Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

Modular Synthesis, Spectroscopic Characterization and In-situ Functionalization using "click" Chemistry of Azide Terminated Amide Containing Self-Assembled Monolayers

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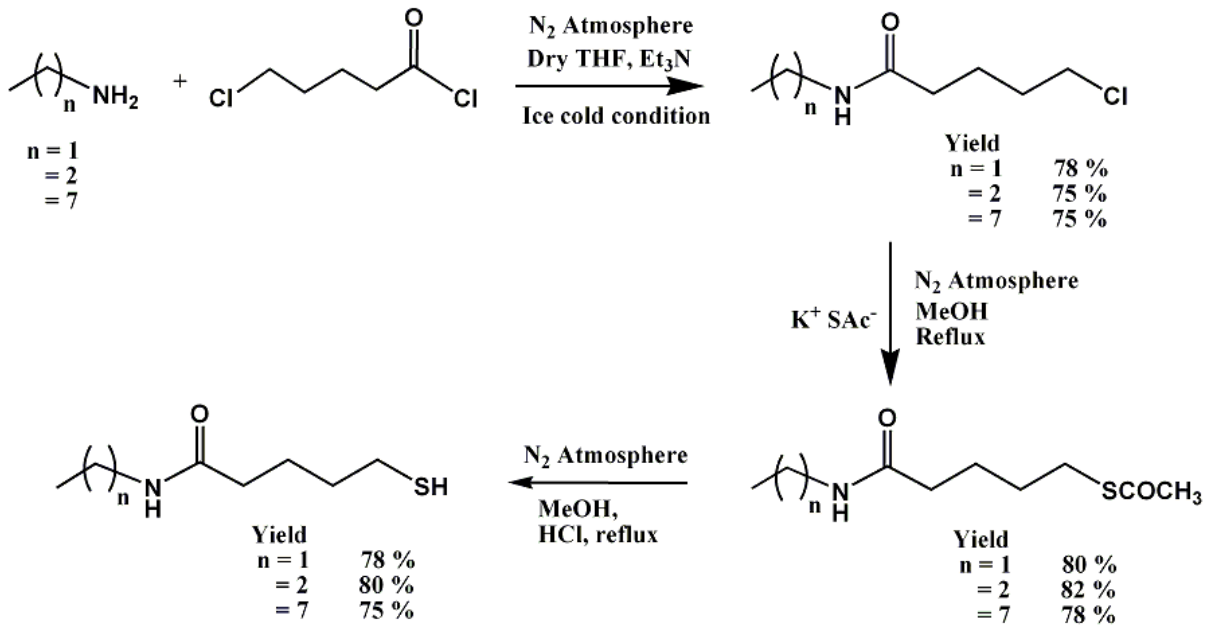
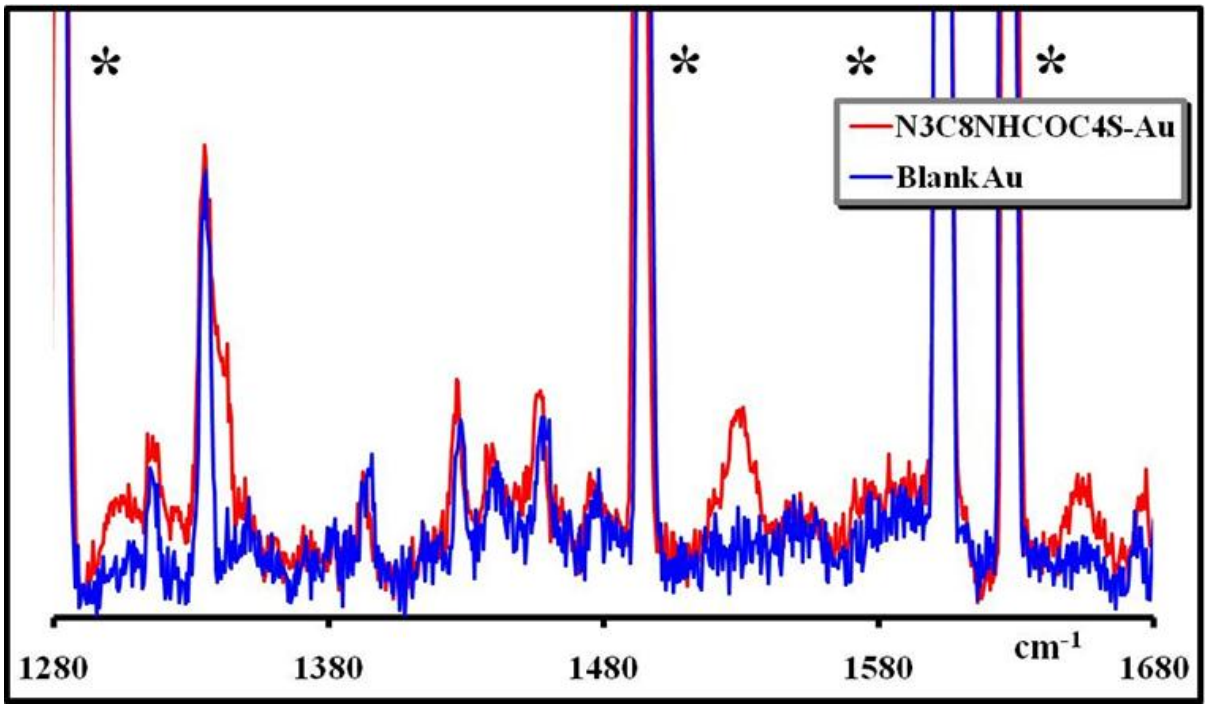
SI 1. Synthetic Scheme:

Scheme of synthesis of Amidealkylthiol (Diluent):



SI 2. Surface Characterization

SERS

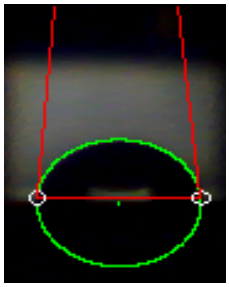


Surface enhanced Raman spectrum (SERS) of $N_3C_8NHCOC_4SH$ SAM on Au disk. The designated peaks at 1306 cm^{-1}, 1342 cm^{-1}, 1530 cm^{-1} and 1654 cm^{-1} are for amide III, azide symmetric stretching frequency, amide II and amide I respectively. * represents the plasma lines.

Contact Angle (CA) Goniometry

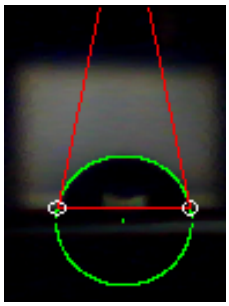
$N_3C_2NHCOC_4SH$

$N_3C_8NHCOC_4SH$



CA ~ 65 ± 1.7°

CA ~ 84 ± 1.6°



$N_3C_{11}SH$

$N_3C_4NHCOC_4SH$

CA ~ 77 ± 1.8°

CA ~ 70 ± 1.5°

SI 3. Synthesis Procedures and Characterization data

SI 3a *1-Azidoethylamine ($N_3C_2NH_2$)*

To a solution of 2-Bromoethylamine hydrobromide (1 gm, 5.0 mmol) in 7 ml water, 1 gm of sodium azide (15 mmol) was added and the reaction was stirred at 85^0C for 12 hours. After cooling the reaction mixture 200 mg of sodium hydroxide was added and stirred for 10 minute. Then diethyl ether and water were added to the reaction vessel and after workup the organic layer was collected, dried over anhydrous Na_2SO_4 and evaporated. The compound was purified by column chromatography on silica gel with 8% MeOH- DCM mixture as the eluent. Light yellow liquid.

Yield : 92% . ^{1}H NMR ($CDCl_3$, 500 MHz) δ (ppm): 3.35 (t, 2H, *J* = 5.5 Hz), 2.87 (t, 2H, *J* = 6 Hz). (^{13}C NMR, $CDCl_3$): 54.8, 41.5. IR spectra (cm^{-1}): 3346 (NH- stretching), 2106 (-N_3 stretching),

SI 3b *N-(4-Azidobutyl)phthalimide (N_3C_4Phth)*

To a solution of *N*-(4-Bromobutyl)phthalimide (1 gm, 3.5 mmol) in 10 ml DMF, 700 mg of sodium azide (10.5 mmol) was added and the reaction was stirred at 85^0C for 12 hours in nitrogen atmosphere. After cooling the reaction mixture water and diethyl ether were added to the reaction vessel and after workup the organic layer was collected, dried over

anhydrous Na_2SO_4 and evaporated. The product was purified by column chromatography on silica gel with DCM as the eluent. White solid product was obtained.

Yield : 86% . IR spectra (cm^{-1}): 2096 (N_3- stretching), 1772, 1710, 1678 (phthalimide). ESI-MS (+ve ion mode, MeOH) m/z = 283.3(100%) [MK^+].

SI 3c *1-Azidobutylamine ($N_3C_4NH_2$)*

To a solution of *N*-(4-Azidobutyl)phthalimide (0.8 gm, 3.0 mmol) in 70 ml EtOH, 3.6 ml of hydrazine hydrate (65 mmol) was added and the reaction was stirred at for 24 hours. After the reaction the precipitate was removed by filtration, the filtrate was evaporated and extracted with chloroform. After evaporating the chloroform the product was purified by column chromatography on silica gel with 2% MeOH- DCM mixture as the eluent. Light yellow oily compound.

Yield : 62% . ^{1}H NMR (CD_3OD, 500 MHz) δ (ppm): 3.3 (t, 2H, *J* = 5.5 Hz), 2.78 (t, 2H, *J* = 6.5 Hz), 1.64 (m, 4H). ^{13}C NMR ($CDCl_3$): 50.8, 40, 27.6, 25.8. IR spectra (cm^{-1}): 3355 (NH-stretching), 2098 (N_3- stretching).

SI 3d *N-(8-phthalimide)-1-octanol (OHC_8Phth)*

To a solution of 8-bromo-1-octanol (1 gm, 4.8 mmol) in 10 ml DMF, 0.9 gm of potassium phthalimide (5.0 mmol) was added and the reaction was stirred at for 2 hours. After the reaction $CHCl_3$ and water were added to the reaction vessel and after workup the organic layer was washed with 0.2 N NaOH and water, dried over anhydrous Na_2SO_4, after evaporating the solvent a colourless viscous liquid compound was obtained.

Yield : 88% . IR spectra (cm^{-1}): 3458 (-OH stretching), 1772, 1714, 1670.

SI 3e *N-(8-phthalimide)-1-methanesulphonate ($OMsC_8Phth$)*

To a solution of *N*-(8-phthalimide)-1-octanol (0.88 gm, 3.2 mmol) in 20 ml dry THF, 0.9 ml of triethylamine (6.5 mmol) was added and stirred for 10 minute at 0^0C in nitrogen atmosphere, then to the reaction mixture 0.5 ml (6.5 mmol) of methanesulfonyl chloride

(OMsCl) (dissolved in THF) was added drop wise and stirred at for 2 hours at low temperature. After the reaction water and diethyl ether were added to the reaction vessel and after workup the organic layer was collected, dried over anhydrous Na_2SO_4 and evaporated. Colourless viscous liquid was obtained.

Yield : 80% . IR spectra (cm^{-1}): 1772, 1714, 1614, 1353, 1174, 943, 721, 530.

SI 3f *N-(8-Azidooctyl)phthalimide (N_3C_8Phth)*

The synthesis procedure of *N*-(8-Azidooctyl)phthalimide was similar as mentioned above. Since here the leaving group was OMs so temperature applied was 60^0C. Light yellow liquid.

Yield : 85%. IR spectra (cm^{-1}): 2096 (-N_3 stretching), 1772, 1714, 1614 (phthalimide). ESI-MS (+ve ion mode, MeOH) m/z = 301.2 (100%) [MH^+].

SI 3g *1-Azidooctylamine ($N_3C_8NH_2$)*

The synthesis procedure of 1-Azidooctylamine was also similar as mentioned above in 1-Azidobutylamine synthesis. Light yellow liquid.

Yield : 68%. ^{1}H NMR ($CDCl_3$, 300 MHz) δ (ppm): 3.27 (t, 2H, *J* = 5.7 Hz), 2.7 (t, 2H, *J* = 6.8 Hz), 1.6 (m, 4H), 1.45 (m, 4H), 1.3 (m, 4H). ^{13}C NMR ($CDCl_3$): 51.5, 42.3, 33.8, 29.4, 29, 28.8, 26.8, 26.6. IR spectra (cm-1): 3355 (NH- stretching), 2098 (N_3- stretching).

Linkers –

Azidoalkylamidechloride [$N_3C_{(n+2)}NHCOC_4Cl$] (n = 0,2,6)

To a solution of Azidoalkylamine in dry THF, two equivalent of triethylamine was added and stirred for 10 minute at 0^0C in nitrogen atmosphere, then to the reaction mixture two equivalent of 5-chlorovaleroyl chloride (dissolved in THF) was added drop wise and stirred for at least 2 hours at low temperature. After the reaction water and diethyl ether were added to the reaction vessel. After workup the organic layer was collected, dried over anhydrous Na_2SO_4 and evaporated

SI 3h *1-Azidoethylamidebutylchloride*

The product was purified by column chromatography on silica gel with 2% MeOH-DCM mixture as the eluent. Light yellow liquid compound was obtained.

Yield : 72%. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 6 (s, 1H), 3.52 (t, 2H, *J* = 5.5 Hz), 3.38-3.44 (m, 4H), 2.22 (t, 2H, *J* = 4.5 Hz), 1.76-1.81 (m, 4H). ^{13}C NMR ($CDCl_3$): 173, 51, 44.7, 39, 35.7, 32, 23. IR spectra (cm^{-1}): 2102 (N_3- stretching), 1647, 1550 (amide stretching & bending). ESI-MS (+ve ion mode, MeOH) m/z = 205.05 (50%) [MH^+], 227.04 (100%) [MNa^+].

SI 3i *1-Azidobutylamidebutylchloride*

The product was purified by column chromatography on silica gel with 40% EtOAc-Hexane mixture as the eluent. Light yellow liquid compound was obtained.

Yield : 65%. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 5.5 (s, 1H), 3.48 (t, 2H, *J* = 6 Hz), 3.2-3.26 (m, 4H), 2.14 (t, 2H, *J* = 6.5 Hz), 1.69-1.76 (m, 4H), 1.51-1.57 (m, 4H). ^{13}C NMR ($CDCl_3$): 172.5, 51, 44.6, 39, 35.8, 32, 27, 26.3, 23.02. IR spectra (cm^{-1}): 2098 (N_3- stretching), 1650, 1554 (amide stretching & bending).

SI 3j *1-Azidooctylamidebutylchloride*

The product was purified by column chromatography on silica gel with 2% MeOH-DCM mixture as the eluent. Light yellow liquid compound was obtained.

Yield : 62%. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 5.53 (s, 1H), 3.48 (t, 2H, *J* = 6 Hz), 3.13-3.21 (m, 4H), 2.13 (t, 2H, *J* = 6.6 Hz), 1.68-1.78 (m, 8H), 1.1-1.5 (m, 8H). ^{13}C NMR ($CDCl_3$): 172.4, 51.5, 44.7, 39.6, 35.8, 32, 29.7, 29.2, 29.1, 28.8, 26.8, 26.7, 23.1. IR spectra (cm^{-1}): 2095 (N_3- stretching), 1637, 1541 (amide stretching & bending). ESI-MS (+ve ion mode, MeOH) m/z = 311.1 (100%) [MNa^+].

Azidoalkylamidethioacetate [$N_3C_{(n+2)}NHCOC_4SAc$]

All thioacetate compounds were synthesised as reported procedure.[1]

SI 3k *1-Azidoethylamidebutylthioacetate*

The product was purified by column chromatography on silica gel with 2% MeOH-DCM mixture as the eluent. Light yellow liquid compound was obtained.

Yield : 85%. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 6 (s, 1H), 3.35 (m, 4H), 2.81 (t, 2H, *J* = 7 Hz), 2.26 (s, 3H), 2.16 (t, 2H, *J* = 7), 1.2-1.6 (m, 4H). ^{13}C NMR ($CDCl_3$): 196.2, 173, 39, 35.8, 29.8, 29.2, 28.6, 23. IR spectra (cm^{-1}): 2102 (N_3- stretching), 1691.5 (carbonyl stretch of thioacetate), 1647, 1544 (amide stretching & bending). ESI-MS (+ve ion mode, MeOH) m/z = 267.1 (100%) [MNa^+].

SI 3l *1-Azidobutylamidebutylthioacetate*

The product was purified by column chromatography on silica gel with 2% MeOH-DCM mixture as the eluent. Light yellow liquid compound was obtained.

Yield : 82%. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 6.1 (s, 1H), 3.47 (t, 2H, *J* = 6 Hz), 3.2 (t, 2H, *J* = 6.5), 2.8 (t, 2H, *J* = 7 Hz), 2.24 (s, 3H), 2.1 (t, 2H, *J* = 7.5), 1.5-1.7 (m, 8H). ^{13}C NMR ($CDCl_3$): 196, 172.6, 51, 44, 38, 35, 32, 30.5, 28.5, 26.2. IR spectra (cm^{-1}): 2096 (N_3-stretching), 1691 (carbonyl stretch of thioacetate), 1647, 1551 (amide stretching & bending).

SI 3m *1-Azidooctylamidebutylthioacetate*

The product was purified by column chromatography on silica gel with 45% EtOAc-Hexane mixture as the eluent. Light yellow liquid compound was obtained.

Yield : 80%. IR spectra (cm^{-1}): 2096.5 (N_3- stretching), 1691.4 (carbonyl stretch of thioacetate), 1645, 1552 (amide stretching & bending). ESI-MS (+ve ion mode, MeOH) m/z = 329.4 (100%) [MH^+], 351.4 (25%) [MNa^+].

Diluents –

Amidealkylchloride [$C_{(n+1)}NHCOC_4Cl$] (n = 1,2,7)

SI 3n *Ethylamidebutylchloride*

Light yellow liquid compound was obtained.

Yield : 78%. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 5.7 (s, 1H), 3.48 (t, 2H, *J* = 4 Hz), 3.18-3.24 (m, 4H), 2.13 (t, 2H, *J* = 7 Hz), 1.7-1.77 (m, 4H), 1.06 (t, 3H, *J* = 5.5). ^{13}C NMR ($CDCl_3$): 172.3, 44.7, 35.8, 34.4, 32, 23, 15. IR spectra (cm^{-1}): 1645, 1553 (amide stretching & bending).

SI 3o *Propylamidebutylchloride*

The product was purified by column chromatography on silica gel with 65% EtOAc-Hexane mixture as the eluent. Light yellow viscous compound was obtained.

Yield : 75%. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 6.2 (s, 1H), 3.57 (t, 2H, *J* = 5 Hz), 3.19 (q, 2H, *J* = 6), 2.22 (t, 2H, *J* = 6.6 Hz), 1.7-1.86 (m, 4H), 1.46-1.58 (m, 4H), 0.92 (t, 3H, *J* = 7.5). ^{13}C NMR ($CDCl_3$): 172.6, 44.6, 41.2, 35.6, 32, 23, 22.8, 11. IR spectra (cm^{-1}): 1645, 1553 (amide stretching & bending). ESI-MS (+ve ion mode, MeOH) m/z = 178.17 (100%) [MH^+].

SI 3p *Octylamidebutylchloride*

The product was purified by column chromatography on silica gel with DCM eluent. Light yellow densed liquid compound was obtained.

Yield : 75%. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 5.8 (s, 1H), 3.55 (t, 2H, *J* = 4 Hz), 3.22 (q, 2H, *J* = 6 Hz), 2.21 (t, 2H, *J* = 7 Hz), 1.75-1.9 (m, 4H), 1.49 (t, 2H, *J* = 6.5), 1.25-1.32 (m, 10H), 0.88 (t, 3H, *J* = 6.5 Hz). ^{13}C NMR ($CDCl_3$): 172.47, 44.6, 39.7, 35.8, 33.25, 32, 29.7, 29.0, 27, 23.1, 22.6, 22.3, 14.2. IR spectra (cm^{-1}): 1645, 1554 (amide stretching & bending). ESI-MS (+ve ion mode, MeOH) m/z = 248.18 (100%) [MH^+], 270.17 (90%) [MNa^+].

Amidealkylthioacetate [$C_{(n+1)}NHCOC_4SAc$]

All thioacetate compounds were synthesised as reported procedure.[1]

SI 3q *Ethylamidebutylthioacetate*

The product was purified by column chromatography on silica gel with 2% MeOH-DCM mixture as the eluent. Light yellow liquid compound was obtained.

Yield : 80%. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 5.7 (s, 1H), 3.52 (t, 2H, *J* = 6 Hz), 3.22-3.28 (m, 4H), 2.81 (t, 2H, *J* = 7.5 Hz), 2.29 (s, 3H), 2.15 (t, 2H, *J* = 8), 1.7-1.8 (m, 4H), 1.1 (t, 3H, *J* =

6 Hz). ^{13}C NMR ($CDCl_3$): 196.2, 172.5, 44.7, 36.2, 35.8, 32.1, 24.8, 23.1, 15. IR spectra (cm^{-1}): 1691.6 (carbonyl stretch of thioacetate), 1645, 1551 (amide stretching & bending).

SI 3r *Propylamidebutylthioacetate*

The product was purified by column chromatography on silica gel with DCM as the eluent. Light yellow liquid compound was obtained.

Yield : 82%. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 5.75 (s, 1H), 3.52 (t, 2H, *J* = 6 Hz), 3.14-3.19 (m, 2H), 2.82 (t, 2H, *J* = 7 Hz), 2.28 (s, 3H), 2.15 (t, 2H, *J* = 7.5), 1.6-1.8 (m, 4H), 0.95 (t, 3H, *J* = 6 Hz). ^{13}C NMR ($CDCl_3$): 196.1, 172.6, 44.7, 41.3, 36.2, 35.8, 32.1, 28.8, 23.1, 11.4. IR spectra (cm^{-1}): 1691.5 (carbonyl stretch of thioacetate), 1645, 1549 (amide stretching & bending). ESI-MS (+ve ion mode, MeOH) m/z = 240.11 (100%) [MNa^+].

SI 3s *Octylamidebutylthioacetate*

The product was purified by column chromatography on silica gel with DCM as the eluent. Light yellow viscous compound was obtained.

Yield : 78%. IR spectra (cm^{-1}): 1693.4 (carbonyl stretch of thioacetate), 1639.4, 1541 (amide stretching & bending).

Amidealkylthiol [$C_{(n+1)}NHCOC_4SH$]

All thiol compounds were synthesised as reported procedure.[1]

SI 3t *Ethylamidebutylthiol*

The product was purified by column chromatography on silica gel with 2% MeOH-DCM mixture as the eluent. Light yellow liquid compound was obtained.

Yield : 78%. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 5.85 (s, 1H), 3.51 (t, 2H, *J* = 5.5 Hz), 3.23 (m, 2H), 2.15 (t, 2H, *J* = 6.5 Hz), 1.7-1.8 (m, 4H), 1.09 (t, 3H, *J* = 7.5). ^{13}C NMR ($CDCl_3$): 172.3, 44.6, 36, 34.4, 32, 24, 14. IR spectra (cm^{-1}): 1645, 1553 (amide stretching & bending). ESI-MS (+ve ion mode, MeOH) m/z = 321.0 (100%) [MH^+], 343.0 (30%) [MNa^+] (Mass of disulfide).

SI 3u *Propylamidebutylthiol*

The product was purified by column chromatography on silica gel with DCM as the eluent. Light yellow liquid compound was obtained.

Yield : 80%. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 6.36, 6.16 (s, 1H), 2.99 (q, 2H, *J* = 6.3 Hz), 2.5 (t, 2H, *J* = 6 Hz), 2.34 (t, 2H, *J* = 7 Hz), 1.32-1.6 (m, 4H), 0.73 (t, 5H, *J* = 7 Hz). ^{13}C NMR ($CDCl_3$): 172.7, 41.1, 38.5, 36, 30.5, 24, 22.7, 11.3. IR spectra (cm^{-1}): 2545 (-SH stretching) 1643, 1553 (amide stretching & bending). ESI-MS (+ve ion mode, MeOH) m/z = 348.95 (60%) [MH^+], 370.91 (100%) [MNa^+] (Mass of disulfide).

SI 3v *Octylamidebutylthiol*

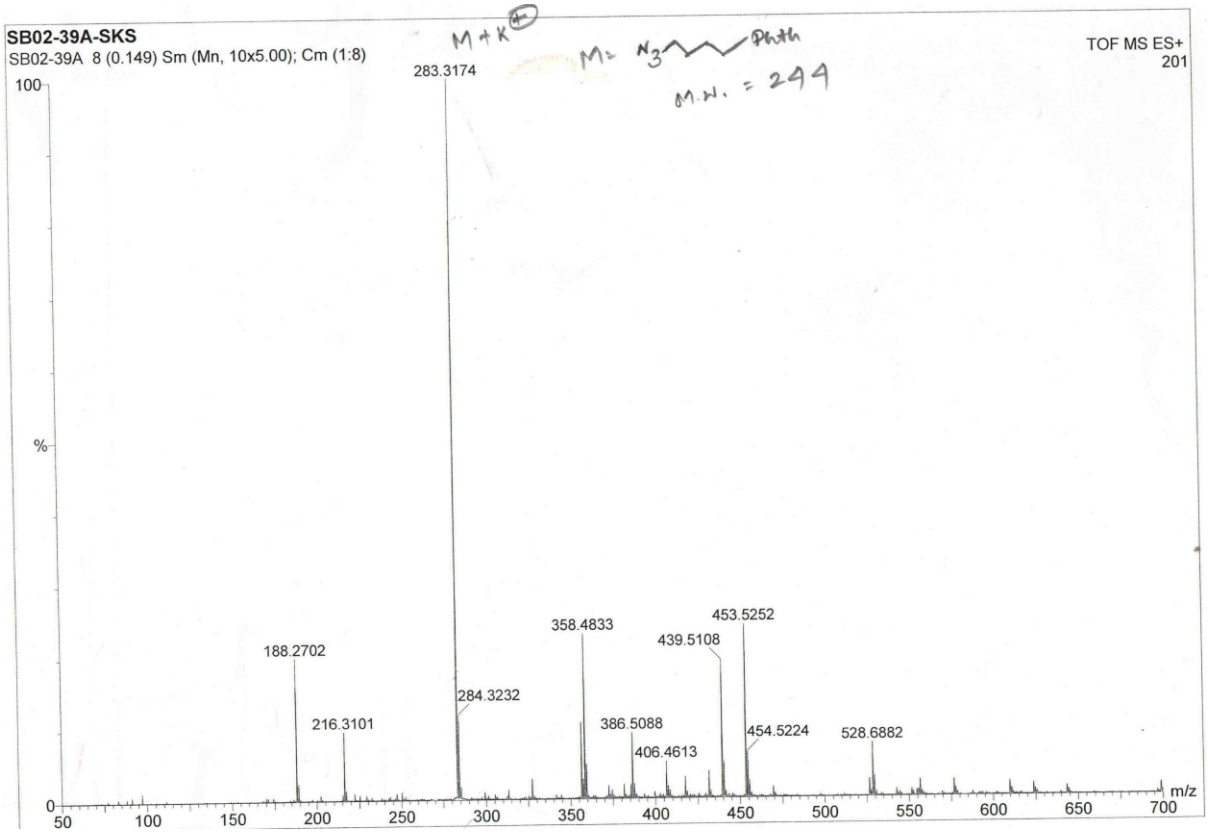
The product was purified by column chromatography on silica gel with 30% EtOAc-Hexane mixture as the eluent. Light yellow viscous compound was obtained.

Yield : 75%. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 5.47 (s, 1H), 3.24 (q, 2H, *J* = 6.9 Hz), 2.53 (t, 2H, *J* = 7 Hz), 2.17 (t, 2H, *J* = 7.5 Hz), 1.6-1.77 (m, 4H), 1.49 (t, 2H, *J* = 6 Hz), 1.27-1.4 (m, 10H), 0.87 (t, 3H, *J* = 6.3 Hz). ^{13}C NMR ($CDCl_3$): 172.55, 39.7, 36.26, 33.64, 31.9, 29.8, 29.4, 29.3, 27, 24.5, 24.4, 22.7, 14.2. IR spectra (cm^{-1}): 1645, 1553 (amide stretching & bending). ESI-MS (+ve ion mode, MeOH) m/z = 246.1 (30%) [MH^+], 268.1 (100%) [MNa^+].

SI 4. Copy of spectra –

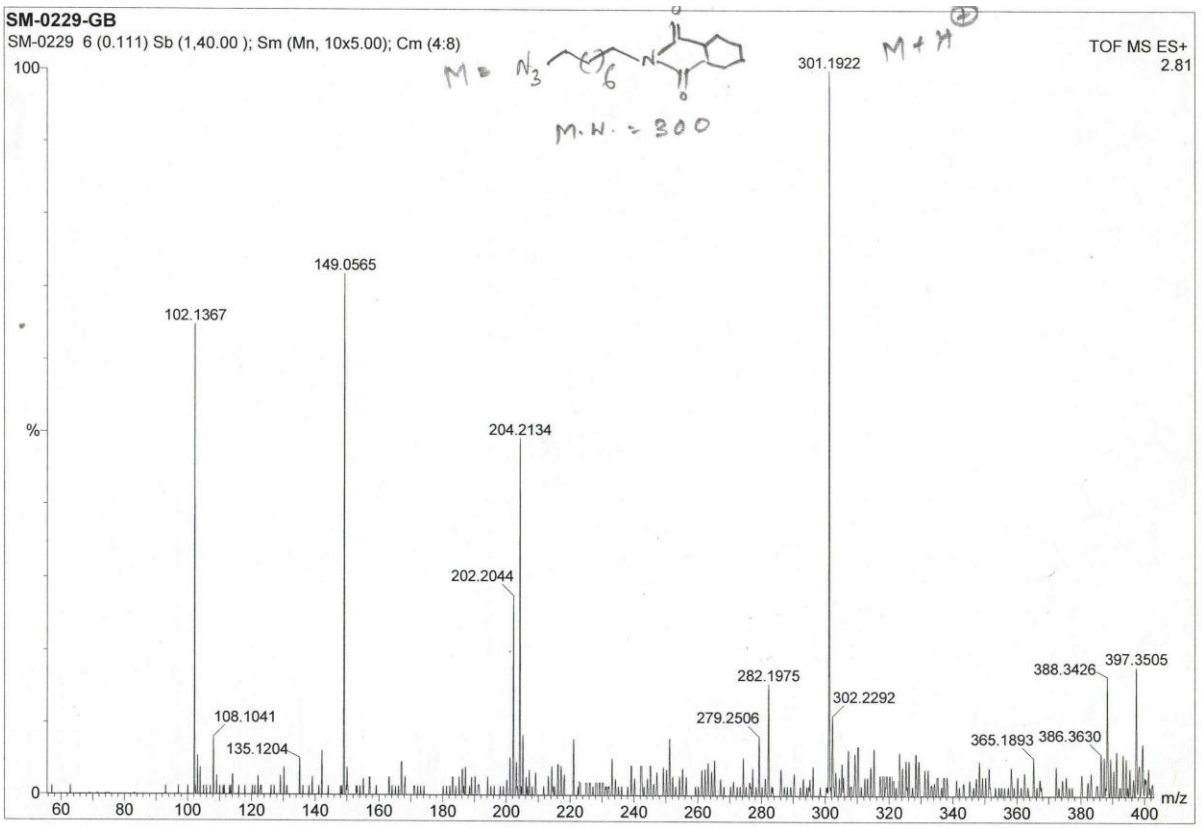
N-(4-Azidobutyl)phthalimide

ESI-MS



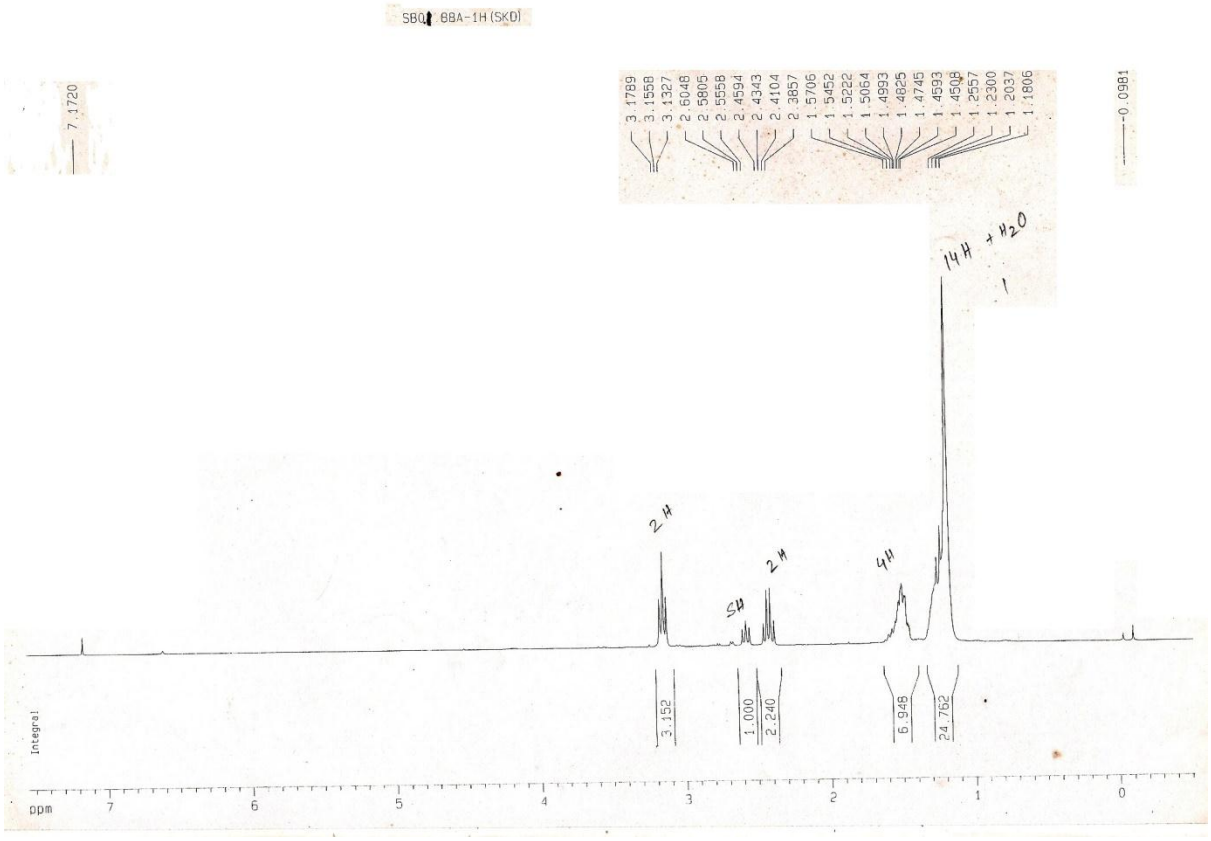
N-(8-Azidooctyl)phthalimide

ESI-MS

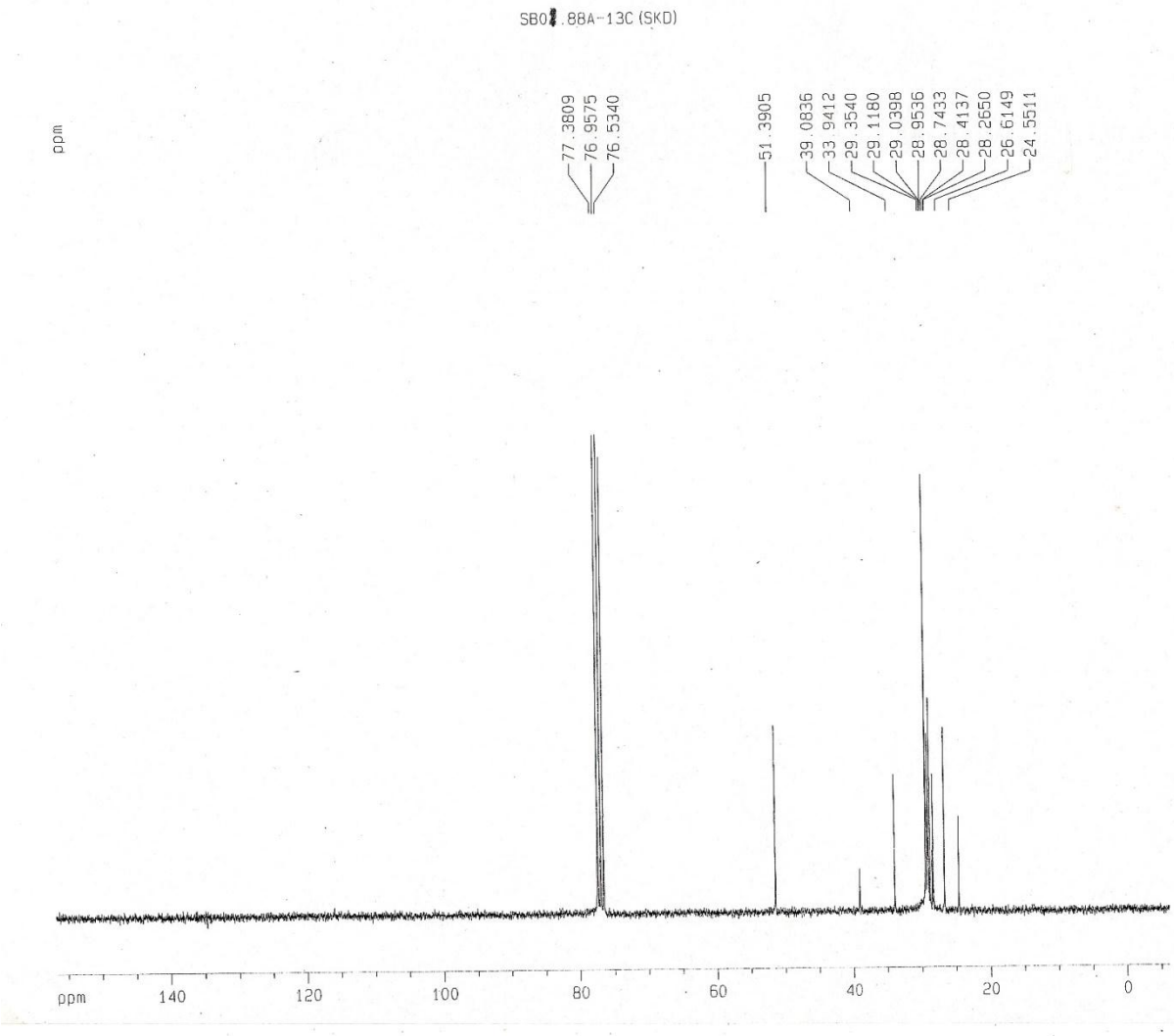


1-Azidoundecanethiol

^{1}H NMR ($CDCl_3$)

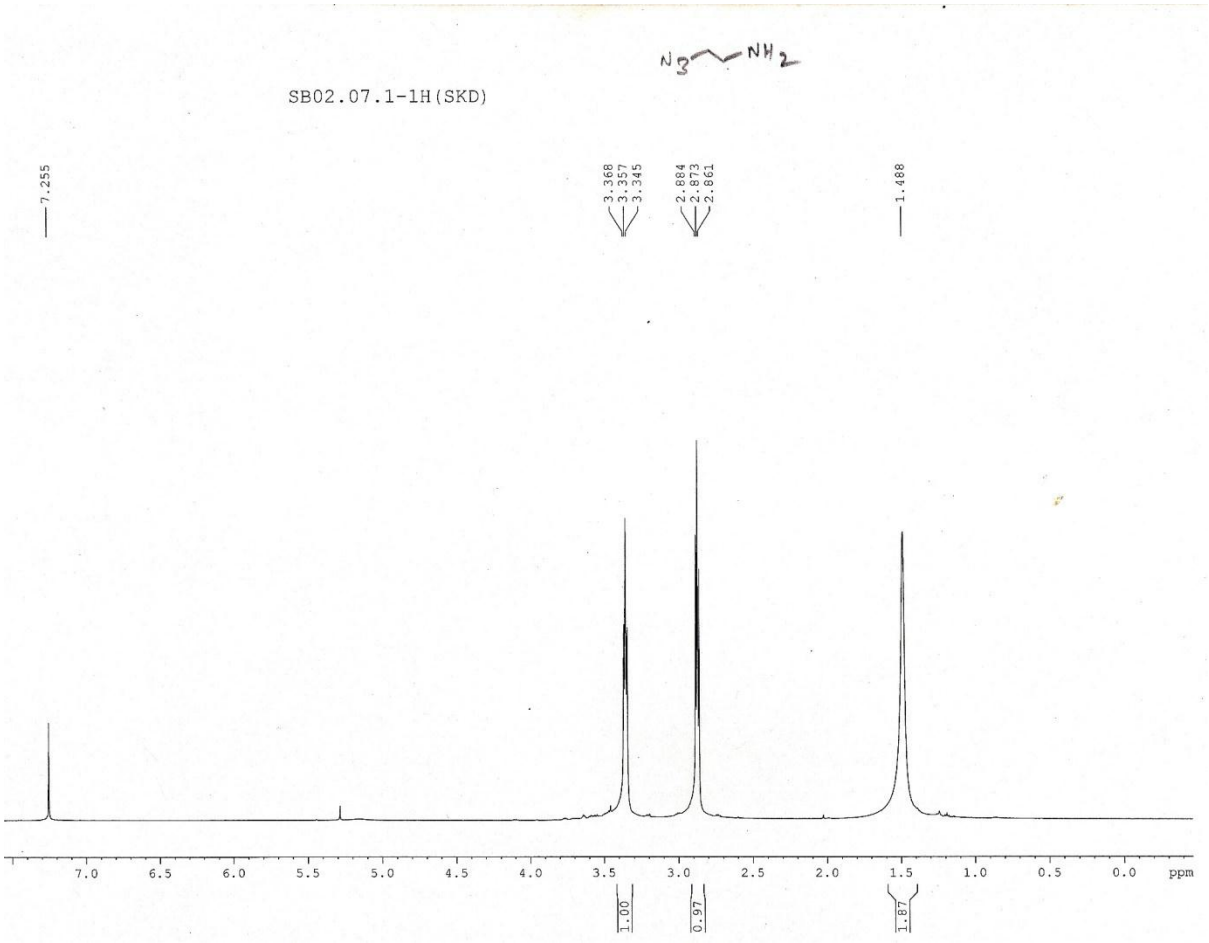


^{13}C NMR

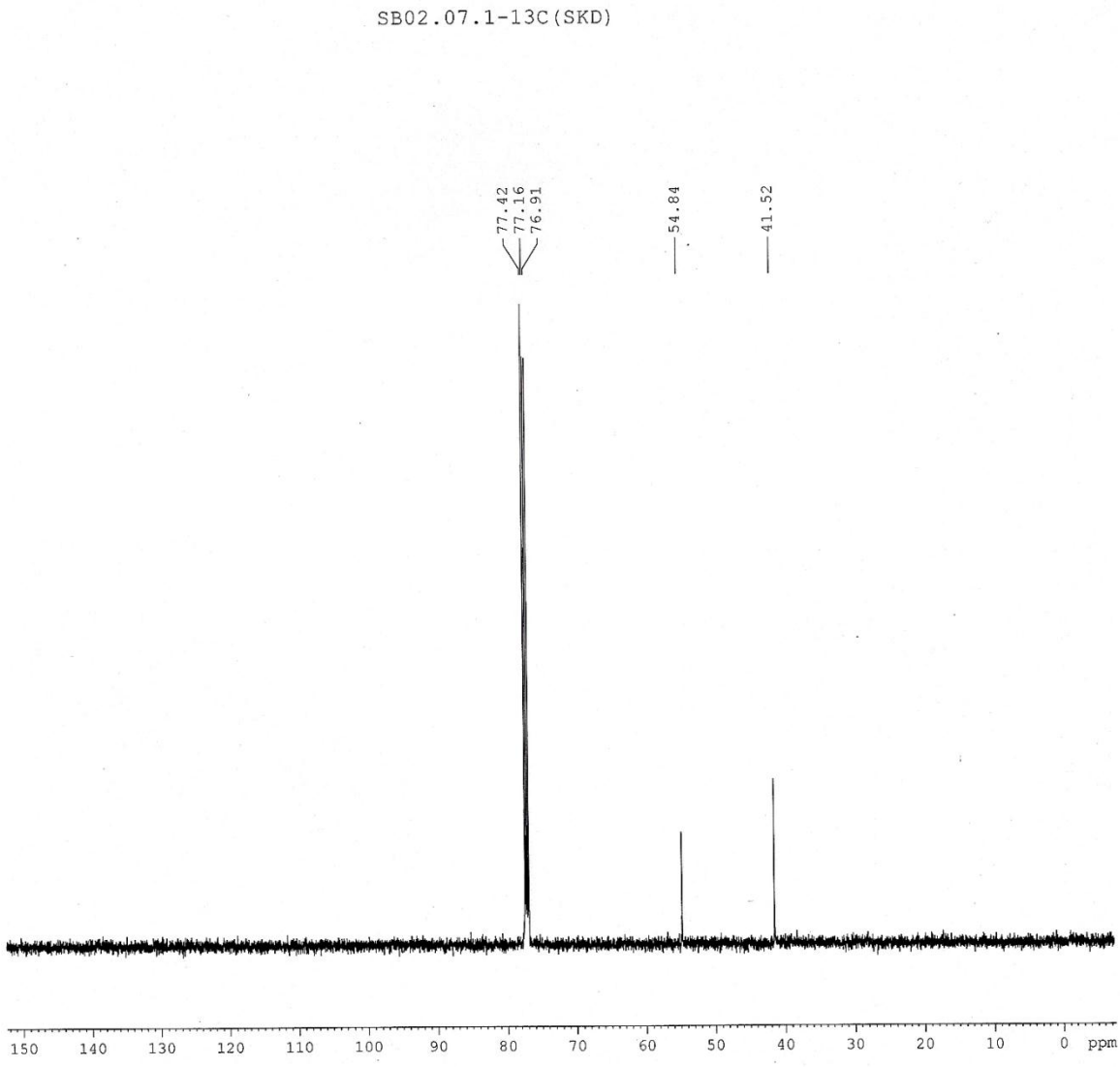


1-Azidoethylamine

^{1}H NMR ($CDCl_3$)

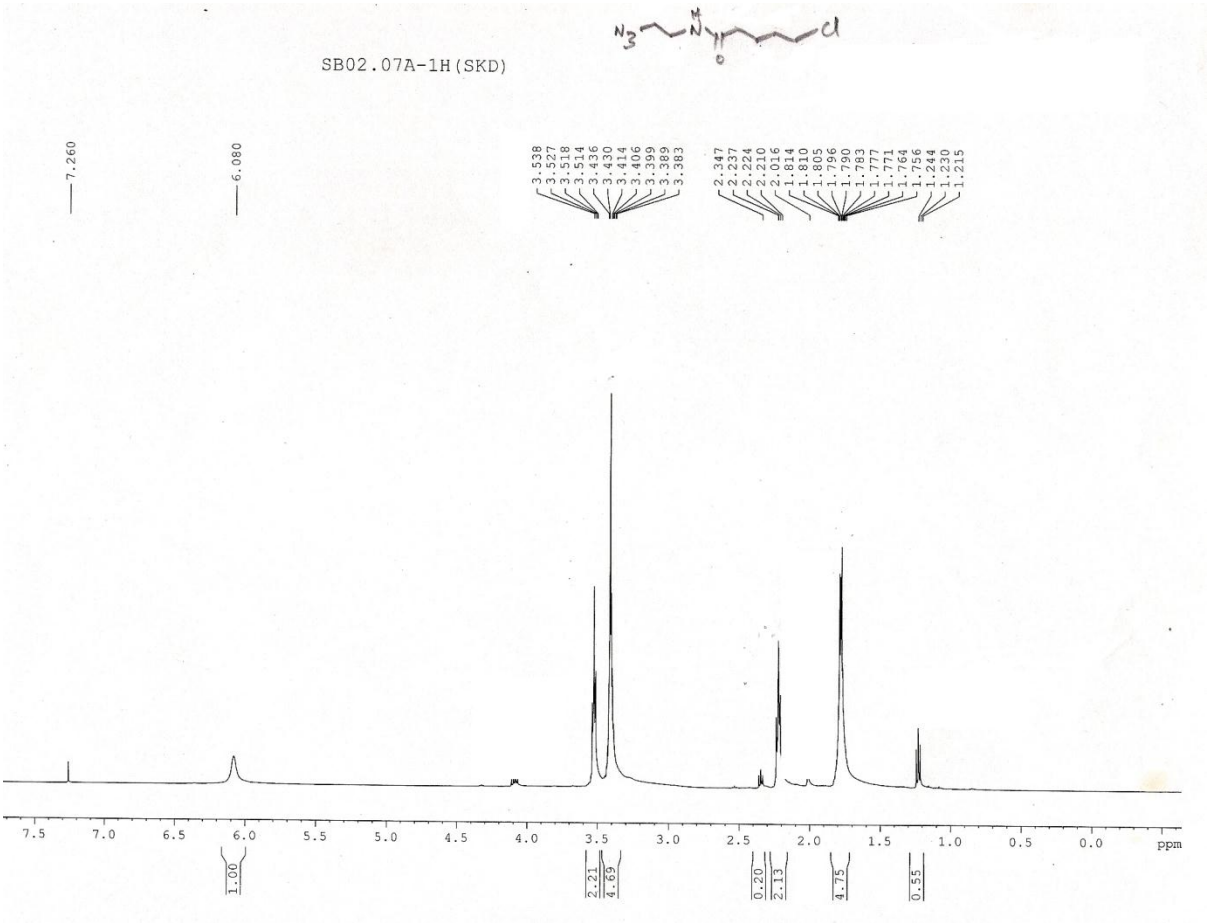


^{13}C NMR

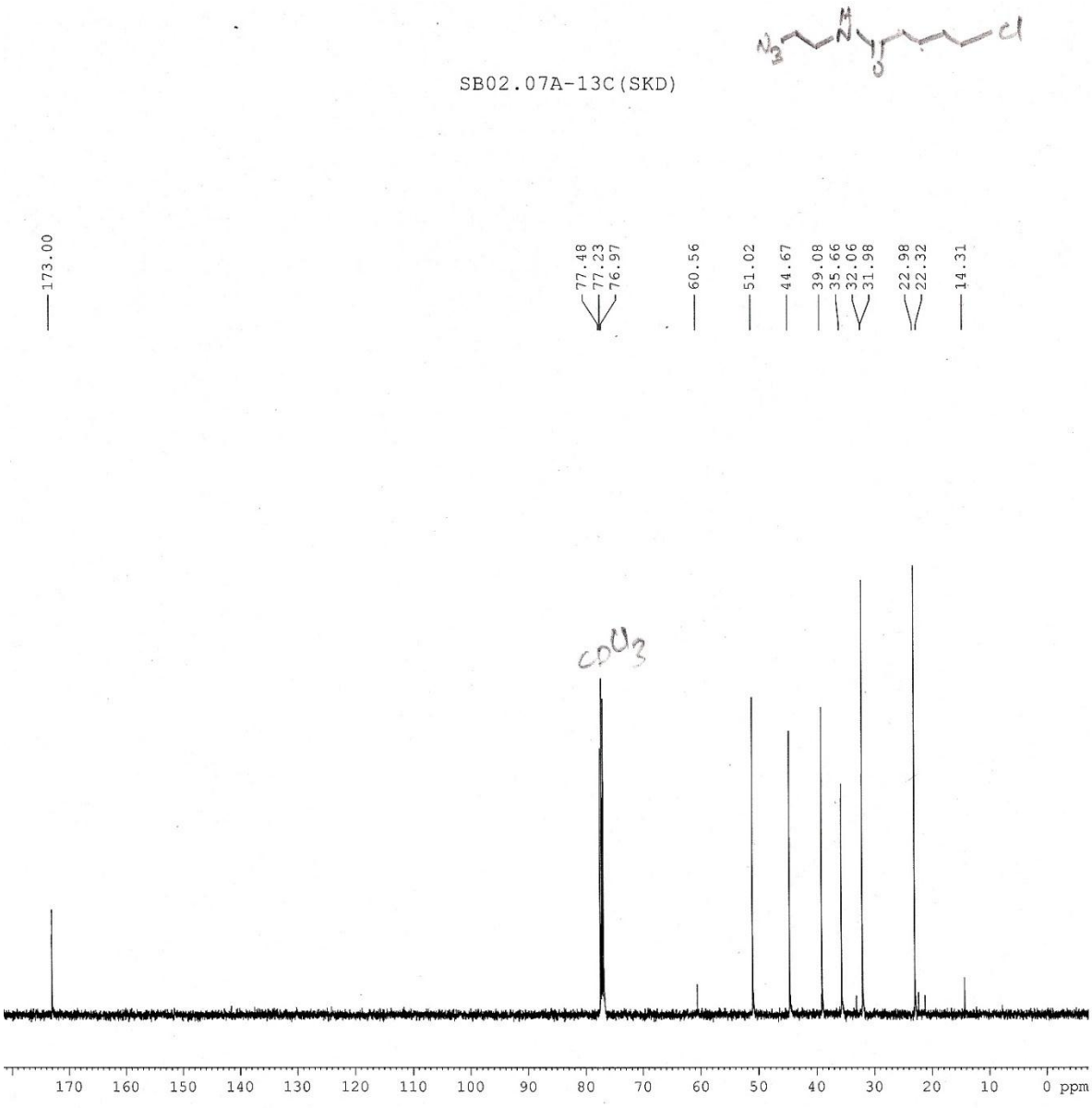


1-Azidoethylamidebutylchloride

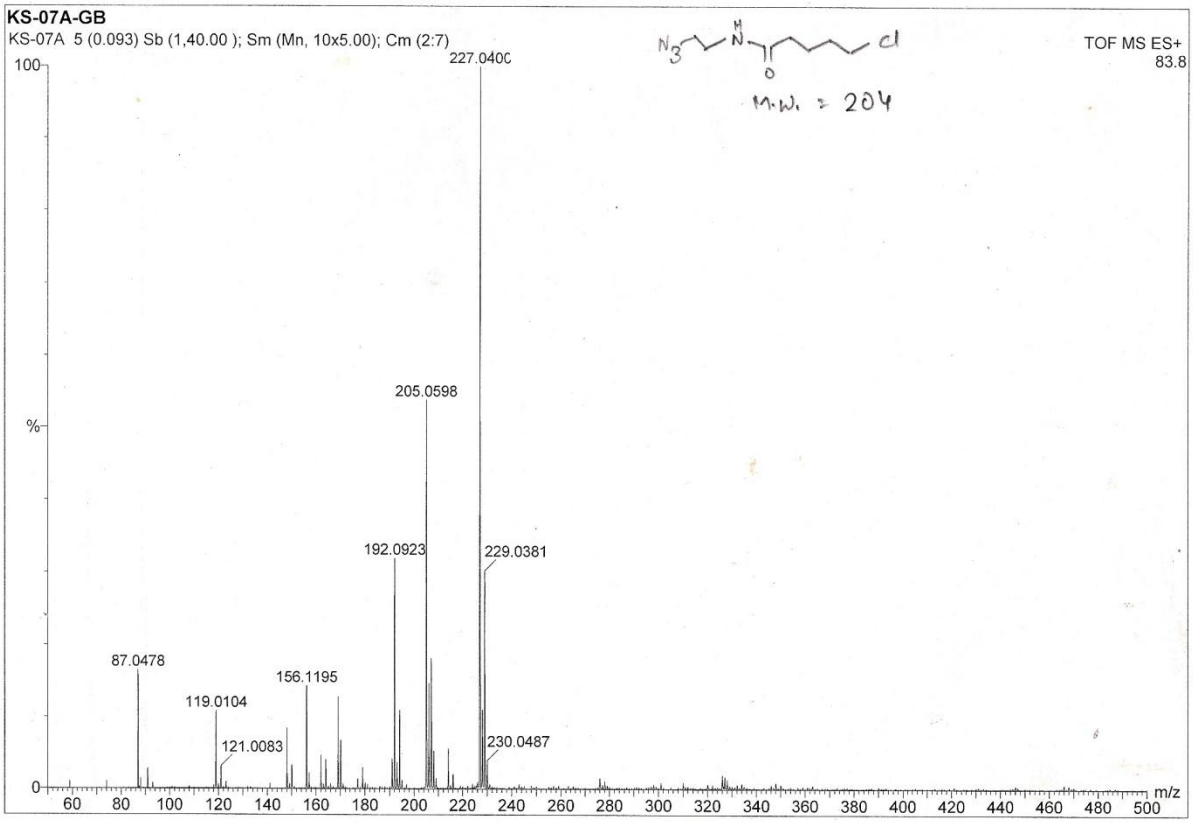
^{1}H NMR ($CDCl_3$)



^{13}C NMR



ESI-MS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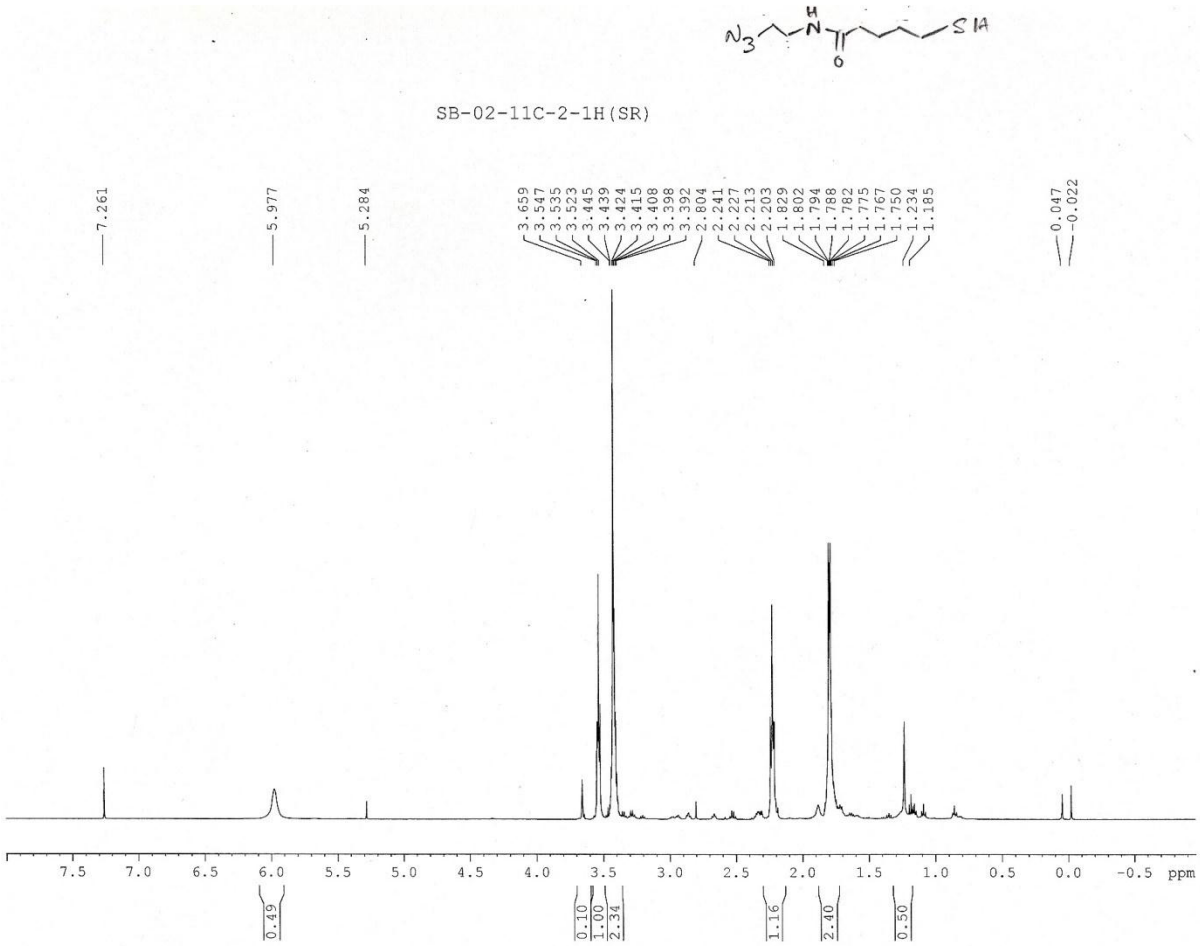
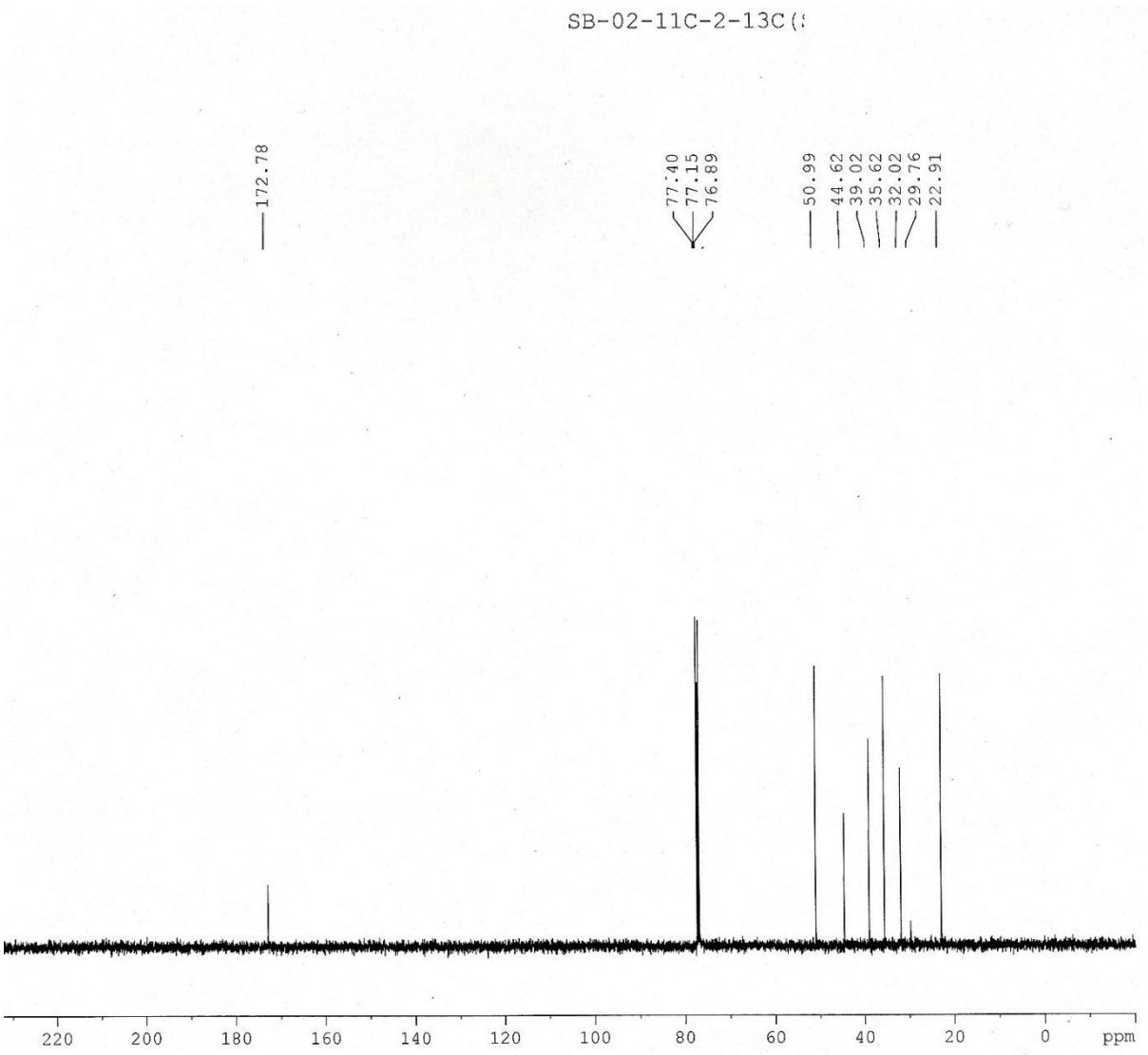
1-Azidoethylamidebutylthiol

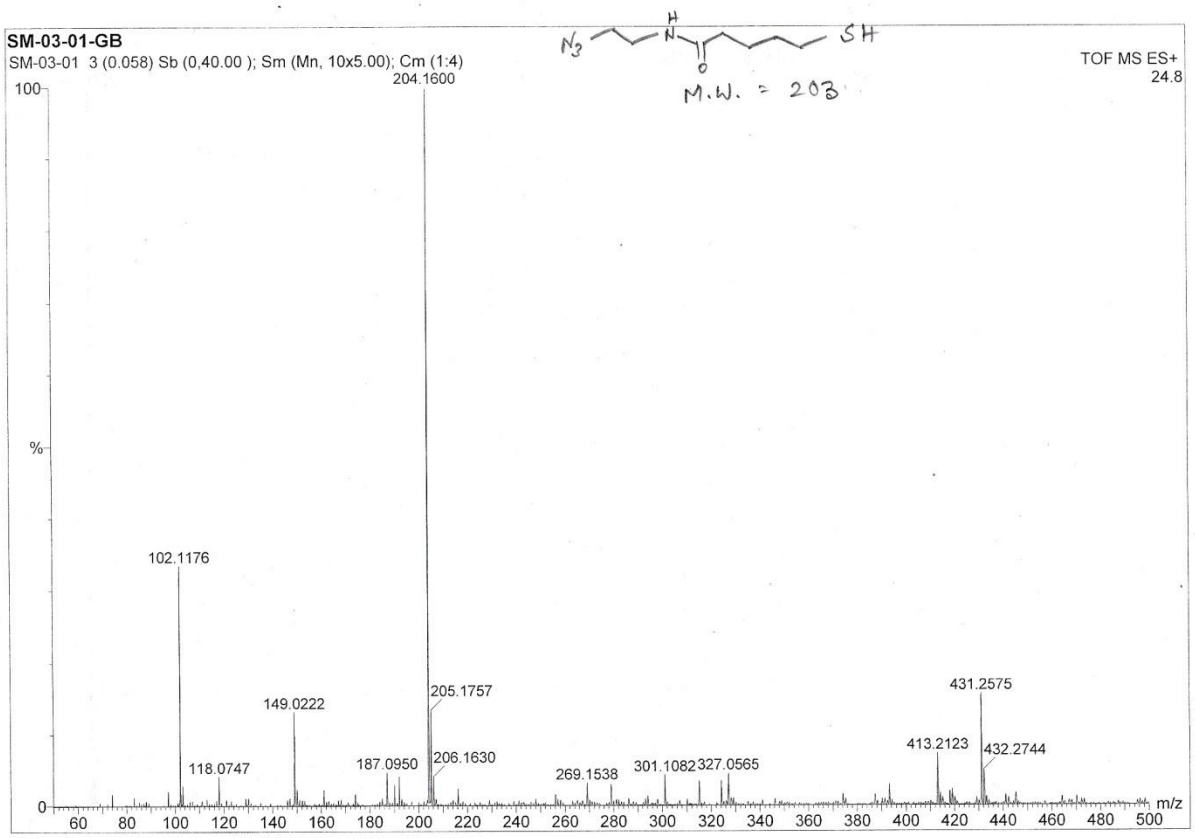
^{1}H NMR ($CDCl_3$)



^{13}C NMR

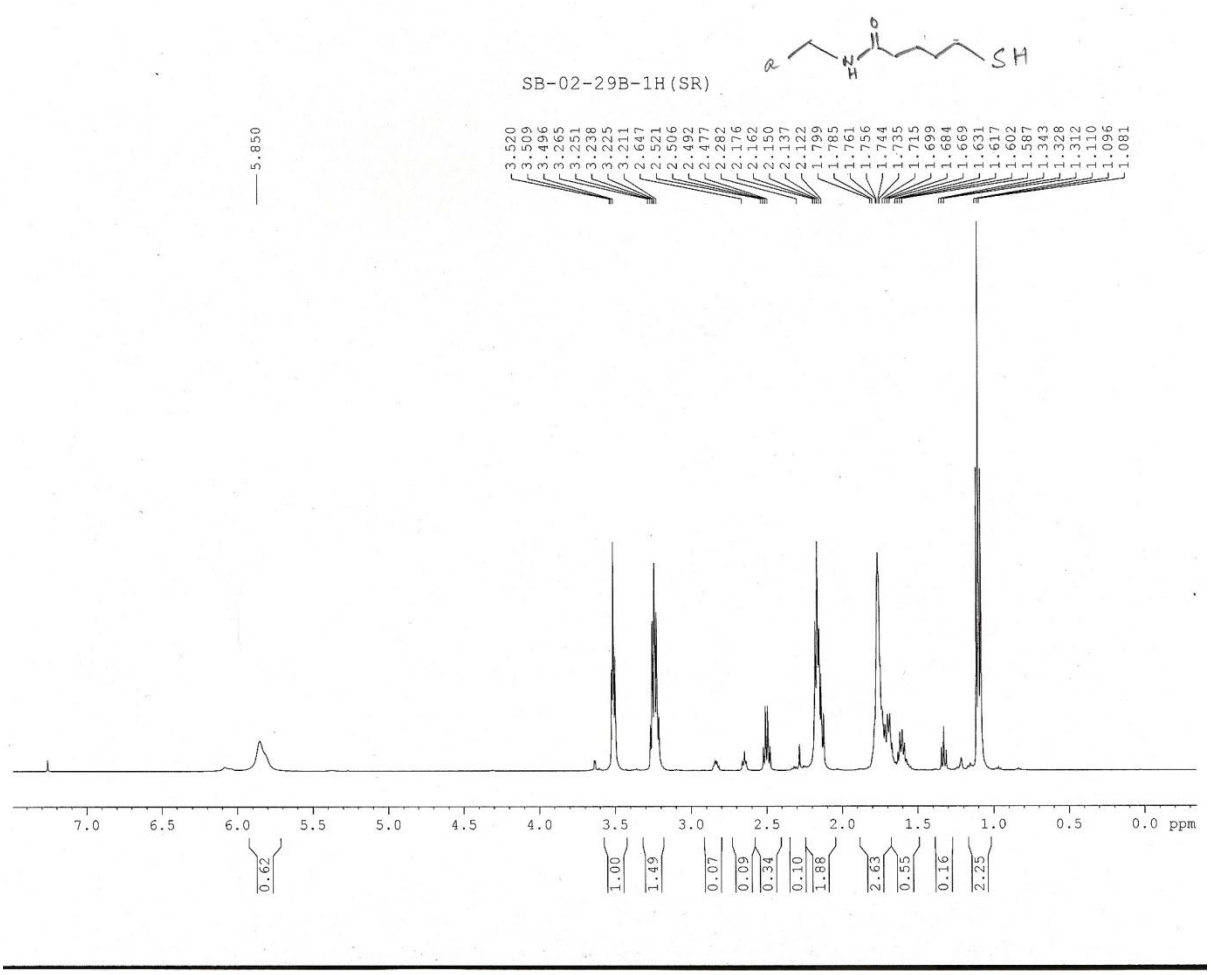


ESI-MS

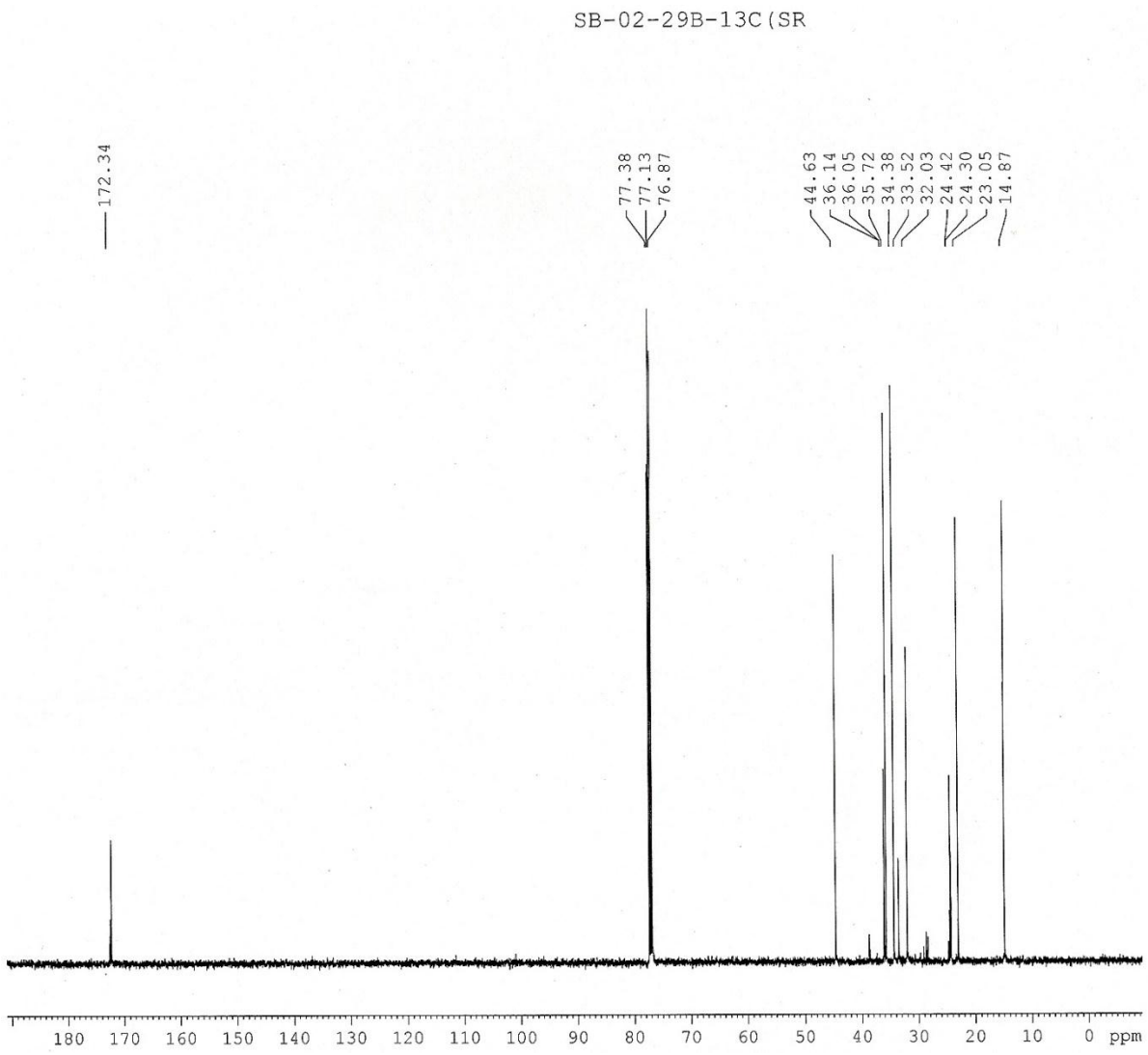


Ethylamidebutylthiol

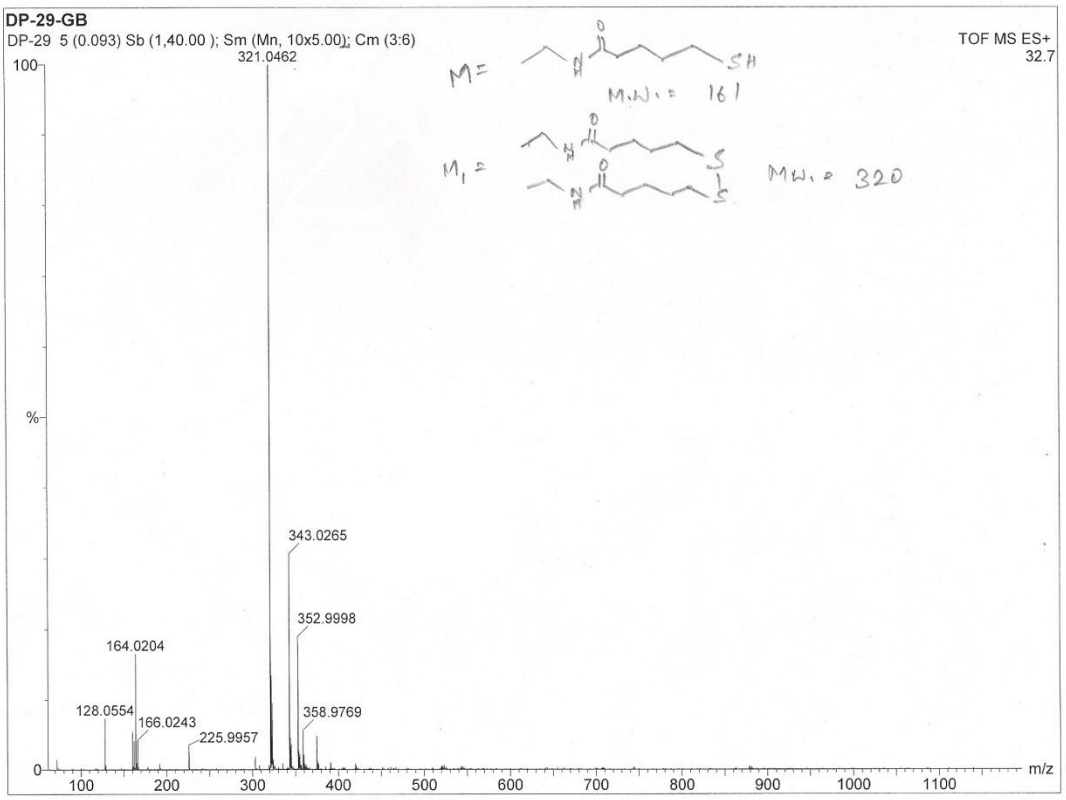
^{1}H NMR ($CDCl_3$)



^{13}C NMR

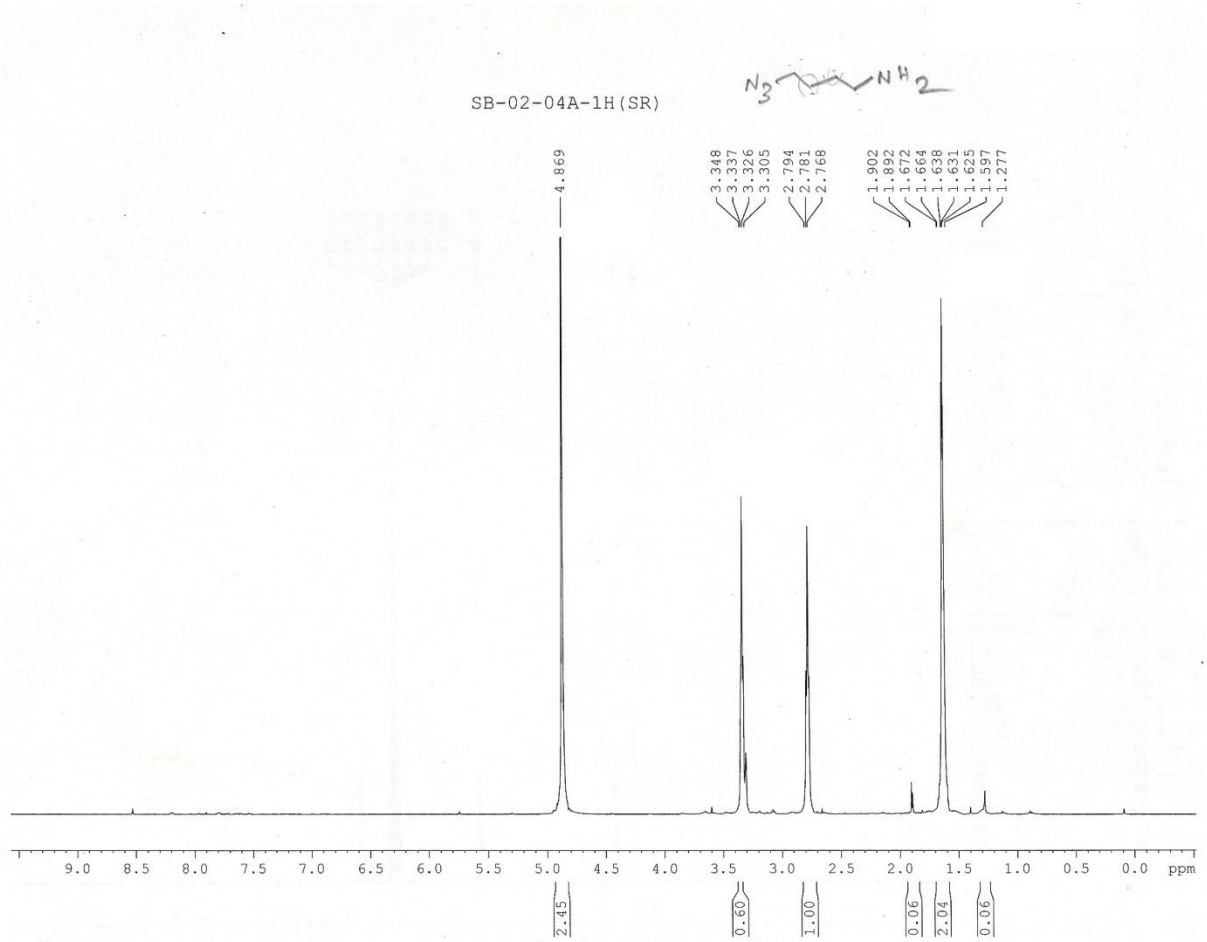


ESI-MS

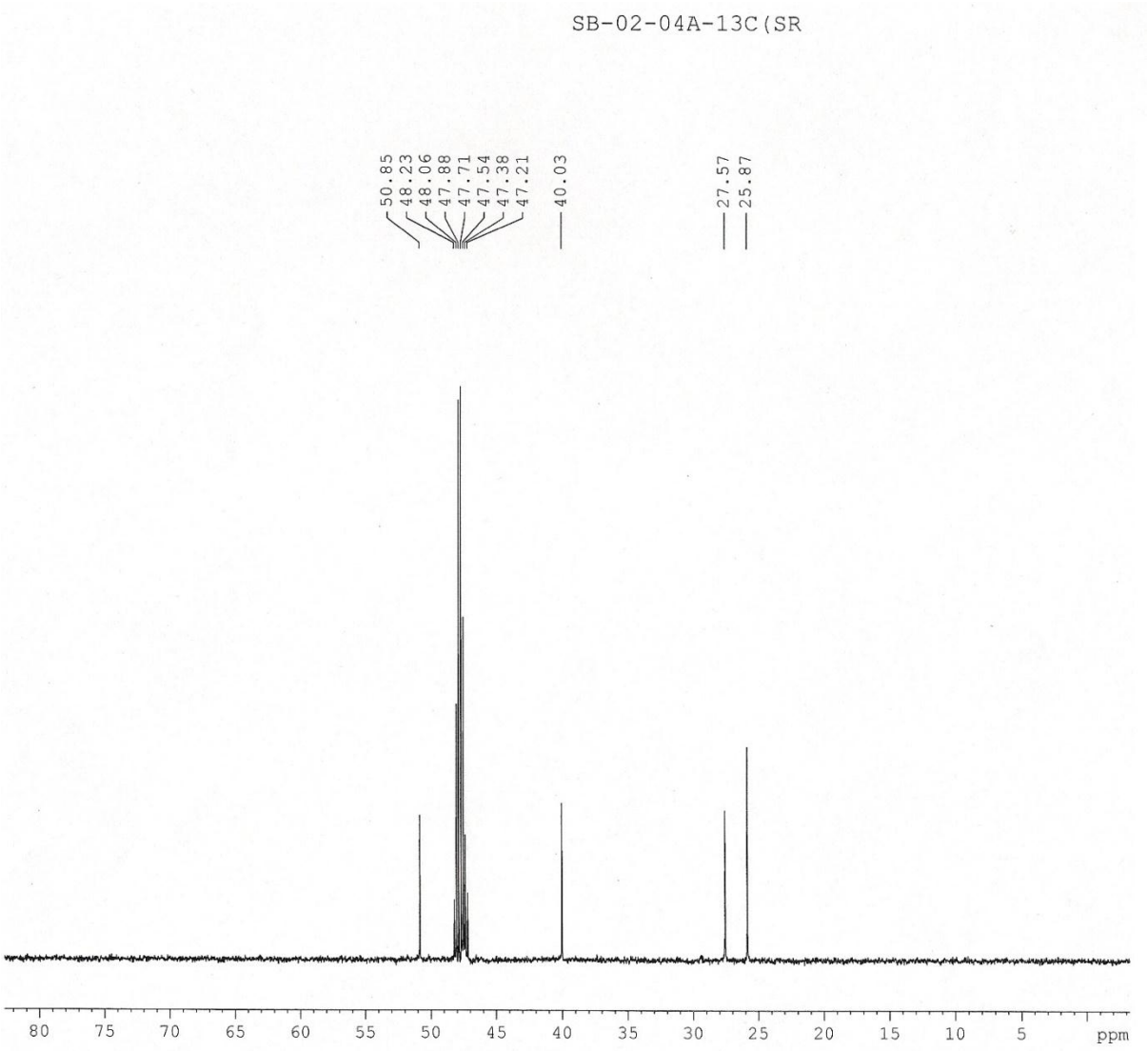


1-Azidobutylamine

^{1}H NMR (CD_3OD)

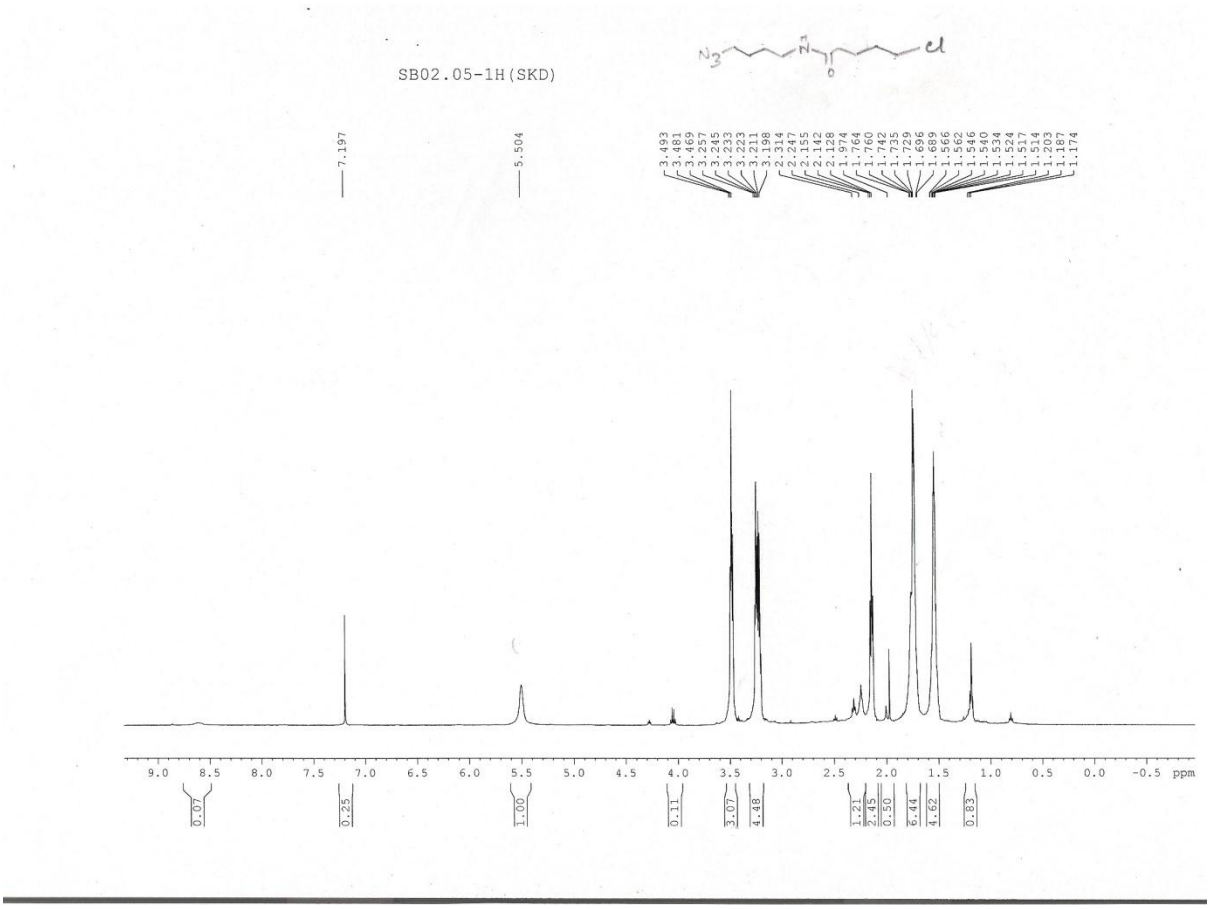


^{13}C NMR

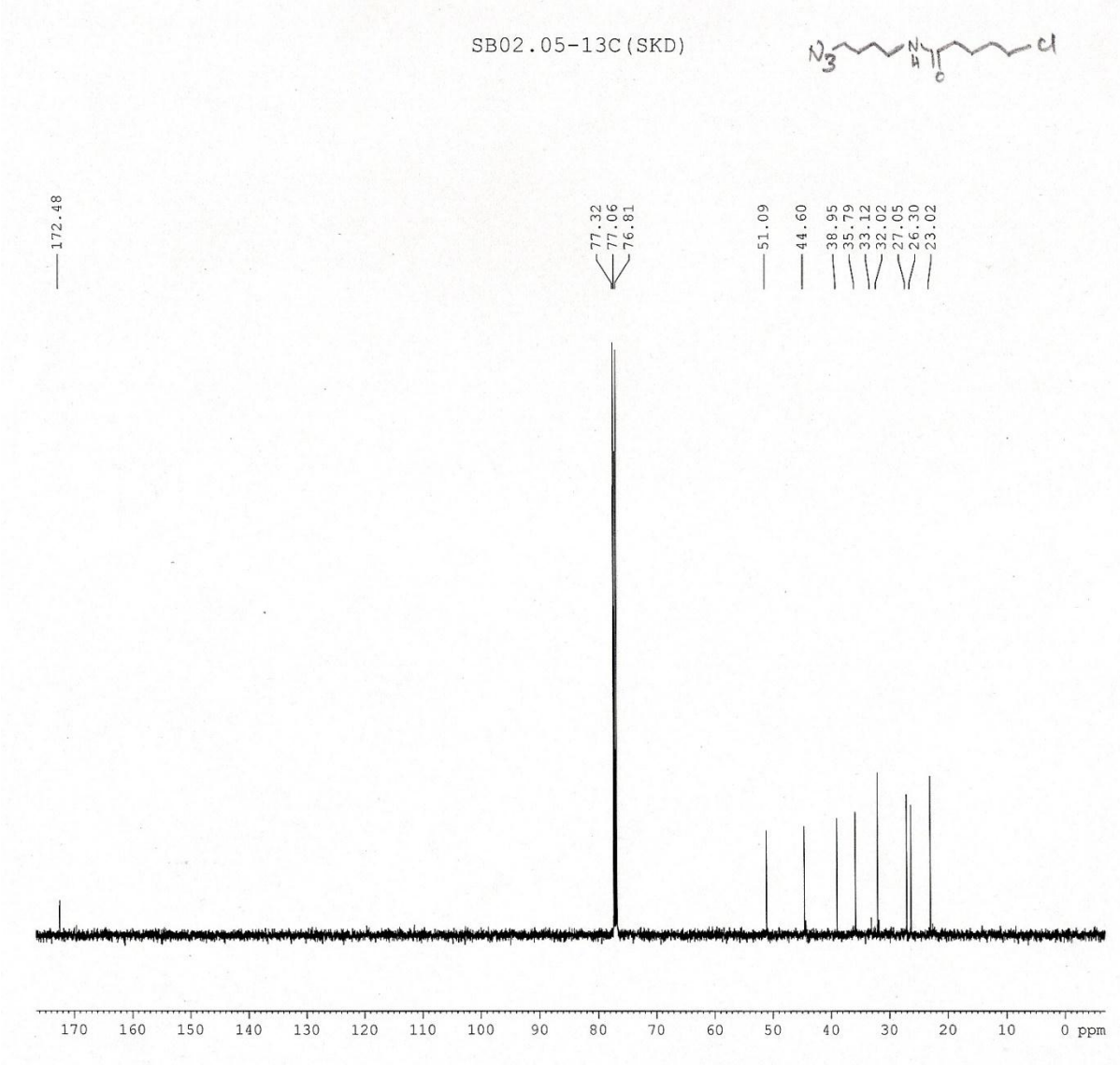


1-Azidobutylamidebutylchloride

^{1}H NMR ($CDCl_3$)

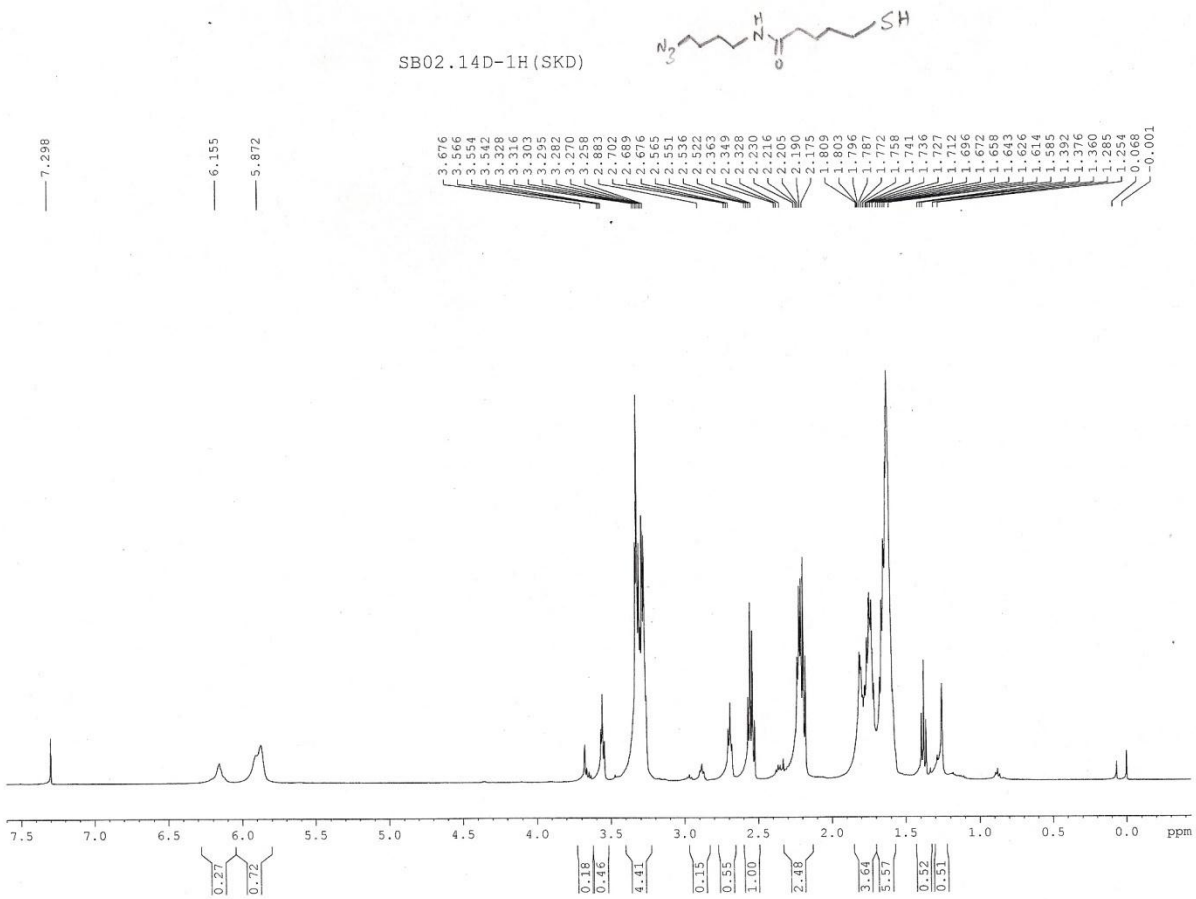


^{13}C NMR

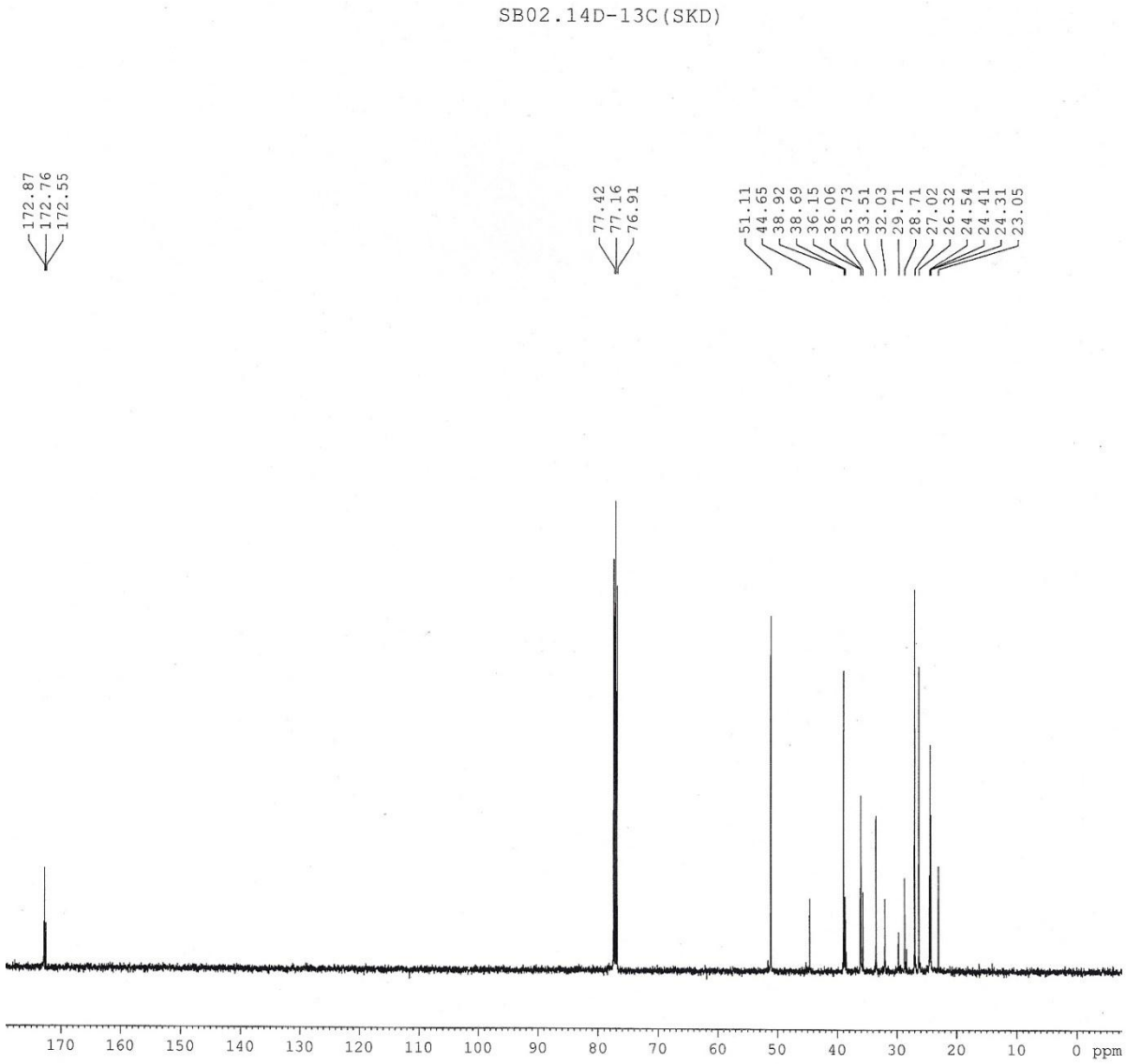


1-Azidobutylamidebutylthiol

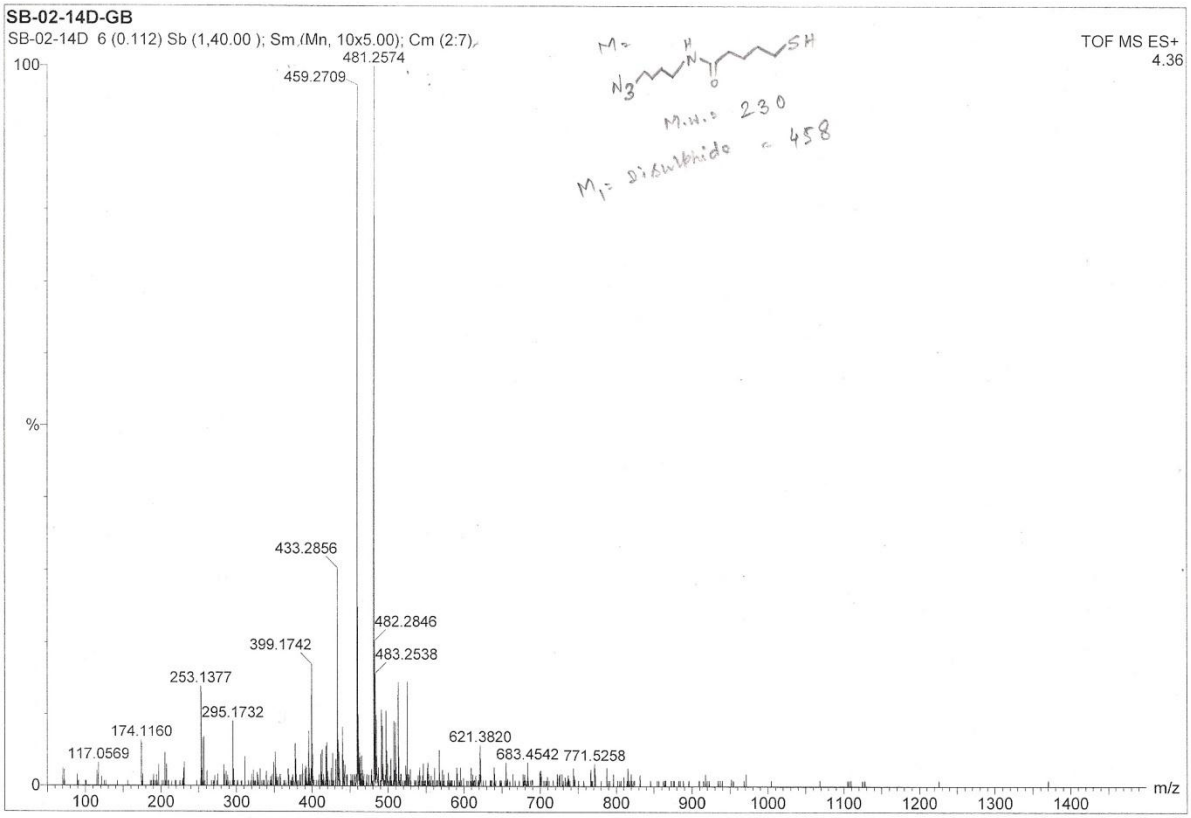
^{1}H NMR ($CDCl_3$)



^{13}C NMR

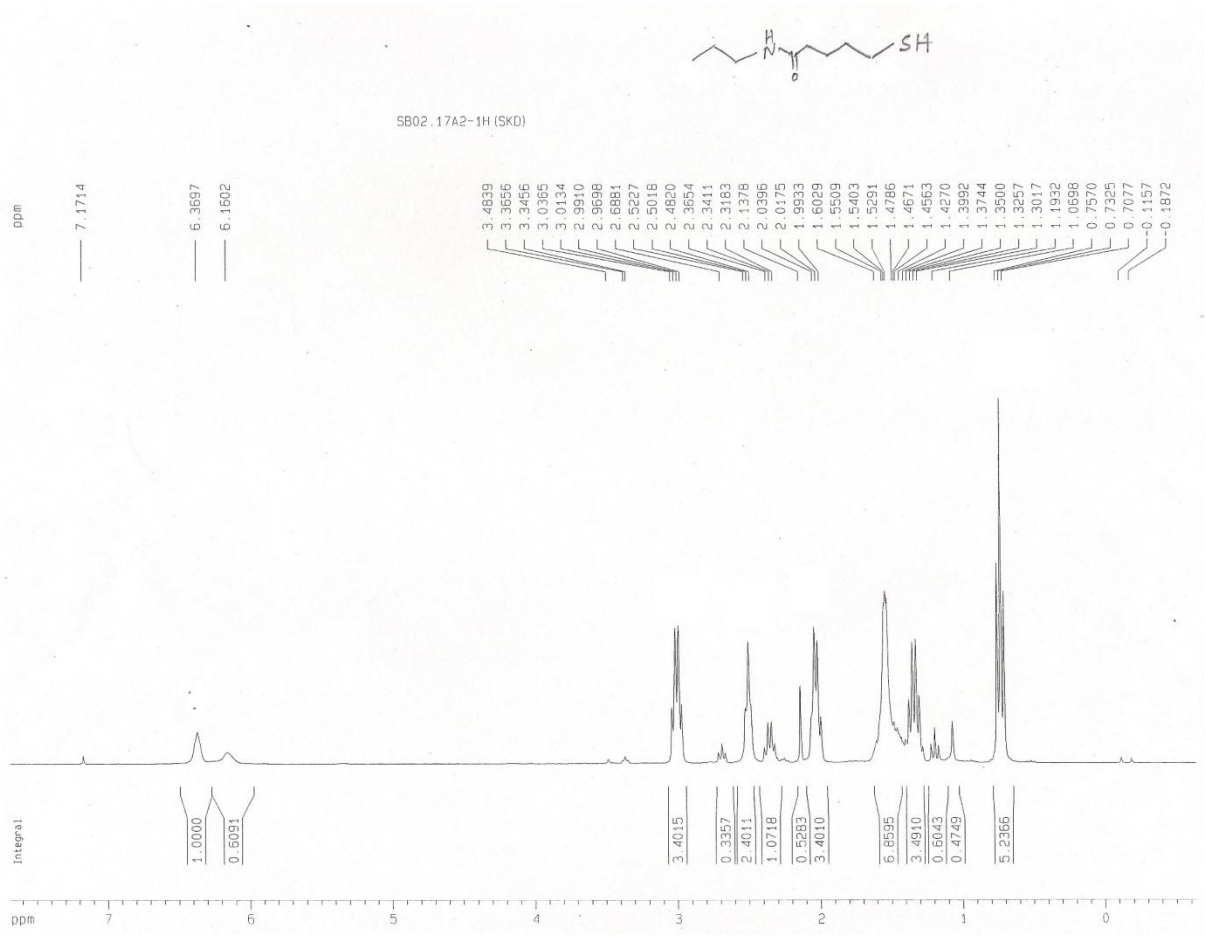


ESI-MS

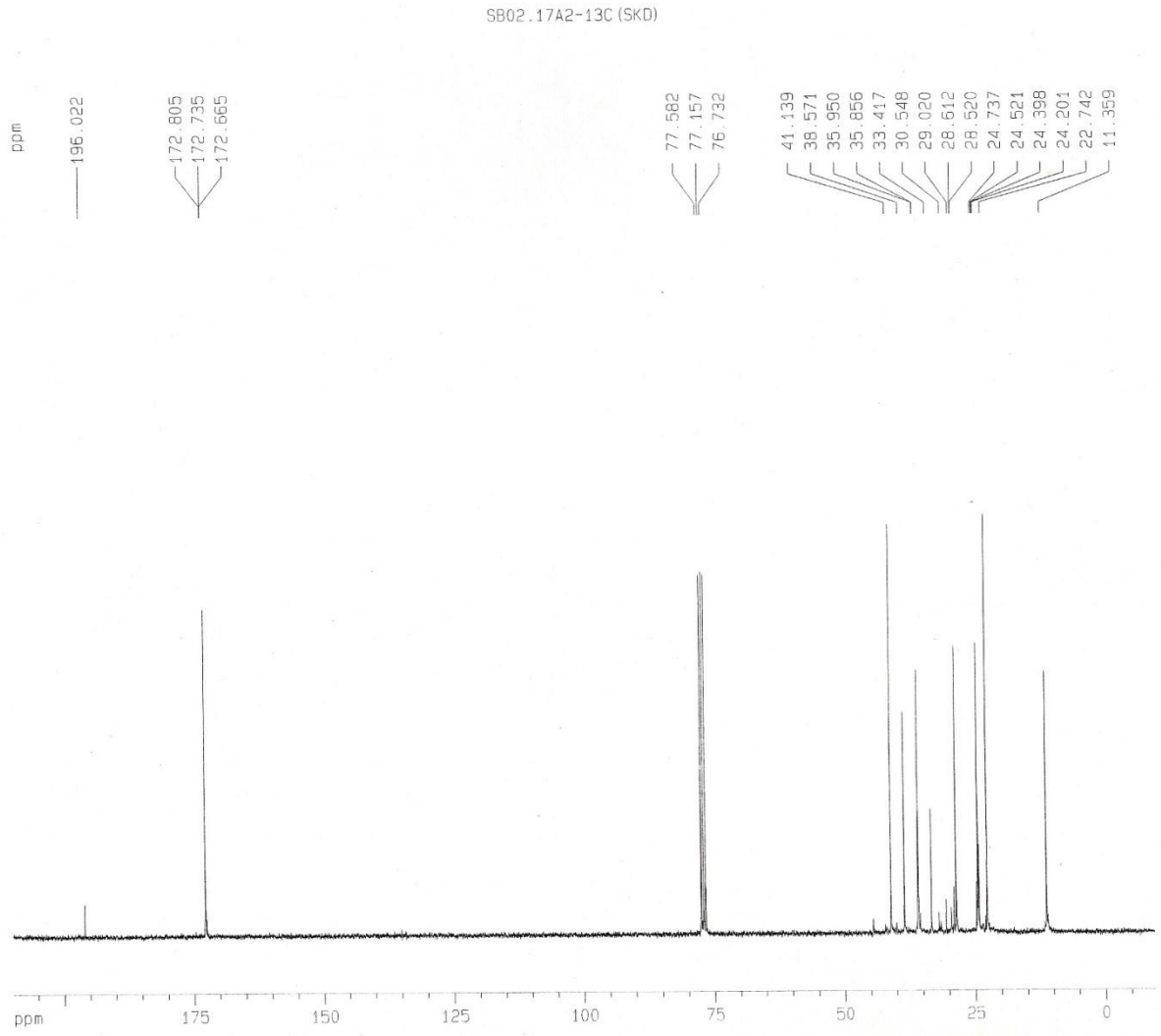

SB-02-14D-GB
SB-02-14D 6 (0.112) Sb (1,40.00); Sm (Mn, 10x5.00); Cm (2:7)
TOF MS ES+
4.36
100
%
0
481.2574
459.2709
433.2856
482.2846
483.2538
399.1742
253.1377
295.1732
174.1160
117.0569
621.3820
683.4542
771.5258
100
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
m/z
M.W.= 230
M= Disulphide = 458

1-Propylamidebutylthiol

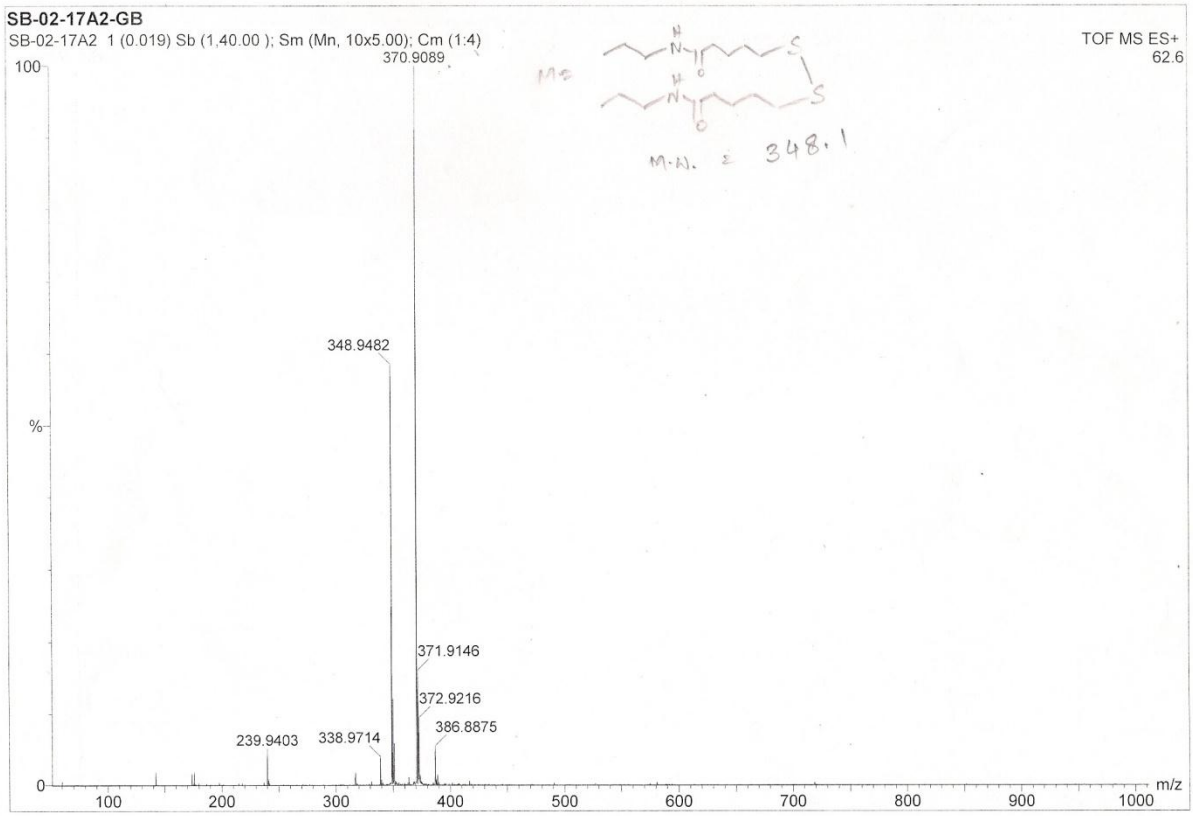
^{1}H NMR ($CDCl_3$)



^{13}C NMR

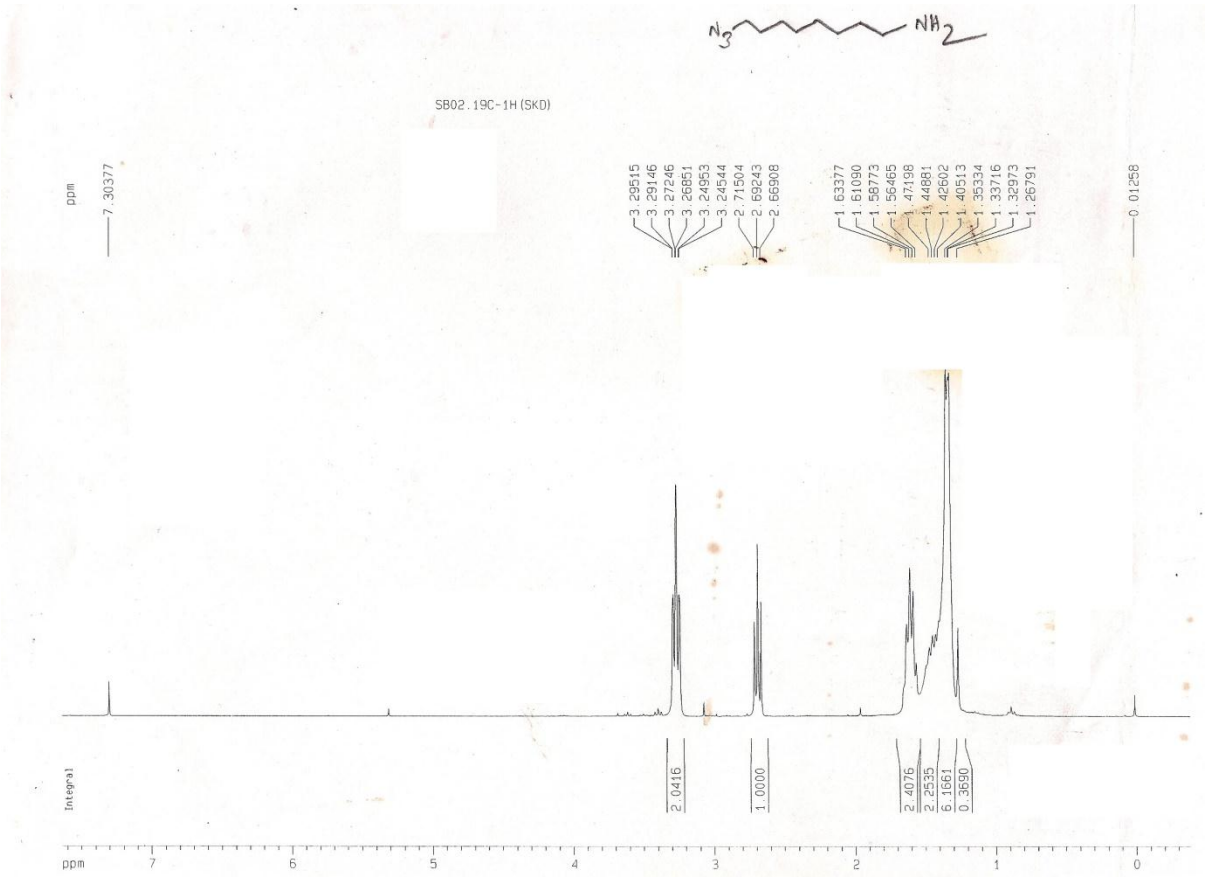

SB02.17A2-13C (SKD)
ppm
196.022
172.805
172.735
172.665
77.582
77.157
76.732
41.139
38.571
35.950
35.856
33.417
30.548
29.020
28.612
28.520
24.737
24.521
24.398
24.201
22.742
11.359
ppm
175
150
125
100
75
50
25
0

ESI-MS

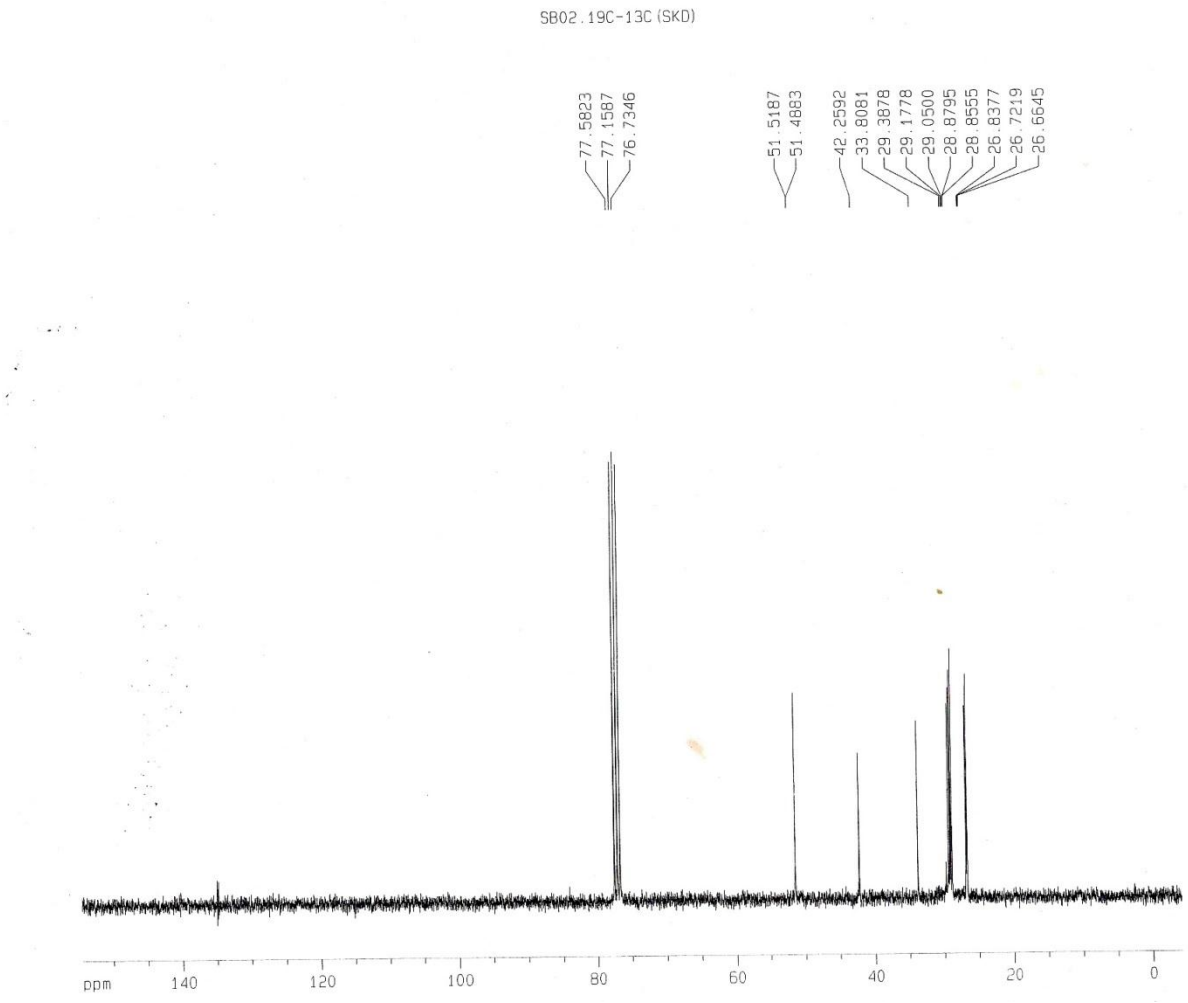

SB-02-17A2-GB
SB-02-17A2 1 (0.019) Sb (1,40.00); Sm (Mn, 10x5.00); Cm (1:4)
TOF MS ES+
62.6
370.9089
348.9482
371.9146
372.9216
386.8875
239.9403
338.9714
100
%
0
m/z
100
200
300
400
500
600
700
800
900
1000
M.W. = 348.1

1-Azidooctylamine

^{1}H NMR ($CDCl_3$)

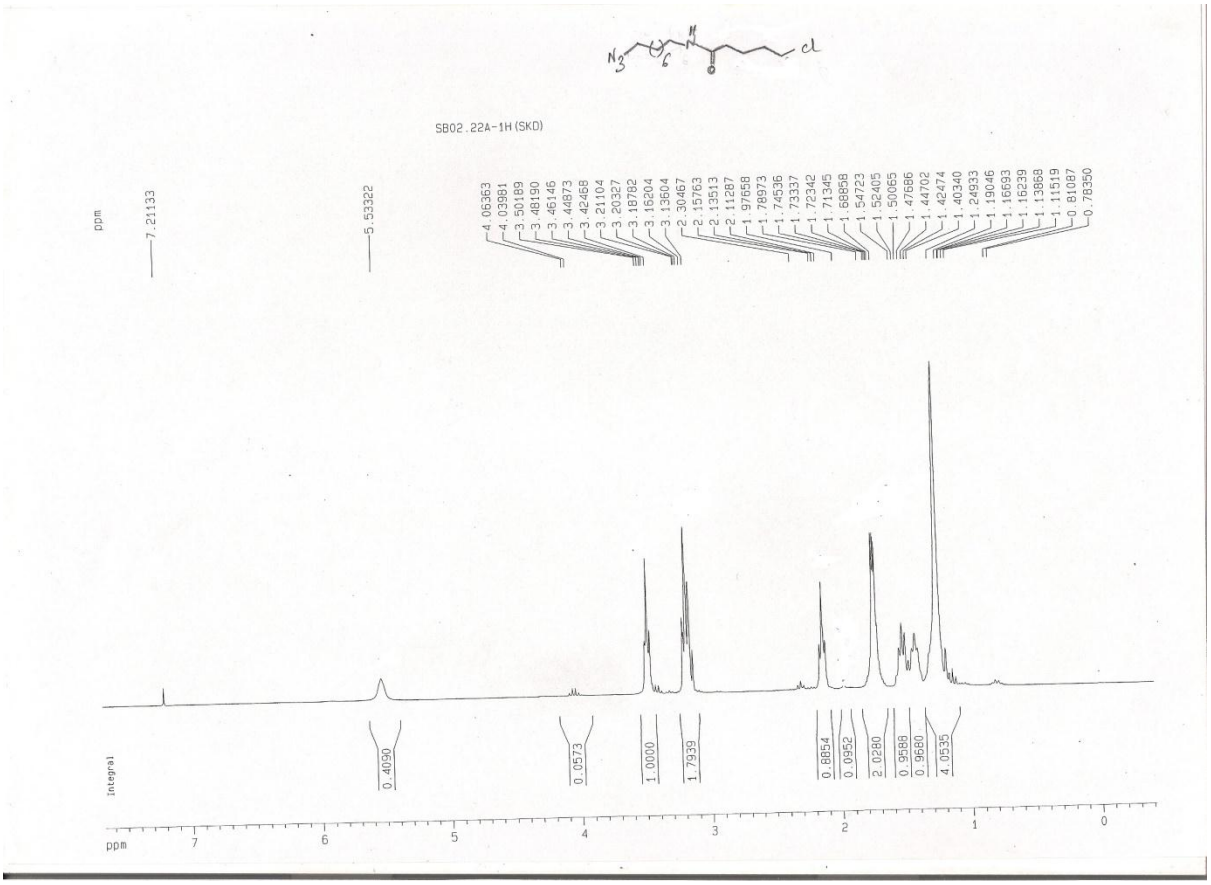


^{13}C NMR

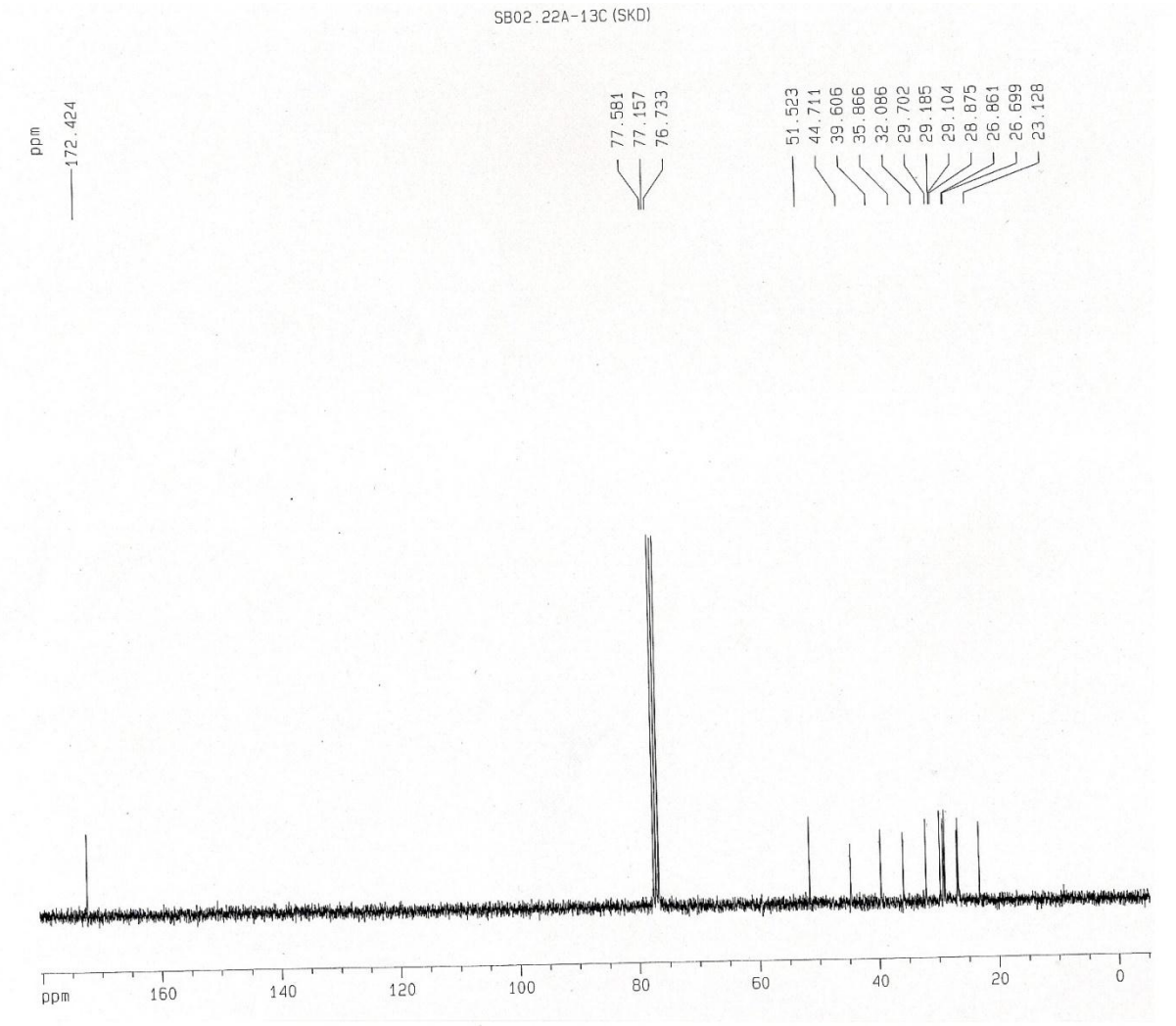

SB02.19C-13C (SKD)
77.5823
77.1587
76.7346
51.5187
51.4883
42.2592
33.8081
29.3878
29.1778
29.0500
28.8795
28.8555
26.8377
26.7219
26.6645
ppm
140
120
100
80
60
40
20
0

1-Azidooctylamidebutylchloride

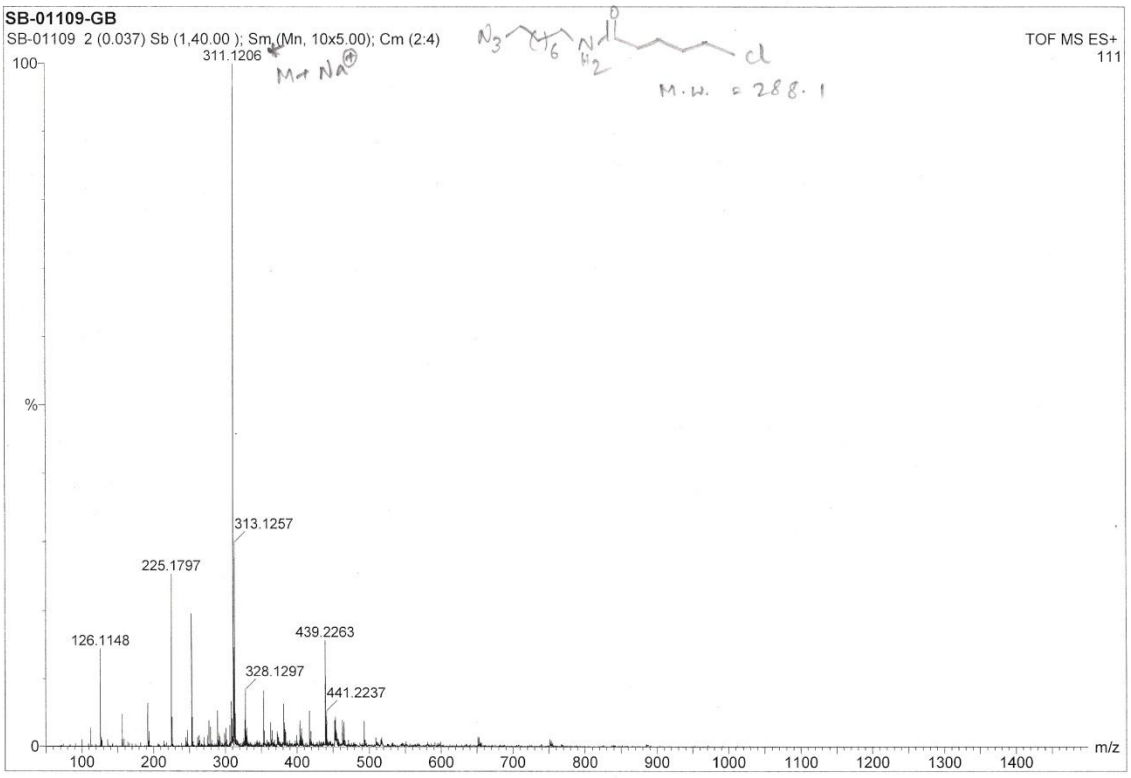
^{1}H NMR ($CDCl_3$)



^{13}C NMR

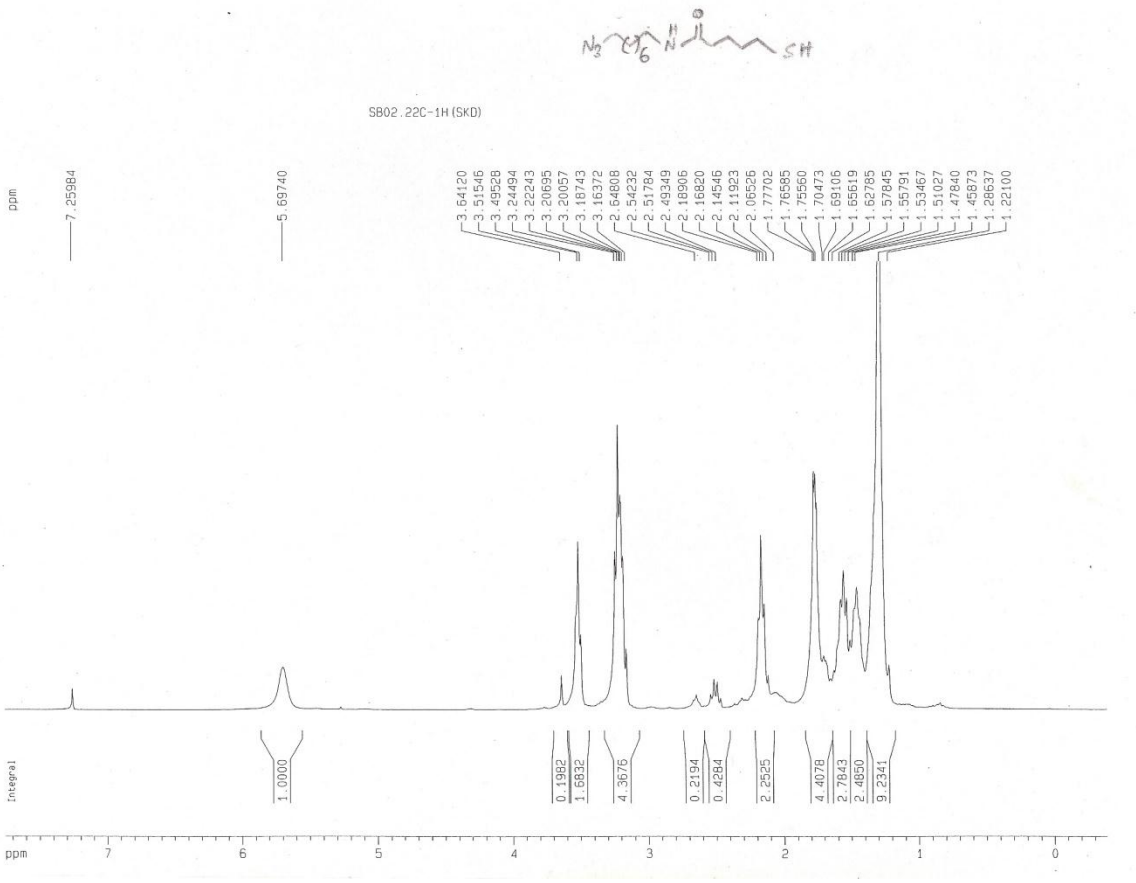

SB02.22A-13C (SKD)
ppm
172.424
77.581
77.157
76.733
51.523
44.711
39.606
35.866
32.086
29.702
29.185
29.104
28.875
26.861
26.699
23.128
ppm
160
140
120
100
80
60
40
20
0

ESI-MS

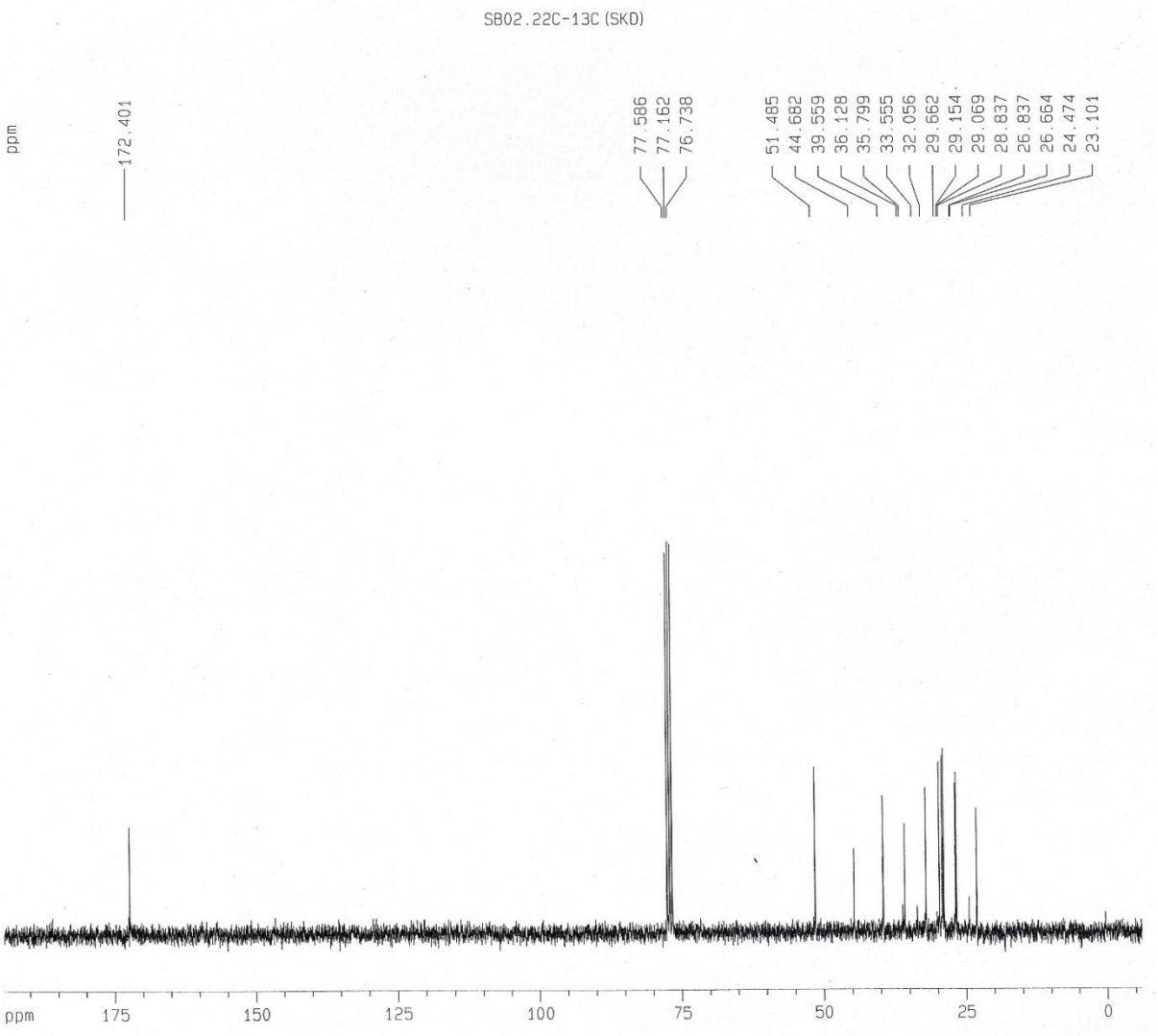

SB-01109-GB
SB-01109 2 (0.037) Sb (1,40.00); Sm (Mn, 10x5.00); Cm (2:4)
TOF MS ES+
111
311.1206
M+ Na+
M.W. = 288.1
100
%
0
313.1257
225.1797
126.1148
439.2263
328.1297
441.2237
100
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
m/z

1-Azidooctylamidebutylthiol

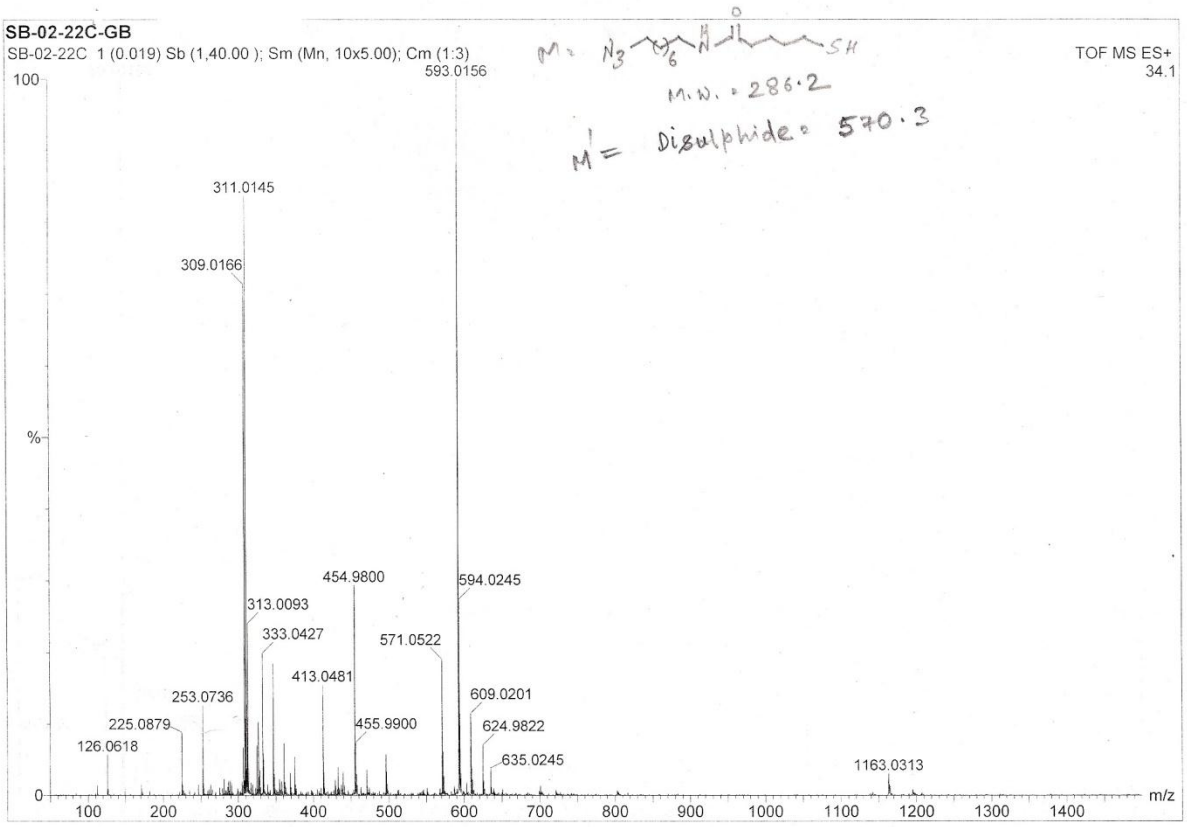
^{1}H NMR ($CDCl_3$)



^{13}C NMR

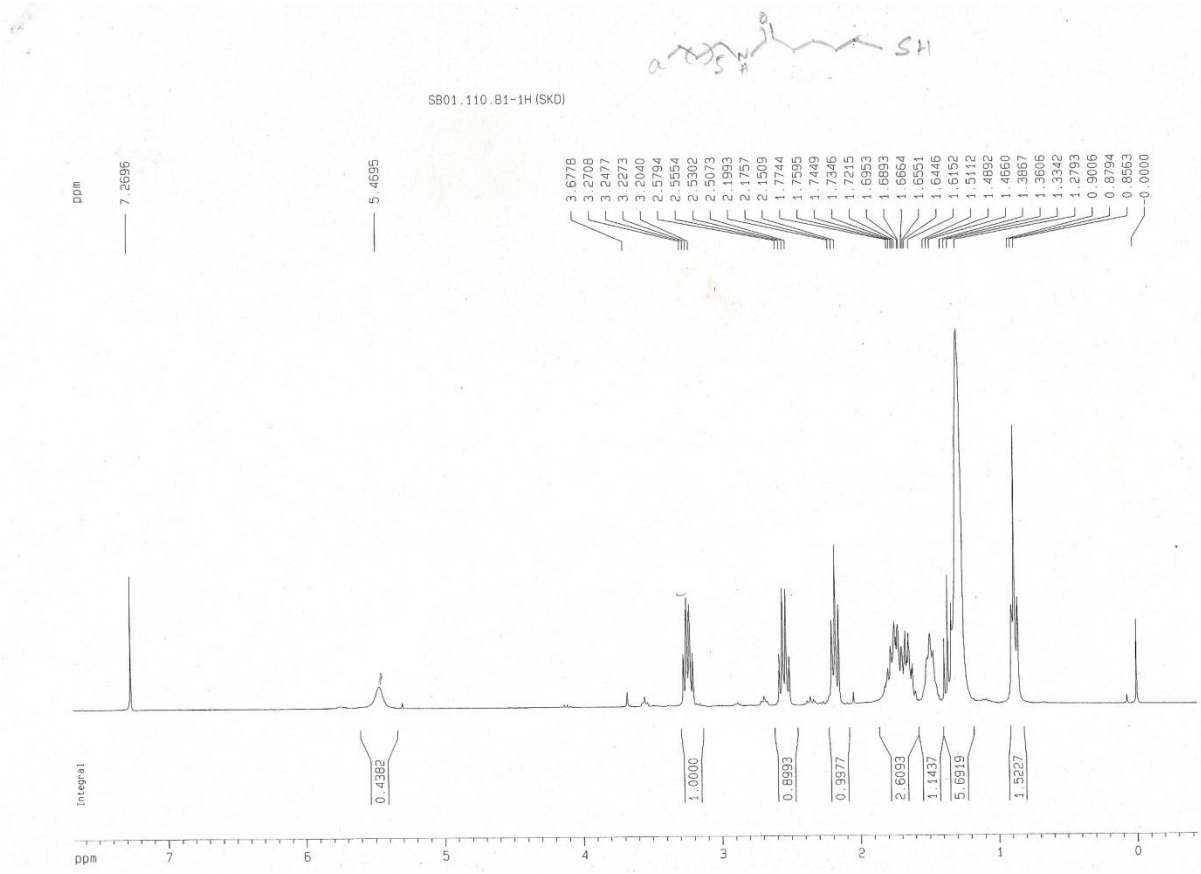


ESI-MS

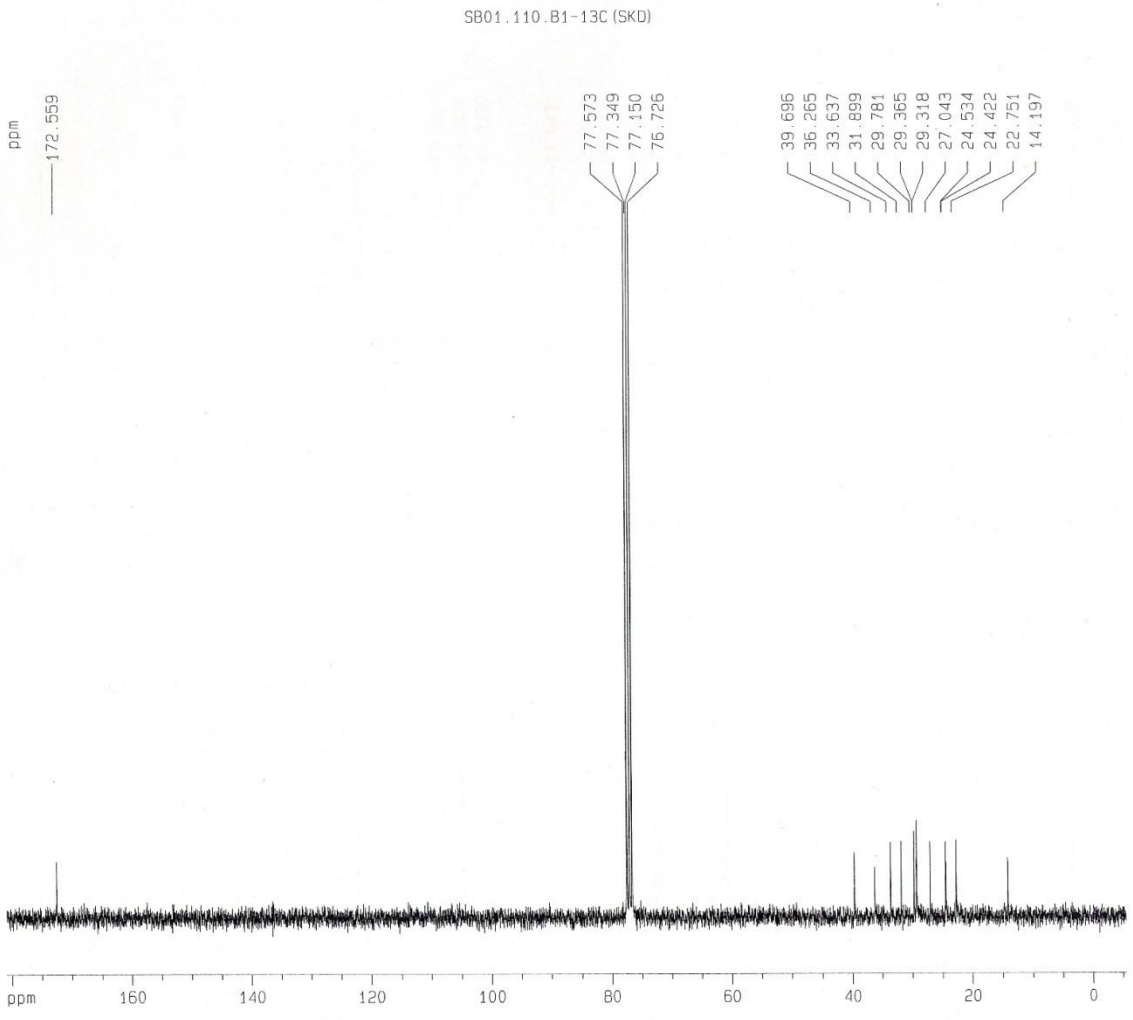


Octylamidebutylthiol

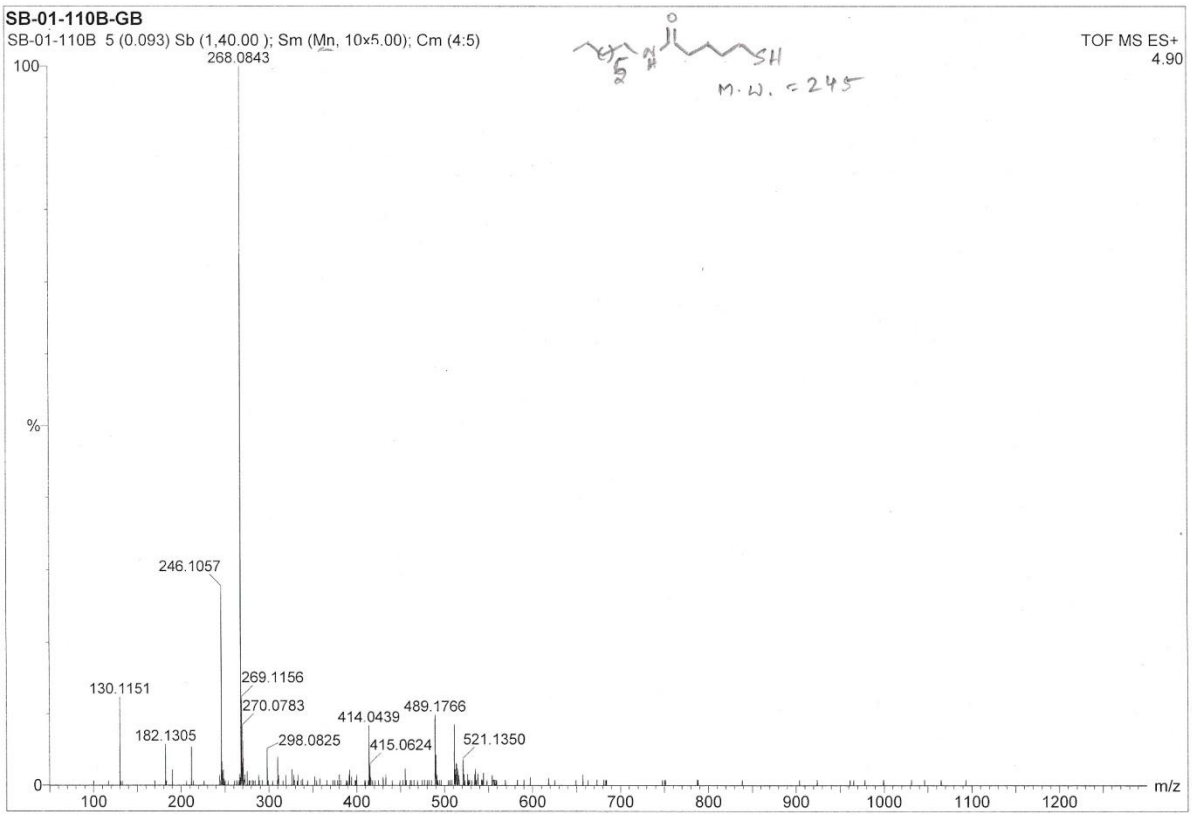
^{1}H NMR ($CDCl_3$)



^{13}C NMR


SB01.110.B1-13C (SKD)
ppm
172.559
77.573
77.349
77.150
76.726
39.696
36.265
33.637
31.899
29.781
29.365
29.318
27.043
24.534
24.422
22.751
14.197
ppm
160
140
120
100
80
60
40
20
0

ESI-MS



Reference:

1 J. P. Collman, N. K. Devaraj and C. E. D. Chidsey, *Langmuir*, 2004, **20**, 1051-1053.