



Supporting Information

for

Rapid construction of tricyclic tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine via isocyanide-based multicomponent reaction

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Beilstein J. Org. Chem. **2024**, *20*, 1436–1443. doi:10.3762/bjoc.20.126

Characterization data and ^1H NMR, ^{13}C NMR, and HRMS spectra of compounds

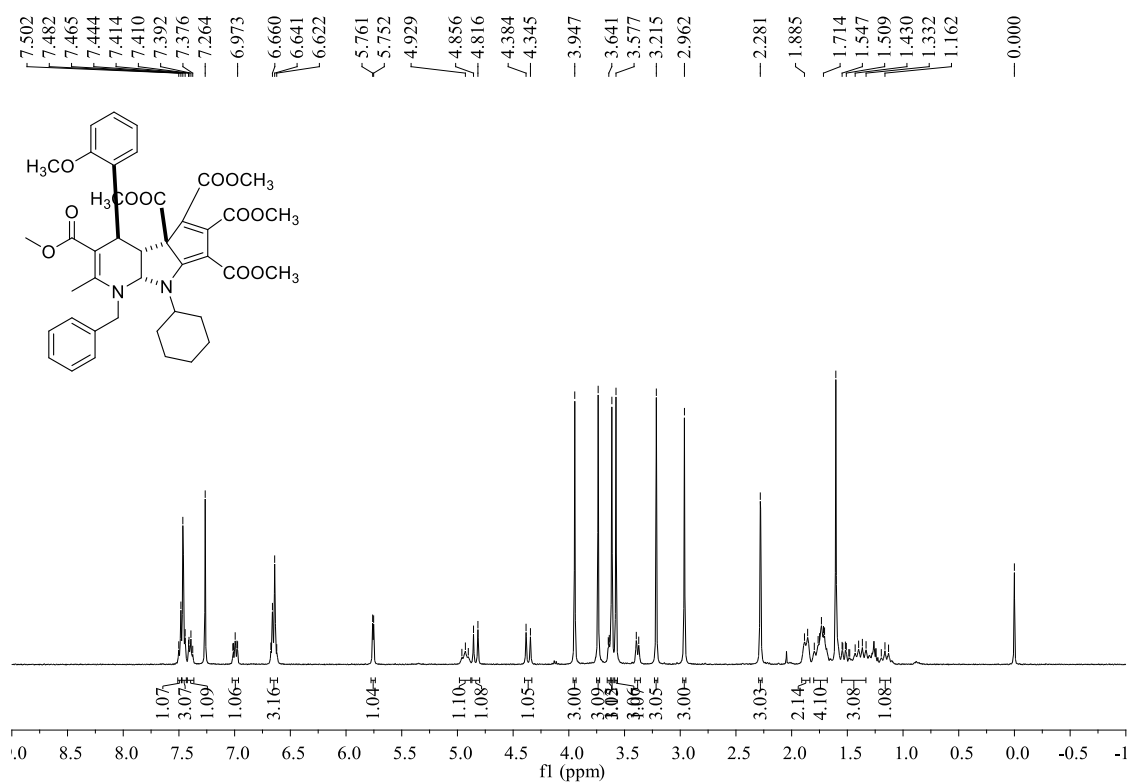
Experiments and general procedure	S2
Characterization data, ^1H NMR, ^{13}C NMR and HRMS of the compounds	S3–S64

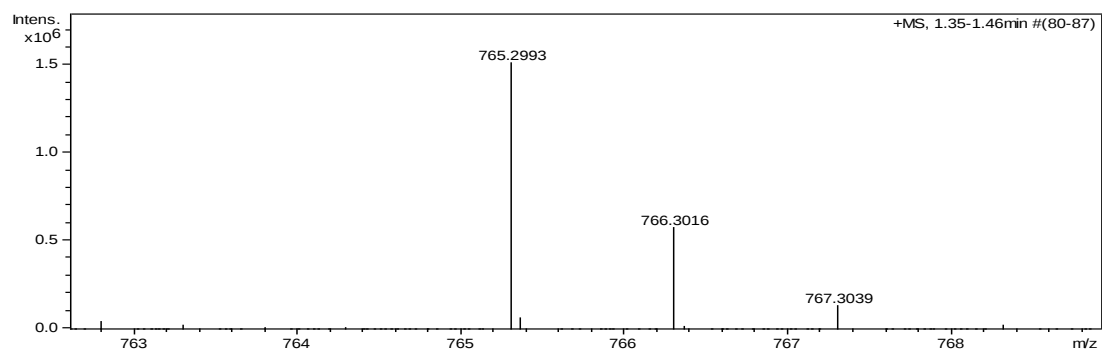
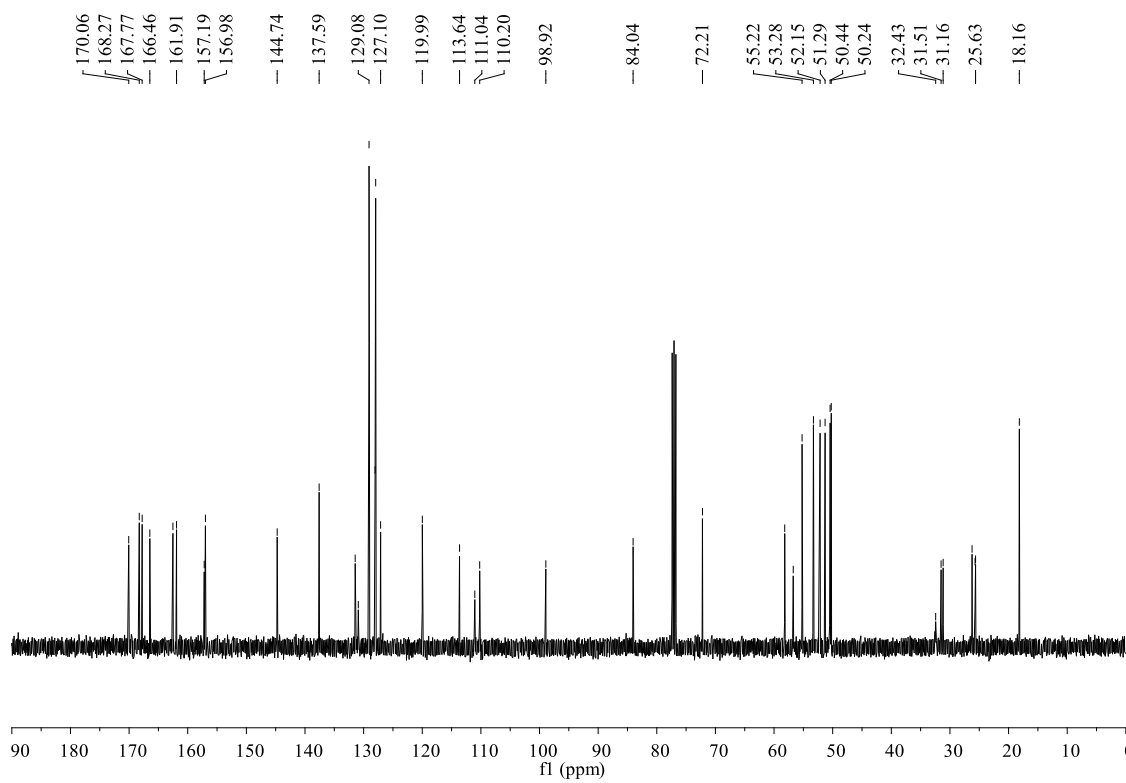
Experimental section

1. General procedure for the multicomponent reaction:

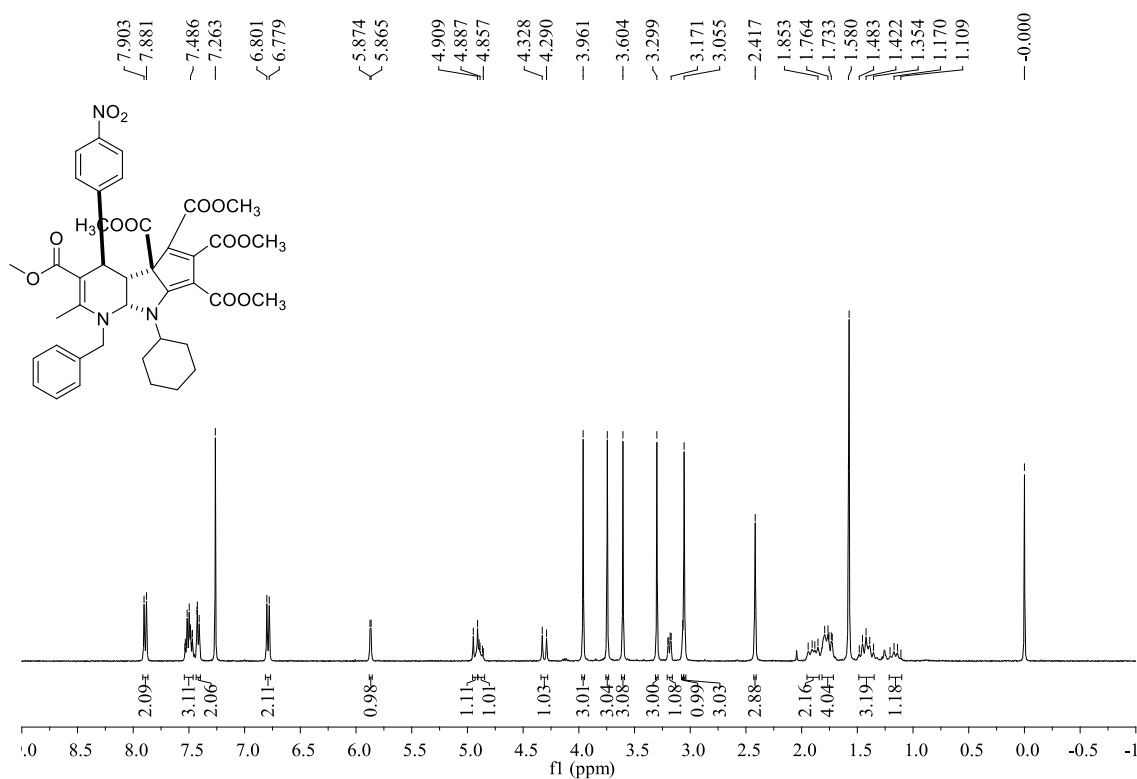
To a round flask was added alkyl isocyanide (0.1 mmol), dialkyl but-2-ynedioate (0.5 mmol), 5,6-unsubstituted 1,4-dihydropyridine (0.1 mmol) and acetonitrile (5.0 mL). The solution was stirred at reflux temperature for nearly one hour. After removing the solvent by rotatory evaporation at reduced pressure, the residue was subjected to column chromatography with a mixture of ethyl acetate and petroleum ether (v/v = 1:4) as eluent to give the pure product for analysis.

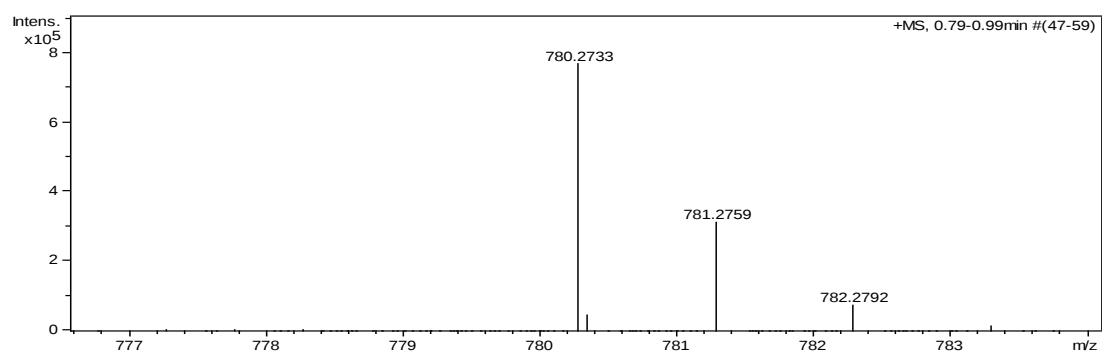
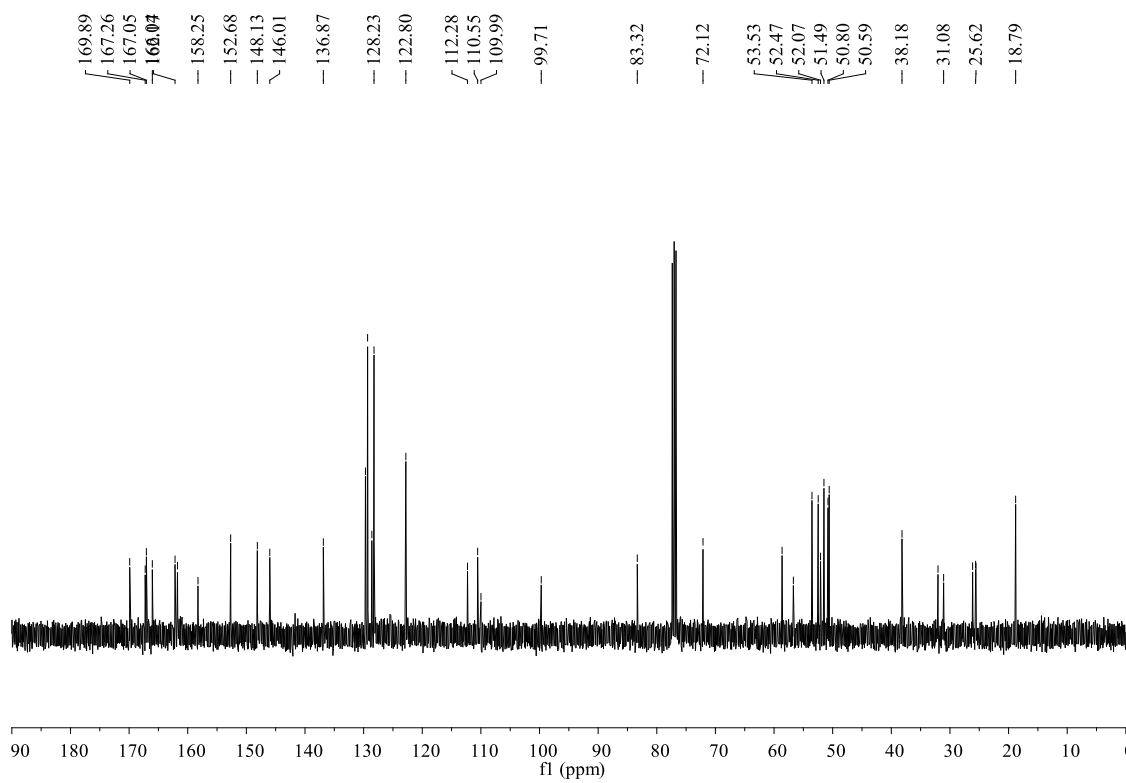
Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-1-benzyl-8-cyclohexyl-4-(2-methoxyphenyl)-2-methyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (4*a*): yellow solid, 89%, m.p. 209-211 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.49 (d, *J* = 8.0 Hz, 1H, ArH), 7.47-7.44 (m, 3H, ArH), 7.41-7.38 (m, 1H, ArH), 7.02-6.97 (m, 1H, ArH), 6.68-6.62 (m, 3H, ArH), 5.76 (d, *J* = 3.6 Hz, 1H, CH), 4.96-4.90 (m, 1H, CH), 4.84 (d, *J* = 16.0 Hz, 1H, CH₂), 4.36 (d, *J* = 15.6 Hz, 1H, CH₂), 3.95 (s, 3H, OCH₃), 3.74 (s, 3H, OCH₃), 3.65-3.63 (m, 1H, CH), 3.61 (s, 3H, OCH₃), 3.58 (s, 3H, OCH₃), 3.38 (d, *J* = 8.4 Hz, 1H, CH), 3.21 (s, 3H, OCH₃), 2.96 (s, 3H, OCH₃), 2.28 (s, 3H, CH₃), 1.89-1.86 (m, 2H, CH₂), 1.80-1.68 (m, 4H, CH₂), 1.55-1.33 (m, 3H, CH₂), 1.20-1.13 (m, 1H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.1, 168.3, 167.8, 166.5, 162.5, 161.9, 157.2, 157.0, 144.7, 137.6, 131.4, 130.9, 129.1, 128.0, 127.9, 127.1, 112.0, 113.6, 111.0, 110.2, 98.9, 84.0, 72.2, 58.2, 56.7, 55.2, 53.3, 52.2, 51.3, 50.4, 50.2, 32.4, 31.5, 31.2, 26.2, 25.7, 25.6, 18.2 ppm. IR (KBr) ν: 3435, 2931, 2862, 2360, 1737, 1698, 1587, 1547, 1435, 1385, 1335, 1251, 1204, 1125, 1092, 1001, 977, 895, 853, 792 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₄₁H₄₆NaN₂O₁₁ ([M+Na]⁺): 765.2994, found: 765.2993.





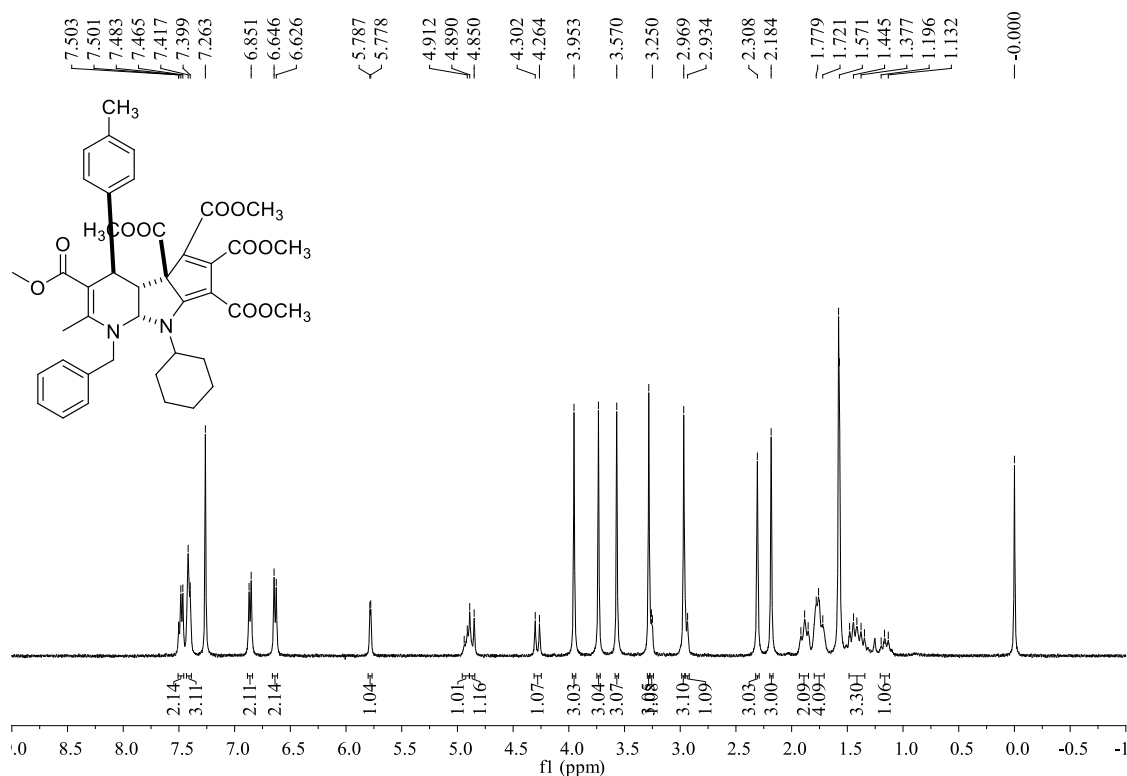
Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-1-benzyl-8-cyclohexyl-2-methyl-4-(4-nitrophenyl)-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (4*b*): yellow solid, 84%, m.p. 211-213 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.89 (d, *J* = 8.8 Hz, 2H, ArH), 7.54-7.47 (m, 3H, ArH), 7.43-7.41 (m, 2H, ArH), 6.79 (d, *J* = 8.8 Hz, 2H, ArH), 5.87 (d, *J* = 3.6 Hz, 1H, CH), 4.93 (d, *J* = 15.6 Hz, 1H, CH₂), 4.90-4.86 (m, 1H, CH), 4.31 (d, *J* = 15.2 Hz, 1H, CH₂), 3.96 (s, 3H, OCH₃), 3.74 (s, 3H, OCH₃), 3.60 (s, 3H, OCH₃), 3.30 (s, 3H, OCH₃), 3.19 (dd, *J*₁ = 8.4 Hz, *J*₂ = 3.6 Hz, 1H, CH), 3.07-3.06 (m, 1H, CH), 3.06 (s, 3H, OCH₃), 2.42 (s, 3H, CH₃), 1.94-1.85 (m, 2H, CH₂), 1.79-1.73 (m, 4H, CH₂), 1.48-1.35 (m, 3H, CH₂), 1.21-1.11 (m, 1H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 169.9, 167.3, 167.1, 166.0, 162.2, 161.7, 158.3, 152.7, 148.1, 146.0, 136.9, 129.7, 129.3, 128.6, 128.2, 122.8, 112.3, 110.6, 110.0, 99.7, 83.3, 72.1, 58.6, 56.7, 53.5, 52.5, 52.1, 51.5, 50.8, 50.6, 38.2, 32.0, 31.1, 26.1, 25.62, 25.56, 18.8 ppm. IR (KBr) ν: 3435, 2949, 2857, 1736, 1698, 1583, 1542, 1434, 1383, 1348, 1233, 1208, 1117, 1091, 1001, 980, 894, 847, 795 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₄₀H₄₃NaN₃O₁₂ ([M+Na]⁺): 780.2739, found: 780.2733.

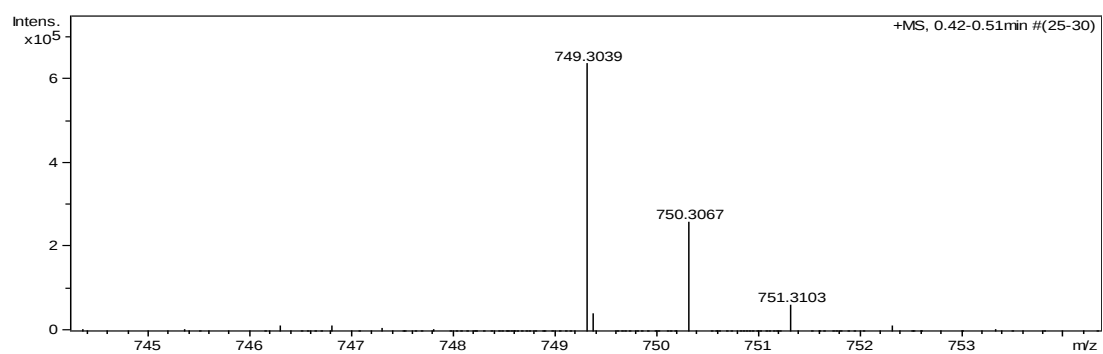
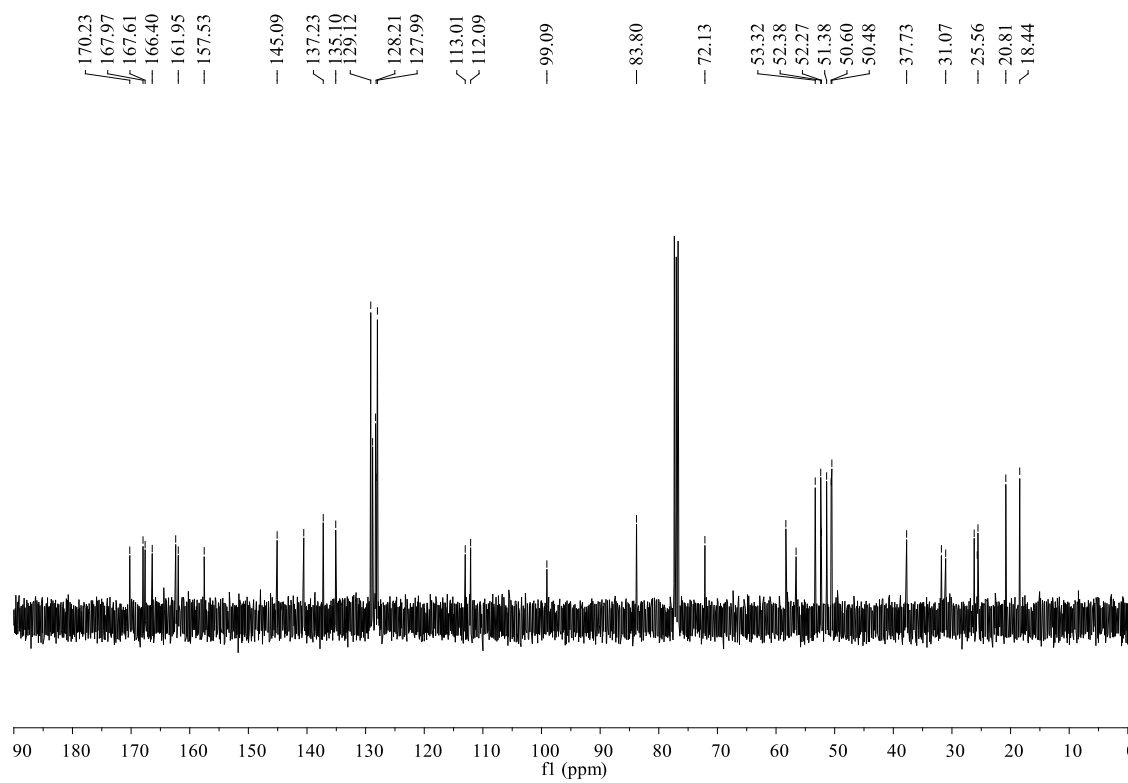




Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-1-benzyl-8-cyclohexyl-2-methyl-4-(*p*-tolyl)-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (4c):

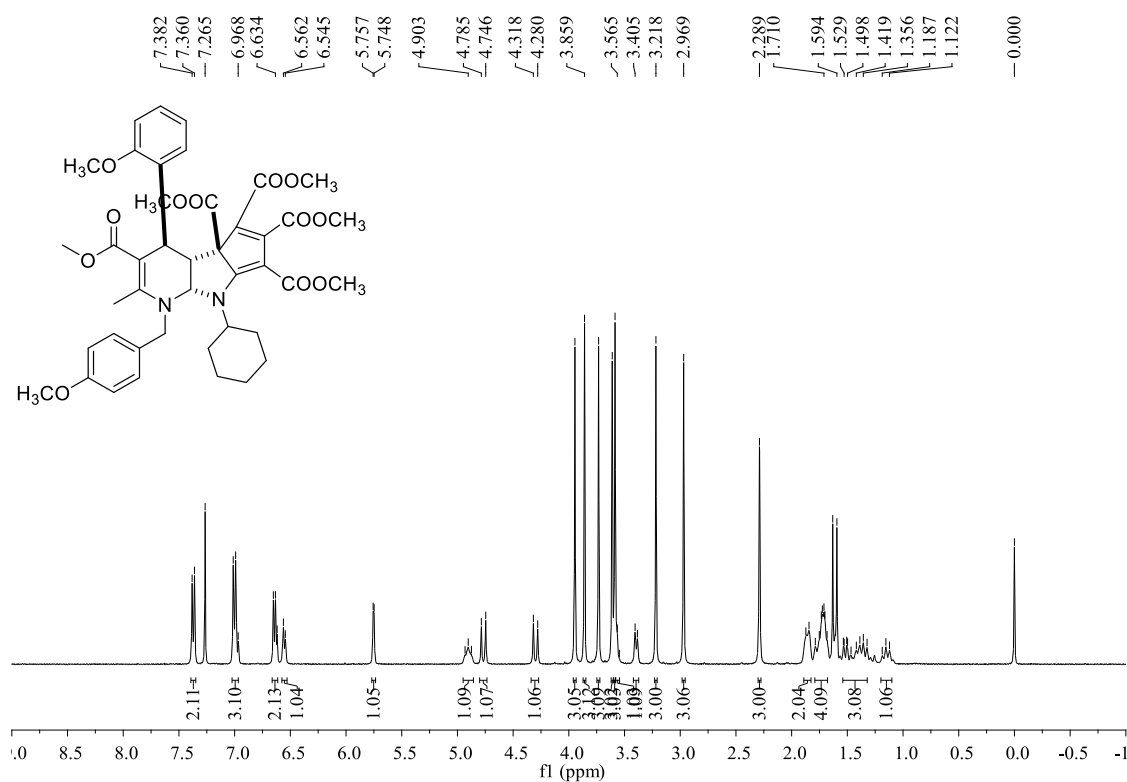
yellow solid, 81%, m.p. 185-187 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.50-7.47 (m, 2H, ArH), 7.42-7.40 (m, 3H, ArH), 6.86 (d, *J* = 7.6 Hz, 2H, ArH), 6.64 (d, *J* = 8.0 Hz, 2H, ArH), 5.78 (d, *J* = 3.6 Hz, 1H, CH), 4.94-4.90 (m, 1H, CH), 4.87 (d, *J* = 16.0 Hz, 1H, CH₂), 4.28 (d, *J* = 15.2 Hz, 1H, CH₂), 3.95 (s, 3H, OCH₃), 3.73 (s, 3H, OCH₃), 3.57 (s, 3H, OCH₃), 3.28 (s, 3H, OCH₃), 3.26-3.25 (m, 1H, CH), 2.97 (s, 3H, OCH₃), 2.96-2.92 (m, 1H, CH), 2.31 (s, 3H, CH₃), 2.18 (s, 3H, CH₃), 1.92-1.85 (m, 2H, CH₂), 1.78-1.72 (m, 4H, CH₂), 1.48-1.35 (m, 3H, CH₂), 1.20-1.13 (m, 1H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.2, 167.9, 167.6, 166.4, 162.4, 162.0, 157.5, 145.1, 140.6, 137.2, 135.1, 129.1, 128.8, 128.3, 128.2, 128.0, 113.0, 112.1, 99.1, 83.8, 72.1, 58.3, 56.6, 53.3, 52.4, 52.3, 51.4, 50.6, 50.5, 37.7, 31.8, 31.1, 26.2, 25.7, 25.6, 20.8, 18.4 ppm. IR (KBr) ν: 3435, 2949, 2859, 1737, 1698, 1581, 1541, 1435, 1387, 1338, 1232, 1205, 1124, 1092, 1001, 978, 894, 852, 788 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₄₁H₄₆NaN₂O₁₀ ([M+Na]⁺): 749.3045, found: 749.3039.

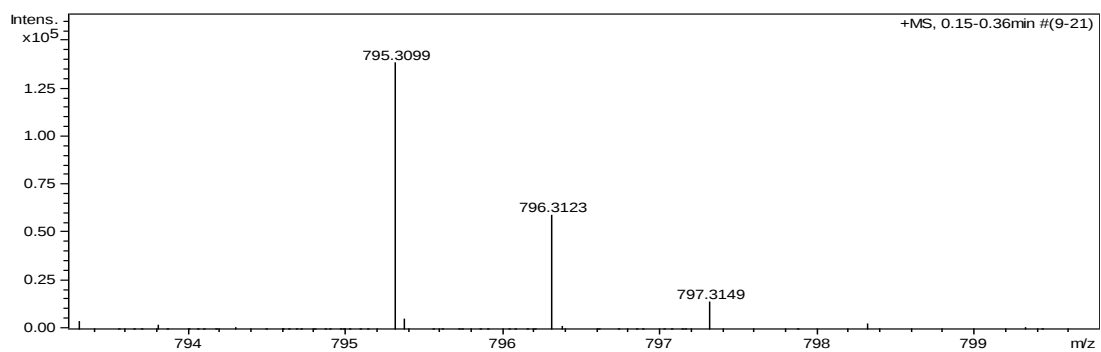
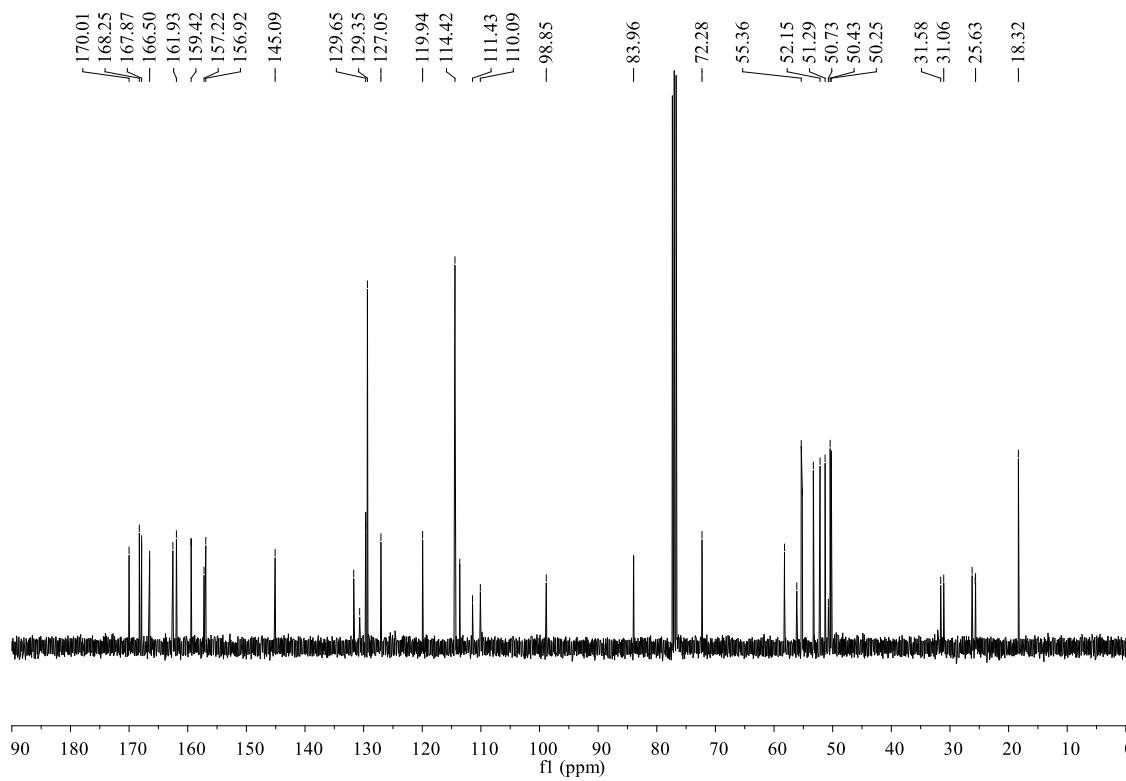




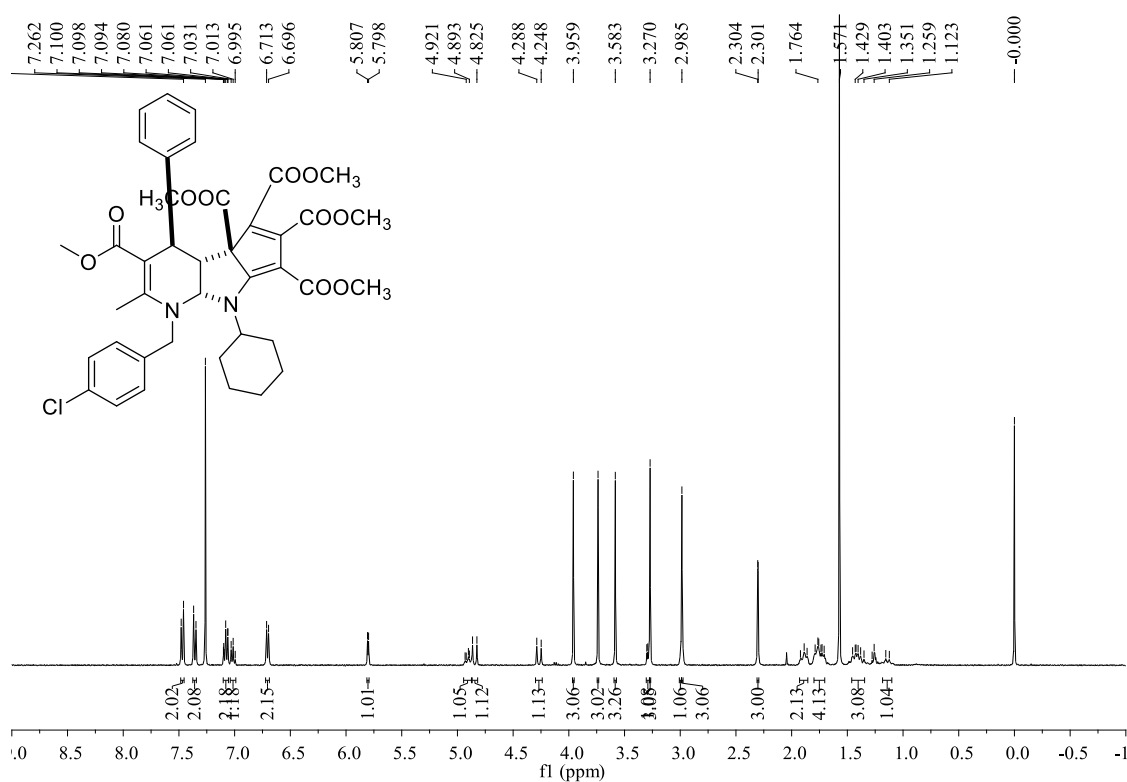
Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-8-cyclohexyl-1-(4-methoxybenzyl)-4-(2-methoxyphenyl)-2-methyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-

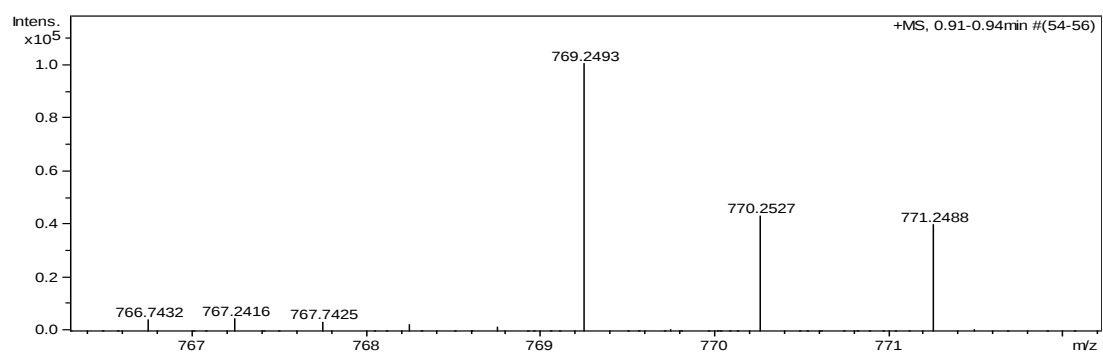
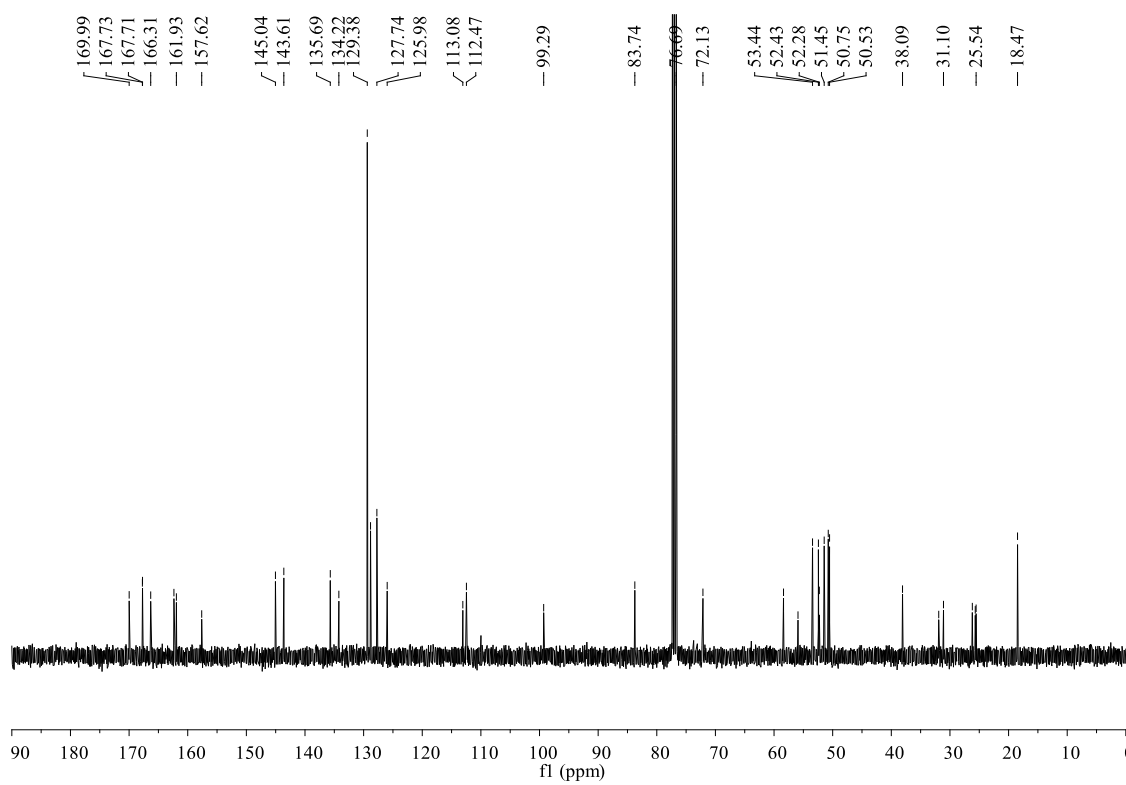
pentacarboxylate (4d): yellow solid, 84%, m.p. 183-185 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.37 (d, *J* = 8.8 Hz, 2H, ArH), 7.01-6.97 (m, 3H, ArH), 6.65-6.62 (m, 2H, ArH), 6.55 (d, *J* = 6.8 Hz, 1H, ArH), 5.75 (d, *J* = 3.6 Hz, 1H, CH), 4.93-4.87 (m, 1H, CH), 4.77 (d, *J* = 15.6 Hz, 1H, CH₂), 4.30 (d, *J* = 15.2 Hz, 1H, CH₂), 3.95 (s, 3H, OCH₃), 3.86 (s, 3H, OCH₃), 3.76 (s, 3H, OCH₃), 3.61 (s, 3H, OCH₃), 3.59 (s, 3H, OCH₃), 3.58-3.55 (m, 1H, CH), 3.39 (d, *J* = 8.4 Hz, 1H, CH), 3.22 (s, 3H, OCH₃), 2.97 (s, 3H, OCH₃), 2.29 (s, 3H, CH₃), 1.87-1.84 (m, 2H, CH₂), 1.79-1.68 (m, 4H, CH₂), 1.54-1.32 (m, 3H, CH₂), 1.19-1.12 (m, 1H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.0, 168.3, 167.9, 166.5, 162.5, 161.9, 159.4, 157.2, 156.9, 145.1, 131.7, 130.7, 129.7, 129.4, 127.1, 119.9, 114.4, 113.6, 111.4, 110.1, 98.9, 84.0, 72.3, 58.2, 56.1, 55.4, 55.2, 53.3, 52.2, 51.3, 50.7, 50.4, 50.3, 31.6, 31.1, 26.2, 25.7, 25.6, 18.3 ppm. IR (KBr) ν: 3435, 2947, 2857, 1733, 1697, 1583, 1549, 1436, 1384, 1334, 1251, 1201, 1108, 1087, 1032, 1000, 894, 819, 791, 756 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₄₂H₄₈NaN₂O₁₂ ([M+Na]⁺): 795.3099, found: 795.3099.



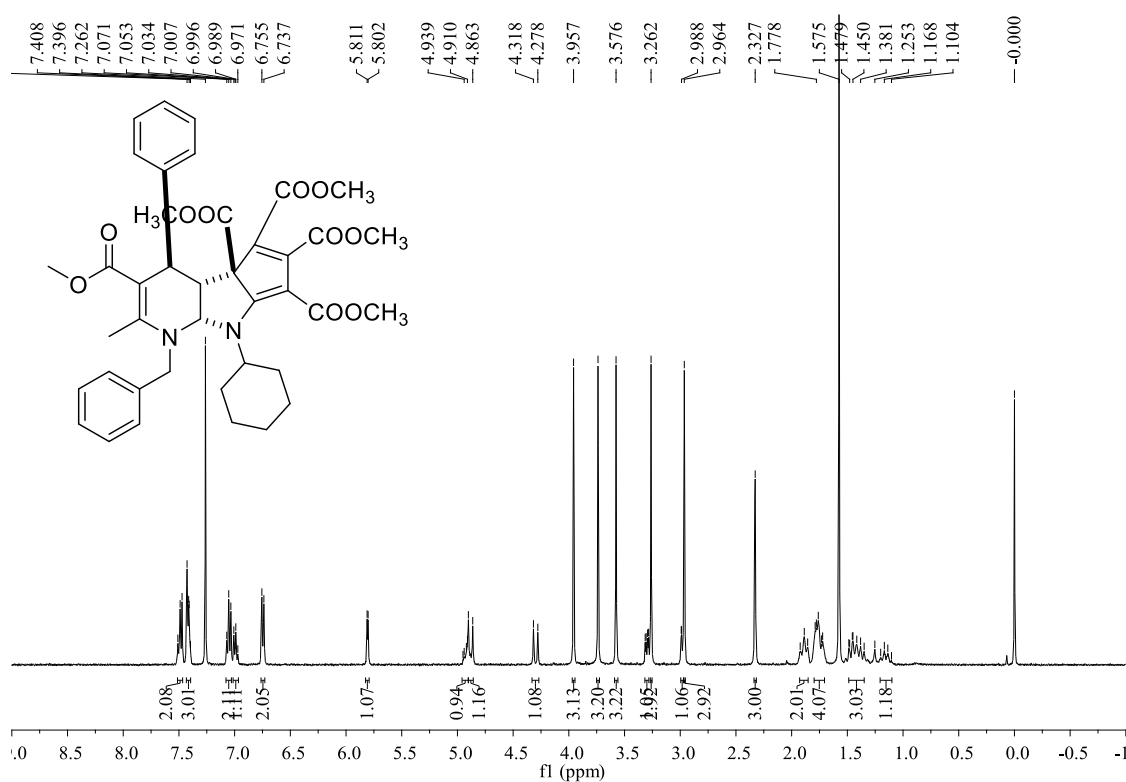


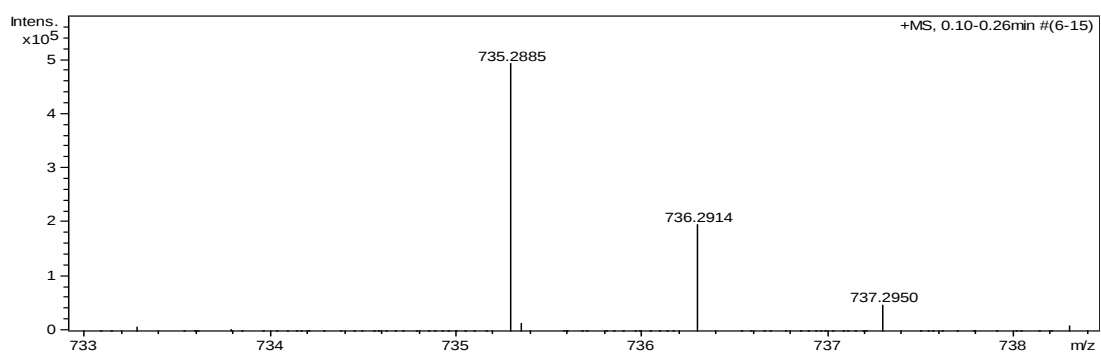
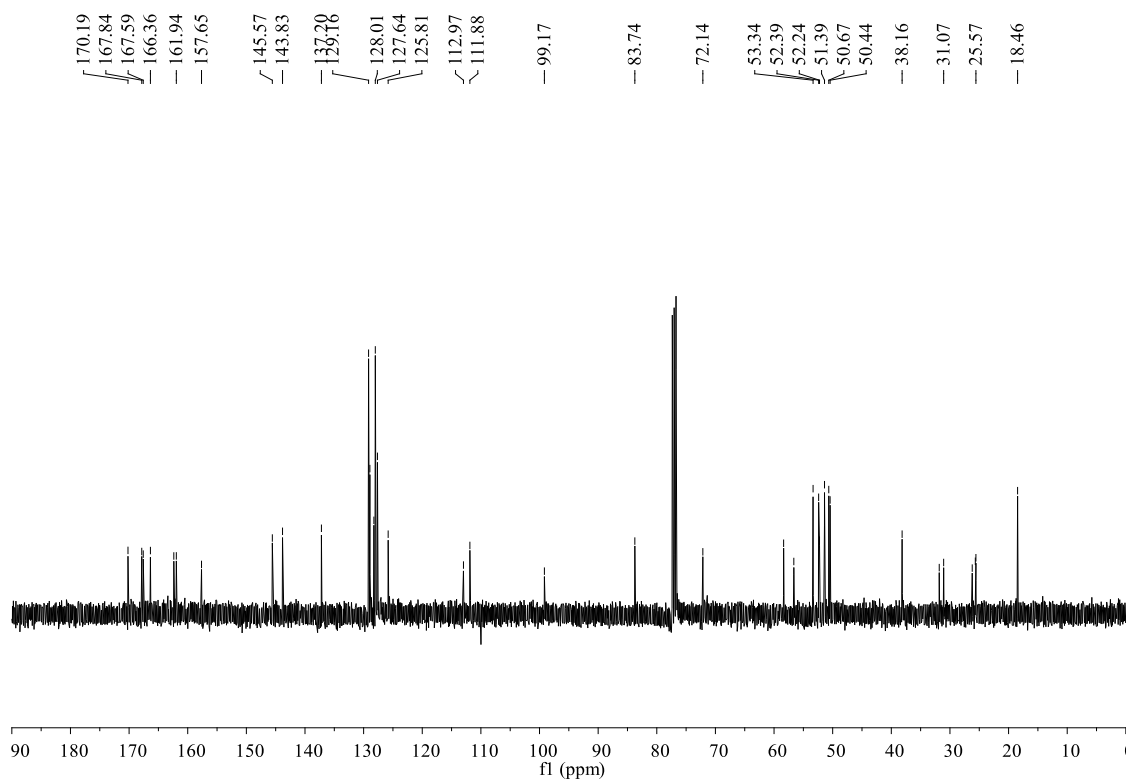
Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-1-(4-chlorobenzyl)-8-cyclohexyl-2-methyl-4-phenyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (4e): yellow solid, 82%, m.p. 206-208 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.47 (d, *J* = 8.4 Hz, 2H, ArH), 7.36 (d, *J* = 8.4 Hz, 2H, ArH), 7.10-7.06 (m, 2H, ArH), 7.03-7.00 (m, 1H, ArH), 6.70 (d, *J* = 6.8 Hz, 2H, ArH), 5.80 (d, *J* = 3.6 Hz, 1H, CH), 4.93-4.89 (m, 1H, CH), 4.84 (d, *J* = 15.6 Hz, 1H, CH₂), 4.27 (d, *J* = 16.0 Hz, 1H, CH₂), 3.96 (s, 3H, OCH₃), 3.74 (s, 3H, OCH₃), 3.58 (s, 3H, OCH₃), 3.30-3.28 (m, 1H, CH), 3.27 (s, 3H, OCH₃), 3.01-2.99 (m, 1H, CH), 2.99 (s, 3H, OCH₃), 2.30 (s, 3H, CH₃), 1.92-1.86 (m, 2H, CH₂), 1.79-1.71 (m, 4H, CH₂), 1.45-1.35 (m, 3H, CH₂), 1.16-1.12 (m, 1H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.0, 167.73, 167.71, 166.3, 162.4, 161.9, 157.6, 145.0, 143.6, 135.7, 134.2, 129.4, 128.8, 127.7, 126.0, 113.1, 112.5, 99.3, 83.7, 77.3, 77.0, 76.7, 72.1, 58.4, 55.9, 53.4, 52.4, 52.3, 51.5, 50.8, 50.5, 38.1, 31.9, 31.1, 26.2, 25.7, 25.5, 18.5 ppm. IR (KBr) ν: 3434, 2950, 2856, 1734, 1692, 1581, 1547, 1435, 1389, 1355, 1228, 1202, 1114, 1090, 1011, 975, 892, 789, 755 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₄₀H₄₃ClNaN₂O₁₀ ([M+Na]⁺): 769.2498, found: 769.2493.



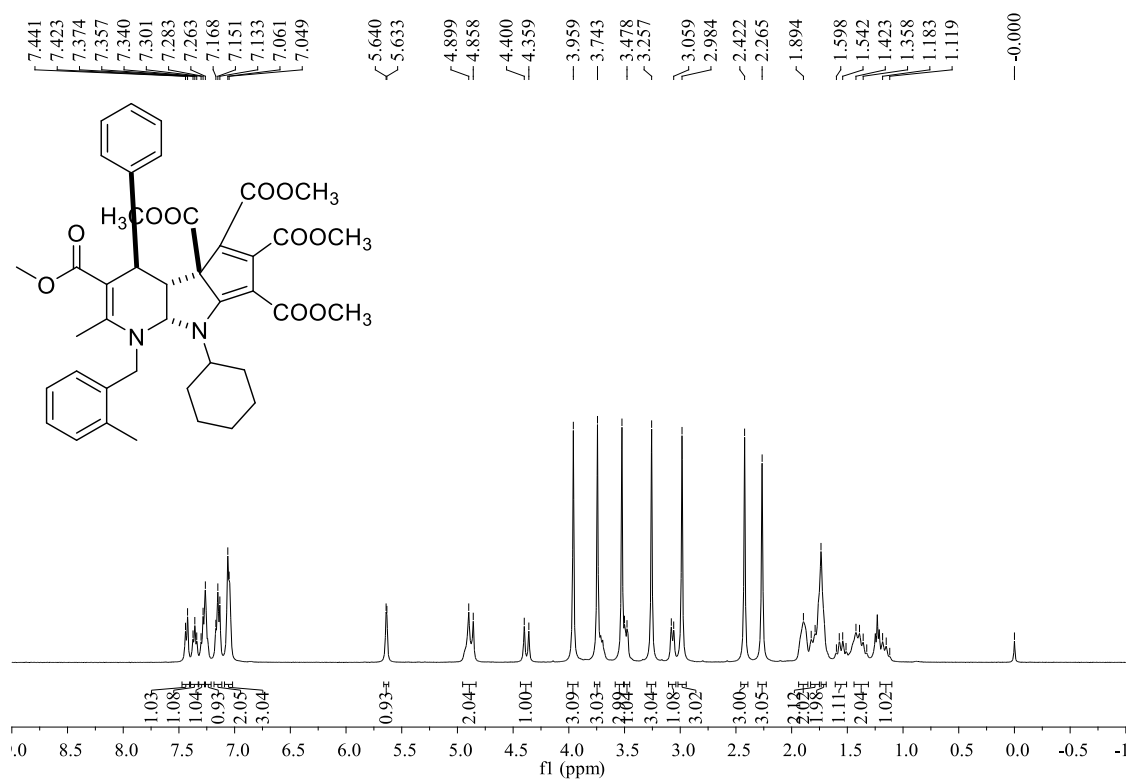


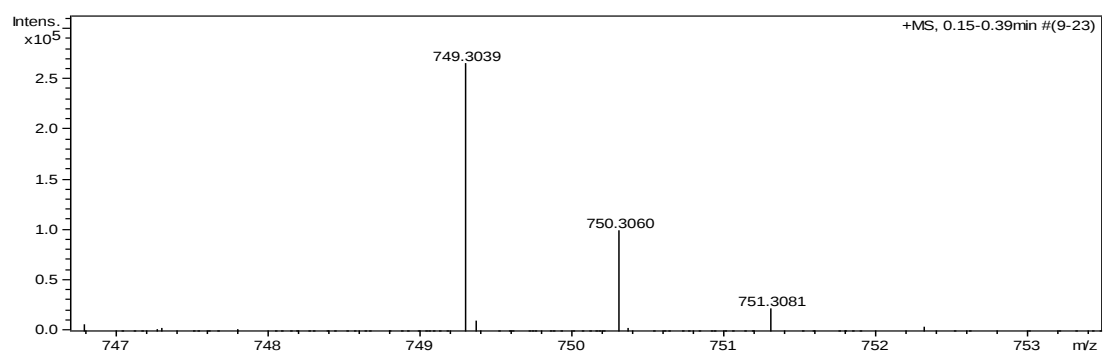
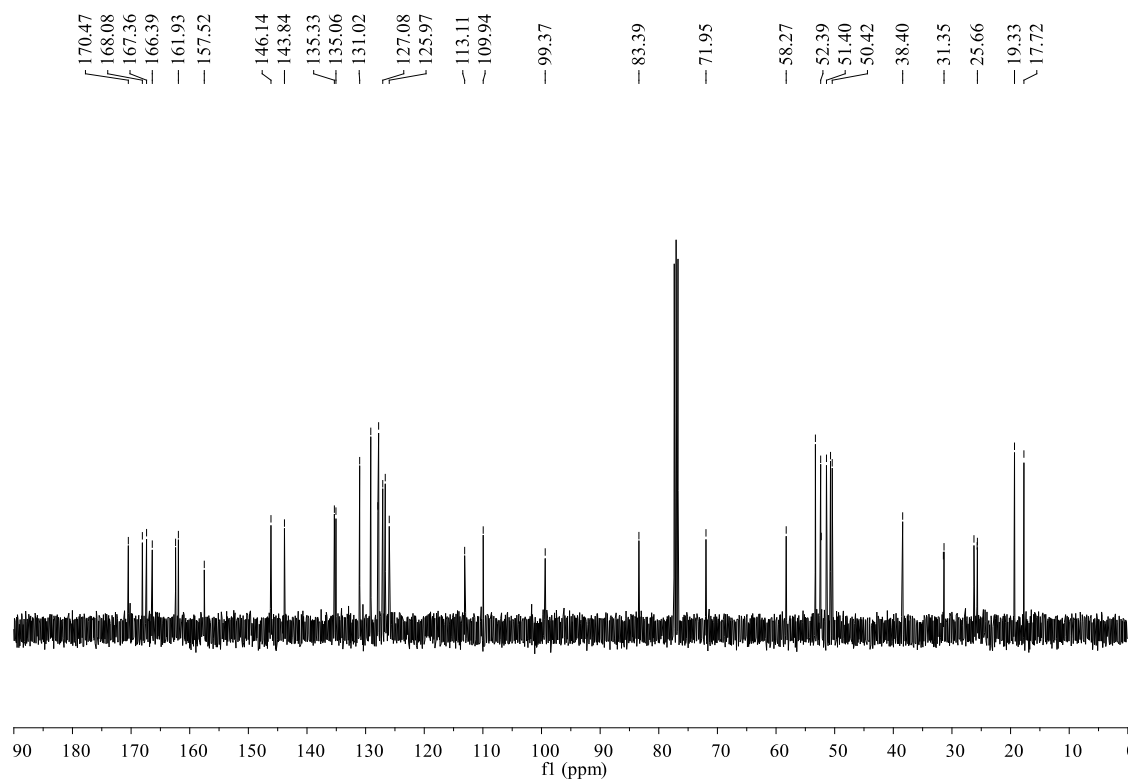
Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-1-benzyl-8-cyclohexyl-2-methyl-4-phenyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (4f):
yellow solid, 90%, m.p. 196-198 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.51-7.47 (m, 2H, ArH), 7.42-7.40 (m, 3H, ArH), 7.07-7.03 (m, 2H, ArH), 7.01-6.97 (m, 1H, ArH), 6.75 (d, *J* = 7.2 Hz, 2H, ArH), 5.81 (d, *J* = 3.6 Hz, 1H, CH), 4.95-4.91 (m, 1H, CH), 4.88 (d, *J* = 15.6 Hz, 1H, CH₂), 4.30 (d, *J* = 16.0 Hz, 1H, CH₂), 3.96 (s, 3H, OCH₃), 3.74 (s, 3H, OCH₃), 3.58 (s, 3H, OCH₃), 3.30 (dd, *J*₁ = 8.8 Hz, *J*₂ = 3.6 Hz, 1H, CH), 3.26 (s, 3H, OCH₃), 2.99-2.97 (m, 1H, CH), 2.96 (s, 3H, OCH₃), 2.33 (s, 3H, CH₃), 1.92-1.86 (m, 2H, CH₂), 1.79-1.72 (m, 4H, CH₂), 1.49-1.35 (m, 3H, CH₂), 1.20-1.10 (m, 1H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.2, 167.8, 167.6, 166.4, 162.4, 161.9, 157.7, 145.6, 143.8, 137.2, 129.2, 128.9, 128.3, 128.0, 127.6, 125.8, 113.0, 111.9, 99.2, 83.7, 72.1, 58.4, 56.6, 53.3, 52.4, 52.2, 51.4, 50.7, 50.4, 38.2, 31.8, 31.1, 26.2, 25.7, 25.6, 18.5 ppm. IR (KBr) ν: 3435, 2952, 2862, 1737, 1698, 1583, 1542, 1435, 1386, 1338, 1239, 1204, 1121, 1092, 1000, 978, 894, 852, 789 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₄₀H₄₄NaN₂O₁₀ ([M+Na]⁺): 735.2888, found: 735.2885.



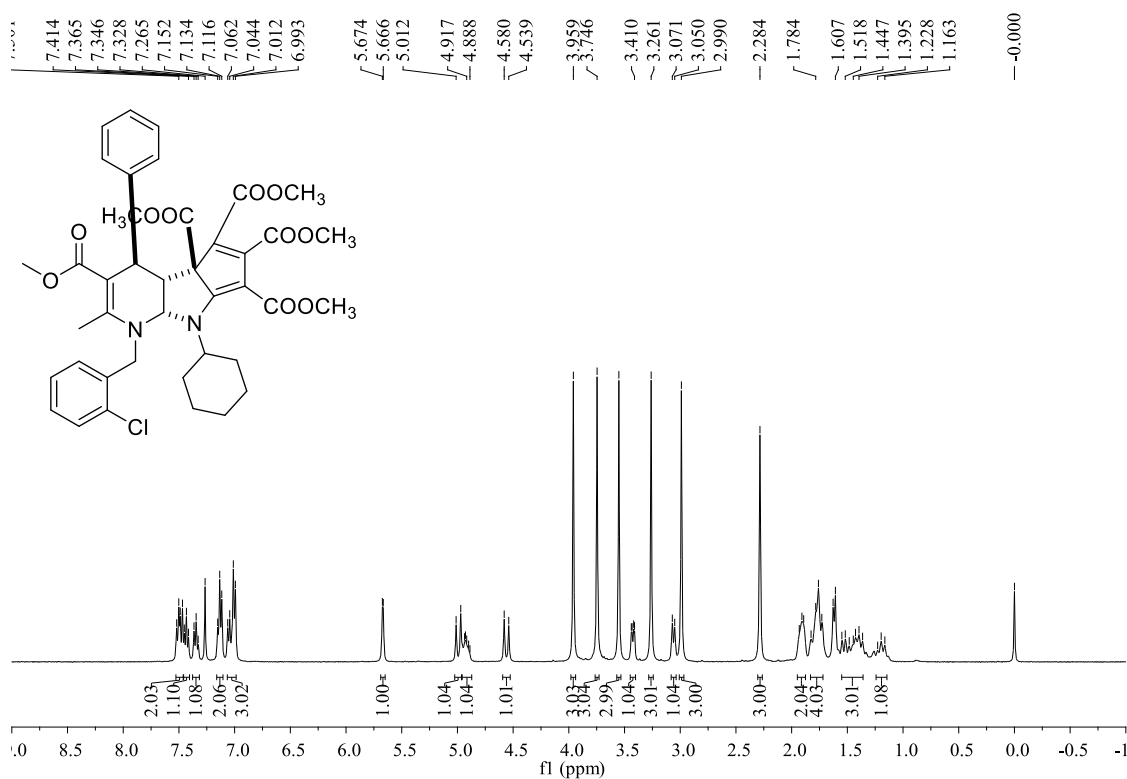


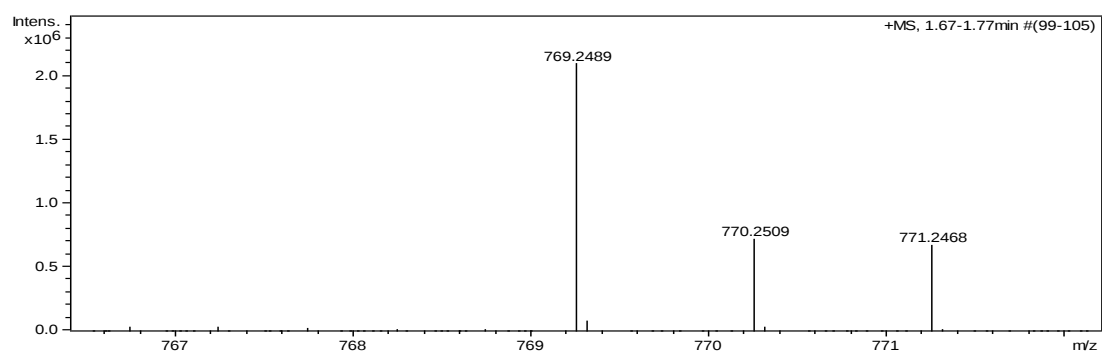
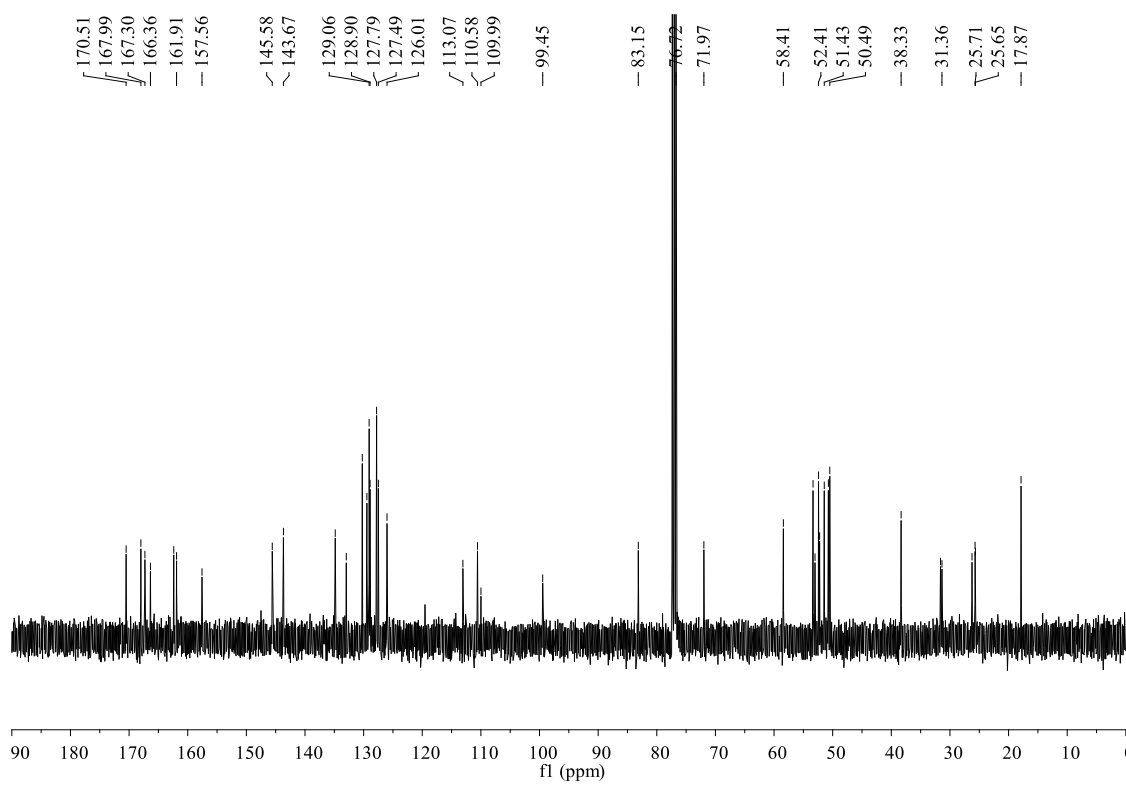
Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-8-cyclohexyl-2-methyl-1-(2-methylbenzyl)-4-phenyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (4g): yellow solid, 81%, m.p. 202-204 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.43 (d, *J* = 7.2 Hz, 1H, ArH), 7.36 (t, *J* = 6.8 Hz, 1H, ArH), 7.30-7.27 (m, 1H, ArH), 7.25-7.22 (m, 1H, ArH), 7.17-7.13 (m, 2H, ArH), 7.09-7.02 (m, 3H, ArH), 5.64 (d, *J* = 2.8 Hz, 1H, CH), 4.95-4.84 (m, 2H, CH, CH₂), 4.38 (d, *J* = 16.4 Hz, 1H, CH₂), 3.96 (s, 3H, OCH₃), 3.74 (s, 3H, OCH₃), 3.52 (s, 3H, OCH₃), 3.50-3.46 (m, 1H, CH), 3.26 (s, 3H, OCH₃), 3.07 (d, *J* = 8.4 Hz, 1H, CH), 2.98 (s, 3H, OCH₃), 2.42 (s, 3H, CH₃), 2.26 (s, 3H, CH₃), 1.94-1.86 (m, 2H, CH₂), 1.83-1.75 (m, 2H, CH₂), 1.74-1.69 (m, 2H, CH₂), 1.60-1.51 (m, 1H, CH₂), 1.42-1.33 (m, 2H, CH₂), 1.18-1.12 (m, 1H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.5, 168.1, 167.4, 166.4, 162.4, 161.9, 157.5, 146.1, 143.8, 135.3, 135.1, 131.0, 129.1, 127.9, 127.8, 127.1, 126.7, 126.0, 113.1, 109.9, 99.4, 83.4, 72.0, 58.3, 53.3, 52.4, 52.3, 51.4, 50.7, 50.4, 38.4, 31.5, 31.4, 26.3, 25.70, 25.66, 19.3, 17.7 ppm. IR (KBr) ν: 3446, 2947, 1733, 1687, 1581, 1545, 1435, 1383, 1339, 1233, 1204, 1131, 1092, 981, 894, 818, 790 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₄₁H₄₆NaN₂O₁₀ ([M+Na]⁺): 749.3045, found: 749.3039.



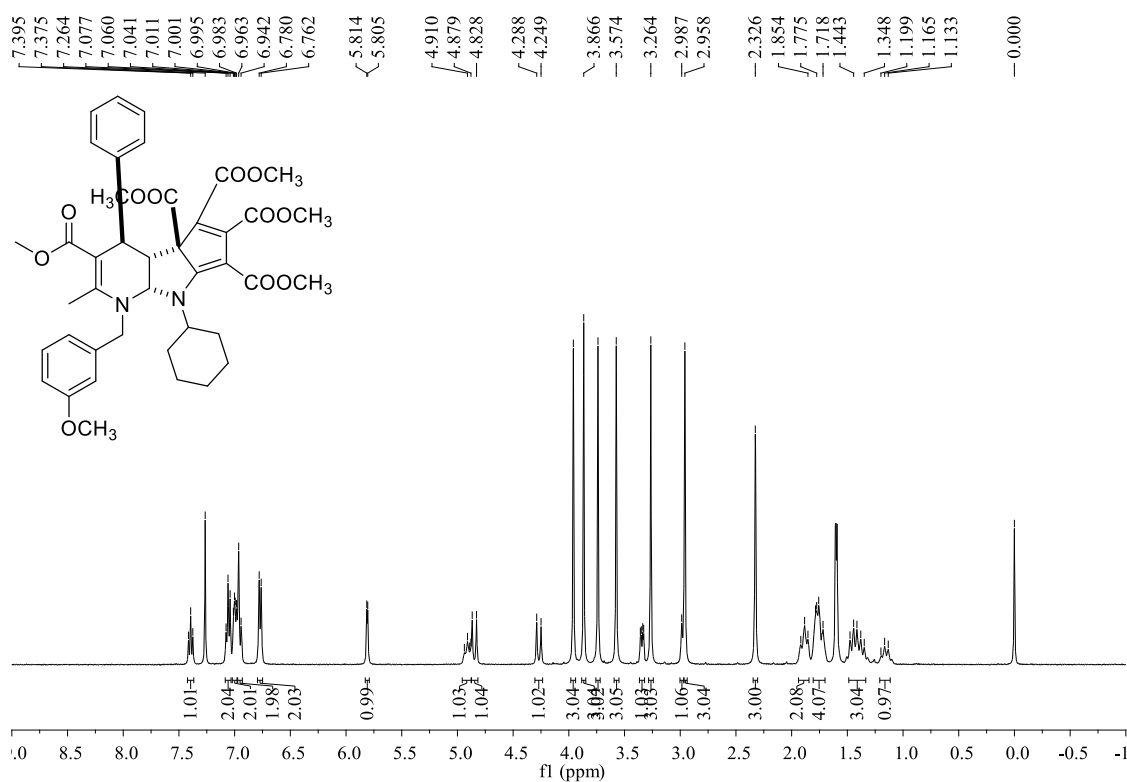


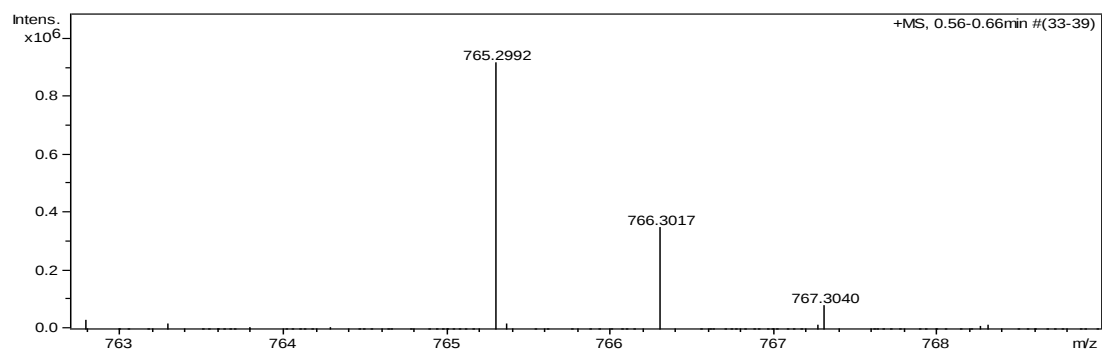
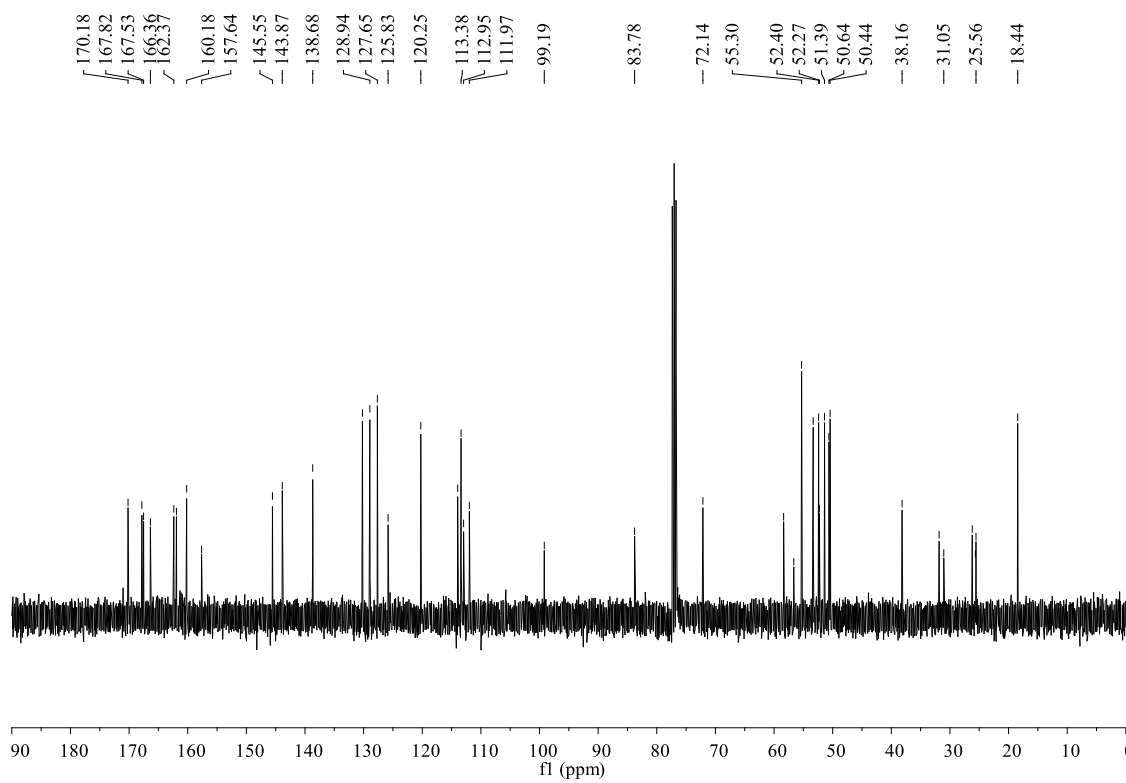
Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-1-(2-chlorobenzyl)-8-cyclohexyl-2-methyl-4-phenyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (4*h*): yellow solid, 80%, m.p. 203-205 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.52-7.47 (m, 2H, ArH), 7.43 (t, *J* = 7.6 Hz, 1H, ArH), 7.35 (t, *J* = 7.6 Hz, 1H, ArH), 7.13 (t, *J* = 7.2 Hz, 2H, ArH), 7.06-6.99 (m, 3H, ArH), 5.67 (d, *J* = 3.2 Hz, 1H, CH), 4.99 (d, *J* = 16.8 Hz, 1H, CH₂), 4.94-4.89 (m, 1H, CH), 4.56 (d, *J* = 16.4 Hz, 1H, CH₂), 3.96 (s, 3H, OCH₃), 3.75 (s, 3H, OCH₃), 3.55 (s, 3H, OCH₃), 3.42 (dd, *J*₁ = 8.4 Hz, *J*₂ = 2.8 Hz, 1H, CH), 3.26 (s, 3H, OCH₃), 3.06 (d, *J* = 8.4 Hz, 1H, CH), 2.99 (s, 3H, OCH₃), 2.28 (s, 3H, CH₃), 1.93-1.89 (m, 2H, CH₂), 1.83-1.73 (m, 4H, CH₂), 1.55-1.36 (m, 3H, CH₂), 1.23-1.16 (m, 1H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.5, 168.0, 167.3, 166.4, 162.4, 161.9, 157.6, 145.6, 143.7, 134.8, 133.0, 130.2, 129.4, 129.1, 128.9, 127.8, 127.5, 126.0, 113.1, 110.6, 110.0, 99.5, 83.2, 77.4, 77.0, 76.7, 72.0, 58.4, 53.4, 53.0, 52.4, 52.2, 51.4, 50.7, 50.5, 38.3, 31.6, 31.4, 26.2, 25.71, 25.65, 17.9 ppm. IR (KBr) ν: 3435, 2949, 2856, 1737, 1695, 1581, 1541, 1435, 1385, 1337, 1240, 1206, 1117, 1091, 999, 978, 895, 854, 790, 755 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₄₀H₄₃ClNaN₂O₁₀ ([M+Na]⁺): 769.2498, found: 769.2489.



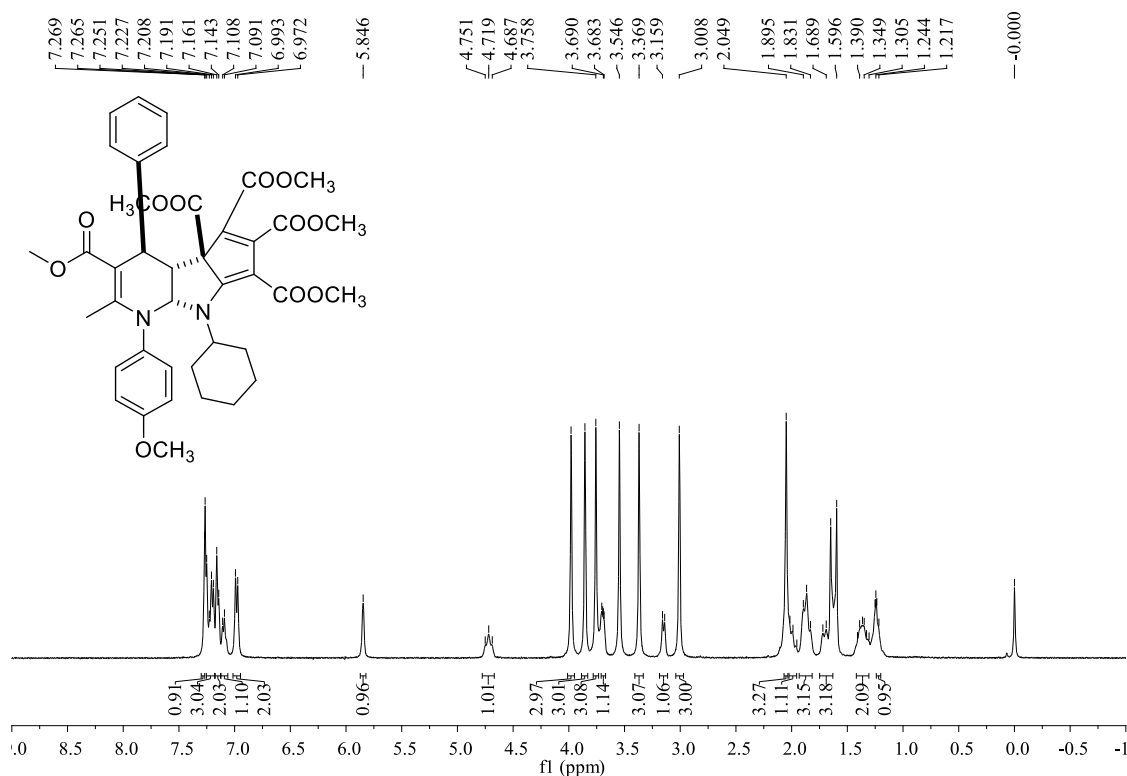


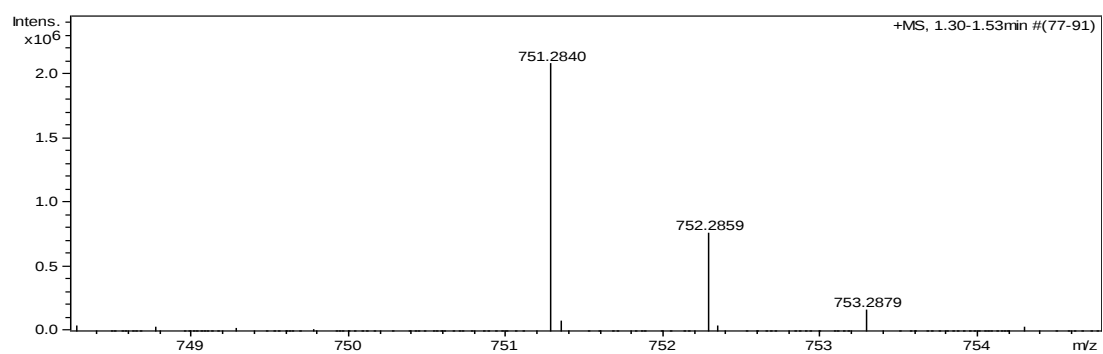
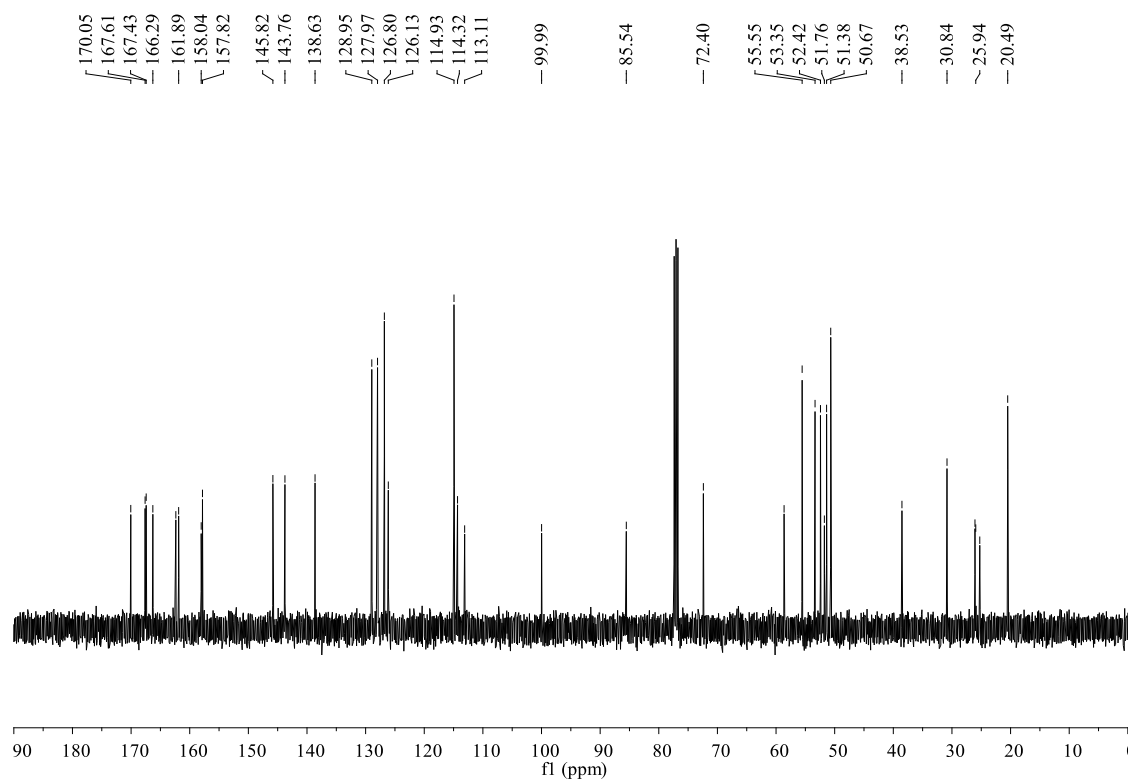
Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-8-cyclohexyl-1-(3-methoxybenzyl)-2-methyl-4-phenyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (4i): yellow solid, 80%, m.p. 201-203 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.39 (t, *J* = 7.6 Hz, 1H, ArH), 7.06 (t, *J* = 6.8 Hz, 2H, ArH), 7.01-6.98 (m, 2H, ArH), 6.97-6.93 (m, 2H, ArH), 6.77 (d, *J* = 7.2 Hz, 2H, ArH), 5.81 (d, *J* = 3.6 Hz, 1H, CH), 4.94-4.88 (m, 1H, CH), 4.85 (d, *J* = 15.6 Hz, 1H, CH₂), 4.27 (d, *J* = 15.6 Hz, 1H, CH₂), 3.96 (s, 3H, OCH₃), 3.87 (s, 3H, OCH₃), 3.74 (s, 3H, OCH₃), 3.57 (s, 3H, OCH₃), 3.34 (dd, *J*₁ = 8.4 Hz, *J*₂ = 3.2 Hz, 1H, CH), 3.26 (s, 3H, OCH₃), 3.00-2.97 (m, 1H, CH), 2.96 (s, 3H, OCH₃), 2.33 (s, 3H, CH₃), 1.92-1.85 (m, 2H, CH₂), 1.79-1.72 (m, 4H, CH₂), 1.48-1.35 (m, 3H, CH₂), 1.20-1.13 (m, 1H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.2, 167.8, 167.5, 166.4, 162.4, 161.9, 160.2, 157.6, 145.6, 143.9, 138.7, 130.2, 128.9, 127.7, 125.8, 120.3, 114.0, 113.4, 113.0, 112.0, 99.2, 83.8, 72.1, 58.4, 56.6, 55.3, 53.3, 52.4, 52.3, 51.4, 50.6, 50.4, 38.2, 31.8, 31.1, 26.2, 25.7, 25.6, 18.4 ppm. IR (KBr) ν: 3446, 2949, 2855, 1733, 1697, 1582, 1542, 1435, 1382, 1347, 1231, 1205, 1113, 1094, 1045, 1001, 893, 867, 789 cm⁻¹ (*m/z*): HRMS (ESI) Calcd. for C₄₁H₄₆NaN₂O₁₁ ([M+Na]⁺): 765.2994, found: 765.2992.



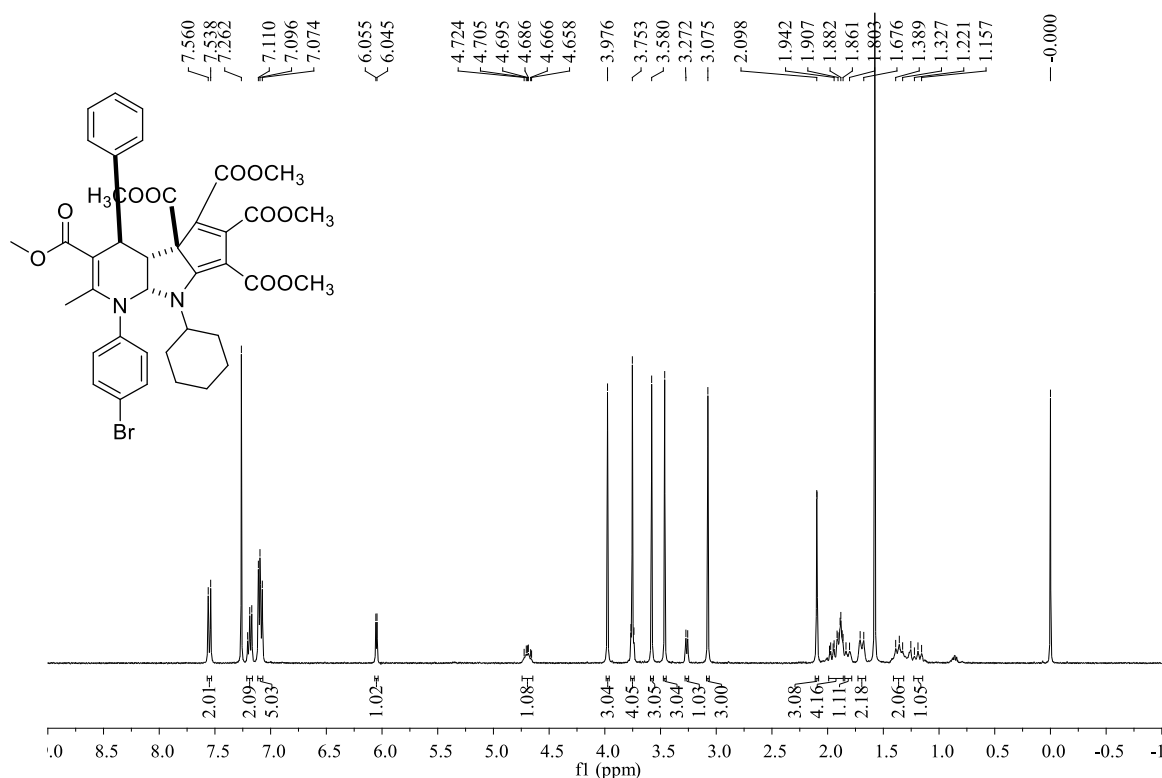


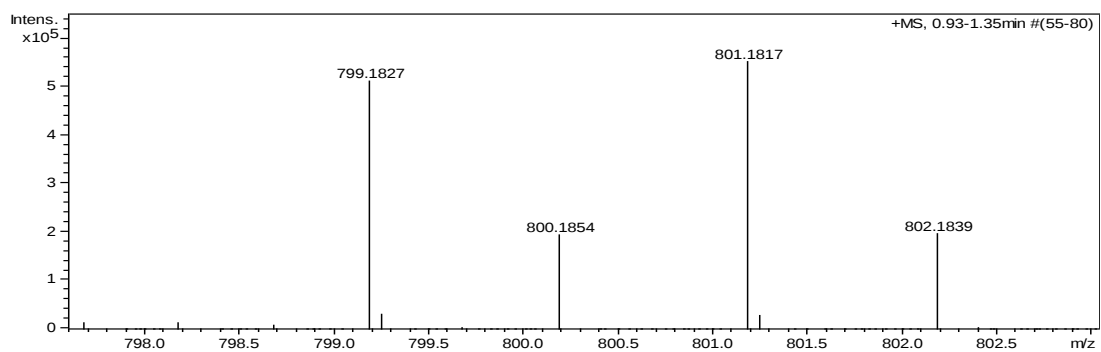
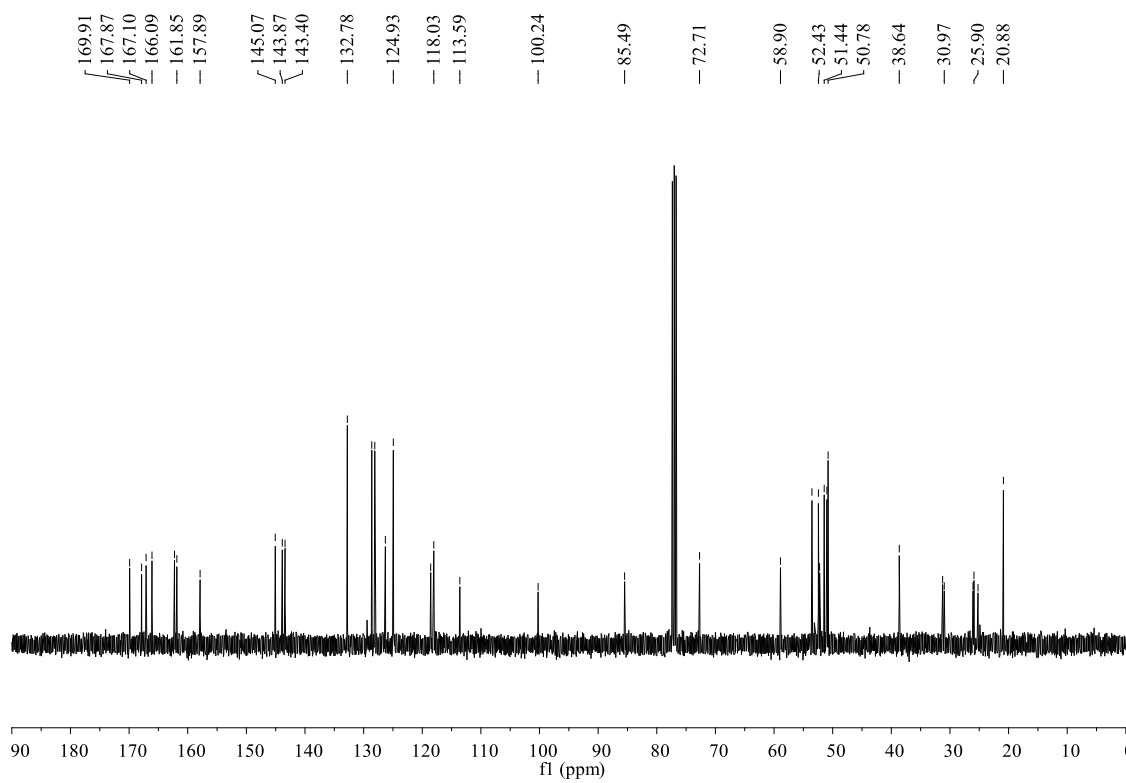
Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aR*)-8-cyclohexyl-1-(4-methoxyphenyl)-2-methyl-4-phenyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (4j): yellow solid, 87%, m.p. 144-146 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.30-7.27 (m, 1H, ArH), 7.25-7.19 (m, 3H, ArH), 7.15 (d, *J* = 7.2 Hz, 2H, ArH), 7.11-7.07 (m, 1H, ArH), 6.98 (d, *J* = 8.4 Hz, 2H, ArH), 5.85 (s, 1H, CH), 4.72 (t, *J* = 12.8 Hz, 1H, CH), 3.98 (s, 3H, OCH₃), 3.86 (s, 3H, OCH₃), 3.76 (s, 3H, OCH₃), 3.71-3.67 (m, 1H, CH), 3.55 (s, 3H, OCH₃), 3.37 (s, 3H, OCH₃), 3.15 (d, *J* = 7.6 Hz, 1H, CH), 3.01 (s, 3H, OCH₃), 2.05 (s, 3H, CH₃), 2.02-1.95 (m, 1H, CH₂), 1.90-1.83 (m, 3H, CH₂), 1.72-1.63 (m, 3H, CH₂), 1.41-1.31 (m, 2H, CH₂), 1.24-1.20 (m, 1H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.1, 167.6, 167.4, 166.3, 162.4, 161.9, 158.0, 157.8, 145.8, 143.8, 138.6, 129.0, 128.0, 126.8, 126.1, 114.9, 114.3, 113.1, 100.0, 85.5, 72.4, 58.6, 55.6, 53.4, 52.4, 51.8, 51.4, 50.7, 38.5, 30.8, 26.1, 25.9, 25.3, 20.5 ppm. IR (KBr) ν: 3434, 2949, 1737, 1694, 1581, 1542, 1509, 1434, 1339, 1231, 1204, 1096, 1067, 1033, 1001, 825, 794, 761 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₄₀H₄₄NaN₂O₁₁ ([M+Na]⁺): 751.2837, found: 751.2840.



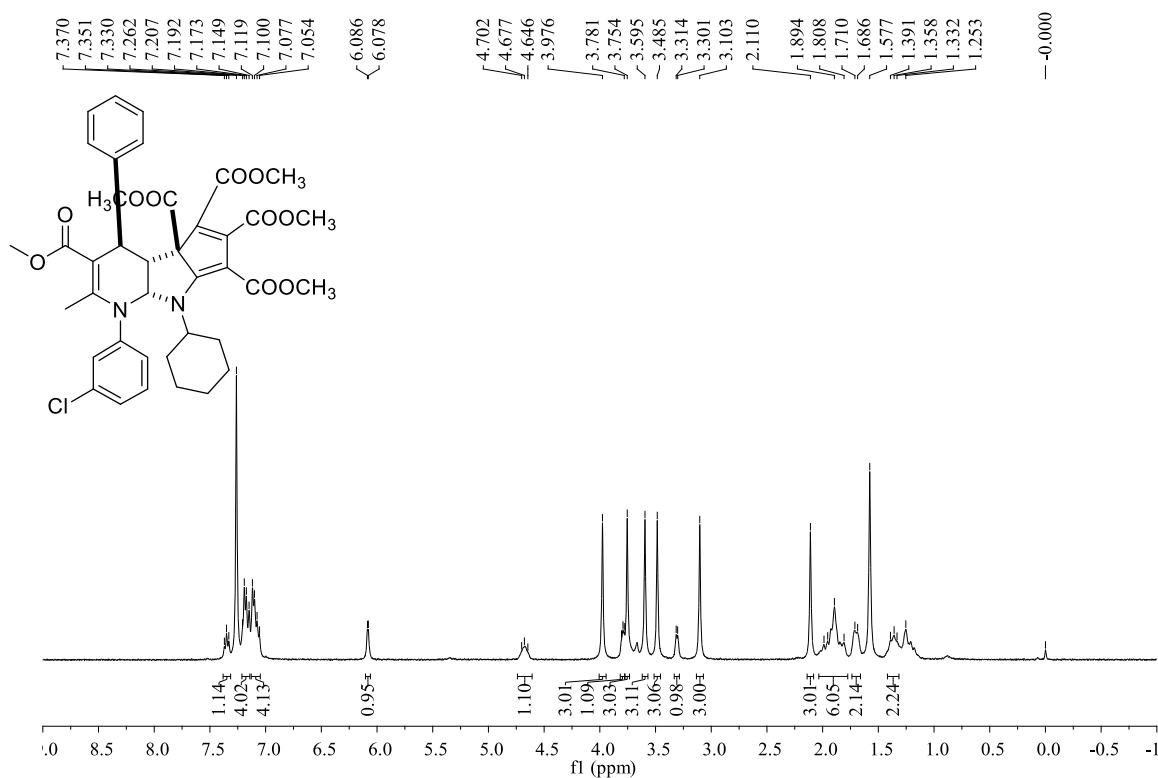


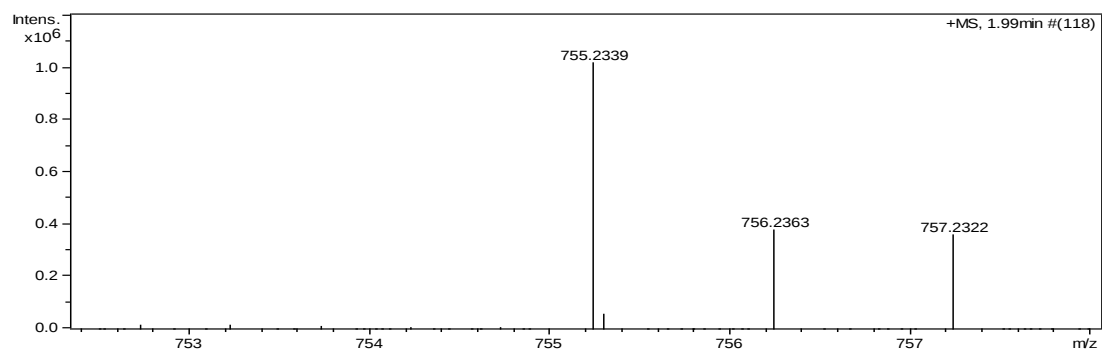
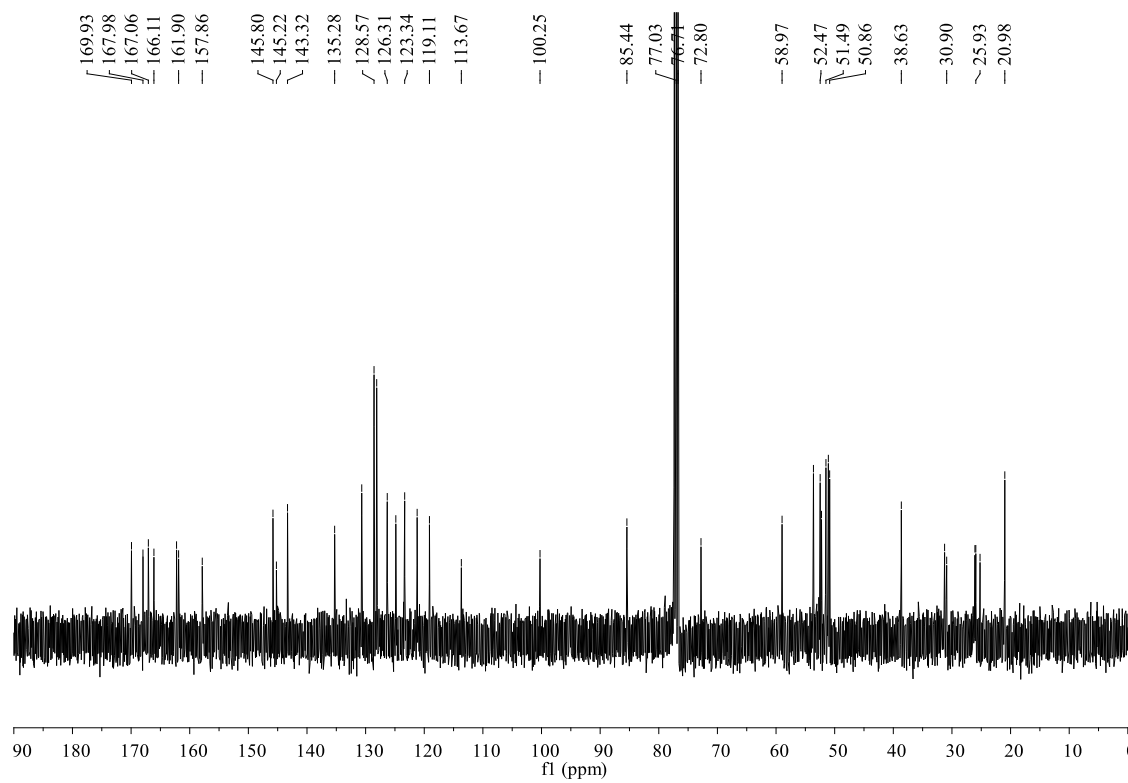
Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aR*)-1-(4-bromophenyl)-8-cyclohexyl-2-methyl-4-phenyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (4k): yellow solid, 93%, m.p. 134-136 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.55 (d, *J* = 8.8 Hz, 2H, ArH), 7.21-7.17 (m, 2H, ArH), 7.11-7.07 (m, 5H, ArH), 6.05 (d, *J* = 4.0 Hz, 1H, CH), 4.72-4.66 (m, 1H, CH), 3.98 (s, 3H, OCH₃), 3.77-3.74 (m, 4H, CH, OCH₃), 3.58 (s, 3H, OCH₃), 3.46 (s, 3H, OCH₃), 3.26 (d, *J* = 6.4 Hz, 1H, CH), 3.08 (s, 3H, OCH₃), 2.10 (s, 3H, CH₃), 1.98-1.86 (m, 4H, CH₂), 1.84-1.80 (m, 1H, CH₂), 1.71-1.68 (m, 2H, CH₂), 1.39-1.33 (m, 2H, CH₂), 1.22-1.16 (m, 1H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 169.9, 167.9, 167.1, 166.1, 162.3, 161.9, 157.9, 145.1, 143.9, 143.4, 132.8, 128.6, 128.1, 126.3, 124.9, 118.6, 118.0, 113.6, 100.2, 85.5, 72.7, 58.9, 53.5, 52.4, 52.2, 51.4, 51.0, 50.8, 38.6, 31.3, 31.0, 26.1, 25.9, 25.2, 20.9 ppm. IR (KBr) ν: 3434, 2949, 2857, 1735, 1698, 1584, 1545, 1489, 1435, 1342, 1235, 1153, 1098, 1071, 1009, 822, 795 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₃₉H₄₁BrNaN₂O₁₀ ([M+Na]⁺): 800.6542, found: 800.1854.



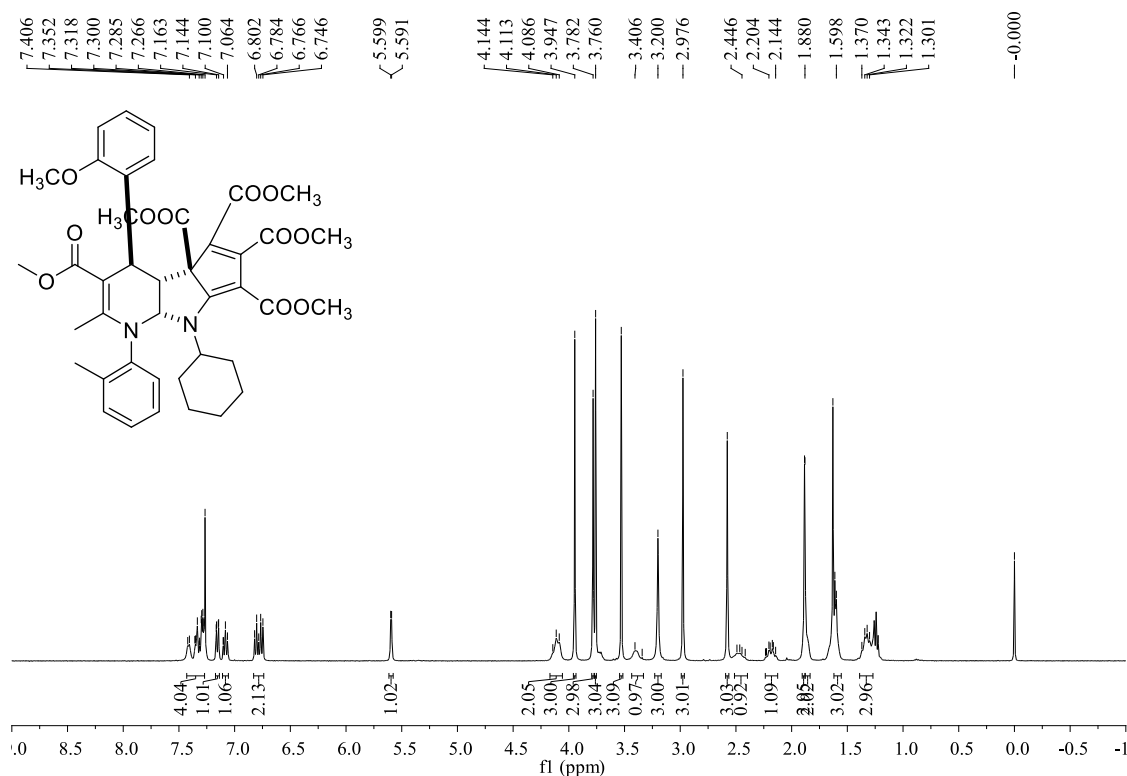


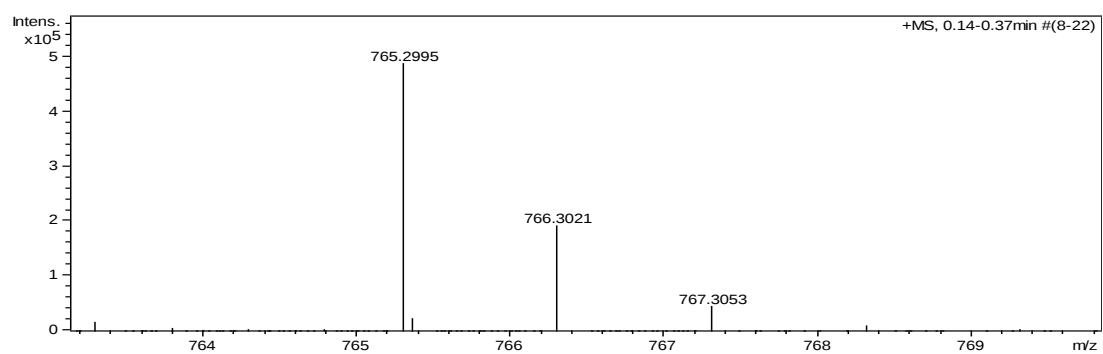
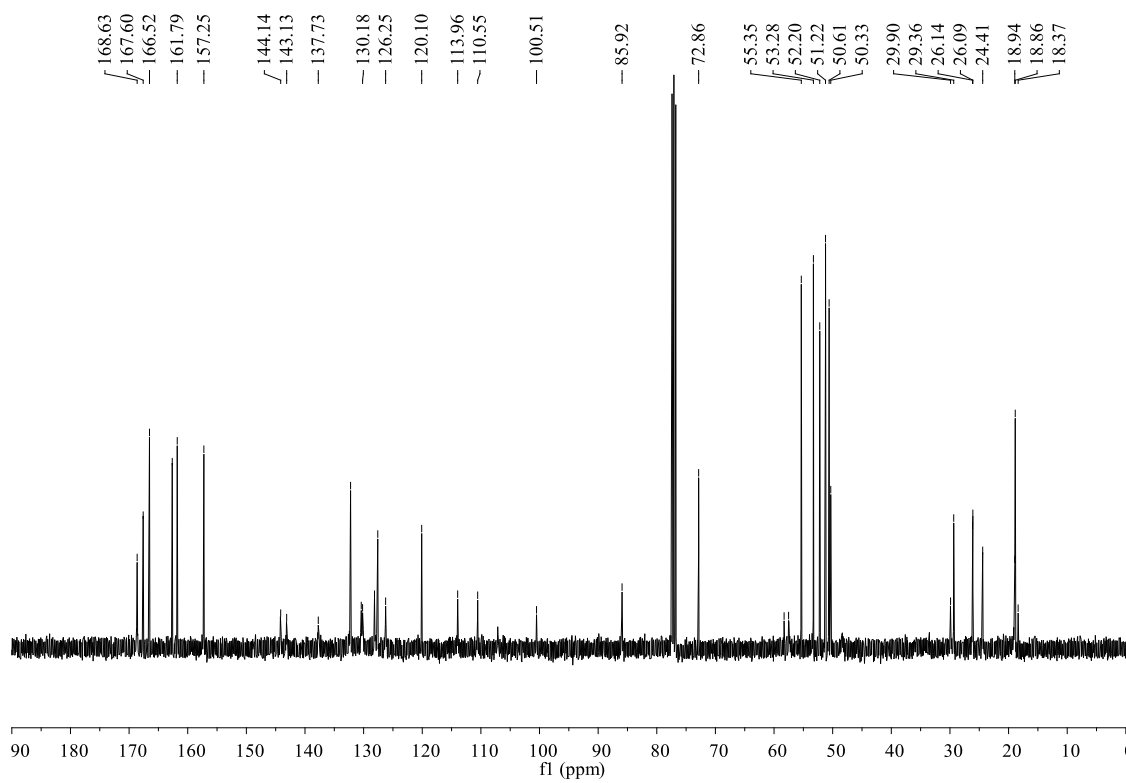
Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aR*)-1-(3-chlorophenyl)-8-cyclohexyl-2-methyl-4-phenyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (4I): yellow solid, 92%, m.p. 184-186 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.37-7.33 (m, 1H, ArH), 7.21-7.15 (m, 4H, ArH), 7.12-7.05 (m, 4H, ArH), 6.08 (d, *J* = 3.2 Hz, 1H, CH), 4.70-4.65 (m, 1H, CH), 3.98 (s, 3H, OCH₃), 3.81-3.78 (m, 1H, CH), 3.75 (s, 3H, OCH₃), 3.59 (s, 3H, OCH₃), 3.48 (s, 3H, OCH₃), 3.31 (d, *J* = 5.2 Hz, 1H, CH), 3.10 (s, 3H, OCH₃), 2.11 (s, 3H, CH₃), 1.99-1.81 (m, 6H, CH₂), 1.71-1.69 (m, 2H, CH₂), 1.39-1.33 (m, 2H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 169.9, 168.0, 167.1, 166.1, 162.3, 161.9, 157.9, 145.8, 145.2, 143.3, 135.3, 130.6, 128.6, 128.1, 126.3, 124.9, 123.3, 121.2, 119.1, 113.7, 100.3, 85.4, 77.4, 77.0, 76.7, 72.8, 59.0, 53.6, 52.5, 52.3, 51.5, 51.1, 50.9, 38.6, 31.3, 30.9, 26.1, 25.9, 25.2, 21.0 ppm. IR (KBr) ν: 3434, 2949, 2855, 1734, 1702, 1589, 1546, 1479, 1435, 1342, 1312, 1229, 1153, 1098, 1067, 1000, 751 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₃₉H₄₁ClNaN₂O₁₀ ([M+Na]⁺): 755.2342, found: 755.2339.





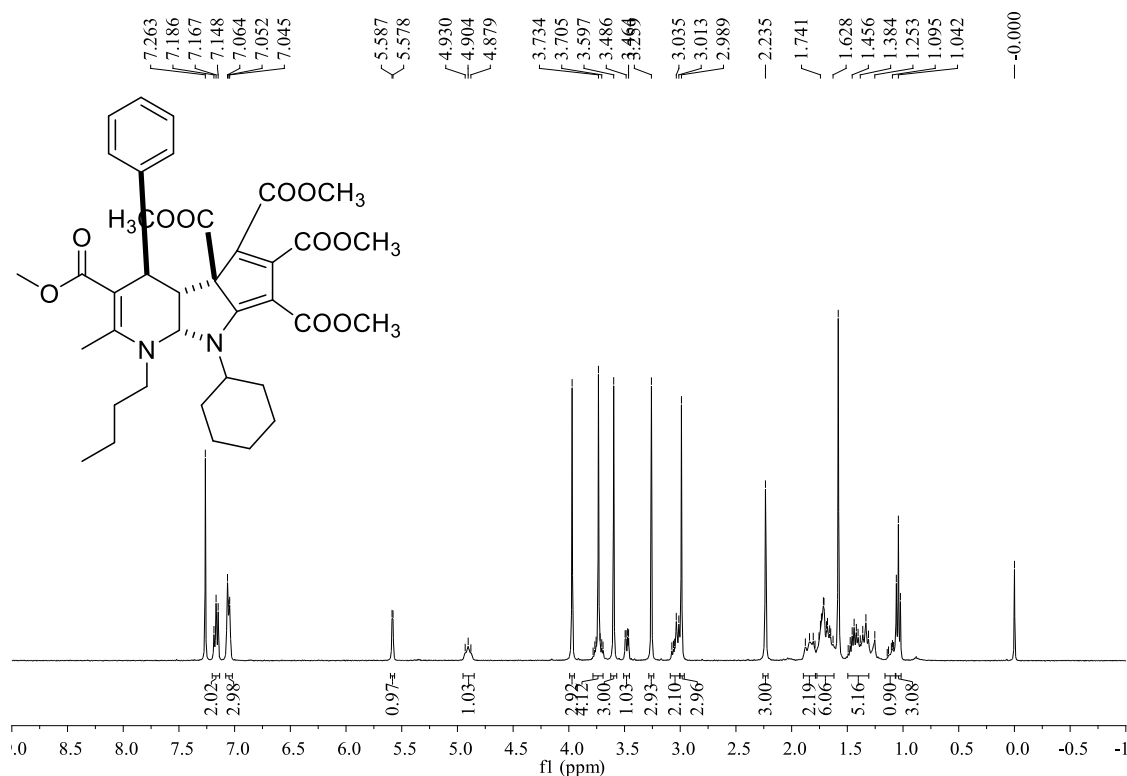
Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aR*)-8-cyclohexyl-4-(2-methoxyphenyl)-2-methyl-1-(*o*-tolyl)-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (4*m*): yellow solid, 93%, m.p. 183-185 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.43-7.27 (m, 4H, ArH), 7.17-7.14 (m, 1H, ArH), 7.10-7.06 (m, 1H, ArH), 6.82-6.75 (m, 2H, ArH), 5.59 (d, *J* = 3.2 Hz, 1H, CH), 4.14-4.09 (m, 2H, CH), 3.95 (s, 3H, OCH₃), 3.78 (s, 3H, OCH₃), 3.76 (s, 3H, OCH₃), 3.53 (s, 3H, OCH₃), 3.41-3.34 (m, 1H, CH), 3.20 (s, 3H, OCH₃), 2.98 (s, 3H, OCH₃), 2.58 (s, 3H, CH₃), 2.49-2.42 (m, 1H, CH₂), 2.24-2.14 (m, 1H, CH₂), 1.88 (s, 3H, CH₃), 1.87-1.83 (m, 2H, CH₂), 1.62-1.56 (m, 3H, CH₂), 1.39-1.27 (m, 3H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 168.6, 167.6, 166.5, 162.6, 161.8, 157.3, 144.1, 143.1, 137.7, 132.2, 130.4, 130.2, 128.1, 127.6, 126.3, 120.1, 114.0, 110.6, 100.5, 85.9, 72.9, 58.3, 57.5, 55.4, 53.3, 52.2, 51.2, 50.6, 50.3, 29.9, 29.4, 26.14, 26.09, 24.4, 18.94, 18.86, 18.4 ppm. IR (KBr) ν: 3435, 2947, 2850, 1734, 1702, 1584, 1542, 1434, 1398, 1337, 1232, 1200, 1118, 1091, 1064, 949, 852, 795, 754 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₄₁H₄₆NaN₂O₁₁ ([*M*+Na]⁺): 765.2994, found: 765.2995.

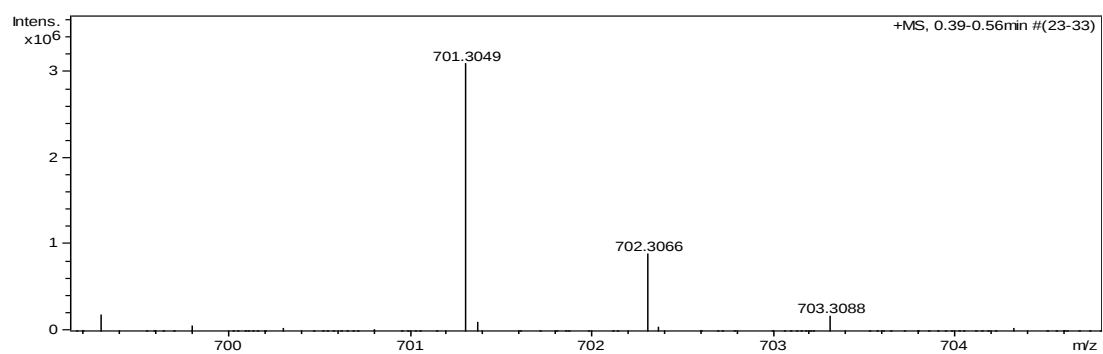
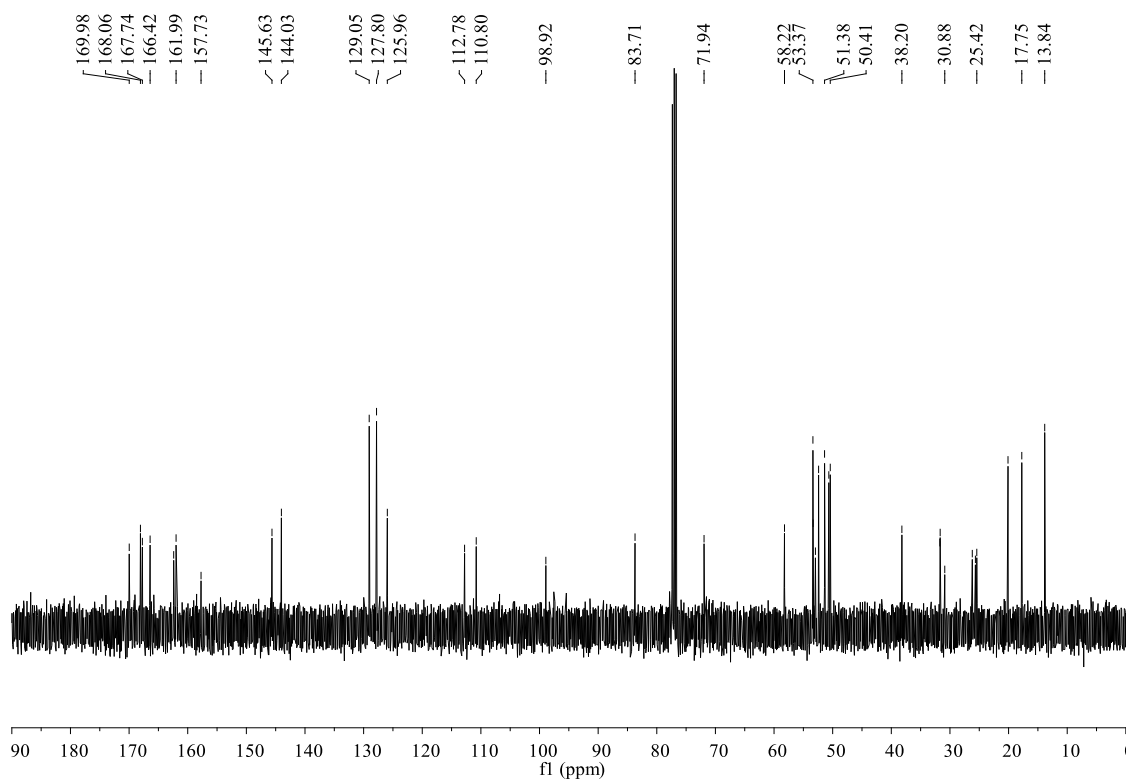




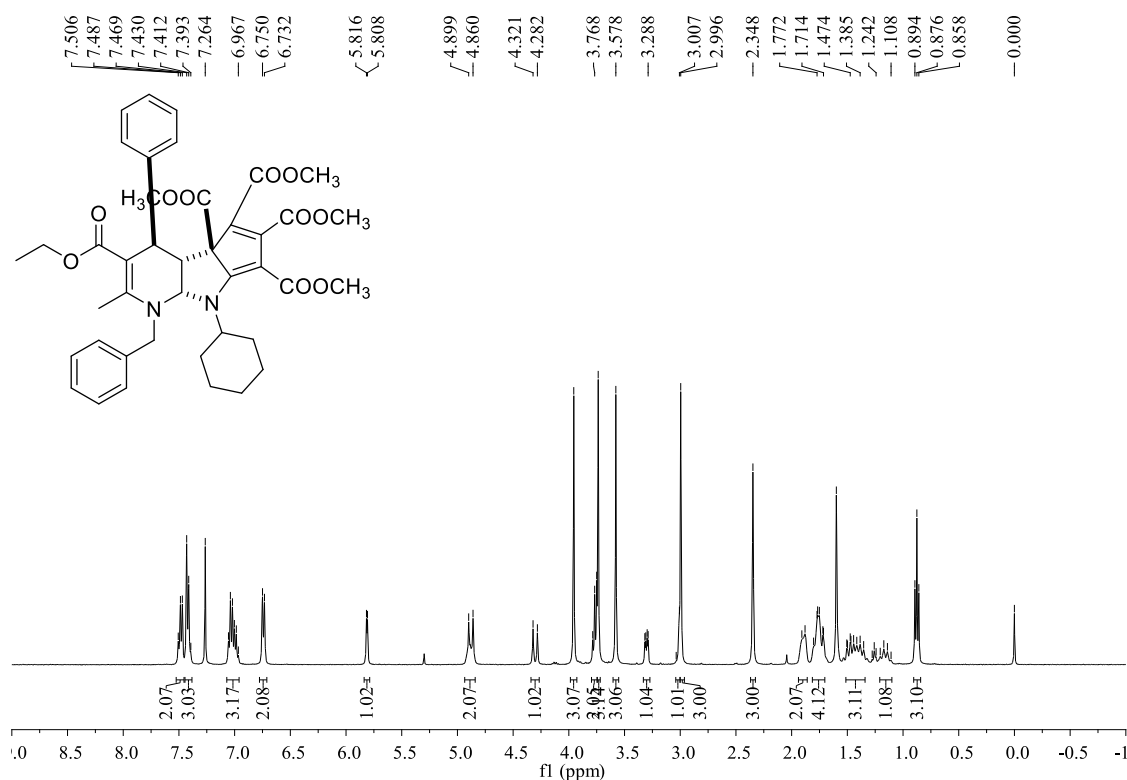
Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-1-butyl-8-cyclohexyl-4-phenyl-2-methyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (**4n**):

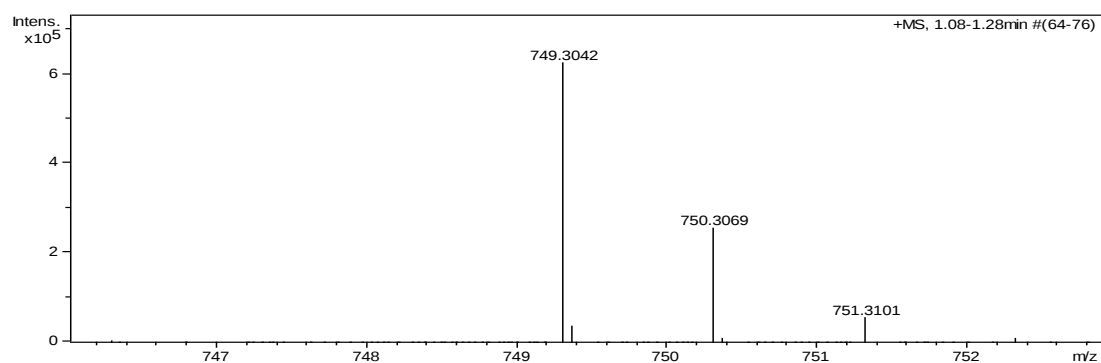
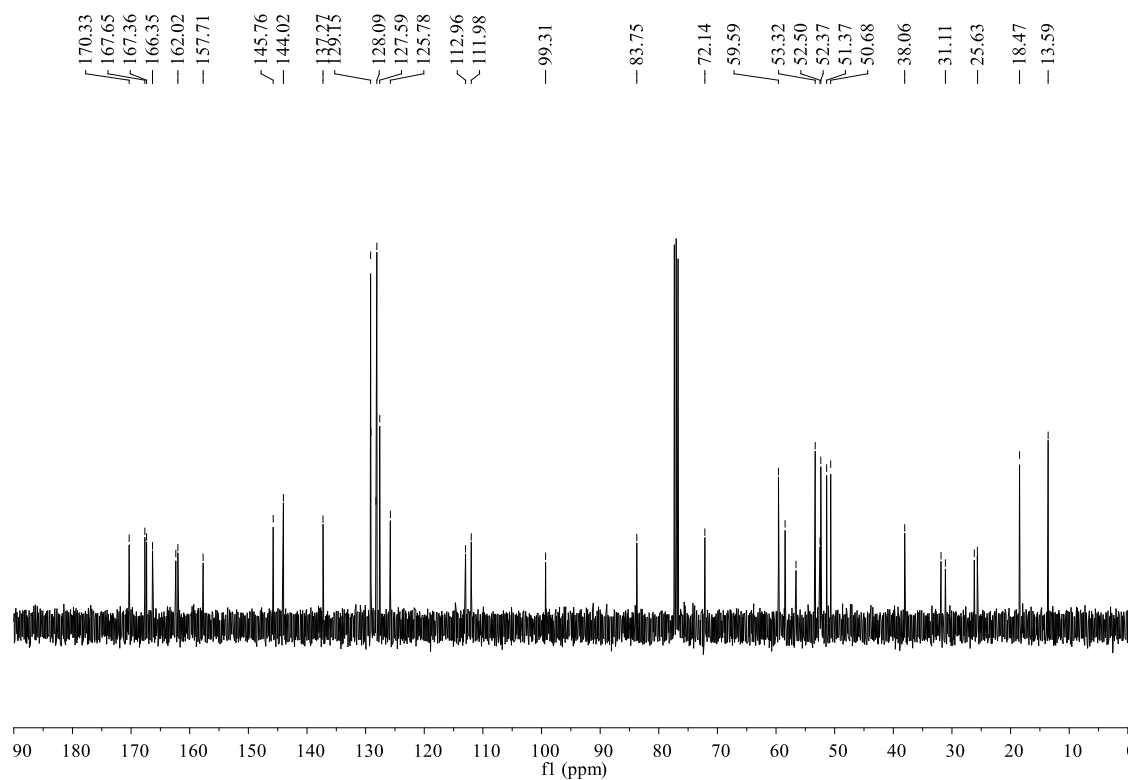
yellow solid, 80%, m.p. 177-179 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.17 (t, *J* = 7.6 Hz, 2H, ArH), 7.08-7.02 (m, 3H, ArH), 5.58 (d, *J* = 3.6 Hz, 1H, CH), 4.90 (d, *J* = 10.4 Hz, 1H, CH), 3.97 (s, 3H, OCH₃), 3.78-3.69 (m, 4H, CH₂, OCH₃), 3.60 (s, 3H, OCH₃), 3.48 (dd, *J*₁ = 9.2 Hz, *J*₂ = 3.6 Hz, 1H, CH), 3.26 (s, 3H, OCH₃), 3.08-3.01 (m, 2H, CH, CH₂), 2.99 (s, 3H, OCH₃), 2.23 (s, 3H, CH₃), 1.88-1.79 (m, 2H, CH₂), 1.73-1.63 (m, 6H, CH₂), 1.49-1.31 (m, 5H, CH₂), 1.14-1.09 (m, 1H, CH₂), 1.04 (t, *J* = 7.2 Hz, 3H, CH₃) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.0, 168.1, 167.7, 166.4, 162.4, 162.0, 157.7, 145.6, 144.0, 129.1, 127.8, 126.0, 112.8, 110.8, 98.9, 83.7, 71.9, 58.2, 53.4, 53.3, 52.9, 52.4, 51.4, 50.7, 50.4, 38.2, 31.71, 31.67, 30.9, 26.21, 26.19, 25.7, 25.4, 20.1, 17.8, 13.8 ppm. IR (KBr) ν: 3434, 2946, 2857, 2360, 1737, 1691, 1584, 1547, 1434, 1379, 1337, 1306, 1227, 1206, 1111, 1082, 1001, 756 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₃₇H₄₆NaN₂O₁₀ ([M+Na]⁺): 701.3045, found: 701.3049.



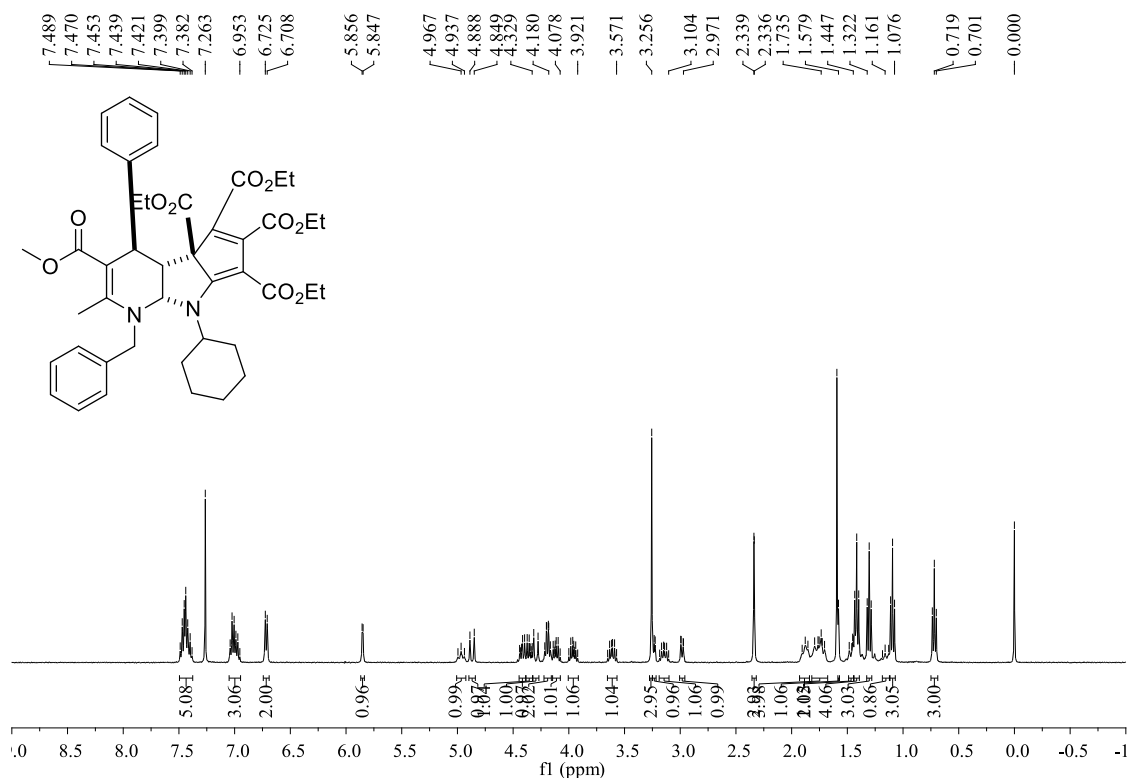


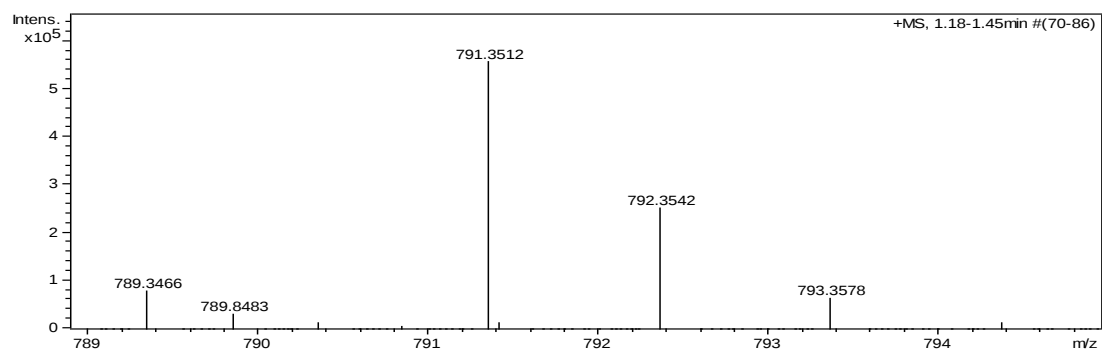
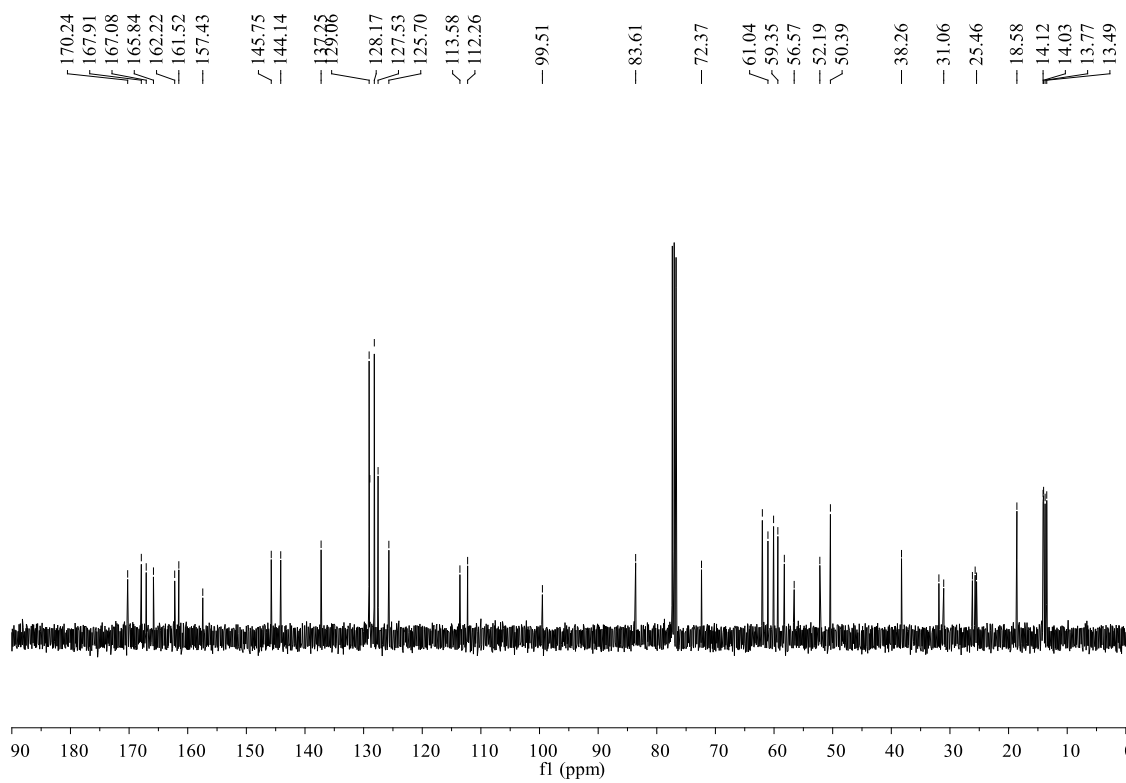
3-Ethyl 4b,5,6,7-tetramethyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-1-benzyl-8-cyclohexyl-2-methyl-4-phenyl-4,4a,8,8a-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4b,5,6,7(1*H*)-pentacarboxylate (4o): yellow solid, 79%, m.p. 204-206 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.51-7.47 (m, 2H, ArH), 7.43-7.39 (m, 3H, ArH), 7.06-6.97 (m, 3H, ArH), 6.74 (d, *J* = 7.2 Hz, 2H, ArH), 5.81 (d, *J* = 3.2 Hz, 1H, CH), 4.90-4.86 (m, 2H, CH, CH₂), 4.30 (d, *J* = 15.6 Hz, 1H, CH₂), 3.96 (s, 3H, OCH₃), 3.79-3.75 (m, 2H, CH₂) 3.74 (s, 3H, OCH₃), 3.58 (s, 3H, OCH₃), 3.30 (dd, *J*₁ = 8.4 Hz, *J*₂ = 3.6 Hz, 1H, CH), 3.04-3.01 (m, 1H, CH), 3.00 (s, 3H, OCH₃), 2.35 (s, 3H, CH₃), 1.91-1.88 (m, 2H, CH₂), 1.80-1.71 (m, 4H, CH₂), 1.51-1.35 (m, 3H, CH₂), 1.17-1.11 (m, 1H, CH₂), 0.88 (t, *J* = 7.2 Hz, 3H, CH₃) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.3, 167.7, 167.4, 166.4, 162.4, 162.0, 157.7, 145.8, 144.0, 137.3, 129.2, 129.1, 128.2, 128.1, 127.6, 125.8, 113.0, 112.0, 99.3, 83.8, 72.1, 59.6, 58.5, 56.6, 53.3, 52.5, 52.4, 51.4, 50.7, 38.1, 31.9, 31.1, 26.2, 25.7, 25.6, 18.5, 13.6 ppm. IR (KBr) ν: 3435, 2949, 2860, 1736, 1698, 1583, 1542, 1434, 1386, 1338, 1236, 1204, 1120, 1091, 1002, 980, 894, 852, 790 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₄₁H₄₆NaN₂O₁₀ ([M+Na]⁺): 749.3045, found: 749.3042.





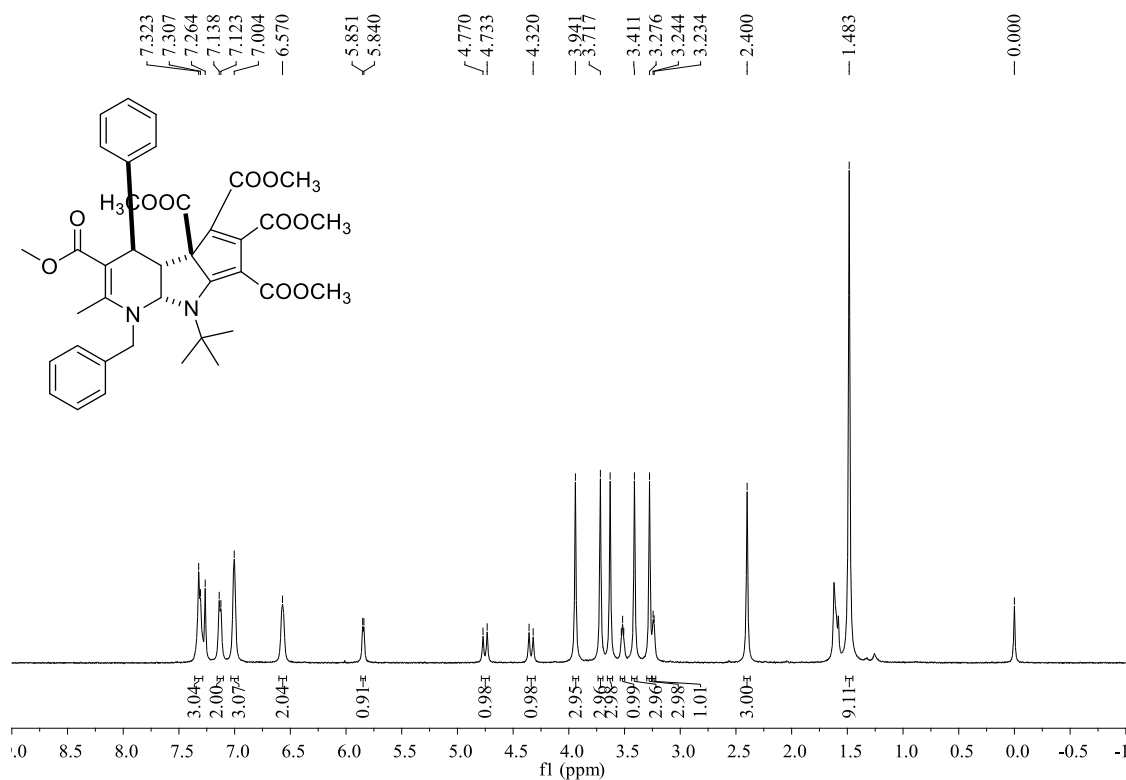
4b,5,6,7-Tetraethyl 3-methyl *rel*-(4R,4aR,4bS,8aS)-1-benzyl-8-cyclohexyl-2-methyl-4-phenyl-4,4a,8,8a-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4b,5,6,7(1*H*)-pentacarboxylate (4p): yellow solid, 72%, m.p. 182-184 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.49-7.38 (m, 5H, ArH), 7.04-6.59 (m, 3H, ArH), 6.72 (t, *J* = 6.8 Hz, 2H, ArH), 5.85 (d, *J* = 3.6 Hz, 1H, CH), 5.00-4.94 (m, 1H, CH), 4.87 (d, *J* = 15.6 Hz, 1H, CH₂), 4.44-4.40 (m, 1H, CH₂), 4.37-4.33 (m, 1H, CH₂), 4.30 (d, *J* = 15.6 Hz, 1H, CH₂), 4.22-4.17 (m, 2H, CH₂), 4.14-4.08 (m, 1H, CH₂), 4.00-3.92 (m, 1H, CH₂), 3.65-3.57 (m, 1H, CH₂), 3.26 (s, 3H, OCH₃), 3.24-3.22 (m, 1H, CH), 3.19-3.10 (m, 1H, CH₂), 3.00-2.97 (m, 1H, CH), 2.34 (s, 3H, CH₃), 1.95-1.85 (m, 2H, CH₂), 1.79-1.71 (m, 4H, CH₂), 1.59-1.57 (m, 1H, CH₂), 1.48-1.45 (m, 1H, CH₂), 1.43-1.40 (m, 4H, CH₂, CH₃), 1.30 (t, *J* = 7.2 Hz, 3H, CH₃), 1.18-1.13 (m, 1H, CH₂), 1.09 (t, *J* = 7.2 Hz, 3H, CH₃), 0.72 (t, *J* = 7.2 Hz, 3H, CH₃) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.2, 167.9, 167.1, 165.8, 162.2, 161.5, 157.4, 145.8, 144.1, 137.3, 129.1, 128.9, 128.2, 127.5, 125.7, 113.6, 112.3, 99.5, 83.6, 72.4, 62.0, 61.0, 60.1, 59.4, 58.3, 56.6, 52.2, 50.4, 38.3, 31.9, 31.1, 26.2, 25.7, 25.5, 18.6, 14.1, 14.0, 13.8, 13.5 ppm. IR (KBr) ν: 3435, 2930, 2858, 1753, 1731, 1684, 1577, 1541, 1445, 1387, 1347, 1327, 1229, 1196, 1126, 1092, 1058, 1027, 984, 895, 757 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₄₄H₅₂NaN₂O₁₀ ([M+Na]⁺): 791.3514, found: 791.3512.

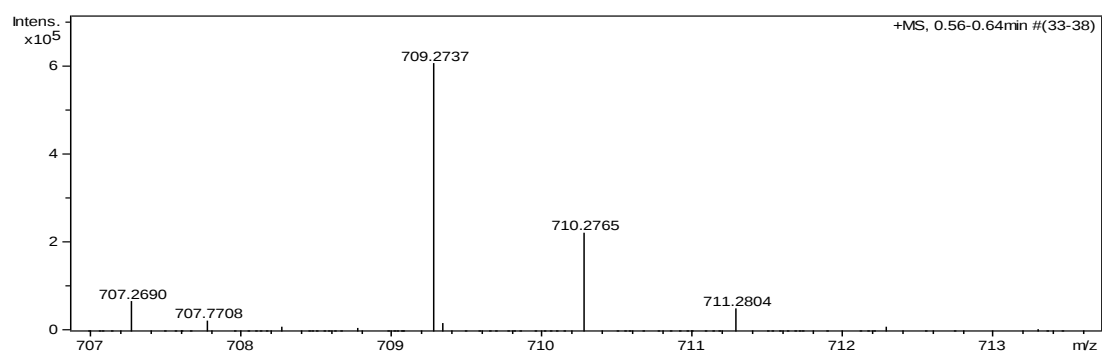
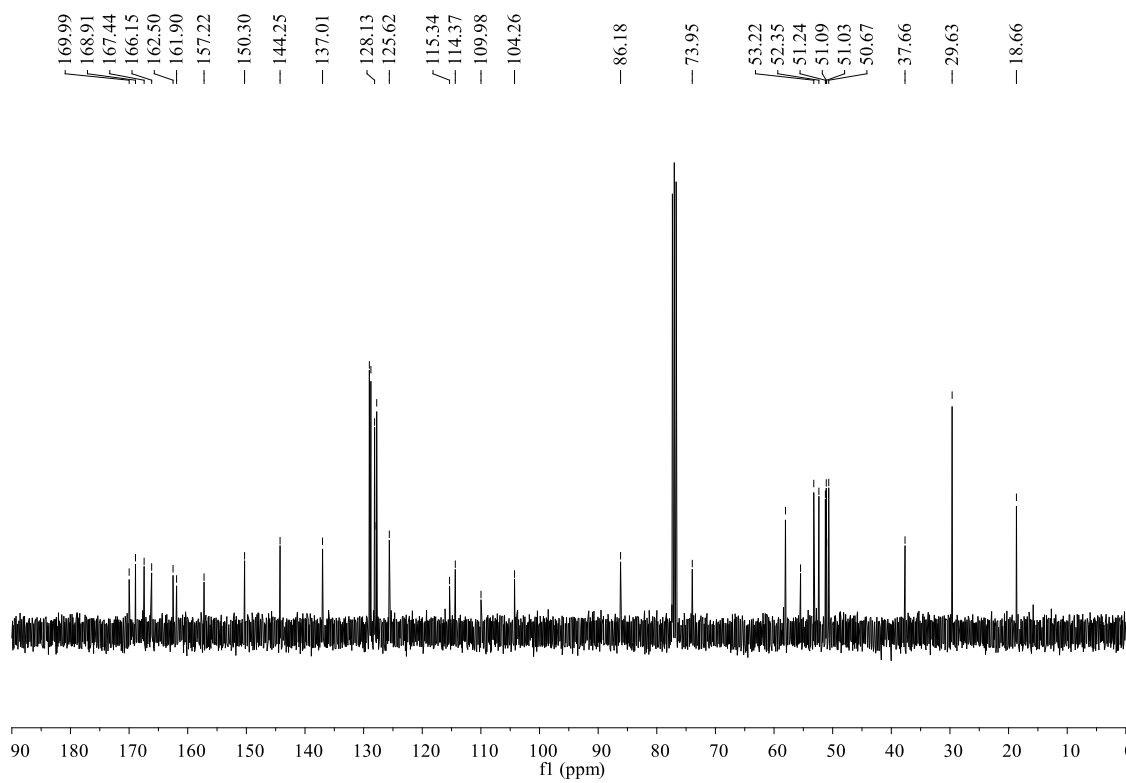




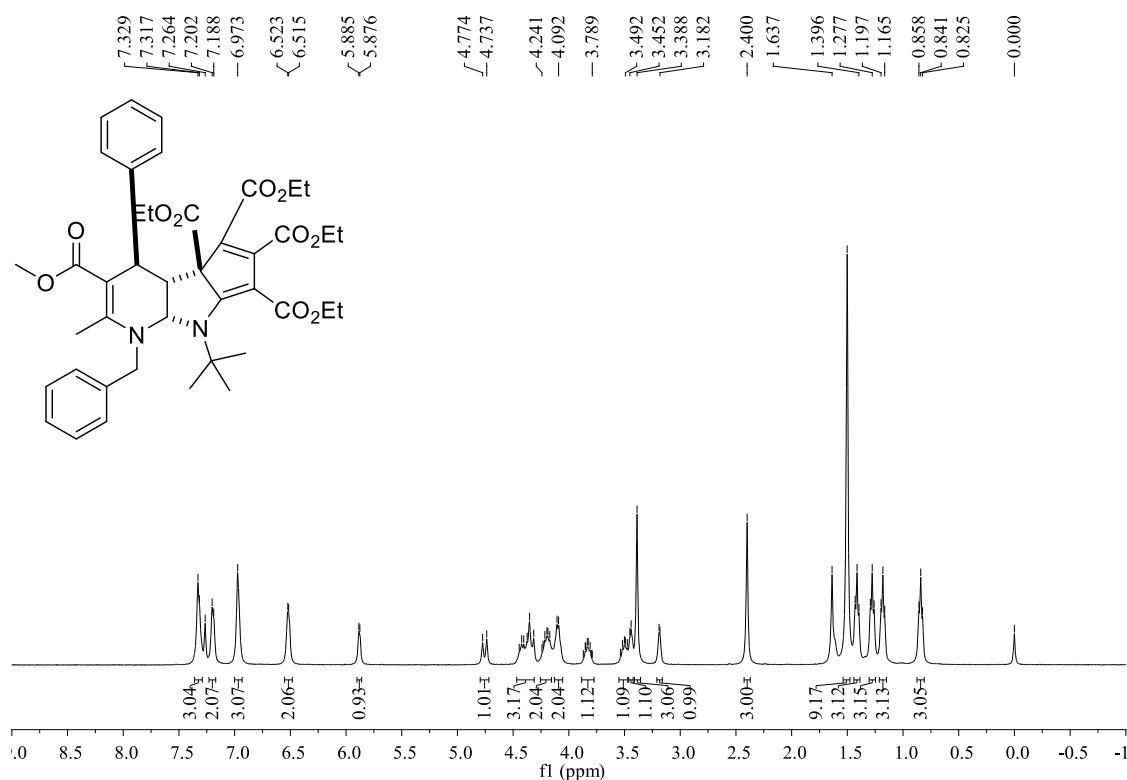
Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-1-benzyl-8-(*tert*-butyl)-2-methyl-4-phenyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (4q):

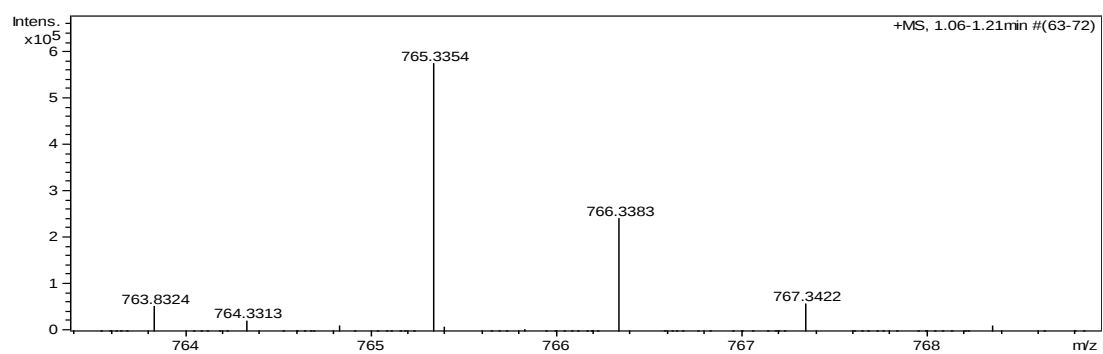
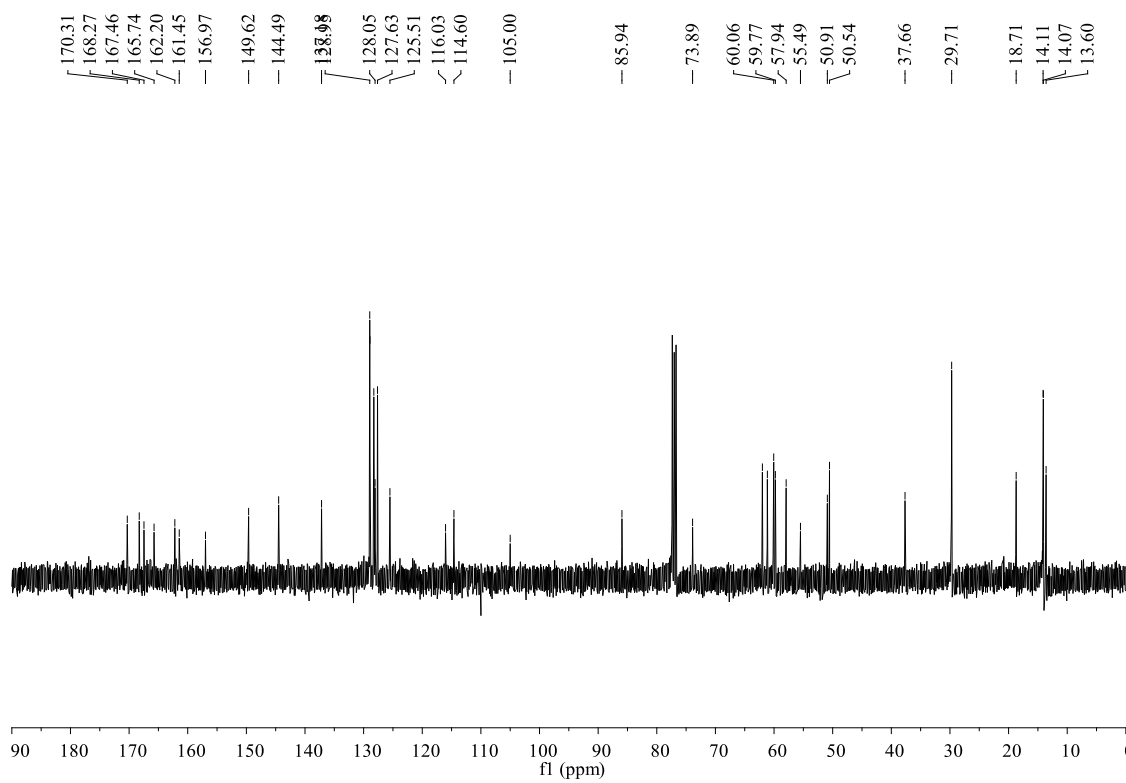
yellow solid, 66%, m.p. 207-209 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.35-7.28 (m, 3H, ArH), 7.16-7.10 (m, 2H, ArH), 7.00 (s, 3H, ArH), 6.57 (s, 2H, ArH) 5.85 (d, *J* = 4.4 Hz, 1H, CH), 4.75 (d, *J* = 14.8 Hz, 1H, CH₂), 4.34 (d, *J* = 14.8 Hz, 1H, CH₂), 3.94 (s, 3H, OCH₃), 3.72 (s, 3H, OCH₃), 3.63 (s, 3H, OCH₃), 3.54-3.50 (m, 1H, CH), 3.41 (s, 3H, OCH₃), 3.28 (s, 3H, OCH₃), 3.25-3.22 (m, 1H, CH), 2.40 (s, 3H, CH₃), 1.48 (s, 9H, CH₃) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.0, 168.9, 167.4, 166.2, 162.5, 161.9, 157.2, 150.3, 144.3, 137.0, 129.0, 128.8, 128.13, 128.07, 127.8, 125.6, 115.3, 114.4, 110.0, 104.3, 86.2, 74.0, 58.1, 55.5, 53.2, 52.4, 51.2, 51.1, 51.0, 50.7, 37.7, 29.6, 18.7 ppm. IR (KBr) ν: 3408, 2951, 2360, 1732, 1707, 1596, 1537, 1433, 1384, 1347, 1225, 1205, 1107, 1012, 1002, 967, 943, 793, 778 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₃₈H₄₂NaN₂O₁₀ ([M+Na]⁺): 709.2732, found: 709.2737.





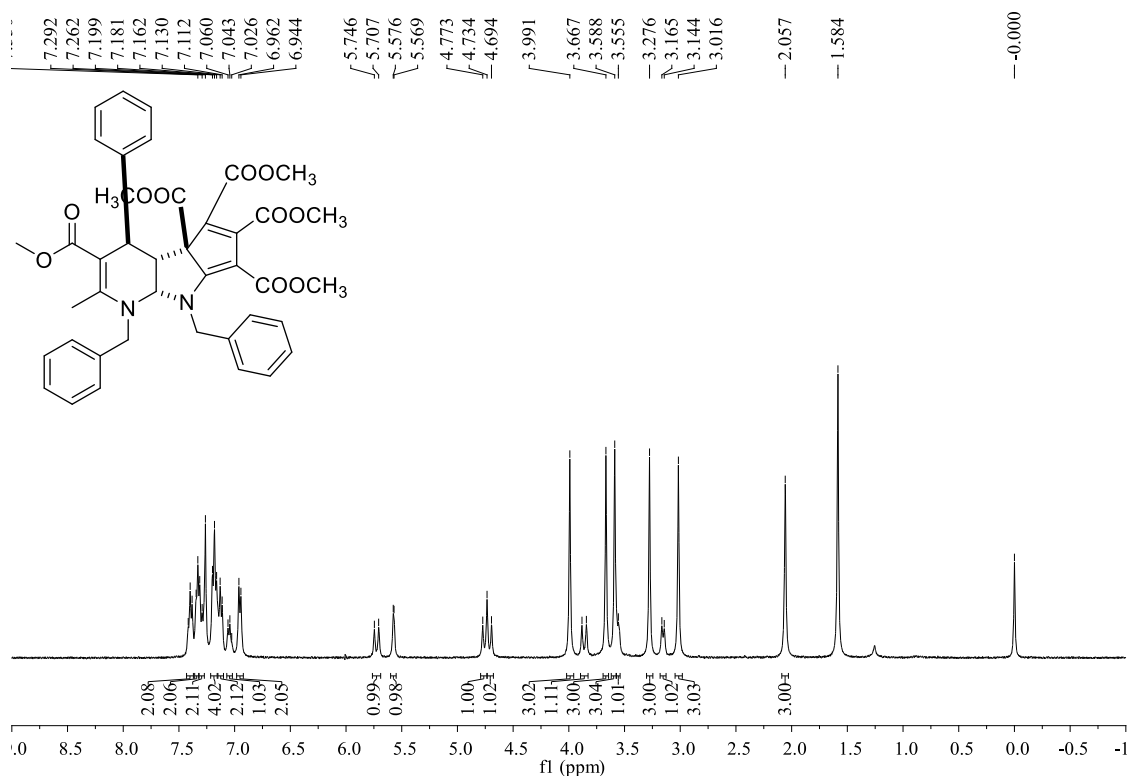
4b,5,6,7-Tetraethyl 3-methyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-1-benzyl-8-(*tert*-butyl)-2-methyl-4-phenyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (4r): yellow solid, 58%, m.p. 141-143 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.36-7.29 (m, 3H, ArH), 7.23-7.17 (m, 2H, ArH), 6.97 (s, 3H, ArH), 6.52 (d, *J* = 4.0 Hz, 2H, ArH), 5.88 (d, *J* = 3.6 Hz, 1H, CH), 4.76 (d, *J* = 14.8 Hz, 1H, CH₂), 4.45-4.32 (m, 3H, CH₂, CH₂), 4.23-4.17 (m, 2H, CH₂), 4.11-4.09 (m, 2H, CH₂), 3.87-3.79 (m, 1H, CH₂), 3.54-3.48 (m, 1H, CH₂), 3.46-3.43 (m, 1H, CH), 3.39 (s, 3H, OCH₃), 3.21-3.16 (m, 1H, CH), 2.40 (s, 3H, CH₃), 1.50 (s, 9H, CH₃), 1.41 (t, *J* = 6.8 Hz, 3H, CH₃), 1.28 (t, *J* = 6.4 Hz, 3H, CH₃), 1.18 (t, *J* = 6.4 Hz, 3H, CH₃), 0.84 (t, *J* = 6.8 Hz, 3H, CH₃) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.3, 168.3, 167.5, 165.7, 162.2, 161.5, 157.0, 149.6, 144.5, 137.2, 129.0, 128.9, 128.3, 128.1, 127.6, 125.5, 116.0, 114.6, 105.0, 85.9, 73.9, 62.0, 61.1, 60.1, 59.8, 57.9, 55.5, 50.9, 50.5, 37.7, 29.7, 18.7, 14.11, 14.07, 13.6 ppm. IR (KBr) ν: 3399, 2980, 2360, 1731, 1701, 1591, 1534, 1455, 1368, 1347, 1330, 1226, 1193, 1111, 1029, 1004, 967, 857, 792, 763 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₄₂H₅₀NaN₂O₁₀ ([M+Na]⁺): 765.3358, found: 765.3354.

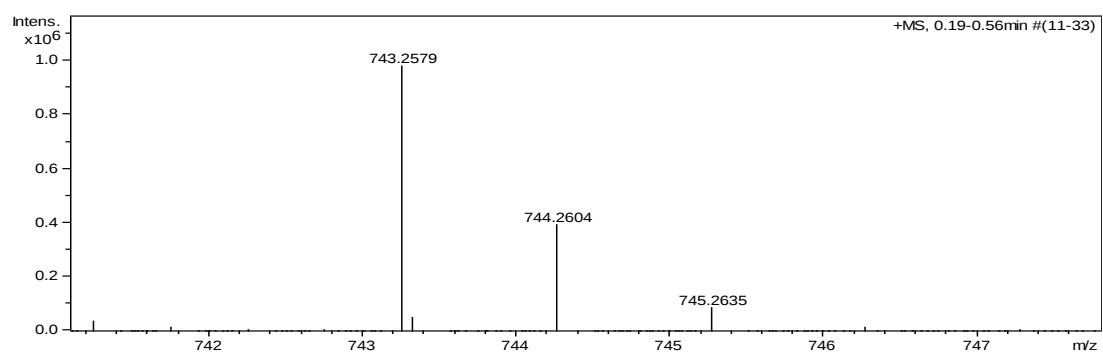
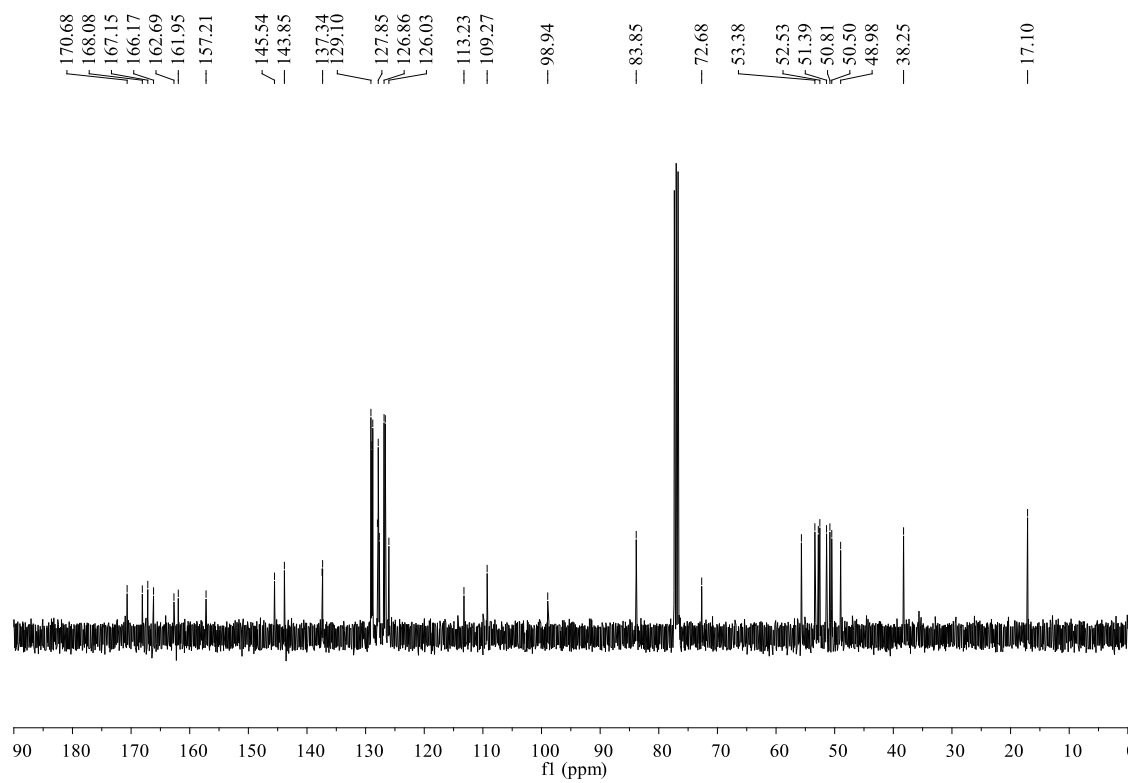




Pentamethyl***rel*-(4*R*,4*aR*,4*bS*,8*aS*)-1,8-dibenzyl-2-methyl-4-phenyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (4*s*):**

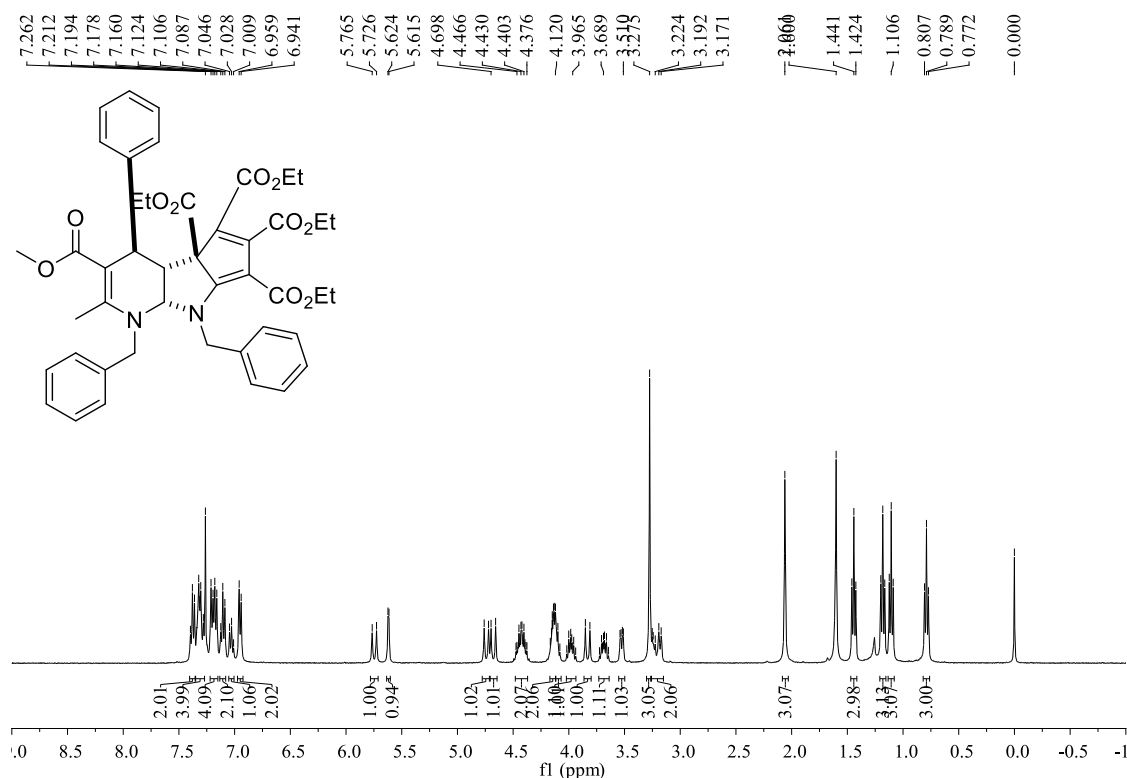
yellow solid, 54%, m.p. 235-237 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.40 (t, *J* = 7.2 Hz, 2H, ArH), 7.34 (t, *J* = 6.0 Hz, 2H, ArH), 7.32-7.27 (m, 2H, ArH), 7.18 (t, *J* = 7.2 Hz, 4H, ArH), 7.15-7.10 (m, 2H, ArH), 7.07-7.02 (m, 1H, ArH), 6.95 (d, *J* = 7.2 Hz, 2H, ArH), 5.73 (d, *J* = 15.6 Hz, 1H, CH₂), 5.59-5.55 (m, 1H, CH), 4.75 (d, *J* = 15.6 Hz, 1H, CH₂), 4.71 (d, *J* = 16.0 Hz, 1H, CH₂), 3.99 (s, 3H, OCH₃), 3.86 (d, *J* = 16.0 Hz, 1H, CH₂), 3.67 (s, 3H, OCH₃), 3.59 (s, 3H, OCH₃), 3.57-3.54 (m, 1H, CH), 3.28 (s, 3H, OCH₃), 3.15 (d, *J* = 8.4 Hz, 1H, CH), 3.02 (s, 3H, OCH₃), 2.06 (s, 3H, CH₃) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.7, 168.1, 167.2, 166.2, 162.7, 162.0, 157.2, 145.5, 143.9, 137.4, 137.3, 129.1, 128.9, 128.8, 128.0, 127.9, 127.7, 126.9, 126.6, 126.0, 113.2, 109.3, 98.9, 83.9, 72.7, 55.7, 53.4, 52.8, 52.5, 51.4, 50.8, 50.5, 49.0, 38.3, 17.1 ppm. IR (KBr) ν: 3391, 2949, 1740, 1692, 1590, 1556, 1438, 1381, 1342, 1226, 1116, 1096, 1073, 1015, 992, 840, 815, 799, 788, 760 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₄₁H₄₀NaN₂O₁₀ ([M+Na]⁺): 743.2575, found: 743.2579.

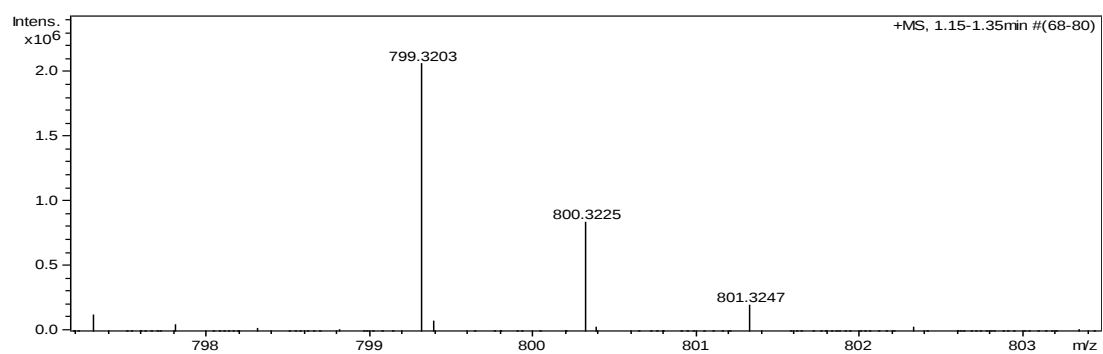
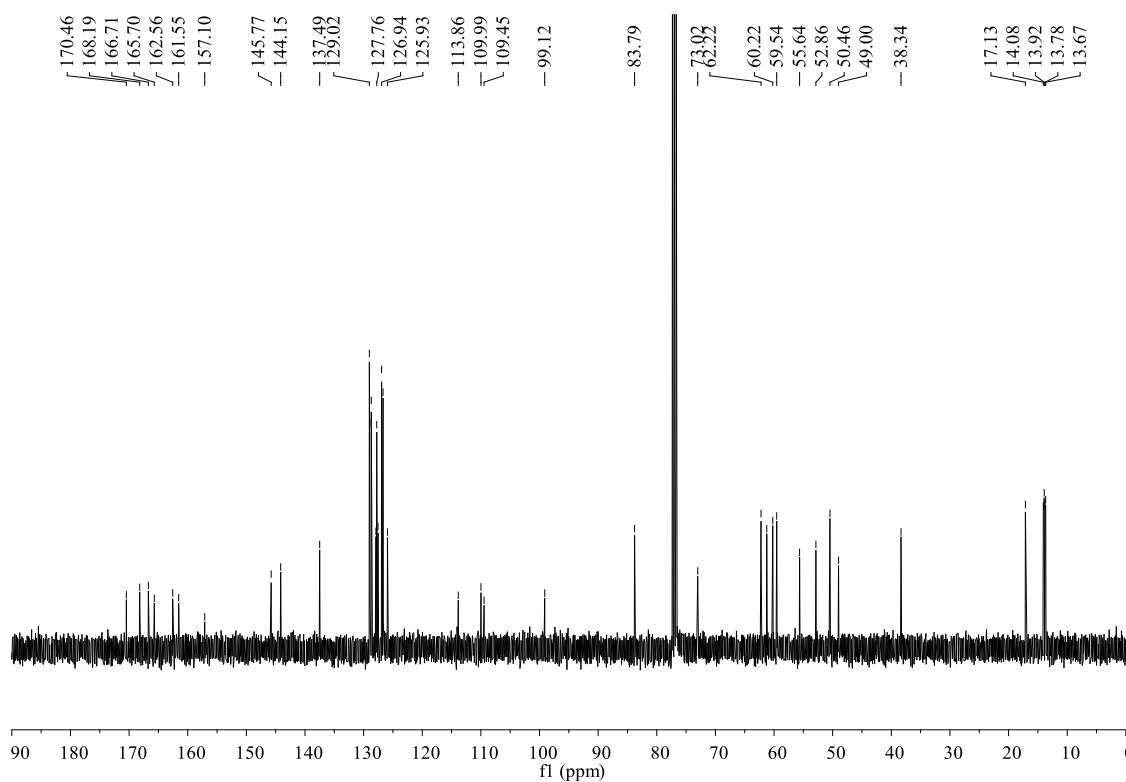




4b,5,6,7-Tetraethyl 3-methyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-1,8-dibenzyl-2-methyl-4-phenyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (4t):

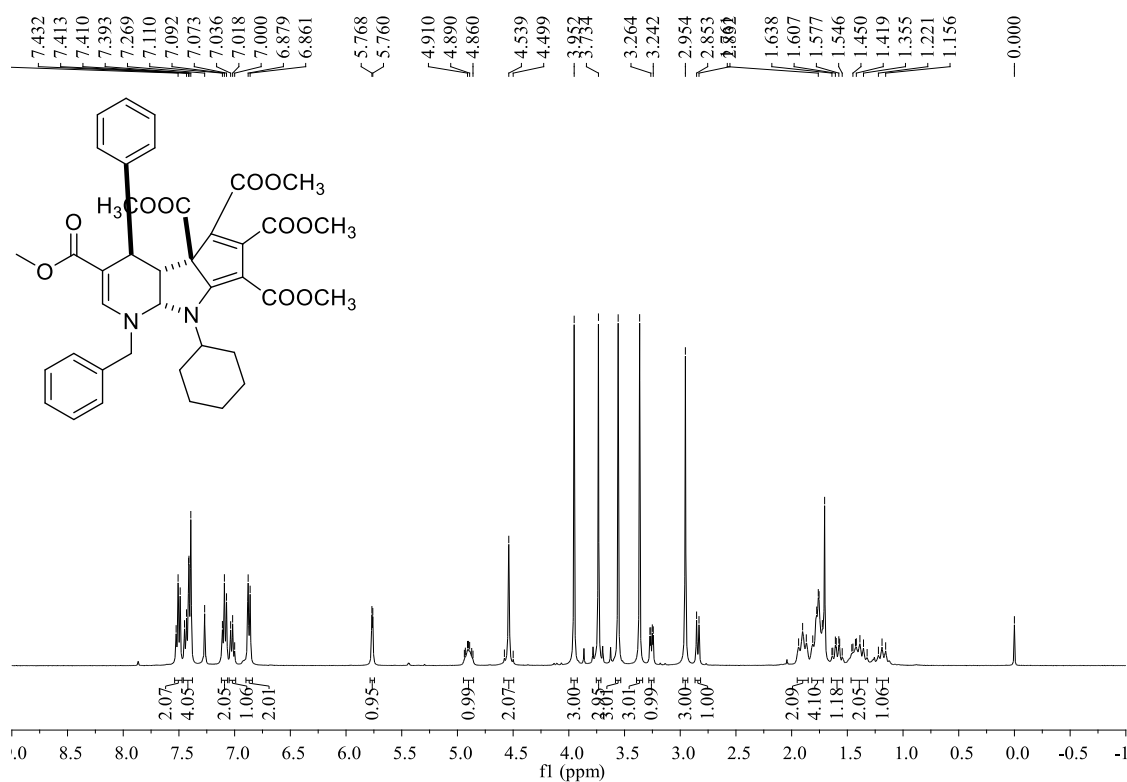
yellow solid, 30%, m.p. 170-172 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.38 (t, *J* = 7.2 Hz, 2H, ArH), 7.35-7.27 (m, 4H, ArH), 7.22-7.15 (m, 4H, ArH), 7.11 (t, *J* = 7.2 Hz, 2H, ArH), 7.03 (t, *J* = 7.2 Hz, 1H, ArH), 6.95 (d, *J* = 7.2 Hz, 2H, ArH), 5.75 (d, *J* = 15.6 Hz, 1H, CH₂), 5.62 (d, *J* = 3.6 Hz, 1H, CH), 4.74 (d, *J* = 15.6 Hz, 1H, CH₂), 4.68 (d, *J* = 16.4 Hz, 1H, CH₂), 4.74-4.38 (m, 2H, CH₂), 4.17-4.13 (m, 2H, CH₂), 4.12-4.07 (m, 1H, CH₂), 4.02-3.94 (m, 1H, CH₂), 3.83 (d, *J* = 16.0 Hz, 1H, CH₂), 3.73-3.65 (m, 1H, CH₂), 3.53(dd, *J*₁ = 8.8 Hz, *J*₂ = 4.0 Hz, 1H, CH), 3.27 (s, 3H, OCH₃), 3.25-3.17 (m, 2H, CH₂,CH), 2.06 (s, 3H, CH₃), 1.44 (t, *J* = 7.2 Hz, 3H, CH₃), 1.18 (t, *J* = 7.2 Hz, 3H, CH₃), 1.11 (t, *J* = 7.2 Hz, 3H, CH₃), 0.79 (t, *J* = 7.2 Hz, 3H, CH₃) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.5, 168.2, 166.7, 165.7, 162.6, 161.6, 157.1, 145.8, 144.2, 137.5, 129.0, 128.9, 128.7, 127.9, 127.8, 127.5, 126.9, 126.7, 125.9, 113.9, 110.0, 109.5, 99.1, 83.8, 73.0, 62.2, 61.2, 60.2, 59.5, 55.6, 52.9, 50.5, 49.0, 38.3, 17.1, 14.1, 13.9, 13.8, 13.7 ppm. IR (KBr) ν: 3390, 2944, 2872, 1729, 1692, 1593, 1563, 1431, 1384, 1334, 1228, 1194, 1100, 1081, 1030, 970, 880, 866, 841, 813, 770, 759 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₄₅H₄₈NaN₂O₁₀ ([M+Na]⁺): 799.3201, found: 799.3203.

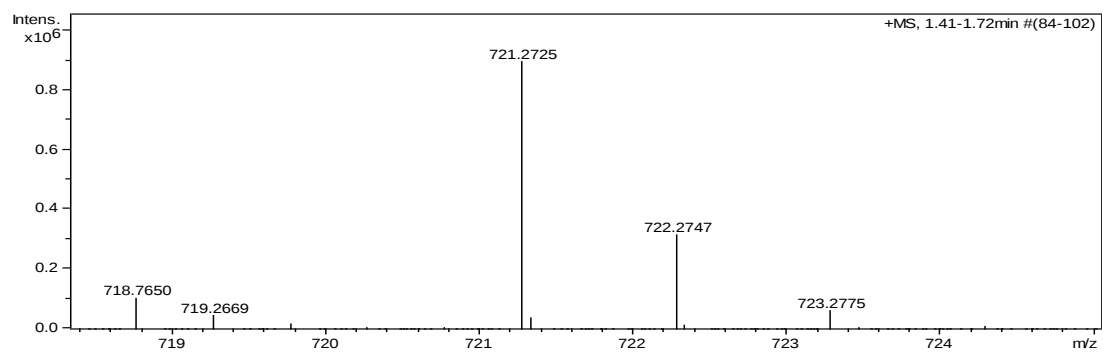
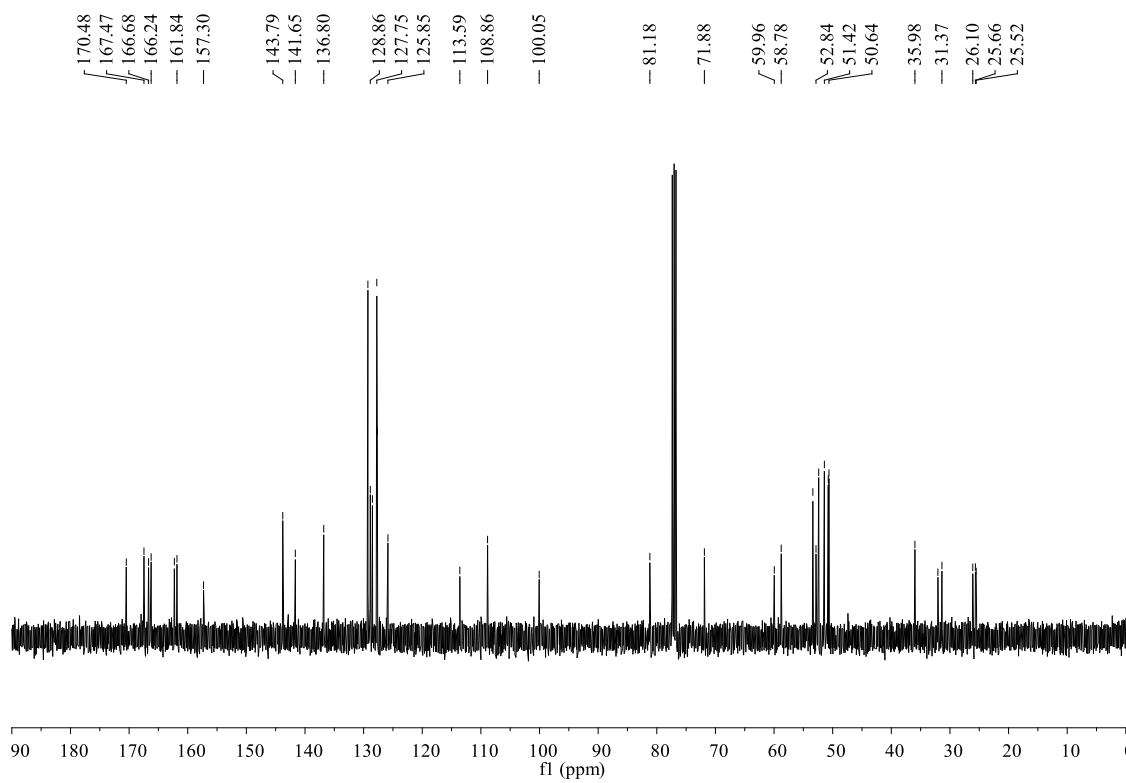




Pentamethyl***rel*-(4*R*,4*aR*,4*bS*,8*aS*)-1-benzyl-8-cyclohexyl-4-phenyl-4,4*a*,8,8*a*-****tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (6a):**

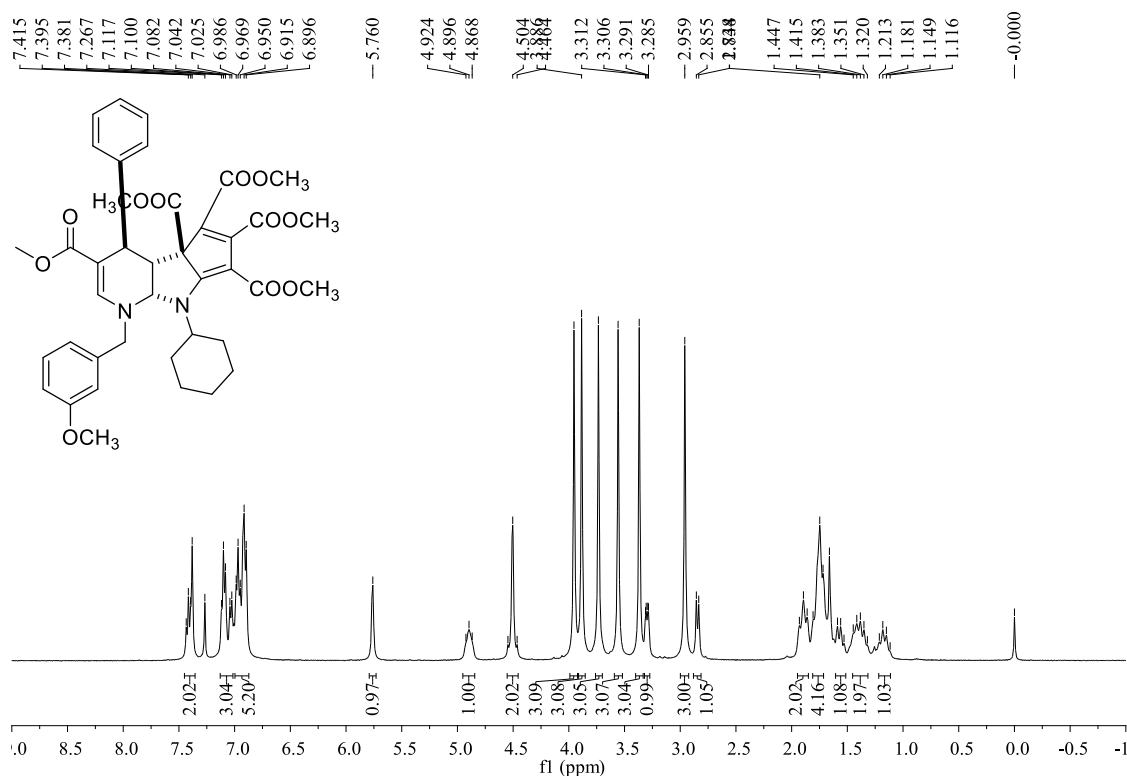
yellow solid, 92%, m.p. 210-212 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.53-7.49 (m, 2H, CH, ArH), 7.45-7.39 (m, 4H, ArH), 7.09 (t, *J* = 7.2 Hz, 2H, ArH), 7.02 (t, *J* = 7.2 Hz, 1H, ArH), 6.87 (d, *J* = 7.2 Hz, 2H, ArH), 5.76 (d, *J* = 3.2 Hz, 1H, CH), 4.94-4.86 (m, 1H, CH), 4.58-4.50 (m, 2H, CH₂), 3.95 (s, 3H, OCH₃), 3.73 (s, 3H, OCH₃), 3.56 (s, 3H, OCH₃), 3.36 (s, 3H, OCH₃), 3.26 (dd, *J*₁ = 8.4 Hz, *J*₂ = 3.2 Hz, 1H, CH), 2.95 (s, 3H, OCH₃), 2.84 (d, *J* = 8.4 Hz, 1H, CH), 1.94-1.87 (m, 2H, CH₂), 1.81-1.72 (m, 4H, CH₂), 1.64-1.55 (m, 1H, CH₂), 1.46-1.32 (m, 2H, CH₂), 1.22-1.16 (m, 1H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.5, 167.5, 166.7, 166.2, 162.3, 161.8, 157.3, 143.8, 141.7, 136.8, 129.3, 128.9, 128.5, 127.8, 127.7, 125.9, 113.6, 108.9, 100.1, 81.2, 71.9, 60.0, 58.8, 53.4, 52.8, 52.4, 51.4, 50.8, 50.6, 36.0, 32.1, 31.4, 26.1, 25.7, 25.5 ppm. IR (KBr) ν: 3435, 2949, 2859, 1740, 1702, 1636, 1585, 1542, 1435, 1345, 1229, 1206, 1111, 1083, 1002, 980, 896, 852, 833, 791, 757 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₃₉H₄₂NaN₂O₁₀ ([M+Na]⁺): 721.2732, found: 721.2725.

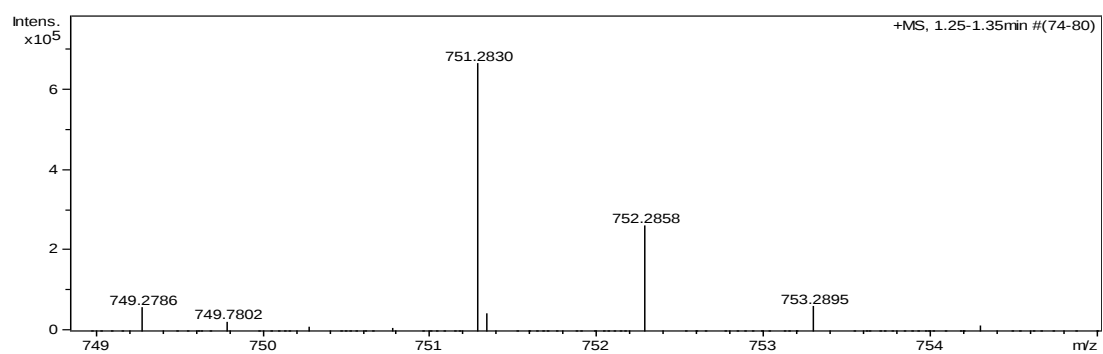
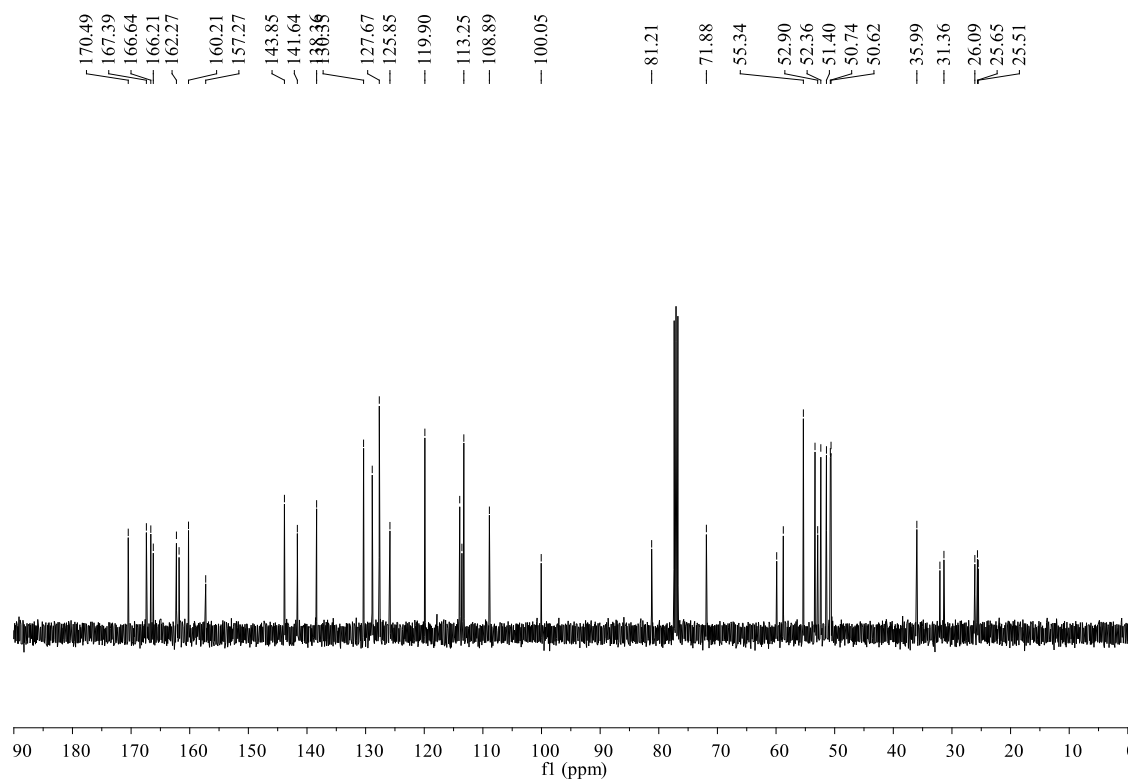




Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-8-cyclohexyl-1-(3-methoxybenzyl)-4-phenyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (6b):

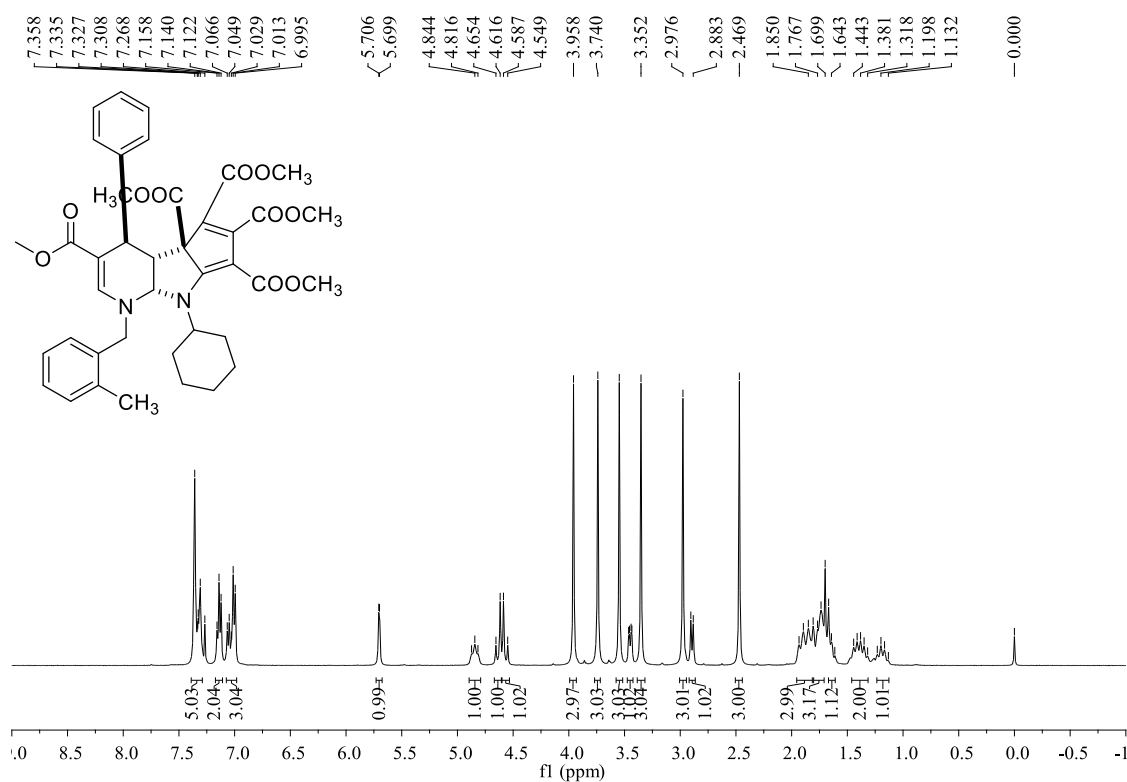
yellow solid, 82%, m.p. 197-199 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.44-7.38 (m, 2H, CH, ArH), 7.12-7.03 (m, 3H, ArH), 6.99-6.90 (m, 5H, ArH), 5.76 (s, 1H, CH), 4.92-4.87 (m, 1H, CH), 4.55-4.46 (m, 2H, CH₂), 3.95 (s, 3H, OCH₃), 3.89 (s, 3H, OCH₃), 3.73 (s, 3H, OCH₃), 3.56 (s, 3H, OCH₃), 3.37 (s, 3H, OCH₃), 3.30 (dd, *J*₁ = 8.4 Hz, *J*₂ = 2.4 Hz, 1H, CH), 2.96 (s, 3H, OCH₃), 2.84 (d, *J* = 8.4 Hz, 1H, CH), 1.93-1.86 (m, 2H, CH₂), 1.81-1.72 (m, 4H, CH₂), 1.59-1.53 (m, 1H, CH₂), 1.45-1.32 (m, 2H, CH₂), 1.21-1.12 (m, 1H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.5, 167.4, 166.6, 166.2, 162.3, 161.8, 160.2, 157.3, 143.9, 141.6, 138.4, 130.4, 128.9, 127.8, 125.9, 119.9, 114.0, 113.6, 113.3, 108.9, 100.1, 81.2, 71.9, 59.9, 58.8, 55.3, 53.4, 52.9, 52.4, 51.4, 50.7, 50.6, 36.0, 32.1, 31.4, 26.1, 25.7, 25.5 ppm. IR (KBr) ν: 3434, 2949, 2858, 1734, 1694, 1586, 1546, 1434, 1391, 1340, 1228, 1203, 1110, 1083, 1013, 981, 895, 852, 791 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₄₀H₄₄NaN₂O₁₁ ([M+Na]⁺): 751.2837, found: 751.2830.

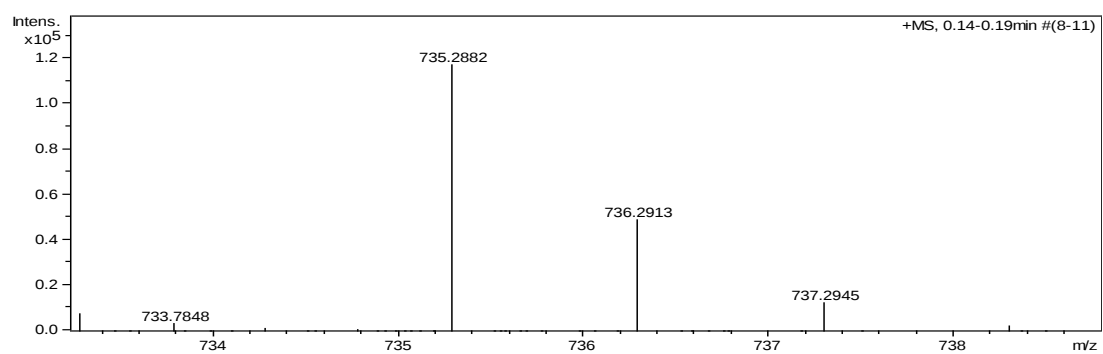
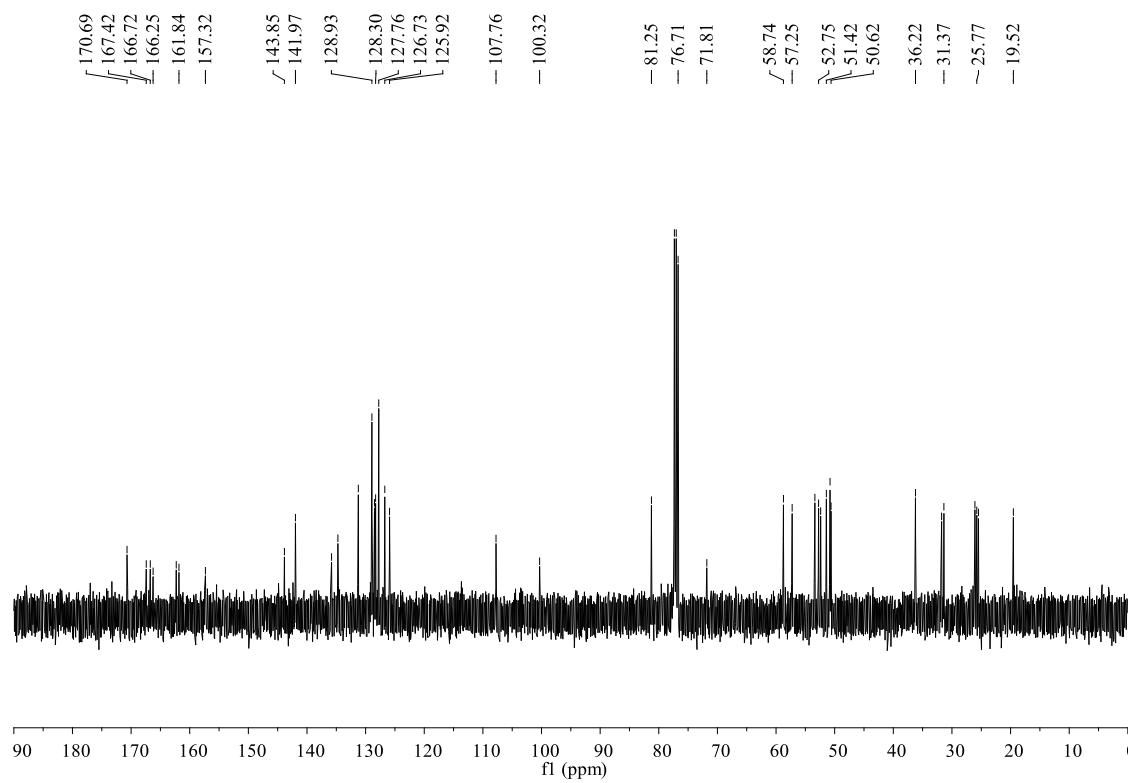




Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-8-cyclohexyl-1-(2-methylbenzyl)-4-phenyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (6c):

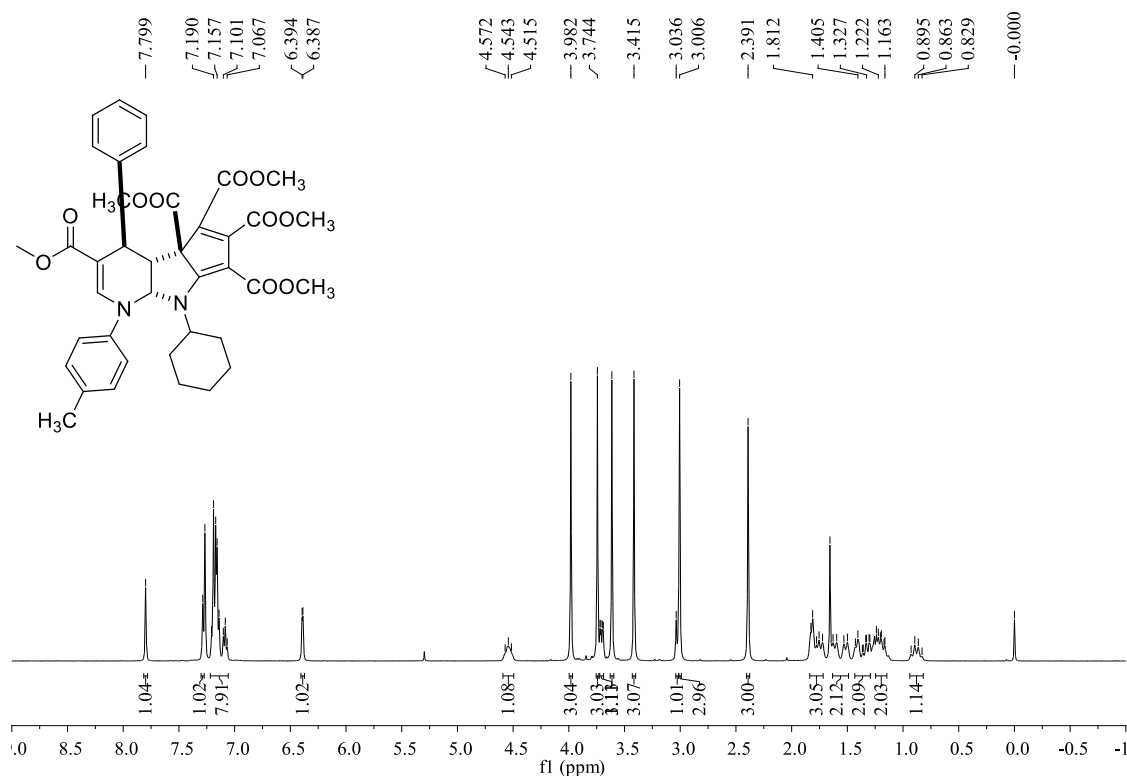
yellow solid, 83%, m.p. 214-216 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.39-7.29 (m, 5H, CH, ArH), 7.14 (t, *J* = 7.2 Hz, 2H, ArH), 7.07-6.98 (m, 3H, ArH), 5.70 (d, *J* = 2.8 Hz, 1H, CH), 4.84 (d, *J* = 11.6 Hz, 1H, CH), 4.64 (d, *J* = 5.2 Hz, 1H, CH₂), 4.57 (d, *J* = 5.2 Hz, 1H, CH₂), 3.96 (s, 3H, OCH₃), 3.74 (s, 3H, OCH₃), 3.55 (s, 3H, OCH₃), 3.45 (dd, *J*₁ = 8.4 Hz, *J*₂ = 2.8 Hz, 1H, CH), 3.35 (s, 3H, OCH₃), 2.98 (s, 3H, OCH₃), 2.89 (d, *J* = 8.8 Hz, 1H, CH), 2.47 (s, 3H, CH₃), 1.93-1.82 (m, 3H, CH₂), 1.81-1.70 (m, 3H, CH₂), 1.67-1.61 (m, 1H, CH₂), 1.44-1.32 (m, 2H, CH₂), 1.23-1.13 (m, 1H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.7, 167.4, 166.7, 166.3, 162.3, 161.8, 157.3, 143.9, 142.0, 135.8, 134.7, 131.2, 128.9, 128.5, 128.3, 127.8, 126.7, 125.9, 107.8, 100.3, 81.3, 77.3, 77.0, 76.7, 71.8, 58.7, 57.3, 53.4, 52.8, 52.4, 51.4, 50.8, 50.6, 36.2, 31.8, 31.4, 26.1, 25.8, 25.5, 19.5 ppm. IR (KBr) ν: 3434, 2948, 2850, 1740, 1701, 1583, 1542, 1434, 1344, 1304, 1227, 1205, 1109, 1081, 1001, 979, 896, 833, 790 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₄₀H₄₄NaN₂O₁₀ ([M+Na]⁺): 735.2888, found: 735.2882.

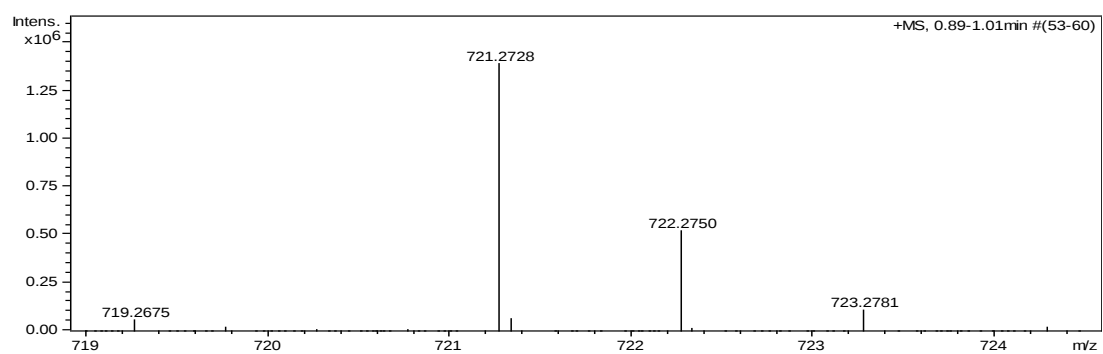
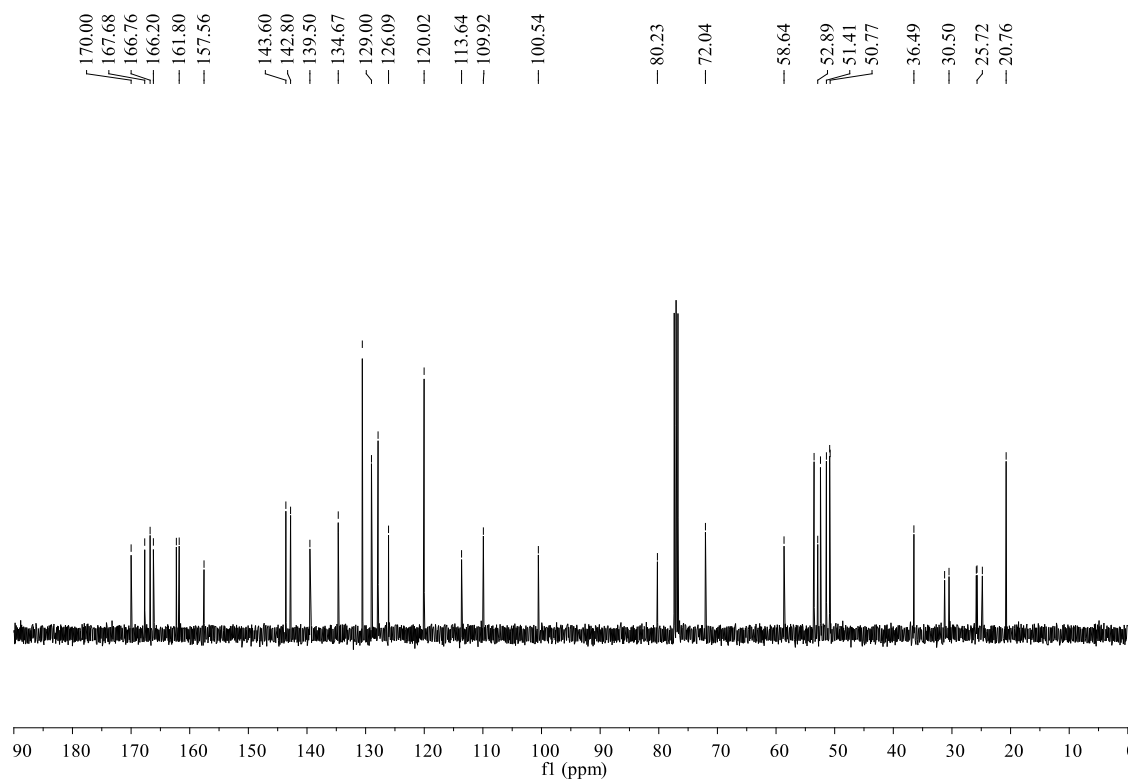




Pentamethyl***rel*-(4*R*,4*aR*,4*bS*,8*aS*)-8-cyclohexyl-4-phenyl-1-(*p*-tolyl)-4,4*a*,8,8*a*-****tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (6d):**

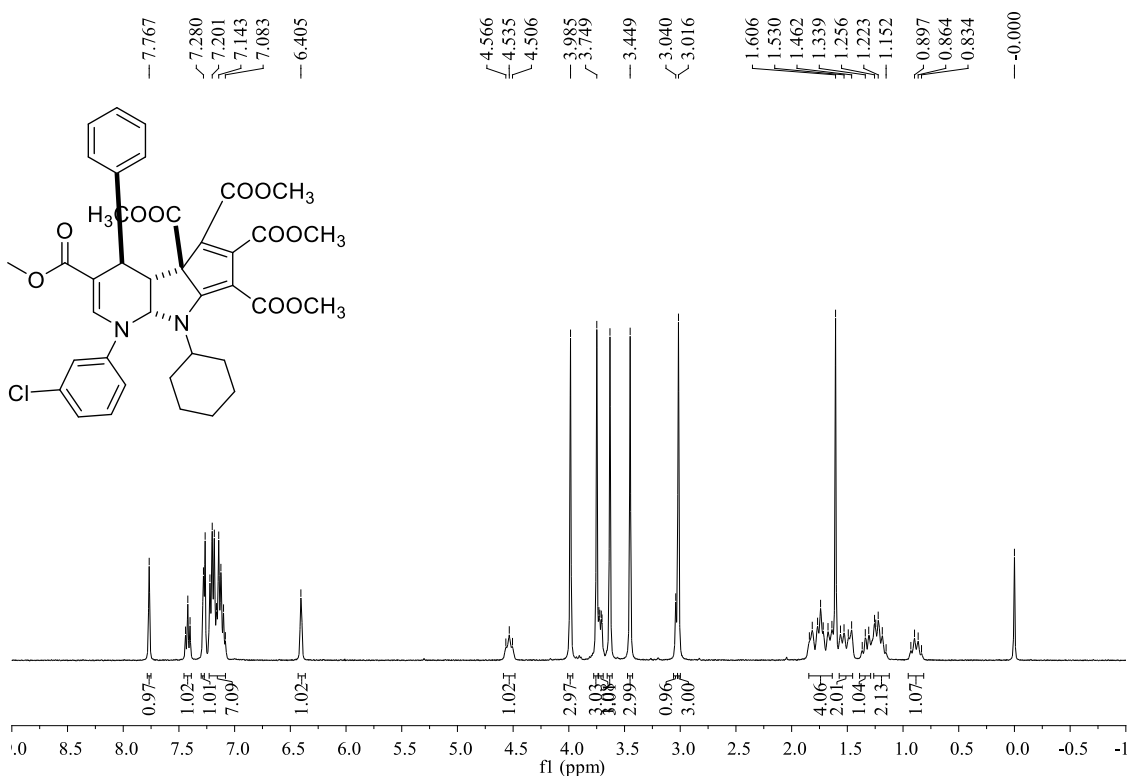
yellow solid, 83%, m.p. 231-233 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.80 (s, 1H, CH), 7.29 (s, 1H, ArH), 7.21-7.07 (m, 8H, ArH), 6.39 (d, *J* = 2.8 Hz, 1H, CH), 4.54 (t, *J* = 11.6 Hz, 1H, CH), 3.98 (s, 3H, OCH₃), 3.74 (s, 3H, OCH₃), 3.71 (dd, *J*₁ = 8.4 Hz, *J*₂ = 3.2 Hz, 1H, CH), 3.61 (s, 3H, OCH₃), 3.42 (s, 3H, OCH₃), 3.04-3.01 (m, 1H, CH), 3.01 (s, 3H, OCH₃), 2.39 (s, 3H, CH₃), 1.83-1.72 (m, 3H, CH₂), 1.66-1.50 (m, 2H, CH₂), 1.43-1.33 (m, 2H, CH₂), 1.24-1.16 (m, 2H, CH₂), 0.93-0.83 (m, 1H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.0, 167.7, 166.8, 166.2, 162.3, 161.8, 157.6, 143.6, 142.8, 139.5, 134.7, 130.6, 129.0, 127.9, 126.1, 120.0, 113.6, 109.9, 100.5, 80.2, 72.0, 58.6, 53.5, 52.9, 52.4, 51.4, 50.9, 50.8, 36.5, 31.3, 30.5, 25.8, 25.7, 24.8, 20.8 ppm. IR (KBr) ν: 3434, 2948, 2861, 1735, 1702, 1579, 1540, 1515, 1437, 1339, 1227, 1201, 1115, 1088, 1004, 981, 889, 819, 782, 757 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₃₉H₄₂NaN₂O₁₀ ([M+Na]⁺): 721.2732, found: 721.2728.

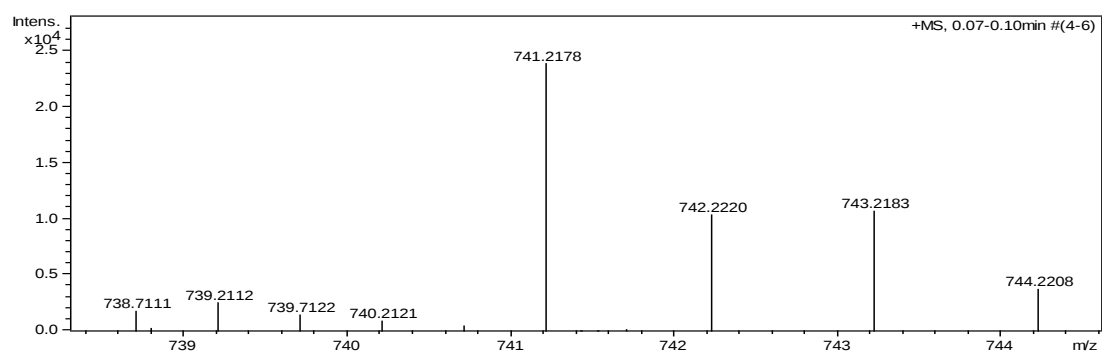
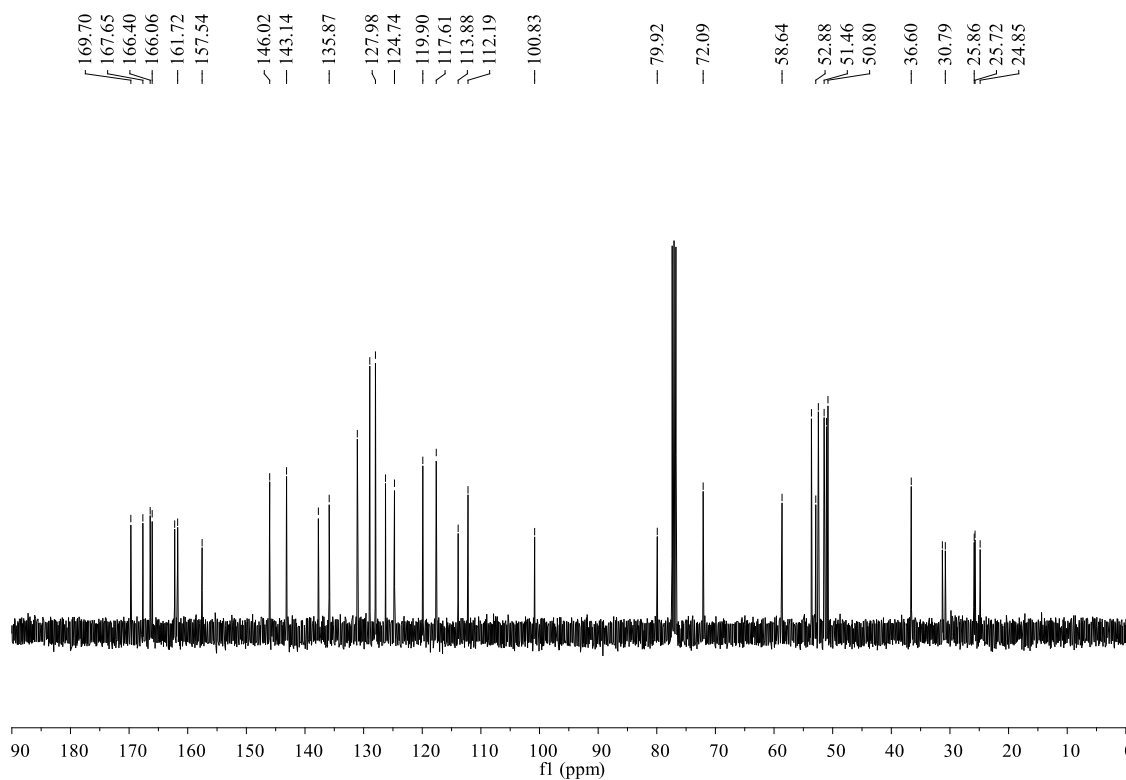




Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-1-(3-chlorophenyl)-8-cyclohexyl-4-phenyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (6e):

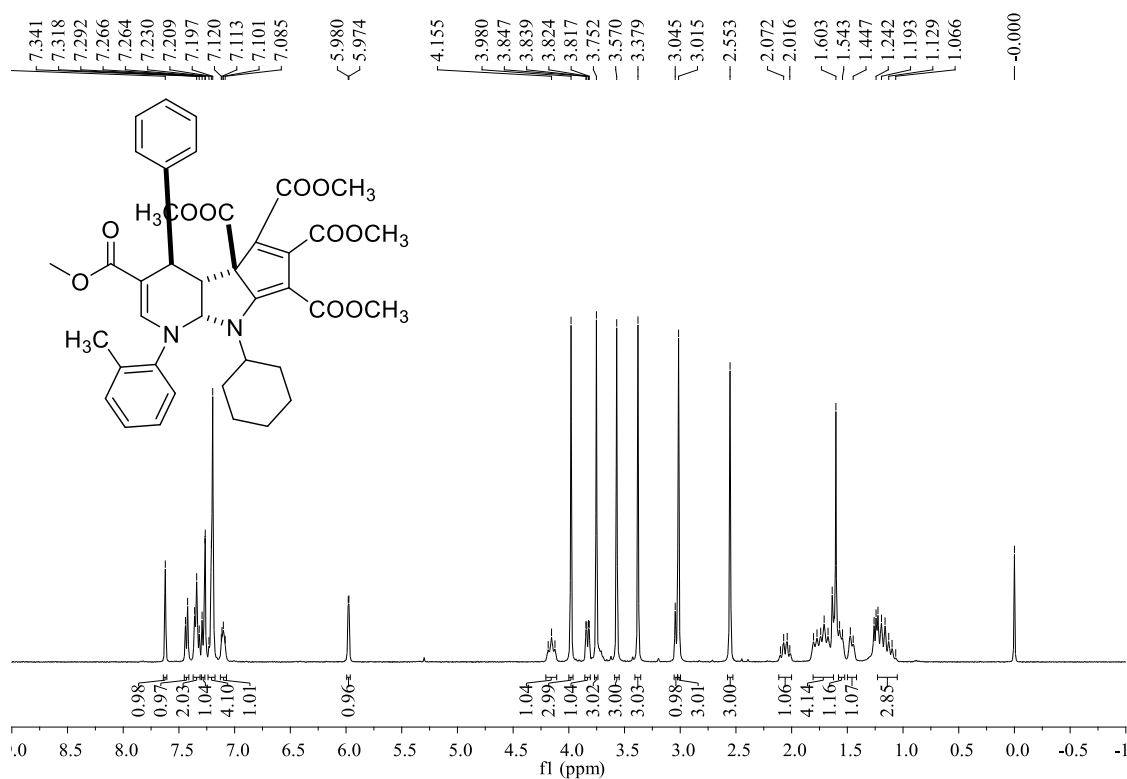
yellow solid, 84%, m.p. 201-203 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.77 (s, 1H, CH), 7.42 (t, *J* = 8.0 Hz, 1H, ArH), 7.28 (s, 1H, ArH), 7.22-7.08 (m, 7H, ArH), 6.41 (s, 1H, CH), 4.54 (t, *J* = 12.4 Hz, 1H, CH), 3.98 (s, 3H, OCH₃), 3.75 (s, 3H, OCH₃), 3.72 (dd, *J*₁ = 8.4 Hz, *J*₂ = 3.2 Hz, 1H, CH), 3.63 (s, 3H, OCH₃), 3.45 (s, 3H, OCH₃), 3.06-3.03 (m, 1H, CH), 3.02 (s, 3H, OCH₃), 1.84-1.64 (m, 4H, CH₂), 1.56-1.46 (m, 2H, CH₂), 1.37-1.31 (m, 1H, CH₂), 1.26-1.15 (m, 2H, CH₂), 0.93-0.83 (m, 1H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 169.7, 167.7, 166.4, 166.1, 162.2, 161.7, 157.5, 146.0, 143.1, 137.7, 135.9, 131.1, 129.0, 128.0, 126.3, 124.7, 119.9, 117.6, 113.9, 112.2, 100.8, 79.9, 72.1, 58.6, 53.6, 52.9, 52.4, 51.5, 51.1, 50.8, 36.6, 31.3, 30.8, 25.9, 25.7, 24.9 ppm. IR (KBr) ν: 3434, 2948, 2860, 1735, 1699, 1590, 1538, 1482, 1436, 1337, 1229, 1200, 1115, 1087, 1006, 833, 788, 770, 751 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₃₈H₃₉ClNaN₂O₁₀ ([M+Na]⁺): 741.2185, found: 741.2178.

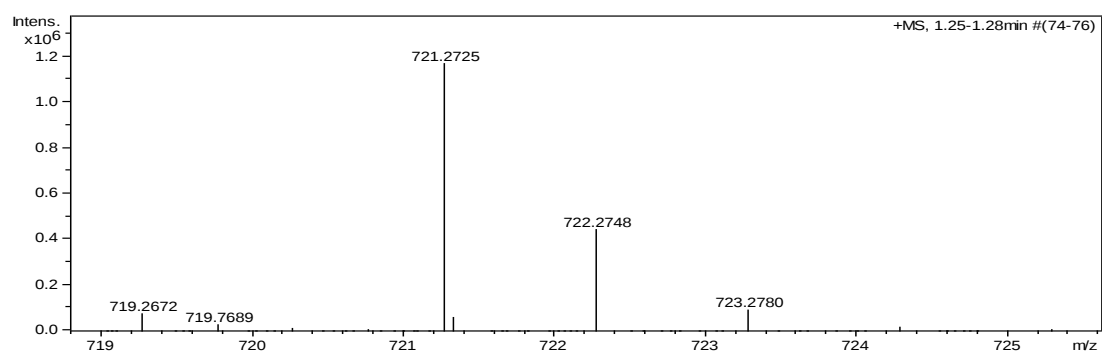
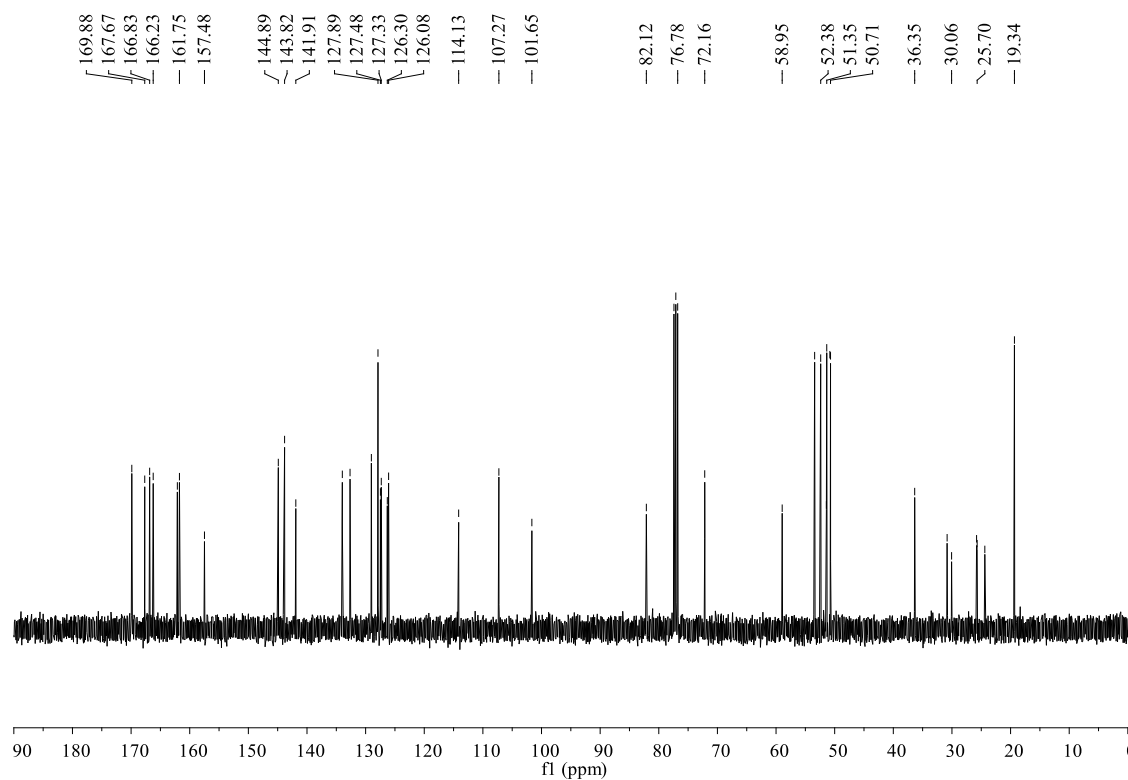




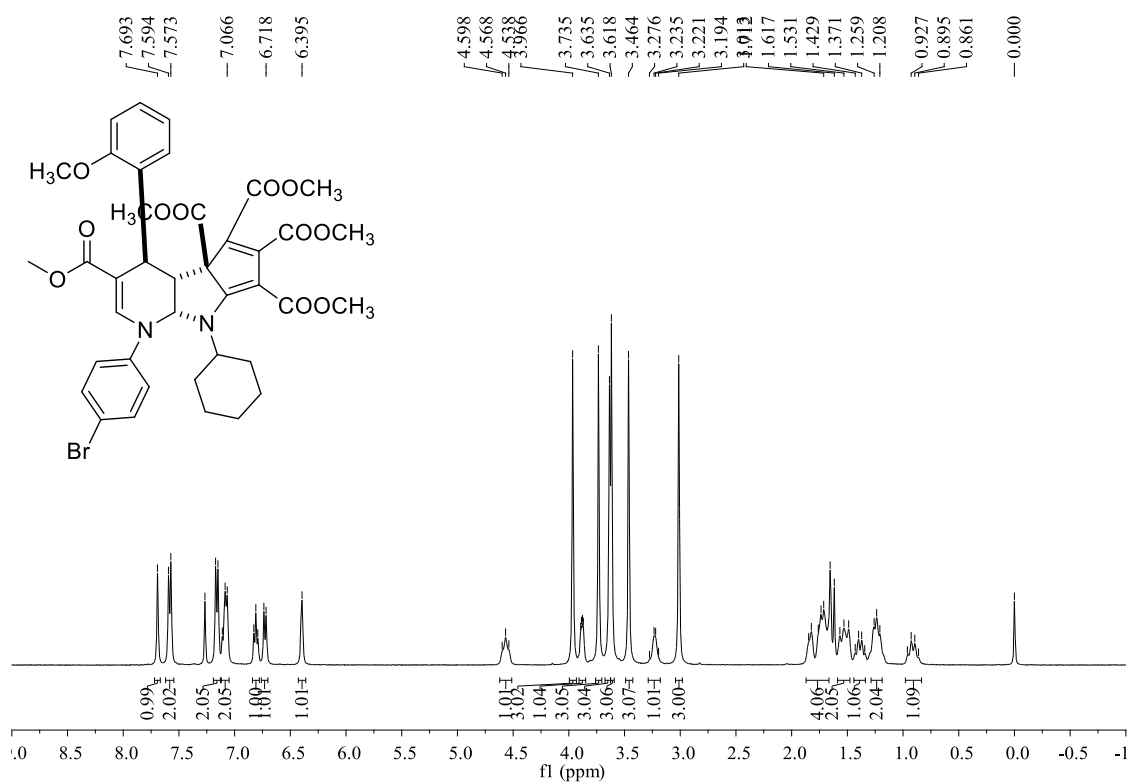
Pentamethyl***rel*-(4*R*,4*aR*,4*bS*,8*aS*)-8-cyclohexyl-4-phenyl-1-(*o*-tolyl)-4,4*a*,8,8*a*-****tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (6f):**

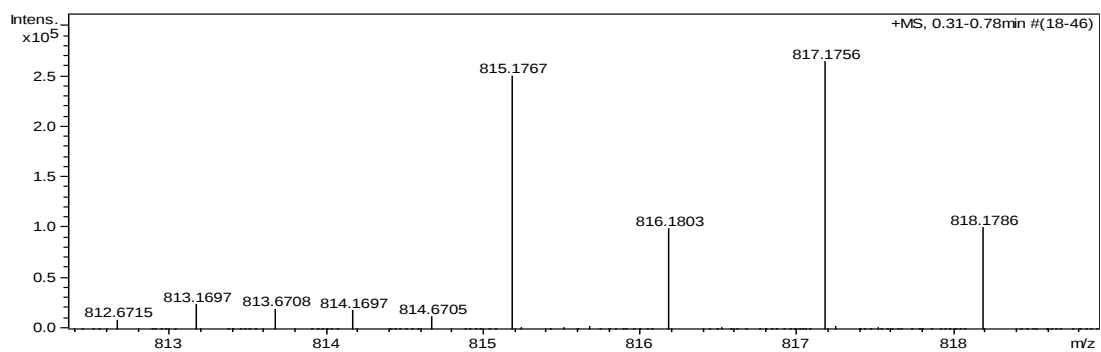
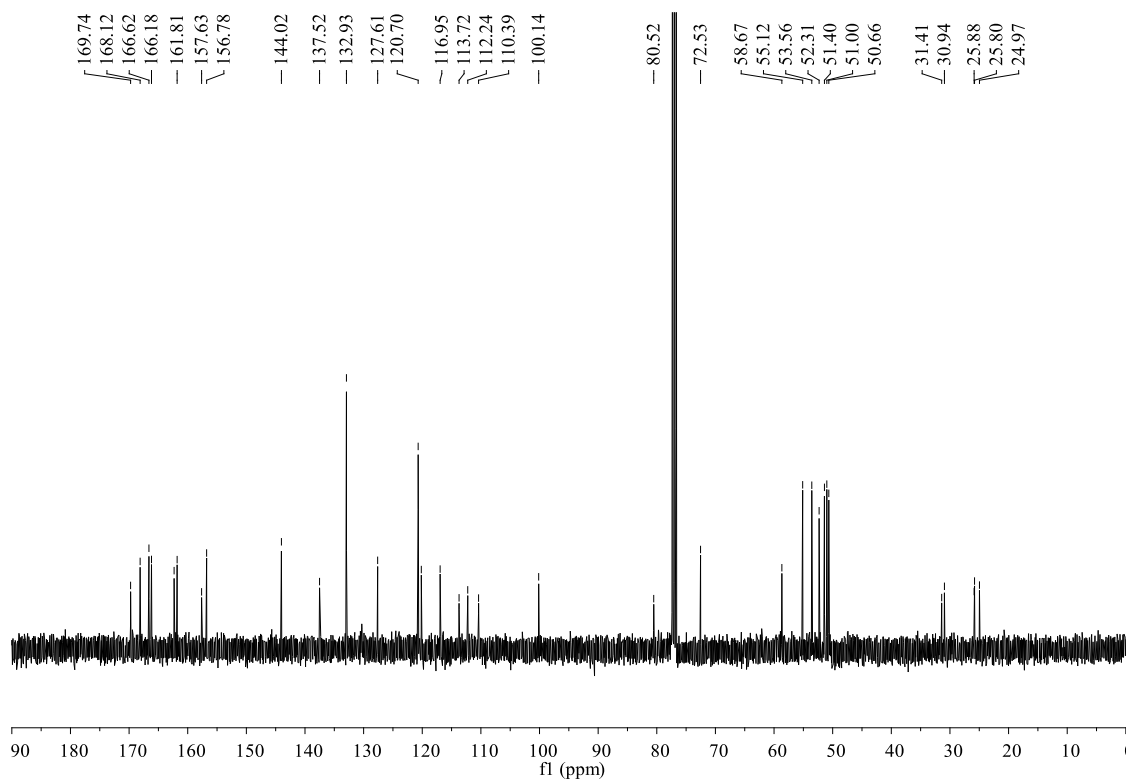
yellow solid, 81%, m.p. 208-210 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.62 (s, 1H, CH), 7.43 (d, *J* = 7.6 Hz, 1H, ArH), 7.36-7.32 (m, 2H, ArH), 7.29-7.27 (m, 1H, ArH), 7.23-7.20 (m, 4H, ArH), 7.12-7.09 (m, 1H, ArH), 5.98 (d, *J* = 2.4 Hz, 1H, CH), 4.16 (t, *J* = 12.0 Hz, 1H, CH), 3.98 (s, 3H, OCH₃), 3.83 (dd, *J*₁ = 9.2 Hz, *J*₂ = 3.2 Hz, 1H, CH), 3.75 (s, 3H, OCH₃), 3.57 (s, 3H, OCH₃), 3.38 (s, 3H, OCH₃), 3.06-3.03 (m, 1H, CH), 3.01 (s, 3H, OCH₃), 2.55 (s, 3H, CH₃), 2.10-2.02 (m, 1H, CH₂), 1.80-1.64 (m, 4H, CH₂), 1.57-1.54 (m, 1H, CH₂), 1.47-1.45 (m, 1H, CH₂), 1.23-1.07 (m, 3H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 169.9, 167.7, 166.8, 166.2, 162.1, 161.8, 157.5, 144.9, 143.8, 141.9, 134.0, 132.7, 129.0, 127.9, 127.5, 127.3, 126.3, 126.1, 114.1, 107.3, 101.7, 82.1, 77.4, 77.1, 76.8, 72.2, 59.0, 53.4, 52.4, 51.41, 51.35, 50.8, 50.7, 36.4, 30.8, 30.1, 25.8, 25.7, 24.4, 19.3 ppm. IR (KBr) ν: 3434, 2947, 2860, 1736, 1700, 1587, 1546, 1494, 1436, 1344, 1229, 1203, 1114, 1096, 1000, 952, 832, 793, 751 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₃₉H₄₂NaN₂O₁₀ ([M+Na]⁺): 721.2732, found: 721.2725.



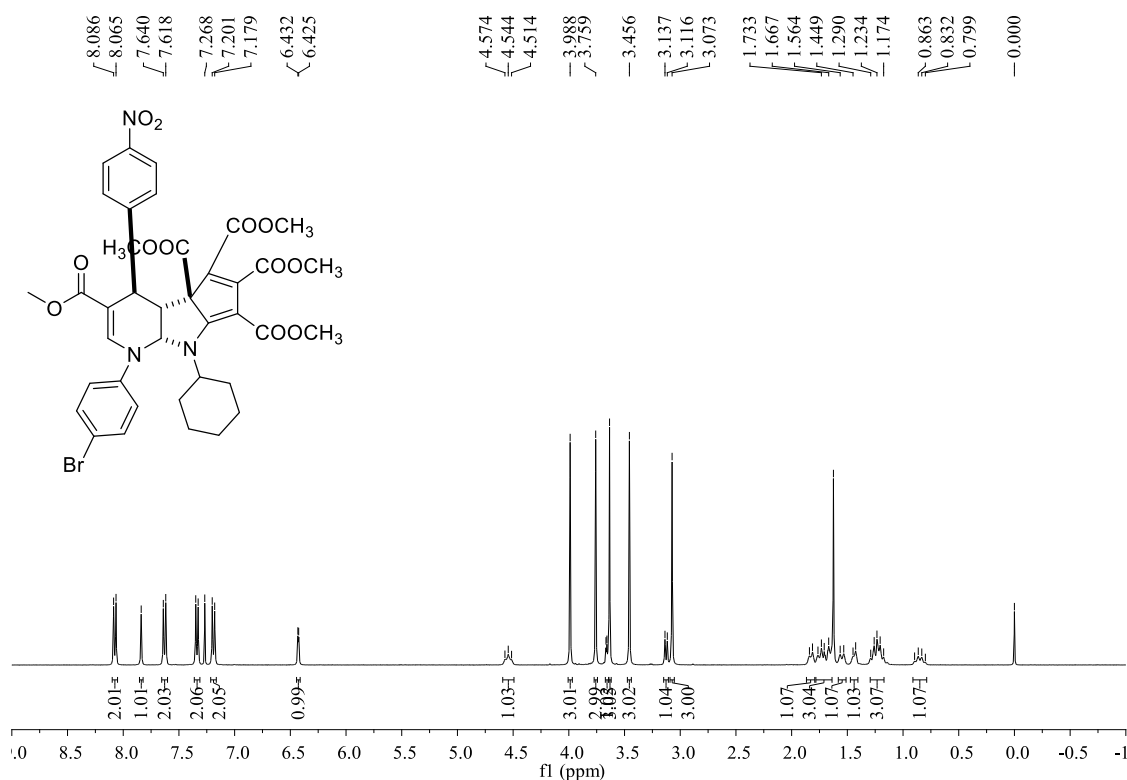


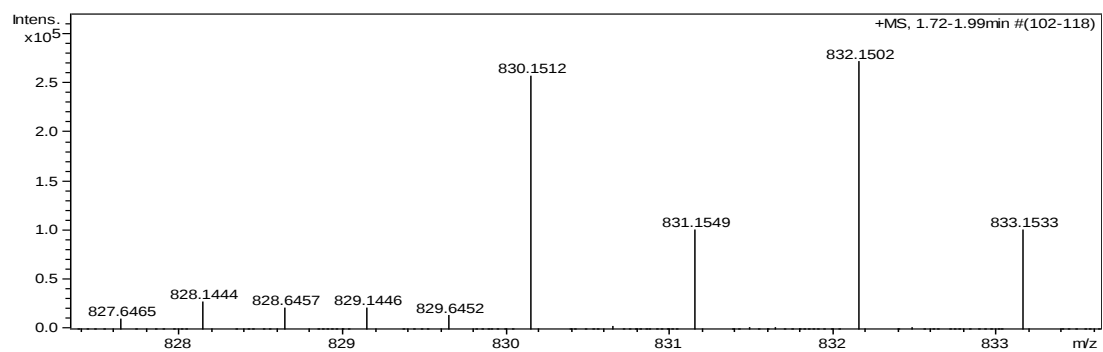
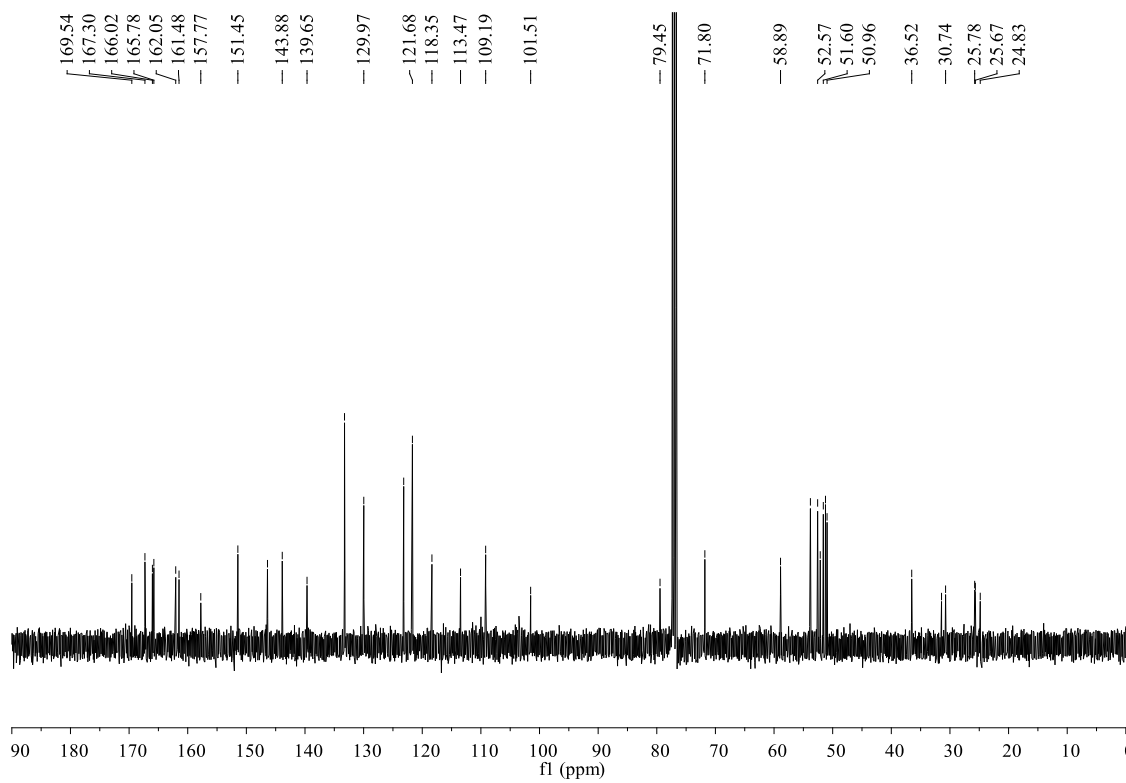
Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-1-(4-bromophenyl)-8-cyclohexyl-4-(2-methoxyphenyl)-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (6g): yellow solid, 88%, m.p. 233-235 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.69 (s, 1H, CH), 7.58 (d, *J* = 8.4 Hz, 2H, ArH), 7.16 (d, *J* = 8.4 Hz, 2H, ArH), 7.11-7.07 (m, 2H, ArH), 6.81 (t, *J* = 7.2 Hz, 1H, ArH), 6.73 (d, *J* = 7.6 Hz, 1H, ArH), 6.39 (s, 1H, CH), 4.57 (t, *J* = 12.0 Hz, 1H, CH), 3.97 (s, 3H, OCH₃), 3.88 (dd, *J*₁ = 6.4 Hz, *J*₂ = 2.4 Hz, 1H, CH), 3.72 (s, 3H, OCH₃), 3.64 (s, 3H, OCH₃), 3.62 (s, 3H, OCH₃), 3.46 (s, 3H, OCH₃), 3.28-3.19 (m, 1H, CH), 3.01 (s, 3H, OCH₃), 1.87-1.67 (m, 4H, CH₂), 1.57-1.49 (m, 2H, CH₂), 1.43-1.34 (m, 1H, CH₂), 1.26-1.21 (m, 2H, CH₂), 0.96-0.86 (m, 1H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 169.7, 168.1, 166.6, 166.2, 162.3, 161.8, 157.6, 156.8, 144.0, 137.5, 132.9, 127.6, 120.7, 120.2, 117.0, 113.7, 112.2, 110.4, 100.1, 80.5, 72.5, 58.7, 55.1, 53.6, 52.3, 51.4, 51.0, 50.7, 31.4, 30.9, 25.9, 25.8, 25.0 ppm. IR (KBr) ν: 3448, 2948, 2857, 1736, 1706, 1655, 1584, 1544, 1435, 1399, 1341, 1312, 1230, 1155, 1113, 1075, 1002, 967, 923, 852, 823, 756 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₃₉H₄₁BrNaN₂O₁₁ ([M+Na]⁺): 815.1786, found: 815.1767.



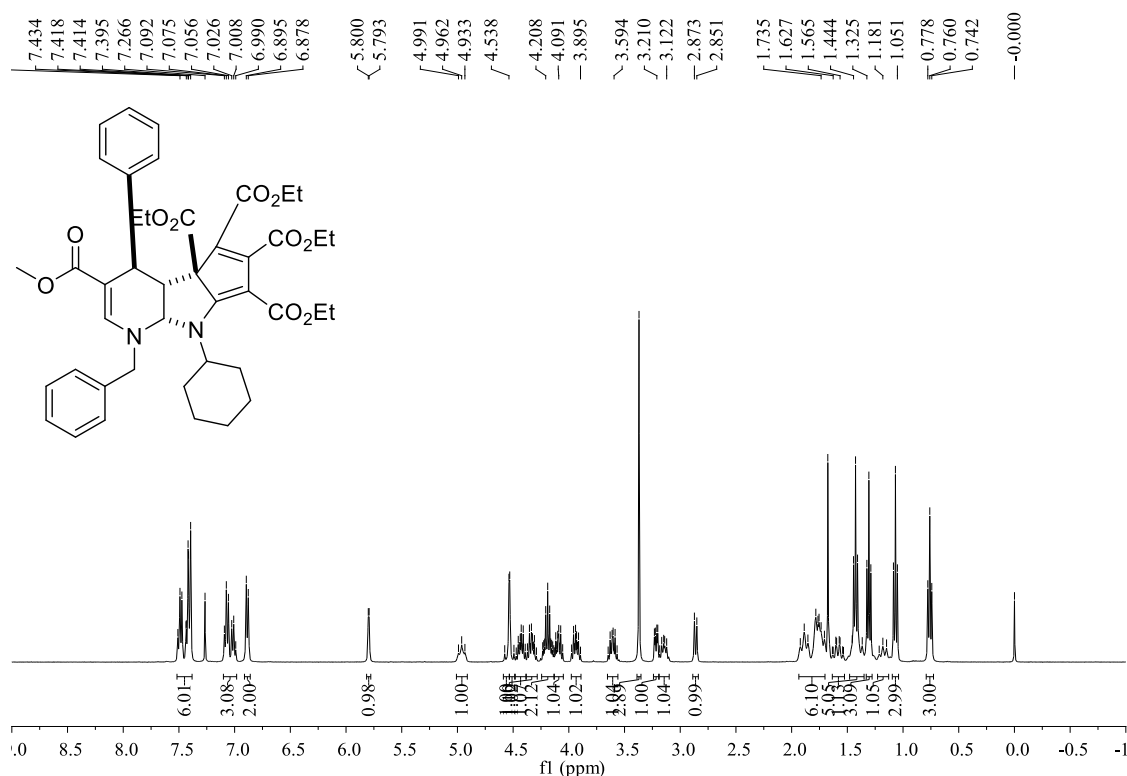


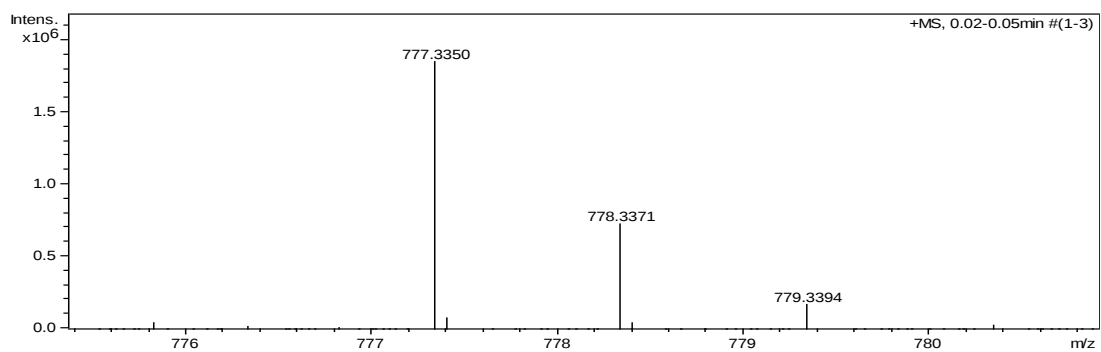
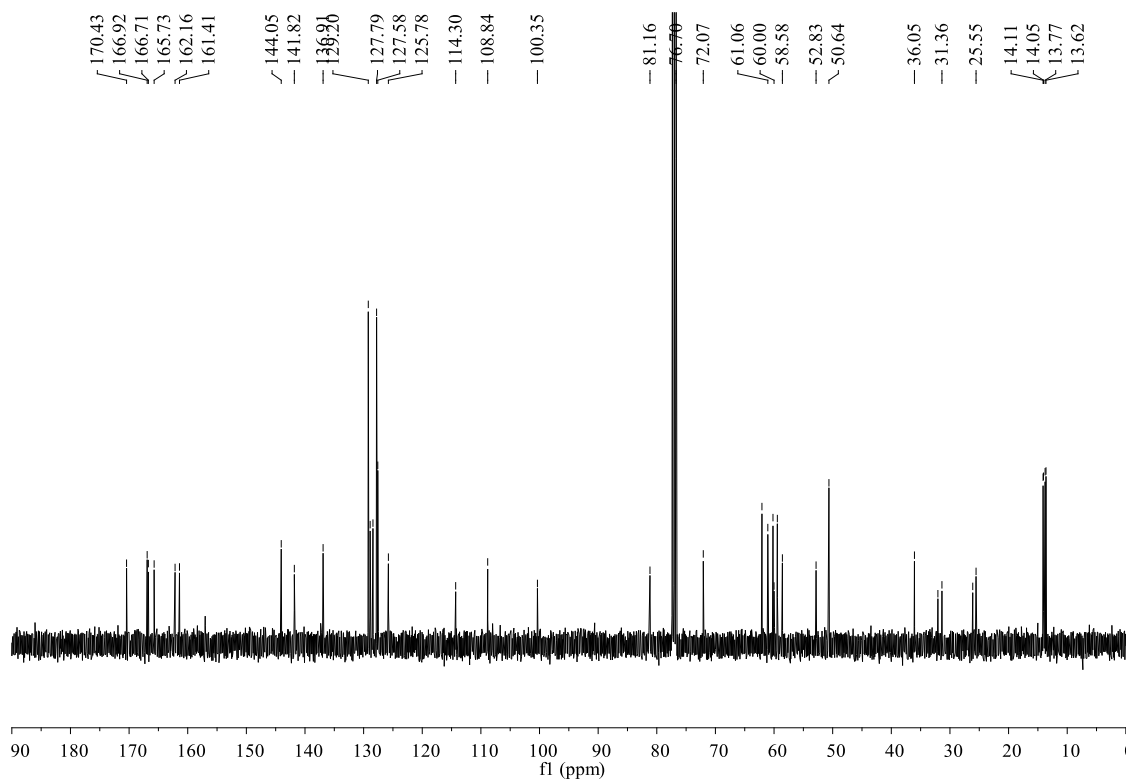
Pentamethyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-1-(4-bromophenyl)-8-cyclohexyl-4-(4-nitrophenyl)-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (6h): yellow solid, 82%, m.p. 230-232 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.08 (d, *J* = 8.4 Hz, 2H, ArH), 7.84 (s, 1H, CH), 7.63 (d, *J* = 8.8 Hz, 2H, ArH), 7.34 (d, *J* = 8.8 Hz, 2H, ArH), 7.19 (d, *J* = 8.8 Hz, 2H, ArH), 6.43 (d, *J* = 2.8 Hz, 1H, CH), 4.54 (t, *J* = 12.0 Hz, 1H, CH), 3.99 (s, 3H, OCH₃), 3.76 (s, 3H, OCH₃), 3.67-3.64 (m, 1H, CH), 3.63 (s, 3H, OCH₃), 3.46 (s, 3H, OCH₃), 3.13 (d, *J* = 8.4 Hz, 1H, CH), 3.07 (s, 3H, OCH₃), 1.87-1.79 (m, 1H, CH₂), 1.78-1.64 (m, 3H, CH₂), 1.58-1.51 (m, 1H, CH₂), 1.47-1.40 (m, 1H, CH₂), 1.29-1.17 (m, 3H, CH₂), 0.90-0.80 (m, 1H, CH₂) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 169.5, 167.3, 166.0, 165.8, 162.1, 161.5, 157.8, 151.5, 146.4, 143.9, 139.7, 133.3, 130.0, 123.2, 121.7, 118.4, 113.5, 109.2, 101.5, 79.5, 71.8, 58.9, 53.8, 52.6, 52.1, 51.6, 51.2, 51.0, 36.5, 31.4, 30.7, 25.8, 25.7, 24.8 ppm. IR (KBr) ν: 3430, 2950, 2854, 1738, 1699, 1583, 1542, 1435, 1401, 1345, 1232, 1206, 1111, 1045, 1002, 979, 831, 786 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₃₈H₃₈BrNaN₃O₁₂ ([M+Na]⁺): 830.1531, found: 830.1512.





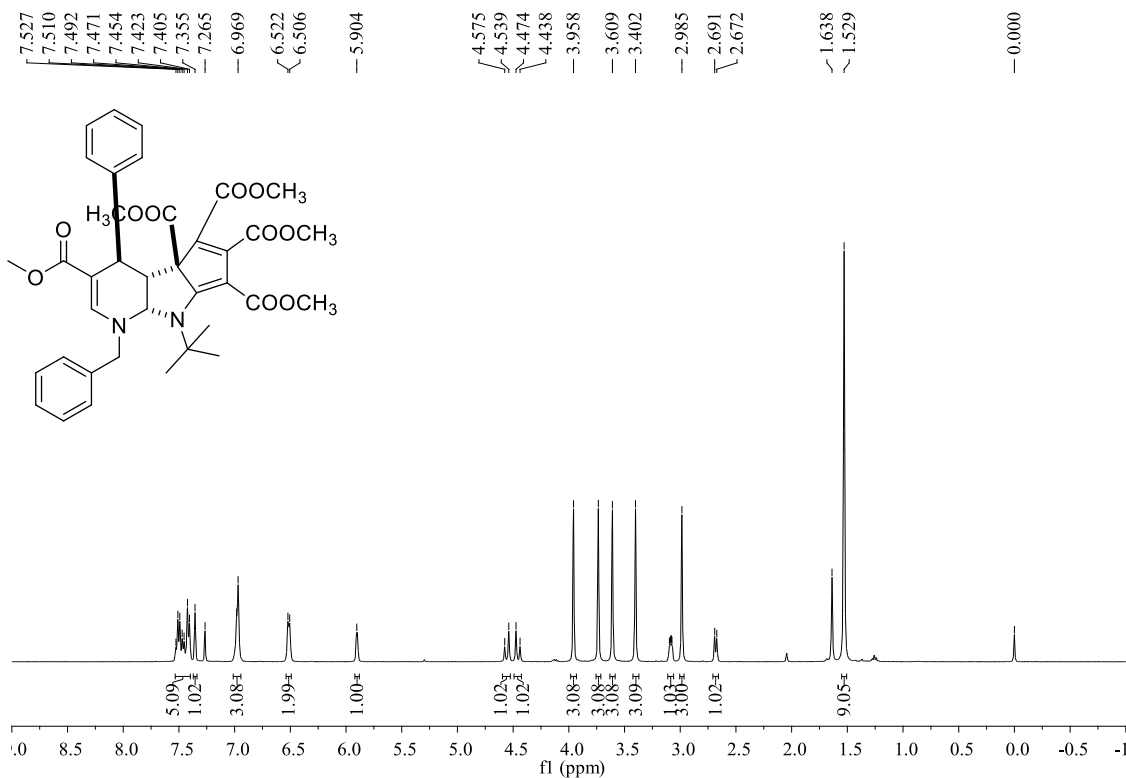
4b,5,6,7-Tetraethyl 3-methyl *rel*-(4*R*,4*aR*,4*bS*,8*aS*)-1-benzyl-8-cyclohexyl-4-phenyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (6i): yellow solid, 77%, m.p. 210-212 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.51-7.40 (m, 6H, CH, ArH), 7.09-6.99 (m, 3H, ArH), 6.89 (t, *J* = 6.8 Hz, 2H, ArH), 5.80 (d, *J* = 2.8 Hz, 1H, CH), 4.96 (t, *J* = 11.6 Hz, 1H, CH), 4.56 (d, *J* = 15.2 Hz, 1H, CH₂), 4.51 (d, *J* = 15.2 Hz, 1H, CH₂), 4.47-4.39 (m, 1H, CH₂), 4.37-4.29 (m, 1H, CH₂), 4.23-4.14 (m, 2H, CH₂), 4.13-4.06 (m, 1H, CH₂), 3.98-3.90 (m, 1H, CH₂), 3.65-3.57 (m, 1H, CH₂), 3.37 (s, 3H, OCH₃), 3.22 (dd, *J*₁ = 8.8 Hz, *J*₂ = 3.2 Hz, 1H, CH), 3.18-3.12 (m, 1H, CH₂), 2.86 (t, *J* = 8.8 Hz, 1H, CH), 1.92-1.71 (m, 6H, CH₂), 1.63-1.54 (m, 1H, CH₂), 1.48-1.35 (m, 5H, CH₂, CH₃), 1.31 (t, *J* = 7.2 Hz, 3H, CH₃), 1.21-1.15 (m, 1H, CH₂), 1.07 (t, *J* = 7.2 Hz, 3H, CH₃), 0.76 (t, *J* = 7.2 Hz, 3H, CH₃) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.4, 166.9, 166.7, 165.7, 162.2, 161.4, 144.1, 141.8, 136.9, 129.2, 128.9, 128.4, 127.8, 127.6, 125.8, 114.3, 108.8, 100.4, 81.2, 77.3, 77.0, 76.7, 72.1, 62.1, 61.1, 60.2, 60.0, 59.4, 58.6, 52.8, 50.6, 36.1, 32.1, 31.4, 26.1, 25.6, 14.11, 14.05, 13.8, 13.6 ppm. IR (KBr) ν: 3435, 2940, 2859, 1729, 1702, 1576, 1538, 1448, 1367, 1330, 1229, 1188, 1108, 1080, 1027, 988, 897, 853, 761 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₄₃H₅₀NaN₂O₁₀ ([M+Na]⁺): 777.3358, found: 777.3350.

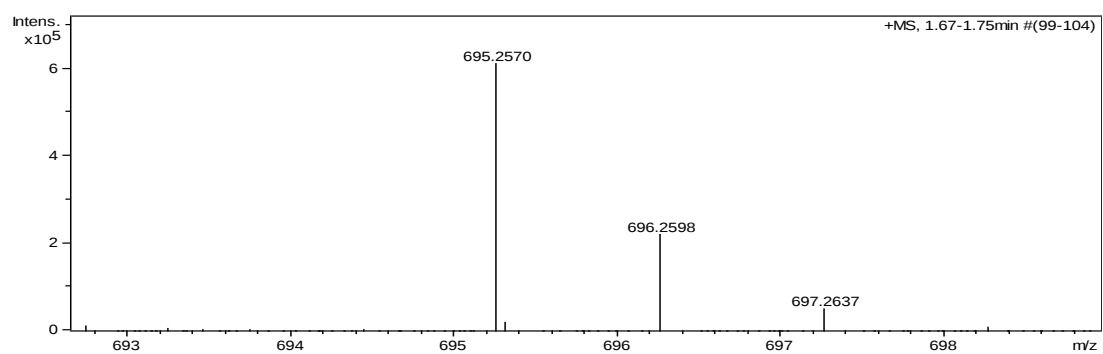
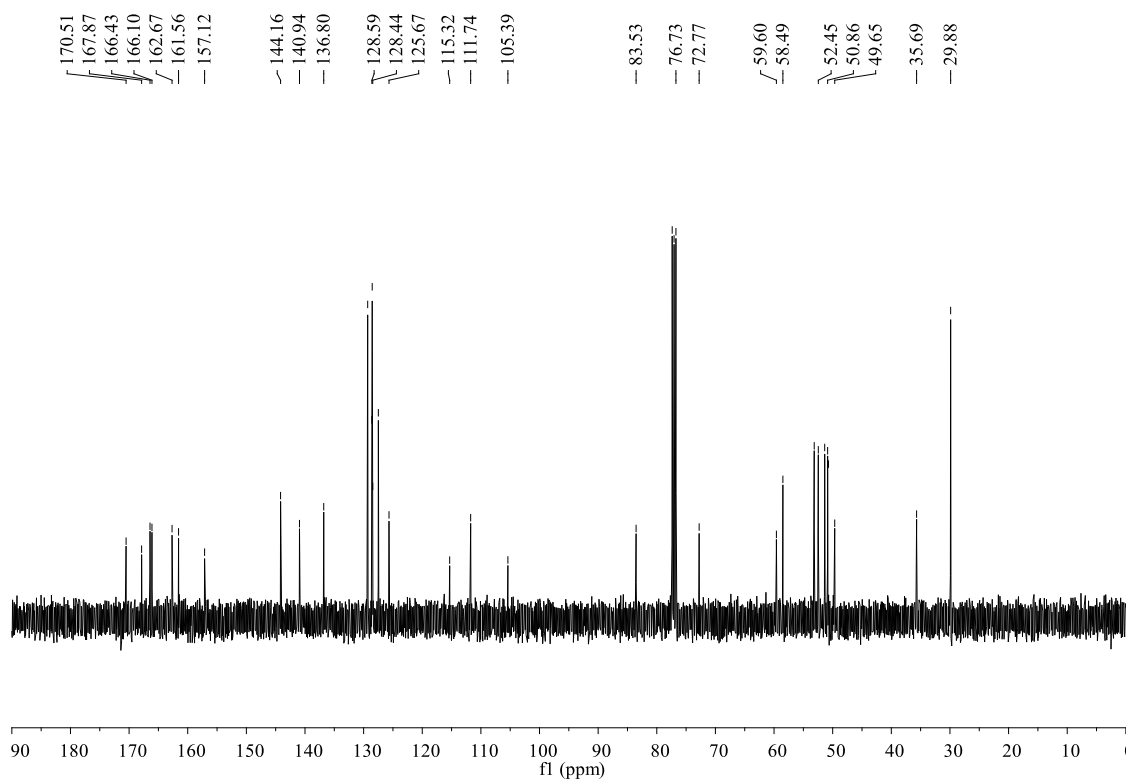




Pentamethyl***rel*-(4*R*,4*aR*,4*bS*,8*aS*)-1-benzyl-8-(*tert*-butyl)-4-phenyl-4,4*a*,8,8*a*-tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (6j):**

yellow solid, 70%, m.p. 205-207 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.53-7.41 (m, 5H, CH, ArH), 7.36 (s, 1H, ArH), 6.98-6.97 (m, 3H, ArH), 6.51 (d, *J* = 6.4 Hz, 2H, ArH), 5.90 (s, 1H, CH), 4.56 (d, *J* = 14.4 Hz, 1H, CH₂), 4.46 (d, *J* = 14.4 Hz, 1H, CH₂), 3.96 (s, 3H, OCH₃), 3.74 (s, 3H, OCH₃), 3.61 (s, 3H, OCH₃), 3.40 (s, 3H, OCH₃), 3.10-3.07 (m, 1H, CH), 2.98 (s, 3H, OCH₃), 2.68 (d, *J* = 7.6 Hz, 1H, CH), 1.53 (s, 9H, CH₃) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.5, 167.9, 166.4, 166.1, 162.7, 161.6, 157.1, 144.2, 140.9, 136.8, 129.3, 128.6, 128.5, 128.4, 127.5, 125.7, 115.3, 111.7, 105.4, 83.5, 77.4, 77.1, 76.7, 72.8, 59.6, 58.5, 53.2, 52.5, 51.4, 50.9, 50.7, 49.7, 35.7, 29.9 ppm. IR (KBr) ν: 3434, 2952, 2360, 1735, 1702, 1642, 1595, 1533, 1435, 1395, 1358, 1233, 1177, 1108, 1080, 1000, 978, 915, 851, 793, 761 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₃₇H₄₀NaN₂O₁₀ ([M+Na]⁺): 695.2575, found: 695.2570.





Pentamethyl

rel-(4*R*,4*aR*,4*bS*,8*aS*)-1,8-dibenzyl-4-phenyl-4,4*a*,8,8*a*-

tetrahydrocyclopenta[4,5]pyrrolo[2,3-*b*]pyridine-3,4*b*,5,6,7(1*H*)-pentacarboxylate (6k):

yellow solid, 58%, m.p. 218-220 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.42-7.31 (m, 7H, CH, ArH), 7.19-7.14 (m, 4H, ArH), 7.11-7.03 (m, 5H, ArH), 6.08 (d, *J* = 16.0 Hz, 1H, CH₂), 5.50 (d, *J* = 2.8 Hz, 1H, CH), 4.51 (d, *J* = 16.0 Hz, 1H, CH₂), 4.39 (d, *J* = 15.2 Hz, 1H, CH₂), 4.04-3.96 (m, 4H, CH₂, CH₃) 3.68 (s, 3H, OCH₃), 3.58 (s, 3H, OCH₃), 3.48 (dd, *J*₁ = 8.8 Hz, *J*₂ = 3.2 Hz, 1H, CH), 3.38 (s, 3H, OCH₃), 3.01-2.99 (m, 1H, CH), 2.98 (s, 3H, OCH₃) ppm. ¹³C NMR (100 MHz, CDCl₃) δ 170.8, 167.0, 166.7, 166.0, 162.7, 161.9, 156.9, 143.7, 141.4, 137.0, 136.6, 129.1, 129.0, 128.9, 128.3, 127.9, 127.1, 126.6, 126.0, 113.6, 107.1, 99.5, 80.9, 77.3, 77.0, 76.7, 72.4, 59.1, 53.7, 53.4, 52.5, 51.4, 50.8, 50.7, 48.5, 35.9 ppm. IR (KBr) ν: 3390, 2949, 1738, 1696, 1585, 1548, 1434, 1383, 1346, 1230, 1116, 1094, 1075, 1011, 988, 847, 810, 795, 780, 763 cm⁻¹; MS (*m/z*): HRMS (ESI) Calcd. for C₄₀H₃₈NaN₂O₁₀ ([M+Na]⁺): 729.2419, found: 729.2414.

