Supporting Information

Design and Synthesis of Betulinic acid Dithiocarbamate conjugates as potential antifungal agents against *Candida albicans*

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1. General information

All the necessary chemicals and solvents were purchased from Sigma Aldrich and TCI. UV cabinet (camag) was used to visualise spots on TLC. All the products were purified using silica gel (60-120) column chromatography. ^{1}HNMR and ^{13}CNMR spectra were recorded in $CDCl_3$ using 400 and 125 MHZ NMR spectrometer respectively. Chemical shifts of ^{1}H and ^{13}C NMR were expressed in parts per million (ppm).

2. Spectral Data of All Compounds

BE: 2-bromoethyl 9-hydroxy-5a,5b,8,8,11a-pentamethyl-1-(prop-1-en-2-yl)icosahydro-3aH-cyclopenta[a]chrysene-3a-carboxylate. The product was purified by column chromatography using Hexane : EtOAc (94:6) to afford **BE** as a pale white solid, with molecular formula $C_{32}H_{51}BrO_3$.^{1}H NMR (400 MHz, $CDCl_3$) δ 4.67 (s, 1H), 4.60 – 4.50 (m, 1H), 4.33 (dd, *J* = 10.9, 5.8 Hz, 2H), 3.47 (t, *J* = 5.9 Hz, 2H), 3.12 (dd, *J* = 11.2, 5.0 Hz, 1H), 3.07 – 2.85 (m, 1H), 2.25 – 2.19 (m, 1H), 2.12 (td, *J* = 12.7, 3.6 Hz, 1H), 1.89 – 1.80 (m, 2H), 1.72 (s, 1H), 1.65 (d, *J* = 2.4 Hz, 1H), 1.62 (s, 3H), 1.58 (d, *J* = 5.2 Hz, 1H), 1.53 (dd, *J* = 7.6, 3.9 Hz, 2H), 1.48 – 1.40 (m, 2H), 1.40 – 1.32 (m, 5H), 1.30 (s, 2H), 1.18 (s, 3H), 1.12 – 1.07 (m, 1H), 0.96 (d, *J* = 12.4 Hz, 1H), 0.90 (d, *J* = 2.6 Hz, 6H), 0.85 (s, 3H), 0.82 (d, *J* = 4.6 Hz, 1H), 0.75 (s, 3H), 0.68 (s, 3H), 0.61 (d, *J* = 9.0 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.76, 150.46, 109.70, 79.02, 63.35, 56.69, 55.34, 50.55, 49.42, 46.96, 42.41, 40.74, 38.86, 38.79, 38.34, 37.19, 37.01, 34.31, 32.07, 30.59, 29.68, 29.19, 27.99, 27.38, 25.53, 20.89, 19.38, 18.29, 16.15, 16.00, 15.37, 14.72.

DTC1: 2-((piperidine-1-carbonothioyl)thio)ethyl-9-hydroxy-5a,5b,8,8,11a-pentamethyl-1-(prop-1-en-2-yl)icosahydro-3aH-cyclopenta[a]chrysene-3a-carboxylate: The product was purified by column chromatography using Hexane : EtOAc (94:6) to afford **DTC 1** as a pale yellow solid with molecular formula $C_{38}H_{61}NO_3S_2$**.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.74 (s, 1H), 4.61 (s, 1H), 4.36 (dt, *J* = 11.2, 5.7 Hz, 4H), 3.66 (t, *J* = 6.2 Hz, 2H), 3.20 (dd, *J* = 11.2, 4.9 Hz, 1H), 3.06 – 2.98 (m, 1H), 2.33 – 2.24 (m, 1H), 2.20 (td, *J* = 12.6, 3.5 Hz, 1H), 2.00 – 1.86 (m, 2H), 1.73 (s, 5H), 1.70 (s, 3H), 1.66 – 1.57 (m, 5H), 1.54 – 1.49 (m, 2H), 1.40 (dd, *J* = 9.6, 6.2 Hz, 8H), 1.28 (d, *J* = 9.3 Hz, 3H), 1.19 – 1.14 (m, 1H), 1.08 – 1.02 (m, 1H), 0.98 (s, 6H), 0.93 (s, 3H), 0.88 (s, 2H), 0.82 (s, 3H), 0.77 (s, 3H), 0.69 (d, *J* = 9.2 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.46, 175.92, 150.61, 109.59, 78.98, 62.07, 56.59, 55.34,

53.22, 51.34, 50.54, 49.42 , 46.99, 42.42, 40.73, 38.86, 38.72, 38.34, 37.18, 37.03, 35.87, 34.33, 32.14 , 30.65 29.68, 27.99 , 27.39, 26.05, 25.55, 25.41, 24.30, 20.89, 19.38, 18.28, 16.15, 16.07, 15.38, 14.72.

DTC2: 2-((pyrrolidine-1-carbonothioyl)thio)ethyl-9-hydroxy-5a,5b,8,8,11apentamethyl-1-(prop-1-en-2-yl)icosahydro-3aH-cyclopenta[a]chrysene-3a-carboxylate: The product was purified by column chromatography using Hexane : EtOAc (94:6) to afford **DTC 2** as a white solid with molecular formula $C_{37}H_{59}NO_3S_2$.^{1}H NMR (400 MHz, $CDCl_3$) δ 4.74 (s, 1H), 4.61 (s, 1H), 4.35 (dt, *J* = 11.4, 6.2 Hz, 4H), 3.91 (s, 2H), 3.66 (t, *J* = 6.2 Hz, 2H), 3.20 (dd, *J* = 11.2, 4.9 Hz, 1H), 3.10 – 2.98 (m, 1H), 2.44 – 2.15 (m, 2H), 1.95 – 1.89 (m, 2H), 1.66 (dt, *J* = 11.5, 9.3 Hz, 16H), 1.47 – 1.33 (m, 8H), 1.27 (s, 3H), 1.20 – 1.13 (m, 1H), 0.98 (s, 6H), 0.93 (s, 3H), 0.82 (s, 3H), 0.77 (s, 3H), 0.69 (d, *J* = 9.2 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.46, 175.94 , 150.69 , 109.59, 79.16, 62.07, 56.59, 55.34, 50.54, 49.42, 47.00, 42.42, 40.73, 38.86, 38.72, 38.34, 37.18, 37.03, 35.87, 34.33, 32.15, 30.65, 29.68 27.99, 27.40, 25.55, 24.30, 20.89, 19.38, 18.28, 16.14, 16.07, 15.37, 14.72.

DTC3: 2-**((4-cyanopiperidine-1-carbonothioyl)thio)ethyl9-hydroxy-5a,5b,8,8,11apenta-**

methyl-1-(prop-1-en-2-yl)icosahydro-3aH-cyclopenta[a]chrysene-3a-carboxylate: The product was purified by column chromatography using Hexane : EtOAc (83:17) to afford **DTC 3** as a yellowish solid with molecular formula $C_{39}H_{60}N_2O_3S_2$. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.73 (s, 1H), 4.60 (s, 1H), 4.39 – 4.29 (m, 2H), 3.63 (t, *J* = 6.2 Hz, 2H), 3.19 – 3.13 (m, 1H), 3.05 – 2.98 (m, 2H), 2.93 (d, *J* = 31.7 Hz, 1H), 2.27 – 2.16 (m, 3H), 2.03 – 1.96 (m, 4H), 1.92 – 1.87 (m, 2H), 1.68 (s, 3H), 1.65 – 1.49 (m, 5H), 1.38 (dd, *J* = 17.4, 6.7 Hz, 10H), 1.29 – 1.19 (m, 4H), 1.16 (d, *J* = 10.7 Hz, 1H), 1.02 (dd, *J* = 12.9, 4.1 Hz, 1H), 0.96 (s, 6H), 0.91 (s, 3H), 0.81 (s, 3H), 0.75 (s, 3H), 0.68 (d, *J* = 9.4 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.14, 196.14, 175.86, 175.86, 150.50, 150.50, 120.34, 120.34, 109.69, 109.69, 78.93, 78.93, 61.71, 56.58, 55.31, 50.49 , 49.37, 47.00, 42.40, 40.70, 38.77 , 38.32, 37.08, 36.15 , 34.32, 32.10, 31.53, 30.59 , 29.67, 28.13, 27.35, 26.18, 25.50, 20.88, 19.34, 18.28, 16.12, 15.40, 14.72.

DTC5: 2-((piperazine-1-carbonothioyl)thio)ethyl-9-hydroxy-5a,5b,8,8,11a-pentamethyl-1-(prop-1-en-2-yl)icosahydro-3aH-cyclopenta[a]chrysene-3a-carboxylate: The product was purified by column chromatography using Hexane : EtOAc (40:60) to afford **DTC 5** as a light brown gelwith molecular formula $C_{37}H_{60}N_2O_3S_2$. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.75 (s,

1H), 4.62 (s, 1H), 4.38 (td, *J* = 11.4, 5.4 Hz, 3H), 4.15 (s, 1H), 3.68 (t, *J* = 6.1 Hz, 2H), 3.20 (dd, *J* = 11.1, 4.8 Hz, 1H), 3.02 (t, *J* = 8.8 Hz, 1H), 2.41 – 2.13 (m, 3H), 1.93 (dd, *J* = 11.0, 7.7 Hz, 3H), 1.70 (s, 3H), 1.61 (t, *J* = 11.4 Hz, 3H), 1.55 (s, 1H), 1.40 (dd, *J* = 18.1, 8.0 Hz, 8H), 1.32 – 1.24 (m, 6H), 1.18 (d, *J* = 10.3 Hz, 2H), 0.98 (s, 6H), 0.93 (s, 3H), 0.87 (d, *J* = 6.5 Hz, 2H), 0.83 (s, 3H), 0.77 (s, 3H), 0.71 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.90 , 175.81, 150.48, 109.71, 78.99 , 61.63 , 56.61, 55.35 , 50.53, 49.42 , 47.01 , 42.43 , 40.74, 38.87 , 38.73, 38.34 , 37.20, 37.00 , 35.96, 34.37, 32.11, 30.62, 29.71, 29.37, 27.99 , 27.40 , 25.53, 22.70, 20.91 , 19.35, 18.32, 16.17, 16.11, 15.38, 14.72, 14.13.

DTC7: 2-((morpholine-4-carbonothioyl)thio)ethyl-9-hydroxy-5a,5b,8,8,11a-pentamethyl-1-(prop-1-en-2-yl)icosahydro-3aH-cyclopenta[a]chrysene-3a-carboxylate: The product was purified by column chromatography using Hexane : EtOAc (88:12) to afford **DTC 7** as yellowish viscous liquid with molecular formula $C_{37}H_{59}NO_4S_2$.^{1}H NMR (400 MHz, $CDCl_3$) δ 4.74 (s, 1H), 4.62 (s, 1H), 4.39 (d, *J* = 6.2 Hz, 3H), 3.79 (s, 4H), 3.67 (d, *J* = 6.2 Hz, 2H), 3.20 (dd, *J* = 11.2, 4.8 Hz, 1H), 3.04 – 2.89 (m, 1H), 2.28 (dd, *J* = 8.9, 2.6 Hz, 1H), 2.25 – 2.15 (m, 1H), 1.92 (dd, *J* = 7.2, 4.2 Hz, 2H), 1.70 (s, 3H), 1.67 – 1.58 (m, 4H), 1.56 – 1.51 (m, 2H), 1.46 – 1.35 (m, 9H), 1.31 (s, 4H), 1.27 (s, 1H), 1.17 (d, *J* = 10.8 Hz, 1H), 1.07 – 1.01 (m, 1H), 0.98 (s, 6H), 0.93 (s, 3H), 0.89 (d, *J* = 7.1 Hz, 1H), 0.83 (s, 3H), 0.77 (s, 3H), 0.69 (d, *J* = 9.4 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.44, 175.87, 150.55, 109.67, 78.98, 61.81 , 56.59, 55.32 , 50.52, 49.39, 47.00, 42.41, 40.72, 38.86, 38.71, 38.33, 37.18, 37.02 , 35.74 , 34.33, 32.12, 30.61, 29.69 , 27.98, 27.39, 25.52, 20.89, 19.36, 18.28, 16.17, 16.09, 15.38 , 14.72.

DTC8: 2-((4-allylpiperazine-1-carbonothioyl)thio)ethyl-9-hydroxy-5a,5b,8,8,11a-penta-

methyl-1-(prop-1-en-2-yl)icosahydro-3aH-cyclopenta[a]chrysene-3a-carboxylate: The product was purified by column chromatography using Hexane : EtOAc (88:12) to afford **DTC 8** as brownish yellow viscous liquid with molecular formula $C_{40}H_{64}N_2O_3S_2$. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.92 – 5.69 (m, 1H), 5.37 – 5.08 (m, 2H), 4.66 (d, *J* = 2.0 Hz, 1H), 4.53 (d, *J* = 1.3 Hz, 1H), 4.37 – 4.24 (m, 3H), 4.05 (d, *J* = 7.1 Hz, 1H), 3.91 (s, 1H), 3.58 (t, *J* = 6.2 Hz, 2H), 3.11 (dd, *J* = 11.2, 5.0 Hz, 1H), 2.99 (d, *J* = 6.6 Hz, 2H), 2.92 (d, *J* = 6.2 Hz, 1H), 2.49 (s, 3H), 2.25 – 2.14 (m, 3H), 1.98 (d, *J* = 2.0 Hz, 1H), 1.89 – 1.79 (m, 2H), 1.61 (s, 3H), 1.52 (t, *J* = 11.4 Hz, 4H), 1.45 (dd, *J* = 6.5, 4.1 Hz, 1H), 1.36 – 1.27 (m, 8H), 1.23 – 1.15 (m, 4H), 1.09 (dd, *J* = 9.0, 5.8 Hz, 1H), 0.95 (dd, *J* = 12.8, 4.5 Hz, 1H), 0.89 (s, 6H),

0.84 (s, 3H), 0.74 (s, 3H), 0.63 (s, 3H), 0.61 (d, *J* = 9.2 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.78, 175.87, 150.55, 133.78, 119.14, 109.63, 78.97, 61.92, 61.08, 56.60, 55.34, 52.23, 50.54, 49.42, 47.00, 42.42, 40.73, 38.86, 38.72, 38.34, 37.18, 37.02, 35.90, 34.33, 32.13, 30.64, 29.69, 27.99, 27.39, 25.54, 20.90, 19.37, 18.31, 16.16, 16.10, 15.38, 14.72

DTC9: 2-((thiomorpholine-4-carbonothioyl)thio)ethyl-9-hydroxy-5a,5b,8,8,11a-pentame

thyl-1-(prop-1-en-2-yl)icosahydro-3aH-cyclopenta[a]chrysene-3a-carboxylate: The product was purified by column chromatography using Hexane : EtOAc (94:6) to afford **DTC 9** as brownish yellow viscous liquid with molecular formula $C_{37}H_{59}NO_3S_3$. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.66 (s, 1H), 4.53 (s, 1H), 4.28 (dt, *J* = 11.3, 5.8 Hz, 3H), 4.05 (q, *J* = 7.1 Hz, 1H), 3.58 (t, *J* = 6.2 Hz, 2H), 3.11 (dd, *J* = 11.2, 4.9 Hz, 1H), 2.93 (td, *J* = 10.8, 4.5 Hz, 1H), 2.68 (s, 3H), 2.24 – 2.16 (m, 1H), 2.11 (td, *J* = 12.7, 3.6 Hz, 1H), 1.86 – 1.78 (m, 2H), 1.61 (s, 3H), 1.59 – 1.49 (m, 4H), 1.48 – 1.41 (m, 2H), .138 – 1.28 (m, 8H), 1.25 – 1.15 (m, 5H), 1.11 – 1.05 (m, 1H), 1.00 – 0.92 (m, 1H), 0.89 (s, 6H), 0.85 (s, 3H), 0.80 (d, *J* = 7.0 Hz, 1H), 0.74 (s, 3H), 0.68 (s, 3H), 0.61 (d, *J* = 9.3 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.72, 176.08, 150.53, 109.86, 79.38, 61.78 , 60.420, 56.60, 55.34, 50.54, 49.41, 47.01, 42.43, 40.73 , 38.86, 38.73, 38.35, 37.19, 37.02, 35.96, 34.35, 32.13, 30.63, 29.70,27.99 , 27.40, 25.55 , 21.07 , 20.98, 19.36, 18.29, 16.16, 16.08, 15.38, 14.73.

DTC10: 2-((4-methylpiperazine-1-carbonothioyl)thio)ethyl 9-hydroxy-5a,5b,8,8,11a-pentamethyl-1-(prop-1-en-2-yl)icosahydro-3aH-cyclopenta[a]chrysene-3a-carboxylate.
The product was purified by column chromatography using Hexane :EtOAc (25:75) to afford **DTC 10**as brownish gel with molecular formula $C_{38}H_{62}N_2O_3S_2$. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.66 (s, 1H), 4.53 (s, 1H), 4.28 (td, *J* = 6.1, 4.4 Hz, 3H), 3.98 (s, 1H), 3.57 (t, *J* = 6.2 Hz, 2H), 3.35 (s, 1H), 3.16 – 3.10 (m, 1H), 2.96 (d, *J* = 4.7 Hz, 1H), 2.60 – 2.54 (m, 4H), 2.35 (s, 1H), 2.37 – 2.31 (m, 3H), 2.22 – 2.10 (m, 2H), 1.98 – 1.93 (m, 1H), 1.86 – 1.82 (m, 2H), 1.61 (s, 3H), 1.52 (s, 3H), 1.48 – 1.42 (m, 1H), 1.36 – 1.27 (m, 7H), 1.22 – 1.17 (m, 4H), 1.09 (d, *J* = 3.4 Hz, 1H), 0.96 (d, *J* = 4.4 Hz, 1H), 0.89 (s, 6H), 0.84 (s, 3H), 0.79 (s, 1H), 0.74 (s, 3H), 0.68 (s, 3H), 0.62 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.16, 175.61, 150.54 , 109.65 , 79.03, 61.83, 56.59 , 55.32, 53.78, 50.53, 49.40, 47.00, 44.89, 42.41, 40.72, 38.84 , 38.71, 38.33, 37.17, 37.01, 35.95, 34.32, 32.12, 30.62, 29.68, 27.97, 27.33, 25.77, 25.56 20.92 , 19.35, 18.29 , 17.63 , 16.15, 16.08 , 15.37 , 14.71.

DTC11: **2-((4-cyclopropylpiperazine-1-carbonothioyl)thio)ethyl-9-hydroxy-5a,5b,8,8,11a-pentamethyl-1-(prop-1-en-2-yl)icosahydro-3aH-cyclopenta[a]chrysene-3a-**

carboxylate: The product was purified by column chromatography using Hexane:EtOAc (94:6) to afford **DTC 11** as brownish solid with molecular formula $C_{40}H_{64}N_2O_3S_2$. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.66 (s, 1H), 4.53 (s, 1H), 4.35 – 4.24 (m, 4H), 3.85 (s, 1H), 3.58 (s, 2H), 3.11 (dd, *J* = 11.0, 4.9 Hz, 1H), 2.95 (dd, *J* = 14.1, 7.1 Hz, 1H), 2.69 (d, *J* = 34.1 Hz, 5H), 2.14 (ddd, *J* = 24.2, 11.8, 5.9 Hz, 3H), 1.91 – 1.77 (m, 3H), 1.61 (s, 4H), 1.52 (s, 3H), 1.32 (d, *J* = 16.7 Hz, 8H), 1.19 (s, 4H), 1.11 – 1.05 (m, 2H), 0.95 (d, *J* = 11.3 Hz, 1H), 0.89 (s, 6H), 0.85 (s, 3H), 0.74 (s, 3H), 0.68 (s, 3H), 0.60 (d, *J* = 9.1 Hz, 1H), 0.43 (dd, *J* = 7.1, 5.2 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.63, 175.87 , 150.54, 109.63 , 78.92, 61.94, 56.58, 55.33, 52.60, 50.52, 49.41, 46.98, 42.40, 40.72, 38.85, 38.72, 38.32, 38.02, 37.17, 37.01, 35.88, 34.32, 32.12, 30.63, 29.68, 28.00, 27.39, 25.53, 20.89, 19.38, 18.29, 16.16, 16.09, 15.40, 14.72, 5.94.

DTC12: 2-((4-(4-nitrophenyl)piperazine-1-carbonothioyl)thio)ethyl-9-hydroxy-5a,5b,8, 8,11a-pentamethyl-1-(prop-1-en-2-yl)icosahydro-3aH-cyclopenta[a]chrysene-3a-carboxylate: The product was purified by column chromatography using Hexane: EtOAc (73:27) to afford **DTC12**as brownish solid with molecular formula $C_{43}H_{63}N_3O_5S_2$**.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 9.3 Hz, 2H), 6.71 (d, *J* = 9.3 Hz, 2H), 4.65 (s, 1H), 4.53 (s, 1H), 4.30 (dd, *J* = 12.4, 6.1 Hz, 3H), 4.05 (dd, *J* = 14.3, 7.1 Hz, 2H), 3.58 (dd, *J* = 11.6, 5.8 Hz, 6H), 3.11 (dd, *J* = 11.1, 4.8 Hz, 1H), 2.93 (dd, *J* = 10.5, 6.9 Hz, 1H), 2.17 – 2.11 (m, 2H), 1.99 (d, *J* = 12.0 Hz, 1H), 1.87 – 1.80 (m, 2H), 1.61 (s, 3H), 1.52 (t, *J* = 11.5 Hz, 3H), 1.40 (d, *J* = 10.9 Hz, 2H), 1.35 – 1.26 (m, 8H), 1.19 (t, *J* = 7.1 Hz, 4H), 1.09 (d, *J* = 10.6 Hz, 1H), 0.97 – 0.92 (m, 1H), 0.88 (s,3H), 0.87 (s, 3),0.84 (s, 3H), 0.73 (s, 3H), 0.66 (s, 3H), 0.60 (d, *J* = 10.3 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.47 , 175.84, 153.65 , 150.49 , 138.96 , 126.05 , 112.21, 109.70, 78.93, 61.71 , 56.59 , 55.30, 53.49, 50.50, 49.40 , 47.02, 45.71, 42.41, 40.72, 38.83, 38.70 , 38.33, 37.17, 37.00, 35.87, 34.34, 32.11, 30.61, 29.70, 27.97, 27.33 , 25.51, 25.51, 20.89 , 19.33, 18.30, 16.16, 16.10, 15.38, 14.72.

DTC13: 2-((4-(4-bromophenyl)piperazine-1-carbonothioyl)thio)ethyl-9-hydroxy-5a,5b, 8,8,11a-pentamethyl-1-(prop-1-en-2-yl)icosahydro-3aH-cyclopenta[a]chrysene-3a-carboxylate: The product was purified by column chromatography using Hexane : EtOAc (85:15) to afford **DTC 13**as yellowish solidwith molecular formula $C_{43}H_{63}BrN_2O_3S_2$. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.8 Hz, 2H), 6.71 (d, *J* = 8.9 Hz, 2H), 4.66 (s, 1H), 4.53 (s, 1H), 4.35 – 4.25 (m, 3H), 4.05 (dd, *J* = 14.3, 7.1 Hz, 1H), 3.60 (t, *J* = 6.1 Hz, 2H), 3.21 (t, *J* = 4.9 Hz, 5H), 3.13 – 3.07 (m, 1H), 2.98 – 2.92 (m, 1H), 2.23 – 2.07 (m, 2H), 1.98 (s, 1H), 1.88 – 1.75 (m, 2H), 1.61 (s, 3H), 1.51 (d, *J* = 11.5 Hz, 3H), 1.41 (d, *J* = 7.8 Hz, 2H),

1.33 (dd, J = 12.9, 4.6 Hz, 8H), 1.19 (dd, J = 8.0, 6.1 Hz, 4H), 1.11 – 1.06 (m, 1H), 0.95 (d, J = 12.8 Hz, 1H), 0.89 (s, 3H), 0.88 (s, 3H), 0.84 (s, 3H), 0.73 (s, 3H), 0.67 (s, 3H), 0.60 (d, J = 10.5 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.16, 175.86 ,150.55 , 149.25 , 132.15 , 117.82 , 112.85, 109.66 , 78.97 , 61.82 , 56.61, 55.33 , 50.53, 49.96,49.60, 48.54 , 47.02 , 42.43 , 40.74, 38.86 , 38.72, 38.35 , 37.19, 37.01 , 35.93, 34.35 , 32.13, 30.64, 29.71, 27.98 , 27.40, 25.54 , 20.91 , 19.36 , 18.30 , 16.16 , 16.11, 15.36 , 14.73 .

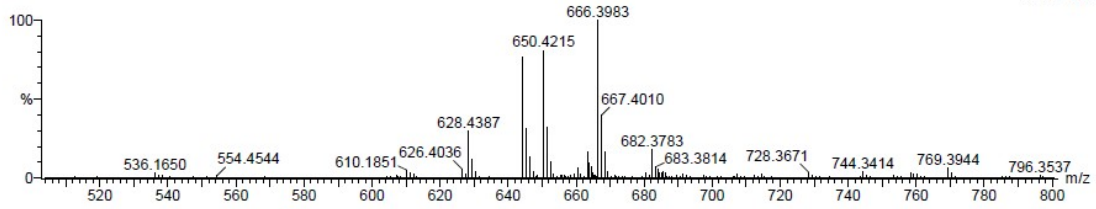
3. HRMS Data of Some products

DTC1

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
25 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-38 H: 0-100 N: 0-1 O: 0-3 S: 0-2

DTC-1 — QMI DIVISION, CSIR-IIIM JAMMU — Xevo G2-XS QTOF YFC2015 — 28-Aug-2024 12:28:58
280824_06 4 (0.104) — 1: TOF MS ES+ 7.77e+005



Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
644.4167	644.4171	-0.4	-0.6	8.5	639.0	n/a	n/a	C38 H62 N O3 S2

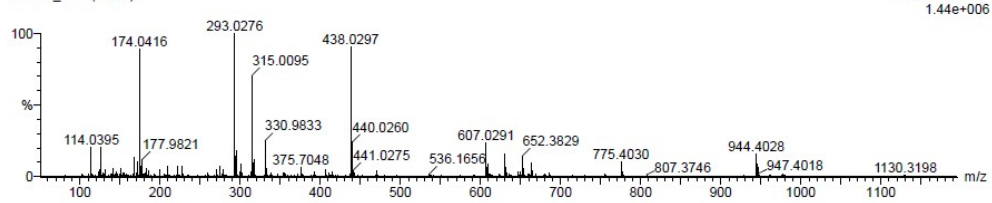
DTC2

Elemental Composition Report — **Page 1**

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
25 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-37 H: 0-100 N: 0-1 O: 0-3 S: 0-2

DTC-2 — QMI DIVISION, CSIR-IIIM JAMMU — Xevo G2-XS QTOF YFC2015 — 28-Aug-2024 12:26:16
280824_05 4 (0.104) — 1: TOF MS ES+ 1.44e+006



Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
630.4012	630.4015	-0.3	-0.5	8.5	689.0	n/a	n/a	C37 H60 N O3 S2

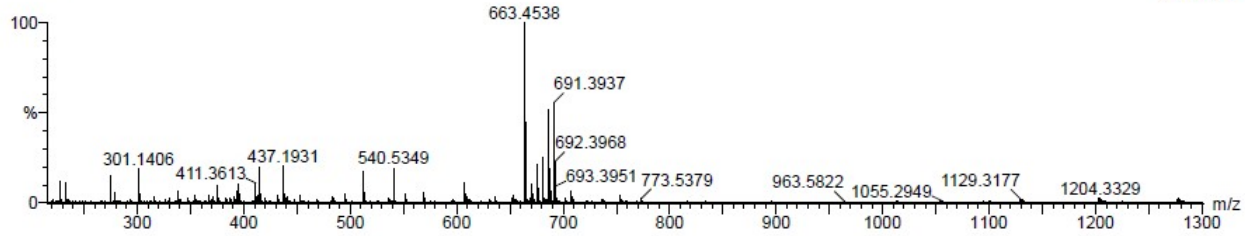
DTC3

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
76 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-39 H: 0-100 N: 0-2 O: 0-3 S: 0-2 Na: 0-1

DTC-3 QMI DIVISION, CSIR-IIIM JAMMU 29-Aug-2024
Xevo G2-XS QTOF YFC2015 12:32:25
290824_03 4 (0.104) 1: TOF MS ES+
8.57e+005



Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
691.3937	691.3943	-0.6	-0.9	10.5	747.9	n/a	n/a	C39 H60 N2 O3 S2 Na

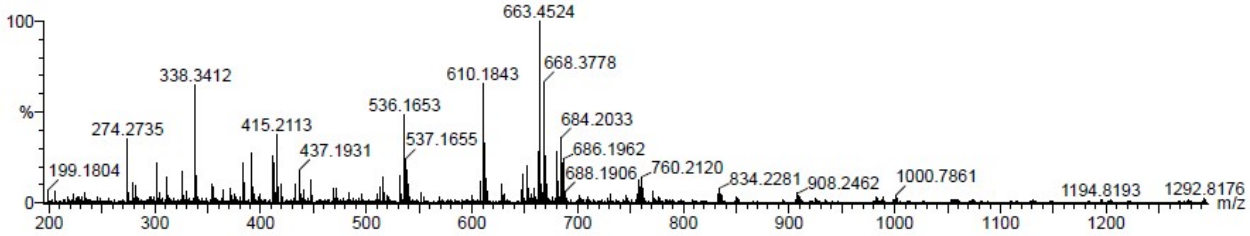
DTC7

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
61 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-37 H: 0-100 N: 0-1 O: 0-4 Na: 0-1 S: 0-2

DTC-7 QMI DIVISION, CSIR-IIIM JAMMU 29-Aug-2024
Xevo G2-XS QTOF YFC2015 12:37:50
290824_05 5 (0.121) 1: TOF MS ES+
1.07e+006



Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
668.3778	668.3783	-0.5	-0.7	8.5	708.5	n/a	n/a	C37 H59 N O4 Na S2

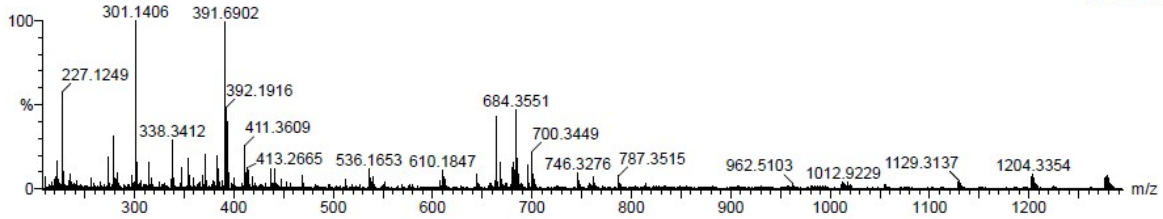
DTC9

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
65 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-37 H: 0-100 N: 0-1 O: 0-3 Na: 0-1 S: 0-3

DTC-9 QMI DIVISION, CSIR-IIIM JAMMU 29-Aug-2024
Xevo G2-XS QTOF YFC2015 12:35:07
290824_04 4 (0.104) 1: TOF MS ES+
1.72e+005



Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
684.3551	684.3555	-0.4	-0.6	8.5	592.7	n/a	n/a	C37 H59 N O3 Na S3

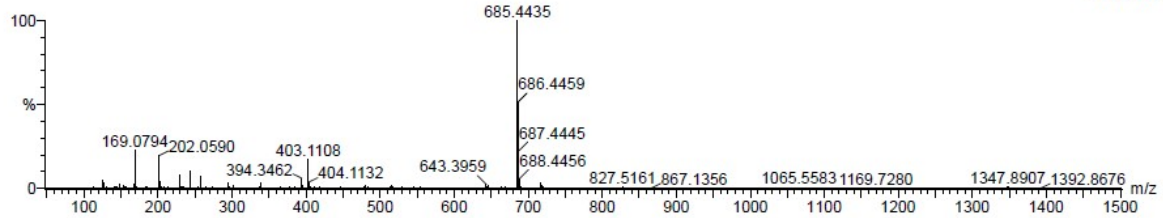
DTC11

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
39 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-40 H: 0-100 N: 0-2 O: 0-3 S: 0-2

DTC-11 QMI DIVISION, CSIR-IIIM JAMMU 29-Aug-2024
Xevo G2-XS QTOF YFC2015 12:29:52
290824_02 6 (0.138) 1: TOF MS ES+
3.64e+007



Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
685.4435	685.4437	-0.2	-0.3	9.5	713.2	n/a	n/a	C40 H65 N2 O3 S2

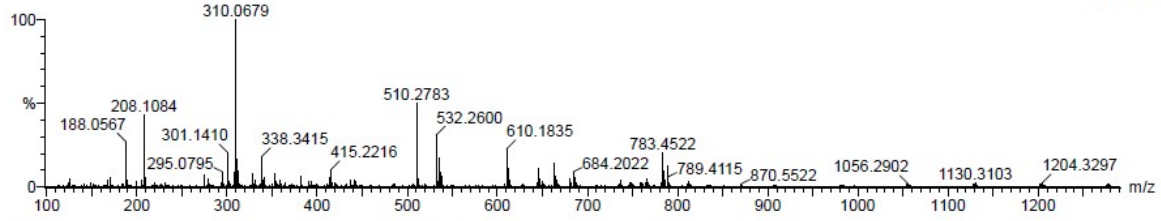
DTC12

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
94 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-43 H: 0-100 N: 0-4 O: 0-5 S: 0-2

DTC-12 QMI DIVISION, CSIR-IIIM JAMMU 28-Aug-2024
Xevo G2-XS QTOF YFC2015 12:20:58
280824_03 5 (0.121) 1: TOF MS ES+
3.03e+006



Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
783.4522	783.4553	-3.1	-4.0	12.5	601.2	n/a	n/a	C43 H67 N4 O5 S2

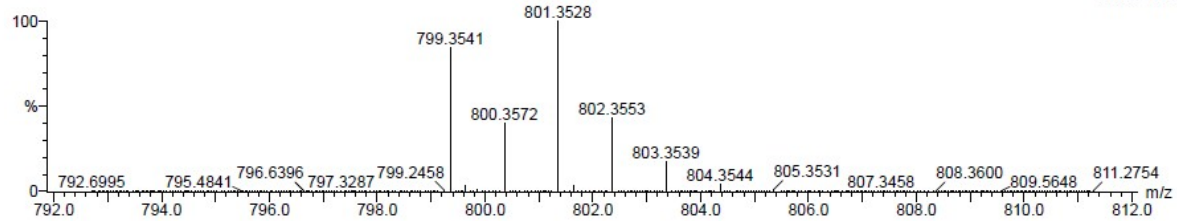
DTC13

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
76 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-43 H: 0-100 N: 0-2 O: 0-3 S: 0-2 Br: 0-1

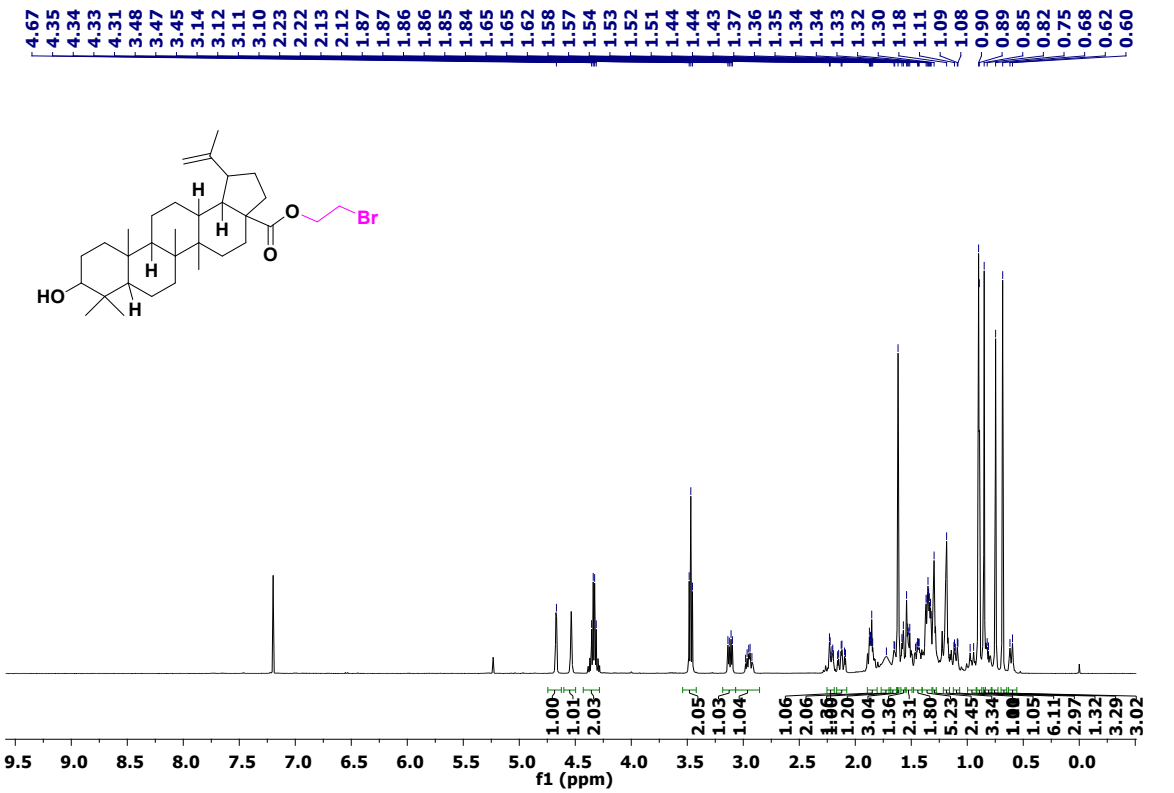
DTC-13 QMI DIVISION, CSIR-IIIM JAMMU 28-Aug-2024
Xevo G2-XS QTOF YFC2015 12:18:18
280824_02 4 (0.104) 1: TOF MS ES+
7.56e+006

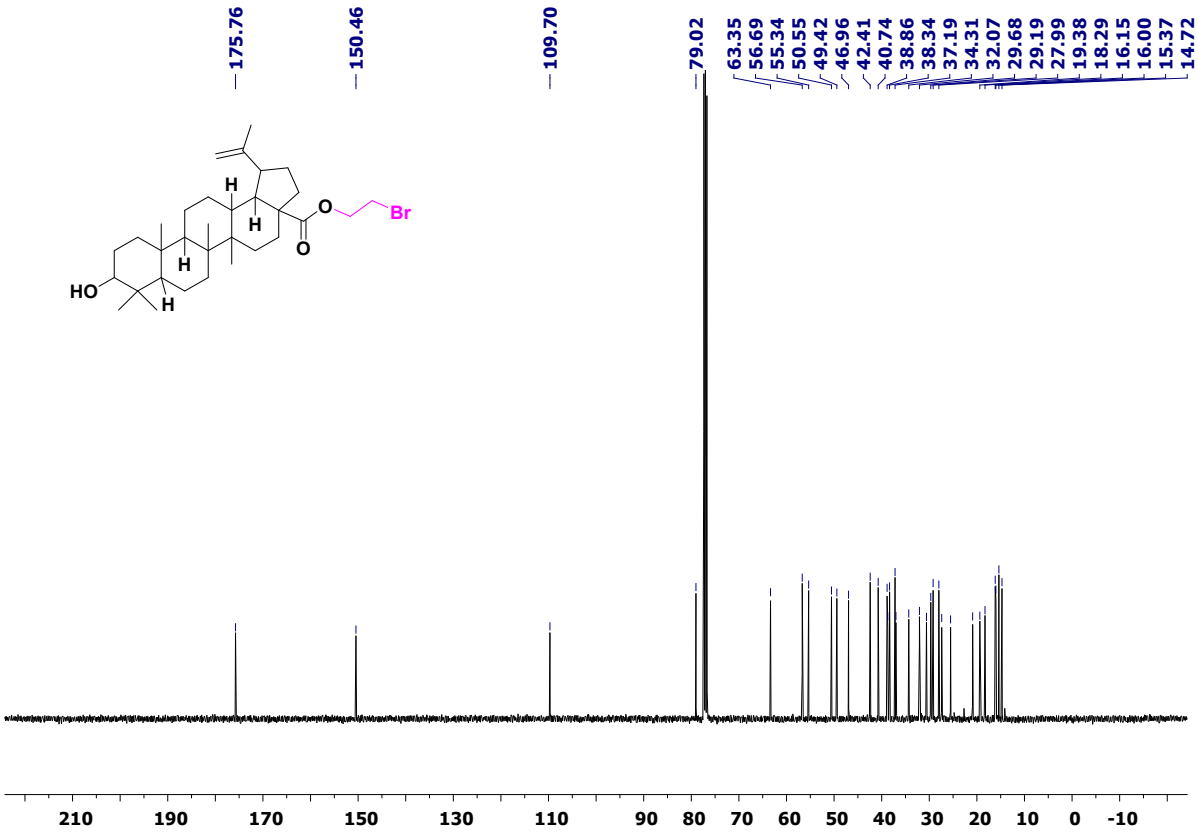


Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
799.3541	799.3542	-0.1	-0.1	12.5	592.2	n/a	n/a	C43 H64 N2 O3 S2 Br

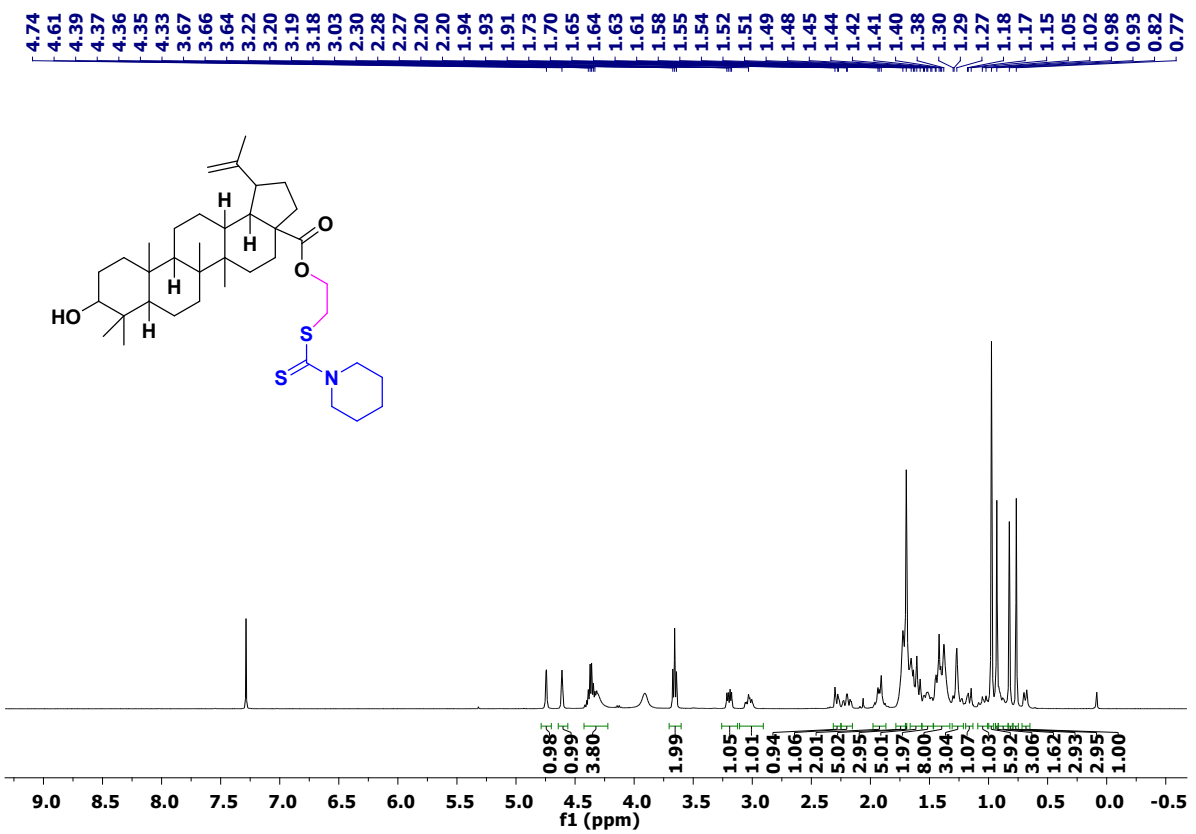
4. ^{1}H and ^{13}C NMR of Products

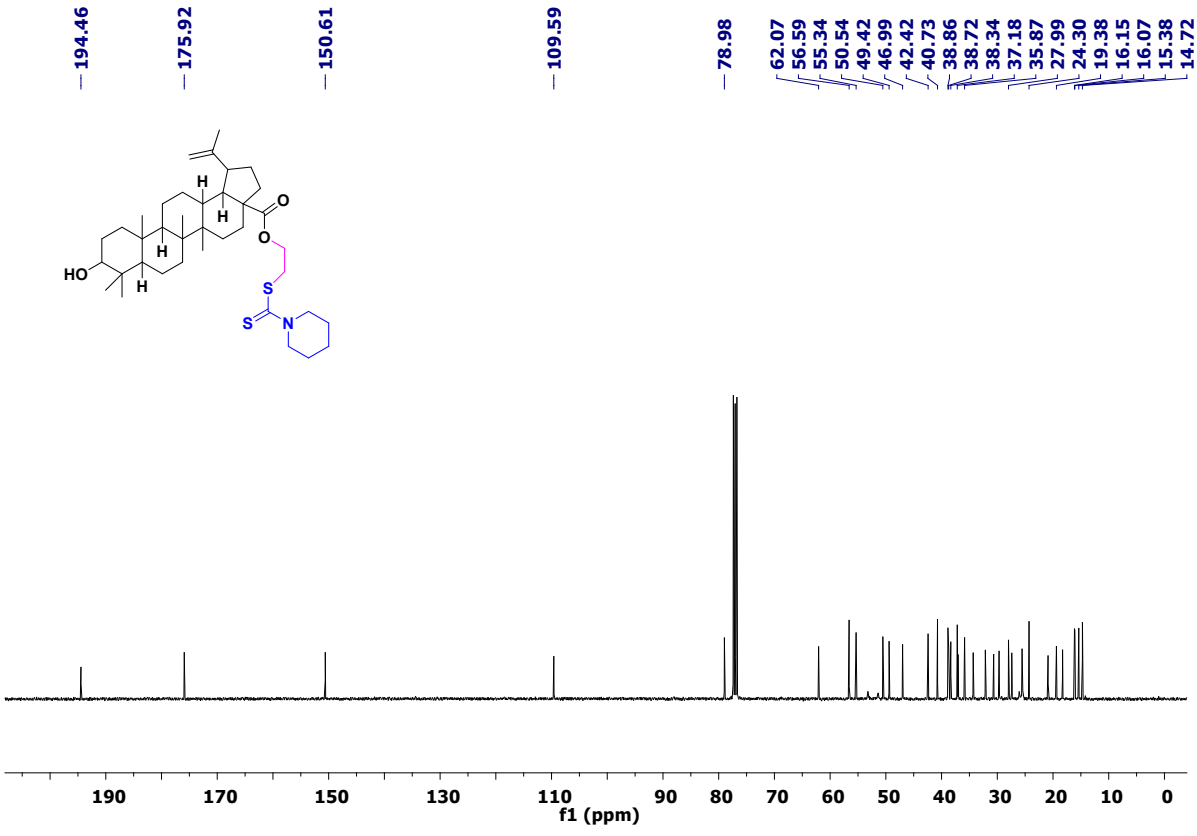
^{1}H NMR and ^{13}C NMR ($CDCl_3$) of **BE**



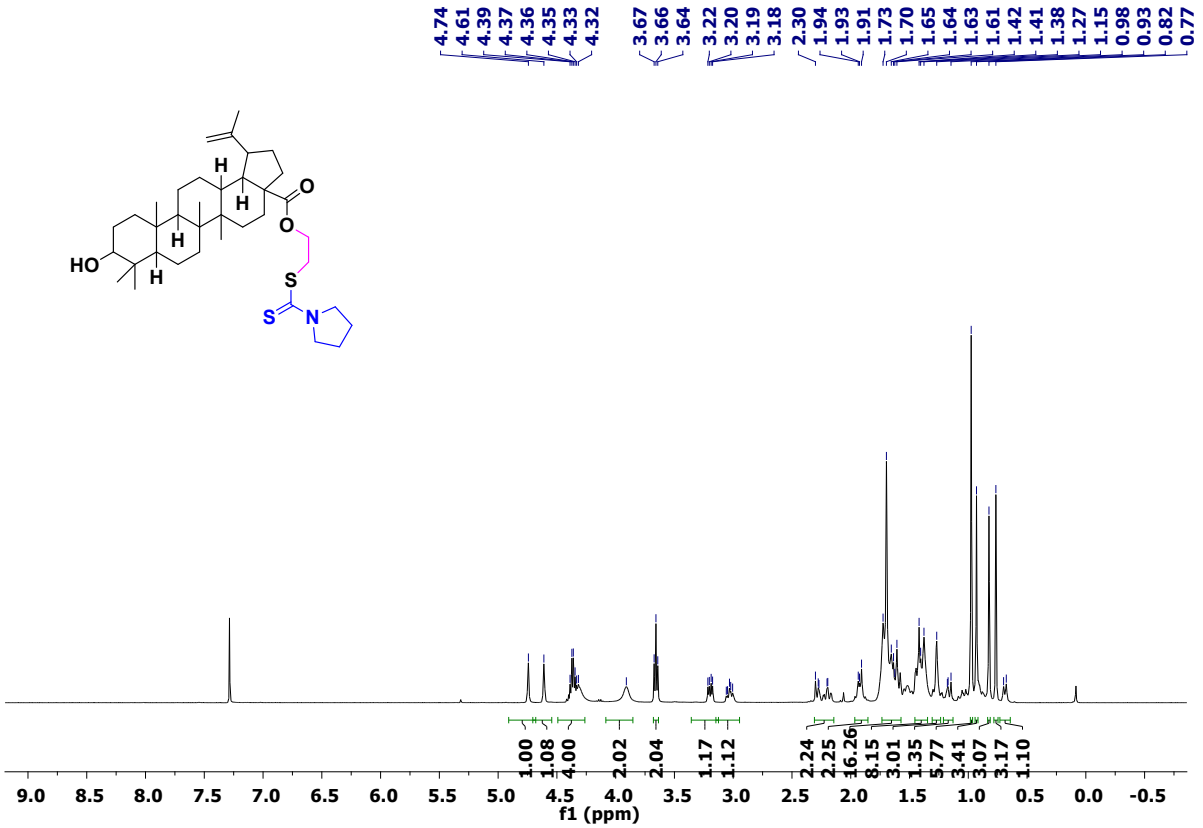


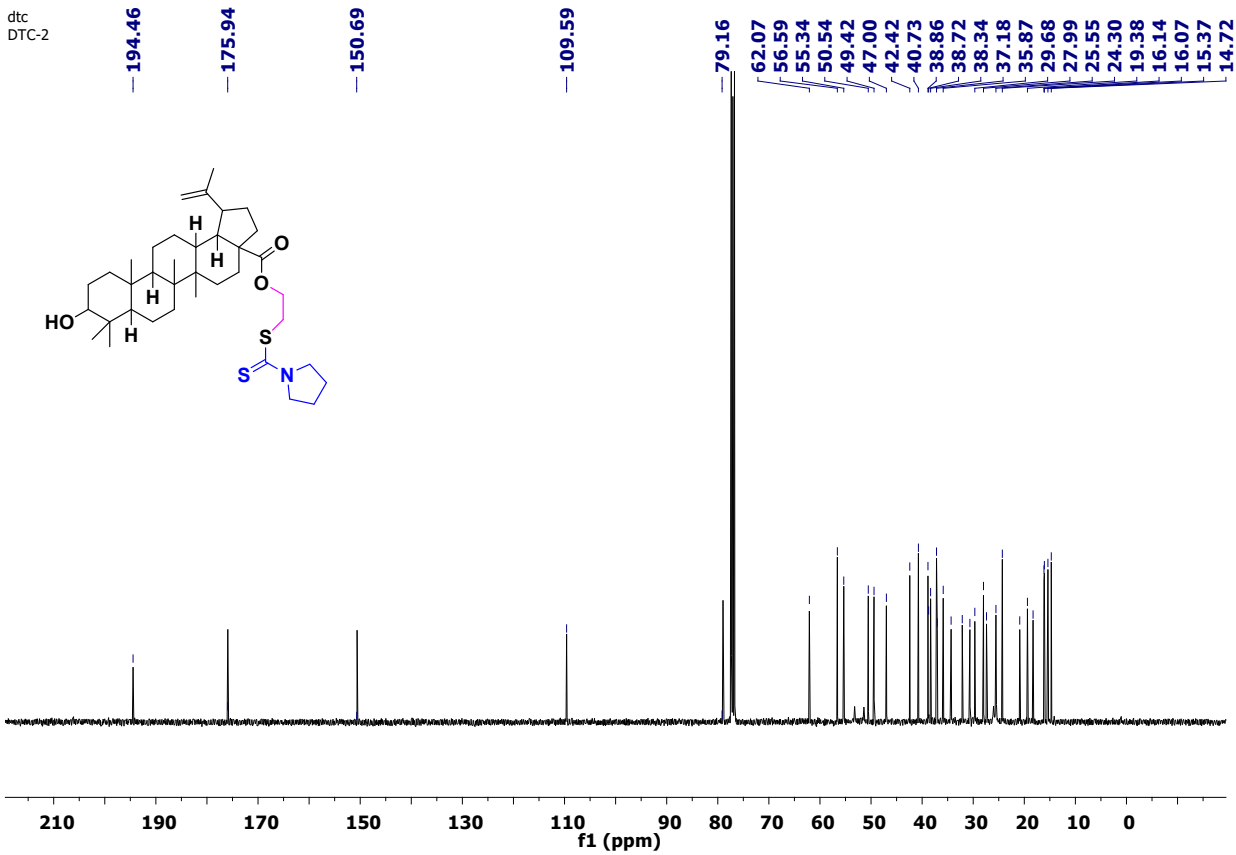
^{1}H NMR and ^{13}C NMR ($CDCl_3$) of **DTC1**



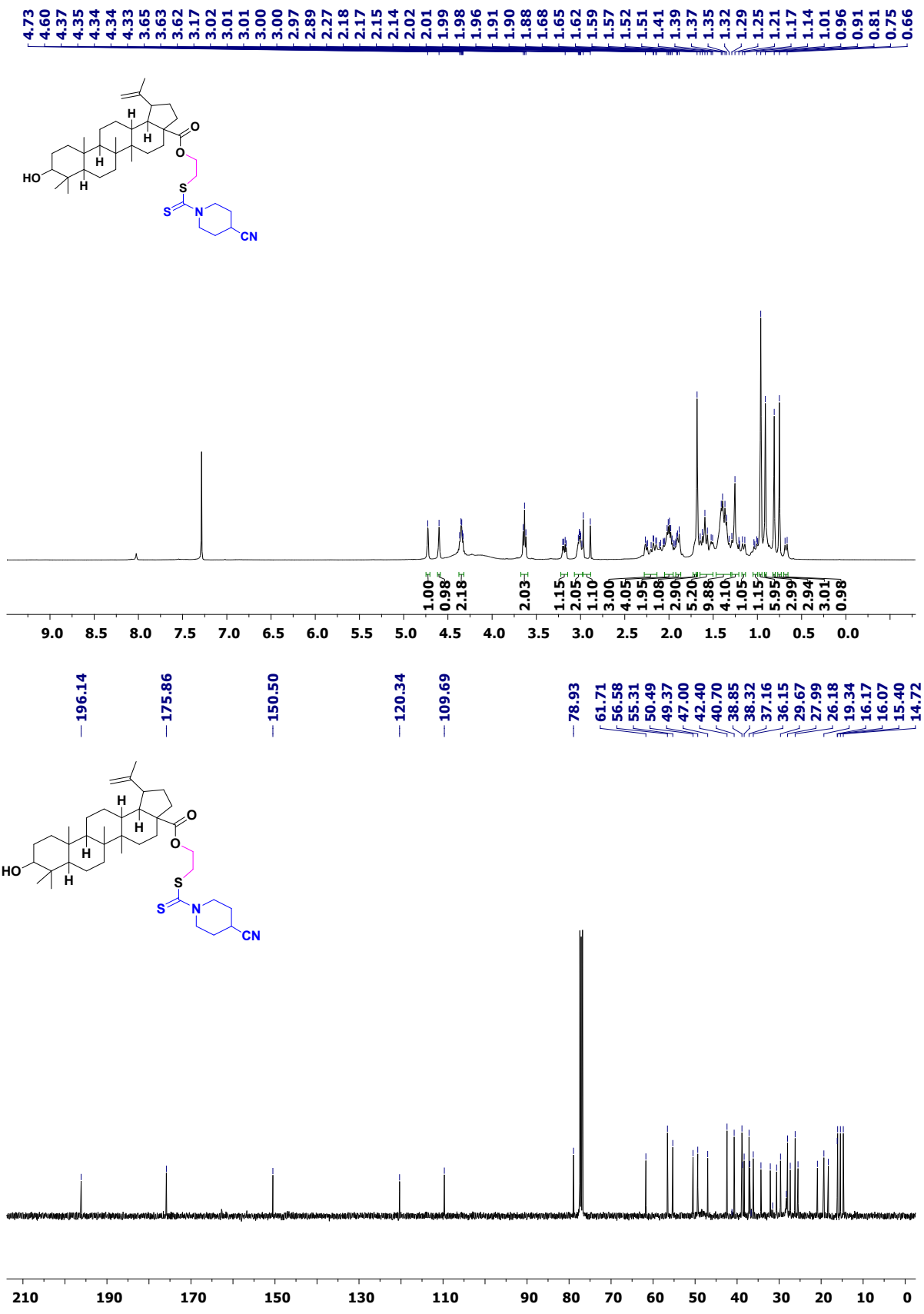


^{1}H NMR and ^{13}C NMR ($CDCl_3$) of **DTC2**

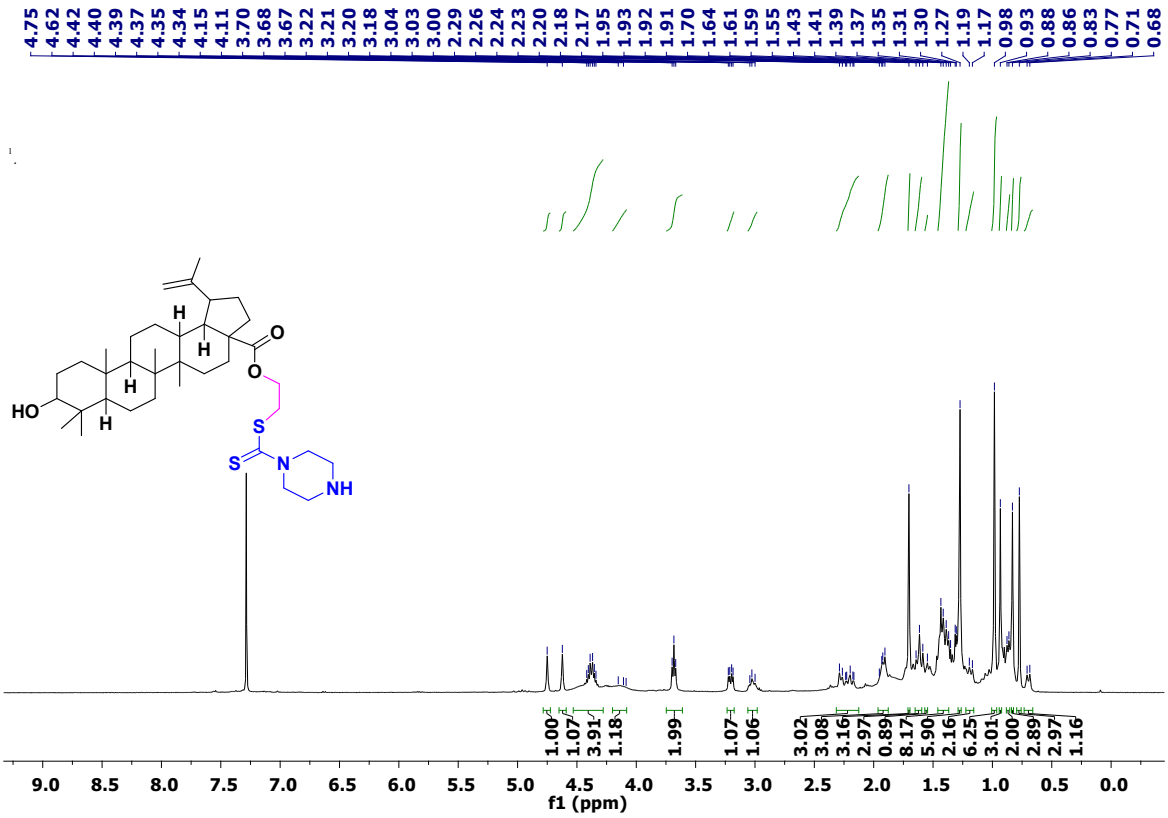


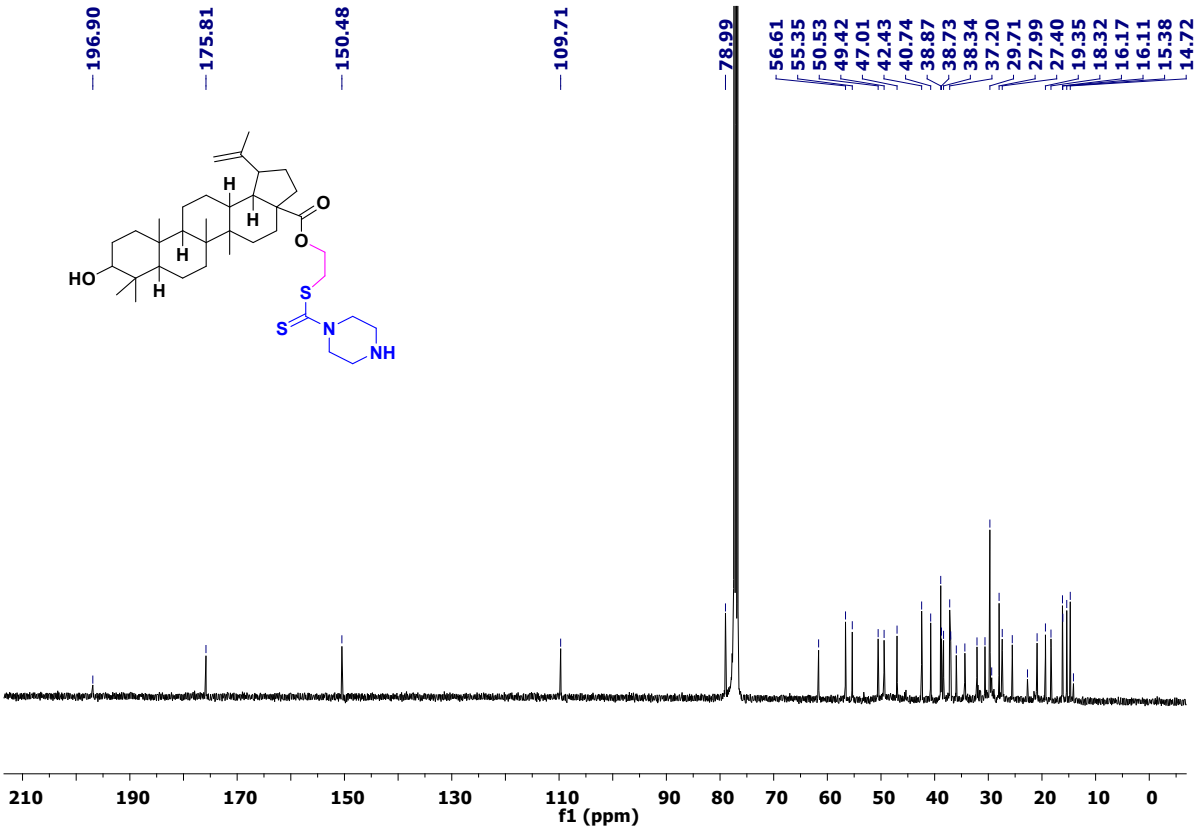


^{1}H NMR and ^{13}C NMR ($CDCl_3$) of **DTC3**

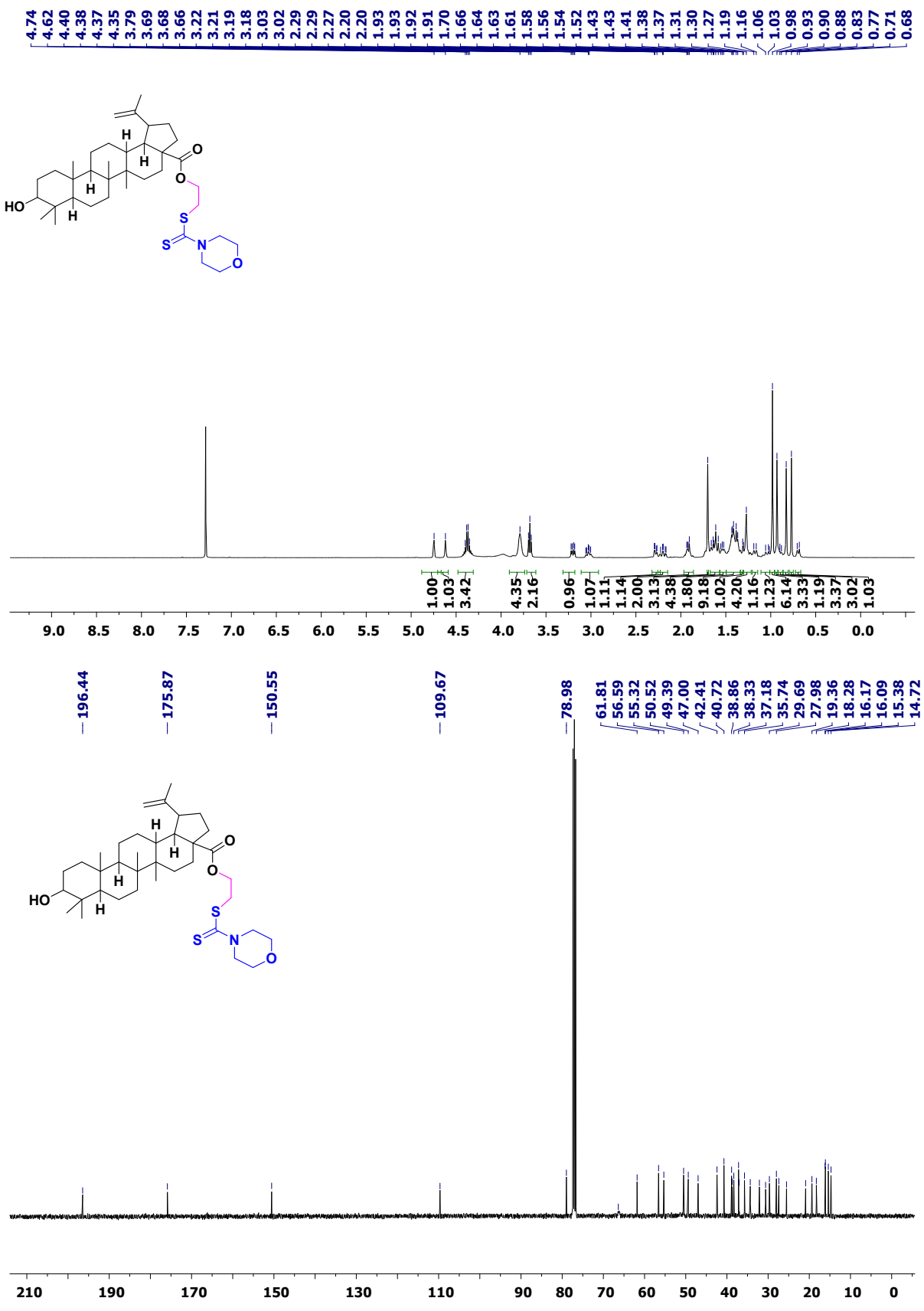


^{1}H NMR and ^{13}C NMR ($CDCl_3$) of **DTC5**

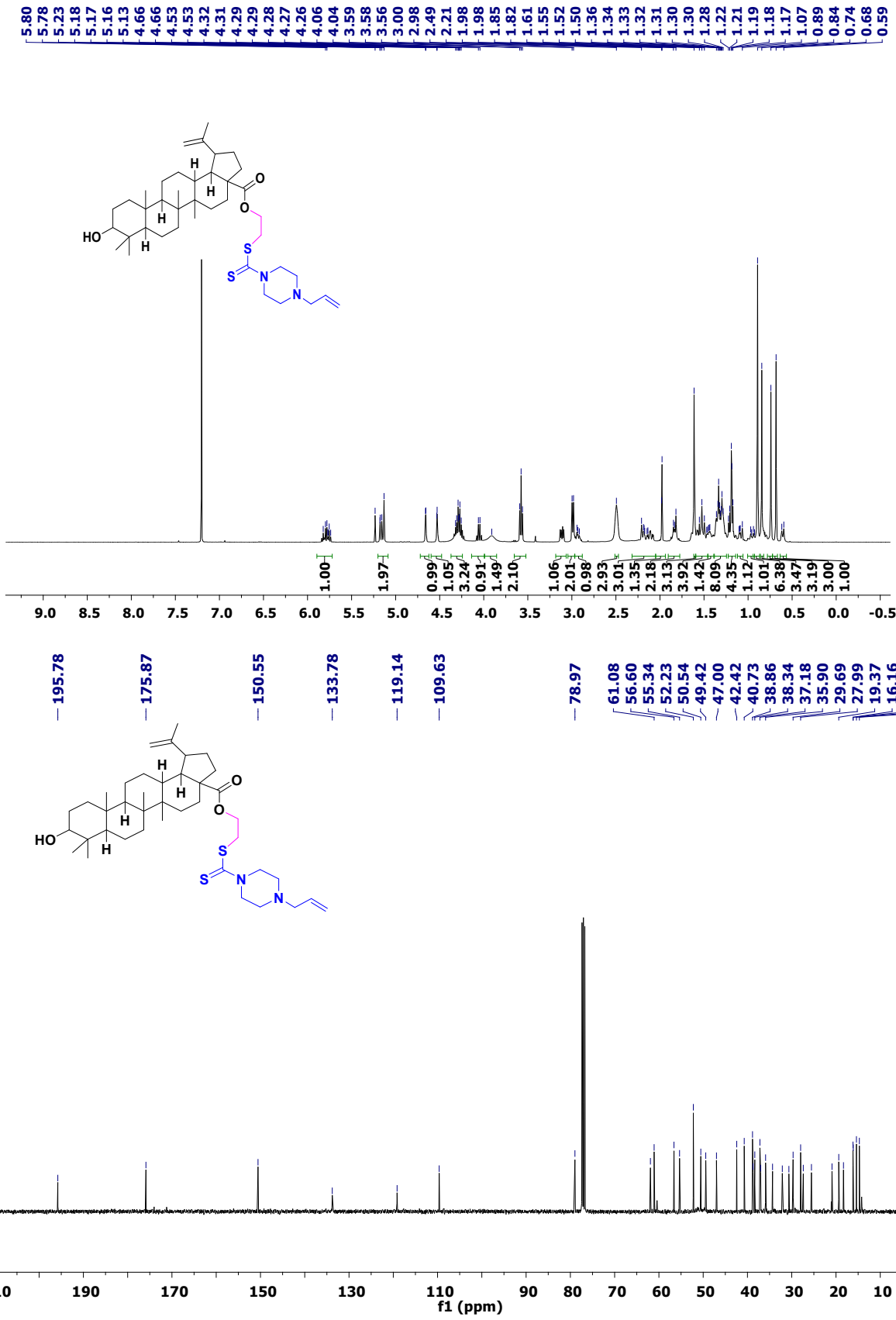




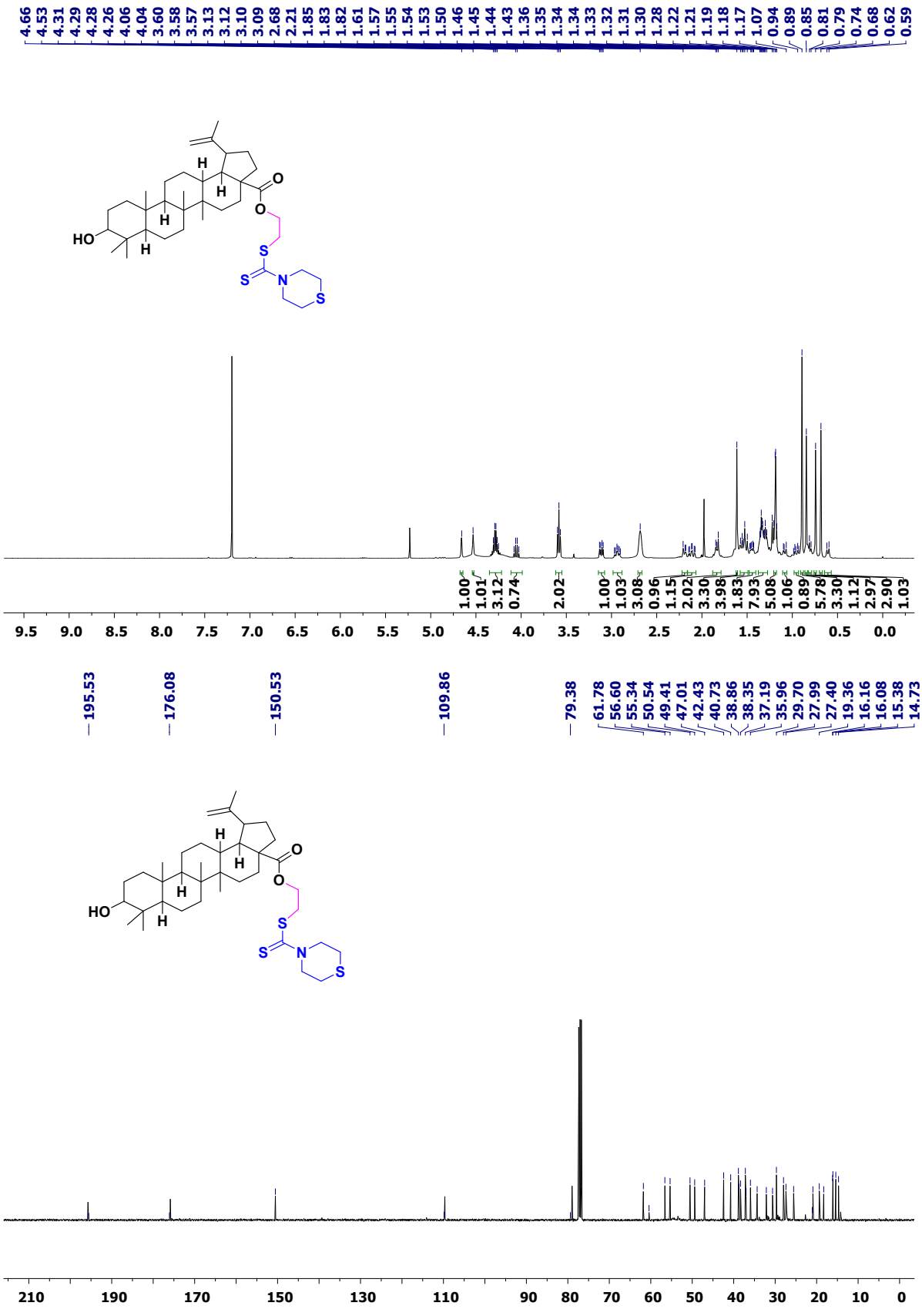
^{1}H NMR and ^{13}C NMR ($CDCl_3$) of **DTC7**



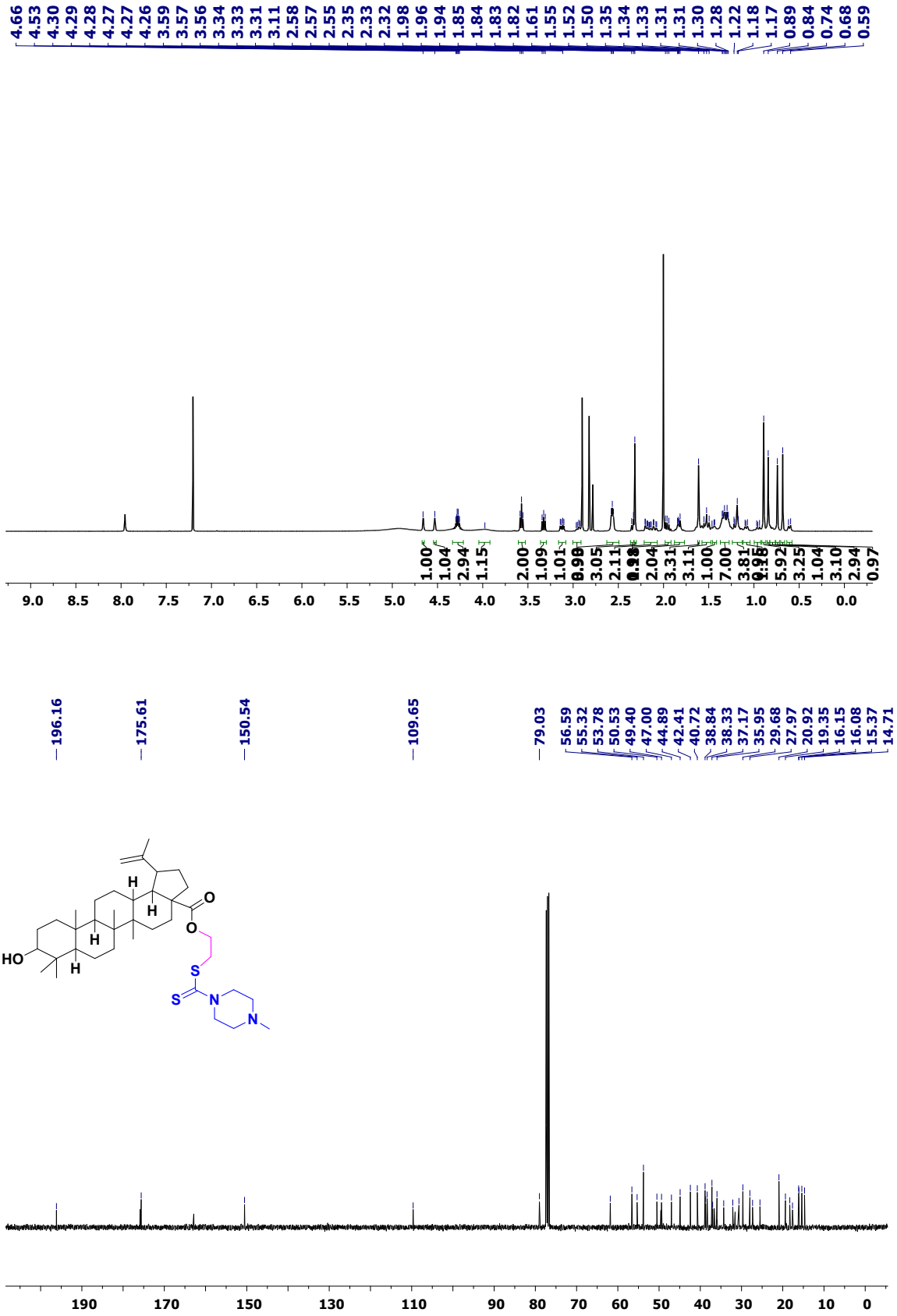
^{1}H NMR and ^{13}C NMR ($CDCl_3$) of **DTC8**



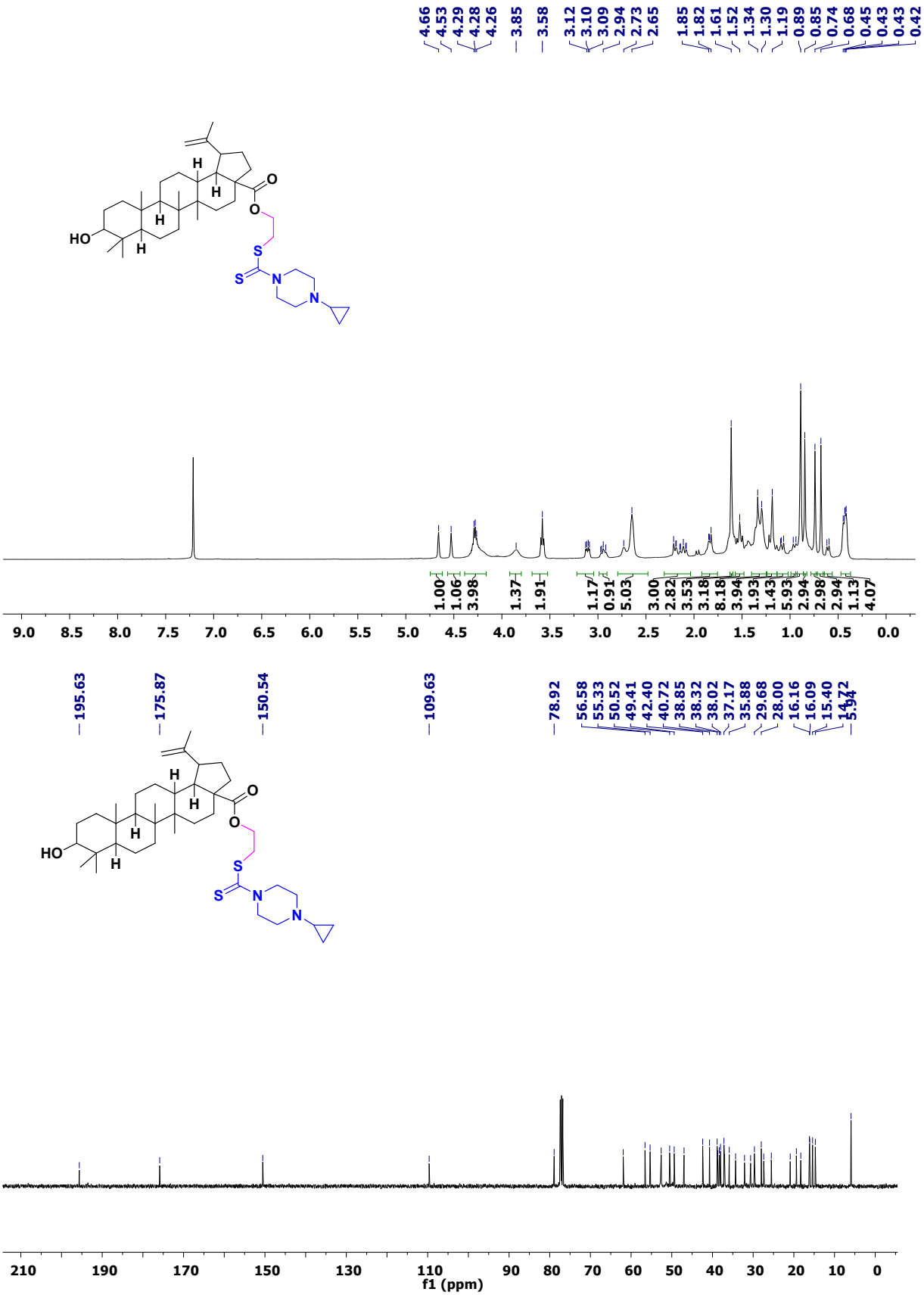
^{1}H NMR and ^{13}C NMR ($CDCl_3$) of **DTC9**



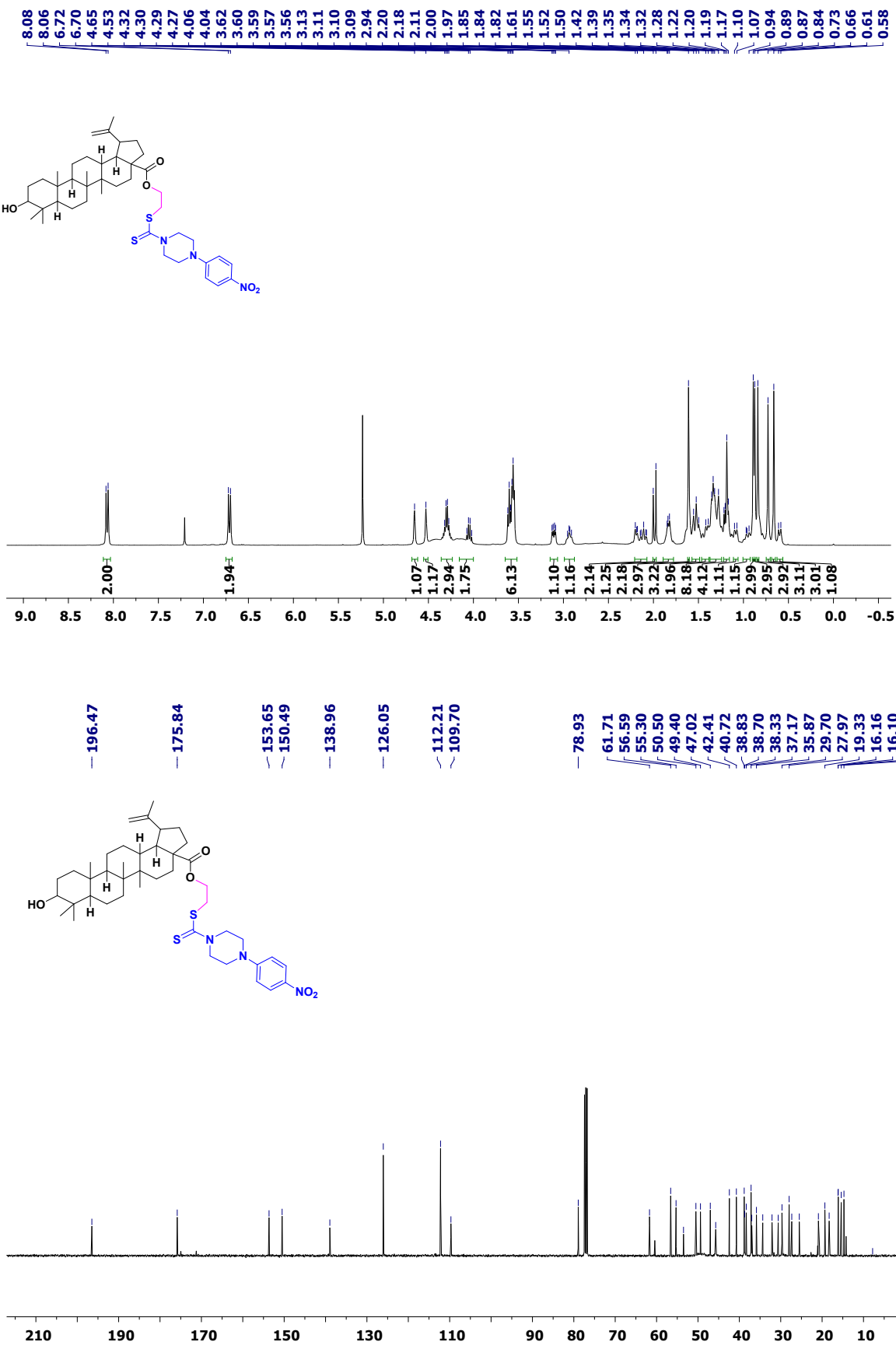
^{1}H NMR and ^{13}C NMR ($CDCl_3$) of **DTC10**



^{1}H NMR and ^{13}C NMR ($CDCl_3$) of **DTC11**



^{1}H NMR and ^{13}C NMR ($CDCl_3$) of **DTC12**



^{1}H NMR and ^{13}C NMR ($CDCl_3$) of **DTC13**