

Supplementary information

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

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RvD1 analogue 1:

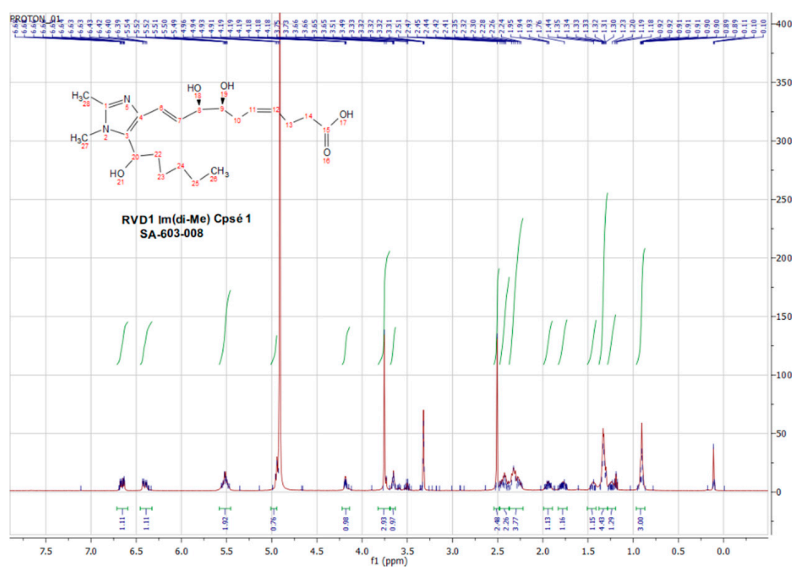


Figure S1: ^1H NMR spectrum analogue 1

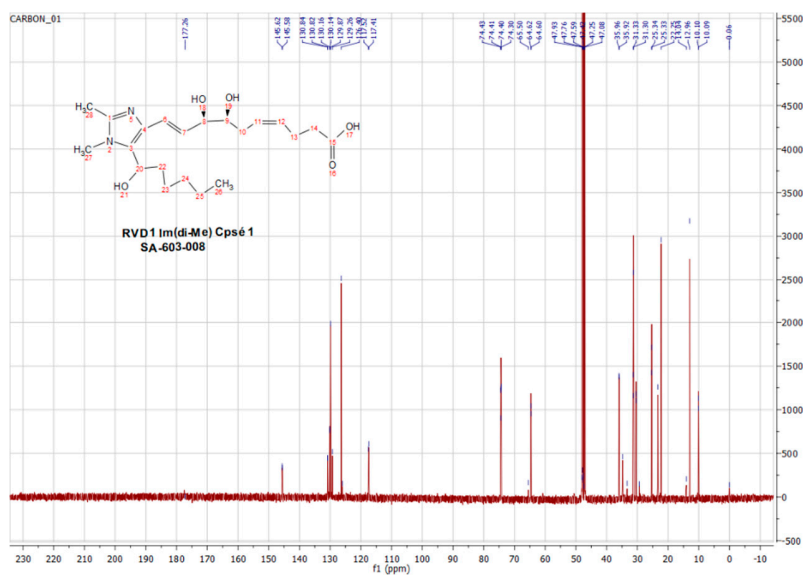


Figure S2: ^{13}C NMR spectrum analogue 1

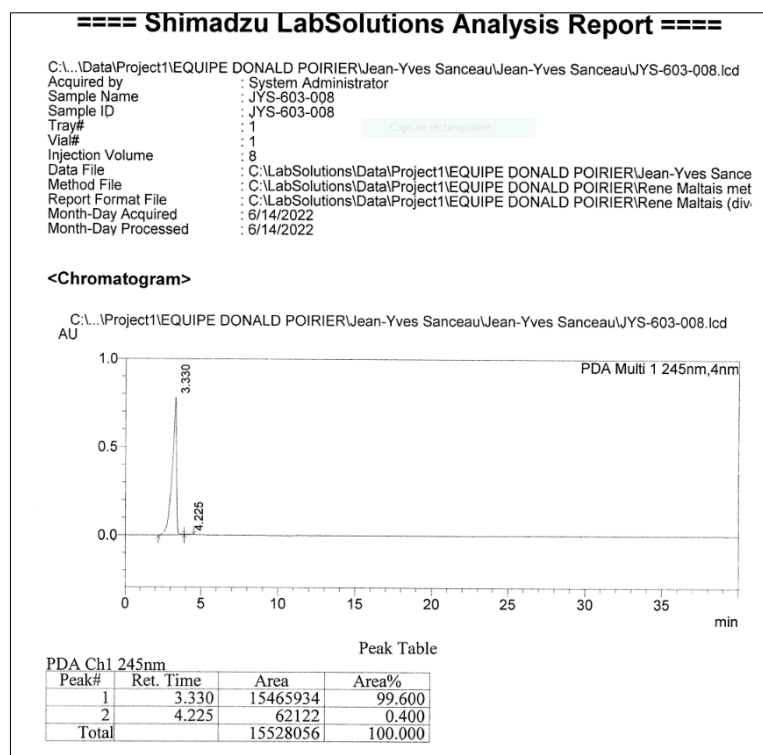


Figure S3: LCMS chromatogram analogue 1

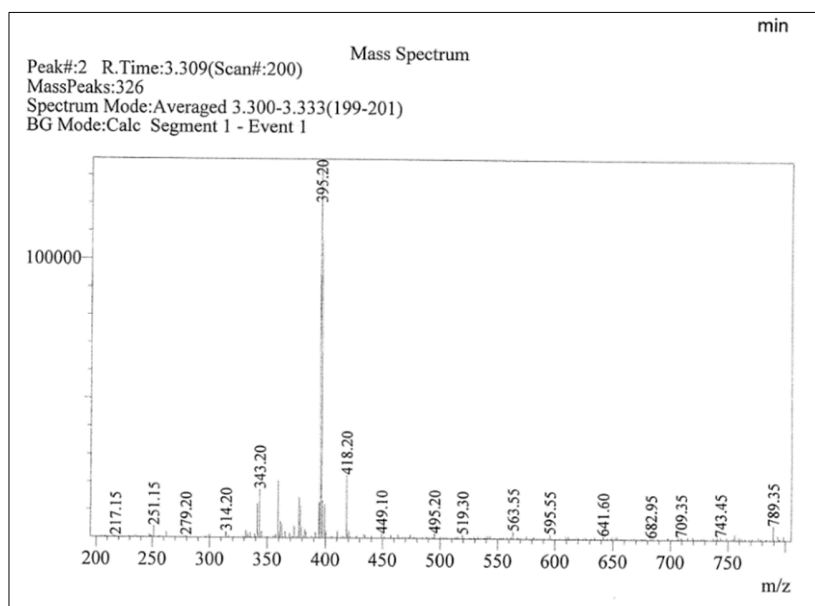


Figure S4: Mass spectrum analogue 1

RvD1 analogue 2:

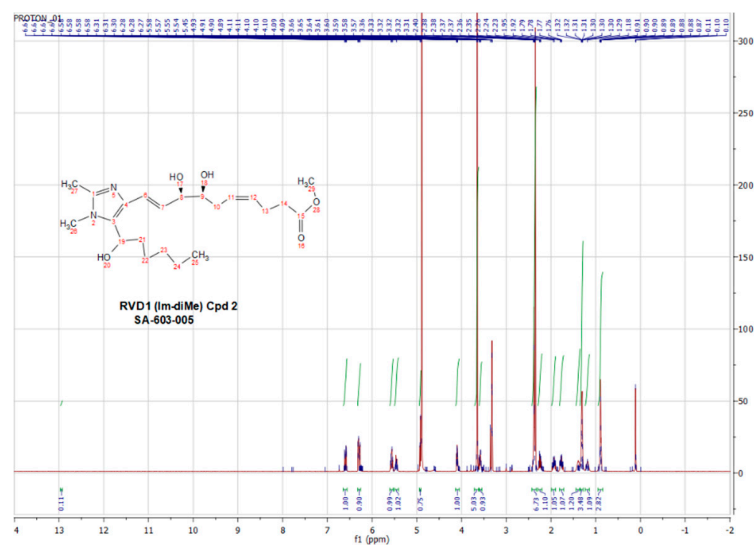


Figure S5: ^1H NMR spectrum analogue 2

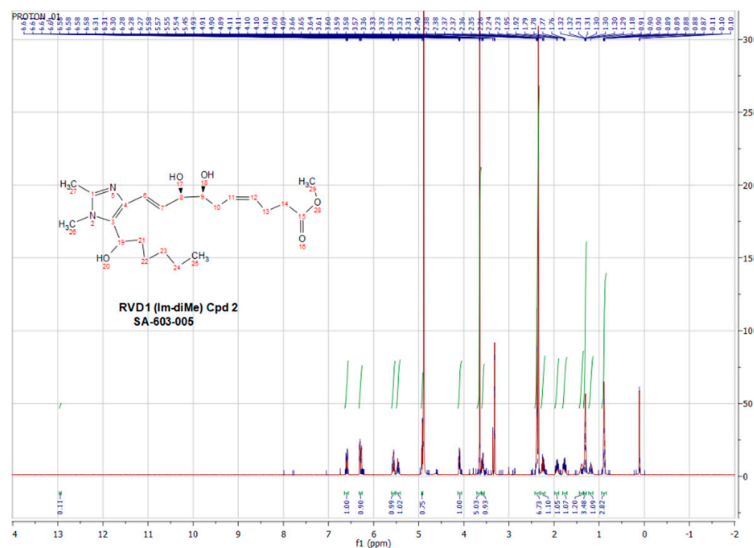


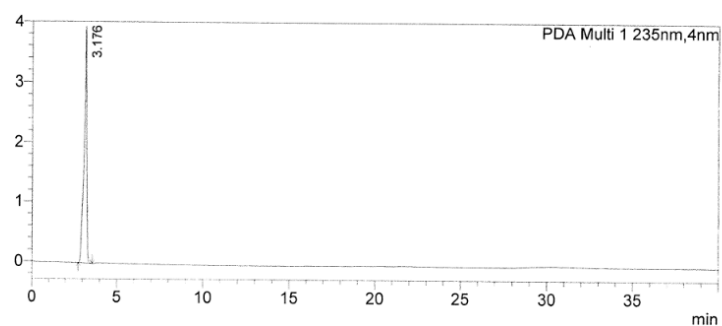
Figure S6: ^{13}C NMR spectrum analogue 2

==== Shimadzu LabSolutions Analysis Report ====

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 Acquired by : System Administrator
 Sample Name : JYS-603-005
 Sample ID : JYS-603-005
 Tray# : 1
 Vial# : 1
 Injection Volume : 7
 Data File : C:\LabSolutions\Data\Project1\EQUIPE DONALD POIRIER\Jean-Yves Sanceau\Jean-Yves Sanceau\JYS-603-005.lcd
 Method File : C:\LabSolutions\Data\Project1\EQUIPE DONALD POIRIER\Rene Maltais met
 Report Format File : C:\LabSolutions\Data\Project1\EQUIPE DONALD POIRIER\Rene Maltais met
 Month-Day Acquired : 6/13/2022
 Month-Day Processed : 6/13/2022

<Chromatogram>

C:\...Data\Project1\EQUIPE DONALD POIRIER\Jean-Yves Sanceau\Jean-Yves Sanceau\JYS-603-005.lcd
 AU



Peak Table

Peak#	Ret. Time	Area	Area%
1	3.176	41400132	100.000
Total		41400132	100.000

Figure S7: LCMS chromatogram analogue 2

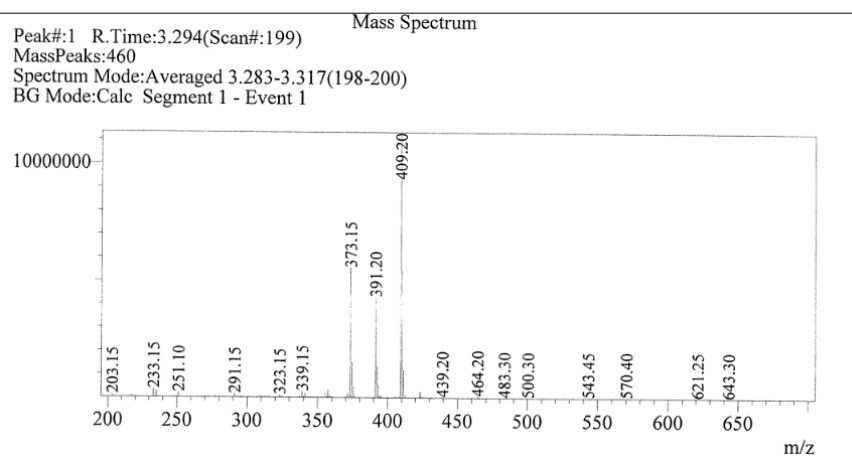


Figure S8: Mass spectrum analogue 2

Mulliken Charge Distribution:

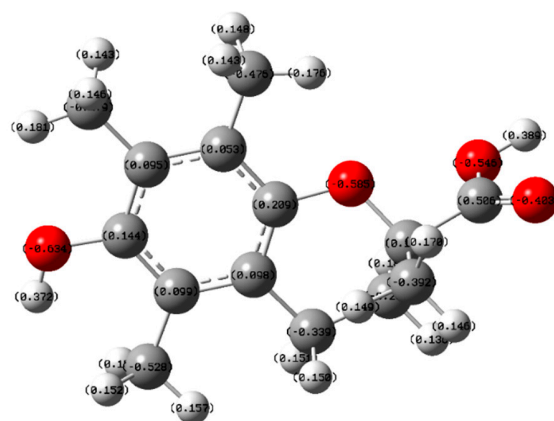


Figure S9: Mulliken charge distribution for Trolox

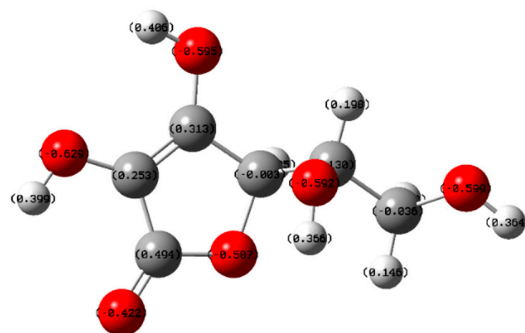


Figure S10: Mulliken charge distribution for Ascorbic Acid

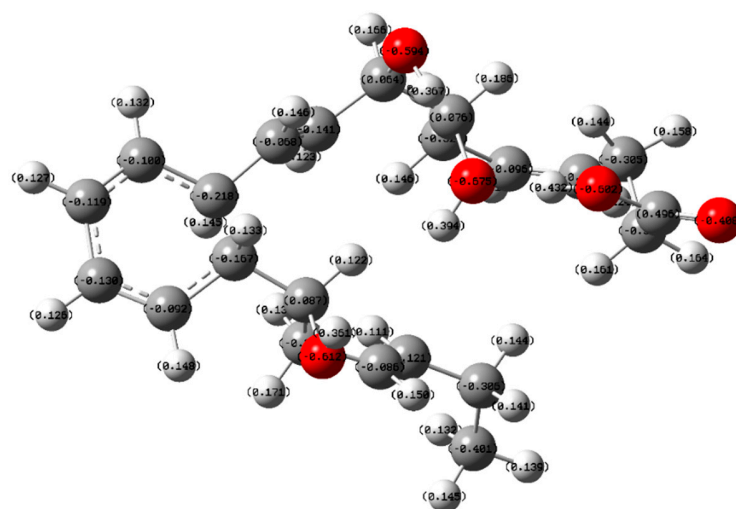


Figure S11: Mulliken charge distribution for ResolvinD1

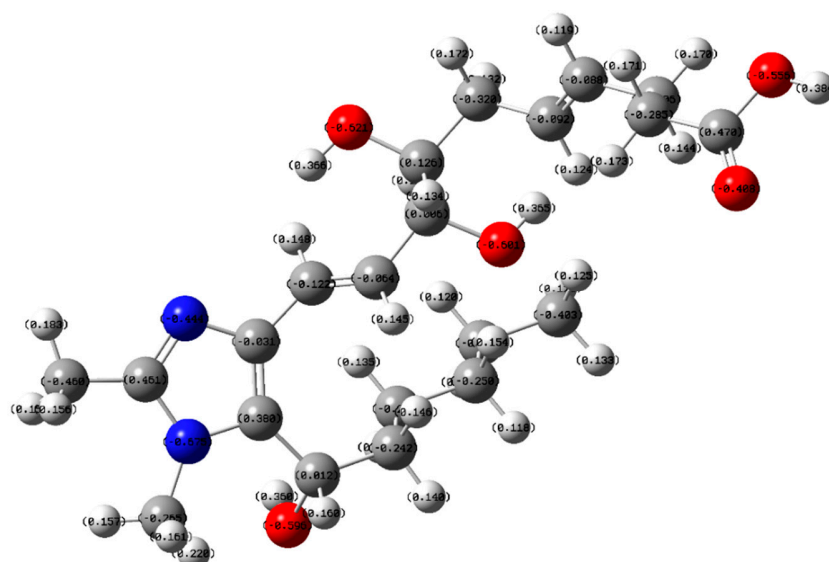


Figure S12: Mulliken charge distribution for analogue 1

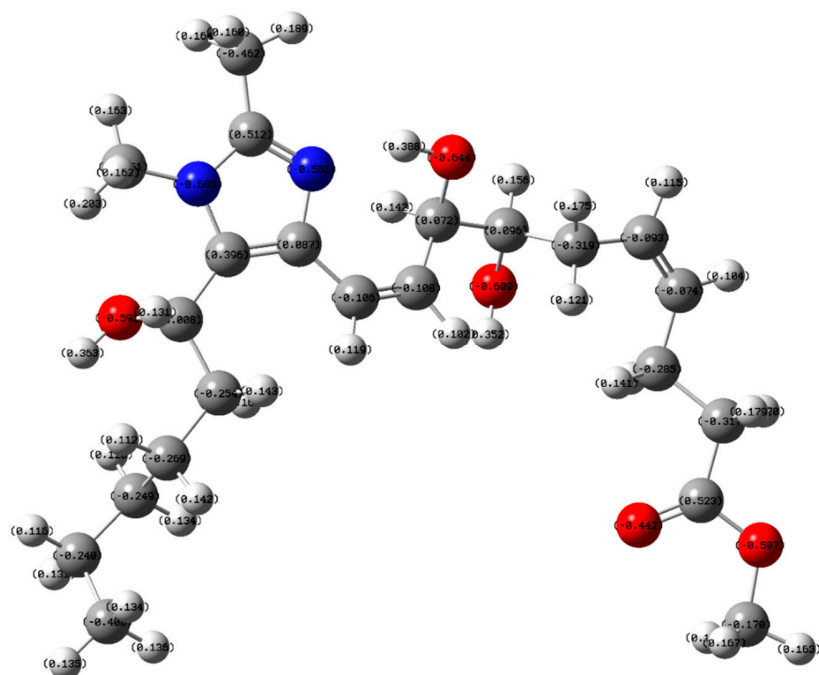


Figure S13: Mulliken charge distribution for analogue 2