**Supplementary information**

**Development of New Resolvin D1 Analogues: Acellular and Computational Approaches to Study Their Antioxidant Activities**

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**RvD1 analogue 1:**

**A graph with different colored lines

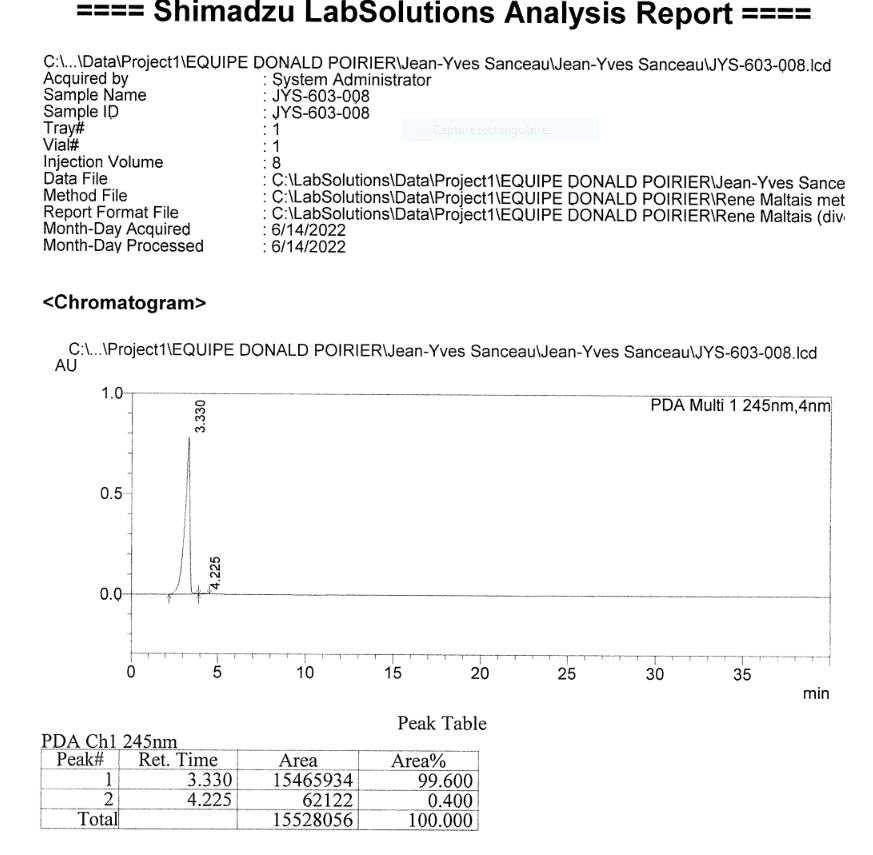
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**Figure S1:** 1H NMR spectrum analogue 1

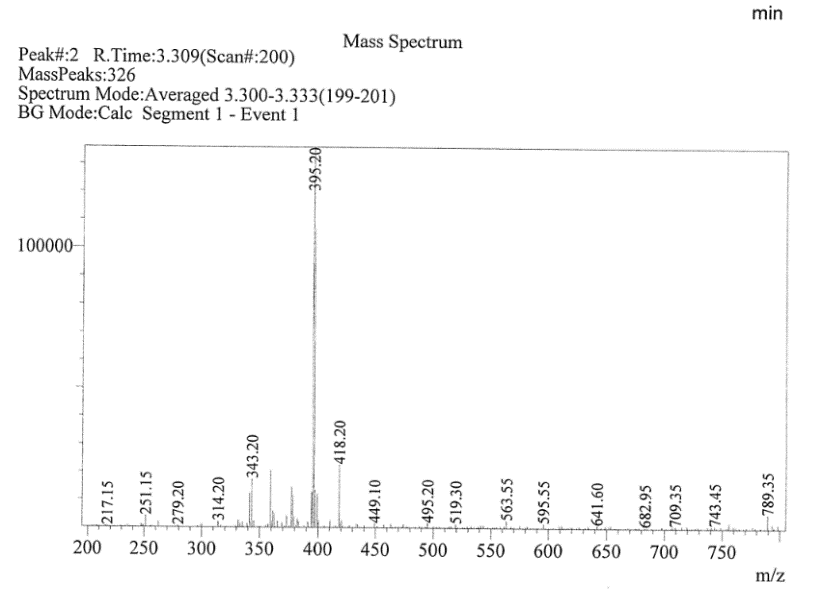
**A graph of a chemical reaction

Description automatically generated**

**Figure S2:** 13C NMR spectrum analogue 1



**Figure S3:** LCMS chromatogram analogue 1



**Figure S4:** Mass spectrum analogue 1

**RvD1 analogue 2:**



**Figure S5:** 1H NMR spectrum analogue 2



**Figure S6:** 13C NMR spectrum analogue 2

A graph on a paper

Description automatically generated

**Figure S7:** LCMS chromatogram analogue 2

A graph with numbers and lines

Description automatically generated

**Figure S8**: Mass spectrum analogue 2

**Mulliken Charge Distribution:**

A molecule structure with white and grey spheres

Description automatically generated

**Figure S9:** Mulliken charge distribution for Trolox

A molecule structure with numbers and spheres

Description automatically generated

**Figure S10:** Mulliken charge distribution for Ascorbic Acid

A molecule structure with red and grey balls

Description automatically generated

**Figure S11:** Mulliken charge distribution for ResolvinD1

A molecule structure with white and red balls

Description automatically generated with medium confidence

**Figure S12:** Mulliken charge distribution for analogue 1

A structure of a molecule

Description automatically generated

**Figure S13:** Mulliken charge distribution for analogue 2