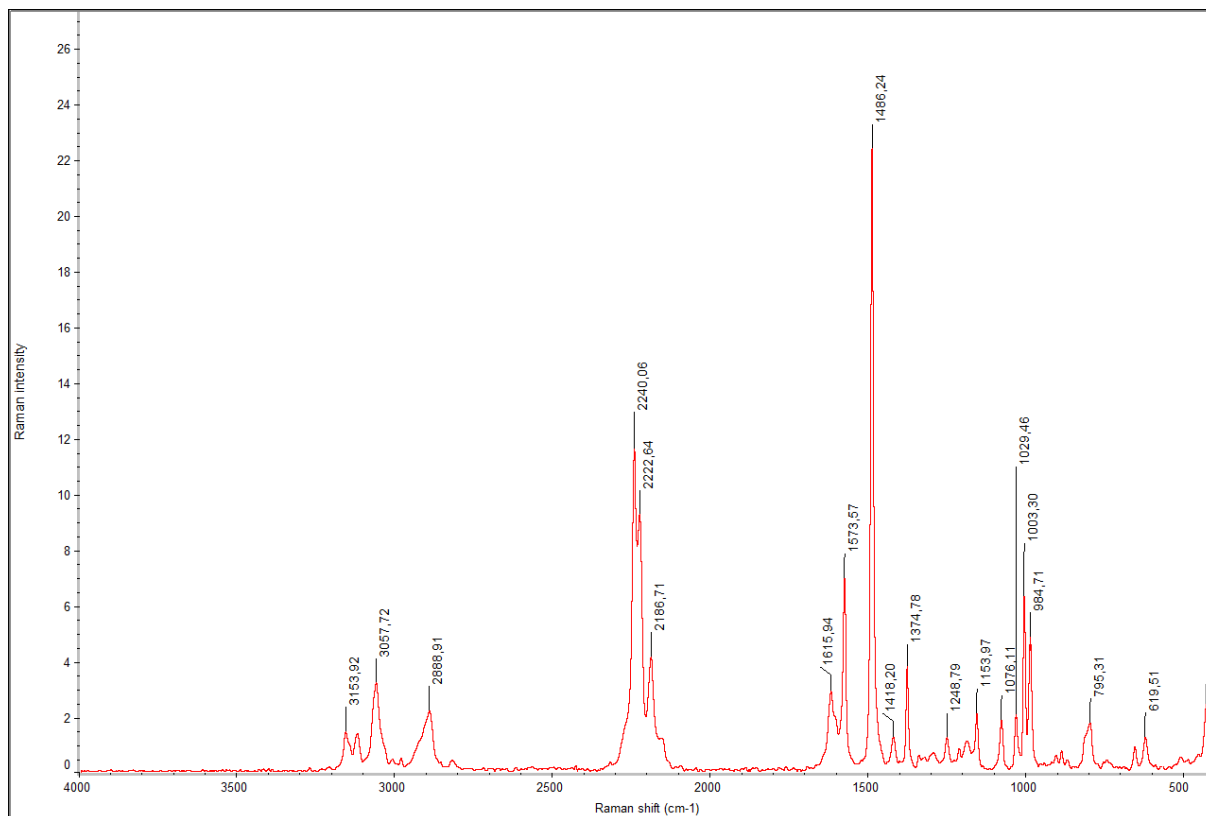


Figure S2. Raman spectrum of extracted essential oil.

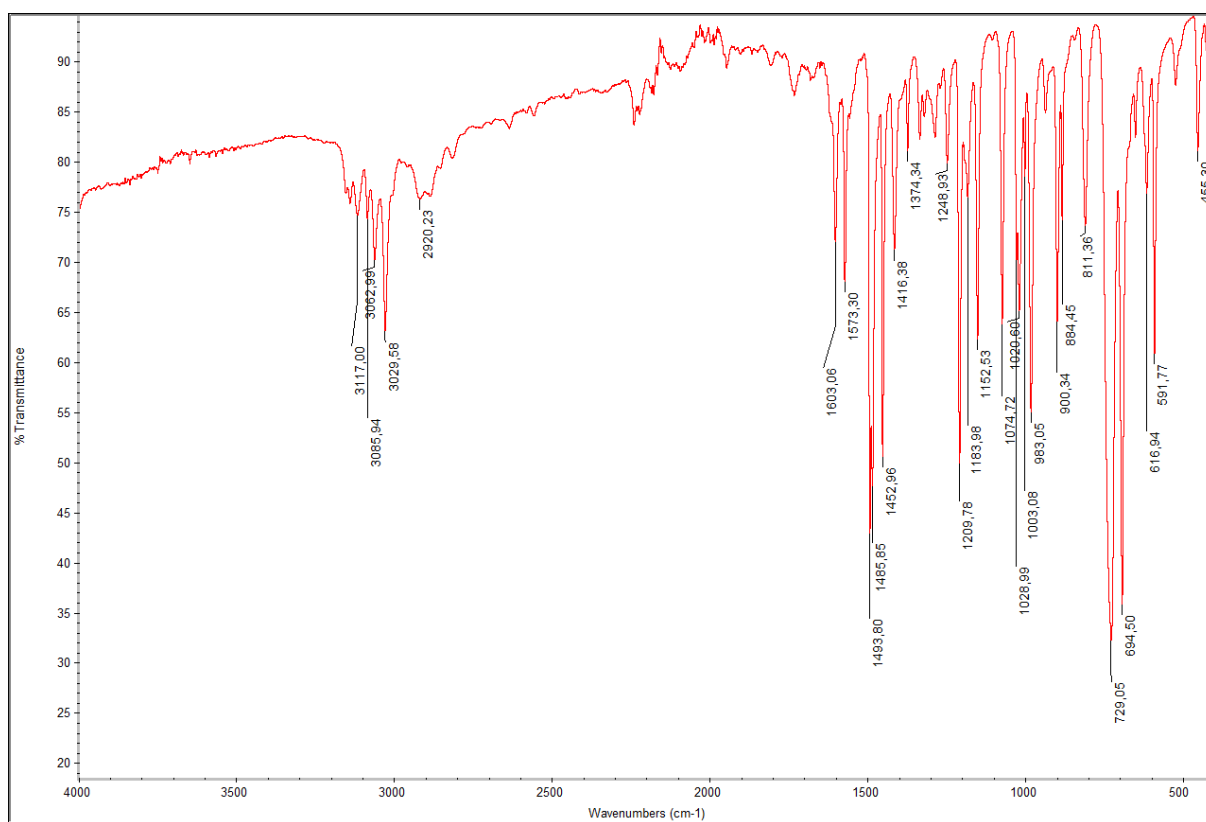


Figure S3. IR spectrum of extracted essential oil.

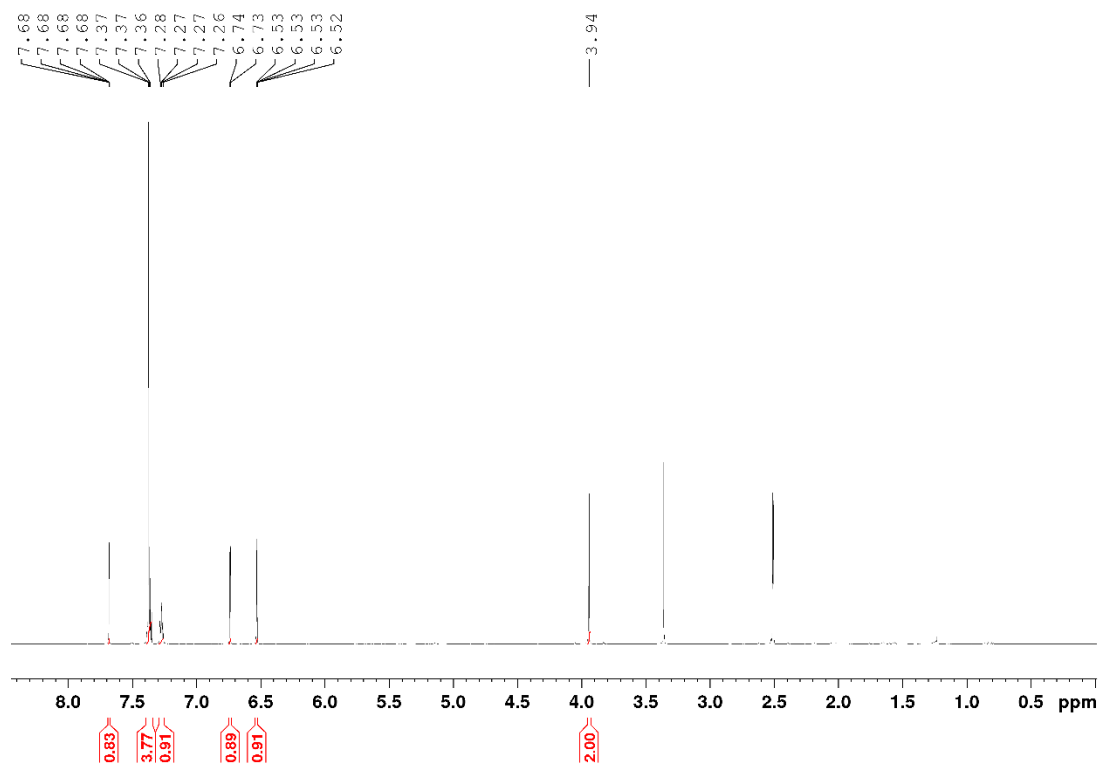


Figure S4. ^1H NMR ($\text{DMSO-}d_6$) spectrum of extracted essential oil.

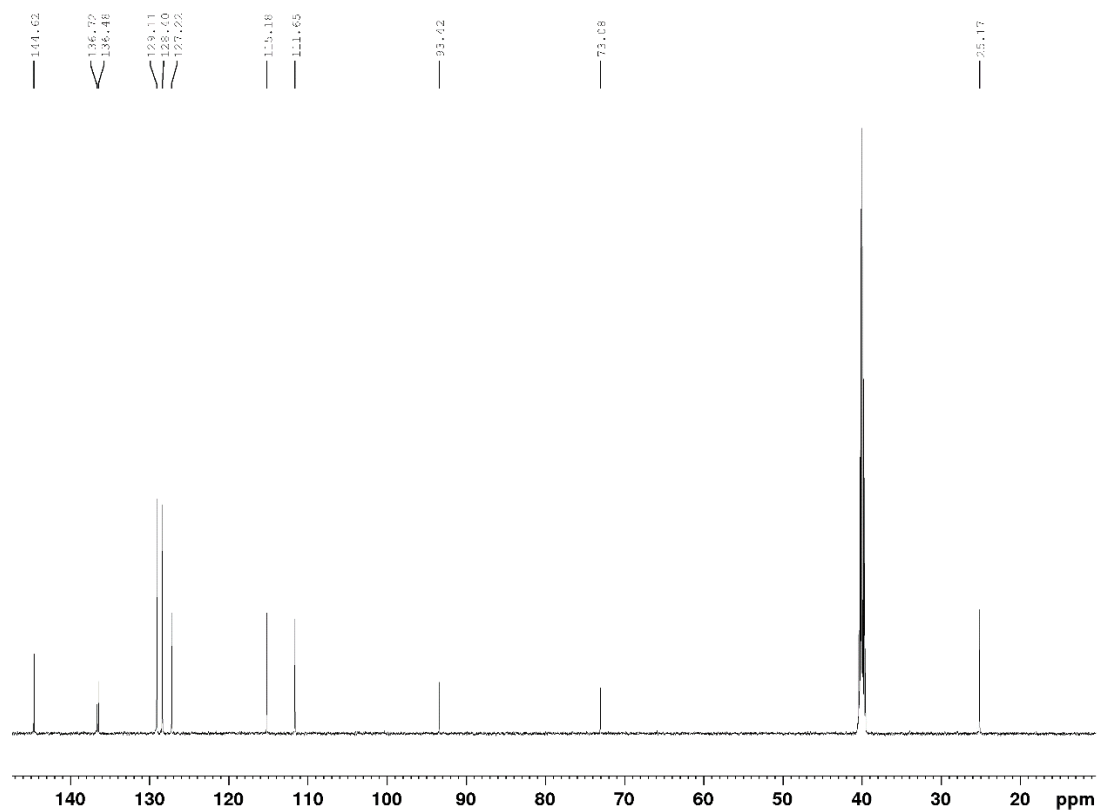


Figure S5. ^{13}C NMR ($\text{DMSO-}d_6$) spectrum of extracted essential oil.

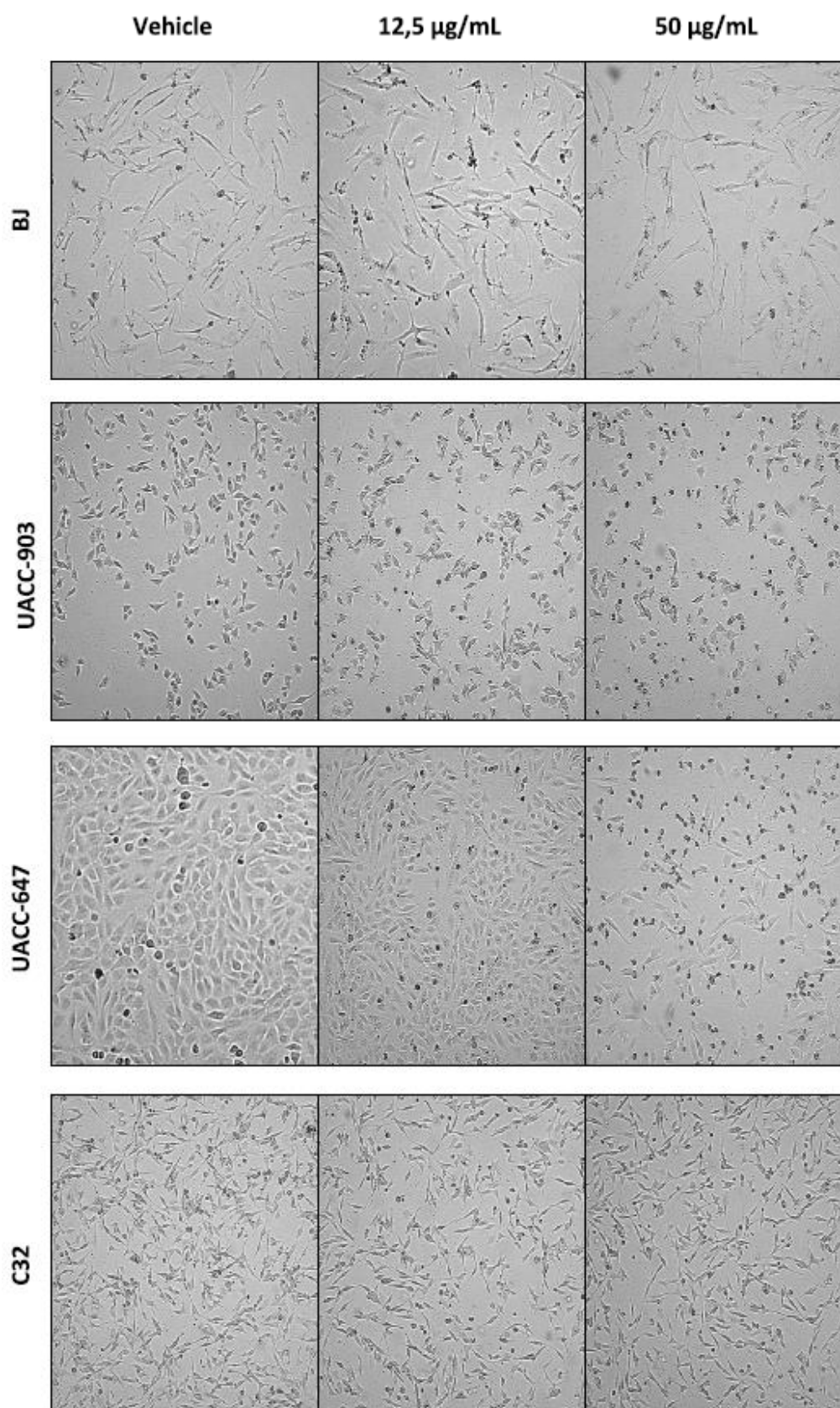


Figure S6. Representative microscopic images the BJ, UACC-903, UACC-647 and C32 cells exposed to either vehicle or carlina oxide (12,5 or 50 $\mu\text{g/mL}$) for 24 h.

References

1. Strzemiński, M.; Wójciak-Kosior, M.; Sowa, I.; Agacka-Mołdoch, M.; Drączkowski, P.; Matusiuk, D.; Kurach, Ł.; Kocjan, R.; Dresler, S. Application of Raman spectroscopy for direct analysis of *Carlina acanthifolia* subsp. *utzka* root essential oil. *Talanta* **2017**, *174*, 633–637.