**Electronic supplementary materials** *Mendeleev Commun.*, 2025, **35**, 447–449

# Trithiacrown ethers incorporating tetrahydropyridine subunit: synthesis, *in vitro* and *in silico* studies of inhibitory activity against α-glucosidase

**Dat T. Nguyen, Nhung T. Dao, Van T. T. Tran, Tien Q. Le, Linh M. Nguyen and Anh T. Le**

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## 1. Chemicals and solvents

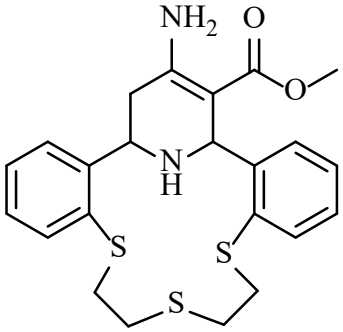
All chemical reagents were purchased from commercial source (Sigma Aldrich, Merck, China) and used directly without any further purification. Solvents for reactions, extraction, recrystallization and column chromatography such as acetonitrile, ethanol, methanol, dichloromethane, *n*-hexane, and ethyl acetate were purchased from China and DEAJUNG (Korea).

## 2. Instrumentation

TLC analysis was performed on commercially prepared silica gel plates (Merck, F254) and visualized by either UV irradiation or staining with $I_2$. Silica gel (0.063–0.2 mm) was used for column chromatography. The melting point of the synthetic molecule was determined in capillary tubes on a digital Stuart SMP3 apparatus. The LC/MS analysis was performed using an Agilent 1100 series chromatograph equipped with Agilent 1100 series DAD (wavelength 254±4 nm was used for detection), Sedex 75 ELSD and Agilent LC/MSD VL mass spectrometer (ionization in ESI mode). IR spectra were recorded on FTIR Affinity – 1S SHIMADZU instrument in the range of 400 and 4000 $cm^{-1}$. $^1H$ &$^{13}C$-NMR spectra were recorded on the Bruker Avance Neo 600 spectrometer (600 and 125 MHz, respectively) in $CDCl_3$ at 25 $^0C$ with TMS used as internal standard.

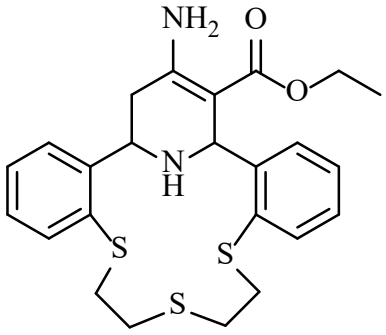
## 3. Spectral data analysis of the synthesized compounds 3a-e

### 3.1. Spectral data analysis compound 3a



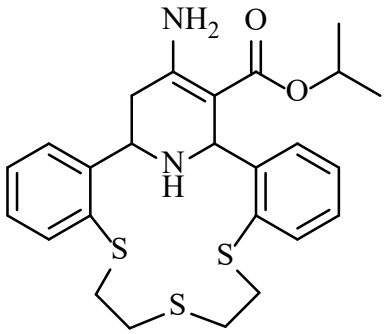

Yield 42 %, white crystals, M.p. 192-194 ºC, $R_f$ = 0.52 (H/E 3/1). IR (KBr), $\nu_{max}$, $cm^{-1}$: 3299 & 3252($NH_2$); 1633 (C=O); 1296 (C-O). $^1$H-NMR ([D1] $CDCl_3$, 298 K) $\delta_H$ (ppm): 2.20-2.23 (4H, m, 2x $SCH_2$), 2.37-2.40 (1H, m, $CH_{tetrahydropyridine}$), 2.51-2.54 (4H, m, 2x $SCH_2$), 2.63-2.72 (2H,m, 2x$CH_{tetrahydropyridine}$), 3.47 (3H, s, $CH_3$), 3.52- 3.56 (1H, m, $CH_{tetrahydropyridine}$), 4.59 (1H, s, NH), 5.85 (1H, s, *NH*-H), 5.92 (1H, s, *NH*-H), 7.24-7.25 (2H, m, $H_{Ar}$), 7.36 (1H, t.d, $J$ = 7.8 Hz, 1.8 Hz; $H_{Ar}$), 7.415-7.436 (2H, m, $H_{Ar}$), 7.49 (1H, d.d, $J$ = 7.8 Hz, $J$ = 1.2 Hz, $H_{Ar}$), 7.59 (2H, d.d, $J$ = 7.2 Hz, 1.2 Hz, $H_{Ar}$). $^{13}$C-NMR, $CDCl_3$: $\delta_C$ (ppm): 167.58 (-C=O ester), 152.65, 146.87, 144.08, 137.16, 136.74, 132.35, 131.55, 129.69, 129.50, 128.99, 128.26, 127.13, 126.55, 95.34, 61.17, 53.39, 50.45, 35.95, 32.64, 31.38, 30.60, 29.01, 28.22, 27.69, 22.97, 21.47, 14.03, 11.10. HRMS (ESI, M + H), m/z Calc. for $[C_{23}H_{27}N_2O_2S_3]^+$: 459.1235 $[M+H]^+$. Found: 459.1462 $[M+H]^+$.

**3.2. Spectral data analysis compound 3b**



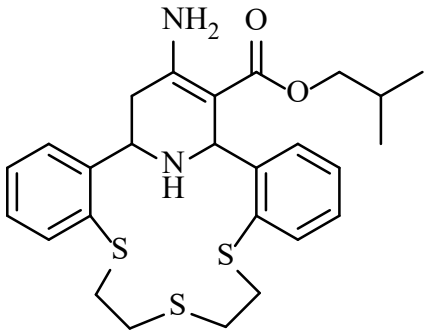
Yield 36 %, white crystals, M.p. 198-200 ºC ($R_f$ = 0.48, H/E 3/1). IR (KBr), $\nu_{max}$, $cm^{-1}$: 3336 ($NH_2$); 1671 (C=O); 1243 (C-O). $^1$H-NMR ([D1] $CDCl_3$, 298 K) $\delta_H$ ppm: 0.94 (3H, d, $J$ = 7.2 Hz, $CH_3$), 2.12-2.17 (2H, m, $SCH_2$), 2.219-2.22 (1H, m, $CH_{tetrahydropyridine}$), 2.398-2.42 (1H, m, $CH_{tetrahydropyridine}$), 2.419-2.510 (4H, m, 2x$SCH_2$), 2.61-2.69 (2H, m, $SCH_2$), 3.55 (1H, d.d, $J$= 10.5 Hz, $CH_{tetrahydropyridine}$), 3.9 (2H, q, $J$= 7.1 Hz, -$CH_2(CH_3)$), 4.58 (1H, s, $CH_{tetrahydropyridine}$), 5.89 (1H, s, *NH*-H), 5.94(1H, s, *NH*-H), 7.22-7.268 (2H, m, $H_{Ar}$), 7.36 (1H, t.d, $J$ = 7.2 Hz, 1.2 Hz, $H_{Ar}$), 7.05-7.46 (2H, m, $H_{Ar}$), 7.06 (1H, d, $J$ = 7.2 Hz, $H_{Ar}$), 7.573-7.596 (2H, m, $H_{Ar}$). $^{13}$C-NMR, $CDCl_3$: $\delta_C$ ppm: 167.07 (-C=O ester), 137.38, 136.98, 131.46, 129.76, 129.57, 128.95, 128.40, 127.02, 126.53, 122.76, 61.15, 58.69, 53.45, 32.65, 31.27, 30.92, 28.11, 27.58, 21.24, 14.12. HRMS (ESI, M+H), m/z Calc. for $[C_{24}H_{29}N_2O_2S_3]^+$: 473.1391 $[M+H]^+$. Found: 473.1380 $[M+H]^+$ .

**3.3. Spectral data analysis compound 3c**



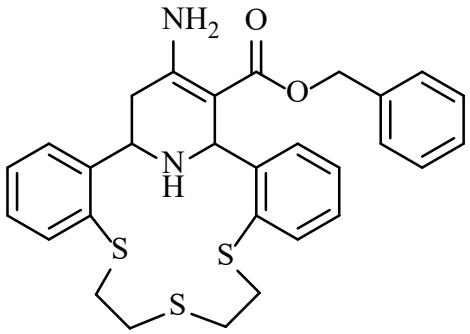
Yield 35 %, white crystals, M.p. 201-203 ºC ($R_f$ = 0.45, H/E 3/1). IR (KBr), $\nu_{max}$, $cm^{-1}$: 3327 ($NH_2$); 1658 (C=O); 1246 (C-O). $^1$H-NMR ([D1] $CDCl_3$, 298 K) $\delta_H$ ppm: 0.66 (3H, d, $J$ = 6 Hz, $CH_3$),1.115 (3H, d, $J$ = 6 Hz, $CH_3$), 2.13-2.24 (2H, m, $SCH_2$), 2.194-2.248 (1H, m, $CH_{tetrahydropyridine}$), 2.48-2.51 (5H, m, 2x$SCH_2$ and $CH_{tetrahydropyridine}$), 2.59- 2.67 (3H, m, $SCH_2$ and $CH_{tetrahydropyridine}$), 3.57 (1H, s, $CH_{tetrahydropyridine}$), 4.77 (1H, q, $J$ = 12.6 Hz, 6 Hz, -*CH*$(CH_3)_2$), 5.91 (2H, d, $J$ = 14Hz, $NH_2$), 7.216-7.259 (2H, m, $H_{Ar}$), 7.35 (1H, t.d, $J$ = 7.2 Hz, 1.2 Hz, $H_{Ar}$), 7.414-7.508 (3H, m, $H_{Ar}$), 7.566-7.580 (2H, m, $H_{Ar}$). $^{13}$C-NMR, $CDCl_3$: $\delta_C$ ppm: 166.51 (-C=O ester), 152.27, 147.83, 144.33, 137.47, 137.10, 132.21, 131.39, 129.79, 129.62, 128.91, 126.90, 126.49, 96.49, 65.52, 61.11, 53.53, 32.64, 31.17, 30.91, 29.71, 28.02, 27.50, 22.15, 21.40, 21.05. HRMS (ESI, M+H), m/z Calc. for $[C_{25}H_{31}N_2O_2S_3]^+$: 487.1548 $[M+H]^+$. Found: 487.1520 $[M+H]^+$.

### 3.4. Spectral data analysis compound 3d



Yield 37 %, white crystals, M.p. 222-224 ºC ($R_f$ = 0.41, H/E 3/1). IR (KBr), $\nu_{max}$, $cm^{-1}$: 3273 ($NH_2$); 1654 (C=O); 1246 (C-O). $^1$H -NMR ([D1] $CDCl_3$, 298 K) $\delta_H$ ppm: 0.625 (6H, d, $J$ = 7.2 Hz, 2x$CH_3$), 1.605-1.63 (1H, m, -$CH(CH_3)_2$), 2.137-2.233 (4H, m, 2x$SCH_2$), 2.348-2.394 (1H, m, $CH_{tetrahydropyridine}$), 2.479-2.52 (4H, m, 2x$SCH_2$), 2.62-2.71 (2H, m, $CH_2$(CH)), 3.57 (1H, ddd, $J$ = 13.2, 10.9, 3.7 Hz, $CH_{tetrahydropyridine}$), 3.61 (1H, dd, $J$ = 10.7, 6.0 Hz, $CH_{tetrahydropyridine}$), 3.70 (1H, dd, $J$ = 10.6, 6.5 Hz, $CH_{tetrahydropyridine}$), 4.588 (1H, s, NH) , 5.85 (1H, brs, *NH*-H), 5.94 (1H, brs, *NH*-H), 7.24 (1H, d.t, $J$= 7.2 Hz, 1.2 Hz, $H_{Ar}$), 7.253- 7.268 (2H, m, $H_{Ar}$), 7.35 (1H, d.t, $J$= 7.2 Hz, 1.2 Hz, $H_{Ar}$), 7.42 (1H, d.t, $J$= 7.2 Hz, 1.2 Hz, $H_{Ar}$), 7.45 (1H, d.d, $J$= 7.2 Hz, 1.2 Hz, $H_{Ar}$), 7.49 (1H, d.d, $J$= 7.2 Hz, 1.2 Hz, $H_{Ar}$), 7.565- 7.599 (2H, m, $H_{Ar}$). $^{13}$C-NMR, $CDCl_3$: $\delta_C$ ppm: 167.16 (-C=O ester), 152.76, 147.27, 144.11, 137.36, 136.73, 132.18, 131.45, 129.69, 129.64, 128.95, 128.30, 127.05, 126.61, 95.43, 69.25, 61.01, 53.51, 32.56, 31.21, 28.10, 27.74, 27.63, 21.36, 18.98, 18.89. HRMS (ESI, M+H), m/z Calc. for $[C_{26}H_{33}N_2O_2S_3]^+$: 501.1704 $[M+H]^+$. Found: 501.1673 $[M+H]^+$ .

### 3.5. Spectral data analysis compound 3e



Yield 35 %, white crystals, M.p. 226-228 ºC ($R_f$ = 0.39, H/E 3/1). IR (KBr), $\nu_{max}$, $cm^{-1}$: 3294 ($NH_2$); 1654 (C=O); 1246 (C-O). $^1$H-NMR ([D1] $CDCl_3$, 298 K) $\delta_H$ ppm: 2.115-2.198 (4H, m, 2x$SCH_2$), 2.362-2.381 (1H, m, $CH_{tetrahydropyridine}$), 2.459- 2.500 (1H, m, $CH_{tetrahydropyridine}$), 2.257- 2.596 (4H, m, 2x$SCH_2$), 2.638-2.685 (1H, m, $CH_{tetrahydropyridin}$), 3.547 (1H, m, $CH_{tetrahydropyridine}$), 4.656 (1H, s, NH) , 4.85 and 4.99 (AB system, 2H, d, $J$=13 Hz, $CH_2$Ph), 5.89 (1H, s, *NH*-H), 5.99 (1H, s, *NH*-H), 6.88 (2H, d.d, $J$ = 7.8 Hz, 1.8Hz $H_{Ar}$), 7.169-7.186 (3H, m, $H_{Ar}$), 7.242- 7.267(2H, m, $H_{Ar}$), 7.37(1H, t.d, $J$= 7.2 Hz; 1.2 Hz, $H_{Ar}$), 7.42 (1H, t, $J$ = 7.6, 1.4 Hz, $H_{Ar}$), 7.464-7.503 (2H, m, $H_{Ar}$), 7.569-7.580 (2H, m, $H_{Ar}$). $^{13}$C-NMR, $CDCl_3$: $\delta_C$ ppm: 166.60 (-C=O ester), 153.27, 137.71, 127.03, 139.96, 131.33, 129.79, 129.73, 129.01, 128.49, 128.12, 127.28, 127.12, 126.55, 64.63, 61.08, 53.48, 32.55, 31.21, 20.91, 28.02, 27.53, 27.43, 21.43. HRMS (ESI, M+H), m/z Calc. for $[C_{29}H_{31}N_2O_2S_3]^+$: 535.1548 $[M+H]^+$. Found: 535.1535 $[M+H]^+$.

**4. Glucosidase inhibition assay**

The standard deviation σ is calculated according to Duncan's formula as follows:

$$\sigma = \sqrt{\frac{(\sum x_i - \bar{x})^2}{n-1}}$$

**Table S1**. Percentage of glucosidase inhibition

| **N₀** | **Entry** | **Concentration (μg/ml)** | **Inhibition (%)** | **$IC_{50}$ (μg/ml)** | **$IC_{50}$ (μM)** |
|---|---|---|---|---|---|
| 1 | **3a** | 256 | 0 | >256 | > 559 |
| | | 3a | 0 | | |
| | | 16 | 0 | | |
| | | 4 | 0 | | |
| | | 1 | 0 | | |
| 2 | **3b** | 256 | 91 | 2.42±0.26 | 5.13± 0.55 |
| | | 64 | 89 | | |
| | | 16 | 87.5 | | |
| | | 4 | 67 | | |
| | | 1 | 35 | | |
| 3 | **3c** | 256 | 0 | >256 | > 526 |
| | | 64 | 0 | | |
| | | 16 | 0 | | |
| | | 4 | 0 | | |
| 4 | **3d** | 256 | 32 | >256 | >512 |
| | | 64 | 0 | | |
| | | 16 | 0 | | |
| | | 4 | 0 | | |
| 5 | **3e** | 256 | 88 | 27.37±1.78 | 51.20 ± 3.33 |
| | | 64 | 79 | | |
| | | 16 | 41 | | |
| | | 4 | 31 | | |
| | | 1 | 4 | | |
| 6 | **Acarbose** | 256 | 63 | 156.16 ± 5.43 | 242.11 ± 8.42 |
| | | 64 | 38 | | |
| | | 16 | 0 | | |
| | | 4 | 0 | | |

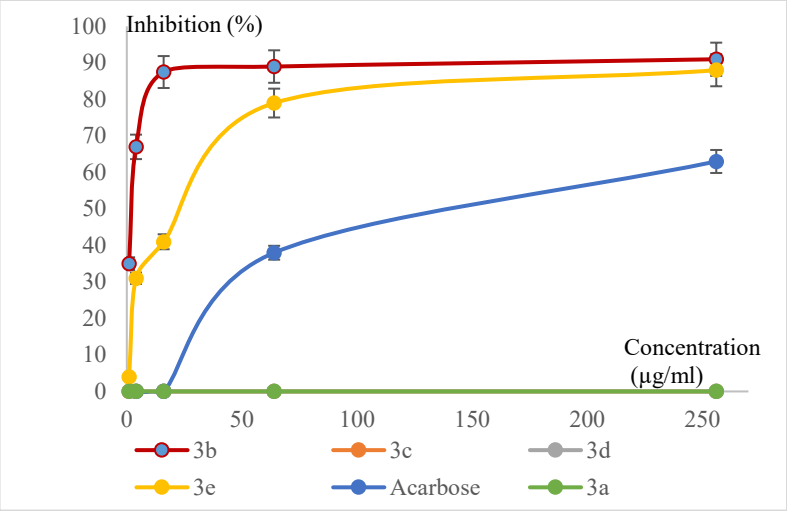



**Figure S1.** α -glucosidase inhibitory activities of the synthetic compounds **3a-e** and acarbose at five concentrations (256, 64, 16, 4, and 1 µg/ml)

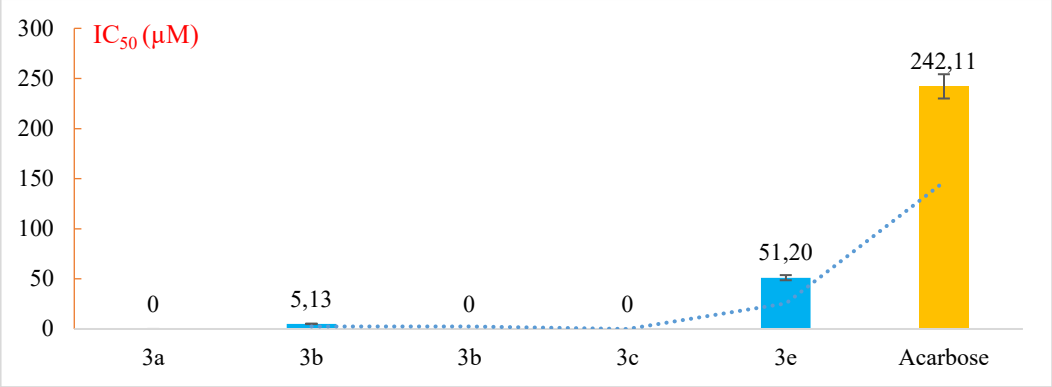
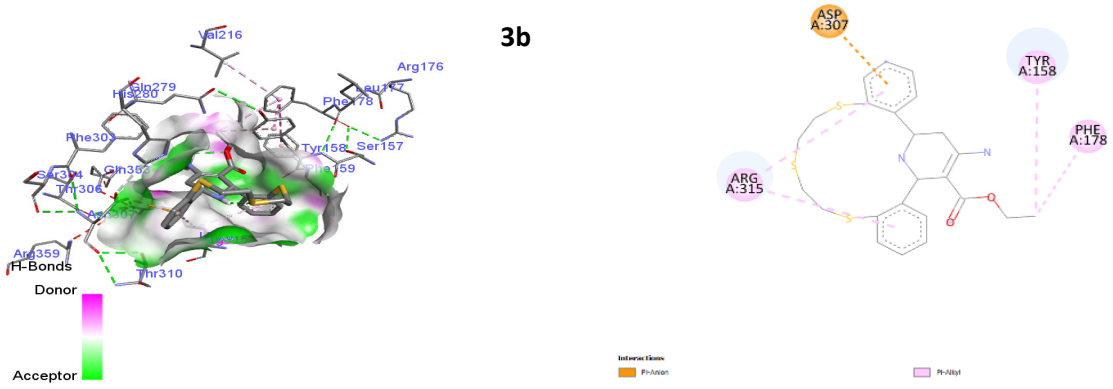



**Figure S2.** The comparation of $IC_{50}$ values (µM) between the synthesized compounds **3a-e** and Acarbose

## 5. Docking studies and ADMET prediction



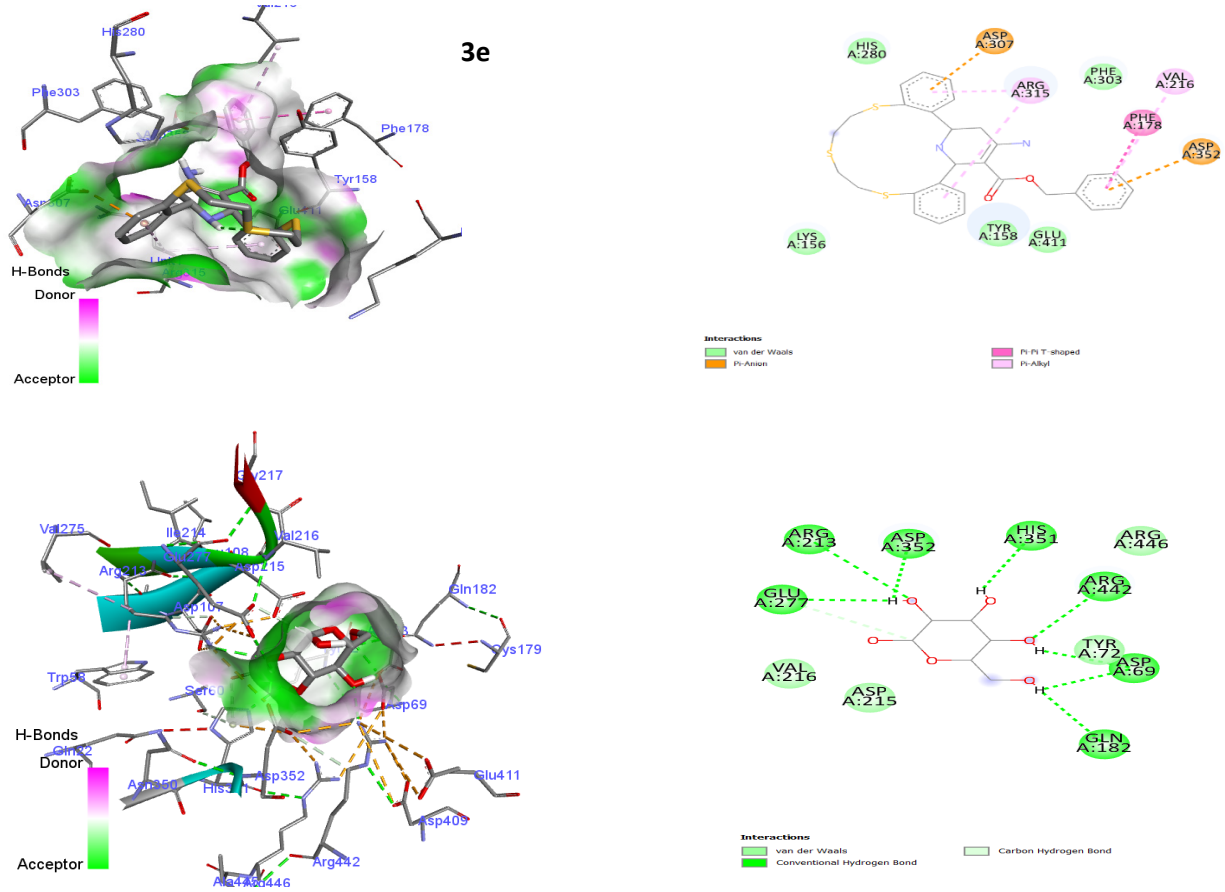



**Figure S3**. The interactions of the potent inhibitors **3b, 3e** and co-crystallized ligand docked into the **3A4A**: 3D (left) and 2D (right)

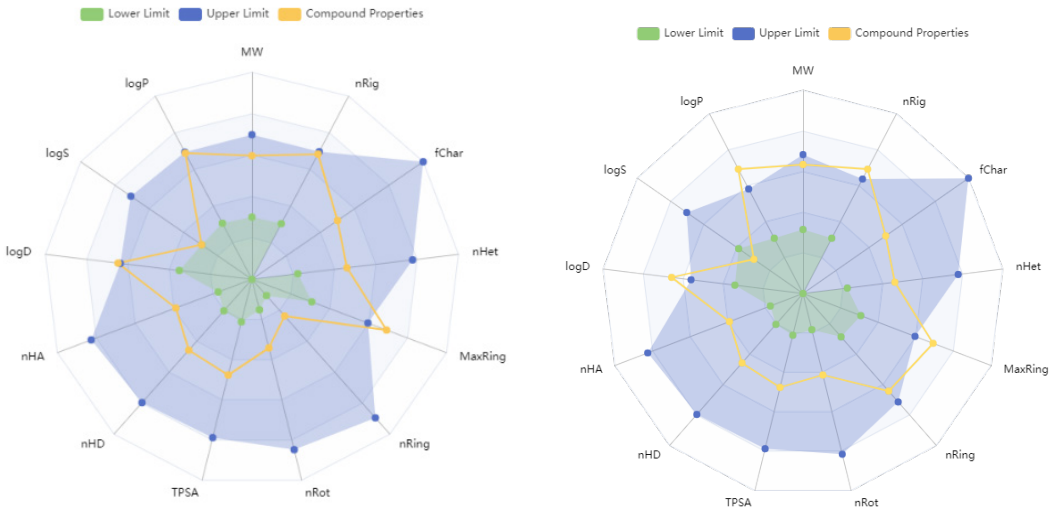
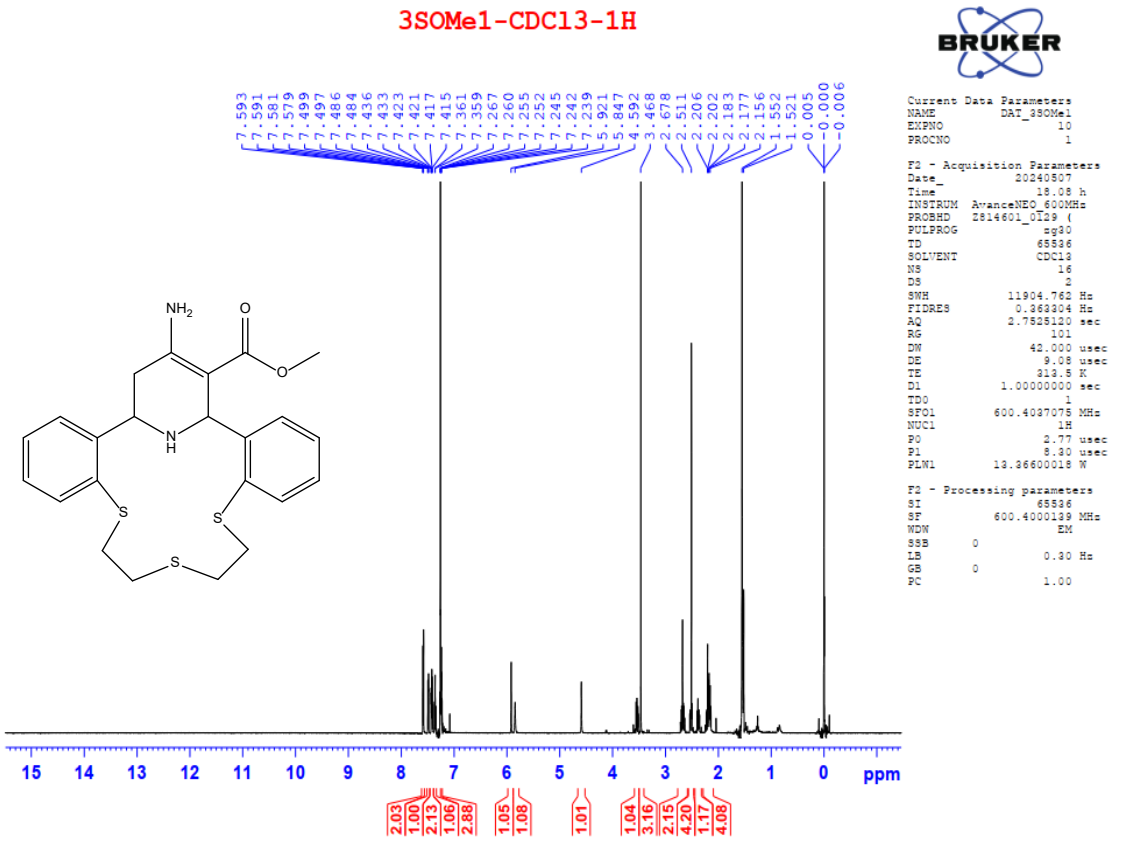
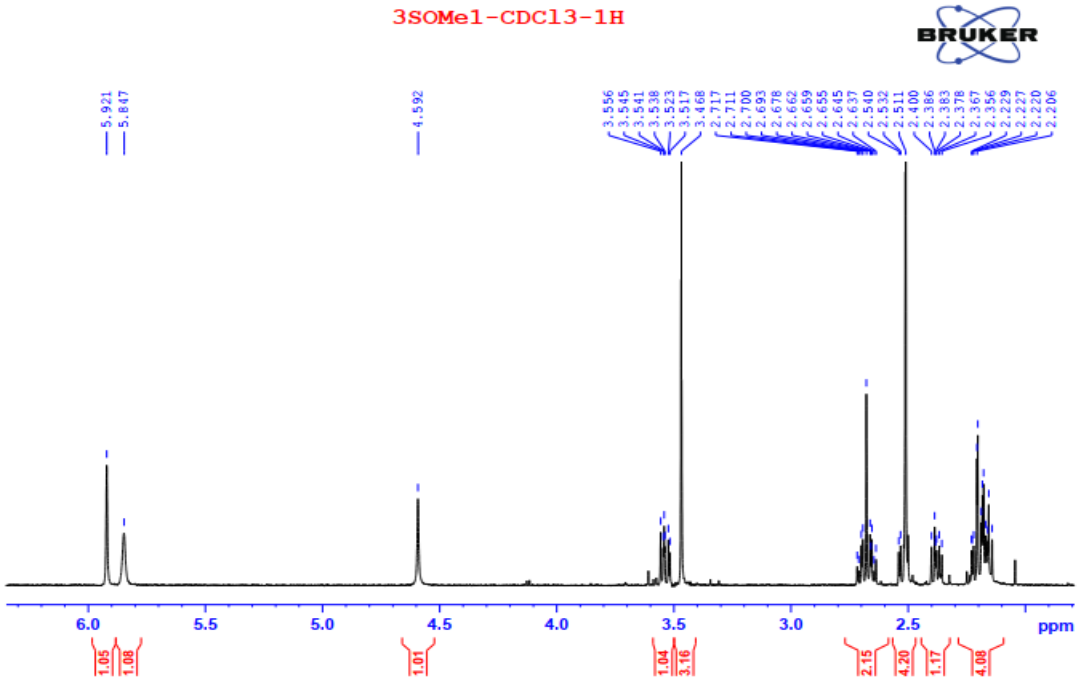


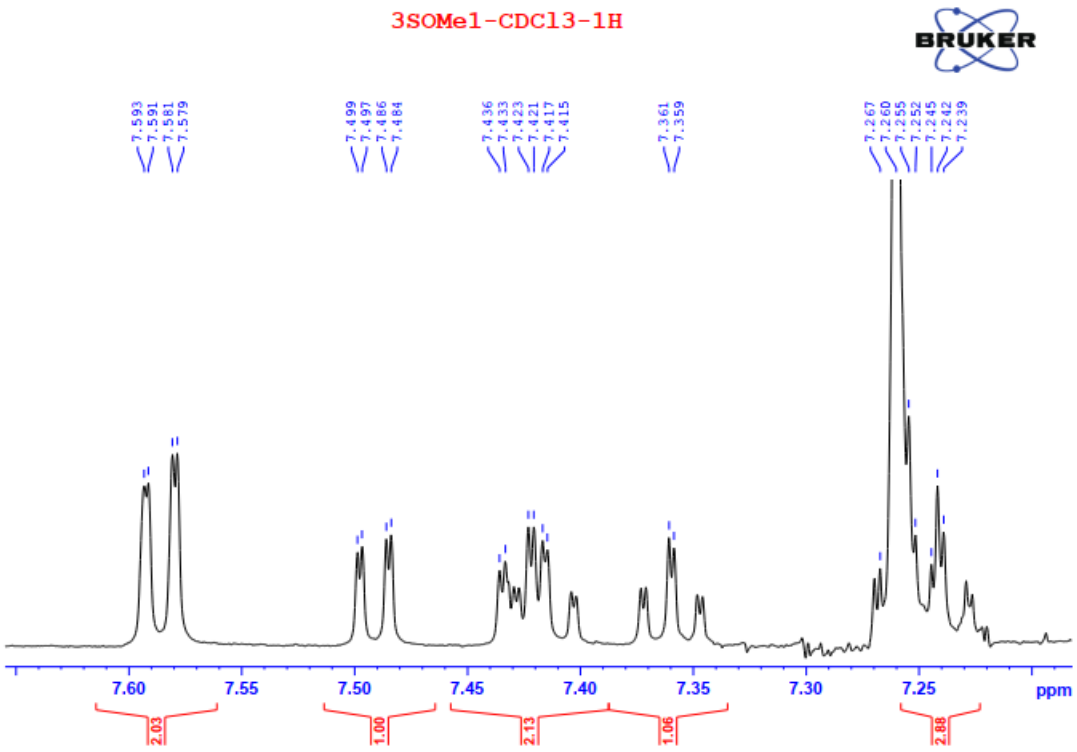

**Figure S4**. Physicochemical property of compounds **3b** (left) and **3e** (right)

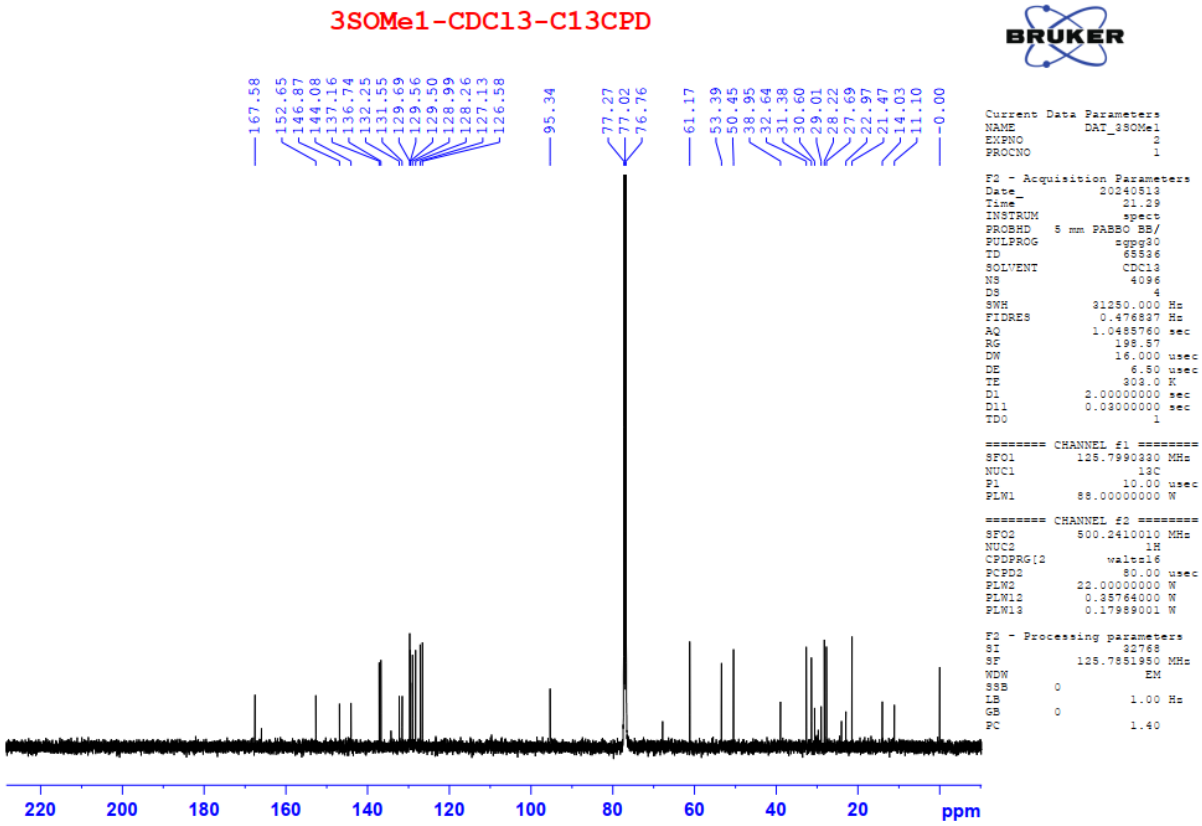
## 6. Spectra of synthesized compounds

### 6.1. Spectra of compound 3a



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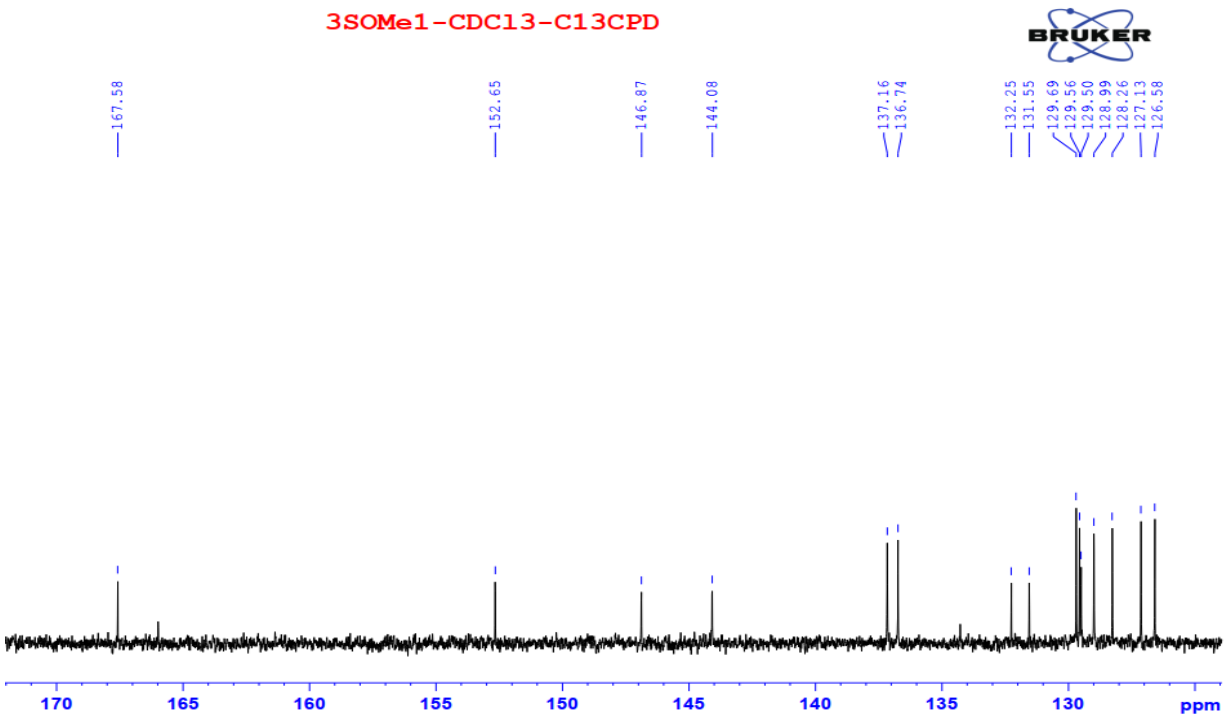
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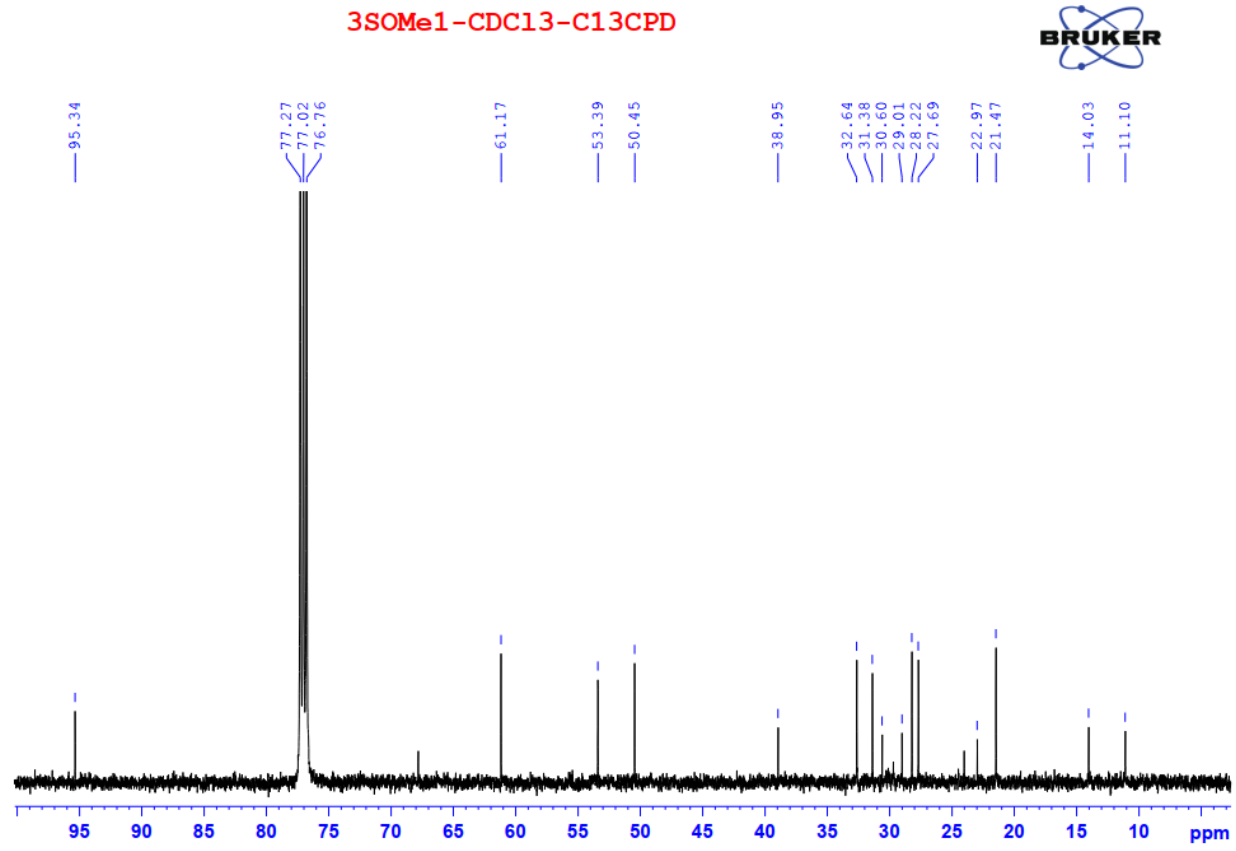
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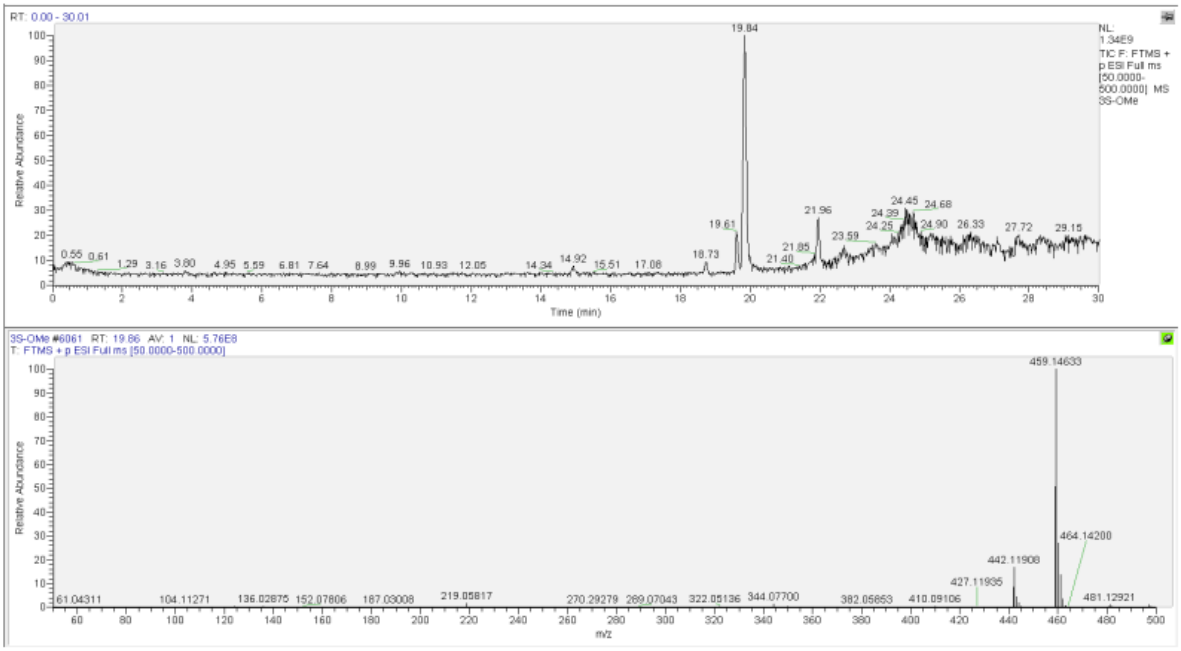
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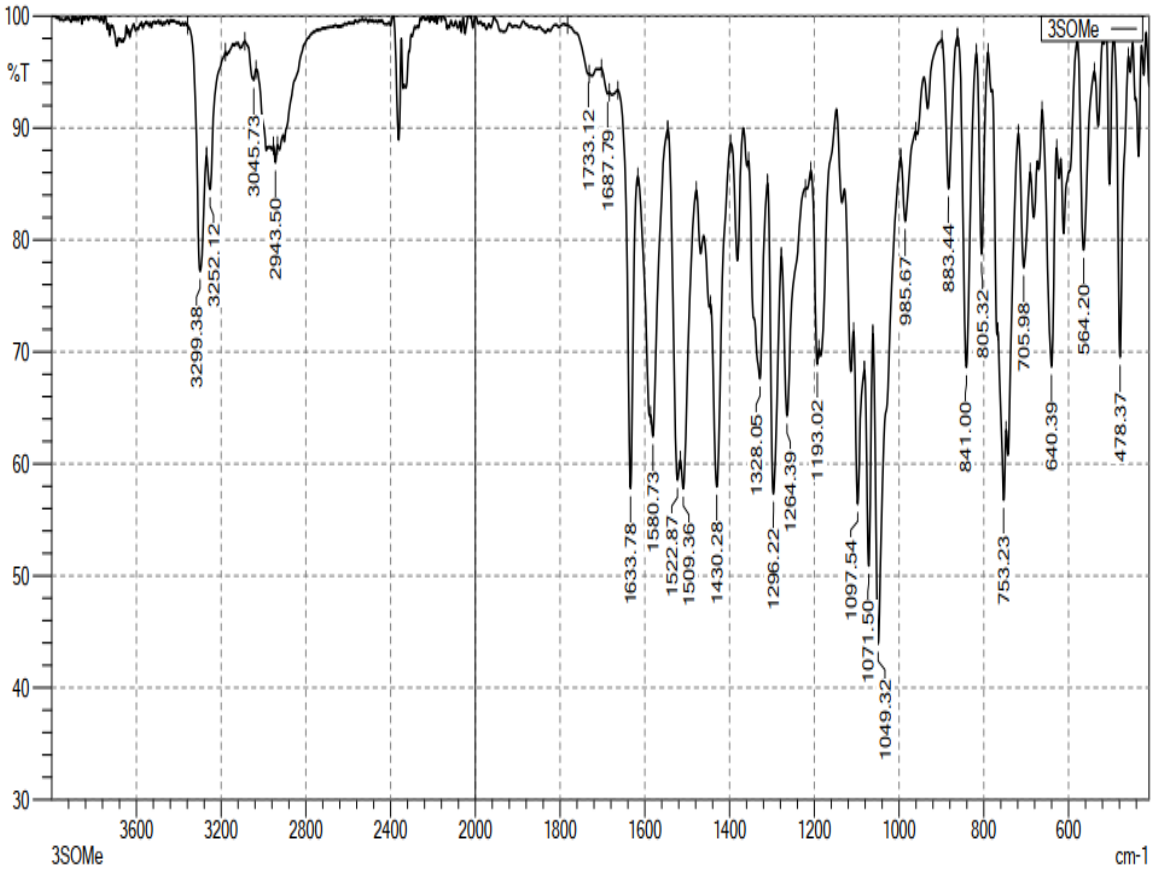
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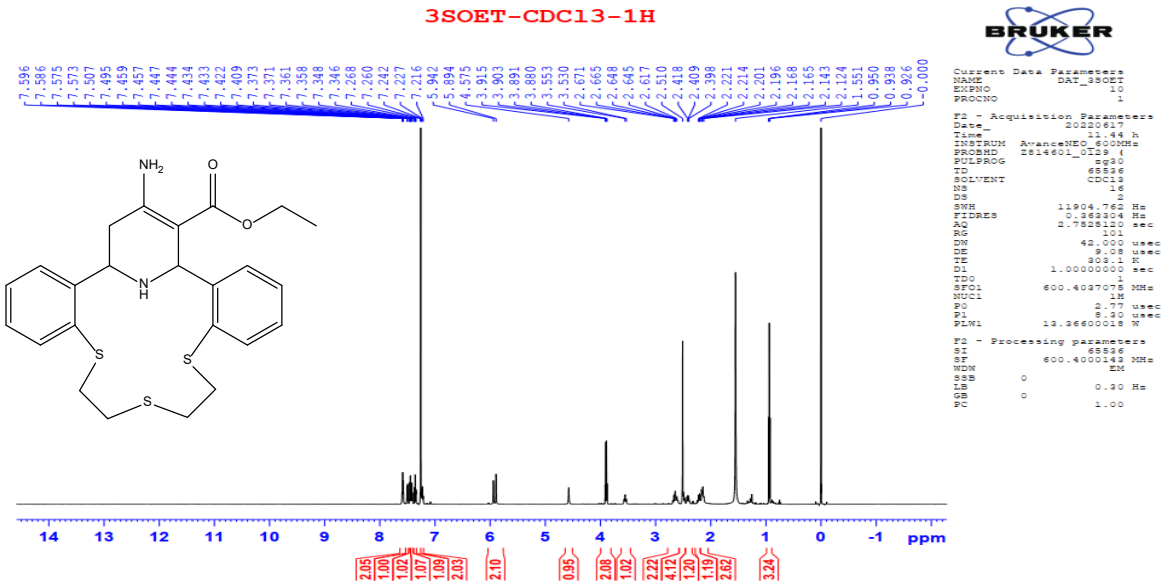
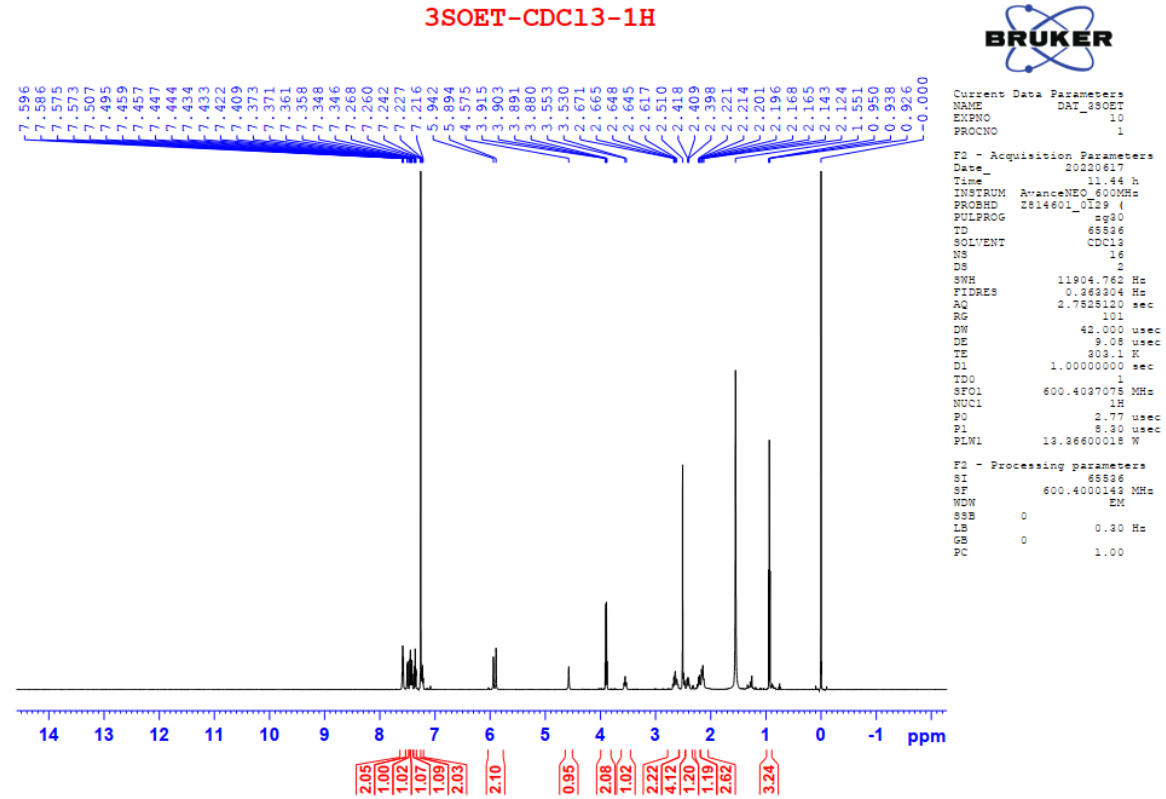
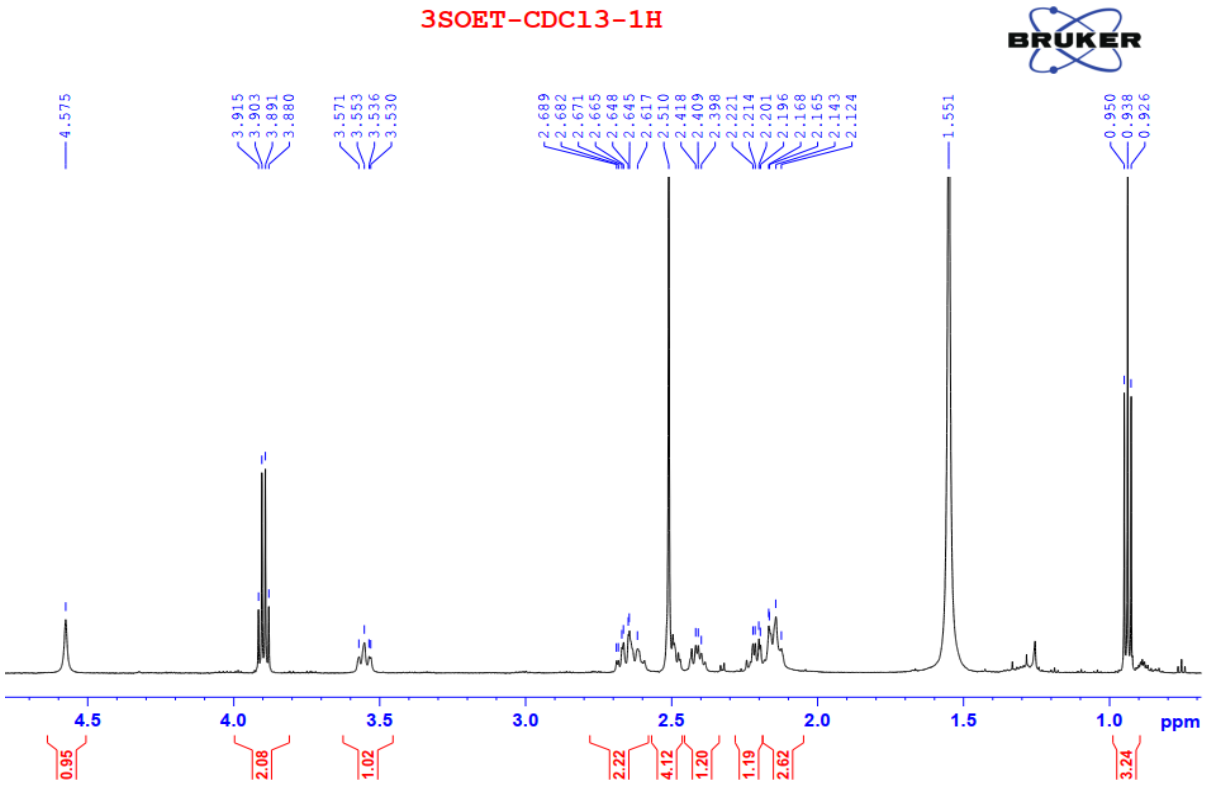
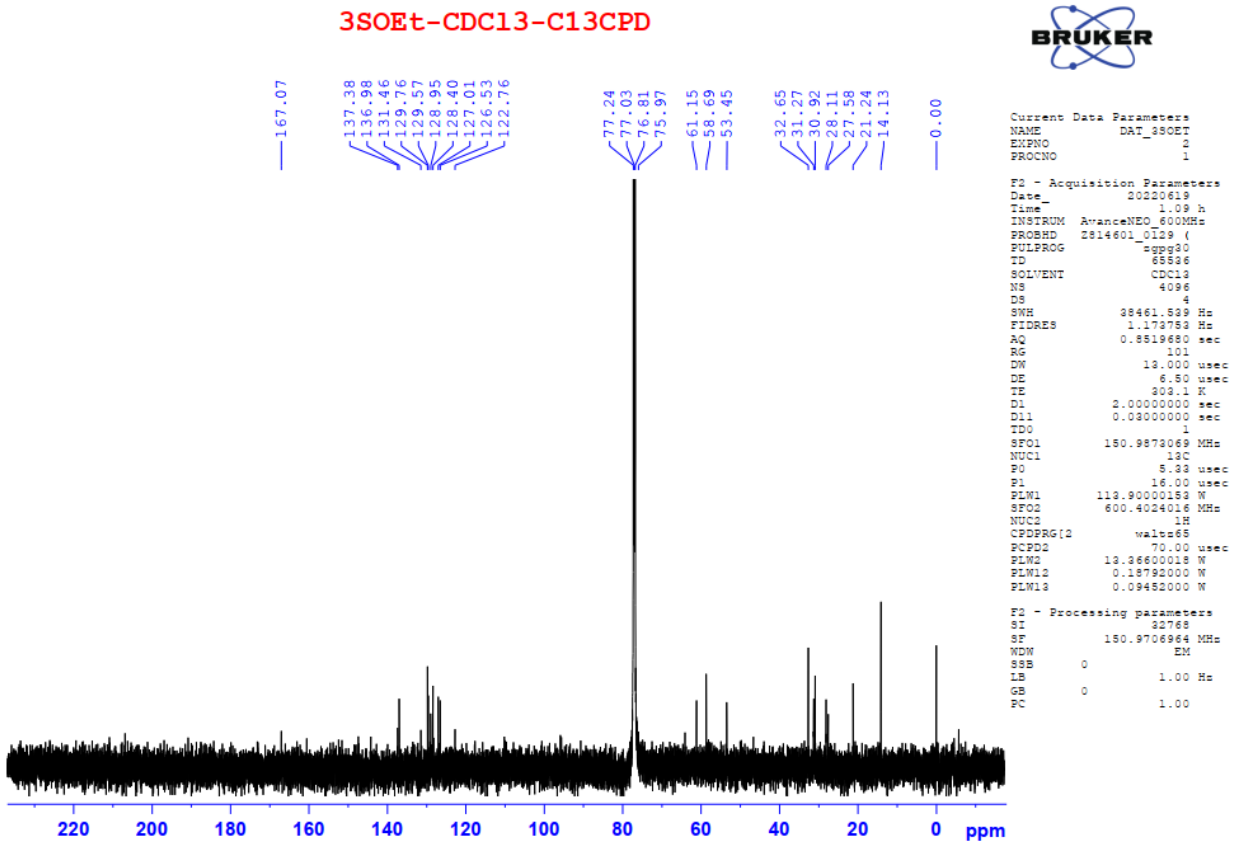
**6.2. Spectra of compound 3b**

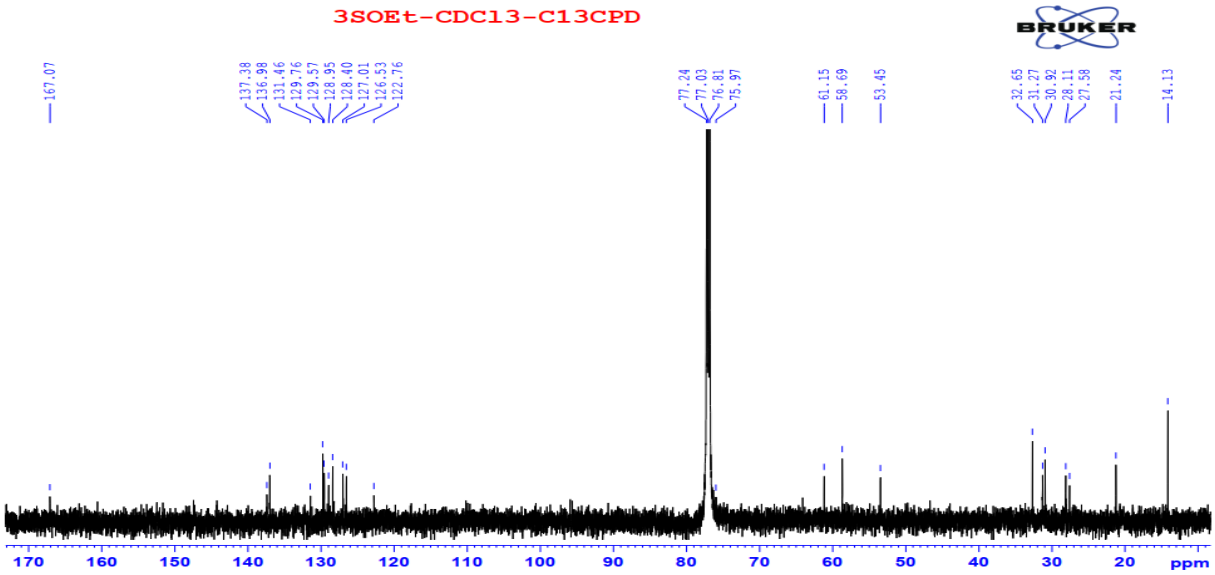


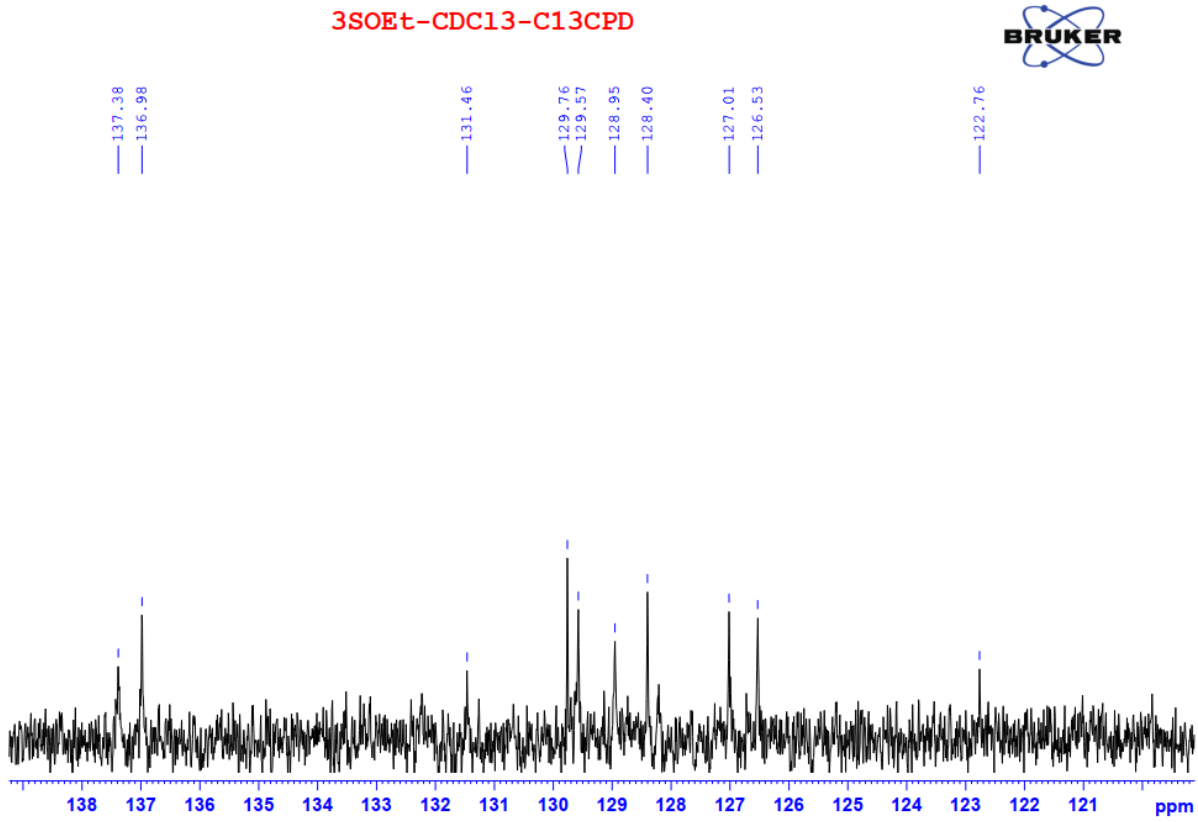





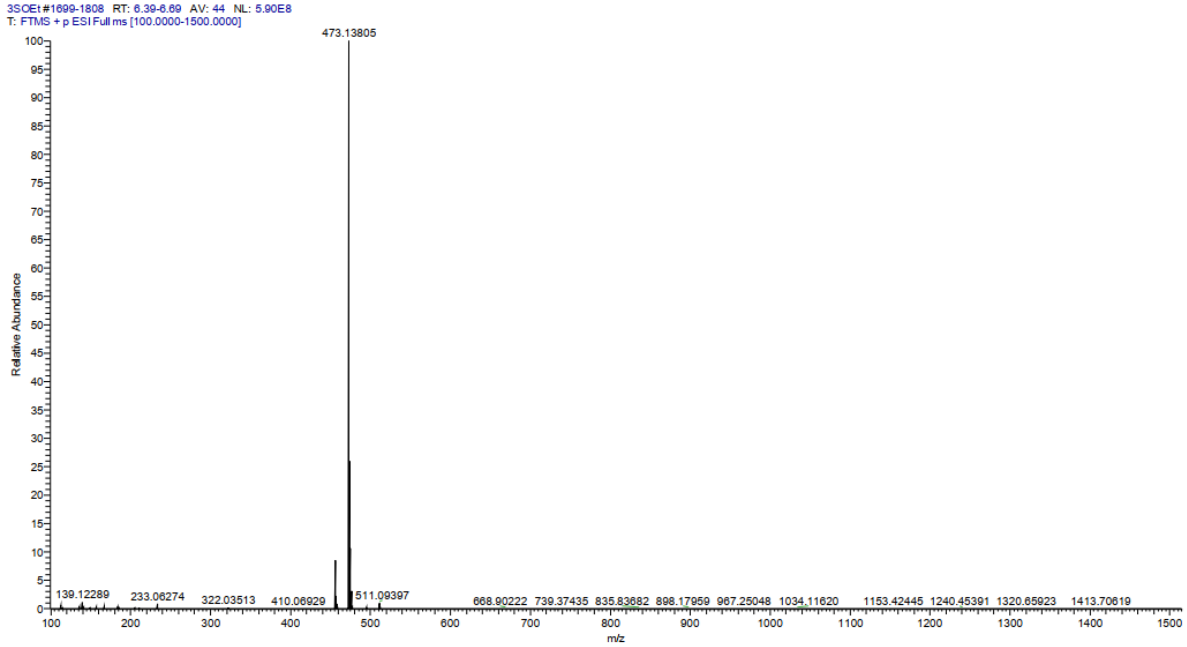

```
Current Data Parameters
NAME                  DAT_3SOET
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20220619
Time                      1.09 h
INSTRUM   AvanceNEO_600MHz
PROBHD    Z814601_0129 (
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        4096
DS                           4
SWH                  38461.529 Hz
FIDRES                1.173752 Hz
AQ                    0.8519680 sec
RG                         101
DW                      13.000 usec
DE                        6.50 usec
TE                       303.1 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                          1
SFO1               150.9873069 MHz
NUC1                        13C
P0                        5.33 usec
P1                       16.00 usec
PLW1           113.90000153 W
SFO2               600.4024016 MHz
NUC2                        1H
CPDPRG[2                waltz65
PCPD2                    70.00 usec
PLW2            13.26600018 W
PLW12            0.18792000 W
PLW13            0.09452000 W

F2 - Processing parameters
SI                       32768
SF                 150.9706964 MHz
WDW                         EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.00
```

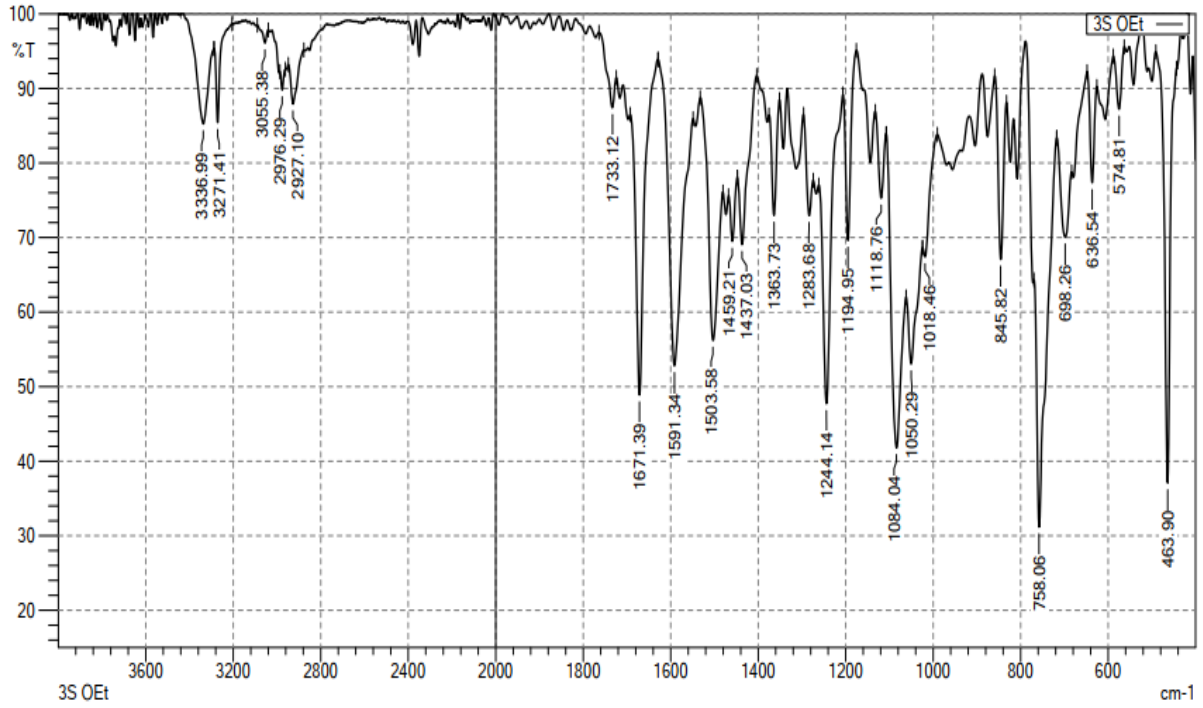

3SOEt-CDCl3-C13CPD
BRUKER
167.07
137.38
136.98
131.46
129.76
129.57
128.95
128.40
127.01
126.53
122.76
77.24
77.03
76.81
75.97
61.15
58.69
53.45
32.65
31.27
30.92
28.11
27.58
21.24
14.13
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


3SOEt-CDCl3-C13CPD
BRUKER
137.38
136.98
131.46
129.76
129.57
128.95
128.40
127.01
126.53
122.76
138 137 136 135 134 133 132 131 130 129 128 127 126 125 124 123 122 121 ppm

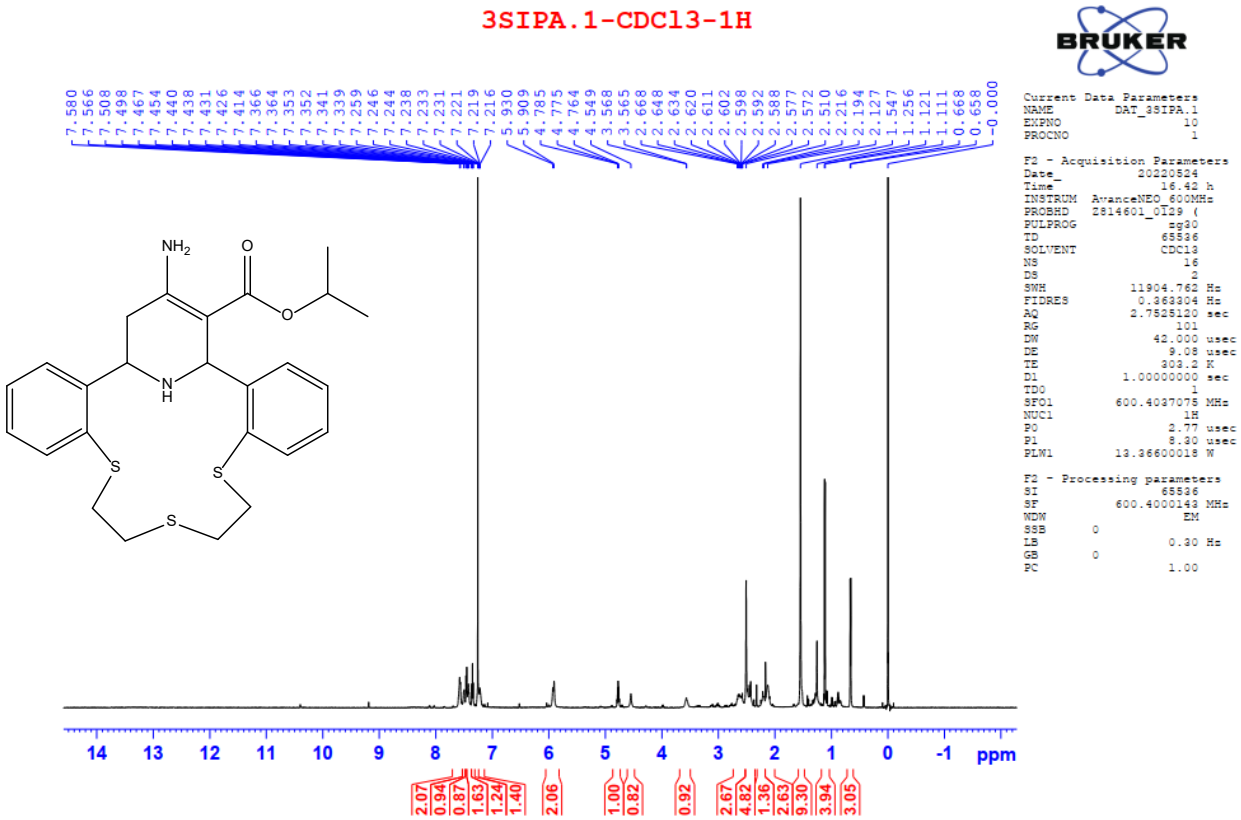
3SOEt:

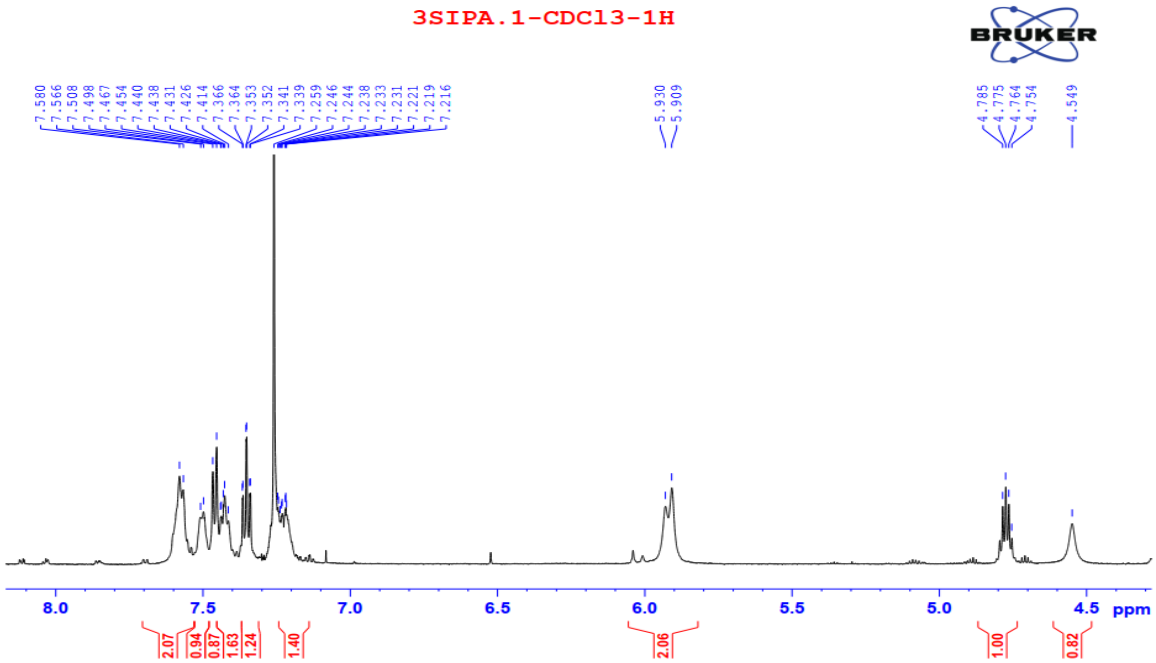
TIC:

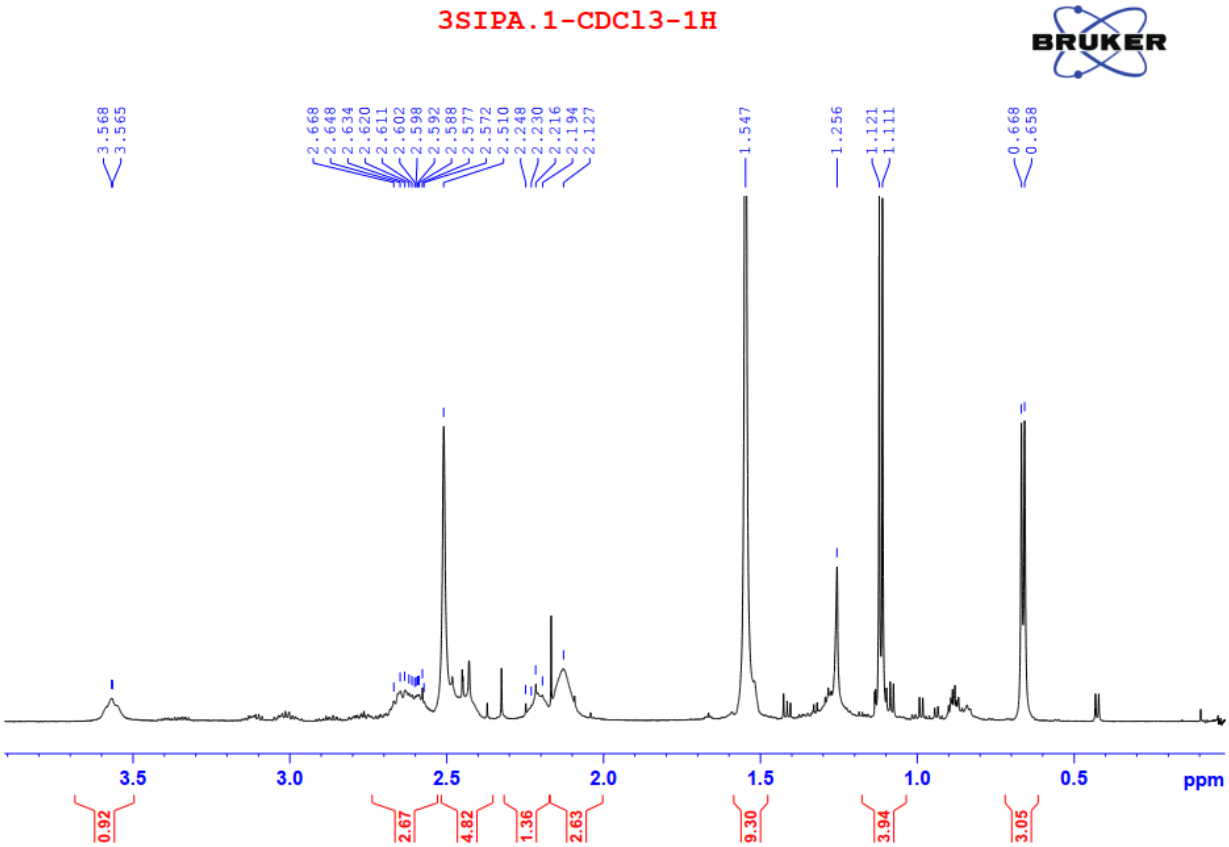

3SOEt#1699-1808 RT: 6.39-6.69 AV: 44 NL: 5.90E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]
473.13805
Relative Abundance
m/z

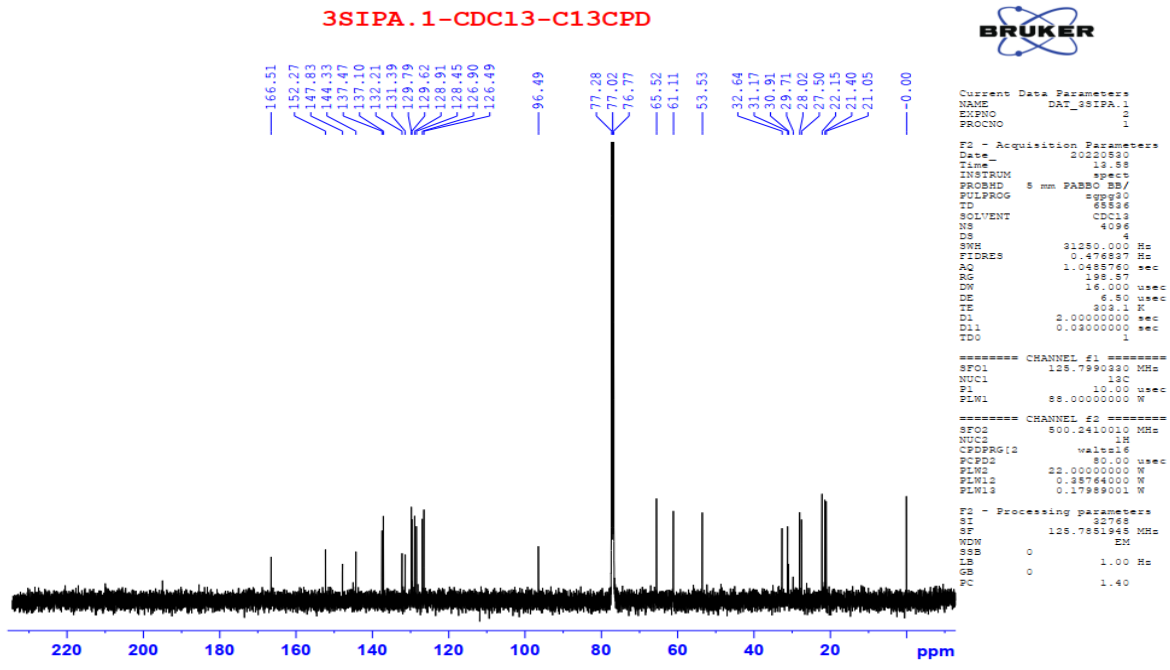

3S OEt
%T
3336.99
3271.41
3055.38
2976.29
2927.10
1733.12
1671.39
1591.34
1503.58
1459.21
1437.03
1363.73
1283.68
1244.14
1194.95
1118.76
1084.04
1050.29
1018.46
845.82
758.06
698.26
636.54
574.81
463.90
3S OEt
cm-1

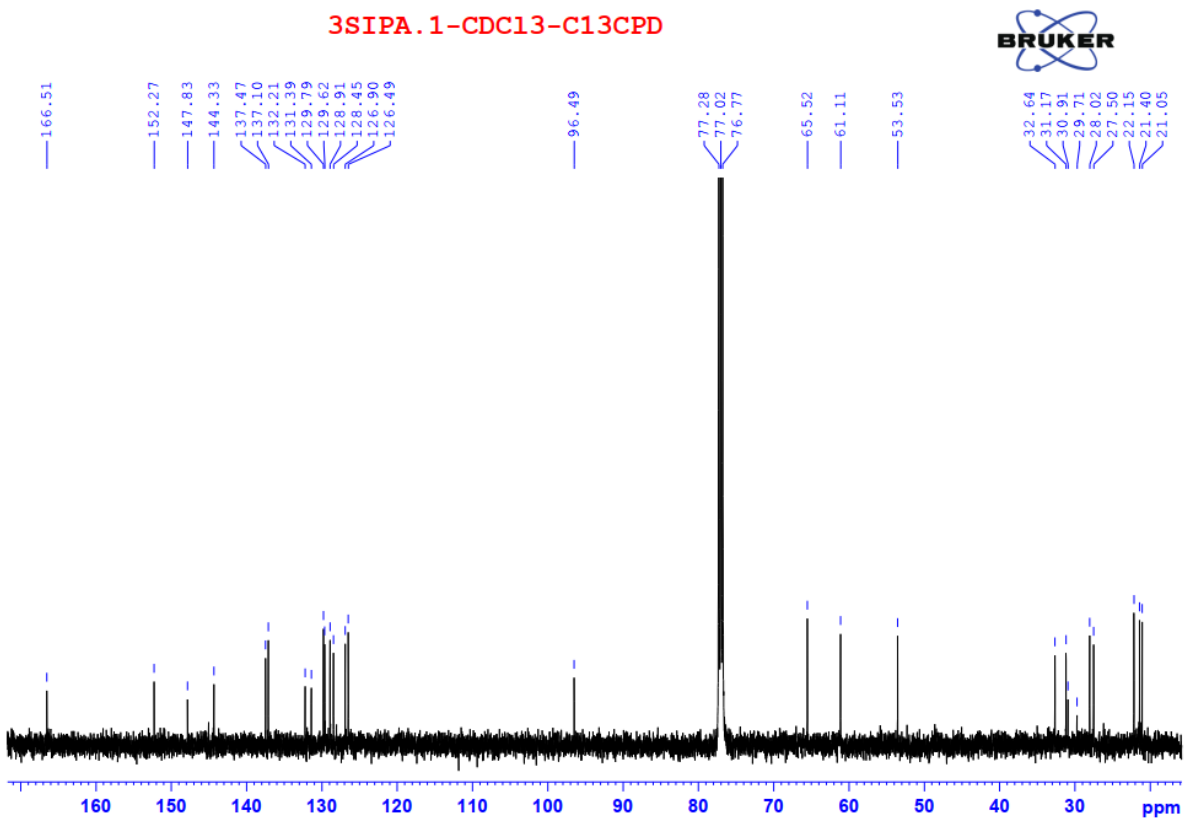
**6.3. Spectra of compound 3c**

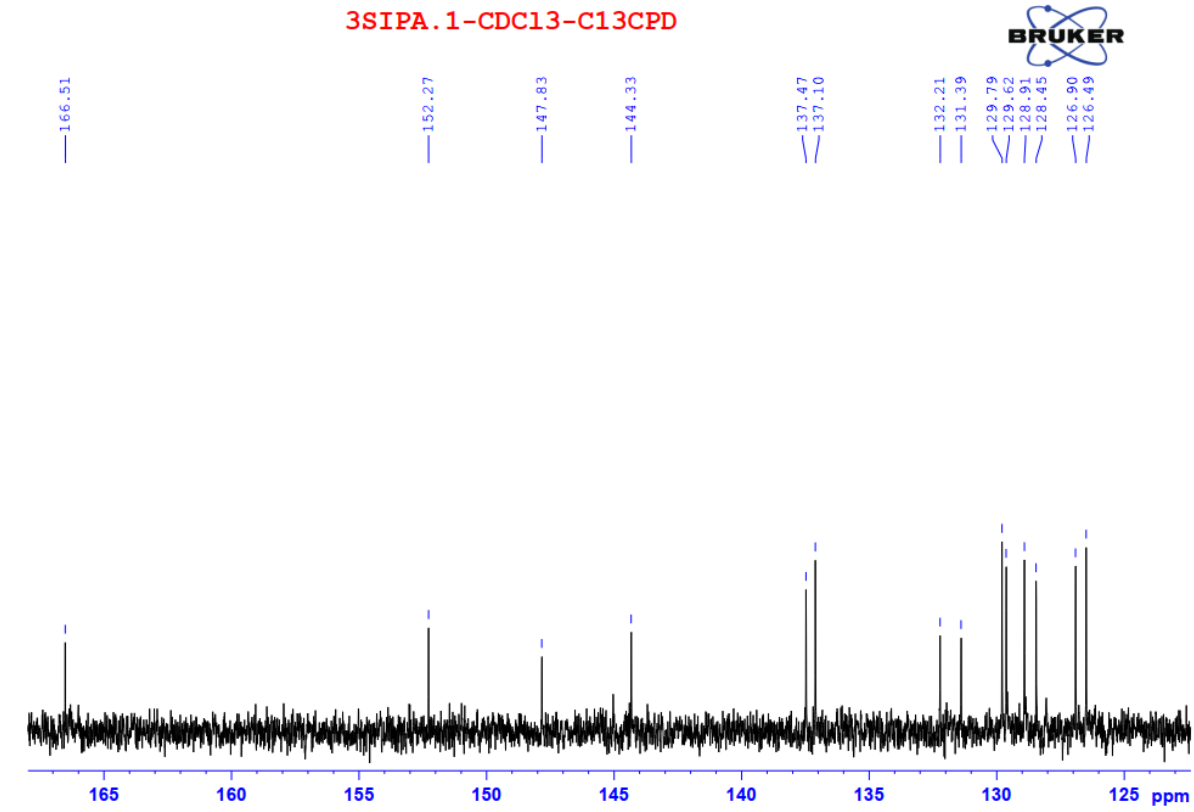


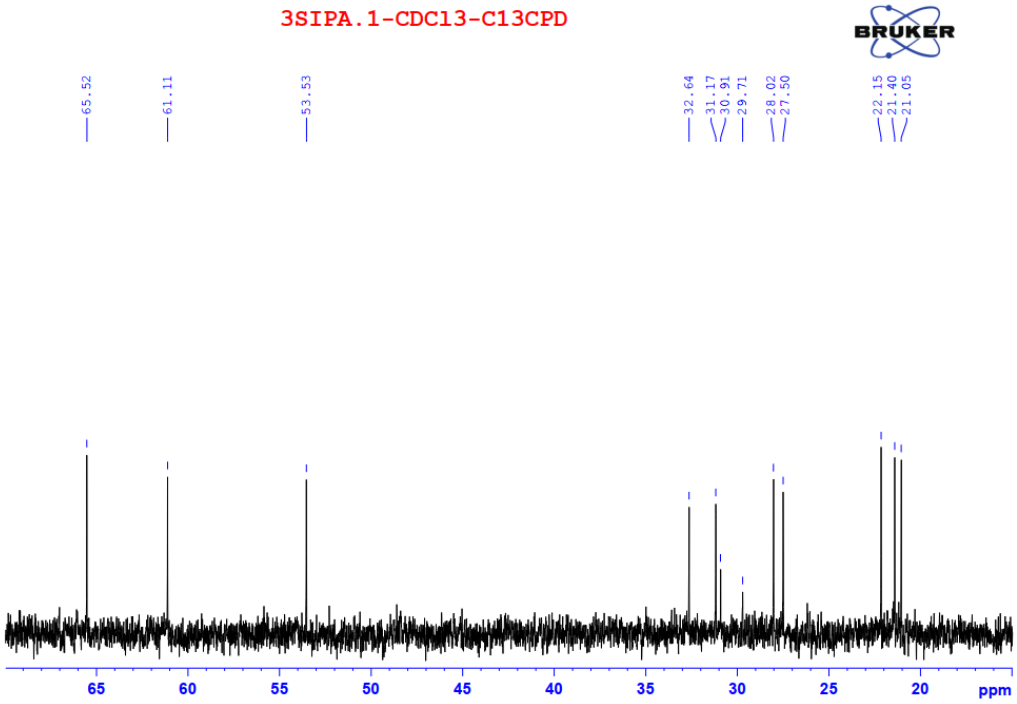



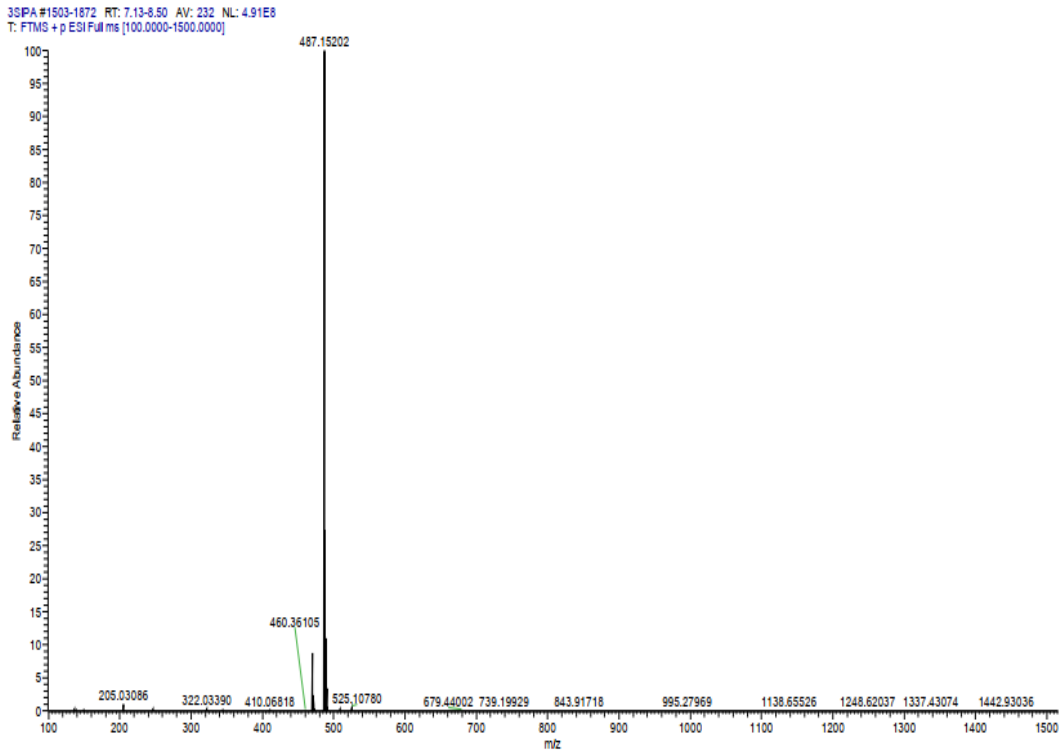

3SIPA.1-CDCl3-1H
3.568
3.565
2.668
2.648
2.634
2.620
2.611
2.602
2.598
2.592
2.588
2.577
2.572
2.510
2.248
2.230
2.216
2.194
2.127
1.547
1.256
1.121
1.111
0.668
0.658
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.92
2.67
4.82
1.36
2.63
9.30
3.94
3.05

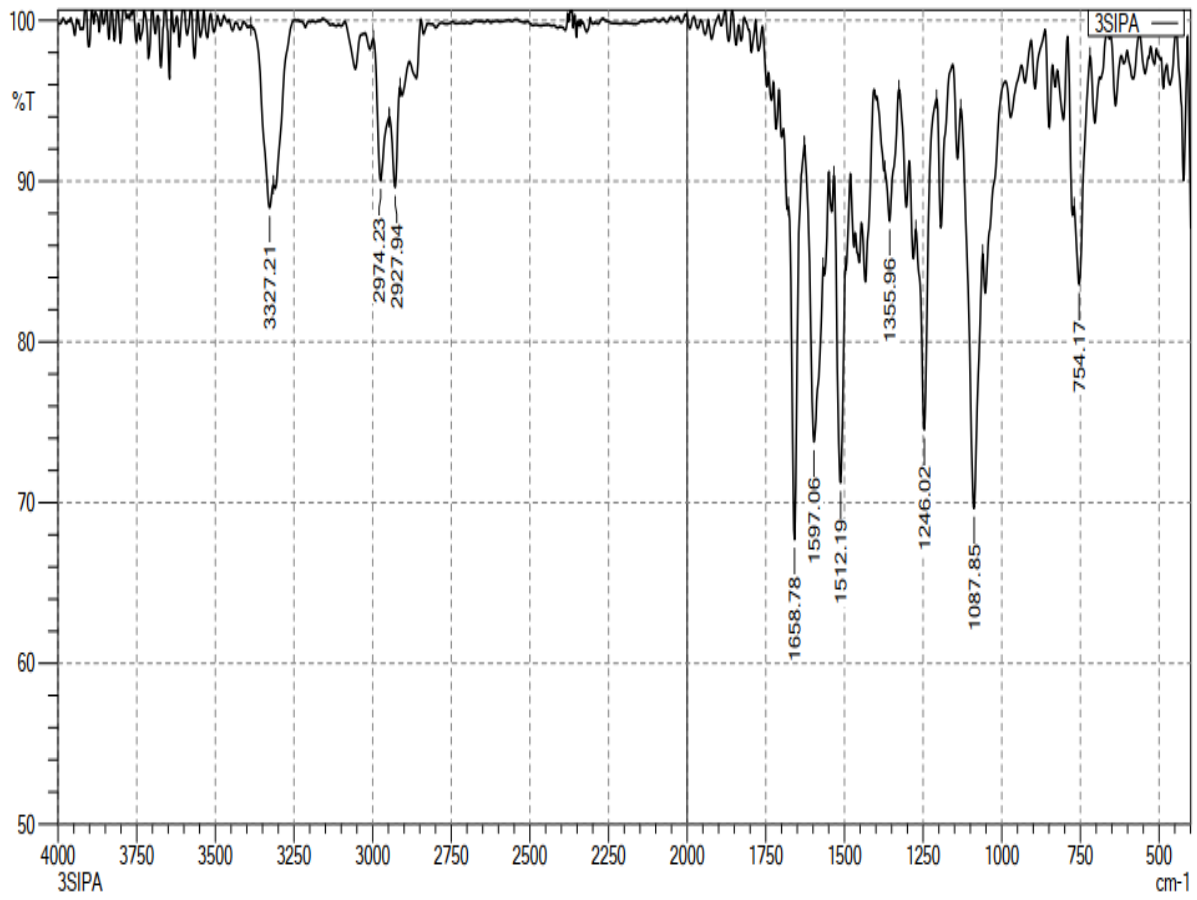

3SIPA.1-CDCl3-C13CPD
166.51
152.27
147.83
144.33
137.47
137.10
132.21
131.39
129.79
129.62
128.91
128.45
126.90
126.49
96.49
77.28
77.02
76.77
65.52
61.11
53.53
32.64
31.17
30.91
29.71
28.02
27.50
22.15
21.40
21.05
-0.00
220
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME DAT_3SIPA.1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220530
Time 12.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4096
DS 4
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 198.57
DW 16.000 usec
DE 6.50 usec
TE 303.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7990330 MHz
NUC1 13C
P1 10.00 usec
PLW1 88.00000000 W
======== CHANNEL f2 ========
SFO2 500.2410010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 22.00000000 W
PLW12 0.35764000 W
PLW13 0.17989001 W
F2 - Processing parameters
SI 32768
SF 125.7851945 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


3SIPA.1-CDCl3-C13CPD
BRUKER
166.51
152.27
147.83
144.33
137.47
137.10
132.21
131.39
129.79
129.62
128.91
128.45
126.90
126.49
96.49
77.28
77.02
76.77
65.52
61.11
53.53
32.64
31.17
30.91
29.71
28.02
27.50
22.15
21.40
21.05
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm

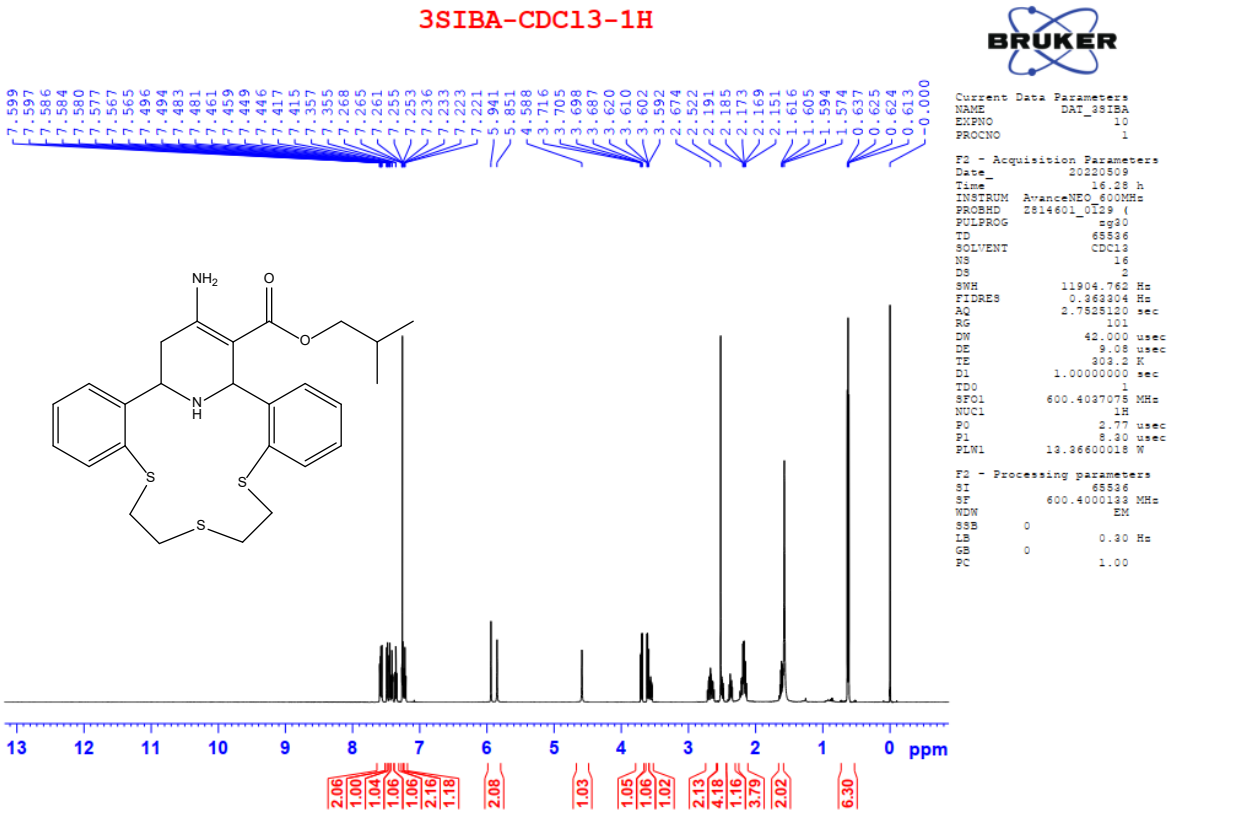

3SIPA.1-CDCl3-C13CPD
BRUKER
166.51
152.27
147.83
144.33
137.47
137.10
132.21
131.39
129.79
129.62
128.91
128.45
126.90
126.49
165
160
155
150
145
140
135
130
125
ppm

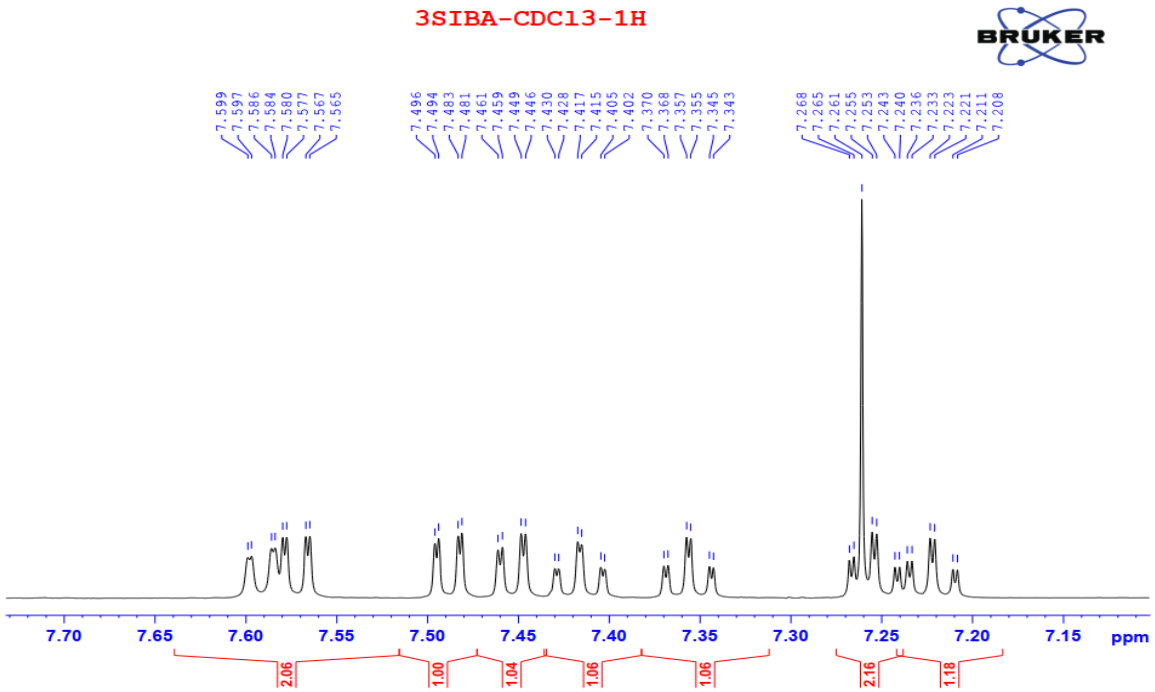

3SIPA.1-CDC13-C13CPD
BRUKER
65.52
61.11
53.53
32.64
31.17
30.91
29.71
28.02
27.50
22.15
21.40
21.05
65
60
55
50
45
40
35
30
25
20
ppm

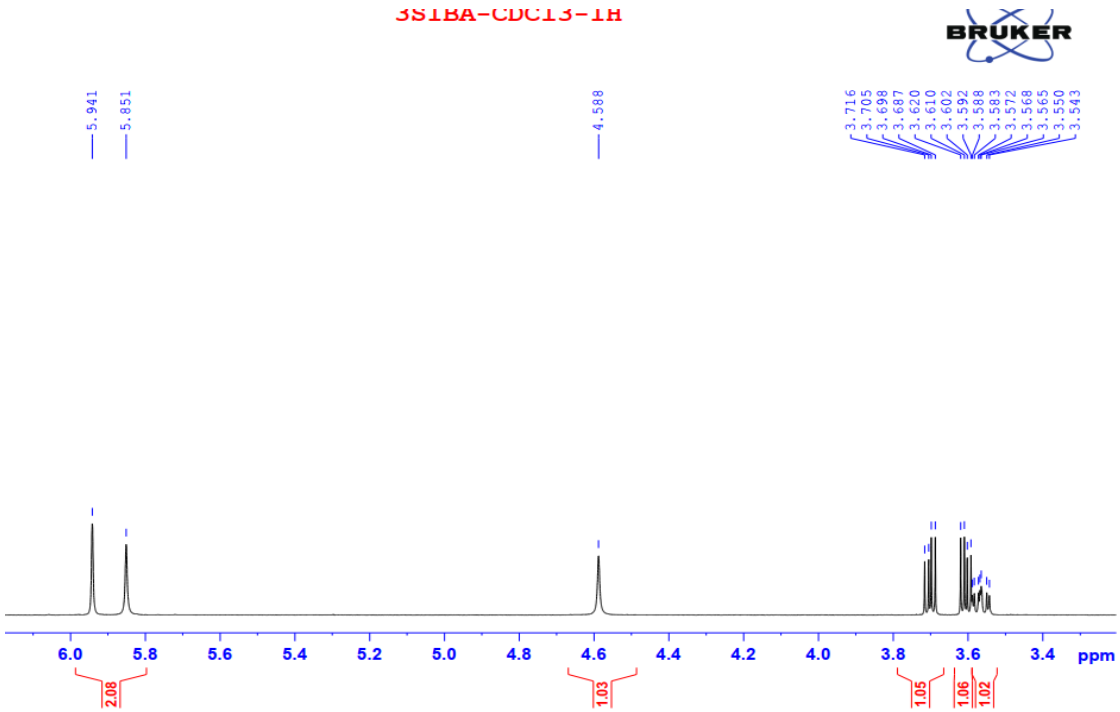

3SIPA #1503-1872 RT: 7.13-8.50 AV: 232 NL: 4.91E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]
487.15202
460.36105
205.03086
322.03390
410.06818
525.10780
679.44002
739.19929
843.91718
995.27969
1138.65526
1248.62037
1337.43074
1442.93036
Relative Abundance
m/z

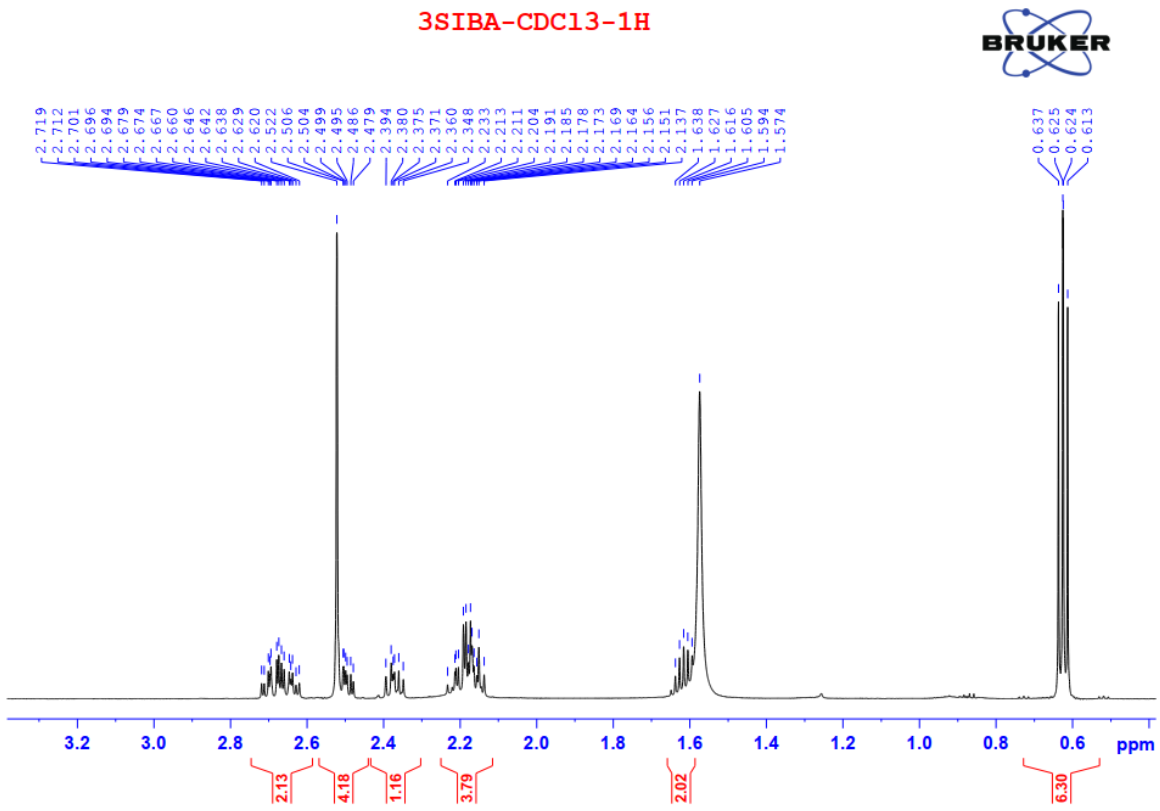

3SIPA
%T
100
90
80
70
60
50
3327.21
2974.23
2927.94
1658.78
1597.06
1512.19
1355.96
1246.02
1087.85
754.17
4000
3750
3500
3250
3000
2750
2500
2250
2000
1750
1500
1250
1000
750
500
cm-1
3SIPA

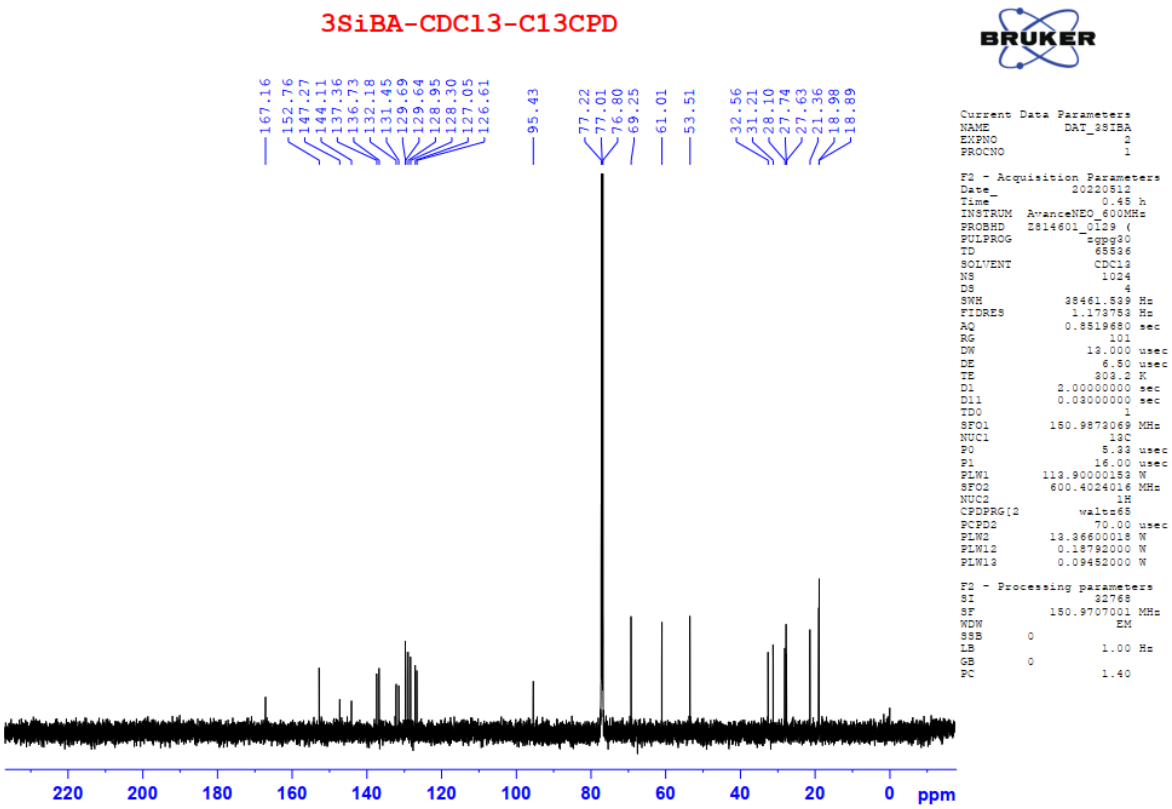
**6.4.** Spectra of compound **3d**



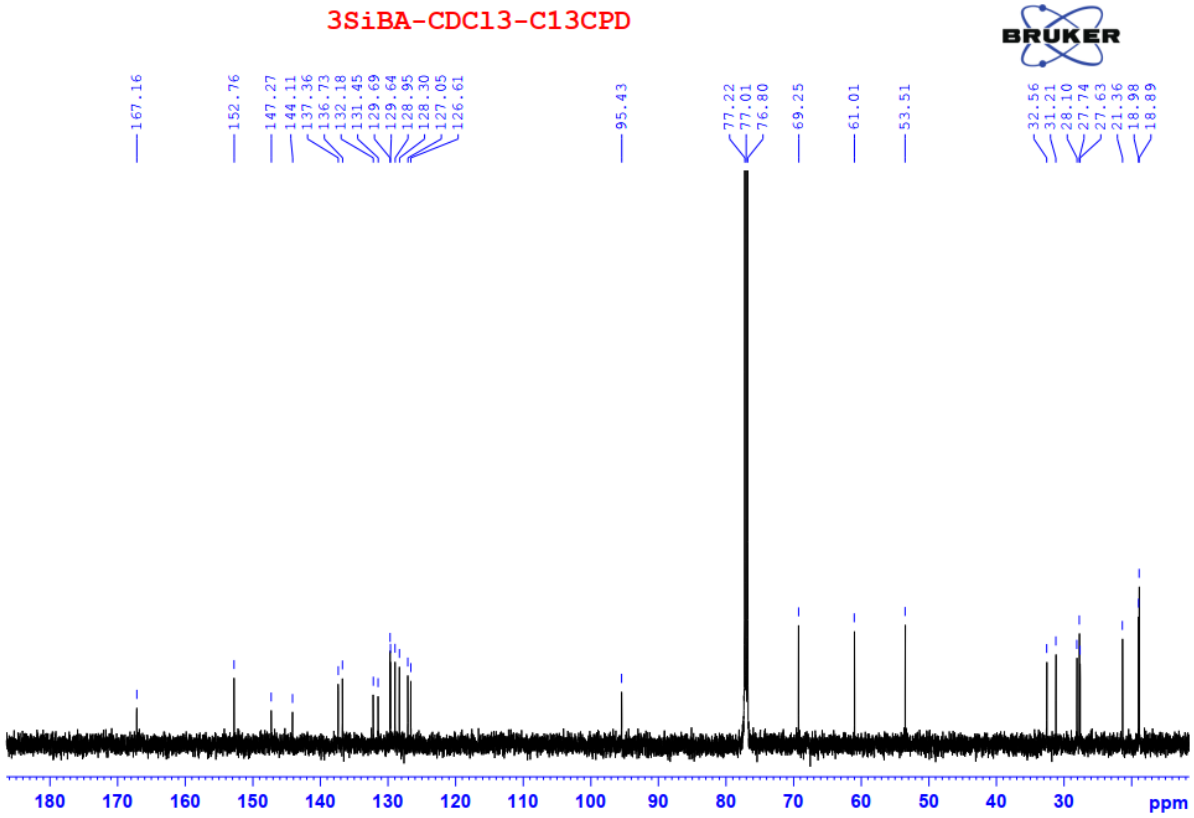



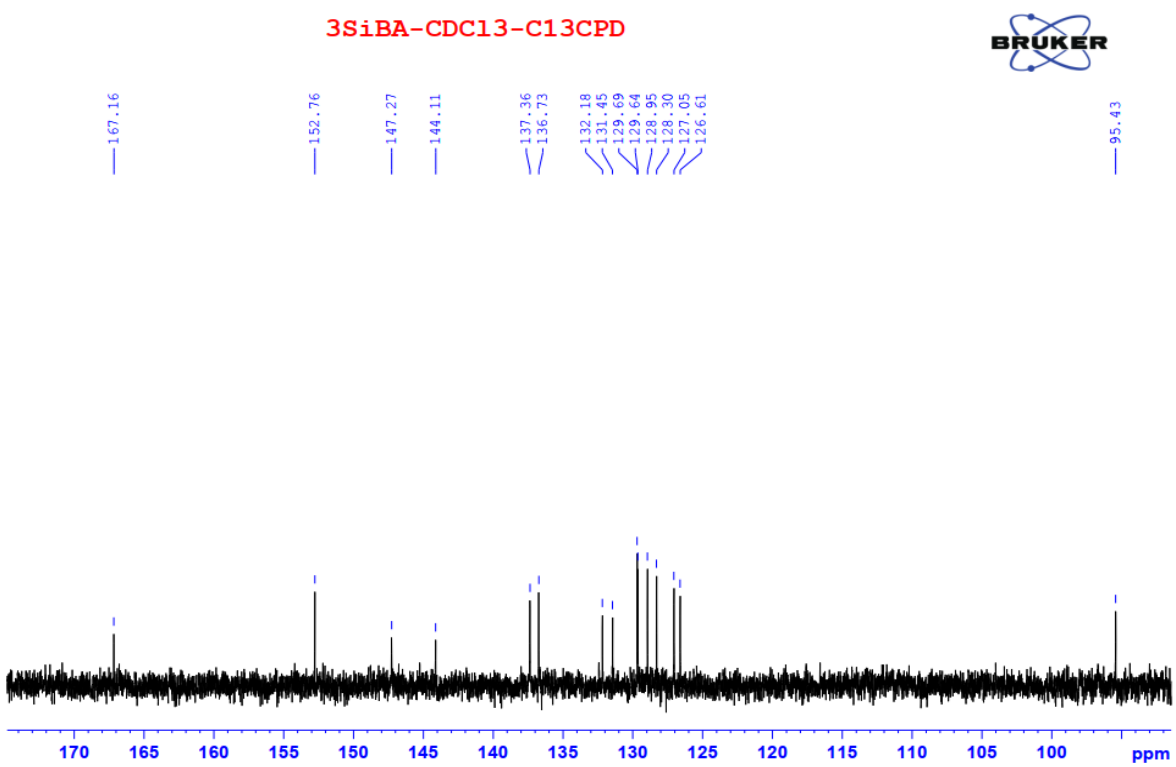

3SIBA-CDC13-1H
BRUKER
5.941
5.851
4.588
3.716
3.705
3.698
3.687
3.620
3.610
3.602
3.592
3.588
3.583
3.572
3.568
3.565
3.550
3.543
6.0
5.8
5.6
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4
ppm
2.08
1.03
1.05
1.06
1.02

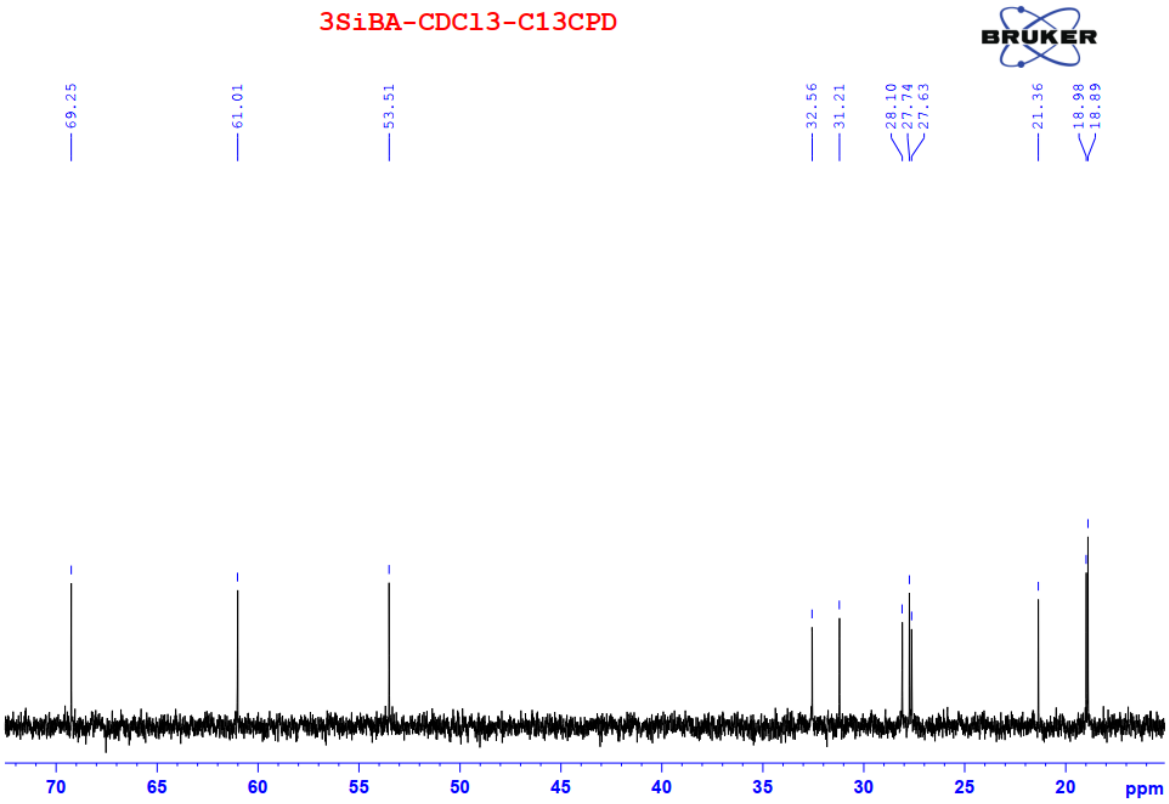

3SIBA-CDC13-1H
BRUKER
2.719
2.712
2.701
2.696
2.694
2.679
2.674
2.667
2.660
2.646
2.642
2.638
2.629
2.620
2.522
2.506
2.504
2.499
2.495
2.486
2.479
2.394
2.380
2.375
2.371
2.360
2.348
2.233
2.213
2.211
2.204
2.191
2.185
2.178
2.173
2.169
2.164
2.156
2.151
2.137
1.638
1.627
1.616
1.605
1.594
1.574
0.637
0.625
0.624
0.613
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
ppm
2.13
4.18
1.16
3.79
2.02
6.30

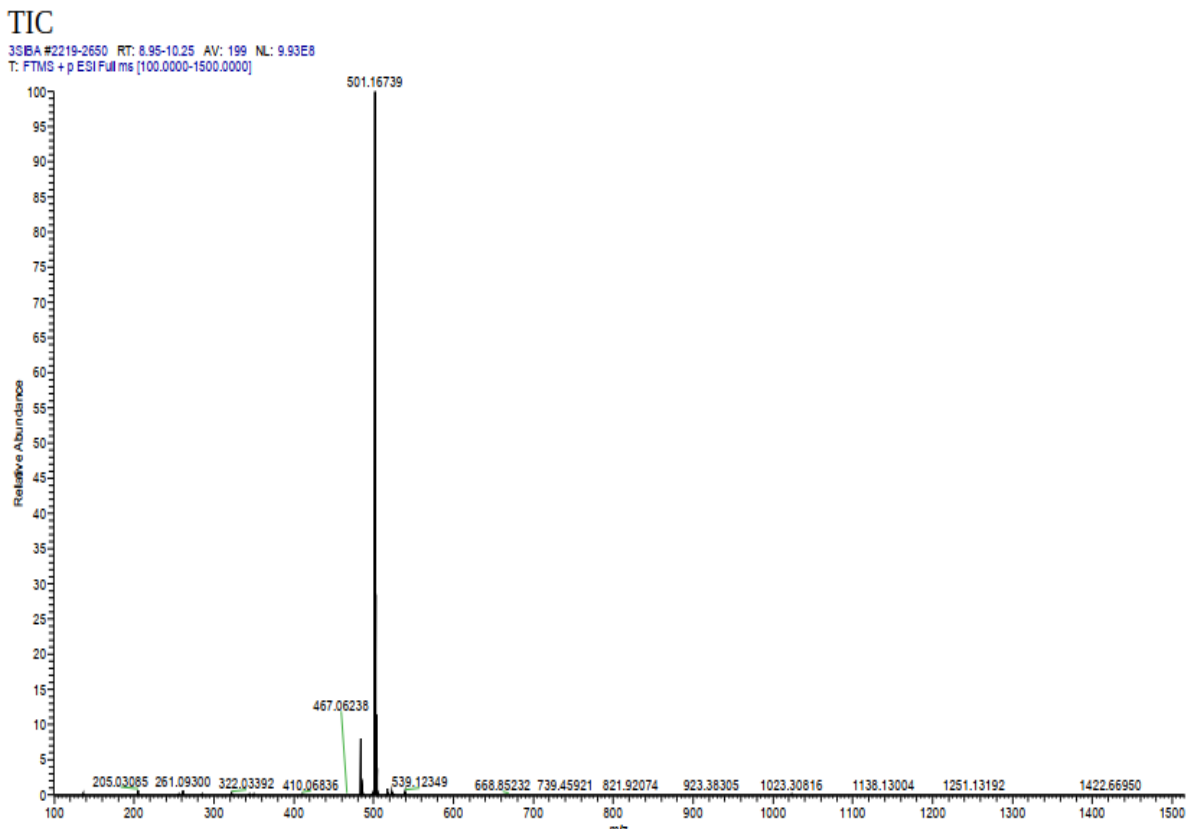


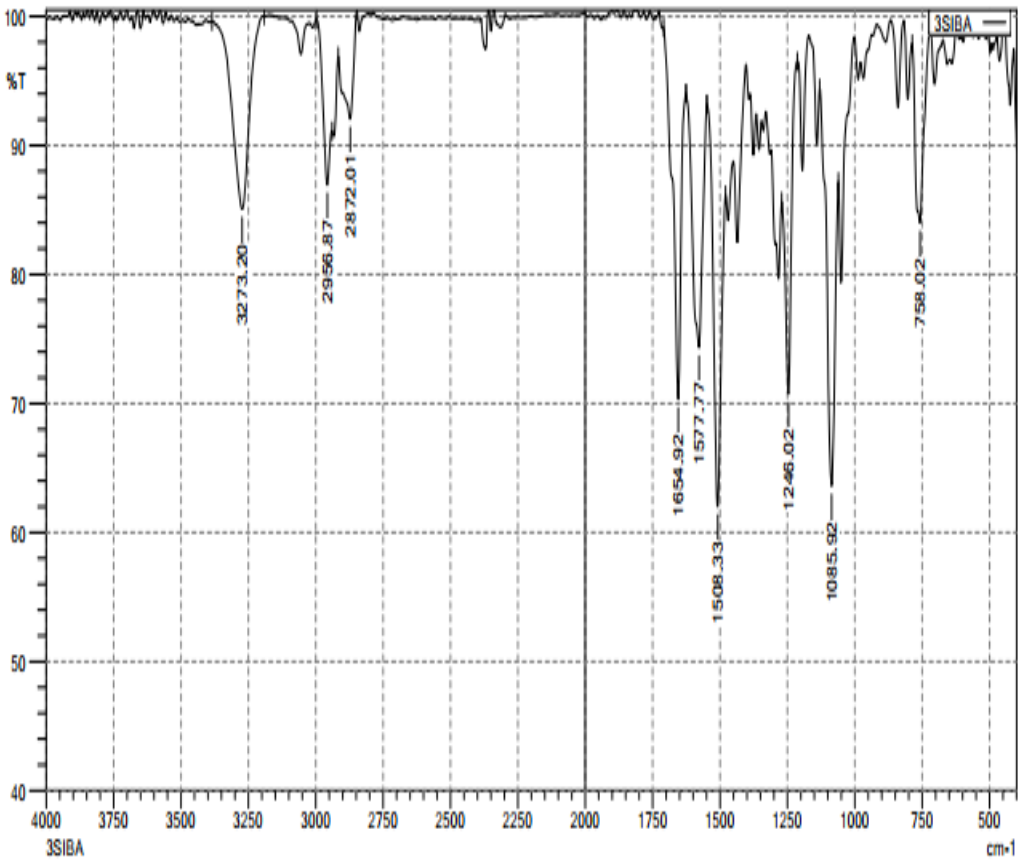

```
Current Data Parameters
NAME              DAT_3SIBA
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20220512
Time_                 0.45 h
INSTRUM  AvanceNEO_600MHz
PROBHD   Z814601_0129 (
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH             38461.539 Hz
FIDRES          1.173753 Hz
AQ              0.8519680 sec
RG                     101
DW                13.000 usec
DE                 6.50 usec
TE                 303.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1
SFO1          150.9878069 MHz
NUC1                   13C
P0                    5.33 usec
P1                   16.00 usec
PLW1         113.90000153 W
SFO2          600.4024016 MHz
NUC2                   1H
CPDPRG[2           waltz65
PCPD2                70.00 usec
PLW2          13.36600018 W
PLW12          0.18792000 W
PLW13          0.09452000 W

F2 - Processing parameters
SI                    32768
SF            150.9707001 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```



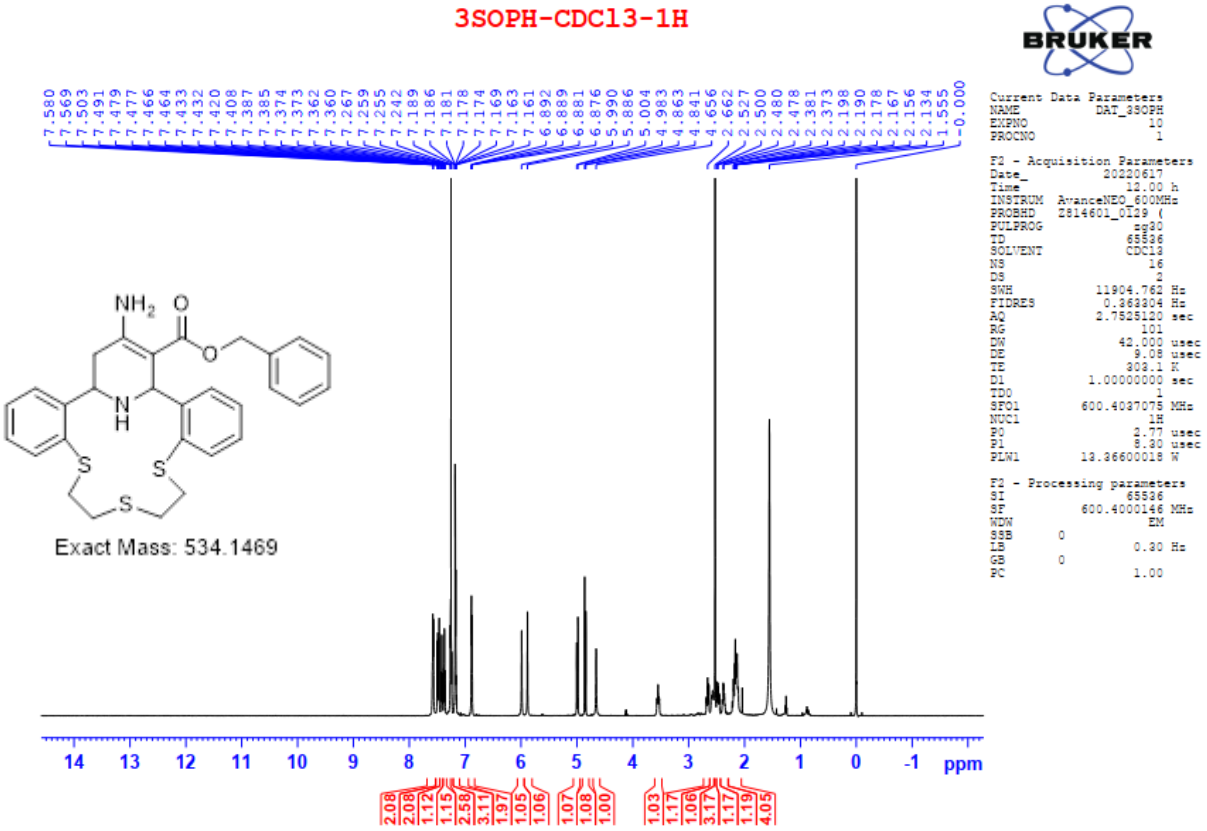

3SiBA-CDCl3-C13CPD
BRUKER
167.16
152.76
147.27
144.11
137.36
136.73
132.18
131.45
129.69
129.64
128.95
128.30
127.05
126.61
95.43
170
165
160
155
150
145
140
135
130
125
120
115
110
105
100
ppm

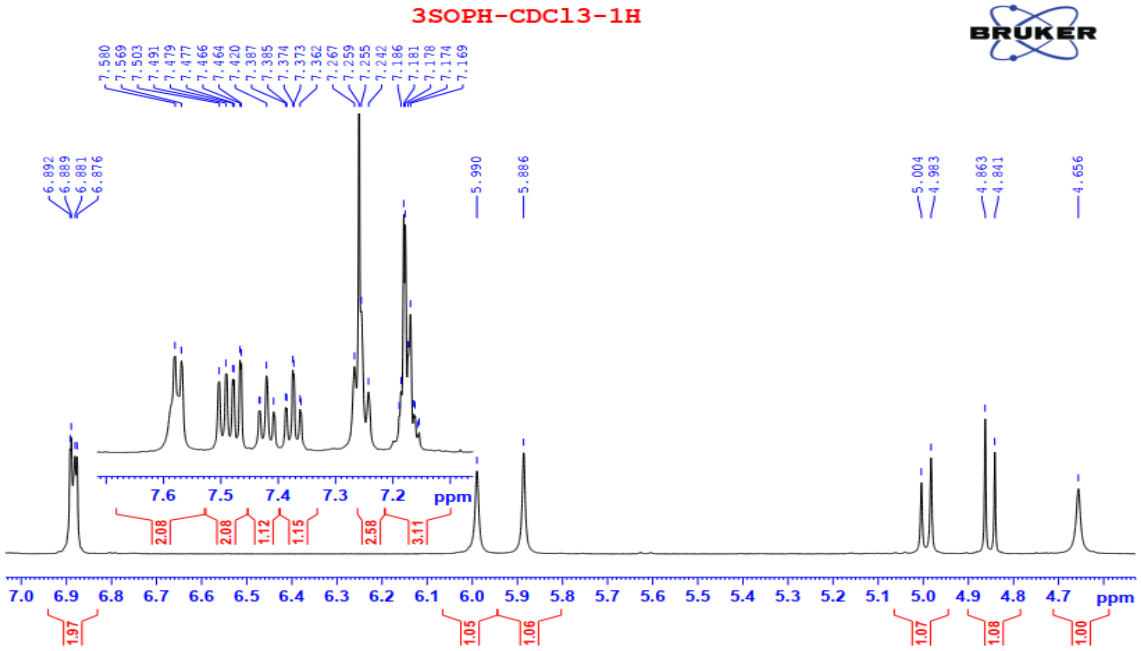

3SiBA-CDCl3-C13CPD
BRUKER
69.25
61.01
53.51
32.56
31.21
28.10
27.74
27.63
21.36
18.98
18.89
70
65
60
55
50
45
40
35
30
25
20
ppm

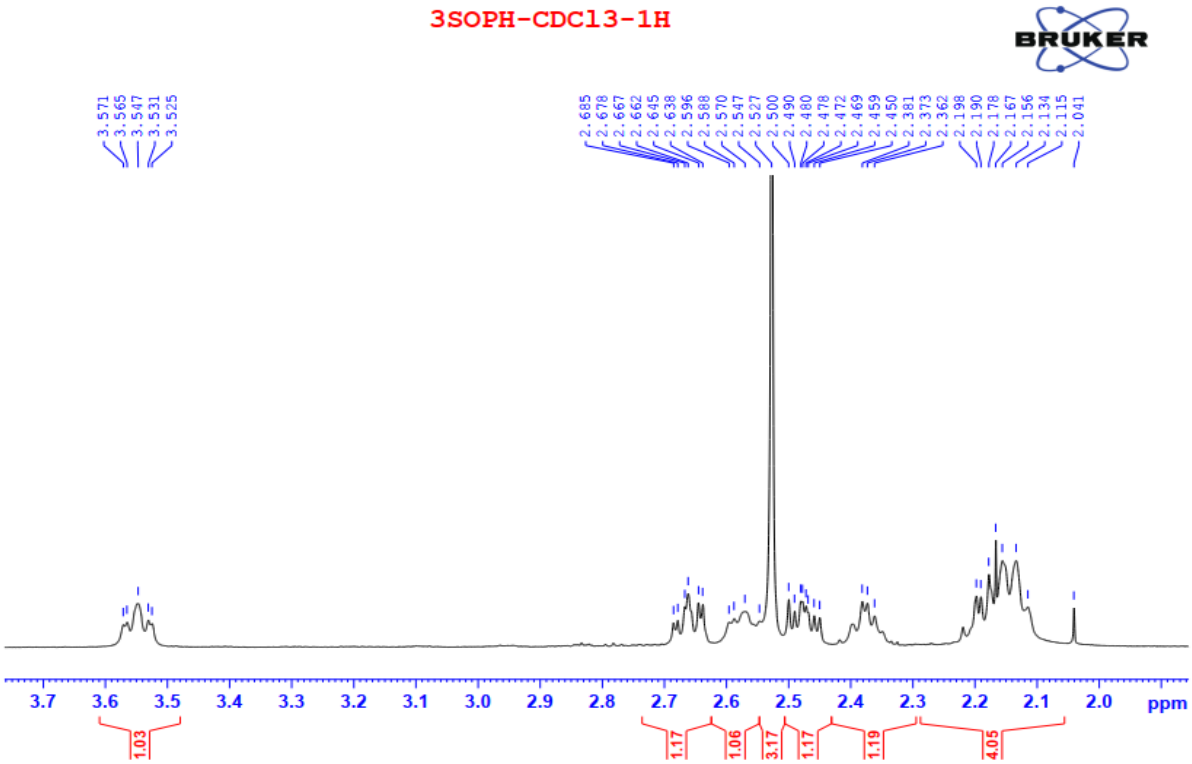

TIC
3SIBA #2219-2650 RT: 8.95-10.25 AV: 199 NL: 9.93E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]
501.16739
467.06238
205.03085
261.09300
322.03392
410.06836
539.12349
668.85232
739.45921
821.92074
923.38305
1023.30816
1138.13004
1251.13192
1422.66950
Relative Abundance
m/z

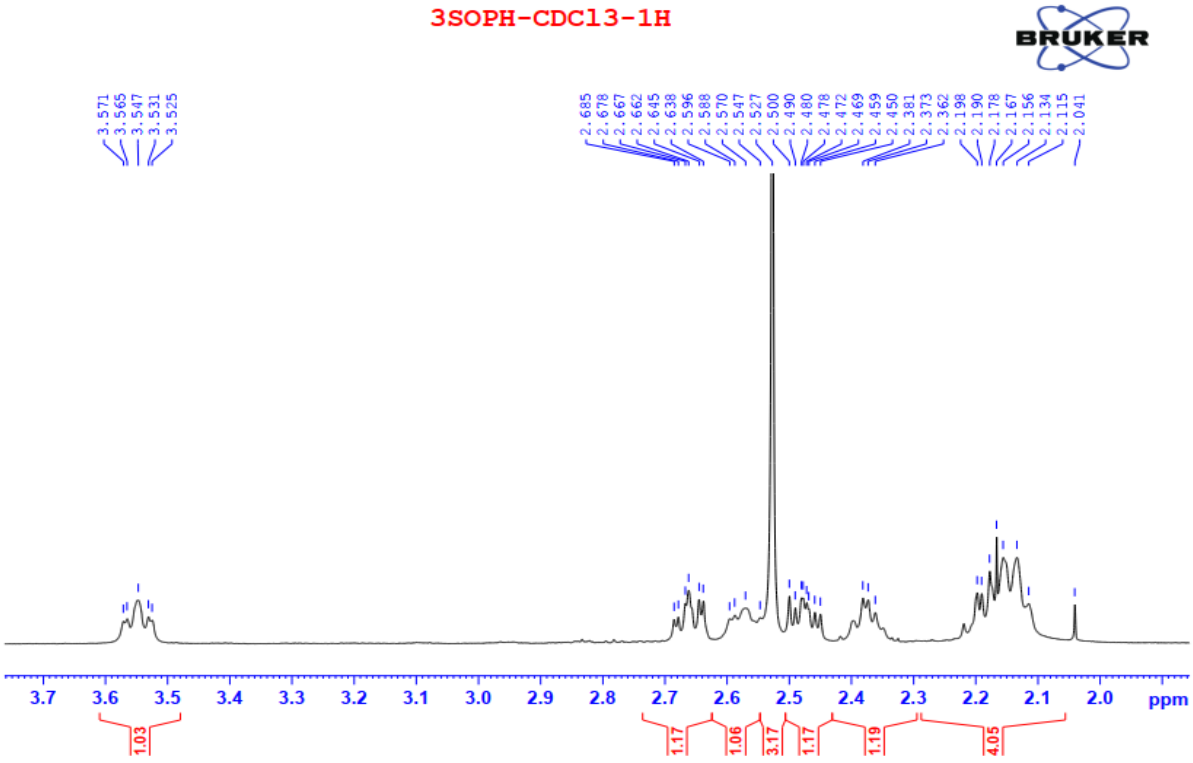

3SIBA
%T
3273.20
2956.87
2872.01
1654.92
1577.77
1508.33
1246.02
1085.92
758.02
cm-1

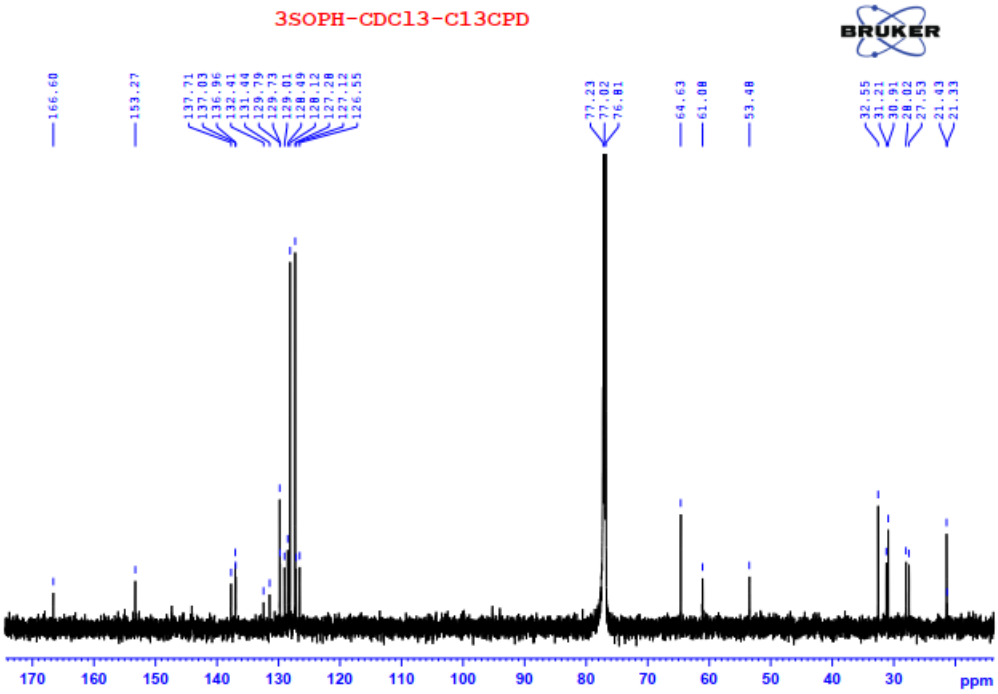
## 6.5. Spectra of compound 3e

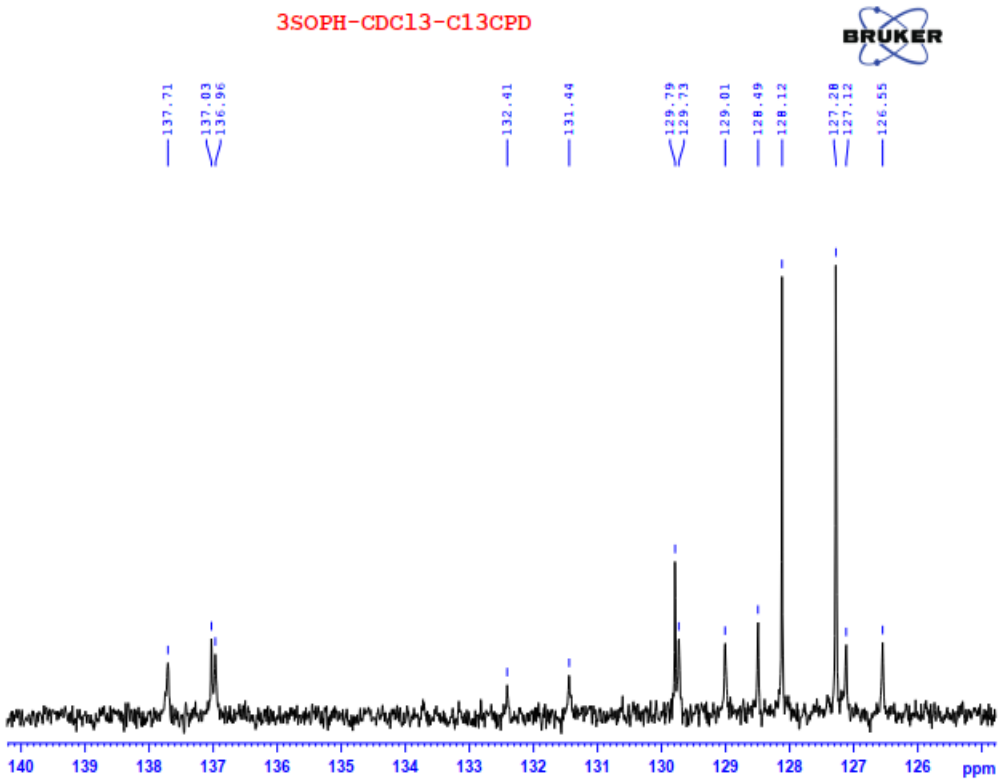


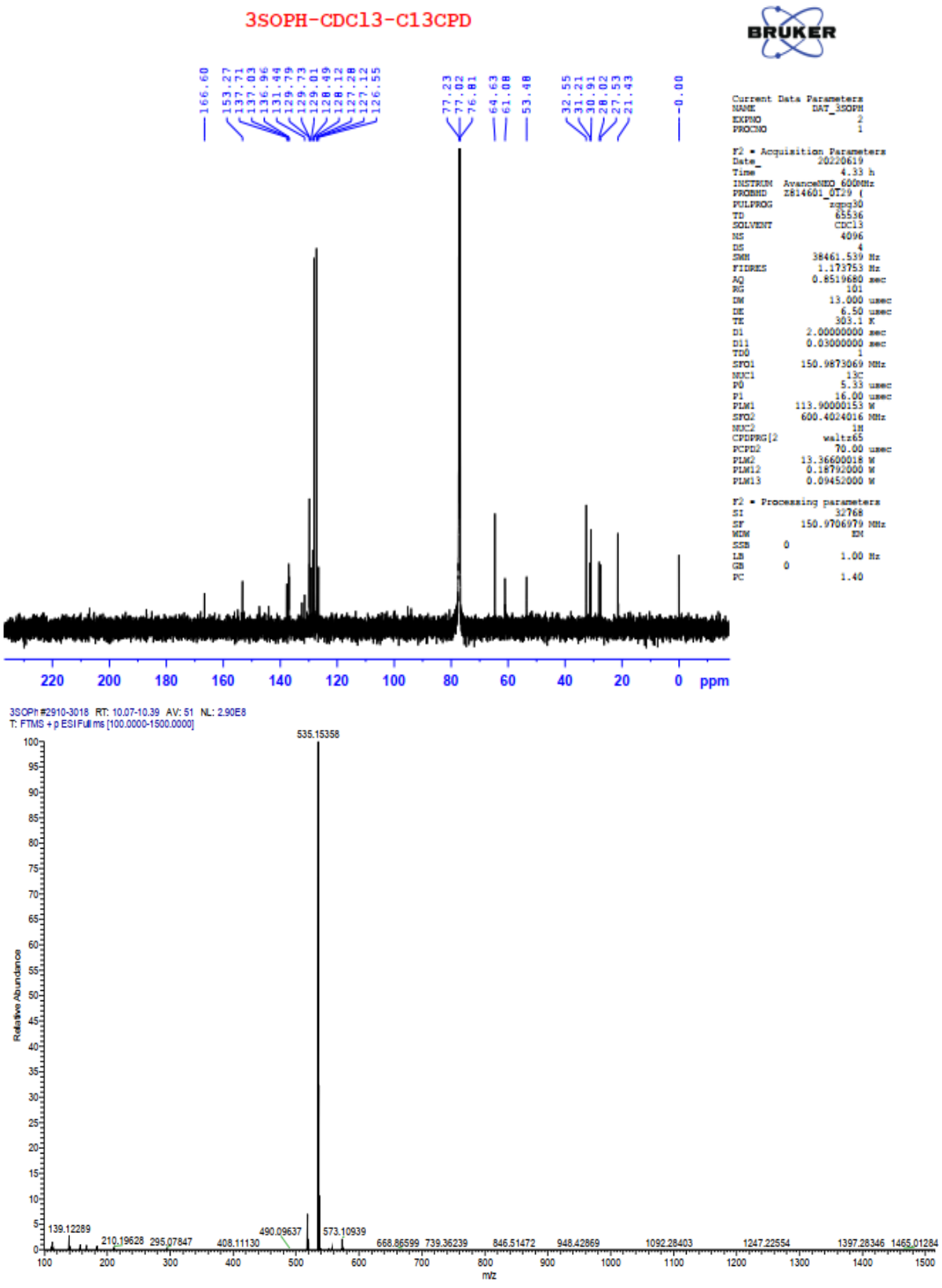



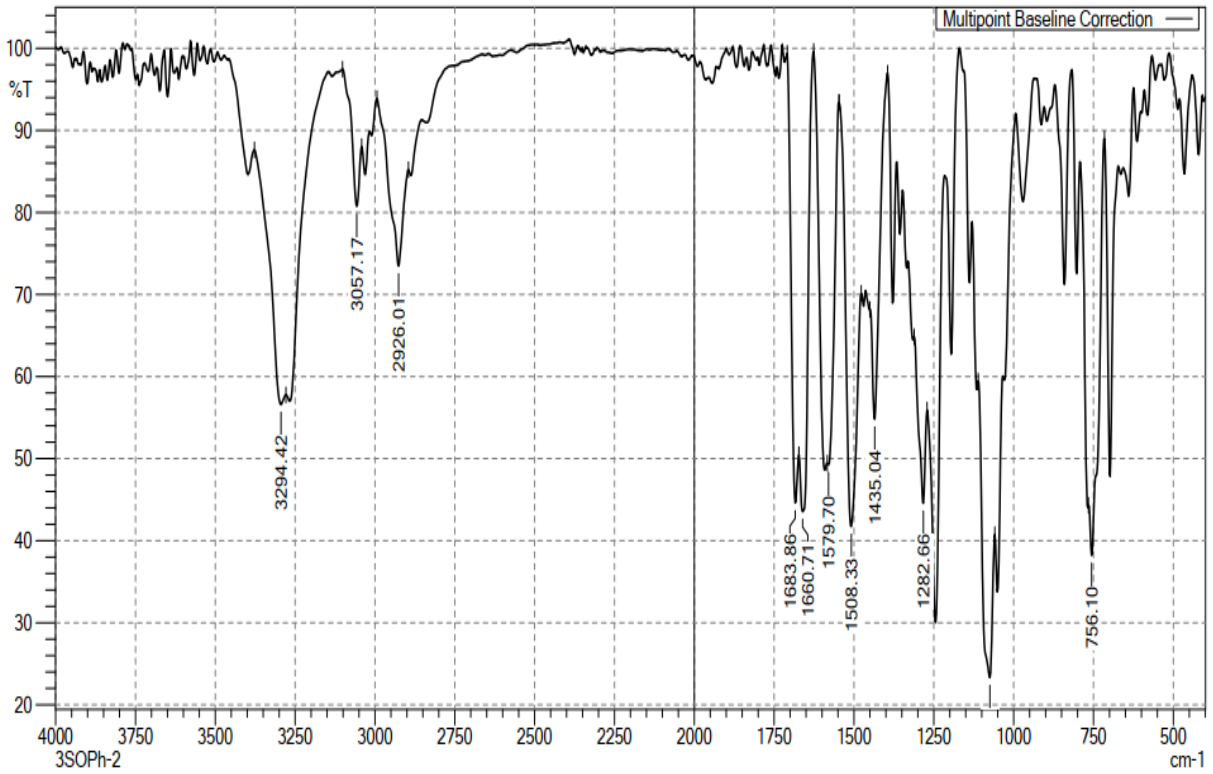

3SOPH-CDCl3-1H
BRUKER
3.571
3.565
3.547
3.531
3.525
2.685
2.678
2.667
2.662
2.645
2.638
2.596
2.588
2.570
2.547
2.527
2.500
2.490
2.480
2.478
2.472
2.469
2.459
2.450
2.381
2.373
2.362
2.198
2.190
2.178
2.167
2.156
2.134
2.115
2.041
3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 ppm
1.03
1.17
1.06
3.17
1.17
1.19
4.05


3SOPH-CDCl3-1H
BRUKER
3.571
3.565
3.547
3.531
3.525
2.685
2.678
2.667
2.662
2.645
2.638
2.596
2.588
2.570
2.547
2.527
2.500
2.490
2.480
2.478
2.472
2.469
2.459
2.450
2.381
2.373
2.362
2.198
2.190
2.178
2.167
2.156
2.134
2.115
2.041
3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 ppm
1.03
1.17
1.06
3.17
1.17
1.19
4.05


3SOPH-CDCl3-C13CPD
BRUKER
166.60
153.27
137.71
137.03
136.96
132.41
131.44
129.79
129.73
129.01
128.49
128.12
127.28
127.12
126.55
77.23
77.02
76.81
64.63
61.08
53.48
32.55
31.21
30.91
28.02
27.53
21.43
21.33
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm


3SOPH-CDCl3-C13CPD
BRUKER
137.71
137.03
136.96
132.41
131.44
129.79
129.73
129.01
128.49
128.12
127.28
127.12
126.55
140 139 138 137 136 135 134 133 132 131 130 129 128 127 126 ppm


3SOPH-CDCl3-C13CPD
166.60
153.27
137.71
137.03
136.96
131.44
129.79
129.73
129.01
128.49
128.12
127.28
127.12
126.55
77.23
77.02
76.81
64.63
61.08
53.48
32.55
31.21
30.91
28.02
27.53
21.43
0.00
Current Data Parameters
NAME DAT_3SOPH
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220619
Time 4.33 h
INSTRUM AvanceNEO_600MHz
PROBHD Z814601_0T29 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4096
DS 4
SWH 38461.539 Hz
FIDRES 1.173753 Hz
AQ 0.8519680 sec
RG 101
DW 13.000 usec
DE 6.50 usec
TE 303.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9873069 MHz
NUC1 13C
P0 5.33 usec
P1 16.00 usec
PLW1 113.90000153 W
SFO2 600.4024016 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 70.00 usec
PLW2 13.36600018 W
PLW12 0.16792000 W
PLW13 0.09452000 W
F2 - Processing parameters
SI 32768
SF 150.9706979 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
220
200
180
160
140
120
100
80
60
40
20
0
ppm
3SOPH #2910-3018 RT: 10.07-10.39 AV: 51 NL: 2.90E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]
535.15358
Relative Abundance
m/z
139.12289
210.19628
295.07847
408.11130
490.09637
573.10939
668.86599
739.36239
846.51472
948.42869
1092.28403
1247.22554
1397.28346
1465.01284


Multipoint Baseline Correction
100
%T
90
80
70
60
50
40
30
20
3294.42
3057.17
2926.01
1683.86
1660.71
1579.70
1508.33
1435.04
1282.66
756.10
4000
3750
3500
3250
3000
2750
2500
2250
2000
1750
1500
1250
1000
750
500
cm-1
3SOPh-2