

Benzoic Acid Derivatives of *Ifloga spicata* (Forssk.) Sch.Bip. as Potential anti-Leishmanials against *Leishmania tropica*

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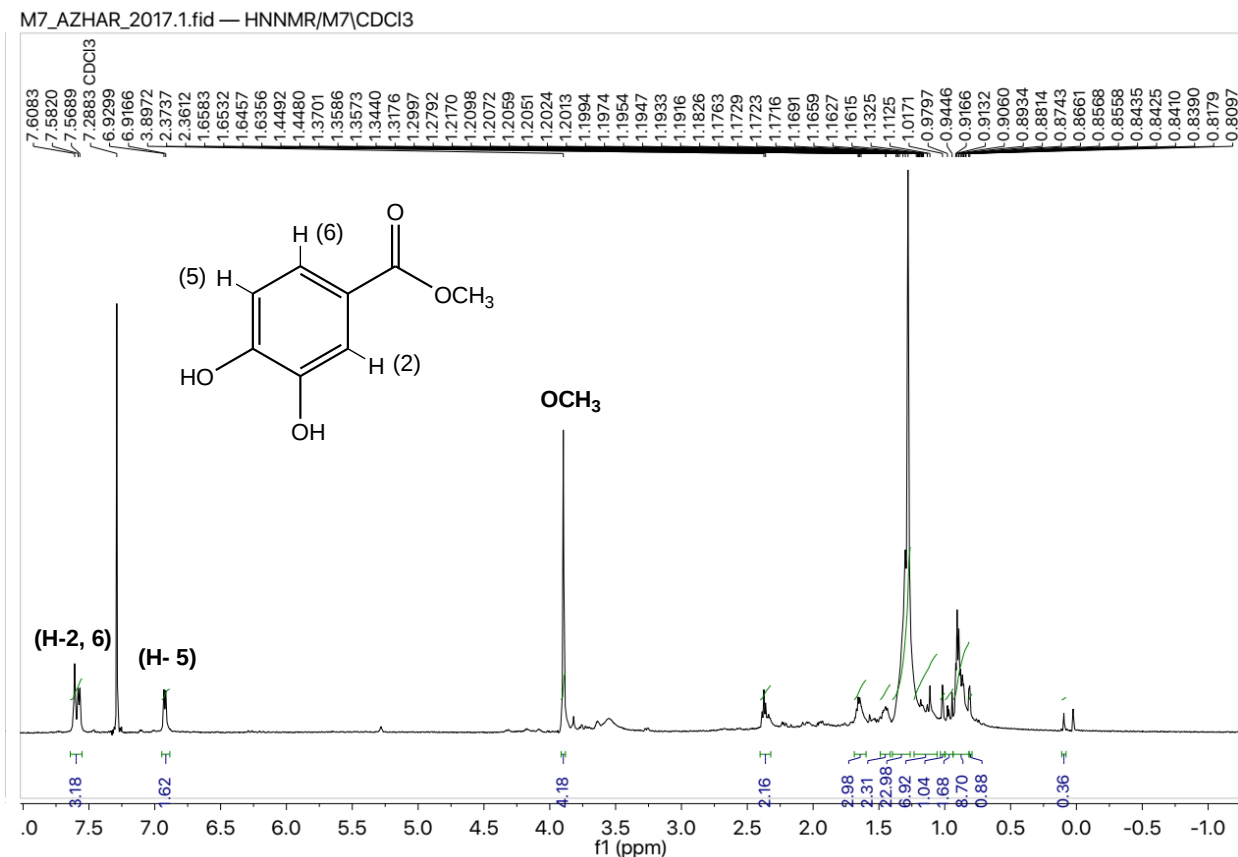


Figure (S1): ¹H NMR Spectrum of Methyl-3,4-dihydroxybenzoate(Compound1)

Assignments of ¹H NMR

H-2 (1H, S, 7.61 ppm): The singlet peak appears at 7.61ppm indicating H-2, which is comparatively highly deshielded proton.

H-6 (1H, d, 7.57 ppm): A doublet peak appears at 7.56ppm indicating H-6, having one proton in the neighbor position with J= 8Hz.

H-5 (1H, d, 6.90 ppm): A doublet peak appears at 6.90 ppm is assigned to H-5, having one proton in the neighbor position with J= 8Hz.

OCH₃ (3H, s, 3.89 ppm): A singlet appears at 3.89 ppm is assigned to OCH₃.

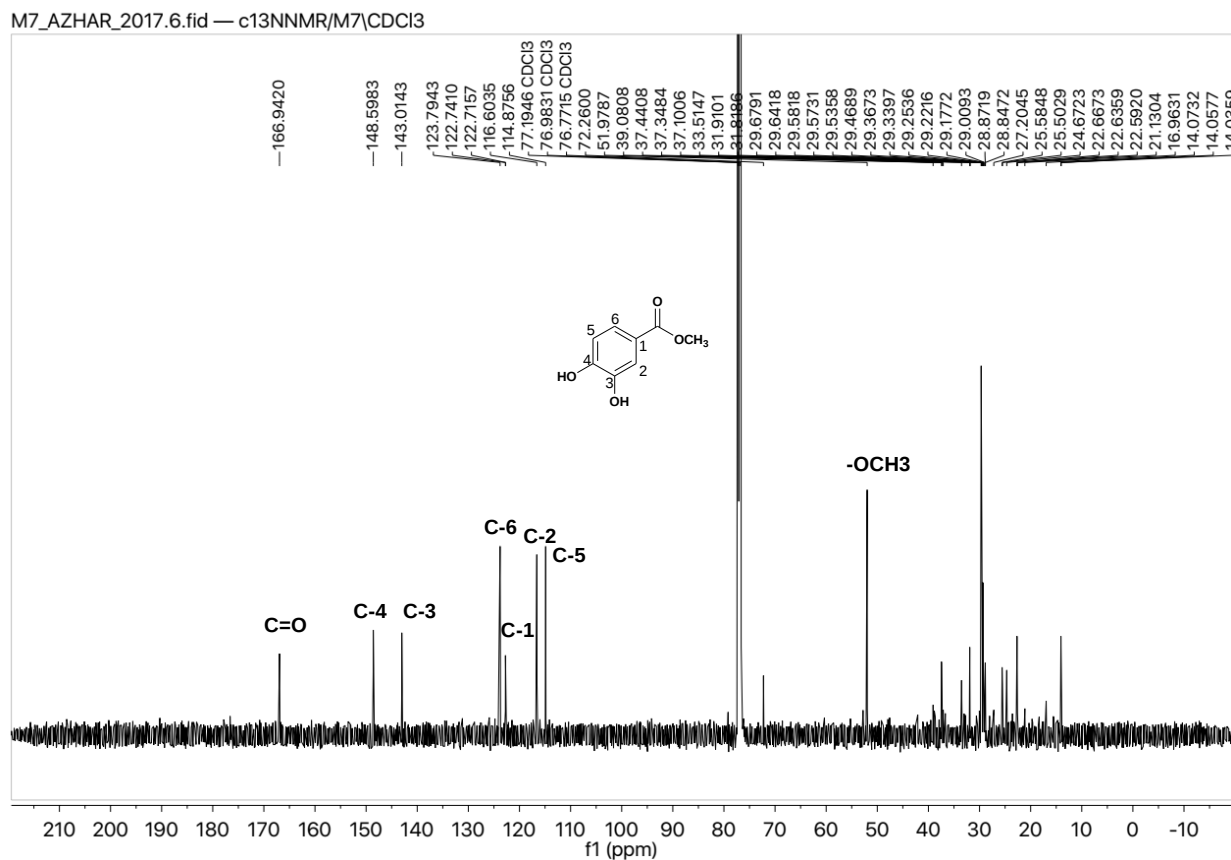


Figure (S2): ¹³C NMR Spectrum of Methyl-3,4-dihydroxybenzoate(Compound1)

M7_AZHAR_2017.3.ser — hmbcNNMR/M7\CDCl3

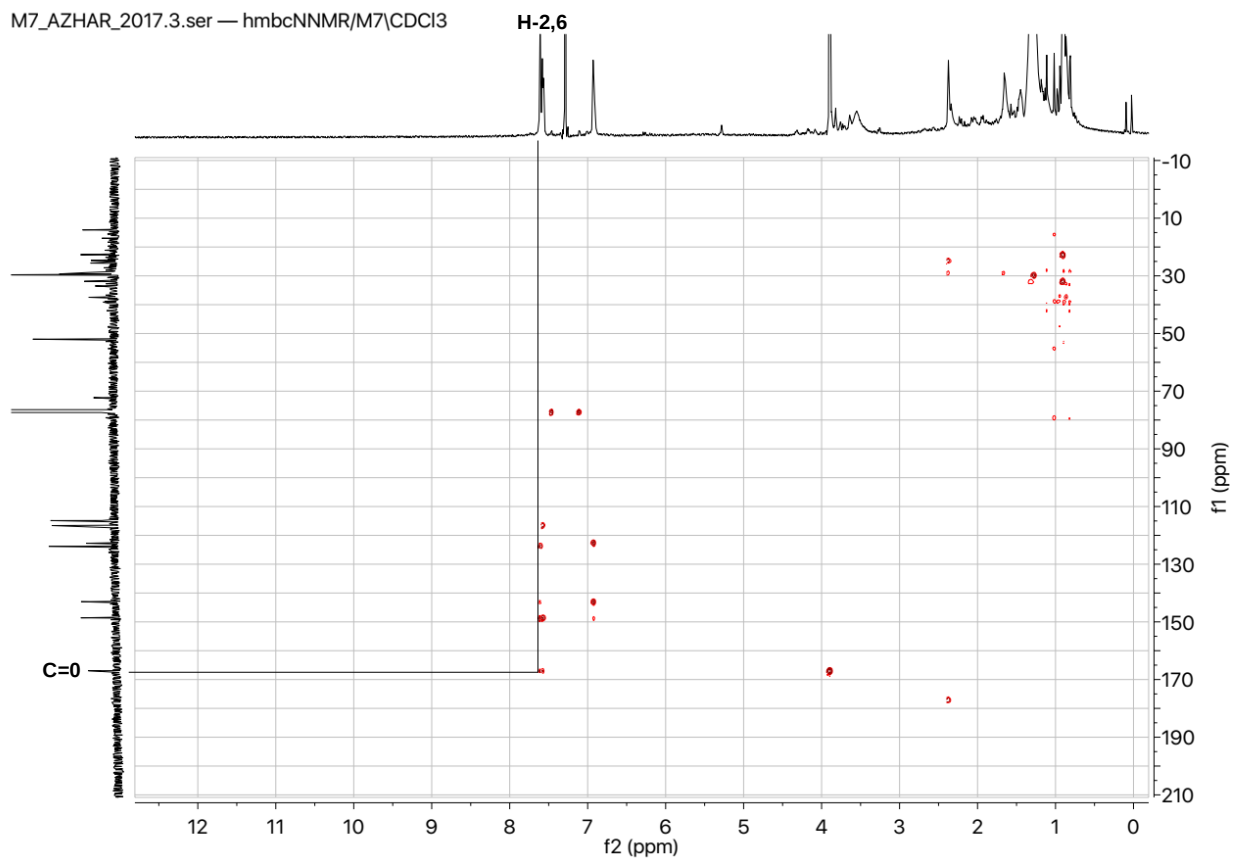


Figure (S3):HMBC Spectrum of Methyl-3,4-dihydroxybenzoate (indication the correlation) **Compound1)**

12_AZHAR_2017.5.fid — DEPTNMR/M2\CDCl3

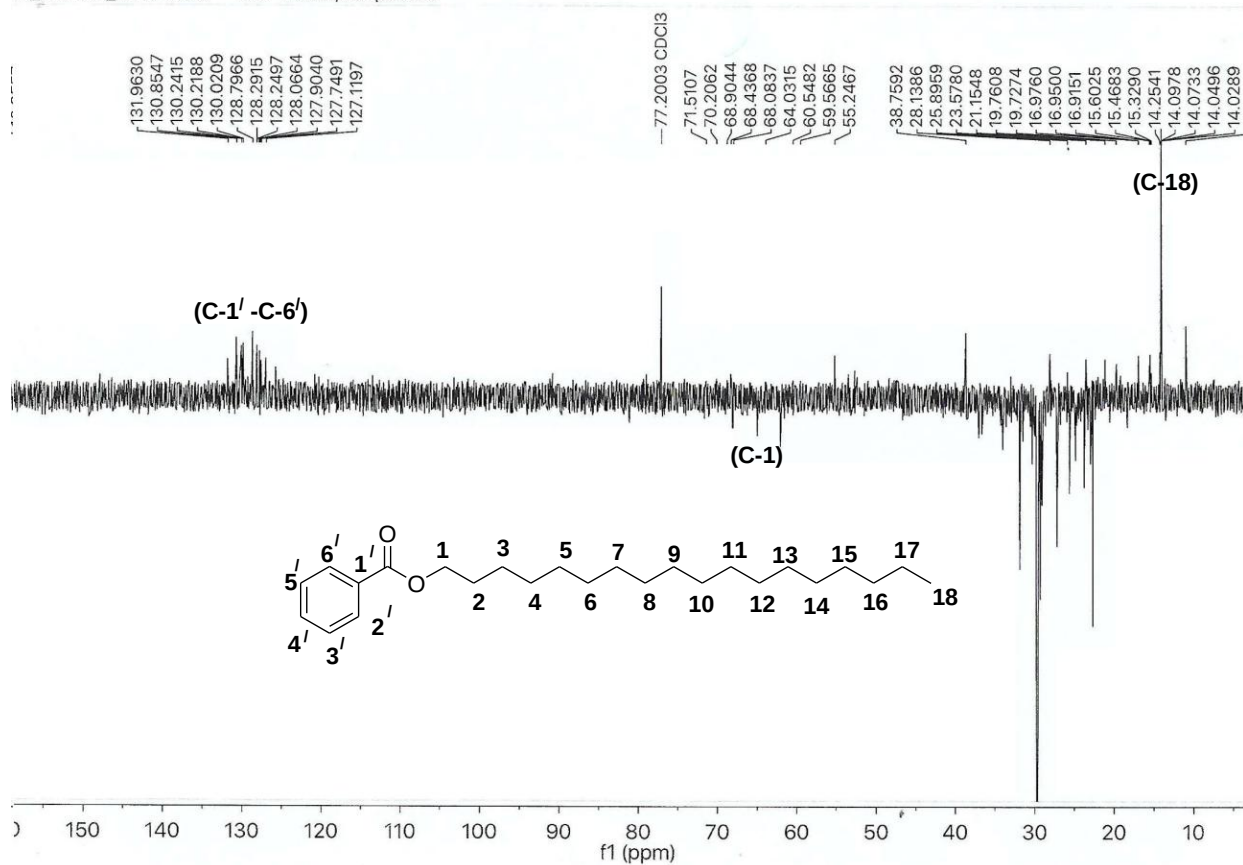


Figure (S4):DEPT-NMR spectrum of Benzoic Acid Octadecyle ester (**Compound2**)

Chemical structure of the polymer repeat unit: *c1ccc(cc1)C(=O)OCC(CCCCCCCCCCCC)C*

¹H NMR spectrum (CDCl₃) showing peaks for the polymer repeat unit. The x-axis is chemical shift (f1) in ppm, ranging from 0 to 16. The y-axis is intensity.

Key peaks and assignments:

- Ar-H: Aromatic protons, multiplet at ~7.4 ppm.
- 1: Benzylic methylene protons, multiplet at ~4.3 ppm.
- 2: Internal methylene protons, multiplet at ~1.8 ppm.
- 3: Methylene protons adjacent to the ester group, multiplet at ~1.3 ppm.
- (CH₂): Long alkyl chain methylene protons, broad multiplet between 0.8 and 1.2 ppm.

Integration values (from left to right): 0.08, 0.01, 0.01, 0.02, 0.01, 0.04, 0.10, 0.14, 0.23, 0.05, 0.10, 1.24, 0.23, 0.11, 0.48, 0.06, 0.01.

Figure (S5): ^1H NMR Spectrum of Benzoic Acid Octadecyle ester (Compound2)