

Supporting Information

Effect-directed discovery of bioactive compounds followed by
highly targeted characterization, isolation and identification,
exemplarily shown for *Solidago virgaurea*

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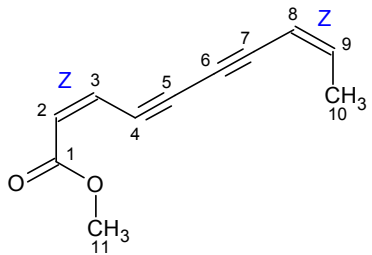
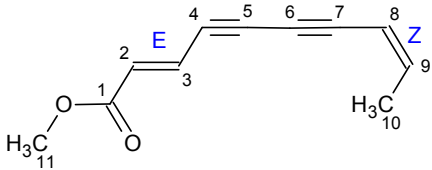
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Table S-1. NMR spectral data and structure of Sv1 and Sv2

	Sv1		Sv2	
no.	¹ H (ppm)	¹³ C (ppm)	¹ H (ppm)	¹³ C (ppm)
1	-	166.36	-	167.27
2	6.29 (d, <i>J</i> = 11.7 Hz, 1H)	131.84	6.38 (d, <i>J</i> = 15.9 Hz, 1H)	133.40
3	6.38 (dd, <i>J</i> = 11.7, 0.7 Hz, 1H)	123.17	6.86 (dd, <i>J</i> = 15.9, 0.7 Hz, 1H)	124.95
4	-	78.87	-	78.98
5	-	85.90	-	82.81
6	-	78.50	-	78.00
7	-	83.92	-	83.26
8	5.66 (m, 1H)	109.66	5.64 (m, 1H)	109.42
9	6.29 (m, 1H)	145.14	6.30 (m, 1H)	145.69
10	1.93 (dd, <i>J</i> = 6.9, 1.7 Hz, 3H)	16.64	1.92 (dd, <i>J</i> = 6.6, 1.7 Hz, 3H)	16.76
11	3.762 (s, 3H)	52.10	3.758 (s, 3H)	52.50
structure and name	 <p>2Z,8Z-matricaria ester</p>		 <p>2E,8Z-matricaria ester</p>	

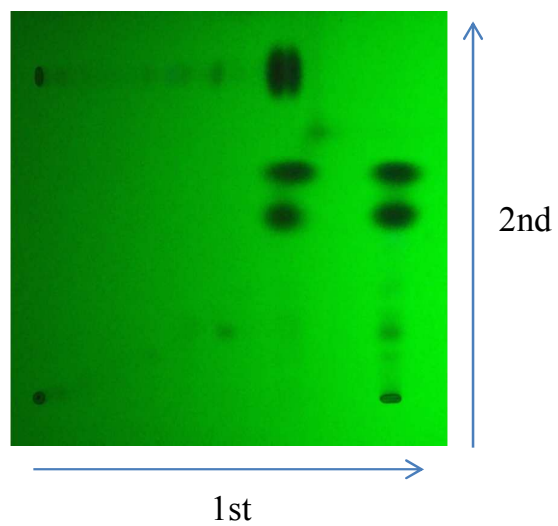


Figure S-1. 2D-HPTLC separation for compound assignment with *n*-hexane – isopropyl acetate – acetic acid (83:14:3, v/v) for the first dimension and *n*-hexane – acetone (17:3, v/v) for the second dimension, documented at UV 254 nm.

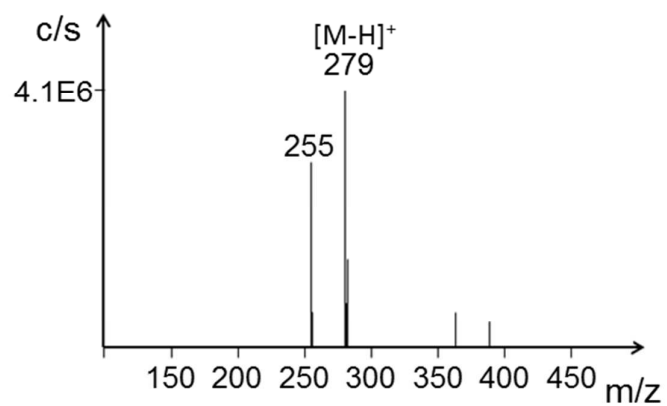


Figure S-2. Mass spectrum of the Sv4 zone in the negative ionization mode, showing the deprotonated molecule at m/z 279.

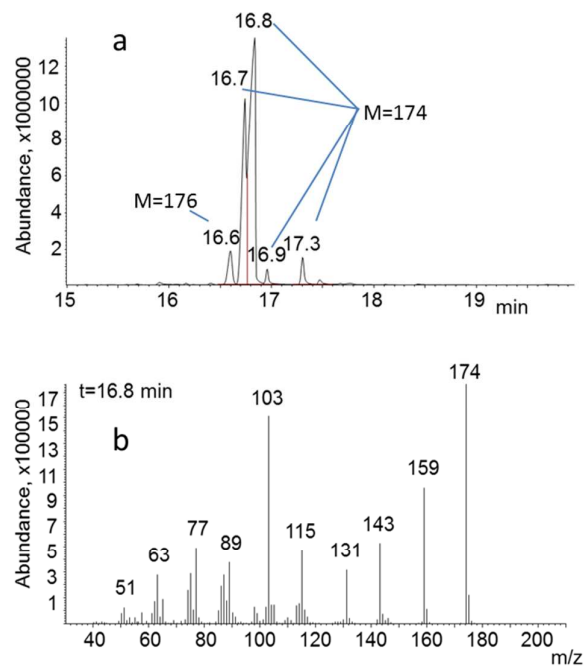


Figure S-3. SPME-GC-EI-MS (a) TIC chromatogram of European golden rod root extract and (b) mass spectrum at 16.8 min that was identical to those at 16.7, 16.9 and 17.3 min.

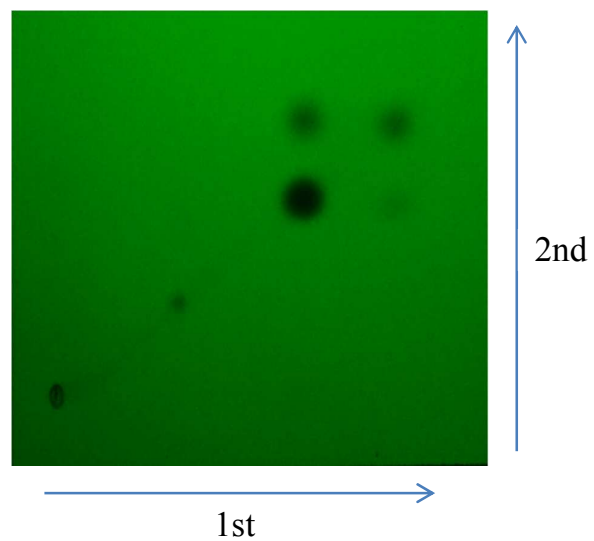


Figure S-4. 2D-HPTLC separation for isomer proof (artefact) using *n*-hexane – acetone 17:3 (v/v) in both dimensions, documented at UV 254 nm.

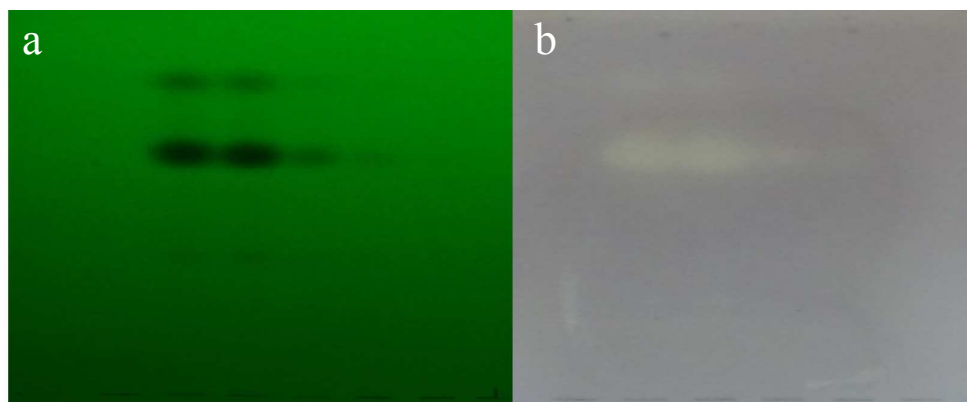


Figure S-5. HPTLC separation of the flash chromatography fractions, detected at (a) UV 254 nm and (b) after the *B. subtilis* bioassay.

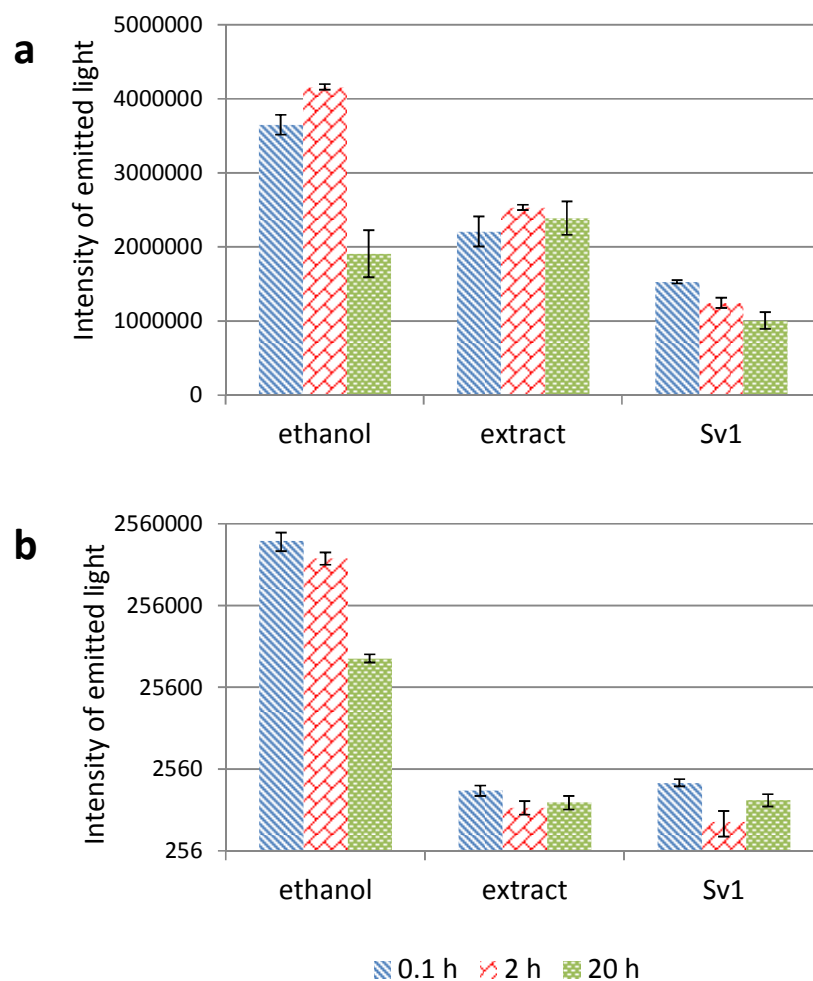
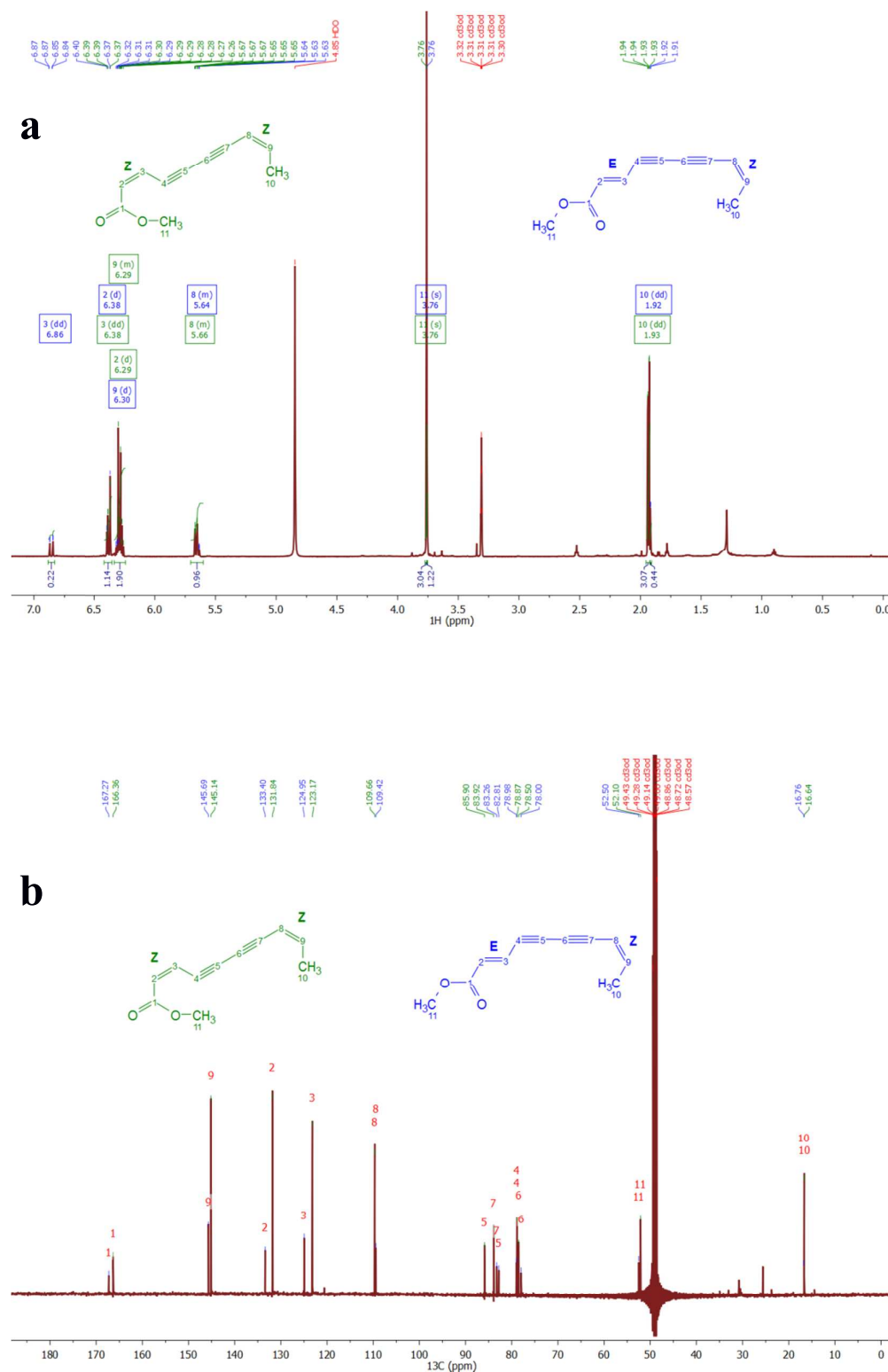


Figure S-6. Luminometric detection ($n = 3$) of the inhibiting activity of European golden rod root extract and its main bioactive component Sv1 against (a) luminescent *Pseudomonas syringae* pv. *maculicola* and (b) *Aliivibrio fischeri*; their solvent ethanol was used as negative control.



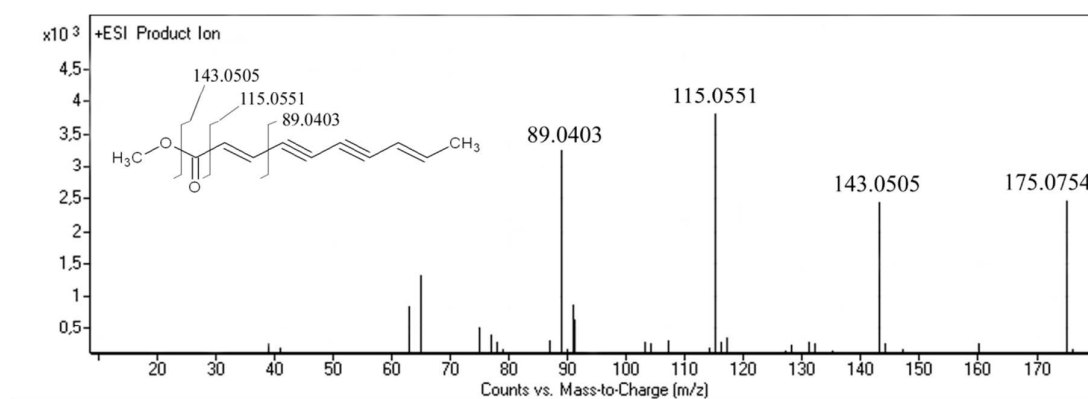


Figure S-8. Positive ion MS² spectrum and proposed fragmentation pattern of matricaria ester.