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Supporting Information

Nickel-Catalyzed Transesterification of Methyl Esters

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1. General Information

1.1. General experimental details

Unless otherwise indicated, reactions were conducted under an atmosphere of argon in 8 mL screw-capped vials that were oven dried (120 °C). Column chromatography was performed manually using Silicycle F60 40−63 µm silica gel. Analytical thin layer chromatography (TLC) was conducted with aluminum-backed EMD Millipore Silica Gel 60 F254 pre-coated plates. Visualization of developed plates was performed under UV light (254 nm) and/or using $KMnO_4$.

1.2. Instrumentation

^1H NMR and ^{13}C NMR were recorded on a Bruker AVANCE 400 or 300 MHz spectrometer. ^1H NMR spectra were internally referenced to the residual solvent signal (e.g., $CDCl_3$ = 7.26 ppm). ^{13}C NMR spectra were internally referenced to the residual solvent signal (e.g., $CDCl_3$ = 77.00 ppm). Data for ^1H NMR are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, m = multiplet), coupling constant (Hz), integration. NMR yields for optimization studies were obtained by ^1H NMR analysis of the crude reaction mixture using 1,1,2,2-tetrachloroethane as an internal standard. IR spectra were obtained using a Nicolet 6700 FT-IR spectrometer with a diamond ATR crystal (ThermoScientific) and are reported in terms of frequency of absorption (cm^{-1}). Melting point ranges were determined on a Canlab GallenKamp Melting Point Apparatus. GC yields for optimization studies were obtained via a 5-point calibration curve using FID analysis (1,3,5-trimethoxybenzene as an internal standard) on an Agilent Technologies 7890B GC with 30 m × 0.25 mm HP-5 column. Accurate mass data (EI) was obtained from an Agilent 5977A GC/MSD using MassWorks 4.0 from CERNO Bioscience. HRMS data was obtained from a Micromass Q-TOF 2 quadrupole – time-of-flight mass spectrometer with ESI source.

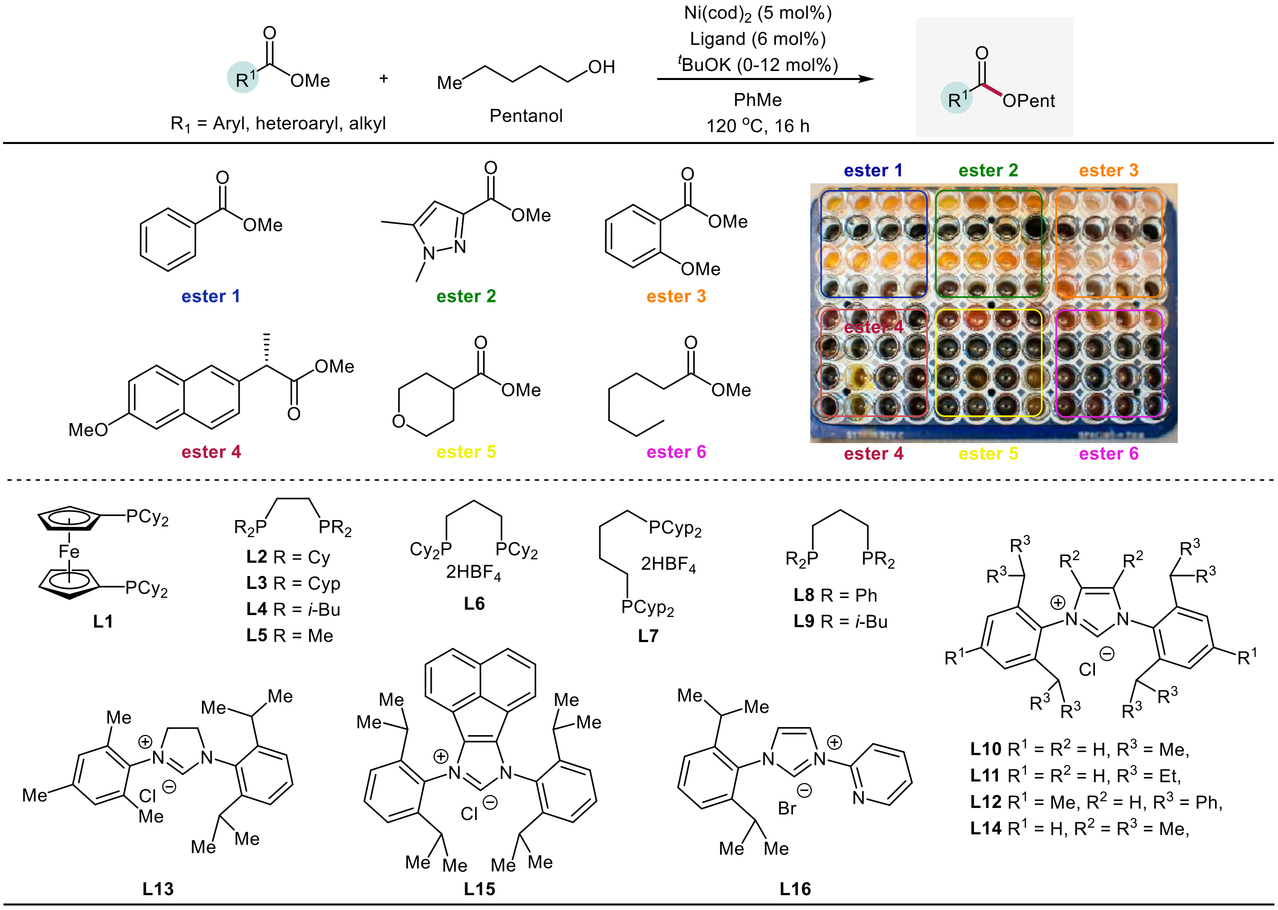
1.3. Materials

Organic solvents were purified by rigorous degassing with nitrogen before passing through a PureSolv solvent purification system. Low water content was confirmed by Karl Fischer titration (<20 ppm for all solvents). Unless otherwise noted, esters, alcohols, and other starting materials were obtained commercially from Sigma-Aldrich, Combi-Blocks and Oakwood Chemicals. $Ni(cod)_2$ was purchased from Sigma-Aldrich.

2. Reaction development and optimization

2.1 General considerations on the high throughput experimentation (HTE) optimizations

Six different esters were selected (ester 1-6) and each of them was tested with sixteen different ligands (L1-L16). In addition to methyl benzoate, a heteroaromatic ester (ester 2), *ortho*-substituted ester (ester 3), benzylic ester (ester 4), secondary aliphatic ester (ester 5), and primary aliphatic ester (ester 6) were screened. For quick analysis, the 96-well plate was run on the GC/MS, and, for each ester, the highest integration of product over integration of internal standard was normalized to 100% "relative performance". This normalization was deemed sufficient to evaluate the efficiency different ligands for a given ester. However, it should be noted that it does not allow us to compare reaction efficiency between different esters, nor does it provide the absolute value of the yield. Since our goal was to identify the optimal ligand for each class of substrates, this normalization technique provides useful information without necessitating isolation of individual products and rigorous quantification using a calibration curve.



Scheme S1: High-throughput experimentation (HTE) optimization for nickel-catalyzed transesterification reaction

Standard procedure for screening the transesterification reaction: 0.05 mmol of ester, 0.1 mmol pentanol, 5 mol% of Ni(cod)$_2$, 6 mol% of ligand (6 mol% ^{t}BuOK for NHC precursors or 12 mol% ^{t}BuOK for bidentate phosphonium tetrafluoroborates were required to release the active ligands via deprotonation. No base was included for free phosphines), 0.25 mL solvent at 120 ℃ for 16 h. After cooling, a consistent volume of internal standard (1,3,5-trimethoxybenzene) was distributed across all plates during plate workup. The aliquots were flushed through silica on a multi-well filtration plate with ethyl acetate solution to a total volume of about 0.5 mL. The relative yield was reported as:

$$\frac{\text{Integration ester of interest / integration of internal standard with ester of interest}}{\text{Integration of highest yielding example/integration of IS for highest yielding example}} * 100\%.$$

2.2 The relative yields for various esters

Table S1. Relative yields for ester 1

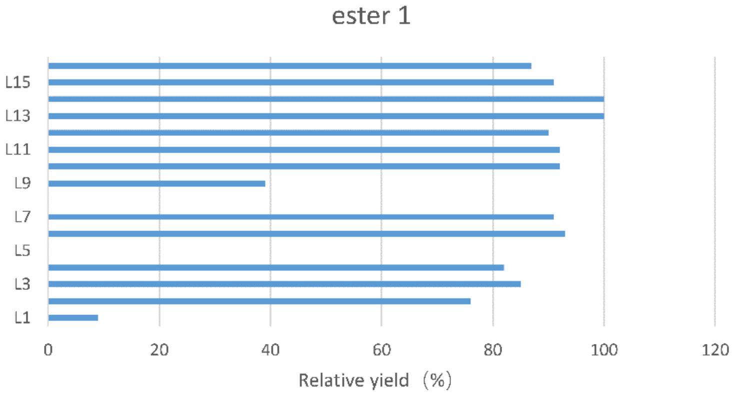


Table S2. Relative yields for ester 2

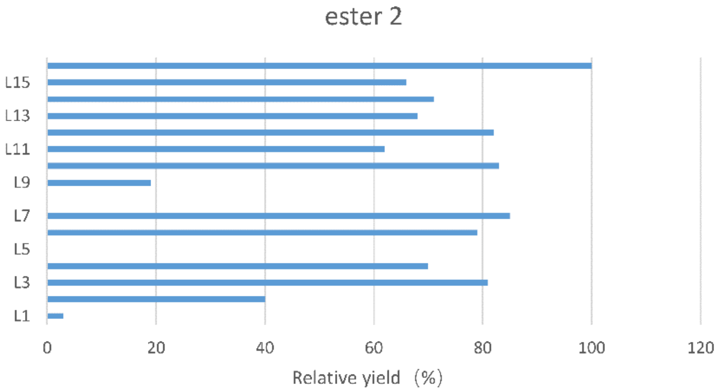


Table S3. Relative yields for ester 3

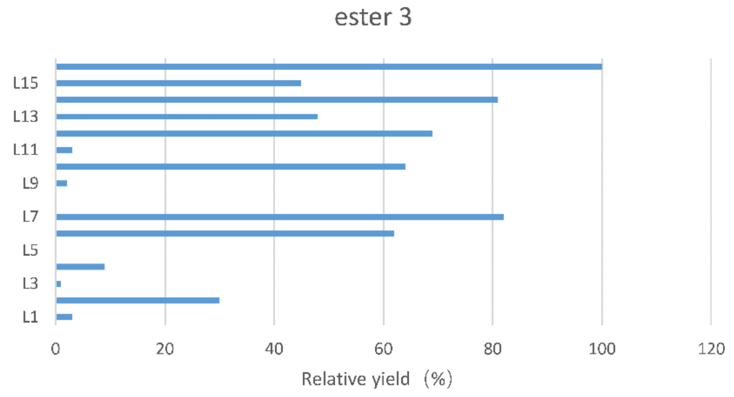


Table S4. Relative yields for ester 4

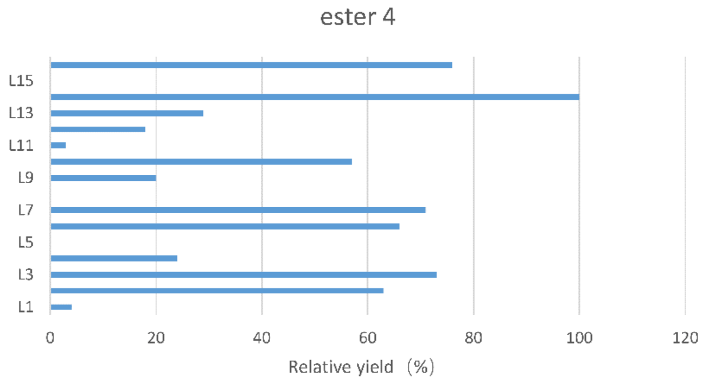


Table S5. Relative yields for ester 5

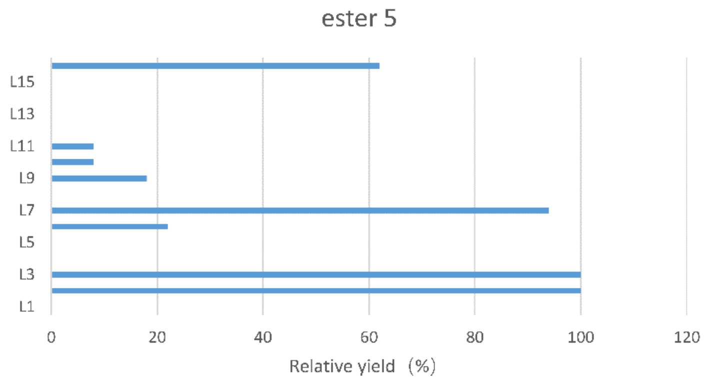
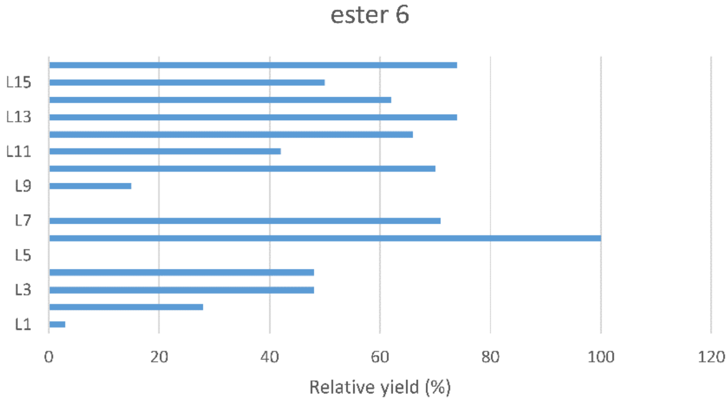
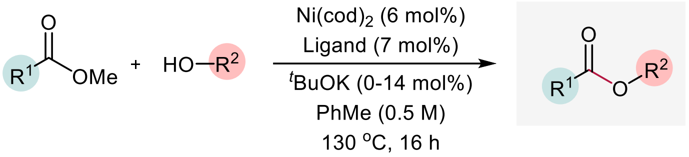


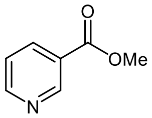
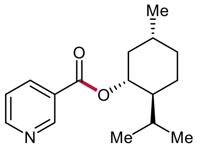
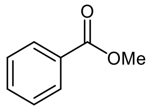
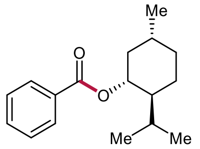
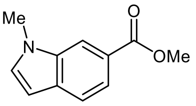
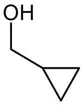
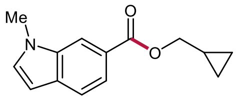
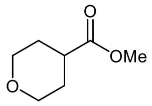
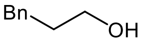
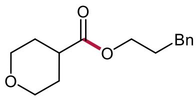
Table S6. Relative yields for ester 6



2.3 Additional experiments

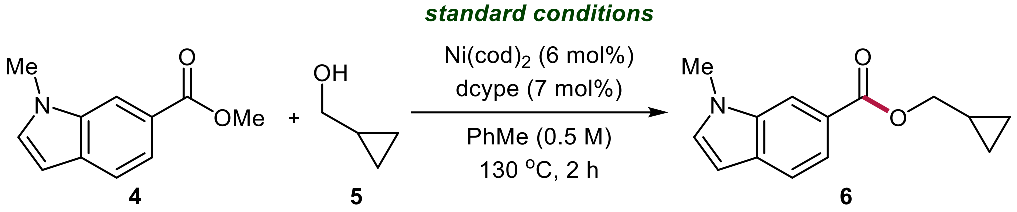
Table S7. Comparing the reactivity of L2 (dcype) with L7 and L16 for the esterification reaction in batch.



Entry	Esters	Alcohol	Product	Yield (%)[a]		
				L2 (dcype)	L7	L16
1		L-menthol		95	75	99
2		L-menthol		95	96	91
3				65	61	99
4				35	94	90

General conditions: Ester (0.2 mmol), alcohol (0.3 mmol), Ni(cod)$_2$ (3.3 mg, 6 mol%), L2 (5.9 mg, 7 mol%), L7 (8.0 mg, 7 mol%) or L16 (5.4 mg, 7 mol%), ^{t}BuOK (0-14 mol%, no base was need for dcype ligand), PhMe (0.4 mL) at 130 °C for 2 h. [a]Yields were determined by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard.

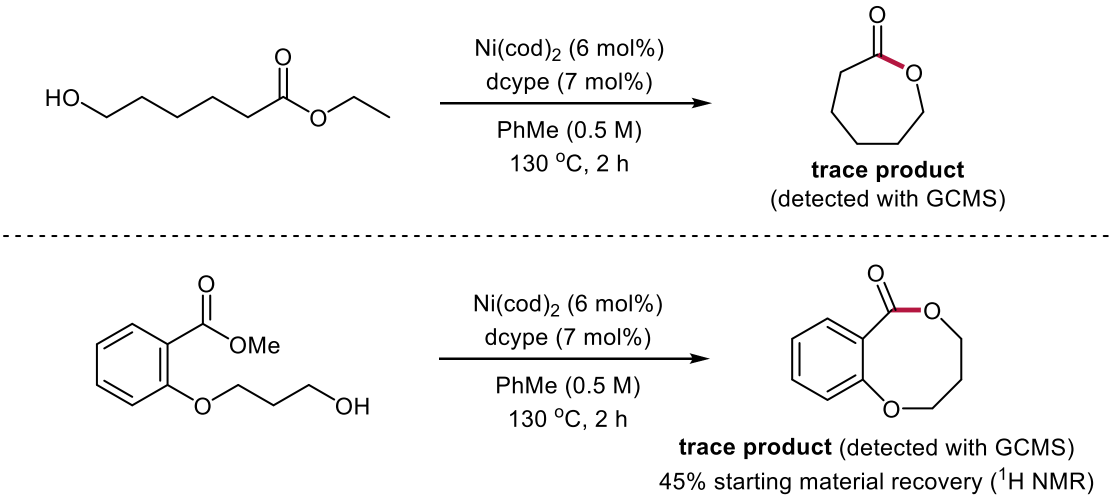
Table S8. Evaluation of air-stable nickel precatalysts and cobalt catalysts for the traneseterification reaction.



Entry	Deviation from standard conditions	Yield (%)[a]
1	none	65
2	Ni(cod)(dq) (6 mol%) instead of $Ni(cod)_2$	9
3	$NiBr_2$·glyme (6 mol%) + Zn (2.0 equiv) instead of $Ni(cod)_2$	38
4	$NiBr_2$·glyme (6 mol%) + Mn (2.0 equiv) instead of $Ni(cod)_2$	91
5	$CoBr_2$ (10 mol%) + Zn (2.0 equiv) instead of $Ni(cod)_2$	56
6	$CoBr_2$ (10 mol%) + Mn (2.0 equiv) instead of $Ni(cod)_2$	90

General conditions: methyl 1-methylindole-6-carboxylate **4** (0.20 mmol), cyclopropylmethanol **5** (0.30 mmol), PhMe (0.40 mL), 130 °C for 2 h. [a]Yield were determined by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachlorethane as an internal standard. Ni(cod)(dq): bis(1,5-cyclooctadiene)(duroquinone) nickel(0).

Figure S1. Evaluation of (macro)lactonization with alcohol containing methyl ester starting materials.

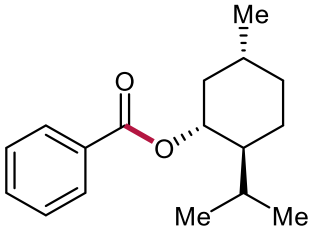


3. Analytical data for transesterification products

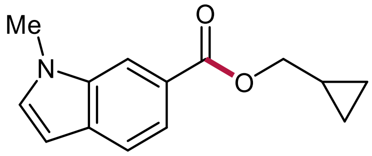
General procedure for Ni-catalyzed transesterification reaction

In a glovebox, an oven dried (120 °C) screw-capped vial was charged with a magnetic stir bar, $Ni(cod)_2$ (3.3 mg, 6 mol%), and 1,2-bis(dicyclohexylphosphino)ethane (dcype, 5.9 mg, 7 mol%). Thoroughly degassed toluene (0.4 mL, 0.5 M) obtained from a solvent purification system was then added. Then, ester (0.2 mmol) and alcohol

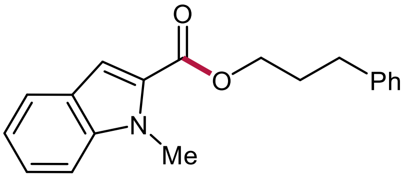
(0.3 mmol, 1.5 equiv) were subsequently added. The vial was sealed with a Teflon-lined screw cap and shipped outside of the glovebox. The reaction was stirred vigorously (650 rpm) in a pre-heated silicone oil bath at 130 °C for 2 hours. After cooling to room temperature, the reaction mixture was quenched with ethyl acetate and filtered through a plug of silica gel and celite (10 mL of ethyl acetate eluent). The crude mixture was then concentrated under reduced pressure, followed by purification via column chromatography.



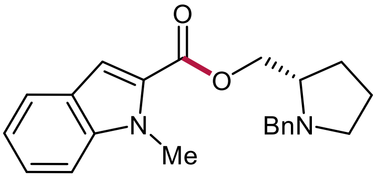
3, (1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl benzoate, hexanes/EtOAc = 10:1, coreless oil, (42.2 mg, 81% yield), Spectral data is in accordance with established literature.[1] **^{1}H NMR** (CDCl$_3$, 400 MHz): δ 8.09 – 8.02 (m, 2H), 7.58 – 7.52 (m, 1H), 7.48 – 7.41 (m, 2H), 4.94 (td, *J* = 11.2, 4.4 Hz, 1H), 2.18 – 2.10 (m, 1H), 2.02 – 1.93 (m, 1H), 1.78 – 1.69 (m, 2H), 1.60 – 1.51 (m, 2H), 1.19 – 1.05 (m, 2H), 0.96 – 0.89 (m, 7H), 0.80 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (100 MHz, CDCl$_3$) δ 166.1, 132.7, 130.9, 129.5, 128.3, 74.8, 47.3, 41.0, 34.3, 31.4, 26.5, 23.6, 22.0, 20.8, 16.5.



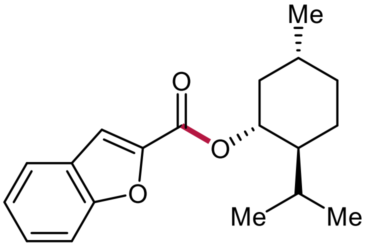
6, Cyclopropylmethyl 1-methyl-1*H*-indole-6-carboxylate, hexanes/EtOAc = 8:1, brown solid (27.5 mg, 60% yield). **^{1}H NMR** (400 MHz, CDCl$_3$) δ 8.13 (s, 1H), 7.85 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.65 (d, *J* = 8.4 Hz, 1H), 7.20 (d, *J* = 3.2 Hz, 1H), 6.53 (d, *J* = 2.8 Hz, 1H), 4.20 (d, *J* = 7.2 Hz, 2H), 3.86 (s, 3H), 1.38 – 1.26 (m, 1H), 0.70 – 0.59 (m, 2H), 0.47 – 0.36 (m, 2H). **^{13}C NMR** (100 MHz, CDCl$_3$) δ 167.9, 136.1, 132.02, 131.95, 123.5, 120.4, 120.3, 111.7, 101.3, 69.4, 33.0, 10.0, 3.3. **Accurate mass (EI)**: m/z calcd for $C_{14}H_{15}NO_2$: 229.1097; found 229.1062, spectral accuracy = 98.2 %.



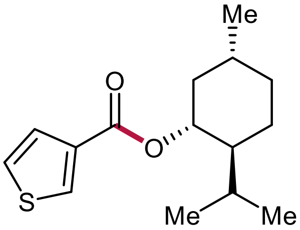
7, 3-Phenylpropyl 1-methyl-1*H*-indole-2-carboxylate, hexanes/EtOAc = 10:1, red oil (49.9 mg, 85% yield). **^{1}H NMR** (400 MHz, CDCl$_3$) δ 7.70 (m, 1H), 7.41 – 7.36 (m, 2H), 7.34 – 7.29 (m, 3H), 7.26 – 7.21 (m, 3H), 7.17 (m, 1H), 4.35 (t, *J* = 6.5 Hz, 2H), 4.09 (s, 3H), 2.82 (t, *J* = 8.5, 2H), 2.19 – 2.03 (m, 2H). **^{13}C NMR** (100 MHz, CDCl$_3$) δ 162.3, 141.2, 139.7, 128.55, 128.52, 127.9, 126.1, 125.9, 125.03, 122.6, 120.6, 110.3, 110.2, 63.8, 32.3, 31.7, 30.4. **Accurate mass (EI)**: m/z calcd for $C_{19}H_{19}NO_2$: 293.1410; found 293.1411, spectral accuracy 98.9%.



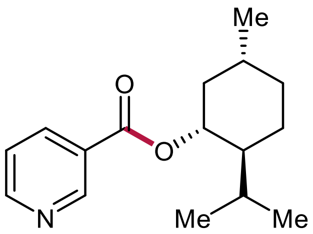
8, (*S*)-(1-Benzylpyrrolidin-2-yl)methyl 1-methyl-1*H*-indole-2-carboxylate, hexanes/EtOAc = 8:1, light yellow oil (43.9 mg, 63% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.67 (dt, *J* = 8.0, 1.2 Hz, 1H), 7.42 – 7.28 (m, 7H), 7.26 – 7.20 (m, 1H), 7.15 (ddd, *J* = 8.0, 6.4, 1.2 Hz, 1H), 4.38 – 4.27 (m, 2H), 4.19 (d, *J* = 13.2 Hz, 1H), 4.09 (s, 3H), 3.48 (d, *J* = 12.8 Hz, 1H), 3.05 – 2.92 (m, 2H), 2.36 – 2.24 (m, 1H), 2.12 – 1.99 (m, 1H), 1.86 – 1.72 (m, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.1, 139.7, 128.8, 128.2, 127.9, 126.9, 125.9, 125.0, 122.6, 120.5, 110.21, 110.18, 67.2, 62.1, 59.5, 54.5, 31.6, 28.6, 23.0. **HRMS** (ESI-TOF): m/z calcd for $C_{22}H_{25}N_2O_2$ $[M+H]^+$: 349.1921, found 349.1912.



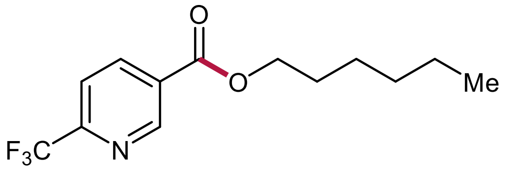
9, (1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl benzofuran-2-carboxylate, hexanes/EtOAc = 8:1, white solid (18.6 mg, 31% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.71 – 7.64 (m, 1H), 7.63 – 7.55 (m, 1H), 7.51 (d, *J* = 0.8 Hz, 1H), 7.43 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.33 – 7.25 (m, 1H), 5.00 (td, *J* = 10.8, 4.4 Hz, 1H), 2.20 – 2.11 (m, 1H), 2.03 – 1.91 (m, 1H), 1.79 – 1.69 (m, 2H), 1.65 – 1.51 (m, 2H), 1.25 – 1.07 (m, 2H), 1.02 – 0.87 (m, 7H), 0.82 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.2, 155.7, 146.0, 127.4, 127.0, 123.7, 122.7, 113.5, 112.4, 75.6, 47.1, 40.9, 34.2, 31.5, 26.5, 23.7, 22.0, 20.7, 16.5. **HRMS** (ESI-TOF): m/z calcd for $C_{19}H_{24}O_3Na$ $[M+Na]^+$: 323.1628, found 323.1623.



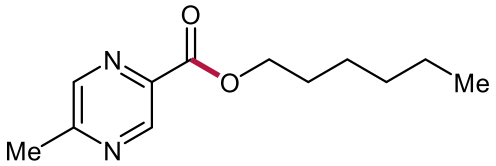
10, (1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl thiophene-3-carboxylate, hexanes/EtOAc = 60:1, coreless oil (24.0 mg, 45% yield). Spectral data was in accordance with established literature.[2] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.08 (dd, *J* = 3.2, 1.2 Hz, 1H), 7.52 (dd, *J* = 5.2, 1.2 Hz, 1H), 7.29 (dd, *J* = 5.2, 3.2 Hz, 1H), 4.87 (td, *J* = 10.8, 4.4 Hz, 1H), 2.15 – 2.06 (m, 1H), 2.00 – 1.89 (m, 1H), 1.76 – 1.68 (m, 2H), 1.59 – 1.46 (m, 2H), 1.16 – 1.04 (m, 2H), 0.95 – 0.88 (m, 7H), 0.79 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.3, 134.4, 132.3, 128.0, 125.8, 74.5, 47.2, 41.0, 34.3, 31.4, 26.5, 23.7, 22.0, 20.7, 16.6.



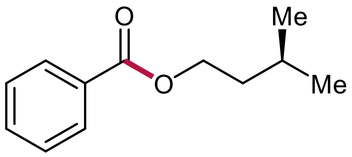
11, (1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl nicotinate, hexanes/EtOAc = 25:1, coreless oil (48.1 mg, 92% yield). Spectral data was in accordance with established literature.[3] **^{1}H NMR** (400 MHz, CDCl$_3$) *δ* 9.25 (s, 1H), 8.79 (s, 1H), 8.28 (d, *J* = 8.0 Hz, 1H), 7.38 (t, *J* = 6.4 Hz, 1H), 4.95 (td, *J* = 10.8, 4.4 Hz, 1H), 2.16 – 2.07 (m, 1H), 1.98 – 1.87 (m, 1H), 1.77 – 1.67 (m, 2H), 1.62 – 1.49 (m, 2H), 1.18 – 1.06 (m, 2H), 0.97 – 0.88 (m, 7H), 0.78 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (100 MHz, CDCl$_3$) *δ* 164.8, 153.1, 150.8, 137.0, 75.5, 47.2, 40.9, 34.2, 31.4, 26.5, 23.6, 22.0, 20.7, 16.5.



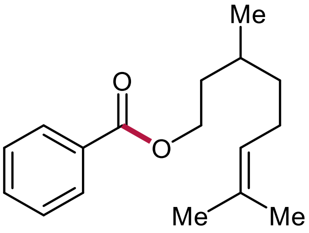
12, Hexyl 6-(trifluoromethyl)nicotinate, hexanes:EtOAc = 10:1, colourless oil (37.4 mg, 68% yield). **^{1}H NMR** (400 MHz, CDCl$_3$) δ 9.30 (d, *J*= 2.0 Hz, 1H), 8.47 (ddd, *J* = 8.1, 2.0, 0.8 Hz, 1H), 7.77 (dd, *J* = 8.1, 0.9 Hz, 1H), 4.38 (t, *J* = 6.7 Hz, 2H), 1.78 (m, 2H), 1.44 (m, 2H), 1.33 (m, 4H), 0.95 – 0.84 (m, 3H). **^{13}C NMR** (100 MHz, CDCl$_3$) δ 163.5, 144.7 (q, *J* = 1300.2 Hz), 138.1, 128.3, 120.7 (q, *J* = 275.2 Hz), 119.6 (q, *J* = 2.8 Hz), 119.2, 65.6, 30.8, 28.0, 25.0, 22.0, 13.4. **^{19}F NMR** (377 MHz, CDCl$_3$) δ -68.27. **HRMS** (ESI-TOF): m/z calcd for C$_{13}$H$_{17}$F$_3$NO$_2$ [M+H]$^+$: 276.1206, found 276.1207.



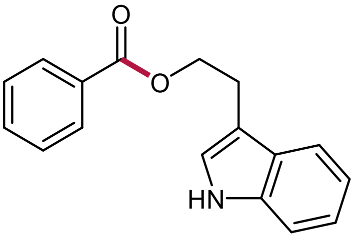
13, Hexyl 5-methylpyrazine-2-carboxylate, PhMe:EtOAc = 10:1, colourless oil (31.1 mg, 70% yield). **^{1}H NMR** (400 MHz, CDCl$_3$) δ 9.17 (d, *J* = 1.4 Hz, 1H), 8.58 (d, *J* = 1.4 Hz, 1H), 4.42 (t, *J* = 6.9 Hz, 2H), 2.66 (s, 3H), 1.85 – 1.76 (m, 2H), 1.49 – 1.25 (m, 7H), 0.93 – 0.83 (m, 3H). **^{13}C NMR** (100 MHz, CDCl$_3$) δ 164.3, 157.6, 145.3, 144.3, 140.8, 66.3, 31.4, 28.6, 25.5, 22.5, 21.9, 14.0. **HRMS** (ESI-TOF): m/z calcd for C$_{12}$H$_{19}$N$_2$O$_2$ [M+H]$^+$: 223.1441, found 223.1443.



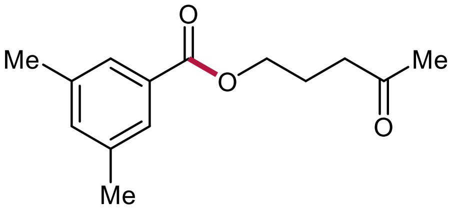
14, Isopentyl benzoate, hexanes:EtOAc = 30:1, colourless oil (32.7 mg, 85% yield). ^{1}**H NMR** (400 MHz, $CDCl_3$) δ 8.09 – 8.02 (m, 1H), 7.60 – 7.51 (m, 1H), 7.44 (m, 1H), 4.21 (dd, *J* = 10.7, 6.0 Hz, 1H), 4.13 (dd, *J* = 10.7, 6.6 Hz, 1H), 1.95 – 1.79 (m, 1H), 1.54 (m, 1H), 1.29 (m, 1H), 1.02 (d, *J* = 6.8 Hz, 1H), 0.96 (t, *J* = 7.5 Hz, 2H). ^{13}**C NMR** (100 MHz, $CDCl_3$) δ 166.8, 132.9, 130.7, 129.7, 128.5, 69.7, 34.4, 26.3, 16.7, 11.44. **HRMS** (ESI-TOF): m/z calcd for $C_{12}H_{16}O_2Na$ $[M+Na]^+$: 215.1053, found 215.1048.



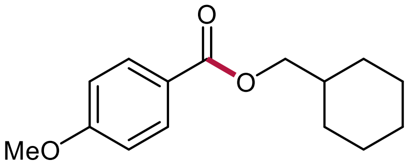
15, 3,7-Dimethyloct-6-en-1-yl benzoate, hexanes:EtOAc = 30:1, colourless oil (43.2 mg, 83% yield), Spectral data is in accordance with established literature.[4] ^{1}**H NMR** (400 MHz, $CDCl_3$) δ 8.07 – 7.99 (m, 2H), 7.58 – 7.49 (m, 1H), 7.42 (m, 2H), 5.08 (m, 1H), 4.42 – 4.27 (m, 2H), 2.09 – 1.89 (m, 2H), 1.85 – 1.75 (m, 1H), 1.70 – 1.50 (m, 8H), 1.44 – 1.33 (m, 1H), 1.27 – 1.16 (m, 1H), 0.95 (d, *J* = 6.5 Hz, 3H). ^{13}**C NMR** (100 MHz, $CDCl_3$) δ 166.2, 132.3 132.2, 130.8, 129.0, 127.8, 124.0, 62.9, 36.4, 34.9, 29.0, 25.1, 24.8, 18.9, 17.1.



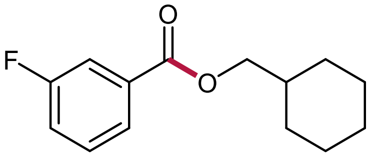
16, 2-(1H-Indol-3-yl)ethyl benzoate, hexanes:EtOAc = 10:1, yellow solid (47 mg, 89% yield). Spectral data is in accordance with established literature.[5] ^{1}**H NMR** (400 MHz, $CDCl_3$) δ 8.12 – 8.00 (m, 3H), 7.70 (d, *J* = 7.6 Hz, 1H), 7.59 – 7.53 (m, 1H), 7.46-7.42 (m, 2H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.25 – 7.20 (m, 1H), 7.18 – 7.13 (m, 1H), 7.11 (s, 1H), 4.62 (t, *J* = 7.2 Hz, 2H), 3.26 (t, *J* = 7.2 Hz, 2H). ^{13}**C NMR** (100 MHz, $CDCl_3$) δ 166.7, 136.2, 132.9, 130.4, 129.6, 128.3, 127.4, 122.12, 122.06, 119.5, 118.8, 112.1, 111.1, 65.0, 24.9.



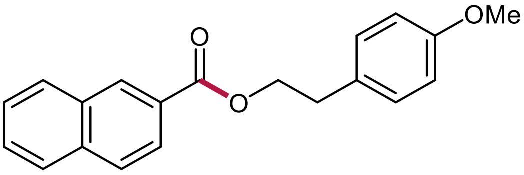
17, 4-Oxopentyl 3,5-dimethylbenzoate, hexanes:EtOAc = 10:1, white solid (21 mg, 44%yield). ^{1}**H NMR** (400 MHz, $CDCl_3$) δ 7.63 (s, 2H), 7.19 (s, 1H), 4.31 (t, *J* = 6.4 Hz, 2H), 2.60 (t, *J* = 7.2 Hz, 2H), 2.36 (s, 6H), 2.18 (s, 3H), 2.09 – 2.02 (m, 2H). ^{13}**C NMR** (100 MHz, CDCl3) δ 207.8, 166.9, 138.0, 134.6, 130.0, 127.2, 64.0, 40.0, 30.1, 22.9, 21.2. **HRMS** (ESI-TOF): m/z calcd for $C_{14}H_{19}O_3$ $[M+H]^+$: 235.1329, found 235.1327.



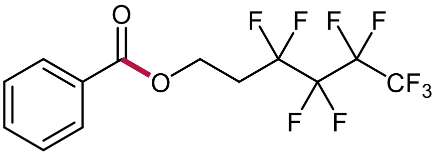
18, Cyclohexylmethyl 4-methoxybenzoate, hexanes:EtOAc = 30:1, colourless oil (40.2 mg, 81% yield). Spectral data is in accordance with established literature.[6] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.04 – 7.95 (m, 2H), 6.95 – 6.87 (m, 2H), 4.10 (d, *J* = 6.4 Hz, 1H), 3.85 (s, 3H), 1.88 – 1.64 (m, 6H), 1.36 – 1.13 (m, 3H), 1.12 – 1.00 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 166.5, 163.2, 131.5, 123.0, 113.6, 69.8, 55.4, 37.3, 29.8, 26.4, 25.7.



19, Cyclohexylmethyl 3-fluorobenzoate, hexanes:EtOAc = 30:1, colourless oil (42.5 mg, 90% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.84 (dt, *J* = 7.7, 1.2 Hz, 1H), 7.72 (ddd, *J* = 9.4, 2.7, 1.5 Hz, 1H), 7.41 (td, *J* = 8.0, 5.5 Hz, 1H), 7.30 – 7.20 (m, 1H), 4.14 (d, *J* = 6.3 Hz, 2H), 1.87 – 1.65 (m, 6H), 1.40 – 1.17 (m, 3H), 1.15 – 0.88 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.5 (d, *J* = 3.2 Hz), 163.8, 132.7 (d, *J* = 7.4 Hz), 128.0 (d, *J* = 7.8 Hz), 125.3 (d, *J* = 3.0 Hz), 119.9 (d, *J* = 21.3 Hz), 116.4 (d, *J* = 22.9 Hz), 70.4, 37.2, 29.7, 26.4, 25.7. **^{19}F NMR** (377 MHz, $CDCl_3$) δ -112.49. **HRMS** (ESI-TOF): m/z calcd for $C_{14}H_{17}FO_2Na$ $[M+Na]^+$: 259.1116, found 259.1110.

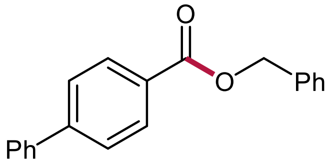


20, 4-Methoxyphenethyl 2-naphthoate, hexanes:EtOAc = 30:1, white solid (39.8 mg, 65% yield), Spectral data is in accordance with established literature.[7] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.60 – 8.55 (s, 1H), 8.04 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.94 (d, *J* = 8.0, 1H), 7.86 (d, *J* = 8.3 Hz, 2H), 7.62 – 7.49 (m, 2H), 7.27 – 7.19 (m, 2H), 6.91 – 6.83 (m, 2H), 4.55 (t, *J* = 7.1 Hz, 2H), 3.79 (s, 3H), 3.07 (t, *J* = 7.0 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 166.1, 157.8, 135.0, 131.9, 130.5, 129.41, 129.38, 128.8, 127.65, 127.57, 127.2, 127.1, 126.0, 124.7, 113.4, 65.3, 54.7, 33.9.

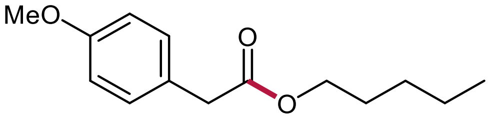


21, 3,3,4,4,5,5,6,6,6-Nonafluorohexyl benzoate, hexanes:EtOAc = 30:1, colourless oil (31.7 mg, 43% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.09 – 8.01 (m, 1H), 7.63 – 7.54 (m, 1H), 7.50 – 7.41 (m, 1H), 4.63 (t, *J* = 6.4 Hz, 1H), 2.70 – 2.53 (m, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 166.1, 133.3, 129.7, 129.5, 128.5, 56.8 (t, *J* = 4.5 Hz), 30.5 (t, *J* = 21.7 Hz). Note: The low signal:noise and multiplicity of fluorine-bearing carbons prevented identification of these atoms. **^{19}F NMR** (377 MHz, $CDCl_3$) δ -81.04 (tt, *J* = 9.1, 3.3 Hz), -113.75 – -133.87 (m), -124.4 – -124.57

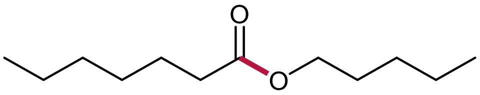
(m), - 125.91 – -126.12 (m). **Accurate mass (EI)**: m/z calcd for $C_{13}H_9F_9O_2$: 368.0453; found 368.0486, spectral accuracy 99.1%.



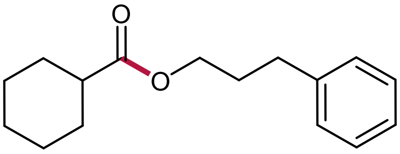
22, Benzyl [1,1'-biphenyl]-4-carboxylate, hexanes:EtOAc = 20:1, white solid (43.3 mg, 75% yield), which included inseparable benzyl alcohol contaminants. Spectral data is in accordance with established literature.[8] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.17 – 8.09 (m, 2H), 7.64 – 7.58 (m, 4H), 7.50 – 7.31 (m, 8H), 5.39 (s, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 166.3, 145.8, 140.0, 136.1, 130.2, 130.1, 128.9, 128.6, 128.3, 128.19, 128.17, 127.3, 127.1, 66.7.



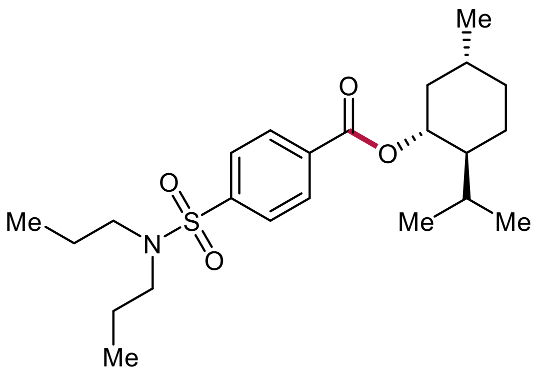
23, Pentyl 2-(4-methoxyphenyl)acetate, hexanes:EtOAc = 30:1, colourless oil (37.8 mg, 80% yield). Spectral data is in accordance with established literature.[9] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.22 – 7.18 (m, 2H), 6.90 – 6.83 (m, 2H), 4.07 (t, *J* = 6.7 Hz, 2H), 3.79 (s, 3H), 3.55 (s, 2H), 1.68 – 1.56 (m, 2H), 1.38 – 1.22 (m, 4H), 0.93 – 0.84 (m, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.1, 158.7, 130.4, 126.4, 114.0, 65.1, 55.3, 40.7, 28.4, 28.1, 22.4, 14.1.



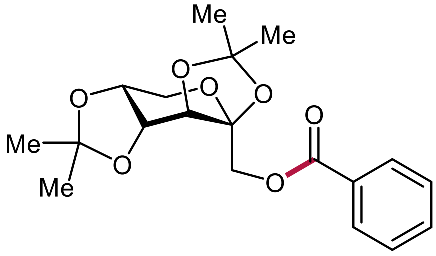
24, Pentyl octanoate, hexanes:EtOAc = 50:1, colourless oil (37.3 mg, 87% yield). Spectral data is in accordance with established literature.[10] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.05 (t, *J* = 6.7 Hz, 2H), 2.28 (t, *J* = 7.5 Hz, 2H), 1.68 – 1.55 (m, 4H), 1.37 – 1.22 (m, 12H), 0.94 – 0.83 (m, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 174.1, 64.5, 34.5, 31.8, 29.2, 29.1, 28.5, 28.2, 25.1, 22.7, 22.4, 14.2, 14.1.



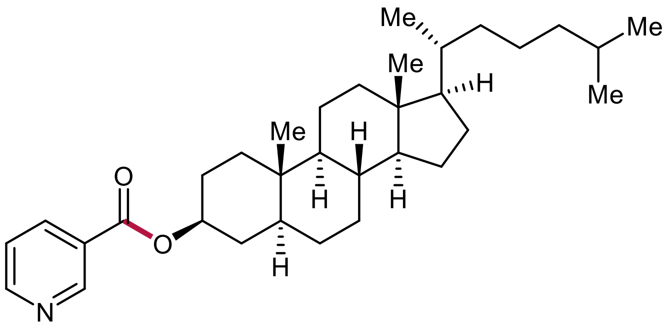
25, 3-Phenylpropyl cyclohexanecarboxylate, hexanes:EtOAc = 100:1, colorless oil (44 mg, 89% yield). Spectral data is in accordance with established literature.[11] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32 – 7.25 (m, 2H), 7.19 (t, *J* = 7.2 Hz, 3H), 4.07 (t, *J* = 6.4 Hz, 2H), 2.69 (t, *J* = 7.8 Hz, 2H), 2.27 – 2.34 (m, 1H), 2.02 – 1.86 (m, 4H), 1.80 – 1.73 (m, 2H), 1.67 – 1.63 (m, 1H), 1.50 – 1.40 (m, 2H), 1.35 – 1.17 (m, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 176.1, 141.3, 128.40, 128.39, 126.0, 63.4, 43.2, 32.2, 30.3, 29.0, 25.8, 25.4.



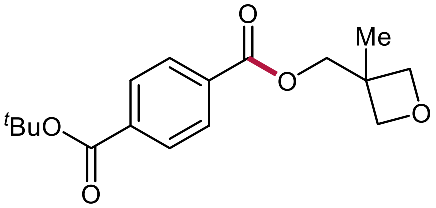
26, (1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl 4-(*N*,*N*-dipropylsulfamoyl)benzoate, hexanes/EtOAc = 25:1, coreless oil (49.1 mg, 58% yield).**^{1}H NMR** (400 MHz, CDCl$_3$) *δ* 8.17 – 8.12 (m, 2H), 7.90 – 7.84 (m, 2H), 4.96 (td, *J* = 10.8, 4.4 Hz, 1H), 3.13 – 3.05 (m, 4H), 2.17 – 2.07 (m, 1H), 1.99 – 1.88 (m, 1H), 1.79 – 1.69 (m, 2H), 1.63 – 1.50 (m, 6H), 1.18 – 1.06 (m, 2H), 0.93 (dd, *J* = 6.8, 3.6 Hz, 6H), 0.90 – 0.85 (m, 7H), 0.80 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, CDCl$_3$) *δ* 164.8, 144.0, 134.1, 130.13, 130.09, 127.0, 75.7, 50.0, 47.2, 40.9, 34.2, 31.5, 26.5, 23.6, 22.0, 20.8, 16.5, 11.2. **HRMS** (ESI-TOF): m/z calcd for C$_{23}$H$_{37}$NO$_4$SNa [M+Na]$^+$: 446.2346, found 446.2341.



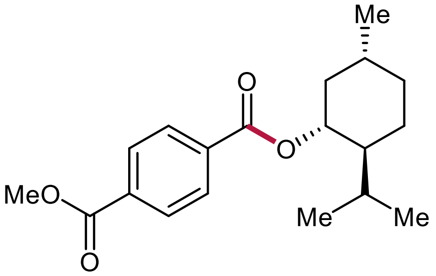
27, ((3aS,5aR,8aR,8bS)-2,2,7,7-Tetramethyltetrahydrobenzo[1,2-d:3,4-d']bis([1,3]dioxole)-3a(4H)-yl)methyl benzoate, Hexane/EtOAc = 10:1, coreless oil, 36.4 mg, 50%. Spectral data is in accordance with established literature.[12] **^{1}H NMR** (400 MHz, CDCl$_3$) δ 8.10 – 8.05 (m, 2H), 7.59 – 7.54 (m, 1H), 7.47 – 7.41 (m, 2H), 4.69 (d, *J* = 11.6 Hz, 1H), 4.64 (dd, *J* = 8.0, 2.8 Hz, 1H), 4.48 (d, *J* = 2.8 Hz, 1H), 4.33 (d, *J* = 12.0 Hz, 1H), 4.29 – 4.24 (m, 1H), 3.96 (dd, *J* = 13.2, 2.0 Hz, 1H), 3.81 (dd, *J* = 12.8, 0.8 Hz, 1H), 1.55 (s, 3H), 1.47 (s, 3H), 1.38 (s, 3H), 1.35 (s, 3H). **^{13}C NMR** (100 MHz, CDCl$_3$) δ 165.9, 133.0, 129.9, 129.7, 128.3, 109.1, 108.8, 101.6, 70.8, 70.5, 70.1, 65.2, 61.3, 26.5, 25.8, 25.5, 24.0.



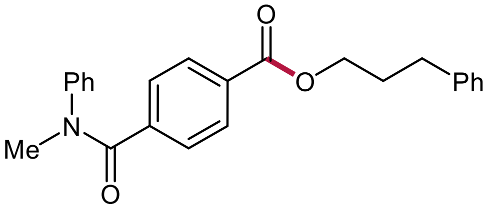
28, (3*S*,5*S*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)hexadecahydro-1*H*-cyclopenta[a]phenanthren-3-yl nicotinate, hexanes/EtOAc = 20:1 to 10:1, light yellow solid (73.1 mg, 74% yield). **^{1}H NMR** (400 MHz, CDCl$_3$) *δ* 9.21 (d, *J* = 1.6 Hz, 1H), 8.76 (dd, *J* = 4.8, 1.6 Hz, 1H), 8.29 (dt, *J* = 8.0, 2.0 Hz, 1H), 7.38 (ddd, *J* = 8.0, 4.8, 0.8 Hz, 1H), 5.03 – 4.92 (m, 1H), 2.03 – 1.90 (m, 2H), 1.87 – 1.62 (m, 5H), 1.60 – 1.45 (m, 4H), 1.43 – 1.20 (m, 10H), 1.16 – 1.05 (m, 6H), 1.04 – 0.94 (m, 3H), 0.94 – 0.83 (m, 14H), 0.72 – 0.63 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) *δ* 164.7, 153.1, 150.8, 136.9, 126.7, 123.1, 75.0, 56.4, 56.2, 54.2, 44.6, 42.5, 39.9, 39.5, 36.7, 36.1, 35.7, 35.44, 35.42, 34.0, 31.9, 28.6, 28.2, 27.9, 27.5, 24.2, 23.8, 22.8, 22.5, 21.2, 18.6, 12.2, 12.0. **HRMS** (ESI-TOF): m/z calcd for $C_{33}H_{52}NO_2$ $[M+H]^+$: 494.3993, found 494.4003.



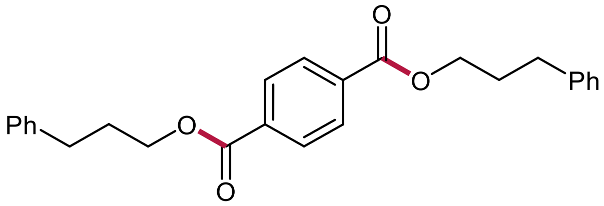
31, Tert-butyl ((3-methyloxetan-3-yl)methyl) terephthalate, 68% yield was determined by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The product was purified by preparative thin layer chromatography. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.10 – 8.04 (m, 4H), 4.64 (d, *J* = 6.0 Hz, 2H), 4.47 (d, *J* = 6.0 Hz, 2H), 4.41 (s, 2H), 1.60 (s, 9H), 1.43 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.8, 164.8, 136.0, 133.1, 129.42, 129.39, 81.8, 79.5, 69.3, 39.3, 28.1, 21.2. **HRMS** (ESI-TOF): m/z calcd for $C_{17}H_{23}O_5$ $[M+H]^+$: 307.1540, found 307.1545.



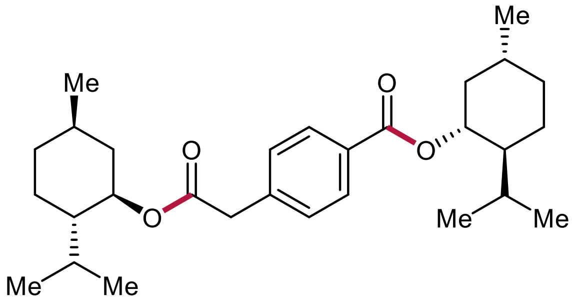
34, (1R,2S,5R)-2-Isopropyl-5-methylcyclohexyl methyl terephthalate, 56% yield was determined by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The product was purified by preparative thin layer chromatography. Spectral data is in accordance with established literature.[13] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.09 (s, 4H), 4.95 (td, *J* = 10.8, 4.4 Hz, 1H), 3.94 (s, 3H), 2.15 – 2.09 (m, 1H), 1.94 – 1.89 (m, 1H), 1.76 – 1.71 (m, 2H), 1.6 – 1.53(m, 2H), 1.18 – 1.06 (m, 2H), 0.92 (dd, *J* = 6.4, 4.0 Hz, 7H), 0.79 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 166.4, 165.3, 134.6, 133.7, 129.5, 75.4, 52.4, 47.2, 40.9, 34.2, 31.4, 26.5, 23.5, 22.0, 20.8, 16.5.



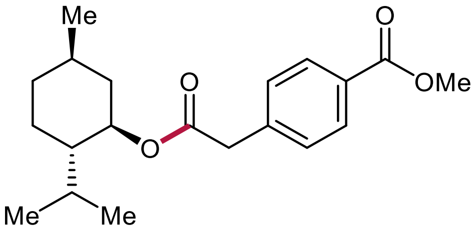
38, 3-Phenylpropyl 4-(methyl(phenyl)carbamoyl)benzoate, 88% yield was determined by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The product was purified by preparative thin layer chromatography. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.82 – 7.79 (m, 2H), 7.33 (d, *J* =8.4 Hz, 2H), 7.30 – 7.21 (m, 4H), 7.20 – 7.12 (m, 4H), 7.02 (d, *J* = 7.6 Hz, 2H), 4.27 (t, *J* = 6.4 Hz, 2H), 3.51 (s, 3H), 2.72 (t, *J* =7.6 Hz, 2H), 2.10 – 2.03 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.7, 165.9, 144.3, 141.1, 140.2, 131.0, 129.31, 129.29, 129.01,128.98, 128.6, 128.5, 128.4, 126.9, 126.0, 64.5, 38.3, 32.3, 30.1. **HRMS** (ESI-TOF): m/z calcd for $C_{24}H_{24}NO_3$ $[M+H]^+$: 374.1751, found 374.1749.



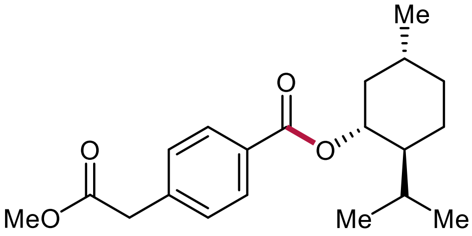
39, Bis(3-phenylpropyl) terephthalate, 10% yield was determined by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The product was purified by preparative thin layer chromatography. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.08 – 8.07 (m, 4H), 7.28 – 7.32 (m, 4H), 7.23 – 7.18 (m, 6H), 4.42 – 4.32 (m, 4H), 2.78 (t, *J* = 7.6 Hz, 4H), 2.16 – 2.09 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.8, 141.0, 134.1, 129.5, 128.5, 128.4, 126.1, 64.8, 32.3, 30.2. **HRMS** (ESI-TOF): m/z calcd for $C_{26}H_{27}O_4$ $[M+H]^+$: 403.1904, found 403.1912.



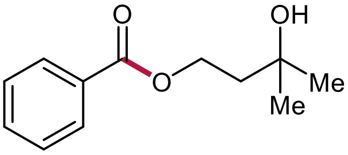
41, (1R,2S,5R)-2-Isopropyl-5-methylcyclohexyl 4-(2-(((1R,2S,5R)-2-isopropyl-5-methylcyclohexyl)oxy)-2-oxoethyl)benzoate, 47% yield was determined by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The product was purified by preparative thin layer chromatography. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 2H), 4.92 (td, *J* = 11.2, 4.4 Hz, 1H), 4.67 (td, *J* = 10.8, 4.4 Hz, 1H), 3.65 (s, 2H), 2.14 – 2.09 (m, 1H), 1.98 – 1.91 (m, 2H), 1.75 – 1.60 (m, 6H), 1.59 – 1.41 (m, 3H), 1.38 – 1.30 (m, 1H), 1.15 – 1.07 (m, 2H), 1.05 – 0.98 (m, 1H), 0.97 – 0.87 (m, 11H), 0.83 (d, *J* = 7.2 Hz, 3H), 0.78 (d, *J* = 7.2 Hz, 3H), 0.68 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.5, 165.9, 139.3, 129.8, 129.6, 129.2, 75.0, 74.8, 47.2, 46.9, 41.7, 40.9, 40.7, 34.3, 34.2, 31.4, 31.3, 26.5, 26.1, 23.6, 23.3, 22.03, 21.97, 20.73, 20.66, 16.5, 16.2. **HRMS** (ESI-TOF): m/z calcd for $C_{29}H_{45}O_4$ $[M+H]^+$: 457.3312, found 457.3321.



42, Methyl 4-(2-(((1R,2S,5R)-2-Isopropyl-5-methylcyclohexyl)oxy)-2-oxoethyl)benzoate, 35% yield was determined by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The product was purified by preparative thin layer chromatography. Spectral data is in accordance with established literature.[14] **^{1}H NMR** (400 MHz, CDCl$_3$) δ 8.00 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 4.67 (td, *J* = 10.8, 4.4 Hz, 1H), 3.91 (s, 3H), 3.65 (s, 2H), 1.97 – 1.92 (m, 1H), 1.77 – 1.61 (m, 4H), 1.52 – 1.40 (m, 1H), 1.38 – 1.30 (m, 1H), 1.07 – 0.99 (m, 1H), 0.98 – 0.91 (m, 1H), 0.88 (d, *J* = 6.4 Hz, 3H), 0.83 (d, *J* = 7.2 Hz, 3H), 0.68 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (100 MHz, CDCl$_3$) δ 170.4, 166.9, 139.5, 129.8, 129.2, 128.9, 75.0, 52.1, 46.9, 41.8, 40.7, 34.1, 31.3, 26.1, 23.3, 22.0, 20.7, 16.2.



43, (1R,2S,5R)-2-Isopropyl-5-methylcyclohexyl 4-(2-methoxy-2-oxoethyl)benzoate, 18% yield was determined by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The product was purified by preparative thin layer chromatography. **^{1}H NMR** (400 MHz, CDCl$_3$) δ 8.02 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 4.92 (td, *J* = 10.8, 4.4 Hz, 1H), 3.70 (s, 3H), 3.69 (s, 2H), 2.14 – 2.08 (m, 1H), 1.98 – 1.91 (m, 1H), 1.75 – 1.69 (m, 2H), 1.59 – 1.54 (m, 3H), 1.15 – 1.02 (m, 2H), 0.92 (t, *J* = 6.4 Hz, 6H), 0.78 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (100 MHz, CDCl$_3$) δ 171.3, 165.8, 138.8, 129.9, 129.8, 129.3, 74.8, 52.2, 47.3, 41.1, 40.9, 34.3, 31.4, 26.5, 23.6, 22.0, 20.8, 16.5. **HRMS** (ESI-TOF): m/z calcd for $C_{20}H_{29}O_4$ $[M+H]^+$: 333.2060, found 333.2066.



45, 3-Hydroxy-3-methylbutyl benzoate, 96% yield was determined by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. The product was purified by preparative thin layer chromatography (Hexane/EtOAc = 5:1). Spectral data is in accordance with established literature.[15] **^{1}H NMR** (400 MHz, CDCl$_3$) δ 8.06 – 7.99 (m, 2H), 7.60 – 7.50 (m, 1H), 7.47 – 7.38 (m, 2H), 4.50 (t, J = 6.8 Hz, 2H), 1.98 (t, *J* = 6.8 Hz, 2H), 1.32 (s, 6H). **^{13}C NMR** (100 MHz, CDCl$_3$) δ 166.6, 132.9, 130.2, 129.5, 128.4, 70.0, 61.9, 41.7, 29.7.

4. References

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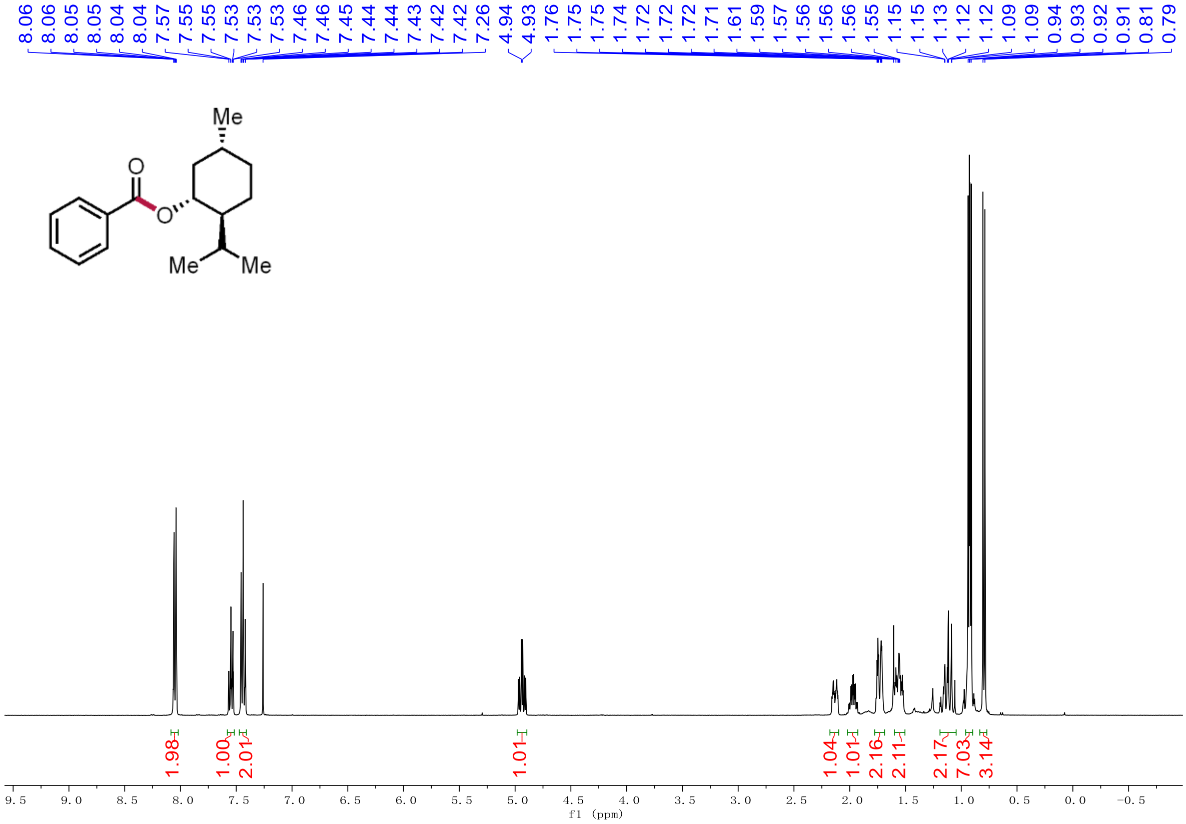
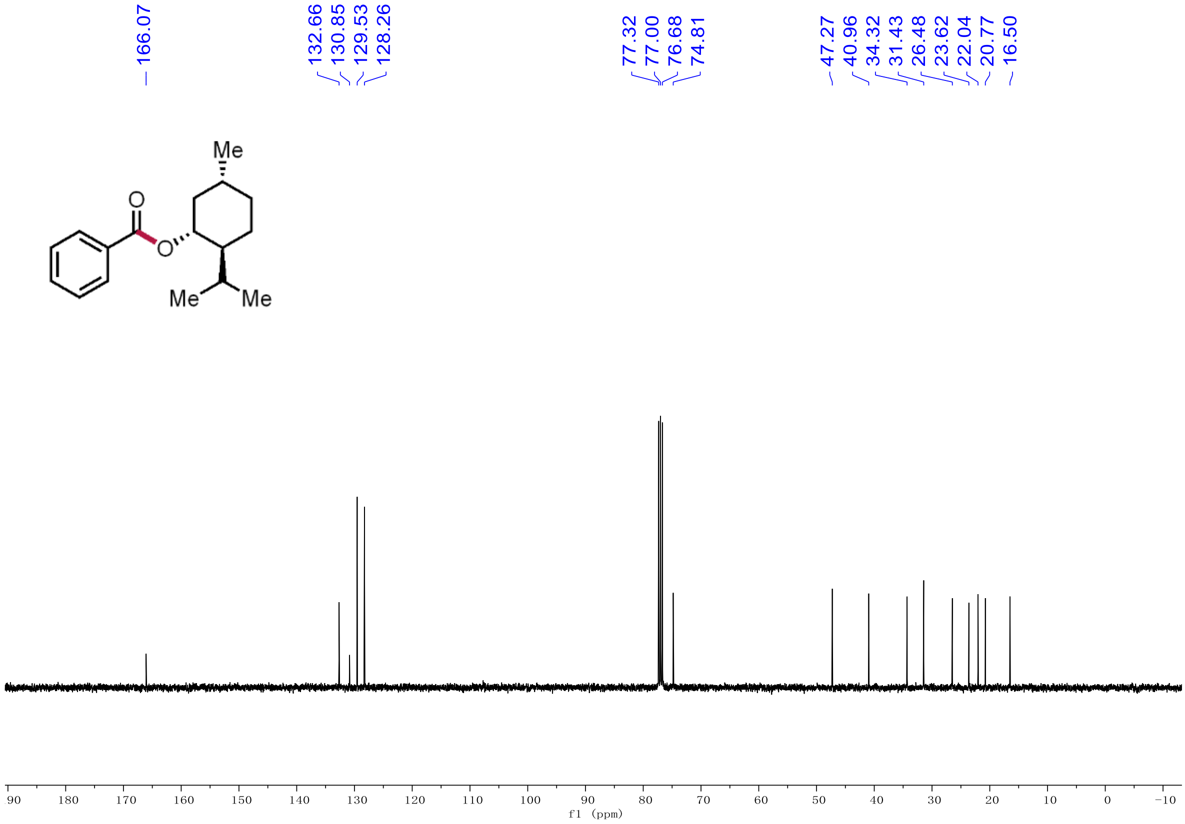
5. NMR spectra

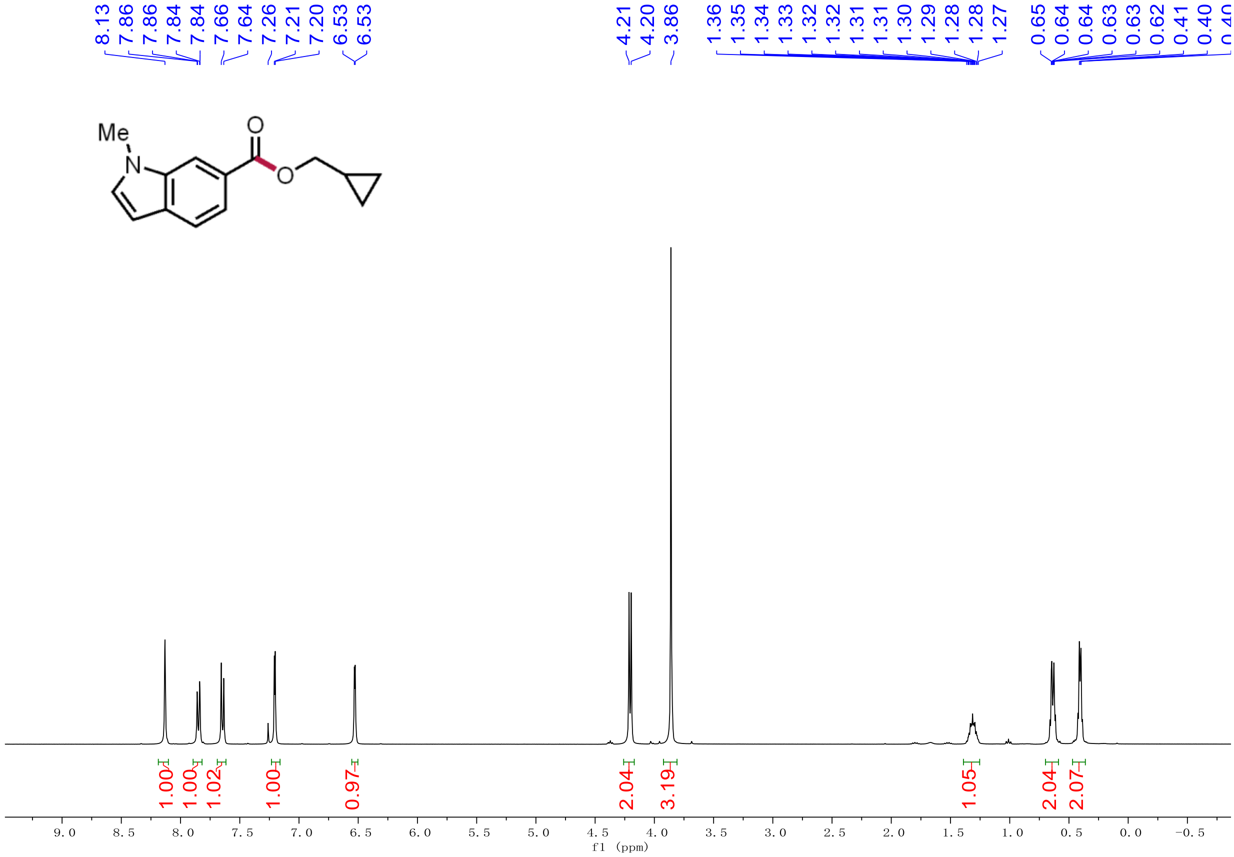
3: (1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl benzoate (^{1}H NMR, CDCl$_3$, 400 MHz)



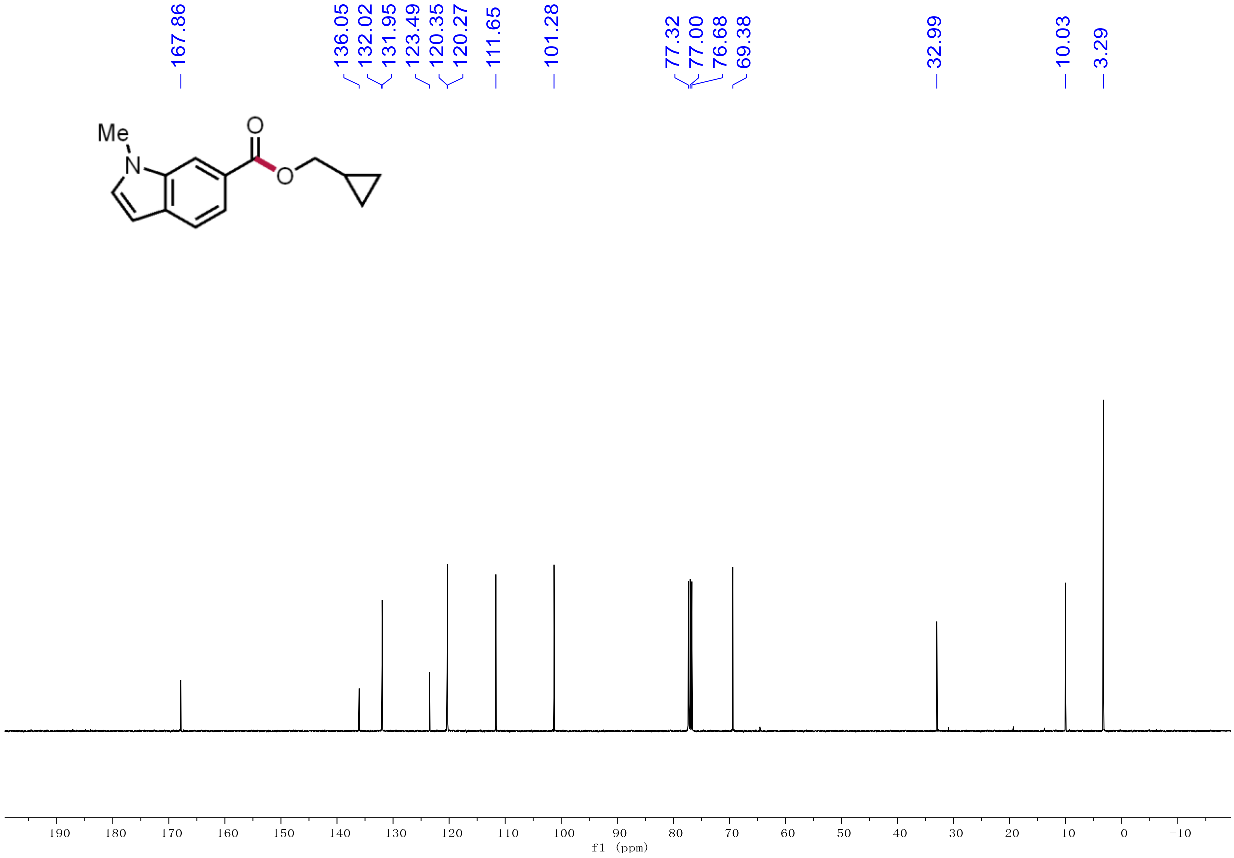
3: (1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl benzoate (^{13}C NMR, CDCl$_3$, 100 MHz)



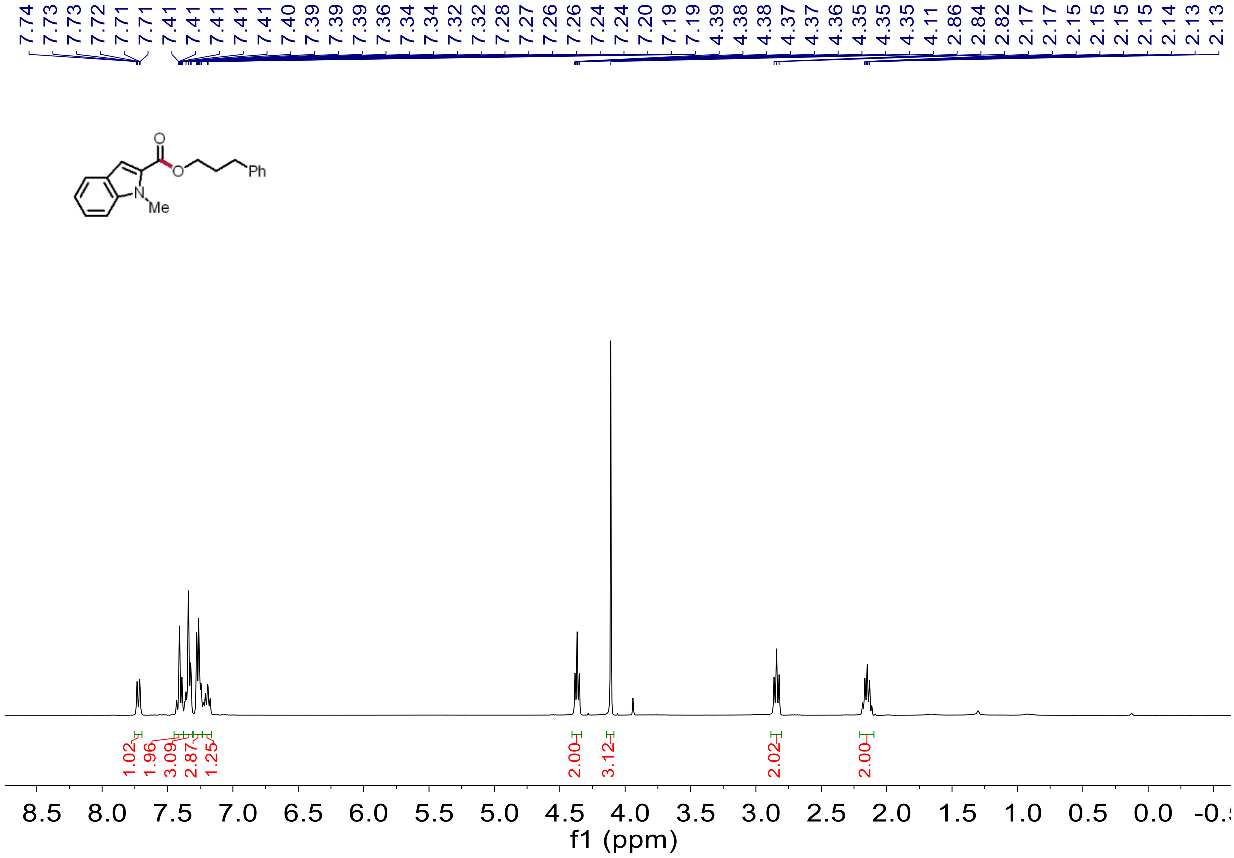
6: Cyclopropylmethyl 1-methyl-1*H*-indole-6-carboxylate (^{1}H NMR, CDCl$_3$, 400 MHz)



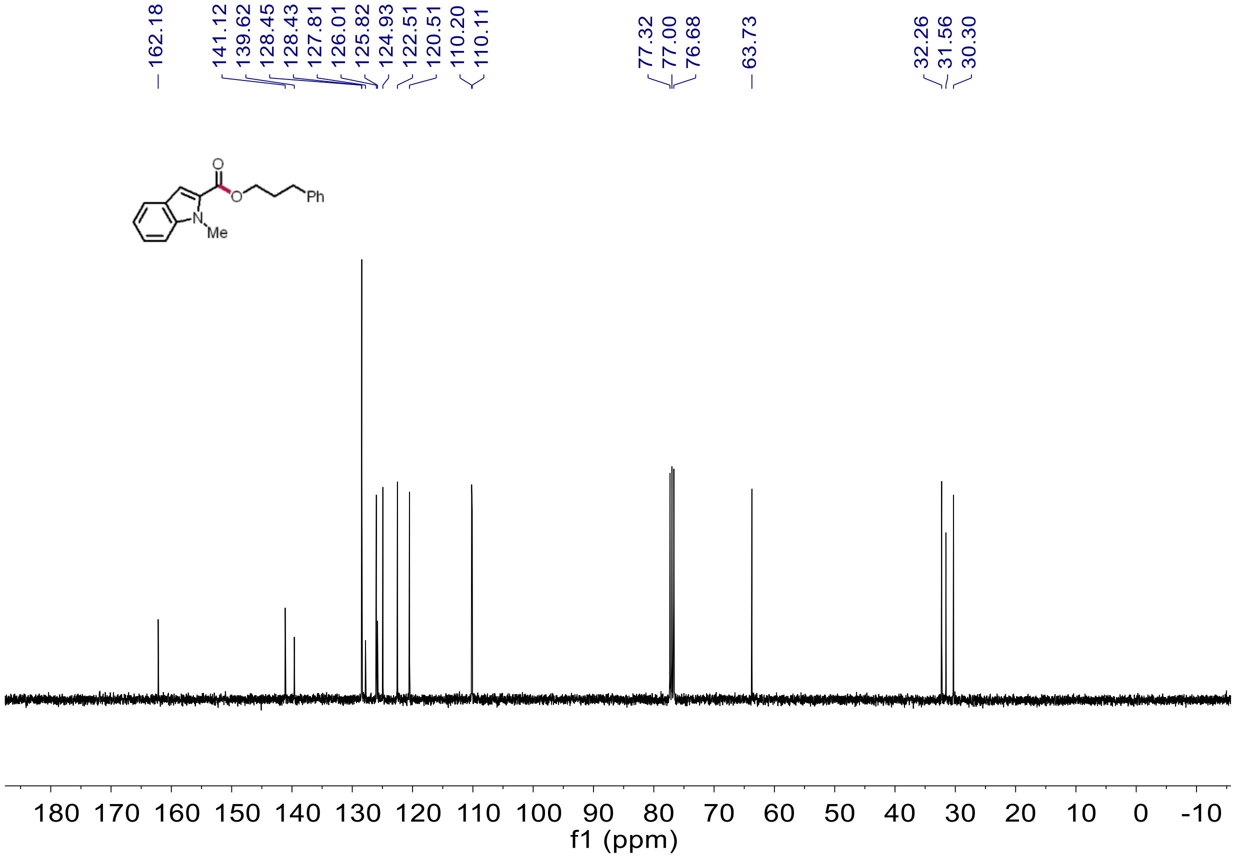
6: Cyclopropylmethyl 1-methyl-1*H*-indole-6-carboxylate (^{13}C NMR, CDCl$_3$, 100 MHz)



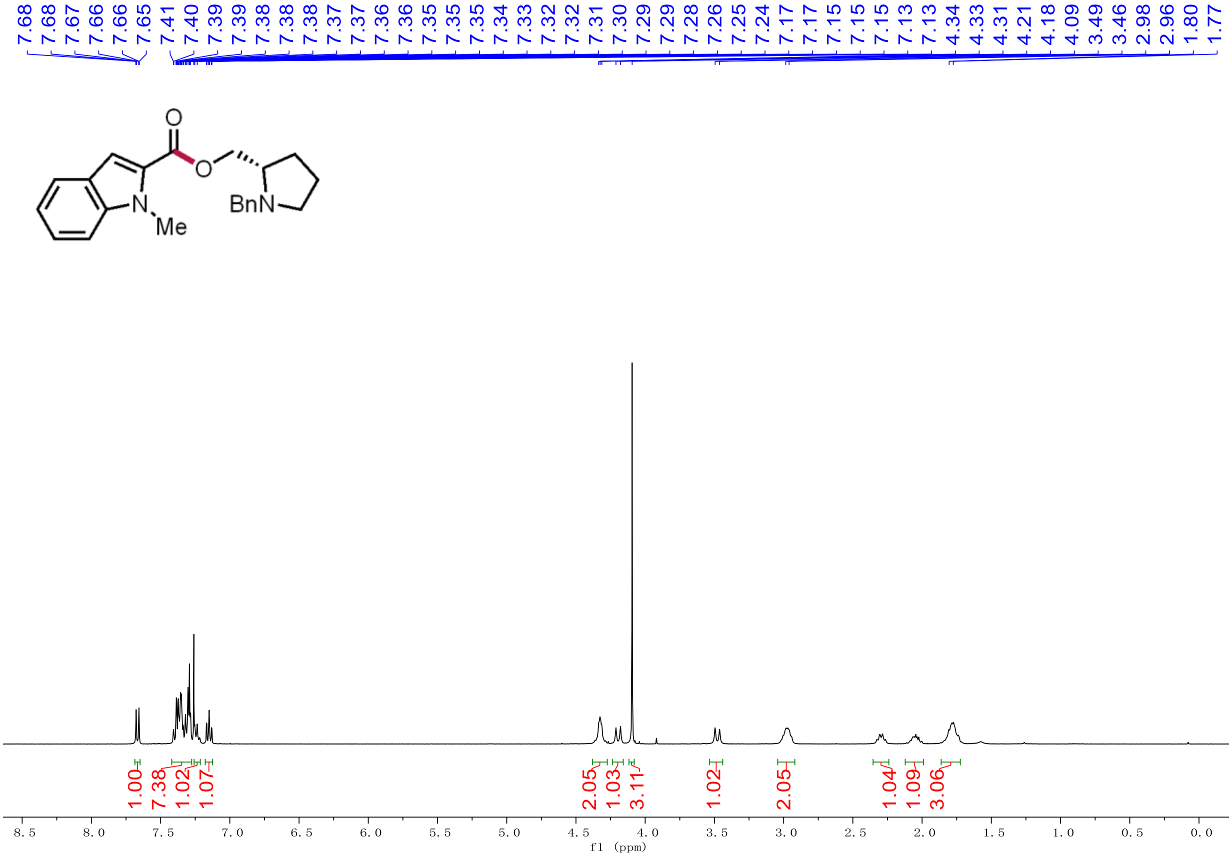
7: 3-Phenylpropyl 1-methyl-1*H*-indole-2-carboxylate (^{1}H NMR, $CDCl_3$, 400 MHz)



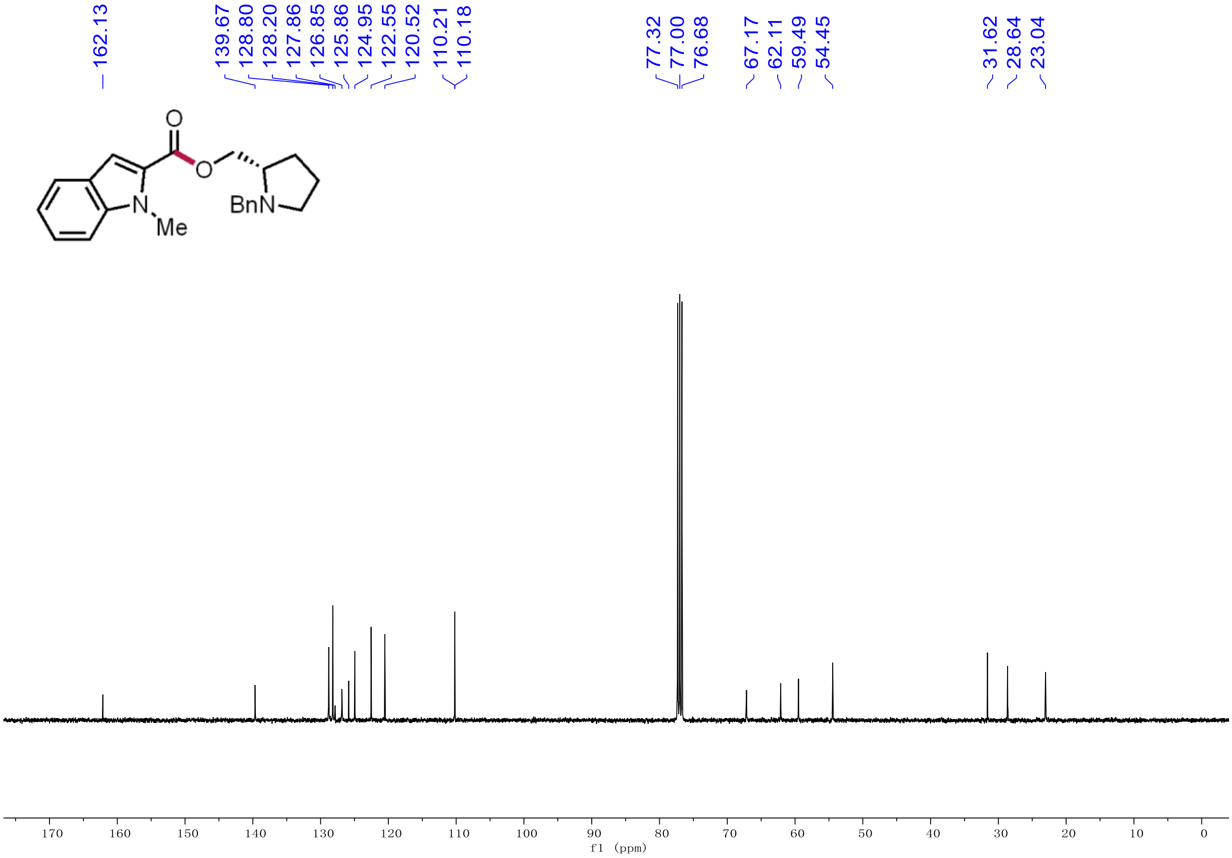
7: 3-Phenylpropyl 1-methyl-1*H*-indole-2-carboxylate (^{13}C NMR, $CDCl_3$, 100 MHz)



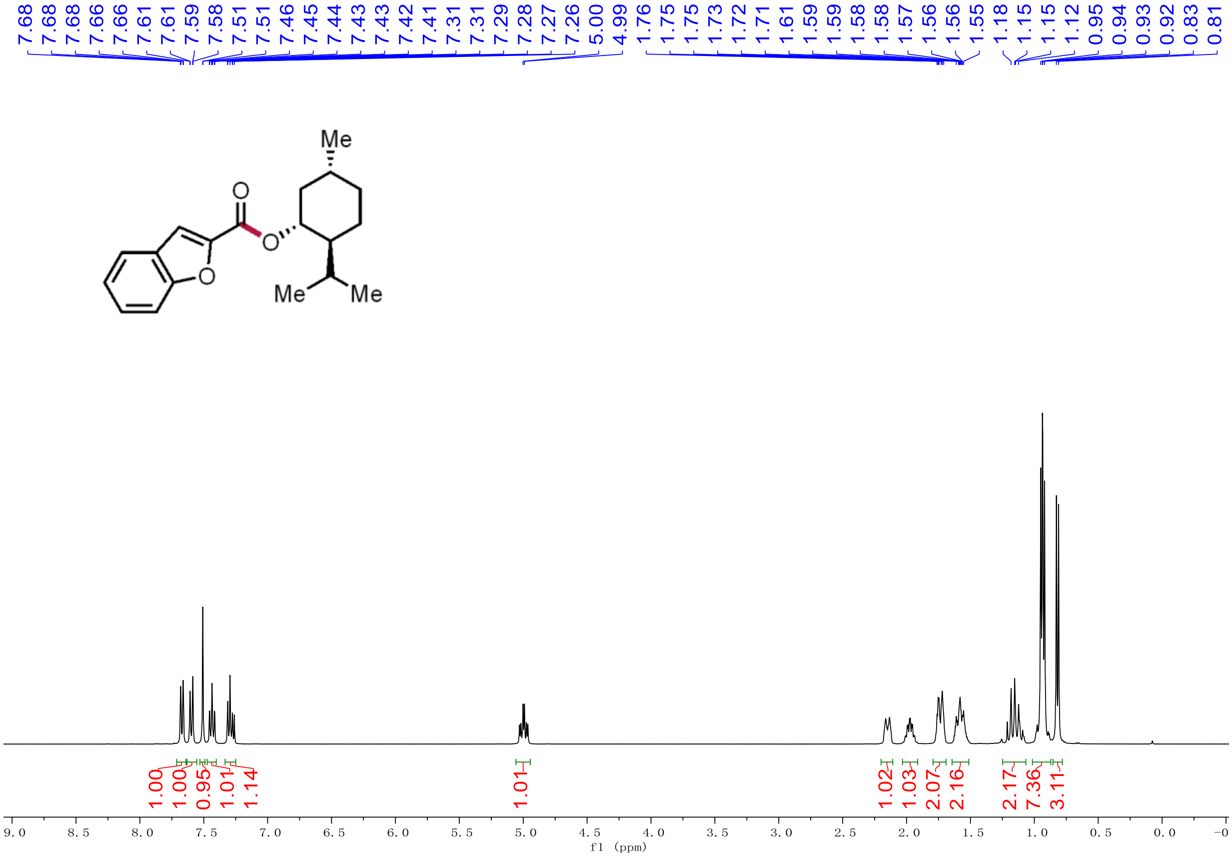
8: (*S*)-(1-Benzylpyrrolidin-2-yl)methyl 1-methyl-1*H*-indole-2-carboxylate (^{1}H NMR, $CDCl_3$, 400 MHz)



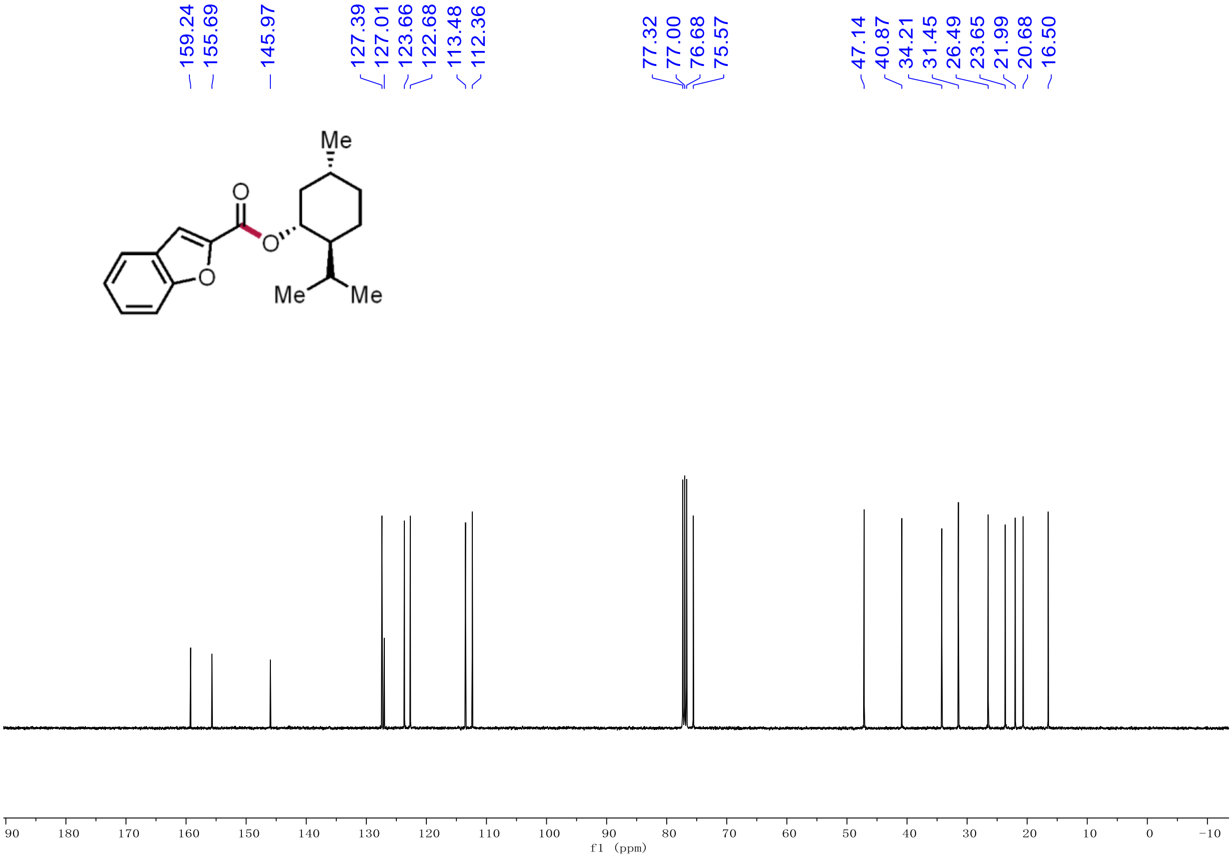
8: (*S*)-(1-Benzylpyrrolidin-2-yl)methyl 1-methyl-1*H*-indole-2-carboxylate (^{13}C NMR, $CDCl_3$, 100 MHz)



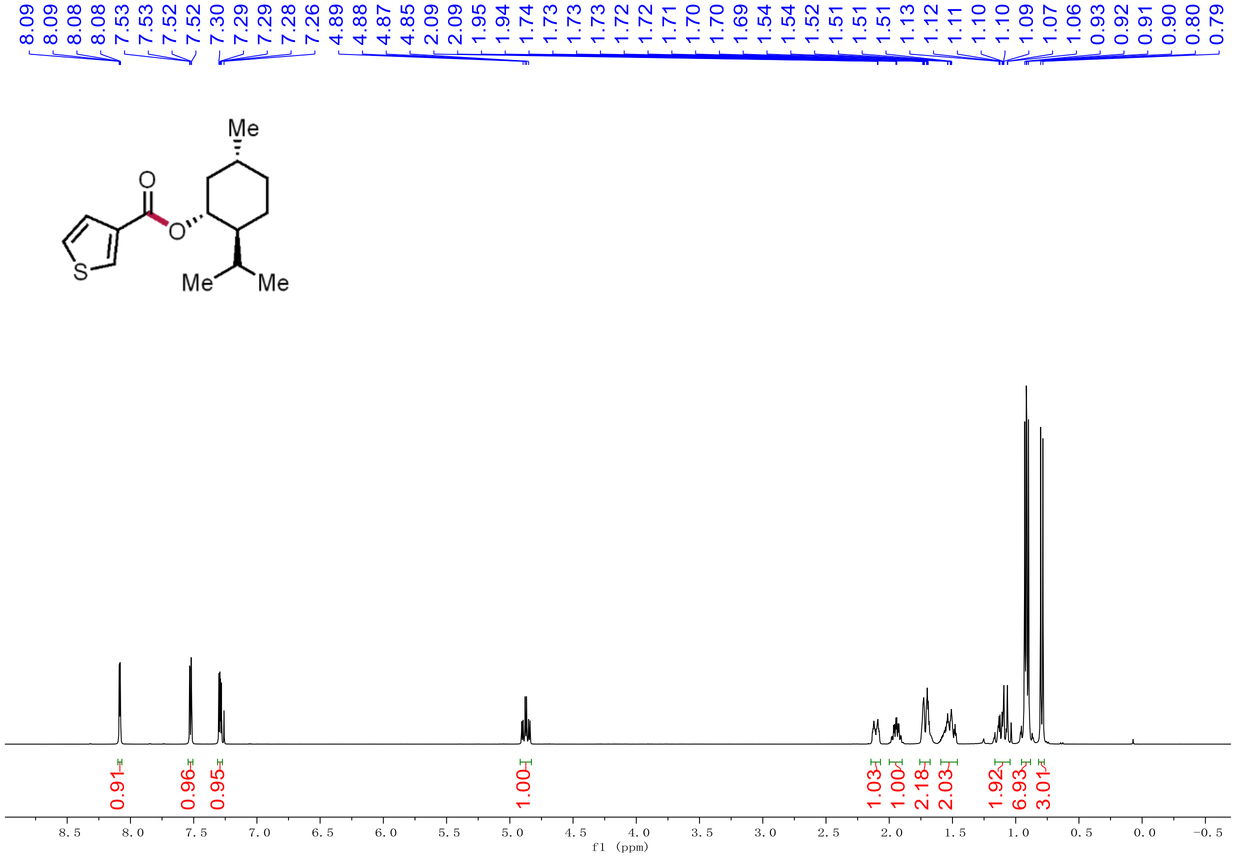
9: (1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl benzofuran-2-carboxylate (^{1}H NMR, CDCl$_3$, 400 MHz)



9: (1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl benzofuran-2-carboxylate (^{13}C NMR, CDCl$_3$, 100 MHz)

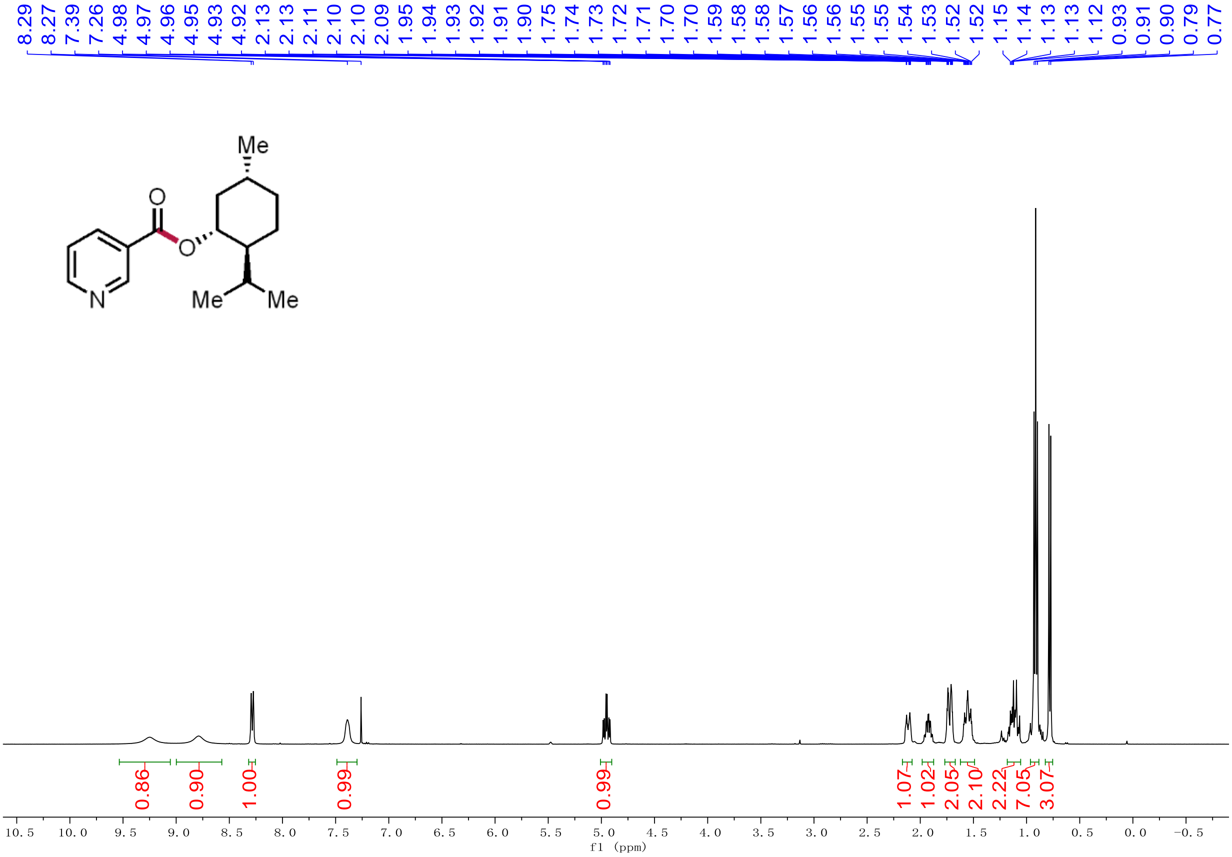


10: (1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl thiophene-3-carboxylate (^{1}H NMR, $CDCl_3$, 400 MHz)

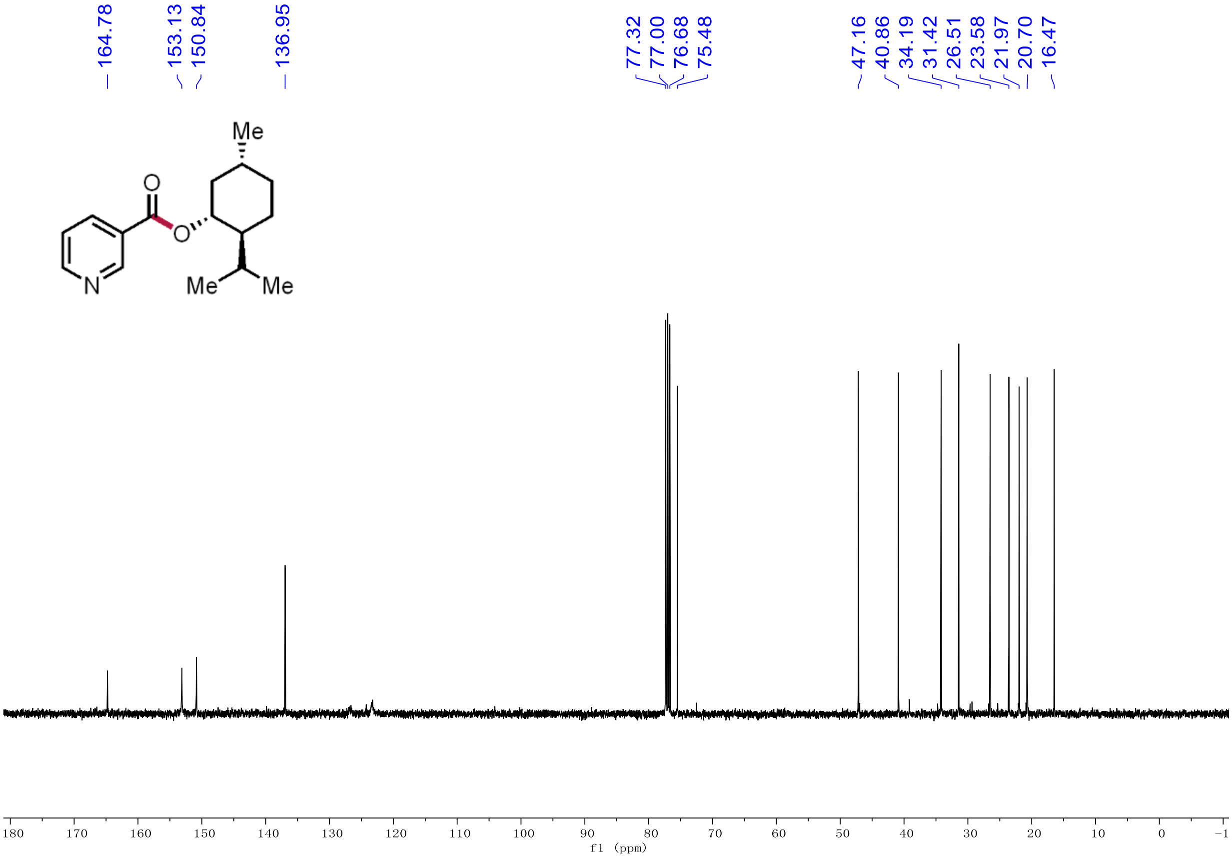


10: (1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl thiophene-3-carboxylat (^{13}C NMR, $CDCl_3$, 100 MHz)

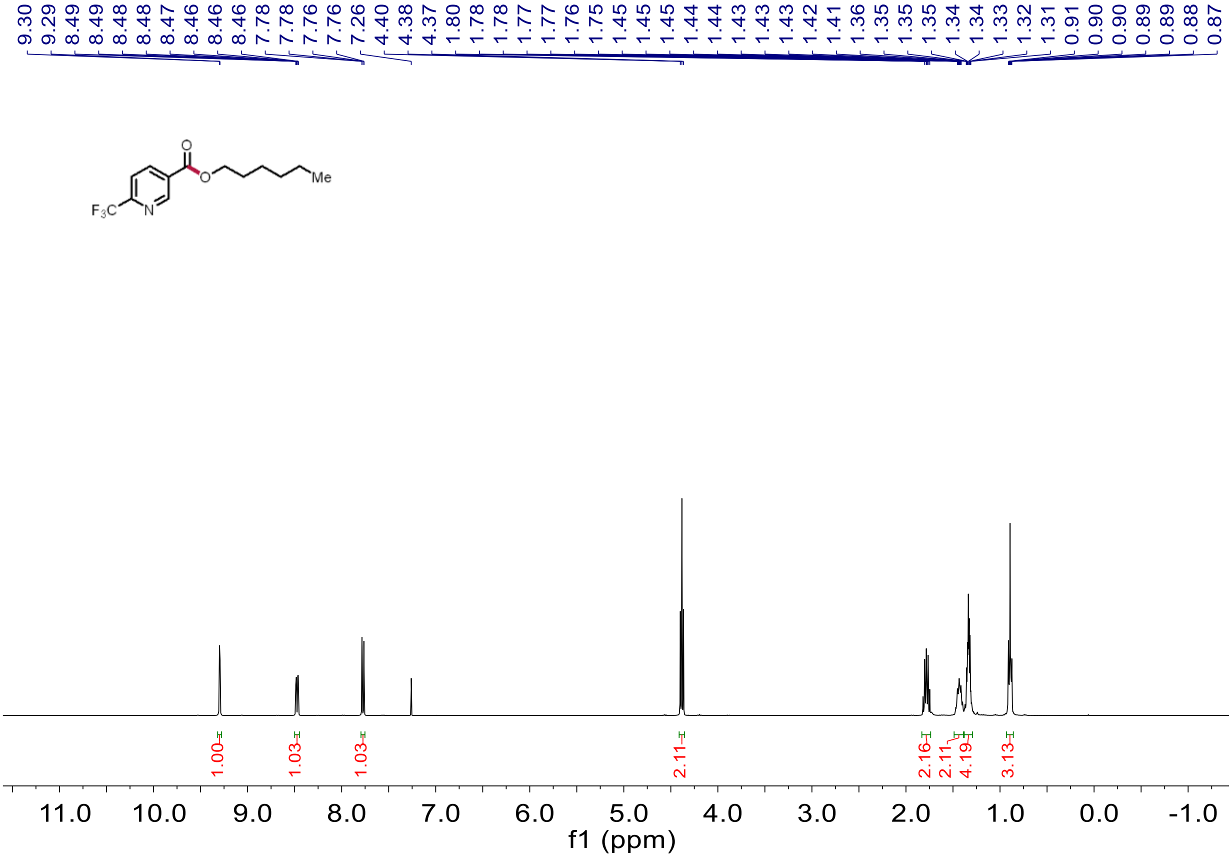
11: (1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl nicotinate (^{1}H NMR, CDCl$_3$, 400 MHz)



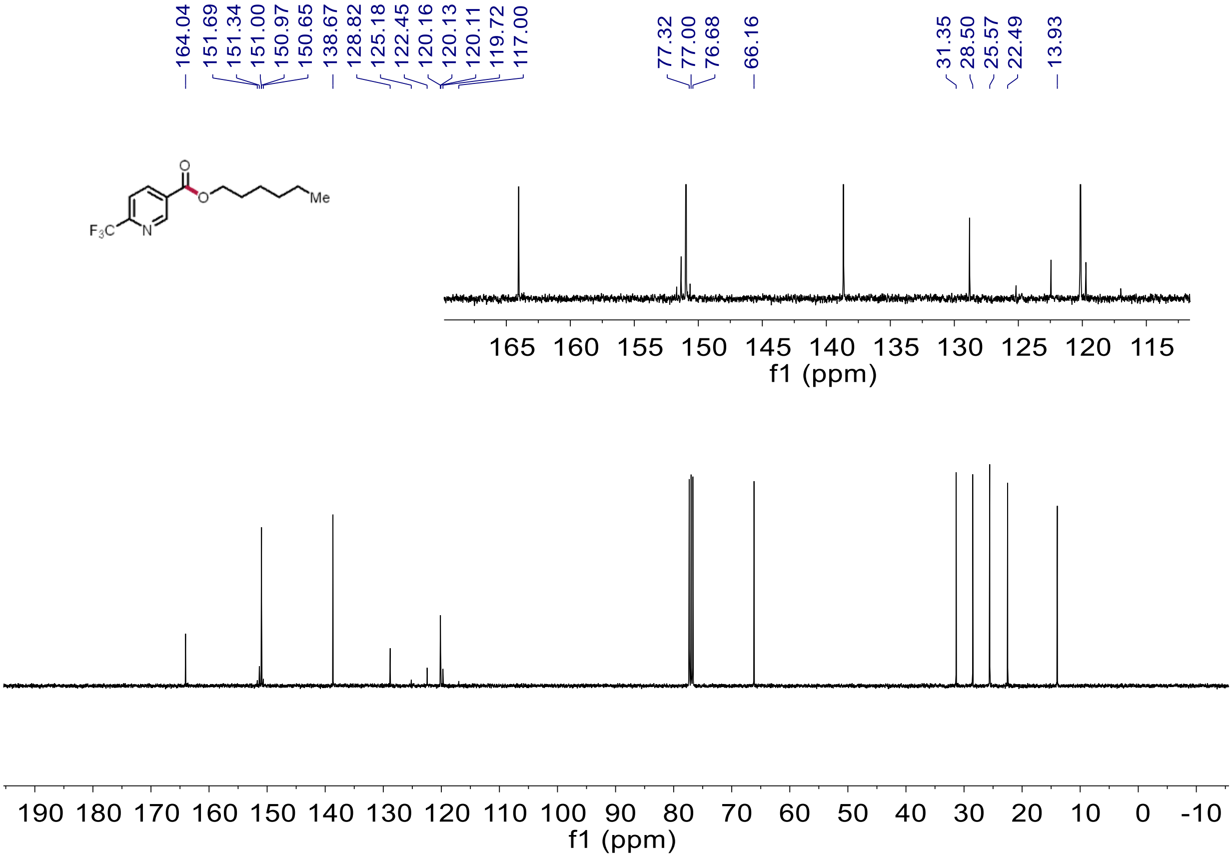
11: (1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl nicotinate (^{13}C NMR, CDCl$_3$, 100 MHz)



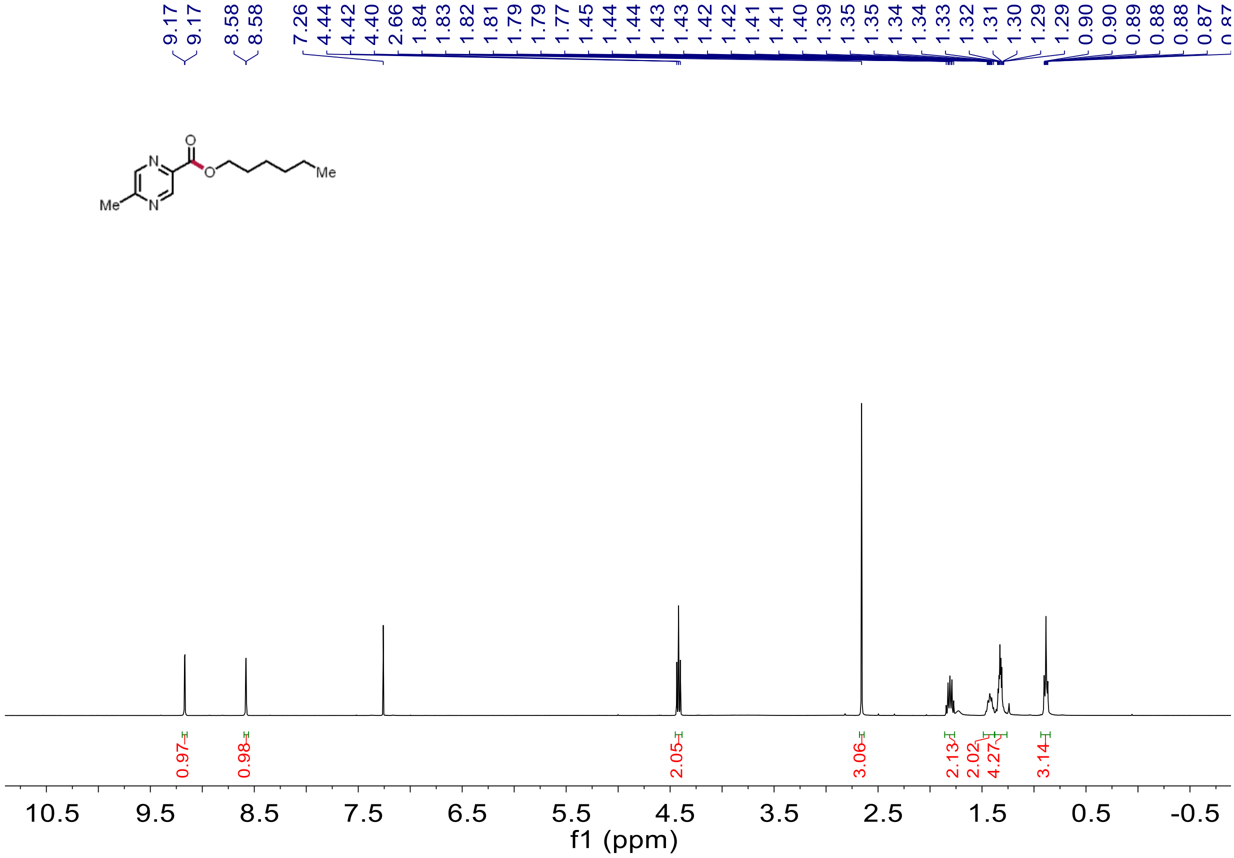
12: Hexyl 6-(trifluoromethyl)nicotinate (^{1}H NMR, CDCl$_3$, 400 MHz)



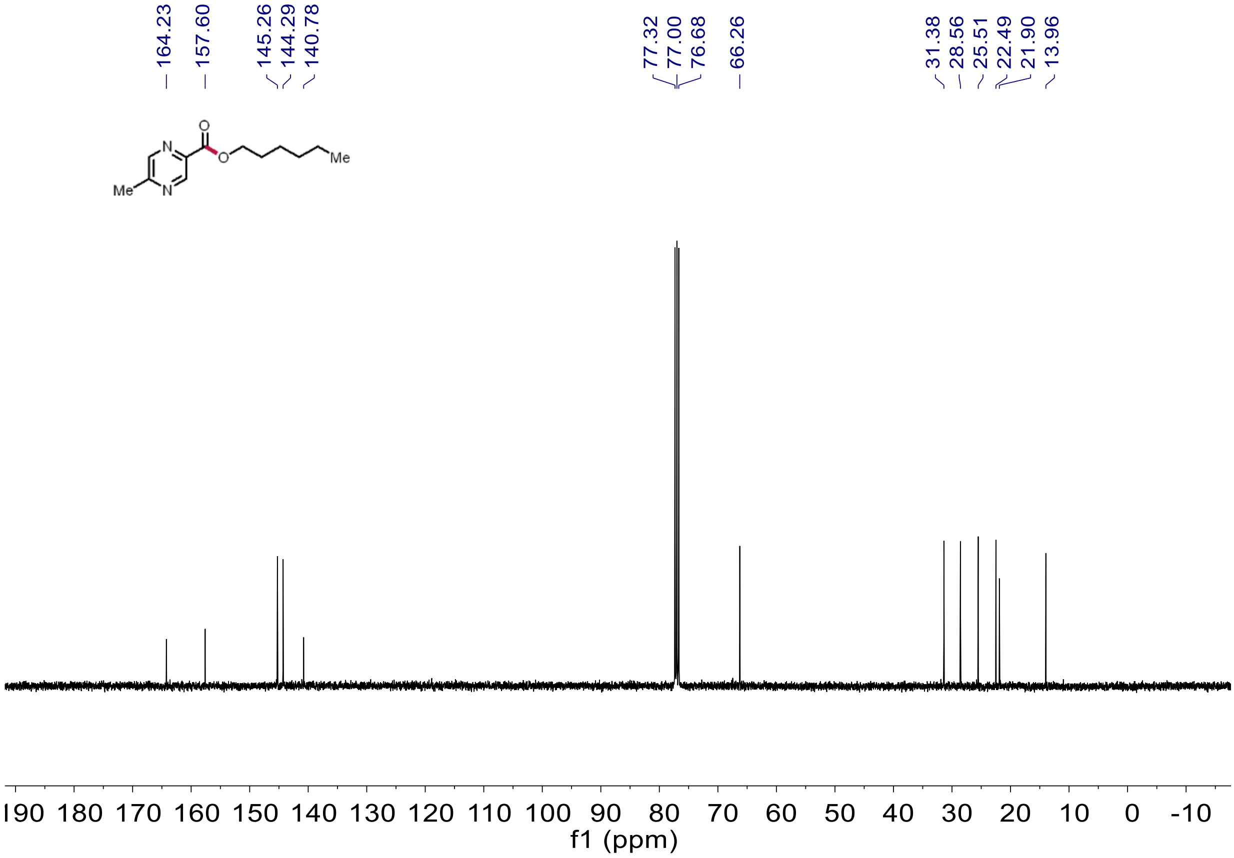
12: Hexyl 6-(trifluoromethyl)nicotinate (^{13}C NMR, CDCl$_{3,}$ 100 MHz)



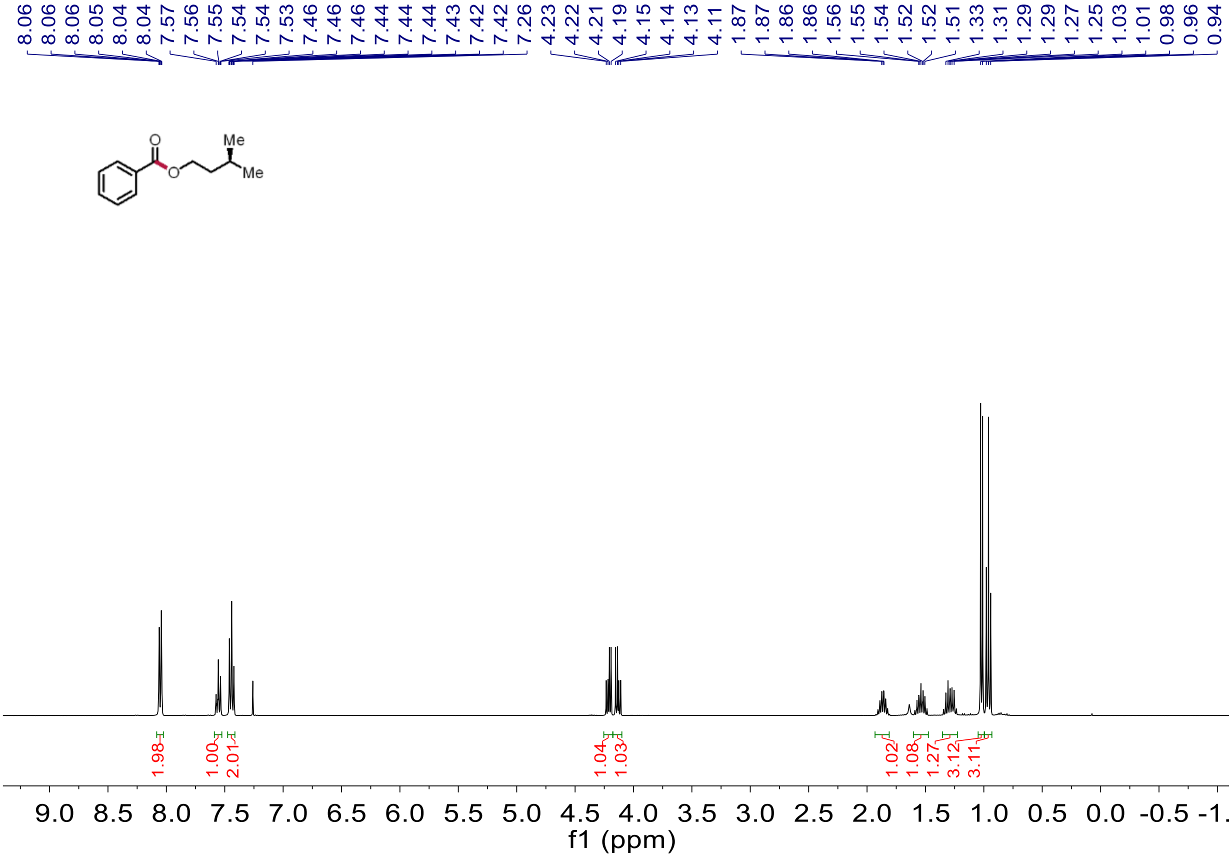
13: Hexyl 5-methylpyrazine-2-carboxylate (^{1}H NMR, $CDCl_3$, 400 MHz)



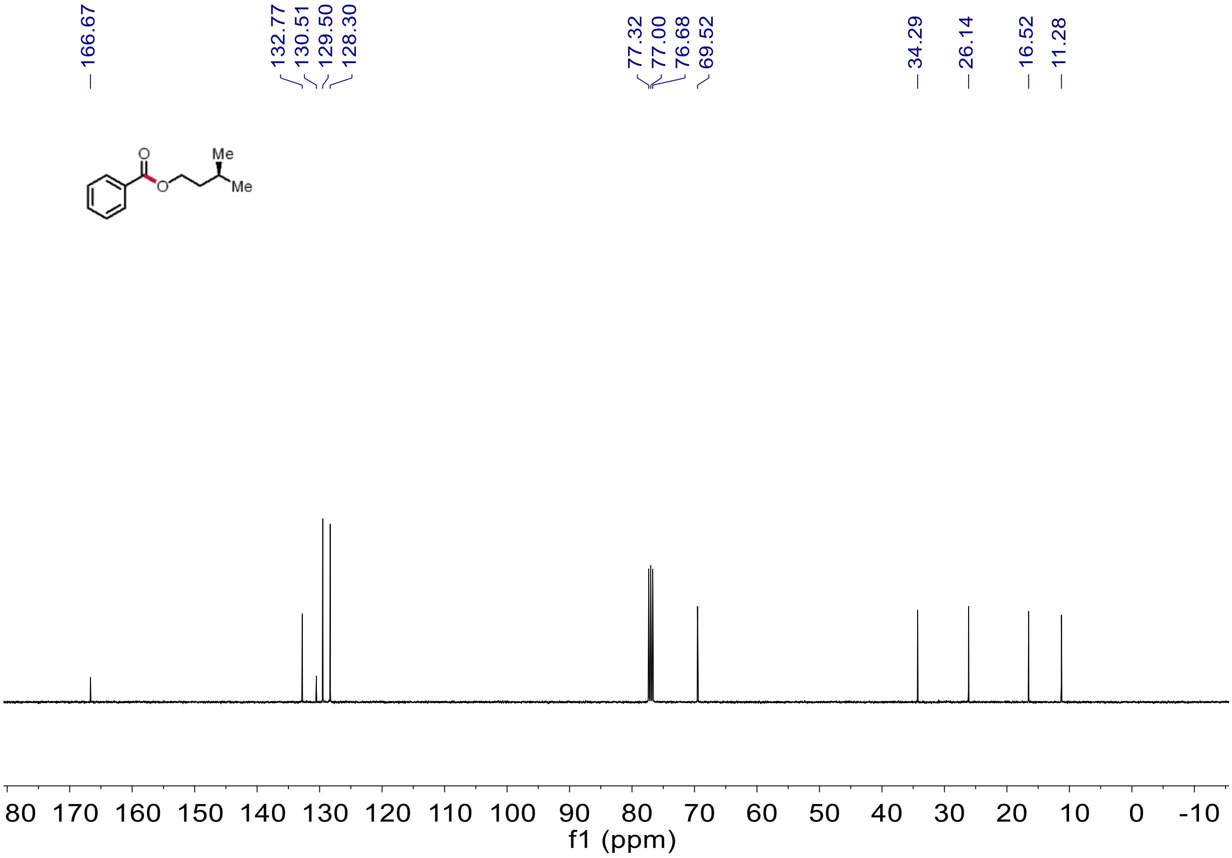
13: Hexyl 5-methylpyrazine-2-carboxylate (^{13}C NMR, $CDCl_3$, 100 MHz)



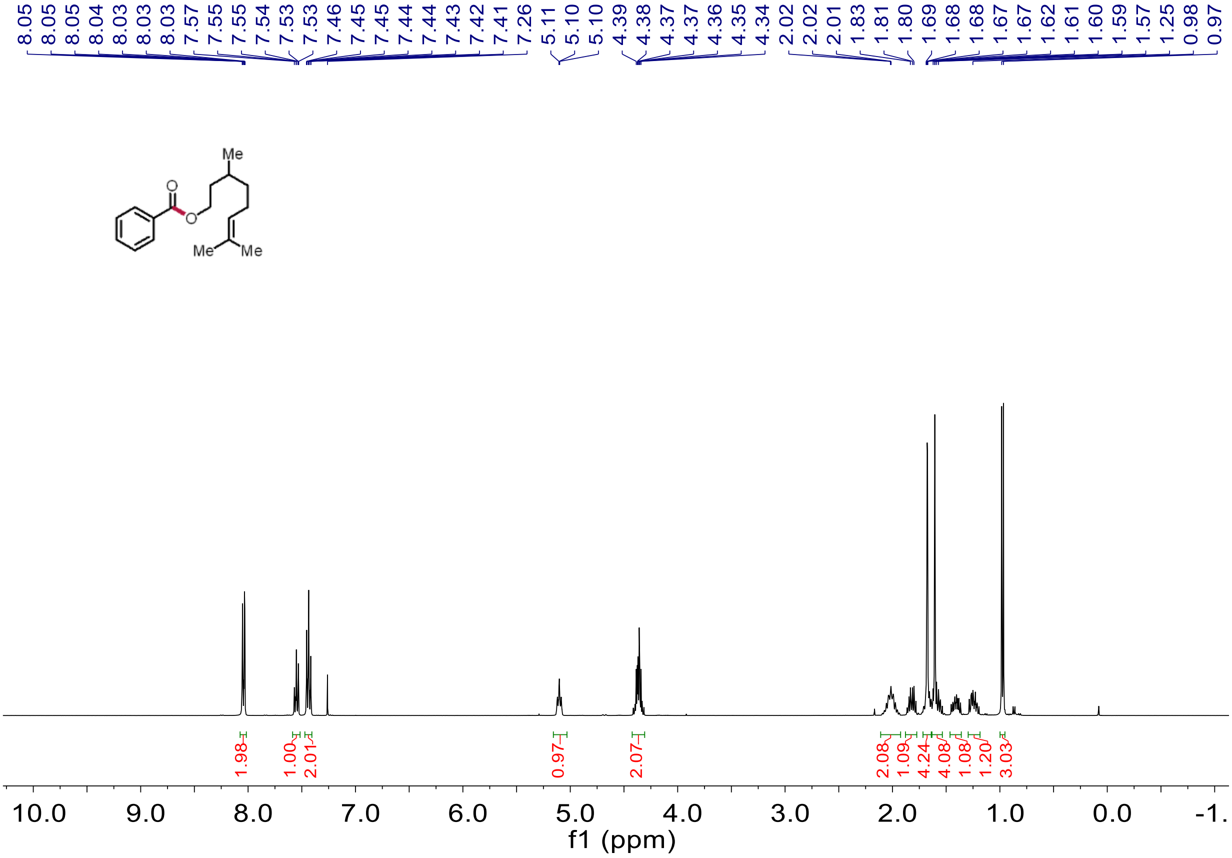
14: Isopentyl benzoate (^{1}H NMR, CDCl$_3$, 400 MHz)



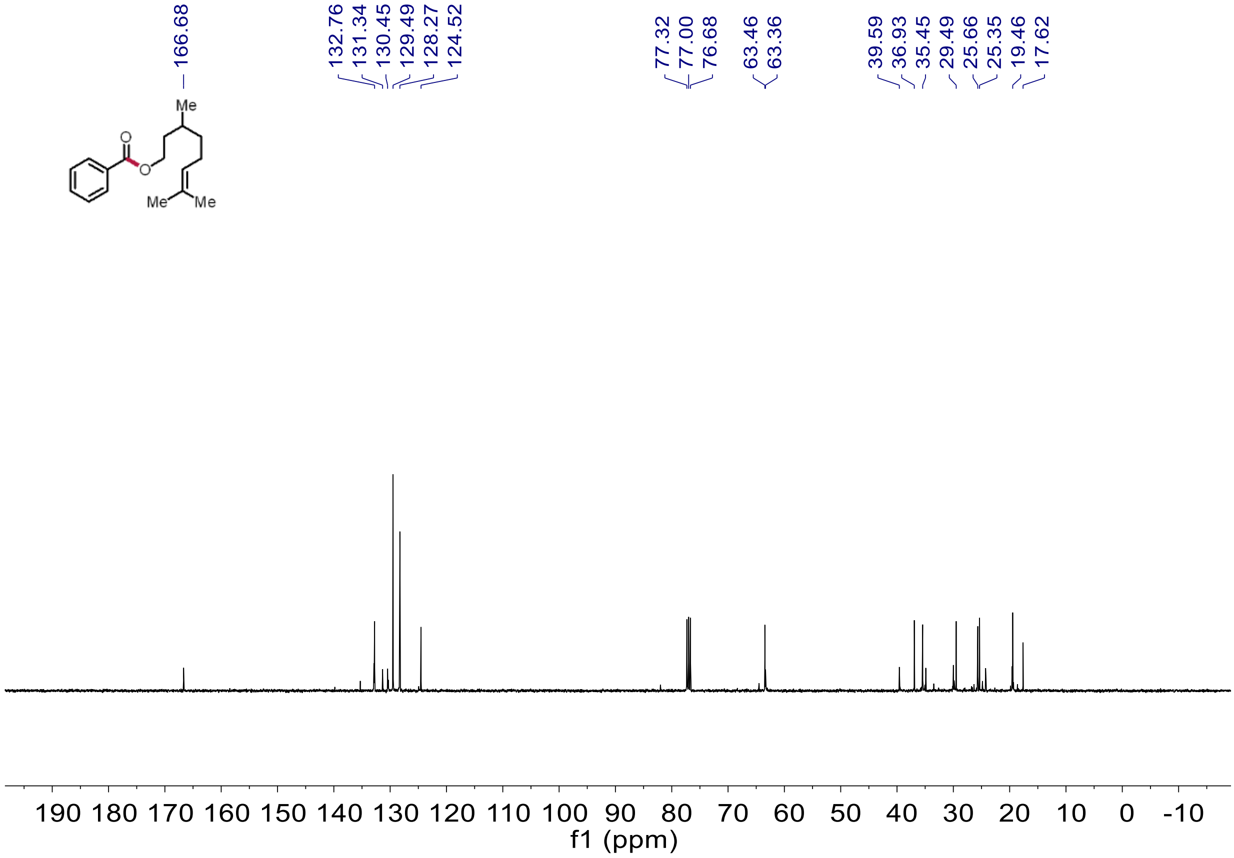
14: Isopentyl benzoate (^{13}C NMR, CDCl$_3$, 100 MHz)



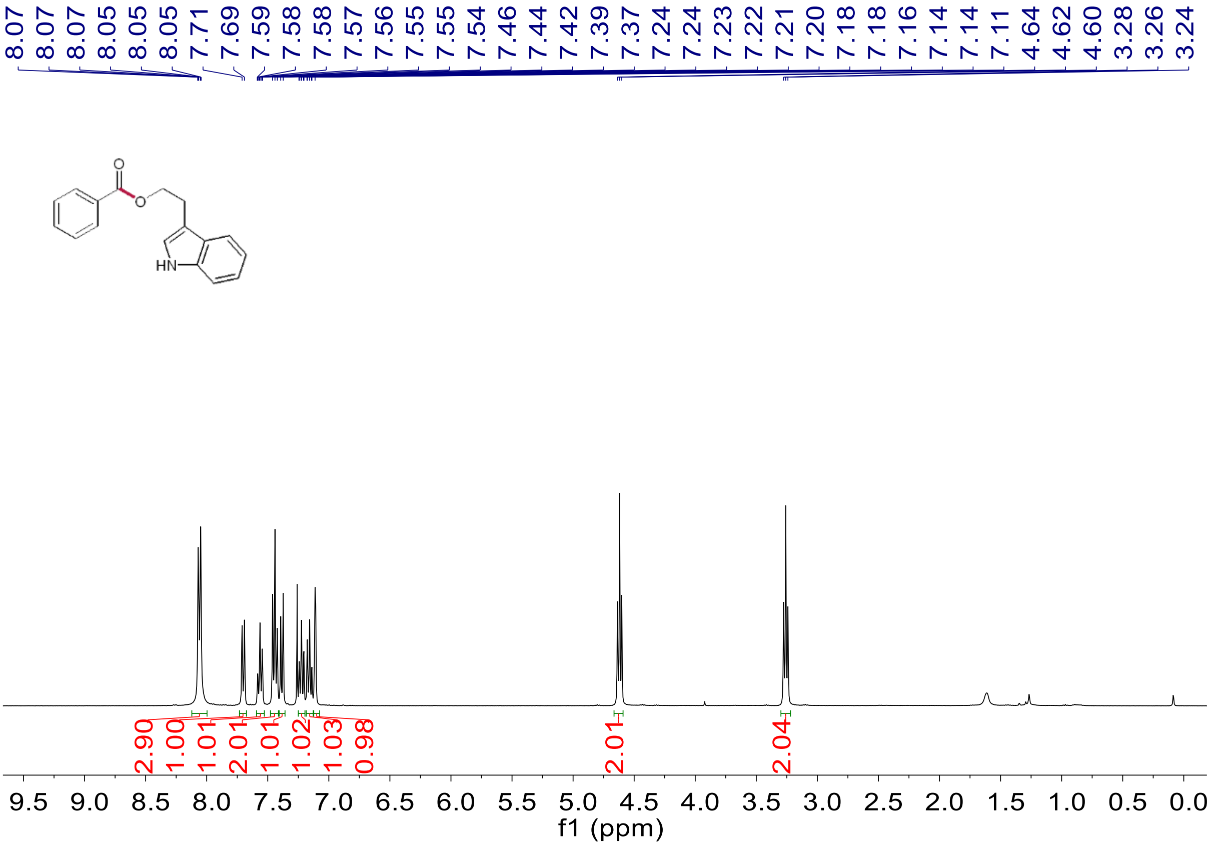
15: 3,7-Dimethyloct-6-en-1-yl benzoate (^{1}H NMR, CDCl$_3$, 400 MHz)



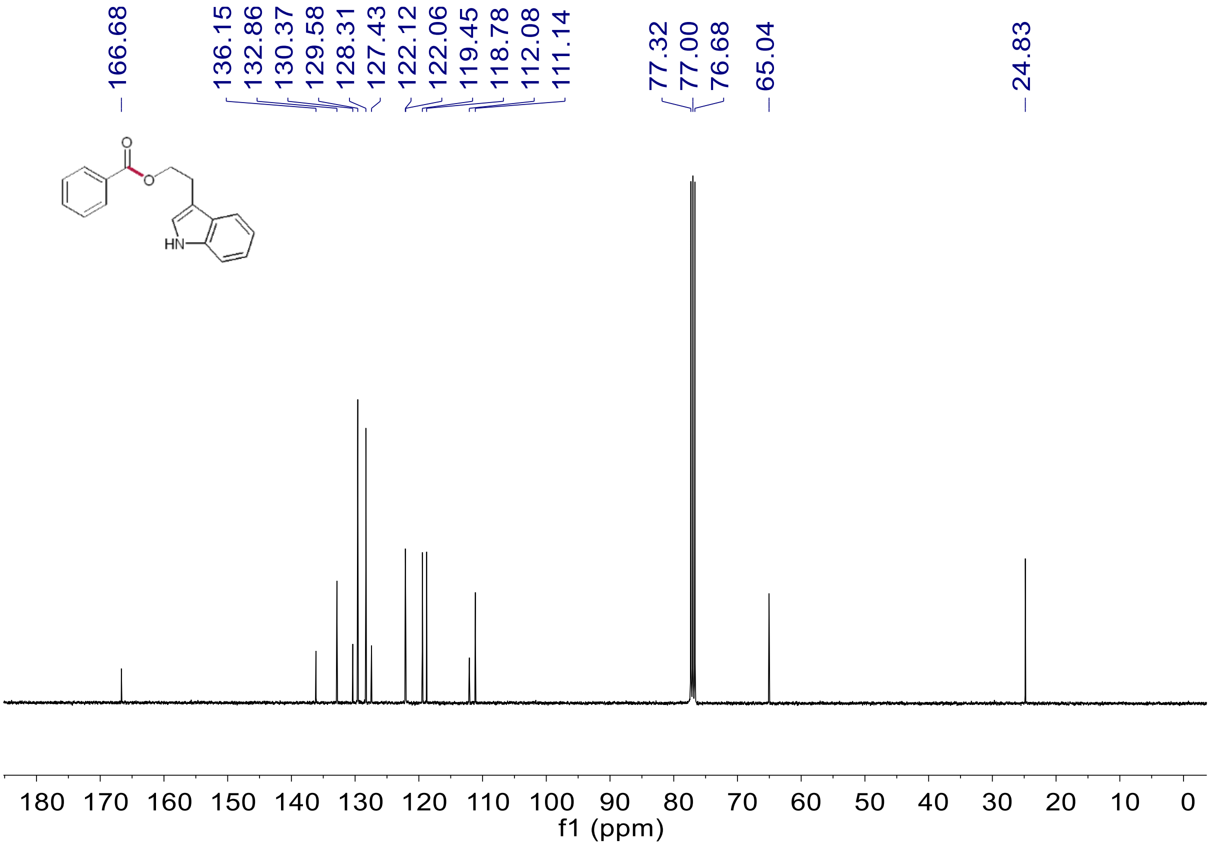
15: 3,7-Dimethyloct-6-en-1-yl benzoate (^{13}C NMR, CDCl$_3$, 100 MHz)



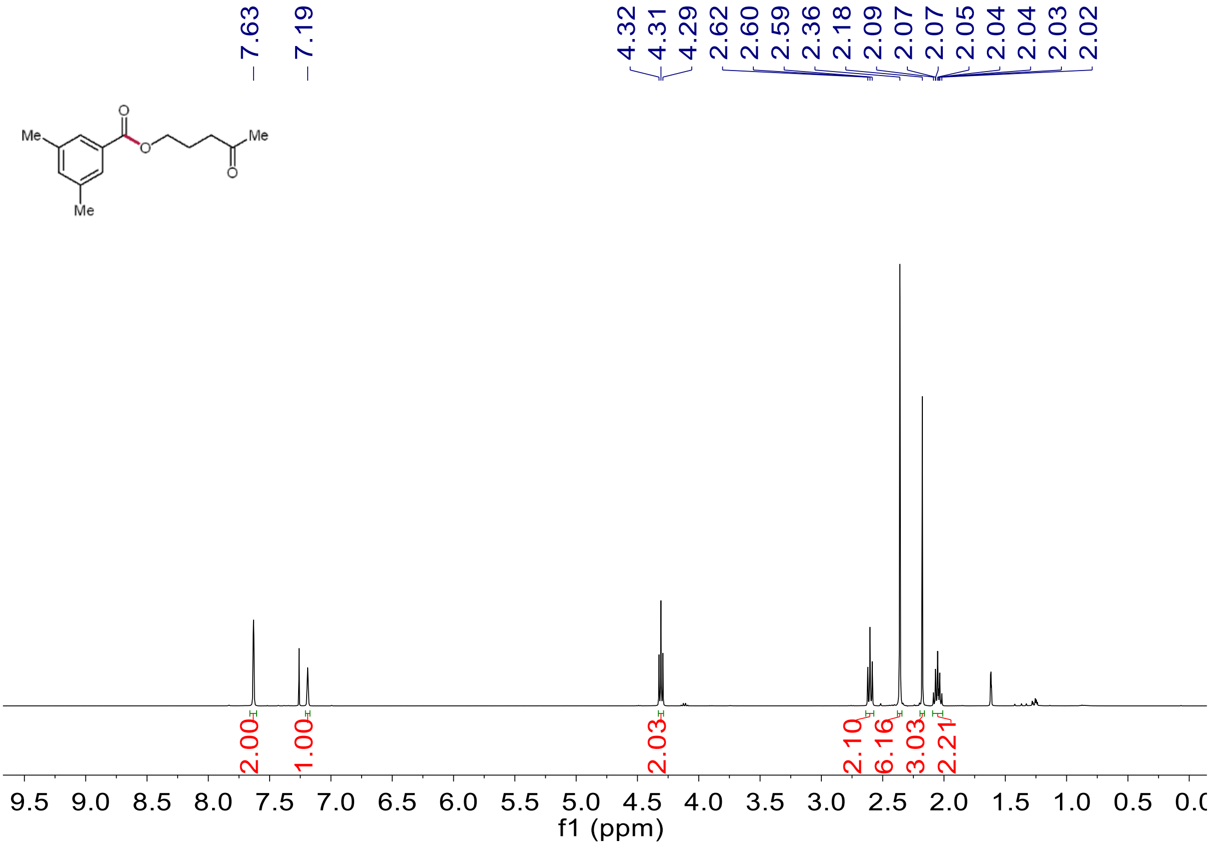
16: 2-(1H-Indol-3-yl)ethyl benzoate (^{1}H NMR, CDCl$_3$, 400 MHz)



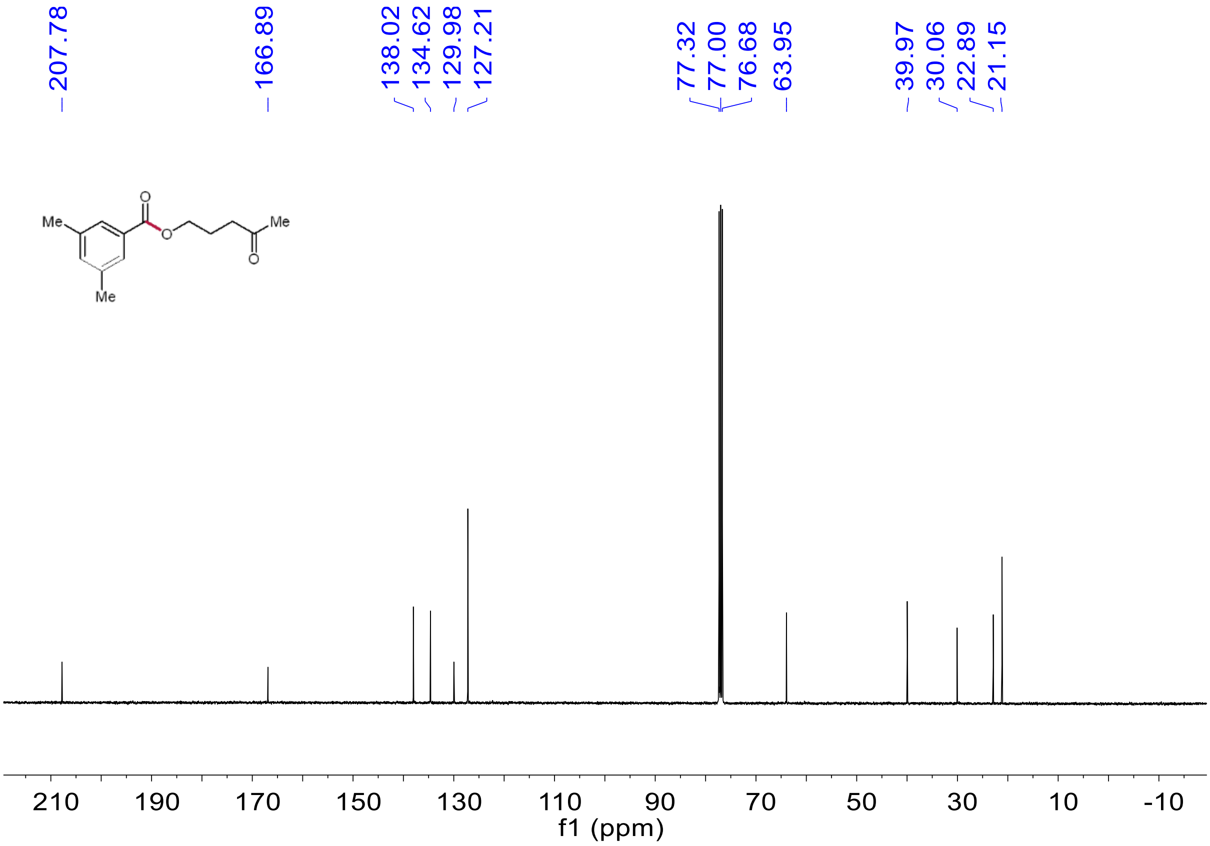
16: 2-(1H-Indol-3-yl)ethyl benzoate (^{13}C NMR, CDCl$_3$, 100 MHz)



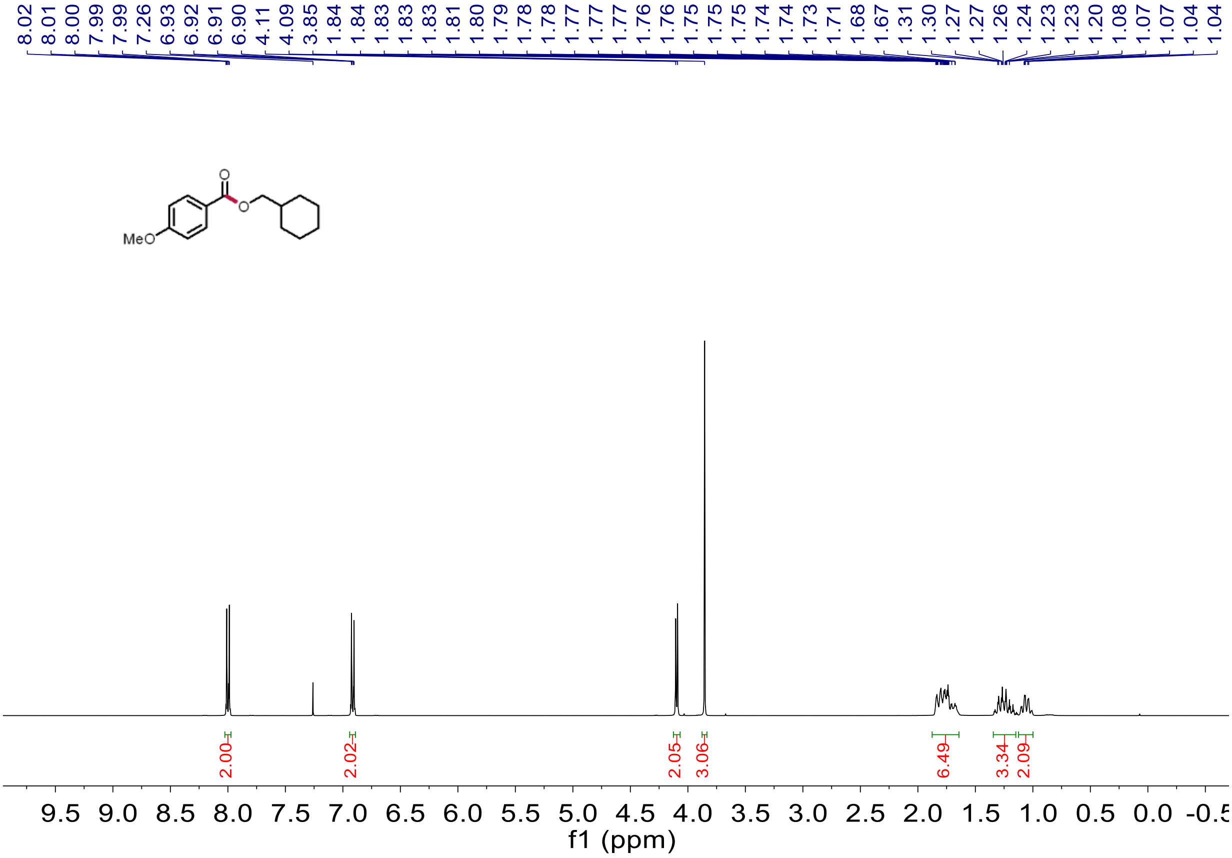
17: 4-Oxopentyl 3,5-dimethylbenzoate (^{1}H NMR, CDCl$_3$, 400 MHz)



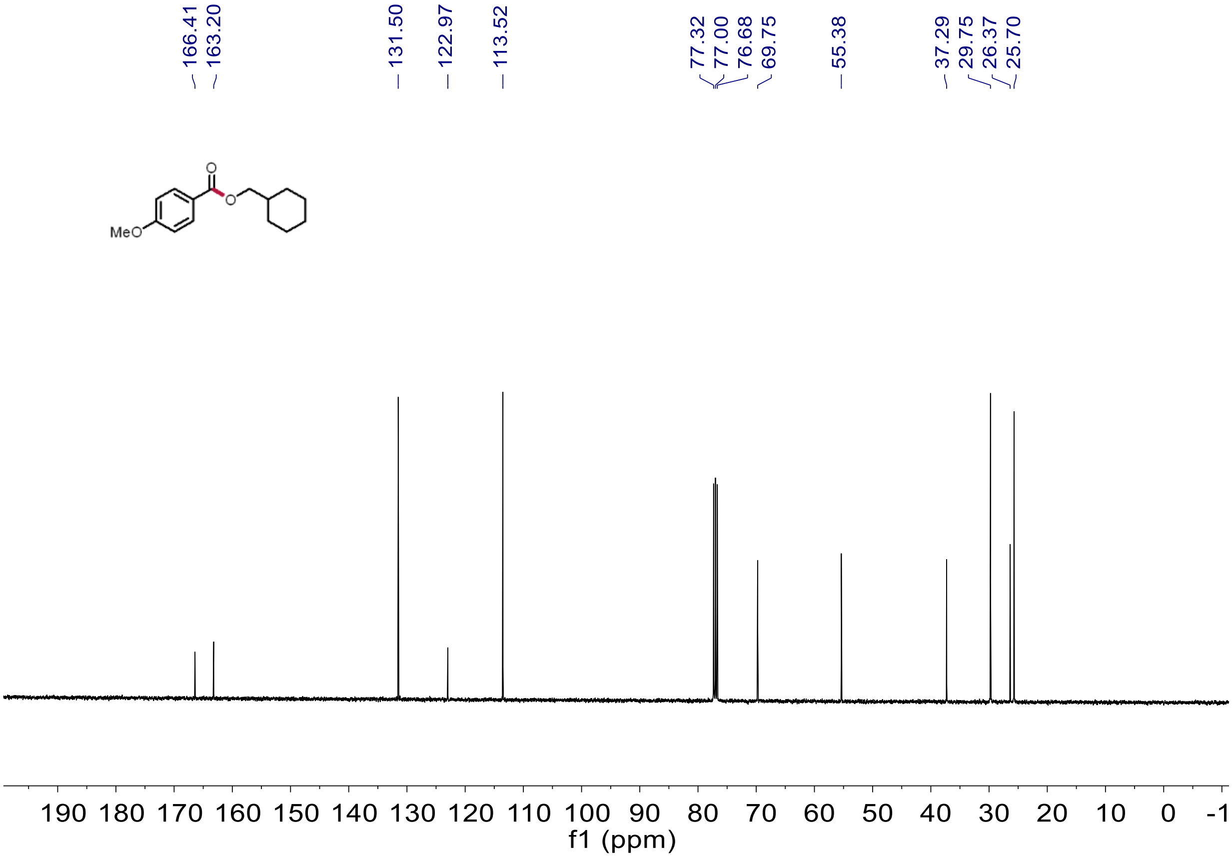
17: 4-Oxopentyl 3,5-dimethylbenzoate (^{13}C NMR, CDCl$_3$, 100 MHz)



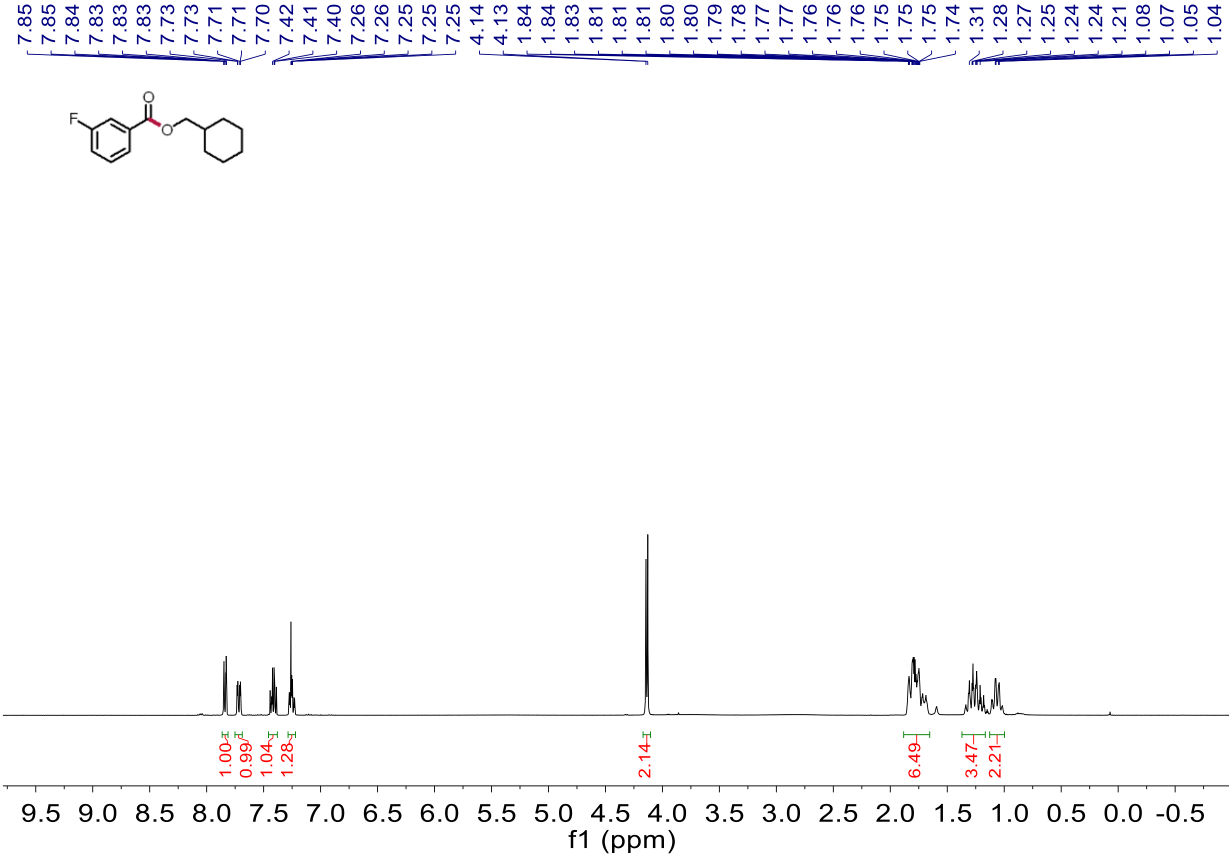
18: Cyclohexylmethyl 4-methoxybenzoate (^{1}H NMR, CDCl$_3$, 400 MHz)



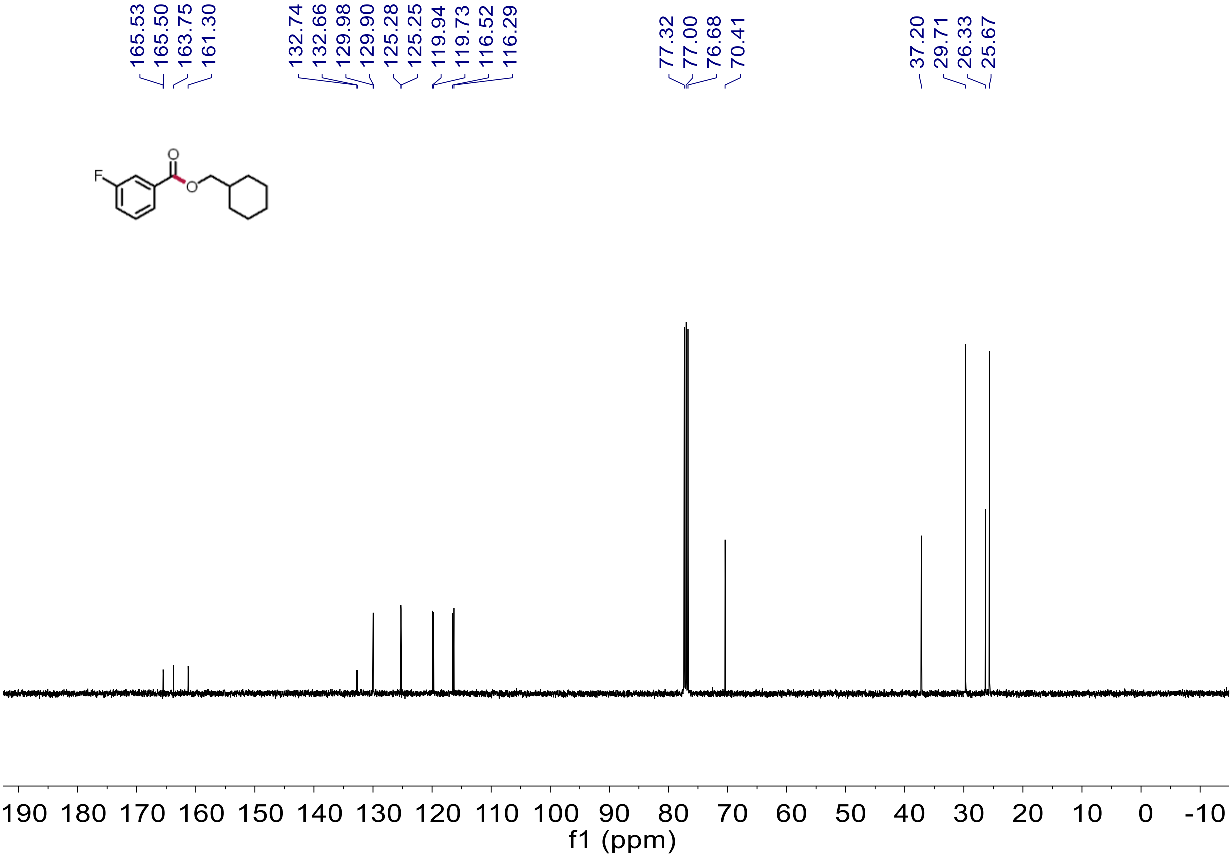
18: Cyclohexylmethyl 4-methoxybenzoate (^{13}C NMR, CDCl$_3$, 100 MHz)



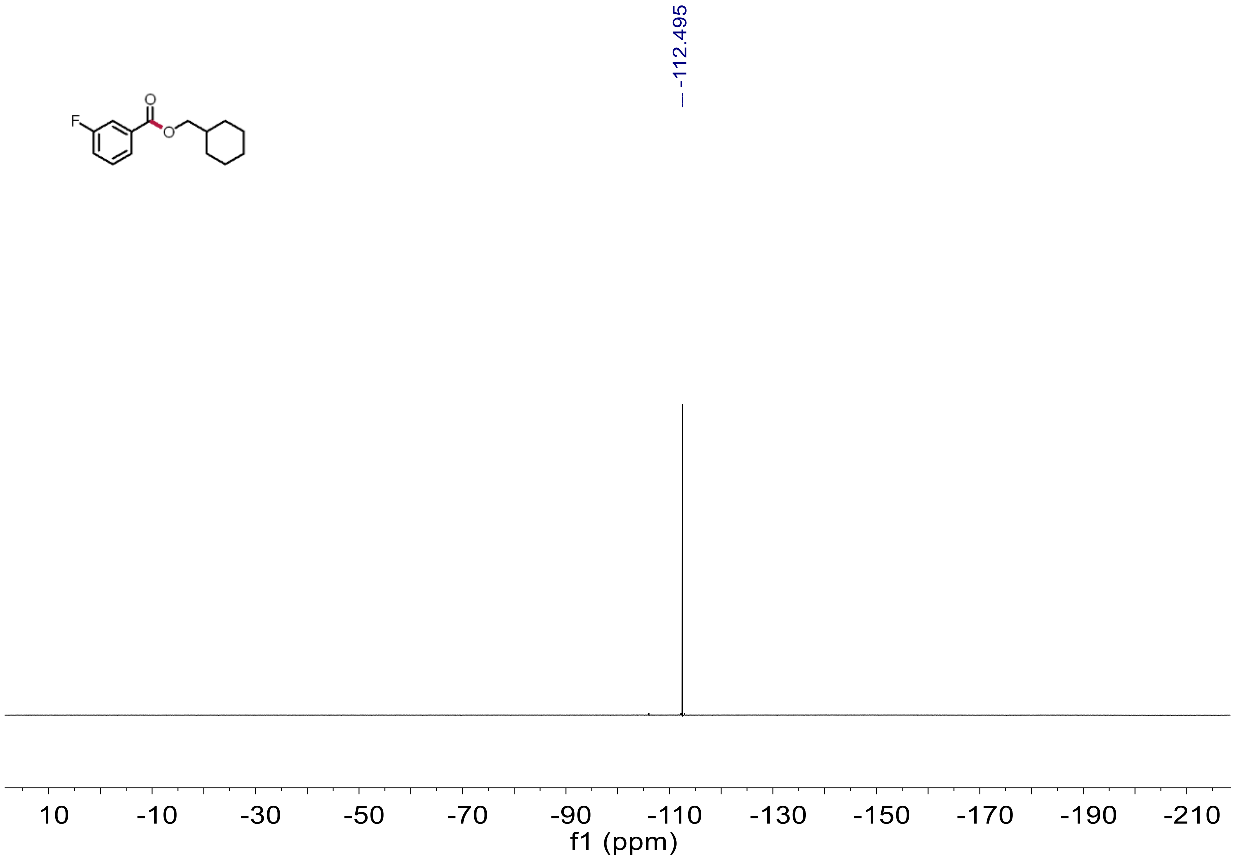
19: Cyclohexylmethyl 3-fluorobenzoate (^{1}H NMR, CDCl$_3$, 400 MHz)



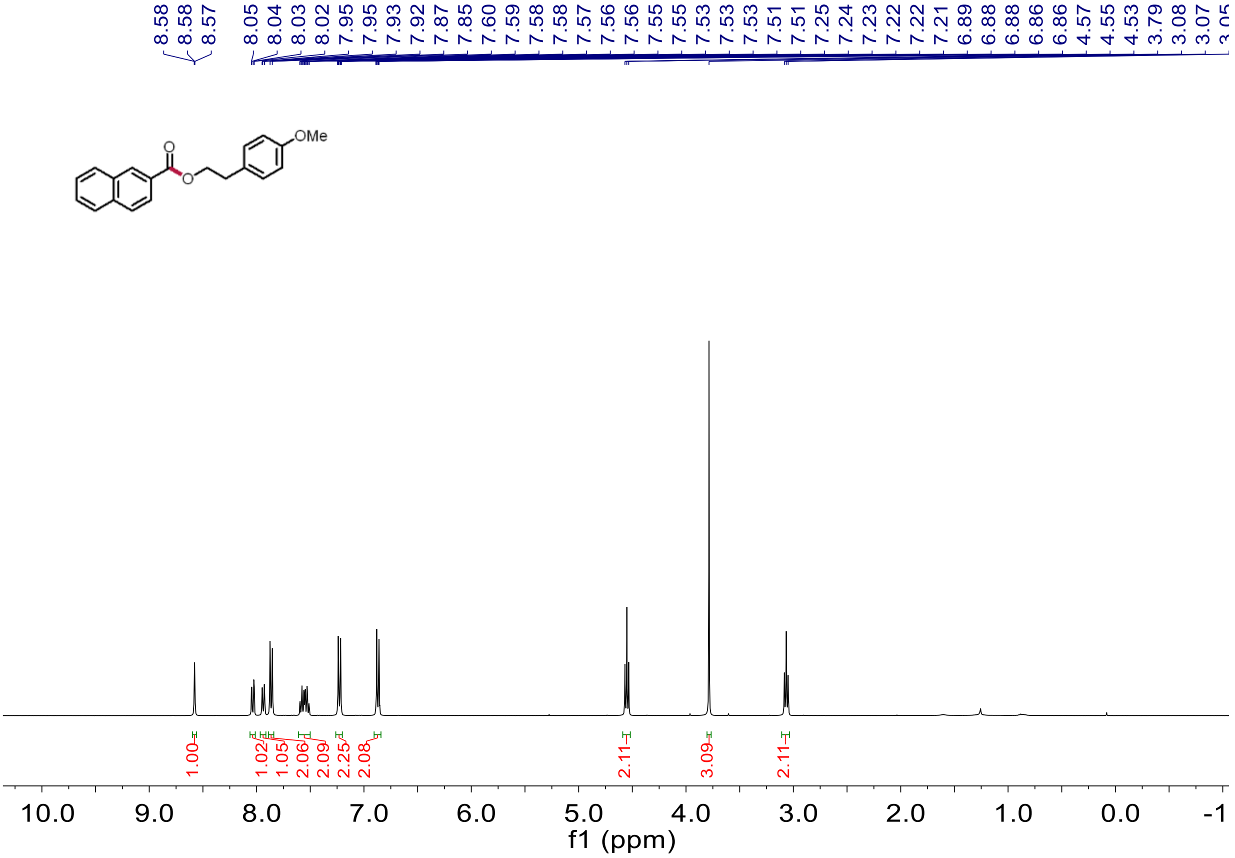
19: Cyclohexylmethyl 3-fluorobenzoate (^{13}C NMR, CDCl$_3$, 100 MHz)



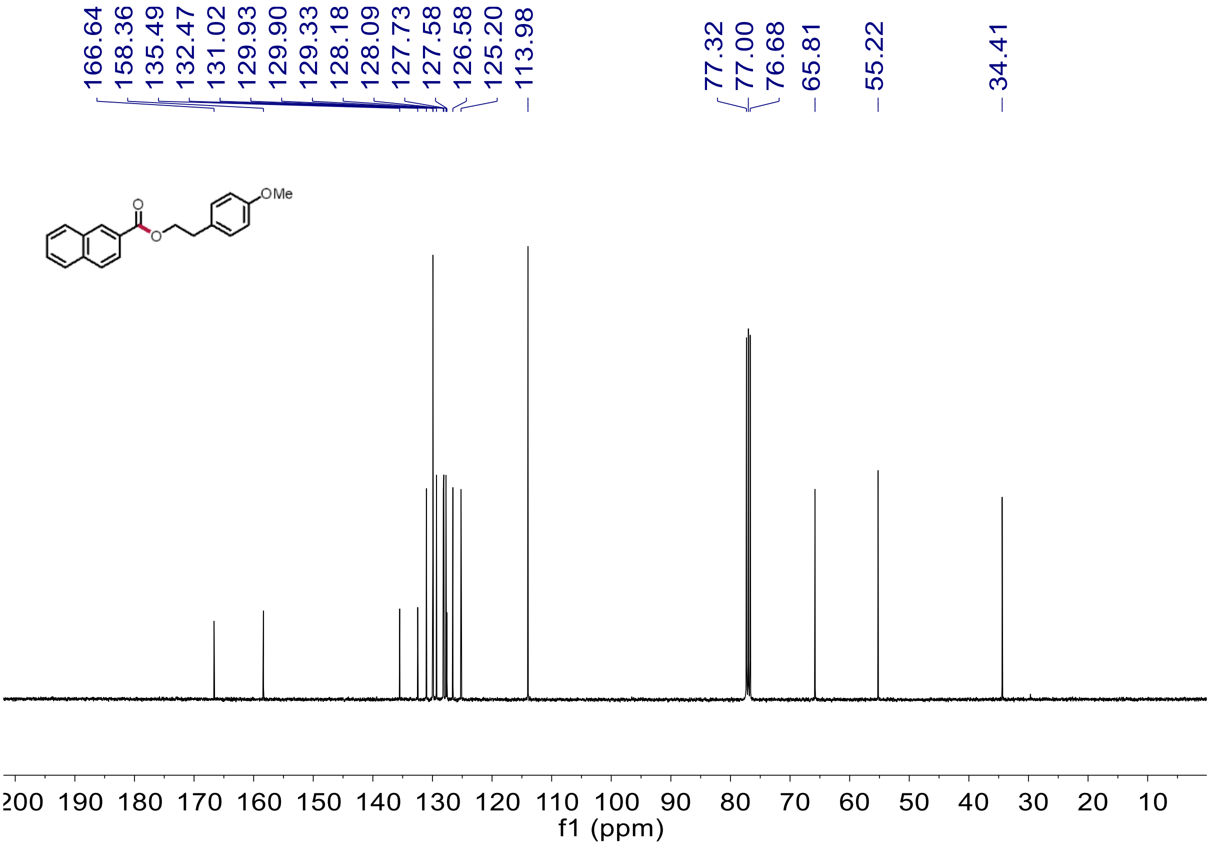
19: Cyclohexylmethyl 3-fluorobenzoate (^{19}F NMR, CDCl$_{3,}$ 377 MHz)



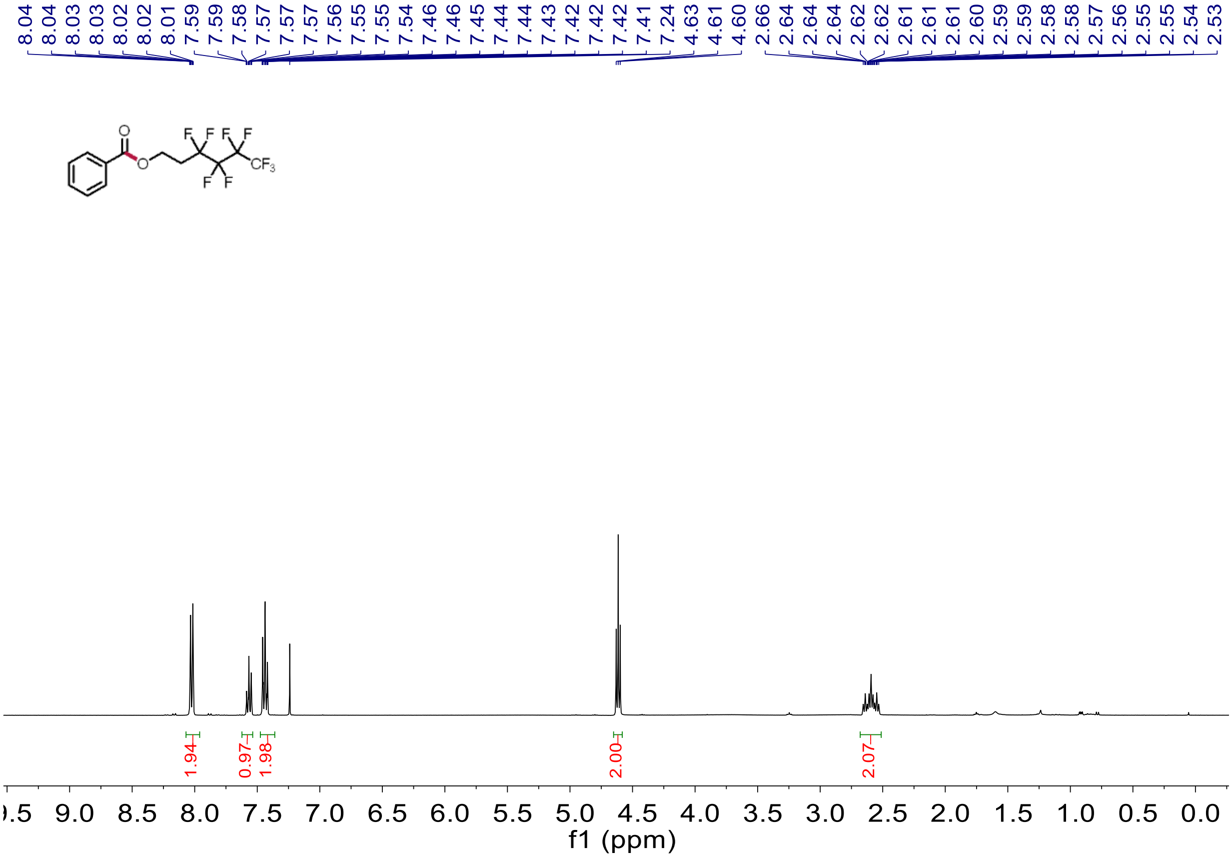
20: 4-Methoxyphenethyl 2-naphthoate (^{1}H NMR, CDCl$_3$, 400 MHz)



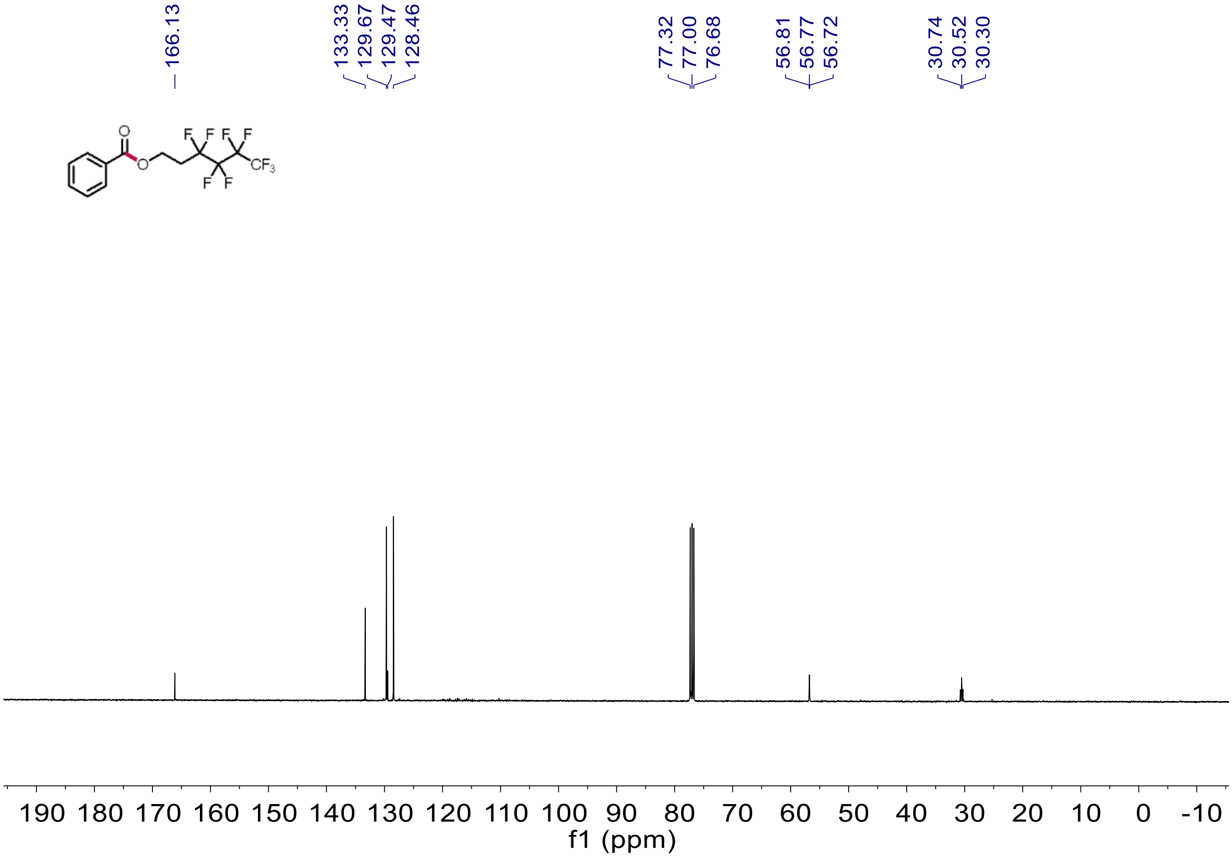
20: 4-Methoxyphenethyl 2-naphthoate (^{13}C NMR, CDCl$_3$, 100 MHz)



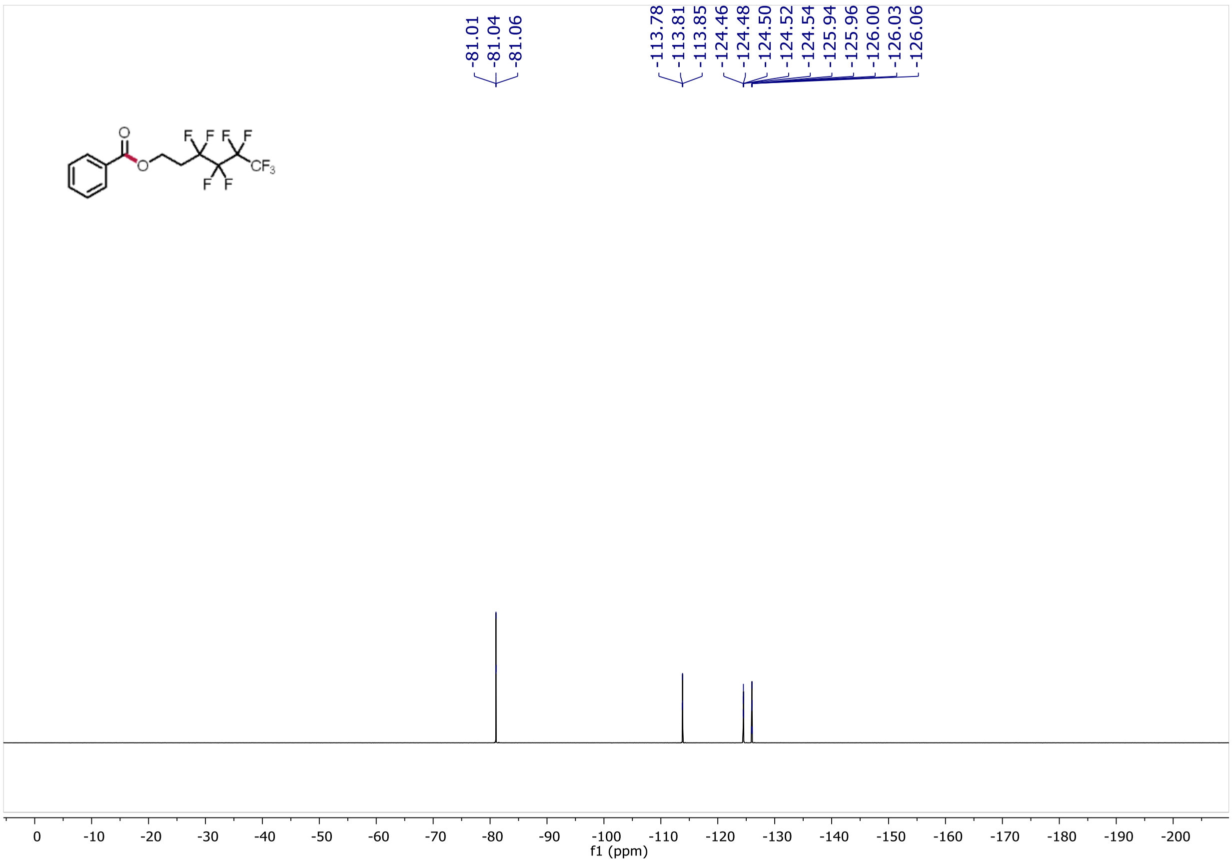
21: 3,3,4,4,5,5,6,6,6-Nonafluorohexyl benzoate (^{1}H NMR, $CDCl_3$, 400 MHz)



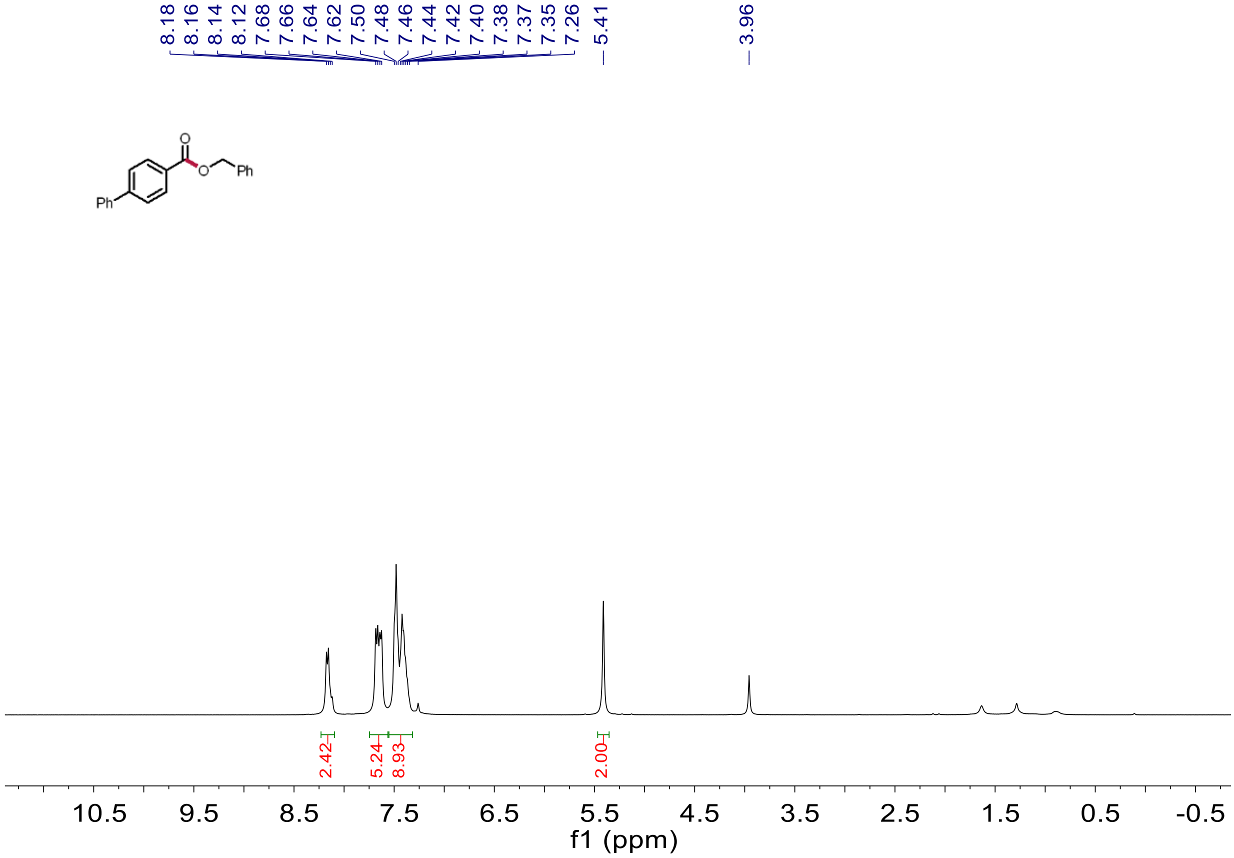
21: 3,3,4,4,5,5,6,6,6-Nonafluorohexyl benzoate (^{13}C NMR, $CDCl_3$, 100 MHz)



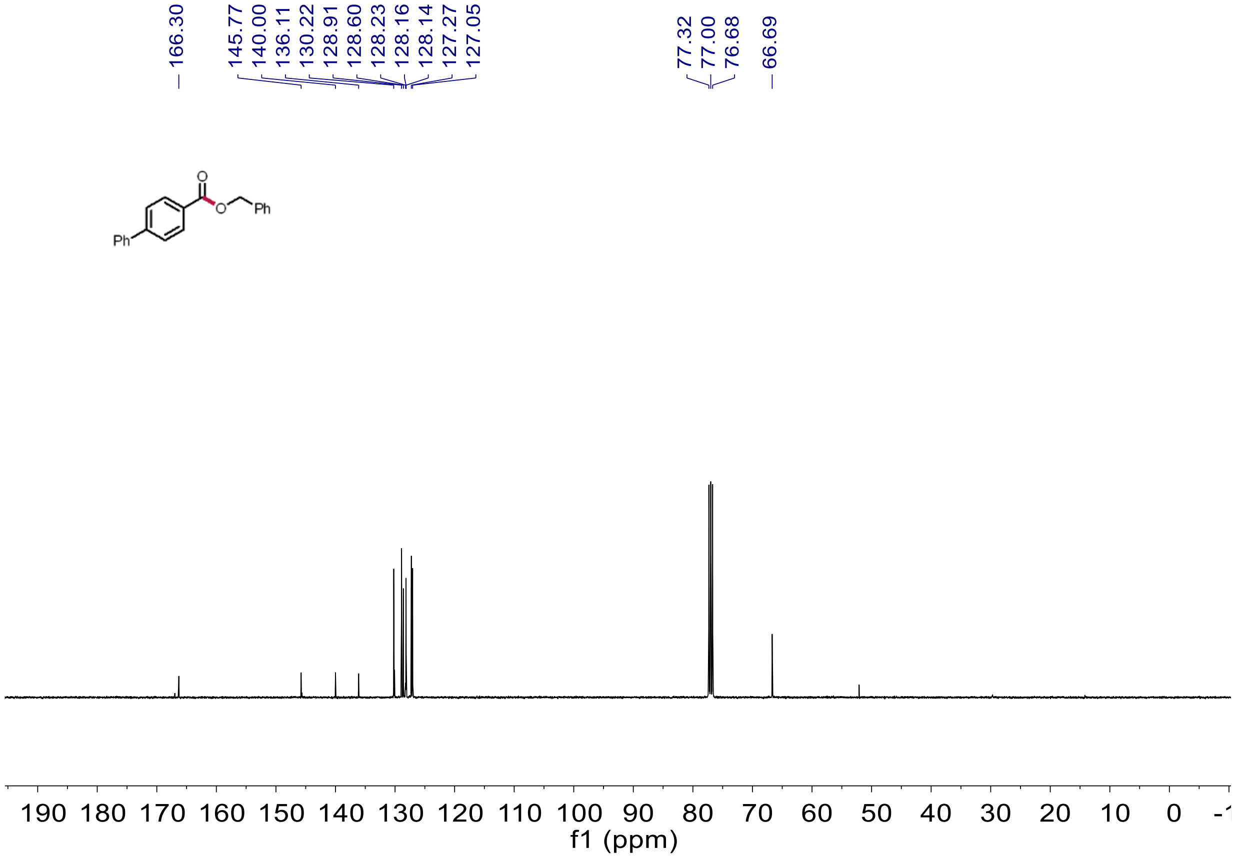
21: 3,3,4,4,5,5,6,6,6-Nonafluorohexyl benzoate (^{19}F NMR, $CDCl_3$, 377 MHz)



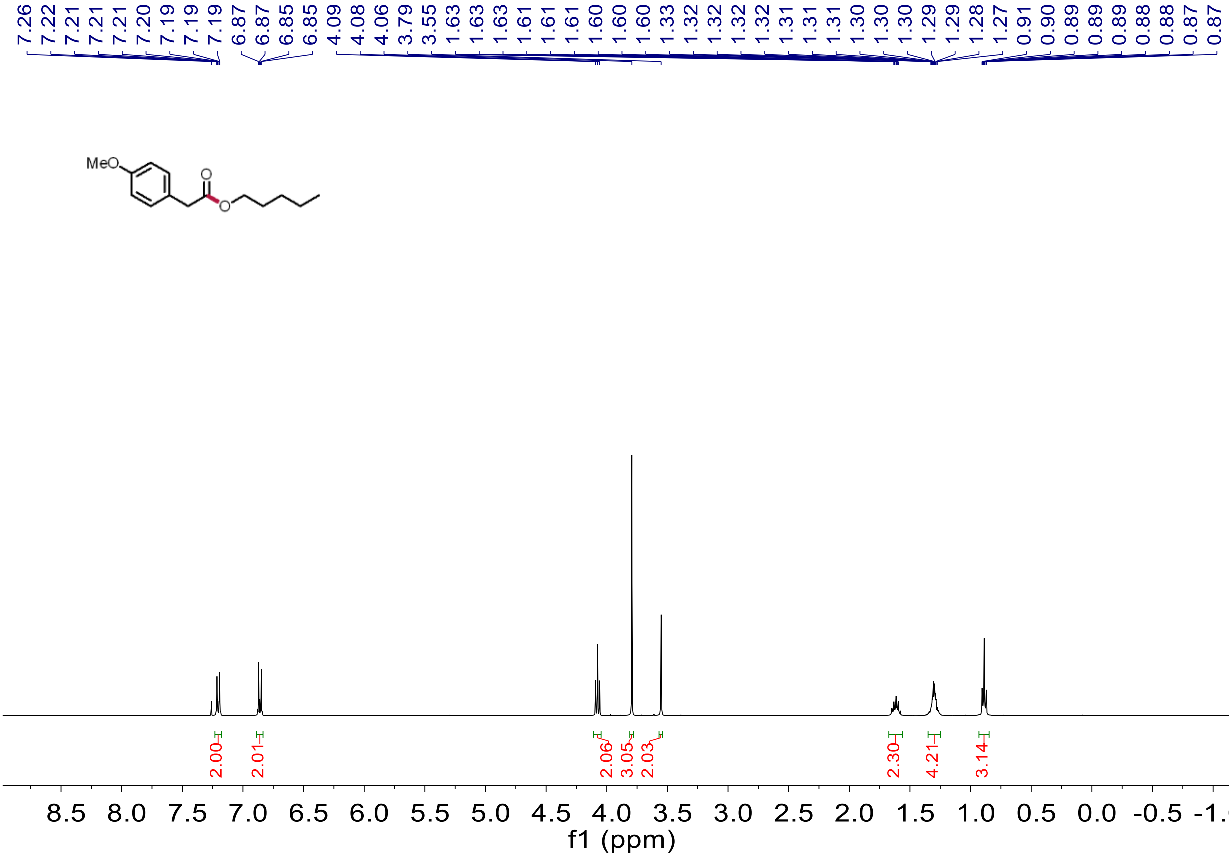
22: Benzyl [1,1’-biphenyl]-4-carboxylate (^{1}H NMR, $CDCl_3$, 400 MHz)



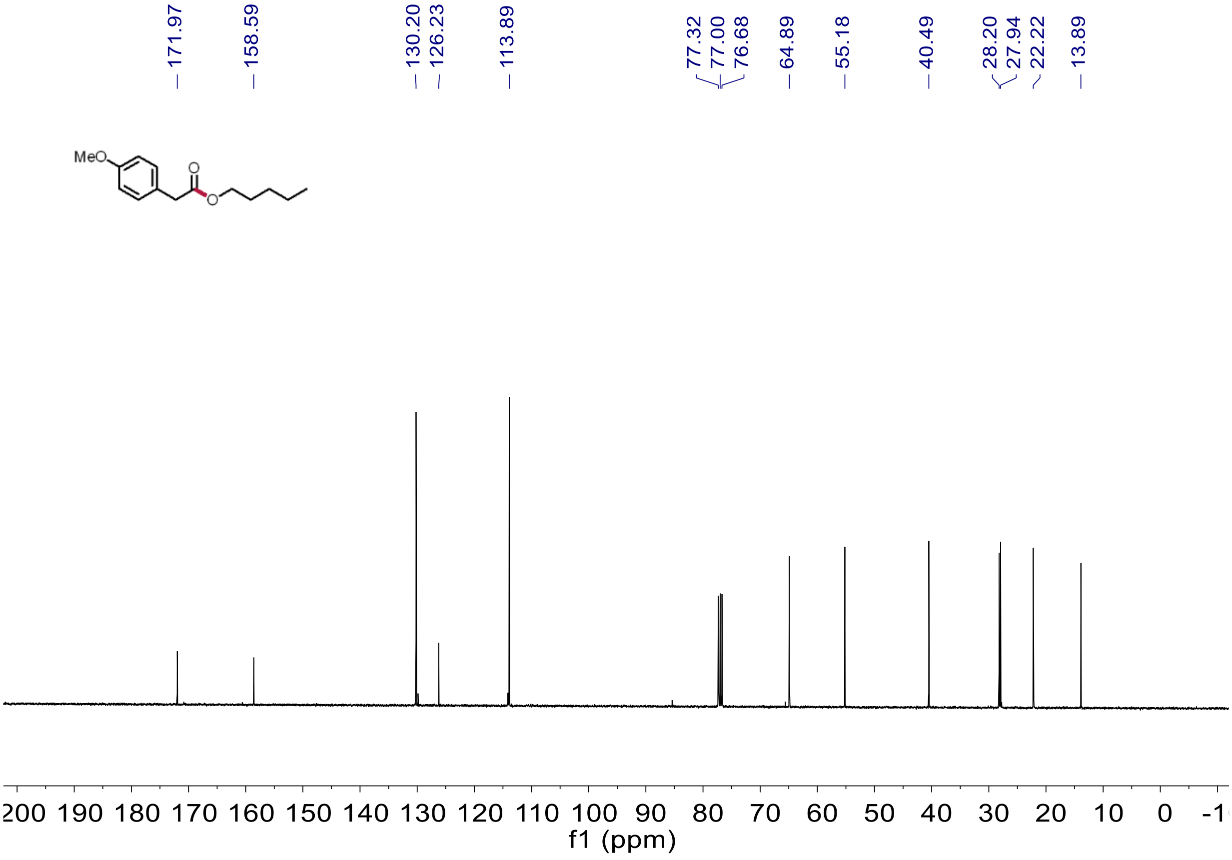
22: Benzyl [1,1’-biphenyl]-4-carboxylate (^{13}C NMR, $CDCl_3$, 100 MHz)



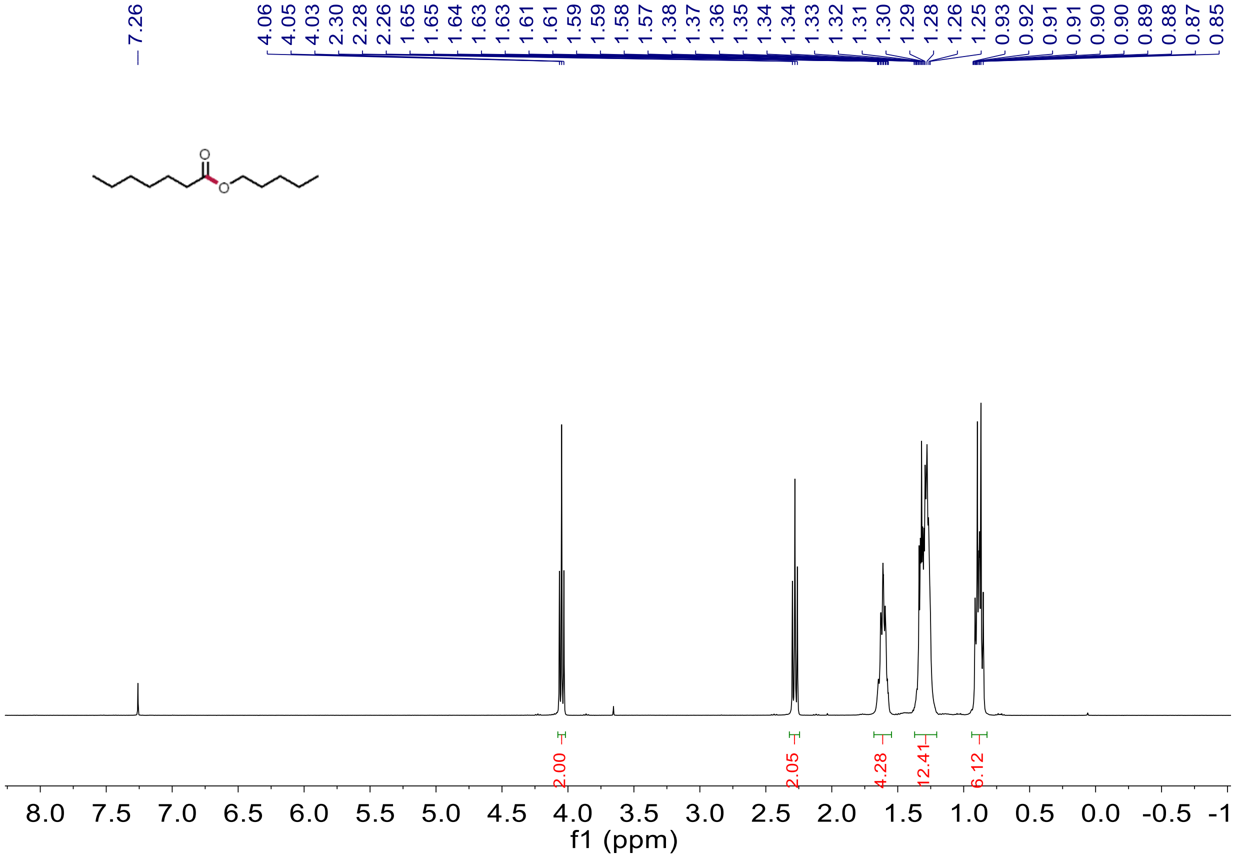
23: Pentyl 2-(4-methoxyphenyl)acetate (^{1}H NMR, $CDCl_3$, 400 MHz)



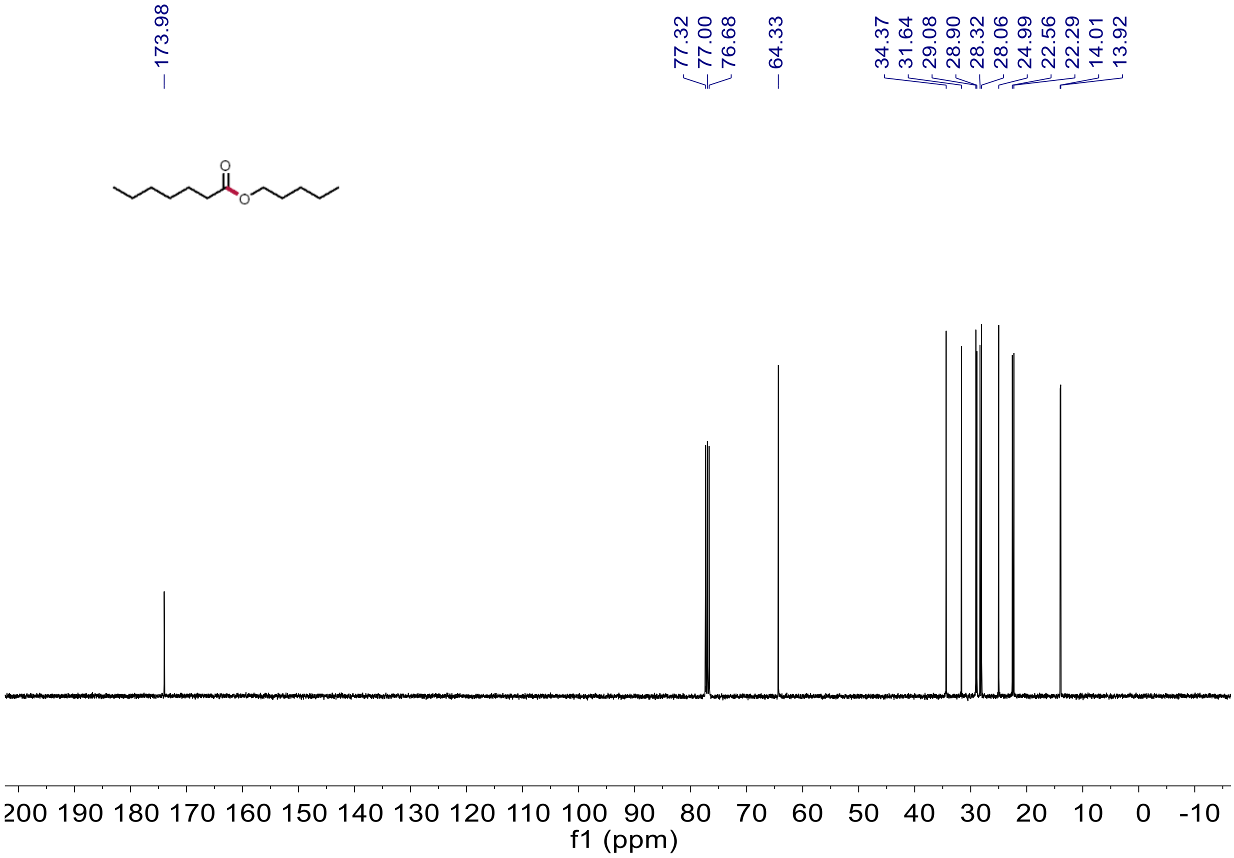
23: Pentyl 2-(4-methoxyphenyl)acetate (^{13}C NMR, $CDCl_3$, 100 MHz)



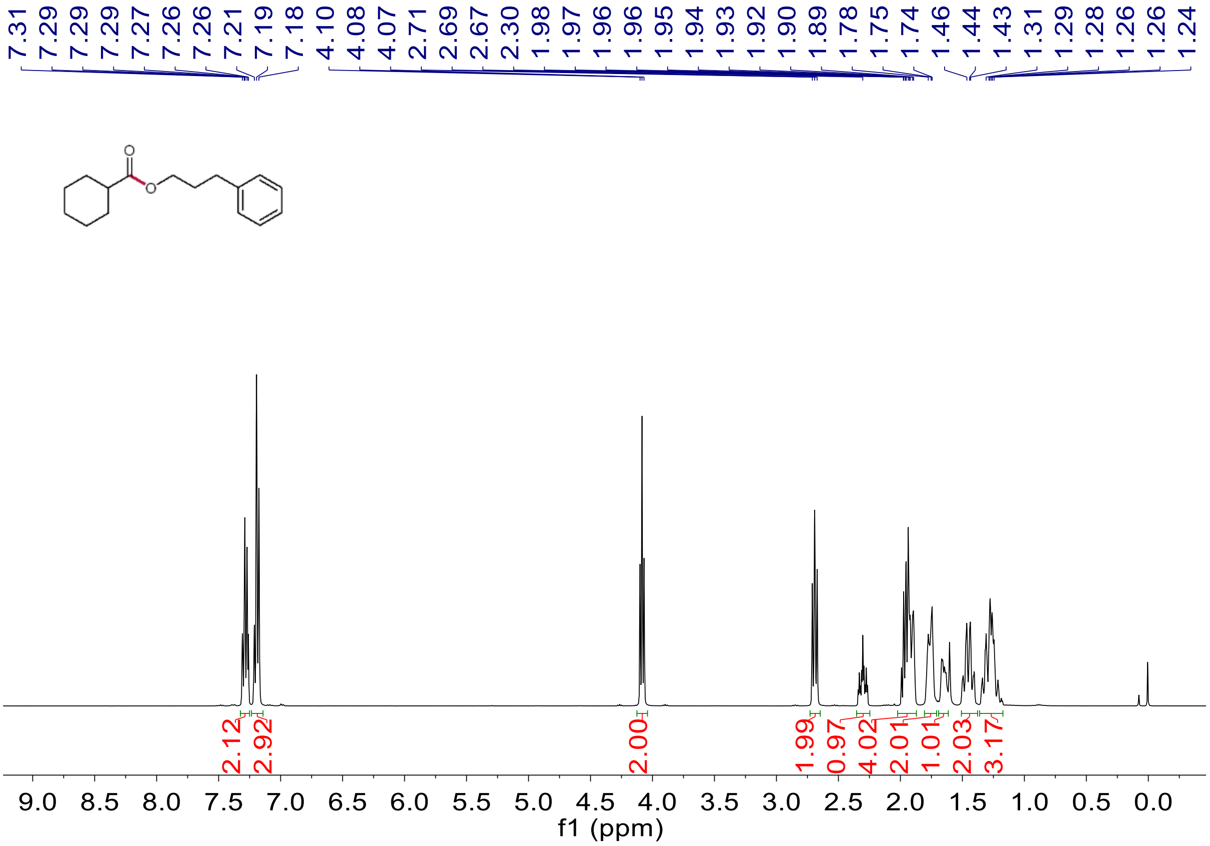
24: Pentyl octanoate (^{1}H NMR, $CDCl_3$, 400 MHz)



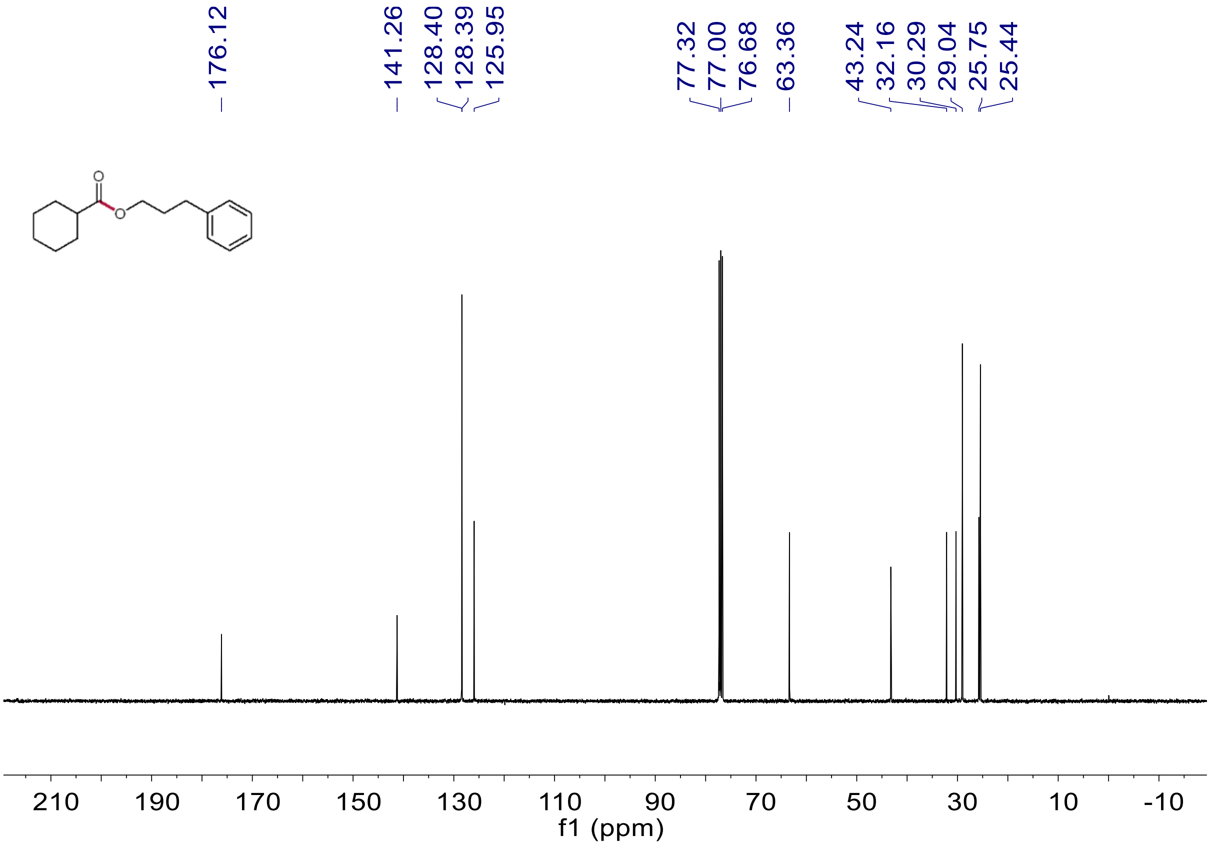
24: Pentyl octanoate (^{13}C NMR, $CDCl_3$, 100 MHz)



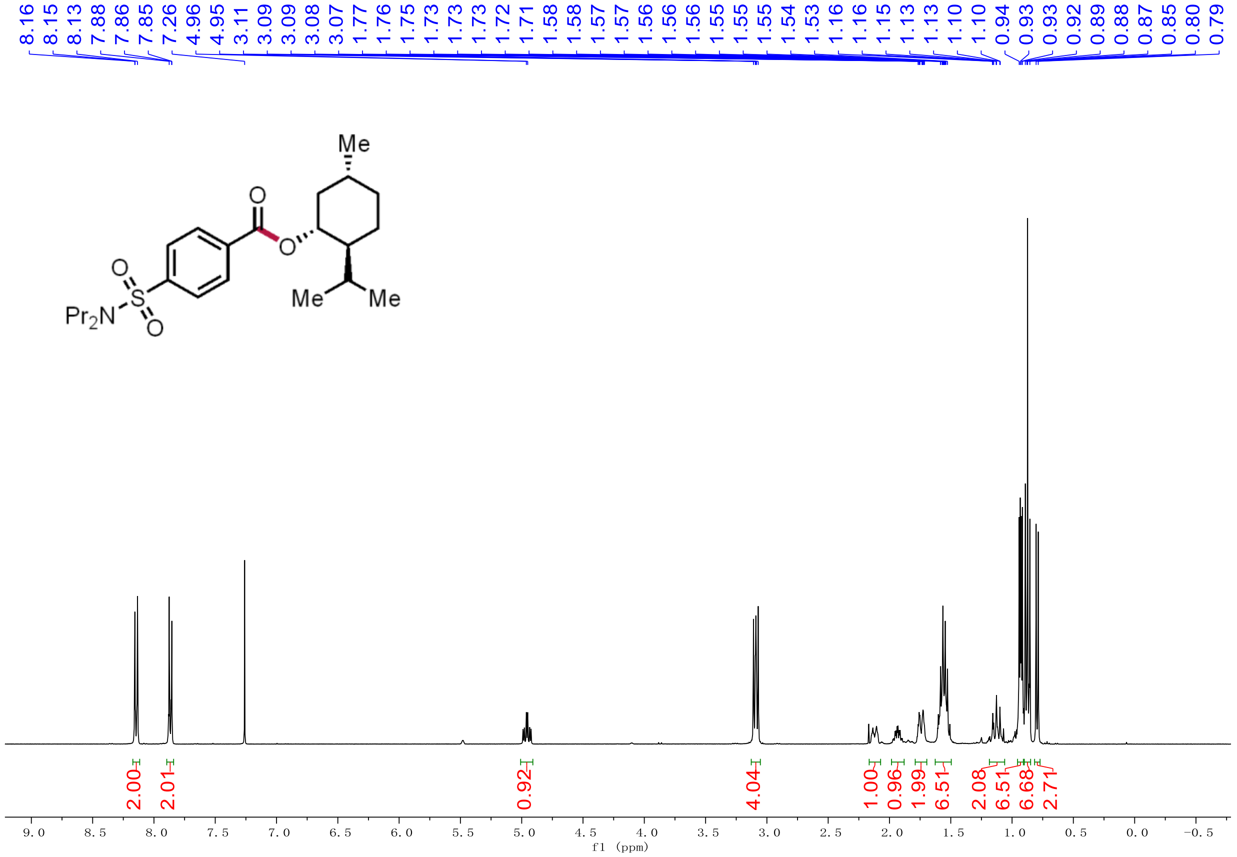
25: 3-Phenylpropyl cyclohexanecarboxylate (^{1}H NMR, $CDCl_3$, 400 MHz)



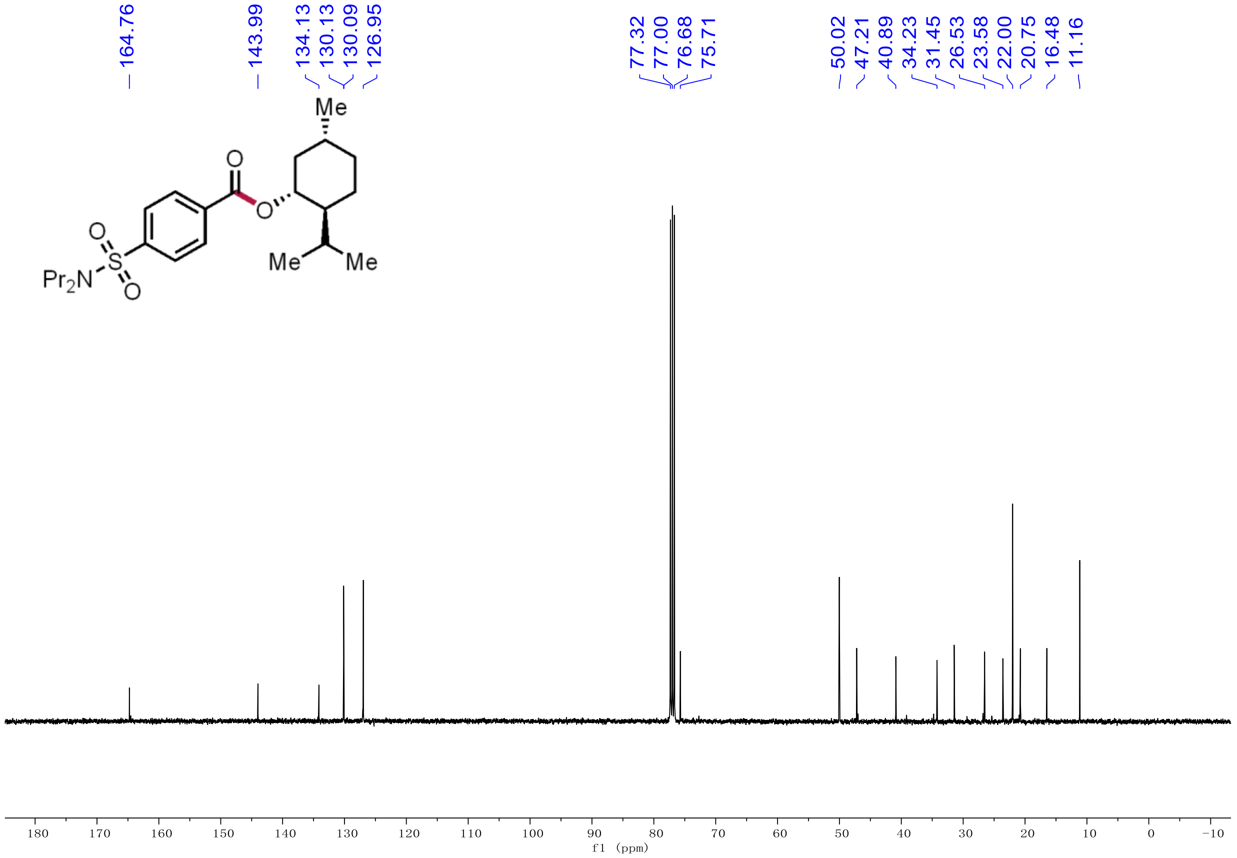
25: 3-Phenylpropyl cyclohexanecarboxylate (^{13}C NMR, $CDCl_3$, 100 MHz)



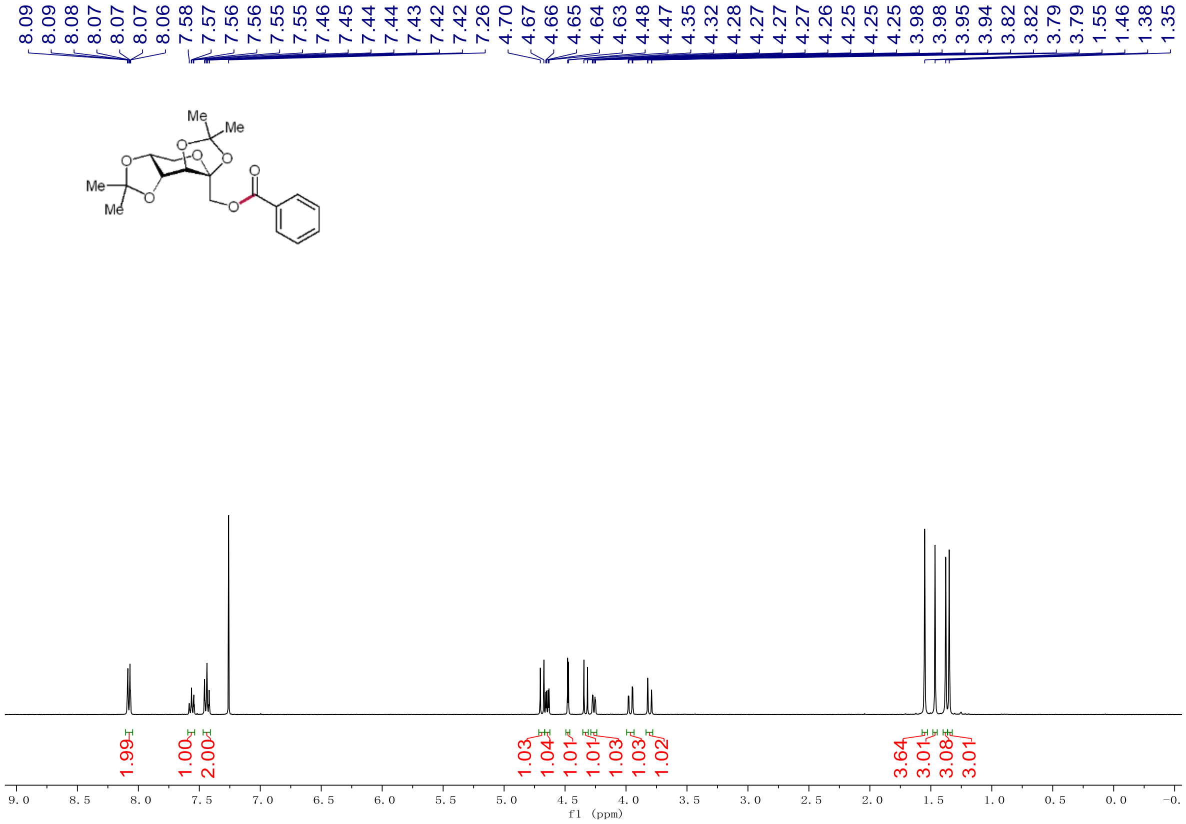
26: (1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl 4-(*N*,*N*-dipropylsulfamoyl)benzoate (^{1}H NMR, CDCl$_3$, 400 MHz)



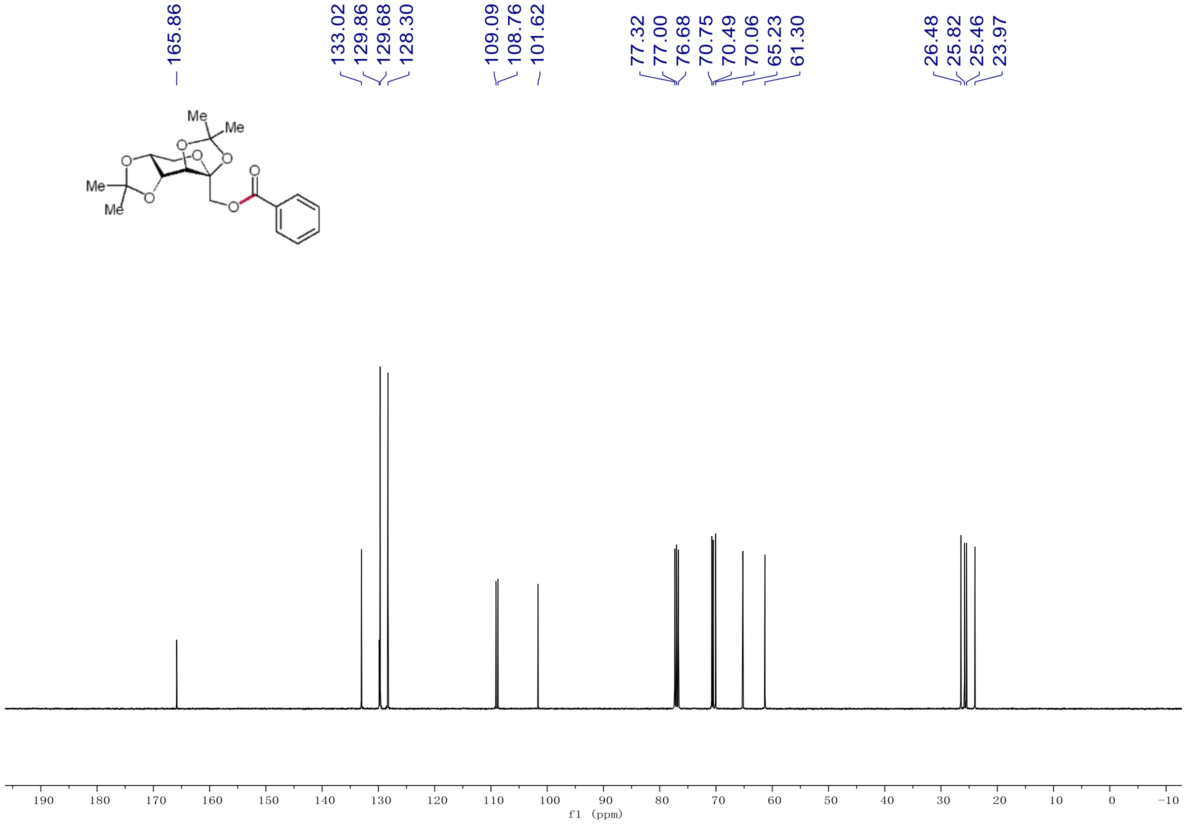
26: (1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl 4-(*N*,*N*-dipropylsulfamoyl)benzoate (^{13}C NMR, CDCl$_3$, 100 MHz)



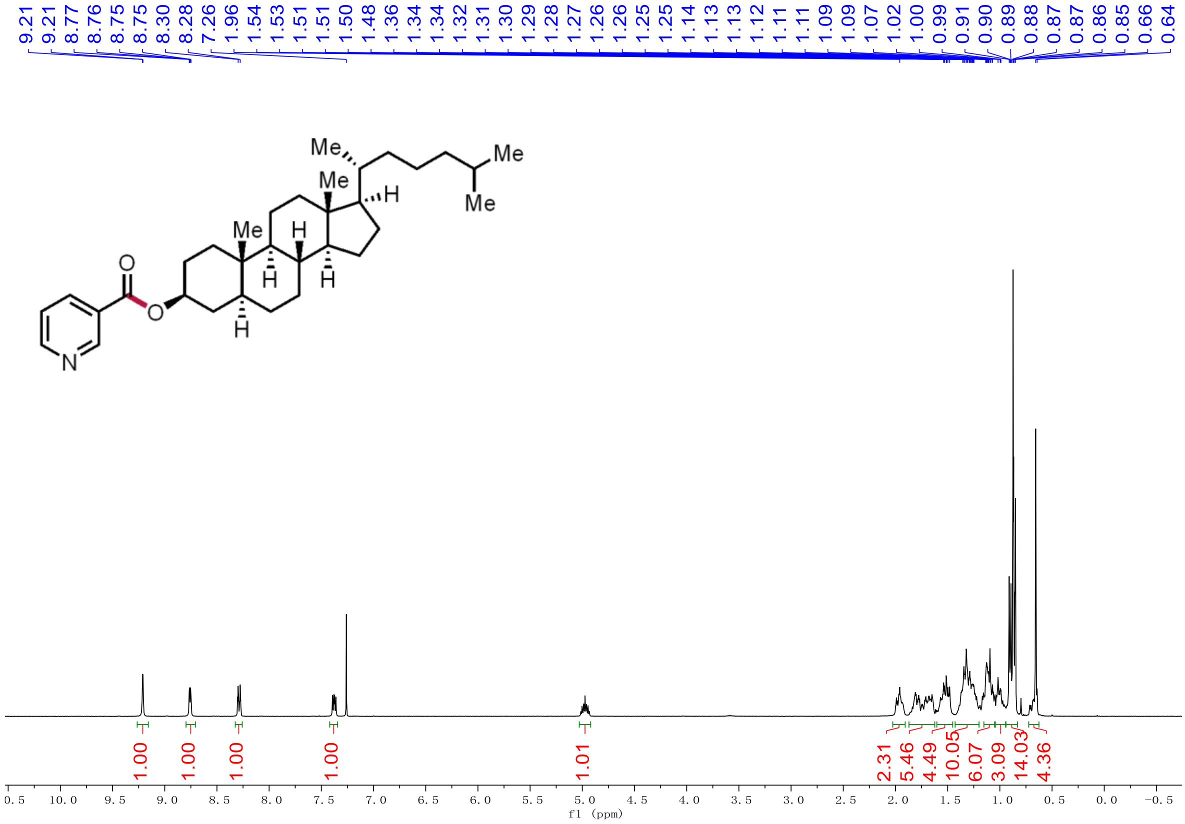
27: ((3aS,5aR,8aR,8bS)-2,2,7,7-Tetramethyltetrahydrobenzo[1,2-d:3,4-d']bis([1,3]dioxole)-3a(4H)-yl)methyl benzoate (^{1}H NMR, CDCl$_3$, 400 MHz)



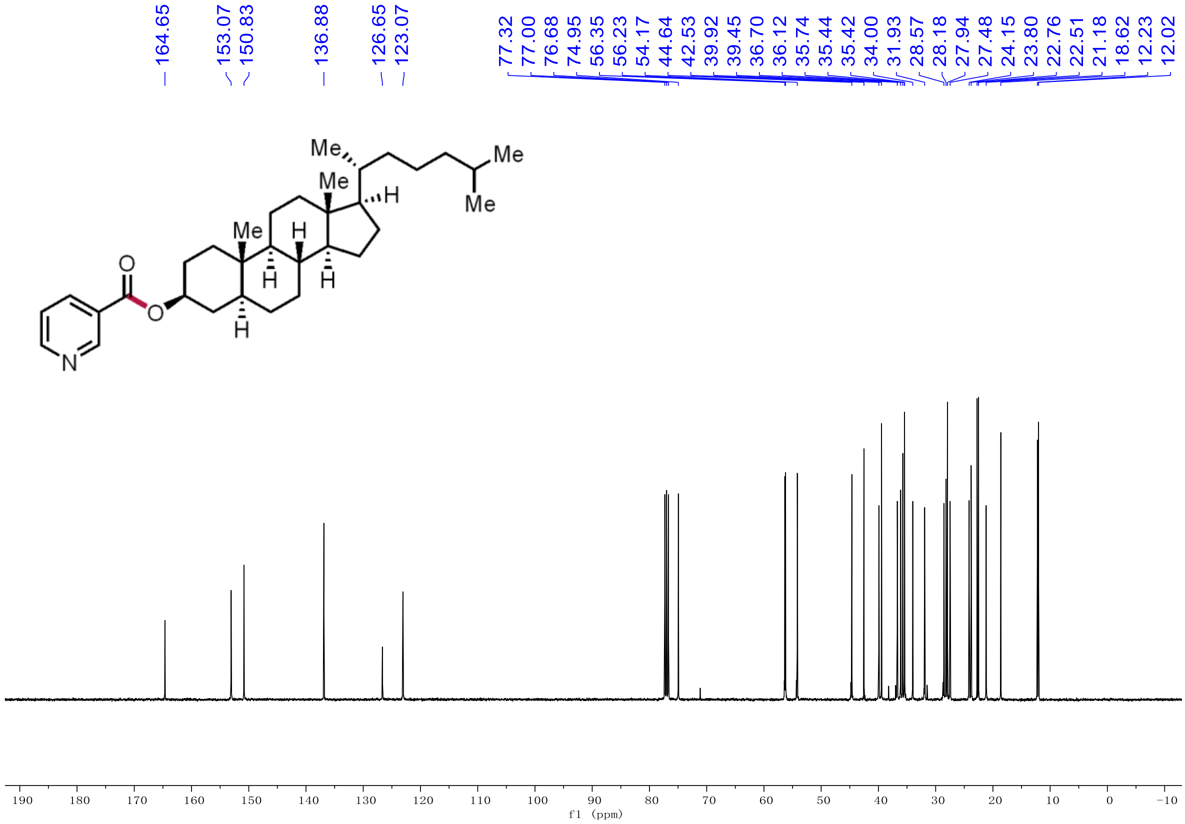
27: ((3aS,5aR,8aR,8bS)-2,2,7,7-Tetramethyltetrahydrobenzo[1,2-d:3,4-d']bis([1,3]dioxole)-3a(4H)-yl)methyl benzoate (^{13}C NMR, CDCl$_3$, 100 MHz)



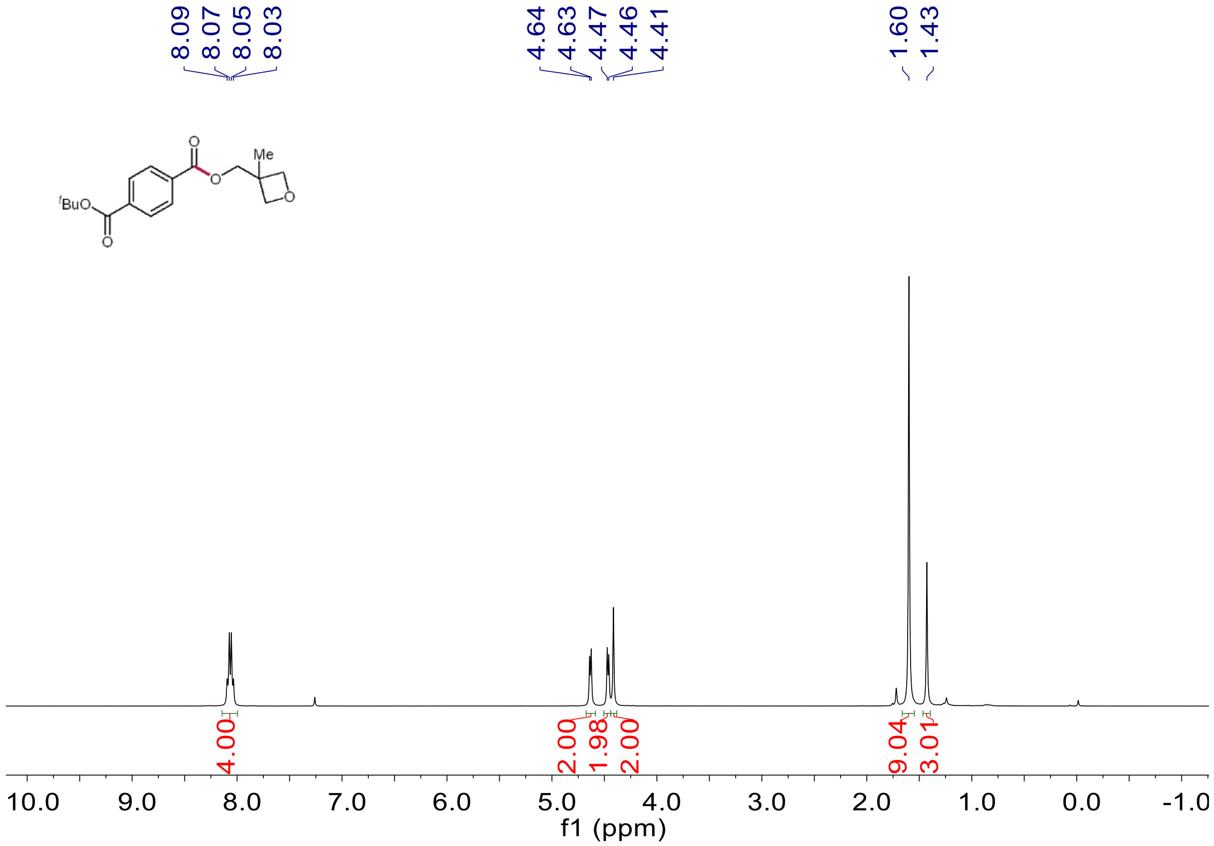
28: (3*S*,5*S*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)hexadecahydro-1*H*-cyclopenta[a]phenanthren-3-yl nicotinate (^{1}H NMR, CDCl$_3$, 400 MHz)



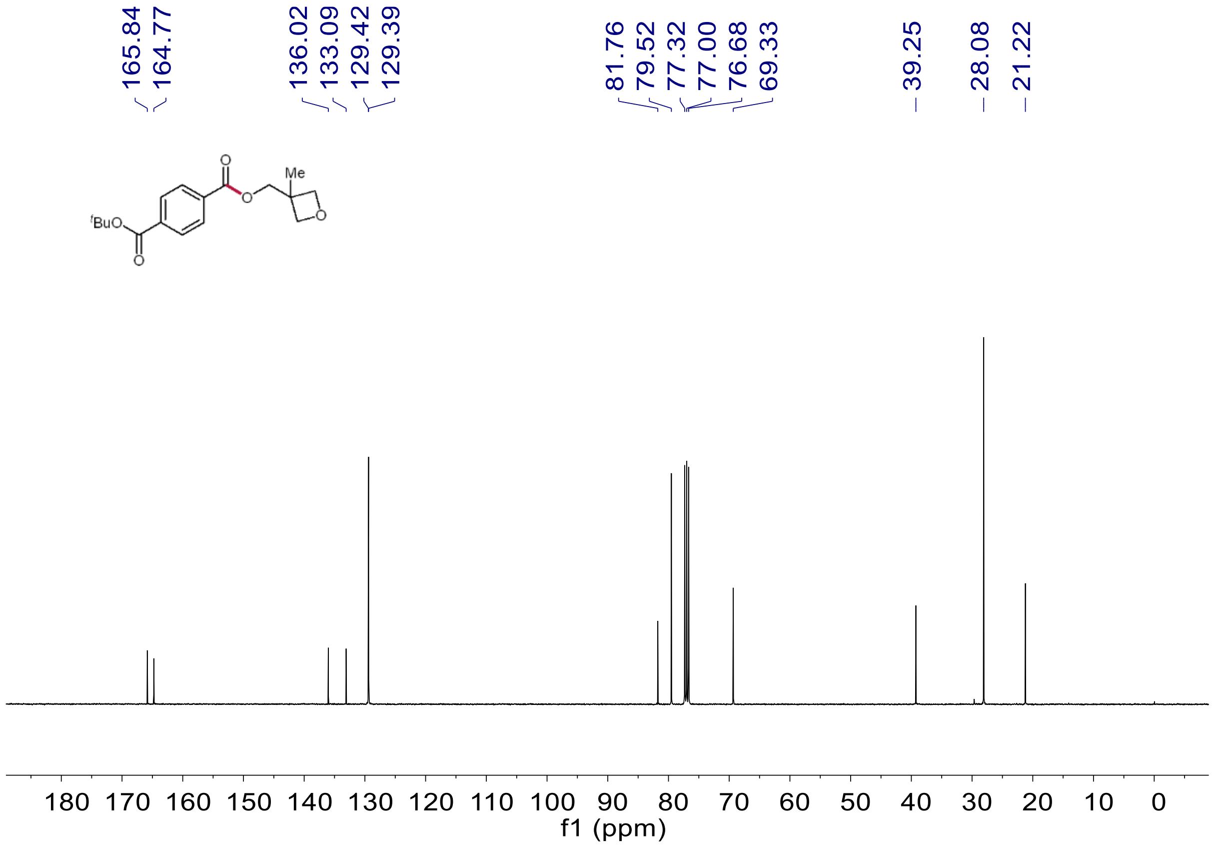
28: (3*S*,5*S*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)hexadecahydro-1*H*-cyclopenta[a]phenanthren-3-yl nicotinate (^{13}C NMR, CDCl$_3$, 100 MHz)



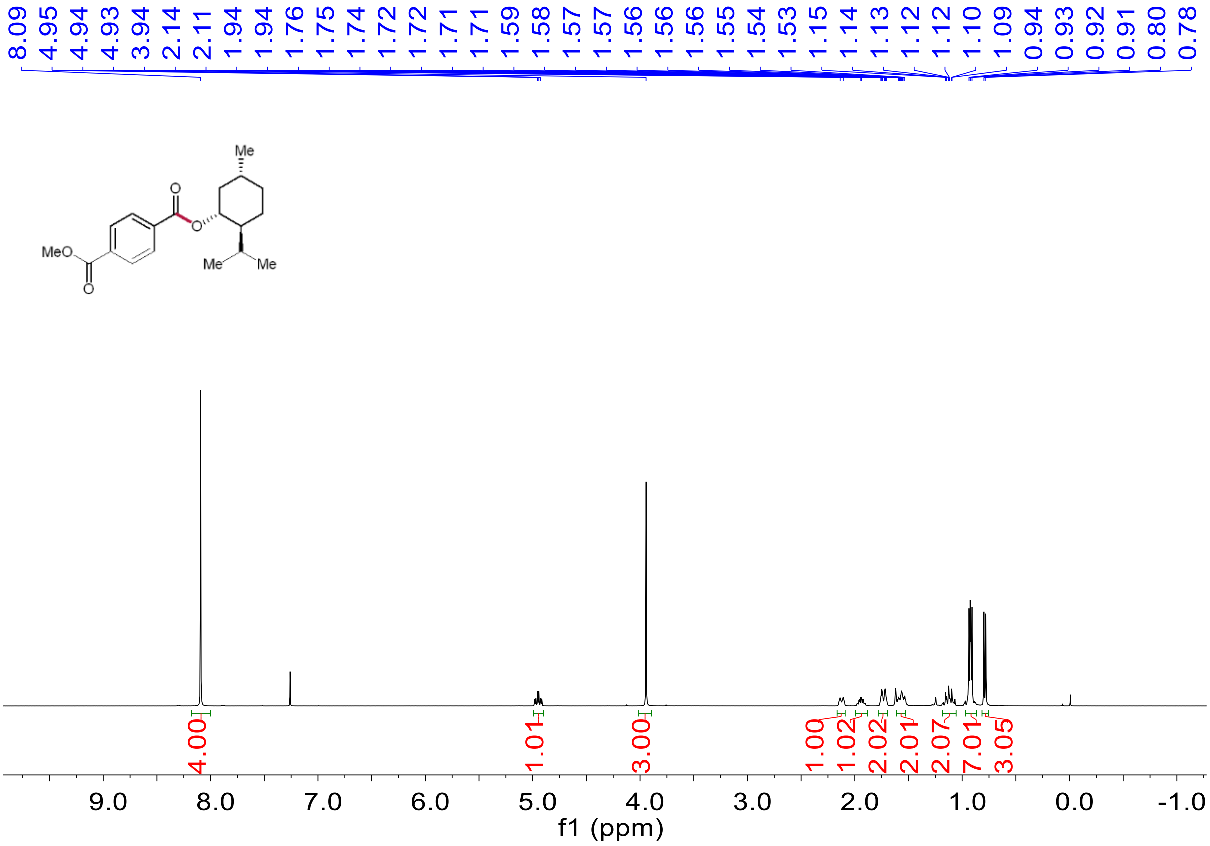
31: Tert-butyl ((3-methyloxetan-3-yl)methyl) terephthalate (^{1}H NMR, CDCl$_3$, 400 MHz)



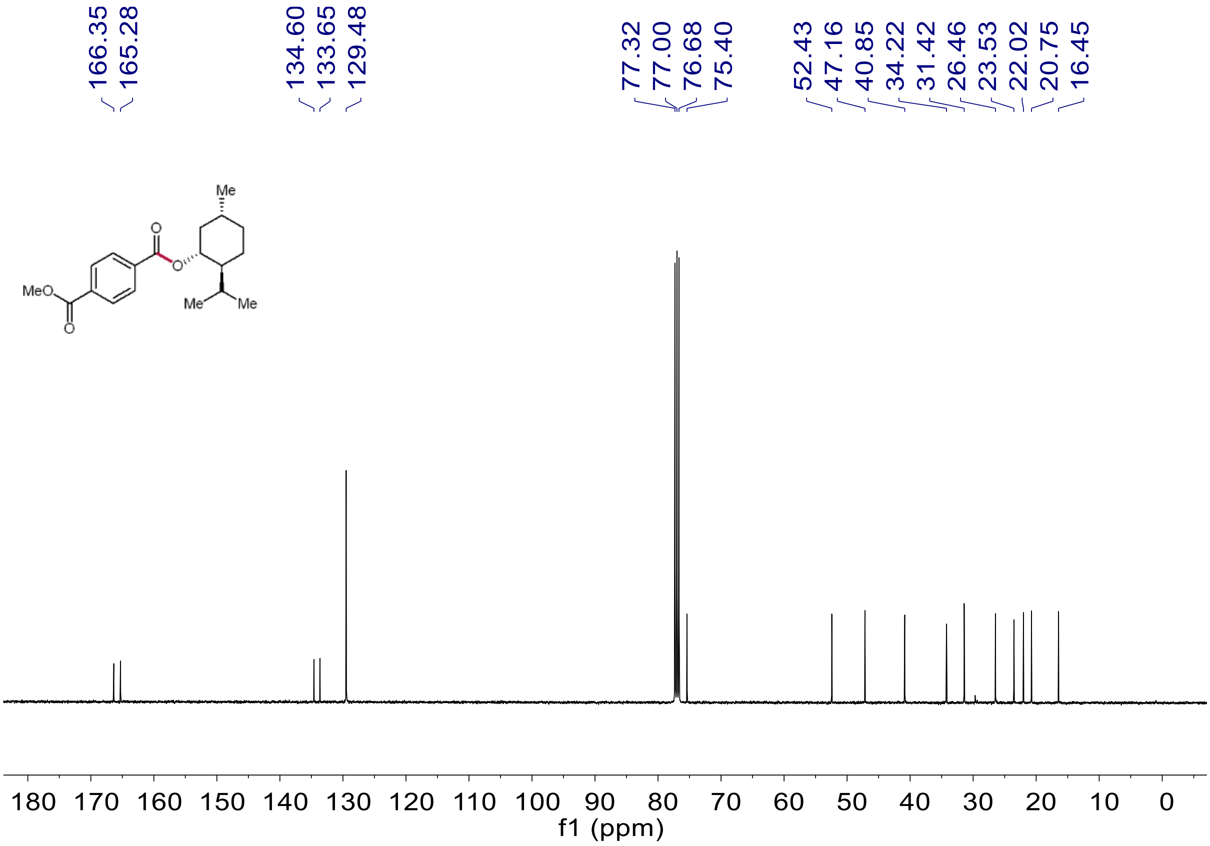
31: Tert-butyl ((3-methyloxetan-3-yl)methyl) terephthalate (^{13}C NMR, CDCl$_3$, 100 MHz)



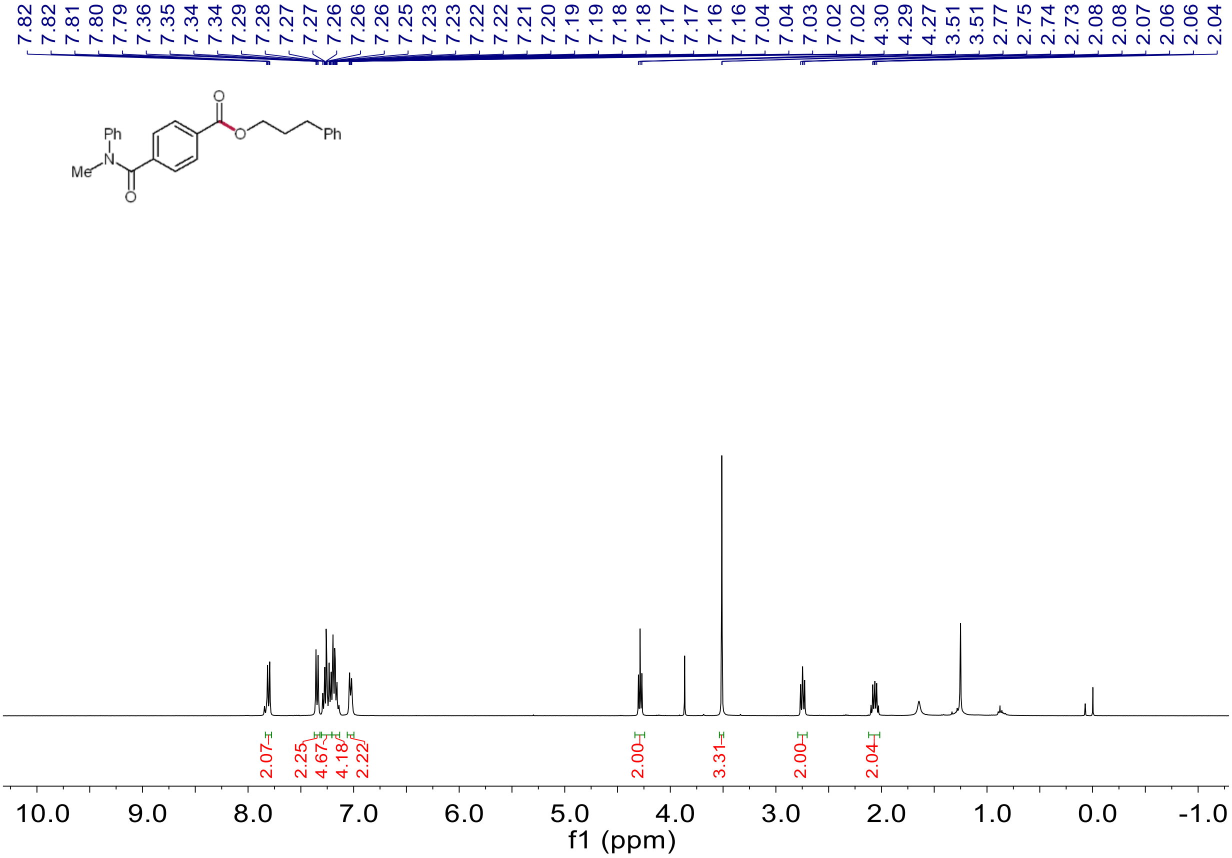
34: (1R,2S,5R)-2-Isopropyl-5-methylcyclohexyl methyl terephthalate (^{1}H NMR, $CDCl_3$, 400 MHz)



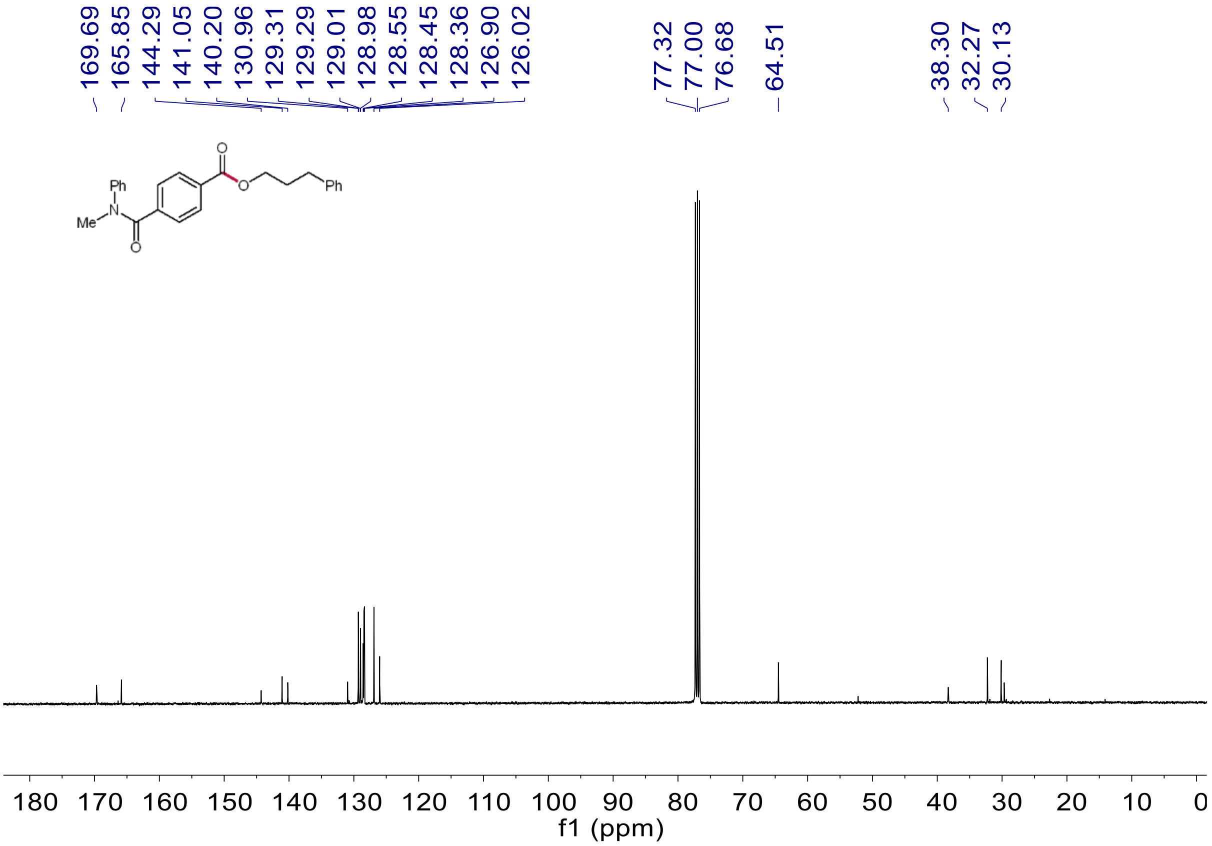
34: (1R,2S,5R)-2-Isopropyl-5-methylcyclohexyl methyl terephthalate (^{13}C NMR, $CDCl_3$, 100 MHz)



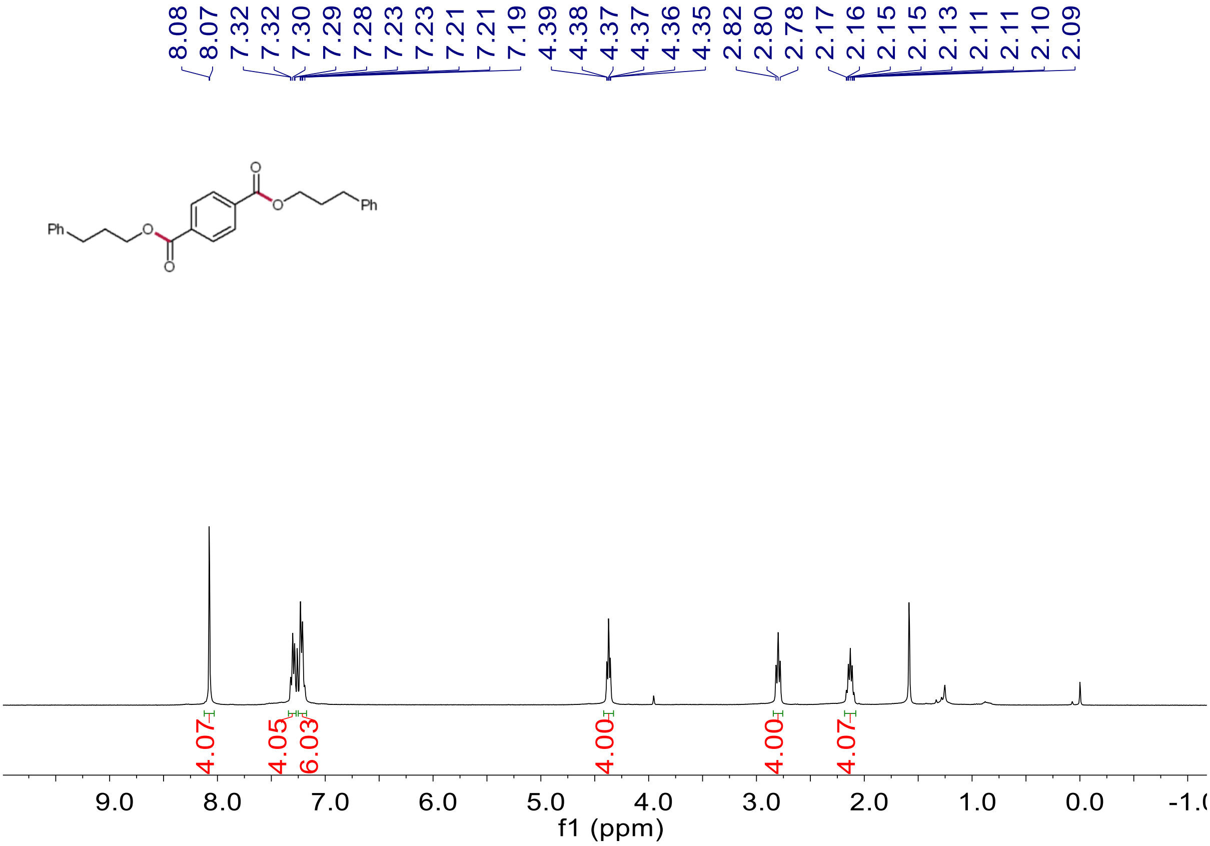
38: 3-Phenylpropyl 4-(methyl(phenyl)carbamoyl)benzoate (^{1}H NMR, CDCl$_3$, 400 MHz)



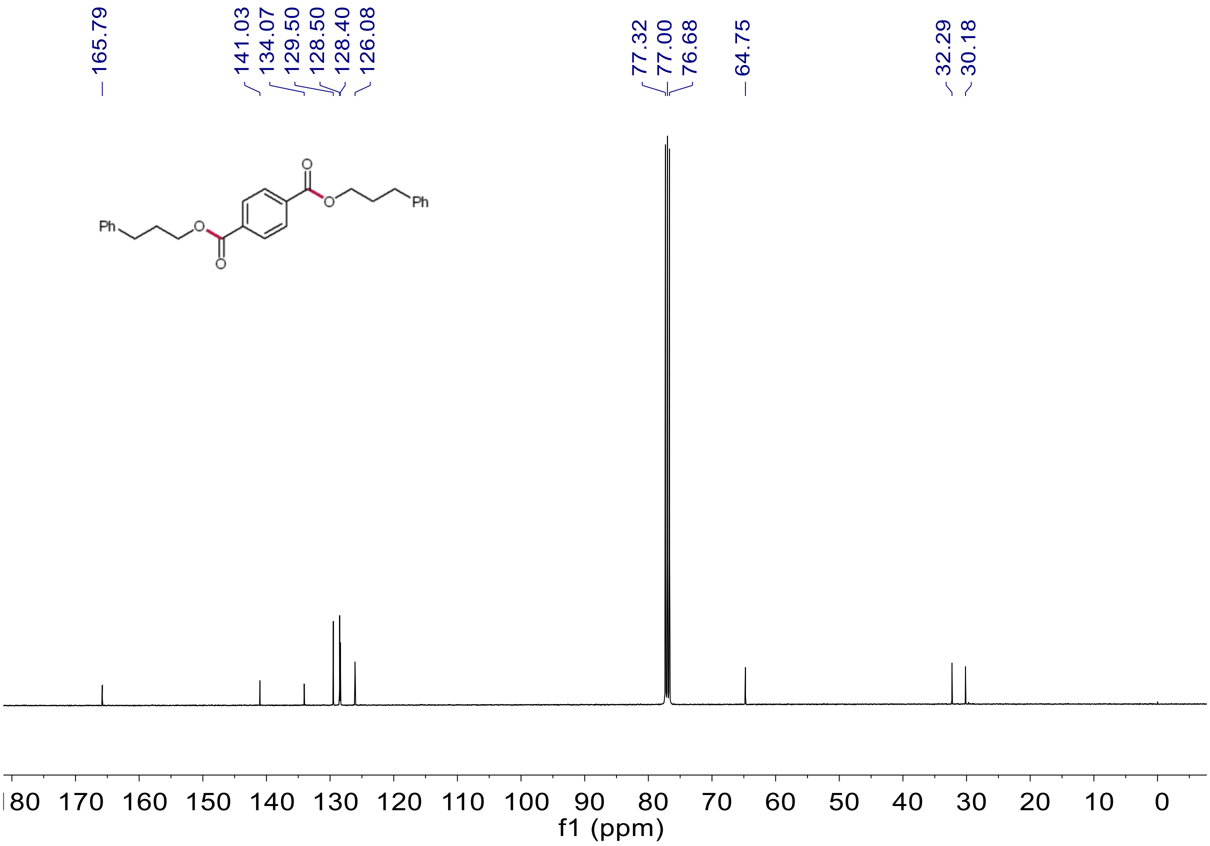
38: 3-Phenylpropyl 4-(methyl(phenyl)carbamoyl)benzoate (^{13}C NMR, CDCl$_3$, 100 MHz)



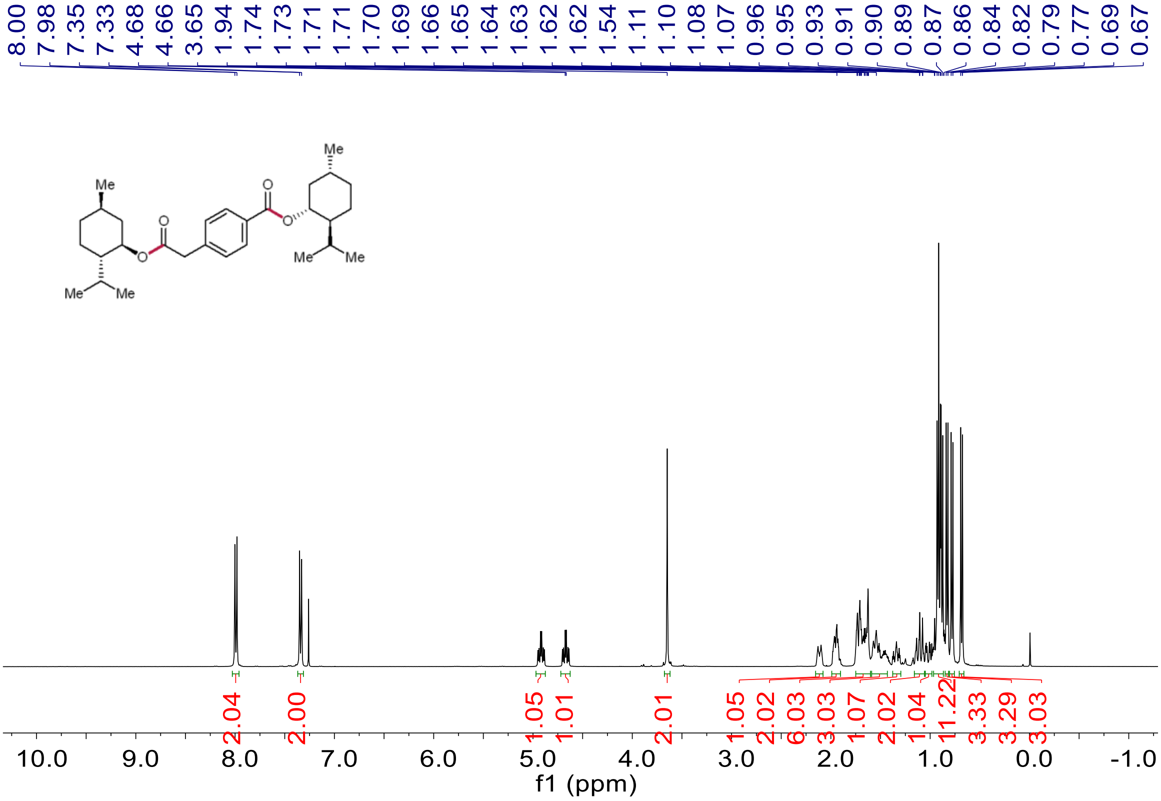
39: Bis(3-phenylpropyl) terephthalate (^{1}H NMR, CDCl$_3$, 400 MHz)



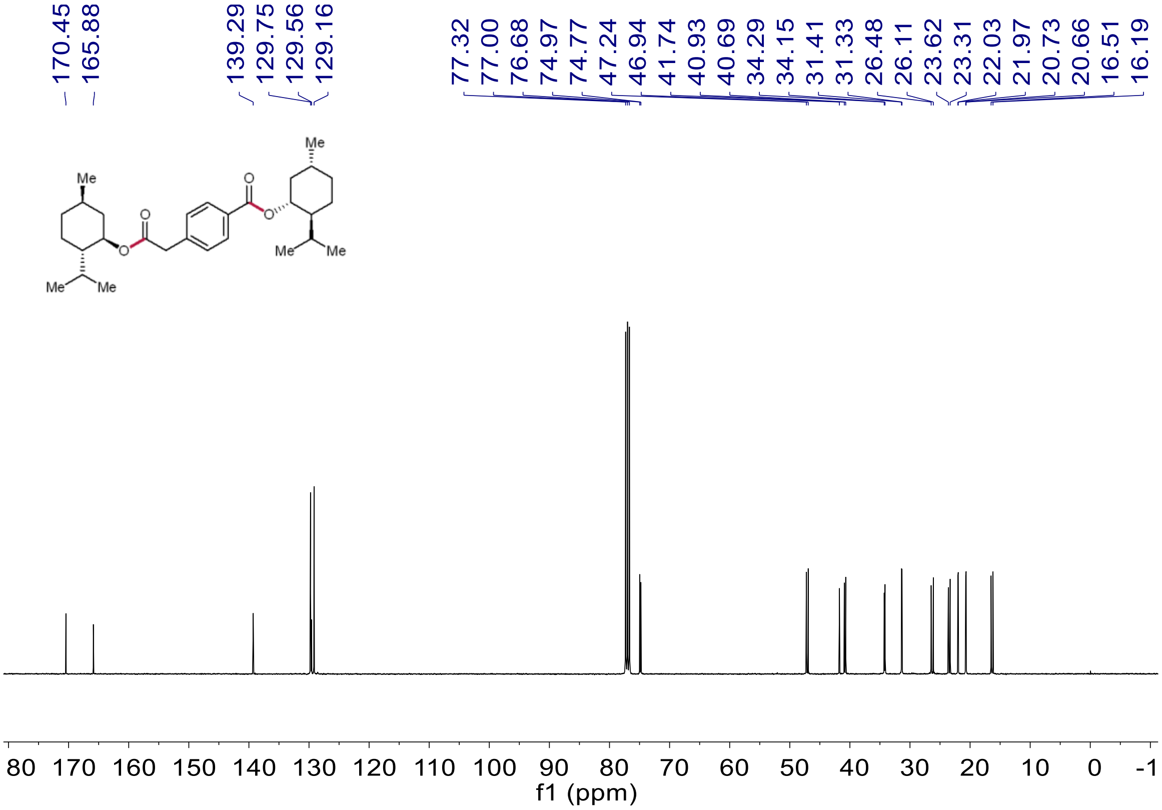
39: Bis(3-phenylpropyl) terephthalate (^{13}C NMR, CDCl$_3$, 100 MHz)



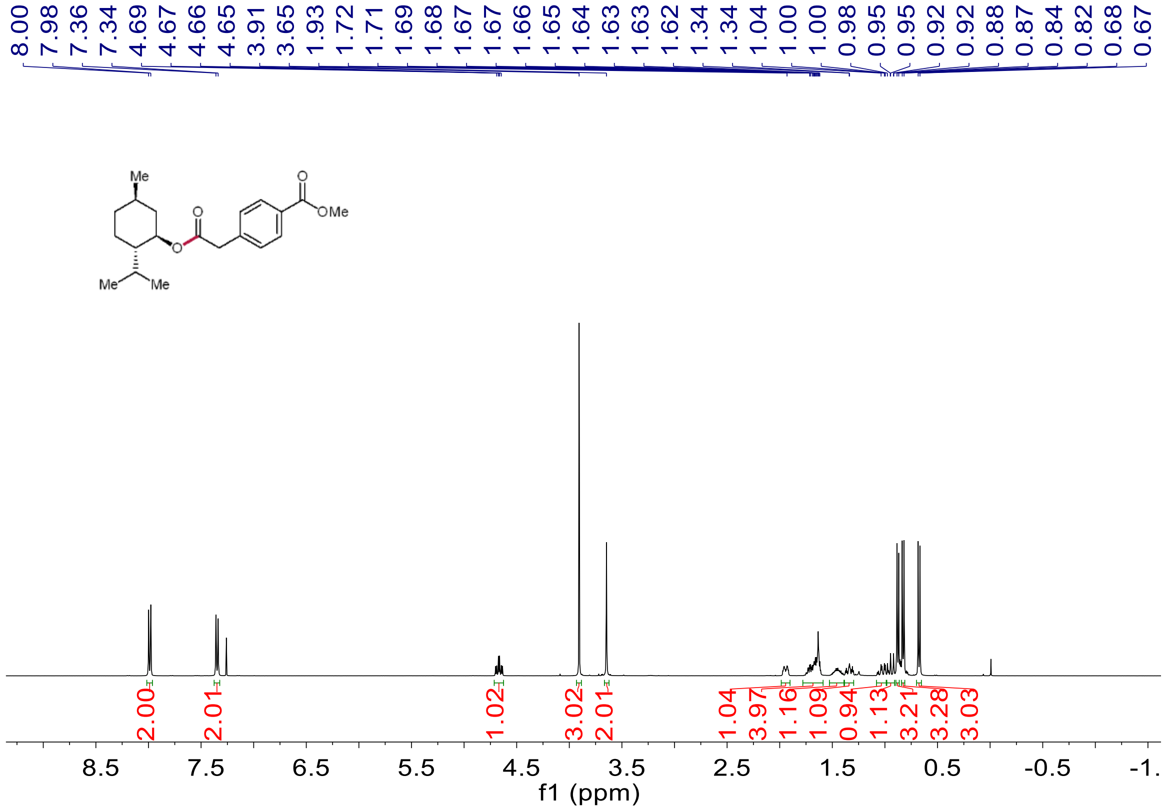
41: (1R,2S,5R)-2-Isopropyl-5-methylcyclohexyl 4-(2-(((1R,2S,5R)-2-isopropyl-5-methylcyclohexyl)oxy)-2-oxoethyl)benzoate (^{1}H NMR, CDCl$_3$, 400 MHz)



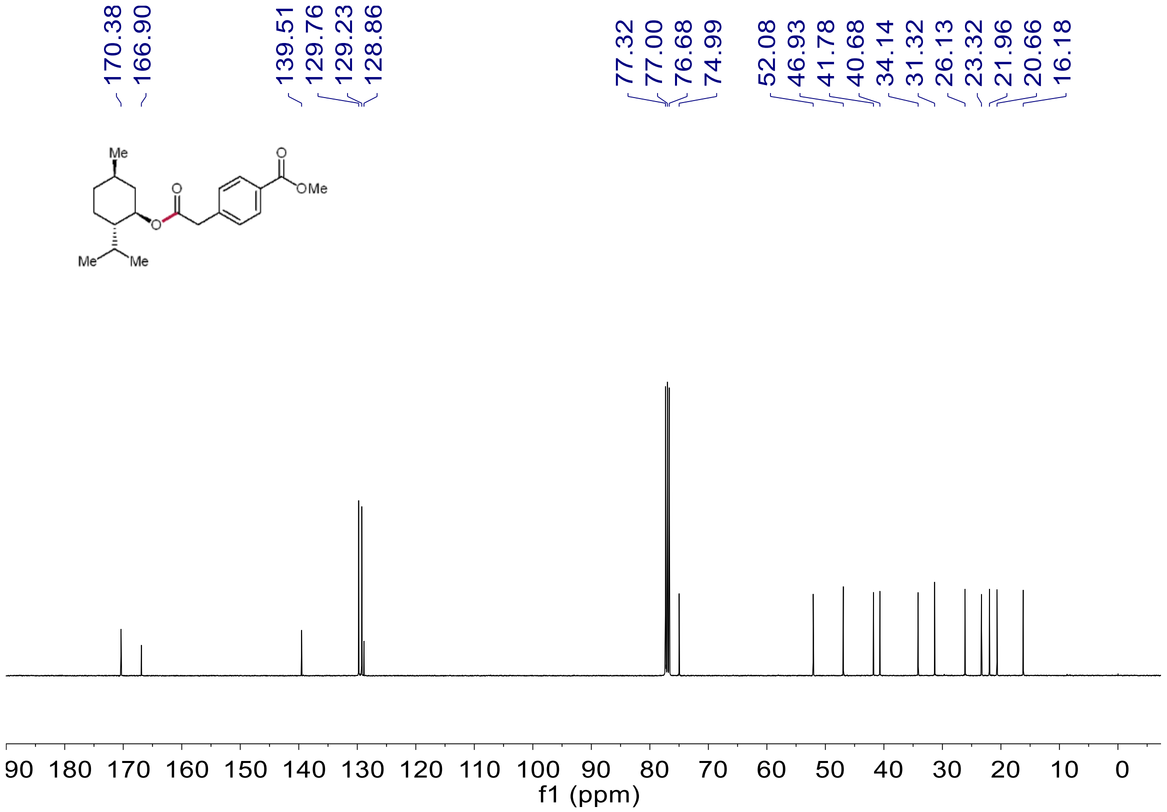
41: (1R,2S,5R)-2-Isopropyl-5-methylcyclohexyl 4-(2-(((1R,2S,5R)-2-isopropyl-5-methylcyclohexyl)oxy)-2-oxoethyl)benzoate (^{13}C NMR, CDCl$_3$, 100 MHz)



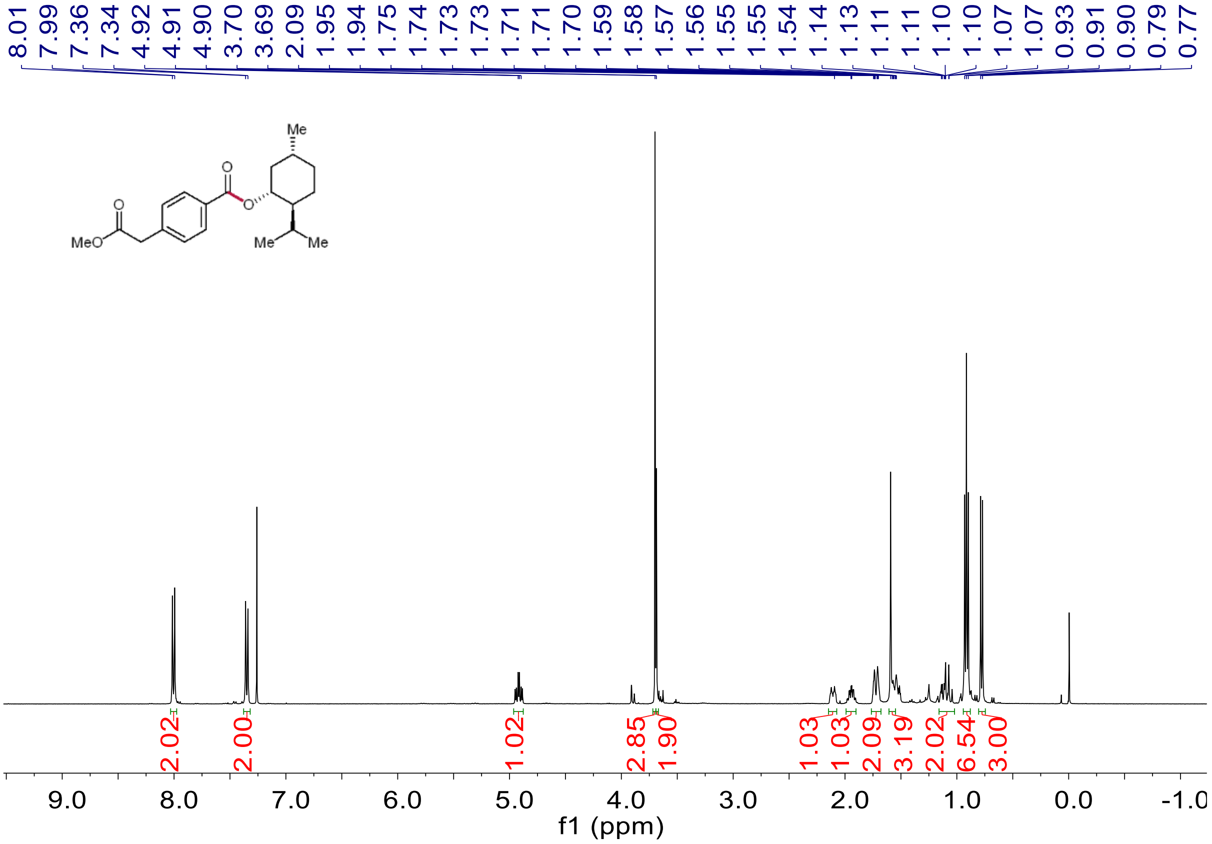
42: Methyl 4-(2-(((1R,2S,5R)-2-Isopropyl-5-methylcyclohexyl)oxy)-2-oxoethyl)benzoate (^{1}H NMR, CDCl$_3$, 400 MHz)



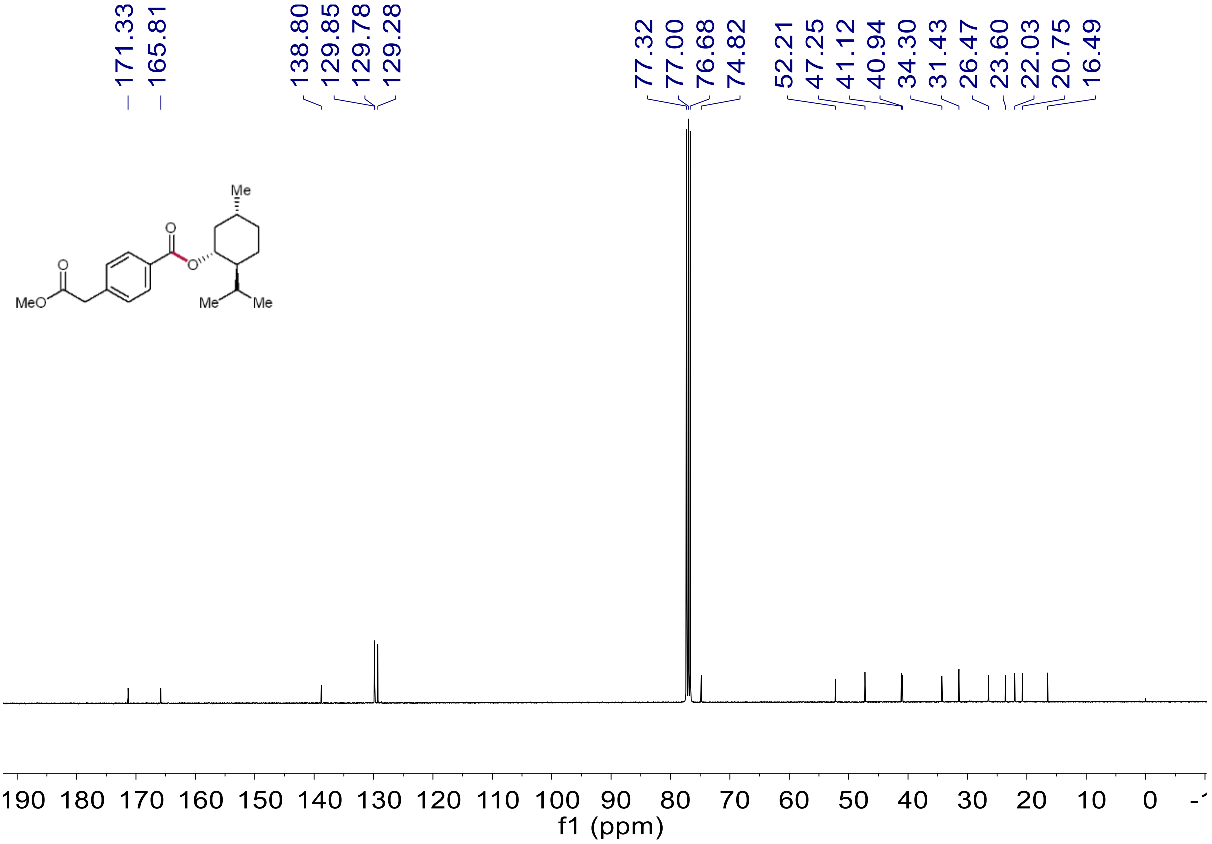
42: Methyl 4-(2-(((1R,2S,5R)-2-Isopropyl-5-methylcyclohexyl)oxy)-2-oxoethyl)benzoate (^{13}C NMR, CDCl$_3$, 100 MHz)



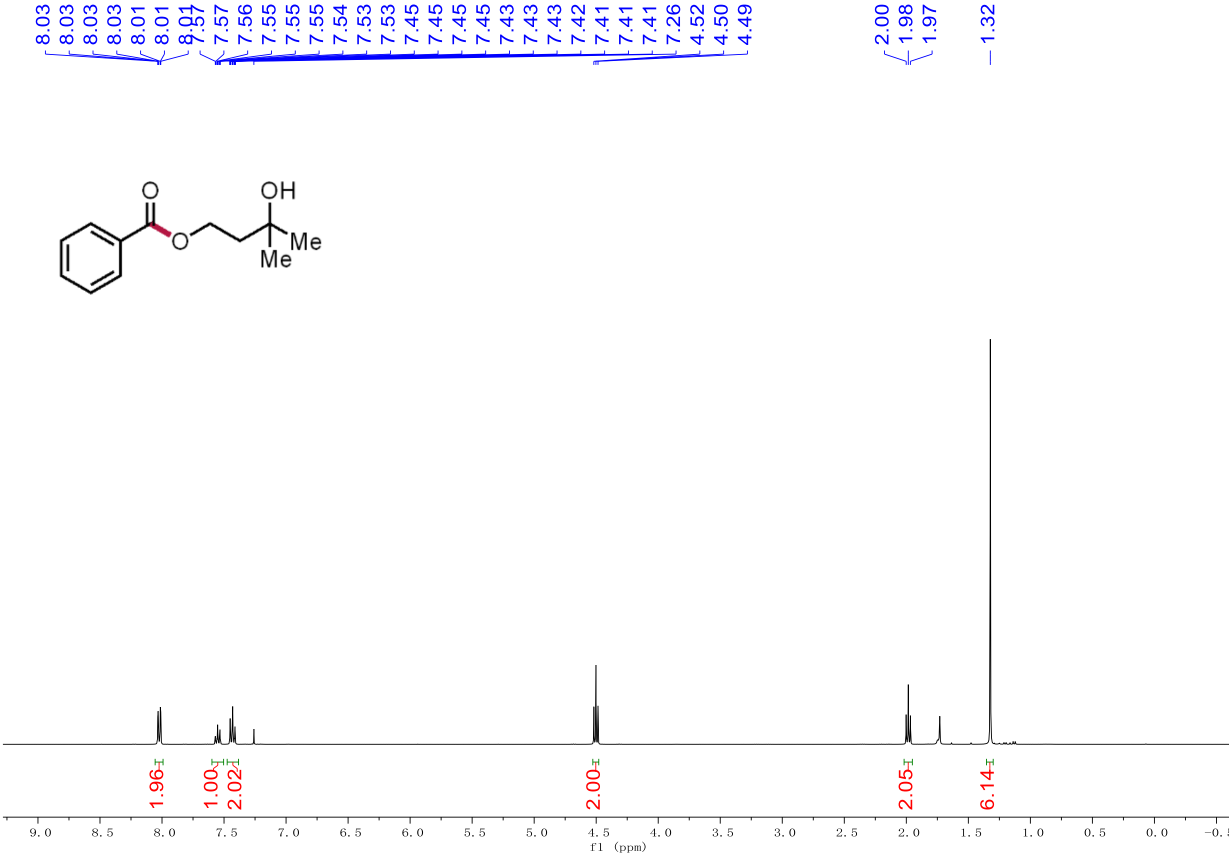
43: (1R,2S,5R)-2-Isopropyl-5-methylcyclohexyl 4-(2-methoxy-2-oxoethyl)benzoate (^{1}H NMR, $CDCl_3$, 400 MHz)



43: (1R,2S,5R)-2-Isopropyl-5-methylcyclohexyl 4-(2-methoxy-2-oxoethyl)benzoate (^{13}C NMR, $CDCl_3$, 100 MHz)



45: 3-Hydroxy-3-methylbutyl benzoate (^{1}H NMR, CDCl$_3$, 400 MHz)



45: 3-Hydroxy-3-methylbutyl benzoate (^{13}C NMR, CDCl$_3$, 100 MHz)