Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Amine-catalyzed site- and stereo-selective coupling of epoxy amine and carbon dioxide to construct oxazolidinones

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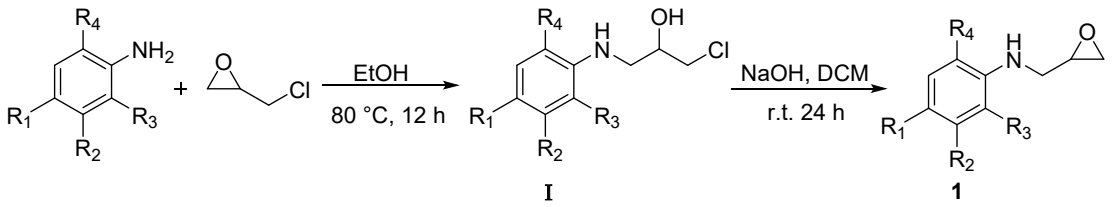
1. General information.

NMR spectra were recorded on a Bruker AVANCE III HD-400 spectrometer. X-ray crystallographic data were collected with an AXS D8 X-ray diffractometer. High resolution mass spectra (HRMS) were obtained on Bruker ESI-QTOF LC/MS instrument (source type: ESI; mass analyzer type: TOF) and Water EI-GCT-TOF MS. All starting materials were purchased from Tianping Epistar, Aladdin, Enox, and used as received.

2. Synthesis and characterization of epoxy amines.

Scheme S1 Preparation of epoxy amine **1**.



Following reported procedures,[1] aniline (20.0 mmol) and epichlorohydrin (22.0 mmol) were dissolved in ethanol (50 mL). The mixture was heated under reflux for 12 hours. After reaction, all volatiles were removed in vacuo, and the γ-chloro-β-hydroxyaniline **I** was isolated by column chromatography (eluent: petroleum ether: ethyl acetate, from 100: 0 to 80: 20). It was then dissolved in dichloromethane (100 mL), and a 0.3 M sodium hydroxide aqueous solution (100 mL) was added. After overnight reaction at room temperature, the organic layer was separated, washed with brine (3 × 100 mL) and dried over Na_2SO_4. Epoxy amine was obtained after removal of solvent.

Characterization data

***N*-(oxiran-2-ylmethyl)aniline (1a)**[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 – 7.15 (m, 2H, Ar-H), 6.76 – 6.72 (m, 1H, Ar-H), 6.69 – 6.61 (m, 2H, Ar-H), 3.94 (s, 1H, NH),

3.60 – 3.49 (m, 1H, NC*H*H), 3.30 – 3.18 (m, 2H, NCH*H*+CH), 2.86 – 2.79 (m, 1H, OC*H*H), 2.71 (dd, *J* = 4.8, 2.4 Hz, 1H, OCH*H*).

4-fluoro-*N*-(oxiran-2-ylmethyl)aniline (1b)[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.93 – 6.86 (m, 2H, Ar-H), 6.61 – 6.55 (m, 2H, Ar-H), 3.76 (s, 1H, NH), 3.55 – 3.46 (m, 1H, NC*H*H), 3.24 – 3.11 (m, 2H, NCH*H*+CH), 2.82 (dd, *J* = 4.9, 3.8 Hz, 1H, OC*H*H), 2.69 (dd, *J* = 4.9, 2.4 Hz, 1H, OCH*H*).

4-chloro-*N*-(oxiran-2-ylmethyl)aniline (1c)[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 – 7.08 (m, 2H, Ar-H), 6.59 – 6.51 (m, 2H, Ar-H), 3.92 (s, 1H, NH), 3.56 – 3.46 (m, 1H, NC*H*H), 3.17 (d, *J* = 11.8 Hz, 2H, NCH*H*+ CH), 2.81 (t, *J* = 4.3 Hz, 1H, OC*H*H), 2.67 (dd, *J* = 5.1, 2.0 Hz, 1H, OCH*H*).

4-bromo-*N*-(oxiran-2-ylmethyl)aniline (1d)[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 – 7.23 (m, 2H, Ar-H), 6.55 – 6.48 (m, 2H, Ar-H), 3.91 (s, 1H, NH), 3.57 – 3.48 (m, 1H, NC*H*H), 3.23 – 3.13 (m, 2H, NCH*H*+CH), 2.84 – 2.78 (m, 1H, OC*H*H), 2.70 – 2.64 (m, 1H, OCH*H*).

4-nitro-*N*-(oxiran-2-ylmethyl)aniline (1e) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 – 8.01 (m, 2H, Ar-H), 6.66 – 6.53 (m, 2H, Ar-H), 4.79 (s, 1H, NH), 3.74 – 3.64 (m, 1H, NC*H*H), 3.38 – 3.26 (m, 1H, NCH*H*), 3.25 – 3.18 (m, 1H, CH), 2.85 (t, *J* = 4.3 Hz, 1H, OC*H*H), 2.67 (dd, *J* = 4.8, 2.6 Hz, 1H, OCH*H*). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.4, 138.3, 126.4, 111.4 (Ar-C), 50.5 (NCH_2), 45.1 (CH), 44.4 (OCH_2). HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_9H_{10}N_2O_3Na$ 217.0589; Found 217.0575.

***N*-(oxiran-2-ylmethyl)-4-(trifluoromethyl)aniline (1f)** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.36 (m, 2H, Ar-H), 6.70 – 6.60 (m, 2H, Ar-H), 4.21 (s, 1H, NH), 3.60 (dd, *J* = 13.9, 2.6 Hz, 1H, NC*H*H), 3.32 – 3.12 (m, 2H, NCH*H*+CH), 2.84 (t, *J* = 4.4 Hz, 1H, OC*H*H), 2.68 (dd, *J* = 4.9, 2.6 Hz, 1H, OCH*H*). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.5 (Ar-C), 126.8 (t, *J* = 3.8 Hz) (Ar-C), 129.1 – 123.7 (d, *J* = 271.7 Hz) (CF_3), 119.4 (q, *J* = 32.4 Hz) (Ar-C), 112.2 (Ar-C), 50.8 (NCH_2), 45.3 (CH), 44.5 (OCH_2). ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.13. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{10}H_{11}F_3NO$ 218.0794; Found 218.0779.

4-methyl-*N*-(oxiran-2-ylmethyl)aniline (1g)[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.06 – 6.97 (m, 2H, Ar-H), 6.62 – 6.56 (m, 2H, Ar-H), 3.77 (s, 1H, NH), 3.58 – 3.46 (m, 1H, NC*H*H), 3.27 – 3.16 (m, 2H, NCH*H*+CH), 2.82 (dd, *J* = 4.9, 3.8 Hz, 1H, OC*H*H), 2.70 (dd, *J* = 5.0, 2.4 Hz, 1H, OCH*H*), 2.26 (s, 3H, CH_3).

4-(*tert*-butyl)-*N*-(oxiran-2-ylmethyl)aniline (1h) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.21 (m, 2H, Ar-H), 6.69 – 6.59 (m, 2H, Ar-H), 3.80 (s, 1H, NH), 3.60 – 3.48 (m, 1H, NC*H*H), 3.32 – 3.20 (m, 2H, NCH*H*+CH), 2.84 (t, *J* = 4.3 Hz, 1H, OC*H*H), 2.73 (dd, *J* = 5.0, 2.2 Hz, 1H, OCH*H*), 1.32 (s, 9H, $C(CH_3)_3$). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.5, 140.7, 126.1, 112.8 (Ar-C), 51.2 (NCH_2), 45.4 (CH), 45.4 (OCH_2), 33.9 ($C(CH_3)_3$), 31.6 (CH_3). HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{13}H_{20}NO$ 206.1545; Found 206.1537.

2-fluoro-*N*-(oxiran-2-ylmethyl)aniline (1i) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.04 – 6.94 (m, 2H, Ar-H), 6.78 – 6.72 (m, 1H, Ar-H), 6.69 – 6.62 (m, 1H, Ar-H), 4.15 (s, 1H, NH), 3.56 (dd, *J* = 13.9, 3.1 Hz, 1H, NC*H*H), 3.33 – 3.16 (m, 2H, NCH*H*+CH), 2.83 (dd, *J* = 5.0, 3.9 Hz, 1H, OC*H*H), 2.70 (dd, *J* = 4.9, 2.6 Hz, 1H, OCH*H*). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.6 (d, *J* = 238.6 Hz), 136.4 (d, *J* = 11.6 Hz), 124.6 (d, *J* = 3.6 Hz), 117.2 (d, *J* = 7.0 Hz), 114.6 (d, *J* = 18.5 Hz), 112.3 (d, *J* = 3.2 Hz) (Ar-C), 50.9 (NCH_2), 45.2 (CH), 44.9 (OCH_2). ^{19}F NMR (376 MHz, $CDCl_3$) δ -136.16. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_9H_{11}FNO$ 168.0825; Found 168.0839.

2-chloro-*N*-(oxiran-2-ylmethyl)aniline (1j) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.25 (m, 1H, Ar-H), 7.21 – 7.14 (m, 1H, Ar-H), 6.78 – 6.65 (m, 2H, Ar-H), 4.56 (t, *J* = 6.1 Hz, 1H, NH), 3.66 – 3.55 (m, 1H, NC*H*H), 3.38 – 3.28 (m, 1H, NCH*H*), 3.24 (p, *J* = 3.4 Hz, 1H, CH), 2.86 (dd, *J* = 4.4, 2.7 Hz, 1H, OC*H*H), 2.72 (dd, *J* = 4.9, 2.7 Hz, 1H, OCH*H*). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.8, 129.3, 127.9, 119.4, 117.8, 111.4 (Ar-C), 50.9 (NCH_2), 45.3 (CH), 44.9 (OCH_2). HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_9H_{10}ClNONa$ 206.0349; Found 206.0330.

2-bromo-*N*-(oxiran-2-ylmethyl)aniline (1k) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.30 (m, 1H, Ar-H), 7.13 – 7.04 (m, 1H, Ar-H), 6.65 – 6.58 (m, 1H, Ar-H), 6.54 – 6.46 (m, 1H, Ar-H), 4.44 (s, 1H, NH), 3.52 – 3.41 (m, 1H, NC*H*H), 3.25 – 3.17 (m,

1H, NCH*H*), 3.15 – 3.09 (m, 1H, CH), 2.73 (dd, *J* = 4.9, 4.0 Hz, 1H, OC*H*H), 2.60 (dd, *J* = 4.9, 2.6 Hz, 1H, OCH*H*). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.7, 132.6, 128.6, 118.4, 111.5, 110.0 (Ar-C), 50.9 (NCH_2), 45.3 (CH), 45.0 (OCH_2). HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_9H_{10}BrNONa$ 249.9843; Found 249.9836.

2-methyl-*N*-(oxiran-2-ylmethyl)aniline (1l)[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 – 7.07 (m, 2H, Ar-H), 6.77 – 6.65 (m, 2H, Ar-H), 3.77 (s, 1H, NH), 3.61 (d, *J* = 11.8 Hz, 1H, NC*H*H), 3.34 – 3.25 (m, 2H, NCH*H*+CH), 2.86 (dd, *J* = 4.3, 2.2 Hz, 1H, OC*H*H), 2.73 (dd, *J* = 5.1, 2.2 Hz, 1H, OCH*H*), 2.19 (s, 3H, CH_3).

2-ethyl-*N*-(oxiran-2-ylmethyl)aniline (1m) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 – 7.06 (m, 2H, Ar-H), 6.84 – 6.66 (m, 2H, Ar-H), 3.85 (s, 1H, NH), 3.61 (d, *J* = 13.3 Hz, 1H, NC*H*H), 3.38 – 3.19 (m, 2H, NCH*H*+CH), 2.85 (dd, *J* = 4.4, 2.4 Hz, 1H, OC*H*H), 2.72 (dd, *J* = 5.0, 2.4 Hz, 1H, OCH*H*), 2.52 (q, *J* = 7.5 Hz, 2H, CH_2), 1.27 (t, *J* = 7.5 Hz, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.3, 128.2, 128.1, 127.1, 117.8, 110.3 (Ar-C), 51.1 (NCH_2), 45.5 (CH), 45.0 (OCH_2), 23.9 (CH_2), 13.0 (CH_3). HRMS (EI) *m/z*: [M] Calcd for $C_{11}H_{15}NO$ 177.1154; Found 177.1152.

2-isopropyl-*N*-(oxiran-2-ylmethyl)aniline (1n) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 – 7.09 (m, 2H, Ar-H), 6.82 – 6.75 (m, 1H, Ar-H), 6.71 – 6.66 (m, 1H, Ar-H), 3.93 (s, 1H, NH), 3.68 – 3.54 (m, 1H, NC*H*H), 3.40 – 3.22 (m, 2H, NCH*H*+CH), 2.95 – 2.83 (m, 2H, OCH_2), 2.73 (sep, 1H, $CH(CH_3)_2$), 1.27 (dd, *J* = 6.8, 4.0 Hz, 6H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.6, 132.8, 126.8, 125.3, 118.0, 110.8 (Ar-C), 51.1 (NCH_2), 45.6 (CH), 45.2 (OCH_2), 27.3 ($CH(CH_3)_2$), 22.4 (CH_3). HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{12}H_{18}NO$ 192.1388; Found 192.1388.

2-methoxy-*N*-(oxiran-2-ylmethyl)aniline (1o) ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 – 6.86 (m, 1H, Ar-H), 6.83 – 6.77 (m, 1H, Ar-H), 6.71 – 6.64 (m, 2H, Ar-H), 4.48 (s, 1H, NH), 3.86 (s, 3H, CH_3), 3.59 – 3.47 (m, 1H, NC*H*H), 3.33 – 3.21 (m, 2H, NCH*H*+CH), 2.83 (dd, *J* = 4.4, 2.5 Hz, 1H, OC*H*H), 2.70 (dd, *J* = 5.0, 2.5 Hz, 1H, OCH*H*). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.0, 137.9, 121.3, 117.1, 110.0, 109.6 (Ar-C), 55.5 (NCH_2), 51.1 (OCH_3), 45.5 (CH), 45.1 (OCH_2). HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{10}H_{14}NO$ 180.1025; Found 180.1024.

3-chloro-*N*-(oxiran-2-ylmethyl)aniline (1p)[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12 – 7.04 (m, 1H, Ar-H), 6.72 – 6.67 (m, 1H, Ar-H), 6.63-6.59 (m, 1H, Ar-H), 6.53 – 6.47 (m, 1H, Ar-H), 3.98 (s, 1H, NH), 3.58-3.46 (m, 1H, NC*H*H), 3.24 – 3.15 (m, 2H, NCH*H*+CH), 2.82 (dd, *J* = 4.9, 3.8 Hz, 1H, OC*H*H), 2.67 (dd, *J* = 4.8, 2.4 Hz, 1H, OCH*H*).

3-methyl-*N*-(oxiran-2-ylmethyl)aniline (1q)[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15 – 7.05 (m, 1H, Ar-H), 6.63 – 6.54 (m, 1H, Ar-H), 6.51 – 6.45 (m, 2H, Ar-H), 3.85 (s, 1H, NH), 3.59 – 3.47 (m, 1H, NC*H*H), 3.30 – 3.19 (m, 2H, NCH*H*+CH), 2.83 (dd, *J* = 5.7, 3.0 Hz, 1H, OC*H*H), 2.71 (dd, *J* = 5.0, 2.2 Hz, 1H, OCH*H*), 2.31 (s, 3H, CH_3).

2,6-difluoro-*N*-(oxiran-2-ylmethyl)aniline (1r) ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.86 – 6.75 (m, 2H, Ar-H), 6.71 – 6.60 (m, 1H, Ar-H), 3.82 (s, 1H, NH), 3.75 – 3.67 (m, 1H, NC*H*H), 3.43 – 3.28 (m, 1H, NCH*H*), 3.23 – 3.15 (m, 1H, CH), 2.80 (dd, *J* = 4.4, 2.7 Hz, 1H, OC*H*H), 2.68 (dd, *J* = 4.9, 2.7 Hz, 1H, OCH*H*). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.4 (dd, *J* = 240.9, 7.5 Hz), 125.5, 117.8 (t, *J* = 9.5 Hz), 112.1 – 110.4 (m) (Ar-C), 51.4 (NCH_2), 47.6 (t, *J* = 4.1 Hz, CH), 45.1 (OCH_2). ^{19}F NMR (376 MHz, $CDCl_3$) δ -128.9. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_9H_9F_2NONa$ 208.0550; Found 208.0546.

2,6-dichloro-*N*-(oxiran-2-ylmethyl)aniline (1s) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25-7.21 (m, 2H, Ar-H), 6.82-6.77 (m, 1H, Ar-H), 4.20 (s, 1H, NH), 3.69 (dd, *J* = 14.0, 5.6 Hz, 1H, NC*H*H), 3.35 (dd, *J* = 14.1, 5.6 Hz, 1H, NCH*H*), 3.20 – 3.10 (m, 1H, CH), 2.80 (dd, *J* = 4.4, 2.7 Hz, 1H, OC*H*H), 2.70 (dd, *J* = 4.9, 2.7 Hz, 1H, OCH*H*). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.2, 128.9, 126.6, 122.3 (Ar-C), 51.5 (NCH_2), 48.8 (CH), 45.5 (OCH_2). HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_9H_9Cl_2NONa$ 239.9959; Found 239.9952.

2,6-dibromo-*N*-(oxiran-2-ylmethyl)aniline (1t) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.39 (m, 2H, Ar-H), 6.73 – 6.66 (m, 1H, Ar-H), 4.11 (s, 1H, NH), 3.66 – 3.56 (m, 1H, NC*H*H), 3.34 – 3.25 (m, 1H, NCH*H*), 3.24 – 3.15 (m, 1H, CH), 2.81 (dd, *J* = 4.4, 2.6 Hz, 1H, OC*H*H), 2.72 (dd, *J* = 4.9, 2.6 Hz, 1H, OCH*H*). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.5, 132.9, 124.2, 117.6 (Ar-C), 51.7 (NCH_2), 49.6 (CH), 45.6 (OCH_2).

HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_9H_9Br_2NONa$ 327.8949; Found 327.8961.

2,6-dimethyl-*N*-(oxiran-2-ylmethyl)aniline (1u) ^1H NMR (400 MHz, $CDCl_3$) δ 7.08 – 7.00 (m, 2H, Ar-H), 6.94 – 6.83 (m, 1H, Ar-H), 3.43 – 3.36 (m, 1H, NC*H*H), 3.34 (s, 1H, NH), 3.20 – 3.13 (m, 1H, CH), 3.04 – 2.95 (m, 1H, NCH*H*), 2.84 (dd, *J* = 4.5, 2.6 Hz, 1H, OC*H*H), 2.73 (dd, *J* = 5.0, 2.6 Hz, 1H, OCH*H*), 2.35 (d, *J* = 2.7 Hz, 6H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.3, 129.9, 128.9, 122.4 (Ar-C), 51.7 (NCH_2), 50.0 (CH), 45.7 (OCH_2), 18.4 (CH_3). HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{11}H_{15}NONa$ 208.0550; Found 208.0541.

2,6-diisopropyl-*N*-(oxiran-2-ylmethyl)aniline (1v) ^1H NMR (400 MHz, $CDCl_3$) δ 7.14 – 7.05 (m, 3H, Ar-H), 3.36 – 3.18 (m, 5H, NH+CH+NC*H*H+$CH(CH_3)_2$), 2.91 (dd, *J* = 12.8, 5.6 Hz, 1H, NCH*H*), 2.85 (dd, *J* = 5.0, 3.8 Hz, 1H, OC*H*H), 2.77 (dd, *J* = 5.0, 2.5 Hz, 1H, OCH*H*), 1.25 (dd, *J* = 6.9, 1.2 Hz, 12H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.8, 142.3, 124.2, 123.6 (Ar-C), 53.1 (NCH_2), 51.6 (CH), 45.5 (OCH_2), 27.6 (*C*H$(CH_3)_2$), 24.3 (CH_3). HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{15}H_{24}NO$ 234.1858; Found 234.1855.

***N*-(oxiran-2-ylmethyl)-3,5-bis(trifluoromethyl)aniline (1w)** ^1H NMR (400 MHz, $CDCl_3$) δ 7.20 (s, 1H, Ar-H), 7.00 (s, 2H, Ar-H), 4.19 – 4.02 (m, 1H, CH), 3.76 – 3.61 (m, 2H, NCH_2), 3.44 (dd, *J* = 13.0, 4.1 Hz, 1H, OC*H*H), 3.28 (dd, *J* = 13.0, 7.2 Hz, 1H, OCH*H*), 2.50 (s, 1H, NH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.5 (Ar-C), 131.5 (q, *J* = 32.8 Hz) (Ar-C), 122.5 (q, *J* = 272.7 Hz) (CF_3), 111.3 (d, *J* = 4.0 Hz) (Ar-C), 110.2 – 109.7 (m) (Ar-C), 68.7 (NCH_2), 46.4 (CH), 45.4 (OCH_2). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.3. HRMS (EI) *m/z*: [M] Calcd for $C_{11}H_9F_6NO$ 285.0588; Found 285.0594.

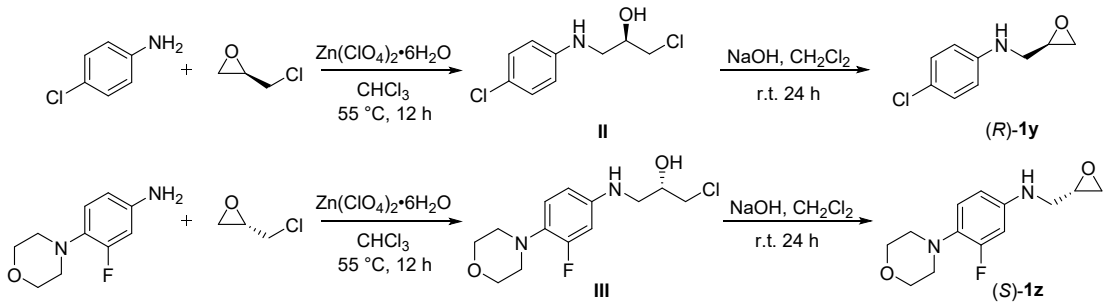
2,3,4,5,6-pentafluoro-*N*-(oxiran-2-ylmethyl)aniline (1x) ^1H NMR (400 MHz, $CDCl_3$) δ 3.85 – 3.69 (m, 2H, NH, NC*H*H), 3.38 – 3.28 (m, 1H, CH), 3.23-3.15 (m, 1H, NCH*H*), 2.84 (dd, *J* = 4.7, 4.0 Hz, 1H, OC*H*H), 2.69 (dd, *J* = 4.7, 2.6 Hz, 1H, OCH*H*). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.7 – 138.3 (m), 138.1 – 135.5 (m), 135.1 (t, *J* = 13.9 Hz), 132.7 (d, *J* = 4.2 Hz), 123.6 (t, *J* = 11.9 Hz) (Ar-C), 51.3 (NCH_2), 47.4 (t, *J* = 4.0 Hz, CH), 45.2 (OCH_2). ^{19}F NMR (376 MHz, $CDCl_3$) δ -159.4 (dd, *J* =

17.0, 5.9 Hz), -163.7 – -165.6 (m), -170.4 – -172.5 (m). HRMS (EI) *m/z*: [M] Calcd for $C_9H_6F_5NO$ 239.0370; Found 239.0372.

(*R*)-4-chloro-*N*-(oxiran-2-ylmethyl) aniline (1y)[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 – 6.97 (m, 2H, Ar-H), 6.60 – 6.43 (m, 2H, Ar-H), 3.90 (s, 1H, NH), 3.48 (dd, *J* = 13.3, 2.1 Hz, 1H, NC*H*H), 3.24 – 3.04 (m, 2H, CH, NCH*H*), 2.79 (dd, *J* = 4.8, 3.8 Hz, 1H, OC*H*H), 2.65 (dd, *J* = 4.9, 2.4 Hz, 1H, OCH*H*).

3-fluoro-4-morpholino-*N*-(oxiran-2-ylmethyl)aniline (1z)[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.85 – 6.70 (m, 1H, Ar-H), 6.37 – 6.28 (m, 2H, Ar-H), 3.91 (s, 1H, NH), 3.79 (t, *J* = 4.6 Hz, 4H, OCH_2CH_2N), 3.43 (d, *J* = 13.4 Hz, 1H, NC*H*H), 3.18 – 3.03 (m, 2H, CH, NCH*H*), 2.91 (dd, *J* = 5.8, 3.5 Hz, 4H, OCH_2CH_2N), 2.76 (dd, *J* = 4.3, 2.5 Hz, 1H, OC*H*H), 2.62 (dd, *J* = 5.0, 2.5 Hz, 1H, OCH*H*).

Scheme S2 Preparation of chiral epoxy amine (*R*)-**1y** and (*S*)-**1z**.

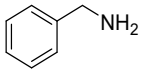
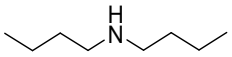
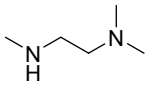
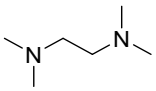
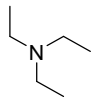
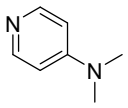
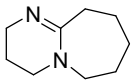


Following reported procedures,[1] 4-chloroaniline (20.0 mmol), (*R*)-epichlorohydrin (22.0 mmol) and $Zn(ClO_4)_2 \cdot 6H_2O$ (0.4 mmol, 2 mol%) were dissolved in $CHCl_3$ (50 mL). The mixture was heated under reflux for 12 hours. After reaction, all volatiles were removed in vacuo, and the (*R*)-γ-chloro-β-hydroxyaniline **II** was isolated by column chromatography (eluent: petroleum ether: ethyl acetate, from 100: 0 to 80: 20). It was then dissolved in dichloromethane (100 mL), and a 0.3 M sodium hydroxide aqueous solution (100 mL) was added. After overnight reaction at room temperature, the organic layer was separated, washed with brine (3 × 100 mL) and dried over Na_2SO_4. (*R*)-**1y** (2.06 g, 11.2 mmol, 56% yield) was obtained after removal of solvent.

(*S*)-Epoxy amine was synthesized following the same procedure from 3-fluoro-4-morpholinoaniline (20.0 mmol) and (*S*)-epichlorohydrin (22.0 mmol). (*S*)-**1z** was isolated in 2.62 g, 10.4 mmol, 52% yield.

3. Coupling reactions between epoxy amines and CO_2.

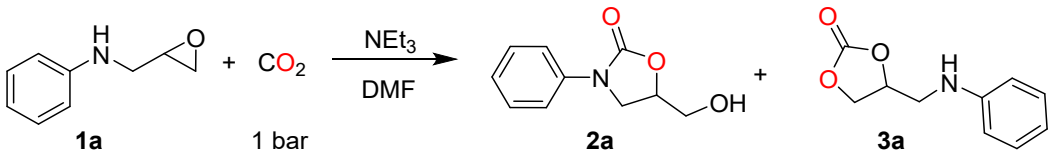
Table S1 pK_b value of various amines[a]

Entry	base	pK_b
1		8.3
2		13.75
3		(4.41)
4		(3.6)
5		6.2 (3.25)
6		7
7		1.1

[a] pK_b value of the conjugated acid in acetonitrile[2, 3] or water[4] (in parenthesis).

General procedure: epoxy amine (0.5 mmol) and amine (5 mol%) were dissolved in DMF (0.5 mL), and the flask was connected with a CO_2 balloon. The mixture was heated at 60-80 ℃ for 20 h, during which period slight blackening was observed. After reaction, the mixture was analyzed by ^1H NMR (0.1 mmol of tetraethylsilane was added as the internal standard) to determine the NMR yield, and purified by flash chromatography (eluent: petroleum ether: ethyl acetate, from 60: 40 to 0: 100) to determine the isolated yield.

Table S2 Condition optimization for the reaction of CO_2 and epoxy amine **1a**.[a]

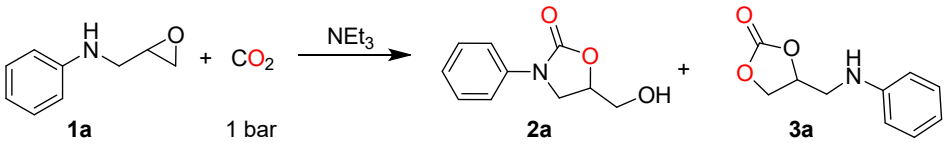


1a 1 bar **2a** **3a**

Entry	Catalyst loading (mol %)	Temp. (°C)	T (h)	Yield (%)	2a:3a
1	5	60	20	99	>99:1
2	5	50	20	76	>99:1
3	5	60	19	89	>99:1
4	5	60	18	85	>99:1
5	4	60	20	90	>99:1
6	3	60	20	88	>99:1
7	2	60	24	99	>99:1
8	-	60	20	n.d.	n.d.

[a]Reaction conditions: epoxy amine (0.5 mmol), DMF (0.5 mL) and CO_2 (1 bar). Yields and selectivity were determined by NMR spectroscopy with tetraethylsilane as an internal standard.

Table S3 Solvent optimization for the reaction of CO_2 and epoxy amine **1a**.[a]

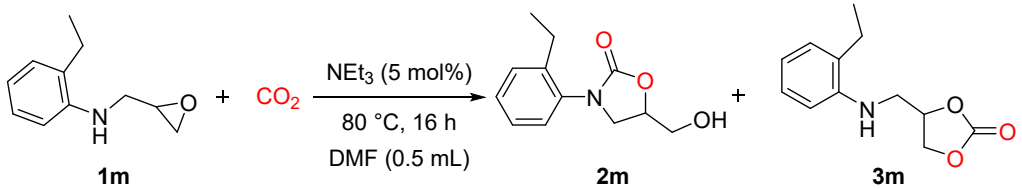


1a **2a** **3a**

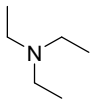
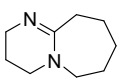
Entry	Solvent	Yield (%)	2a:3a
1	CH_3CN	72	>99:1
2	CH_2Cl_2	56	>99:1
3	EA	52	3:10
4	C_2H_5OH	80	8:1
5	Tol	26	>99:1
6	CH_3COCH_3	72	>99:1
7	PhCl	66	>99:1
8	THF	36	>99:1
9	DMF	99	>99:1
10	C_2H_5OH:DMF 9:1	82	40:1
11	C_2H_5OH:DMF 4:1	88	11:1
12	C_2H_5OH:DMF 1:1	94	47:3

[a]Reaction conditions: epoxy amine (0.5 mmol), NEt_3 (5 mol%), solvent (0.5 mL) and CO_2 (1 bar), temperature (60 °C), 20 h reaction. Yields and selectivity were determined by NMR spectroscopy with tetraethylsilane as an internal standard.

Table S4 Amine-catalyzed reaction of 2,6-dimethyl substituted amine epoxy with CO_2.[a]

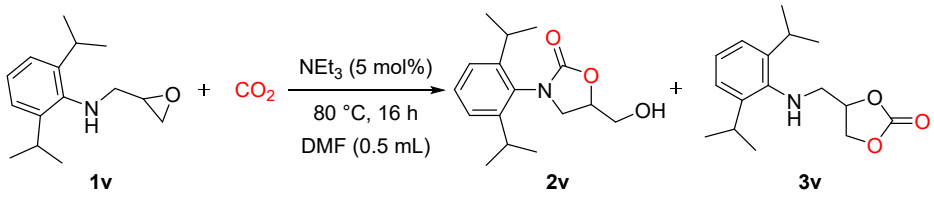


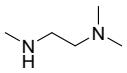
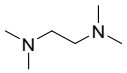
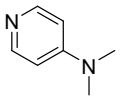
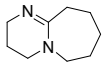
1m **2m** **3m**

Entry	Cat. (5 mol%)	Conversion (%)	Yield (%) of **2m**	**2m**:**3m**
1		96	96	>99:1
2		99	64	2:1

[a]Reaction conditions: **1m** (0.5 mmol), NEt_3 (5 mol%), DMF (0.5 mL), and CO_2 (1 bar) at 80 ºC for 16 h. Yields, conversions and selectivity were determined by NMR spectroscopy with mesitylene as an internal standard.

Table S5 Amine-catalyzed reaction of 2,6-diisopropyl substituted amine epoxy with CO_2.[a]

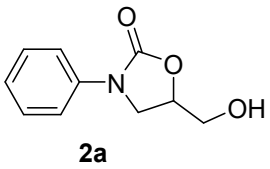


Entry	Cat. (5 mol%)	Conversion (%)	Yield (%) of **2v**	**2v**:**3v**
1		80	80	>99:1
2		82	82	>99:1
3		94	94	>99:1
4		76	76	>99:1
5		90	70	4:1

[a]Reaction conditions: **1v** (0.5 mmol), NEt_3 (5 mol%), DMF (0.5 mL), and CO_2 (1 bar) at 80 ºC for 16 h. Yields, conversions and selectivity were determined by NMR spectroscopy with tetraethylsilane as an internal standard.

Characterization data:

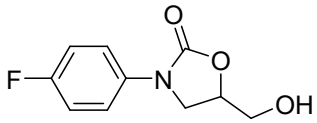
5-(hydroxymethyl)-3-phenyloxazolidin-2-one (2a)[1]



2a

White solid, isolated in 96.0 mg, 0.5 mmol, 99% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.51 (m, 2H, Ar-H), 7.41 – 7.32 (m, 2H, Ar-H), 7.17 – 7.10 (m, 1H, Ar-H), 4.77 – 4.68 (m, 1H, CH), 4.09 – 3.92 (m, 3H, NCH_2+C*H*HOH), 3.80 – 3.76 (m, 1H, CH*H*OH), 2.65 (br-s, J = 6.2 Hz, 1H, OH).

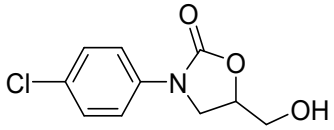
(4-fluorophenyl)-5-(hydroxymethyl)oxazolidin-2-one (2b)[1]



2b

White solid, isolated in 100.0 mg, 0.47 mmol, 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.42 (m, 2H, Ar-H), 7.11 – 7.02 (m, 2H, Ar-H), 4.79 – 4.65 (m, 1H, CH), 4.08 – 3.89 (m, 3H, NCH_2+C*H*HOH), 3.75 (dd, *J* = 12.6, 3.9 Hz, 1H, CH*H*OH), 2.59 (br-s, 1H, OH).

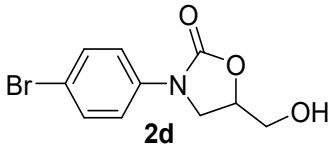
(4-chlorophenyl)-5-(hydroxymethyl)oxazolidin-2-one (2c)[1]



2c

Pale yellow solid, isolated in 100.1 mg, 0.44 mmol, 88% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.44 (m, 2H, Ar-H), 7.35 – 7.29 (m, 2H, Ar-H), 4.73 (tt, *J* = 7.3, 3.5 Hz, 1H, CH), 4.06 – 3.90 (m, 3H, NCH_2+C*H*HOH), 3.74 (dd, *J* = 12.7, 3.8 Hz, 1H, CH*H*OH), 2.74 (br-s, 1H, OH).

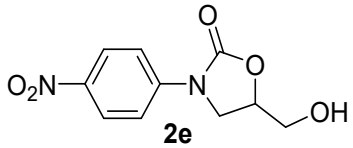
(4-bromophenyl)-5-(hydroxymethyl)oxazolidin-2-one (2d)[1]



2d

Yellow solid, isolated in 114.3 mg, 0.42 mmol, 81%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.37 (m, 4H, Ar-H), 4.78 – 4.68 (m, 1H, CH), 4.06 – 3.92 (m, 3H, NCH_2+C*H*HOH), 3.73 (dd, *J* = 12.7, 3.8 Hz, 1H, CH*H*OH), 2.74 (br-s, 1H, OH).

5-(hydroxymethyl)-3-(4-nitrophenyl)oxazolidin-2-one (2e)

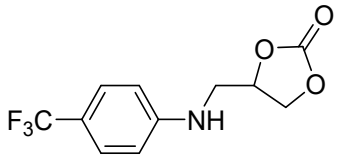


2e

Yellow solid, isolated in 120.4 mg, 0.43 mmol, 86% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.33 – 8.22 (m, 2H, Ar-H), 7.87 – 7.76 (m, 2H, Ar-H), 5.25 (t, *J* = 5.6 Hz, 1H, OH), 4.83 – 4.70 (m, 1H, CH), 4.18 (dd, *J* = 9.1, 6.0 Hz, 1H, NC*H*H), 3.92 (dd, *J* = 9.0, 6.0 Hz, 1H, NCH*H*), 3.76-3.64 (m, 1H, C*H*HOH), 3.64-3.52 (m, 1H,

CH*H*OH). ^{13}C NMR (101 MHz, DMSO-d_6) δ 154.2 (C=O), 144.4, 142.1, 124.9, 117.4 (Ar-C), 73.6 (CH), 61.5 (NCH_2), 46.0 (CH_2OH). HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{10}H_{10}N_2O_5Na$ 261.0487; Found 261.0499.

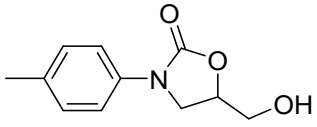
4-(((4-(trifluoromethyl)phenyl)amino)methyl)-1,3-dioxolan-2-one (3f)



3f

White solid, isolated in 99.3 mg, 0.38 mmol, 76%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.33 (m, 2H, Ar-H), 6.72 – 6.57 (m, 2H, Ar-H), 4.99 – 4.83 (m, 1H, CH), 4.60 – 4.46 (m, 2H, NCH_2), 4.26 (dd, *J* = 8.7, 6.7 Hz, 1H, NH), 3.62 – 3.38 (m, 2H, C*H*$_2$OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.9 (C=O), 149.5 (Ar-C), 126.9 (q, *J* = 4.0 Hz) (Ar-C), 128.7 – 123.3 (t, *J* = 271.7 Hz) (CF_3), 120.4 (q, *J* = 30.3 Hz) (Ar-C), 112.4 (Ar-C), 75.4 (CH), 67.1 (NCH_2), 45.3 (CH_2OH). ^{19}F NMR (376 MHz, $CDCl_3$) δ -118.25. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{11}H_{10}F_3NO_3Na$ 284.0510; Found 284.0505.

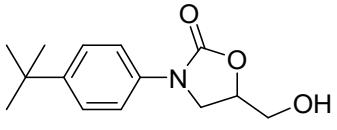
5-(hydroxymethyl)-3-(p-tolyl)oxazolidin-2-one (2g)[1]



2g

White solid, isolated in 102.4 mg, 0.49 mmol, 96%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.36 (m, 2H, Ar-H), 7.22 – 7.12 (m, 2H, Ar-H), 4.80 – 4.61 (m, 1H, CH), 4.05 – 3.89 (m, 3H, NCH_2+C*H*HOH), 3.75 (dd, *J* = 12.6, 4.2 Hz, 1H, CH*H*OH), 2.33 (s, 3H, CH_3), 1.93 (br-s, 1H, OH).

4-(4-(*tert*-butyl)phenyl)-5-(hydroxymethyl)oxazolidin-2-one (2h)

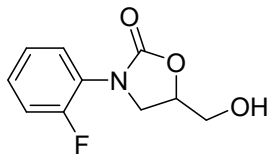


2h

Pale yellow solid, isolated in 114.6 mg, 0.46 mmol, 92%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.44 (m, 2H, Ar-H), 7.42 – 7.34 (m, 2H, Ar-H), 4.79 – 4.65 (m, 1H, CH),

4.10 – 3.89 (m, 3H, NCH_2+C*H*HOH), 3.75 (dd, *J* = 12.6, 4.2 Hz, 1H, CH*H*OH), 1.31 (s, 9H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.2 (C=O), 147.3, 135.6, 126.0, 118.3 (Ar-C), 73.1 (CH), 62.9 (NCH_2), 46.6 (CH_2OH), 34.5 ($C(CH_3)_3$), 31.4 (CH_3). HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{14}H_{19}NO_3Na$ 272.1263; Found 272.1261.

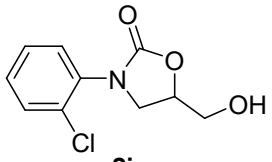
3-(2-fluorophenyl)-5-(hydroxymethyl)oxazolidin-2-one (2i)



2i

White solid, isolated in 100.4 mg, 0.48 mmol, 95%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.48 (m, 1H, Ar-H), 7.29 – 7.22 (m, 1H, Ar-H), 7.20 – 7.10 (m, 2H, Ar-H), 4.84 – 4.71 (m, 1H, CH), 4.07 (t, *J* = 8.8 Hz, 1H, NC*H*H), 4.00 – 3.93 (m, 2H, NCH*H*+ C*H*HOH), 3.76 (dd, *J* = 12.6, 4.3 Hz, 1H, CH*H*OH), 2.65 (br-s, 1H, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.3 (C=O), 156.0 (d, *J* = 44.3 Hz), 128.5 (d, *J* = 7.8 Hz), 127.4 (d, *J* = 1.4 Hz), 125.2 (d, *J* = 11.0 Hz), 124.8 (d, *J* = 3.7 Hz), 116.8 (d, *J* = 20.0 Hz) (Ar-C), 74.3 (CH), 63.0 (NCH_2), 48.2 (CH_2OH). ^{19}F NMR (376 MHz, $CDCl_3$) δ -120.71. HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{10}H_{10}FNO_3Na$ 234.0543; Found 234.0558.

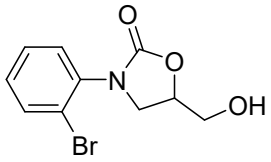
3-(2-chlorophenyl)-5-(hydroxymethyl)oxazolidin-2-one (2j)



2j

White solid, isolated in 103.5 mg, 0.46 mmol, 91%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.40 (m, 1H, Ar-H), 7.39 – 7.34 (m, 1H, Ar-H), 7.33 – 7.23 (m, 2H, Ar-H), 4.82 – 4.70 (m, 1H, CH), 3.98 (dd, *J* = 8.7, 6.4 Hz, 1H, NC*H*H), 3.89 (dd, *J* = 12.6, 3.4 Hz, 1H, C*H*HOH), 3.84 (dd, *J* = 8.5, 6.4 Hz, 1H, NCH*H*), 3.71 (dd, *J* = 12.6, 4.4 Hz, 1H, CH*H*OH), 3.27 (br-s, 1H, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.8 (C=O), 134.7, 132.5, 130.6, 129.7, 129.6, 128.1 (Ar-C), 74.6 (CH), 62.9 (NCH_2), 48.3 (CH_2OH). HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{10}H_{10}ClNO_3Na$ 250.0247; Found 250.0260.

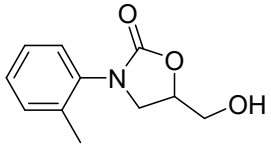
3-(2-bromophenyl)-5-(hydroxymethyl)oxazolidin-2-one (2k)



2k

White solid, isolated in 115.6 mg, 0.43 mmol, 85%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.53 (m, 1H, Ar-H), 7.36 – 7.26 (m, 2H, Ar-H), 7.22 – 7.11 (m, 1H, Ar-H), 4.78 – 4.66 (m, 1H, CH), 3.95 (t, *J* = 8.7 Hz, 1H, NC*H*H), 3.90 – 3.75 (m, 2H, NCH*H*+ C*H*HOH), 3.73-3.65 (m, 1H, CH*H*OH), 3.44 (br-s, 1H, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.8 (C=O), 136.2, 133.7, 130.0, 129.9, 128.8, 122.6 (Ar-C), 74.7 (CH), 62.8 (NCH_2), 48.5 (CH_2OH). HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{10}H_{10}BrNO_3Na$ 293.9742; Found 293.9749.

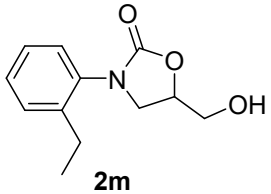
5-(hydroxymethyl)-3-(o-tolyl)oxazolidin-2-one (2l)[1]



2l

White solid, isolated in 100.0 mg, 0.46 mmol, 96%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 – 7.10 (m, 4H, Ar-H), 4.72 – 4.62 (m, 1H, CH), 3.90 – 3.76 (m, 3H, NCH_2+C*H*HOH), 3.60 (dd, *J* = 12.7, 3.6 Hz, 1H, CH*H*OH), 3.33 (br-s, 1H, OH), 2.23 (s, 3H, CH_3).

3-(2-ethylphenyl)-5-(hydroxymethyl)oxazolidin-2-one (2m)

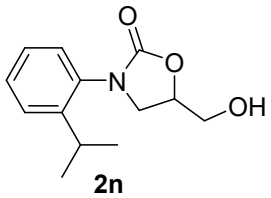


2m

White solid, isolated in 110.6 mg, 0.43 mmol, 86%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.27 (m, 2H, Ar-H), 7.27 – 7.20 (m, 2H, Ar-H), 4.81 – 4.65 (m, 1H, CH), 3.99 – 3.81 (m, 3H, NCH_2+C*H*HOH), 3.68 (dd, *J* = 12.6, 3.8 Hz, 1H, CH*H*OH), 3.42 (br-s, 1H, OH), 2.65 (q, *J* = 7.6 Hz, 2H, CH_2), 1.23 (t, *J* = 7.6 Hz, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.1 (C=O), 142.2, 135.4, 129.4, 128.7, 127.3, 127.0 (Ar-C), 74.1

(CH), 62.8 (NCH_2), 49.7 (CH_2OH), 24.0 (CH_2), 14.5 (CH_3). HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{12}H_{15}NO_3Na$ 244.0950; Found 244.0944.

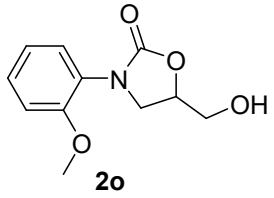
4-(hydroxymethyl)-3-(2-isopropylphenyl)oxazolidin-2-one (2n)



2n

White solid, isolated in 117.6 mg, 0.5 mmol, 97%. ^1H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.22 (m, 2H, Ar-H), 7.18 – 7.09 (m, 2H, Ar-H), 4.71 – 4.57 (m, 1H, CH), 3.87 – 3.48 (m, 5H, NCH_2+CH_2OH, OH), 3.04 (hept, *J* = 7.0 Hz, 1H, C*H*(CH_3)$_2$), 1.15 (t, *J* = 6.5 Hz, 6H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.6 (C=O), 147.2, 134.7, 129.0, 127.7, 127.0, 126.9 (Ar-C), 74.2 (CH), 62.8 (NCH_2), 50.3 (CH_2OH), 28.1 (*C*H(CH_3)$_2$), 23.9 (CH_3). HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{13}H_{17}NO_3Na$ 258.1101; Found 258.1103.

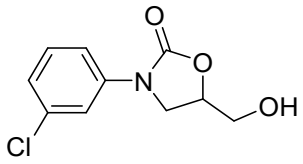
5-(hydroxymethyl)-3-(2-methoxyphenyl)oxazolidin-2-one (2o)



2o

White solid, isolated in 101.5 mg, 0.45 mmol, 91%. ^1H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.24 (m, 2H, Ar-H), 7.00 – 6.88 (m, 2H, Ar-H), 4.79 – 4.60 (m, 1H, CH), 3.97 (t, *J* = 8.8 Hz, 1H, NC*H*H), 3.87 – 3.70 (m, 6H, NCH*H*+C*H*$_2$OH+CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.2 (C=O), 155.0, 129.1, 128.5, 125.8, 121.0, 112.1 (Ar-C), 74.4 (CH), 63.2 (NCH_2), 55.7 (CH_2OH), 48.4 (OCH_3). HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{11}H_{13}NO_4Na$ 246.0742; Found 246.0738.

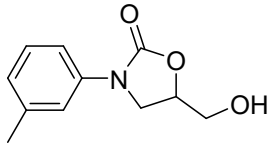
3-(3-chlorophenyl)-5-(hydroxymethyl)oxazolidin-2-one (2p)[1]



2p

Pale yellow solid, isolated in 110.0 mg, 0.48 mmol, 97%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.46 (m, 1H, Ar-H), 7.29 – 7.23 (m, 1H, Ar-H), 7.20 – 7.12 (m, 1H, Ar-H), 7.01 – 6.94 (m, 1H, Ar-H), 4.68 – 4.55 (m, 1H, CH), 3.93 – 3.79 (m, 3H, NCH_2+C*H*HOH), 3.75 (s, 1H, CH*H*OH), 3.67 – 3.56 (m, 1H, OH).

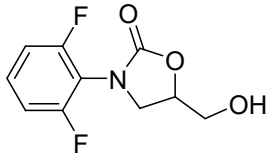
5-(hydroxymethyl)-3-(m-tolyl)oxazolidin-2-one (2q)[1]



2q

Dark solid, isolated in 103.6 mg, 0.38 mmol, 75%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.35 (m, 1H, Ar-H), 7.32 – 7.27 (m, 1H, Ar-H), 7.26 – 7.21 (m, 1H, Ar-H), 6.97 – 6.92 (m, 1H, Ar-H), 4.79 – 4.63 (m, 1H, CH), 4.07 – 3.90 (m, 3H, NCH_2+C*H*HOH), 3.73 (dd, *J* = 12.6, 4.2 Hz, 1H, CH*H*OH), 2.40 – 2.30 (m, 3H, CH_3).

3-(2,6-difluorophenyl)-5-(hydroxymethyl)oxazolidin-2-one (2r)

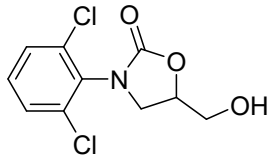


2r

White solid, isolated in 101.8 mg, 0.44 mmol, 89%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.21 (m, 1H, Ar-H), 7.01 – 6.89 (m, 2H, Ar-H), 4.86 – 4.72 (m, 1H, CH), 3.94 (t, *J* = 8.6 Hz, 1H, NC*H*H), 3.88 (dd, *J* = 12.5, 3.7 Hz, 1H, C*H*HOH), 3.81 (dd, *J* = 8.4, 6.5 Hz, 1H, NCH*H*), 3.73 (dd, *J* = 12.5, 4.5 Hz, 1H, CH*H*OH), 3.32 (br-s, 1H, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.3 (d, *J* = 253.3 Hz) (Ar-C), 156.0 (C=O), 129.7 (d, *J* = 10.1 Hz) (Ar-C), 112.4 (d, *J* = 3.6 Hz) (Ar-C), 112.2 (d, *J* = 3.5 Hz) (Ar-C), 75.1 (CH), 62.9 (NCH_2), 47.8 (CH_2OH). ^{19}F NMR (376 MHz, $CDCl_3$) δ -117.35.

HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{10}H_9F_2NO_3Na$ 252.0448; Found 252.0444.

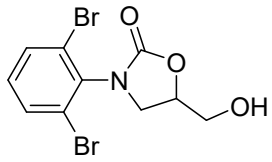
3-(2,6-dichlorophenyl)-5-(hydroxymethyl)oxazolidin-2-one (2s)



2s

White solid, isolated in 115.4 mg, 0.44 mmol, 88%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.29 (m, 2H, Ar-H), 7.24 – 7.16 (m, 1H, Ar-H), 4.85 – 4.72 (m, 1H, CH), 3.94 – 3.83 (m, 2H, NCH_2), 3.80 – 3.70 (m, 2H, C*H*$_2$OH), 3.00 (br-s, 1H, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.6 (C=O), 135.7, 135.7, 132.0, 130.4, 128.9, 128.9 (Ar-C), 74.9 (CH), 63.1 (NCH_2), 46.5 (CH_2OH). HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{10}H_9Cl_2NO_3Na$ 283.9857; Found 283.9862.

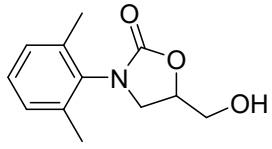
3-(2,6-dibromophenyl)-5-(hydroxymethyl)oxazolidin-2-one (2t)



2t

Pale yellow solid, isolated in 150.9 mg, 0.43 mmol, 86%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.50 (m, 2H, Ar-H), 7.17 – 7.01 (m, 1H, Ar-H), 4.92 – 4.74 (m, 1H, CH), 3.97 – 3.86 (m, 2H, NCH_2), 3.85 – 3.76 (m, 2H, C*H*$_2$OH), 3.74 – 3.58 (m, 1H, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.6 (C=O), 134.5, 132.8, 132.7, 131.4, 125.3, 125.3 (Ar-C), 75.1 (CH), 63.0 (NCH_2), 46.5 (CH_2OH). HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{10}H_9Br_2NO_3Na$ 371.8847; Found 371.8842.

3-(2,6-dimethylphenyl)-5-(hydroxymethyl)oxazolidin-2-one (2u)

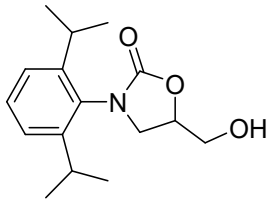


2u

White solid, isolated in 90.2 mg, 0.41 mmol, 82%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 – 7.16 (m, 1H, Ar-H), 7.14 – 7.09 (m, 2H, Ar-H), 4.87 – 4.77 (m, 1H, CH), 4.02 (dd, *J* = 12.7, 3.0 Hz, 1H, NC*H*H), 3.89 – 3.69 (m, 3H, NCH*H*+CH_2OH), 2.96 (br-s, 1H, OH), 2.31 (s, 6H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.5 (C=O), 137.1,

136.7, 133.8, 128.9, 128.7, 128.7 (Ar-C), 74.1 (CH), 62.8 (NCH_2), 47.1 (CH_2OH), 17.8, 17.7 (CH_3). HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{12}H_{15}NO_3Na$ 244.0950; Found 244.0961.

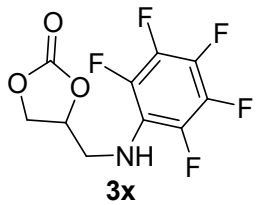
3-(2,6-diisopropylphenyl)-5-(hydroxymethyl)oxazolidin-2-one (2v)



2v

Dark solid, isolated in 120.6 mg, 0.44 mmol, 87%. ^1H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.31 (m, 1H, Ar-H), 7.24-7.15 (m, 2H, Ar-H), 4.84 – 4.73 (m, 1H, CH), 3.96 (dd, *J* = 12.5, 3.2 Hz, 1H, NC*H*H), 3.83 – 3.74 (m, 2H, CH_2OH), 3.69 (dd, *J* = 12.6, 3.8 Hz, 1H, NCH*H*), 3.43 (br-s, 1H, OH), 3.19 – 2.88 (m, 2H, C*H*$(CH_3)_2$), 1.24 (q, *J* = 7.5 Hz, 12H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.5 (C=O), 146.7, 146.3, 130.2, 128.4, 123.3, 123.2 (Ar-C), 72.9 (CH), 61.7 (NCH_2), 48.9 (CH_2OH), 27.7, 27.4 (*C*H$(CH_3)_2$), 23.5, 23.3, 23.2, 23.1 (CH_3). HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{16}H_{23}NO_3Na$ 300.1570; Found 300.1564.

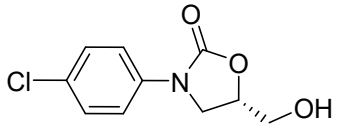
4-(((perfluorophenyl)amino)methyl)-1,3-dioxolan-2-one (3x)



3x

Dark solid, isolated in 107.6 mg, 0.38 mmol, 76%. ^1H NMR (400 MHz, $CDCl_3$) δ 4.93 – 4.82 (m, 1H, CH), 4.03 – 3.95 (m, 2H, NC*H*H+OC*H*H), 3.90 (dd, *J* = 8.1, 6.5 Hz, 1H, NCH*H*), 3.75 (dd, *J* = 12.8, 3.9 Hz, 1H, OCH*H*), 3.01 (s, 1H, NH). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.5 (C=O), 146.05 – 143.02 (m), 141.34 (m), 139.45 – 136.05 (m), 112.56 – 111.80 (m) (Ar-C), 75.4 (CH), 62.4 (NCH_2), 47.4 (CH_2OH). ^{19}F NMR (376 MHz, $CDCl_3$) δ -144.31 (d, *J* = 21.0 Hz), -153.57 (t, *J* = 21.4 Hz), -161.09 – -161.41 (m). HRMS (ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{10}H_6F_5NO_3$ 306.0166; Found 306.0169.

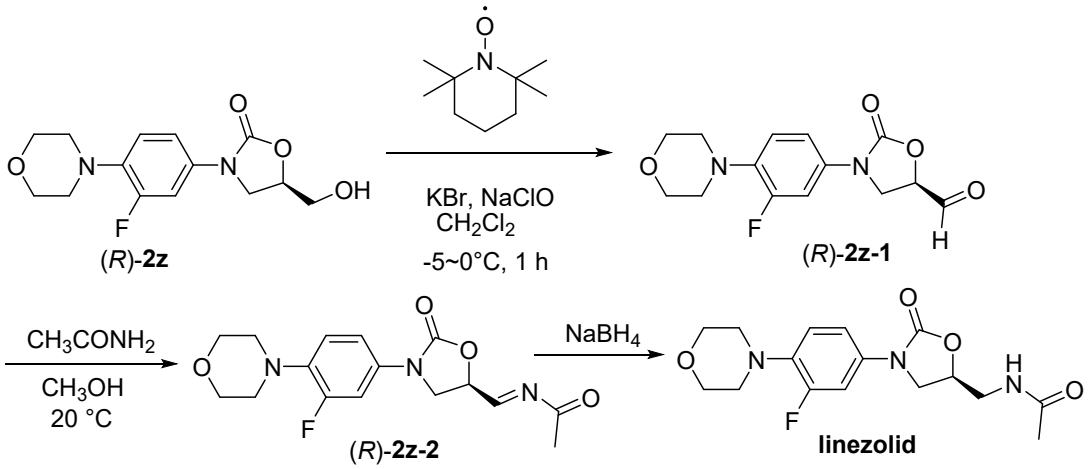
(*S*)-**3-(4-chlorophenyl)-5-(hydroxymethyl)oxazolidin-2-one ((*S*)-2y)**[1]



(*S*)-**2y**

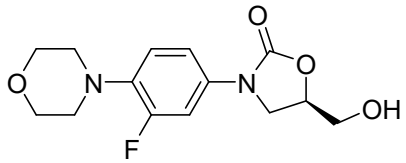
White solid, isolated in 99.0 mg, 0.44 mmol, 87%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.45 (m, 2H, Ar-H), 7.34 – 7.28 (m, 2H, Ar-H), 4.81 – 4.66 (m, 1H, CH), 4.07 – 3.92 (m, 3H, NCH_2+C*H*HOH), 3.74 (dd, *J* = 12.7, 3.8 Hz, 1H, CH*H*OH), 2.74 (br-s, 1H, OH).

Scheme S3 Preparation of linezolid.



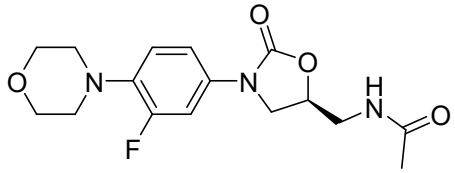
Following a reported procedure,[5] (*R*)-**2z** (1 g, 3.4 mmol) was dissolved in dichloromethane (5 mL). 20% potassium bromide aqueous solution (0.05 g) was added. The mixture was cooled to -5 ℃, and 2,2,6,6-tetramethylpiperidinooxy (0.01 g, 0.05 mmol) was added, followed by dropwise addition of 6.5% sodium hypochlorite solution (10 g). The mixture was left at 0 ℃ for 1 hour, which was then extracted by dichloromethane (3 × 15 mL). The organic phase was combined, and dried with anhydrous sodium sulfate. The crude product (*R*)-**2z-1** (0.73 g, 2.5 mmol, 90%) was obtained after removal of solvent.

The crude (*R*)-**2z-1** (0.73 g) was dissolved in methanol (12 mL), and acetamide (0.15 g, 2.5 mmol) was added slowly. The reaction was monitored by liquid chromatography. After 24 h reaction, sodium borohydride (0.113 g, 3 mmol) was added, and linezolid (0.40 g, 1.1 mmol, 54% yield) was collected as a precipitate.



(*R*)-**2z**

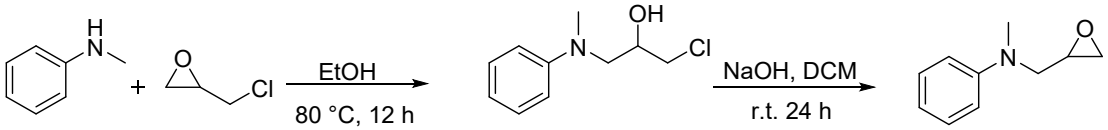
White solid.[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.36 (m, 1H, Ar-H), 7.17 – 7.07 (m, 1H, Ar-H), 6.99 – 6.82 (m, 1H, Ar-H), 4.87 – 4.58 (m, 1H, CH), 4.03 – 3.90 (m, 3H, NCH_2+C*H*HOH), 3.89 – 3.84 (m, 4H, O*C*H_2CH_2N), 3.74 (dd, *J* = 12.6, 4.0 Hz, 1H, CH*H*OH), 3.08 – 3.01 (m, 4H, OCH_2C*H*$_2$N), 2.64 (br-s, 1H, OH).



linezolid

White solid.[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (m, 1H), 7.09 (m, 1H), 6.92 (m, 1H), 4.78 (m, 1H, CH), 4.05 (dd, *J* = 8.8, 6.3 Hz, 1H, NHC*H*H), 3.93 – 3.81 (m, 4H, O*C*H_2CH_2N), 3.65 (dd, *J* = 9.1, 6.3 Hz, 1H, NHCH*H*), 3.31 (t, *J* = 5.4 Hz, 2H, NCH_2), 3.10 – 3.02 (m, 4H, OCH_2C*H*$_2$N), 2.39 (s, 3H, CH_3).

Scheme S4 Preparation of *N*-methyl-*N*-(oxiran-2-ylmethyl)aniline.



III

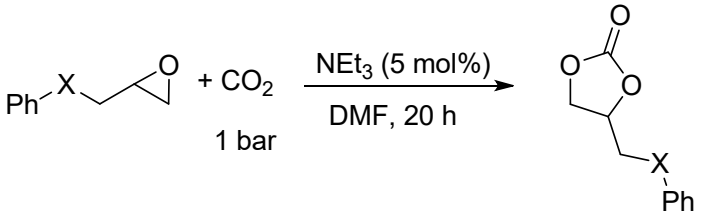
N-methyl aniline (20.0 mmol) and epichlorohydrin (22.0 mmol) were dissolved in ethanol (50 mL). The mixture was heated under reflux for 12 hours. After reaction, all volatiles were removed in vacuo, and the γ-chloro-β-hydroxyaniline **III** was isolated by column chromatography (eluent: petroleum ether: ethyl acetate, from 100: 0 to 80: 20). It was then dissolved in dichloromethane (100 mL), and a 0.3 M sodium hydroxide aqueous solution (100 mL) was added. After overnight reaction at room temperature, the organic layer was separated, washed with brine (3 × 100 mL) and dried over Na_2SO_4. Epoxy amine was obtained after removal of solvent.

***N*-methyl-*N*-(oxiran-2-ylmethyl)aniline**[6]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (t, *J* = 8.0 Hz, 2H, Ar-H), 6.82 (dd, *J* = 13.4, 7.5 Hz, 3H, Ar-H), 3.71 (dd, *J* = 15.7, 3.1 Hz, 1H, CH), 3.45 (dd, *J* = 15.7, 4.9 Hz, 1H, NC*H*H), 3.21 (t, *J* = 3.9 Hz, 1H, NCH*H*), 3.06 (d, *J* = 1.7 Hz, 3H, CH_3), 2.84 (t, *J* = 4.5 Hz, 1H, OC*H*H), 2.63 (dd, *J* = 5.1, 2.6 Hz, 1H, OCH*H*).

Reaction of phenylglycidylether and *N*-methyl epoxy amine with CO_2.

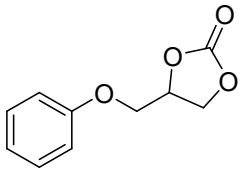
Table S6 Reaction of alkylene oxide with CO_2[a].



Entry	X	Tempeture (°C)	Yield (%)
1	O	80	60
2[b]	CH_3N	80	-
3[b]	CH_3N	120	14

[a]Reaction conditions: alkylene oxide (1 mmol), NEt_3 (5 mol%), DMF (1 mL), and CO_2 (1 bar). Isolated yields. [b]Yields were determined by ^{1}H NMR spectroscopy with mesitylene as an internal standard.

4-(phenoxymethyl)-1,3-dioxolan-2-one[7]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.27 (m, 2H, Ar-H), 7.01 (t, *J* = 7.4 Hz, 1H, Ar-H), 6.94 – 6.87 (m, 2H, Ar-H), 5.02 (m, 1H, CH), 4.60 (t, *J* = 8.4 Hz, 1H, OC*H*H), 4.52 (dd, *J* = 8.5, 5.9 Hz, 1H, OCH*H*), 4.23 (dd, *J* = 10.6, 4.1 Hz, 1H, PhOC*H*H), 4.13 (dd, *J* = 10.6, 3.6 Hz, 1H, PhOCH*H*).

4. Kinetic study

Determination of rate order of CO_2

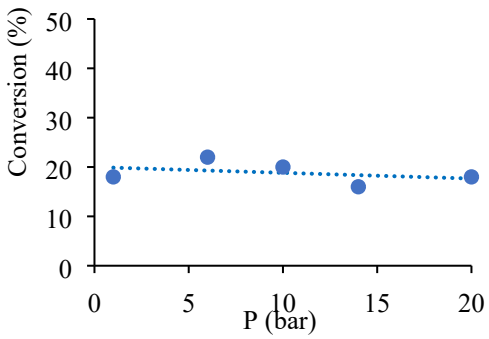


Fig. S1 Plot of conversion of epoxy amine versus pressure (bar) for the reaction of *N*-(oxiran-2-ylmethyl)aniline (**1a**) and CO_2 catalyzed by NEt_3. Conditions: *N*-(oxiran-2-ylmethyl)aniline (0.5 mmol), NEt_3 (5 mol %), 60 °C, 4 h.

Determination of rate order of epoxy amine

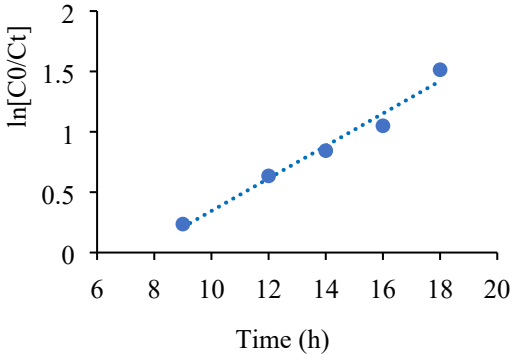


Fig. S2 Plot of $\ln[C_0/C_t]$ versus time (h) for the reaction of *N*-(oxiran-2-ylmethyl)aniline (**1a**) and CO_2 catalyzed by NEt_3. Conditions: *N*-(oxiran-2-ylmethyl)aniline (0.5 mmol), NEt_3 (5 mol %), 60 °C.

Assuming that the reaction volume remains constant during the reaction, in the presence of 5 mol% NEt_3, epoxy amine (1 mmol, 0.1492 g) and CO_2 (1 bar) reacted in DMF (1 mL) at 60 °C. The plot of the conversion rate of epoxy amine against time gave Fig. S3 (a), and $t_{1/2}$ was determined to be 12.82 h. Changing the amount of epoxy amine to 1.25 mmol (0.1865 g), and keeping other conditions unchanged, $t_{1/2}$'

was determined to be 12.05 h (Fig. S3 (b)). According to $n = 1 + \frac{lg\frac{t_{1/2}}{t'_{1/2}}}{lg\frac{c_{1/2}}{c'_{1/2}}} = 1.27$, the rate order of epoxy amine was determined to be first-order.

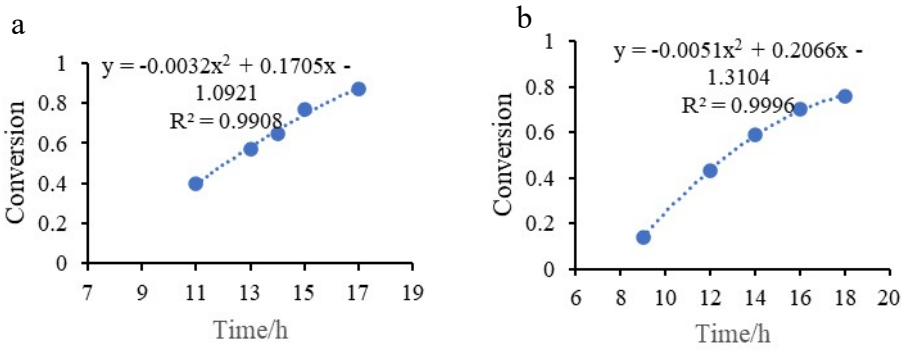


Fig. S3 Plot of conversion of epoxy amine versus time (h) for the reaction of *N*-(oxiran-2-ylmethyl)aniline (**1a**) and CO_2 catalyzed by NEt_3. a: **1a** (1 mmol), 0.5 mol% NEt_3, 1 bar CO_2. b: **1a** (1.25 mmol), 0.5 mol% NEt_3, 1 bar CO_2.

Determination of rate order of NEt_3

Catalyst loading of 4 mol%:

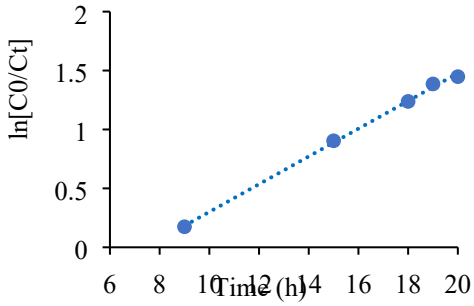


Fig. S4 Plot of $\ln[C_0/C_t]$ versus time (h) for the reaction of *N*-(oxiran-2-ylmethyl)aniline (**1a**) and CO_2 catalyzed by NEt_3. Conditions: *N*-(oxiran-2-ylmethyl)aniline (0.5 mmol), NEt_3 (4 mol%), 60 °C.

Catalyst loading of 3 mol%:

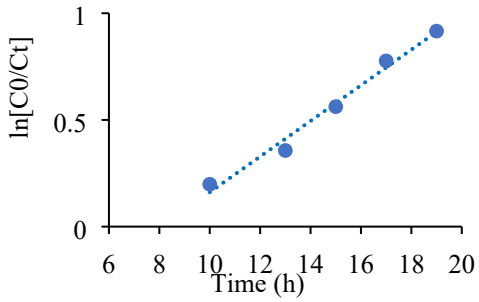


Fig. S5 Plot of $\ln[C_0/C_t]$ versus time (h) for the reaction of *N*-(oxiran-2-ylmethyl)aniline (**1a**) and CO_2 catalyzed by NEt_3. Conditions: *N*-(oxiran-2-ylmethyl)aniline (0.5 mmol), NEt_3 (3 mol%), 60 °C.

Catalyst loading of 2 mol%:

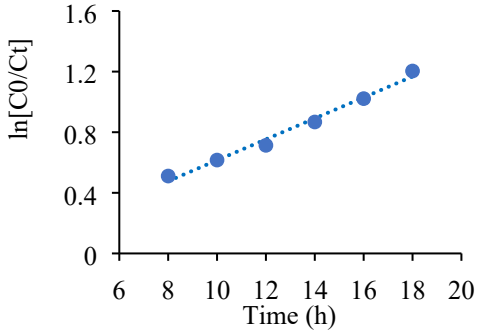


Fig. S6 Plot of $\ln[C_0/C_t]$ versus time (h) for the reaction of *N*-(oxiran-2-ylmethyl)aniline (**1a**) and CO_2 catalyzed by NEt_3. Conditions: *N*-(oxiran-2-ylmethyl)aniline (0.5 mmol), NEt_3 (2 mol%), 60 °C.

Catalyst loading of 1 mol%:

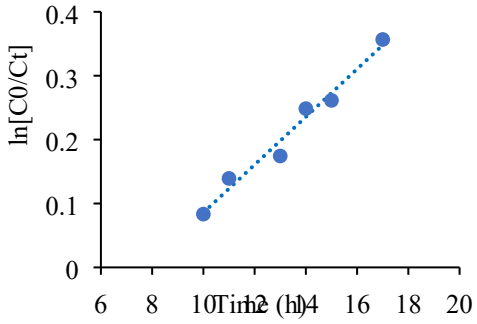


Fig. S7 Plot of $\ln[C_0/C_t]$ versus time (h) for the reaction of *N*-(oxiran-2-ylmethyl)aniline (**1a**) and CO_2 catalyzed by NEt_3. Conditions: *N*-(oxiran-2-ylmethyl)aniline (0.5 mmol), NEt_3 (1 mol%), 60 °C.

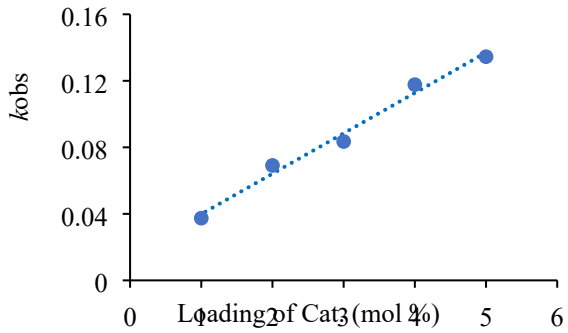


Fig. S8 Plot of k_{obs} versus NEt_3 (mol%) for the reaction of *N*-(oxiran-2-ylmethyl)aniline (**1a**) and CO_2. catalyzed by NEt_3. Conditions: *N*-(oxiran-2-ylmethyl)aniline (0.5 mmol), CO_2 (1 bar); loadings of NEt_3: 4, 3, 2 and 1 mol%; 60 °C.

Table S7 Cycloaddition of epoxy amine and CO_2 catalyzed by NEt_3 at different temperature.[a]

Entry	T (°C)	Time (h)	Yield (%)
1	40	10	10
2	40	14	18
3	40	16	24
4	40	18	28
5	40	19	32
7	50	8	16
8	50	10	26
9	50	12	29
10	50	14	37
12	50	18	45
13	50	19	50
14	60	9	21
15	60	12	47
16	60	14	57
17	60	16	65
18	60	18	78
20	70	6	34
21	70	8	50
22	70	12	72
23	70	14	78
24	70	16	82
25	70	17	86
27	80	6	57

28	80	8	70
29	80	10	80
30	80	12	87
31	80	14	91
32	80	16	96

[a]Reaction conditions: epoxy amine C_0 = 1.000 mol/L, 50.00 mM NEt_3, 1 bar CO_2. Yields and selectivity were determined by ^1H NMR spectroscopy with tetraethylsilane as an internal standard.

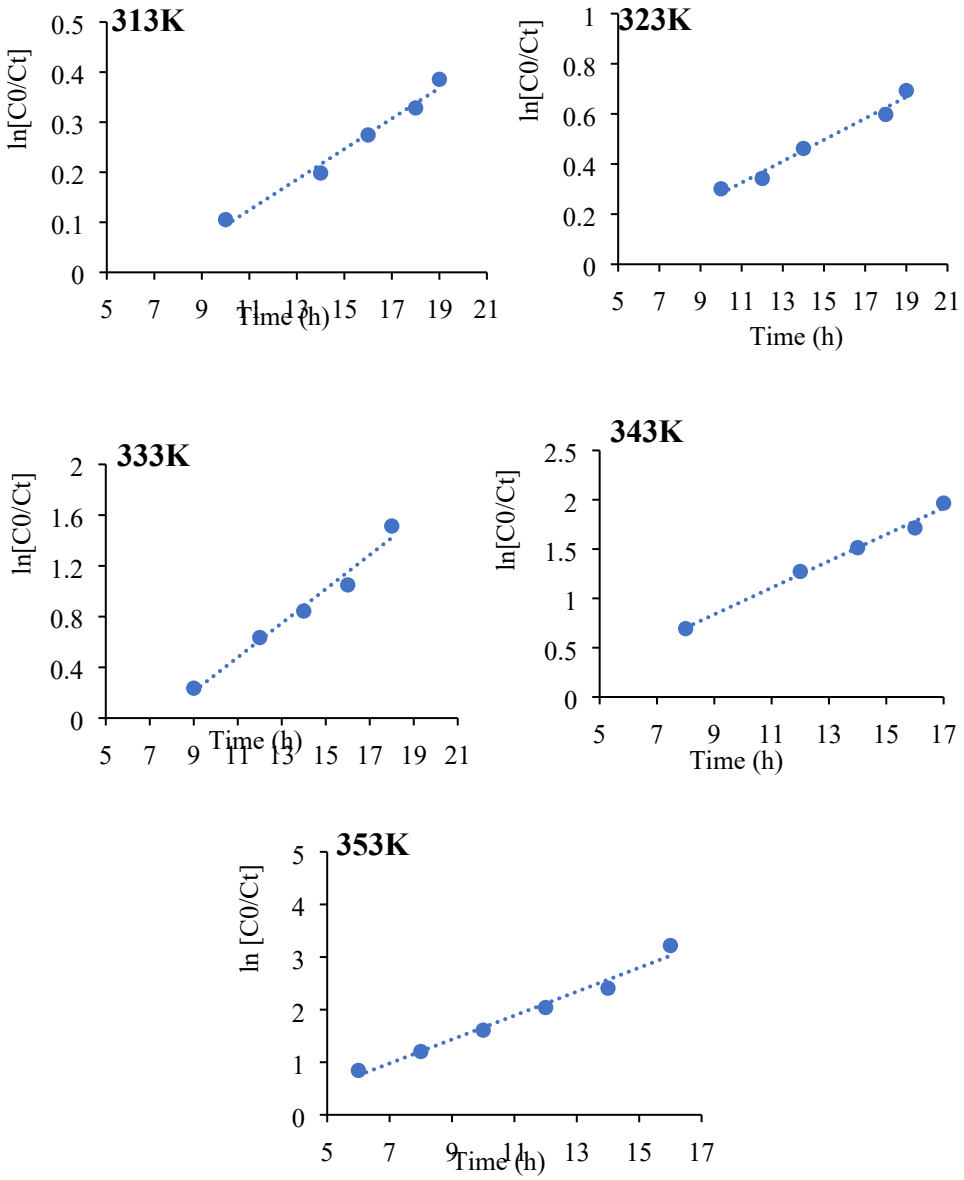


Fig. S9 Plot of $\ln[C_0/C_t]$ versus Time for the reaction of *N*-(oxiran-2-ylmethyl)aniline (**1a**) and CO_2 catalyzed by NEt_3. Conditions: *N*-(oxiran-2-ylmethyl)aniline (0.5 mmol), CO_2 (1 bar); NEt_3 (5 mol%), temperature: 40, 50, 60, 70 and 80 °C.

Table S8 Data for Eyring plot.

Entry	T (k)	k_{obs} (h^{-1})	k_{obs} (^10^{-5} s^{-1})	k (10^{-4})[a]	ln(k/T)	1/T (k^{-1})
1	313	0.0305	0.8472	1.6944	-14.4292	0.00319
2	323	0.0427	1.1861	2.3722	-14.1241	0.00310
3	333	0.1345	3.7361	7.4722	-13.0073	0.00300
4	343	0.1352	3.7556	7.5111	-13.0317	0.00292
5	353	0.2247	6.2417	12.4833	-12.5524	0.00283

[a]Calculated on the basis of the kinetic equation $k_{obs} = k[Cat.]$

$$\ln\frac{k}{T} = -\frac{\Delta H}{R}\times\frac{1}{T} + \ln\frac{k_B}{h} + \frac{\Delta S}{R}$$

$$-\frac{\Delta H}{R} = -5376.4 \rightarrow \Delta H = (10.68 \pm 1.87)\ \text{kcal/mol}$$

$$\ln\frac{k_B}{h} + \frac{\Delta S}{R} = 2.7455 \rightarrow \Delta S = (-42.99 \pm 5.65)\ \text{cal/(mol·K)}$$

$$\Delta G_{333K} = \Delta H - T\Delta S = (25.00 \pm 3.75)\ \text{kcal/mol}$$

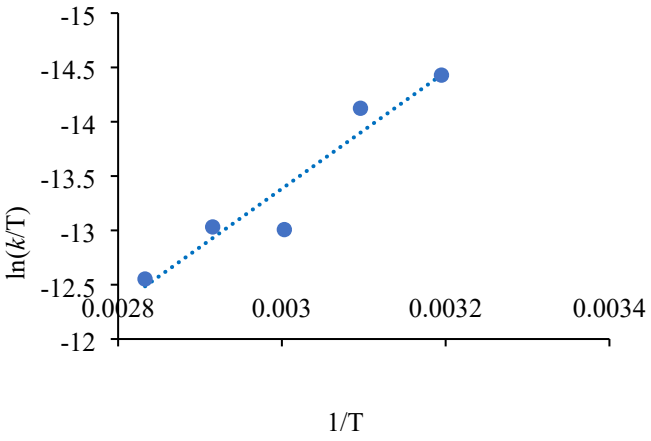


Fig. S10 Plot of ln(k/T) versus ln(1/T) for the reaction of *N*-(oxiran-2-ylmethyl)aniline (**1a**) and CO_2 catalyzed by NEt_3. Conditions: *N*-(oxiran-2-ylmethyl)aniline (0.5 mmol), CO_2 (1 bar); NEt_3 (5 mol%), temperture: 40, 50, 60, 70 and 80 ℃.

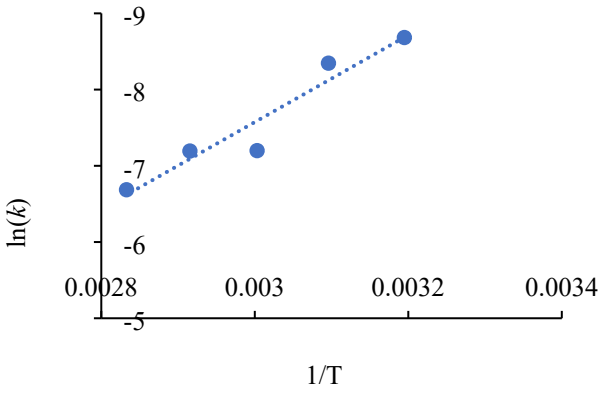


Fig. S11 Plot of ln(k) versus ln(1/T) for the reaction of *N*-(oxiran-2-ylmethyl)aniline (**1a**) and CO_2 catalyzed by NEt_3. Conditions: *N*-(oxiran-2-ylmethyl)aniline (0.5 mmol), CO_2 (1 bar); NEt_3 (5 mol%), temperture: 40, 50, 60, 70 and 80 °C.

5. Control experiments

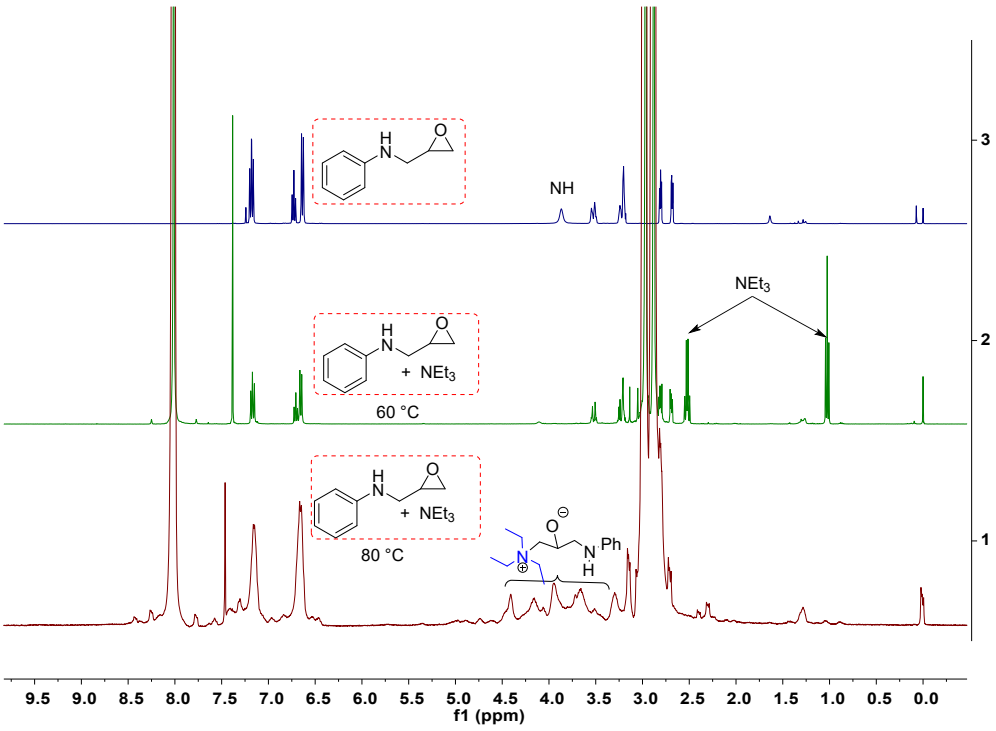


Fig. **S12** Reaction of epoxy amine with NEt_3 at different temperatures.

After epoxy amine **1a** (0.5 mmol), NEt_3 (0.5 mmol) and DMF (0.5 mL) were heated at 60 °C for 20 h without CO_2, NMR monitoring reveals disappearance of NH signal of 1a, which may be due to the formation of hydrogen bond. Other peaks of 1a did not change significantly (2nd spectrum, Fig. S12). Further reacting at 80 °C for 20 h led to

appearance of some new signals at 3.2-4.5 ppm (3rd spectrum, Fig. S12), which can be assigned to the ring-opened product.[8,] 错误!未找到引用源。

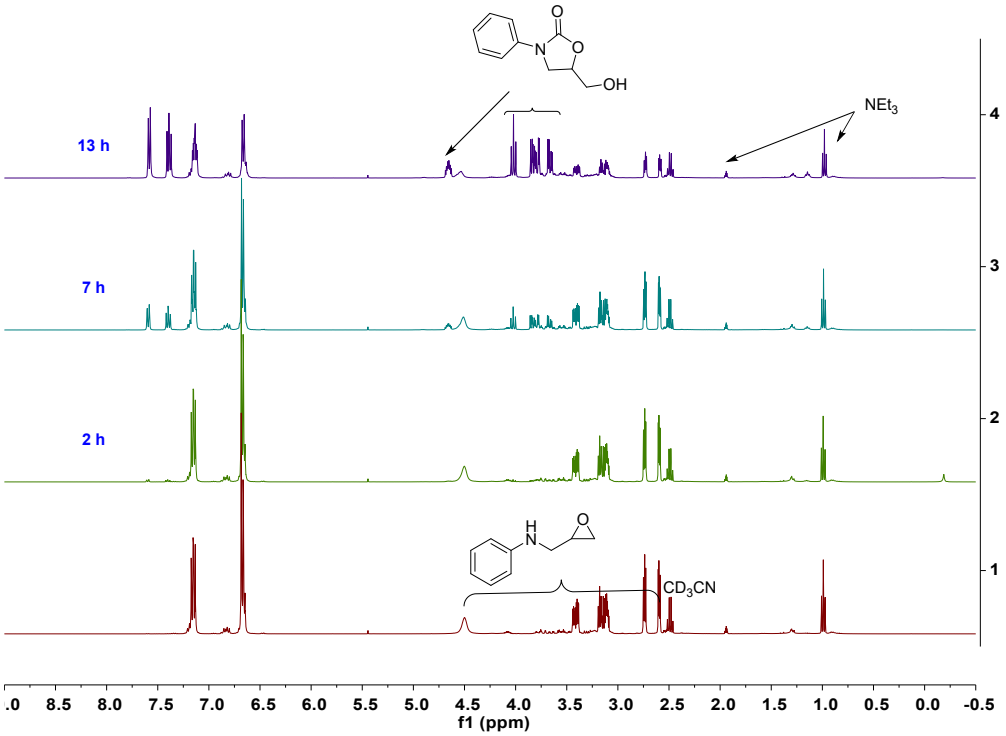


Fig. S13. NMR tube reaction between *N*-(oxiran-2-ylmethyl)aniline **1a** and CO_2 (CD_3CN).

6. DFT study.

Computational Details:

The B3LYP density functional method[10] combined with 6-31G(d) basis set[11] was employed to carry out all the geometry optimizations. Vibrational frequency analyses at the same level of theory were performed on all the optimized geometries to characterize stationary points as local minima (no imaginary frequency) or transition states (one imaginary frequency). In addition, intrinsic reaction coordinate (IRC) calculations were used to verify that the transition state connects with appropriate reactant and product.[12] The gas-phase Gibbs free energies for all species were obtained at 298.15 K and 1 atm at their respective optimized structures. The M06-2X functional[13,1413] with larger basis set 6-311++G(d,p) was used in subsequent single-point energy calculations at the optimized structures with SMD solvation method,[15]

which was employed to consider the effect of solvation in N,N-Dimethylformamide solvent. The solvation Gibbs free energy was used for discussion and its value was obtained via the sum of solvation single-point energy and gas phase thermal correction to Gibbs free energy. All calculations were carried out with the Gaussian 09 suite of programs.[16]

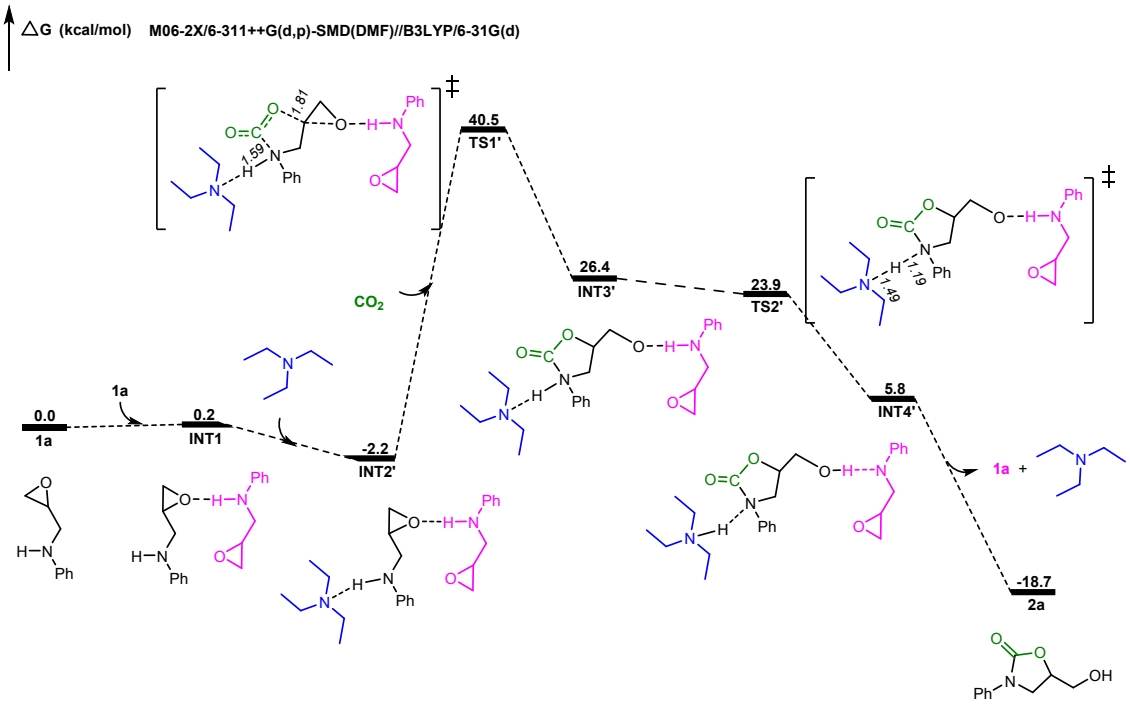


Fig. S14. Energy profile for the formation of the product **2a** via direct nucleophilic attack of CO_2 with **1a** in the presence of NEt_3 H-bonded with **1a**.

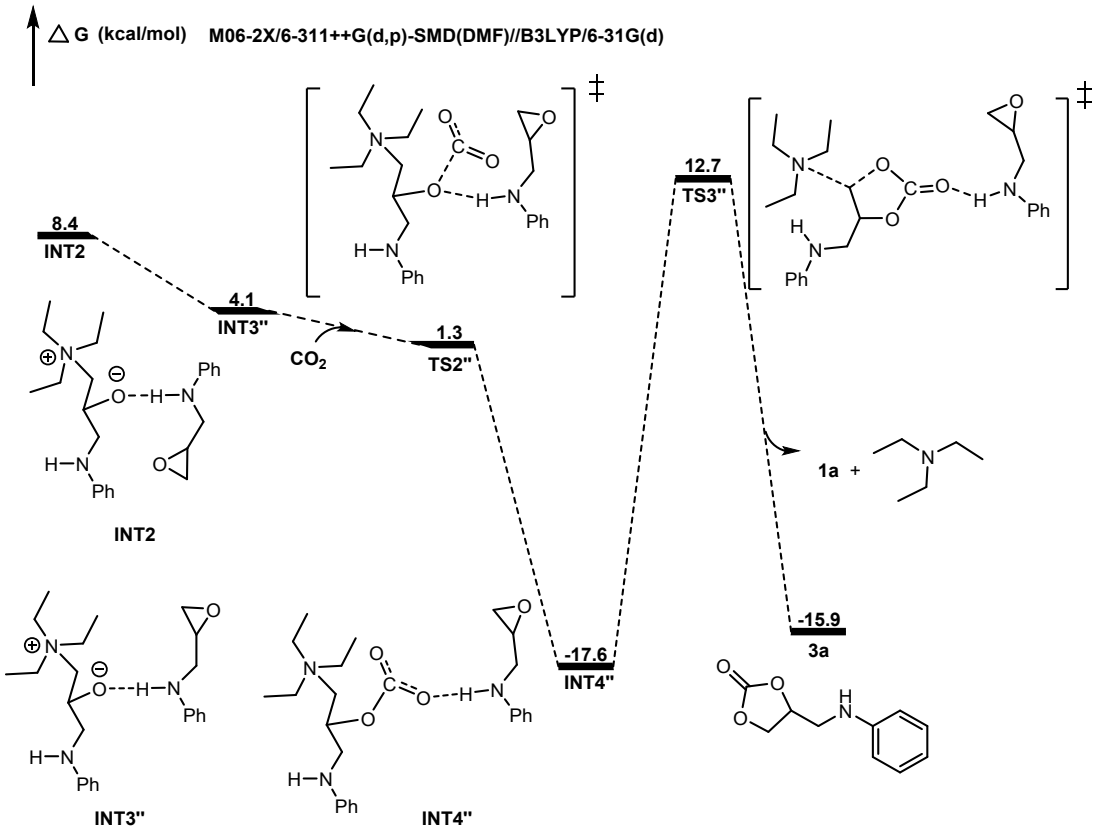


Fig. S15. Energy profile for the formation of **3a** via the CO_2 adduct with **INT2**.

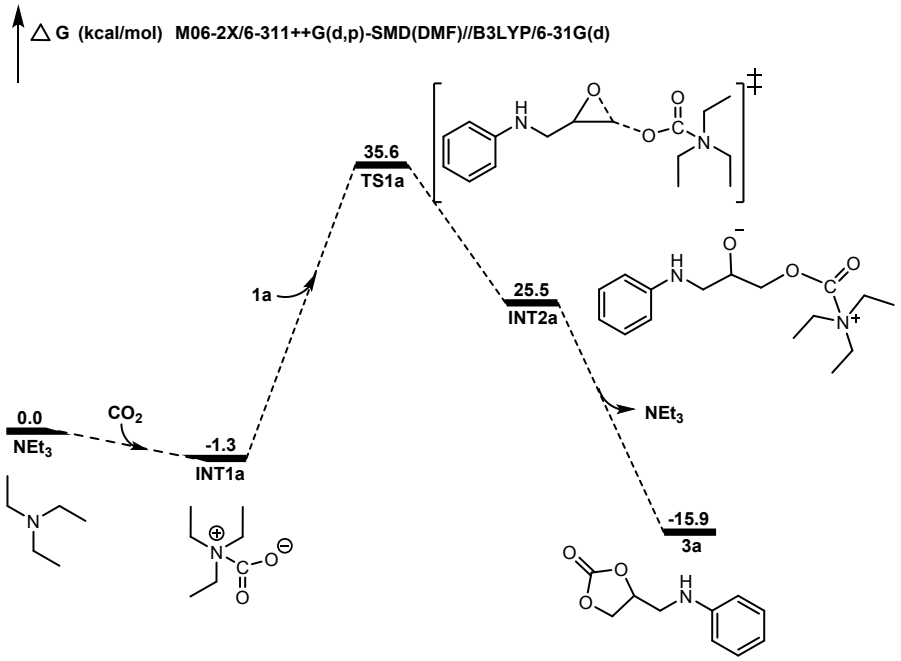


Fig. S16. Energy profile for the formation of **3a** via the CO_2 adduct with NEt_3.

Cartesian Coordinates and Energies

1a

C	3.11399900	-1.10432500	-0.11168300
C	1.74625700	-1.28271600	0.05932000
C	0.88006100	-0.17507500	0.15243500
C	1.43402900	1.11399300	0.06196400
C	2.81046000	1.27955300	-0.10381200
C	3.66192800	0.17982300	-0.19315800
H	3.75814700	-1.97734300	-0.18213500
H	1.33179300	-2.28647000	0.12943200
H	0.79740800	1.99084500	0.11765400
H	3.21467500	2.28676700	-0.17037700
H	4.73096300	0.31700500	-0.32632900
N	-0.48311500	-0.39773900	0.36835900
H	-0.79793400	-1.30083000	0.03116400
C	-1.46954500	0.64105900	0.12740700
H	-1.46915900	0.99557200	-0.91805800
H	-1.24949000	1.50564800	0.76618900
C	-2.83819900	0.11589100	0.48575700
C	-4.01788200	0.39731300	-0.34153500
H	-2.98371400	-0.12137700	1.54107000
H	-3.91685800	1.01905700	-1.23143000
H	-5.00869800	0.39403200	0.11264300
O	-3.36899800	-0.87898000	-0.40856200

Zero-point correction= 0.185025 (Hartree/Particle)
Thermal correction to Energy= 0.194792
Thermal correction to Enthalpy= 0.195737
Thermal correction to Gibbs Free Energy= 0.148717
Sum of electronic and zero-point Energies= -479.318909
Sum of electronic and thermal Energies= -479.309141
Sum of electronic and thermal Enthalpies= -479.308197
Sum of electronic and thermal Free Energies= -479.355217
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -479.44998640

INT1

C	-0.89412700	-1.07132900	1.33254700
C	-0.95091900	-0.87558200	-0.17451600
H	-0.88277100	0.19311400	-0.39675300
H	-0.07661000	-1.34943100	-0.63540900
N	-2.14745800	-1.42396700	-0.78960100
C	-3.41457800	-0.85740900	-0.62217900
C	-3.60342700	0.46878600	-0.18908100
C	-4.55194100	-1.62484500	-0.94276700
C	-4.89143500	0.99754200	-0.09520700
H	-2.75397200	1.09042000	0.07518100
C	-5.82917000	-1.08407100	-0.84183100
H	-4.42159800	-2.65147700	-1.28074200
C	-6.01362300	0.23456700	-0.41715400
H	-5.01193900	2.02419100	0.24223400
H	-6.68766000	-1.70082900	-1.09641500
H	-7.01155100	0.65531000	-0.33665000
C	-0.06065200	-2.11549400	1.94644200
O	0.35221200	-0.73721600	1.97113700
H	-2.16025400	-2.43460800	-0.84378400
H	-1.77085200	-0.72517000	1.88057700
H	-0.32440700	-2.52978000	2.91898800
H	0.54010500	-2.76527800	1.30915700

C	4.66179300	-2.00247800	0.06144700
C	3.67231900	-1.15604800	0.54657000
C	3.45563300	0.11128000	-0.03671200
C	4.26486500	0.48863100	-1.12501500
C	5.25905900	-0.37046400	-1.59743000
C	5.46841600	-1.61952600	-1.01577000
H	4.80743900	-2.97223300	0.53185900
H	3.05840300	-1.45484300	1.39255700
H	4.12157900	1.44927800	-1.60892700
H	5.87106100	-0.05360900	-2.43873300
H	6.24187700	-2.28297500	-1.39148700
N	2.47715000	0.94216400	0.50111200
H	1.74764300	0.44648200	1.00793300
C	2.03399100	2.13385700	-0.19307700
H	1.62563700	1.92326000	-1.19795000
H	2.88913400	2.81085000	-0.33072900
C	0.99022800	2.86280300	0.61620400
C	-0.05009700	3.67362100	-0.02907600
H	1.28462800	3.11077800	1.63709200
H	-0.08201200	3.74343300	-1.11654900
H	-0.48478400	4.51927300	0.50328200
O	-0.36533100	2.38264500	0.51065200

Zero-point correction= 0.371212 (Hartree/Particle)
Thermal correction to Energy= 0.392807
Thermal correction to Enthalpy= 0.393751
Thermal correction to Gibbs Free Energy= 0.314879
Sum of electronic and zero-point Energies= -958.644815
Sum of electronic and thermal Energies= -958.623219
Sum of electronic and thermal Enthalpies= -958.622275
Sum of electronic and thermal Free Energies= -958.701147
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -958.90570307

NEt_3

N	0.04269800	-0.27272600	0.56130400
C	-1.32397200	-0.77820900	0.63884500
H	-1.25654700	-1.85512500	0.85026100
H	-1.79354700	-0.32275400	1.52072800
C	-2.25131600	-0.58696800	-0.57813200
H	-3.20298000	-1.10575000	-0.40750300
H	-2.47773300	0.46819000	-0.76206000
H	-1.80762800	-1.00118900	-1.49072300
C	0.88235900	-0.92814800	-0.43532500
H	0.61133400	-1.99184300	-0.42849400
H	0.69409000	-0.57438600	-1.46669500
C	2.37951100	-0.80632000	-0.13570900
H	2.59736500	-1.16073300	0.87750400
H	2.95549400	-1.40852200	-0.84763500
H	2.73552400	0.22641500	-0.21864600
C	0.22808100	1.16719000	0.72704200
H	1.23497300	1.33569600	1.13206400
H	-0.46706200	1.49094000	1.51162900
C	0.05550300	2.07497200	-0.50707800
H	-0.96045100	2.03898600	-0.91206900
H	0.27105500	3.11521800	-0.23337000
H	0.74622900	1.79883500	-1.31197000

Zero-point correction= 0.206960 (Hartree/Particle)
Thermal correction to Energy= 0.216410

Thermal correction to Enthalpy= 0.217354
Thermal correction to Gibbs Free Energy= 0.172966
Sum of electronic and zero-point Energies= -292.205724
Sum of electronic and thermal Energies= -292.196274
Sum of electronic and thermal Enthalpies= -292.195330
Sum of electronic and thermal Free Energies= -292.239718
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -292.34363588

TS1

C	0.38097200	-0.17398900	-0.76024300
C	0.24655800	0.36651500	0.67556300
H	-0.43980300	1.22266800	0.63352300
H	-0.24405300	-0.39913200	1.28644200
N	1.51569200	0.71353600	1.32982300
C	2.13039600	1.96781500	1.13811700
C	1.71460300	2.88420300	0.15757200
C	3.23597300	2.30013600	1.94547000
C	2.39971400	4.09065000	-0.00277000
H	0.84321800	2.68619200	-0.45683400
C	3.90430700	3.50856200	1.77882400
H	3.56548700	1.59689800	2.70888800
C	3.49541200	4.41490000	0.79635100
H	2.05498400	4.78931800	-0.76111000
H	4.75078500	3.74213900	2.42022000
H	4.01818600	5.35775400	0.66344100
C	0.77450500	-1.61675100	-0.94616000
O	-0.82187300	-0.48333000	-1.33590000
H	1.52682600	0.45060500	2.30823400
H	1.01957000	0.51110000	-1.34993800
H	0.82691900	-1.90355700	-1.99010900
H	0.23115500	-2.30253200	-0.30608000
N	2.56201700	-2.27099200	-0.53950200
C	3.43936200	-1.15045200	-1.00598200
H	3.02622100	-0.83011900	-1.96875700
H	3.28101700	-0.32866500	-0.30483900
C	4.93701800	-1.42126300	-1.18849400
H	5.40150000	-0.49391100	-1.54146900
H	5.44095700	-1.70517800	-0.26175100
H	5.13984400	-2.19038500	-1.94034700
C	2.76585400	-3.49834700	-1.35725000
H	2.67390700	-3.18642100	-2.40404800
H	3.79343900	-3.85753200	-1.22630500
C	1.79242200	-4.64292900	-1.07559000
H	0.75055000	-4.35334700	-1.23350300
H	2.01608600	-5.46461400	-1.76411700
H	1.89267200	-5.03515400	-0.05888800
C	2.58906400	-2.50629000	0.93283200
H	1.70199400	-3.10224600	1.16839400
H	2.44192600	-1.52254900	1.38422400
C	3.81966900	-3.19485400	1.53248700
H	4.71872000	-2.57683300	1.47618400
H	3.62255200	-3.38811400	2.59311600
H	4.03521500	-4.15965400	1.06173800
C	-4.70694900	-2.55975800	1.24650900
C	-3.81306700	-1.69333300	0.63182900
C	-4.20409100	-0.38164100	0.27278500
C	-5.53133300	0.01017200	0.54787400

C	-6.41660300	-0.87368300	1.16659600
C	-6.02054900	-2.16199700	1.52455500
H	-4.37789900	-3.56382400	1.50729300
H	-2.79916500	-2.00980800	0.39848800
H	-5.86860800	1.00849400	0.28624700
H	-7.43333800	-0.54330700	1.36909000
H	-6.71679600	-2.84369100	2.00482100
N	-3.27966400	0.45970500	-0.30546800
H	-2.39881200	0.03036800	-0.62283400
C	-3.65998700	1.67377500	-0.99381500
H	-4.01861400	2.43865400	-0.28807100
H	-4.48240800	1.49265000	-1.71180800
C	-2.48151100	2.23623000	-1.75304700
C	-2.37146800	3.67102800	-2.04240200
H	-1.97275100	1.52534400	-2.40392500
H	-3.14503700	4.35540700	-1.69113800
H	-1.82791600	4.00626300	-2.92641000
O	-1.57268300	3.07568000	-1.01181300

Zero-point correction= 0.580767 (Hartree/Particle)
Thermal correction to Energy= 0.612038
Thermal correction to Enthalpy= 0.612983
Thermal correction to Gibbs Free Energy= 0.513660
Sum of electronic and zero-point Energies= -1250.808673
Sum of electronic and thermal Energies= -1250.777402
Sum of electronic and thermal Enthalpies= -1250.776457
Sum of electronic and thermal Free Energies= -1250.875780
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -1251.22622626

INT2

C	-0.34175600	-0.42539900	0.61481000
C	-0.18731900	0.08011400	-0.84476900
H	0.60040100	0.84390200	-0.82009300
H	0.19839600	-0.74713600	-1.45167700
N	-1.40626500	0.58007000	-1.51048400
C	-1.88292700	1.89280500	-1.28837900
C	-1.37283500	2.73845300	-0.28937200
C	-2.94558000	2.35812900	-2.08796900
C	-1.92434100	4.00844700	-0.10476100
H	-0.53152900	2.43897000	0.32543900
C	-3.48054000	3.62831100	-1.89737600
H	-3.34635000	1.71070600	-2.86673600
C	-2.97762100	4.46474500	-0.89677700
H	-1.50328800	4.64943300	0.66556900
H	-4.29530600	3.96515000	-2.53401800
H	-3.39487200	5.45633400	-0.74566500
C	-1.10435600	-1.79216000	0.79062300
O	0.85024600	-0.75242900	1.14713500
H	-1.39623800	0.37710600	-2.50489700
H	-0.90961800	0.35404500	1.17730100
H	-0.96162300	-2.04152200	1.84273800
H	-0.59913200	-2.53835400	0.17675900
N	-2.66299500	-2.03065000	0.55586100
C	-3.37288500	-0.78490800	1.08537500
H	-2.80505500	-0.48840500	1.96960300
H	-3.21317400	-0.01537100	0.32930000
C	-4.84986500	-0.90072100	1.46123100
H	-5.17866000	0.10176300	1.75571900

H	-5.49342900	-1.22543400	0.64180100
H	-5.01880900	-1.55836300	2.31856200
C	-3.08527500	-3.24300200	1.36199900
H	-2.91251100	-2.97420700	2.40799400
H	-4.16106100	-3.36974000	1.22762600
C	-2.36361300	-4.54547100	1.02879400
H	-1.28446300	-4.47788300	1.18186100
H	-2.74719400	-5.32003900	1.70122900
H	-2.55454100	-4.88142700	0.00529100
C	-2.87742600	-2.23097700	-0.93359400
H	-2.20447900	-3.04175800	-1.21909500
H	-2.50613700	-1.30739100	-1.38475900
C	-4.29254300	-2.53535100	-1.41684200
H	-4.96358800	-1.67889800	-1.32111200
H	-4.22747700	-2.77336700	-2.48433200
H	-4.74995900	-3.39880300	-0.92299500
C	4.64707200	-2.58353600	-1.39610500
C	3.75765800	-1.74258100	-0.74195500
C	4.17517700	-0.47610400	-0.26434400
C	5.52400300	-0.10853300	-0.45824600
C	6.40433800	-0.96781500	-1.11797100
C	5.98209600	-2.20778800	-1.59656700
H	4.29907200	-3.55300200	-1.74858300
H	2.72817500	-2.03940600	-0.55641200
H	5.88045100	0.85376400	-0.10292300
H	7.43802700	-0.65689000	-1.25697200
H	6.67454500	-2.87051200	-2.10841600
N	3.25109000	0.34084700	0.34536500
H	2.34212400	-0.10022900	0.59394600
C	3.63855700	1.44913900	1.18881300
H	4.05868400	2.28211200	0.60346700
H	4.41545400	1.15269400	1.92022300
C	2.43566300	1.95720400	1.95042900
C	2.38121500	3.32607300	2.47596000
H	1.83797200	1.17792700	2.42370100
H	3.21728700	4.00593600	2.30331400
H	1.79015500	3.54386200	3.36675600
O	1.63519900	2.97219400	1.30502200

Zero-point correction= 0.583245 (Hartree/Particle)
Thermal correction to Energy= 0.614165
Thermal correction to Enthalpy= 0.615109
Thermal correction to Gibbs Free Energy= 0.516293
Sum of electronic and zero-point Energies= -1250.811515
Sum of electronic and thermal Energies= -1250.780595
Sum of electronic and thermal Enthalpies= -1250.779651
Sum of electronic and thermal Free Energies= -1250.878466
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -1251.25333989

INT3

C	0.42404600	-0.00715700	-1.19272700
C	0.80161000	0.51936200	0.21353300
H	1.23447500	1.51490700	0.06589500
H	-0.09410400	0.65251000	0.82538600
N	1.72290400	-0.36682900	0.94547100
C	3.11401900	-0.32026200	0.68315200
C	3.66486400	0.38352500	-0.40043300
C	3.97669400	-1.04505600	1.52660900

C	5.04289100	0.34715400	-0.62695700
H	3.03508900	0.98159900	-1.04987600
C	5.34858000	-1.06347200	1.29652300
H	3.55846700	-1.59343900	2.36920700
C	5.89395100	-0.37151500	0.21125700
H	5.44976200	0.90391700	-1.46716200
H	5.99456100	-1.62367500	1.96811100
H	6.96446700	-0.38874800	0.02849700
C	-0.74265100	-1.03459600	-1.30855000
O	0.00312700	1.02642100	-2.03339900
H	1.55215600	-0.33771400	1.94511600
H	1.32365000	-0.45018100	-1.64004600
H	-0.81144700	-1.28178000	-2.37060600
H	-1.66718800	-0.54044300	-1.00771600
N	-0.73096400	-2.40409900	-0.57579600
C	0.66698600	-2.99776900	-0.75507000
H	0.85678300	-2.94422000	-1.83090700
H	1.33933900	-2.30174000	-0.25211700
C	0.91164100	-4.41668800	-0.25224900
H	1.92822400	-4.68883200	-0.55613700
H	0.87579200	-4.48851700	0.83685500
H	0.23609600	-5.16245800	-0.68079000
C	-1.74632200	-3.30860500	-1.25852300
H	-1.33617400	-3.51066100	-2.25244500
H	-1.74948300	-4.24839300	-0.70588400
C	-3.16052900	-2.75067000	-1.36976700
H	-3.22040500	-1.90065600	-2.05128800
H	-3.80033000	-3.54689800	-1.76581400
H	-3.57244500	-2.43166000	-0.40931900
C	-1.07984100	-2.16709600	0.90084900
H	-1.80370400	-1.35010600	0.91389600
H	-0.15336700	-1.80351300	1.34522000
C	-1.64188700	-3.34485500	1.69367500
H	-0.98056300	-4.21246300	1.73072000
H	-1.77995000	-2.99252800	2.72162300
H	-2.62340300	-3.66664800	1.33626600
C	-4.47102300	0.31001800	-0.07592700
C	-3.44873600	1.05216500	-0.65166900
C	-2.55944300	1.86699500	0.12828800
C	-2.81868700	1.86849800	1.54000400
C	-3.84075700	1.10267900	2.09920100
C	-4.67710100	0.30225000	1.31388100
H	-5.14182600	-0.25619800	-0.72230500
H	-3.32881800	1.08303200	-1.73311300
H	-2.20902400	2.48433700	2.19440800
H	-3.99282600	1.14021200	3.17782800
H	-5.48877800	-0.26749000	1.75824400
N	-1.56678300	2.53663500	-0.49994700
H	-0.63777100	1.65512800	-1.49807500
C	-0.85944900	3.52330900	0.28076000
H	-0.29264000	3.11801300	1.14757000
H	-1.55498700	4.26911400	0.71612500
C	0.13190200	4.27490700	-0.57872100
C	1.27934000	4.98503200	0.00152600
H	-0.26677000	4.62557400	-1.53188800
H	1.44123000	4.95386300	1.08045200
H	1.69283300	5.86219400	-0.49830500

O	1.47017100	3.74054100	-0.68381400

Zero-point correction= 0.583476 (Hartree/Particle)
Thermal correction to Energy= 0.613676
Thermal correction to Enthalpy= 0.614621
Thermal correction to Gibbs Free Energy= 0.520224
Sum of electronic and zero-point Energies= -1250.801084
Sum of electronic and thermal Energies= -1250.770883
Sum of electronic and thermal Enthalpies= -1250.769939
Sum of electronic and thermal Free Energies= -1250.864335
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -1251.26194212

CO_2

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16915600
O	0.00000000	0.00000000	-1.16915600

Zero-point correction= 0.011593 (Hartree/Particle)
Thermal correction to Energy= 0.014240
Thermal correction to Enthalpy= 0.015184
Thermal correction to Gibbs Free Energy= -0.009126
Sum of electronic and zero-point Energies= -188.569347
Sum of electronic and thermal Energies= -188.566700
Sum of electronic and thermal Enthalpies= -188.565756
Sum of electronic and thermal Free Energies= -188.590066
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -188.57624548

TS2

C	0.38278900	0.02878600	-1.12106200
C	0.67122200	0.57634100	0.30037300
H	0.94620200	1.62956400	0.17778400
H	-0.23826700	0.55470200	0.90779000
N	1.71428600	-0.17164000	1.02635200
C	3.08361400	0.08585500	0.77020000
C	3.52613700	0.89219100	-0.29145700
C	4.04263200	-0.52647200	1.59900800
C	4.89488900	1.06527600	-0.51061800
H	2.81556000	1.40856500	-0.92739400
C	5.40275400	-0.33652600	1.37643900
H	3.70768700	-1.15344500	2.42390400
C	5.84159100	0.45723000	0.31287600
H	5.21668300	1.69845800	-1.33347800
H	6.12332800	-0.81363800	2.03629800
H	6.90327300	0.60273300	0.13534800
C	-0.58177600	-1.19491400	-1.23452700
O	-0.24301900	0.96338900	-1.92447700
H	1.54111400	-0.17591100	2.02623500
H	1.34949200	-0.24913200	-1.57154400
H	-0.65861900	-1.40158100	-2.30418100
H	-1.56077300	-0.88742200	-0.86762200
N	-0.30163300	-2.58542900	-0.58053500
C	1.16550500	-2.91209400	-0.85401500
H	1.29110800	-2.75013200	-1.92812400
H	1.73181900	-2.14473100	-0.32601500
C	1.67585000	-4.29842500	-0.47332300
H	2.70894900	-4.36450100	-0.83127800
H	1.70312600	-4.45597900	0.60680900
H	1.12032100	-5.11781000	-0.93842800
C	-1.18543600	-3.61016900	-1.27222700

H	-0.81217500	-3.67499900	-2.29841600
H	-0.99503200	-4.57009300	-0.79127900
C	-2.67892700	-3.29901500	-1.27020500
H	-2.92376600	-2.42380200	-1.87407000
H	-3.19981500	-4.16168700	-1.69940500
H	-3.07799400	-3.13308900	-0.26622500
C	-0.60818800	-2.48642100	0.91653600
H	-1.47210400	-1.82397000	0.99917600
H	0.25286200	-1.96574500	1.33678700
C	-0.89910700	-3.78244200	1.67118200
H	-0.07783100	-4.50133200	1.65500400
H	-1.07078500	-3.50655200	2.71741900
H	-1.80687500	-4.28137400	1.32153500
C	-4.51969300	-0.21948700	0.05297000
C	-3.54587400	0.54944500	-0.57251600
C	-2.86450500	1.61051900	0.10638300
C	-3.27813700	1.84578000	1.45370200
C	-4.25722700	1.06278800	2.06318100
C	-4.88527000	0.01320700	1.38723900
H	-5.02943700	-0.99550900	-0.51818500
H	-3.31462400	0.39976800	-1.62513700
H	-2.82175200	2.65060800	2.02167600
H	-4.53599500	1.28124100	3.09346500
H	-5.65673200	-0.58158600	1.86871800
N	-1.89453000	2.29610000	-0.55263800
H	-1.01768100	1.56878800	-1.33226500
C	-1.34934200	3.46737000	0.08999700
H	-0.82994500	3.26608300	1.05116000
H	-2.14859400	4.19361900	0.33496700
C	-0.35824400	4.16827600	-0.81294900
C	0.64112500	5.10248100	-0.27696100
H	-0.69249600	4.30066400	-1.84283100
H	0.69331700	5.27511800	0.79949100
H	1.00806000	5.92587600	-0.89137500
O	1.03092400	3.79255300	-0.70801400

Zero-point correction= 0.579483 (Hartree/Particle)
Thermal correction to Energy= 0.609474
Thermal correction to Enthalpy= 0.610418
Thermal correction to Gibbs Free Energy= 0.516017
Sum of electronic and zero-point Energies= -1250.804247
Sum of electronic and thermal Energies= -1250.774255
Sum of electronic and thermal Enthalpies= -1250.773311
Sum of electronic and thermal Free Energies= -1250.867712
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -1251.25824398

INT4

C	-0.59893800	-0.14301700	-1.04208700
C	-0.82539400	-0.65141900	0.40227700
H	-0.62628500	-1.72876200	0.38394800
H	-0.09812700	-0.20583500	1.08609000
N	-2.17153300	-0.35778600	0.92131200
C	-3.26658300	-1.18637800	0.57291600
C	-3.18849800	-2.18268100	-0.41405400
C	-4.49747200	-0.97085400	1.22058400
C	-4.32280800	-2.93033900	-0.73995700
H	-2.24776200	-2.40163100	-0.90724600
C	-5.61640600	-1.73043400	0.89447800

H	-4.56612600	-0.19995700	1.98644400
C	-5.54012500	-2.71405600	-0.09589600
H	-4.24015500	-3.70126500	-1.50173600
H	-6.55366300	-1.55064600	1.41537700
H	-6.41437800	-3.30446800	-0.35439400
C	-0.16797500	1.33990300	-1.24768500
O	0.42758800	-0.84680700	-1.68091100
H	-2.15732300	-0.19226100	1.92212300
H	-1.51952400	-0.32353900	-1.61146800
H	-0.07922800	1.47209400	-2.32842500
H	0.81593300	1.47521300	-0.79810000
N	-1.02549000	2.53825300	-0.76202300
C	-2.47784000	2.22990000	-1.12816500
H	-2.44516900	1.94682200	-2.18418000
H	-2.73600800	1.34649000	-0.54290400
C	-3.52039300	3.32267900	-0.91486600
H	-4.46481400	2.93887100	-1.31560300
H	-3.69004700	3.54407500	0.14097200
H	-3.30094800	4.25448200	-1.44367900
C	-0.57132200	3.77504300	-1.52304800
H	-0.87475500	3.60812300	-2.56074600
H	-1.15562500	4.61095700	-1.13842700
C	0.91903800	4.08832500	-1.44844300
H	1.52787400	3.34725000	-1.96942900
H	1.07914300	5.05677200	-1.93469600
H	1.28750100	4.16051800	-0.42242600
C	-0.82740800	2.69337200	0.75370900
H	0.21239700	2.42690000	0.95293000
H	-1.46345500	1.92364700	1.19108100
C	-1.11748100	4.06128300	1.36695800
H	-2.14030500	4.40985000	1.21287800
H	-0.96249500	3.95939800	2.44640600
H	-0.42697200	4.83477600	1.02050700
C	3.24310800	2.38022700	0.81717000
C	3.00550500	1.17661200	0.16546100
C	2.63616000	-0.01745000	0.87224500
C	2.55956900	0.12271200	2.29766700
C	2.78435300	1.34509600	2.92994100
C	3.11544500	2.49739700	2.21101200
H	3.56421200	3.24179600	0.23157700
H	3.15218800	1.09660400	-0.90873800
H	2.33215100	-0.74311900	2.91082900
H	2.70973200	1.39284800	4.01606400
H	3.31707400	3.43755300	2.71730300
N	2.37162400	-1.14770500	0.16621400
H	1.21633200	-0.96304300	-1.02260900
C	2.17543800	-2.35044600	0.94941600
H	1.37926900	-2.26524700	1.71761400
H	3.09285800	-2.62301700	1.50775800
C	1.80578500	-3.53132500	0.08018300
C	1.10789000	-4.69840600	0.63592900
H	2.43628500	-3.68314400	-0.79516600
H	0.82667700	-4.70511800	1.69050500
H	1.25157000	-5.68534700	0.19399400
O	0.40184300	-3.75597800	-0.18161600
C	4.52103100	-1.63403100	-1.70068400
O	4.30860300	-0.68409000	-2.35023100

O	4.82842800	-2.61165700	-1.13390600

Zero-point correction= 0.596173 (Hartree/Particle)
Thermal correction to Energy= 0.630768
Thermal correction to Enthalpy= 0.631712
Thermal correction to Gibbs Free Energy= 0.525206
Sum of electronic and zero-point Energies= -1439.376854
Sum of electronic and thermal Energies= -1439.342259
Sum of electronic and thermal Enthalpies= -1439.341315
Sum of electronic and thermal Free Energies= -1439.447821
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -1439.84352089

TS3

C	-0.59099000	-0.14860400	-1.03235400
C	-0.74211000	-0.64830200	0.42397000
H	-0.52197100	-1.72199900	0.40714400
H	0.00571800	-0.18097100	1.07074200
N	-2.06913700	-0.37064900	0.99535500
C	-3.16401000	-1.22021900	0.69207800
C	-3.09980200	-2.23600300	-0.27538900
C	-4.37889800	-1.00433800	1.36853000
C	-4.23396000	-3.00273000	-0.55528000
H	-2.16989100	-2.45704800	-0.78811000
C	-5.49706900	-1.78348200	1.08907500
H	-4.43574800	-0.21790600	2.11932600
C	-5.43565700	-2.78641100	0.11719600
H	-4.16276200	-3.78854600	-1.30276500
H	-6.42199900	-1.60368700	1.63143800
H	-6.30953000	-3.39183700	-0.10519300
C	-0.19103800	1.33676500	-1.26631400
O	0.41687700	-0.84151000	-1.71512800
H	-2.01646100	-0.20491400	1.99499100
H	-1.52919400	-0.35309500	-1.56150100
H	-0.11140000	1.45094600	-2.34943100
H	0.79267800	1.49781700	-0.82650600
N	-1.06955100	2.52306800	-0.79494900
C	-2.51650000	2.17801400	-1.15239500
H	-2.47713300	1.86020400	-2.19818700
H	-2.76079100	1.30973600	-0.53932800
C	-3.57884100	3.25864500	-0.98021900
H	-4.51574200	2.84092900	-1.36430600
H	-3.75288100	3.52015800	0.06541900
H	-3.37716100	4.17124800	-1.54776100
C	-0.63803200	3.75561200	-1.57730200
H	-0.93769300	3.56569800	-2.61202700
H	-1.23664200	4.58775400	-1.20663800
C	0.84721700	4.09701200	-1.50930400
H	1.47184400	3.35483200	-2.00998400
H	0.99042000	5.05386500	-2.02262800
H	1.21006200	4.21051500	-0.48449600
C	-0.87189300	2.70557300	0.71688700
H	0.17755900	2.47652200	0.91298100
H	-1.47865500	1.91900200	1.16660400
C	-1.20449100	4.07077300	1.31389600
H	-2.24142000	4.37899500	1.16950000
H	-1.03282200	3.99057500	2.39272500
H	-0.54872200	4.86512300	0.94738800
C	3.09720700	2.36642900	1.14009800

C	2.95839800	1.25254900	0.31808000
C	2.74585900	-0.05652000	0.85029400
C	2.71399700	-0.14251600	2.27270500
C	2.83354700	0.98923400	3.08069500
C	3.01517400	2.26066900	2.53550400
H	3.30205800	3.33446600	0.68331300
H	3.07471500	1.34664100	-0.75587000
H	2.61241000	-1.10716400	2.75656800
H	2.79875600	0.86488600	4.16189100
H	3.12966000	3.13331400	3.17282400
N	2.55816100	-1.11845100	-0.01453100
H	1.23940800	-0.90862800	-1.11928100
C	2.45497200	-2.43478500	0.60418100
H	1.77902300	-2.42974300	1.47361800
H	3.43848000	-2.78118500	0.96386300
C	1.90820000	-3.47820800	-0.34624900
C	1.32350600	-4.72218100	0.17198900
H	2.34930900	-3.49758600	-1.34019400
H	1.26368500	-4.88140200	1.25021600
H	1.36347200	-5.63458700	-0.42402700
O	0.47662000	-3.68714100	-0.34400000
C	4.00771000	-1.21976900	-1.50498600
O	3.86264200	-0.23055400	-2.15973500
O	4.55987100	-2.25754000	-1.28810500

Zero-point correction= 0.597680 (Hartree/Particle)
Thermal correction to Energy= 0.630876
Thermal correction to Enthalpy= 0.631820
Thermal correction to Gibbs Free Energy= 0.530210
Sum of electronic and zero-point Energies= -1439.372314
Sum of electronic and thermal Energies= -1439.339118
Sum of electronic and thermal Enthalpies= -1439.338174
Sum of electronic and thermal Free Energies= -1439.439784
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -1439.84480722

INT5

C	-1.22250600	-0.18125600	1.29444800
C	-0.45941100	0.77887400	0.34205400
H	0.08096100	1.50231800	0.96812200
H	0.27978000	0.23497300	-0.25146800
N	-1.34670100	1.46099300	-0.59885500
C	-2.08853200	2.58899200	-0.20716000
C	-2.28667700	2.93502100	1.14154800
C	-2.68991500	3.38493700	-1.20131300
C	-3.07207100	4.04218200	1.47129000
H	-1.82567400	2.35468300	1.93411700
C	-3.46265000	4.48867800	-0.85836500
H	-2.54140200	3.12767100	-2.24843400
C	-3.66546300	4.82625300	0.48347700
H	-3.20985300	4.29349900	2.52008800
H	-3.90899000	5.09068600	-1.64605900
H	-4.27077800	5.68767100	0.75021200
C	-1.20063900	-1.69479100	0.93714100
O	-0.70973600	-0.11456400	2.61916000
H	-0.91397500	1.58264100	-1.50741700
H	-2.25769100	0.16620700	1.36566700
H	-1.50161000	-2.21591900	1.84907400
H	-0.19218500	-2.02191000	0.66910800

N	-2.16155700	-2.22942300	-0.14705600
C	-3.57636900	-1.77928700	0.23560400
H	-3.59630000	-1.75732900	1.32797300
H	-3.65949000	-0.74962600	-0.11575000
C	-4.76309600	-2.60767200	-0.25530800
H	-5.66945900	-2.06572200	0.03686500
H	-4.79263700	-2.73447300	-1.33858300
H	-4.81097700	-3.59300100	0.21535700
C	-2.06963700	-3.75569400	-0.12271500
H	-2.27614900	-4.03915000	0.91390800
H	-2.89296300	-4.12259600	-0.73531100
C	-0.75239200	-4.35606600	-0.60564200
H	0.14350000	-3.91258600	-0.15493200
H	-0.78038200	-5.42409100	-0.35953800
H	-0.64632100	-4.27198400	-1.69084700
C	-1.73357800	-1.66972300	-1.50717800
H	-0.65321200	-1.84830300	-1.58346300
H	-1.87866000	-0.59075900	-1.42060300
C	-2.47973000	-2.19812100	-2.72725600
H	-3.52101000	-1.86694200	-2.77809900
H	-1.96889100	-1.79118700	-3.60653400
H	-2.45052800	-3.28780700	-2.82001300
C	3.87780100	1.41233200	-2.92730000
C	3.50306200	0.28388200	-2.20336200
C	3.37091300	0.34564800	-0.80357200
C	3.61723500	1.57319300	-0.16424300
C	4.00988400	2.69463900	-0.89747200
C	4.14330700	2.62465900	-2.28338400
H	3.97740400	1.33878500	-4.00802000
H	3.29635400	-0.65126100	-2.70731600
H	3.46624900	1.65429400	0.90746800
H	4.19543800	3.63140300	-0.37683900
H	4.44418800	3.49905500	-2.85452400
N	3.02631500	-0.80716900	-0.05663100
H	0.25595600	0.06424700	2.59926600
C	3.66705400	-1.05632400	1.23265200
H	4.49129200	-0.34804100	1.34751500
H	4.08327600	-2.07108700	1.24053700
C	2.71895100	-0.95480400	2.41217000
C	3.00709800	-0.17388600	3.62227100
H	2.01600600	-1.77859900	2.48793000
H	3.94027100	0.38300100	3.69974300
H	2.55143700	-0.45063400	4.57248400
O	2.09587200	0.34106200	2.62976300
C	1.98536500	-1.71345700	-0.45819200
O	1.33235400	-1.42289700	-1.49354800
O	1.79433400	-2.68087500	0.33399400

Zero-point correction= 0.602278 (Hartree/Particle)
Thermal correction to Energy= 0.634759
Thermal correction to Enthalpy= 0.635703
Thermal correction to Gibbs Free Energy= 0.537241
Sum of electronic and zero-point Energies= -1439.411159
Sum of electronic and thermal Energies= -1439.378678
Sum of electronic and thermal Enthalpies= -1439.377733
Sum of electronic and thermal Free Energies= -1439.476196
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -1439.87470946

TS4

C	-1.59656400	1.80427500	0.50775900
C	-1.77856500	1.31379400	-0.94545000
H	-2.35994200	2.09675700	-1.45097300
H	-0.80406300	1.29371500	-1.43934700
N	-2.40547600	-0.00124200	-1.08989300
C	-3.80834000	-0.15381800	-1.07120600
C	-4.68184400	0.85432000	-0.63118000
C	-4.35406700	-1.38790400	-1.47401000
C	-6.05937300	0.62301200	-0.59584300
H	-4.30075200	1.82514800	-0.33422200
C	-5.72740500	-1.60337900	-1.44038300
H	-3.68750600	-2.17684800	-1.81769900
C	-6.59393800	-0.59999700	-0.99601500
H	-6.71694100	1.41969700	-0.25771700
H	-6.12331900	-2.56227500	-1.76480500
H	-7.66604200	-0.76991000	-0.96845100
C	-0.48902000	1.15986600	1.39901100
O	-1.25180400	3.16805000	0.50004600
H	-1.98878300	-0.54266700	-1.83864300
H	-2.55754100	1.72659700	1.02781400
H	-0.46036800	1.78877400	2.29086400
H	0.46485700	1.24983500	0.88798800
N	-0.53983400	-0.29001800	1.92551800
C	-1.98782500	-0.60123700	2.30849600
H	-2.37546900	0.32391500	2.74259300
H	-2.50749600	-0.76844000	1.36406400
C	-2.24044600	-1.74182400	3.29251500
H	-3.32734600	-1.84516800	3.38101600
H	-1.84659900	-2.70350200	2.96258600
H	-1.85430200	-1.52927400	4.29274900
C	0.34632800	-0.35801600	3.17146500
H	-0.16611700	0.25325700	3.92072400
H	0.31584200	-1.39344400	3.51080900
C	1.79073900	0.10178600	3.00305100
H	1.87753100	1.16093900	2.75145400
H	2.28638400	-0.03841300	3.96970600
H	2.36408100	-0.46815800	2.26889000
C	-0.00643100	-1.20714600	0.81837100
H	0.97675100	-0.81186000	0.56345200
H	-0.68022600	-1.03525300	-0.02058200
C	0.09962900	-2.69807100	1.11241600
H	-0.87392000	-3.19014700	1.17850400
H	0.64146500	-3.14128700	0.27039700
H	0.68037700	-2.92535400	2.01103000
C	3.56368400	-3.37830600	-0.63733400
C	3.65557700	-2.04240000	-0.25648500
C	3.08942400	-1.02342600	-1.06055300
C	2.46183900	-1.41929500	-2.26465400
C	2.37277800	-2.76521000	-2.62423800
C	2.91206300	-3.76249400	-1.81355000
H	4.01812500	-4.13313000	0.00090800
H	4.18748500	-1.75017700	0.63789100
H	2.06650500	-0.67845600	-2.94969300
H	1.88825900	-3.02612500	-3.56261500
H	2.84888900	-4.80840600	-2.10084400
N	3.10487600	0.32585800	-0.67099100

H	-0.50698600	3.31078100	-0.16696100
C	2.42676400	1.32628000	-1.48274600
H	1.47264000	0.92701000	-1.83280000
H	3.01122200	1.61362200	-2.37107500
C	2.18046800	2.54725400	-0.63324500
C	1.95495200	3.86710100	-1.20628900
H	1.85033600	2.42829600	0.38468300
H	2.45902800	4.08443100	-2.15698500
H	2.02733400	4.72442100	-0.52509600
O	0.67823000	3.27929100	-1.33952600
C	4.03583900	0.93709500	0.28449300
O	4.65655400	0.22808400	1.08083000
O	4.02352700	2.20899300	0.18384700

Zero-point correction= 0.599686 (Hartree/Particle)
Thermal correction to Energy= 0.632286
Thermal correction to Enthalpy= 0.633230
Thermal correction to Gibbs Free Energy= 0.532137
Sum of electronic and zero-point Energies= -1439.368512
Sum of electronic and thermal Energies= -1439.335912
Sum of electronic and thermal Enthalpies= -1439.334968
Sum of electronic and thermal Free Energies= -1439.436062
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -1439.83952351

2a

C	3.63323500	0.57811300	-0.00524400
C	2.28935700	0.93649300	0.06548200
C	1.30038100	-0.06310200	0.05503400
C	1.69121900	-1.40984900	-0.02313700
C	3.04265600	-1.74936000	-0.09039600
C	4.02369300	-0.76027000	-0.08252600
H	4.38421400	1.36365200	0.00310000
H	1.99817000	1.97580300	0.11885200
H	0.95018000	-2.20144300	-0.03447500
H	3.32145300	-2.79803500	-0.15046600
H	5.07537300	-1.02640500	-0.13527300
N	-0.07811600	0.24966100	0.14479200
H	-3.47331000	-2.32309100	-0.49271500
C	-1.10789700	-0.77560300	0.21878100
H	-0.92387300	-1.47066200	1.04307400
H	-1.15231400	-1.35648900	-0.71685300
C	-2.37915500	0.06308700	0.44065800
C	-3.58349200	-0.37287400	-0.39072300
H	-2.65560300	0.07116700	1.50126500
H	-3.33446700	-0.30584000	-1.45988800
H	-4.41947000	0.30589600	-0.19992800
O	-4.01121400	-1.67497000	-0.01420200
C	-0.64093800	1.50800000	-0.02892500
O	-0.09132100	2.56328200	-0.22999400
O	-2.00220100	1.39794000	0.06366300

Zero-point correction= 0.201623 (Hartree/Particle)
Thermal correction to Energy= 0.213766
Thermal correction to Enthalpy= 0.214710
Thermal correction to Gibbs Free Energy= 0.161801
Sum of electronic and zero-point Energies= -667.910473
Sum of electronic and thermal Energies= -667.898330
Sum of electronic and thermal Enthalpies= -667.897386
Sum of electronic and thermal Free Energies= -667.950295

M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -668.06687474

INT2'

C	0.23207500	1.21216100	1.86757000
C	0.05895000	0.95158100	0.37782000
H	0.65509300	1.68818400	-0.17194000
H	0.47555200	-0.03303200	0.13940500
N	-1.31638700	0.98510300	-0.06901300
C	-2.04721500	2.14993000	-0.23966000
C	-1.46429000	3.43307900	-0.17565000
C	-3.42872000	2.06461400	-0.51988600
C	-2.23983000	4.57200500	-0.39368900
H	-0.40621500	3.54661800	0.03869900
C	-4.18719500	3.21004900	-0.73184000
H	-3.89637500	1.08442200	-0.57563800
C	-3.60339900	4.47911300	-0.67199700
H	-1.76239200	5.54776400	-0.33916800
H	-5.24868800	3.10884400	-0.94662600
H	-4.19906800	5.37218600	-0.83648600
C	0.41952300	0.12098900	2.83268900
O	1.53742100	0.92491700	2.41210400
H	-1.83341500	0.10703000	-0.00945700
H	-0.19412600	2.14664600	2.23300700
H	0.13026700	0.25253700	3.87499900
H	0.43652700	-0.91033200	2.47959800
N	-2.56245200	-1.95067200	0.01234600
C	-2.78875400	-2.13532500	1.45192500
H	-1.87259300	-1.80152400	1.95824700
H	-3.57590700	-1.43124400	1.74960000
C	-3.14136000	-3.53818500	1.97898700
H	-3.16663600	-3.51943400	3.07537900
H	-4.12242100	-3.87840800	1.63414700
H	-2.39802100	-4.28497100	1.67973100
C	-1.42699700	-2.72403500	-0.51090100
H	-0.60358500	-2.60557000	0.20482500
H	-1.64003200	-3.80629400	-0.55305800
C	-0.95068200	-2.25347000	-1.88711500
H	-0.78369700	-1.17127600	-1.89371600
H	-0.00634800	-2.74939300	-2.13531200
H	-1.66976600	-2.49058300	-2.67895000
C	-3.76660200	-1.95047000	-0.83371600
H	-3.53553400	-1.37037900	-1.73563800
H	-4.53262200	-1.37989800	-0.29443400
C	-4.35753700	-3.30203300	-1.27389400
H	-4.71152800	-3.90185300	-0.43073800
H	-5.21124900	-3.12436600	-1.93875600
H	-3.62900400	-3.90116600	-1.83063100
C	2.75191300	-3.39311200	0.53440200
C	2.94028600	-2.05296200	0.85290200
C	3.41173800	-1.13776400	-0.11490900
C	3.69033100	-1.62444400	-1.40654200
C	3.50176600	-2.97431000	-1.71011300
C	3.02840500	-3.87008700	-0.75213000
H	2.39406100	-4.07542800	1.30210300
H	2.74501400	-1.69436600	1.86021500
H	4.05161800	-0.95315600	-2.17839300
H	3.72688900	-3.32332900	-2.71517700

H	2.88543800	-4.91862200	-0.99637200
N	3.60252200	0.19141800	0.24781500
H	3.01339000	0.49297600	1.02210300
C	3.83835600	1.21127800	-0.75721500
H	3.06071600	1.22607900	-1.54108400
H	4.79642000	1.01285100	-1.25940900
C	3.91038200	2.57669600	-0.11988600
C	3.50245200	3.78310600	-0.85094900
H	4.64197200	2.67751500	0.68355000
H	3.12995100	3.69464400	-1.87178900
H	3.95309900	4.74399700	-0.60326200
O	2.65456200	3.22395300	0.16104400

Zero-point correction= 0.579664 (Hartree/Particle)
Thermal correction to Energy= 0.612595
Thermal correction to Enthalpy= 0.613539
Thermal correction to Gibbs Free Energy= 0.507391
Sum of electronic and zero-point Energies= -1250.857701
Sum of electronic and thermal Energies= -1250.824769
Sum of electronic and thermal Enthalpies= -1250.823825
Sum of electronic and thermal Free Energies= -1250.929973
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -1251.26139021

TS1'

O	1.79012900	-0.42859800	2.99820300
C	0.64746200	-1.60020100	2.21684600
C	0.39677700	-0.76425200	0.97573700
H	0.17522000	-1.35587000	0.09270900
H	-0.44366900	-0.09008500	1.15300400
C	2.09465000	0.50316600	2.19885600
O	2.64821800	1.57055600	2.31485300
N	1.59495900	0.10479300	0.74034000
C	2.71899800	-0.47212400	-0.03739600
C	2.66222900	-1.75835200	-0.57390000
C	3.84975300	0.33162900	-0.21986700
C	3.75478300	-2.23403600	-1.30537200
H	1.79199600	-2.39395700	-0.46280200
C	4.92935400	-0.15939400	-0.95102700
H	3.88822000	1.31790100	0.22716300
C	4.88586400	-1.44371900	-1.49727600
H	3.70719100	-3.23388200	-1.72660400
H	5.80689200	0.46571300	-1.08852200
H	5.72860800	-1.82407200	-2.06729500
C	-0.52878700	-1.88306400	3.06830600
O	-1.06196500	-2.66437900	2.06430800
H	1.25330100	1.00947300	0.26423700
H	1.34032800	-2.42806300	2.11971700
H	-0.27890600	-2.41077600	4.00632900
H	-1.09230000	-0.96575500	3.33711600
N	0.48972300	2.47592600	-0.41494400
C	-0.17108400	3.04138800	0.78937700
H	-0.85733700	2.26671100	1.15332800
H	0.60873800	3.16307700	1.54884800
C	-0.97404600	4.34347900	0.65437800
H	-1.48048300	4.54264400	1.60589500
H	-0.34159100	5.20811900	0.43470700
H	-1.74766200	4.26965600	-0.11650100
C	-0.48052700	2.10302000	-1.46969000

H	-1.30663100	1.57997100	-0.97598400
H	-0.91883800	2.99590100	-1.93996700
C	0.10690900	1.20120100	-2.55582500
H	0.52978700	0.28028600	-2.13986200
H	-0.68866300	0.91388000	-3.25135900
H	0.88878200	1.70107200	-3.13756400
C	1.66369600	3.24369500	-0.89954600
H	2.29739300	2.54563300	-1.45900600
H	2.23323700	3.53007800	-0.00857200
C	1.42505300	4.47598100	-1.78576300
H	0.85073700	5.25786100	-1.28369000
H	2.39589300	4.90270100	-2.06378900
H	0.90549100	4.21904100	-2.71482900
C	-4.08934900	1.45596600	1.06960500
C	-3.41340900	0.24134900	1.09001400
C	-3.38251700	-0.59706100	-0.05455000
C	-4.08302600	-0.16069700	-1.20286100
C	-4.75112600	1.06424600	-1.20510000
C	-4.76009300	1.88980900	-0.08021700
H	-4.10239700	2.06744200	1.96942400
H	-2.92258600	-0.09849600	1.99900000
H	-4.11567500	-0.78448700	-2.09034500
H	-5.28144500	1.36957900	-2.10467000
H	-5.29122600	2.83702100	-0.08947000
N	-2.66672500	-1.76474000	-0.00752100
H	-2.19652600	-2.03289000	0.87749600
C	-2.61116100	-2.73604600	-1.07431800
H	-2.48046000	-2.24149200	-2.04720400
H	-3.53726500	-3.33745200	-1.14250800
C	-1.43695000	-3.66564300	-0.86451500
C	-0.79922200	-4.34658400	-1.99688000
H	-1.34983700	-4.09815000	0.13104600
H	-1.17375000	-4.18355400	-3.00820600
H	-0.29020900	-5.29775200	-1.84128200
O	-0.17081100	-3.20525500	-1.39226400

Zero-point correction= 0.594264 (Hartree/Particle)
Thermal correction to Energy= 0.628399
Thermal correction to Enthalpy= 0.629343
Thermal correction to Gibbs Free Energy= 0.524215
Sum of electronic and zero-point Energies= -1439.362509
Sum of electronic and thermal Energies= -1439.328374
Sum of electronic and thermal Enthalpies= -1439.327430
Sum of electronic and thermal Free Energies= -1439.432558
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -1439.78411793

INT3'

O	1.57896300	-0.54419200	2.92792500
C	0.74078600	-1.56251100	2.20522600
C	0.41137700	-0.83622700	0.90643200
H	0.25619600	-1.47785500	0.04722800
H	-0.47728200	-0.21564800	1.04094300
C	1.98461200	0.42390400	2.15138700
O	2.57262900	1.43149500	2.43165400
N	1.56638700	0.10913000	0.71128600
C	2.74157100	-0.37540800	-0.06739300
C	2.74409200	-1.62472100	-0.68730200
C	3.84228800	0.48174800	-0.16736800

C	3.87194200	-2.00827300	-1.41953300
H	1.89779300	-2.30013700	-0.63808200
C	4.95787800	0.08023600	-0.89945800
H	3.83378400	1.43930100	0.33954100
C	4.97629500	-1.16584700	-1.52879800
H	3.87349000	-2.97905800	-1.90604900
H	5.81330200	0.74531900	-0.97284800
H	5.84643300	-1.47659500	-2.09966000
C	-0.54388300	-1.96289200	2.95137200
O	-1.26294500	-2.71285600	2.08669100
H	1.17420400	1.05191100	0.25765800
H	1.39315900	-2.42568800	2.05609000
H	-0.24913200	-2.47969500	3.89381400
H	-1.01646900	-0.99927800	3.28363100
N	0.43988400	2.41313500	-0.32227400
C	-0.17459900	2.97285600	0.91591300
H	-0.76854600	2.16147600	1.35397800
H	0.64800600	3.18050600	1.60830900
C	-1.08684900	4.20051100	0.80106900
H	-1.50569100	4.41152200	1.79164800
H	-0.55445900	5.09778700	0.47455800
H	-1.92855100	4.02162300	0.12559500
C	-0.58559000	2.01865400	-1.32394400
H	-1.36895500	1.47677900	-0.78545900
H	-1.06588200	2.90784500	-1.75368900
C	-0.04370800	1.14046400	-2.45117000
H	0.42384500	0.22454500	-2.07429100
H	-0.87771400	0.83964700	-3.09321900
H	0.68635800	1.66346800	-3.07815100
C	1.56010100	3.21876000	-0.87963600
H	2.17136300	2.53940600	-1.48364600
H	2.17920000	3.51766400	-0.02632600
C	1.22916100	4.44986500	-1.73499400
H	0.69038700	5.22104100	-1.18027200
H	2.16799400	4.89091700	-2.08939600
H	0.63740600	4.19093700	-2.61891500
C	-4.02002400	1.47058200	0.96345800
C	-3.38839400	0.23432900	1.03006400
C	-3.32105200	-0.61787500	-0.10734500
C	-3.94267700	-0.16225700	-1.29669400
C	-4.56412100	1.08591800	-1.34360600
C	-4.60748000	1.92177700	-0.22605300
H	-4.06701700	2.08704900	1.85914400
H	-2.96604600	-0.12091000	1.96716300
H	-3.95482200	-0.79358700	-2.17956200
H	-5.03410500	1.40153000	-2.27308400
H	-5.10833900	2.88461000	-0.26954600
N	-2.64941200	-1.80057100	-0.00230300
H	-2.20752500	-2.07158800	0.92201000
C	-2.53021200	-2.77948600	-1.05655100
H	-2.40965000	-2.29733800	-2.03709000
H	-3.42279600	-3.42949500	-1.12761200
C	-1.31226300	-3.64573800	-0.81298300
C	-0.66646600	-4.37102600	-1.91148400
H	-1.17891200	-3.98208400	0.21490300
H	-1.06876900	-4.29583400	-2.92279400
H	-0.10940400	-5.28522500	-1.70581700

O	-0.07459500	-3.16204500	-1.40768500

Zero-point correction= 0.594609 (Hartree/Particle)
Thermal correction to Energy= 0.628502
Thermal correction to Enthalpy= 0.629446
Thermal correction to Gibbs Free Energy= 0.525436
Sum of electronic and zero-point Energies= -1439.368894
Sum of electronic and thermal Energies= -1439.335002
Sum of electronic and thermal Enthalpies= -1439.334058
Sum of electronic and thermal Free Energies= -1439.438068
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -1439.80784425

TS2'

O	1.53799700	-0.49414500	2.93511400
C	0.68858700	-1.51342100	2.23556300
C	0.39046600	-0.81737100	0.91368500
H	0.22337400	-1.48141200	0.07457600
H	-0.48900300	-0.17853000	1.02403300
C	1.98451600	0.43051300	2.12292100
O	2.60644700	1.42465100	2.38762400
N	1.56599600	0.09576300	0.70203100
C	2.72460600	-0.43264300	-0.06719200
C	2.67322000	-1.66943800	-0.71251700
C	3.87185300	0.36556700	-0.14554700
C	3.78499100	-2.09682300	-1.44493400
H	1.79797000	-2.30742600	-0.67673800
C	4.97165900	-0.07938900	-0.87657400
H	3.91145300	1.31171000	0.38016900
C	4.93238300	-1.31153800	-1.53134900
H	3.74012100	-3.05822200	-1.94800500
H	5.86100300	0.54200000	-0.92885700
H	5.79016500	-1.65583700	-2.10171900
C	-0.61284800	-1.86118100	2.98005400
O	-1.35119700	-2.61628000	2.13571900
H	1.16180100	1.09948900	0.20386100
H	1.32209100	-2.39564400	2.11656400
H	-0.33916300	-2.35791100	3.93959300
H	-1.06065100	-0.87527900	3.28169900
N	0.54410500	2.34348700	-0.32991700
C	-0.05020700	2.96182700	0.89812000
H	-0.59681000	2.15920600	1.40712700
H	0.78869600	3.23786100	1.54367500
C	-1.01364800	4.14139200	0.73208600
H	-1.35318800	4.44350300	1.72925900
H	-0.54897000	5.01369500	0.26623100
H	-1.90318400	3.86422700	0.15928300
C	-0.50431100	1.96918000	-1.32329100
H	-1.29592100	1.45519000	-0.77045500
H	-0.95827600	2.87359800	-1.74591600
C	-0.00256700	1.07202600	-2.45356900
H	0.45789700	0.15049200	-2.08266000
H	-0.85980100	0.78156700	-3.06908000
H	0.71796100	1.57799400	-3.10485400
C	1.69624100	3.09606900	-0.90800800
H	2.23557700	2.39324100	-1.55008200
H	2.36168300	3.32526000	-0.06893900
C	1.41222600	4.37105100	-1.70991100
H	0.99451800	5.17322400	-1.09750400

H	2.35785300	4.73476100	-2.12779800
H	0.73336000	4.19096800	-2.54951100
C	-3.97676700	1.61142500	0.90834200
C	-3.38595300	0.35735800	1.00658400
C	-3.34282100	-0.52421800	-0.11007700
C	-3.94405300	-0.07503000	-1.31311500
C	-4.52289200	1.19165900	-1.39216400
C	-4.54383900	2.05463500	-0.29439300
H	-4.00870900	2.24891900	1.78991500
H	-2.97978900	0.01007500	1.95366600
H	-3.97527800	-0.72614800	-2.18098000
H	-4.97871900	1.50049800	-2.33096000
H	-5.01499900	3.03100300	-0.36198900
N	-2.71329100	-1.72535700	0.02789500
H	-2.27416900	-1.98385100	0.95962700
C	-2.62484500	-2.73739500	-0.99810700
H	-2.51227200	-2.28796300	-1.99460800
H	-3.52816800	-3.37506000	-1.03462500
C	-1.41566400	-3.61364100	-0.74639400
C	-0.80355400	-4.39102700	-1.82838600
H	-1.26693800	-3.91165600	0.29148100
H	-1.22586500	-4.34978100	-2.83352900
H	-0.25569000	-5.30491700	-1.59799100
O	-0.18428600	-3.17217900	-1.38533200

Zero-point correction= 0.592269 (Hartree/Particle)
Thermal correction to Energy= 0.625629
Thermal correction to Enthalpy= 0.626574
Thermal correction to Gibbs Free Energy= 0.524540
Sum of electronic and zero-point Energies= -1439.371029
Sum of electronic and thermal Energies= -1439.337669
Sum of electronic and thermal Enthalpies= -1439.336725
Sum of electronic and thermal Free Energies= -1439.438758
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -1439.81099115

INT4'

O	3.07263100	-0.82195800	3.16491000
C	0.02993800	-1.55571100	1.85732300
C	0.12251200	-0.92395300	0.47960900
H	-0.24649600	-1.64564700	-0.26108200
H	-0.54593300	-0.05736900	0.44849300
C	3.41582400	0.11489700	2.55681900
O	3.78161100	1.06831300	1.98531200
N	1.47190000	-0.47114400	0.16718800
C	2.37942400	-1.29784500	-0.50188300
C	2.19121600	-2.68752200	-0.63107200
C	3.55464600	-0.73284500	-1.04078700
C	3.14595800	-3.47088800	-1.28177300
H	1.30135400	-3.16317100	-0.23162400
C	4.49577500	-1.52659300	-1.68761200
H	3.72268900	0.33605700	-0.93841400
C	4.30284800	-2.90531500	-1.81616500
H	2.97491900	-4.54141000	-1.36782000
H	5.39008600	-1.06127300	-2.09553800
H	5.04065700	-3.52309600	-2.31976800
C	-0.43656600	-0.79760600	3.02332700
O	-1.30427800	-1.74589500	2.37079600
H	1.50535500	0.51462400	-0.10320700

H	0.69032700	-2.40367700	2.03603300
H	-0.11903800	-1.08408600	4.02490900
H	-0.72179000	0.24790500	2.90325500
N	1.06332900	2.60743700	-0.50277600
C	0.82693500	3.06497300	0.87463800
H	0.03311300	2.42490600	1.28348400
H	1.73441600	2.84275100	1.44840200
C	0.41986800	4.53024500	1.11362200
H	0.18371500	4.67304500	2.17530000
H	1.21982500	5.23169300	0.85871300
H	-0.47174700	4.80377300	0.53921800
C	-0.12801100	2.68883600	-1.35969800
H	-0.97879100	2.34195100	-0.76147000
H	-0.36393600	3.72668900	-1.65121700
C	-0.02709900	1.82878100	-2.62120900
H	0.21686200	0.79078600	-2.37106700
H	-0.98732400	1.83804900	-3.14822900
H	0.73538600	2.19692400	-3.31632600
C	2.31854700	3.06327700	-1.12287100
H	2.58758900	2.33317300	-1.89659100
H	3.09560300	2.98930700	-0.35287900
C	2.36261500	4.46402500	-1.76064500
H	2.19375600	5.26412200	-1.03460900
H	3.35025800	4.62407300	-2.20957800
H	1.62040500	4.57274200	-2.55911800
C	-3.77350700	2.27005000	1.04895700
C	-3.51814300	0.90862400	1.16984600
C	-3.70006300	0.03760900	0.07200400
C	-4.14223400	0.59020800	-1.14604800
C	-4.39918700	1.95881900	-1.25037700
C	-4.21694700	2.81220900	-0.16274400
H	-3.63153200	2.91463000	1.91338100
H	-3.19180100	0.49252000	2.11955000
H	-4.28919500	-0.04505500	-2.01327800
H	-4.74450700	2.35766800	-2.20137700
H	-4.42034300	3.87526200	-0.25215800
N	-3.46080500	-1.32078100	0.23982700
H	-2.81178200	-1.53543000	0.99490900
C	-3.37327900	-2.21257600	-0.90093900
H	-2.64007400	-1.87082700	-1.65272500
H	-4.35013600	-2.25985900	-1.40425800
C	-3.00079600	-3.60497700	-0.45545700
C	-2.22809700	-4.50415800	-1.32193900
H	-3.65911800	-4.04495100	0.29548300
H	-1.90593200	-4.16092700	-2.30533700
H	-2.34525500	-5.58318200	-1.22280500
O	-1.60316300	-3.85004300	-0.20975200

Zero-point correction= 0.597934 (Hartree/Particle)
Thermal correction to Energy= 0.631548
Thermal correction to Enthalpy= 0.632492
Thermal correction to Gibbs Free Energy= 0.529465
Sum of electronic and zero-point Energies= -1439.406021
Sum of electronic and thermal Energies= -1439.372408
Sum of electronic and thermal Enthalpies= -1439.371463
Sum of electronic and thermal Free Energies= -1439.474491
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -1439.84468226

INT3''

C	-0.61354600	0.16270800	-0.98137000
C	0.06189500	1.44391100	-1.56589500
H	1.13381500	1.36803500	-1.34561400
H	-0.03702400	1.40470200	-2.65724300
N	-0.50090400	2.71604800	-1.10464200
C	-0.06627300	3.36378600	0.05283500
C	0.71575300	2.72428100	1.03365200
C	-0.44654700	4.70364200	0.27502000
C	1.09165500	3.40874300	2.18981000
H	1.03965500	1.69939200	0.89044900
C	-0.06424000	5.37363800	1.43225400
H	-1.04762700	5.21557100	-0.47511400
C	0.70758500	4.73249700	2.40547400
H	1.70195900	2.89340400	2.92766200
H	-0.36983000	6.40801800	1.57214200
H	1.00721200	5.25678900	3.30828300
C	-2.10963200	0.22086200	-1.42237600
O	-0.01488900	-0.96372500	-1.41647500
H	-0.73356900	3.36192200	-1.84752200
H	-0.60445700	0.30710900	0.13283900
H	-2.14137800	-0.19941400	-2.43126000
H	-2.50063600	1.24101100	-1.41745600
N	-3.09383900	-0.61454800	-0.57992200
C	-2.37964700	-1.92558500	-0.14768300
H	-1.55730600	-2.04774400	-0.86622800
H	-1.89229500	-1.69089400	0.79791600
C	-3.23274900	-3.17833200	-0.00013200
H	-2.55928600	-3.93495300	0.41486200
H	-4.07393100	-3.07795400	0.69313800
H	-3.61058800	-3.55952700	-0.95375200
C	-4.31065500	-0.93366400	-1.42758700
H	-3.93681100	-1.55529900	-2.24460300
H	-4.97573200	-1.54971400	-0.82191100
C	-5.07471300	0.26449100	-1.98308600
H	-4.45741700	0.89743500	-2.62439600
H	-5.89869700	-0.12163600	-2.59264500
H	-5.51633100	0.88476200	-1.19788700
C	-3.45508600	0.21927900	0.63956000
H	-3.89549600	1.14545900	0.26458100
H	-2.49809000	0.48230500	1.09418200
C	-4.37522700	-0.43547100	1.66191900
H	-3.92258300	-1.31297100	2.13000000
H	-4.56343300	0.29726200	2.45382300
H	-5.34634200	-0.71896200	1.24375500
C	4.41331800	-0.00013300	-2.25269300
C	3.28954600	-0.63536900	-1.74210300
C	3.32108600	-1.24634600	-0.46367600
C	4.52313900	-1.17306400	0.27184400
C	5.64668300	-0.53868200	-0.26392800
C	5.60960800	0.05244700	-1.52500800
H	4.35884100	0.45797000	-3.23845900
H	2.35906500	-0.68095400	-2.30057800
H	4.58511700	-1.59687400	1.26939300
H	6.56000900	-0.50114900	0.32672600
H	6.48684000	0.54752000	-1.93241900
N	2.18433800	-1.89831600	-0.02156000

H	1.29244600	-1.59130700	-0.47592100
C	2.11607600	-2.52051800	1.27336000
H	1.98308800	-1.81104800	2.11381700
H	3.05733200	-3.05639000	1.46578100
C	1.01273200	-3.55086300	1.34176700
C	0.46163200	-3.99804700	2.62796500
H	0.98294800	-4.24088300	0.49751900
H	0.82212100	-3.54634100	3.55296400
H	0.06788000	-5.00957200	2.73150700
O	-0.29523600	-3.12285500	1.77960000

Zero-point correction= 0.583096 (Hartree/Particle)
Thermal correction to Energy= 0.613799
Thermal correction to Enthalpy= 0.614744
Thermal correction to Gibbs Free Energy= 0.517398
Sum of electronic and zero-point Energies= -1250.824512
Sum of electronic and thermal Energies= -1250.793808
Sum of electronic and thermal Enthalpies= -1250.792864
Sum of electronic and thermal Free Energies= -1250.890209
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -1251.26132148

TS2''

C	-0.61140200	0.31239200	-0.75076400
C	0.28543600	1.26484900	-1.60187200
H	1.31429600	0.89466600	-1.52143100
H	-0.00801600	1.15664100	-2.65299400
N	0.18498900	2.68143600	-1.24770400
C	0.97550000	3.27388600	-0.25949800
C	1.72945100	2.52384100	0.66261200
C	1.00024100	4.67969900	-0.15401000
C	2.47344200	3.16921600	1.65098600
H	1.75249700	1.44138800	0.60186100
C	1.74675300	5.30938400	0.83629000
H	0.42460200	5.27477000	-0.86148700
C	2.49004300	4.56035700	1.75302900
H	3.05546400	2.56591800	2.34339000
H	1.74949500	6.39567500	0.88914700
H	3.07451000	5.05271400	2.52487200
C	-2.07834400	0.75559000	-1.01901500
O	-0.38856600	-0.99404600	-1.05881200
H	0.01173200	3.29711800	-2.03113600
H	-0.38055500	0.55660500	0.31535800
H	-2.38765100	0.28441300	-1.95217000
H	-2.14643300	1.84241300	-1.09907600
N	-3.12849700	0.34717600	0.03431700
C	-2.75778700	-1.05056500	0.59625000
H	-2.11448500	-1.50261100	-0.16592900
H	-2.10228000	-0.86017100	1.44531700
C	-3.89937700	-1.96986500	1.01155600
H	-3.41525300	-2.83847500	1.46867600
H	-4.57740100	-1.54361200	1.75778000
H	-4.49278000	-2.32785600	0.16495200
C	-4.48547100	0.29623900	-0.64546700
H	-4.40113100	-0.49802000	-1.39090500
H	-5.21135600	-0.02283400	0.10273100
C	-4.95154200	1.59025000	-1.30579500
H	-4.26703100	1.93529600	-2.08389700
H	-5.91709900	1.38836900	-1.78165200

H	-5.10822600	2.40154700	-0.58871400
C	-3.08395800	1.38910300	1.14029500
H	-3.31674400	2.34801300	0.67334600
H	-2.03738200	1.42905800	1.44956100
C	-3.98998500	1.14571700	2.34038800
H	-3.72344600	0.23798800	2.88671000
H	-3.86443100	1.98990000	3.02680000
H	-5.05066600	1.09909500	2.07358500
C	4.23042700	-0.96691600	-1.94377100
C	3.02063000	-1.37089500	-1.39459300
C	2.92228900	-1.69478300	-0.01965200
C	4.08701400	-1.58506100	0.76851500
C	5.29811900	-1.18793600	0.19580500
C	5.38662400	-0.87421400	-1.15845400
H	4.27553900	-0.72980000	-3.00472500
H	2.12865400	-1.46096700	-2.00631300
H	4.05298300	-1.79561200	1.83287900
H	6.17986500	-1.11503300	0.82926000
H	6.33110500	-0.56234100	-1.59550200
N	1.70020400	-2.12332700	0.47315800
H	0.86835800	-1.77925200	-0.04766800
C	1.53446900	-2.49511400	1.85397300
H	1.50913800	-1.64009600	2.55800500
H	2.38745100	-3.12055400	2.15622600
C	0.28849800	-3.32240100	2.06954400
C	-0.28994800	-3.48965500	3.40925500
H	0.13150200	-4.11242500	1.33429300
H	0.16115600	-2.97292500	4.25729300
H	-0.83227700	-4.40159900	3.65979800
O	-0.92567900	-2.63674800	2.44645100
C	-1.00566800	-2.09221800	-3.08388800
O	-0.11349400	-2.84899000	-3.04545200
O	-1.97767600	-1.47894200	-3.35430600

Zero-point correction= 0.596070 (Hartree/Particle)
Thermal correction to Energy= 0.630097
Thermal correction to Enthalpy= 0.631041
Thermal correction to Gibbs Free Energy= 0.525234
Sum of electronic and zero-point Energies= -1439.405092
Sum of electronic and thermal Energies= -1439.371065
Sum of electronic and thermal Enthalpies= -1439.370121
Sum of electronic and thermal Free Energies= -1439.475928
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -1439.84763013

INT4''

C	1.20923300	0.50902300	1.22337400
C	2.47956600	0.56555800	2.09667100
H	2.66324100	1.62029600	2.33899400
H	2.25014700	0.06046700	3.04032400
N	3.65722500	-0.07551700	1.52099400
C	4.54092000	0.60538200	0.67189300
C	4.18946500	1.79506900	0.00876300
C	5.81521000	0.05457600	0.42921900
C	5.09221100	2.40534200	-0.86498600
H	3.22371900	2.25709900	0.18160300
C	6.70499400	0.67406800	-0.44191900
H	6.10352700	-0.86392000	0.93780400
C	6.35129100	1.85548300	-1.10055100

H	4.79988800	3.32783400	-1.35997700
H	7.68466400	0.23148400	-0.60371000
H	7.04730100	2.33832400	-1.77983000
C	0.76287000	-0.94530300	0.88553200
O	0.20711500	1.07596200	2.03750100
H	4.13979900	-0.68526300	2.16817200
H	1.33054200	1.10493900	0.31544800
H	-0.28969900	-1.02436500	1.16107700
H	1.33256300	-1.66566800	1.47502700
N	0.83156000	-1.45890700	-0.56831100
C	0.29470500	-0.36625200	-1.52621500
H	-0.34059500	0.29427100	-0.92720800
H	1.17221000	0.21844200	-1.81015400
C	-0.46287400	-0.82936000	-2.76747700
H	-0.68725300	0.07859200	-3.33820600
H	0.10127800	-1.49768600	-3.42412000
H	-1.42099300	-1.29354200	-2.51962900
C	-0.06421600	-2.69518800	-0.64673400
H	-1.07629900	-2.34764600	-0.43109600
H	-0.03747500	-3.03229000	-1.68207200
C	0.29936200	-3.84907300	0.28096600
H	0.22977900	-3.58317500	1.33787300
H	-0.43709300	-4.63894500	0.10401100
H	1.29016800	-4.26845700	0.07983400
C	2.27925600	-1.78828100	-0.89942700
H	2.61374100	-2.50074800	-0.14390200
H	2.83809000	-0.86822600	-0.73105900
C	2.54934600	-2.32609700	-2.29897500
H	2.30720400	-1.60171800	-3.08025800
H	3.62341400	-2.52844700	-2.36756800
H	2.02649300	-3.26351800	-2.51149400
C	-3.07945700	-2.59825500	1.70689700
C	-3.17069400	-1.21745100	1.58014500
C	-3.66643600	-0.62848000	0.38541000
C	-4.01651700	-1.49610900	-0.67797100
C	-3.91515700	-2.88182800	-0.52951500
C	-3.45059100	-3.45229900	0.65691400
H	-2.72202100	-3.01732300	2.64565400
H	-2.88081700	-0.56078600	2.39611900
H	-4.40888000	-1.08682200	-1.60333100
H	-4.21847200	-3.52138400	-1.35627000
H	-3.39955200	-4.53151800	0.77290400
N	-3.80902300	0.73168700	0.31396100
H	-3.29102900	1.26490100	1.02244300
C	-4.01485200	1.41965500	-0.94627000
H	-5.01461400	1.20118200	-1.34801100
H	-3.27716000	1.09275500	-1.70205600
C	-3.87564000	2.91280600	-0.76970800
C	-4.56939900	3.84404900	-1.66857300
H	-2.94649700	3.22657100	-0.29478200
H	-5.20853900	3.45626100	-2.46447100
H	-4.14006900	4.82764500	-1.86370800
O	-5.04676400	3.62692500	-0.33860500
C	-0.92093400	1.68882500	1.35805800
O	-1.87426100	1.88522100	2.12106500
O	-0.77471800	1.89494000	0.13328900

Zero-point correction= 0.600409 (Hartree/Particle)

Thermal correction to Energy= 0.633684
Thermal correction to Enthalpy= 0.634628
Thermal correction to Gibbs Free Energy= 0.532078
Sum of electronic and zero-point Energies= -1439.411839
Sum of electronic and thermal Energies= -1439.378564
Sum of electronic and thermal Enthalpies= -1439.377620
Sum of electronic and thermal Free Energies= -1439.480169
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -1439.884668

TS3''

C	0.84190300	0.25745800	1.07789300
C	1.99671900	0.65446400	2.02833300
H	1.92477500	1.73629400	2.19882400
H	1.81319200	0.15636200	2.98194900
N	3.31978700	0.27440300	1.55596200
C	4.13331400	1.12446900	0.80344900
C	3.62922900	2.24968900	0.12504100
C	5.50560400	0.82846300	0.67708700
C	4.47791900	3.04522500	-0.64766500
H	2.58018100	2.51521400	0.20486300
C	6.33929700	1.62947000	-0.09547400
H	5.91260900	-0.03689600	1.19729800
C	5.83414600	2.74659100	-0.76787800
H	4.06474400	3.91209900	-1.15721800
H	7.39495200	1.38028000	-0.16884700
H	6.48708600	3.37120500	-1.36993500
C	0.70029500	-1.24356300	0.89825300
O	-0.38257600	0.75174100	1.60939700
H	3.83744600	-0.30535500	2.20223500
H	0.97002300	0.76472100	0.11956000
H	-0.25133900	-1.68321700	0.65192100
H	1.48179100	-1.89190900	1.26356100
N	1.15295700	-1.60265900	-1.08139900
C	0.14107500	-0.77577000	-1.82237200
H	-0.74916200	-0.70788800	-1.18819100
H	0.55898900	0.23158500	-1.90069000
C	-0.30782000	-1.24391100	-3.21252400
H	-0.98389500	-0.48205800	-3.61558500
H	0.51705200	-1.36496100	-3.91984500
H	-0.87002300	-2.18073400	-3.16734700
C	0.86905200	-3.05989900	-1.23858200
H	-0.16645000	-3.20780300	-0.91687900
H	0.91428100	-3.32035400	-2.30241500
C	1.79060100	-4.00813800	-0.47018100
H	1.75530100	-3.85515900	0.61119300
H	1.45690900	-5.03364100	-0.66186500
H	2.83290100	-3.94050000	-0.79685900
C	2.56344500	-1.22714600	-1.36661900
H	3.18164600	-1.71024000	-0.60626700
H	2.64979200	-0.15394900	-1.18309500
C	3.11321200	-1.54773900	-2.76082800
H	2.61675100	-0.96997200	-3.54524900
H	4.17606100	-1.28309500	-2.78264900
H	3.03125600	-2.61042600	-3.01149400
C	-3.77733100	3.79536900	-0.50577900
C	-3.34628200	2.62289500	0.10105800
C	-3.96092400	1.38763800	-0.20049600

C	-5.02163000	1.37929300	-1.12529700
C	-5.43807800	2.56614800	-1.73318800
C	-4.82603800	3.78144700	-1.43347600
H	-3.28892900	4.73354100	-0.25197700
H	-2.52433700	2.63404200	0.81250200
H	-5.53201900	0.45274800	-1.36800900
H	-6.26111200	2.53271200	-2.44370400
H	-5.15979000	4.70114100	-1.90559000
N	-3.46182700	0.23561400	0.40163700
H	-3.00564500	0.40362700	1.29990300
C	-4.17785900	-1.02460800	0.35053900
H	-4.39428200	-1.28401600	-0.69261100
H	-5.14592100	-0.99274600	0.88599300
C	-3.32520600	-2.12200700	0.94211400
C	-3.42608700	-3.51116500	0.48066300
H	-2.95758100	-1.93982000	1.95187500
H	-4.13344700	-3.76927900	-0.30829200
H	-3.17052200	-4.32545500	1.15843800
O	-2.32552500	-2.68868100	0.06014000
C	-0.91255900	-0.14779300	2.56257900
O	-2.00115300	0.14880900	3.04357800
O	-0.18270900	-1.18297800	2.73578500

Zero-point correction= 0.598027 (Hartree/Particle)
Thermal correction to Energy= 0.631411
Thermal correction to Enthalpy= 0.632355
Thermal correction to Gibbs Free Energy= 0.528953
Sum of electronic and zero-point Energies= -1439.393709
Sum of electronic and thermal Energies= -1439.360325
Sum of electronic and thermal Enthalpies= -1439.359381
Sum of electronic and thermal Free Energies= -1439.462783
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -1439.83321631

INT1a

N	0.15739400	-0.16868400	0.02557000
C	-0.29425400	-1.53544600	0.44886400
H	-0.52599100	-2.07628300	-0.47238600
H	0.54614000	-2.04253900	0.93489200
C	-1.50496800	-1.55810600	1.37727600
H	-1.76363900	-2.60524700	1.57108100
H	-1.30333100	-1.08662900	2.34378200
H	-2.38125000	-1.07653000	0.93164500
C	0.57522000	0.64935400	1.20444000
H	-0.32867500	0.82676100	1.78659400
H	1.25663500	0.04552300	1.81611900
C	1.21958000	1.98928700	0.86320700
H	0.58120800	2.58403500	0.20405300
H	1.35429800	2.55125200	1.79459300
H	2.20532200	1.88071300	0.40084200
C	1.21624800	-0.27917600	-1.02877700
H	1.41140700	0.73284800	-1.39135700
H	0.75854300	-0.82977300	-1.85221100
C	2.52479900	-0.94372800	-0.60318300
H	2.39045200	-1.99167500	-0.31847200
H	3.21370200	-0.92192000	-1.45565000
H	3.01129000	-0.41974000	0.22626900
C	-1.31944900	0.60398300	-0.79810100
O	-1.49554700	0.02746900	-1.84712800

O	-1.75831900	1.47915300	-0.08801500

Zero-point correction= 0.221975 (Hartree/Particle)
Thermal correction to Energy= 0.234189
Thermal correction to Enthalpy= 0.235133
Thermal correction to Gibbs Free Energy= 0.184458
Sum of electronic and zero-point Energies= -480.781884
Sum of electronic and thermal Energies= -480.769671
Sum of electronic and thermal Enthalpies= -480.768727
Sum of electronic and thermal Free Energies= -480.819401
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -480.93467870

TS1a

N	3.49163300	-0.47005600	0.14387300
C	3.85336600	-0.02571700	1.56319500
H	2.92636800	-0.08395500	2.13493500
H	4.54963900	-0.77177600	1.94737900
C	4.45914900	1.36756100	1.66320200
H	4.65452200	1.55980000	2.72375500
H	5.41048100	1.45456900	1.13180400
H	3.78089900	2.14953600	1.30820800
C	4.75110100	-0.61468600	-0.69410800
H	5.15831000	0.38859900	-0.79607600
H	5.44295400	-1.21083100	-0.09618600
C	4.54555100	-1.23634900	-2.06914100
H	3.78380300	-0.70855300	-2.64832500
H	5.49438900	-1.15120500	-2.61048100
H	4.28897000	-2.29812900	-2.02170600
C	2.68977000	-1.76961600	0.20684000
H	2.35714700	-1.97046300	-0.81297000
H	1.81061500	-1.53985600	0.80616000
C	3.43522200	-2.96609400	0.77997700
H	3.71567700	-2.82510100	1.82734000
H	2.74985100	-3.81998100	0.73700100
H	4.32776800	-3.23174200	0.20653100
C	2.55925500	0.66219300	-0.46389400
O	1.42841400	0.64721800	0.11099900
O	3.03132800	1.37321200	-1.32356700
C	-6.64589300	-0.29296000	-0.17952800
C	-5.56149100	0.56049800	-0.00479400
C	-4.25478100	0.04837400	0.17391900
C	-4.08671200	-1.35331600	0.16123900
C	-5.18573600	-2.19760300	-0.01229300
C	-6.47265300	-1.68318300	-0.18395100
H	-7.63793100	0.13202100	-0.31648200
H	-5.70759200	1.63895200	-0.00271600
H	-3.09689200	-1.78017500	0.28989300
H	-5.02634000	-3.27381900	-0.01708200
H	-7.32189200	-2.34682800	-0.32106600
N	-3.20382600	0.92078100	0.39163300
H	-3.33651000	1.86771500	0.03261200
C	-1.81305000	0.54986200	0.18279600
H	-1.65721200	0.11385800	-0.82026800
H	-1.48980400	-0.19340900	0.92297400
C	-1.00669600	1.86222000	0.31601500
C	0.25972400	1.91188600	-0.45059400
O	-1.52974400	2.89920000	-0.40376700
H	-0.84979900	2.06161100	1.40209800

H	0.87837200	2.78276700	-0.27081100
H	0.18282500	1.60585200	-1.48766000

Zero-point correction= 0.408608 (Hartree/Particle)
Thermal correction to Energy= 0.430975
Thermal correction to Enthalpy= 0.431919
Thermal correction to Gibbs Free Energy= 0.354859
Sum of electronic and zero-point Energies= -960.066796
Sum of electronic and thermal Energies= -960.044429
Sum of electronic and thermal Enthalpies= -960.043485
Sum of electronic and thermal Free Energies= -960.120545
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -960.33697295

INT2a

N	3.34425100	0.44432800	-0.17307100
C	3.66035700	-0.14281200	-1.56439500
H	2.71131600	-0.15351900	-2.10127200
H	4.32625200	0.57800600	-2.03811500
C	4.28862100	-1.52748100	-1.54463100
H	4.47714700	-1.80429500	-2.58746200
H	5.24597100	-1.55299900	-1.01810700
H	3.62728900	-2.29003500	-1.12166600
C	4.64440800	0.72421600	0.58191100
H	5.10799300	-0.24486300	0.75333200
H	5.26704000	1.28570200	-0.11523700
C	4.47743000	1.47171700	1.89745000
H	3.79926400	0.95840700	2.58335500
H	5.46394100	1.51035000	2.37215400
H	4.13720000	2.50189700	1.76331600
C	2.49568500	1.71920700	-0.33861600
H	2.17198800	1.99449800	0.66602300
H	1.61945800	1.41772700	-0.90958700
C	3.20822900	2.87629400	-1.02215700
H	3.50204400	2.64350900	-2.04904900
H	2.48951300	3.70207500	-1.06641700
H	4.08285600	3.22942600	-0.47019000
C	2.53197400	-0.61125500	0.58540700
O	1.34674300	-0.71216400	0.05496200
O	3.02033400	-1.23216500	1.49212000
C	-6.51081100	0.21124200	0.04003600
C	-5.39612800	-0.59370400	-0.16781300
C	-4.09229400	-0.03989200	-0.20828300
C	-3.96709500	1.35682900	-0.02765600
C	-5.09646100	2.15240600	0.17758000
C	-6.37694900	1.59544000	0.21492200
H	-7.49729000	-0.24700400	0.06899500
H	-5.51296400	-1.66725200	-0.30301400
H	-2.98312100	1.81547000	-0.05400300
H	-4.96737900	3.22440200	0.31319600
H	-7.25062800	2.22072800	0.37711300
N	-3.01266300	-0.85875000	-0.45472400
H	-3.09444700	-1.85287100	-0.18014800
C	-1.64461300	-0.50134800	-0.12739000
H	-1.57313000	-0.07391500	0.89069400
H	-1.24011400	0.24320000	-0.82755400
C	-0.86347600	-1.86851500	-0.18793800
C	0.44148600	-1.77653500	0.60934100
O	-1.58108700	-2.87850700	0.32898100

H	-0.56318100	-1.99263900	-1.27301300
H	0.99252000	-2.71693000	0.55208700
H	0.24925000	-1.52027700	1.65401600

Zero-point correction= 0.409989 (Hartree/Particle)
Thermal correction to Energy= 0.432321
Thermal correction to Enthalpy= 0.433265
Thermal correction to Gibbs Free Energy= 0.356739
Sum of electronic and zero-point Energies= -960.072038
Sum of electronic and thermal Energies= -960.049706
Sum of electronic and thermal Enthalpies= -960.048762
Sum of electronic and thermal Free Energies= -960.125288
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -960.35488021

3a

C	1.82548600	-0.56163000	0.85033200
C	2.95771500	-1.43946200	0.30071200
H	1.73845300	-0.61679800	1.93657600
H	3.66967800	-1.73869100	1.07383900
H	2.60430500	-2.31826300	-0.24080900
C	3.27645200	0.71108800	-0.40007300
O	3.76774400	1.66801100	-0.93854800
O	2.29417700	0.77943800	0.52965600
O	3.63502000	-0.56776000	-0.63456500
C	0.47803200	-0.81317600	0.18815400
H	0.16917600	-1.82564600	0.47114600
H	0.59749200	-0.80147700	-0.90922600
N	-0.50162700	0.15042000	0.65995200
H	-0.13992000	1.09851900	0.68508200
C	-1.83425300	0.09275800	0.24962600
C	-2.41113900	-1.06331500	-0.31077400
C	-2.65573000	1.22460600	0.44173600
C	-3.76665400	-1.08075900	-0.65000000
H	-1.80970000	-1.94945200	-0.48506900
C	-4.00279600	1.19403300	0.09542600
H	-2.22074300	2.12579400	0.86913200
C	-4.57491600	0.03952500	-0.45242300
H	-4.18818700	-1.98610600	-1.08074800
H	-4.61081000	2.08168300	0.25391500
H	-5.62705900	0.01797900	-0.72214700

Zero-point correction= 0.202472 (Hartree/Particle)
Thermal correction to Energy= 0.214186
Thermal correction to Enthalpy= 0.215130
Thermal correction to Gibbs Free Energy= 0.162700
Sum of electronic and zero-point Energies= -667.936250
Sum of electronic and thermal Energies= -667.924537
Sum of electronic and thermal Enthalpies= -667.923593
Sum of electronic and thermal Free Energies= -667.976023
M06-2X/6-311++G(d,p)/SMD//B3LYP/6-31G(d,p) energy= -668.06414391

7. X-ray crystallographic data.

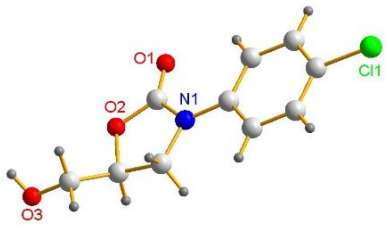


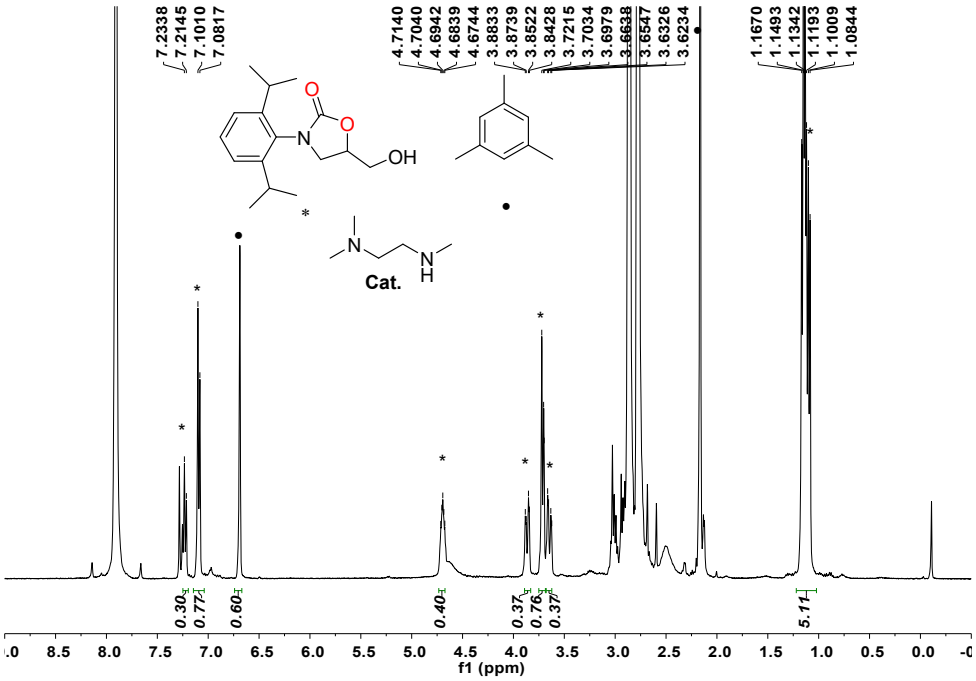
Fig. S17 Crystal structure of (*S*)-**2y** (CCDC 2159922).

Table S9 Crystallographic data of (*S*)-**2y**

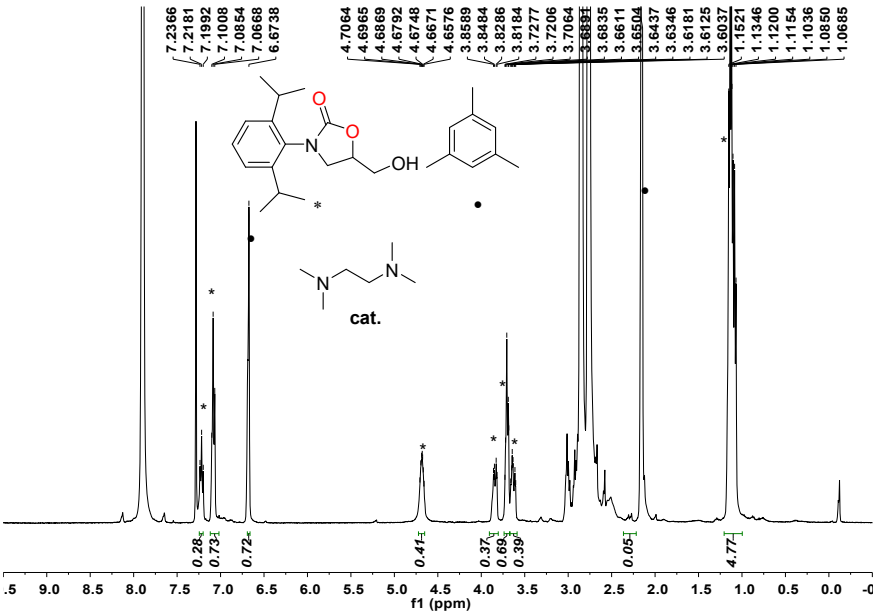
Empirical formula	$C_{10}H_{10}NO_3Cl$
Formula weight	227.64
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	7.3826(10)
b/Å	11.4210(15)
c/Å	11.6800(14)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	984.8(2)
Z	14
ρ_{calc}g/cm^3	1.853
μ/mm^{-1}	9.677
F(000)	546.0
Crystal size/mm^3	0.35 × 0.3 × 0.2
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	10.834 to 154.946
Index ranges	-9 ≤ h ≤ 6, -14 ≤ k ≤ 11, -14 ≤ l ≤ 11
Reflections collected	2560
Independent reflections	1744 [R_{int} = 0.0377, R_{sigma} = 0.0537]
Data/restraints/parameters	1744/0/137
Goodness-of-fit on F^2	1.039
Final R indexes [I>=2σ (I)]	R_1 = 0.0831, wR_2 = 0.2290
Final R indexes [all data]	R_1 = 0.0909, wR_2 = 0.2457
Largest diff. peak/hole / e Å^{-3}	0.56/-0.36
Flack parameter	0.04(4)

8. ^{1}H, ^{13}C and ^{19}F NMR spectra.

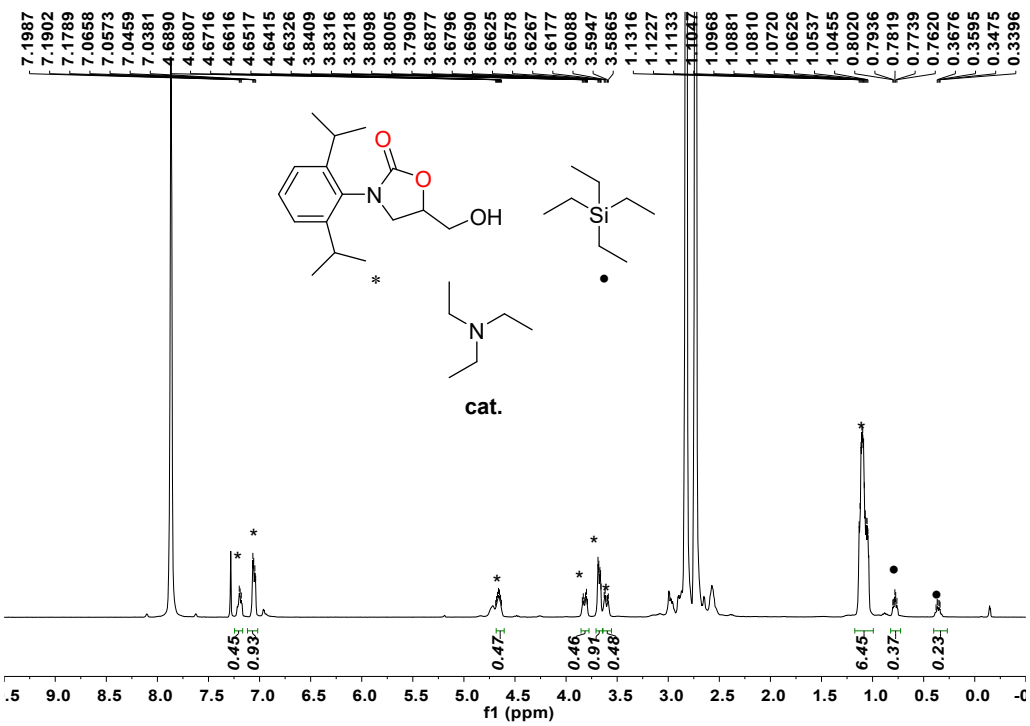
NMR spectra of crude products



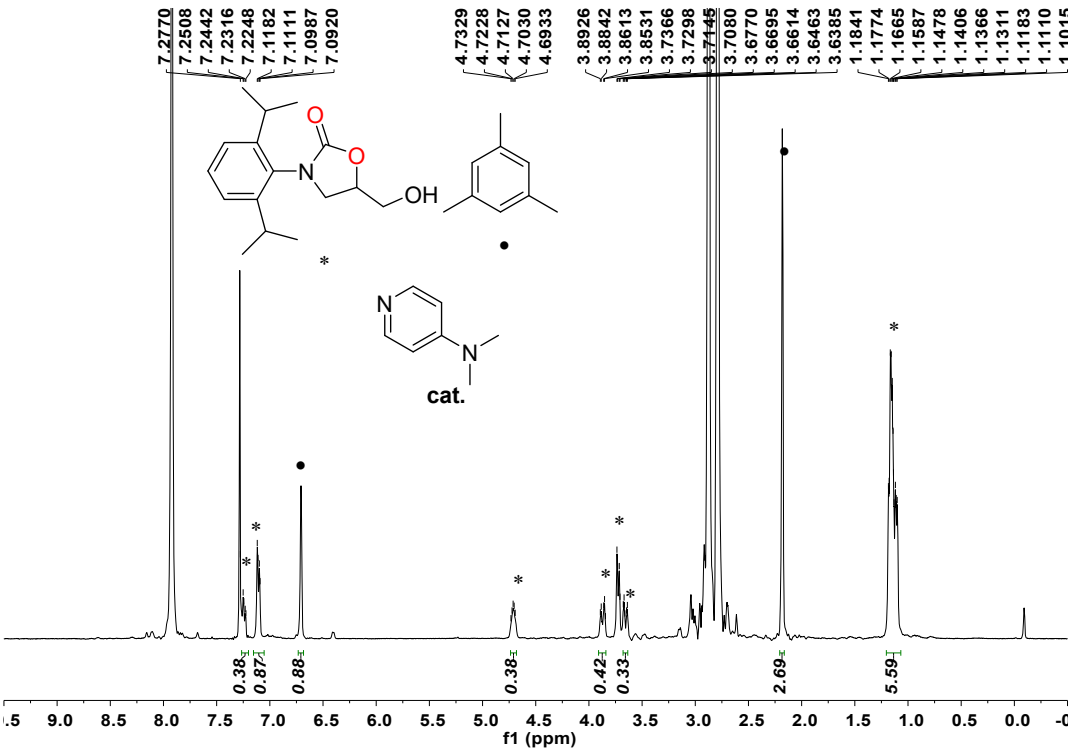
^{1}H NMR spectrum for reaction of **1v** and CO_2 (conditions in Table S4, entry 1; 0.200 mmol internal standard, $CDCl_3$, 400 MHz)



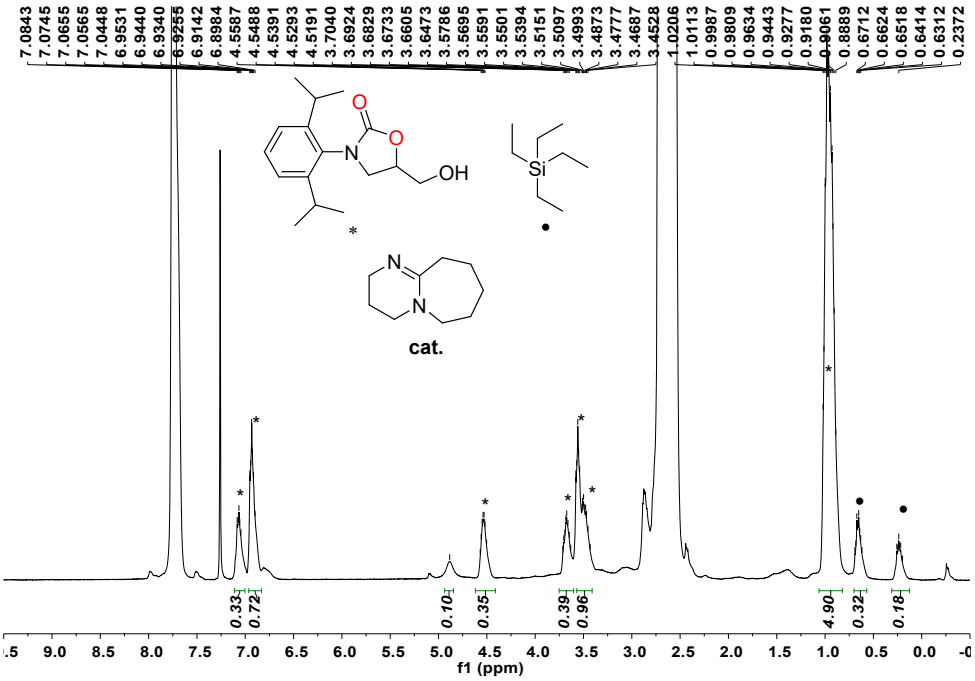
^{1}H NMR spectrum for reaction of **1v** and CO_2 (conditions in Table S4, entry 2; 0.240 mmol internal standard, $CDCl_3$, 400 MHz)



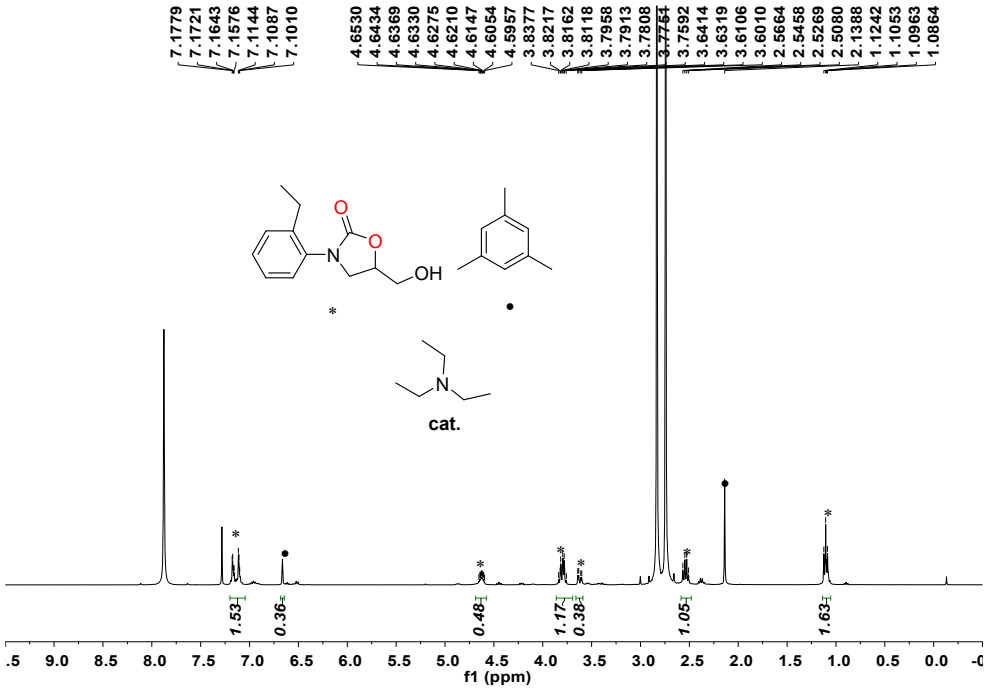
^{1}H NMR spectrum for reaction of **1v** and CO_2 (conditions in Table S4, entry 3; 0.030 mmol internal standard, $CDCl_3$, 400 MHz)



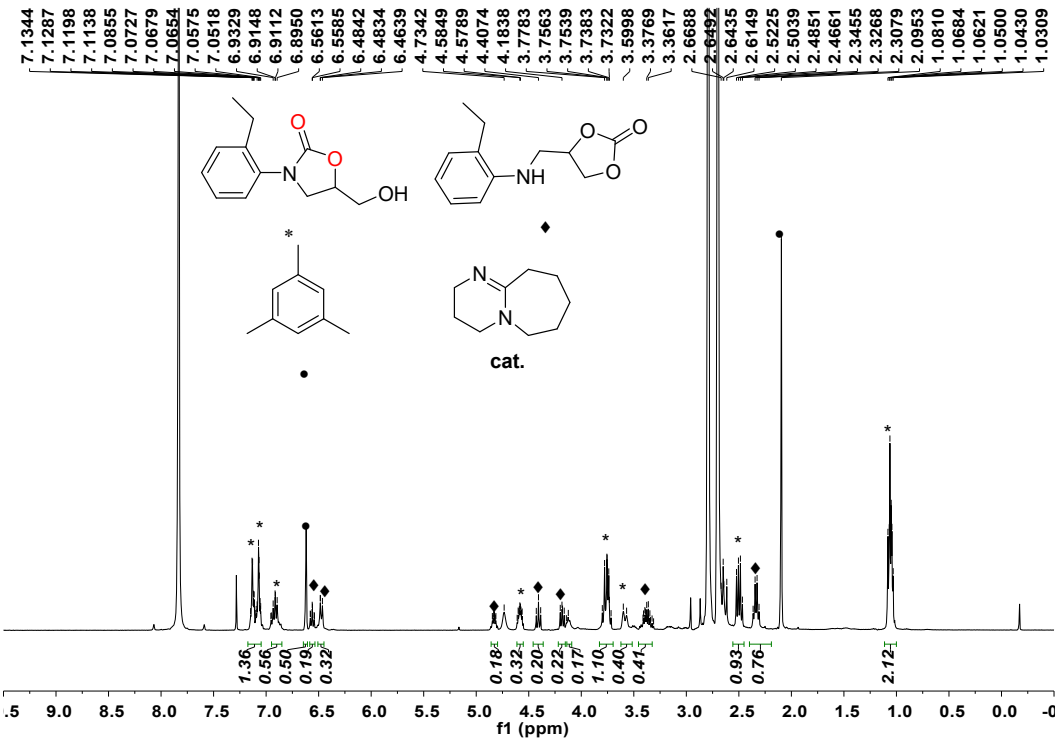
^{1}H NMR spectrum for reaction of **1v** and CO_2 (conditions in Table S4, entry 4; 0.293 mmol internal standard, $CDCl_3$, 400 MHz)



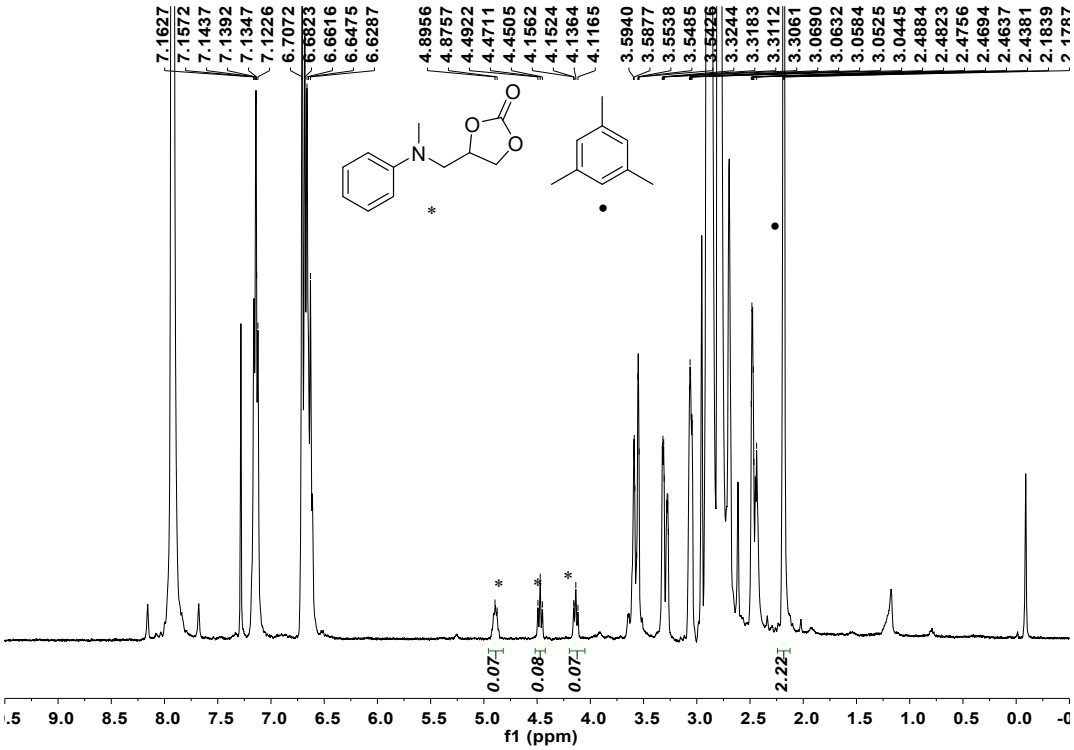
^{1}H NMR spectrum for reaction of **1v** and CO_2 (conditions in Table S4, entry 5; 0.023 mmol internal standard, $CDCl_3$, 400 MHz)



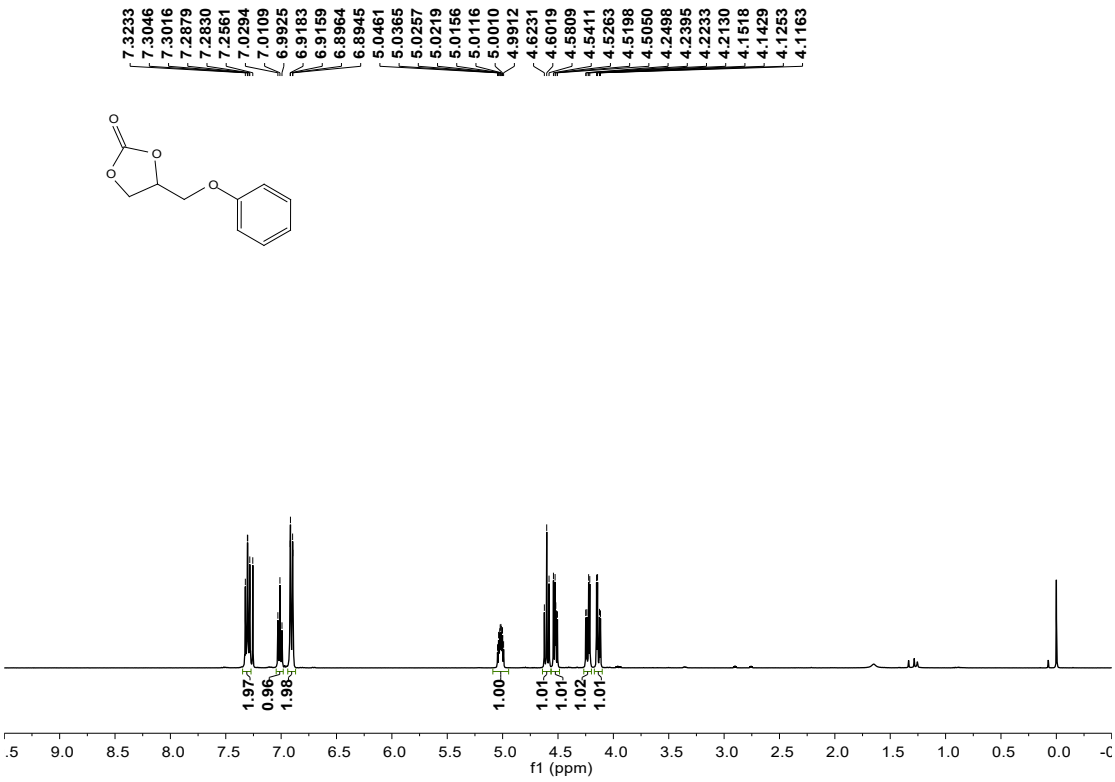
^{1}H NMR spectrum for reaction of **1m** and CO_2 (conditions in Table S5, entry 1; 0.120 mmol internal standard, $CDCl_3$, 400 MHz)



^{1}H NMR spectrum for reaction of **1m** and CO_2 (conditions in Table S5, entry 2; 0.168 mmol internal standard, $CDCl_3$, 400 MHz)

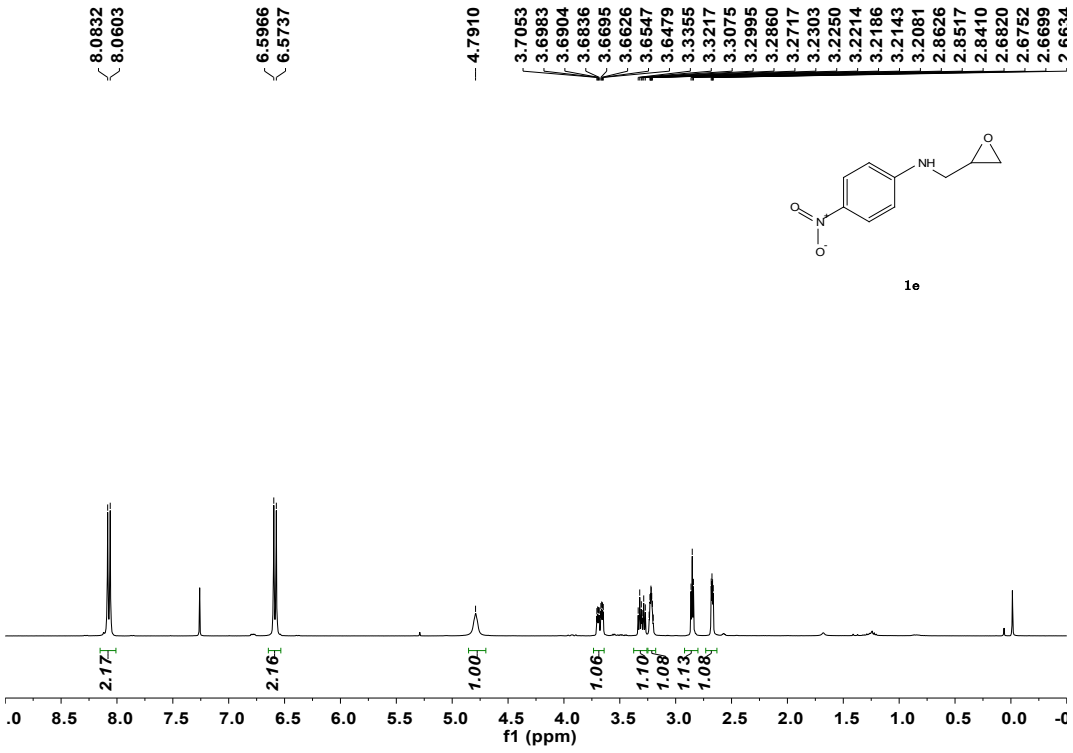


^{1}H NMR spectrum for reaction of *N*-methyl-*N*-(oxiran-2-ylmethyl)aniline and CO_2 (120 °C, 0.247 mmol internal standard, $CDCl_3$, 400 MHz)

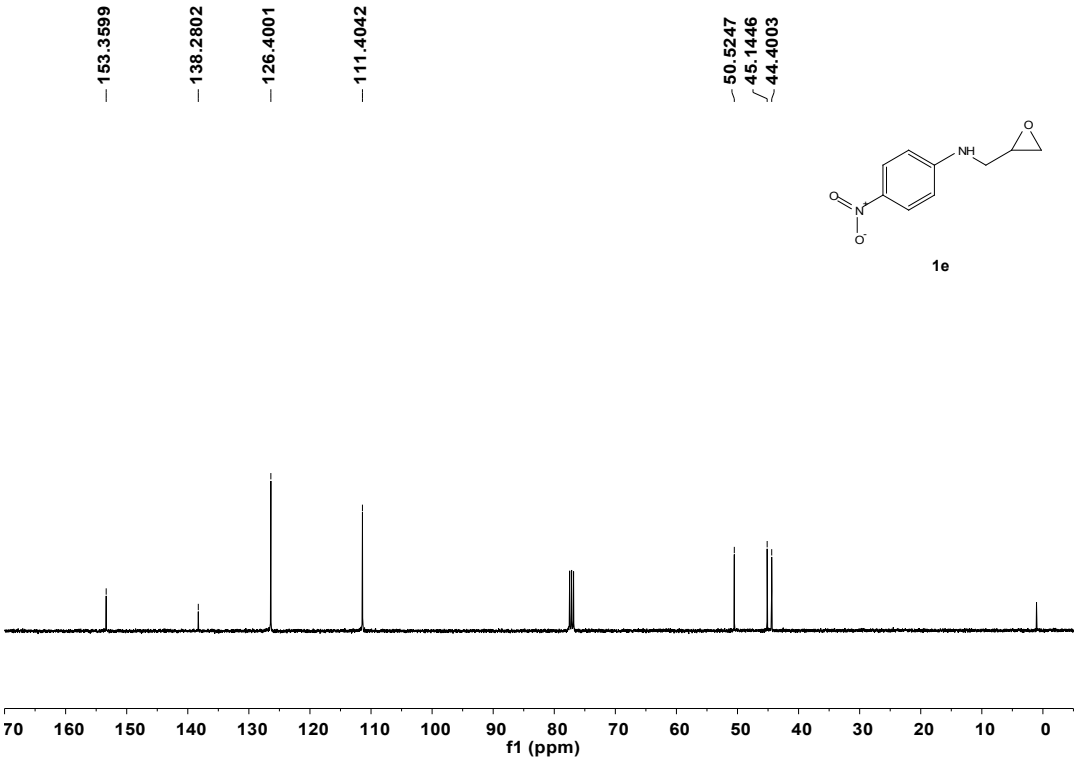


^{1}H NMR spectrum of 4-(phenoxymethyl)-1,3-dioxolan-2-one ($CDCl_3$, 400 MHz)

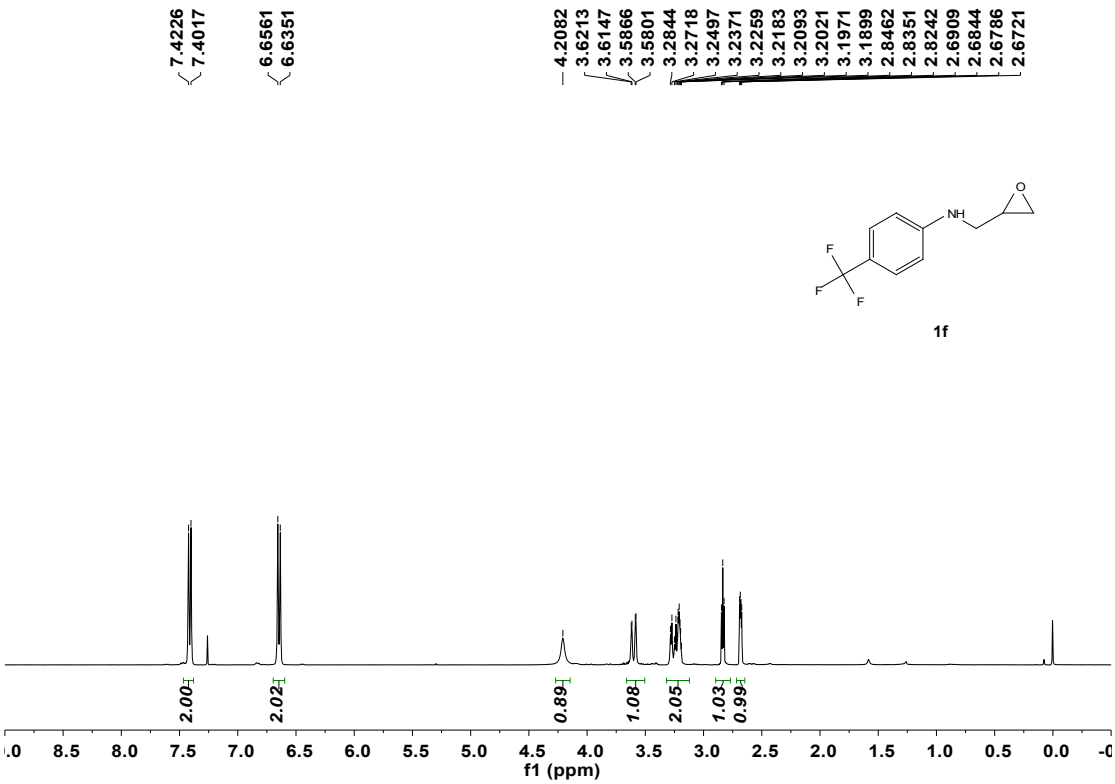
NMR spectra of epoxy amines



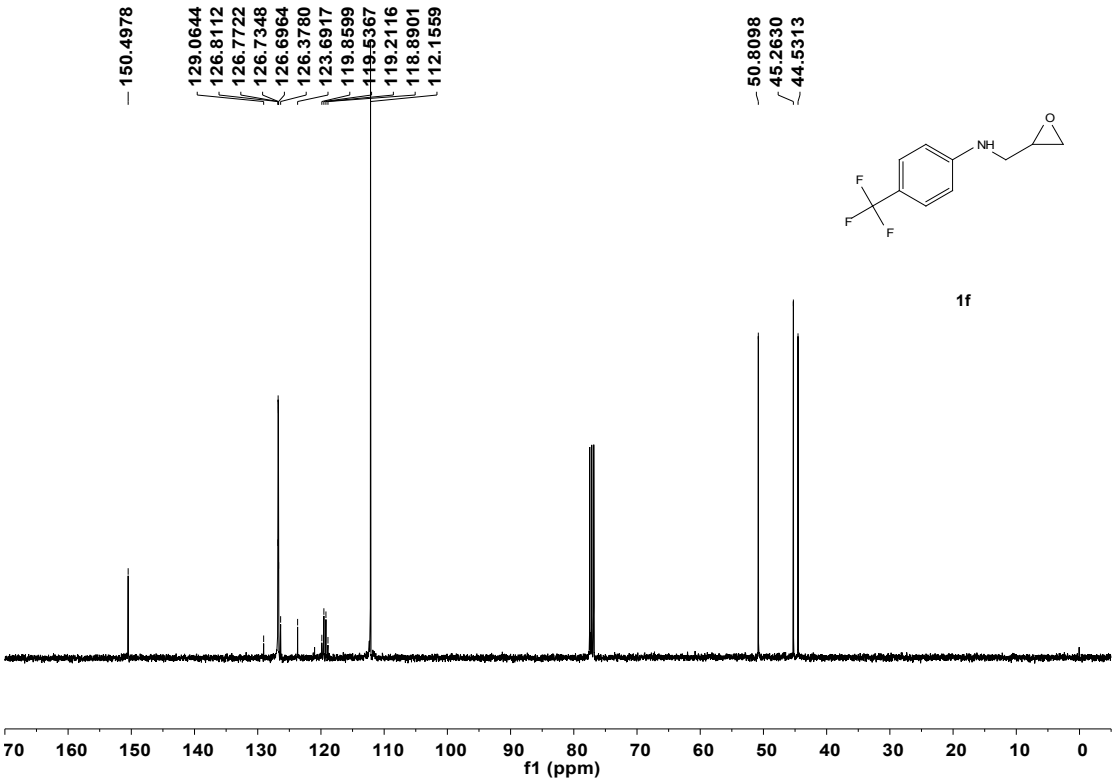
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **1e**



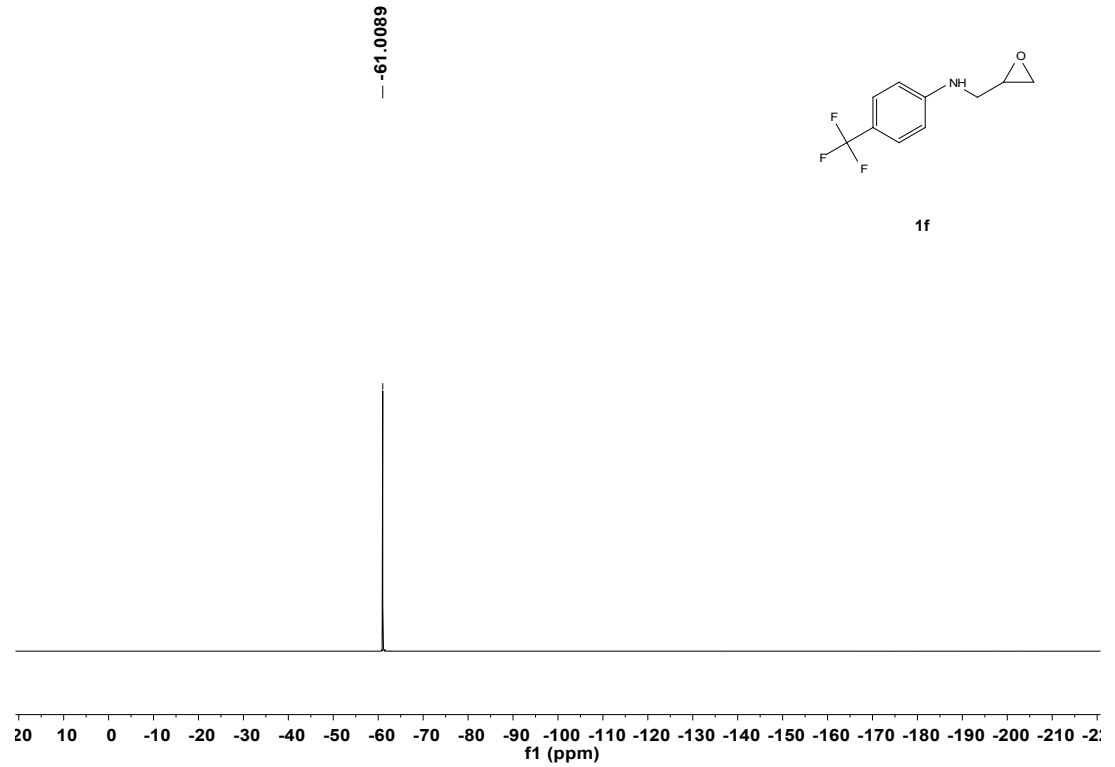
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **1e**



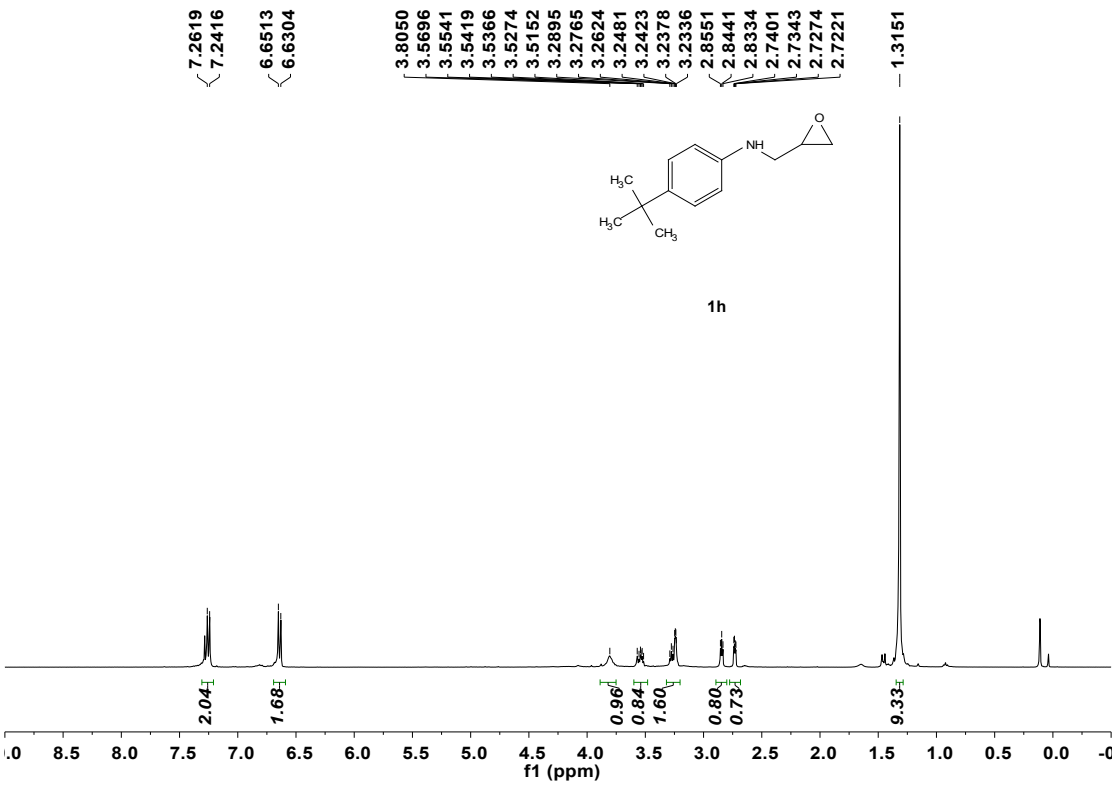
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **1f**



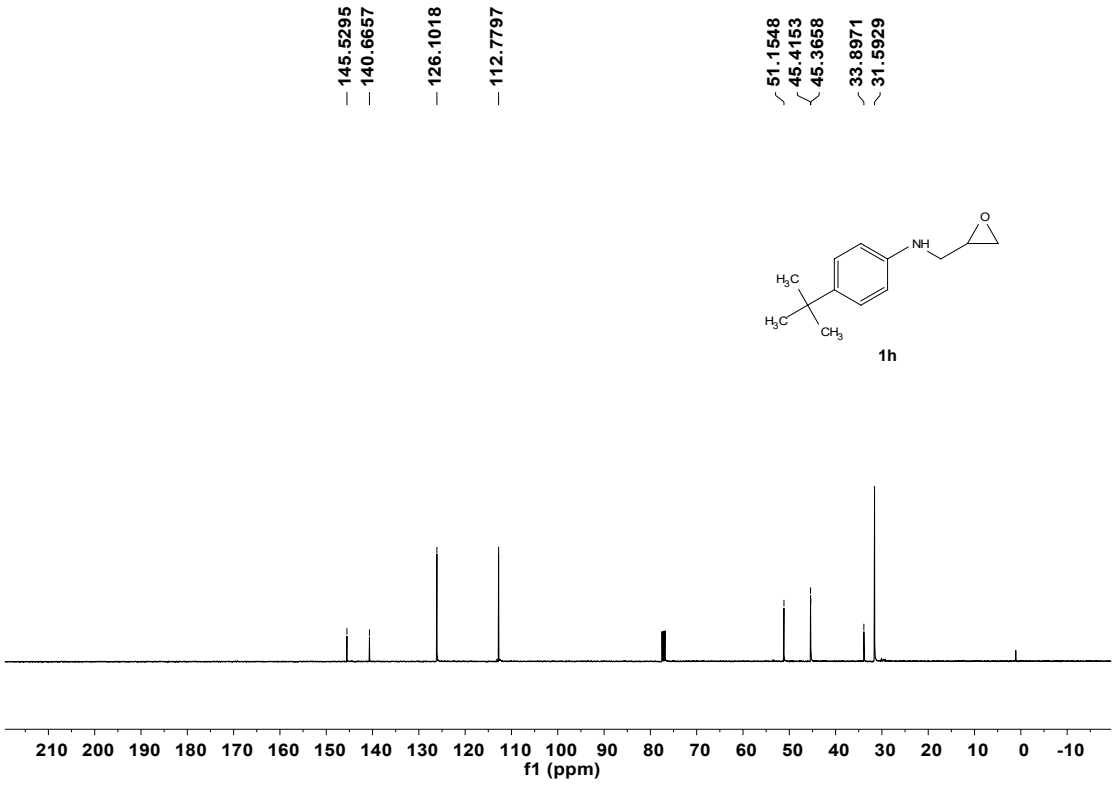
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **1f**



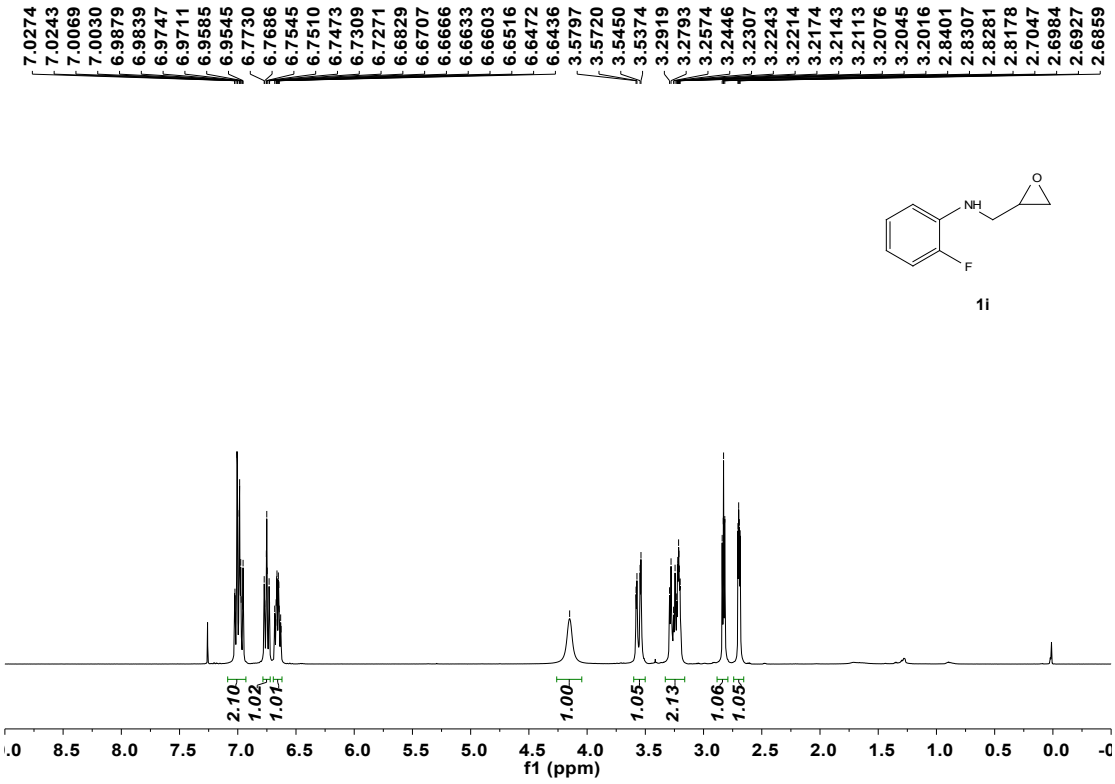
^{19}F NMR spectrum ($CDCl_3$, 376 MHz) of **1f**



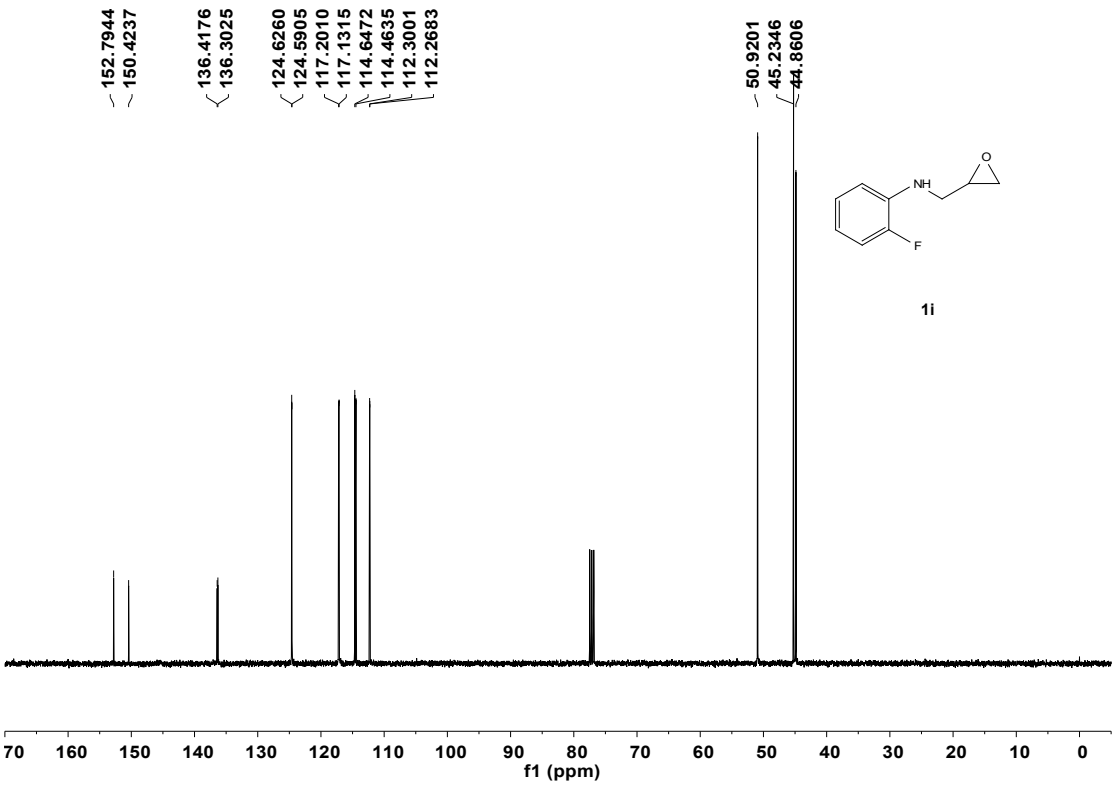
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **1h**



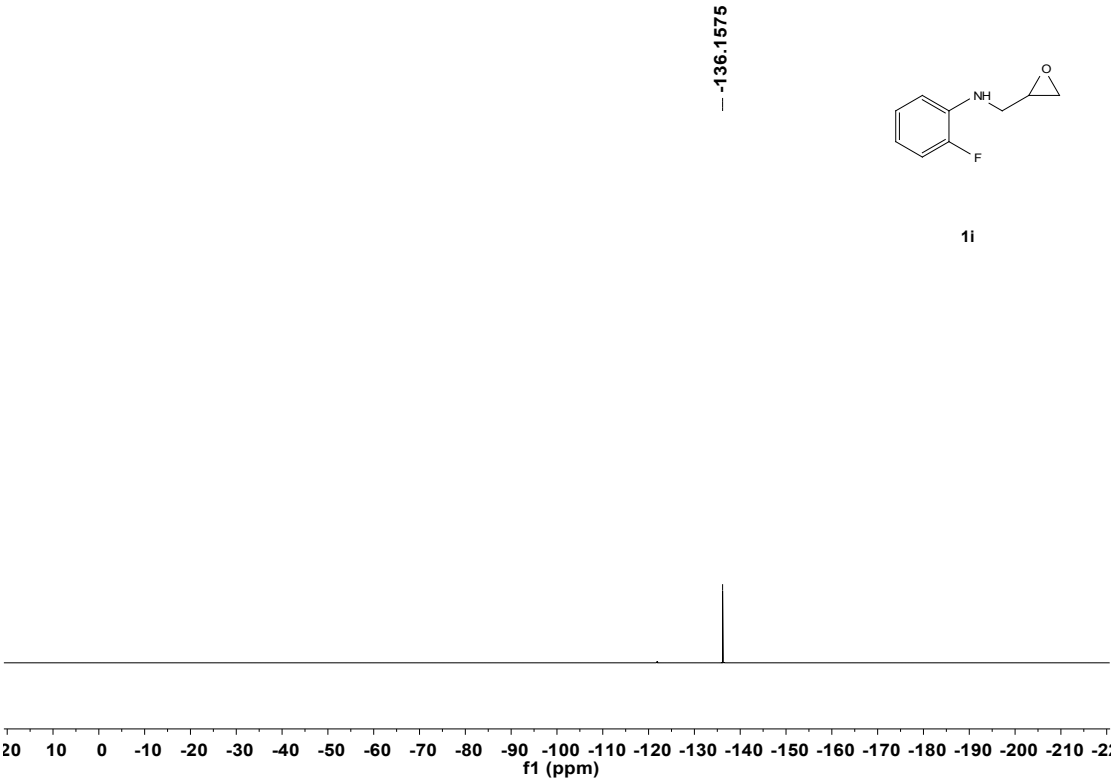
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **1h**



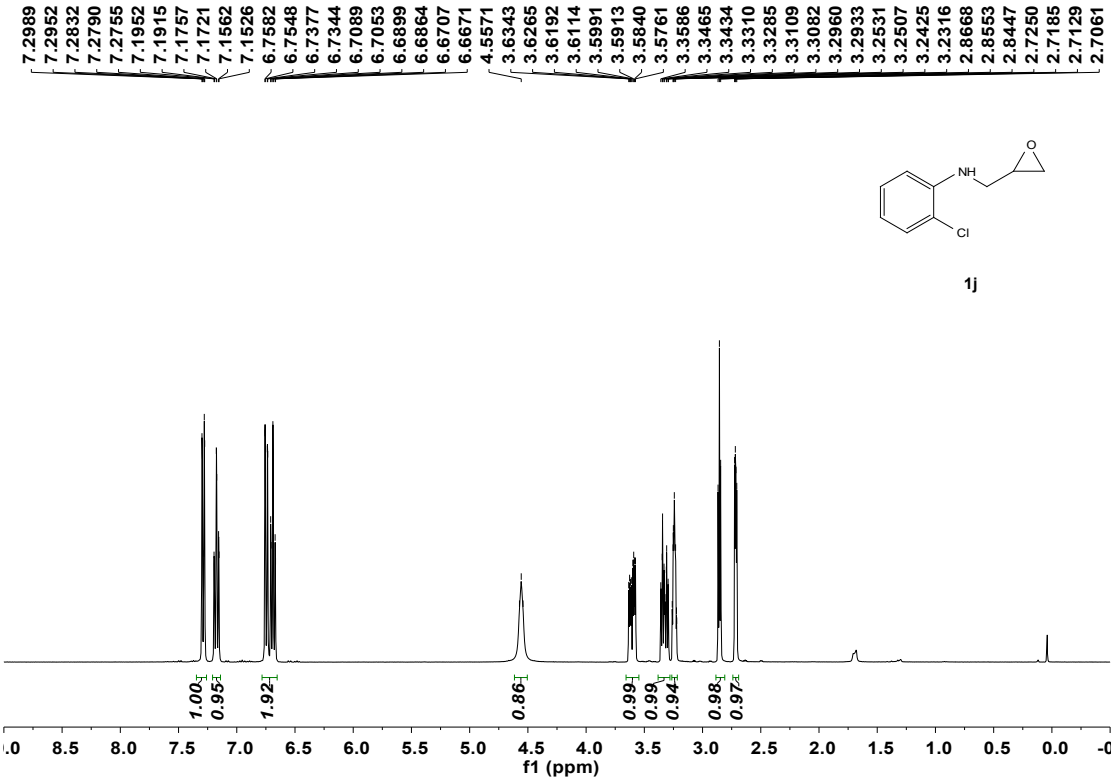
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **1i**



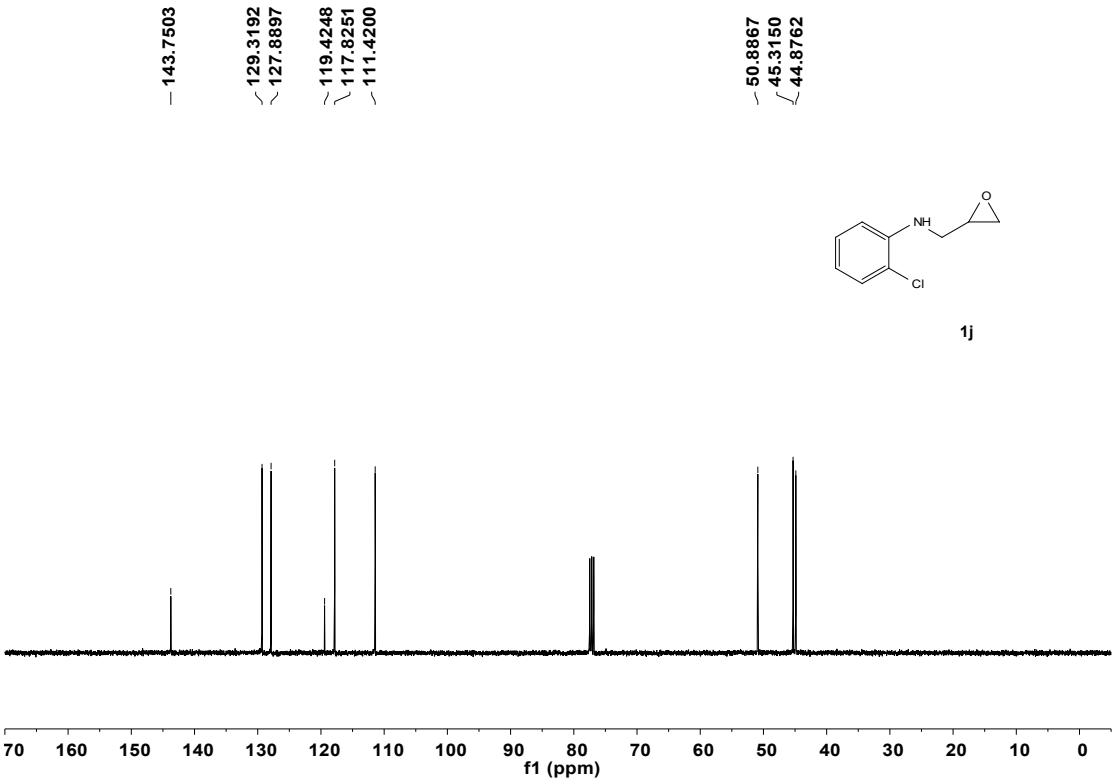
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **1i**



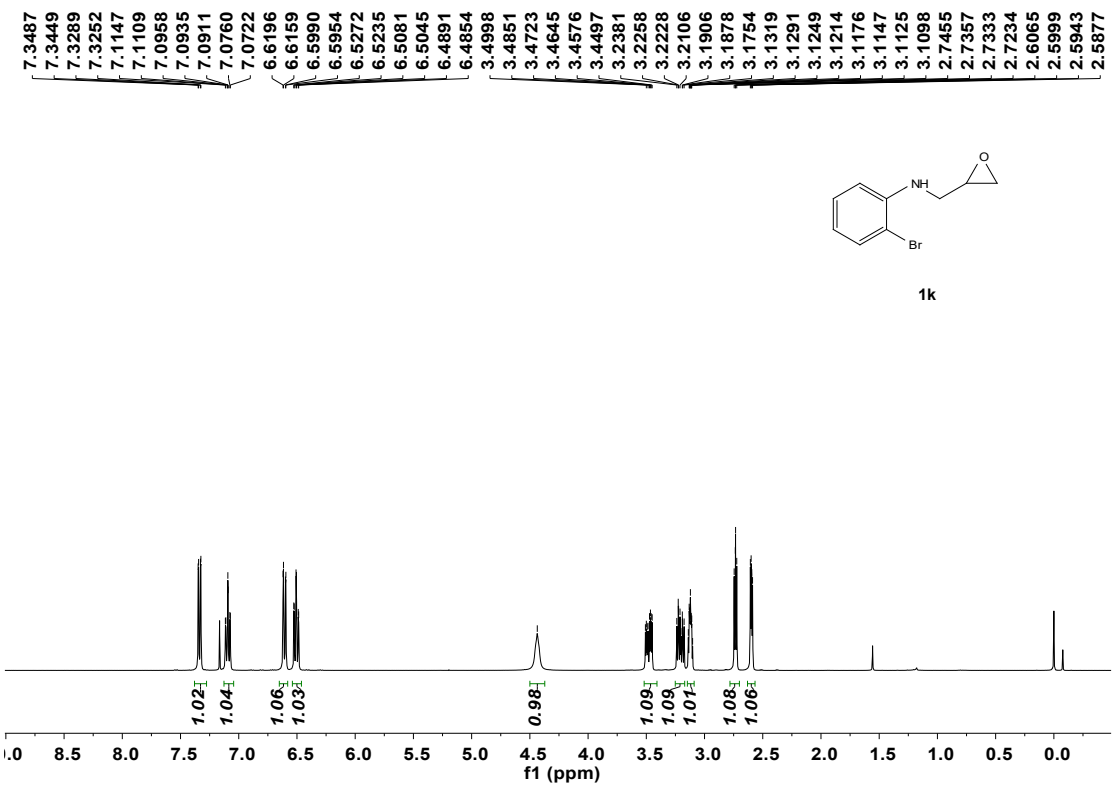
^{19}F NMR spectrum ($CDCl_3$, 376 MHz) of **1i**



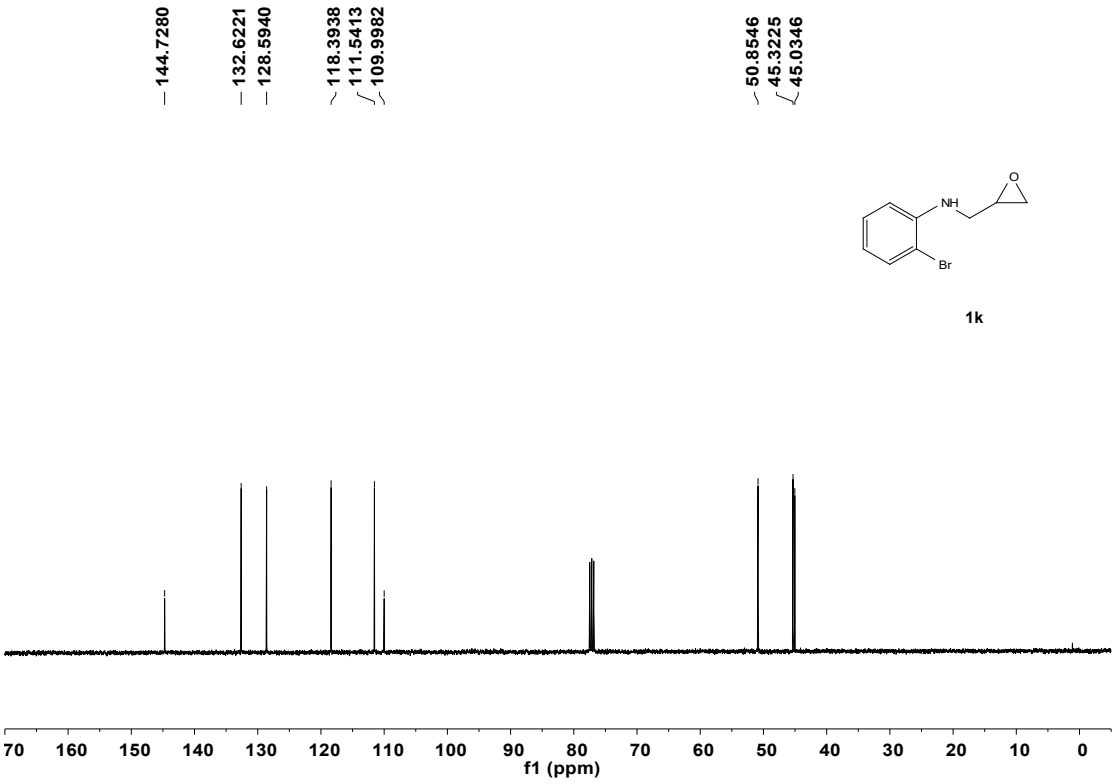
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **1j**



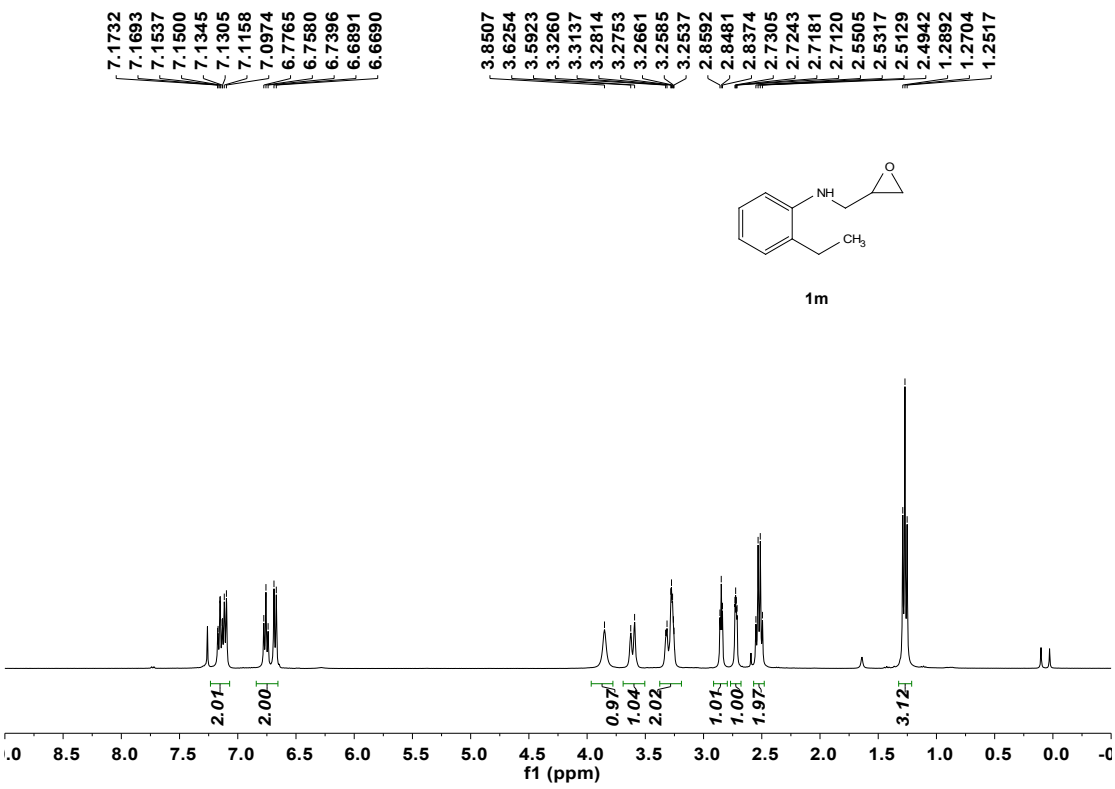
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **1j**



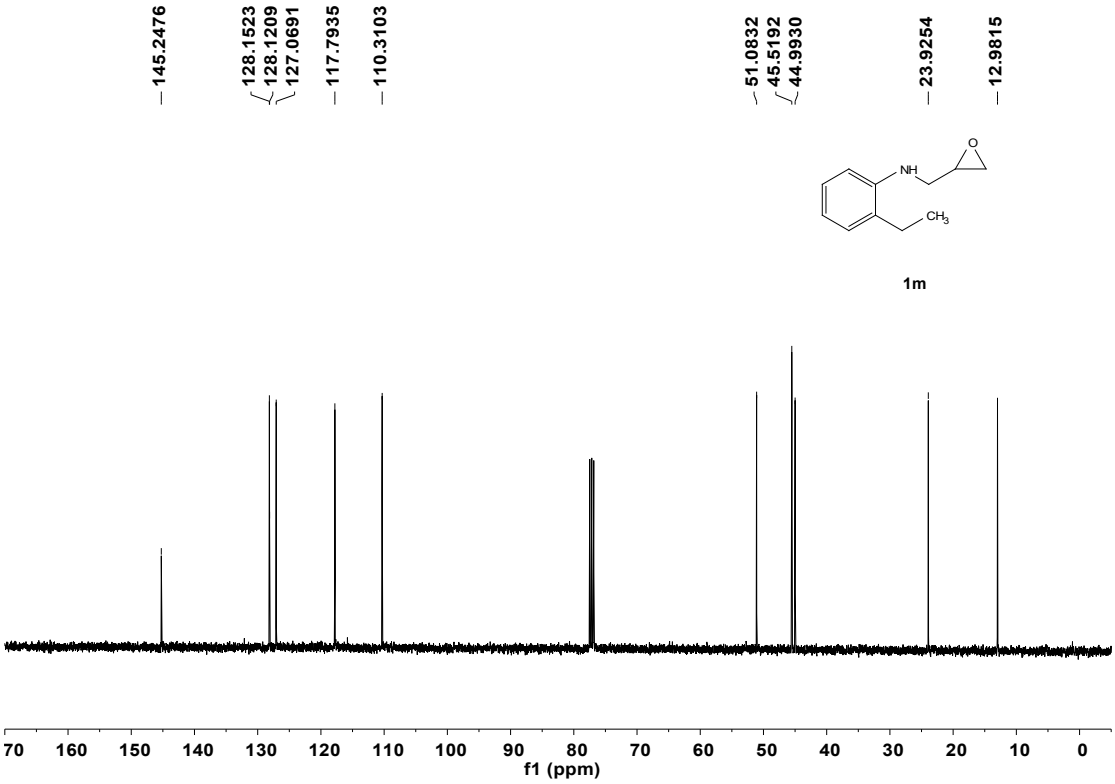
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **1k**



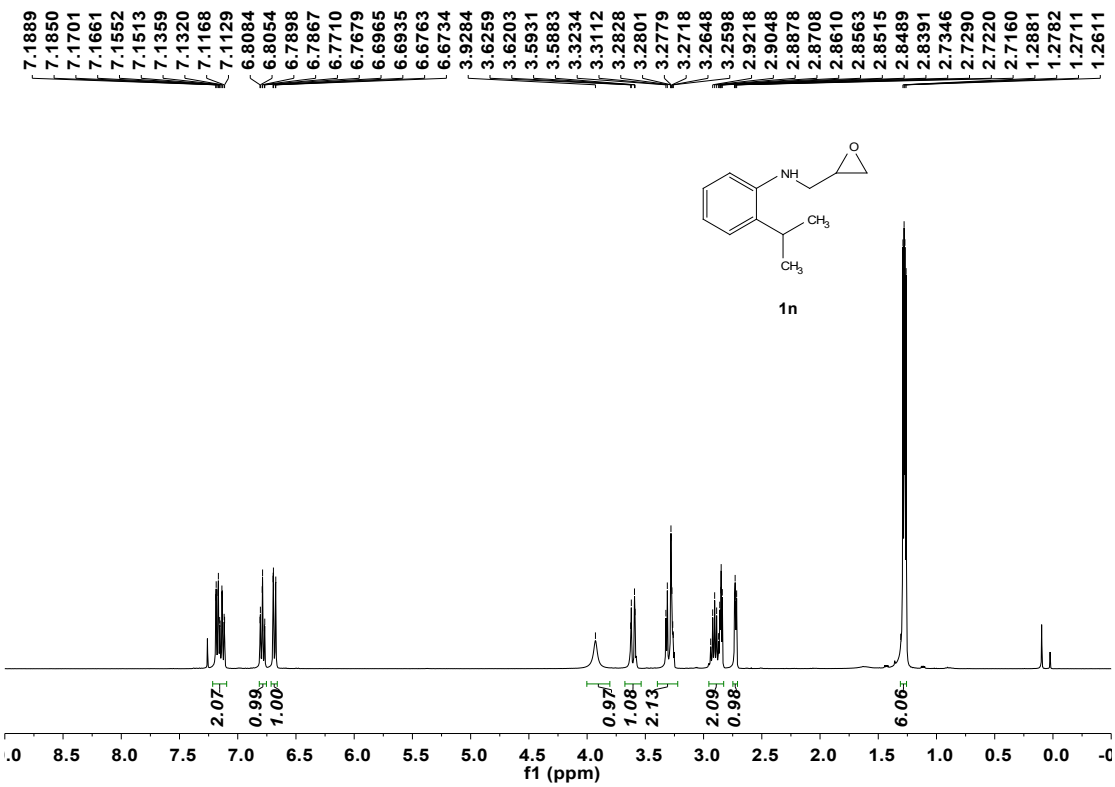
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **1k**



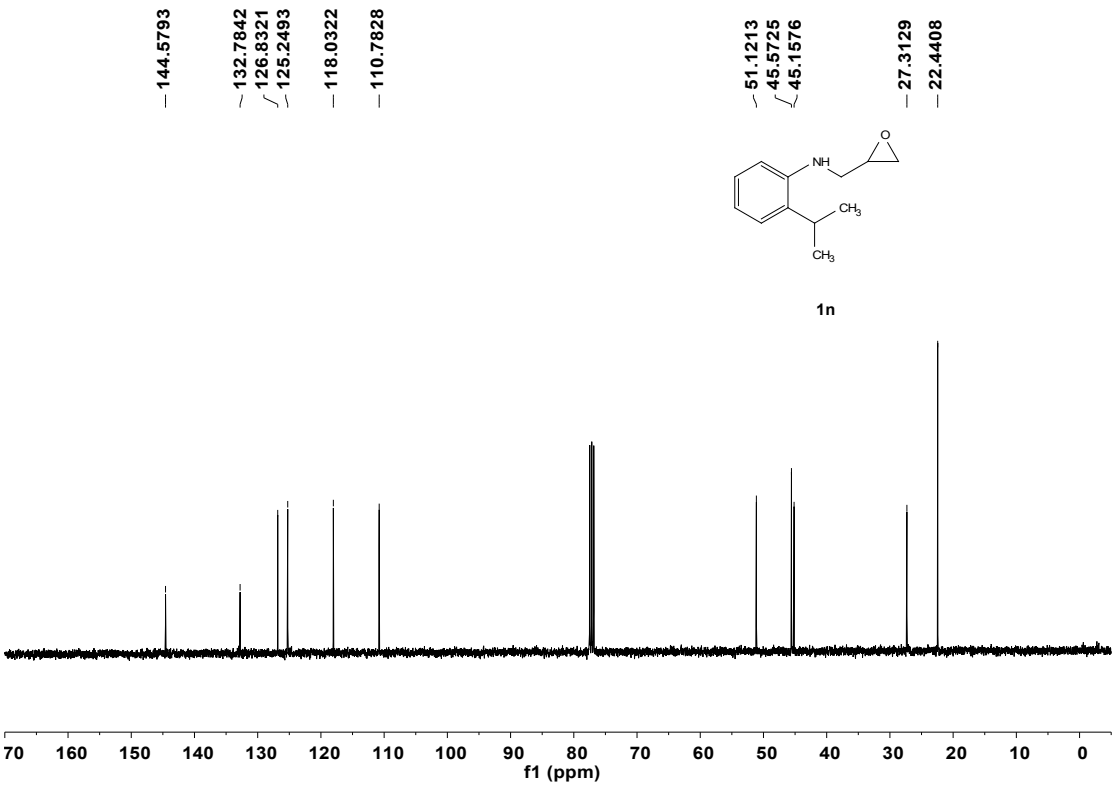
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **1m**



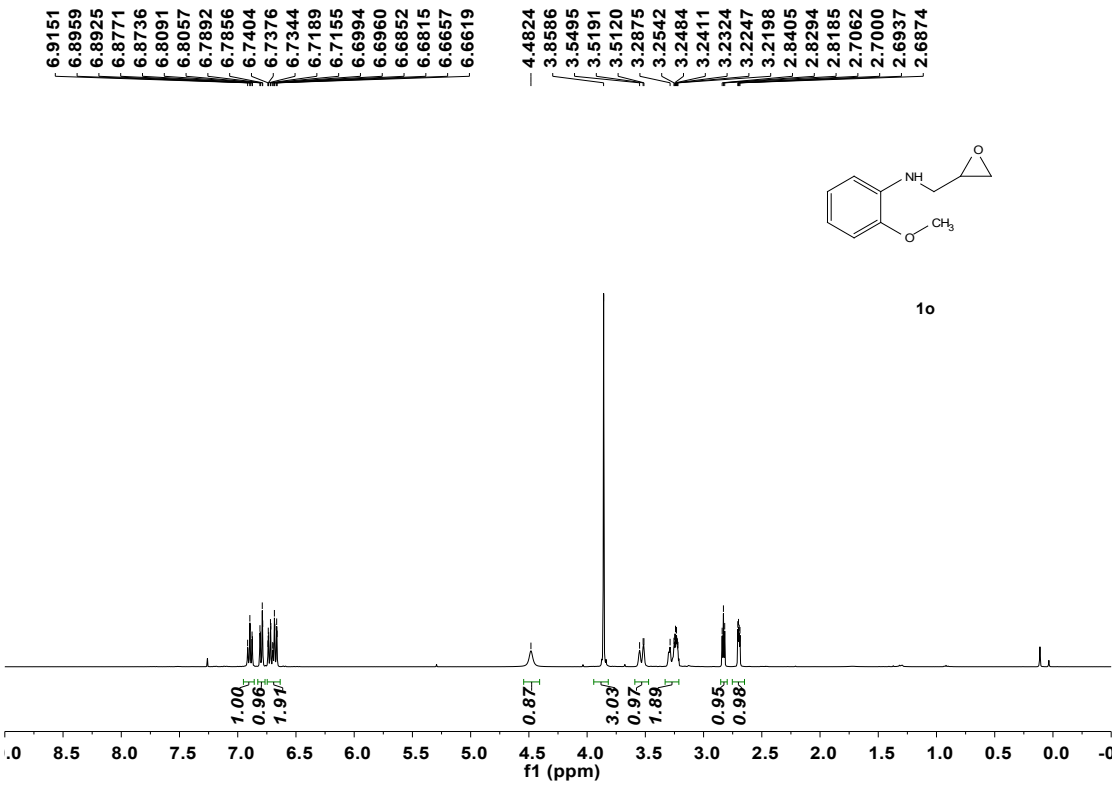
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **1m**



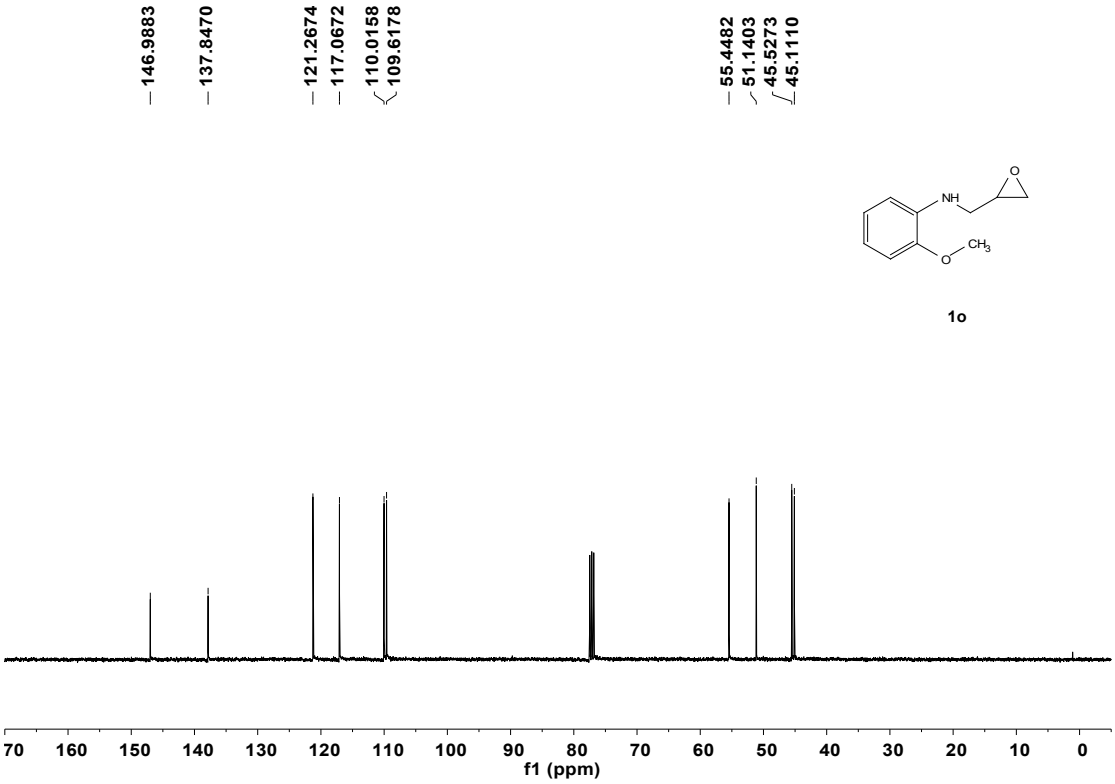
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **1n**



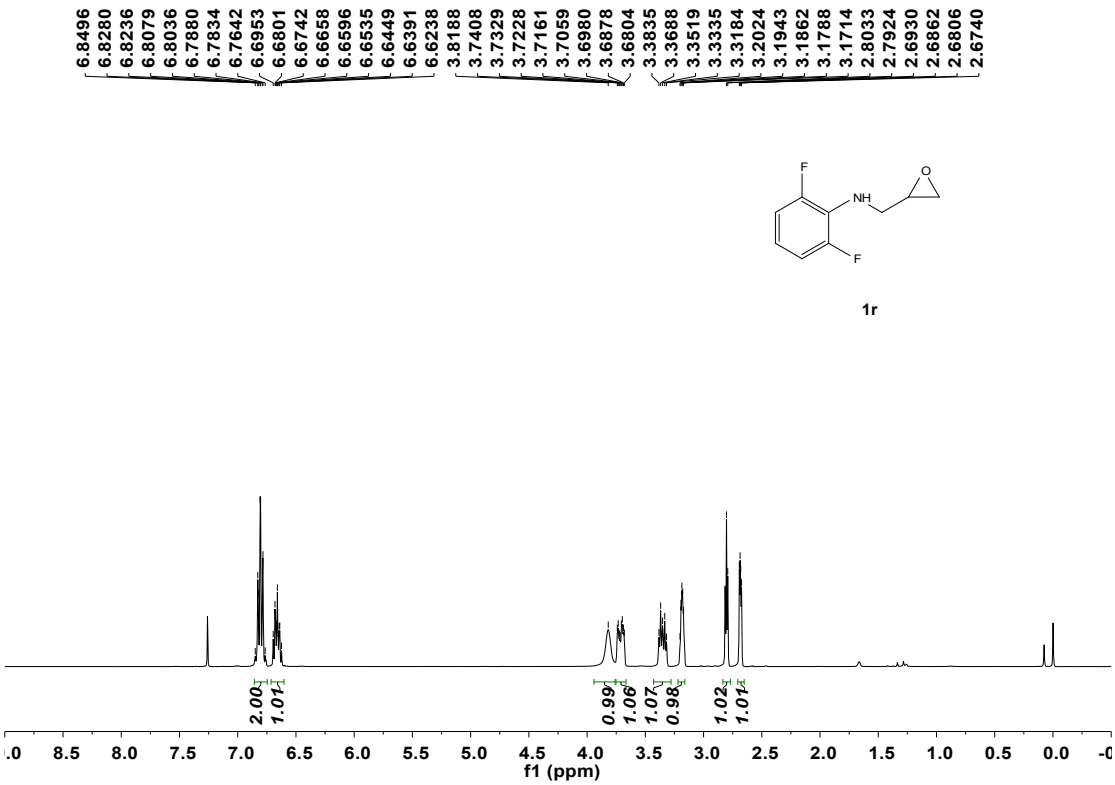
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **1n**



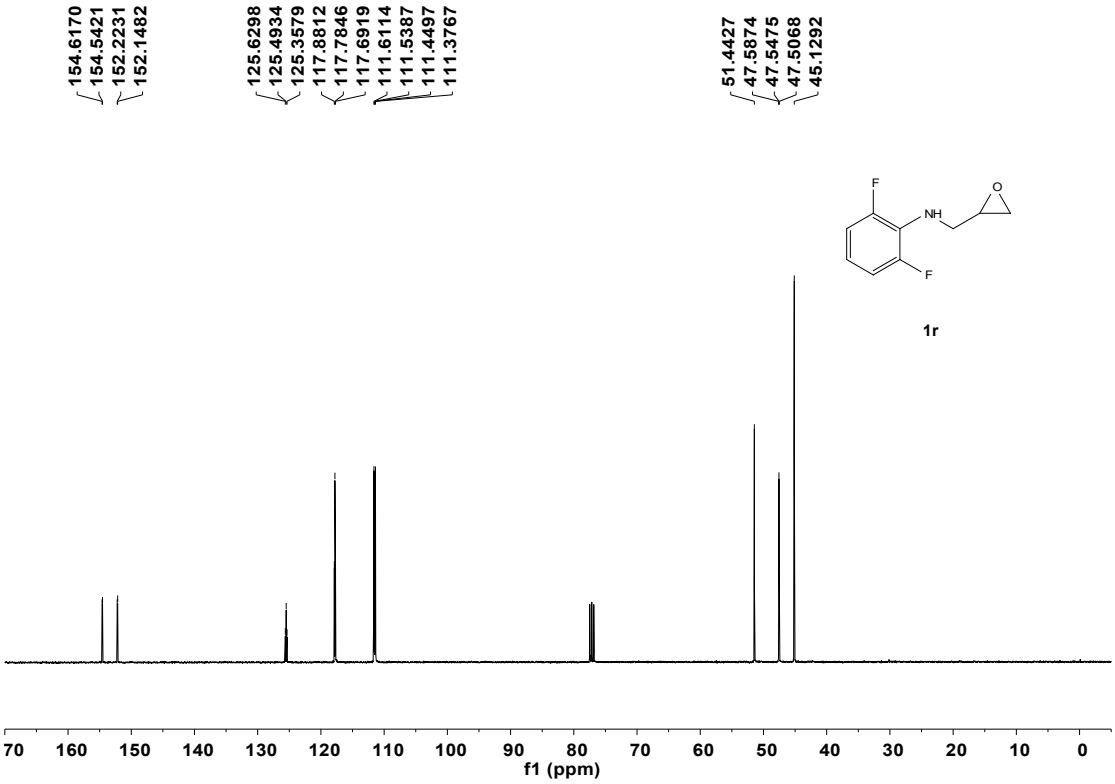
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **1o**



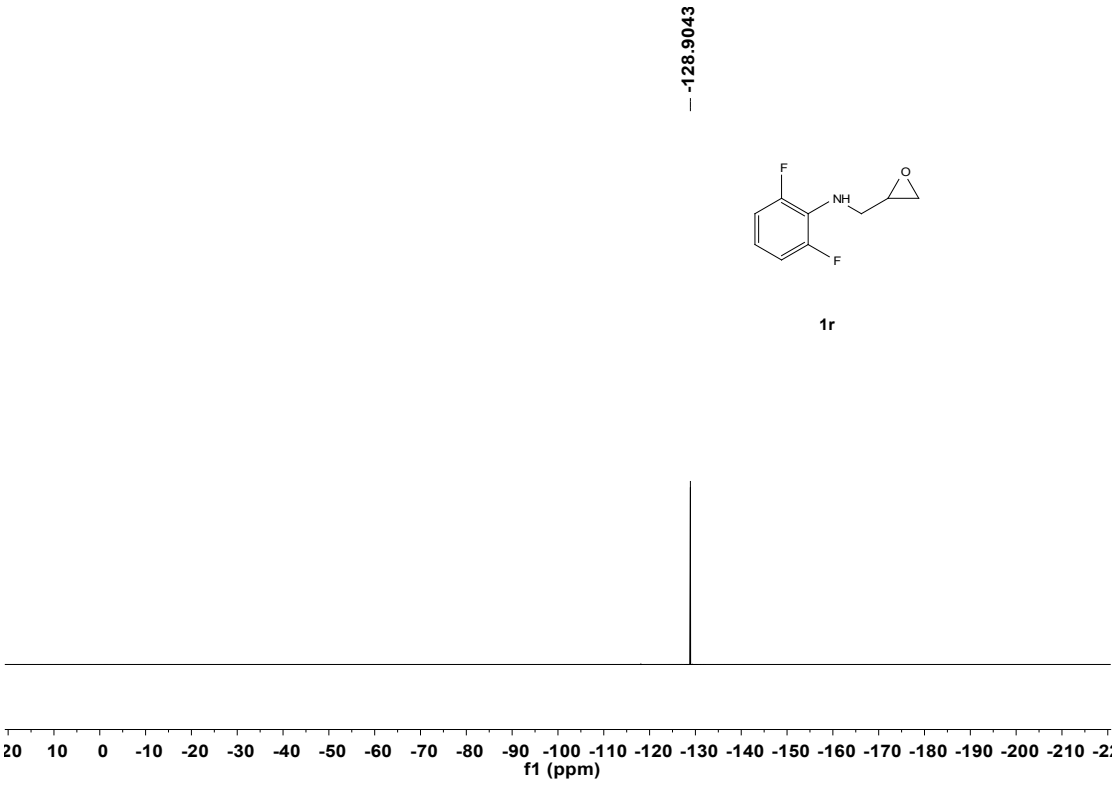
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **1o**



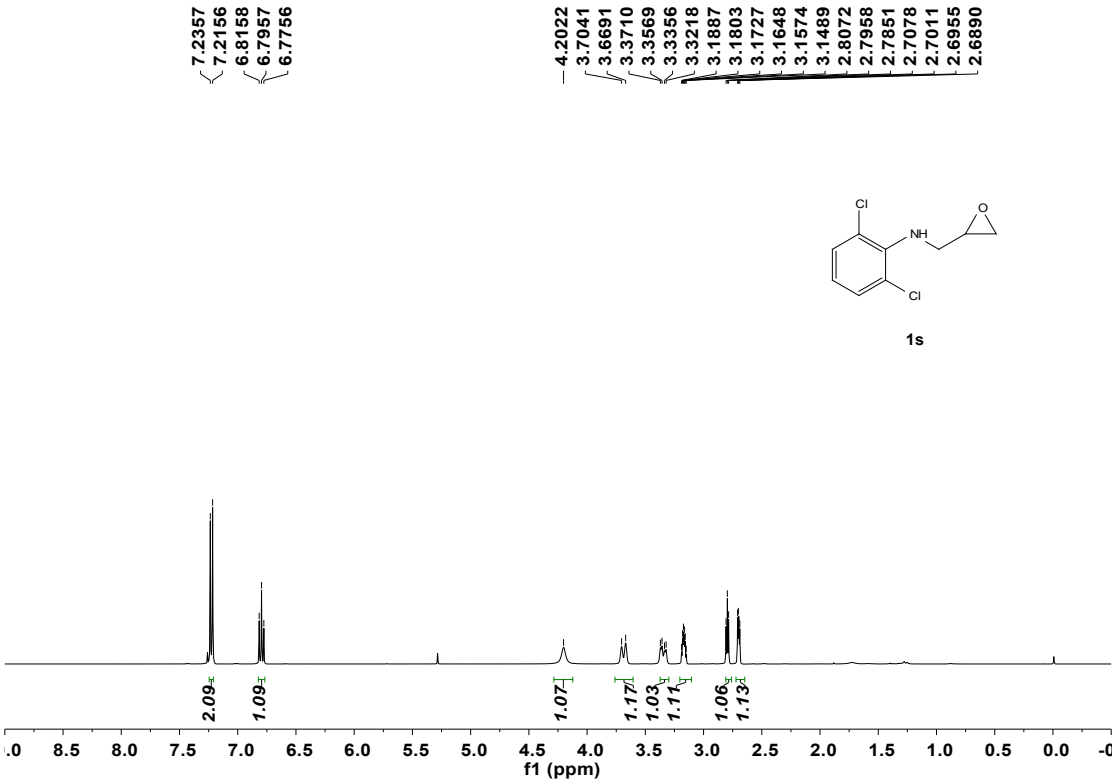
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **1r**



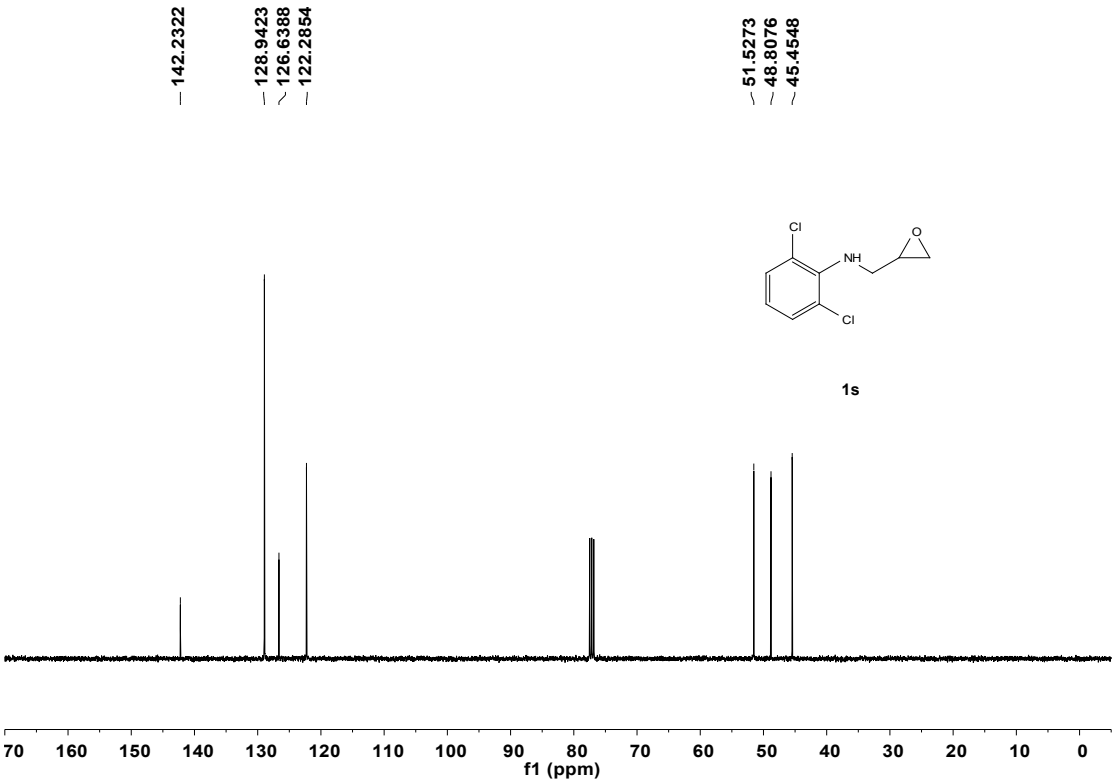
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **1r**



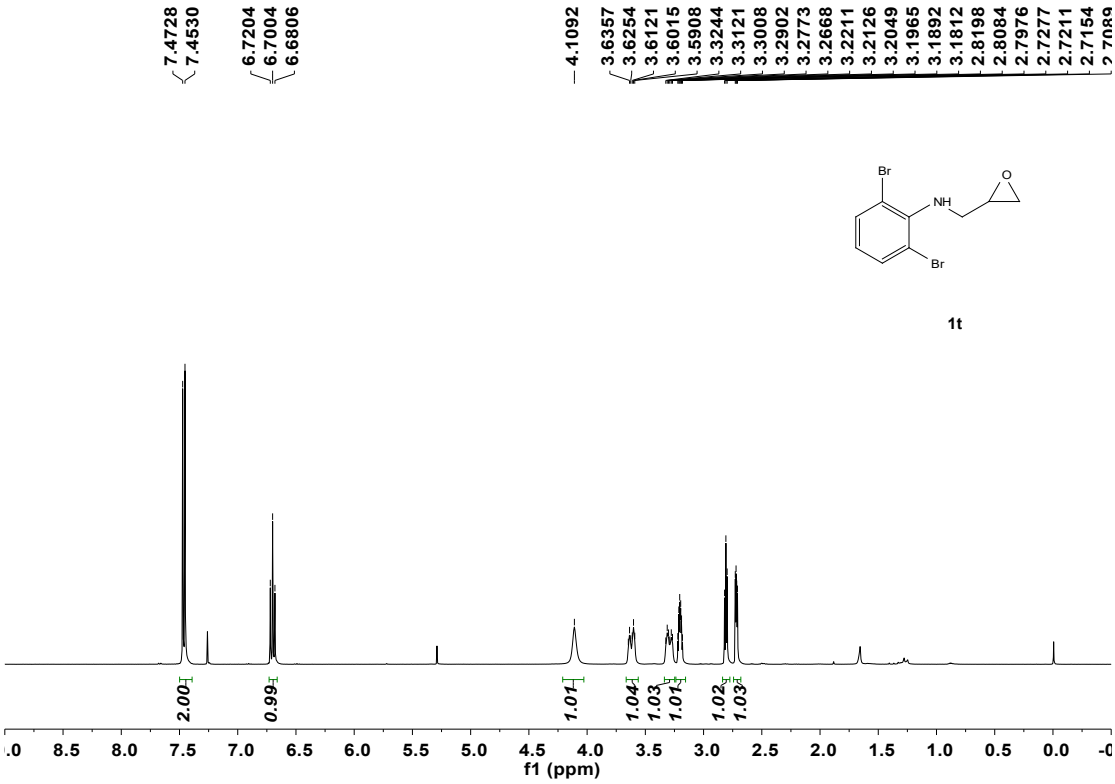
^{19}F NMR spectrum ($CDCl_3$, 376 MHz) of **1r**



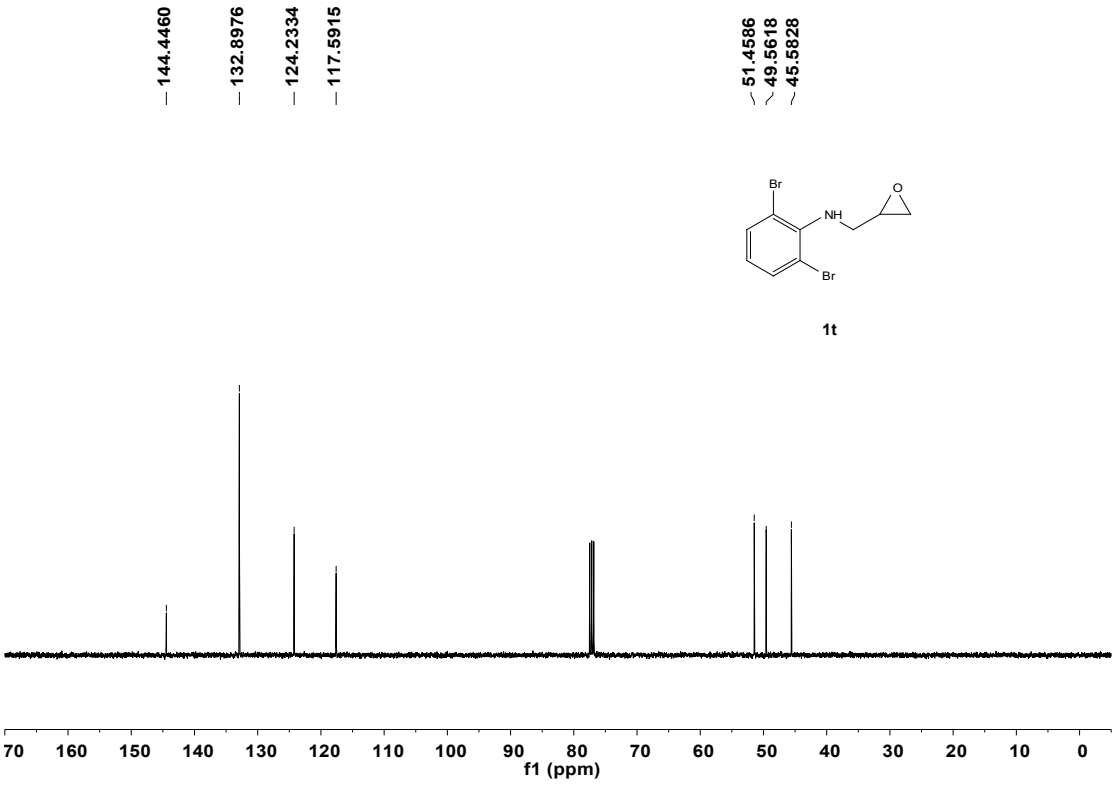
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **1s**



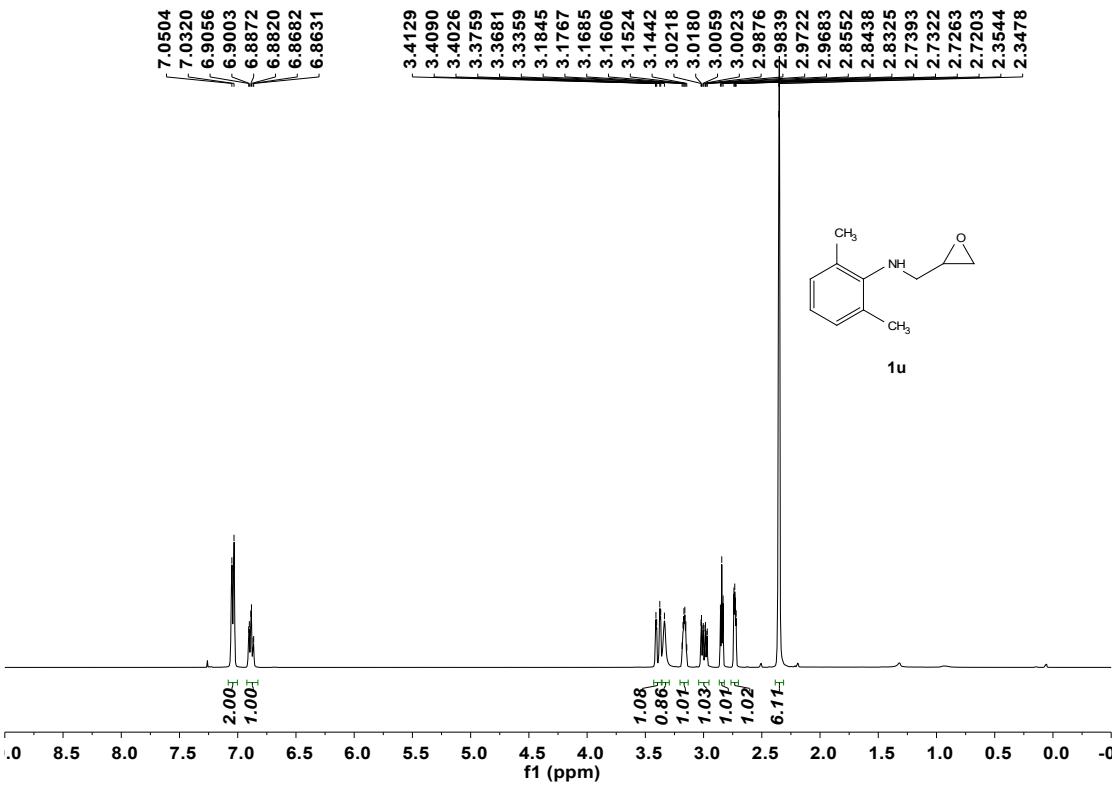
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **1s**



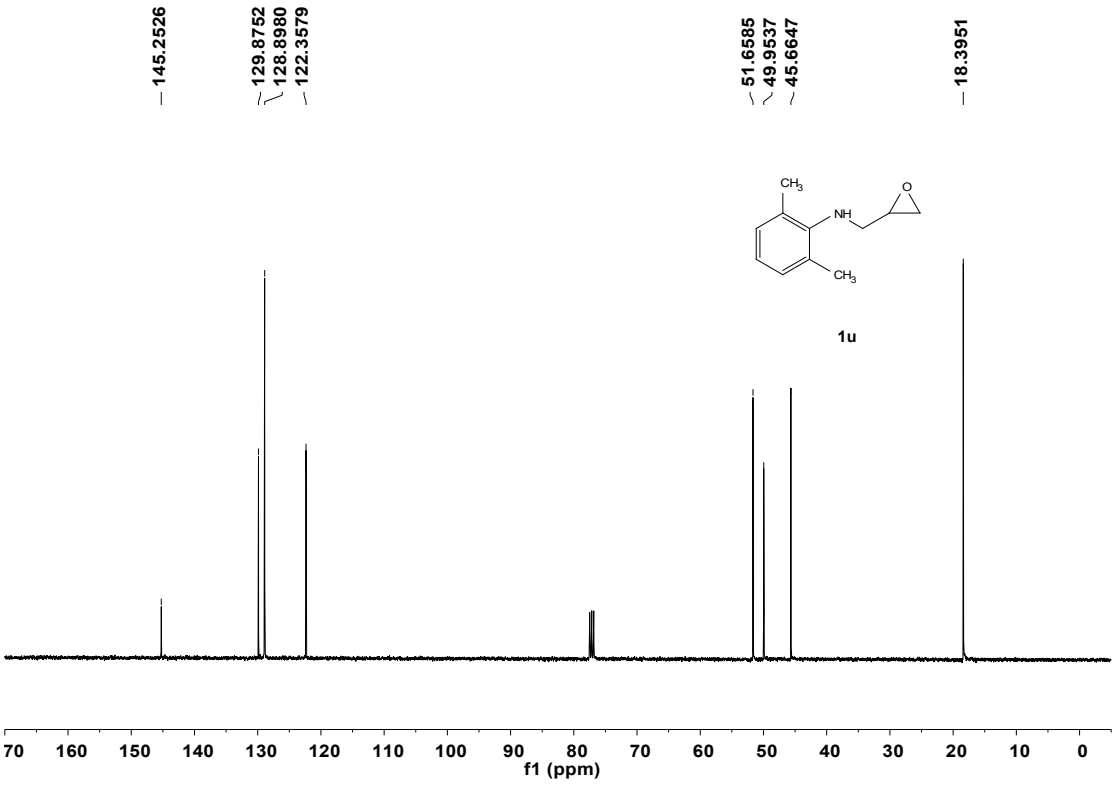
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **1t**



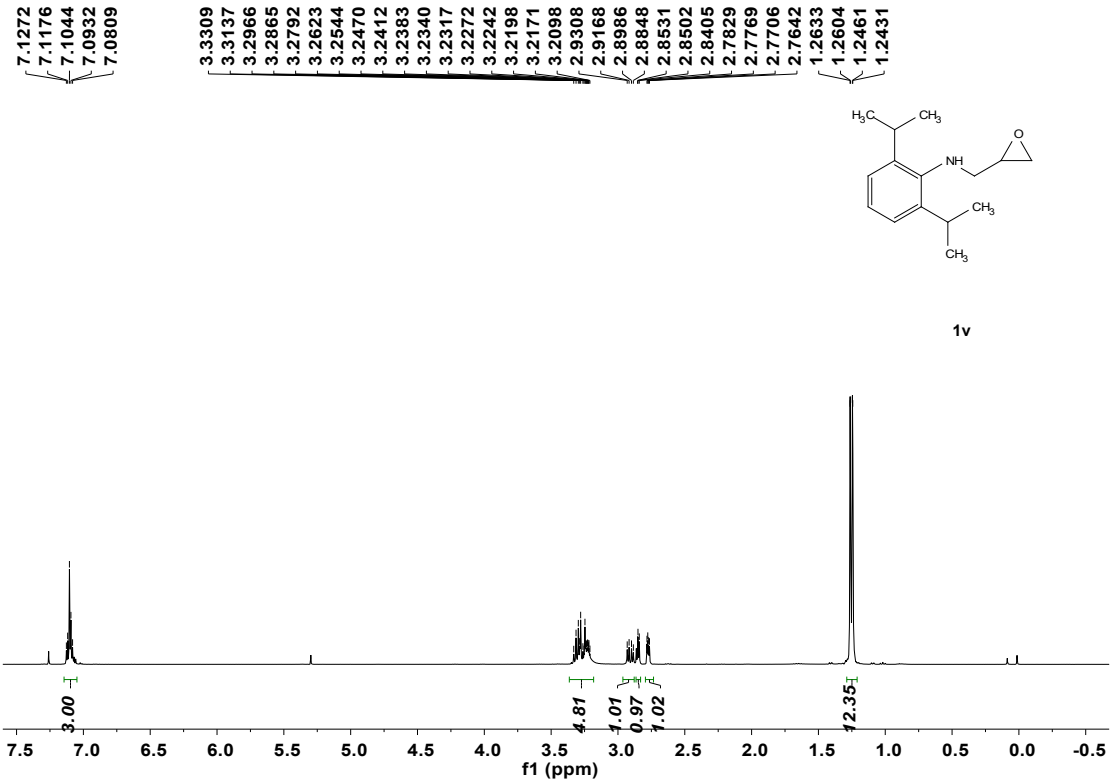
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **1t**



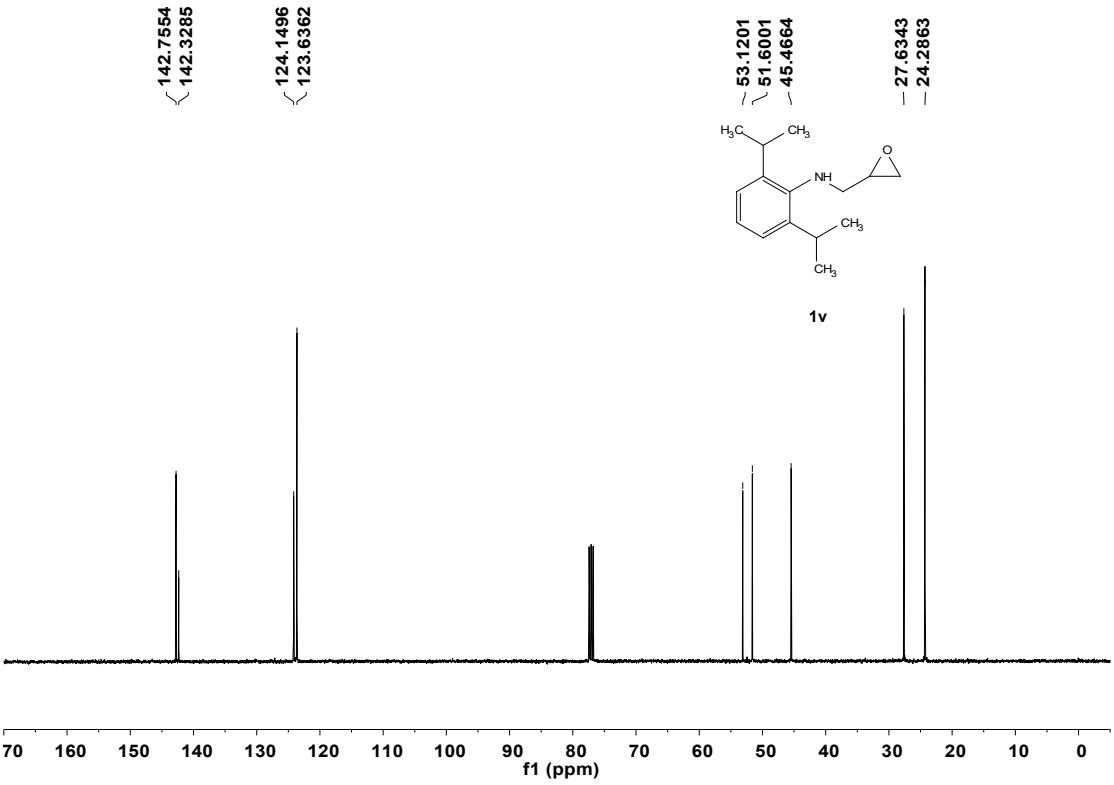
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **1u**



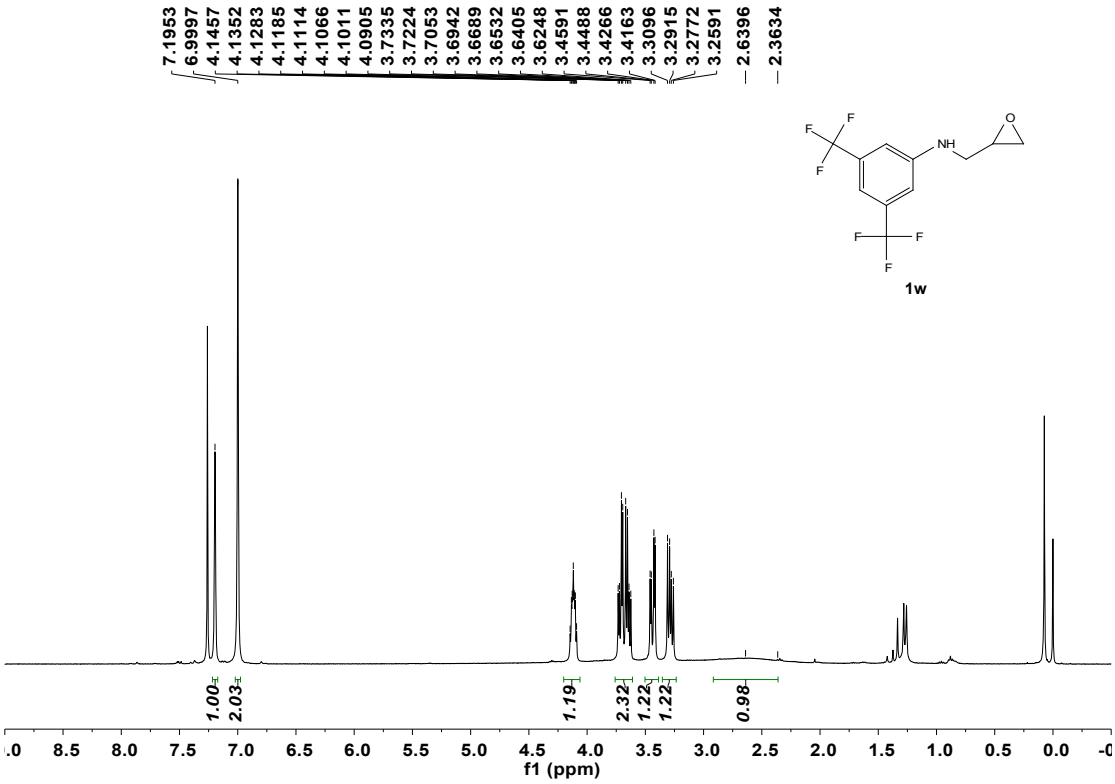
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **1u**



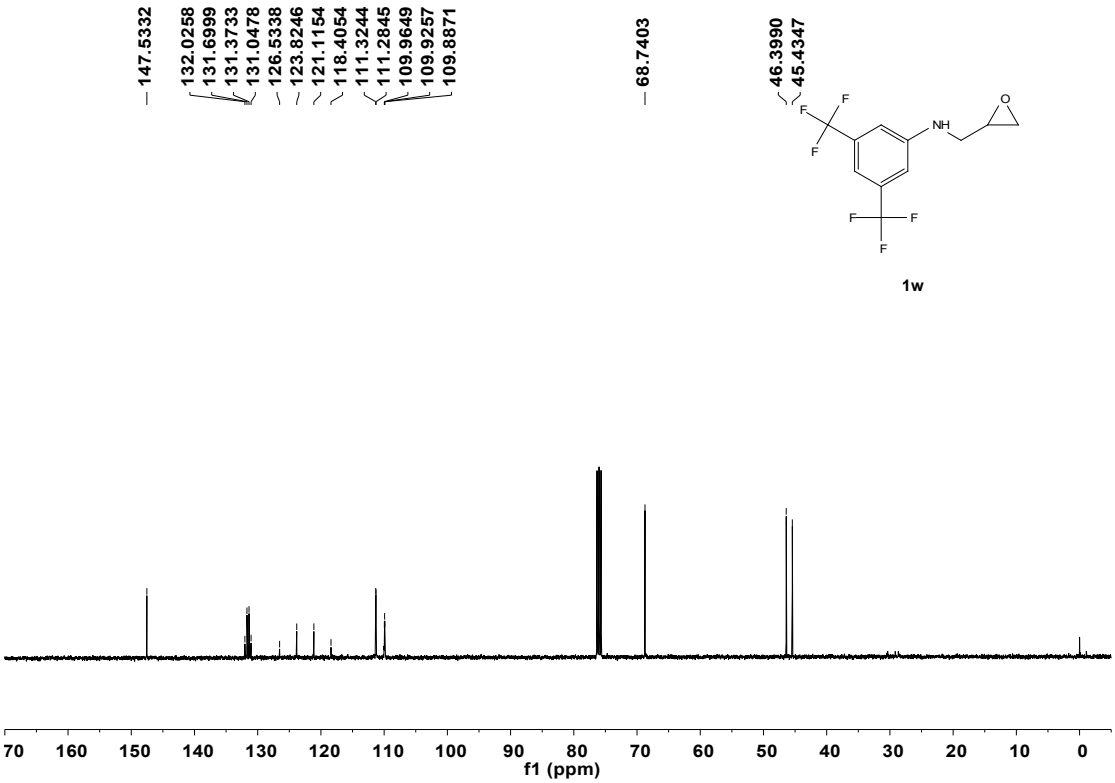
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **1v**



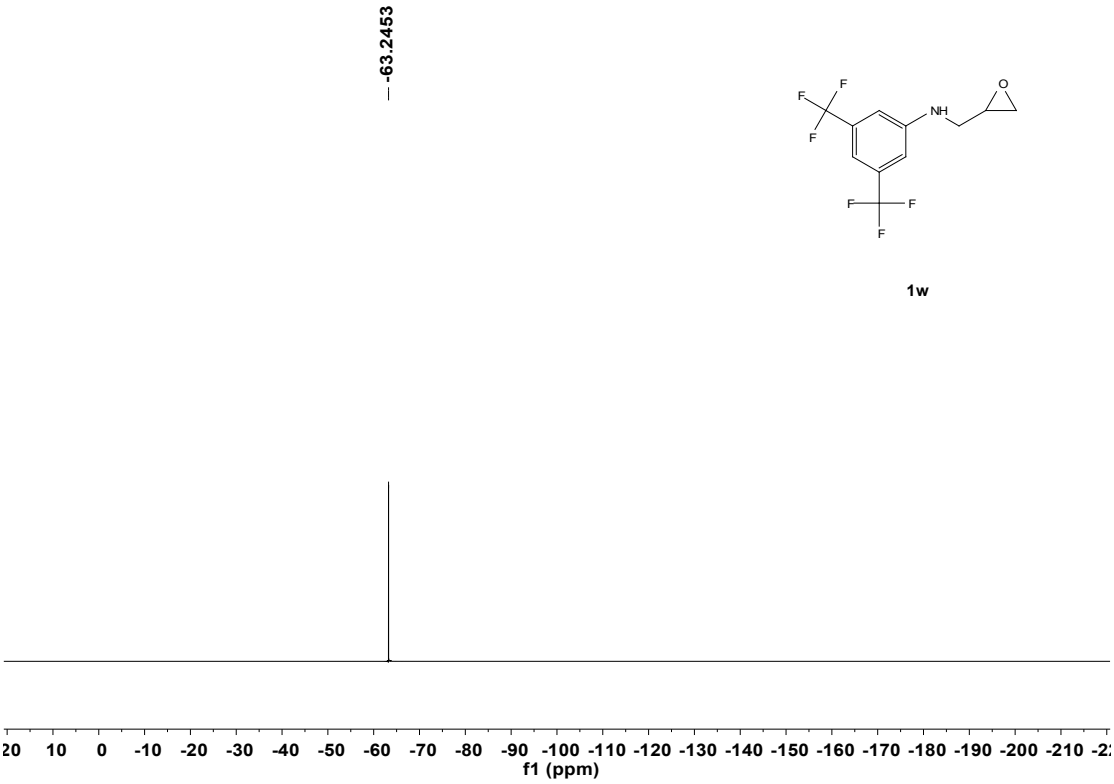
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **1v**



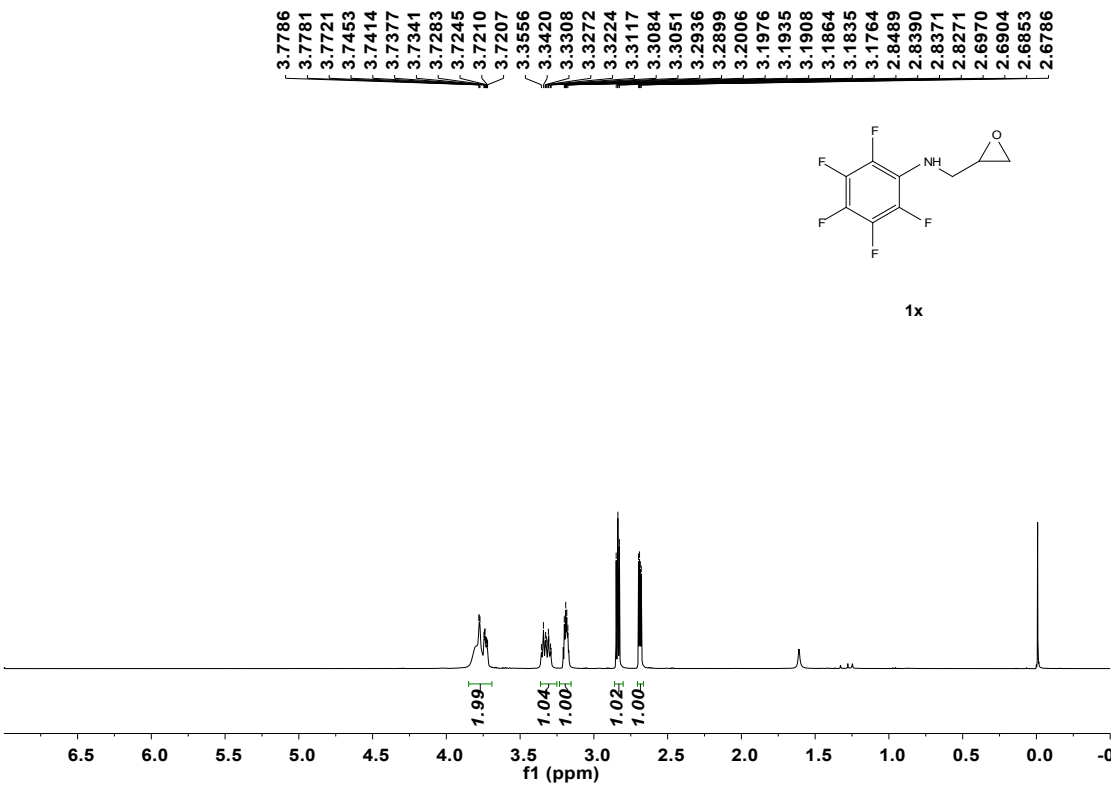
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **1w**



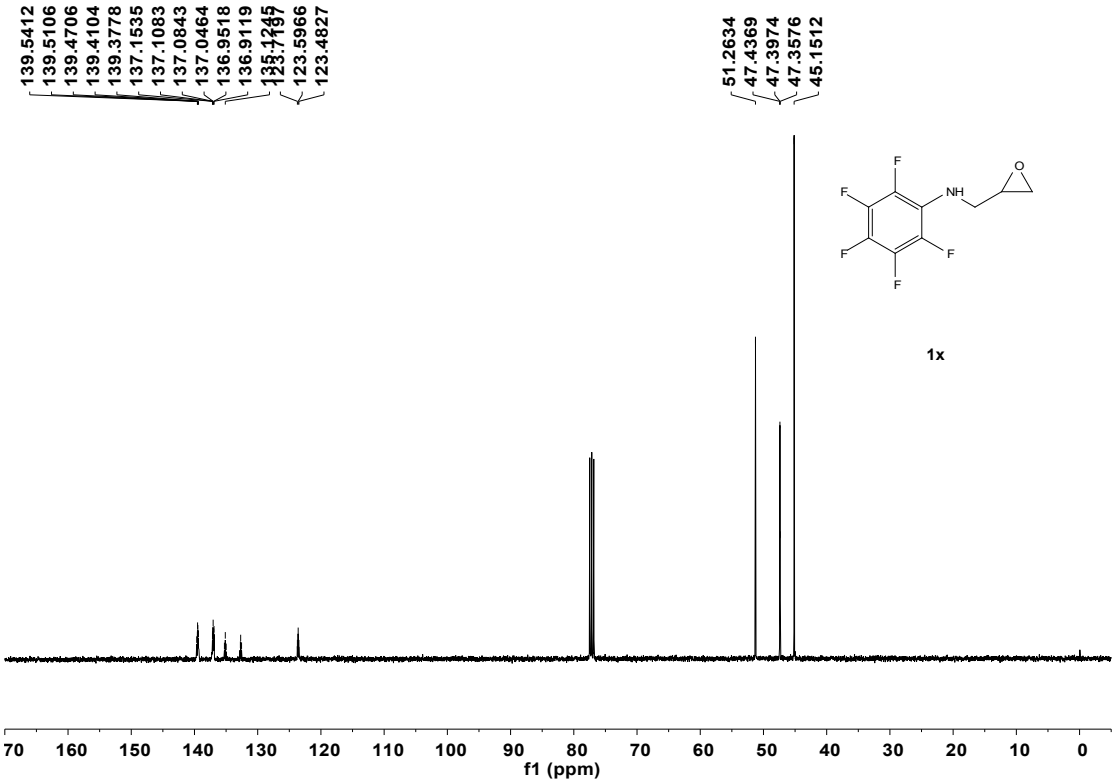
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **1w**



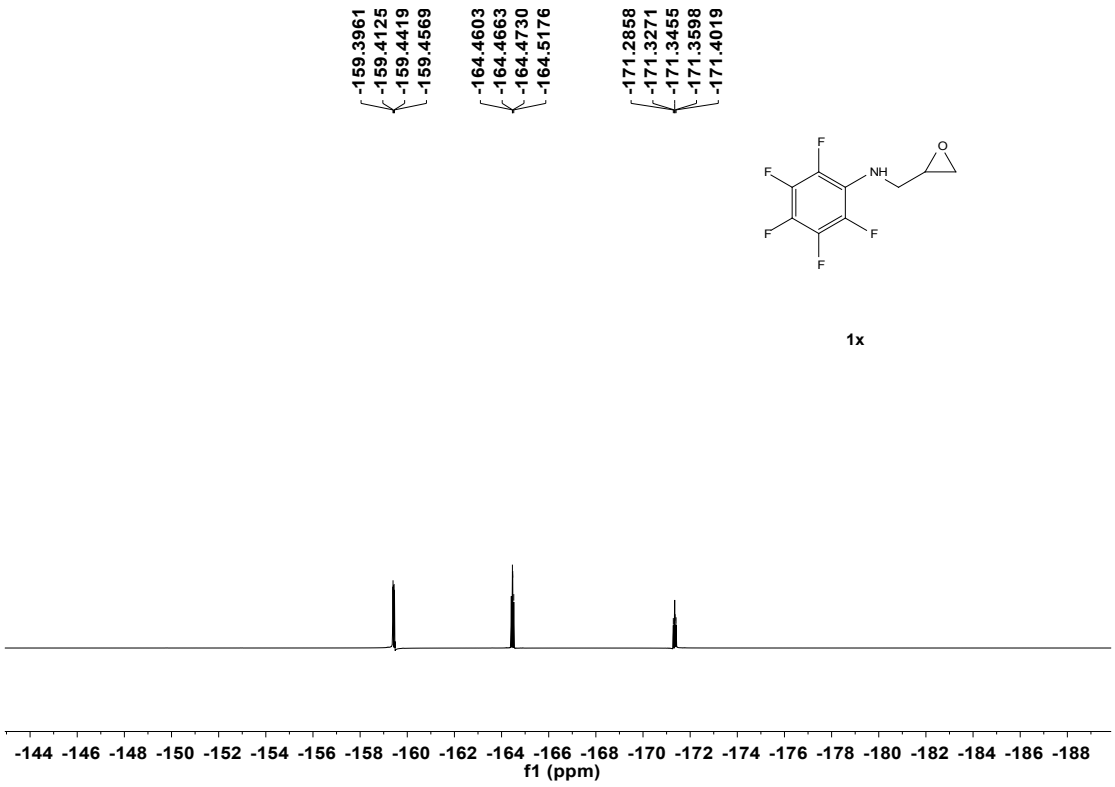
^{19}F NMR spectrum ($CDCl_3$, 376 MHz) of **1w**



^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **1x**

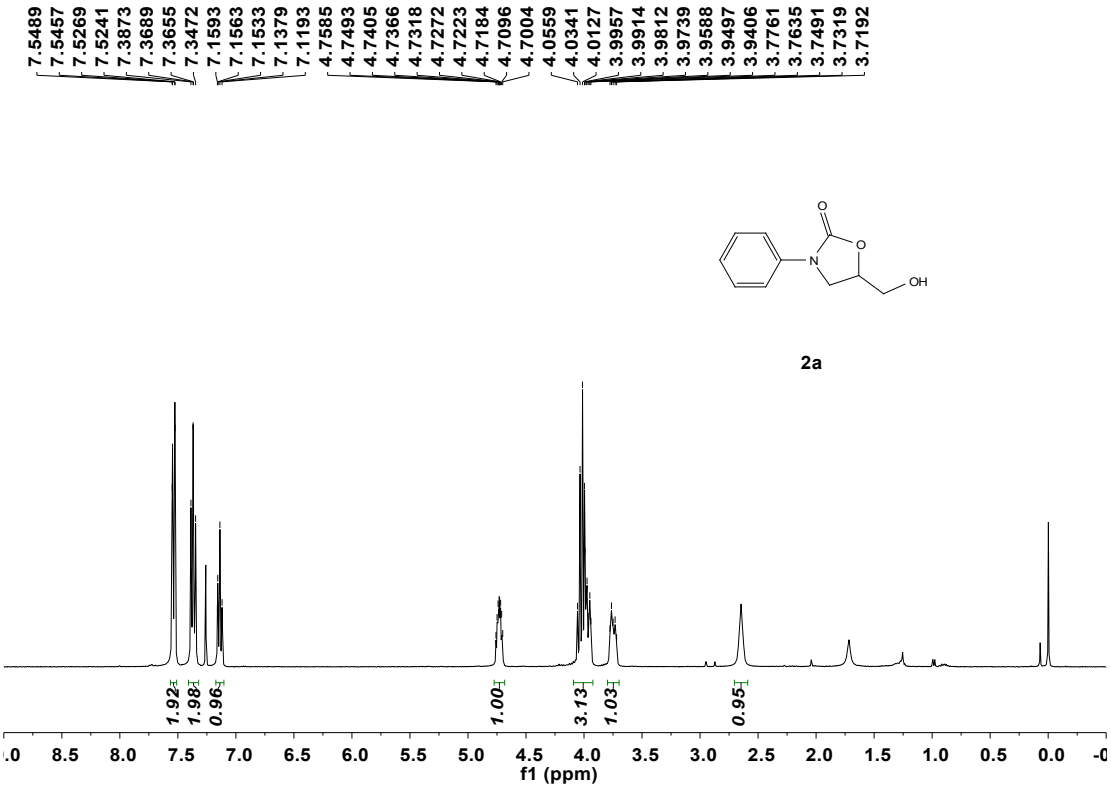


^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **1x**

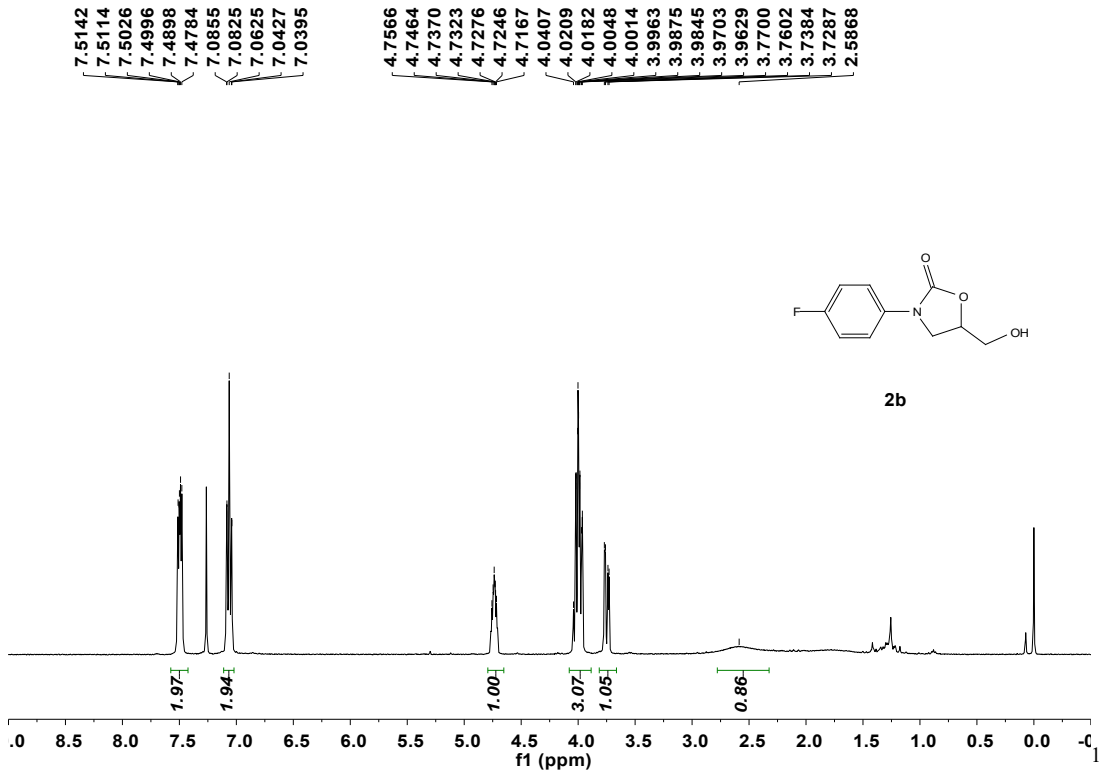


^{19}F NMR spectrum ($CDCl_3$, 376 MHz) of **1x**

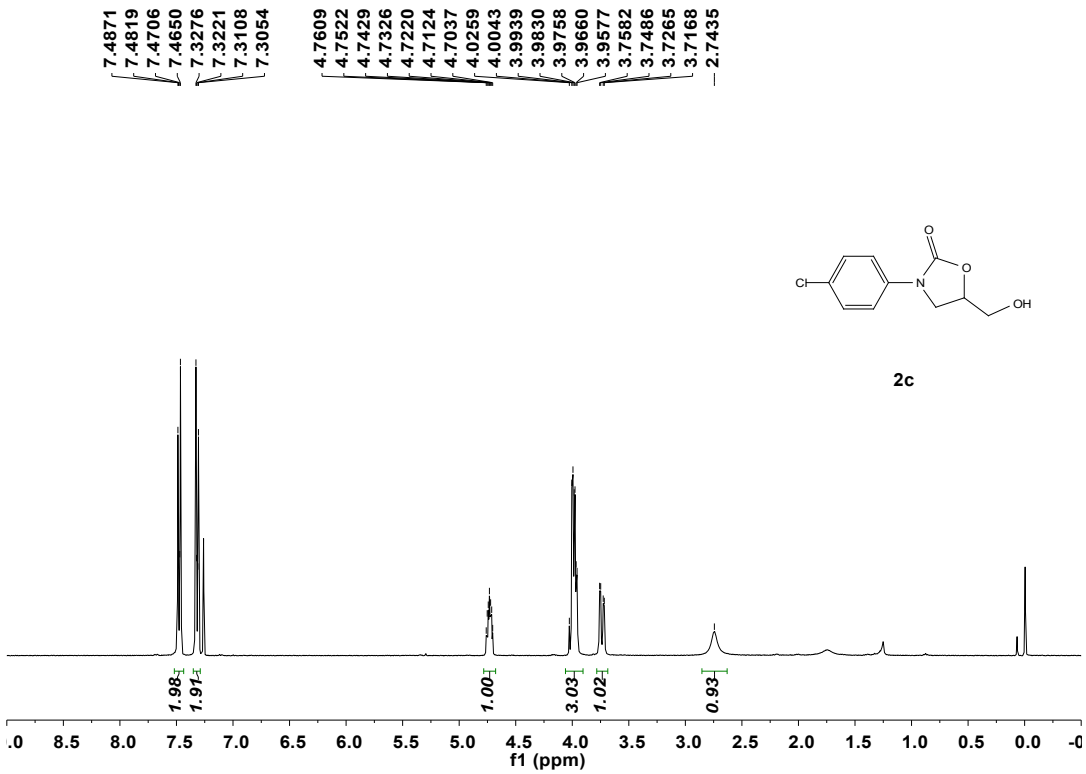
NMR spectra of isolated products



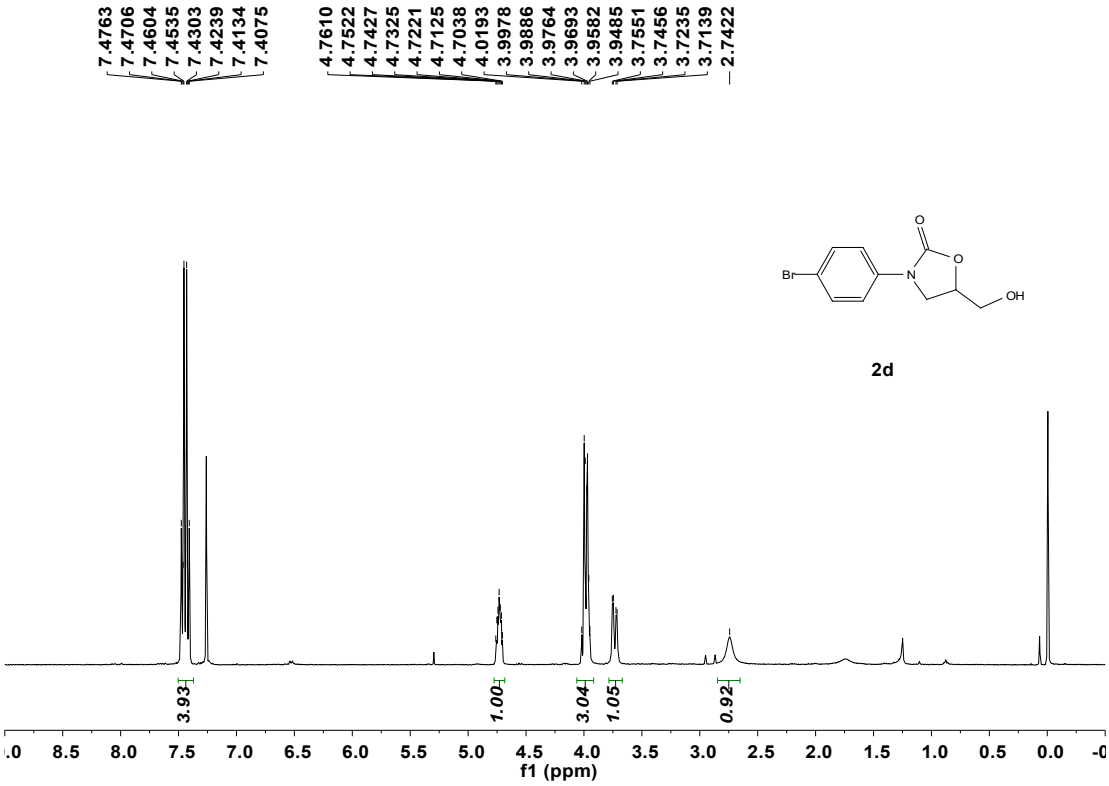
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **2a**



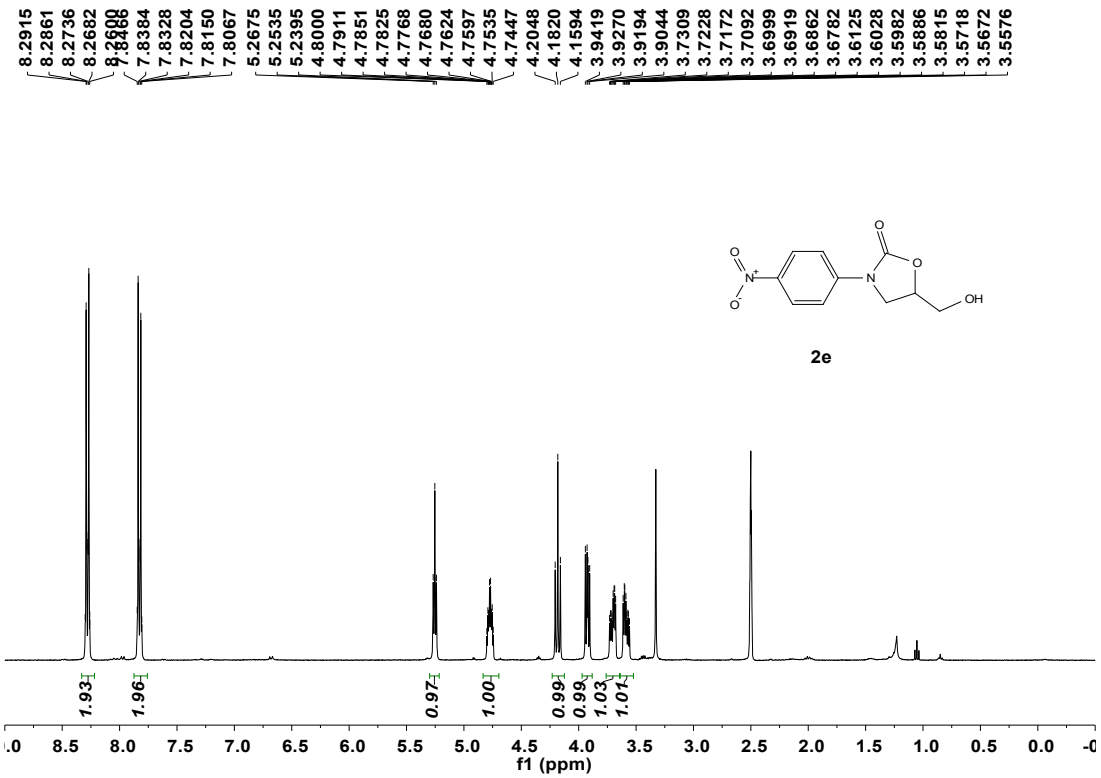
H NMR spectrum ($CDCl_3$, 400 MHz) of **2b**



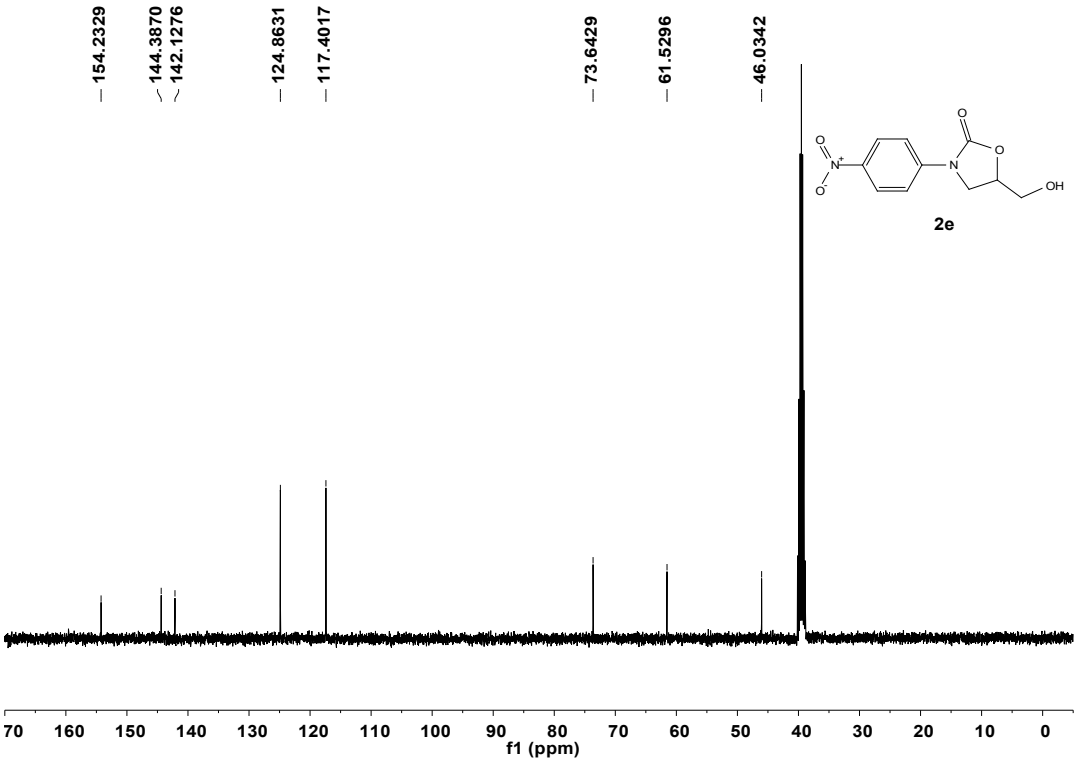
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **2c**



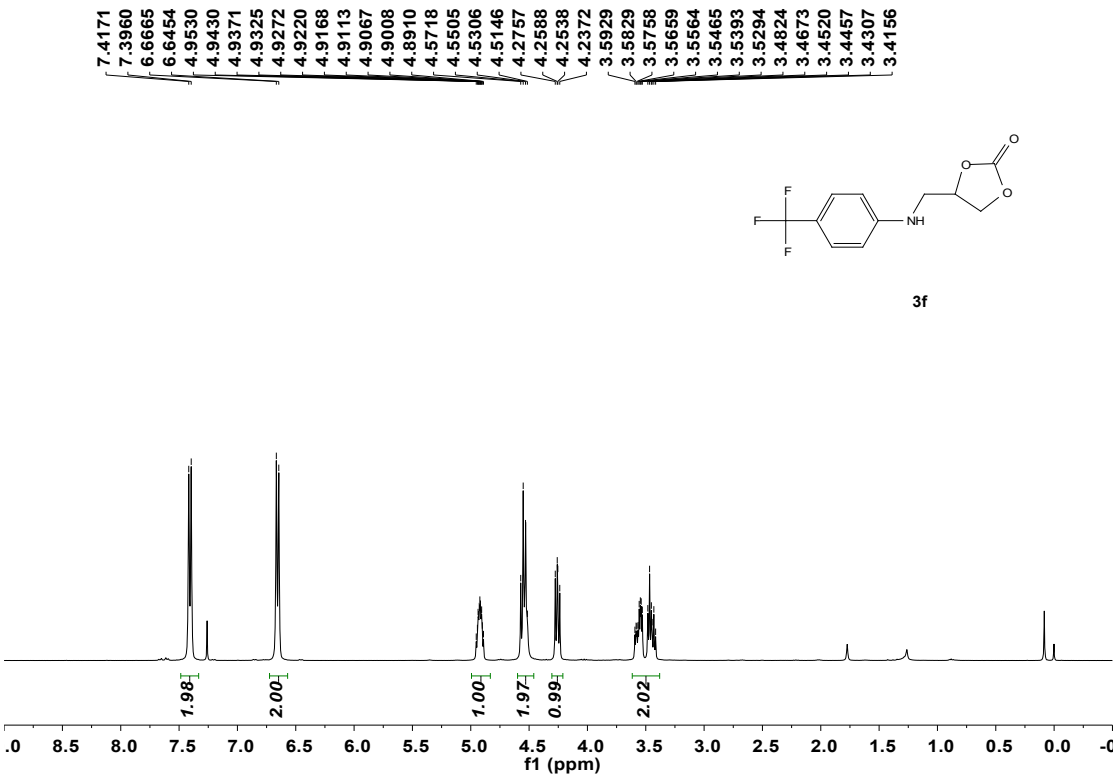
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **2d**



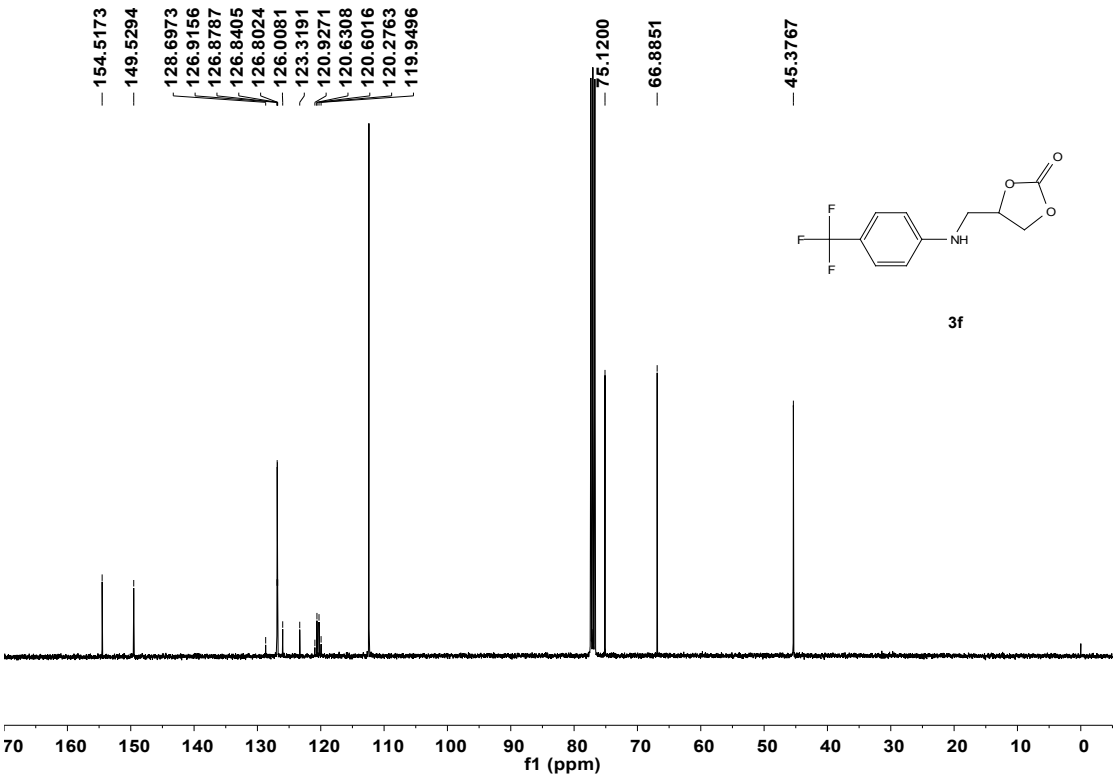
^{1}H NMR spectrum (DMSO, 400 MHz) of **2e**



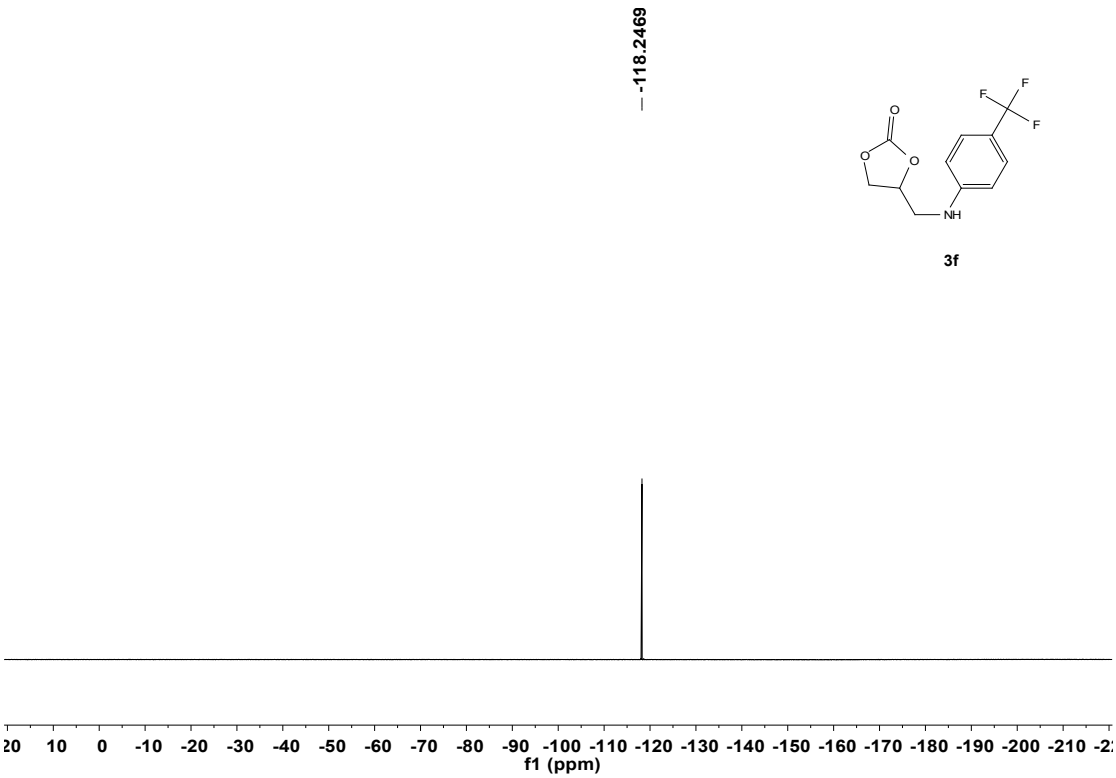
^{13}C NMR spectrum (DMSO, 101 MHz) of **2e**



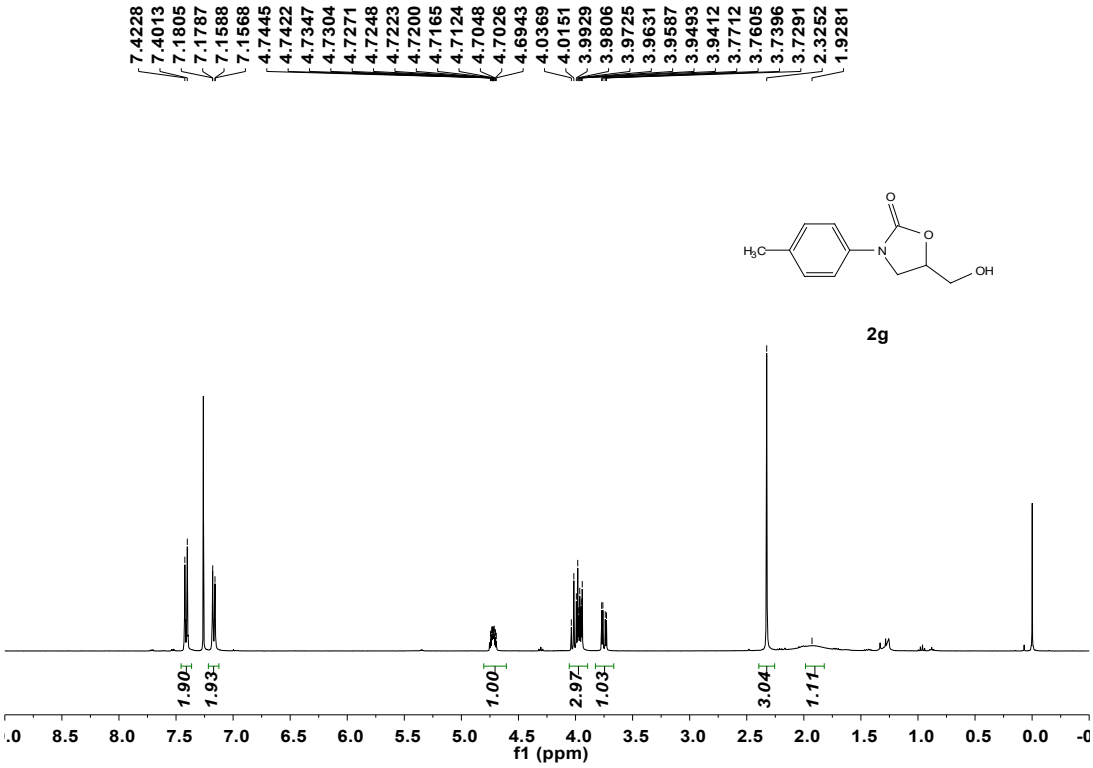
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **3f**



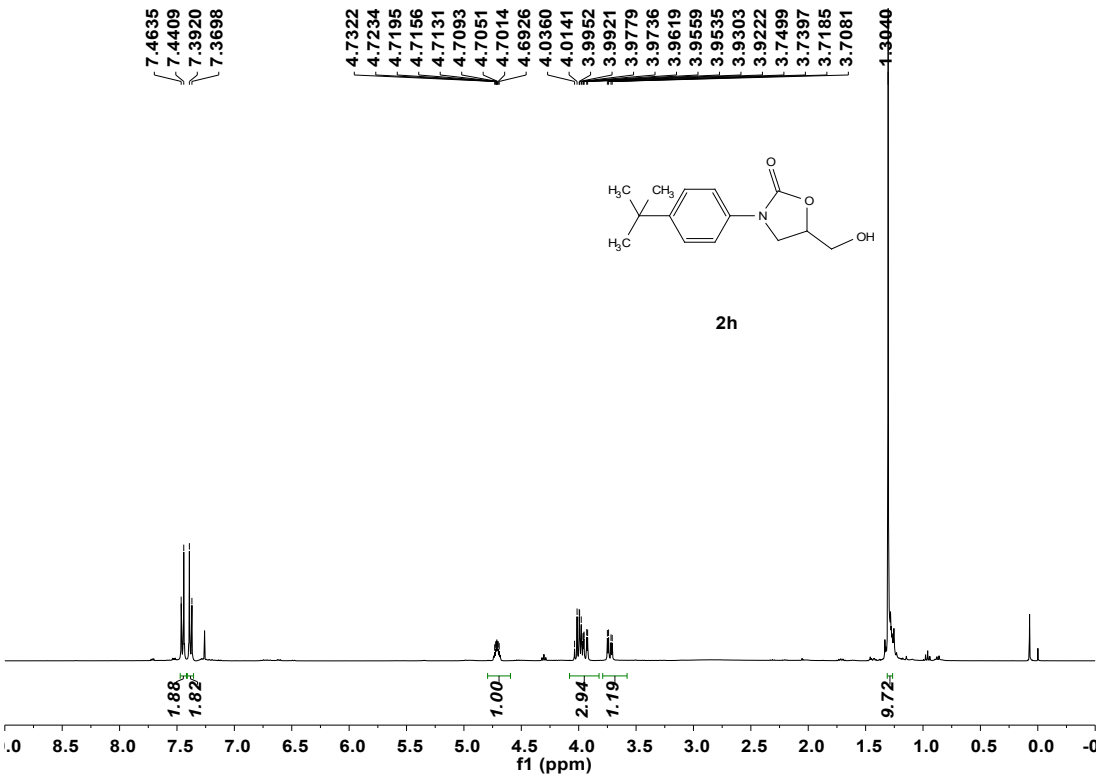
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **3f**



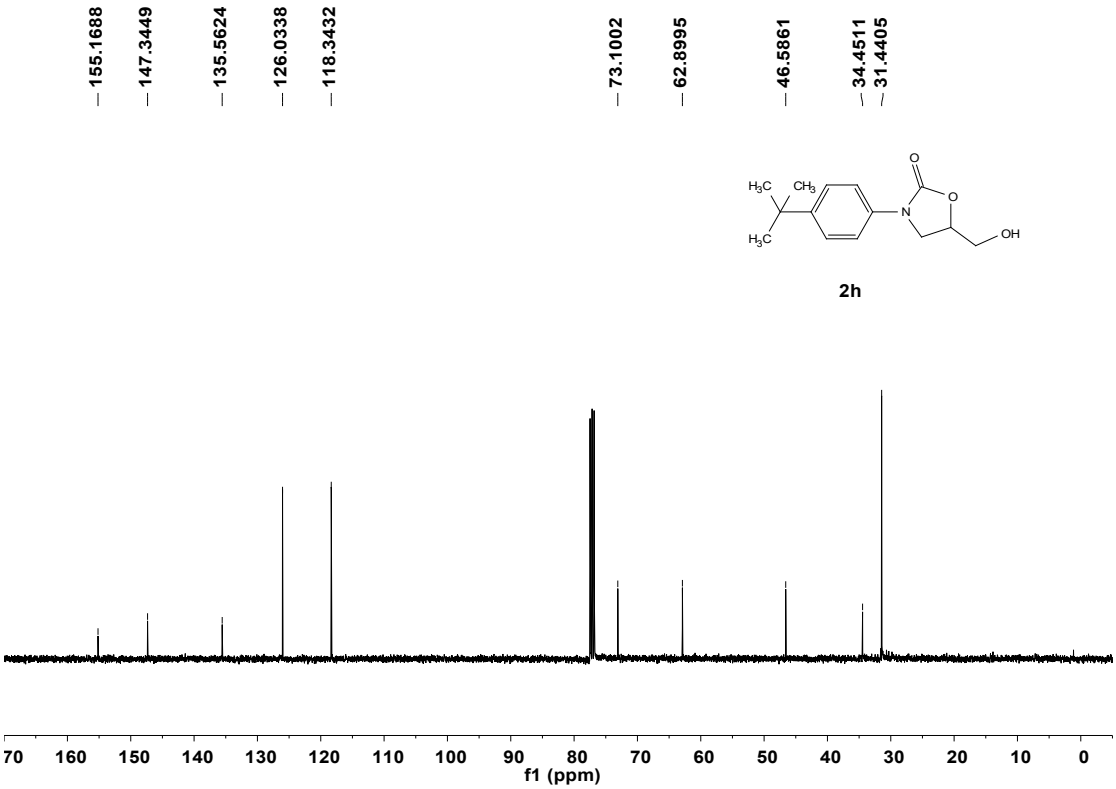
^{19}F NMR spectrum ($CDCl_3$, 376 MHz) of **3f**



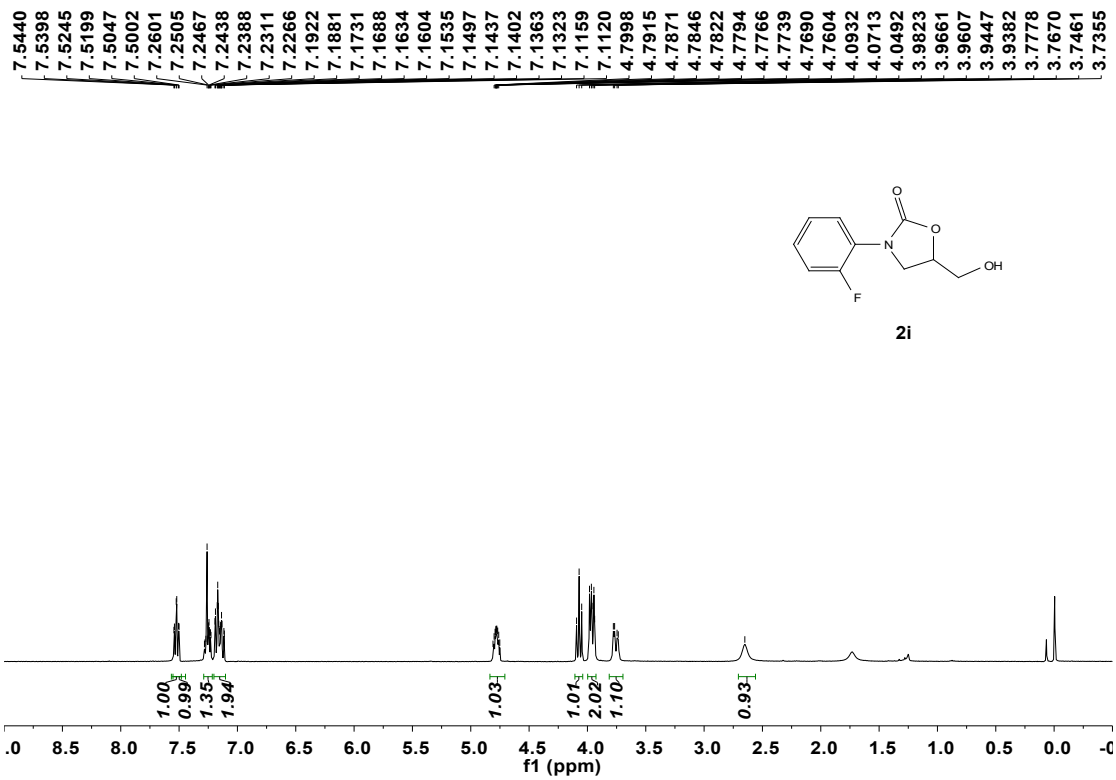
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **2g**



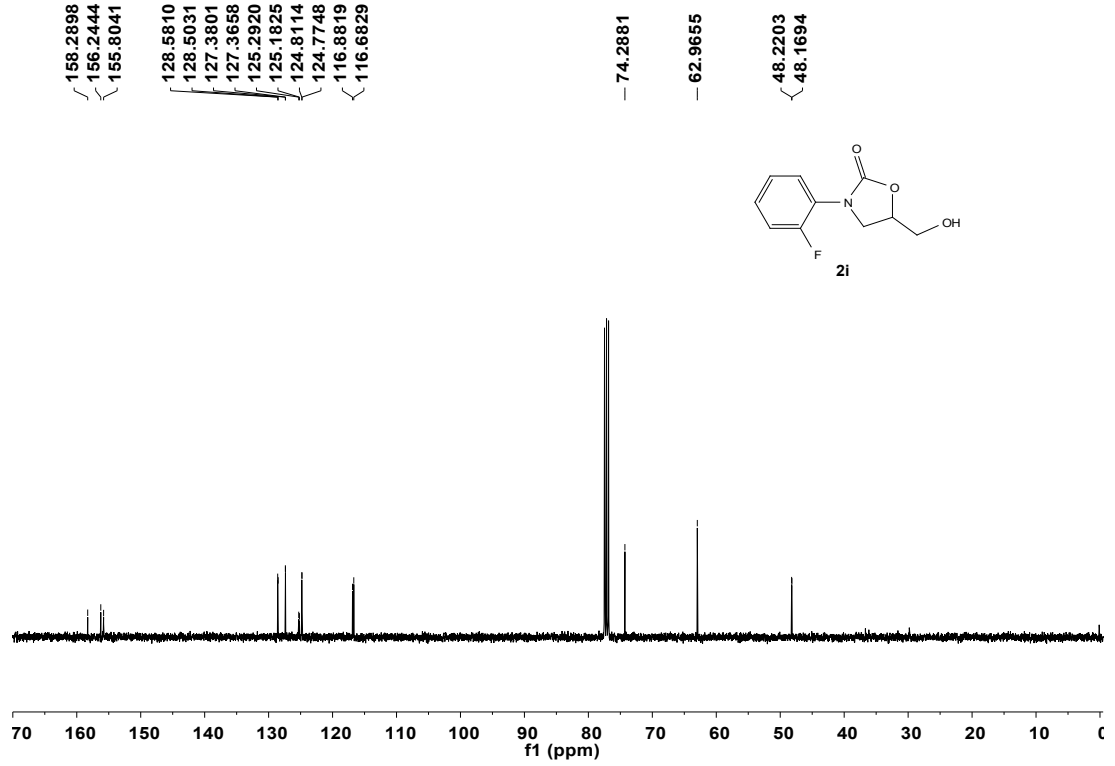
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **2h**



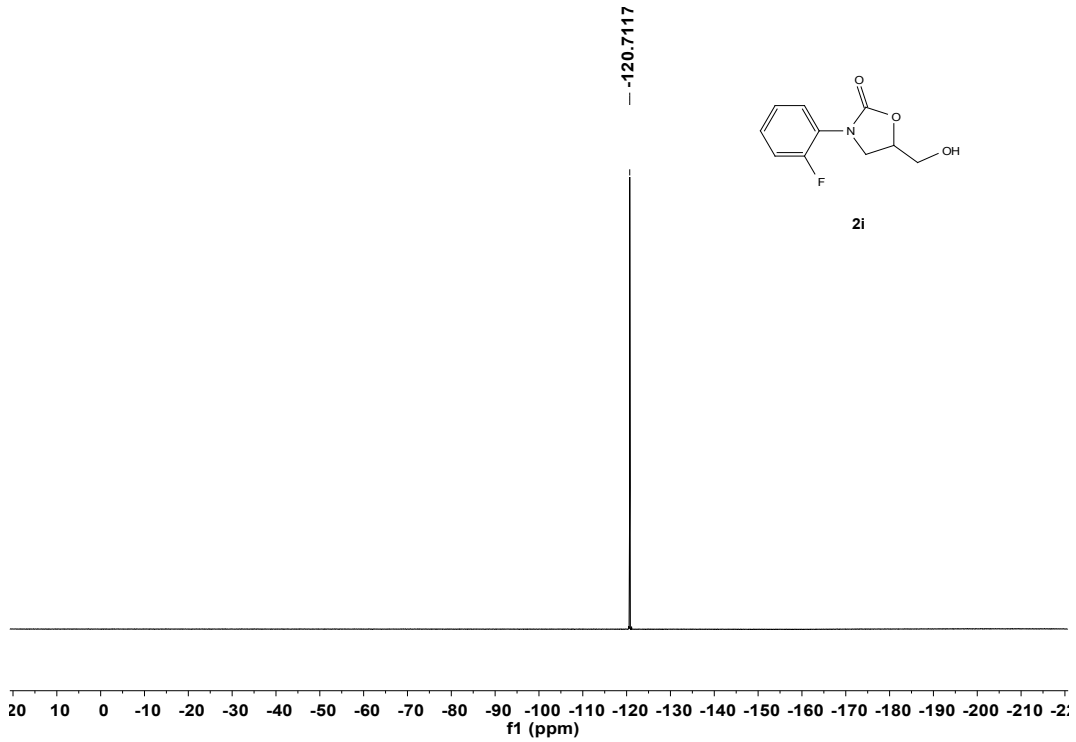
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **2h**



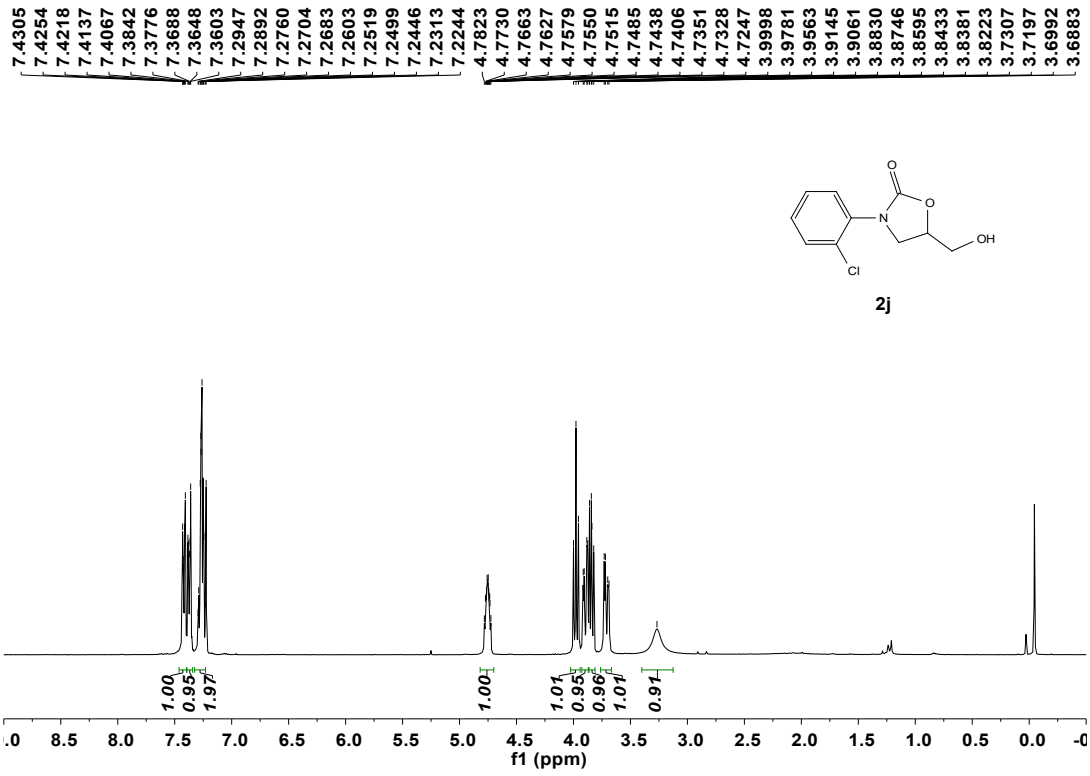
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **2i**



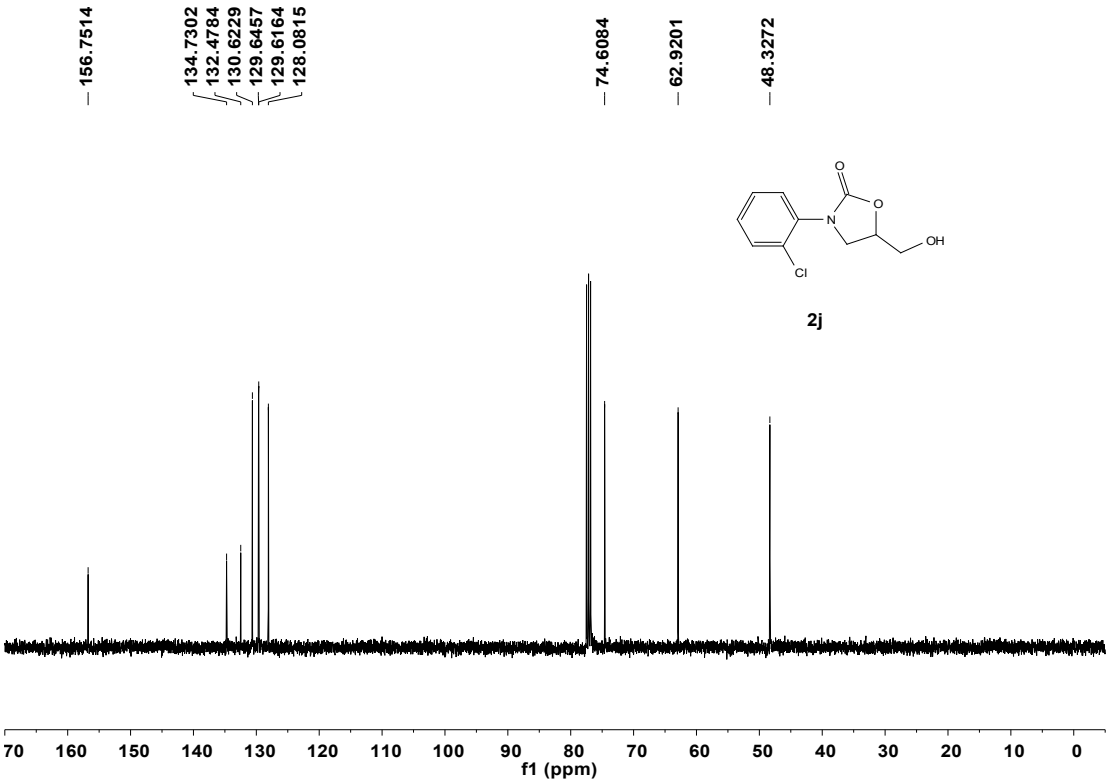
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **2i**



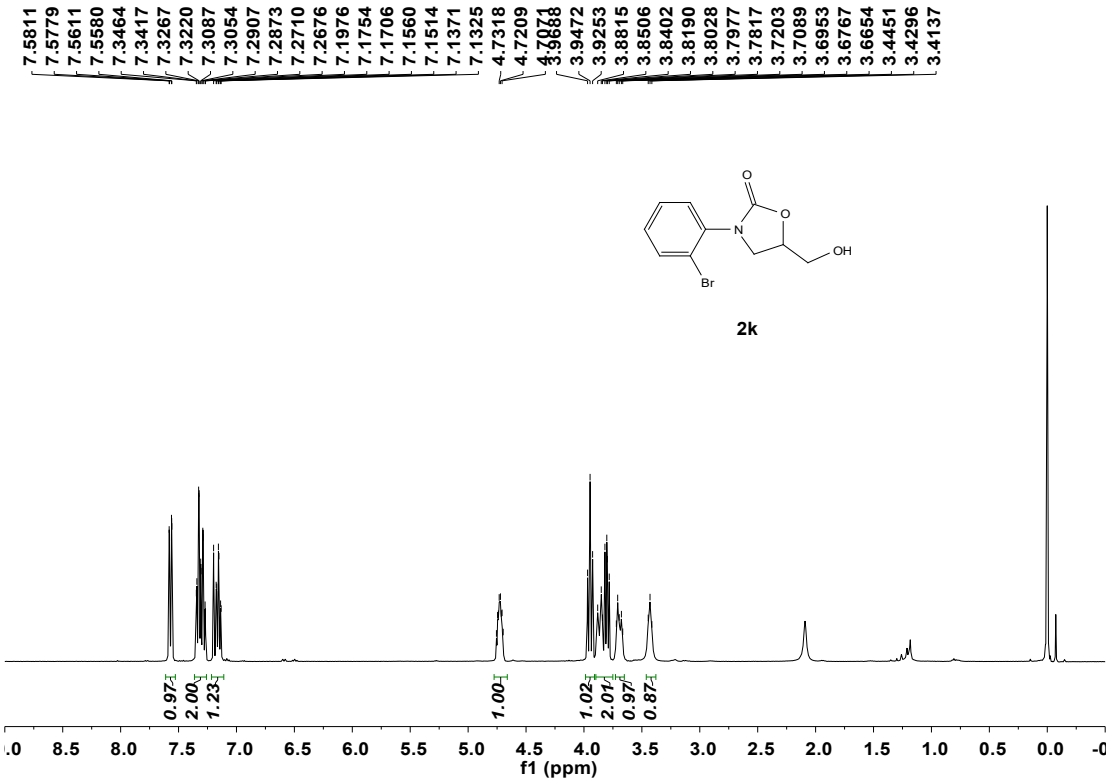
^{19}F NMR spectrum ($CDCl_3$, 376 MHz) of **2i**



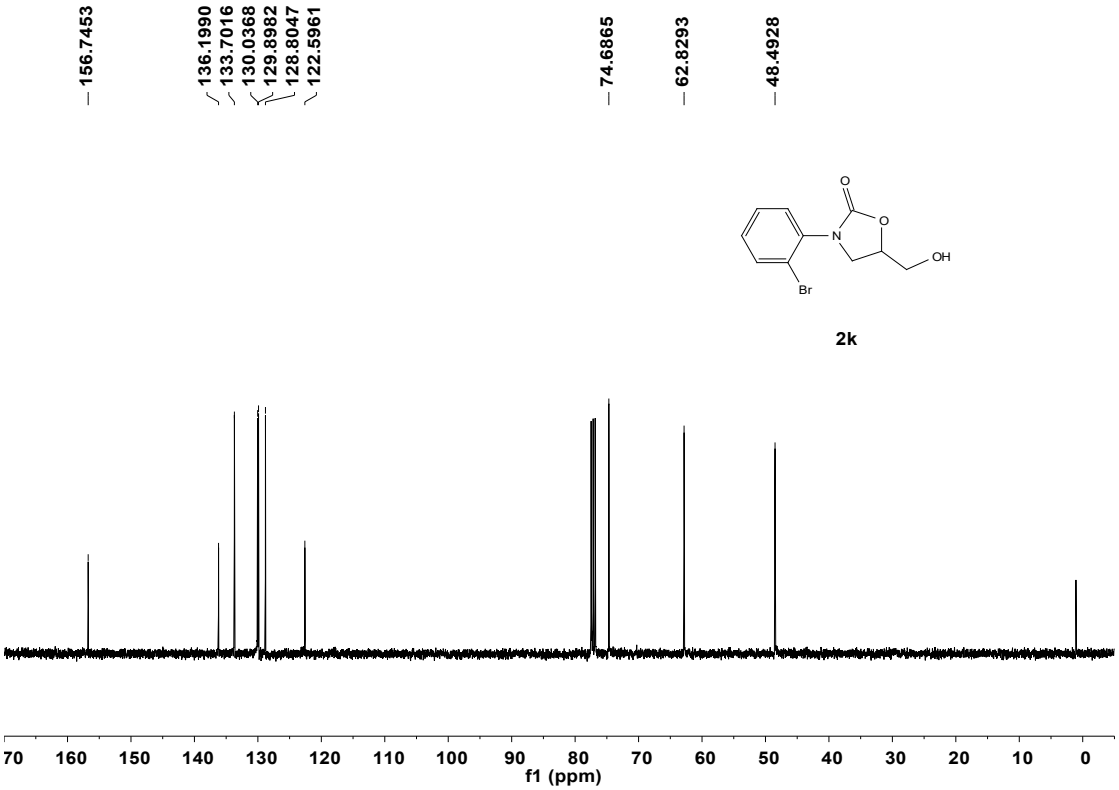
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **2j**



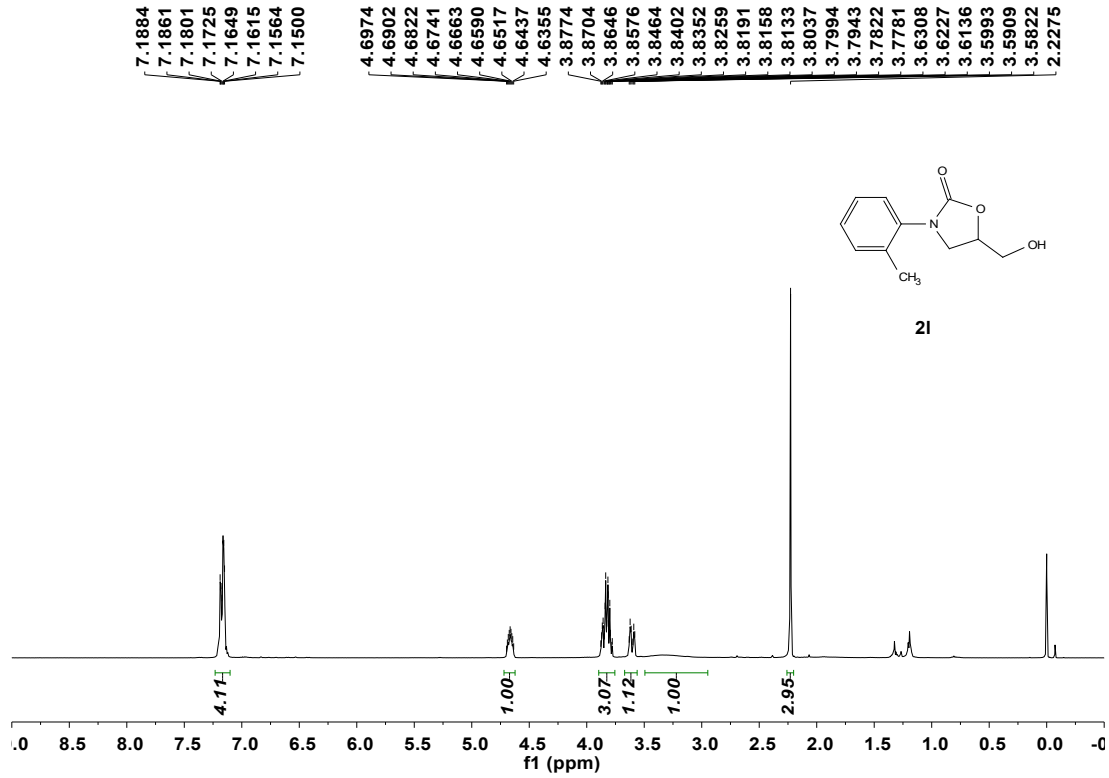
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **2j**



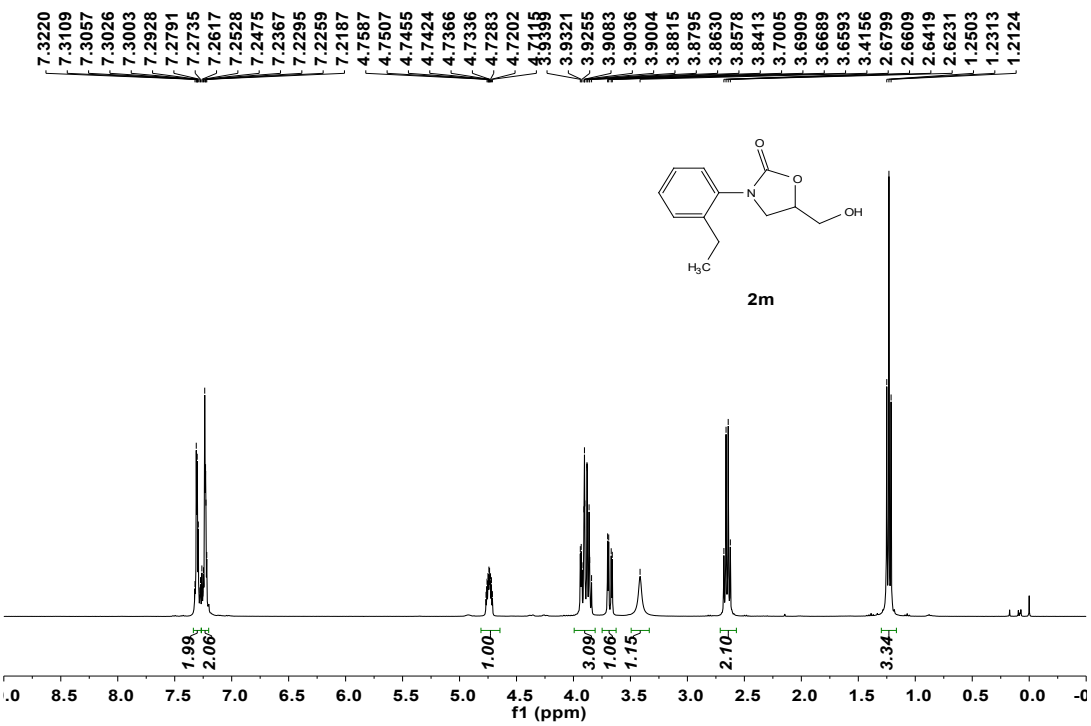
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **2k**



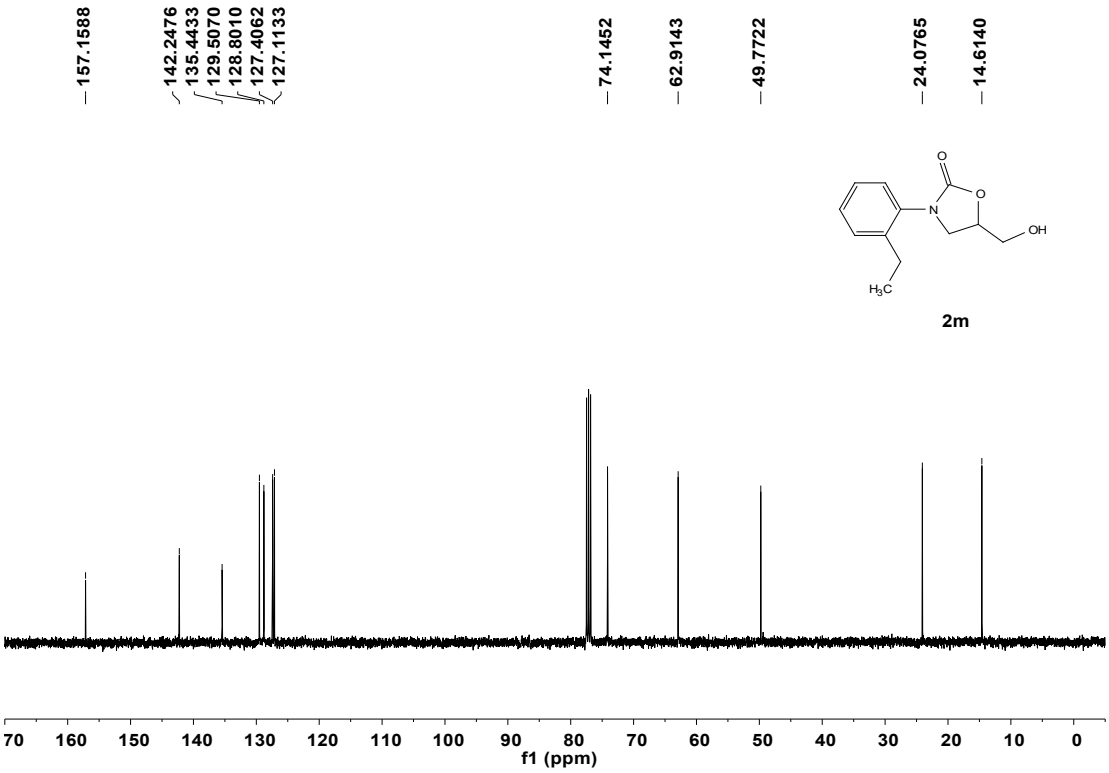
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **2k**



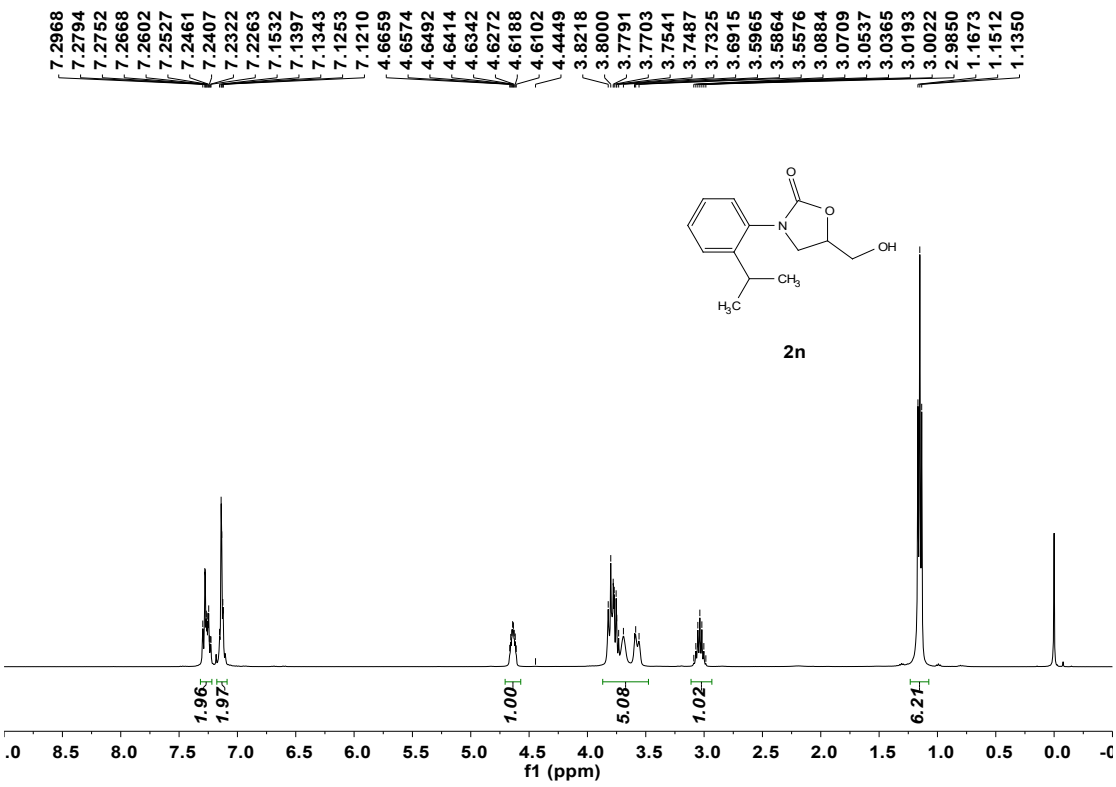
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **2l**



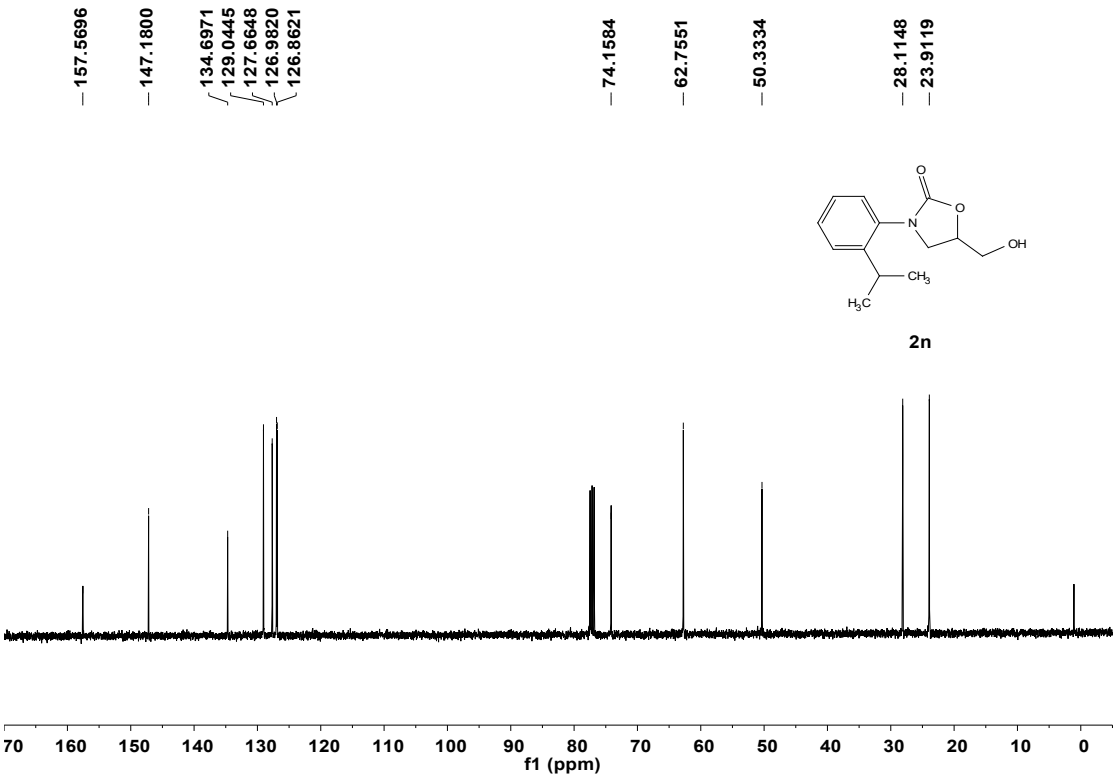
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **2m**



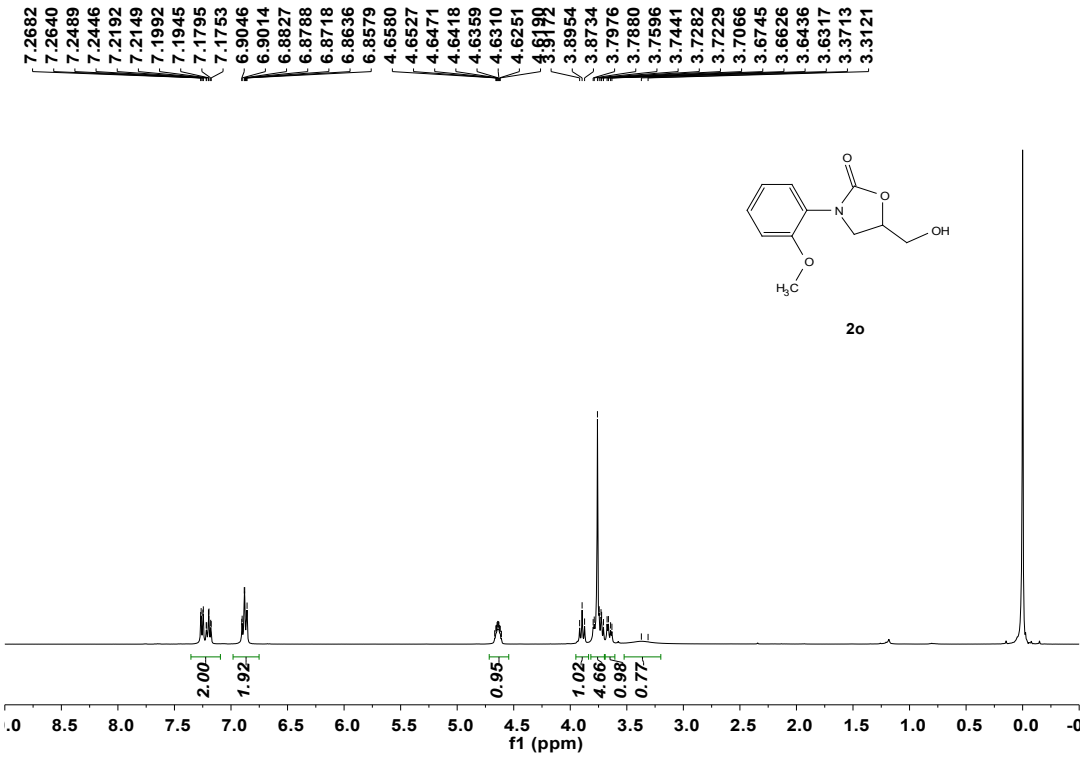
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **2m**



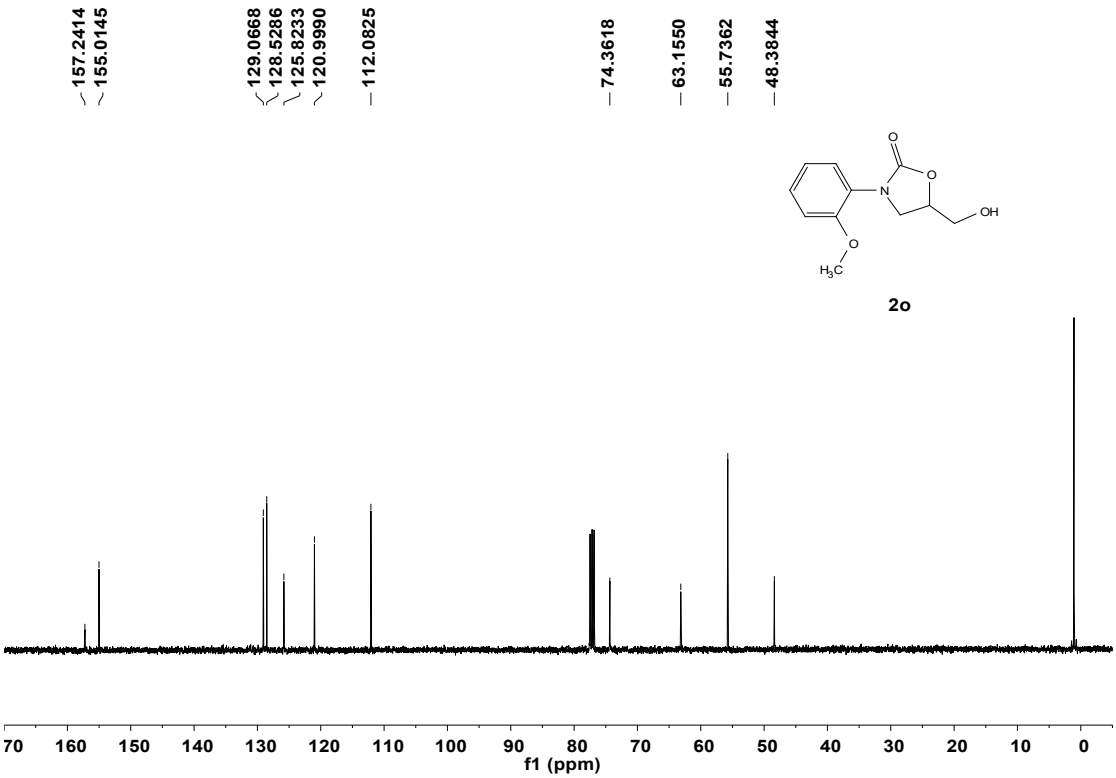
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **2n**



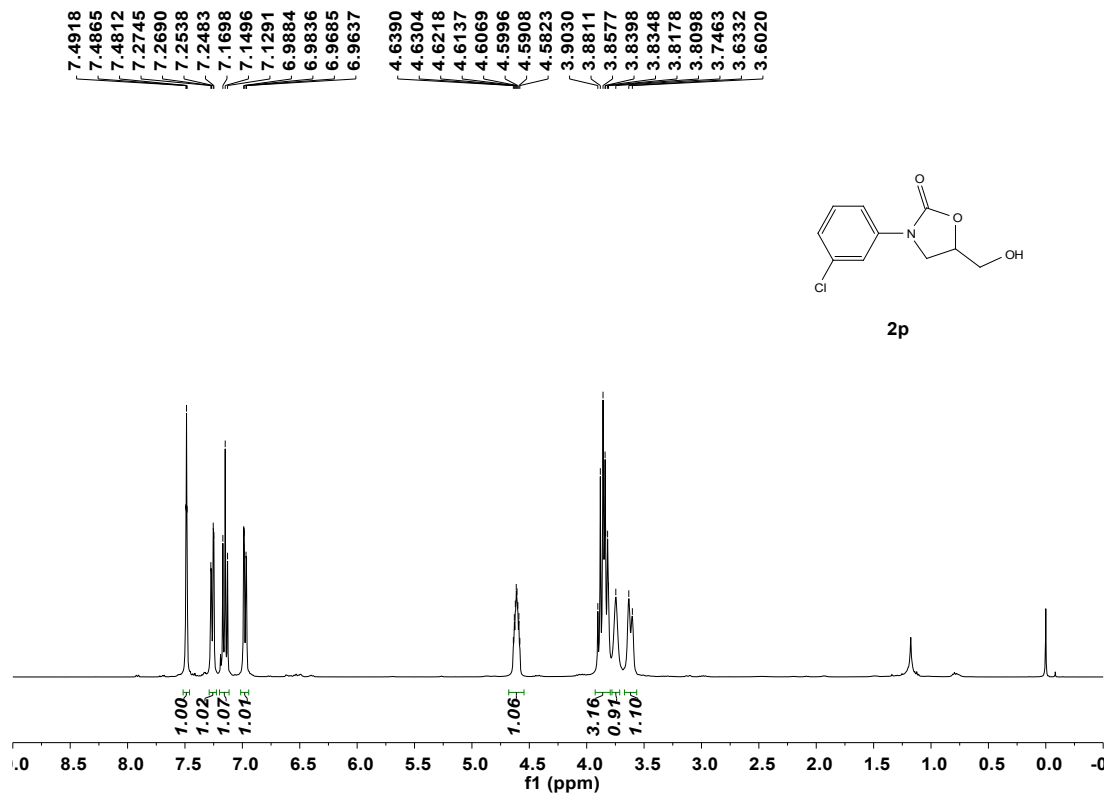
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **2n**



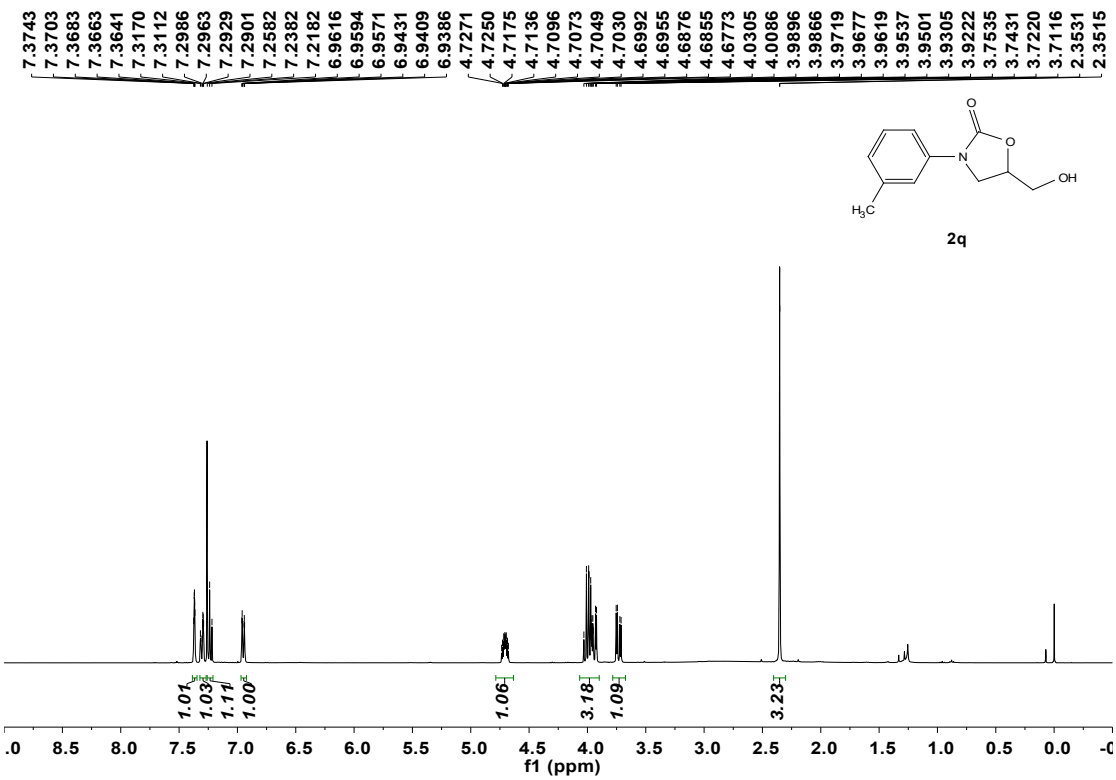
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **2o**



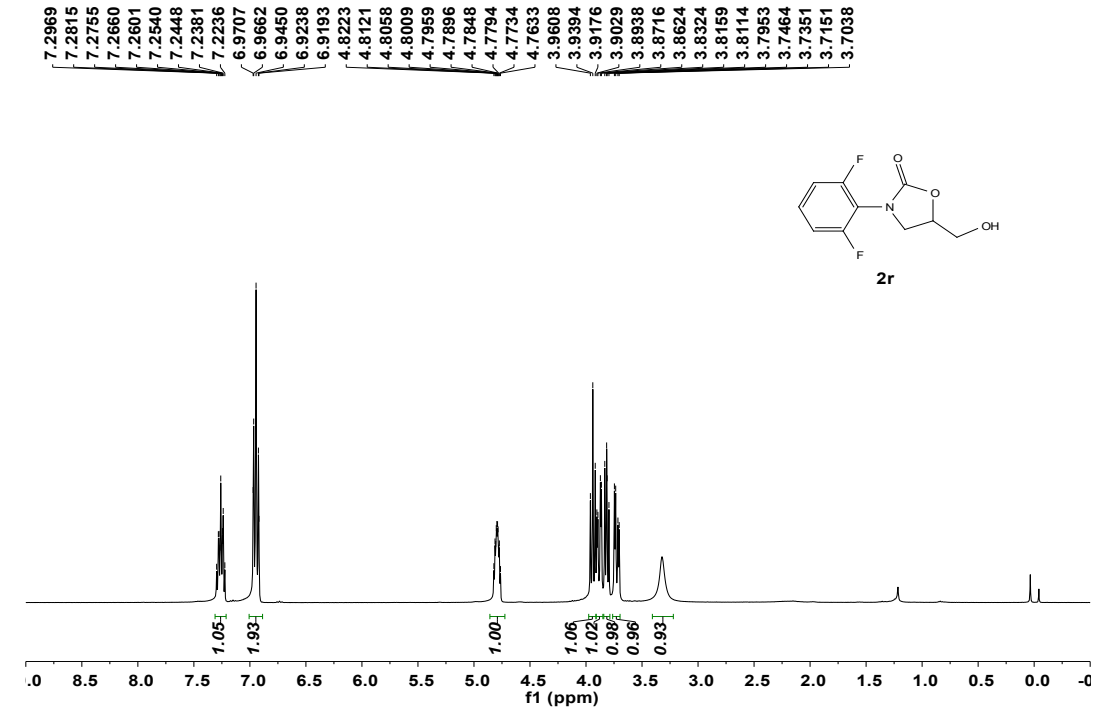
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **2o**



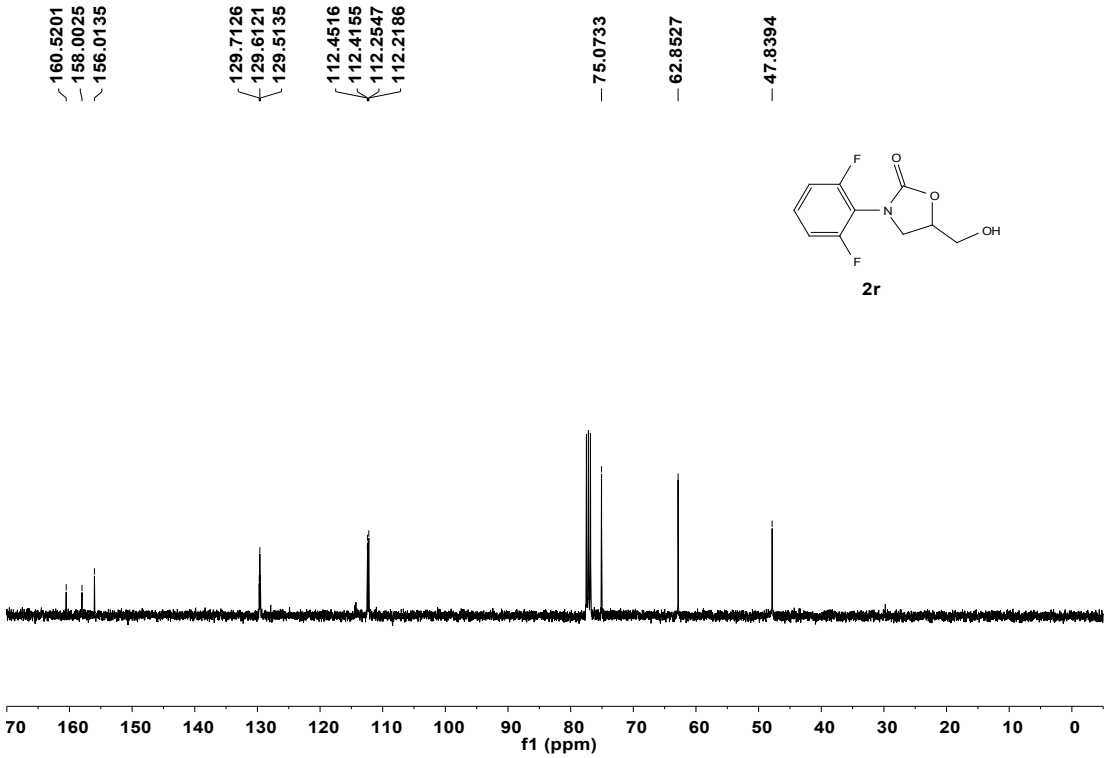
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **2p**



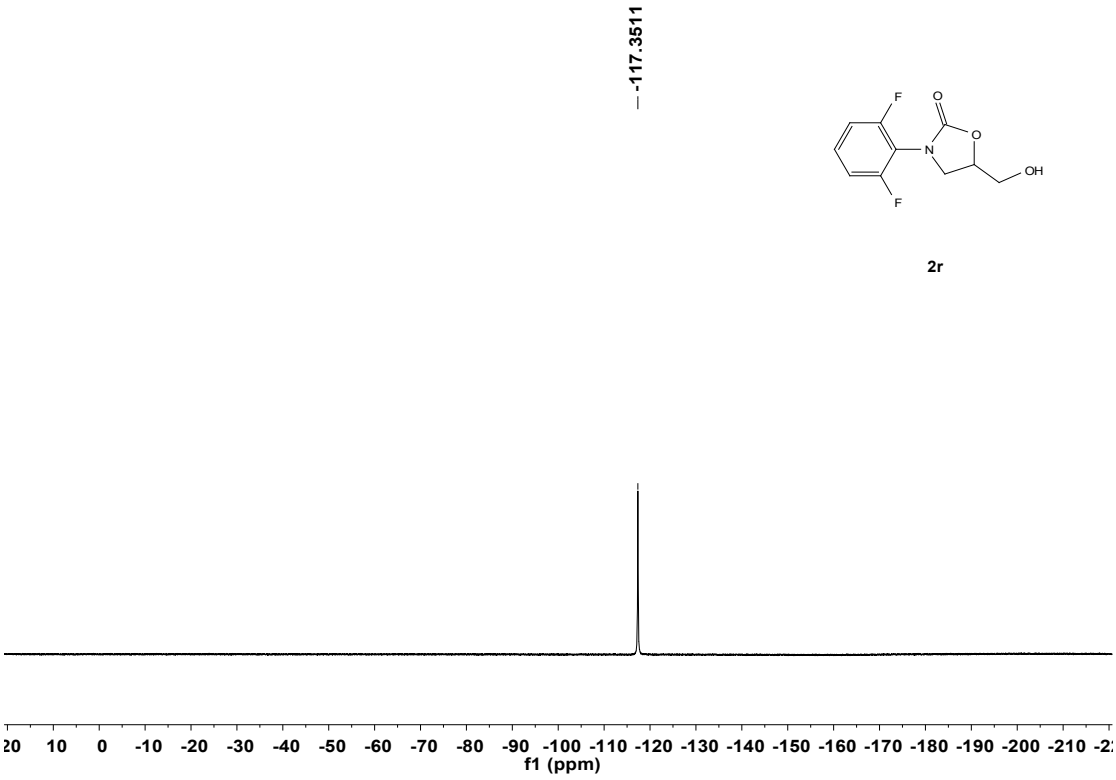
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **2q**



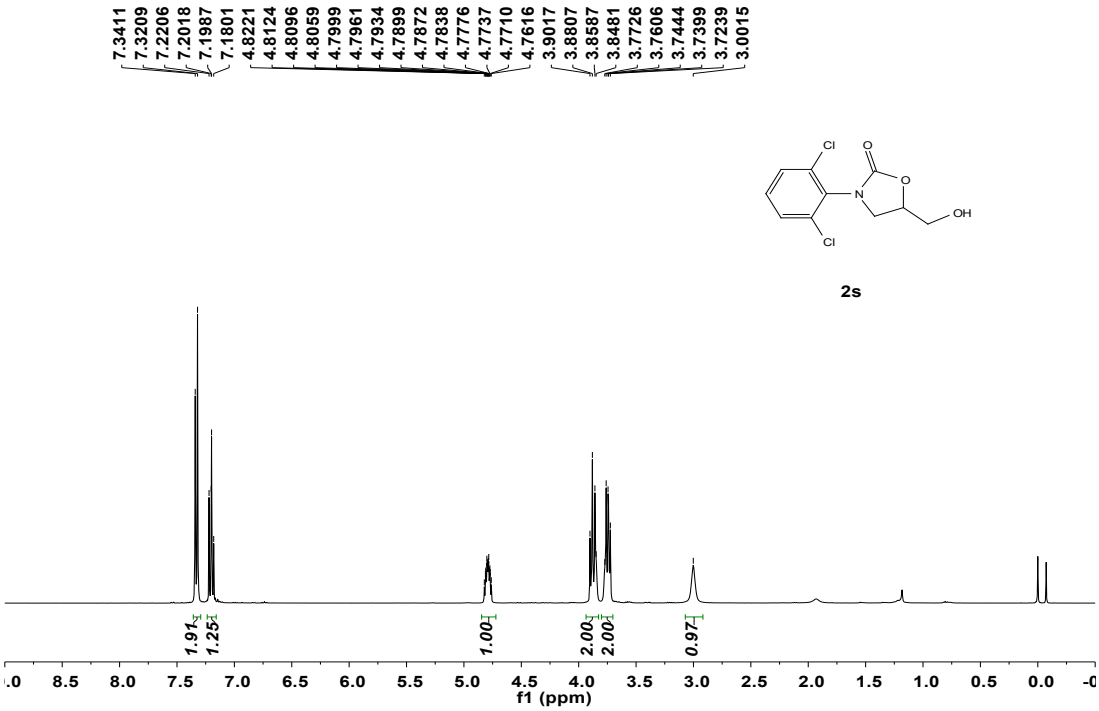
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **2r**



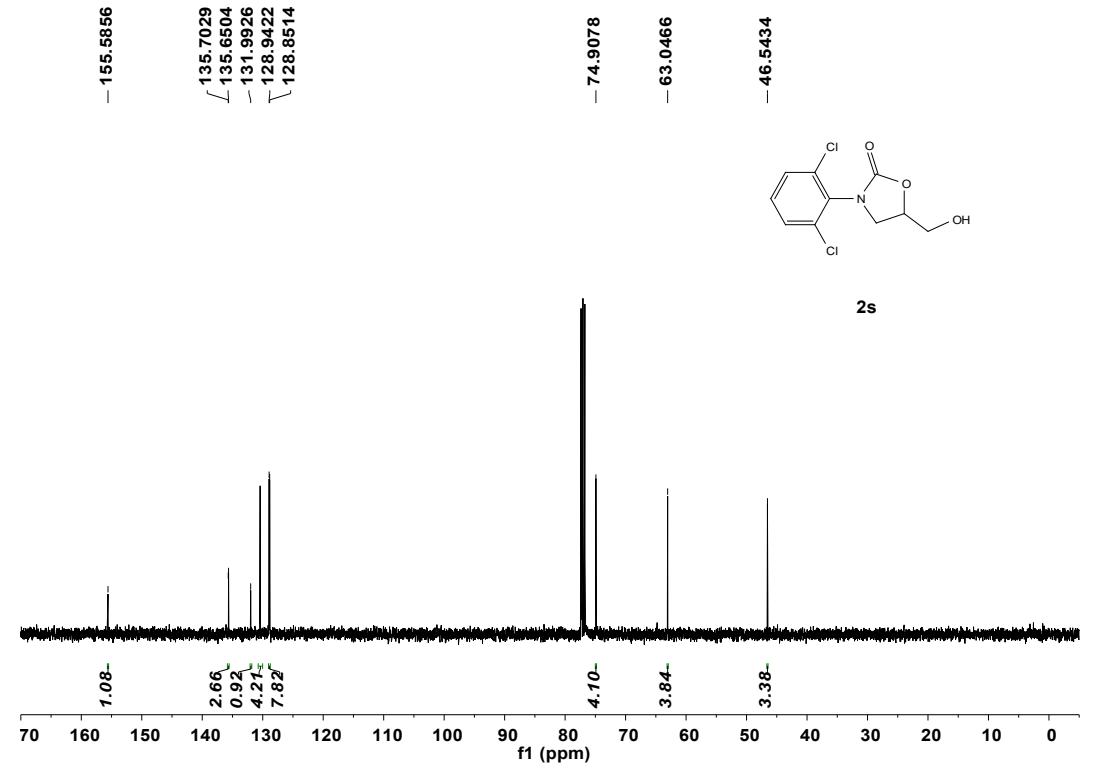
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **2r**



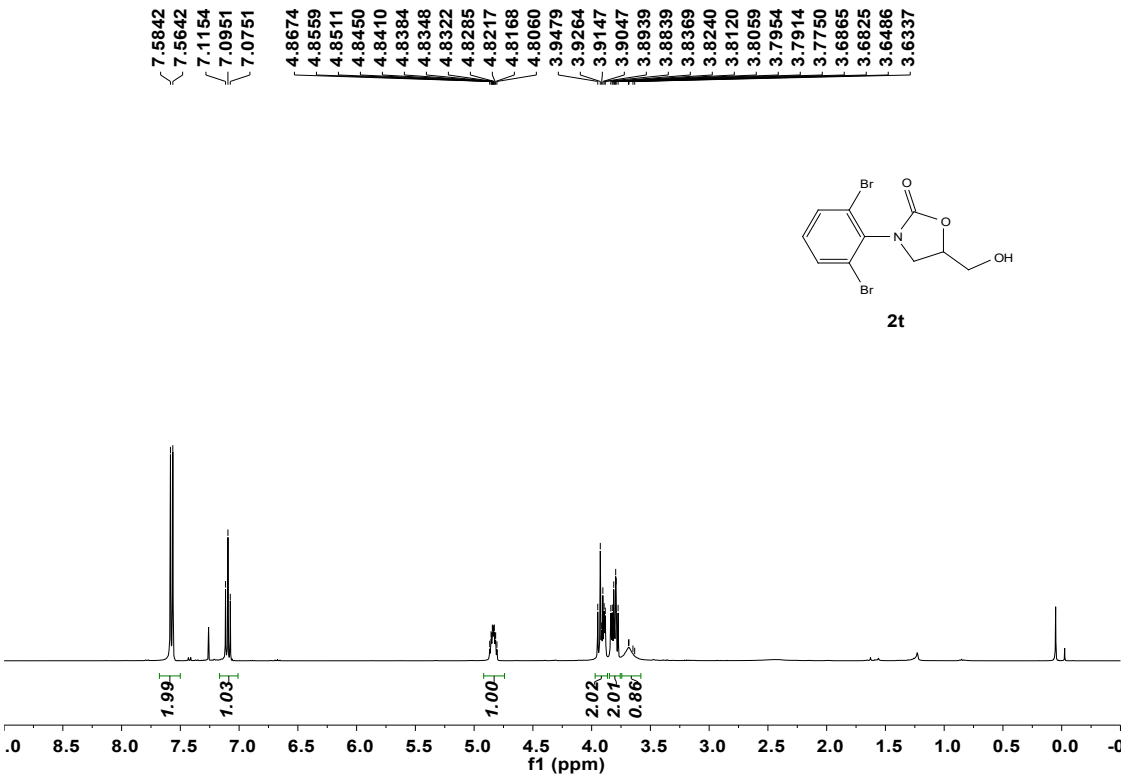
^{19}F NMR spectrum ($CDCl_3$, 376 MHz) of **2r**



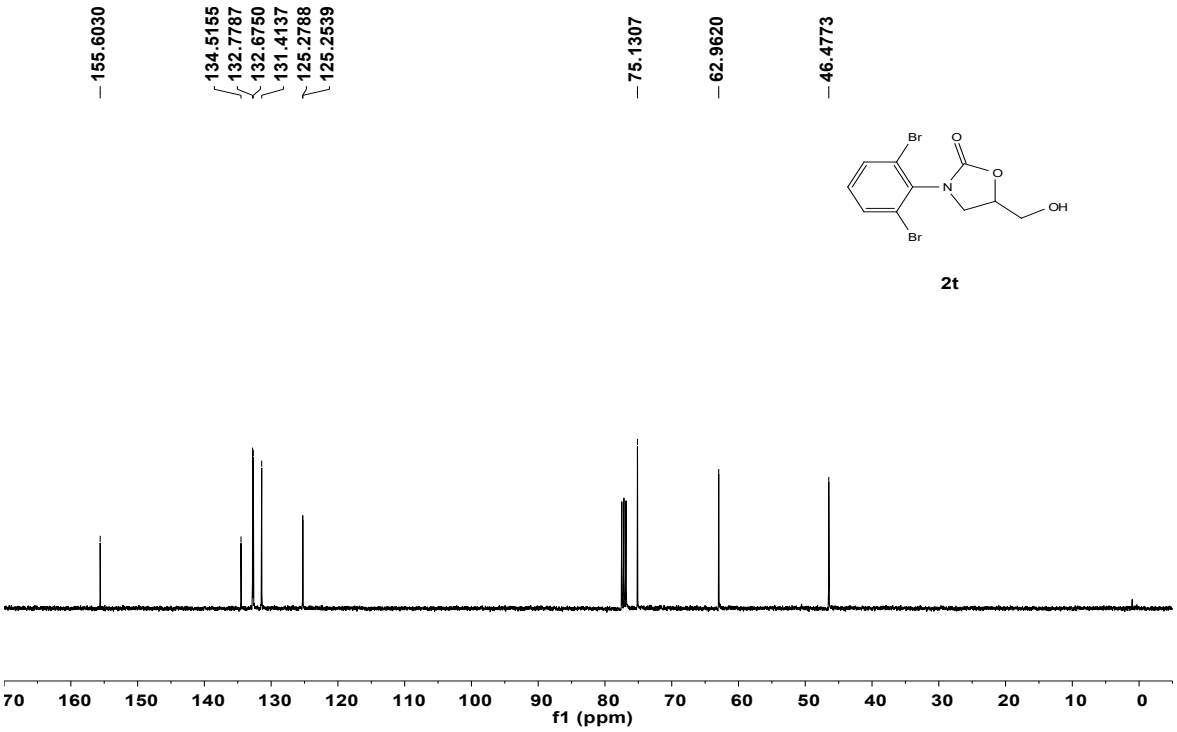
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **2s**



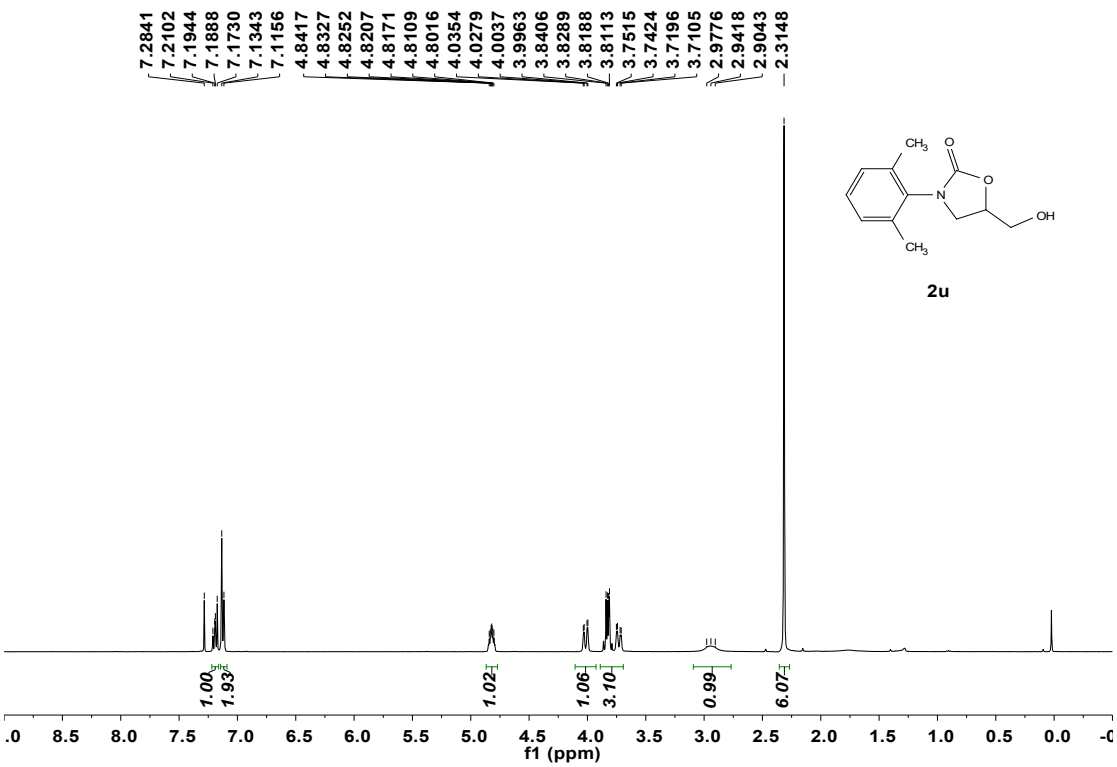
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **2s**



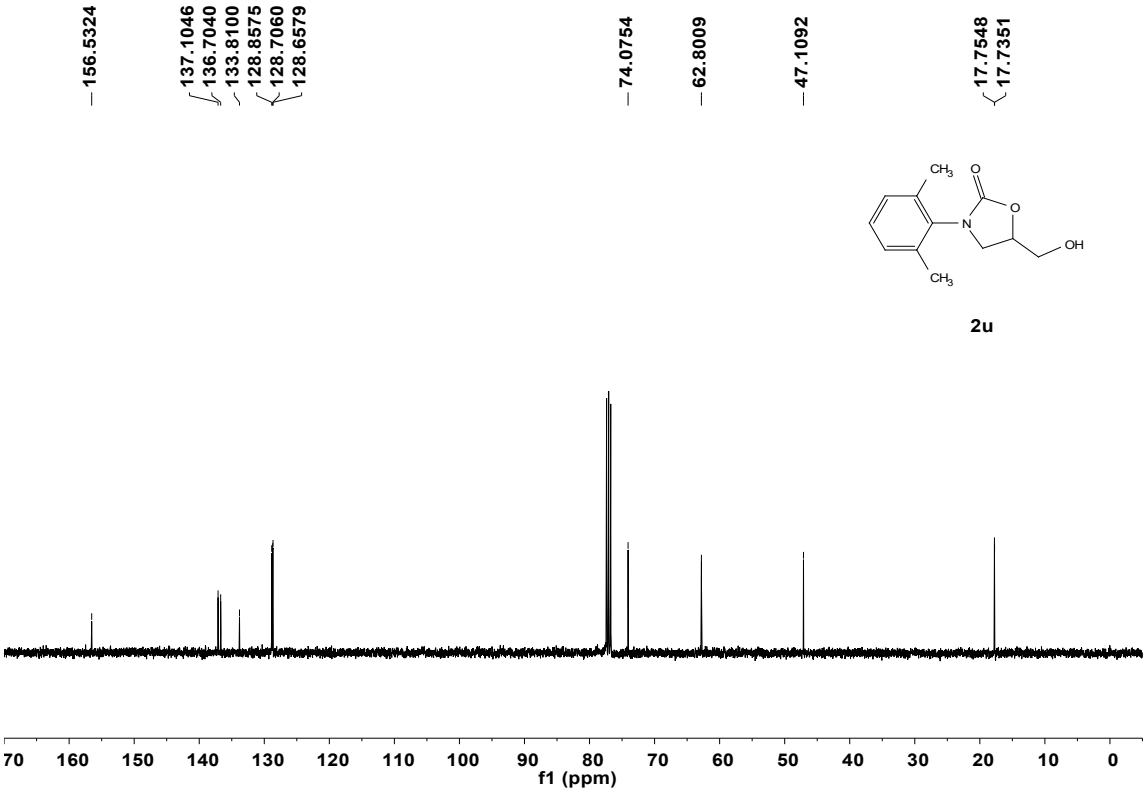
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **2t**



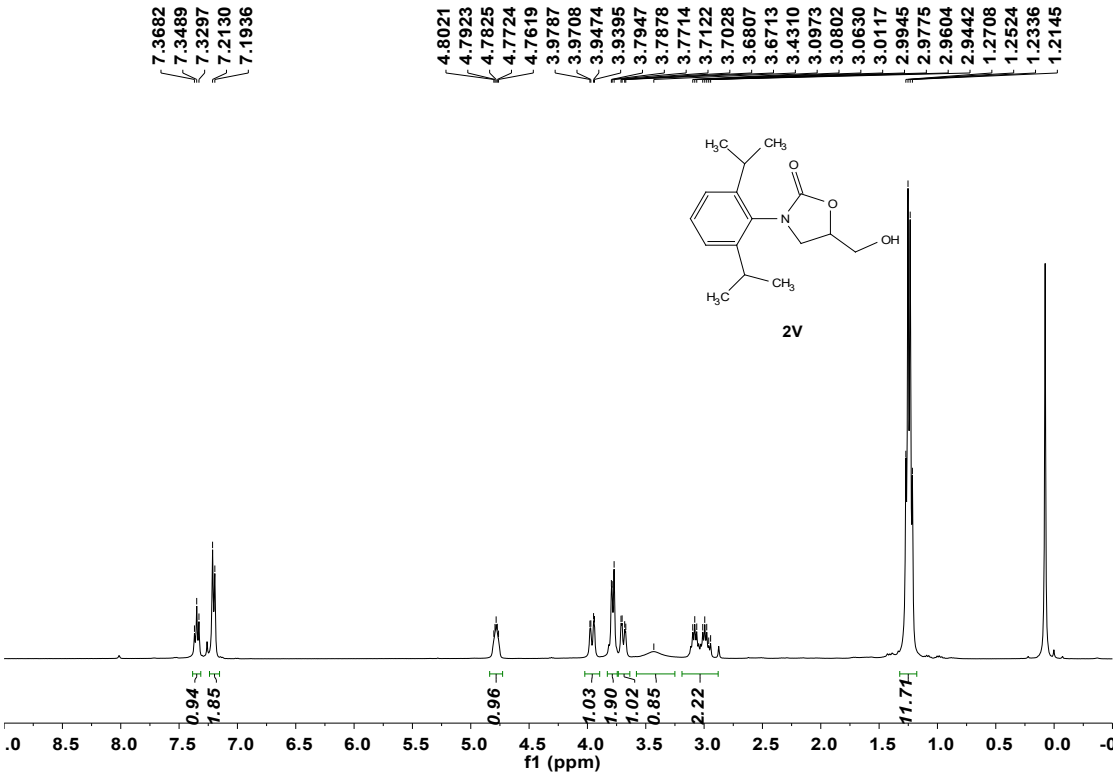
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **2t**



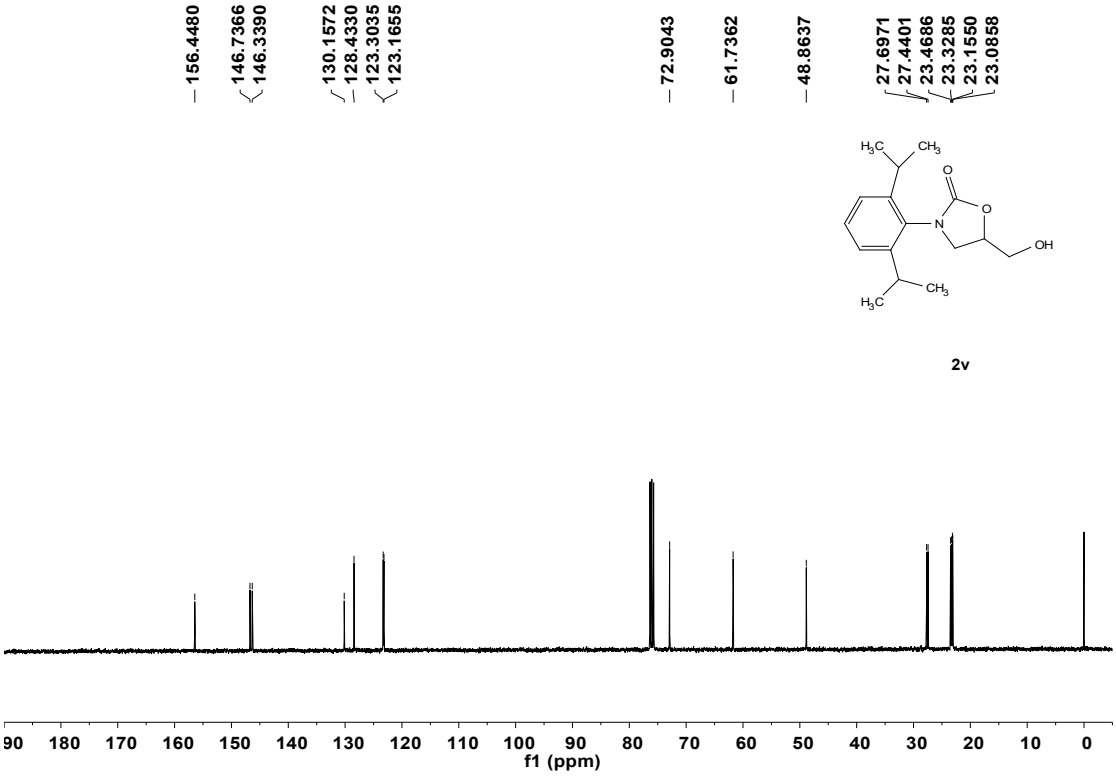
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **2u**



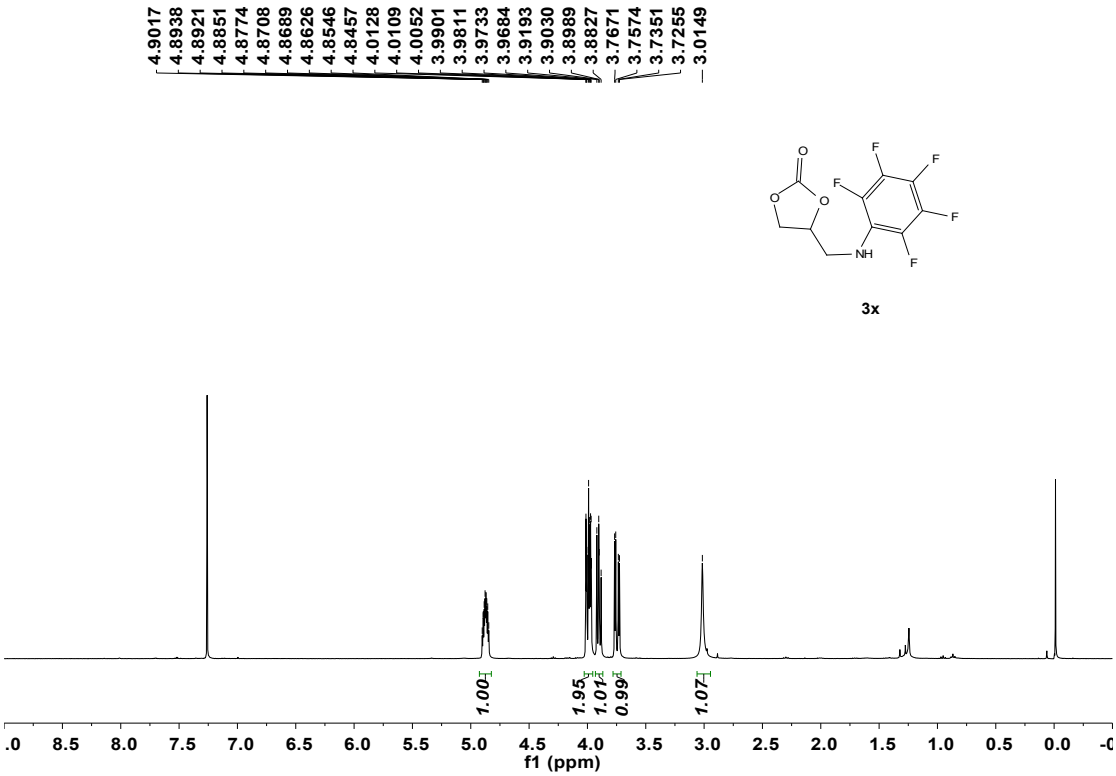
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **2u**



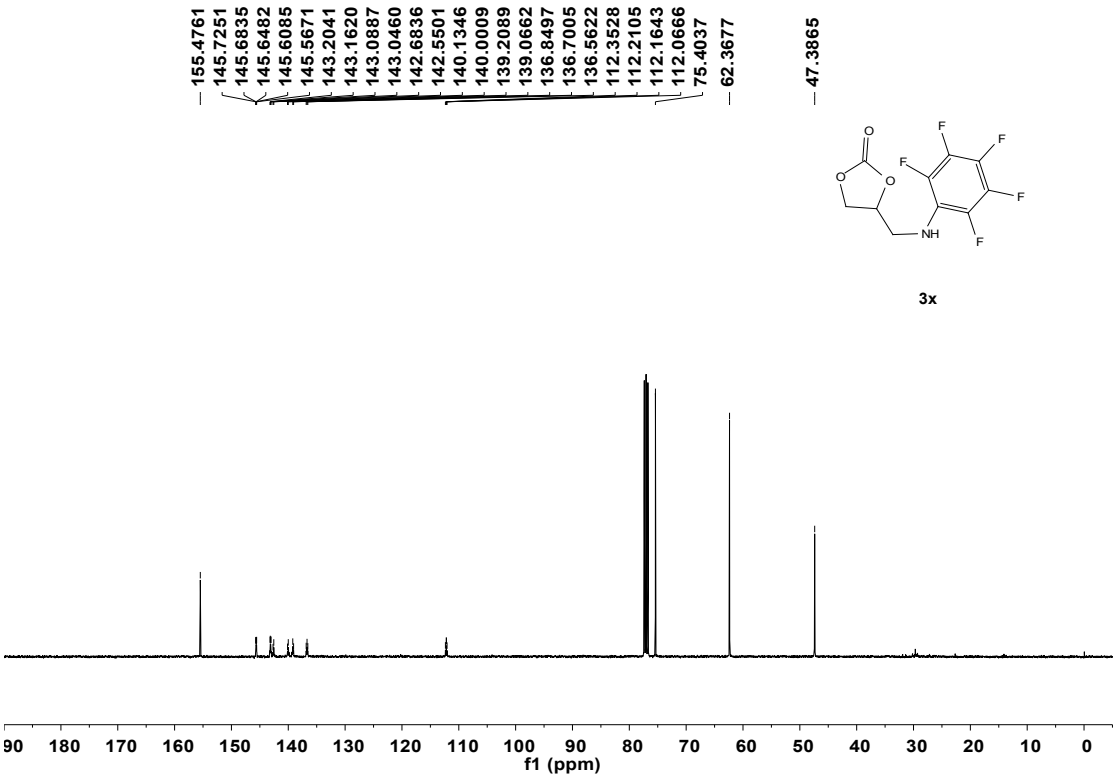
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **2v**



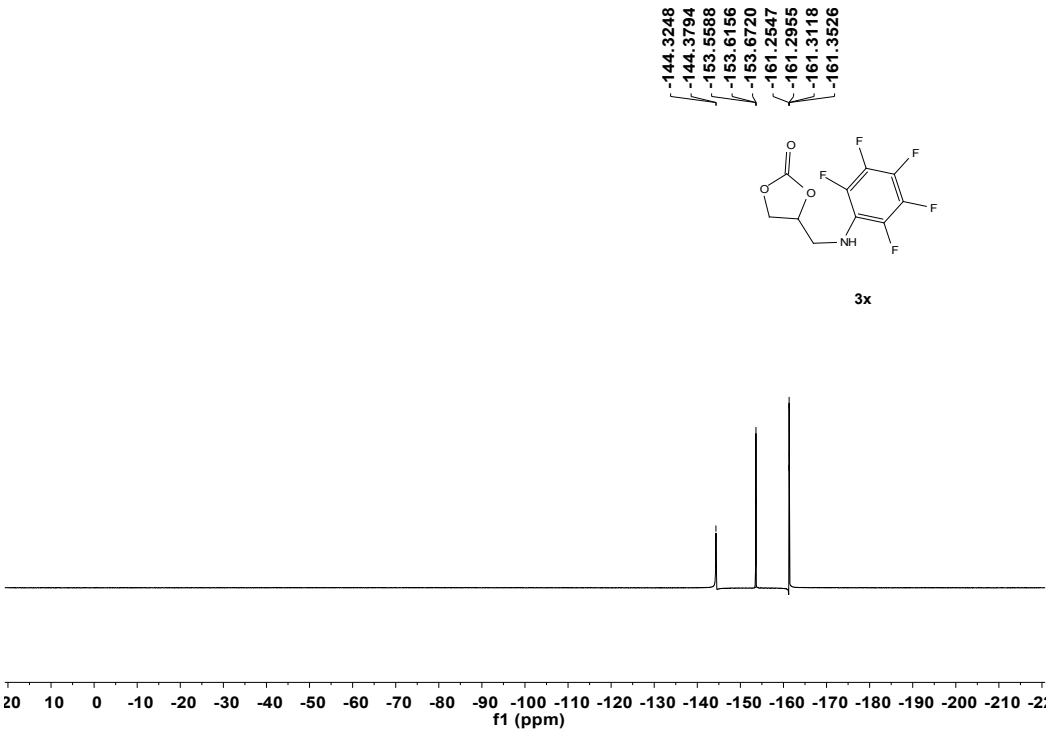
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **2v**



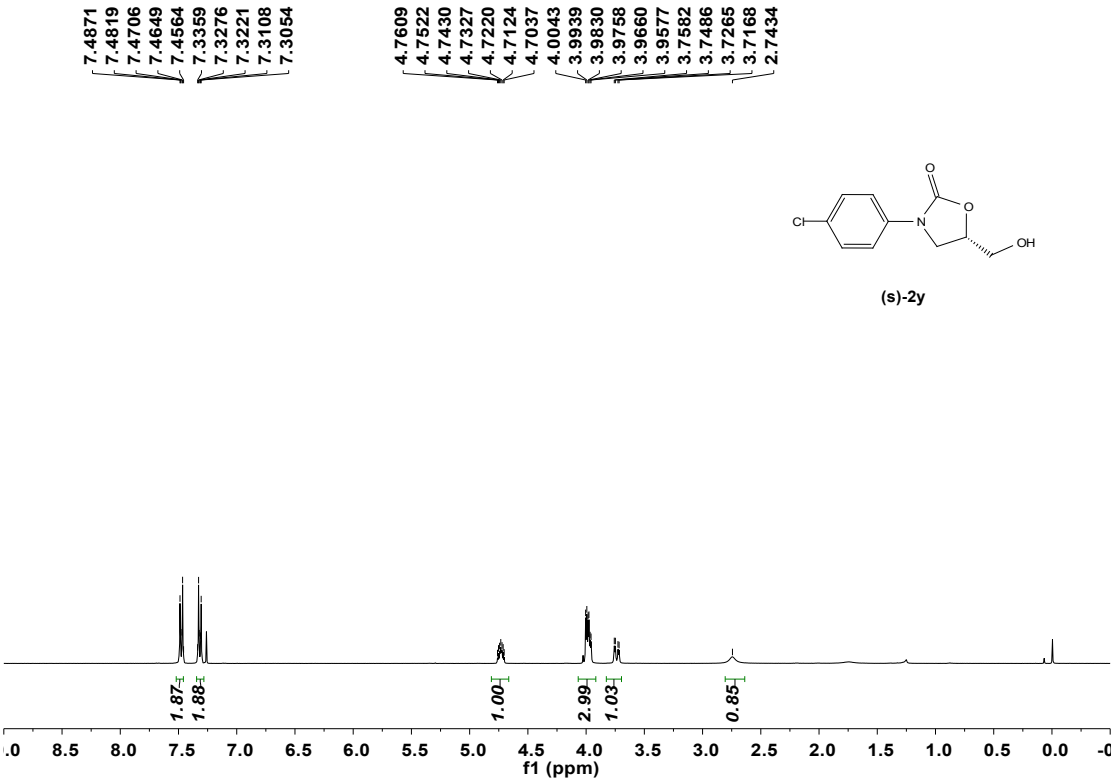
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **3x**



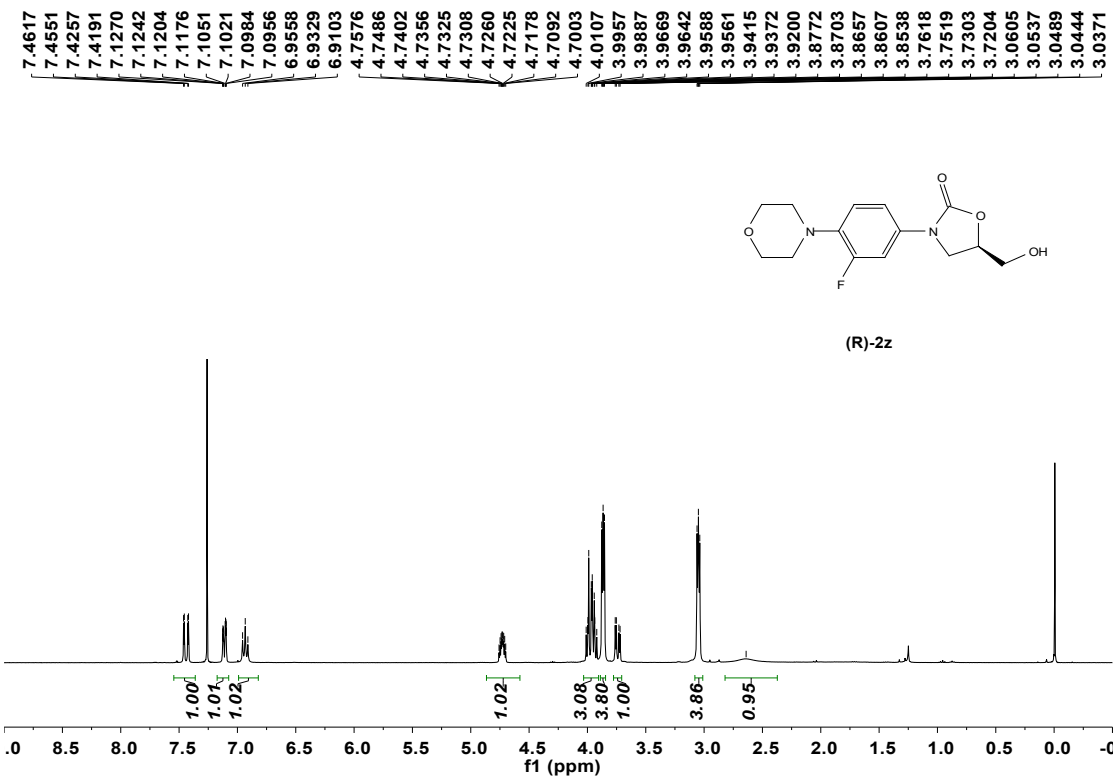
^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of **3x**



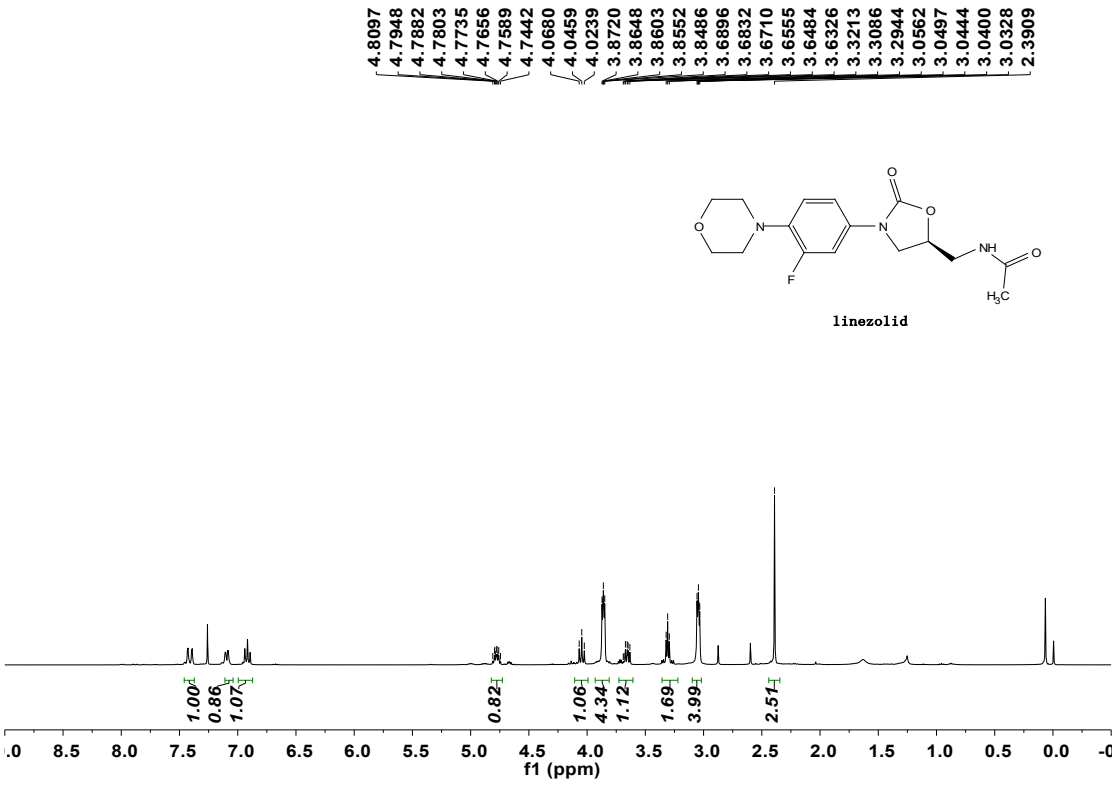
^{19}F NMR spectrum ($CDCl_3$, 376 MHz) of **3x**



^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of (*S*)-**2y**



^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of (*R*)-**2z**



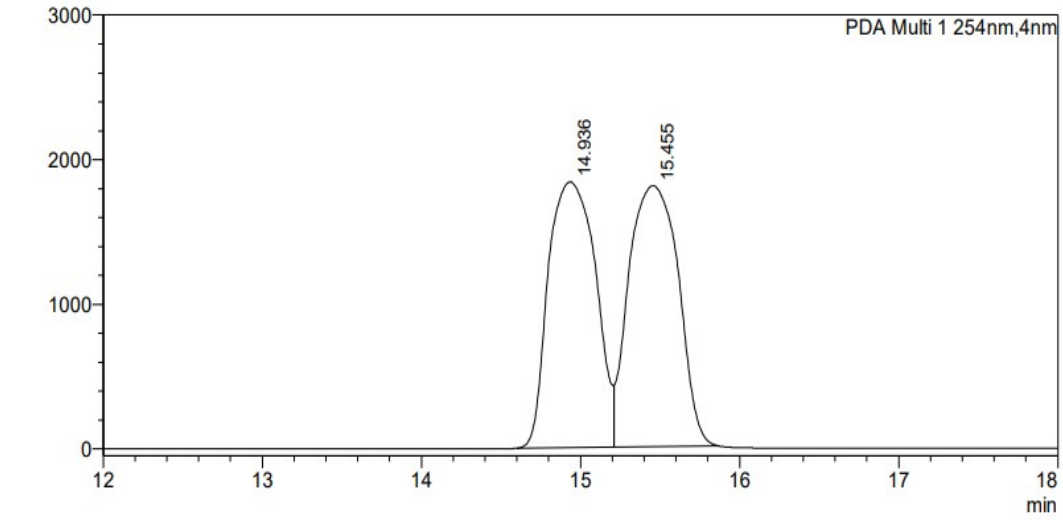
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of linezolid

9. HPLC spectra.

Fig. S18 HPLC spectra of compound **1y**

<Chromatogram>

(a) racemic compound 1y



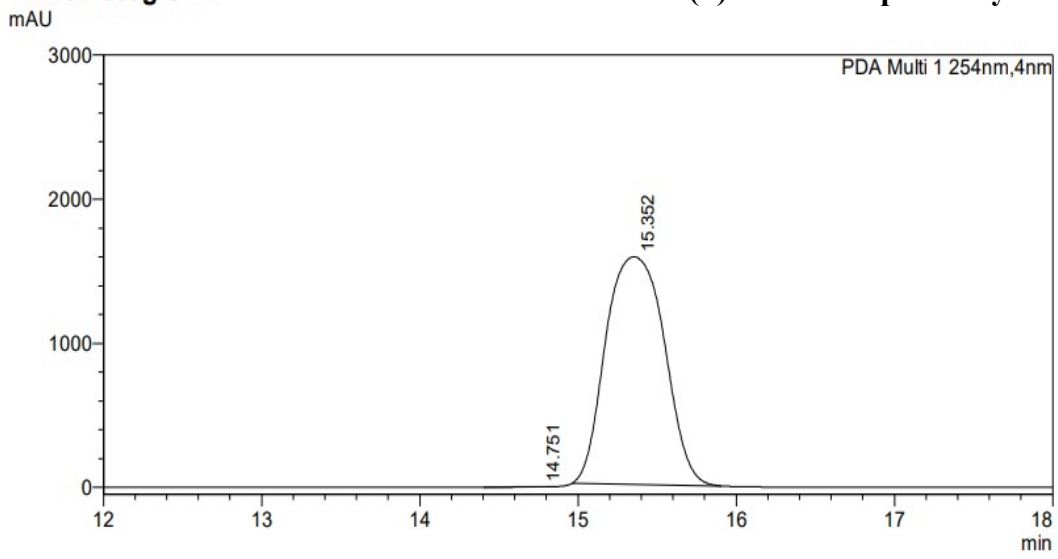
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Height%	Area	Area%
1	14.936	1838020	50.460	38183728	49.359
2	15.455	1804539	49.540	39175986	50.641
Total		3642559	100.000	77359713	100.000

<Chromatogram>

(b) chiral compound 1y



<Peak Table>

PDA Ch1 254nm

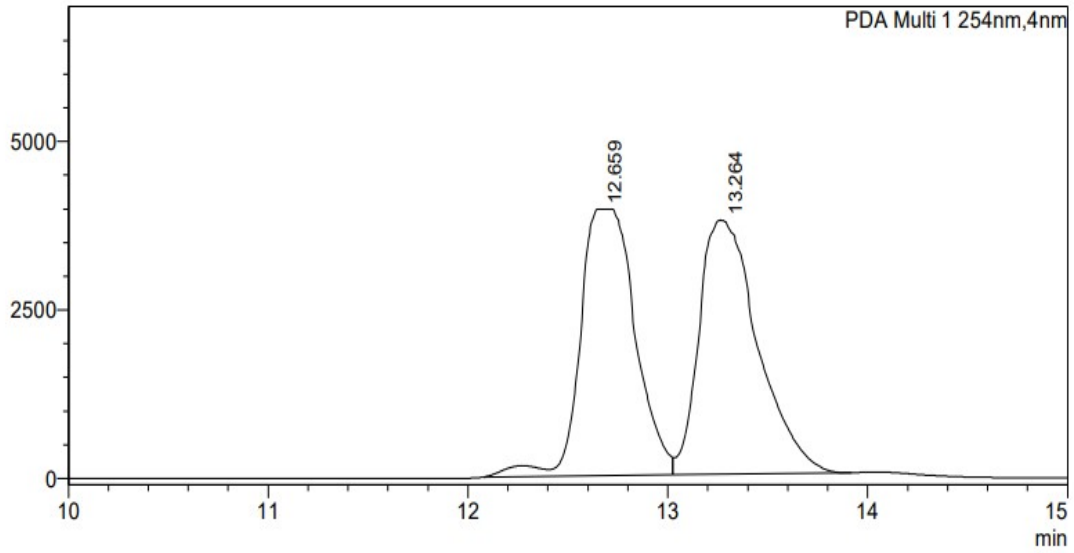
Peak#	Ret. Time	Height	Height%	Area	Area%
1	14.751	1915	0.121	20334	0.050
2	15.352	1577947	99.879	40781243	99.950
Total		1579862	100.000	40801578	100.000

Fig. S19 HPLC spectra of compound **1z**

<Chromatogram>

mAU

(a) racemic compound 1z



<Peak Table>

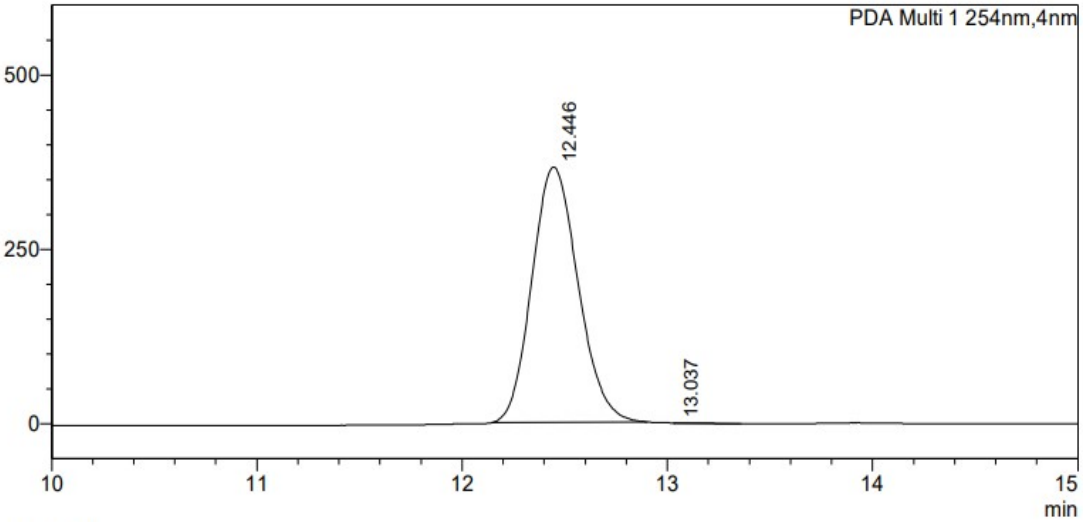
PDA Ch1 254nm

Peak#	Ret. Time	Height	Height%	Area	Area%
1	12.659	3959500	51.219	75687006	49.548
2	13.264	3771036	48.781	77069337	50.452
Total		7730537	100.000	152756344	100.000

<Chromatogram>

mAU

(b) chiral compound 1z



<Peak Table>

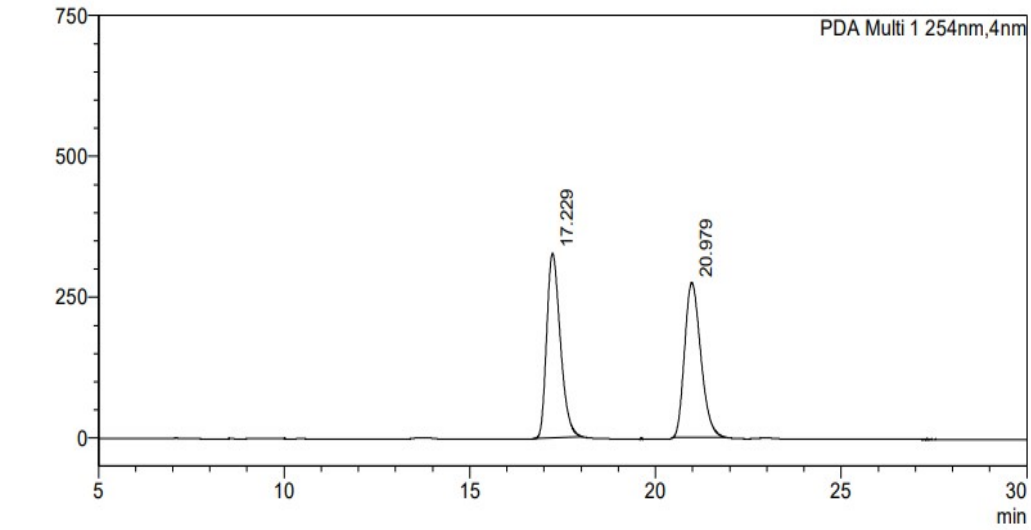
PDA Ch1 254nm

Peak#	Ret. Time	Height	Height%	Area	Area%
1	12.446	365583	99.997	5727033	99.979
2	13.037	9	0.003	1199	0.021
Total		365593	100.000	5728233	100.000

Fig. S20 HPLC spectra of compound **2y**

<Chromatogram>

(a) racemic compound 2y



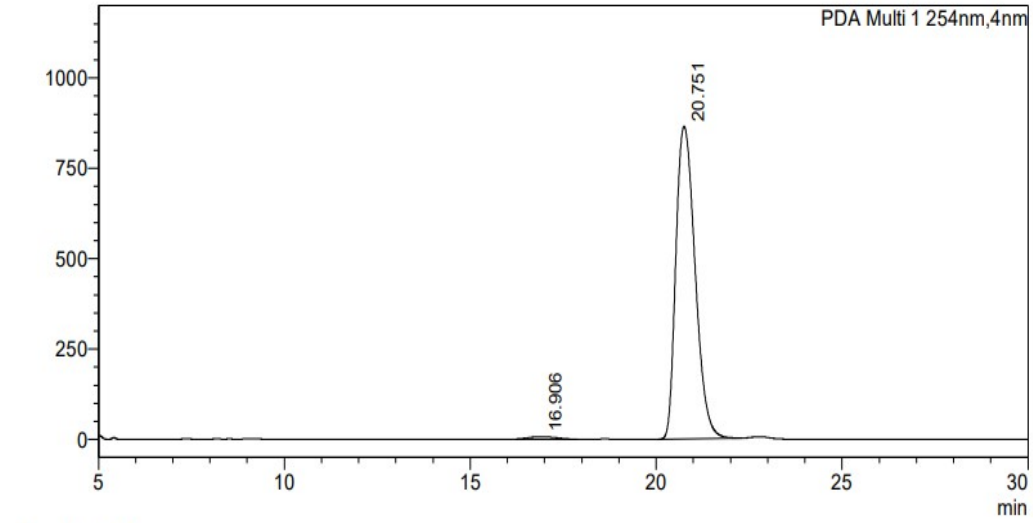
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Height%	Area	Area%
1	17.229	327600	54.428	8376278	50.194
2	20.979	274291	45.572	8311509	49.806
Total		601891	100.000	16687786	100.000

<Chromatogram>

(b) chiral compound 2y



<Peak Table>

PDA Ch1 254nm

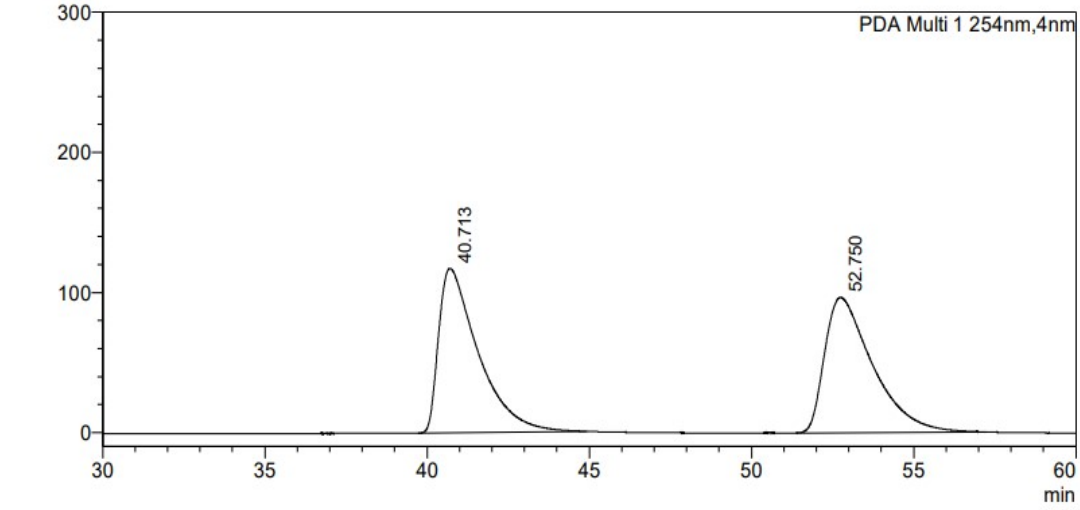
Peak#	Ret. Time	Height	Height%	Area	Area%
1	16.906	6481	0.744	325069	1.035
2	20.751	864709	99.256	31085854	98.965
Total		871190	100.000	31410923	100.000

Fig. S21 HPLC spectra of compound **2z**

<Chromatogram>

(a) racemic compound 2z

mAU



<Peak Table>

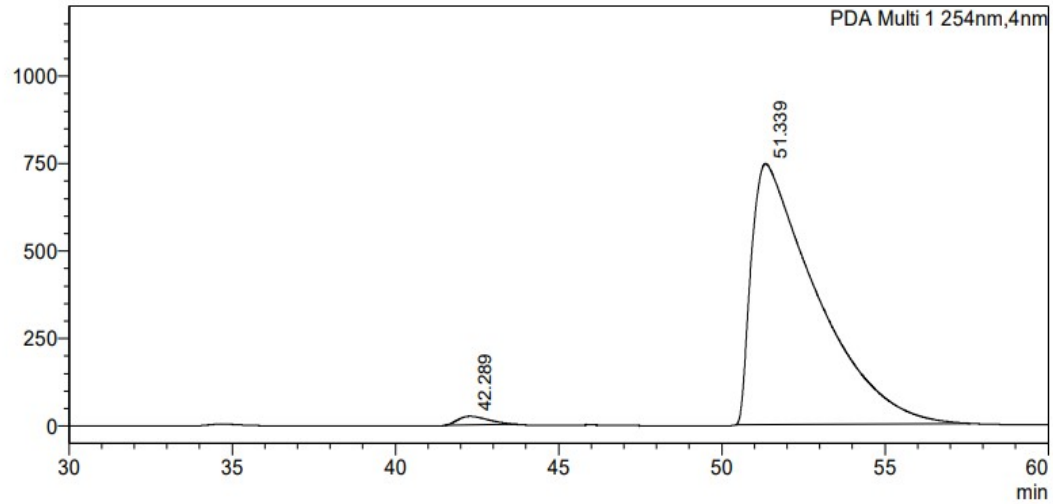
PDA Ch1 254nm

Peak#	Ret. Time	Height	Height%	Area	Area%
1	40.713	117346	54.876	9942096	50.039
2	52.750	96493	45.124	9926731	49.961
Total		213838	100.000	19868828	100.000

(b) chiral compound 2z

<Chromatogram>

mAU



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Height	Height%	Area	Area%
1	42.289	24961	3.238	1621601	1.537
2	51.339	745851	96.762	103872724	98.463
Total		770813	100.000	105494324	100.000

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