Supplementay Material to:

New insights into the Chemical Composition of *Baccharis palustris* Heering (Asteraceae) Essential Oil

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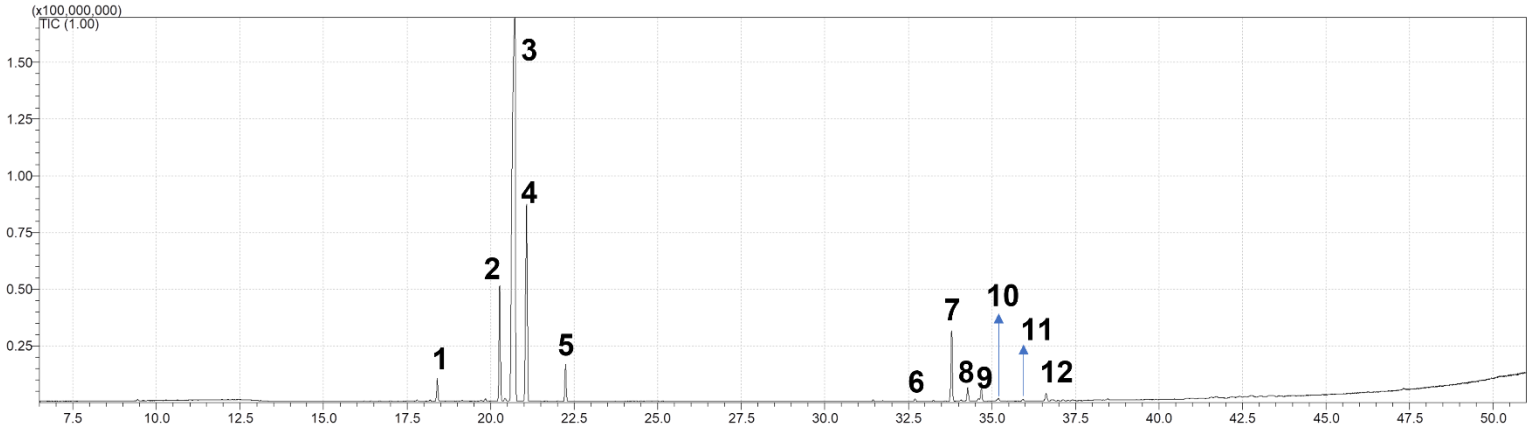

Figure S1. HRGC/qMS profile of *B. palustris* essential oil in Rxi-1MS capillary column (60 m x 0.25 mm x 0.25 µm). Peak identification: **1.** EHM (3-ethylidene-2-methyl-1-hexen-4-yne; tentative), **2.** (*trans*)-β-ocimene, **3.** baccharisdyine, **4.** 7-(*cis*)-dehydrobaccharisdyine, **5.** 7-(*trans*)-dehydrobaccharisdyine, **6.** (*trans*)-β-caryophyllene, **7.** (*cis*)-lachnophyllum acid methyl ester, **8.** germacrene D, **9.** byciclogermacrene, **10.** δ-cadinene, **11.** (*trans*)-nerolidol, **12.** spathulenol + germacrene D-4-ol. Oven program: 50°C (5 min), 5°C/min, 280°C (0 min). Injector temperature: 280°C (Rxi-1MS), interface temperature: 280°C (Rxi-1MS).

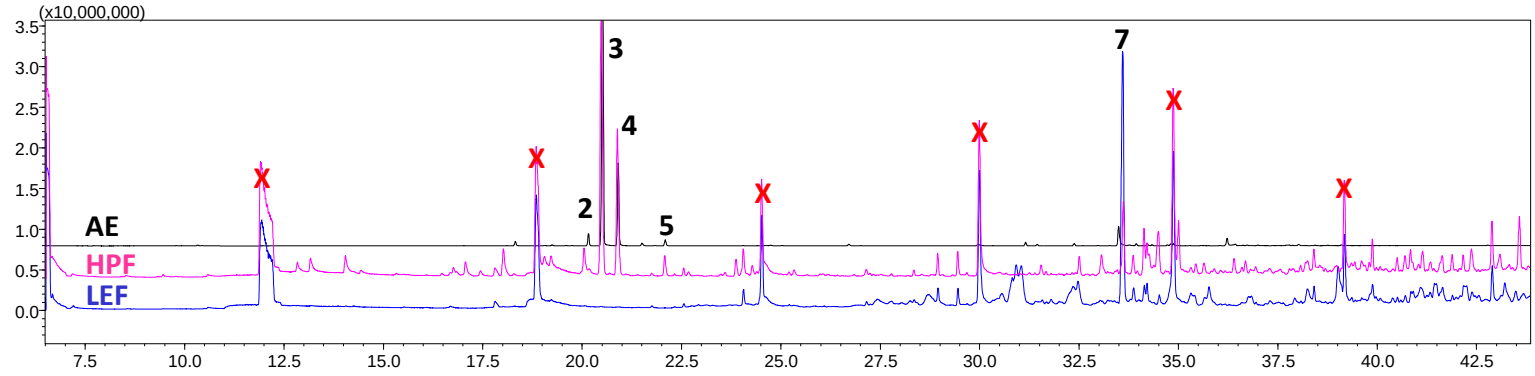

Figure S2. HRGC/qMS chromatogram of *B. palustris* essential oil and its fractions obtained after preparative TLC: HPF (hydrocarbon polyacetylene fraction) and LEF (lachnophyllum acid methyl esters fraction). Experimental conditions and peak numbering as in Figure S1. The peaks with a red cross are silylated by-products (artifacts) from the overnight silica gel extraction and/or column bleeding.

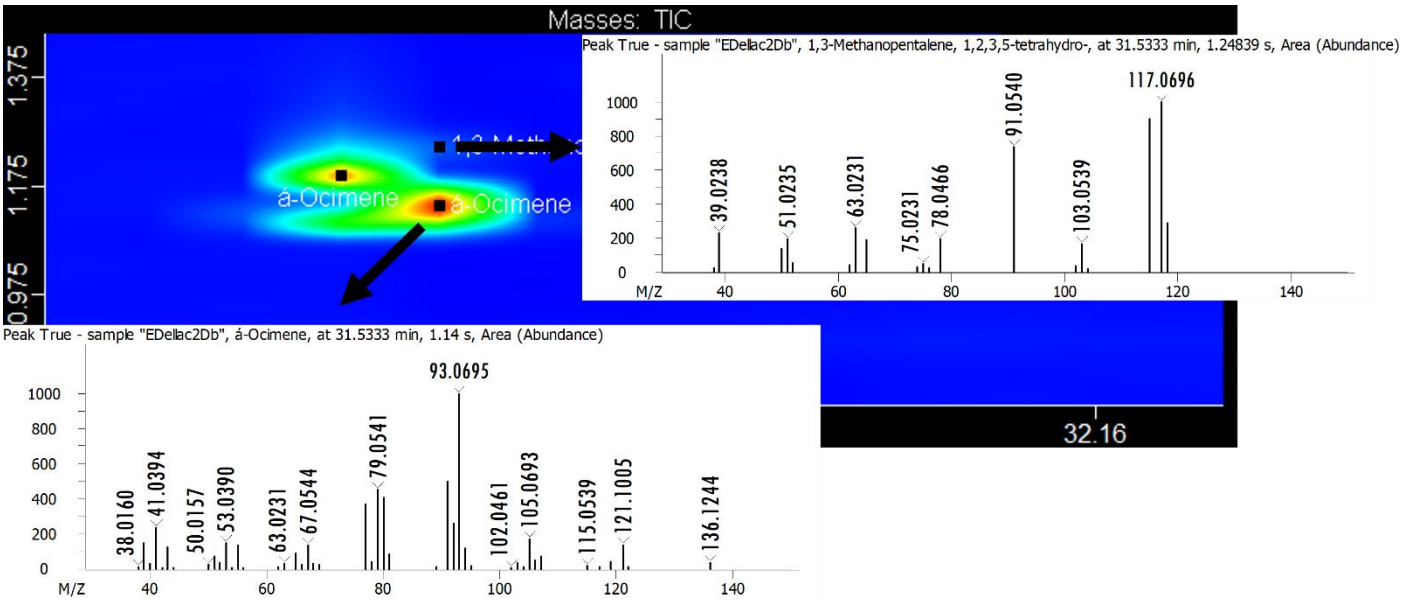

Figure S3. GCxGC/TOF contour plot showing a co-elution of (*trans*)-β-ocimene with an unknown component (molecular ion and base peak at 118 and 117 m/z, respectively), probably a positional isomer of baccharisdyine (see Figure S3 for its mass spectrum).

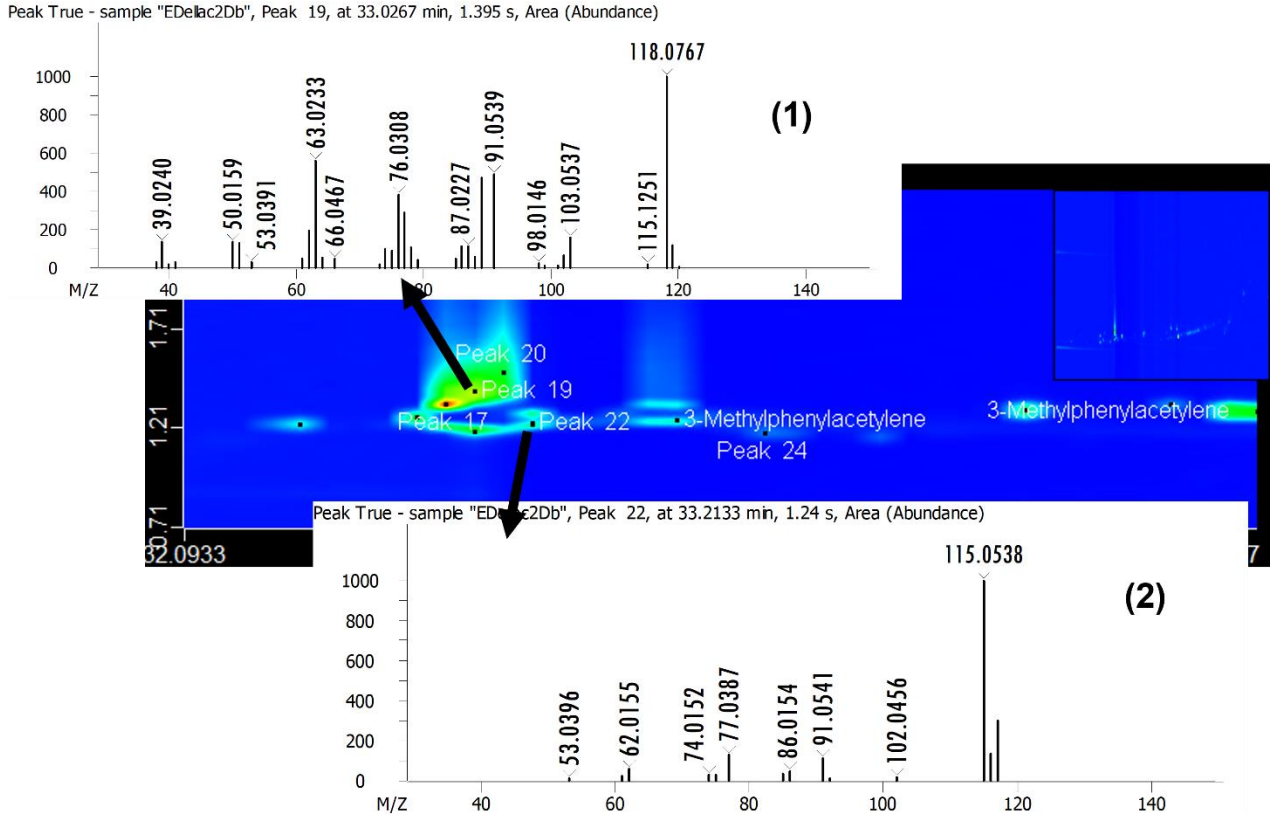

Figure S4. GCxGC/TOF contour plot showing a co-elution of baccharisdyine (**1**, peak #19) and several components, among them, **2** (peak #22, presumably, a polyacetylene).

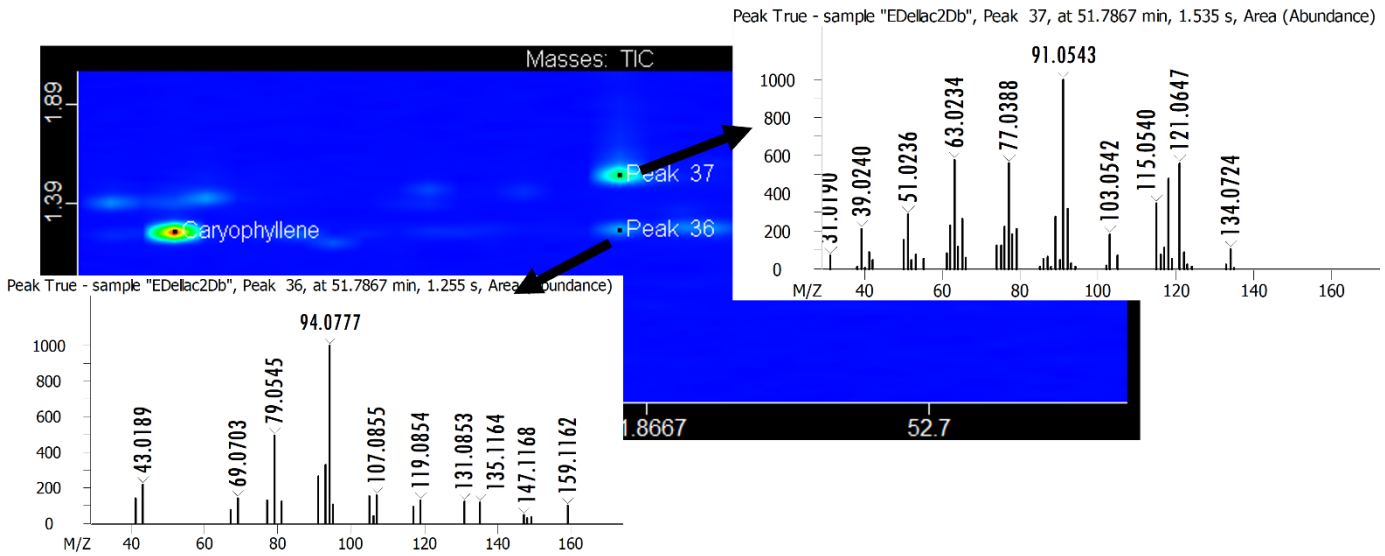

Figure S5. GCxGC/TOF contour plot showing a co-elution of two unknown MinTraCs of *B. palustris* essential oil (peaks #37 and #36.

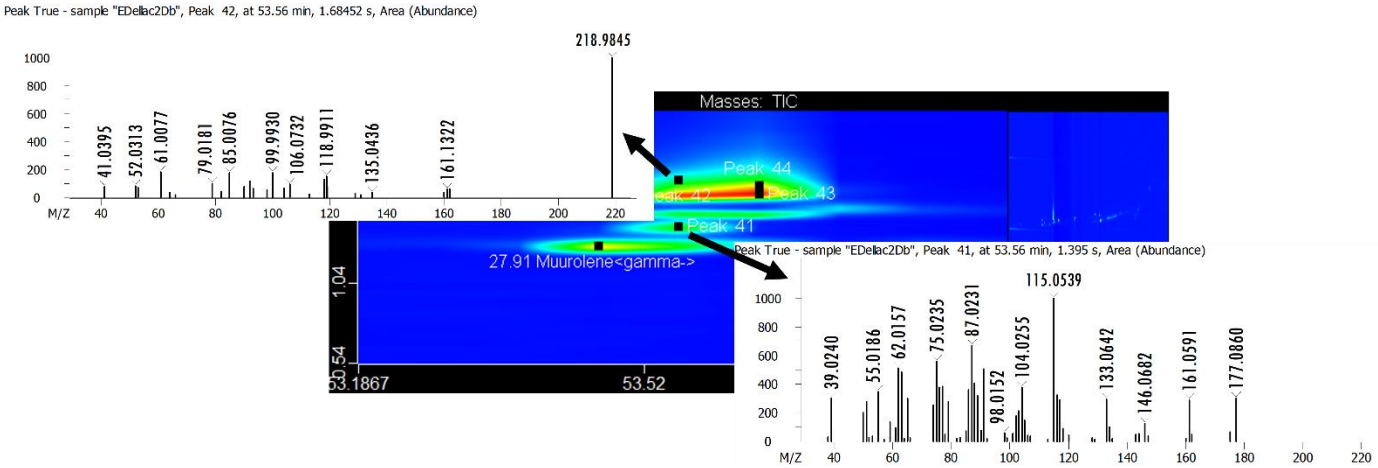

Figure S6. GCxGC/TOF contour plot showing a co-elution of two unknown MinTraCs of *B. palustris* essential oil (peaks #41 and #42). The co-elution of peaks #43 and #44 is shown as Figure 2 in the main text of this article.

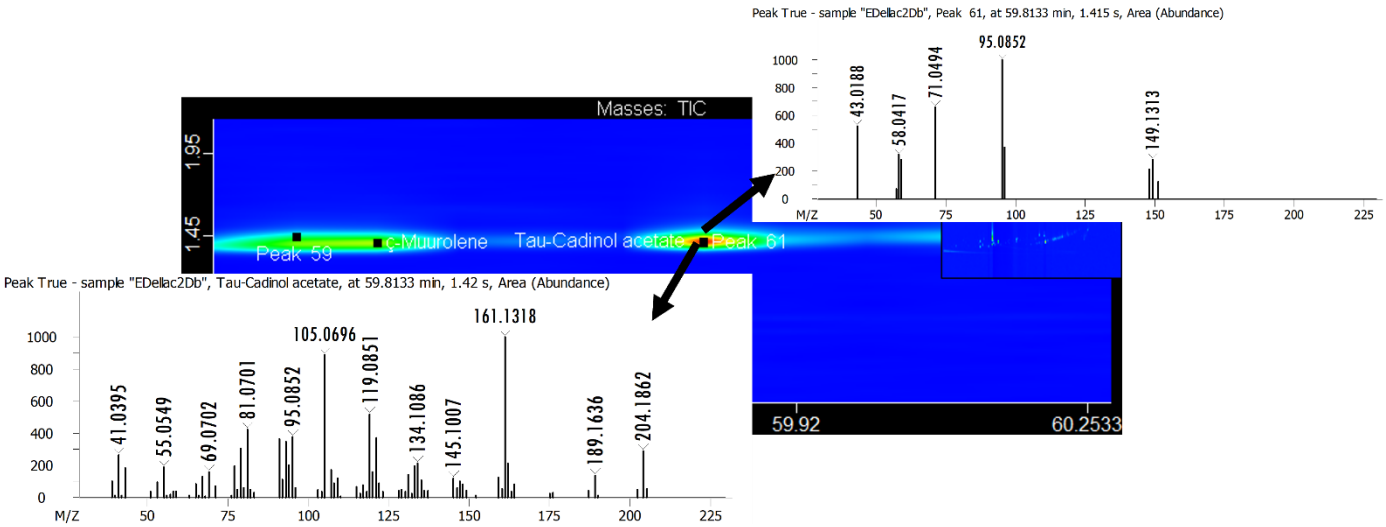

Figure S7. GCxGC/TOF contour plot showing a co-elution of the tentative peak of *epi*-α-cadinol acetate (synonym: ζ-cadinol acetate) and an unknown component of *B. palustris* essential oil (peak #61).

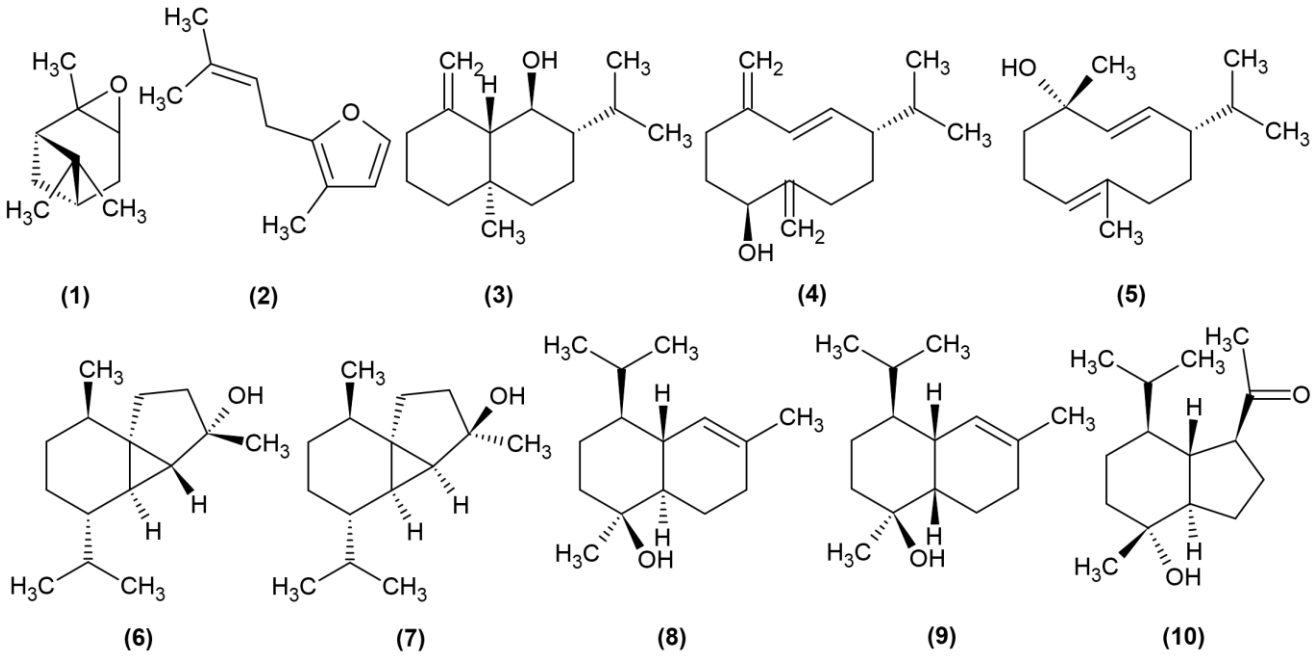

Figure S8. Structure of ten terpenoids identified as MinTraCs (**1-10**) for the first time in *B. palustris* essential oil. **1**: α-pinene oxide, **2:** rosefuran, **3:** junenol, **4:** germacra-4(15),5,10(14)-trien-1-β-ol, **5:** germacrene D-4-ol, **6:** cubebol, **7:** *epi*-cubebol, **8:** *epi*-α-cadinol, **9:** *epi*-α-muurolol, and **10:** oplopanone. Structures according to Adams (2017) [20] and Linstrom & Mallard (2023) [22].

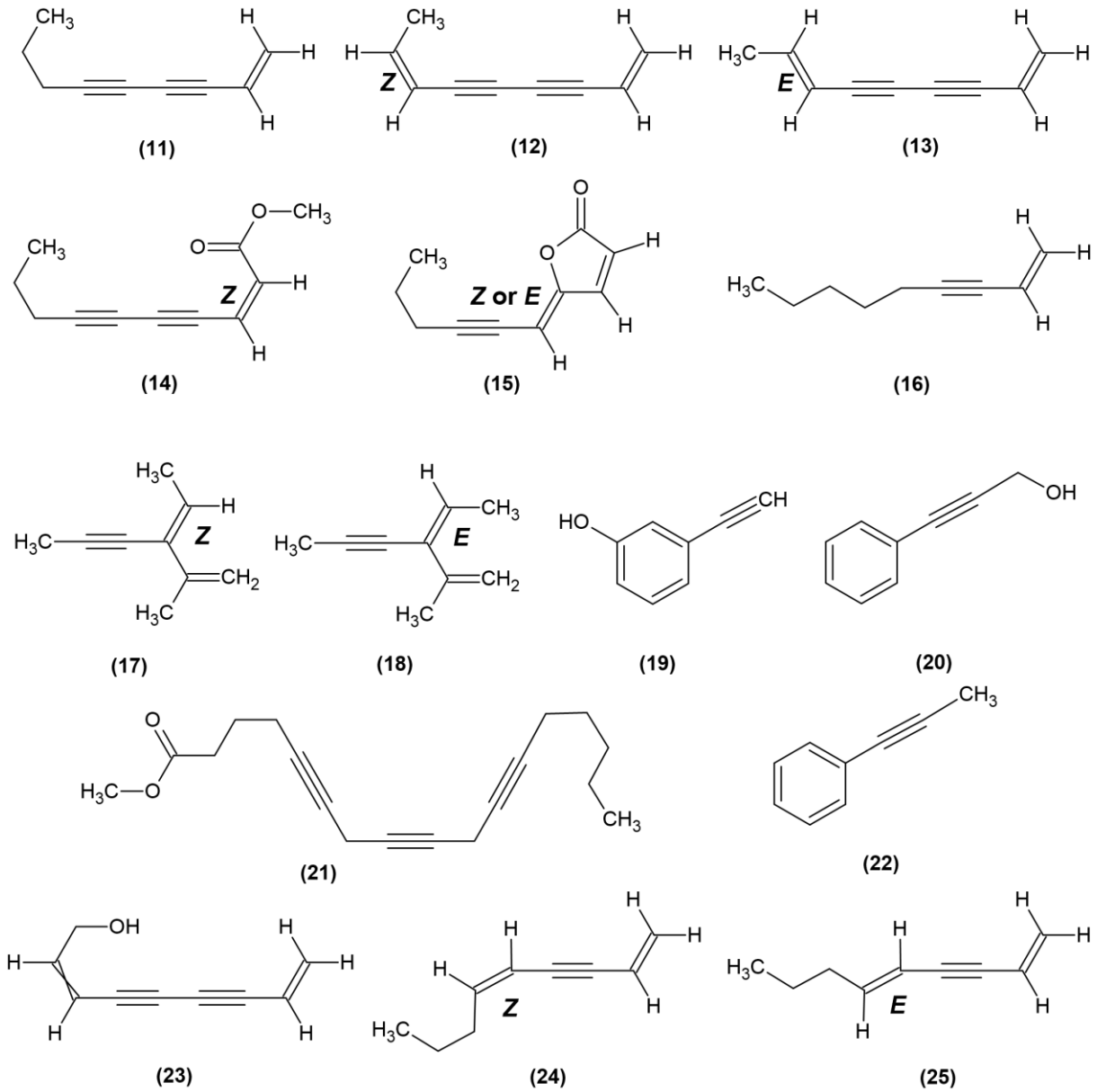

Figure S9. Structure of the polyacetylenes identified (**11-15**), tentatively identified (**16-21**) or hypothesized (**23-25**) as MinTraCs in *B. palustris* essential oil; **22** is a supposed structure which was not confirmed for this oil in our previous study (see the main text) [11]. Structures according to Linstrom & Mallard (2023) [22] and Minteguiaga *et al.* (2022) [11].