

Supplementary Material

Article

Butyl (2,2-dibutoxybutanoyl)-L-tryptophanate

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Content

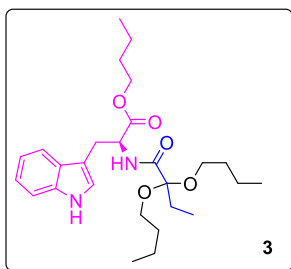
Spectroscopic data for characterization of compounds **3**, **5**, and **6** (Page 2).

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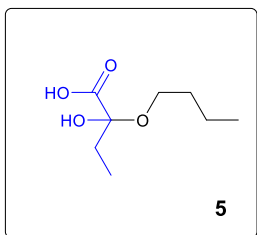
¹H and ¹³C NMR experiments of compound **5** (Page 4-5)

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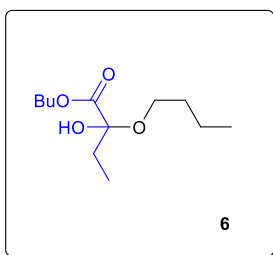
Butyl (2,2-dibutoxybutanoyl)-L-tryptophanate (3, C₂₇H₄₂N₂O₅)

Yellow oil; ¹H NMR (400 MHz, CDCl₃) δ 8.23 (s, 1H), 7.53 (d, *J* = 8.7 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.19 (d, *J* = 8.2 Hz, 1H), 7.13 (d, *J* = 7.0 Hz, 1H), 4.31 – 4.24 (m, 2H), 4.23 – 4.17 (m, 2H), 4.14 – 4.07 (m, 2H), 3.88 (dd, *J* = 11.2, 3.8 Hz, 1H), 3.14 (dd, *J* = 15.1, 3.9 Hz, 1H), 2.84 (d, *J* = 15.1 Hz, 1H), 2.16 (dd, *J* = 13.7, 7.4 Hz, 1H), 2.01 (dd, *J* = 13.7, 7.3 Hz, 1H), 1.76 – 1.60 (m, 6H), 1.49 – 1.33 (m, 6H), 0.99 (t, *J* = 7.4 Hz, 3H), 0.95 – 0.90 (m, 9H).; ¹³C NMR (100 MHz, CDCl₃) δ 174.11, 172.86, 136.70, 131.96, 131.05, 128.96, 126.65, 122.35, 119.69, 118.55, 111.17, 110.59, 65.72, 65.16, 63.24, 54.32, 33.69, 30.77, 30.74, 25.35, 19.27, 14.21, 13.86, 8.17. ESI+-HRMS *m/z* [M+H]⁺, 475.3166 (calcd. 475.3172, C₂₇H₄₃N₂O₅).



2-butoxy-2-hydroxybutanoic acid (5, C₈H₁₆O₄)

White solid; ¹H NMR (400 MHz, CDCl₃) δ 4.20 – 4.10 (m, 2H), 2.27-2.24 (m, 1H), 1.91 – 1.83 (m, 1H), 1.67 – 1.56 (m, 2H), 1.38 – 1.32 (m, 2H), 0.93 – 0.84 (m, 6H).; ¹³C NMR (100 MHz, CDCl₃) δ 169.45, 168.42, 88.01, 66.13, 30.42, 27.05, 18.98, 13.59, 8.87, 6.99.



Butyl 2-butoxy-2-hydroxybutanoate (6, C₁₂H₂₄O₄)

Yellow oil; ¹H NMR (400 MHz, CDCl₃) δ 4.13 (t, *J* = 6.6 Hz, 2H), 3.74 (t, *J* = 6.6 Hz, 2H), 1.67 – 1.59 (m, 6H), 1.46 – 1.33 (m, 6H), 0.95 – 0.89 (m, 6H).

Figure S1. ^1H NMR spectrum of compound **3** (400 MHz, CDCl_3)

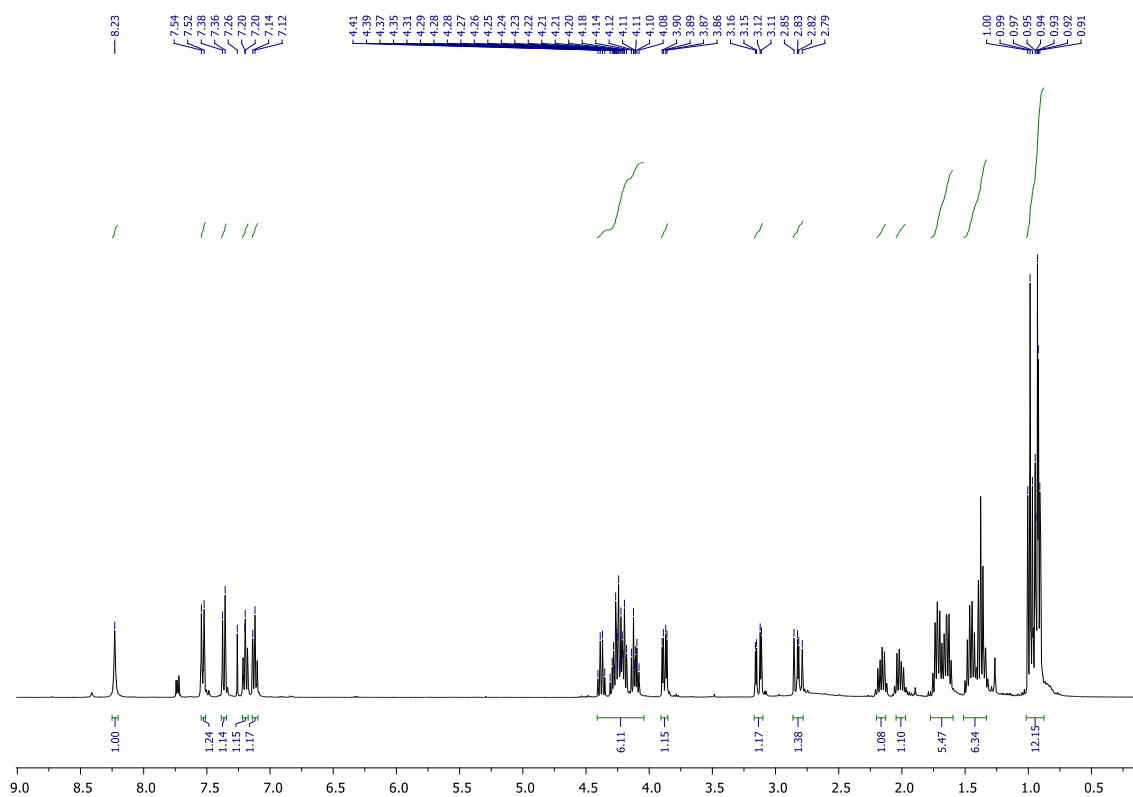


Figure S2. ^{13}C NMR spectrum of compound **3** (100 MHz, CDCl_3)

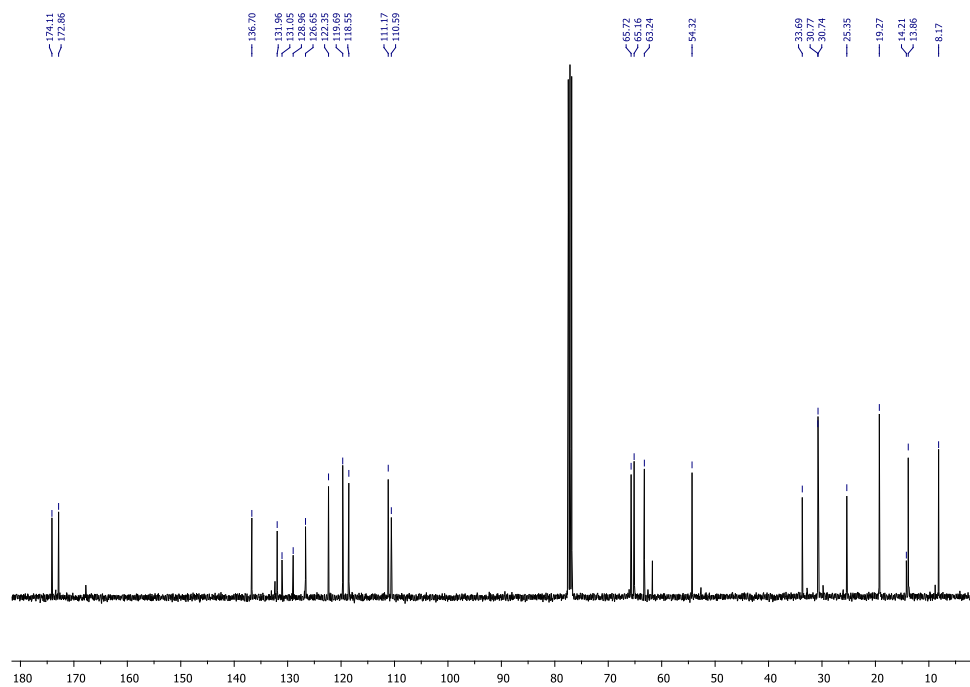


Figure S3. ESI⁺-HRMS spectrum of compound **3**

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MassPeaks:1
Spectrum Mode:Averaged 8.777-8.783(5267-5271)
BG Mode:Calc Segment 1 - Event 1

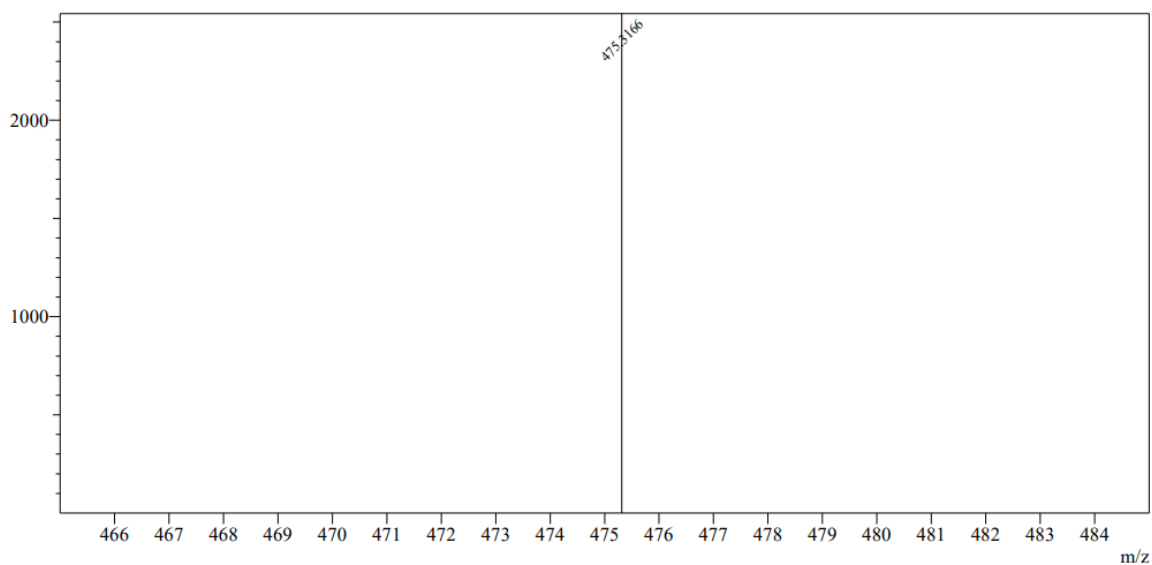


Figure S4. ¹H spectrum of compound **5** (400 MHz, CDCl₃)

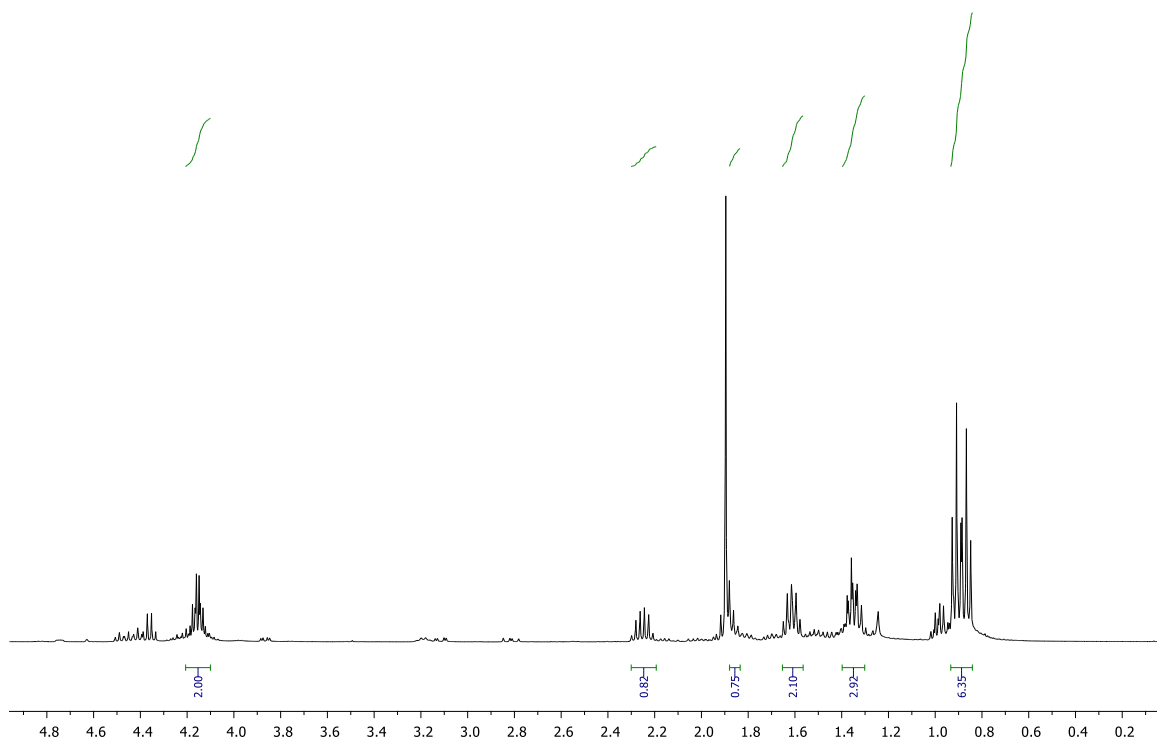


Figure S5. ^{13}C NMR experiments of compound **5** (100 MHz, CDCl_3)

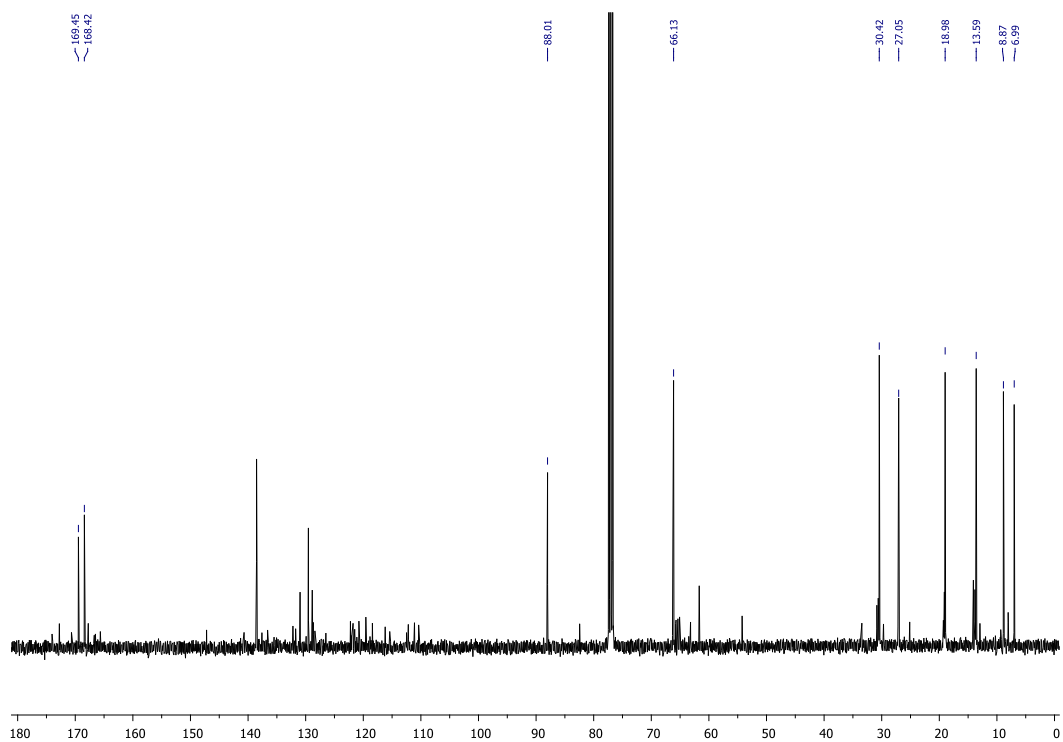


Figure S6. ^1H NMR spectrum of compound **6** (400 MHz, CDCl_3)

