BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

The high potential of methyl laurate as a recyclable competitor to conventional toxic solvents in [3 + 2] cycloaddition reactions

Ayhan Yıldırım and Mustafa Göker

Beilstein J. Org. Chem. **2025,** *21,* 2389–2415. doi:10.3762/bjoc.21.184

Characterization data, copies of NMR spectra, additional Table and Figures

Table of contents

1. Characterization data S2–S14
2. References S14
3. ^{1}H NMR spectra S15–S35
4. ^{13}C NMR spectra S36–S56
5. Figure S1a–m) Results for the 13 other solvents calculated by *ChemFREE* S57–S69
6. Table S1. Polarizabilities of the solvents S70–S71
7. Figure S2. FTIR spectra of recovered methyl laurate S72
8. Figure S3. TLC plate of recovered methyl laurate S73
9. Figure S4. GC chromatogram and MS spectrum of methyl laurate S74

*2,3,5-Triphenyltetrahydro-4H-pyrrolo[3,4-d]isoxazole-4,6(5H)-dione (**3a**)*[1]

White solid, mp 149–150 °C; ^{1}H NMR (400 MHz, $CDCl_3$), mixture of *cis/trans*-diastereoisomers (*28/72*): δ 7.56 (*d*, *J* = 8 Hz, 2H, Ar), 7.47-7.31 (*m*, 15H, Ar), 7.26-7.22 (*m*, 4H, Ar), 7.15-7.11 (*m*, 4H, Ar), 7.05-6.96 (*m*, 3H, Ar), 6.64-6.60 (*m*, 2H, Ar), 5.75 (*s*, 1H, *trans*-H^3), 5.27 (*d*, *J* = 7.8 Hz, 1H, *cis*-H^3), 5.10 (*d*, *J* = 7.6 Hz, 1H, *trans*-H^{6a}), 4.94 (*d*, *J* = 9.2 Hz, 1H, *cis*-H^{6a}), 4.05 (*t*, *J* = 9.2 Hz, 1H, *cis*-H^{3a}), 4.00 (*d*, *J* = 7.5 Hz, 1H, *trans*-H^{3a}); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.11, 173.34, 172.58, 171.28, 148.89, 147.44, 138.68, 134.56, 131.19, 130.99, 129.40, 129.13, 129.04, 129.00, 128.90, 128.85, 128.76, 128.18, 127.61, 126.56, 126.17, 125.98, 124.80, 122.94, 118.79, 114.46, 71.54, 70.07, 57.36, 54.67.

*6-(4,6-Dioxo-2,3-diphenylhexahydro-5H-pyrrolo[3,4-d]isoxazol-5-yl)hexanoic acid (**3b**)*

Oily amber liquid; ^{1}H NMR (400 MHz, $CDCl_3$), mixture of *cis/trans*-diastereoisomers (*29/71*): δ 7.49 (*d*, *J* = 7.3 Hz, 2H, Ar), 7.37 (*t*, *J* = 7.8 Hz, 2H, Ar), 7.32-7.28 (*m*, 3H, Ar), 7.24-7.17 (*m*, 3H, Ar), 7.09-7.02 (*m*, 4H, Ar), 6.92 (*t*, *J* = 7.4 Hz, 1H, Ar), 5.54 (*s*, 1H, *trans*-H^3), 5.08 (*d*, *J* = 7.8 Hz, 1H, *cis*-H^3), 4.98 (*d*, *J* = 7.4 Hz, 1H, *trans*-H^{6a}), 4.81 (*d*, *J* = 9.2 Hz, 1H, *cis*-H^{6a}), 3.90 (*t*, *J* = 9.2 Hz, 1H, *cis*-H^{3a}), 3.83 (*d*, *J* = 7.4 Hz, 1H, *trans*-H^{3a}); 3.20 (*t*, *J* = 7.5 Hz, 2H, -NC$\underline{H}_2$-), 2.26 (*t*, *J* = 7.5 Hz, 2H, -C$\underline{H}_2$COOH), 1.61 (*quin*, *J* = 7.4 Hz, 2H, -CH_2), 1.51 (*quin*, *J* = 6.8 Hz, 2H, -CH_2), 1.29-1.04 (*m*, 6H, -CH_2-); ^{13}C NMR (101 MHz, $CDCl_3$) δ 179.11, 175.06, 174.39, 173.60, 172.38, 170.86, 148.46, 147.31, 138.68, 134.48, 134.08, 129.06, 128.92, 128.83, 128.78, 128.75, 128.10, 127.52, 126.65, 124.82, 122.81, 119.04, 114.50, 71.11, 69.70, 57.24, 54.59, 39.02, 38.78, 37.61, 33.72, 33.65, 33.58, 28.17, 27.17, 26.25, 26.20, 26.15, 26.03, 24.10.

*11-(4,6-Dioxo-2,3-diphenylhexahydro-5H-pyrrolo[3,4-d]isoxazol-5-yl)undecanoic acid (**3c**)*

Oily amber liquid; ^{1}H NMR (400 MHz, $CDCl_3$), mixture of *cis/trans*-diastereoisomers (*29/71*): δ 7.48 (*d*, *J* = 7.6 Hz, 2H, Ar), 7.37 (*t*, *J* = 7.9 Hz, 2H, Ar), 7.32-7.28 (*m*, 4H, Ar), 7.23-7.16 (*m*, 4H, Ar), 7.09-7.01 (*m*, 4H, Ar), 6.90 (*t*, *J* = 7.5 Hz, 1H, Ar), 5.52 (*s*, 1H, *trans*-H^3), 5.07 (*d*, *J* = 7.8 Hz, 1H, *cis*-H^3), 4.98 (*d*, *J* = 7.5 Hz, 1H, *trans*-H^{6a}), 4.79 (*d*, *J* = 9.2 Hz, 1H, *cis*-H^{6a}), 3.89 (*t*, *J* = 9.2 Hz, 1H, *cis*-H^{3a}), 3.82 (*d*, *J* = 7.4 Hz, 1H, *trans*-H^{3a}); 3.19 (*t*, *J* = 7.5 Hz, 2H, -NC$\underline{H}_2$-), 2.34 (*t*, *J* = 7.5 Hz, 4H, 2x -C$\underline{H}_2$COOH), 1.66-1.55 (*m*, 4H, 2x -CH_2-), 1.41-1.01 (*m*, 26H, 13x -CH_2-); ^{13}C NMR (101 MHz, $CDCl_3$) δ 179.47, 175.08, 174.46, 173.63, 172.42, 170.92, 148.40, 147.30, 138.68, 134.49, 134.04, 129.00, 128.90, 128.81, 128.74, 128.71, 128.08, 127.54, 126.69, 124.81, 122.77, 119.14, 114.58, 71.15, 69.73, 57.24, 54.60, 39.35, 39.13, 37.94, 33.97, 29.36, 29.31, 29.25, 29.16, 29.02, 28.51, 27.56, 26.79, 26.71, 26.64, 24.68.

*4-(4,6-Dioxo-2,3-diphenylhexahydro-5H-pyrrolo[3,4-d]isoxazol-5-yl)-N-dodecylbenzamide **(3d)***[2]

Yellowish solid, mp 146–147 °C; ^{1}H NMR (400 MHz, $CDCl_3$), mixture of *cis/trans*-diastereoisomers (*29/71*): δ 7.69 (*d*, *J* = 8.4 Hz, 2H, Ar), 7.56 (*d*, *J* = 7.8 Hz, 2H, Ar), 7.42 (*t*, *J* = 7.4 Hz, 3H, Ar), 7.38-7.34 (*m*, 3H, Ar), 7.23 (*t*, *J* = 7.5 Hz, 4H, Ar), 7.15-7.06 (*m*, 5H, Ar), 6.97 (*t*, *J* = 7.4 Hz, 3H, Ar), 6.69 (*d*, *J* = 8.4 Hz, 2H, Ar), 5.77 (*s*, 1H, *trans*-H^3), 5.29 (*d*, *J* = 7.8 Hz, 1H, *cis*-H^3), 5.12 (*d*, *J* = 7.5 Hz, 1H, *trans*-H^{6a}), 4.94 (*d*, *J* = 9.2 Hz, 1H, *cis*-H^{6a}), 4.07 (*t*, *J* = 8.8 Hz, 1H, *cis*-H^{3a}), 4.04 (*d*, *J* = 7.6 Hz, 1H, *trans*-H^{3a}), 3.45-3.39 (*m*, 4H, 2x -NHC$\underline{H}_2$-), 1.59 (*quin*, *J* = 7.3 Hz, 4H, 2x -NHCH$_2$C$\underline{H}_2$CH$_2$-), 1.36-1.26 (m, 36H, -CH_2-), 0.88 (*t*, *J* = 7 Hz, 6H, 2x -CH_3); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.82, 173.13, 172.28, 171.00, 169.04, 166.36, 148.82, 147.29, 138.50, 135.34,

135.07, 133.40, 129.42, 129.08, 129.02, 128.99, 128.87, 128.24, 127.68, 127.54, 126.52, 126.21, 125.91, 125.58, 124.92, 123.06, 118.85, 114.46, 71.57, 70.07, 57.37, 54.71, 40.23, 31.92, 29.65, 29.63, 29.60, 29.56, 29.47, 29.35, 29.33, 27.00, 22.69, 14.11.

*3-(4-Hydroxyphenyl)-2,5-diphenyltetrahydro-4H-pyrrolo[3,4-d]isoxazole-4,6(5H)-dione (**3e**)*[3]

Cream colored solid, mp 181–182 °C (dec); ^{1}H NMR (400 MHz, DMSO-d_6), mixture of *cis/trans*-diastereoisomers (*47/53*): δ 9.48 (*s*, 1H, Ar-OH), 9.47 (*s*, 1H, Ar-OH), 7.51-7.46 (*m*, 2H, Ar), 7.43-7.32 (*m*, 7H, Ar), 7.28-7.21 (*m*, 6H, Ar), 7.16-7.05 (*m*, 6H, Ar), 6.93 (*t*, *J* = 7.3 Hz, 1H, Ar), 6.77-6.71 (*m*, 4H, Ar), 6.67-6.65 (*m*, 2H, Ar), 5.68 (*s*, 1H, *trans*-H^3), 5.41 (*d*, *J* = 7.4 Hz, 1H, *cis*-H^3), 5.39 (*d*, *J* = 7.8 Hz, 1H, *trans*-H^{6a}), 4.87 (*d*, *J* = 9.2 Hz, 1H, *cis*-H^{6a}), 4.11 (*t*, *J* = 8.1 Hz, 1H, *cis*-H^{3a}), 4.05 (*d*, *J* = 7.4 Hz, 1H, *trans*-H^{3a}); ^{13}C NMR (101 MHz, DMSO-d_6) δ 174.63, 174.31, 173.38, 171.98, 157.22, 156.98, 148.89, 147.71, 131.54, 129.40, 128.95, 128.78, 128.66, 128.47, 128.37, 126.54, 126.40, 125.26, 124.48, 122.10, 119.13, 115.40, 115.20, 114.40, 77.66, 77.24, 70.46, 68.46, 56.54, 54.44.

*6-(3-(4-Hydroxyphenyl)-4,6-dioxo-2-phenylhexahydro-5H-pyrrolo[3,4-d]isoxazol-5-yl)hexanoic acid (**3f**)*

Sticky orange oil; ^{1}H NMR (400 MHz, $CDCl_3$), mixture of *cis/trans*-diastereoisomers (*9/91*): δ 7.32 (*d*, *J* = 8.7 Hz, 2H, Ar), 7.17 (*t*, *J* = 7.3 Hz, 2H, Ar), 7.00 (*d*, *J* = 7.8 Hz, 2H, Ar), 6.91 (*t*, *J* = 7.5 Hz, 2H, Ar), 6.81 (*d*, *J* = 8.5 Hz, 2H, Ar), 5.43 (*s*, 1H, *trans*-H^3), 5.10 (*d*, *J* = 7.9 Hz, 1H, *cis*-H^3), 4.99 (*d*, *J* = 7.4 Hz, 1H, *trans*-H^{6a}), 4.83 (*d*, *J* = 8.9 Hz, 1H, *cis*-H^{6a}), 3.87 (*t*, *J* = 8.7 Hz, 1H, *cis*-H^{3a}), 3.80 (*d*, *J* = 7.4 Hz, 1H, *trans*-H^{3a}), 3.24 (*t*, *J* = 6.6 Hz, 2H, -NCH_2), 2.26 (*t*, *J* = 7.4 Hz, 2H, -CH_2COOH), 1.64-1.12 (*m*,

12H, CH_2); ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.90, 173.79, 155.50, 148.21, 130.67, 128.99, 128.23, 122.80, 115.68, 114.79, 69.34, 57.21, 38.98, 33.34, 26.25, 25.91, 24.06.

*11-(3-(4-Hydroxyphenyl)-4,6-dioxo-2-phenylhexahydro-5H-pyrrolo[3,4-d]isoxazol-5-yl)undecanoic acid (**3g**)*

Sticky orange oil; ^1H NMR (400 MHz, $CDCl_3$), mixture of *cis/trans*-diastereoisomers (37*/63*): δ 7.31 (*d*, *J* = 8.6 Hz, 2H, Ar), 7.23-7.15 (*m*, 4H, Ar), 7.08-7.03 (*m*, 2H, Ar), 6.99 (*d*, *J* = 8.0 Hz, 2H, Ar), 6.89 (*t*, *J* = 7.4 Hz, 1H, Ar), 6.80 (*d*, *J* = 8.6 Hz, 2H, Ar), 6.74 (*d*, *J* = 8.7 Hz, 1H, Ar), 5.42 (*s*, 1H, *trans*-H^3), 5.06 (*d*, *J* = 7.6 Hz, 1H, *cis*-H^3), 4.99 (*d*, *J* = 7.4 Hz, 1H, *trans*-H^{6a}), 4.71 (*d*, *J* = 8.9 Hz, 1H, *cis*-H^{6a}), 3.86 (*t*, *J* = 8.9 Hz, 1H, *cis*-H^{3a}), 3.79 (*d*, *J* = 7.4 Hz, 1H, *trans*-H^{3a}), 3.21 (*t*, *J* = 6.5 Hz, 2H, -NCH_2), 2.35 (*t*, *J* = 7.4 Hz, 2H, -CH_2COOH), 1.62 (*quin*, *J* = 7.4 Hz, 2H, CH_2), 1.34-1.09 (*m*, 38H, CH_2); ^{13}C NMR (101 MHz, $CDCl_3$) δ 178.64, 175.30, 174.77, 173.80, 173.01, 156.10, 155.51, 148.17, 147.24, 132.38, 130.64, 128.95, 128.90, 128.70, 128.25, 125.98, 124.90, 122.79, 119.37, 115.95, 115.82, 115.68, 114.85, 70.92, 69.38, 57.21, 54.53, 51.46, 39.35, 39.25, 34.16, 33.82, 33.75, 31.91, 29.59, 29.45, 29.32, 29.25, 29.20, 29.16, 28.98, 28.81, 27.58, 26.75, 26.70, 26.60, 24.98, 24.67, 24.63, 22.68.

*N-Dodecyl-4-(3-(4-hydroxyphenyl)-4,6-dioxo-2-phenylhexahydro-5H-pyrrolo[3,4-d]isoxazol-5-yl)benzamide (**3h**)*

Orange solid, mp 149–150 °C (dec); ^1H NMR (400 MHz, $CDCl_3$), mixture of *cis/trans*-diastereoisomers (33*/67*): δ 7.65 (*t*, *J* = 8.3 Hz, 4H, Ar), 7.31 (*d*, *J* = 8.4 Hz, 2H, Ar), 7.22-7.17 (*m*, 6H, Ar), 7.09-7.05 (*m*, 6H, Ar), 6.93 (*t*, *J* = 7.6 Hz, 2H, Ar), 6.82-6.75 (*m*, 4H, Ar), 6.66 (*d*, *J* = 8.3 Hz, 2H, Ar), 6.54 (*t*, *J* = 5.1 Hz, 1H, NH), 6.31 (*t*, *J* = 5.9 Hz, 1H, NH), 5.63 (*s*, 1H, *trans*-H^3), 5.23 (*d*, *J* = 7.8 Hz, 1H, *cis*-H^3), 5.08 (*d*, *J* = 7.5 Hz,

1H, *trans*-H^{6a}), 4.82 (*d*, *J* = 9.0 Hz, 1H, *cis*-H^{6a}), 3.97 (*t*, *J* = 8.9 Hz, 1H, *cis*-H^{3a}), 3.95 (*d*, *J* = 7.5 Hz, 1H, *trans*-H^{3a}), 3.43-3.38 (*m*, 4H, 2x -NCH_2), 1.59 (*s*, 4H, 2x CH_2), 1.33-1.25 (*m*, 36H, CH_2), 0.87 (*t*, *J* = 7.0 Hz, 6H, 2x CH_3); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.16, 173.59, 172.61, 171.53, 167.07, 166.81, 156.80, 156.07, 148.71, 147.40, 135.10, 134.75, 133.68, 133.51, 130.09, 129.35, 128.83, 127.98, 127.79, 127.58, 126.30, 126.02, 125.60, 124.86, 123.01, 118.85, 116.14, 115.86, 114.62, 71.35, 69.72, 57.30, 54.72, 40.43, 31.92, 29.64, 29.60, 29.57, 29.52, 29.35, 27.03, 27.00, 22.69, 14.11.

*3-(2-Hydroxyphenyl)-2,5-diphenyltetrahydro-4H-pyrrolo[3,4-d]isoxazole-4,6(5H)-dione (**3i**)*[3]

Yellow solid, mp 186–187 °C (dec); ^{1}H NMR (400 MHz, DMSO-d_6), mixture of *cis/trans*-diastereoisomers (*34/66*): δ 8.06 (*s*, 1H, Ar-OH), 7.97 (*s*, 1H, Ar-OH), 7.52-7.42 (*m*, 4H, Ar), 7.39-7.15 (*m*, 18H, Ar), 7.07-7.03 (*m*, 1H, Ar), 6.98-6.94 (*m*, 1H, Ar), 6.92-6.85 (*m*, 2H, Ar), 6.65-6.62 (*m*, 2H, Ar), 5.91 (*s*, 1H, *trans*-H^3), 5.31 (*d*, *J* = 7.9 Hz, 1H, *cis*-H^3), 5.13 (*d*, *J* = 7.6 Hz, 1H, *trans*-H^{6a}), 4.96 (*d*, *J* = 9.2 Hz, 1H, *cis*-H^{6a}), 4.16 (*t*, *J* = 9.2 Hz, 1H, *cis*-H^{3a}), 4.15 (*d*, *J* = 7.6 Hz, 1H, *trans*-H^{3a}); ^{13}C NMR (101 MHz, DMSO-d_6) δ 174.28, 173.25, 172.07, 171.14, 155.20, 153.99, 150.21, 148.28, 145.94, 130.89, 130.52, 129.69, 129.51, 129.42, 129.18, 129.07, 129.01, 128.90, 128.84, 127.90, 126.55, 126.31, 126.11, 123.88, 123.18, 121.93, 121.00, 120.82, 120.25, 117.43, 116.77, 115.29, 68.16, 56.49, 53.52.

*6-(3-(2-Hydroxyphenyl)-4,6-dioxo-2-phenylhexahydro-5H-pyrrolo[3,4-d]isoxazol-5-yl)hexanoic acid (**3j**)*

Yellowish solid, mp 156–157 °C (dec); ^{1}H NMR (400 MHz, $CDCl_3$), mixture of *cis/trans*-diastereoisomers (*16/84*): δ 7.40 (*d*, *J* = 7.8 Hz, 1H, Ar), 7.24-7.21 (*m*, 3H, Ar), 7.11 (*d*, *J* = 7.6 Hz, 2H, Ar), 6.98 (*t*, *J* = 7.3 Hz, 1H, Ar), 6.94-6.89 (*m*, 2H, Ar), 5.70 (*s*, 1H, *trans*-H^3), 5.11 (*d*, *J* = 7.7 Hz, 1H, *cis*-H^3), 4.99 (*d*, *J* = 7.4 Hz, 1H, *trans*-H^{6a}), 4.89 (*d*, *J* = 9.4 Hz, 1H, *cis*-H^{6a}), 4.01 (*t*, *J* = 8.9 Hz, 1H, *cis*-H^{3a}), 3.96 (*d*, *J* = 7.5 Hz, 1H, *trans*-H^{3a}), 3.21 (t, *J* = 7.4 Hz, 2H, NCH_2), 2.26 (*t*, *J* = 7.4 Hz, 2H, -CH_2COOH), 1.65-1.09 (*m*, 6H, CH_2); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.85, 164.93, 154.04, 147.86, 134.08, 129.67, 129.18, 129.01, 128.03, 123.97, 120.80, 120.19, 116.91, 115.53, 70.34, 68.26, 56.57, 40.78, 38.98, 33.22, 29.69, 28.16, 26.28, 25.96, 24.04.

*11-(3-(2-Hydroxyphenyl)-4,6-dioxo-2-phenylhexahydro-5H-pyrrolo[3,4-d]isoxazol-5-yl)undecanoic acid (**3k**)*

Amber sticky oil; ^{1}H NMR (400 MHz, $CDCl_3$), mixture of *cis/trans*-diastereoisomers (*20/80*): δ 7.41 (*d*, *J* = 7.9 Hz, 1H, Ar), 7.24-7.17 (*m*, 3H, Ar), 7.10 (*d*, *J* = 8.3 Hz, 2H, Ar), 6.97-6.89 (*m*, 3H, Ar), 5.73 (*s*, 1H, *trans*-H^3), 5.09 (*d*, *J* = 7.7 Hz, 1H, *cis*-H^3), 4.98 (*d*, *J* = 7.4 Hz, 1H, *trans*-H^{6a}), 4.93 (*d*, *J* = 9.3 Hz, 1H, *cis*-H^{6a}), 4.03 (*t*, *J* = 9.3 Hz, 1H, *cis*-H^{3a}), 3.96 (*d*, *J* = 7.5 Hz, 1H, *trans*-H^{3a}), 3.18 (t, *J* = 7.3 Hz, 2H, NCH_2), 2.34 (*t*, *J* = 7.6 Hz, 2H, -CH_2COOH), 1.64-1.59 (*m*, 4H, CH_2), 1.26-1.08 (*m*, 26H, CH_2); ^{13}C NMR (101 MHz, $CDCl_3$) δ 179.38, 175.82, 174.48, 173.27, 172.96, 171.34, 154.86, 153.99, 148.20, 146.22, 134.06, 130.02, 129.48, 129.15, 128.91, 128.35, 127.81, 126.05, 123.82, 123.55, 120.69, 120.54, 120.18, 116.81, 116.40, 115.09, 67.34, 60.48, 56.43, 53.12, 39.46, 39.36, 37.96, 33.97, 31.90, 29.35, 29.27, 29.21, 29.14, 28.99, 28.50, 27.33, 26.83, 26.70, 26.62, 24.68, 21.04.

*N-Dodecyl-4-(3-(2-hydroxyphenyl)-4,6-dioxo-2-phenylhexahydro-5H-pyrrolo[3,4-d]isoxazol-5-yl)benzamide (**3l**)*

Yellowish solid, mp 182–183 °C (dec); ^{1}H NMR (400 MHz, DMSO-d_6), mixture of *cis/trans*-diastereoisomers (*33/67*): δ 10.06 (*s*, 2H, Ar-OH), 8.47 (*s*, 2H, C(O)NH), 7.94-7.77 (*m*, 4H, Ar), 7.40-6.85 (*m*, 20H, Ar), 6.64-6.62 (*m*, 2H, Ar), 5.93 (*s*, 1H, *trans*-H^3), 5.41 (*d*, *J* = 7.9 Hz, 1H, *cis*-H^3), 5.33 (*d*, *J* = 7.5 Hz, 1H, *trans*-H^{6a}), 5.08 (*d*, *J* = 8.9 Hz, 1H, *cis*-H^{6a}), 4.19 (*t*, *J* = 8.8 Hz, 1H, *cis*-H^{3a}), 4.13 (*d*, *J* = 7.6 Hz, 1H, *trans*-H^{3a}), 3.35 (*s*, 4H, 2x -NHC$\underline{H}_2$-), 1.50 (*s*, 4H, 2x -NHCH$_2$C$\underline{H}_2$CH$_2$-), 1.28-1.24 (m, 36H, -CH$_2$-), 0.85 (*t*, *J* = 7.2 Hz, 6H, 2x -CH$_3$); ^{13}C NMR (101 MHz, DMSO-d_6) δ 174.49, 173.09, 171.63, 165.31, 165.23, 154.84, 154.49, 149.72, 147.40, 134.86, 134.66, 133.95, 133.59, 129.17, 128.69, 127.76, 127.55, 127.16, 126.16, 126.04, 125.23, 124.71, 122.11, 121.44, 119.49, 119.07, 115.21, 113.70, 78.04, 77.13, 64.44, 62.61, 55.48, 52.86, 31.29, 29.04, 29.00, 28.77, 28.70, 26.46, 22.08, 13.92.

*3-(4-(Dimethylamino)phenyl)-2,5-diphenyltetrahydro-4H-pyrrolo[3,4-d]isoxazole-4,6(5H)-dione **(3m)***[4]

Beige solid, mp 176–177 °C (dec); ^{1}H NMR (400 MHz, $CDCl_3$), mixture of *cis/trans*-diastereoisomers (*40/60*): δ 7.42-7.32 (*m*, 8H, Ar), 7.27-7.21 (*m*, 6H, Ar), 7.13-7.09 (*m*, 6H, Ar), 7.04 (*t*, *J* = 7.3 Hz, 1H, Ar), 6.96 (*t*, *J* = 7.3 Hz, 1H, Ar), 6.73 (*d*, *J* = 8.8 Hz, 2H, Ar), 6.68-6.64 (*m*, 4H, Ar), 5.65 (*s*, 1H, *trans*-H^3), 5.24 (*d*, *J* = 7.8 Hz, 1H, *cis*-H^3), 5.12 (*d*, *J* = 7.5 Hz, 1H, *trans*-H^{6a}), 4.83 (*d*, *J* = 9.2 Hz, 1H, *cis*-H^{6a}), 4.05 (*t*, *J* = 9.2 Hz, 1H, *cis*-H^{3a}), 3.98 (*d*, *J* = 7.5 Hz, 1H, *trans*-H^{3a}), 2.96 (*s*, 6H, 2x -C$\underline{H}_3$), 2.93 (*s*, 6H, 2x -C$\underline{H}_3$); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.39, 173.78, 172.86, 171.66, 150.65, 150.35, 148.98, 147.83, 131.38, 131.09, 129.27, 129.08, 128.98, 128.91, 128.72, 128.65,

128.42, 127.49, 126.22, 126.12, 126.04, 124.52, 122.69, 121.20, 118.85, 114.65, 112.57, 112.50, 71.68, 69.91, 57.33, 54.70, 40.50, 40.33.

*6-(3-(4-(Dimethylamino)phenyl)-4,6-dioxo-2-phenylhexahydro-5H-pyrrolo[3,4-d]isoxazol-5-yl)hexanoic acid (**3n**)*

Orange sticky liquid; ^{1}H NMR (400 MHz, $CDCl_3$), mixture of *cis/trans*-diastereoisomers (*43/57*): δ 7.30 (*d*, *J* = 8.9 Hz, 2H, Ar), 7.22-7.23 (*m*, 6H, Ar), 7.08 (*d*, *J* = 7.6 Hz, 2H, Ar), 7.04-7.00 (*m*, 3H, Ar), 6.89 (*t*, *J* = 7.3 Hz, 1H, Ar), 6.70-6.63 (*m*, 4H, Ar), 5.42 (*s*, 1H, *trans*-H^3), 5.05 (*d*, *J* = 7.8 Hz, 1H, *cis*-H^3), 4.98 (*d*, *J* = 7.4 Hz, 1H, *trans*-H^{6a}), 4.72 (*d*, *J* = 8.9 Hz, 1H, *cis*-H^{6a}), 3.84 (*d*, *J* = 7.6 Hz, 1H, *trans*-H^{3a}), 3.81 (*t*, *J* = 8.9 Hz, 1H, *cis*-H^{3a}), 3.22 (*t*, *J* = 6.6 Hz, 2H, -NCH_2-), 2.93 (*s*, 6H, 2x -C$\underline{H}_3$), 2.92 (*s*, 6H, 2x -C$\underline{H}_3$), 2.31 (*t*, *J* = 7.5 Hz, 2H, -C$\underline{H}_2$COOH), 2.26 (*t*, *J* = 7.5 Hz, 2H, -C$\underline{H}_2$COOH), 1.65-1.48 (*m*, 6H, CH_2), 1.34-1.26 (*m*, 6H, CH_2); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.82, 173.13, 172.28, 171.00, 169.04, 166.36, 148.82, 147.29, 138.50, 135.34, 129.42, 129.02, 128.87, 128.24, 127.68, 127.54, 126.52, 126.21, 125.91, 123.06, 118.85, 114.46, 71.57, 70.07, 57.37, 54.71, 40.23, 31.92, 29.65, 29.63, 29.60, 29.56, 29.35, 29.33, 27.00, 22.69, 14.11.

*11-(3-(4-(Dimethylamino)phenyl)-4,6-dioxo-2-phenylhexahydro-5H-pyrrolo[3,4-d]isoxazol-5-yl)undecanoic acid (**3o**)*

Orange sticky liquid; ^{1}H NMR (400 MHz, $CDCl_3$), mixture of *cis/trans*-diastereoisomers (*31/69*): δ 7.30 (*d*, *J* = 8.8 Hz, 2H, Ar), 7.21-7.12 (*m*, 5H, Ar), 7.09-7.04 (*m*, 2H, Ar), 6.88 (*t*, *J* = 7.5 Hz, 1H, Ar), 6.69 (*d*, *J* = 8.8 Hz, 2H, Ar), 6.63 (*d*, *J* = 8.8 Hz, 1H, Ar), 5.52 (*s*, 1H, *trans*-H^3), 5.04 (*d*, *J* = 7.6 Hz, 1H, *cis*-H^3), 4.98 (*d*, *J* = 7.4 Hz, 1H, *trans*-H^{6a}), 4.68 (*d*, *J* = 9.0 Hz, 1H, *cis*-H^{6a}), 3.83 (*d*, *J* = 7.6 Hz, 1H, *trans*-H^{3a}), 3.79 (*t*, *J* = 9.0 Hz, 1H, *cis*-H^{3a}), 3.23-3.19 (*m*, 2H, -NCH_2-), 2.93 (*s*, 12H, 4x -C$\underline{H}_3$); 2.36-2.32 (*m*,

4H, 2x -C<u>H</u>$_2$COOH), 1.66-1.58 (*m*, 4H, CH_2), 1.28-1.09 (*m*, 28H, CH_2); ^{13}C NMR (101 MHz, $CDCl_3$) δ 179.36, 175.39, 174.85, 173.90, 172.77, 150.44, 150.25, 148.44, 147.72, 128.87, 128.62, 128.35, 127.66, 126.11, 124.51, 122.53, 121.24, 119.12, 114.86, 112.59, 112.31, 71.29, 69.55, 57.22, 54.55, 40.51, 40.29, 39.27, 39.10, 33.97, 29.35, 29.31, 29.26, 29.17, 29.11, 29.02, 27.63, 26.85, 26.74, 26.65, 24.69.

*4-(3-(4-(Dimethylamino)phenyl)-4,6-dioxo-2-phenylhexahydro-5H-pyrrolo[3,4-d]isoxazol-5-yl)-N-dodecylbenzamide (**3p**)*

Yellow solid, mp 147–148 °C (dec); ^{1}H NMR (400 MHz, $CDCl_3$), mixture of *cis/trans*-diastereoisomers (*29/71*): δ 7.74 (*d*, *J* = 8.5 Hz, 3H, Ar), 7.67 (*d*, *J* = 8.5 Hz, 2H, Ar), 7.37 (*d*, *J* = 8.8 Hz, 3H, Ar), 7.23-7.10 (*m*, 11H, Ar), 6.74-6.69 (*m*, 4H, Ar), 6.64 (*d*, *J* = 8.8 Hz, 3H, Ar), 6.25 (*t*, *J* = 5.6 Hz, 1H, NH), 6.20 (*t*, *J* = 5.6 Hz, 1H, NH), 5.65 (*s*, 1H, *trans*-H^3), 5.24 (*d*, *J* = 7.8 Hz, 1H, *cis*-H^3), 5.11 (*d*, *J* = 7.5 Hz, 1H, *trans*-H^{6a}), 4.79 (*d*, *J* = 9.0 Hz, 1H, *cis*-H^{6a}), 3.99 (*d*, *J* = 7.5 Hz, 1H, *trans*-H^{3a}), 3.97 (*t*, *J* = 9.0 Hz, 1H, *cis*-H^{3a}), 3.44-3.38 (*m*, 4H, 2x -NCH_2-), 2.96 (*s*, 6H, 2x -C<u>H</u>$_3$), 2.92 (*s*, 6H, 2x -C<u>H</u>$_3$), 1.61-1.56 (*m*, 6H, CH_2), 1.37-1.21 (*m*, 32H, CH_2), 0.88 (*t*, *J* = 7.0 Hz, 6H, 2x CH_3); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.13, 173.65, 172.59, 171.42, 166.51, 166.42, 150.65, 150.36, 148.91, 147.69, 135.23, 134.95, 133.80, 133.50, 129.29, 128.73, 128.34, 127.67, 127.53, 127.47, 126.23, 126.03, 124.63, 122.80, 120.96, 118.94, 114.65, 112.57, 112.44, 71.71, 69.93, 57.32, 54.77, 40.49, 40.29, 40.24, 31.93, 29.66, 29.64, 29.61, 29.58, 29.35, 27.03, 22.69, 14.11.

*3-(4-((11-Hydroxyundecyl)oxy)phenyl)-2,5-diphenyltetrahydro-4H-pyrrolo[3,4-d]isoxazole-4,6(5H)-dione (**3q**)*[2]

White solid, mp 84–85 °C; ^{1}H NMR (400 MHz, $CDCl_3$), mixture of *cis/trans*-diastereoisomers (*40/60*): δ 7.45-7.32 (*m*, 11H, Ar), 7.26-7.22 (*m*, 5H, Ar), 7.14-7.05 (*m*, 6H, Ar), 6.97 (*t*, *J* = 8.8 Hz, 1H, Ar), 6.91 (*d*, *J* = 8.8 Hz, 2H, Ar), 6.87 (*d*, *J* = 8.6 Hz, 1H, Ar), 6.65-6.63 (*m*, 2H, Ar), 5.68 (*s*, 1H, *trans*-H^3), 5.26 (*d*, *J* = 7.9 Hz, 1H, *cis*-H^3), 5.12 (*d*, *J* = 7.5 Hz, 1H, *trans*-H^{6a}), 4.87 (*d*, *J* = 9.2 Hz, 1H, *cis*-H^{6a}), 4.02 (*t*, *J* = 9.2 Hz, 1H, *cis*-H^{3a}), 3.97 (*d*, *J* = 7.5 Hz, 1H, *trans*-H^{3a}), 3.94-3.90 (*m*, 4H, 2x -C$\underline{H}_2$OAr), 3.63 (*t*, *J* = 6.6 Hz, 4H, 2x -C$\underline{H}_2$OH), 1.81-1.72 (*m*, 4H, 2x -C$\underline{H}_2$-), 1.56 (*quin*, *J* = 6.5 Hz, 6H, 3x -C$\underline{H}_2$-), 1.47-1.42 (m, 6H, 3x -C$\underline{H}_2$-), 1.32-1.26 (m, 20H, 10x -C$\underline{H}_2$-); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.21, 173.56, 172.67, 171.49, 159.50, 159.03, 148.81, 147.49, 131.25, 131.01, 130.42, 129.33, 129.14, 129.00, 128.96, 128.77, 128.74, 127.80, 126.18, 126.00, 125.96, 124.76, 122.87, 118.95, 114.95, 114.88, 114.59, 71.30, 69.73, 68.16, 68.00, 63.09, 57.37, 54.63, 32.83, 29.58, 29.53, 29.50, 29.42, 29.37, 29.24, 26.06, 26.03, 25.76.

6-(3-(4-((11-Hydroxyundecyl)oxy)phenyl)-4,6-dioxo-2-phenylhexahydro-5H-pyrrolo[3,4-d]isoxazol-5-yl)hexanoic acid (***3r**)*

Amber sticky liquid, ^{1}H NMR (400 MHz, $CDCl_3$), mixture of *cis/trans*-diastereoisomers (*42/58*): δ 7.37-7.34 (*m*, 2H, Ar), 7.23-7.16 (m, 6H, Ar), 7.08-7.00 (m, 4H, Ar), 6.92-6.82 (m, 6H, Ar), 5.45 (*s*, 1H, *trans*-H^3), 5.07 (*d*, *J* = 7.6 Hz, 1H, *cis*-H^3), 4.99 (*d*, *J* = 7.4 Hz, 1H, *trans*-H^{6a}), 4.74 (*d*, *J* = 9.0 Hz, 1H, *cis*-H^{6a}), 3.93 (*t*, *J* = 6.9 Hz, 2H, -CH_2OAr), 3.85 (*t*, *J* = 9.2 Hz, 1H, *cis*-H^{3a}), 3.79 (*d*, *J* = 7.4 Hz, 1H, *trans*-H^{3a}), 3.66 (*t*, *J* = 2.1 Hz, 1H, -OH), 3.64 (*t*, *J* = 6.6 Hz, 2H, -CH_2OH), 3.22 (*t*, *J* = 6.5 Hz, 2H, -NCH_2), 2.32 (*t*, *J* = 7.5 Hz, 2H, -CH_2COOH), 2.26 (*t*, *J* = 7.5 Hz, 2H, -CH_2COOH), 1.76 (*quin*,

J = 6.3 Hz, 4H, CH_2), 1.63-1.07 (*m*, 44H, CH_2); ^{13}C NMR (101 MHz, $CDCl_3$) δ 178.36, 178.09, 175.17, 174.56, 173.70, 172.55, 159.36, 158.94, 148.35, 147.43, 130.39, 128.99, 128.72, 128.65, 127.91, 125.90, 124.75, 122.73, 119.09, 114.80, 114.71, 70.90, 69.36, 68.11, 67.95, 63.07, 57.24, 54.52, 51.43, 38.99, 38.79, 34.15, 33.61, 33.52, 32.75, 32.67, 31.91, 29.60, 29.56, 29.52, 29.48, 29.40, 29.34, 29.25, 29.22, 29.16, 27.25, 26.31, 26.27, 26.04, 25.74, 25.68, 24.98, 24.13, 22.68.

*11-(3-(4-((11-Hydroxyundecyl)oxy)phenyl)-4,6-dioxo-2-phenylhexahydro-5H-pyrrolo[3,4-d]isoxazol-5-yl)undecanoic acid (**3s**)*

Yellowish sticky liquid, ^{1}H NMR (400 MHz, $CDCl_3$), mixture of *cis/trans*-diastereoisomers (*37/63*): δ 7.35 (*d*, *J* = 8.6 Hz, 2H, Ar), 7.23-7.15 (m, 4H, Ar), 7.08-6.99 (m, 4H, Ar), 6.91-6.81 (m, 4H, Ar), 5.43 (*s*, 1H, *trans*-H^3), 5.06 (*d*, *J* = 7.6 Hz, 1H, *cis*-H^3), 4.99 (*d*, *J* = 7.4 Hz, 1H, *trans*-H^{6a}), 4.73 (*d*, *J* = 9.1 Hz, 1H, *cis*-H^{6a}), 3.93 (*t*, *J* = 7.4 Hz, 2H, -CH_2OAr), 3.85 (*t*, *J* = 9.2 Hz, 1H, *cis*-H^{3a}), 3.79 (*d*, *J* = 7.4 Hz, 1H, *trans*-H^{3a}), 3.65 (*t*, *J* = 2.1 Hz, 1H, -OH), 3.64 (*t*, 2H, *J* = 6.6 Hz, -CH_2OH), 3.22-3.19 (*m*, 2H, -NCH_2), 2.35-2.28 (m, 4H 2x -CH_2COOH), 1.76 (*quin*, *J* = 7.3 Hz, 4H, CH_2), 1.64-1.08 (*m*, 56H, CH_2); ^{13}C NMR (101 MHz, $CDCl_3$) δ 178.89, 178.67, 175.20, 174.60, 173.73, 172.59, 159.33, 158.93, 148.29, 147.45, 130.39, 128.93, 128.69, 127.96, 125.92, 124.72, 122.70, 119.12, 114.78, 114.69, 70.93, 69.39, 68.10, 67.93, 63.05, 57.23, 54.52, 39.31, 39.12, 33.94, 32.75, 29.60, 29.56, 29.52, 29.48, 29.41, 29.38, 29.35, 29.31, 29.25, 29.22, 29.20, 29.16, 29.08, 29.05, 29.02, 27.62, 26.84, 26.71, 26.63, 26.08, 26.01, 25.74, 24.98, 24.70.

*N-Dodecyl-4-(3-(4-((11-hydroxyundecyl)oxy)phenyl)-4,6-dioxo-2-phenylhexahydro-5H-pyrrolo[3,4-d]isoxazol-5-yl)benzamide (**3t**)*[2]

Yellowish solid, mp 108–109 °C; ^{1}H NMR (400 MHz, $CDCl_3$), mixture of *cis/trans*-diastereoisomers (*44/56*): δ 7.77-775 (*m*, 2H, Ar), 7.69-7.67 (m, 2H, Ar), 7.44-7.42 (m, 3H, Ar), 7.31-7.29 (m, 3H, Ar), 7.25-7.16 (m, 4H, Ar), 7.12-7.05 (m, 4H, Ar), 6.97-6.96 (m, 2H, Ar), 6.92-6.90 (m, 2H, Ar), 6.86-6.84 (m, 2H, Ar), 6.71-6.69 (m, 2H, Ar), 6.25 (*t*, *J* = 5.5 Hz, 1H, NH), 6.19 (*t*, *J* = 5.8 Hz, 1H, NH), 5.69 (*s*, 1H, *trans*-H^3), 5.25 (*d*, *J* = 7.8 Hz, 1H, *cis*-H^3), 5.11 (*d*, *J* = 7.5 Hz, 1H, *trans*-H^{6a}), 4.82 (*d*, *J* = 9.0 Hz, 1H, *cis*-H^{6a}), 4.00 (*t*, *J* = 9.0 Hz, 1H, *cis*-H^{3a}), 3.99 (*d*, *J* = 7.5 Hz, 1H, *trans*-H^{3a}), 3.95 (*t*, *J* = 6.5 Hz, 2H, -CH_2OAr), 3.90 (*t*, *J* = 6.5 Hz, 2H, -CH_2OAr), 3.67-3.61 (*m*, 6H, 2x –OH, 2x -CH_2OH), 3.41 (*quin*, *J* = 5.5 Hz, 4H, 2x -NCH_2), 1.80-1.26 (*m*, 76H, CH_2), 0.88 (*t*, *J* = 7.0 Hz, 6H, 2x CH_3); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.95, 173.47, 172.42, 171.25, 166.40, 159.56, 159.06, 148.75, 147.30, 138.64, 135.29, 135.03, 133.43, 130.24, 129.35, 128.77, 128.66, 127.78, 127.72, 127.55, 126.21, 125.93, 125.78, 124.91, 122.98, 119.14, 114.99, 114.89, 114.59, 71.33, 69.73, 68.16, 68.04, 63.05, 57.36, 54.69, 40.24, 32.82, 31.92, 29.66, 29.63, 29.60, 29.58, 29.54, 29.50, 29.46, 29.43, 29.40, 29.35, 29.24, 27.01, 26.03, 25.76, 25.74, 22.69, 14.11.

*3-(Furan-2-yl)-2,5-diphenyltetrahydro-4H-pyrrolo[3,4-d]isoxazole-4,6(5H)-dione (**3u**)*[1]

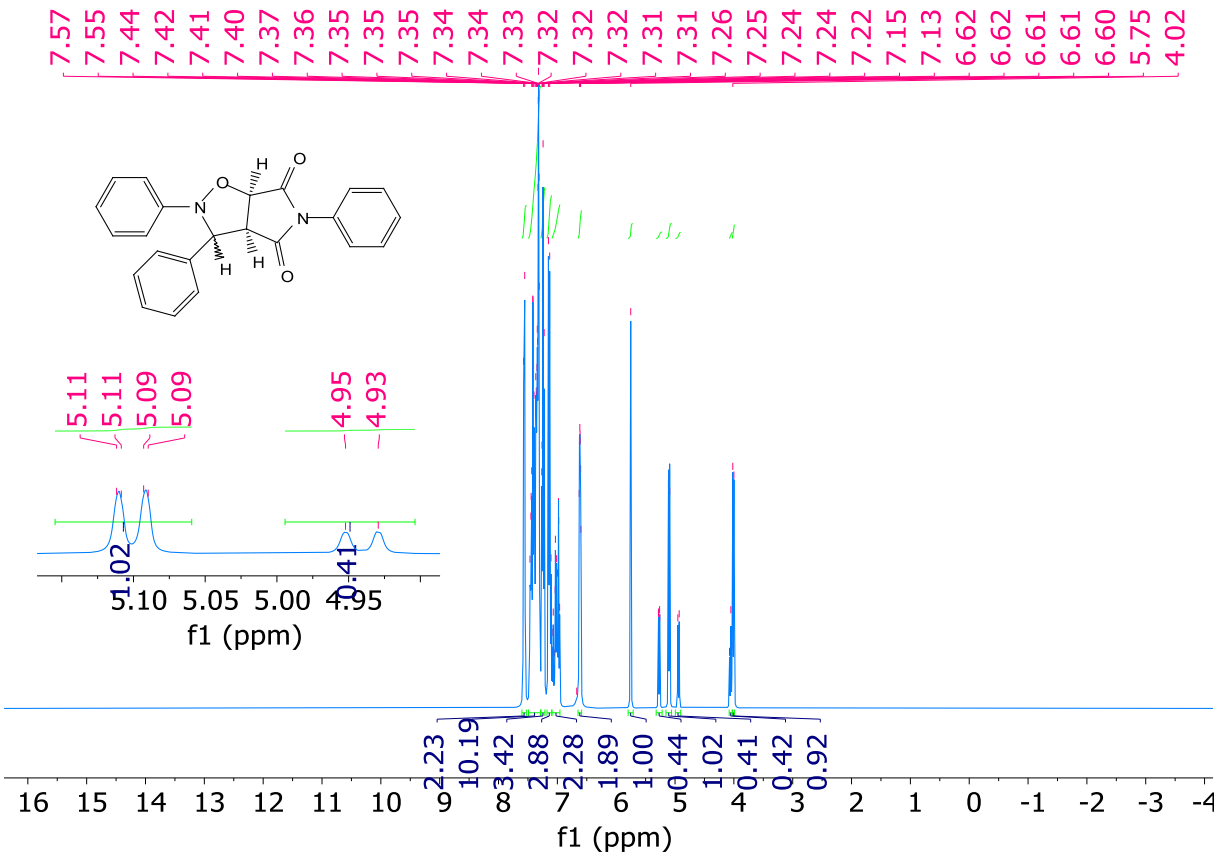
Beige solid, mp 144–145 °C; ^{1}H NMR (400 MHz, $CDCl_3$), mixture of *cis/trans*-diastereoisomers (*33/67*): δ 7.54-7.34 (*m*, 7H, Ar, 1H, furyl), 7.28-7.22 (*m*, 5H, Ar), 7.11 (*d*, *J* = 7.6 Hz, 3H, Ar), 7.05 (*d*, *J* = 8.6 Hz, 1H, Ar), 7.00 (*t*, *J* = 7.4 Hz, 1H, Ar), 6.77-6.75 (*m*, 2H, Ar), 6.37-6.32 (*m*, 3H, furyl), 5.68 (*s*, 1H, *trans*-H^3), 5.26 (*d*, *J* = 7.8 Hz, 1H, *cis*-H^3), 5.20 (*d*, *J* = 7.5 Hz, 1H, *trans*-H^{6a}), 4.86 (*d*, *J* = 9.2 Hz, 1H, *cis*-H^{6a}), 4.18 (*d*, *J* = 7.5 Hz, 1H, *trans*-H^{3a}), 4.00 (*t*, *J* = 9.2 Hz, 1H, *cis*-H^{3a}); ^{13}C NMR (101 MHz,

$CDCl_3$) δ 173.79, 173.20, 172.70, 171.46, 150.33, 147.64, 147.05, 146.85, 143.42, 142.85, 131.46, 131.04, 129.24, 129.22, 129.06, 129.02, 128.87, 128.84, 126.23, 126.21, 125.33, 123.39, 118.82, 115.32, 110.92, 110.82, 110.71, 108.50, 66.73, 64.36, 53.71, 52.77.

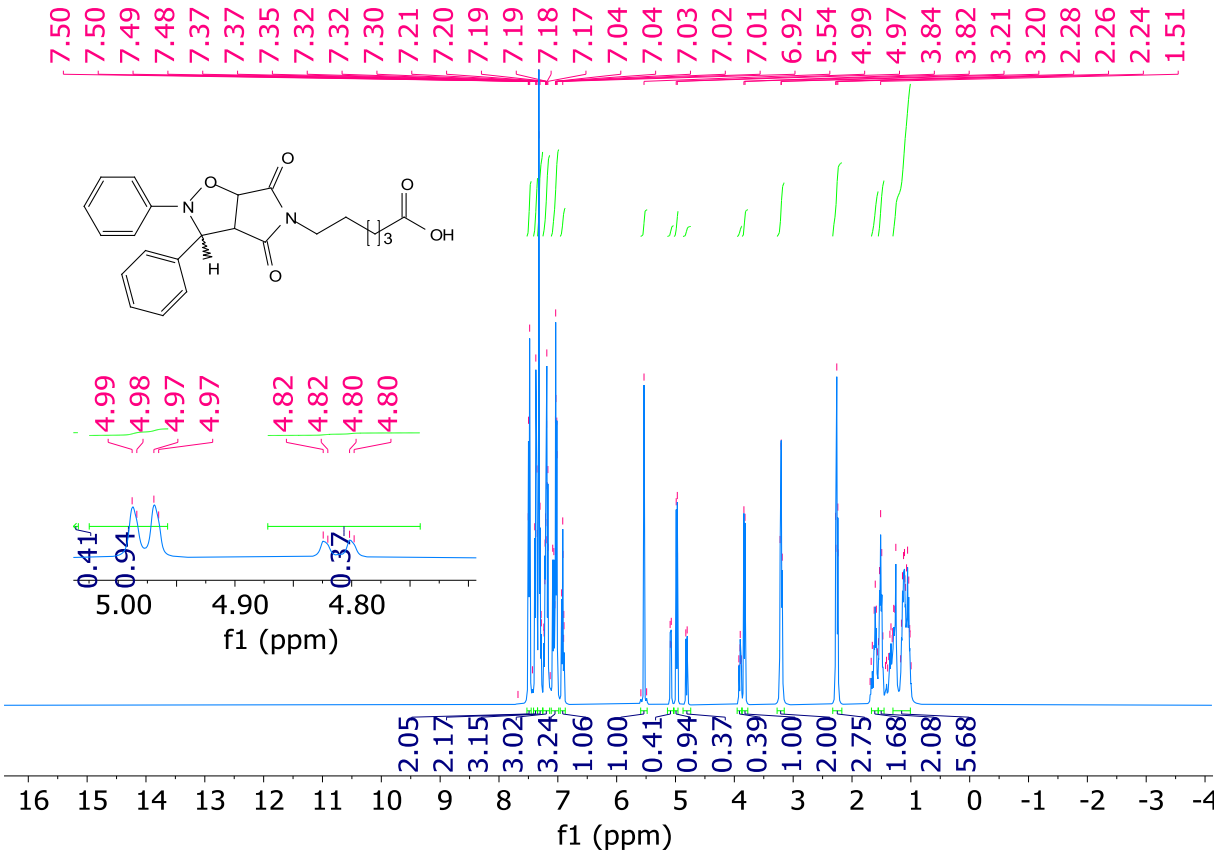
References

1. Iwakura, Y.; Uno, K.; Hongu, T. *Bull. Chem. Soc. Jpn.* **1969**, *42*, 2882–2885. doi: 10.1246/bcsj.42.2882
2. Yıldırım, A.; Kaya, Y. *J. Phys. Org. Chem.* **2017**, *30*, e3629. doi: 10.1002/poc.3629
3. Kaur, M.; Singh, B.; Singh, B. *WJPPS* **2014**, *3*, 1299–1317
4. Singal, K. K.; Giare, R. *Chem. Environ. Res.* **1998**, *7*, 93–98

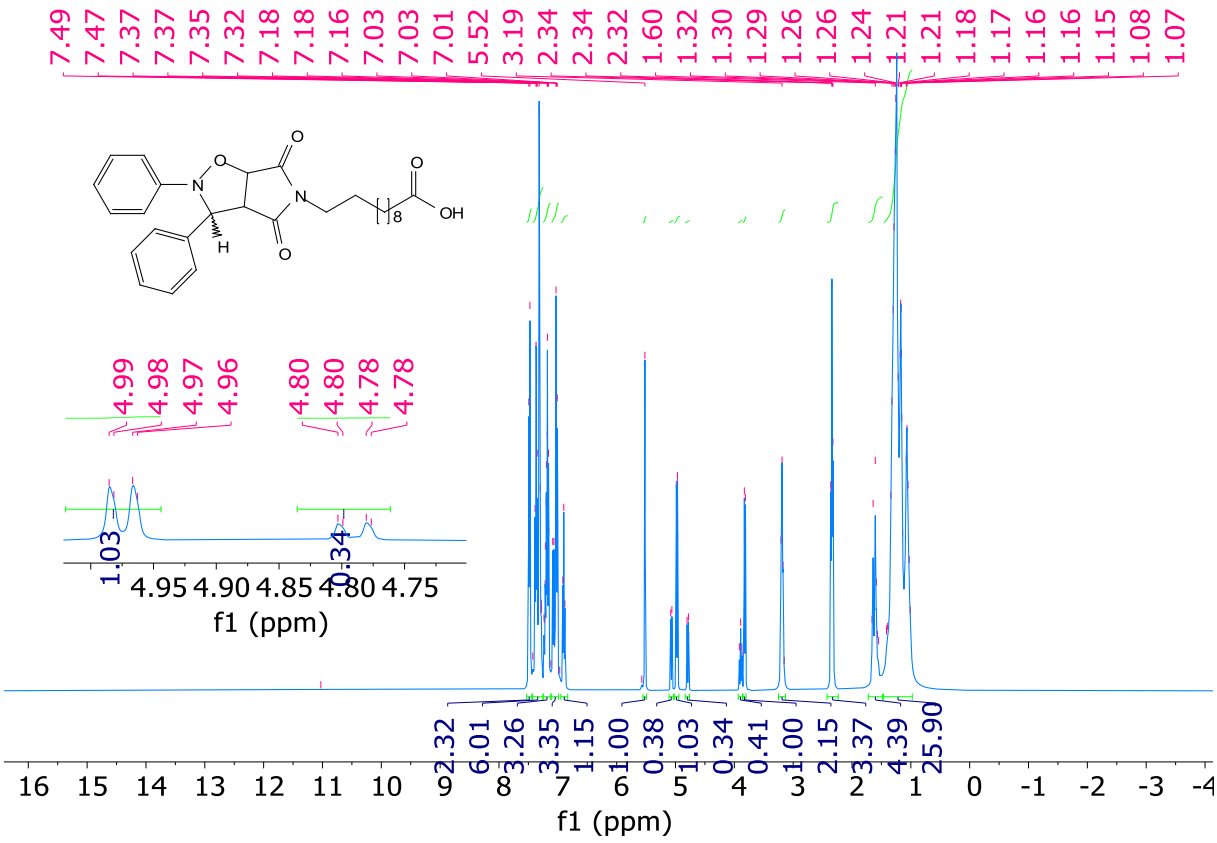
3a


7.57 7.55 7.44 7.42 7.41 7.40 7.37 7.36 7.35 7.35 7.35 7.34 7.34 7.33 7.32 7.32 7.32 7.31 7.31 7.26 7.25 7.24 7.24 7.22 7.15 7.13 6.62 6.62 6.61 6.61 6.60 5.75 4.02
5.11 5.11 5.09 5.09
4.95 4.93
1.02
0.41
5.10 5.05 5.00 4.95
f1 (ppm)
2.23 10.19 3.42 2.88 2.28 1.89 1.00 0.44 1.02 0.41 0.42 0.92
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

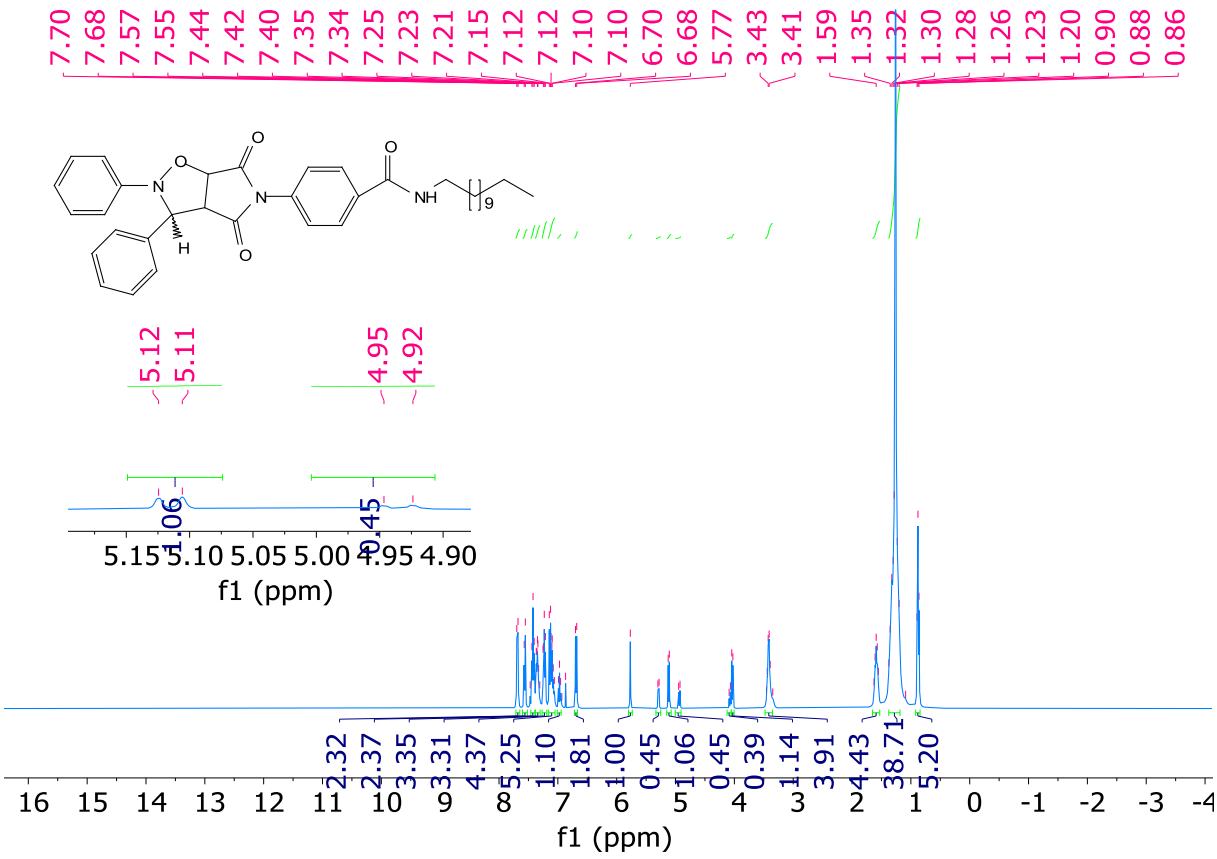
3b


7.50 7.50 7.49 7.48 7.37 7.37 7.35 7.32 7.32 7.30 7.21 7.20 7.19 7.19 7.18 7.17 7.04 7.04 7.03 7.02 7.01 6.92 5.54 4.99 4.97 3.84 3.82 3.21 3.20 2.28 2.26 2.24 1.51
O
O
N
O
N
O
OH
3
H
O
4.99 4.98 4.97 4.97 4.82 4.82 4.80 4.80
0.41 0.94 0.37
5.00 4.90 4.80
f1 (ppm)
2.05 2.17 3.15 3.02 3.24 1.06 1.00 0.41 0.94 0.37 0.39 1.00 2.00 2.75 1.68 2.08 5.68
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

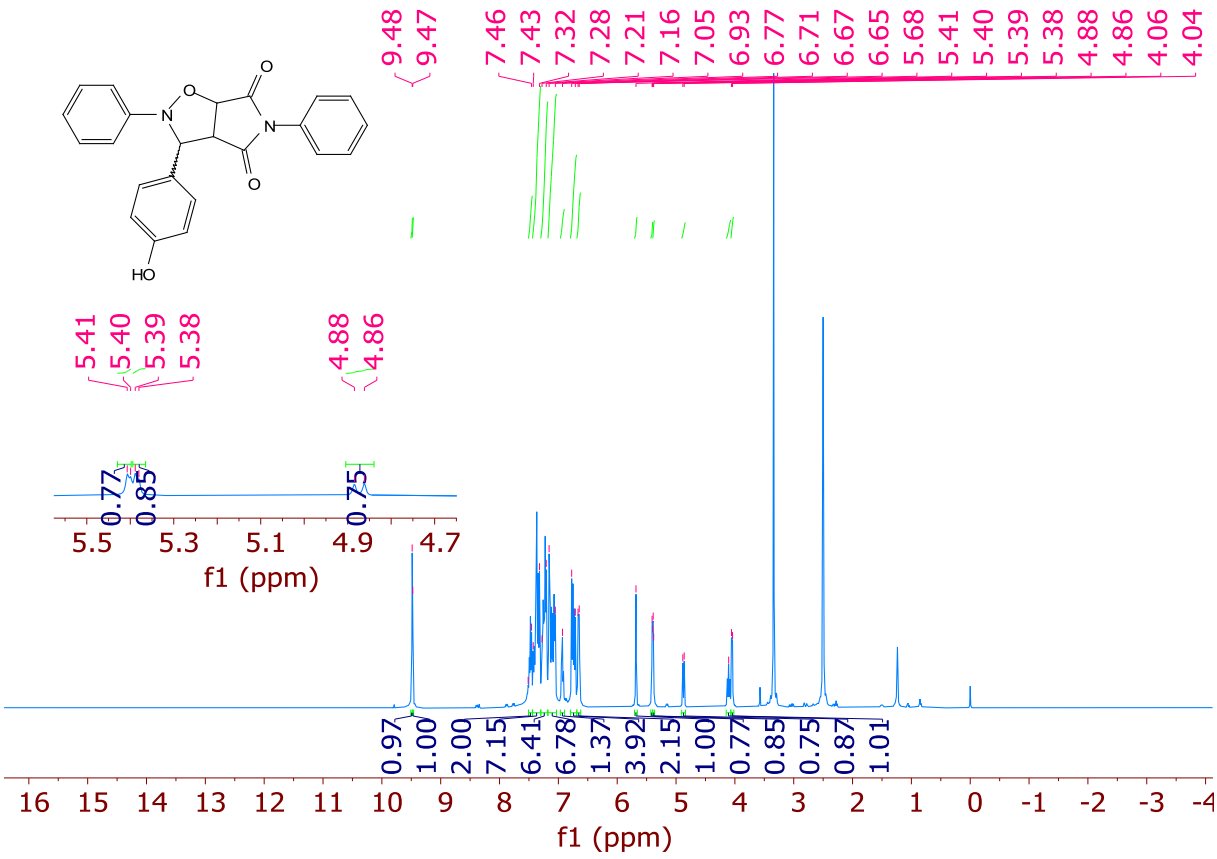
3c


7.49 7.47 7.37 7.37 7.35 7.32 7.18 7.18 7.16 7.03 7.03 7.01 5.52 3.19 2.34 2.34 2.32 1.60 1.32 1.30 1.29 1.26 1.26 1.24 1.21 1.21 1.18 1.17 1.16 1.16 1.15 1.08 1.07
O
N
O
O
N
8
OH
H
O
4.99 4.98 4.97 4.96 4.80 4.80 4.78 4.78
1.03
0.34
4.95 4.90 4.85 4.80 4.75
f1 (ppm)
2.32 6.01 3.26 3.35 1.15 1.00 0.38 1.03 0.34 0.41 1.00 2.15 3.37 4.39 25.90
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

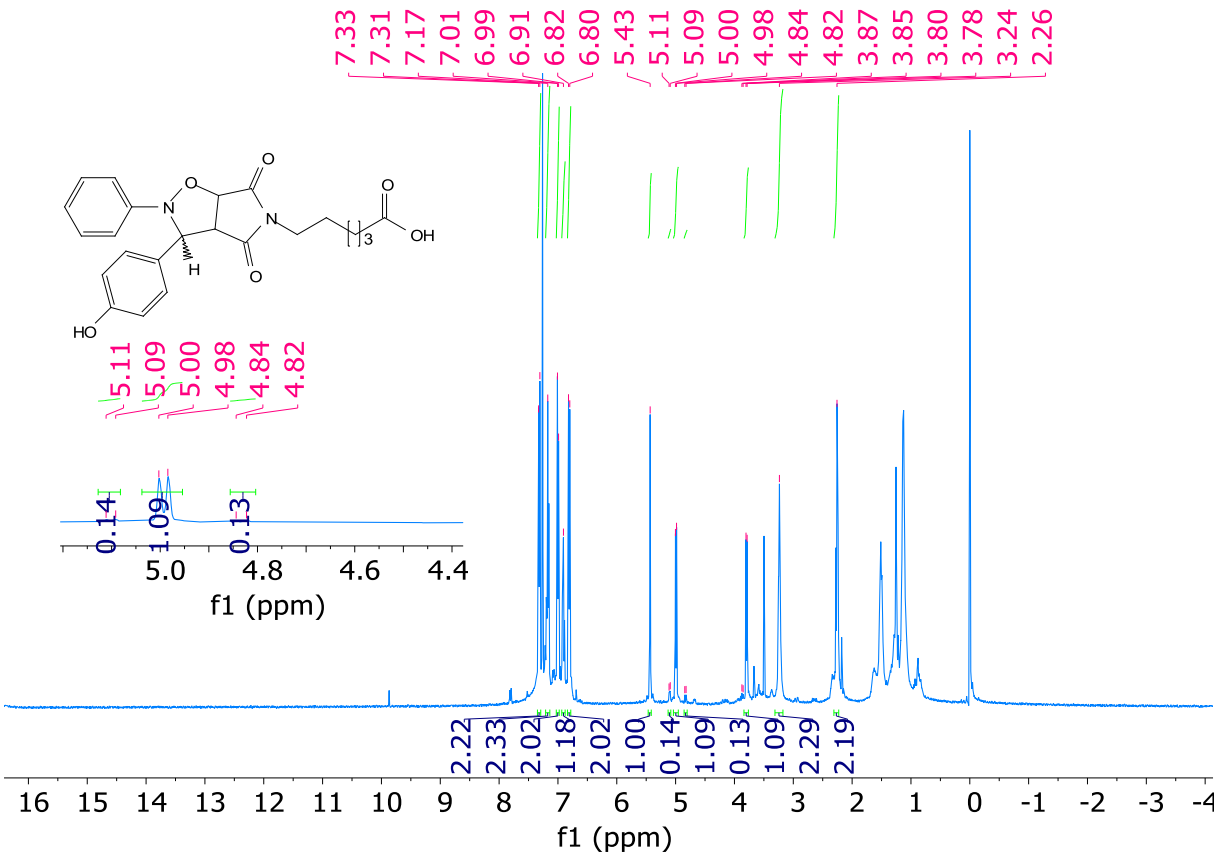
3d


7.70 7.68 7.57 7.55 7.44 7.42 7.40 7.35 7.34 7.25 7.23 7.21 7.15 7.12 7.12 7.10 7.10 6.70 6.68 5.77 3.43 3.41 1.59 1.35 1.32 1.30 1.28 1.26 1.23 1.20 0.90 0.88 0.86
O
O
N
O
N
O
NH
9
H
O
5.12 5.11 4.95 4.92
1.06 0.45
5.15 5.10 5.05 5.00 4.95 4.90
f1 (ppm)
2.32 2.37 3.35 3.31 4.37 5.25 1.10 1.81 1.00 0.45 1.06 0.45 0.39 1.14 3.91 4.43 38.71 5.20
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

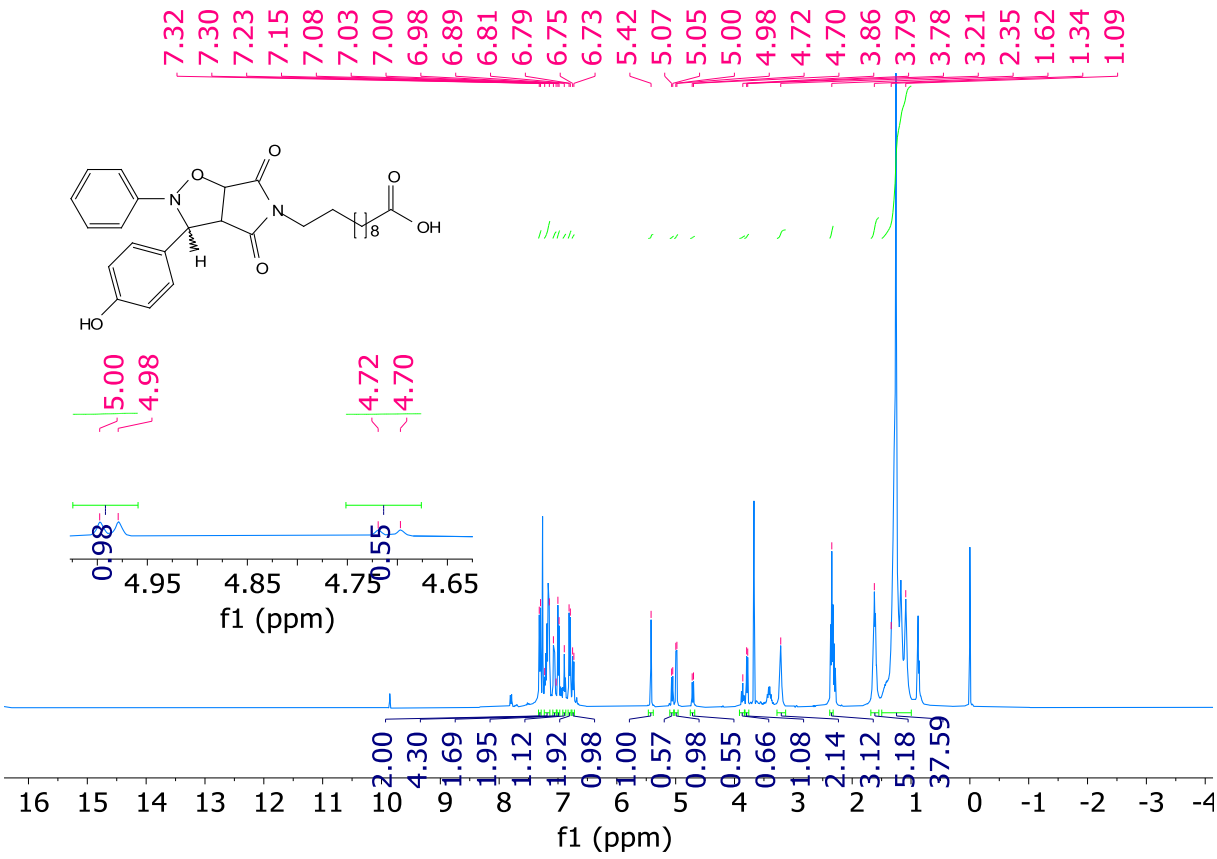
3e


9.48
9.47
7.46
7.43
7.32
7.28
7.21
7.16
7.05
6.93
6.77
6.71
6.67
6.65
5.68
5.41
5.40
5.39
5.38
4.88
4.86
4.06
4.04
HO
O
N
O
N
O
5.41
5.40
5.39
5.38
4.88
4.86
0.77
0.85
0.75
5.5
5.3
5.1
4.9
4.7
f1 (ppm)
0.97
1.00
2.00
7.15
6.41
6.78
1.37
3.92
2.15
1.00
0.77
0.85
0.75
0.87
1.01
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

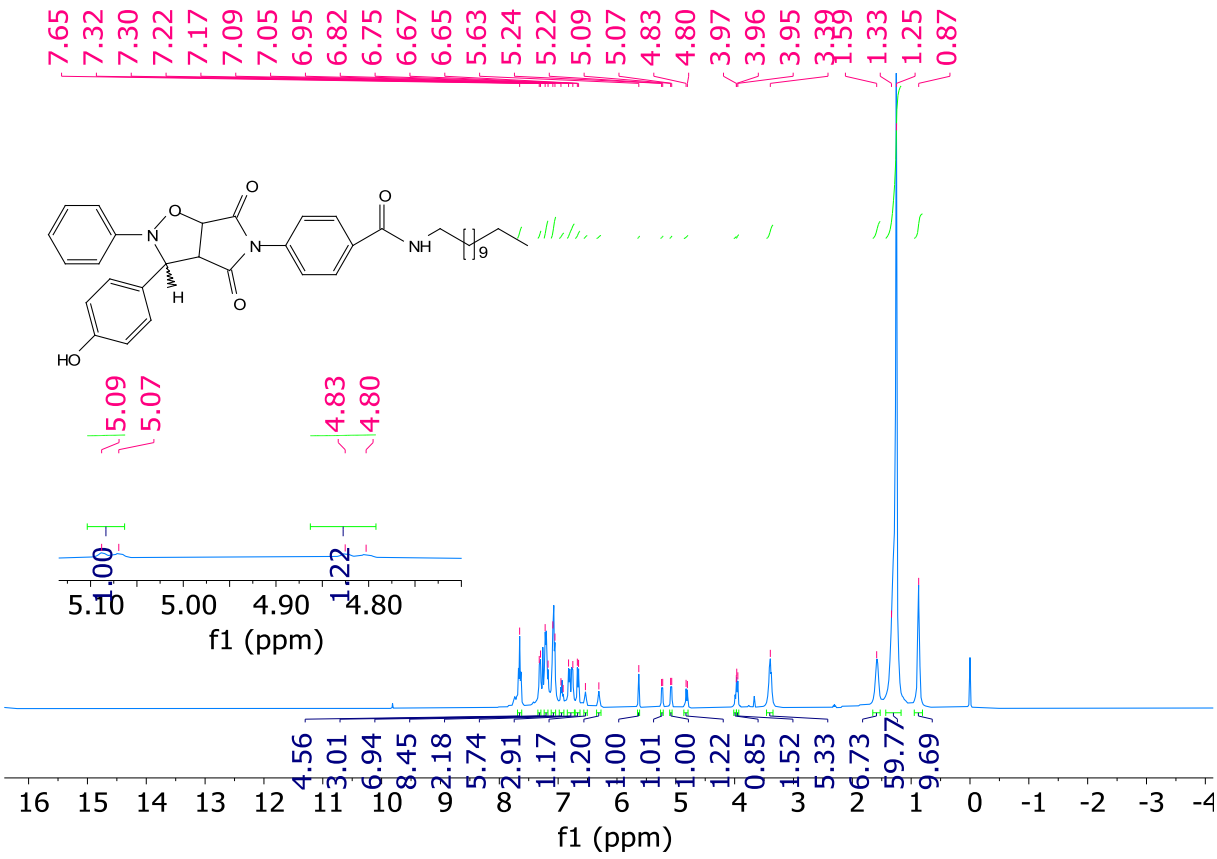
3f


7.33
7.31
7.17
7.01
6.99
6.91
6.82
6.80
5.43
5.11
5.09
5.00
4.98
4.84
4.82
3.87
3.85
3.80
3.78
3.24
2.26
O
N
O
N
O
OH
3
H
O
HO
5.11
5.09
5.00
4.98
4.84
4.82
0.14
1.09
0.13
5.0
4.8
4.6
4.4
f1 (ppm)
2.22
2.33
2.02
1.18
2.02
1.00
0.14
1.09
0.13
1.09
2.29
2.19
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

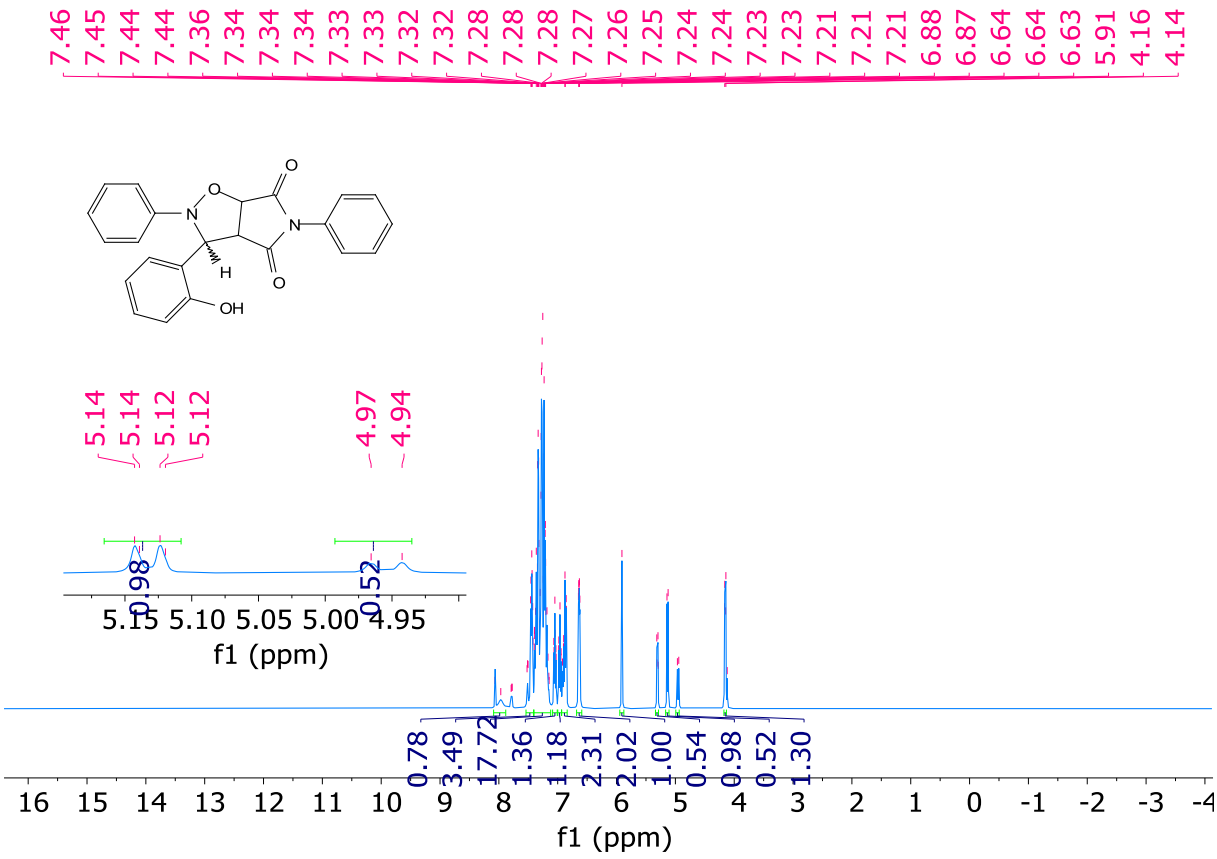
3g


7.32 7.30 7.23 7.15 7.08 7.03 7.00 6.98 6.89 6.81 6.79 6.75 6.73 5.42 5.07 5.05 5.00 4.98 4.72 4.70 3.86 3.79 3.78 3.21 2.35 1.62 1.34 1.09
O
O
N
O
N
O
OH
8
H
HO
5.00 4.98 4.72 4.70
0.98 0.55
4.95 4.85 4.75 4.65
f1 (ppm)
2.00 4.30 1.69 1.95 1.12 1.92 0.98 1.00 0.57 0.98 0.55 0.66 1.08 2.14 3.12 5.18 37.59
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

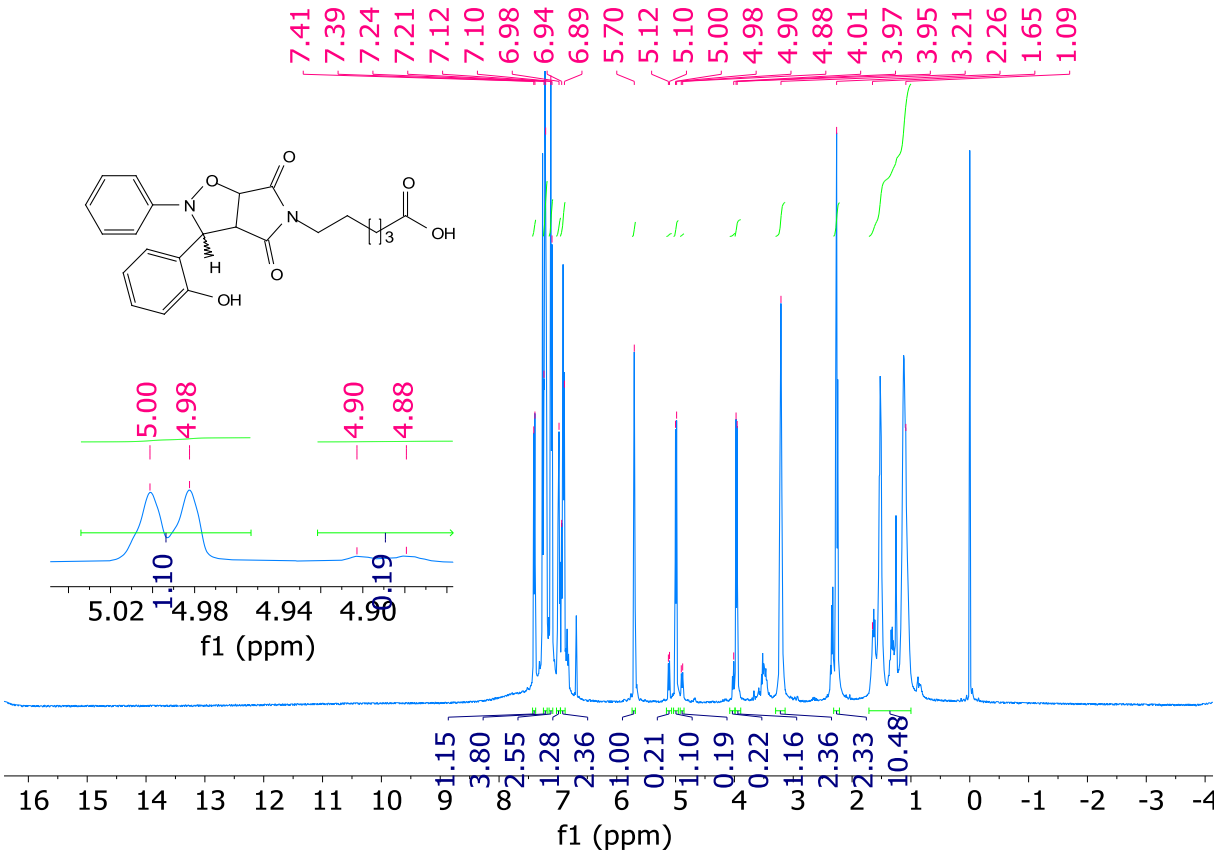
3h


7.65
7.32
7.30
7.22
7.17
7.09
7.05
6.95
6.82
6.75
6.67
6.65
5.63
5.24
5.22
5.09
5.07
4.83
4.80
3.97
3.96
3.95
3.39
3.38
1.59
1.33
1.25
0.87
O
O
N
O
N
O
NH
9
H
O
HO
5.09
5.07
4.83
4.80
1.00
1.22
5.10
5.00
4.90
4.80
f1 (ppm)
4.56
3.01
6.94
8.45
2.18
5.74
2.91
1.17
1.20
1.00
1.01
1.00
1.22
0.85
1.52
5.33
6.73
59.77
9.69
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

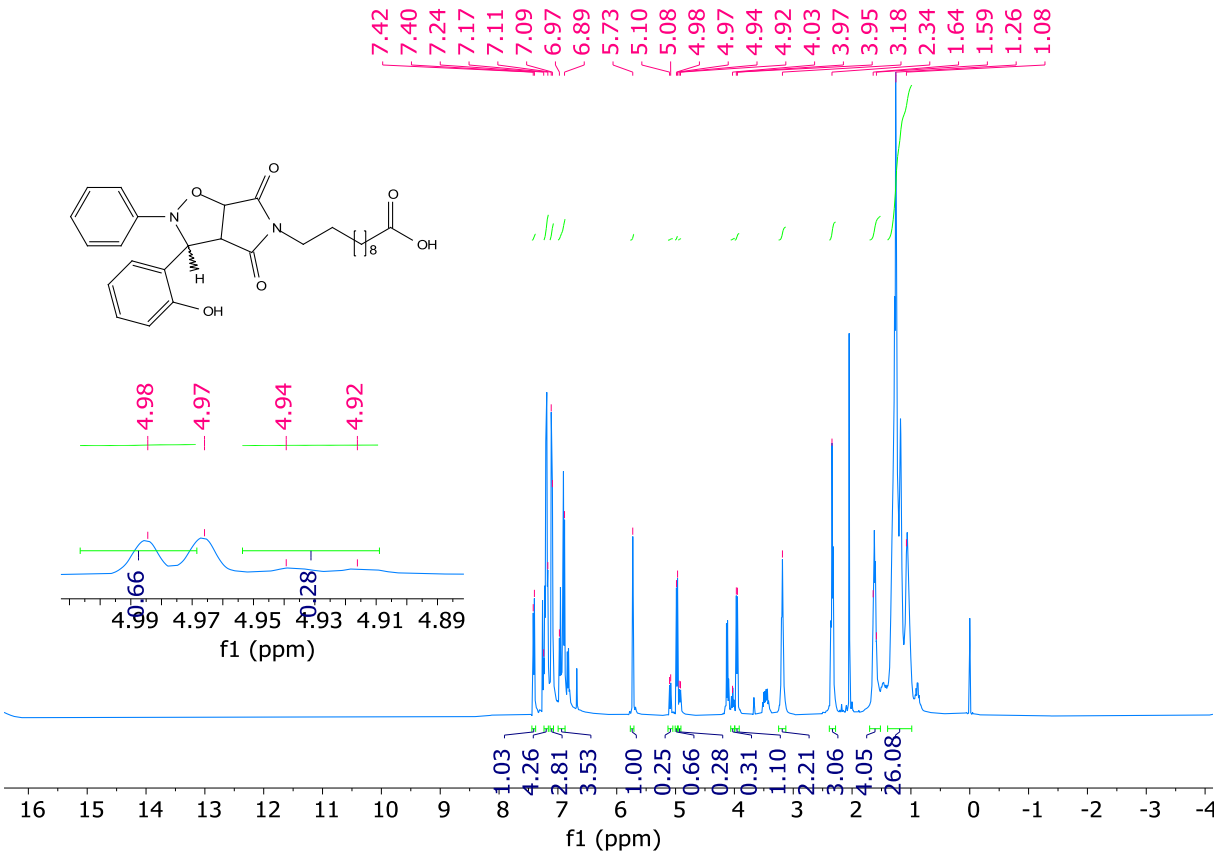
3i


7.46 7.45 7.44 7.44 7.36 7.34 7.34 7.34 7.33 7.33 7.32 7.32 7.28 7.28 7.28 7.27 7.26 7.25 7.24 7.24 7.23 7.23 7.21 7.21 7.21 6.88 6.87 6.64 6.64 6.63 5.91 4.16 4.14
O
O
N
O
N
H
O
OH
5.14 5.14 5.12 5.12
4.97 4.94
0.98
0.52
5.15 5.10 5.05 5.00 4.95
f1 (ppm)
0.78 3.49 17.72 1.36 1.18 2.31 2.02 1.00 0.54 0.98 0.52 1.30
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

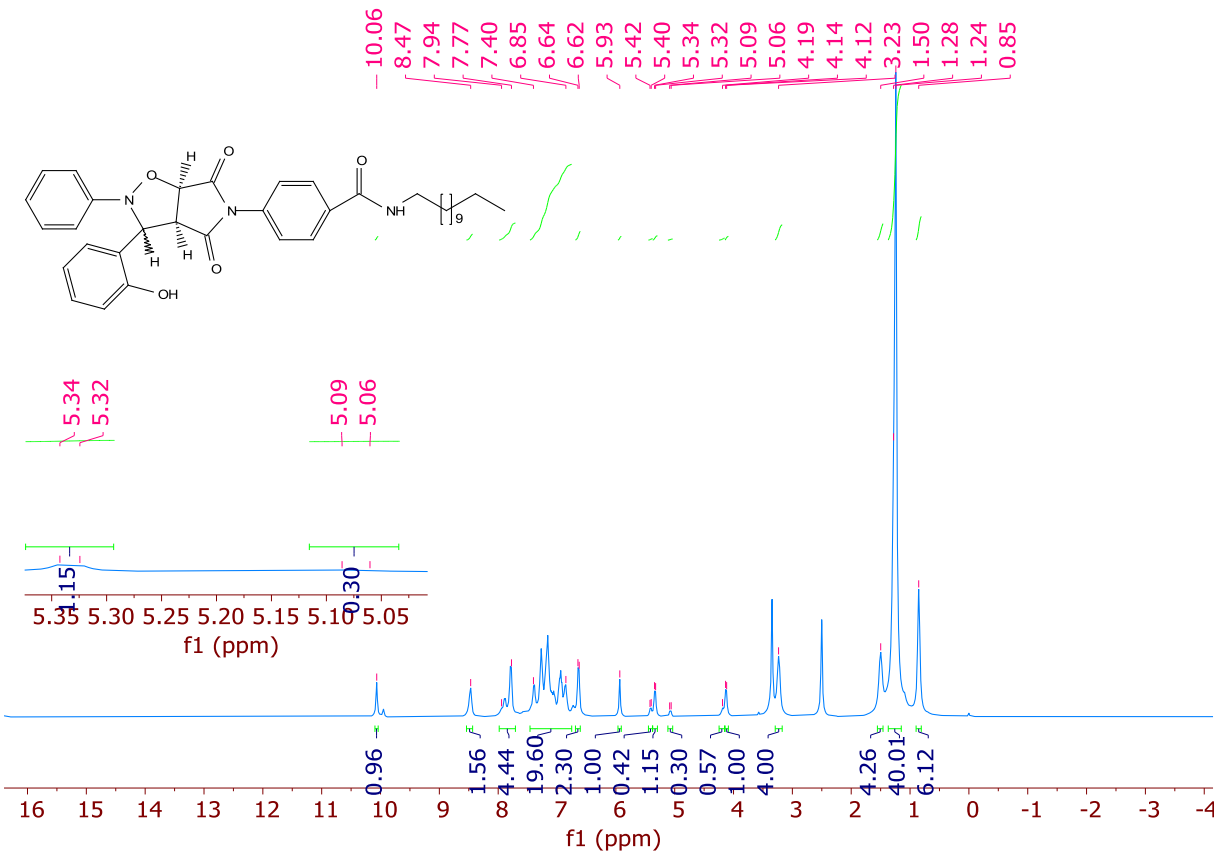
3j


7.41
7.39
7.24
7.21
7.12
7.10
6.98
6.94
6.89
5.70
5.12
5.10
5.00
4.98
4.90
4.88
4.01
3.97
3.95
3.21
2.26
1.65
1.09
O
O
N
O
N
O
OH
3
H
OH
5.00
4.98
4.90
4.88
1.10
0.19
5.02
4.98
4.94
4.90
f1 (ppm)
1.15
3.80
2.55
1.28
2.36
1.00
0.21
1.10
0.19
0.22
1.16
2.36
2.33
10.48
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

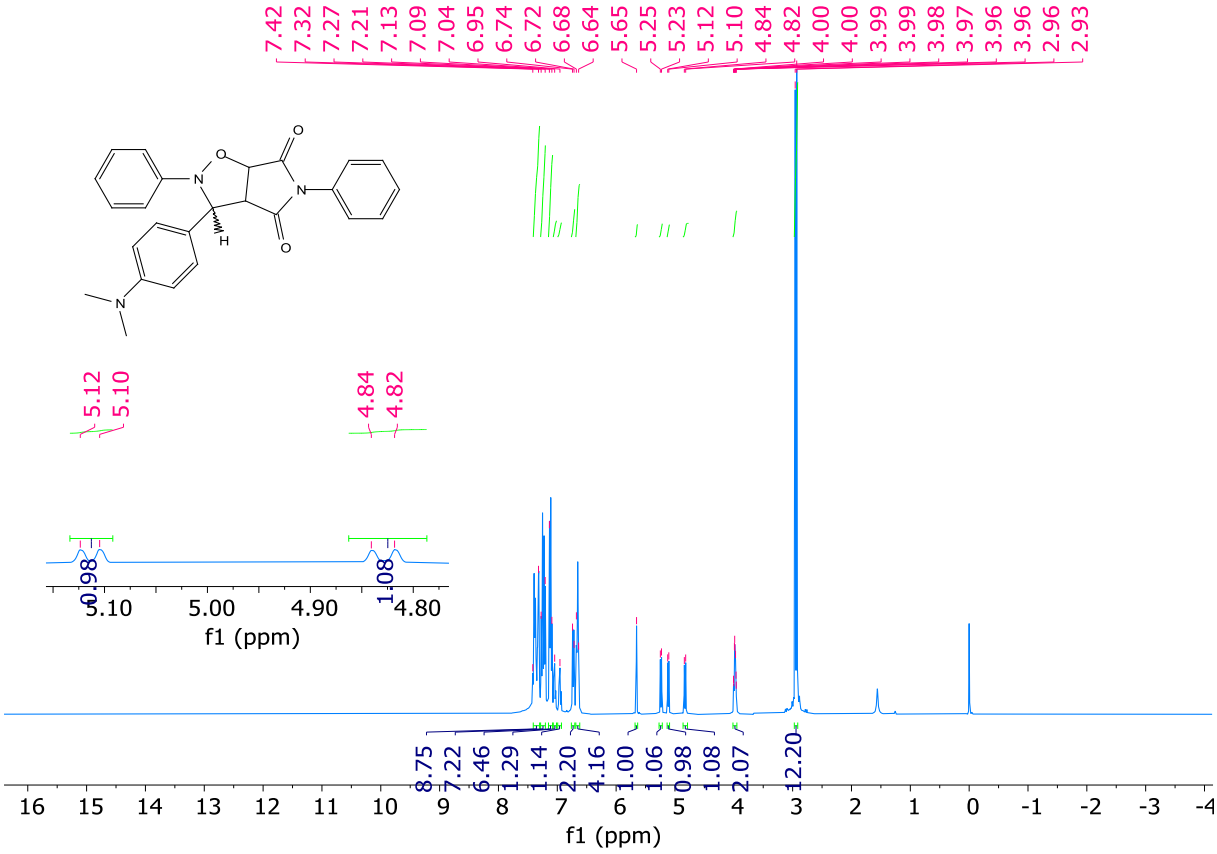
3k


7.42
7.40
7.24
7.17
7.11
7.09
6.97
6.89
5.73
5.10
5.08
4.98
4.97
4.94
4.92
4.03
3.97
3.95
3.18
2.34
1.64
1.59
1.26
1.08
OH
OH
8
4.98
4.97
4.94
4.92
0.66
0.28
4.99 4.97 4.95 4.93 4.91 4.89
f1 (ppm)
1.03
4.26
2.81
3.53
1.00
0.25
0.66
0.28
0.31
1.10
2.21
3.06
4.05
26.08
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

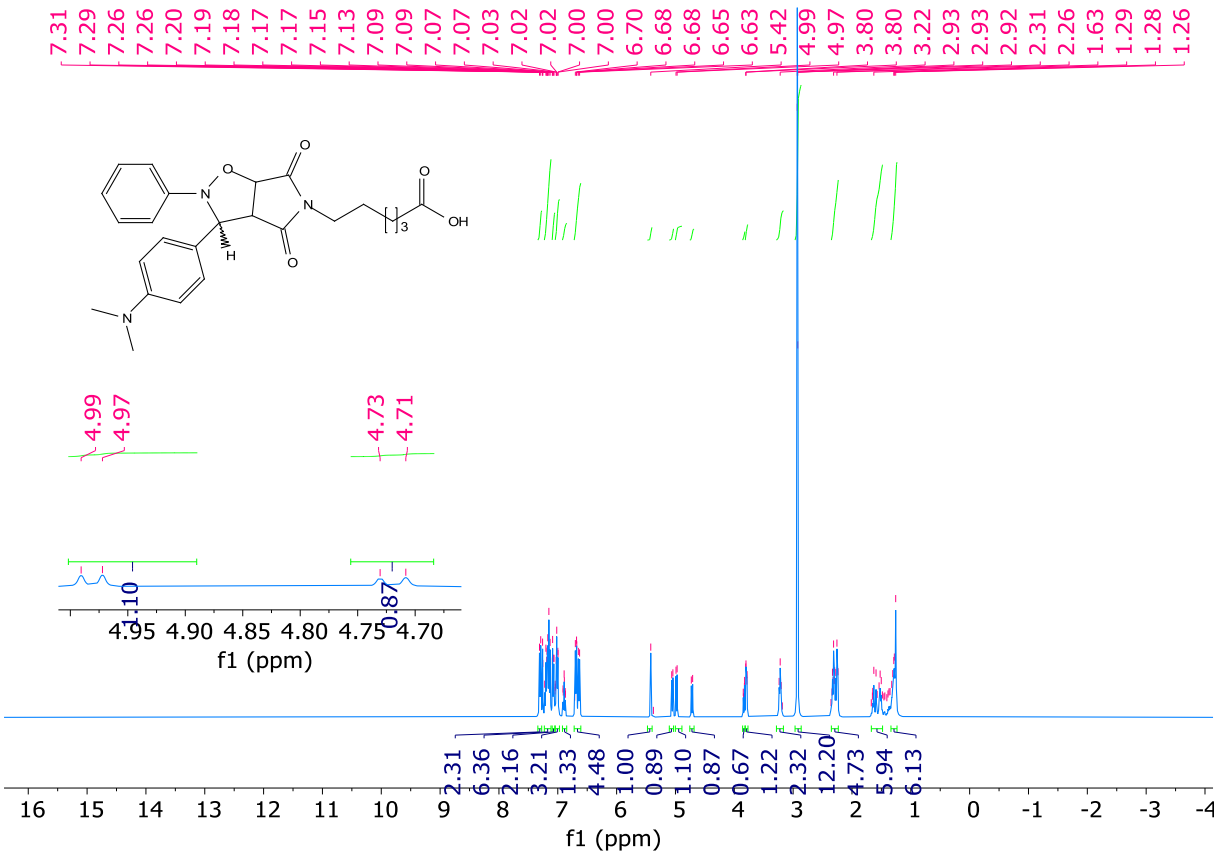
3l


10.06
8.47
7.94
7.77
7.40
6.85
6.64
6.62
5.93
5.42
5.40
5.34
5.32
5.09
5.06
4.19
4.14
4.12
3.23
1.50
1.28
1.24
0.85
OH
NH
9
5.34
5.32
5.09
5.06
1.15
0.30
5.35 5.30 5.25 5.20 5.15 5.10 5.05
f1 (ppm)
0.96
1.56
4.44
19.60
2.30
1.00
0.42
1.15
0.30
0.57
1.00
4.00
4.26
40.01
6.12
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

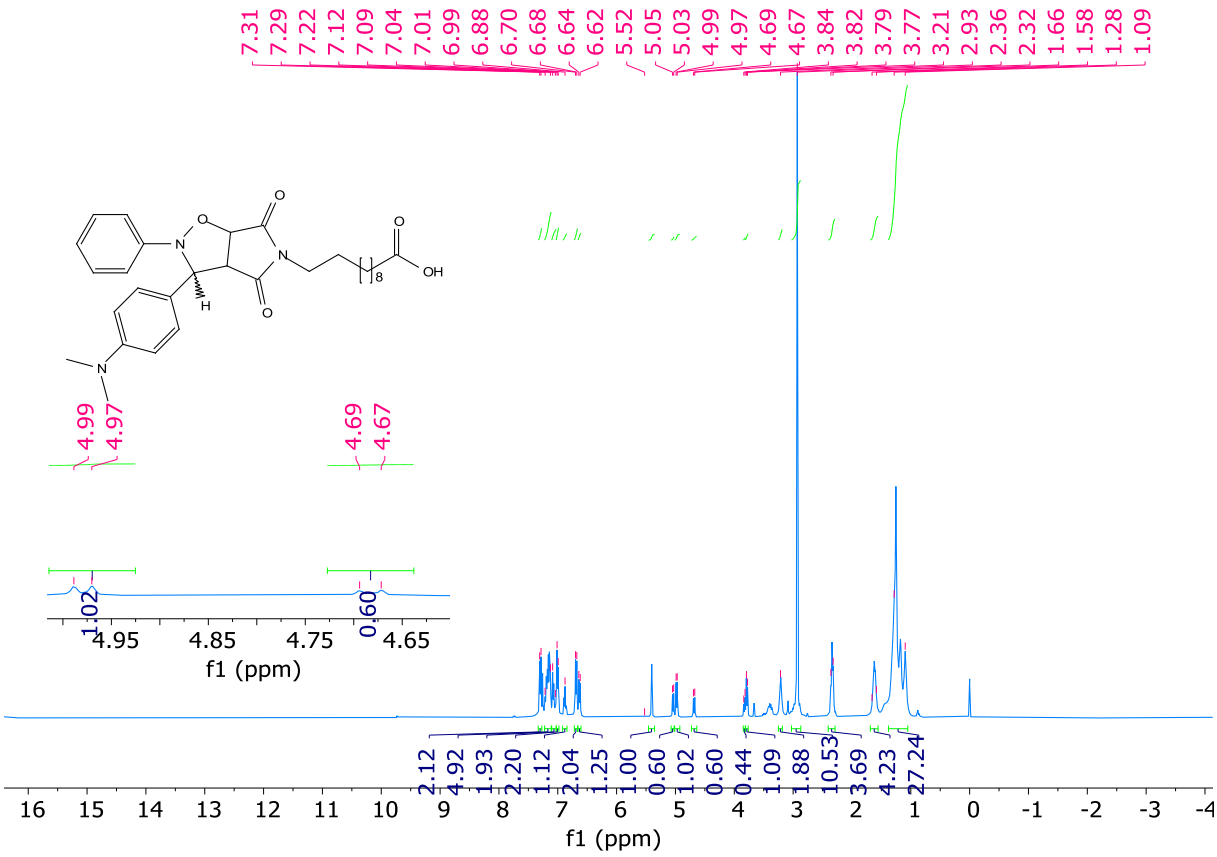
3m


7.42
7.32
7.27
7.21
7.13
7.09
7.04
6.95
6.74
6.72
6.68
6.64
5.65
5.25
5.23
5.12
5.10
4.84
4.82
4.00
4.00
3.99
3.99
3.98
3.97
3.96
3.96
2.96
2.93
O
N
O
N
H
O
N
5.12
5.10
4.84
4.82
0.98
1.08
5.10
5.00
4.90
4.80
f1 (ppm)
8.75
7.22
6.46
1.29
1.14
2.20
4.16
1.00
1.06
0.98
1.08
2.07
12.20
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

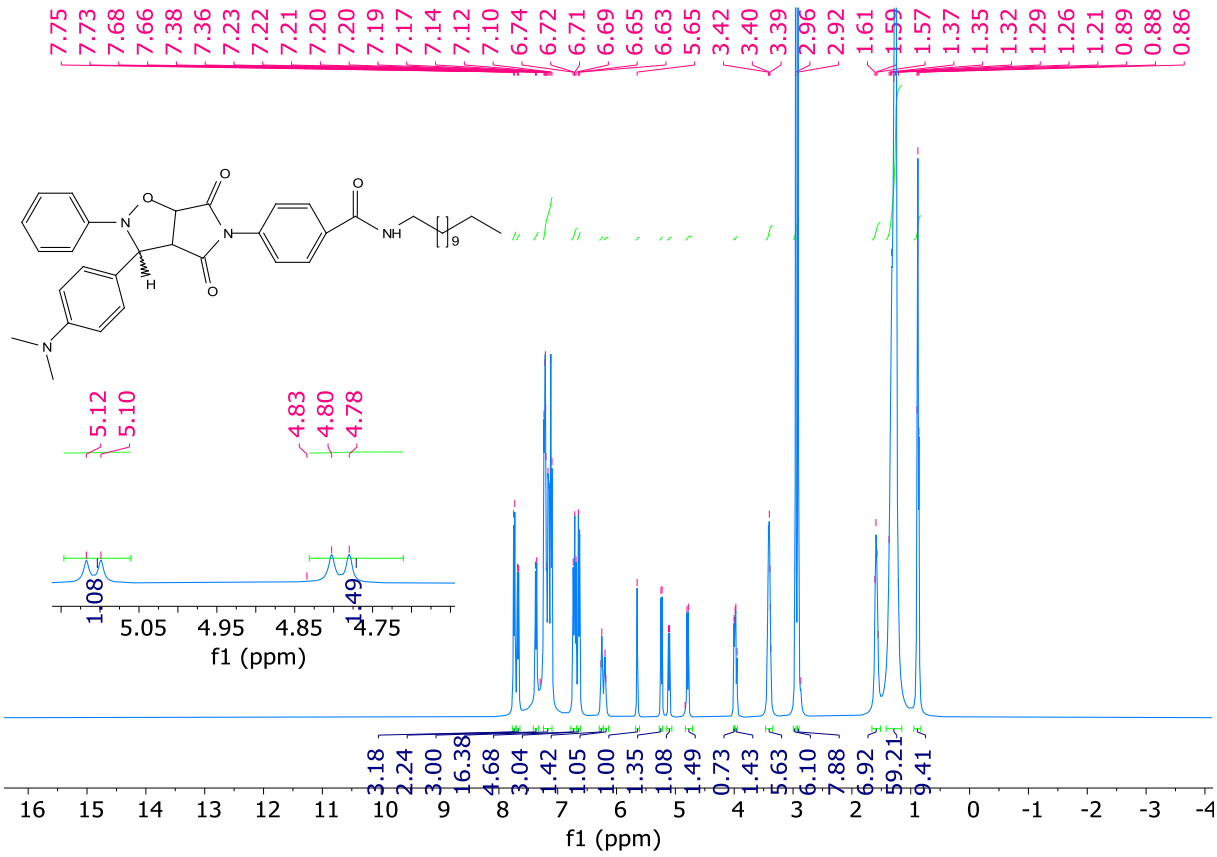
3n


7.31 7.29 7.26 7.26 7.20 7.19 7.18 7.17 7.17 7.15 7.13 7.09 7.09 7.07 7.07 7.03 7.02 7.02 7.00 7.00 6.70 6.68 6.68 6.65 6.63 5.42 4.99 4.97 3.80 3.80 3.22 2.93 2.93 2.92 2.31 2.26 1.63 1.29 1.28 1.26
4.99 4.97 4.73 4.71
1.10 0.87
4.95 4.90 4.85 4.80 4.75 4.70
f1 (ppm)
2.31 6.36 2.16 3.21 1.33 4.48 1.00 0.89 1.10 0.87 0.67 1.22 2.32 12.20 4.73 5.94 6.13
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

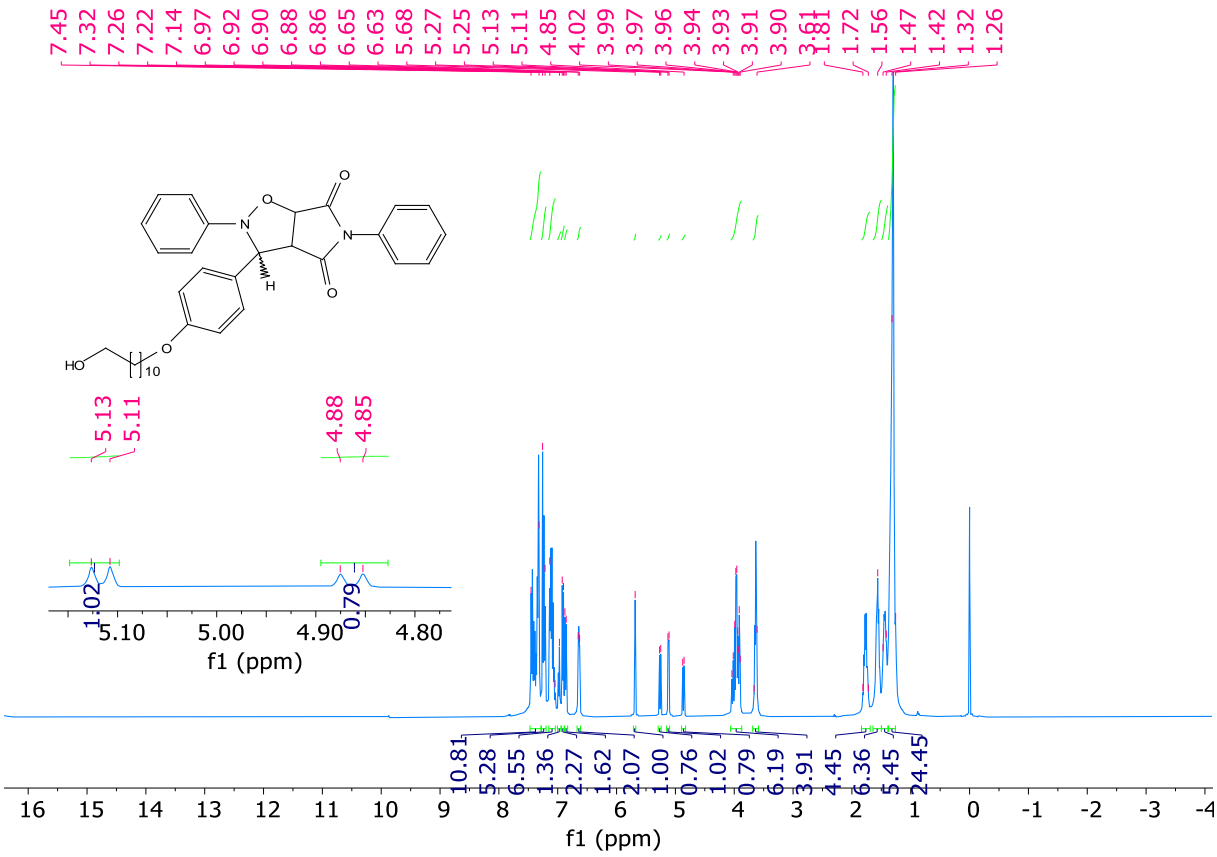
3o


7.31 7.29 7.22 7.12 7.09 7.04 7.01 6.99 6.88 6.70 6.68 6.64 6.62 5.52 5.05 5.03 4.99 4.97 4.69 4.67 3.84 3.82 3.79 3.77 3.21 2.93 2.36 2.32 1.66 1.58 1.28 1.09
OH
4.99 4.97 4.69 4.67
1.02 0.60
4.95 4.85 4.75 4.65
f1 (ppm)
2.12 4.92 1.93 2.20 1.12 2.04 1.25 1.00 0.60 1.02 0.60 0.44 1.09 1.88 10.53 3.69 4.23 27.24
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

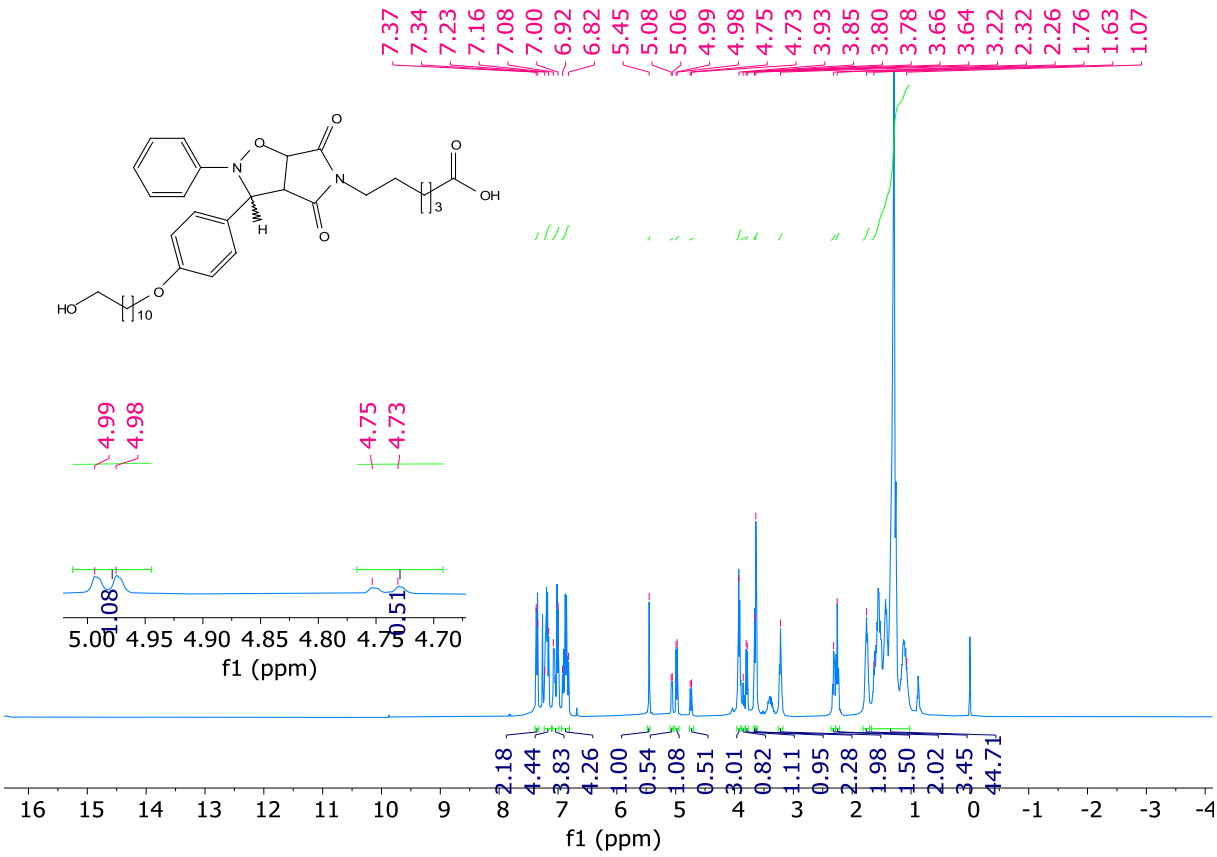
3p


7.75 7.73 7.68 7.66 7.38 7.36 7.23 7.22 7.21 7.20 7.20 7.19 7.17 7.14 7.12 7.10 6.74 6.72 6.71 6.69 6.65 6.63 5.65 3.42 3.40 3.39 2.96 2.92 1.61 1.59 1.57 1.37 1.35 1.32 1.29 1.26 1.21 0.89 0.88 0.86
5.12 5.10 4.83 4.80 4.78
1.08 1.49
5.05 4.95 4.85 4.75
f1 (ppm)
3.18 2.24 3.00 16.38 4.68 3.04 1.42 1.05 1.00 1.35 1.08 1.49 0.73 1.43 5.63 6.10 7.88 6.92 59.21 9.41
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

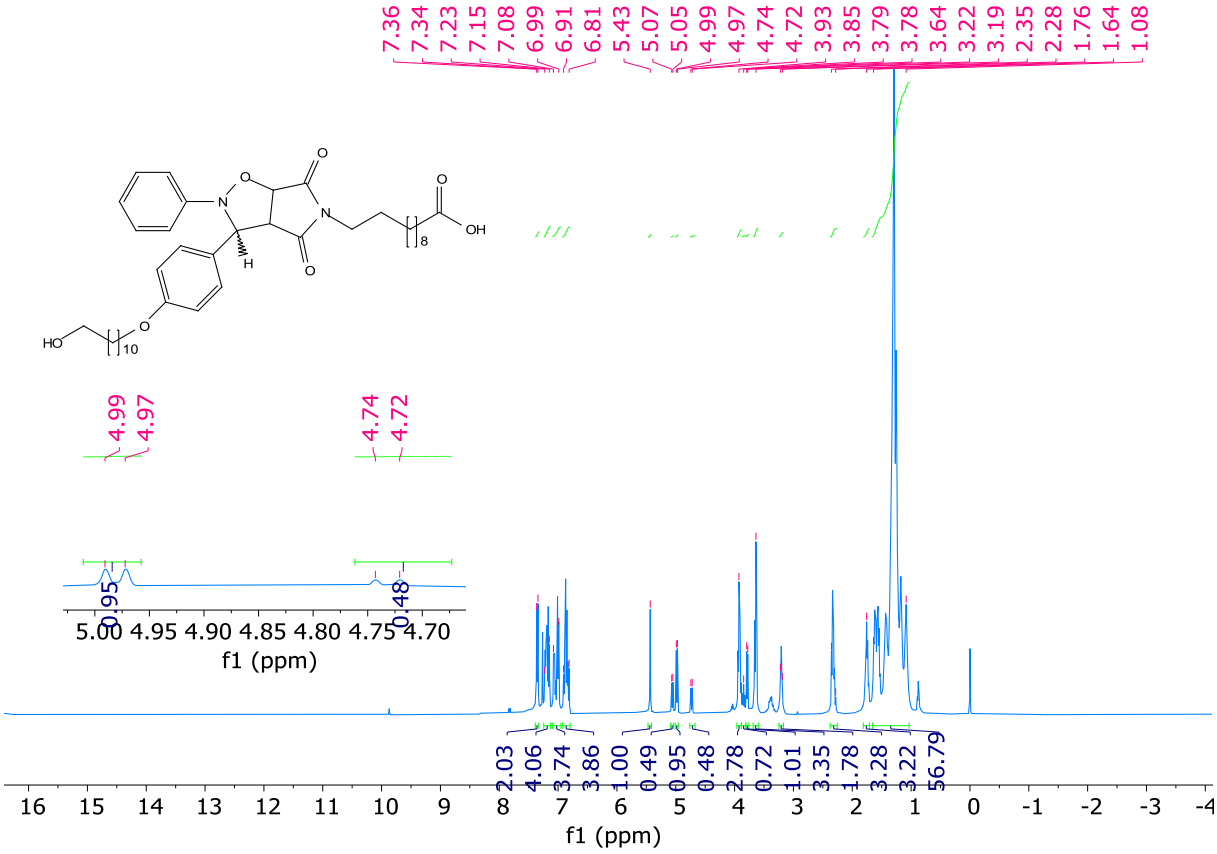
3q


7.45 7.32 7.26 7.22 7.14 6.97 6.92 6.90 6.88 6.86 6.65 6.63 5.68 5.27 5.25 5.13 5.11 4.85 4.02 3.99 3.97 3.96 3.94 3.93 3.91 3.90 3.61 1.81 1.72 1.56 1.47 1.42 1.32 1.26
5.13 5.11 4.88 4.85
1.02 0.79
5.10 5.00 4.90 4.80
f1 (ppm)
10.81 5.28 6.55 1.36 2.27 1.62 2.07 1.00 0.76 1.02 0.79 6.19 3.91 4.45 6.36 5.45 24.45
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

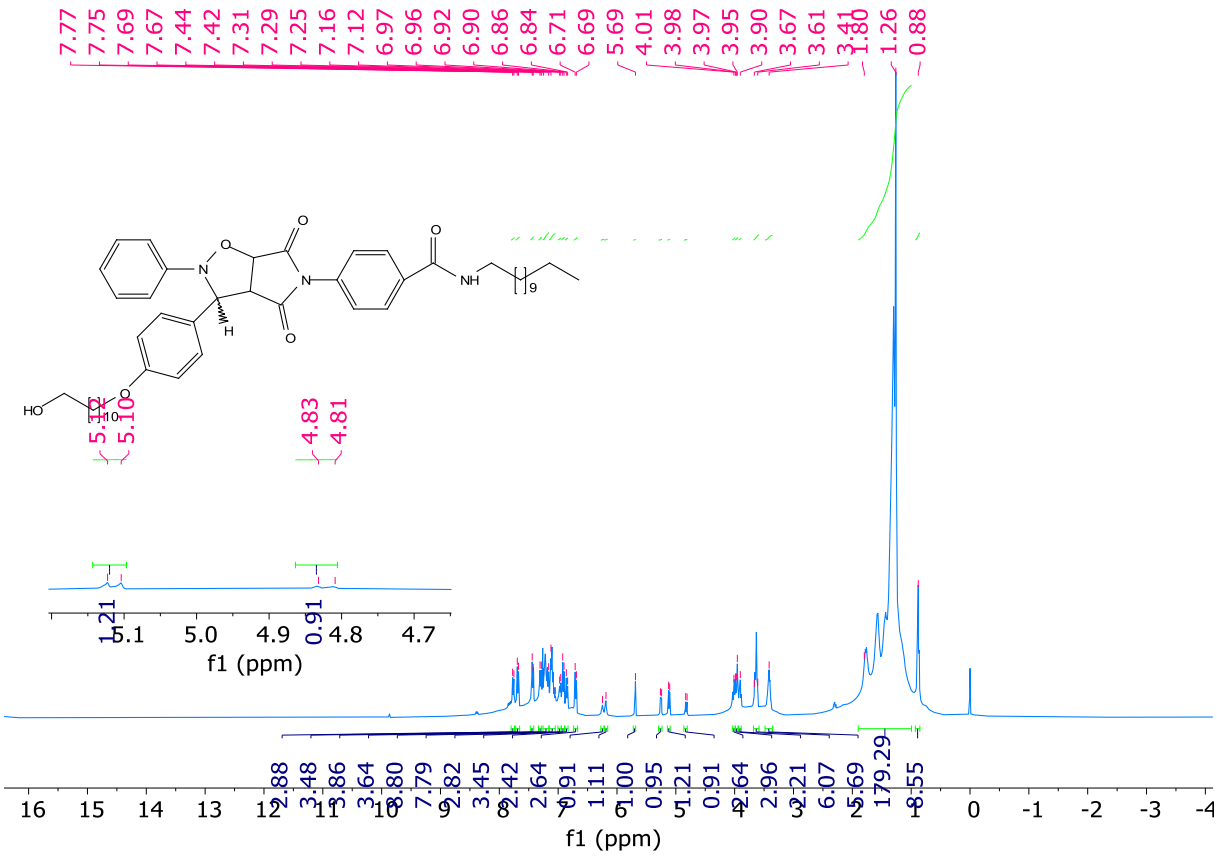
3r


7.37 7.34 7.23 7.16 7.08 7.00 6.92 6.82 5.45 5.08 5.06 4.99 4.98 4.75 4.73 3.93 3.85 3.80 3.78 3.66 3.64 3.22 2.32 2.26 1.76 1.63 1.07
4.99 4.98 4.75 4.73
1.08 0.51
5.00 4.95 4.90 4.85 4.80 4.75 4.70
f1 (ppm)
2.18 4.44 3.83 4.26 1.00 0.54 1.08 0.51 3.01 0.82 1.11 0.95 2.28 1.98 1.50 2.02 3.45 44.71
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

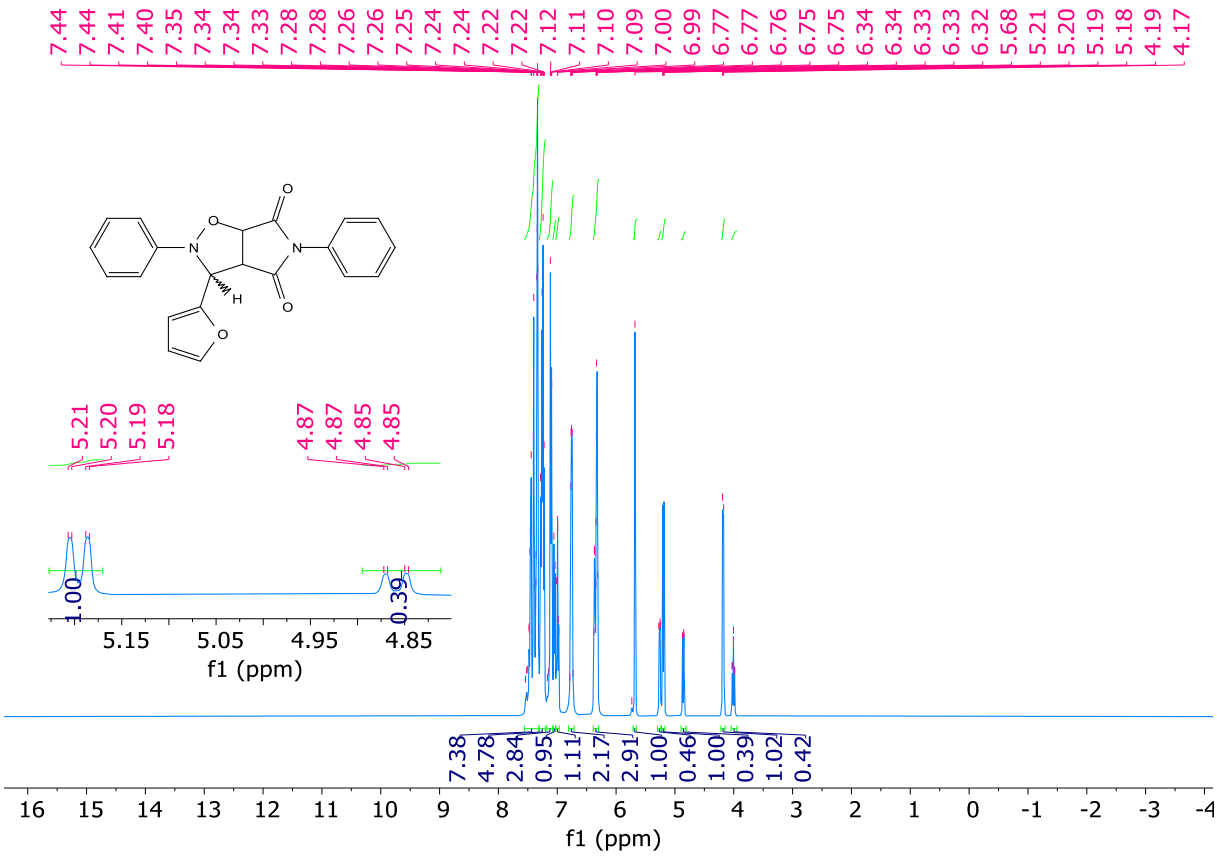
3s


7.36
7.34
7.23
7.15
7.08
6.99
6.91
6.81
5.43
5.07
5.05
4.99
4.97
4.74
4.72
3.93
3.85
3.79
3.78
3.64
3.22
3.19
2.35
2.28
1.76
1.64
1.08
HO
10
H
O
N
O
O
N
O
OH
8
4.99
4.97
4.74
4.72
0.95
0.48
5.00 4.95 4.90 4.85 4.80 4.75 4.70
f1 (ppm)
2.03
4.06
3.74
3.86
1.00
0.49
0.95
0.48
2.78
0.72
1.01
3.35
1.78
3.28
3.22
56.79
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

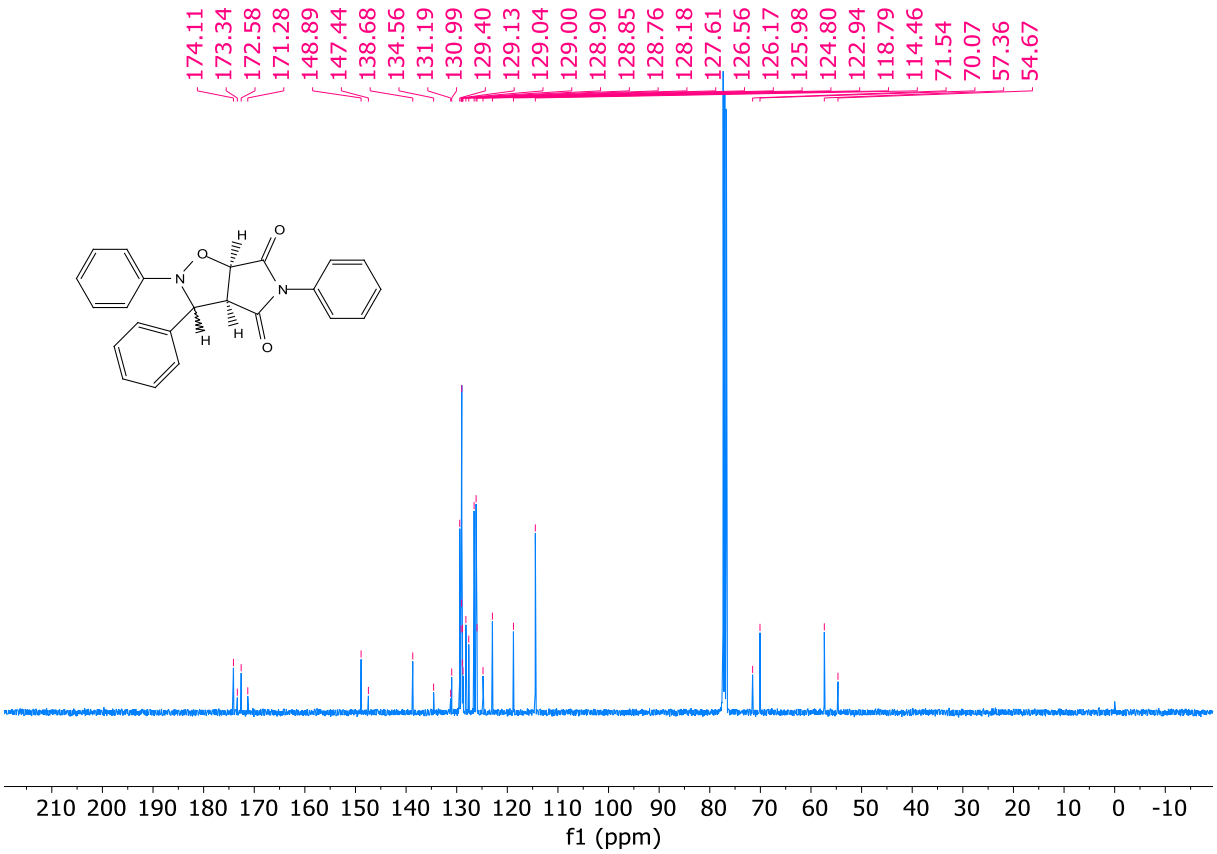
3t


7.77
7.75
7.69
7.67
7.44
7.42
7.31
7.29
7.25
7.16
7.12
6.97
6.96
6.92
6.90
6.86
6.84
6.71
6.69
5.69
4.01
3.98
3.97
3.95
3.90
3.67
3.61
3.41
1.80
1.26
0.88
5.11
5.10
4.83
4.81
1.21
0.91
f1 (ppm)
2.88
3.48
3.86
3.64
3.80
7.79
2.82
3.45
2.42
2.64
0.91
1.11
1.00
0.95
1.21
0.91
2.64
2.96
2.21
6.07
5.69
179.29
8.55
f1 (ppm)

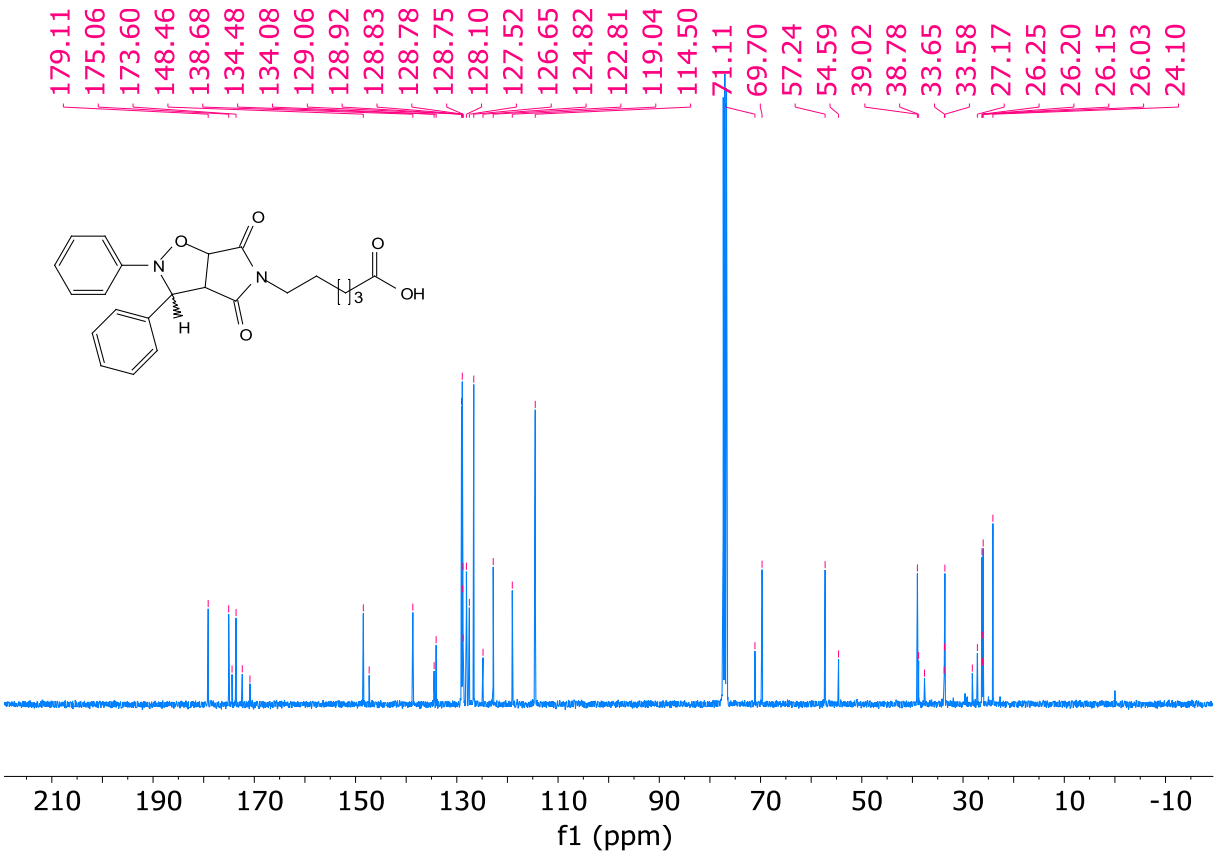
3u


7.44 7.44 7.41 7.40 7.35 7.34 7.34 7.33 7.28 7.28 7.26 7.26 7.25 7.24 7.24 7.22 7.22 7.12 7.11 7.10 7.09 7.00 6.99 6.77 6.77 6.76 6.75 6.75 6.34 6.34 6.33 6.33 6.32 5.68 5.21 5.20 5.19 5.18 4.19 4.17
5.21 5.20 5.19 5.18
4.87 4.87 4.85 4.85
1.00
0.39
5.15 5.05 4.95 4.85
f1 (ppm)
7.38 4.78 2.84 0.95 1.11 2.17 2.91 1.00 0.46 1.00 0.39 1.02 0.42
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

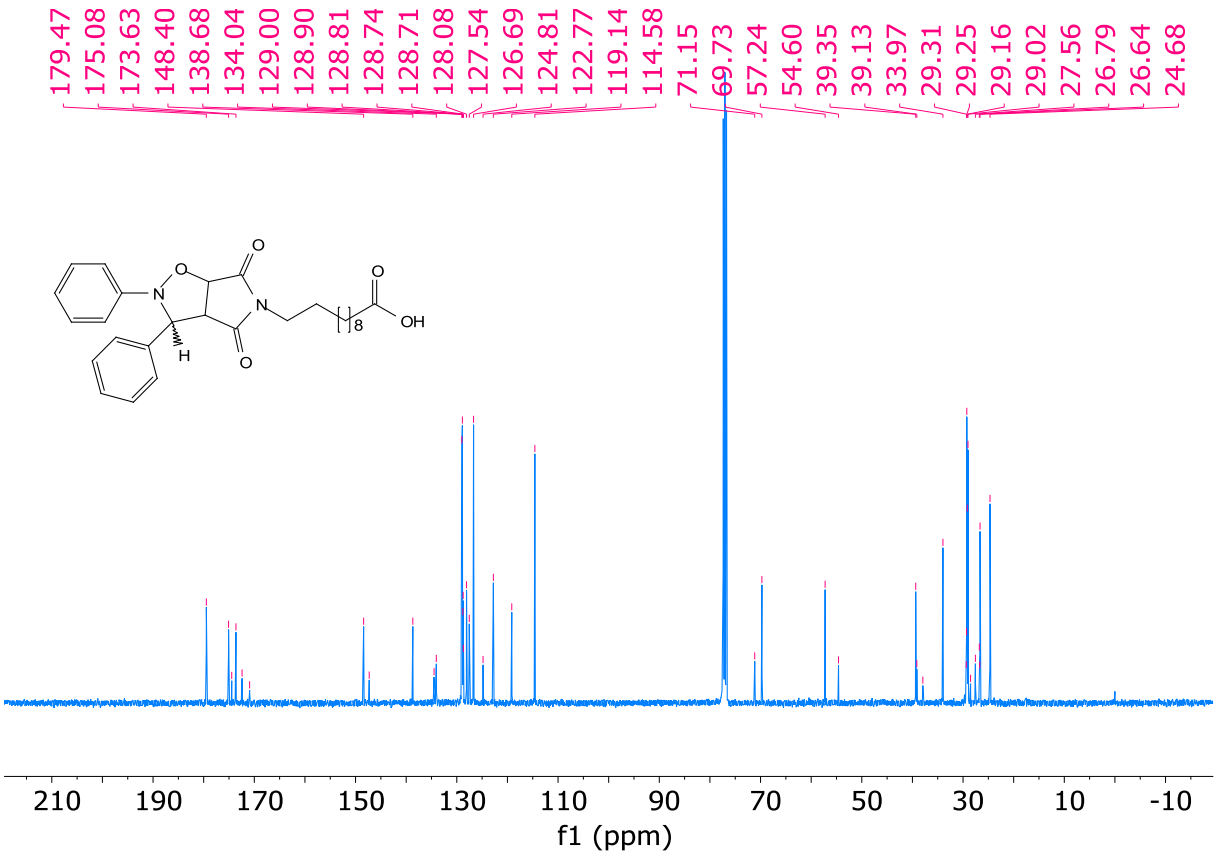
3a


174.11
173.34
172.58
171.28
148.89
147.44
138.68
134.56
131.19
130.99
129.40
129.13
129.04
129.00
128.90
128.85
128.76
128.18
127.61
126.56
126.17
125.98
124.80
122.94
118.79
114.46
71.54
70.07
57.36
54.67
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

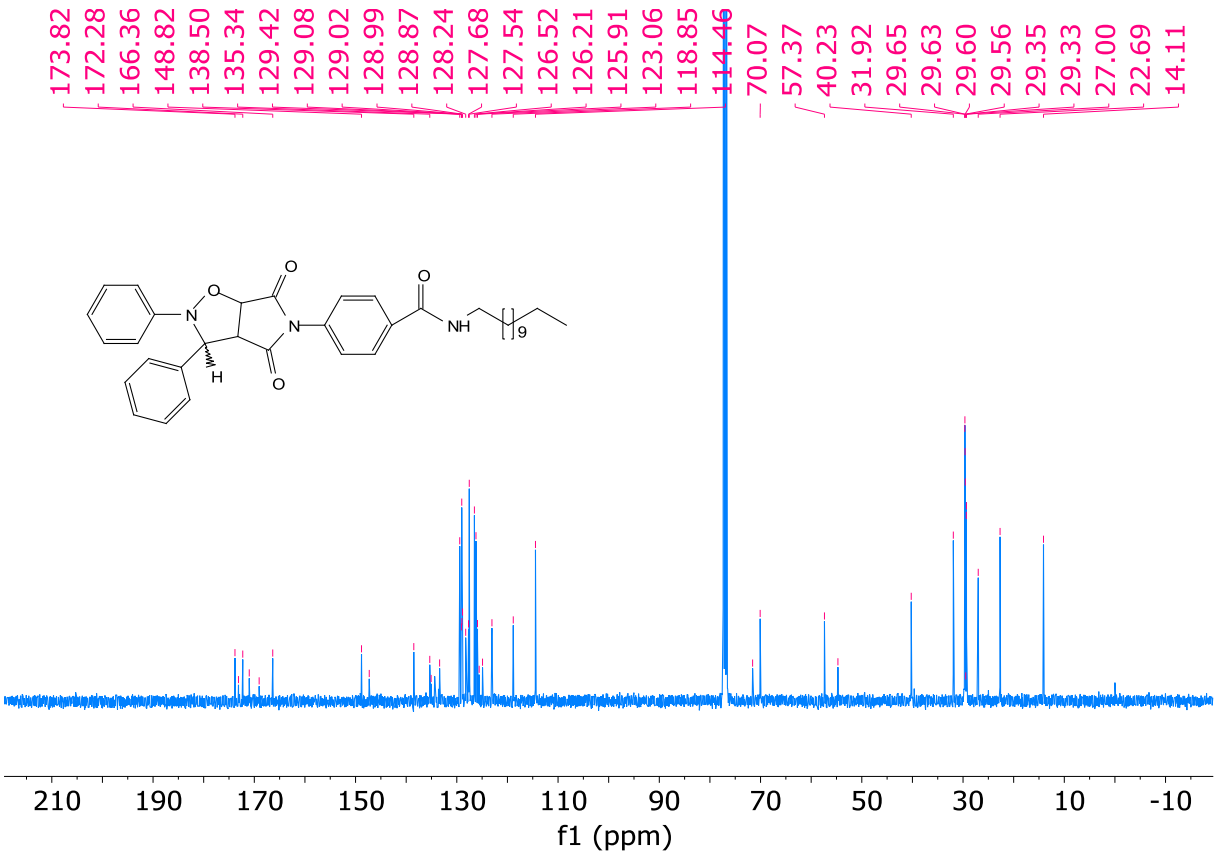
3b


179.11
175.06
173.60
148.46
138.68
134.48
134.08
129.06
128.92
128.83
128.78
128.75
128.10
127.52
126.65
124.82
122.81
119.04
114.50
71.11
69.70
57.24
54.59
39.02
38.78
33.65
33.58
27.17
26.25
26.20
26.15
26.03
24.10
O
O
N
O
N
O
OH
3
H
O
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

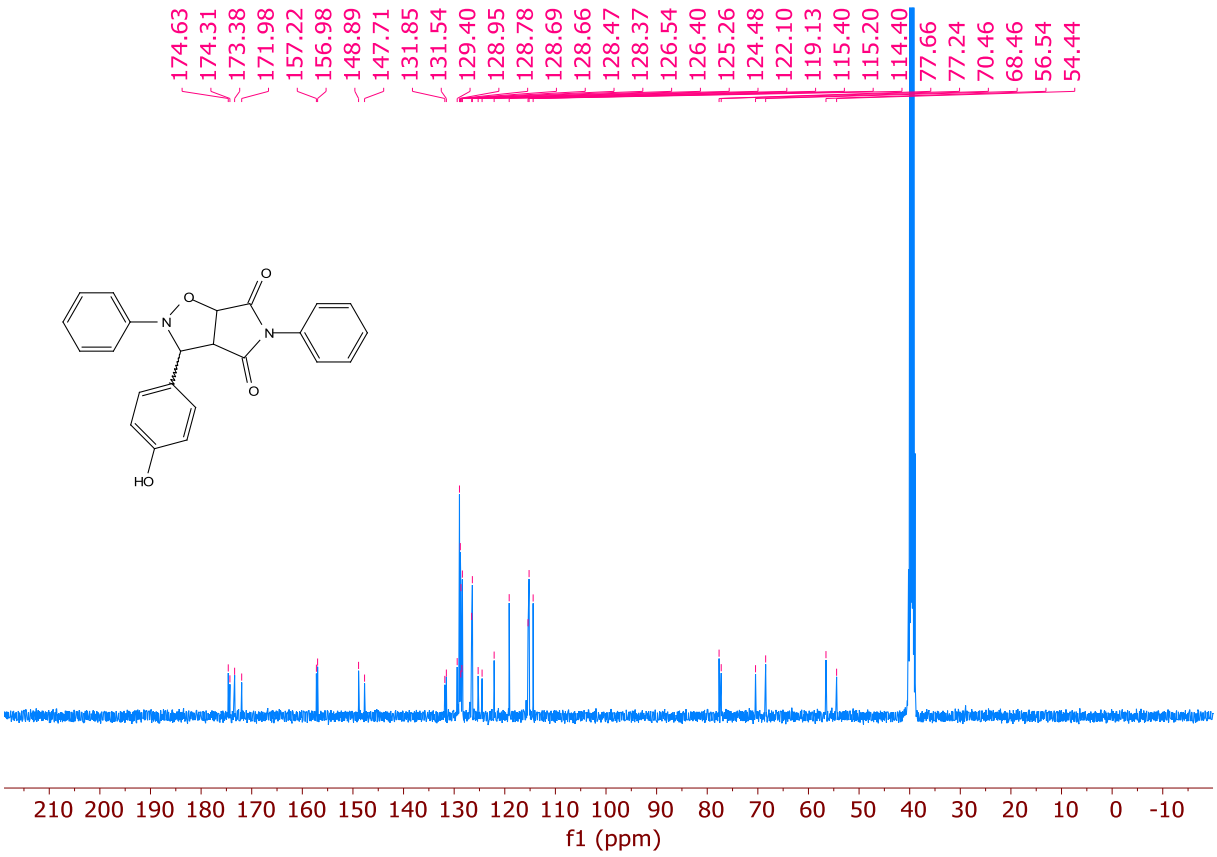
3c


179.47
175.08
173.63
148.40
138.68
134.04
129.00
128.90
128.81
128.74
128.71
128.08
127.54
126.69
124.81
122.77
119.14
114.58
71.15
69.73
57.24
54.60
39.35
39.13
33.97
29.31
29.25
29.16
29.02
27.56
26.79
26.64
24.68
O
O
N
O
N
O
OH
8
H
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

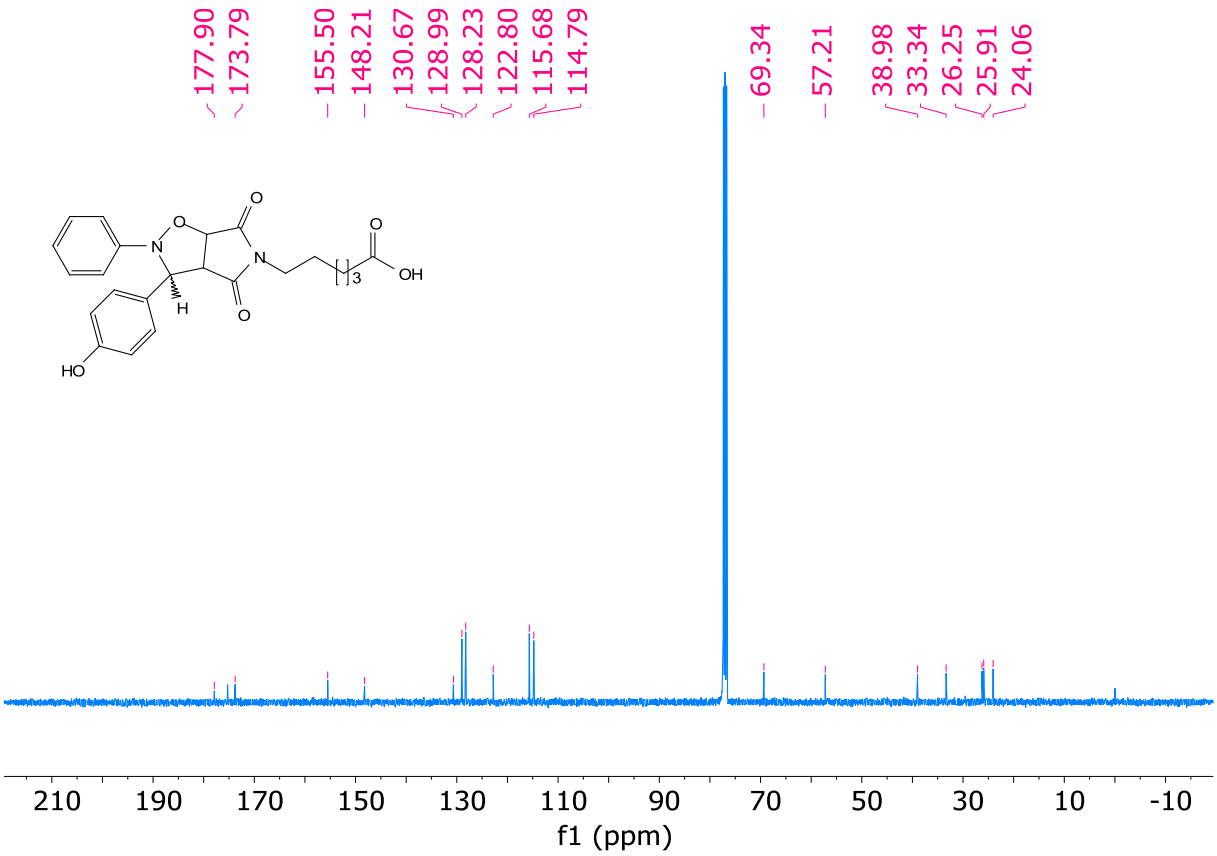
3d


173.82
172.28
166.36
148.82
138.50
135.34
129.42
129.08
129.02
128.99
128.87
128.24
127.68
127.54
126.52
126.21
125.91
123.06
118.85
114.46
70.07
57.37
40.23
31.92
29.65
29.63
29.60
29.56
29.35
29.33
27.00
22.69
14.11
O
O
N
N
O
NH
9
H
O
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

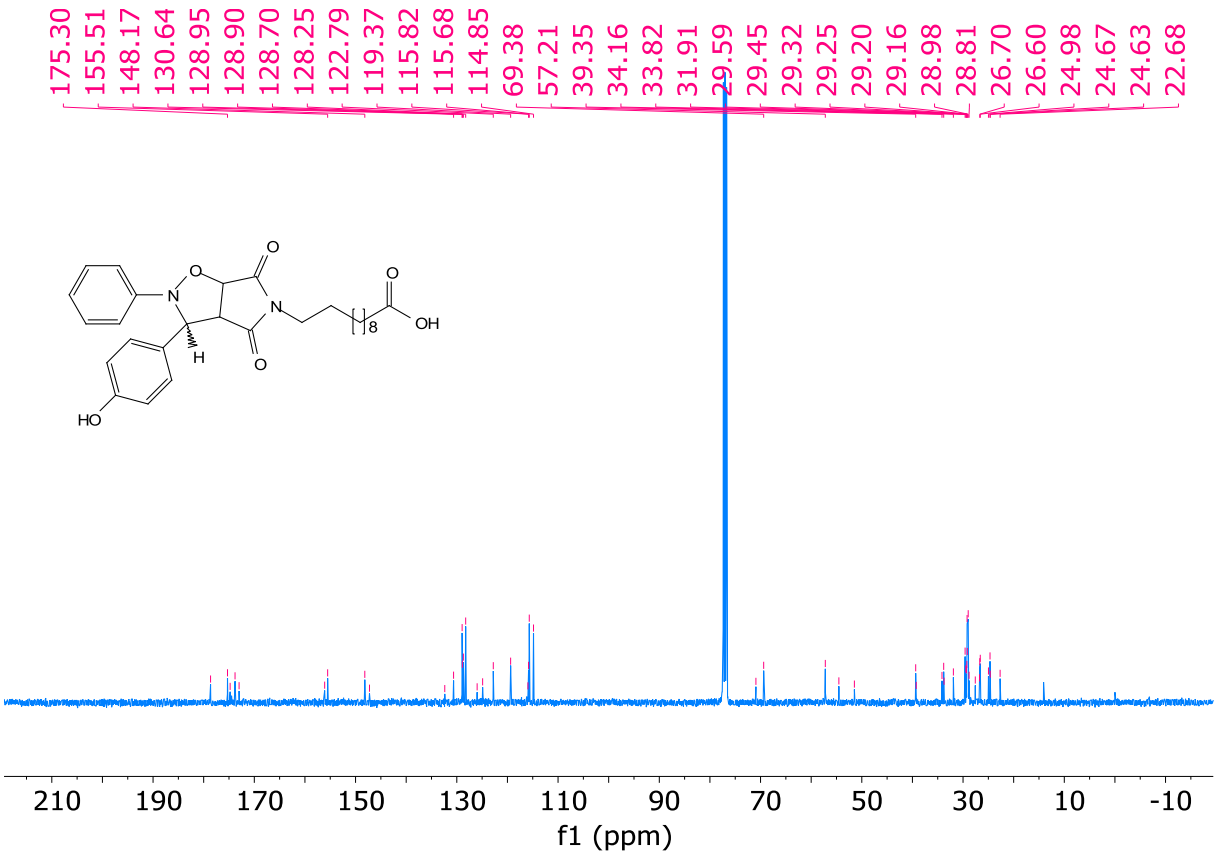
3e


174.63
174.31
173.38
171.98
157.22
156.98
148.89
147.71
131.85
131.54
129.40
128.95
128.78
128.69
128.66
128.47
128.37
126.54
126.40
125.26
124.48
122.10
119.13
115.40
115.20
114.40
77.66
77.24
70.46
68.46
56.54
54.44
O
N
O
N
O
HO
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

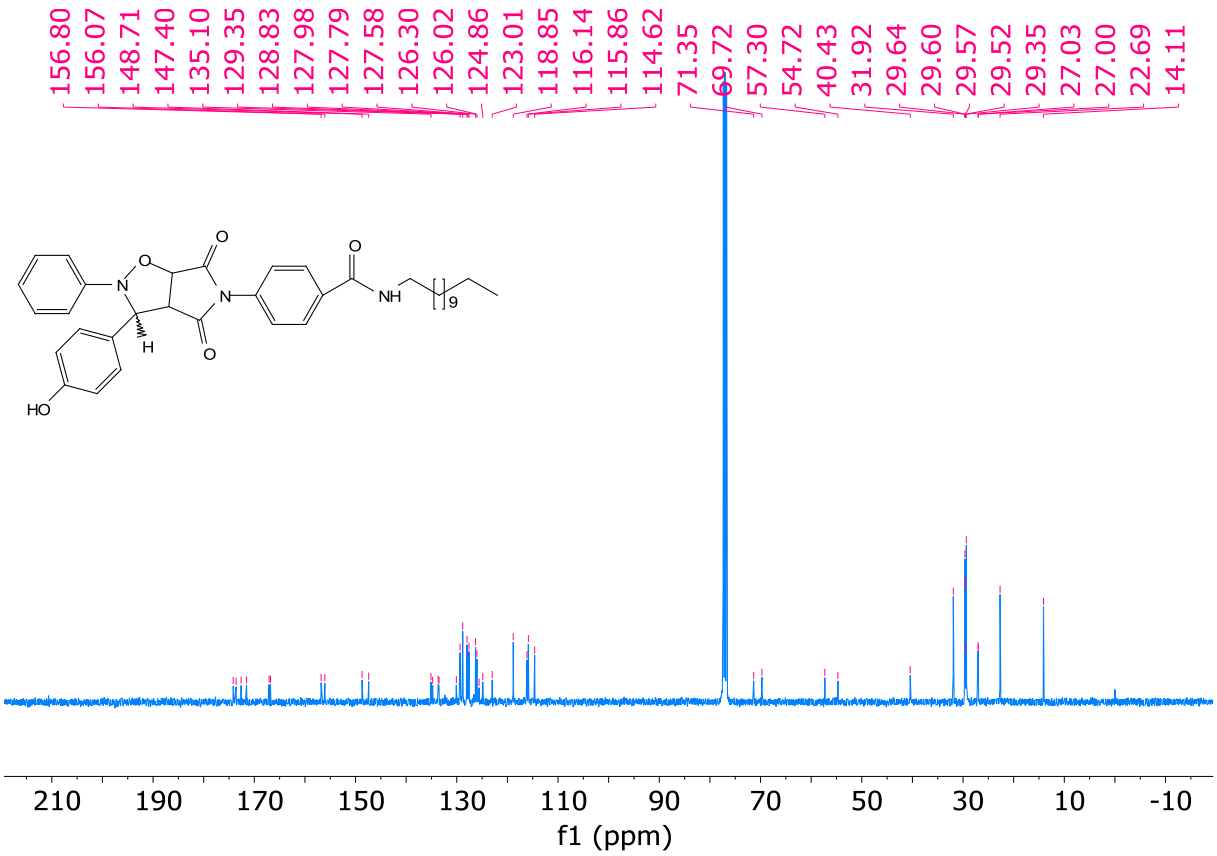
3f


177.90
173.79
155.50
148.21
130.67
128.99
128.23
122.80
115.68
114.79
69.34
57.21
38.98
33.34
26.25
25.91
24.06
O
N
O
N
O
OH
3
H
O
HO
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

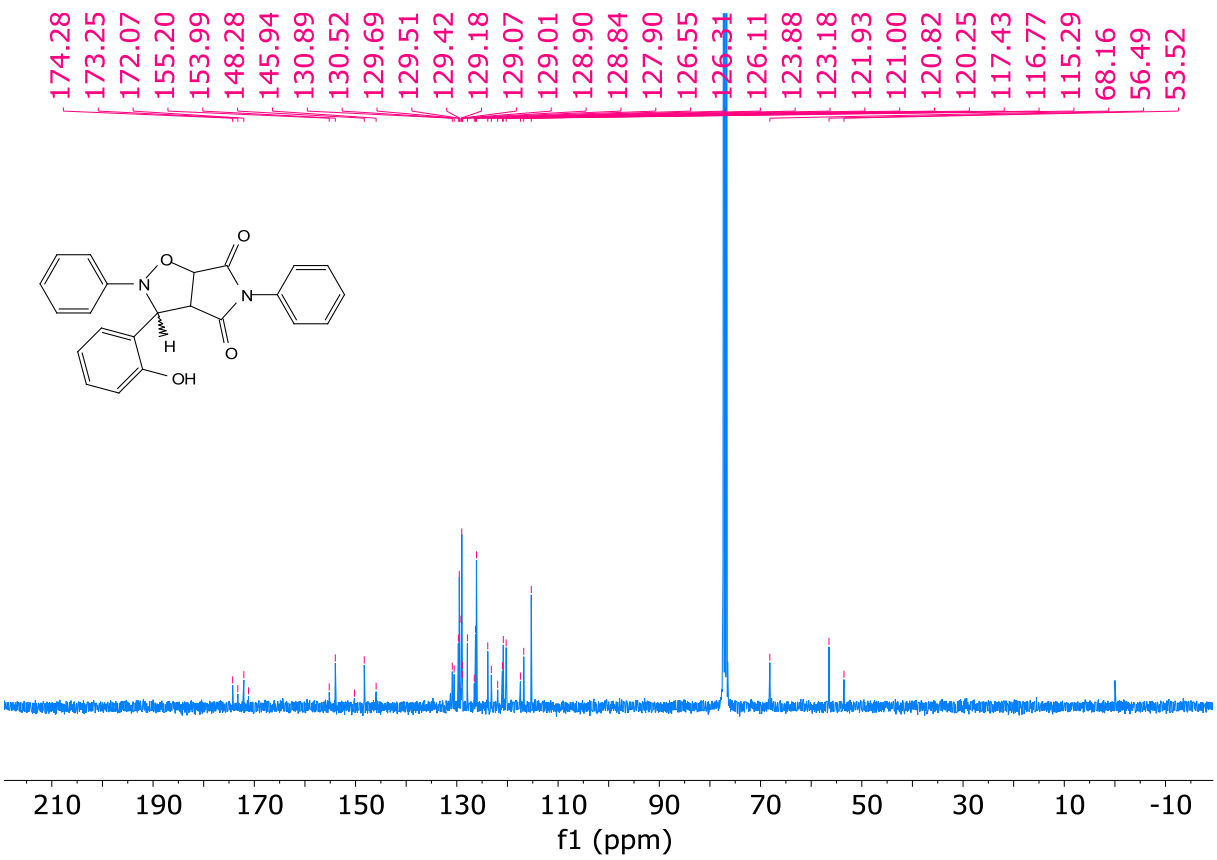
3g


175.30
155.51
148.17
130.64
128.95
128.90
128.70
128.25
122.79
119.37
115.82
115.68
114.85
69.38
57.21
39.35
34.16
33.82
31.91
29.59
29.45
29.32
29.25
29.20
29.16
28.98
28.81
26.70
26.60
24.98
24.67
24.63
22.68
O
O
N
O
N
O
OH
8
H
O
HO
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

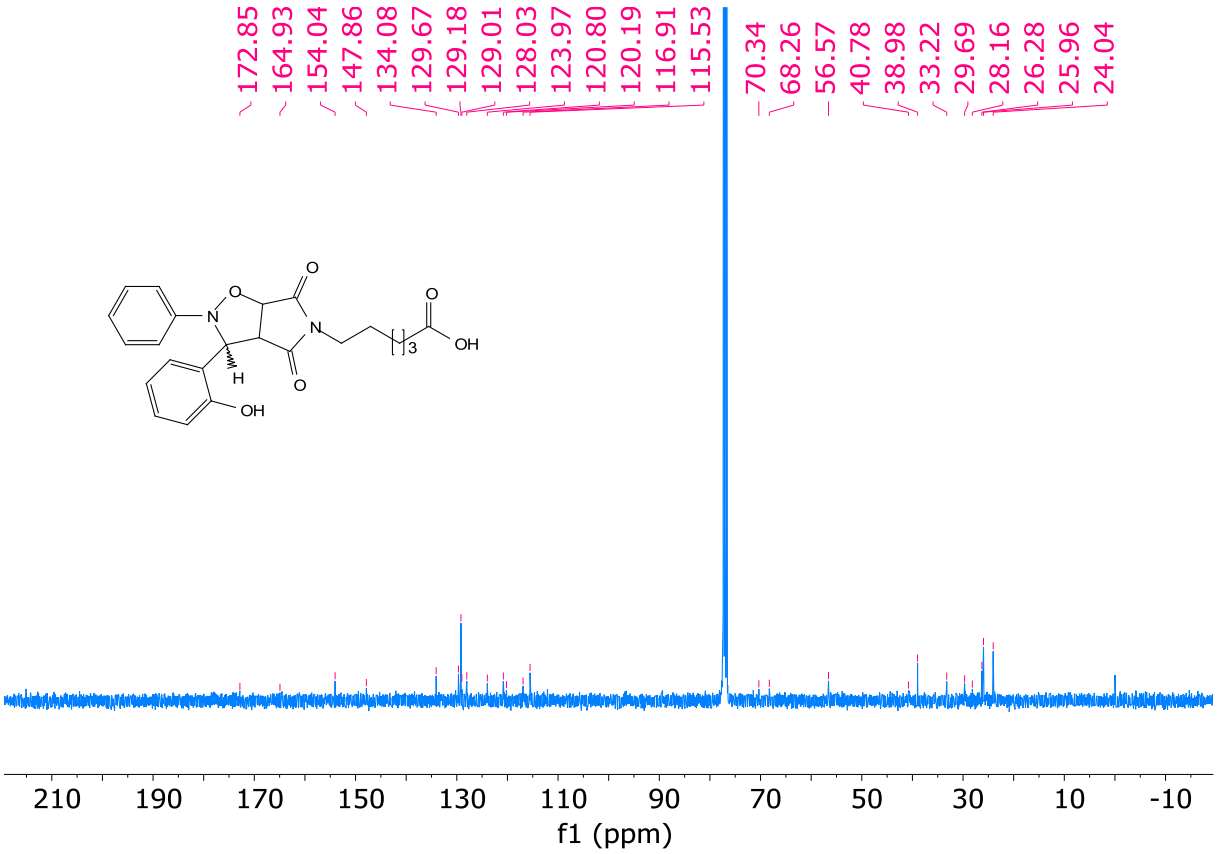
3h


156.80
156.07
148.71
147.40
135.10
129.35
128.83
127.98
127.79
127.58
126.30
126.02
124.86
123.01
118.85
116.14
115.86
114.62
71.35
69.72
57.30
54.72
40.43
31.92
29.64
29.60
29.57
29.52
29.35
27.03
27.00
22.69
14.11
O
O
N
O
N
O
NH
9
H
HO
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

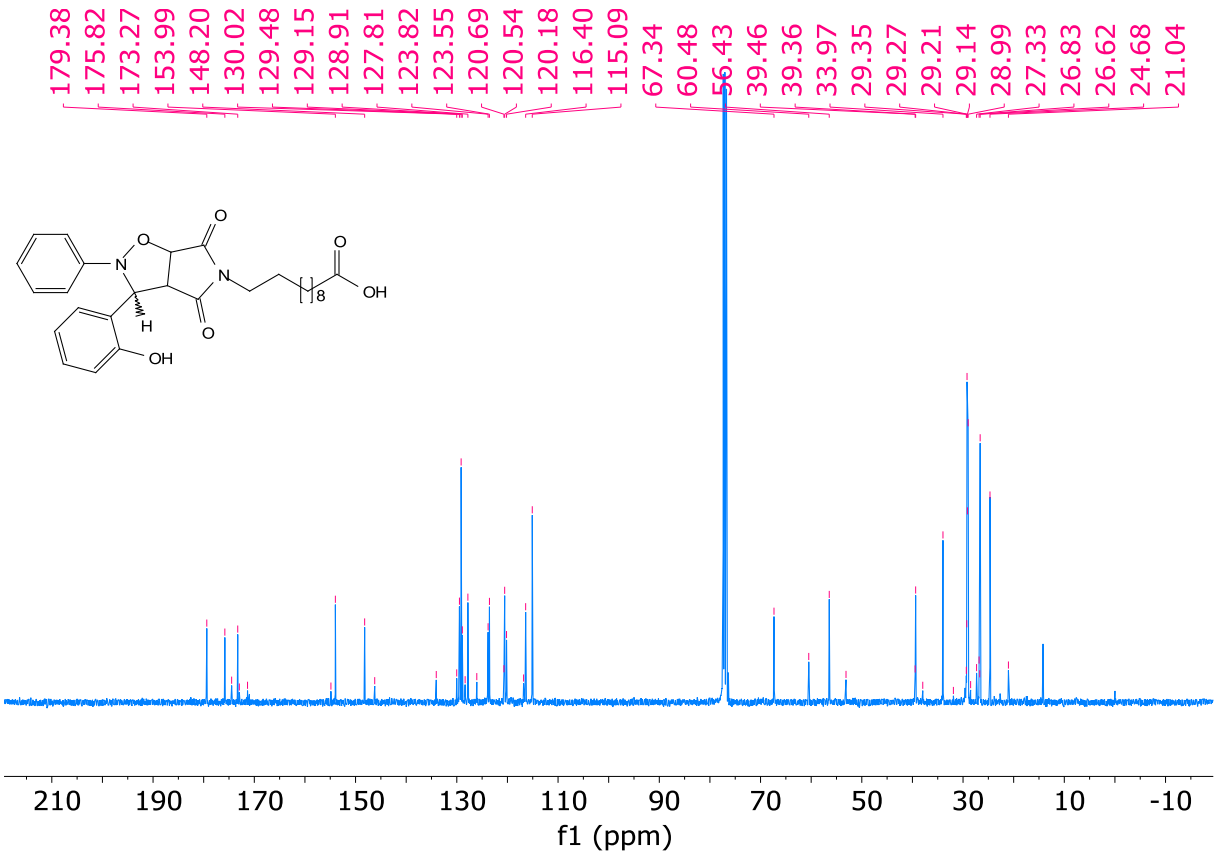
3i


174.28
173.25
172.07
155.20
153.99
148.28
145.94
130.89
130.52
129.69
129.51
129.42
129.18
129.07
129.01
128.90
128.84
127.90
126.55
126.31
126.11
123.88
123.18
121.93
121.00
120.82
120.25
117.43
116.77
115.29
68.16
56.49
53.52
O
N
O
N
O
H
OH
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

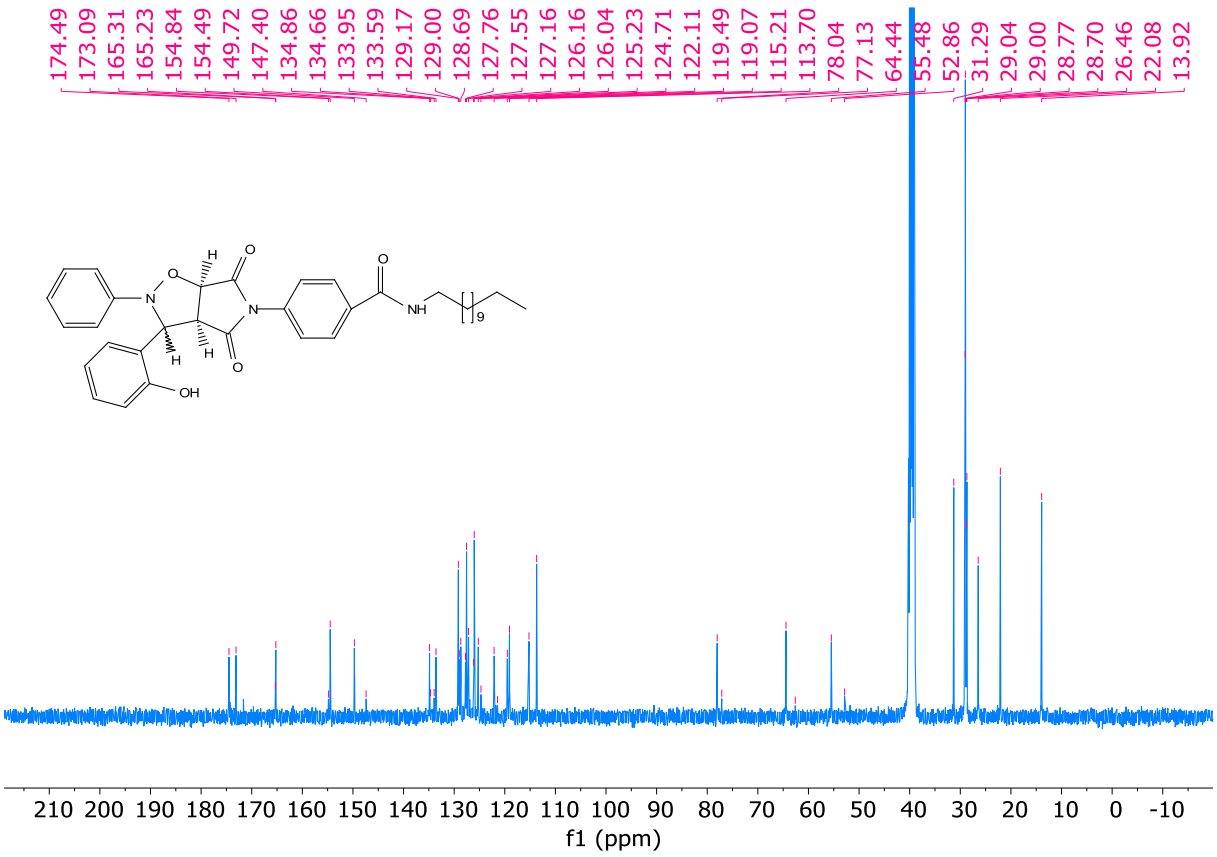
3j


172.85
164.93
154.04
147.86
134.08
129.67
129.18
129.01
128.03
123.97
120.80
120.19
116.91
115.53
70.34
68.26
56.57
40.78
38.98
33.22
29.69
28.16
26.28
25.96
24.04
O
N
O
O
N
O
OH
3
H
OH
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

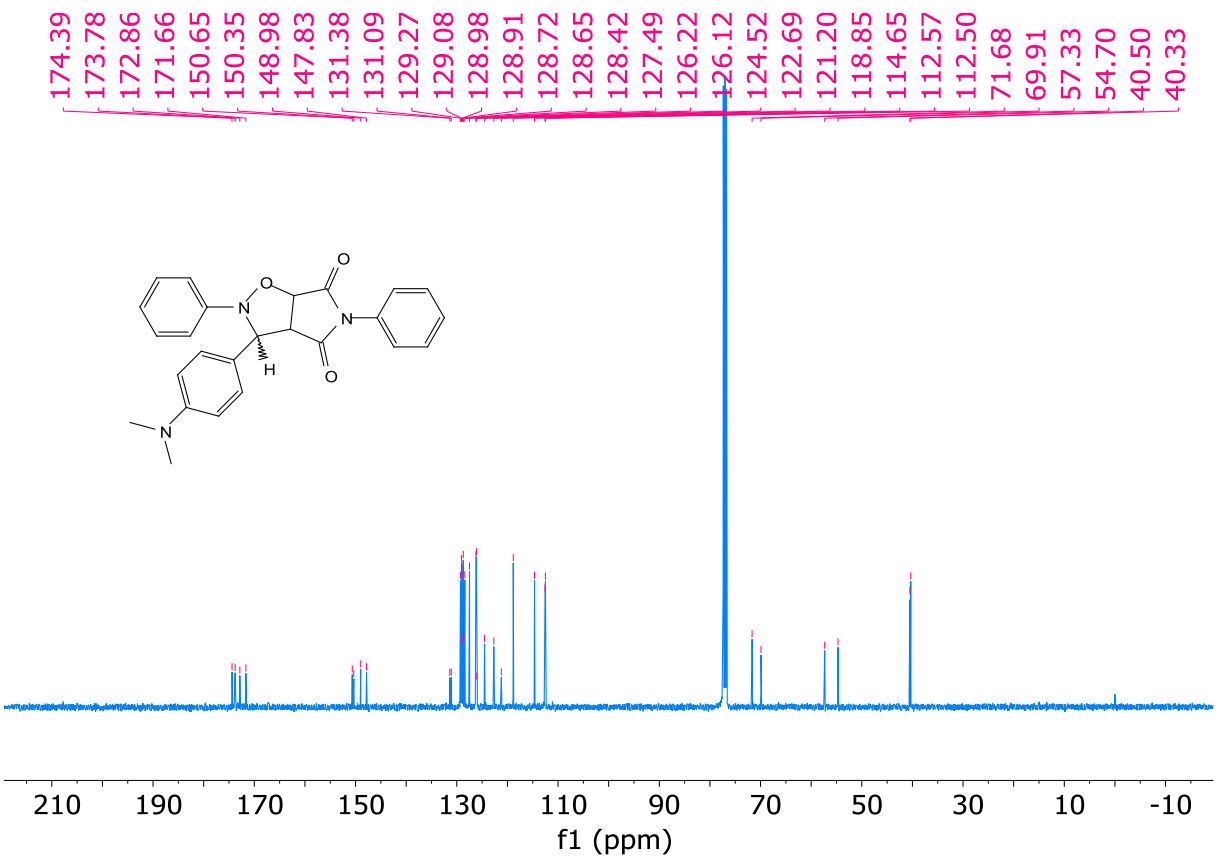
3k


179.38
175.82
173.27
153.99
148.20
130.02
129.48
129.15
128.91
127.81
123.82
123.55
120.69
120.54
120.18
116.40
115.09
67.34
60.48
56.43
39.46
39.36
33.97
29.35
29.27
29.21
29.14
28.99
27.33
26.83
26.62
24.68
21.04
O
O
N
N
O
O
8
OH
H
OH
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

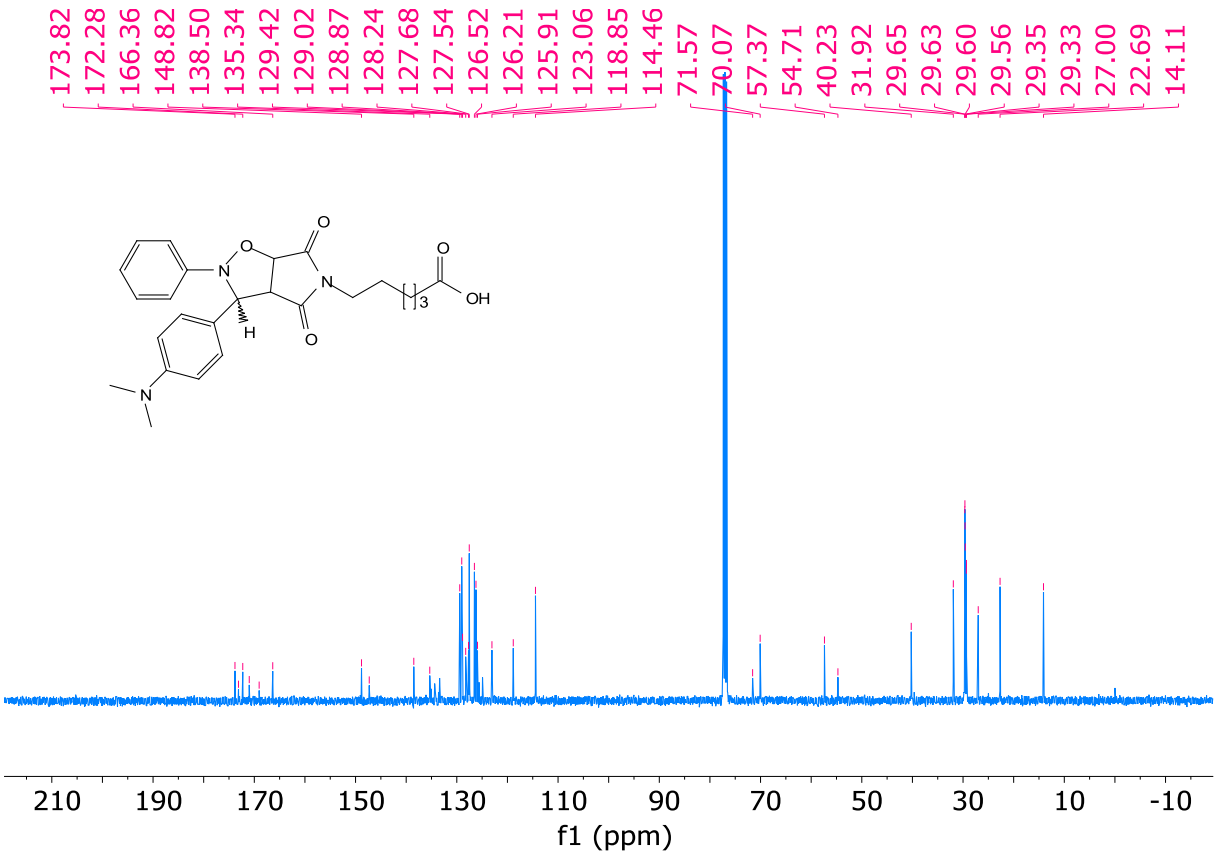
3l


174.49
173.09
165.31
165.23
154.84
154.49
149.72
147.40
134.86
134.66
133.95
133.59
129.17
129.00
128.69
127.76
127.55
127.16
126.16
126.04
125.23
124.71
122.11
119.49
119.07
115.21
113.70
78.04
77.13
64.44
55.48
52.86
31.29
29.04
29.00
28.77
28.70
26.46
22.08
13.92
O
H
O
N
N
O
O
NH
9
H
H
OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

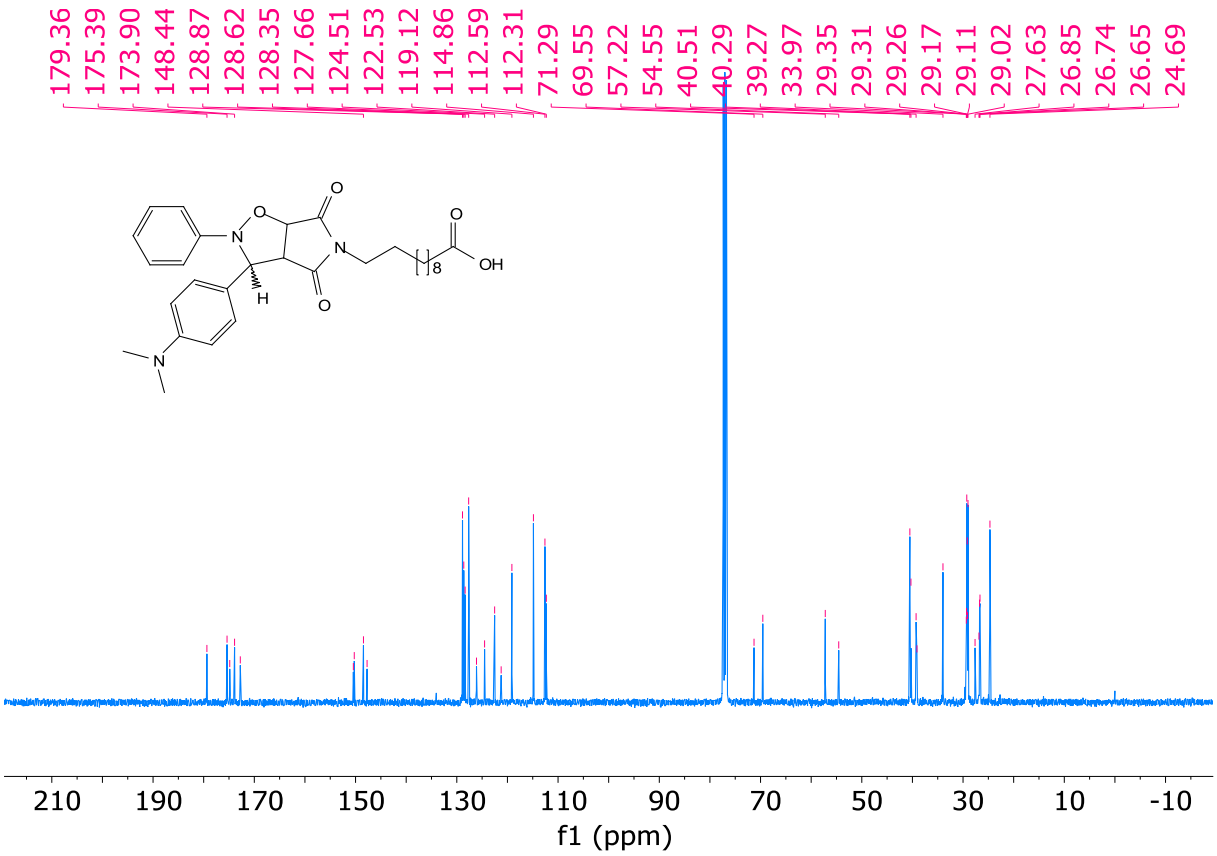
3m


174.39
173.78
172.86
171.66
150.65
150.35
148.98
147.83
131.38
131.09
129.27
129.08
128.98
128.91
128.72
128.65
128.42
127.49
126.22
126.12
124.52
122.69
121.20
118.85
114.65
112.57
112.50
71.68
69.91
57.33
54.70
40.50
40.33
O
N
O
N
O
H
N
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

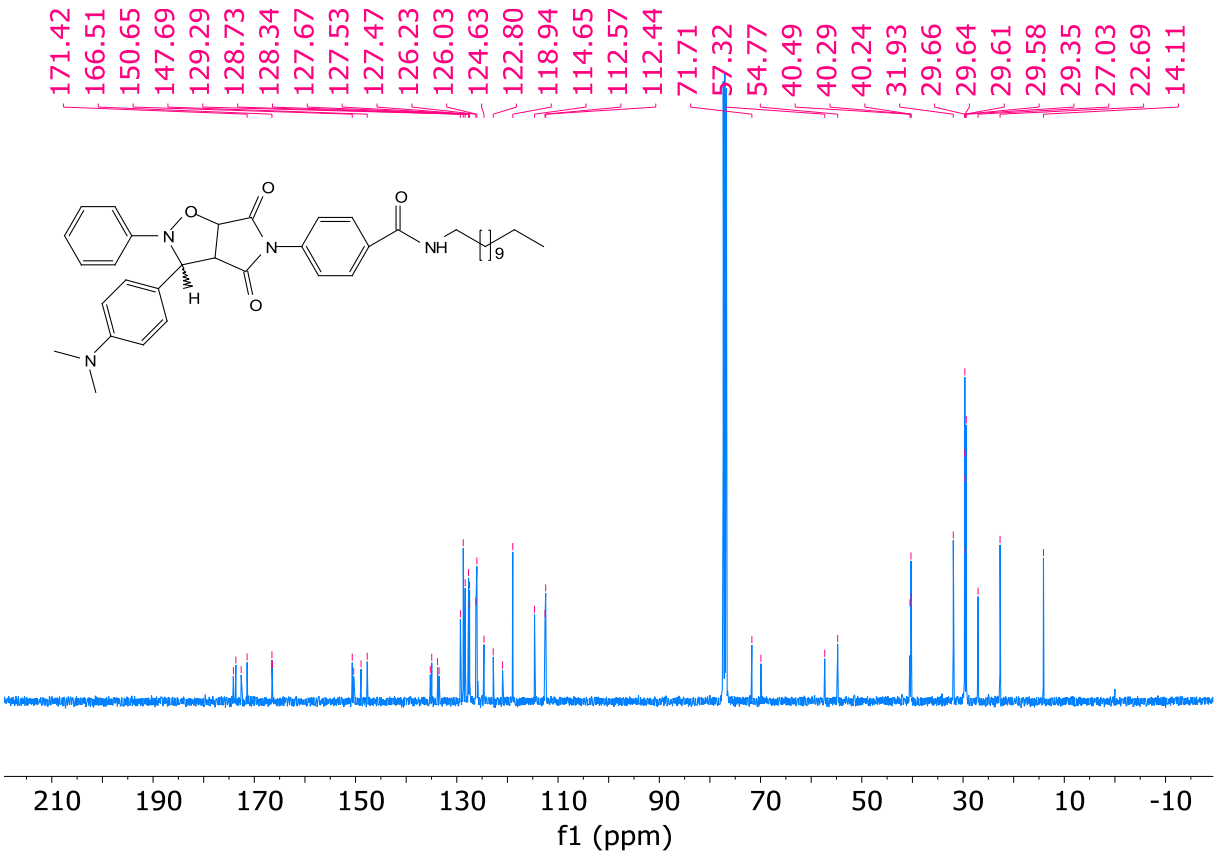
3n


173.82
172.28
166.36
148.82
138.50
135.34
129.42
129.02
128.87
128.24
127.68
127.54
126.52
126.21
125.91
123.06
118.85
114.46
71.57
70.07
57.37
54.71
40.23
31.92
29.65
29.63
29.60
29.56
29.35
29.33
27.00
22.69
14.11
O
N
O
O
N
O
OH
3
H
O
N
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

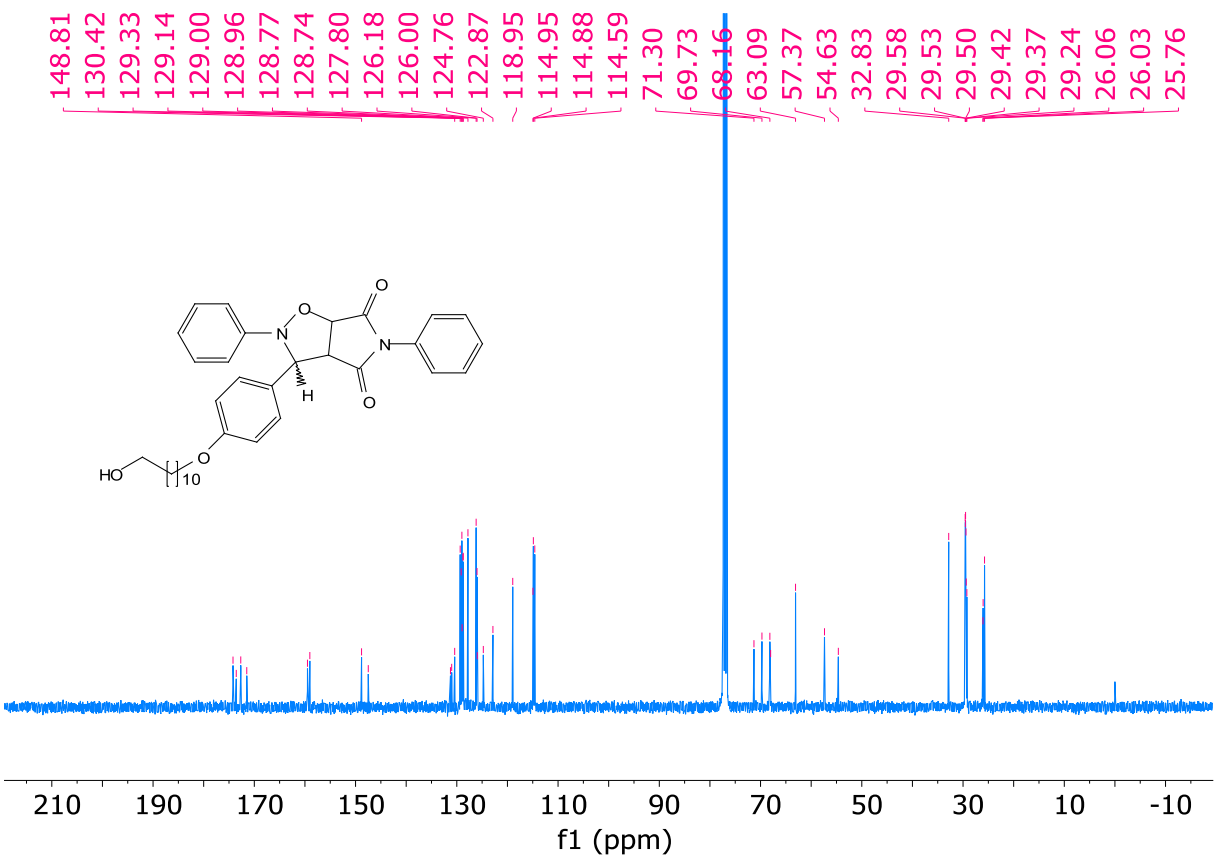
3o


179.36
175.39
173.90
148.44
128.87
128.62
128.35
127.66
124.51
122.53
119.12
114.86
112.59
112.31
71.29
69.55
57.22
54.55
40.51
40.29
39.27
33.97
29.35
29.31
29.26
29.17
29.11
29.02
27.63
26.85
26.74
26.65
24.69
O
O
N
O
N
8
OH
O
H
N
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

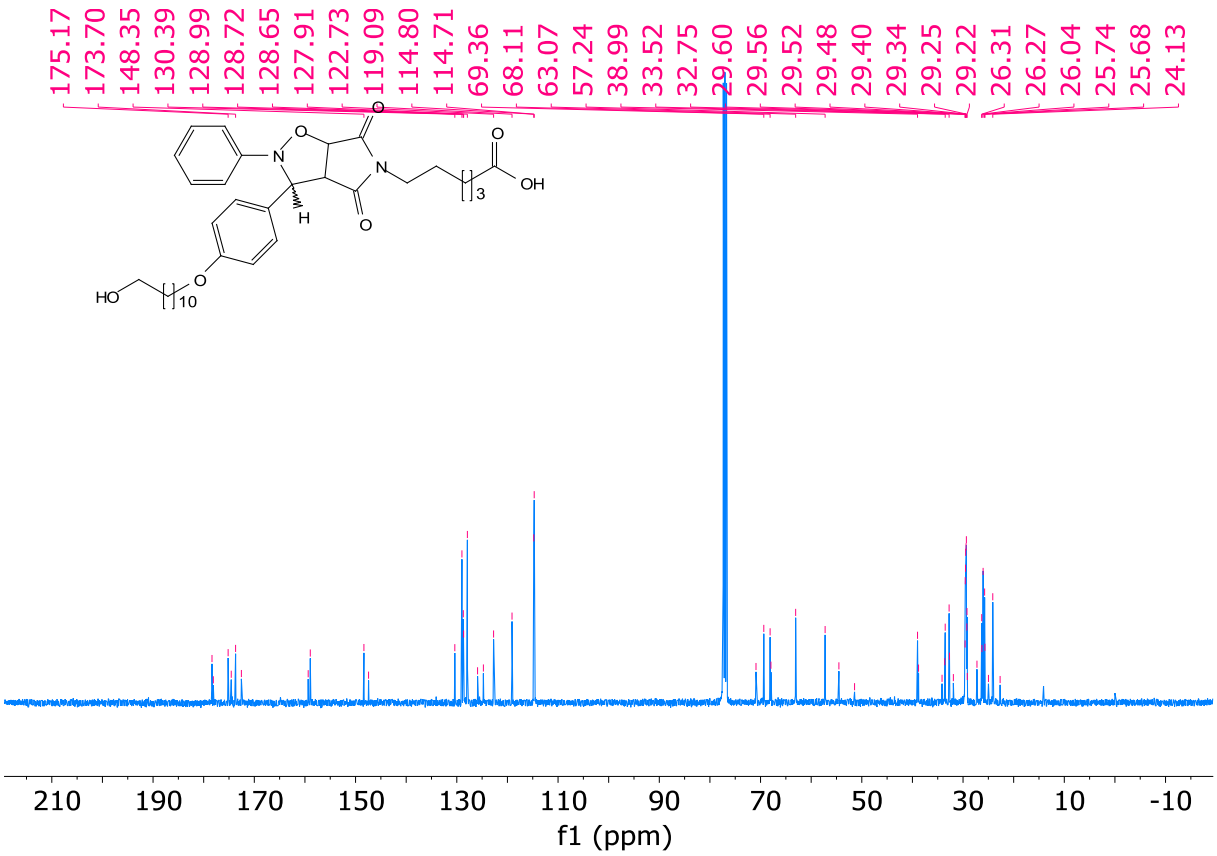
3p


171.42
166.51
150.65
147.69
129.29
128.73
128.34
127.67
127.53
127.47
126.23
126.03
124.63
122.80
118.94
114.65
112.57
112.44
71.71
57.32
54.77
40.49
40.29
40.24
31.93
29.66
29.64
29.61
29.58
29.35
27.03
22.69
14.11
O
O
N
N
O
NH
9
H
O
N
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

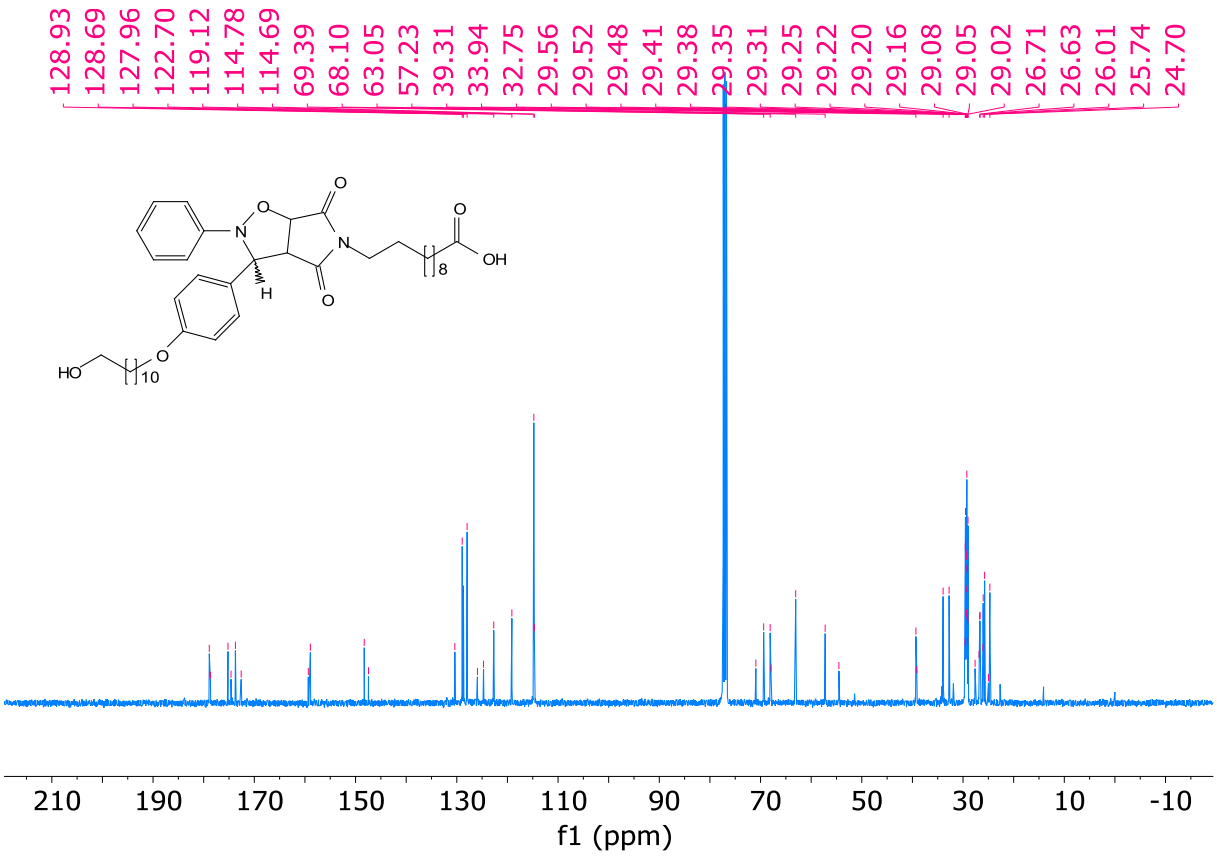
3q


148.81
130.42
129.33
129.14
129.00
128.96
128.77
128.74
127.80
126.18
126.00
124.76
122.87
118.95
114.95
114.88
114.59
71.30
69.73
68.16
63.09
57.37
54.63
32.83
29.58
29.53
29.50
29.42
29.37
29.24
26.06
26.03
25.76
O
N
O
N
O
H
HO
O
10
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

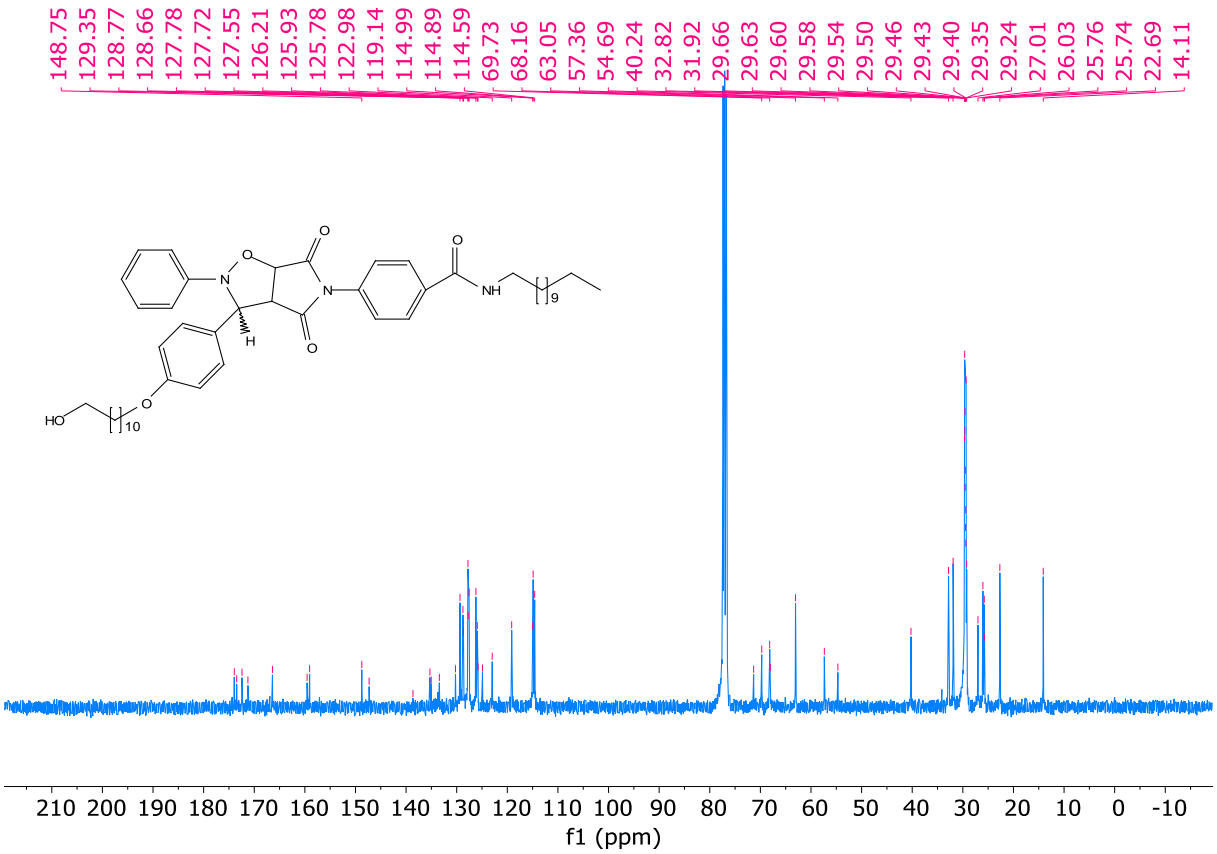
3r


175.17
173.70
148.35
130.39
128.99
128.72
128.65
127.91
122.73
119.09
114.80
114.71
69.36
68.11
63.07
57.24
38.99
33.52
32.75
29.60
29.56
29.52
29.48
29.40
29.34
29.25
29.22
26.31
26.27
26.04
25.74
25.68
24.13
O
N
O
N
O
OH
3
H
O
HO
10
O
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

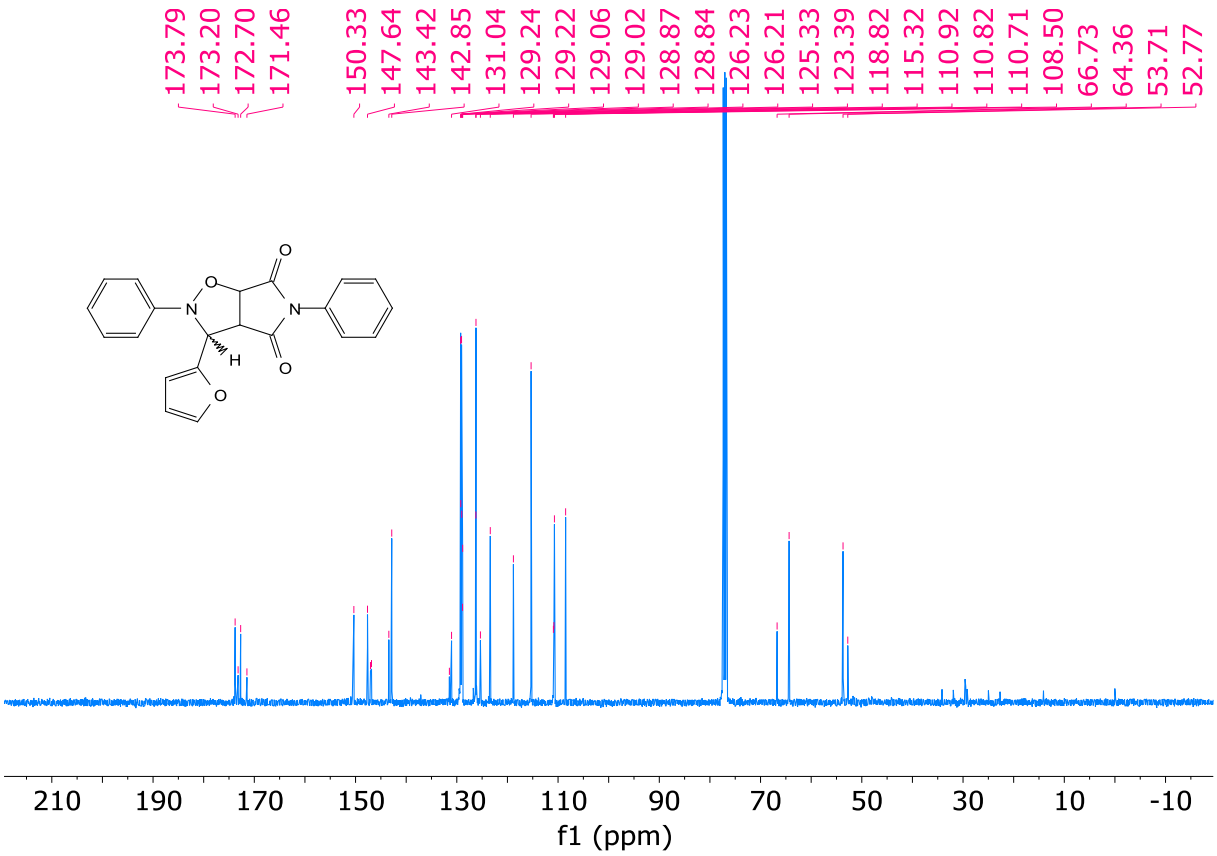
3s


128.93
128.69
127.96
122.70
119.12
114.78
114.69
69.39
68.10
63.05
57.23
39.31
33.94
32.75
29.56
29.52
29.48
29.41
29.38
29.35
29.31
29.25
29.22
29.20
29.16
29.08
29.05
29.02
26.71
26.63
26.01
25.74
24.70
O
N
O
O
N
OH
8
H
O
HO
10
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

3t

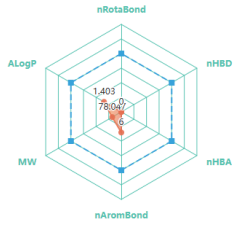

148.75
129.35
128.77
128.66
127.78
127.72
127.55
126.21
125.93
125.78
122.98
119.14
114.99
114.89
114.59
69.73
68.16
63.05
57.36
54.69
40.24
32.82
31.92
29.66
29.63
29.60
29.58
29.54
29.50
29.46
29.43
29.40
29.35
29.24
27.01
26.03
25.76
25.74
22.69
14.11
O
N
O
N
O
O
H
NH
9
HO
10
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3u


173.79
173.20
172.70
171.46
150.33
147.64
143.42
142.85
131.04
129.24
129.22
129.06
129.02
128.87
128.84
126.23
126.21
125.33
123.39
118.82
115.32
110.92
110.82
110.71
108.50
66.73
64.36
53.71
52.77
O
O
N
N
O
H
O
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

Pesticide-likeness

Pesticide-likeness Radar



Pesticide-likeness Score

Type	RDL	QEP	GAU
Fungicide Likeness	3.778	0.473	6.326
Herbicide Likeness	4.179	0.396	4.596
Insecticide Likeness	4.581	0.469	3.312

Environmental Risk

nAromBond	6	Biodegradability	NON Readily Biodegradable
Persistence (air)	0.023	Persistence (soil)	22.917
Persistence (water)	7.122	Persistence (sediment)	332

Ecological Risk

Mammals toxicity	Low Toxic	
Mallard duck toxicity	High Toxic	
Bobwhite quail toxicity	High Toxic	
Zebra finch toxicity	Low Toxic	
Algae toxicity	4.224	
Fish toxicity	3.887	
Daphnia toxicity	24.622	
Bee toxicity	Non Toxic	
Mysid toxicity	5.248	
Earthworm toxicity	4.783	
Fish BCF	0.983	

Figure S1: a) Results for the benzene calculated by *ChemFREE*

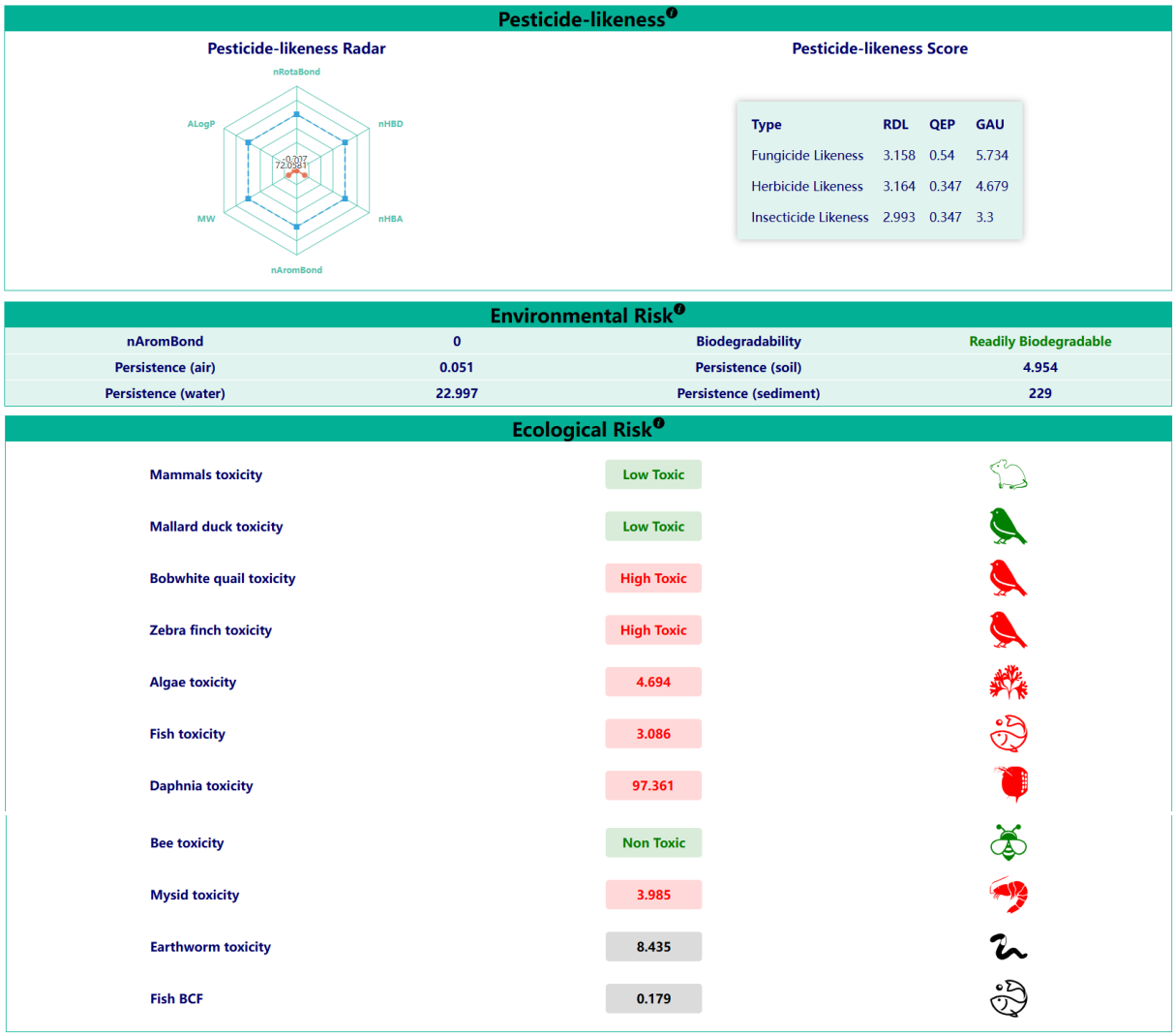
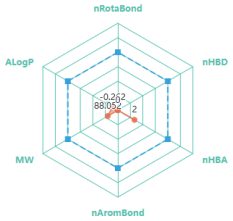


Figure S1: b) Results for the THF calculated by *ChemFREE*

Pesticide-likeness

Pesticide-likeness Radar



Pesticide-likeness Score

Type	RDL	QEP	GAU
Fungicide Likeness	1.795	0.649	5.719
Herbicide Likeness	3.193	0.383	5.306
Insecticide Likeness	3.135	0.436	4.332

Environmental Risk

nAromBond	0	Biodegradability	Readily Biodegradable
Persistence (air)	0.028	Persistence (soil)	16.207
Persistence (water)	22.997	Persistence (sediment)	127

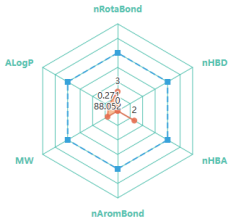
Ecological Risk

Mammals toxicity	Low Toxic	
Mallard duck toxicity	Low Toxic	
Bobwhite quail toxicity	High Toxic	
Zebra finch toxicity	Low Toxic	
Algae toxicity	4.405	
Fish toxicity	2.376	
Daphnia toxicity	110.881	
Bee toxicity	Non Toxic	
Mysid toxicity	4.053	
Earthworm toxicity	4.127	
Fish BCF	0.111	

Figure S1: c) Results for the dioxane calculated by *ChemFREE*

Pesticide-likeness

Pesticide-likeness Radar



Pesticide-likeness Score

Type	RDL	QEP	GAU
Fungicide Likeness	1.915	0.693	5.461
Herbicide Likeness	2.699	0.444	5.575
Insecticide Likeness	2.483	0.574	4.878

Environmental Risk

nAromBond	0	Biodegradability	Readily Biodegradable
Persistence (air)	0.015	Persistence (soil)	10.672
Persistence (water)	2.883	Persistence (sediment)	23

Ecological Risk

Mammals toxicity	Low Toxic	
Mallard duck toxicity	Low Toxic	
Bobwhite quail toxicity	High Toxic	
Zebra finch toxicity	High Toxic	
Algae toxicity	3.334	
Fish toxicity	3.47	
Daphnia toxicity	314.496	
Bee toxicity	Non Toxic	
Mysid toxicity	4.992	
Earthworm toxicity	40.414	
Fish BCF	0.251	

Figure S1: d) Results for the EtOAc calculated by *ChemFREE*

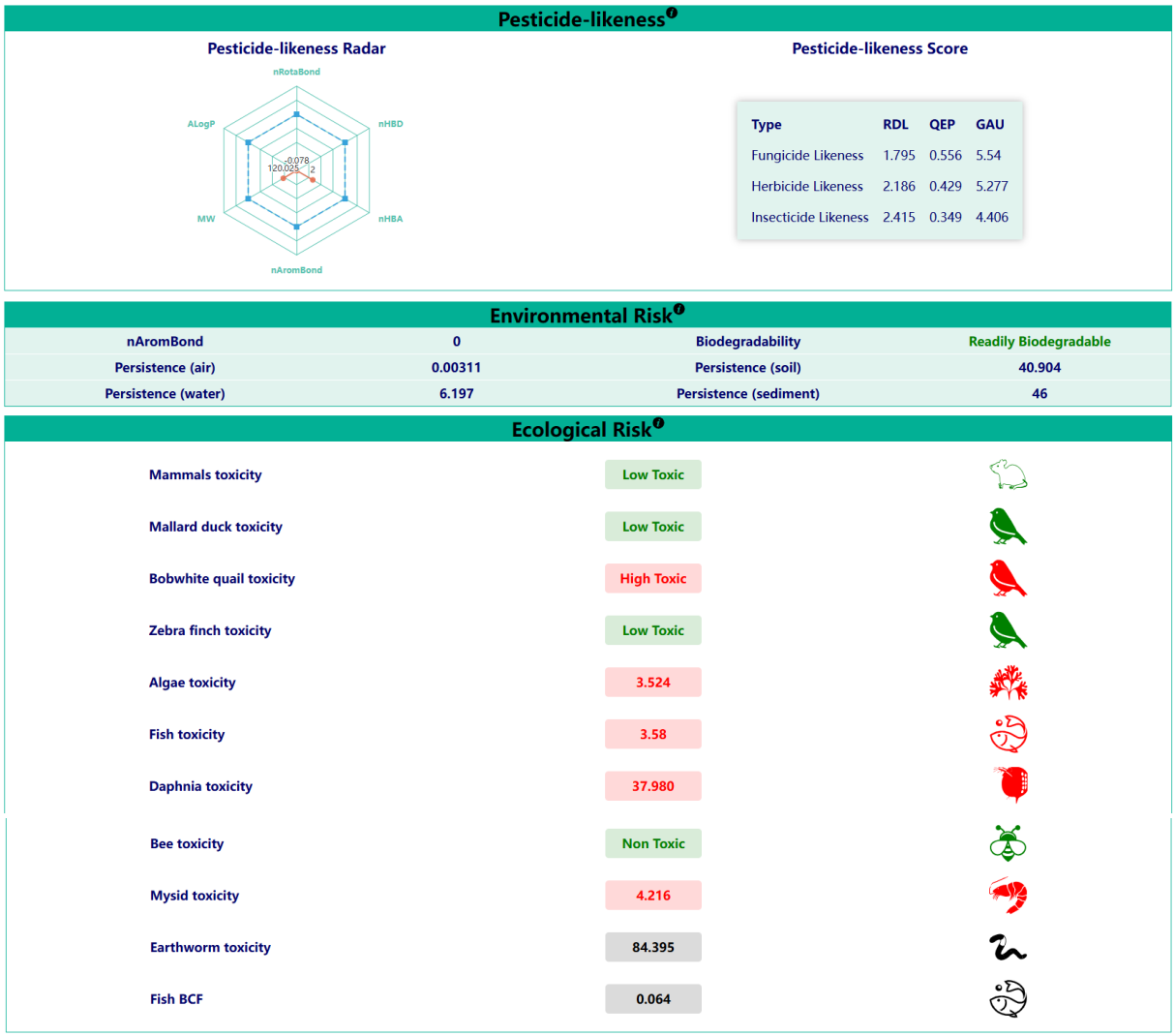
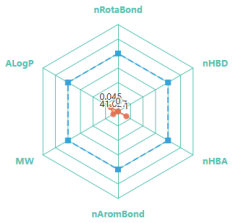


Figure S1: e) Results for the sulfolane calculated by *ChemFREE*

Pesticide-likeness

Pesticide-likeness Radar



Pesticide-likeness Score

Type	RDL	QEP	GAU
Fungicide Likeness	3.465	0.598	6.156
Herbicide Likeness	2.847	0.368	5.025
Insecticide Likeness	3.445	0.425	3.125

Environmental Risk

nAromBond	0	Biodegradability	Readily Biodegradable
Persistence (air)	0.00201	Persistence (soil)	22.917
Persistence (water)	22.997	Persistence (sediment)	46

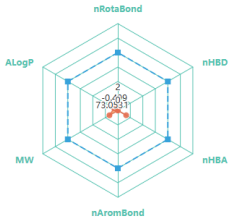
Ecological Risk

Mammals toxicity	Low Toxic	
Mallard duck toxicity	High Toxic	
Bobwhite quail toxicity	High Toxic	
Zebra finch toxicity	Low Toxic	
Algae toxicity	NaN	
Fish toxicity	3.596	
Daphnia toxicity	28.124	
Bee toxicity	Toxic	
Mysid toxicity	5.074	
Earthworm toxicity	16.803	
Fish BCF	0.250	

Figure S1: f) Results for the MeCN calculated by *ChemFREE*

Pesticide-likeness

Pesticide-likeness Radar



Pesticide-likeness Score

Type	RDL	QEP	GAU
Fungicide Likeness	2.734	0.584	5.77
Herbicide Likeness	2.48	0.382	5.415
Insecticide Likeness	1.866	0.413	3.438

Environmental Risk

nAromBond	0	Biodegradability	NON Readily Biodegradable
Persistence (air)	0.013	Persistence (soil)	4.954
Persistence (water)	4.191	Persistence (sediment)	46

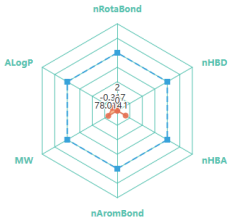
Ecological Risk

Mammals toxicity	Low Toxic	
Mallard duck toxicity	High Toxic	
Bobwhite quail toxicity	High Toxic	
Zebra finch toxicity	High Toxic	
Algae toxicity	4.009	
Fish toxicity	2.644	
Daphnia toxicity	387.173	
Bee toxicity	Toxic	
Mysid toxicity	4.84	
Earthworm toxicity	25.959	
Fish BCF	0.103	

Figure S1: g) Results for the DMFcalculated by *ChemFREE*

Pesticide-likeness

Pesticide-likeness Radar



Pesticide-likeness Score

Type	RDL	QEP	GAU
Fungicide Likeness	2.734	0.614	5.507
Herbicide Likeness	2.48	0.392	4.746
Insecticide Likeness	1.866	0.442	3.571

Environmental Risk

nAromBond	0	Biodegradability	Readily Biodegradable
Persistence (air)	0.021	Persistence (soil)	22.917
Persistence (water)	2.529	Persistence (sediment)	46

Ecological Risk

Mammals toxicity	Low Toxic	
Mallard duck toxicity	High Toxic	
Bobwhite quail toxicity	High Toxic	
Zebra finch toxicity	Low Toxic	
Algae toxicity	5.023	
Fish toxicity	3.359	
Daphnia toxicity	9763.896	
Bee toxicity	Non Toxic	
Mysid toxicity	4.361	
Earthworm toxicity	80.385	
Fish BCF	0.116	

Figure S1: h) Results for the DMSO calculated by *ChemFREE*

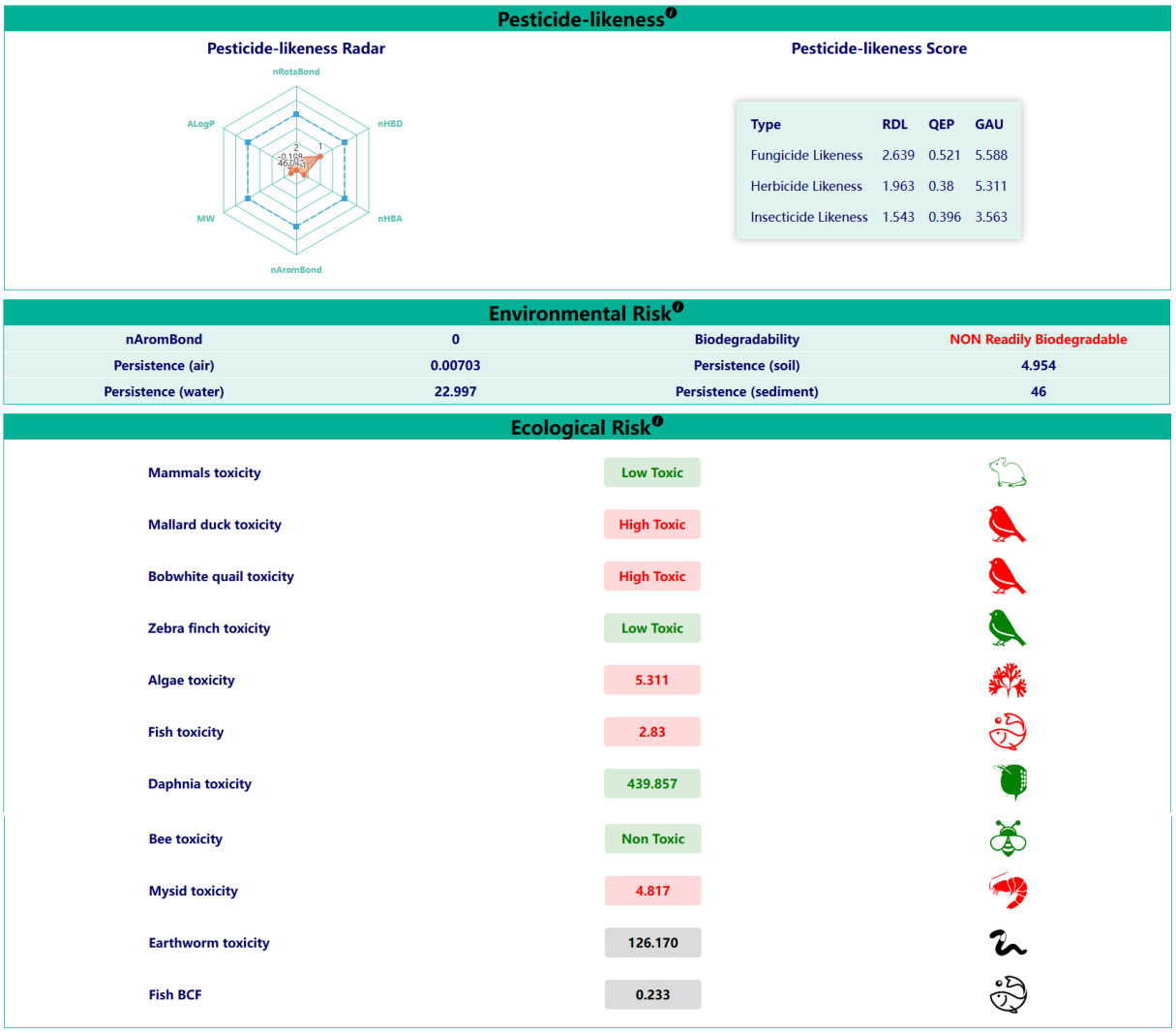


Figure S1: i) Results for the EtOH calculated by *ChemFREE*

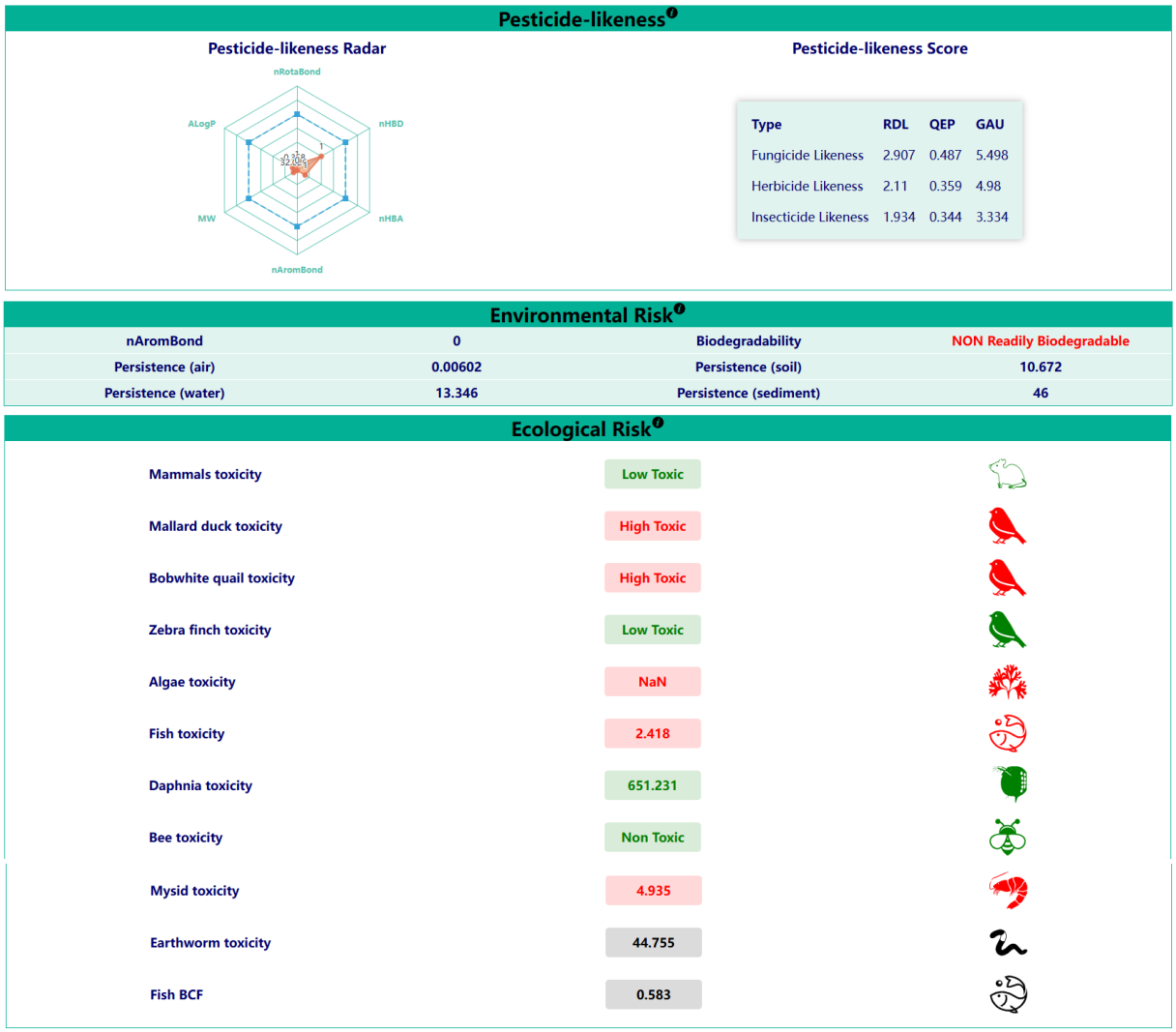
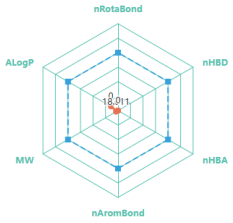


Figure S1: j) Results for the MeOH calculated by *ChemFREE*

Pesticide-likeness

Pesticide-likeness Radar



Pesticide-likeness Score

Type	RDL	QEP	GAU
Fungicide Likeness	0.0	0.436	5.626
Herbicide Likeness	0.0	0.317	4.314
Insecticide Likeness	0.0	0.385	3.254

Environmental Risk

nAromBond	0	Biodegradability	NON Readily Biodegradable
Persistence (air)	0.00676	Persistence (soil)	Not classifiable
Persistence (water)	15.794	Persistence (sediment)	Not classifiable

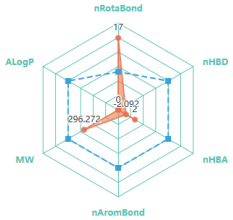
Ecological Risk

Mammals toxicity	Low Toxic	
Mallard duck toxicity	High Toxic	
Bobwhite quail toxicity	High Toxic	
Zebra finch toxicity	High Toxic	
Algae toxicity	NaN	
Fish toxicity	3.412	
Daphnia toxicity	1119.788	
Bee toxicity	Low Toxic	
Mysid toxicity	5.326	
Earthworm toxicity	Not classifiable	
Fish BCF	Not classifiable	

Figure S1: k) Results for the water calculated by *ChemFREE*

Pesticide-likeness

Pesticide-likeness Radar



Pesticide-likeness Score

Type	RDL	QEP	GAU
Fungicide Likeness	0.0	0.0	4.74
Herbicide Likeness	0.0	0.386	4.764
Insecticide Likeness	0.0	0.323	4.84

Environmental Risk

nAromBond	0	Biodegradability	Readily Biodegradable
Persistence (air)	1.019	Persistence (soil)	22.918
Persistence (water)	7.075	Persistence (sediment)	13

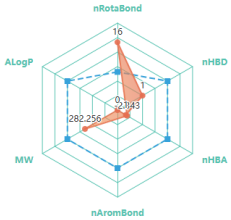
Ecological Risk

Mammals toxicity	Low Toxic	
Mallard duck toxicity	Low Toxic	
Bobwhite quail toxicity	Low Toxic	
Zebra finch toxicity	High Toxic	
Algae toxicity	7.003	
Fish toxicity	5.843	
Daphnia toxicity	0.28840	
Bee toxicity	Non Toxic	
Mysid toxicity	6.773	
Earthworm toxicity	50.969	
Fish BCF	1.633	

Figure S1: l) Results for the methyl oleate calculated by *ChemFREE*

Pesticide-likeness

Pesticide-likeness Radar



Pesticide-likeness Score

Type	RDL	QEP	GAU
Fungicide Likeness	0.734	0.168	4.832
Herbicide Likeness	0.0	0.36	5.139
Insecticide Likeness	0.0	0.267	4.526

Environmental Risk

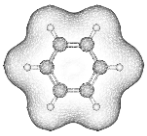
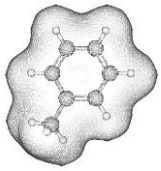
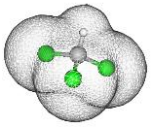
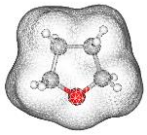
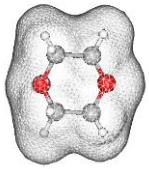
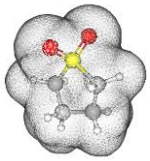
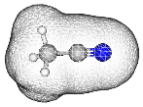
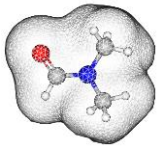
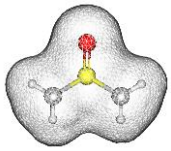
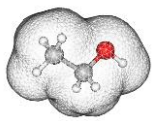
nAromBond	0	Biodegradability	Readily Biodegradable
Persistence (air)	0.837	Persistence (soil)	22.918
Persistence (water)	1071.741	Persistence (sediment)	13

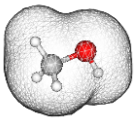
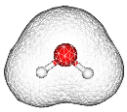
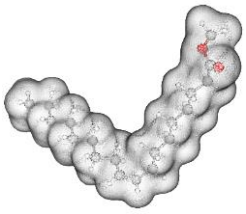
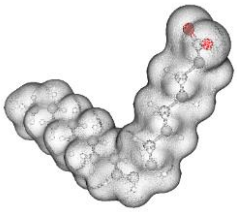
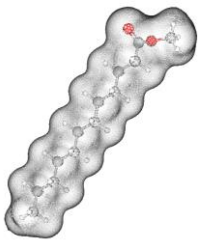
Ecological Risk

Mammals toxicity	Low Toxic	
Mallard duck toxicity	Low Toxic	
Bobwhite quail toxicity	Low Toxic	
Zebra finch toxicity	High Toxic	
Algae toxicity	7.367	
Fish toxicity	5.657	
Daphnia toxicity	0.28962	
Bee toxicity	Non Toxic	
Mysid toxicity	5.8	
Earthworm toxicity	83.958	
Fish BCF	1.860	

Figure S1: m) Results for the oleic acid calculated by *ChemFREE*

Table 1S: Polarizabilities of the solvents.[a]

Entry	Solvent	Displaying	Molecular polarizability	Principal polarizability components		
				α(xx)	α(yy)	α(zz)
1	Benzene		8.89	10.74	10.47	5.19
2	Toluene		10.97	12.08	14.05	6.79
3	Chloroform		8.52	9.34	9.34	6.89
4	THF		8.14	8.16	9.11	7.15
5	Dioxane		8.97	7.58	8.78	10.55
6	EtOAc		9.38	8.82	7.39	11.91
7	Sulfolane		11.48	11.37	10.36	12.70
8	MeCN		4.27	5.51	3.65	3.65
9	DMF		7.69	8.29	8.82	5.95
10	DMSO		7.91	9.04	8.08	6.60
11	EtOH		5.30	6.37	4.91	4.63

12	MeOH		3.38	3.01	3.18	3.96
13	Water		1.51	1.91	1.40	1.21
14	Methyl oleate		39.08	41.85	46.24	29.16
15	Oleic acid		36.60	37.78	44.60	27.44
16	Methyl laurate		27.87	21.37	22.46	39.79

[a] Calculated with *ChemAxon* software.

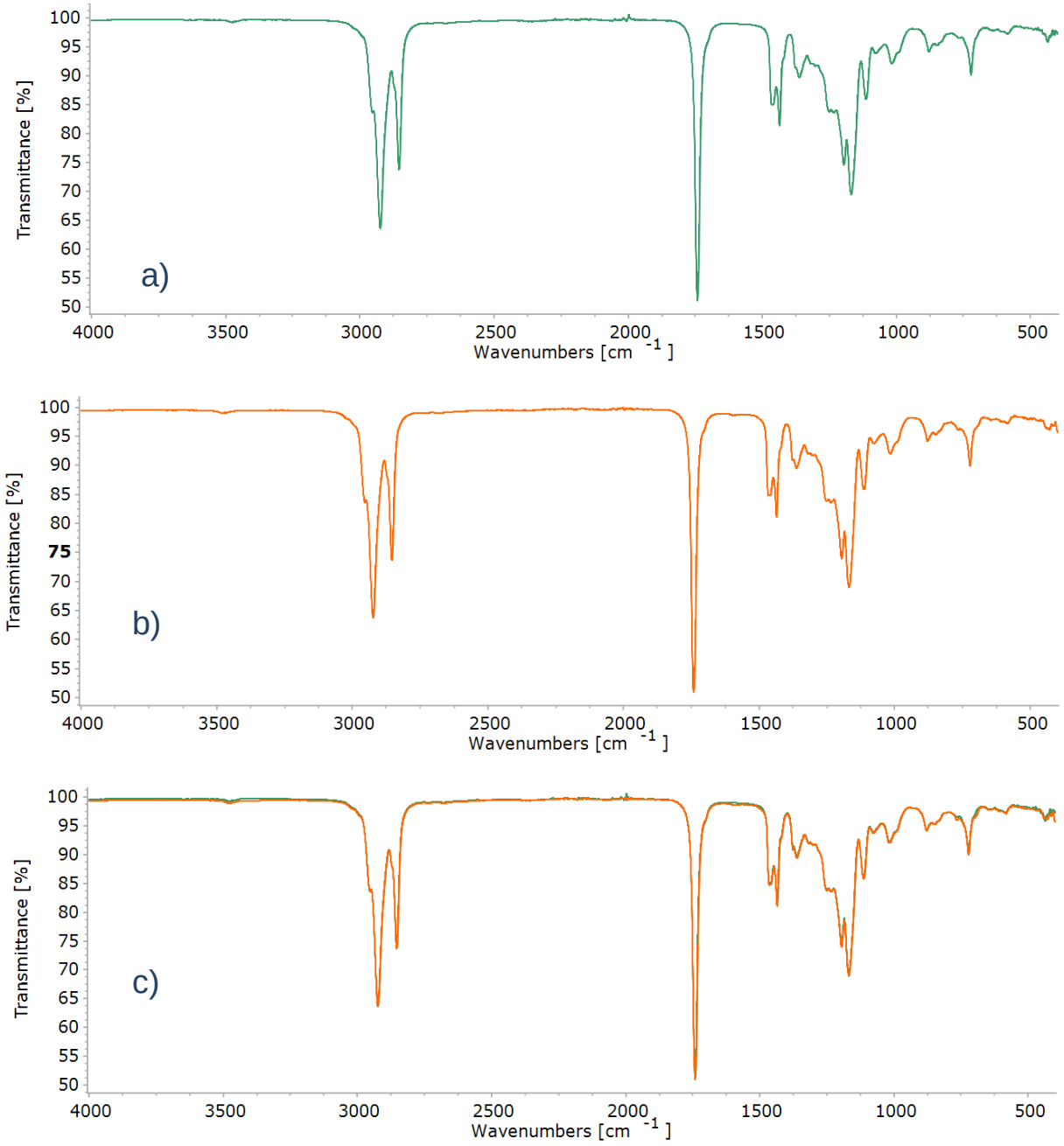


Figure S2: a) FTIR spectrum before reaction, b) Spectrum after reaction, c) Stacked spectra

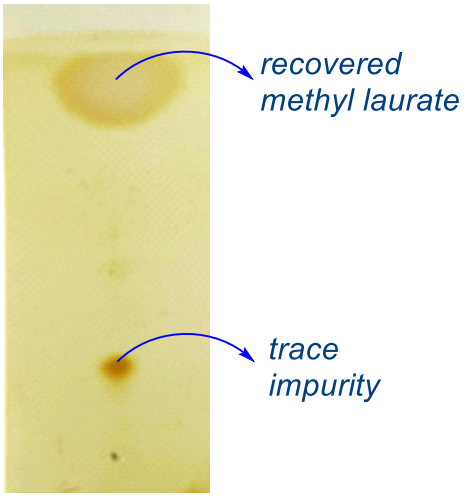


Figure S3: TLC plate of recovered methyl laurate (PE/EtOAc = 8/2, spots were made visible with iodine)

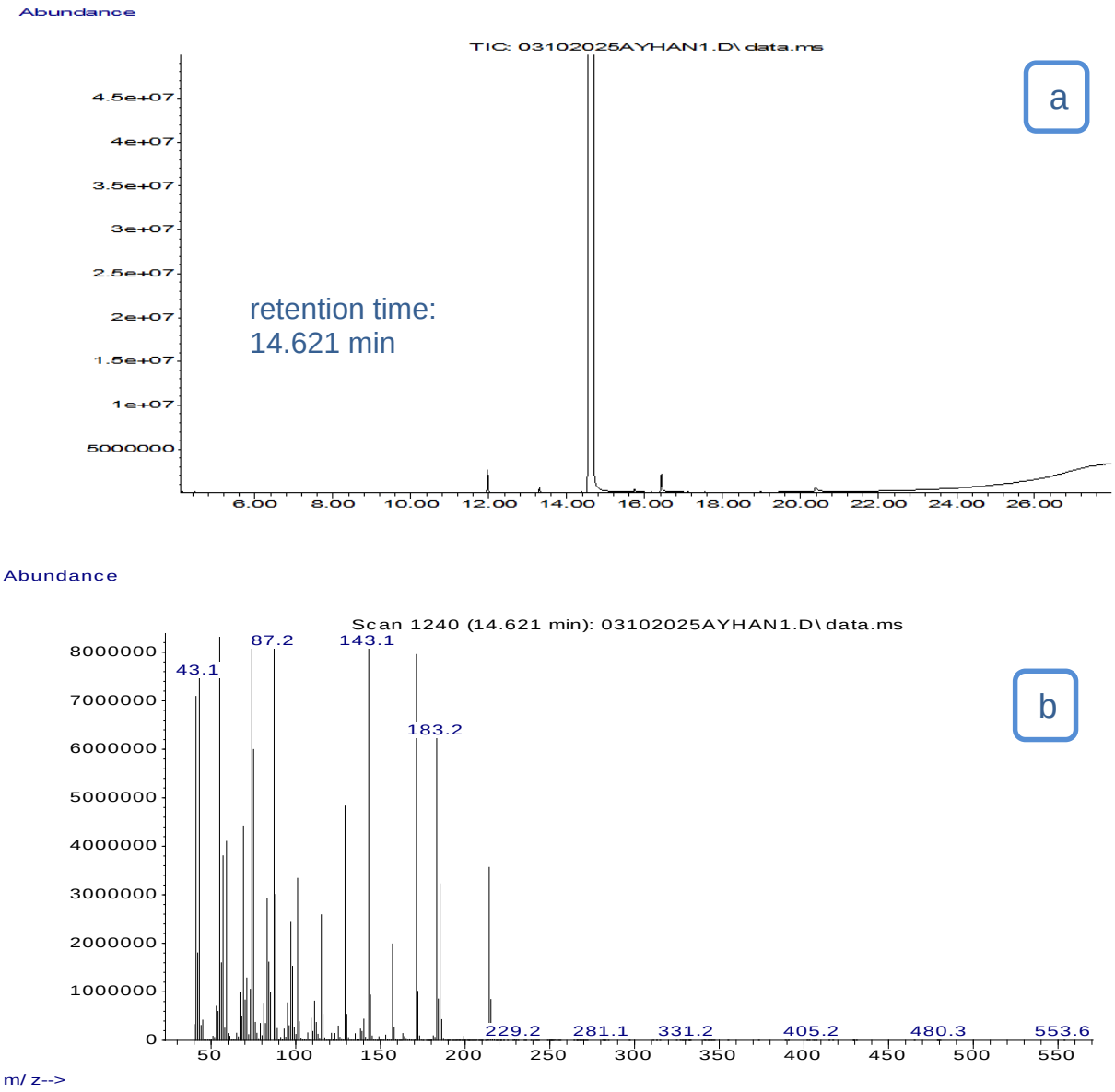


Figure S4: a) GC chromatogram of recovered methyl laurate. b) MS spectrum of recovered methyl laurate