Supporting Information

Investigating Triorthogonal Chemoselectivity. Effect of Azide Substitution on the Triazine Core

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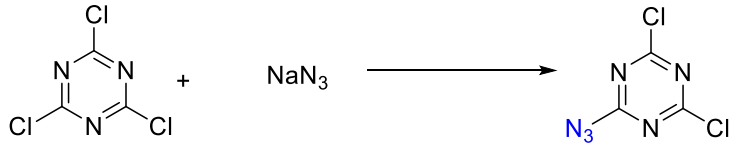
1. General Information

All the chemicals and diisopropylethylamine were purchased from Sigma-Aldrich (Sigma-Aldrich, Germany). The solvents used were of analytical and HPLC reagent grade. Magnetic resonance spectra (^{1}H and ^{13}C) were recorded with Bruker 400 MHz, and chemical shift values are reported in δ units (ppm) using TMS as internal standard. Follow-up of the reactions and checks of the purity of the compound were done by TLC on silica-gel-protected aluminum sheets 60 F254 (Merck), and the spots were detected by exposure to UV light at λ = 254 nm. Analytical HPLC was performed on an Agilent 1100 system using a Phenomenax C18 column (3µm, 4.6×50 mm) by dissolving the sample in CH_3CN only. Chemstation software was used for data processing. Buffer A: 0.1% TFA in H_2O, buffer B: 0.1% TFA in CH_3CN were used in HPLC. High resolution mass spectrometry (HRMS) was performed using a Bruker ESI-QTOF mass spectrometer in positive-ion mode.

2. General procedure for synthesis of mono substituted triazine (m-TA) derivatives

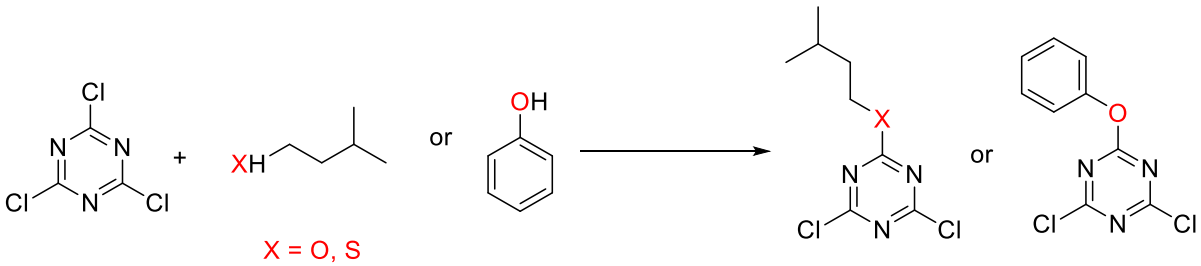
2.1. Synthesis of 2-azido-4,6-dichloro-1,3,5-triazine (2)



The procedure for the synthesis of N_3-TA was modified from the previous published procedures to safely optimize its synthesis at lab scale. 27.3 mmol of s-triazine (TA) was dissolved in 100 mL acetone and cooled to 0ºC. Sodium azide (27.3 mmol) was dissolved in water (50 mL) and was also cooled to 0ºC. A solution of sodium azide was added dropwise to a vigorously stirred solution of TA. The reaction was stirred at 0ºC for 30 min, after which acetone was removed under vacuum under ice cold conditions. After complete removal of acetone, the remaining water layer was extracted using cold DCM (3 x 50 mL). EtOAc can also be used but is slightly slower in separation in separatory funnel. Another disadvantage associated with EtOAc is the removal to obtain crude (EtOAc takes longer time compared to DCM). The organic layer was collected, dried over $MgSO_4$, filtered and concentrated under cold conditions (to avoid explosion due to friction) to afford almost pure TA-N_3. This compound was further purified using silica gel column chromatography and *n*-hexane as mobile phase, affording 4.7 g (90.4%) of pure product, which was confirmed by ^{13}C NMR.

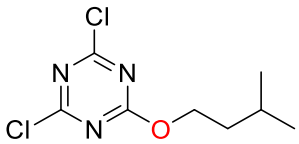
Off white solid: HPLC [30-95 % of CH_3CN (0.1% TFA/ H_2O (0.1 %TFA) over 15 mins] t_R = 3.59 min; IR: 2101-2167 cm^{-1}; ^{13}C NMR (100 MHz, $CDCl_3$): 170.4, 171.6.

2.2. Synthesis of mono nucleophilic substituted derivatives



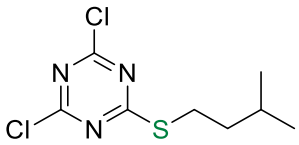
TCT (1 g, 5.4 mmol) was dissolved in DCM (5 mL) and cooled to 0 ºC for 5 min. Nucleophile (5.4 mmol) was then added to the above stirring solution, followed by addition of DIEA (945 µL, 5.4 mmol). The reaction was stirred at 0 ºC (-20 ºC in case of phenol) for 30 min. The progress of the reaction was monitored by TLC (EtOAc/hexane as mobile phase) until no starting material was observed. The solution washed several times with water to remove DIEA salts. The organic layer was collected, dried over $MgSO_4$, filtered and concentrated to afford pure product which was used for the next step without further purification.

2.3. 2,4-dichloro-6-(isopentyloxy)-1,3,5-triazine (3)



Yield = 1.32 g (96.3%); Off-white semi-solid; HPLC [30-95 % of CH_3CN (0.1% TFA/ H_2O (0.1 %TFA) over 15 mins] t_R = 8.44 min; ^1H NMR (400 MHz, $CDCl_3$): 0.99 (d, J = 6.7 Hz, -CH_3), 1.74 (m, -CH_2), 1.83 (m, CH), 4.6 (m, -CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): 22.2, 24.6, 36.8, 69.0, 170.9, 172.3. HRMS: m/z: calcd. for $C_8H_{11}Cl_2N_3O$: 236.0428 $[M+H]^+$; found: 236.0457.

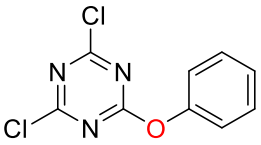
2.4. 2,4-dichloro-6-(isopentylthio)-1,3,5-triazine (4)



Yield = 1.33 g (98.1%); Pale yellow oil; HPLC [30-95 % of CH_3CN (0.1% TFA/ H_2O (0.1 %TFA) over 15 mins] t_R = 10.24 min; ^1H NMR (400 MHz, $CDCl_3$): 0.90 (d, J = 6.5 Hz, -CH_3), 1.55 (m, -CH_2), 1.65 (m, -CH), 3.1 (t, J = 6.3 Hz, -CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): 21.2,

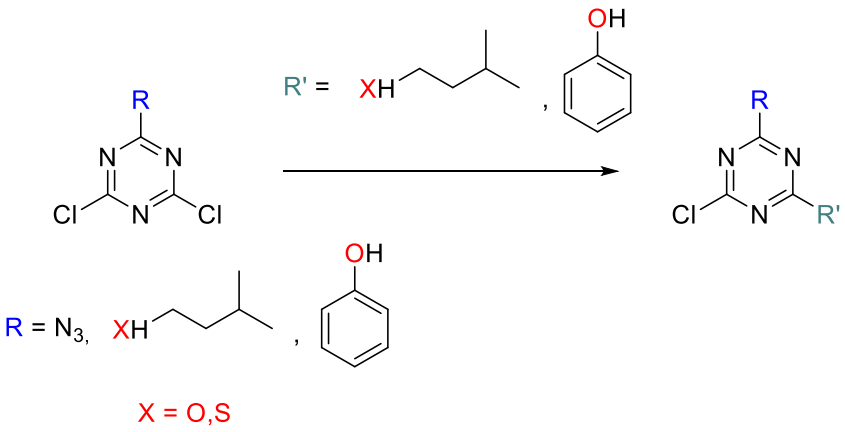
26.5, 28.3, 36.2, 168.9, 185.6. HRMS: m/z: calcd. for $C_8H_{11}Cl_2N_3S$: 252.0251 $[M+H]^+$; found: 252.0246.

2.5. 2,4-dichloro-6-phenoxy-1,3,5-triazine (5)



Yield = 1.28 g (92.6%); Off-white solid; HPLC [30-95 % of CH_3CN (0.1% TFA/ H_2O (0.1 %TFA) over 15 mins] t_R = 6.33 min; ^1H NMR (400 MHz, $CDCl_3$): 7.10 (d, *J* = 1.6 Hz, -CH), 7.30 (t, *J* = 1.6 Hz, -CH), 7.40 (t, *J* = 2.0 Hz, -CH); ^{13}C NMR (100 MHz, $CDCl_3$): 120.0, 125.7, 128.7, 150.7, 170.0, 172.0. HRMS: m/z: calcd. for $C_9H_5Cl_2N_3O$: 241.0904 $[M+H]^+$; found: 241.0886.

3. General procedure for synthesis of dichloro substituted TA (d-TA) derivatives



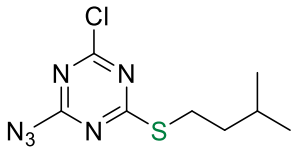
Second substitution in case of mono-azide triazine derivative

TA-N_3 (500 mg, 2.6 mmol) was dissolved in DCM (3 mL) and cooled to 0 ºC for 5 min. Nucleophile (2.6 mmol) was then added to the above stirring solution, followed by addition of DIEA (453 µL, 2.6 mmol). The reaction was stirred at 0 ºC (-20 ºC in case of phenol) for 30 min. The progress of the reaction was monitored by TLC (EtOAc/hexane as mobile phase) until no starting material was observed. The solution washed several times with water to remove DIEA salts. The organic layer was collected, dried over $MgSO_4$, filtered and concentrated to afford pure product which was used for the next step without further purification.

Second substitution in case of m-TA derivatives

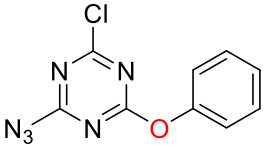
Nucleophile/sodium azide (0.27 mmol) was added to m-TA (0.27 mmol) in DCM (1 mL), followed by addition of DIEA (47 µL, 0.27 mmol). The reaction was stirred at room temperature for 3 h (30 mins at 0 ºC in case of azide and overnight for alcohol). The progress of the reaction was monitored by TLC (EtOAc/hexane as mobile phase) until no starting material was observed. The solution was concentrated to dryness and the residue was dissolved in DCM and washed several times with water to remove DIEA salts. The organic layer was collected, dried over $MgSO_4$, filtered and concentrated to afford pure product, which was used for the next step without further purification.

3.1. 2-azido-4-chloro-6-(isopentylthio)-1,3,5-triazine (6)



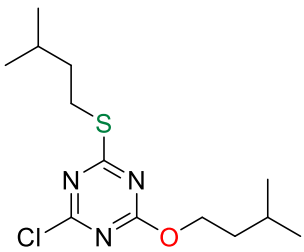
Yield = 648 mg (96.5%); Pale yellow liquid; HPLC [30-95 % of CH_3CN (0.1% TFA/ H_2O (0.1 %TFA) over 15 mins] t_R = 10.02 min; ^{1}H NMR (400 MHz, $CDCl_3$): 0.96 (d, J = 6.6 Hz, -CH_3), 1.62 (m, -CH_2), 1.73 (m, -CH), 3.15 (m, -CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): 22.2, 27.5, 29.0, 37.5, 170.4, 182.9, 186.1. HRMS: m/z: calcd. for $C_8H_{11}ClN_6S$: 259.0527 $[M+H]^+$; found: 259.0568.

3.2. 2-azido-4-chloro-6-phenoxy-1,3,5-triazine (7)



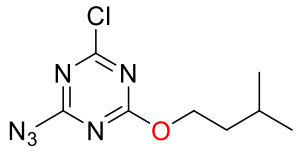
Yield = 618 mg (95.8%); Off white solid; HPLC [30-95 % of CH_3CN (0.1% TFA/ H_2O (0.1 %TFA) over 15 mins] t_R = 6.19 min; ^{1}H NMR (400 MHz, $CDCl_3$): 7.17 (d, J = 8.0 Hz, -CH), 7.30 (t, J = 7.6 Hz, -CH), 7.4 (t, J = 8.0 Hz, -CH); ^{13}C NMR (100 MHz, $CDCl_3$): 121.2, 126.7, 129,8 151.2, 171.7, 172.2, 173.4. HRMS: m/z: calcd. for $C_9H_5ClN_6O$: 249.0684 $[M+H]^+$; found: 249.0693.

3.3. 2-chloro-4-(isopentyloxy)-6-(isopentylthio)-1,3,5-triazine (8)



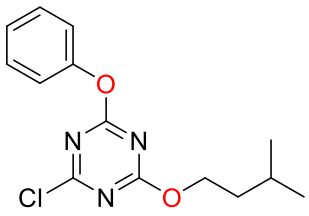
Yield = 76 mg (92.6%); Gummy; HPLC [30-95 % of CH_3CN (0.1% TFA/ H_2O (0.1 %TFA) over 15 mins] t_R = 13.10 min; ^1H NMR (400 MHz, $CDCl_3$): 0.95 (d, J = 6.6 Hz, -CH_3), 1.60 (m, -CH_2), 1.71 (m, -CH), 3.13 (m, -CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): 22.2, 22.4, 24.8, 27.5, 28.4, 37.3, 37.9, 66.5, 167.6, 169.3, 182.4. HRMS: m/z: calcd. for $C_{13}H_{22}ClN_3OS$: 304.1422 $[M+H]^+$; found: 304.1430.

*3.4. 2-azido-4-chloro-6-(isopentyloxy)-1,3,5-triazine (*9)



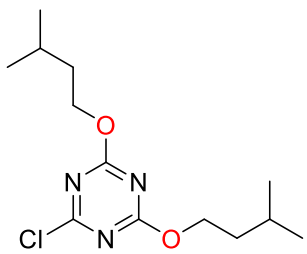
Yield = 63 mg (96.3%); Gummy; HPLC [30-95 % of CH_3CN (0.1% TFA/ H_2O (0.1 %TFA) over 15 mins] t_R = 8.23 min; ^1H NMR (400 MHz, $CDCl_3$): 0.96 (d, J = 6.6 Hz, -CH_3), 1.69 (m, -CH_2), 1.80 (m, -CH), 4.48 (m, -CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): 22.4, 24.7, 31.1, 68.5, 172.0, 172.3, 172.8. LCMS (m/z): 294.21 [M+H]. HRMS: m/z: calcd. for $C_8H_{11}ClN_6O$: 243.0756 $[M+H]^+$; found: 243.0786.

3.5. 2-chloro-4-(isopentyloxy)-6-phenoxy-1,3,5-triazine (10)



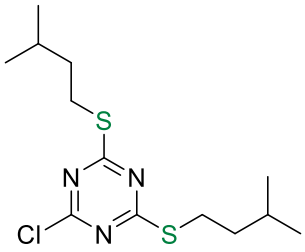
Yield = 70 mg (88.9%); Gummy; ^1H NMR (400 MHz, $CDCl_3$): 0.91 (d, J = 6.6 Hz, -CH_3), 1.62 (m, -CH_2), 1.72 (m, -CH), 4.39 (m, -CH_2), 7.17 (d, J = 8.2 Hz, -CH), 7.28 (m, -CH), 7.4 (m, -CH); ^{13}C NMR (100 MHz, $CDCl_3$): 22.4, 24.7, 36.9, 68.3, 121.3, 126.4, 129.7, 151.5, 172.2, 172.4, 173.2. LCMS (m/z): 294.16 [M+H]. HRMS: m/z: calcd. for $C_{14}H_{16}ClN_3O_2$: 294.1076 $[M+H]^+$; found: 294.1063.

3.6. 2-chloro-4,6-bis(isopentyloxy)-1,3,5-triazine (11)



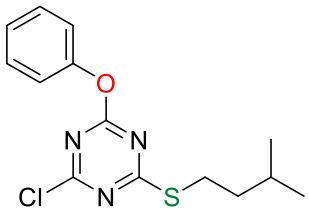
Yield = 75 mg (96.3%); Off white solid; ^1H NMR (400 MHz, $CDCl_3$): 0.96 (d, J = 6.6 Hz, -CH_3), 1.69 (m, -CH_2), 1.81 (m, -CH), 4.50 (m, -CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): 22.4, 24.7, 37.1, 67.9, 172.1, 172.5. HRMS: m/z: calcd. for $C_{13}H_{22}ClN_3O_2$: 288.1473 $[M+H]^+$; found: 288.1501.

3.7. 2-chloro-4,6-bis(isopentylthio)-1,3,5-triazine (12)



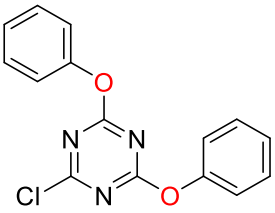
Yield = 80 mg (93.0%); Gummy; ^{1}H NMR (400 MHz, $CDCl_3$): 0.94 (d, *J* = 6.7 Hz, -CH_3), 1.59 (m, -CH_2), 1.72 (m, -CH), 3.10 (m, -CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): 22.3, 27.5, 28.3, 37.9, 179.5, 182.9. HRMS: m/z: calcd. for $C_{13}H_{22}ClN_3S_2$: 320.1039 $[M+H]^+$; found: 320.1027.

3.8. 2-chloro-4-(isopentylthio)-6-phenoxy-1,3,5-triazine (13)



Yield = 81 mg (96.3%); Gummy; ^{1}H NMR (400 MHz, $CDCl_3$): 0.87 (d, *J* = 6.5 Hz, -CH_3), 1.50 (m, -CH_2), 1.60 (m, -CH), 2.99 (m, -CH_2), 7.15 (m, -CH), 7.27 (m, -CH), 7.41 (m, -CH); ^{13}C NMR (100 MHz, $CDCl_3$): 21.1, 26.4, 27.7, 36.9, 120.5, 124.9, 128.4, 150.7, 169.9, 172.6, 185.6.

3.9. 2-chloro-4,6-diphenoxy-1,3,5-triazine (14)



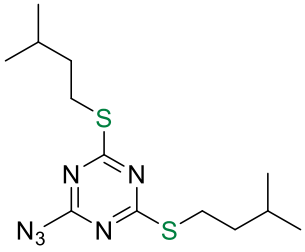
Yield = 75 mg (92.6%); Gummy; ^{1}H NMR (400 MHz, $CDCl_3$): 7.14 (d, *J* = 8.1 Hz, -CH_3), 7.27 (m, -CH), 7.39 (m, -CH); ^{13}C NMR (100 MHz, $CDCl_3$): 121.2, 126.5, 129.7, 151.3, 172.4, 173.7. HRMS: m/z: calcd. for $C_{15}H_{10}ClN_3O_2$: 300.0534 $[M+H]^+$; found: 300.0557.

4. Synthesis of tri-substituted s-triazine from above precursors

To a stirring solution of d-TA (50 mg, 0.26 mmol) in DCM (0.5 mL), nucleophile (0.26 mmol) was added, followed by addition of DIEA (45 µL, 0.26 mmol). The reaction was stirred at room temperature (40 ºC in case of alcohol as substituent) for 12 h. The progress of the reaction was monitored by TLC (EtOAc/hexane as mobile phase) until no starting

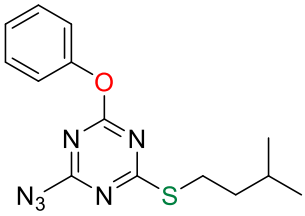
material was observed. The solution washed several times with water to remove DIEA salts. The organic layer was collected, dried over $MgSO_4$, filtered and concentrated to afford pure product.

4.1. 2-azido-4,6-bis(isopentylthio)-1,3,5-triazine (15)



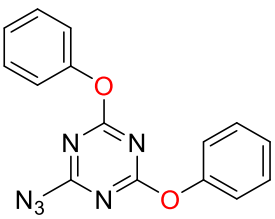
Yield = 75 mg (88.5%); Gummy; HPLC [30-95 % of CH_3CN (0.1% TFA/ H_2O (0.1 %TFA) over 15 mins] t_R = 9.79 min; ^1H NMR (400 MHz, $CDCl_3$): 0.87 (d, J = 6.6 Hz, -CH_3), 1.52 (m, -CH_2), 1.65 (m, -CH), 3.03 (m, -CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): 21.2, 26.5, 27.3, 36.9, 178.5, 178.6.

4.2. 2-azido-4-(isopentylthio)-6-phenoxy-1,3,5-triazine (16)



Yield = 76 mg (93.3%); Gummy; HPLC [30-95 % of CH_3CN (0.1% TFA/ H_2O (0.1 %TFA) over 15 mins] t_R = 11.17 min; ^1H NMR (400 MHz, $CDCl_3$): 0.85 (d, J = 6.2 Hz, -CH_3), 1.49 (m, -CH_2), 1.56 (m, -CH), 2.98 (m, -CH_2), 7.15 (d, J = 7.9 Hz, -CH), 7.26 (m, -CH), 7.39 (m, -CH); ^{13}C NMR (100 MHz, $CDCl_3$): 22.1, 27.5, 28.7, 37.9, 121.5, 126.1, 129.5, 151.6, 170.2, 183.3, 186.3. HRMS: m/z: calcd. for $C_{14}H_{16}N_6OS$: 317.1179 $[M+H]^+$; found: 317.1171.

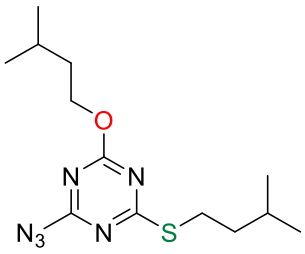
4.3. 2-azido-4,6-diphenoxy-1,3,5-triazine (17)



Yield = 71 mg (88.5%); Off white semi solid; HPLC [30-95 % of CH_3CN (0.1% TFA/ H_2O (0.1 %TFA) over 15 mins] t_R = 8.05 min; ^1H NMR (400 MHz, $CDCl_3$): 7.14 (d, J = 8.3 Hz, -

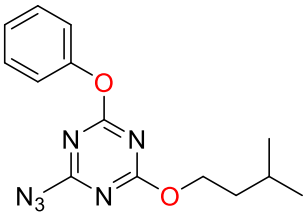
CH_3), 7.25 (m, -CH), 7.36 (m, -CH); ^{13}C NMR (100 MHz, $CDCl_3$): 121.4, 126.3, 129.5, 151.5, 173.1. HRMS: m/z: calcd. for $C_{15}H_{10}N_6O_2$: 307.0978 $[M+H]^+$; found: 307.0968.

4.4. *2-azido-4-(isopentyloxy)-6-(isopentylthio)-1,3,5-triazine* (18)



Yield = 68 mg (84.6%); Gummy; HPLC [30-95 % of CH_3CN (0.1% TFA/ H_2O (0.1 %TFA) over 15 mins] t_R = 13.05 min; ^1H NMR (400 MHz, $CDCl_3$): 0.95 (m, -CH_3), 1.63 (m, -CH_2), 1.76 (m, -CH), 3.14 (m, -CH_2), 4.42 (m, -CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): 22.2, 22.3, 22.5 24.8, 28.7, 37.3, 37.9, 67.3, 170.1, 182.5, 185.5. HRMS: m/z: calcd. for $C_{13}H_{22}N_6OS$: 311.1853 $[M+H]^+$; found: 311.1846.

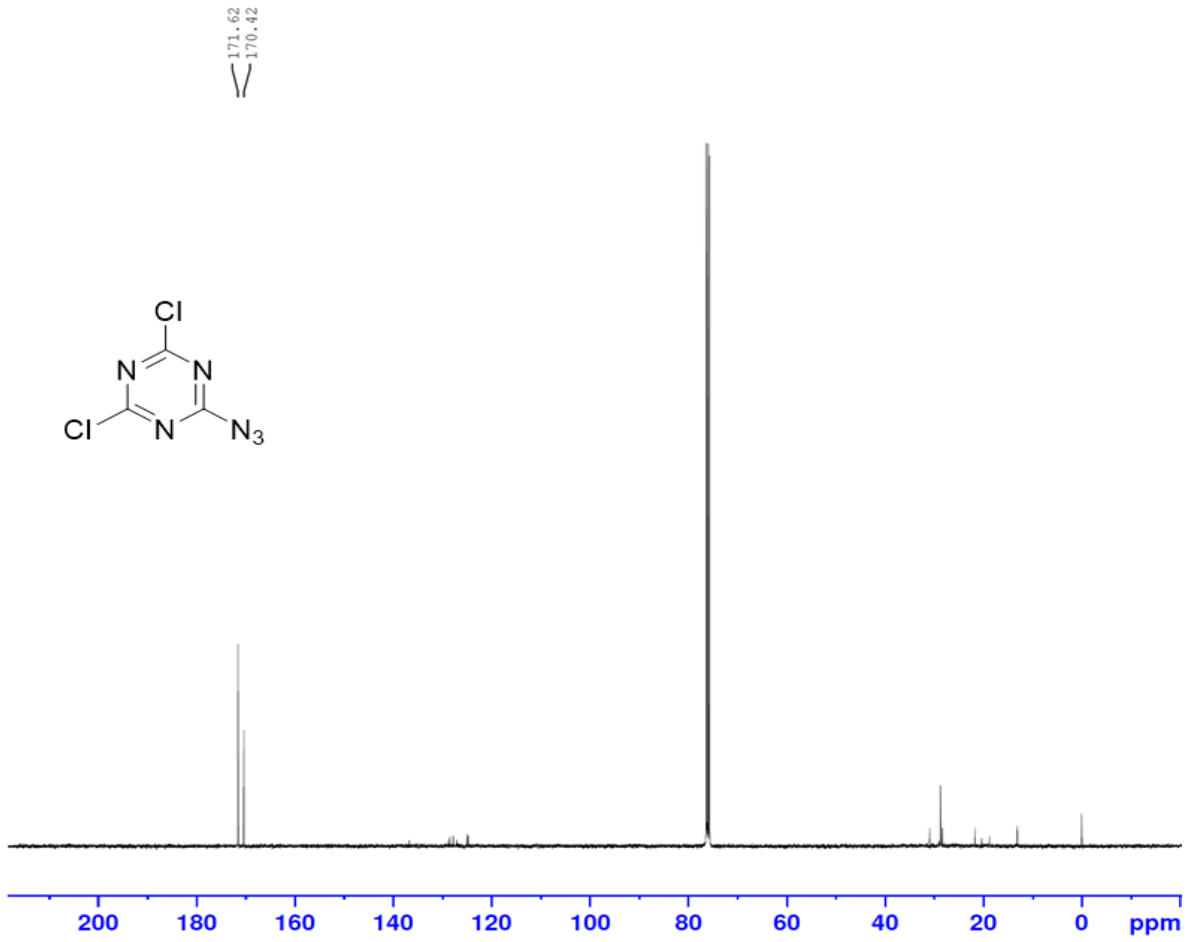
4.5. *2-azido-4-(isopentyloxy)-6-phenoxy-1,3,5-triazine* (19)

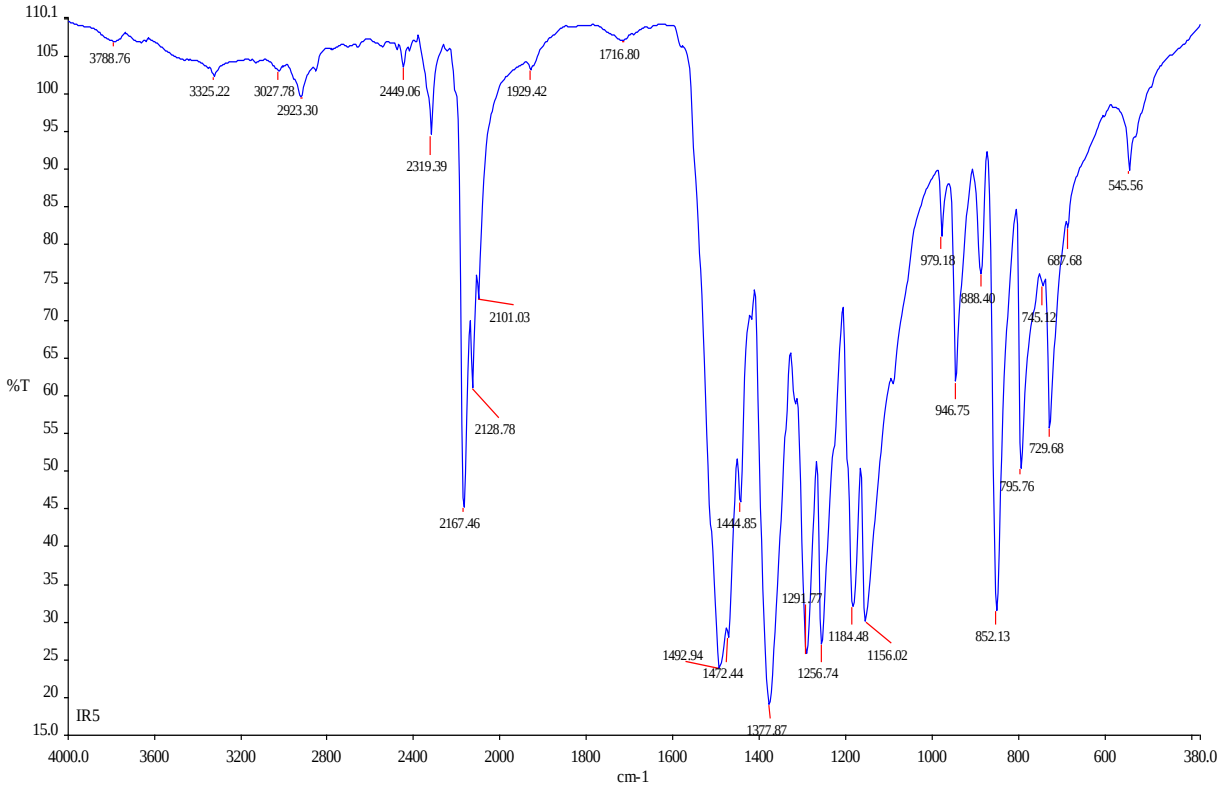


Yield = 72 mg (92.3%); Gummy; HPLC [30-95 % of CH_3CN (0.1% TFA/ H_2O (0.1 %TFA) over 15 mins] t_R = 9.72 min; ^1H NMR (400 MHz, $CDCl_3$): 0.91 (d, J = 6.6 Hz, -CH_3), 1.62 (m, -CH_2), 1.73 (m, -CH), 4.38 (t, J = 6.8 Hz, -CH_2), 7.17 (d, J = 8.4 Hz, -CH), 7.26 (m, -CH), 7.40 (m, -CH); ^{13}C NMR (100 MHz, $CDCl_3$): 22.4, 24.8, 37.1, 67.7, 121.5, 126.1, 129.5, 151.6, 172.6, 172.9, 173.1. HRMS: m/z: calcd. for $C_{14}H_{16}N_6O_2$: 301.1408 $[M+H]^+$; found: 301.1431.

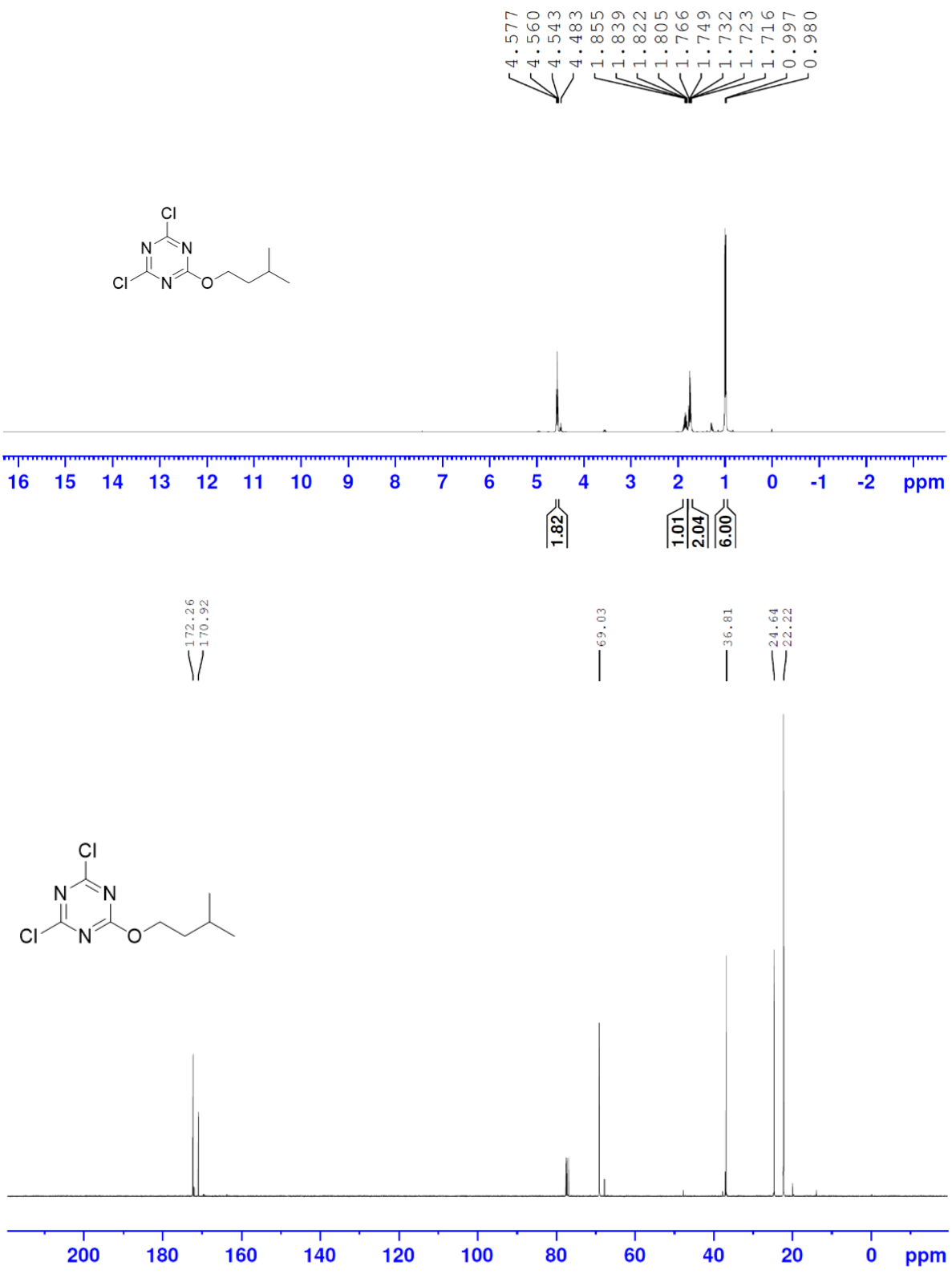
5. Characterization

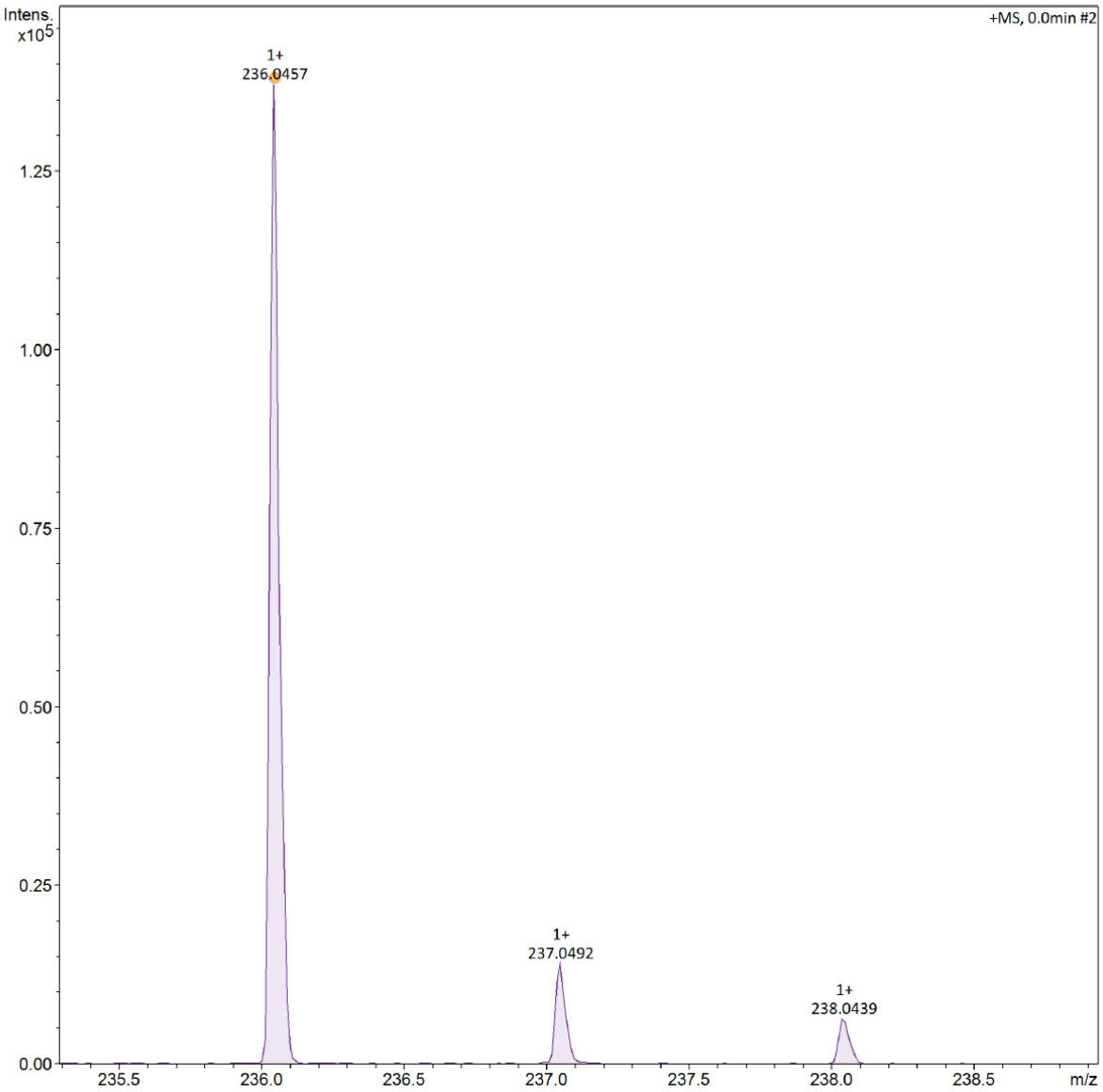
5.1. Characterization of *2-azido-4,6-dichloro-1,3,5-triazine* (2)


171.62
170.42
Cl
N
N
Cl
N
N3
200
180
160
140
120
100
80
60
40
20
0
ppm

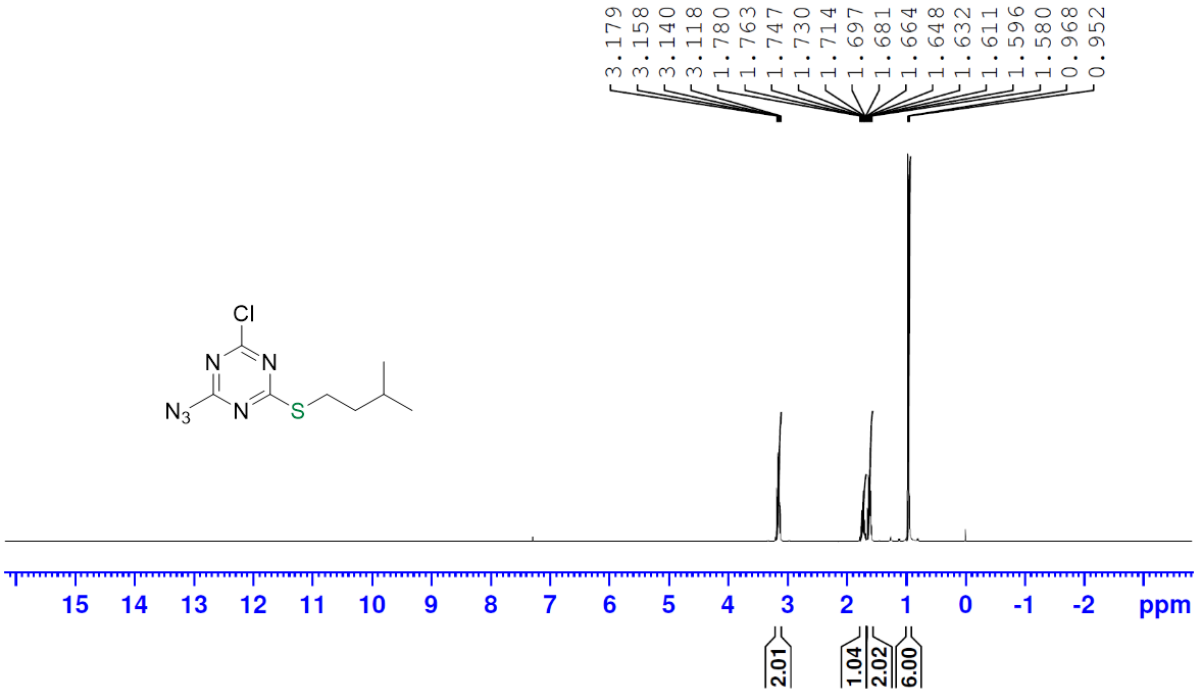

%T
cm-1
IR5
3788.76
3325.22
3027.78
2923.30
2449.06
2319.39
2167.46
2128.78
2101.03
1929.42
1716.80
1492.94
1472.44
1444.85
1377.87
1291.77
1256.74
1184.48
1156.02
979.18
946.75
888.40
852.13
795.76
745.12
729.68
687.68
545.56

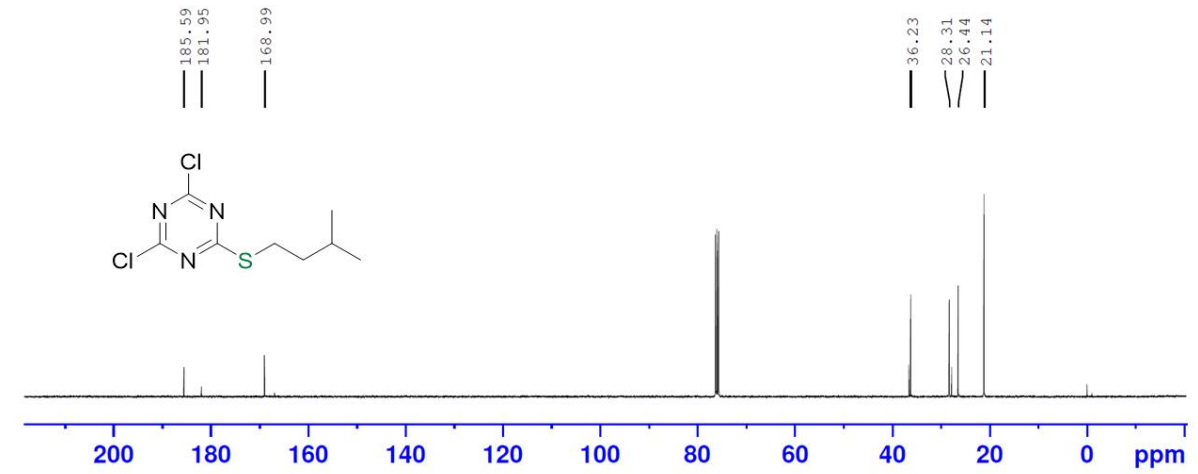
5.2. Characterization of *2,4-dichloro-6-(isopentyloxy)-1,3,5-triazine* (3)

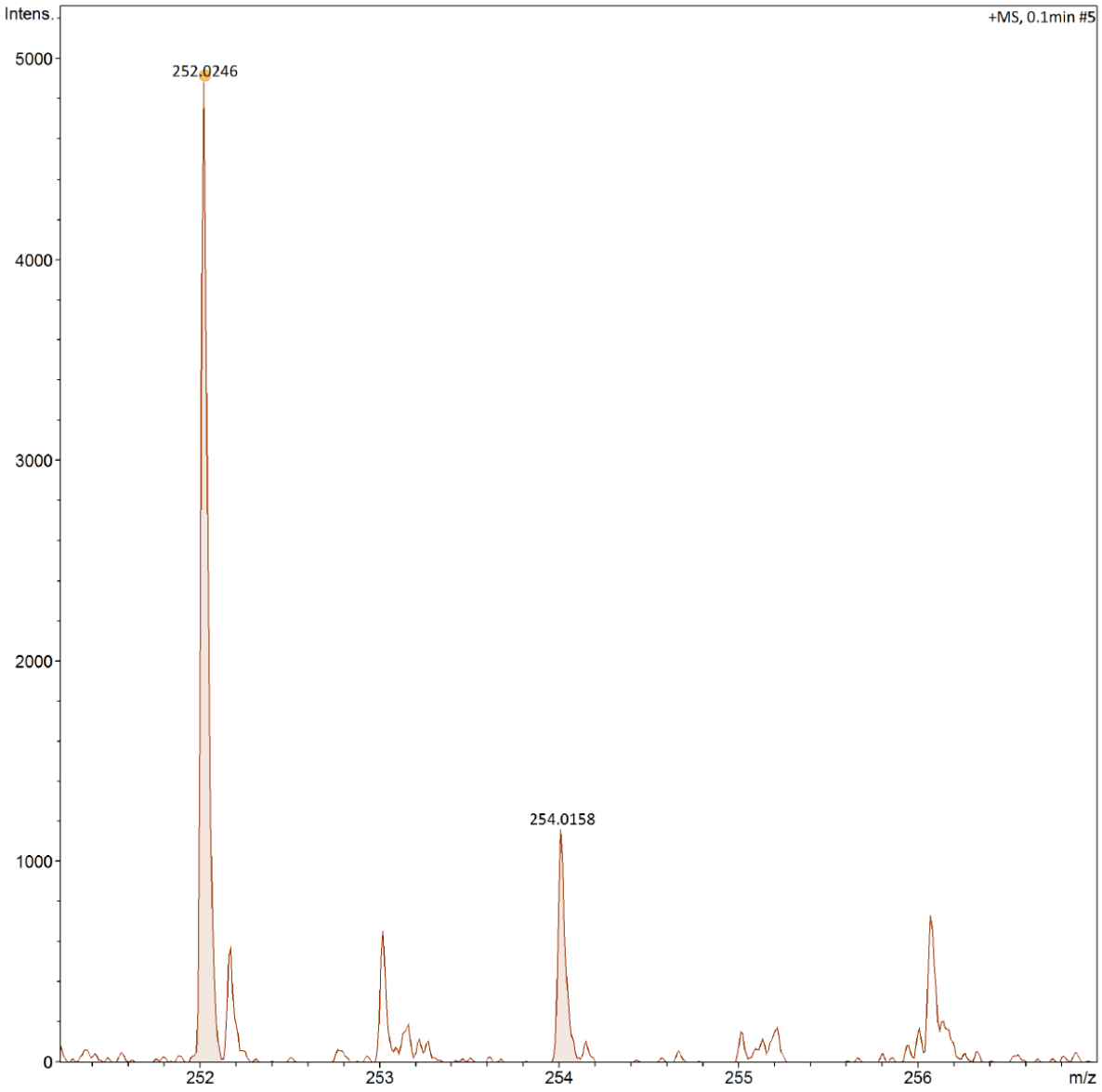




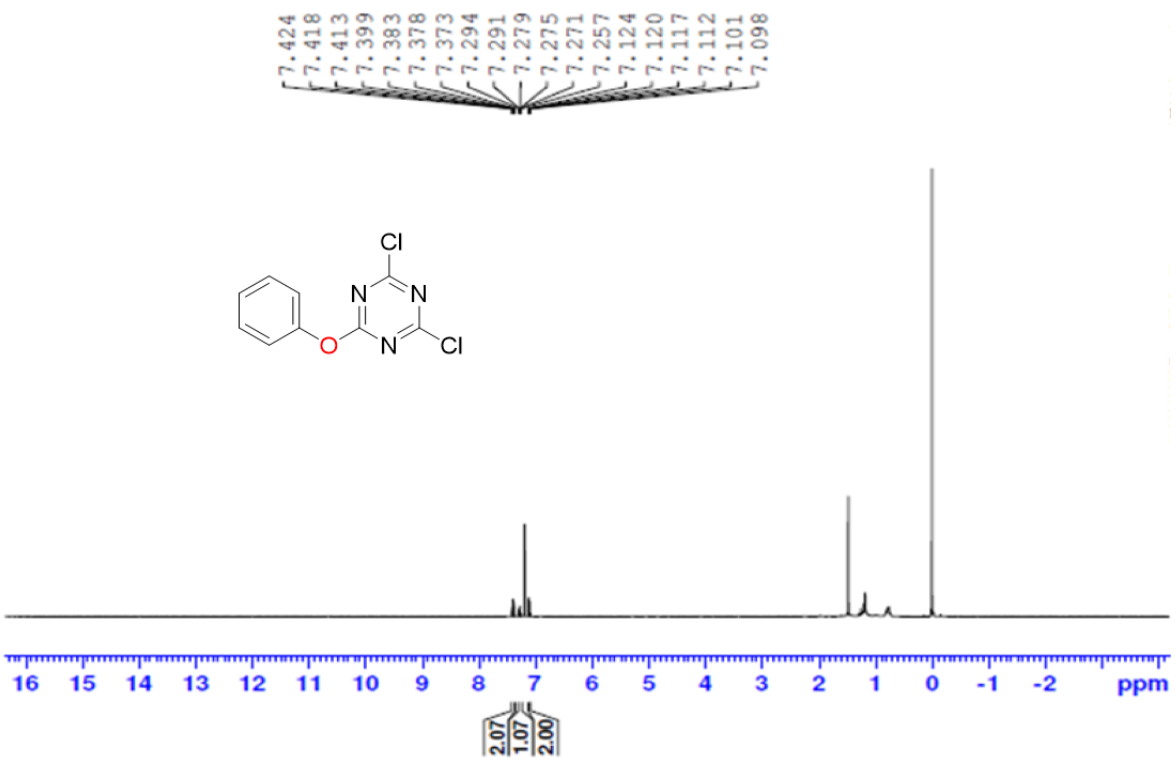
5.3. Characterization of *2,4-dichloro-6-(isopentylthio)-1,3,5-triazine* (4)

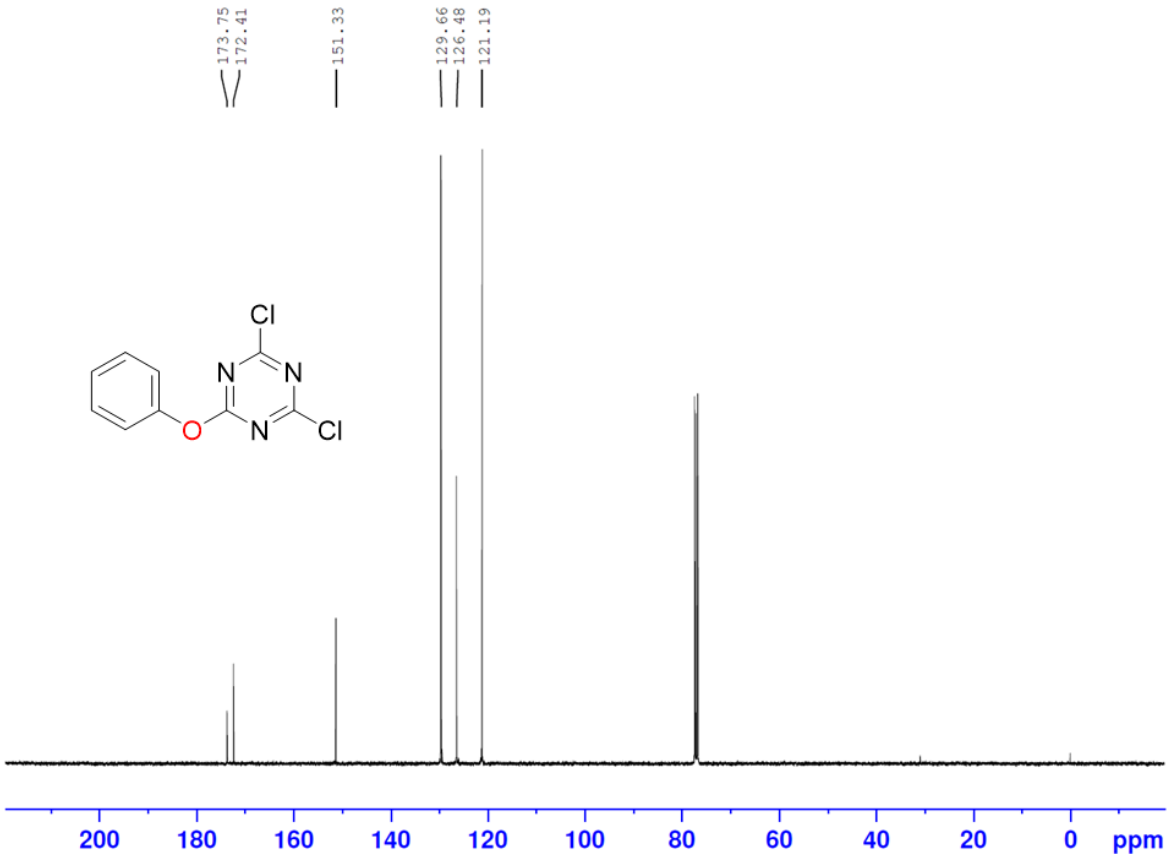

3.179
3.158
3.140
3.118
1.780
1.763
1.747
1.730
1.714
1.697
1.681
1.664
1.648
1.632
1.611
1.596
1.580
0.968
0.952
Cl
N
N
N3
N
S
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
2.01
1.04
2.02
6.00

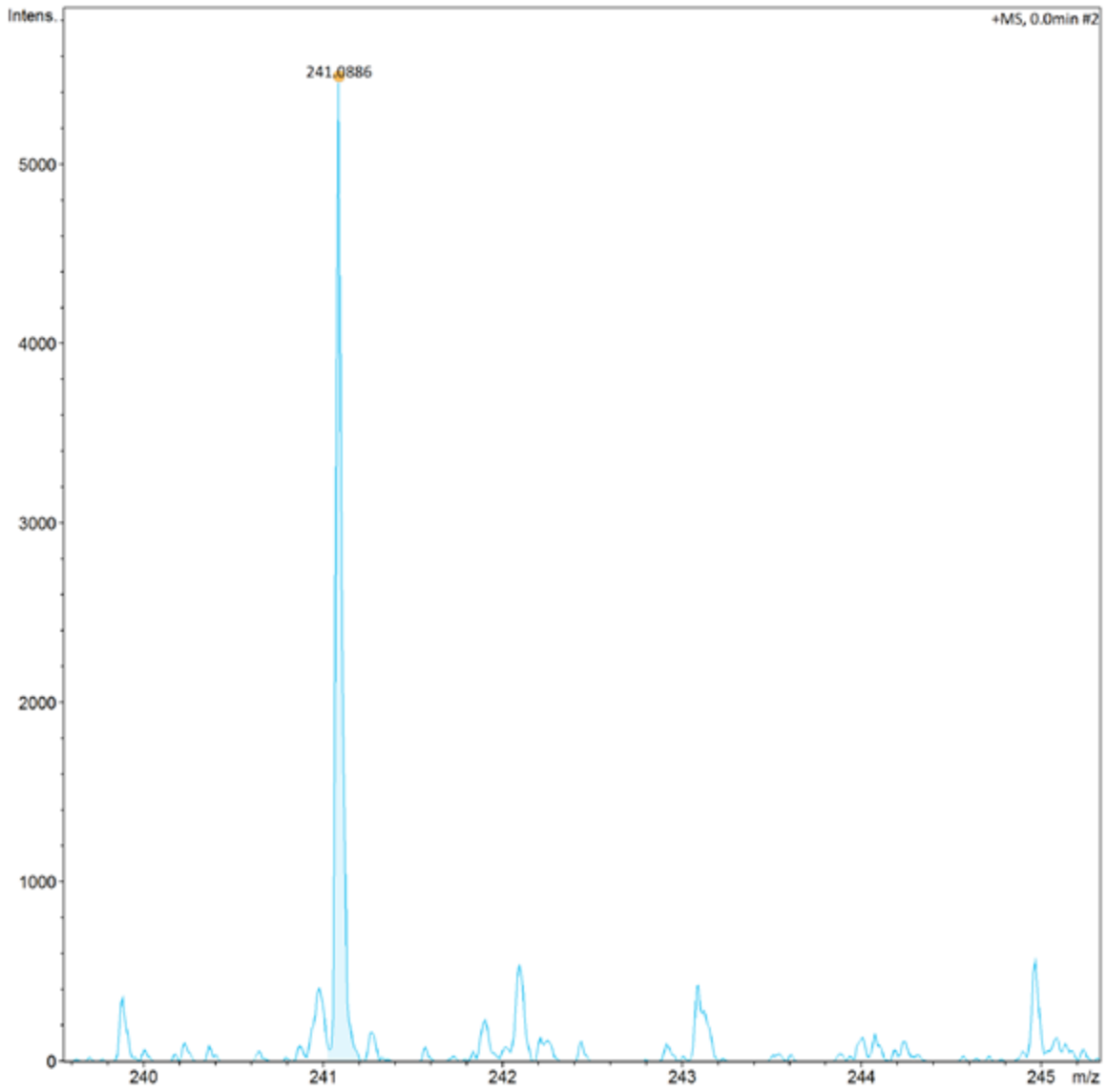

185.59
181.95
168.99
36.23
28.31
26.44
21.14
Cl
N
N
Cl
N
S
200 180 160 140 120 100 80 60 40 20 0 ppm



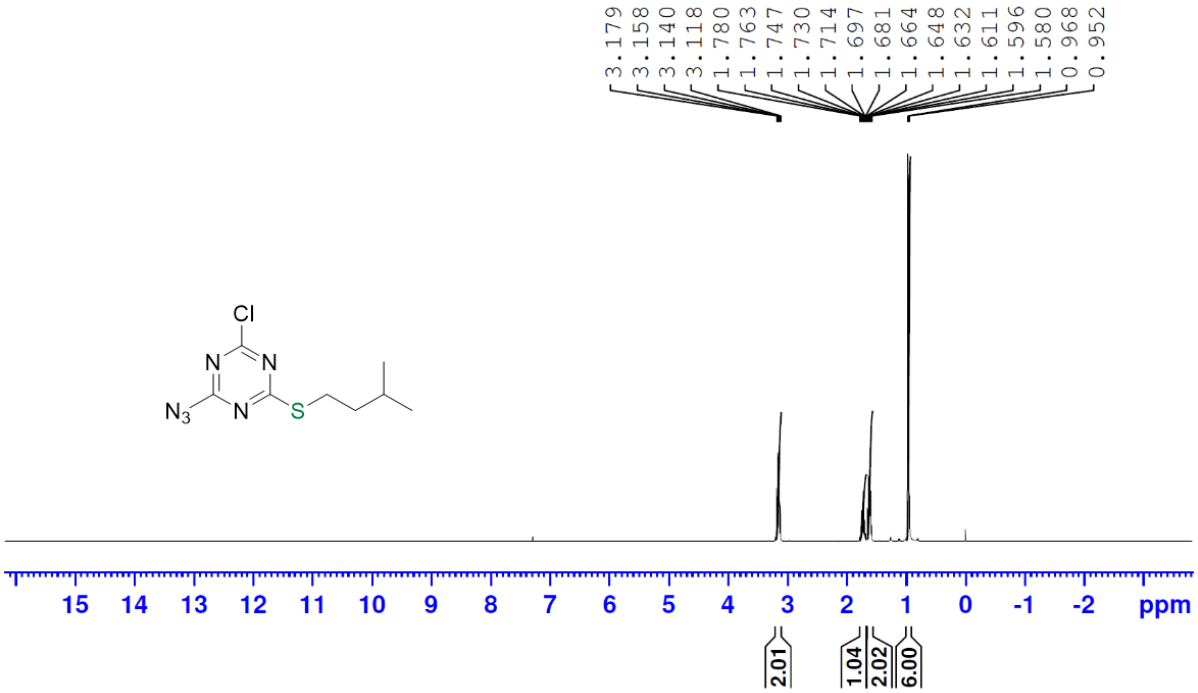
5.4. Characterization of *2,4-dichloro-6-phenoxy-1,3,5-triazine* (5)

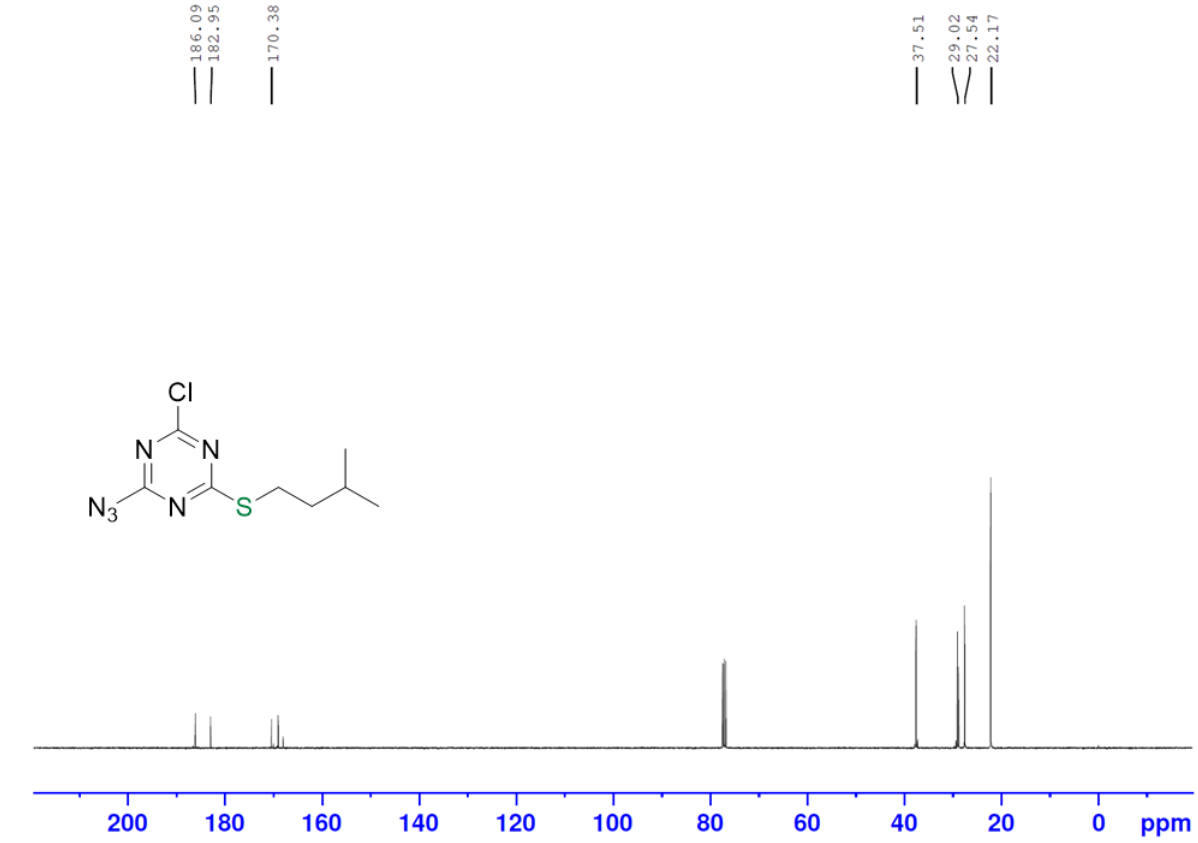

7.424
7.418
7.413
7.399
7.383
7.378
7.373
7.294
7.291
7.279
7.275
7.271
7.257
7.124
7.120
7.117
7.112
7.101
7.098
Cl
N
N
O
N
Cl
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
2.07
1.07
2.00

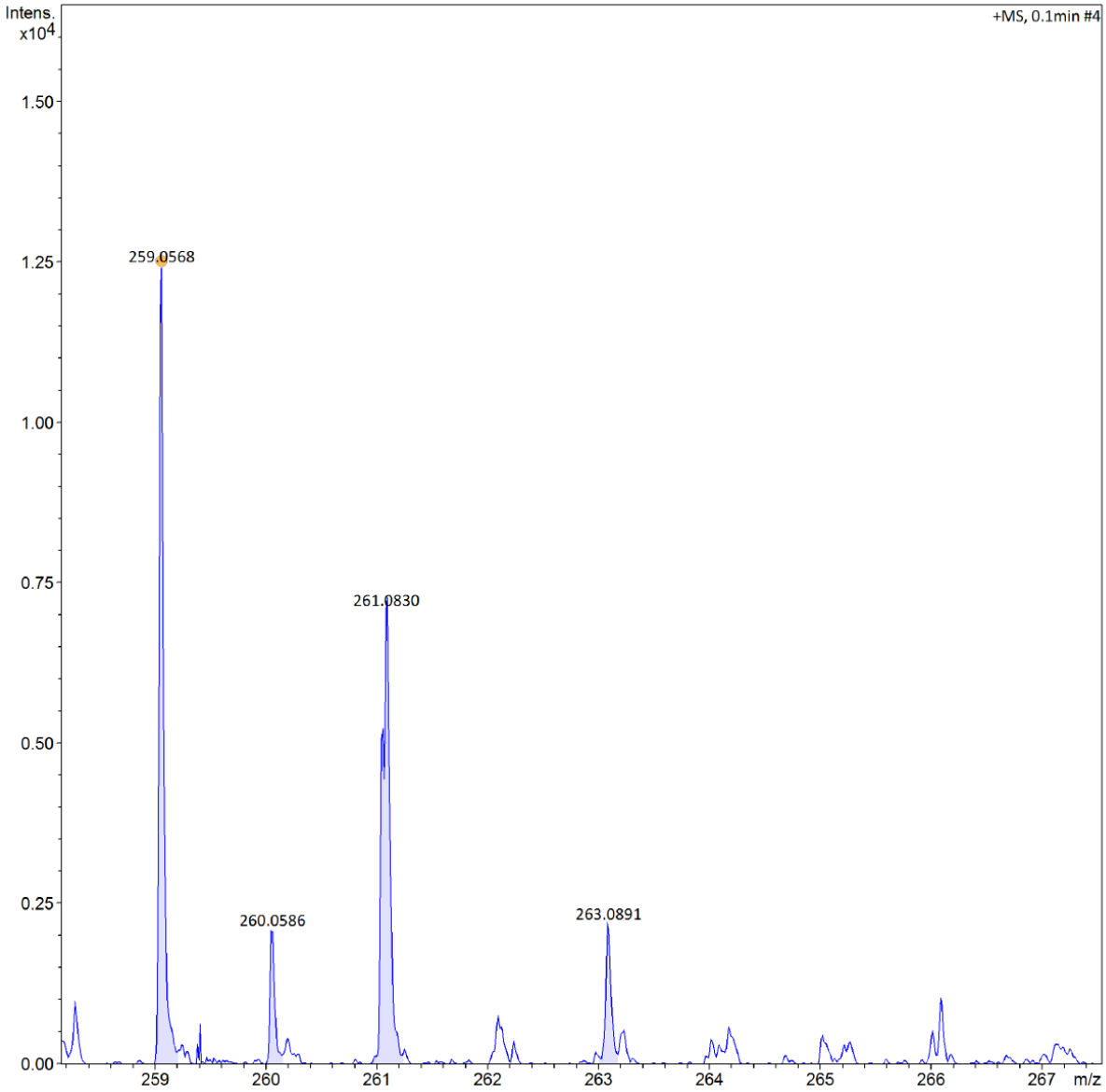

173.75
172.41
151.33
129.66
126.48
121.19
Cl
N
N
O
N
Cl
200 180 160 140 120 100 80 60 40 20 0 ppm



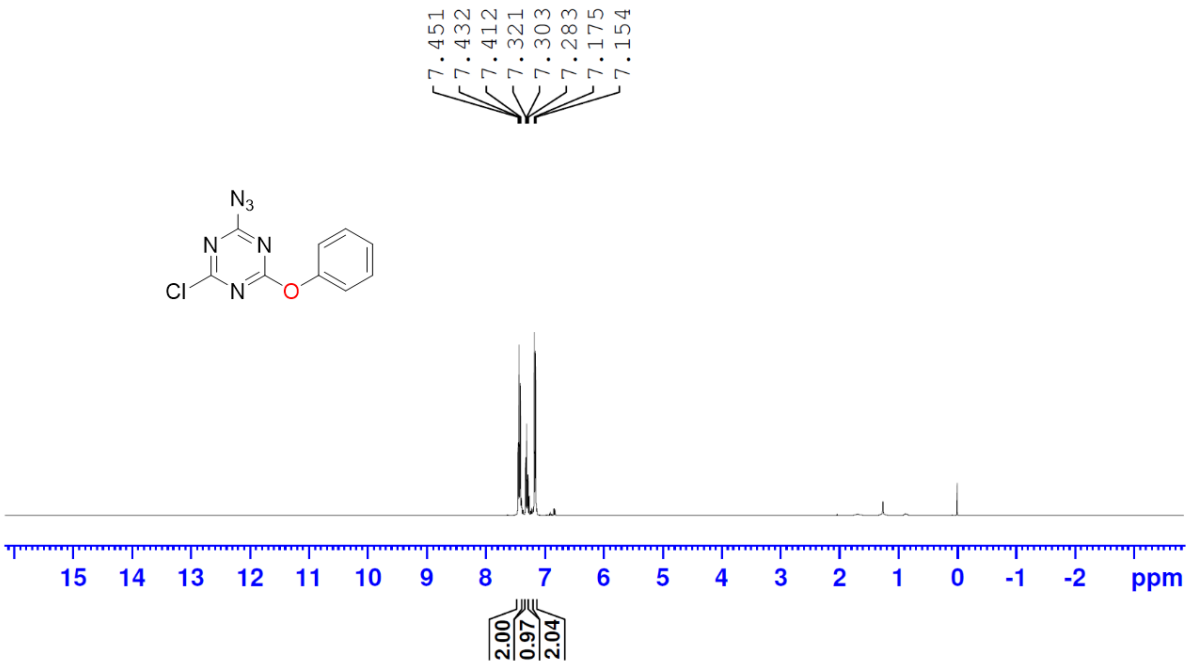
5.5. Characterization of *2-azido-4-chloro-6-(isopentylthio)-1,3,5-triazine* (6)

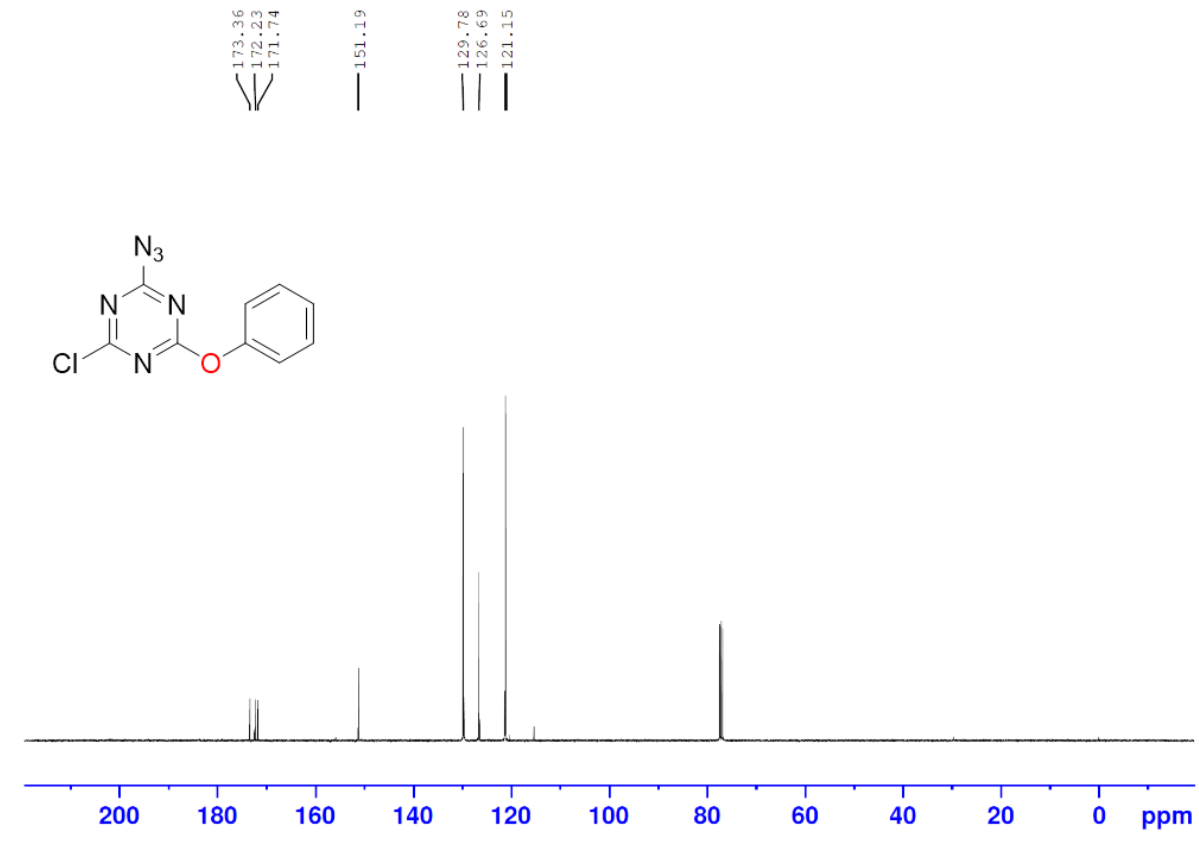

3.179
3.158
3.140
3.118
1.780
1.763
1.747
1.730
1.714
1.697
1.681
1.664
1.648
1.632
1.611
1.596
1.580
0.968
0.952
Cl
N
N
N3
N
S
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
2.01
1.04
2.02
6.00

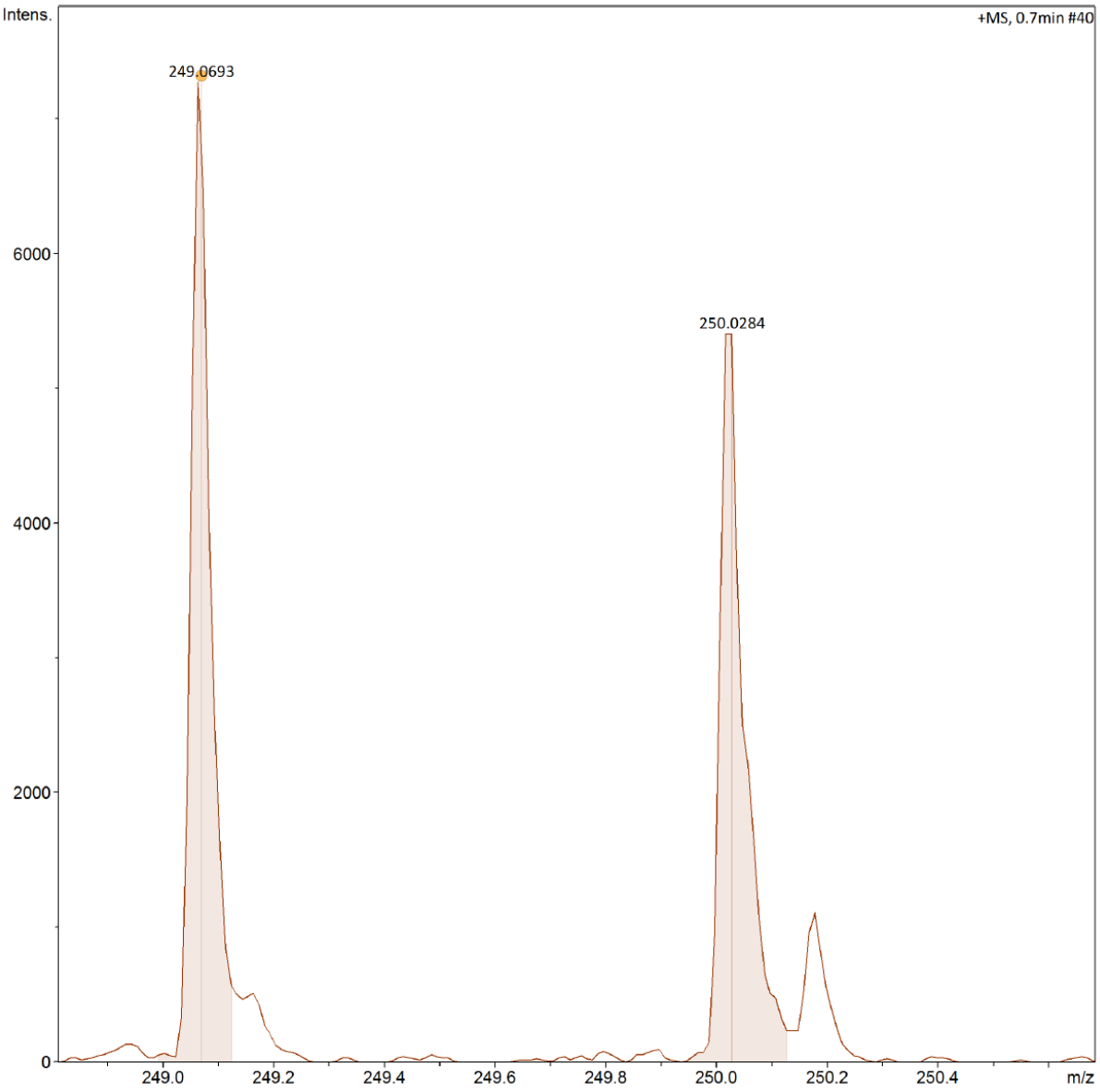

186.09
182.95
170.38
37.51
29.02
27.54
22.17
Cl
N
N
N3
N
S
200 180 160 140 120 100 80 60 40 20 0 ppm



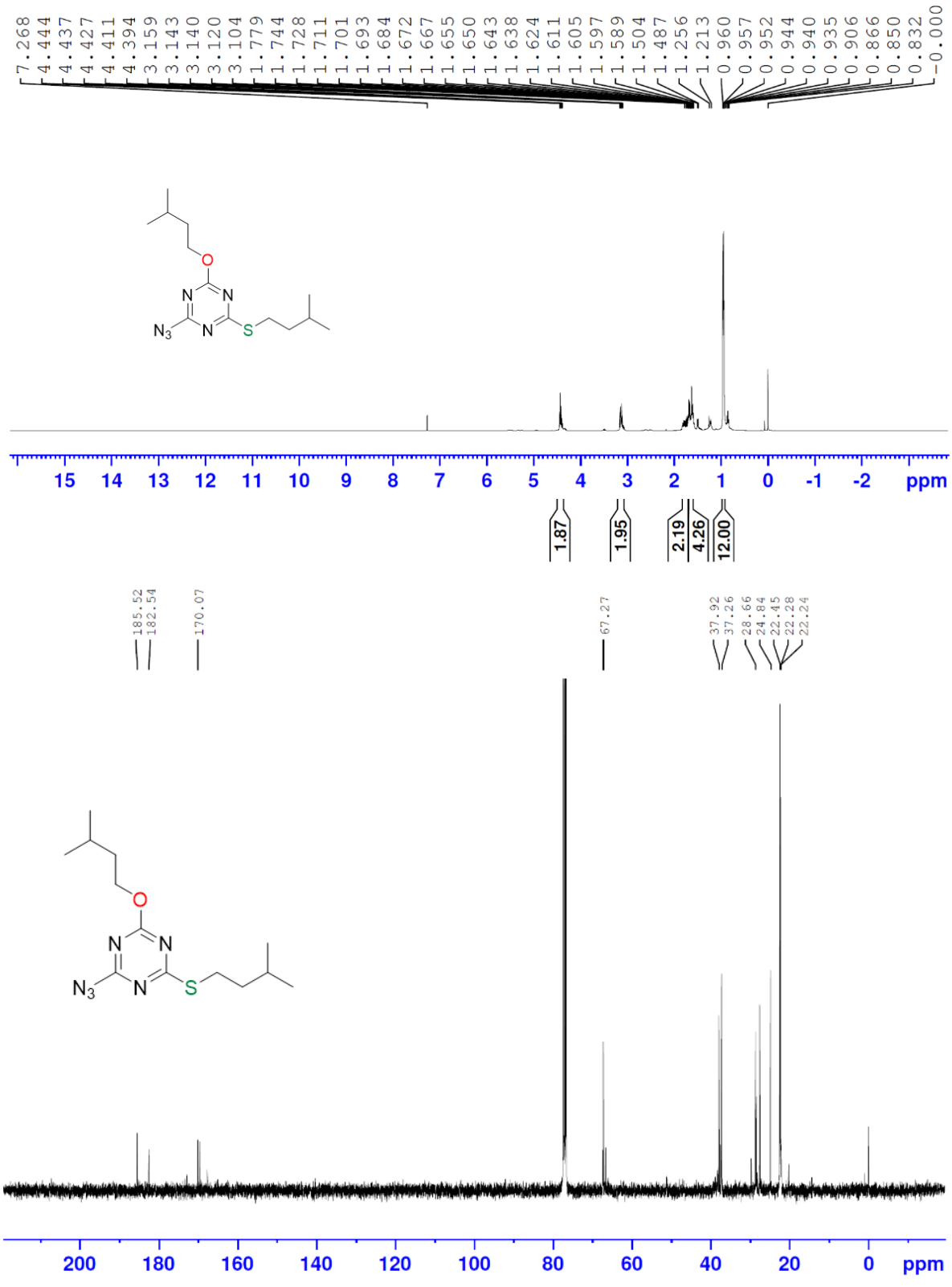
5.6. Characterization of *2-azido-4-chloro-6-phenoxy-1,3,5-triazine* (7)

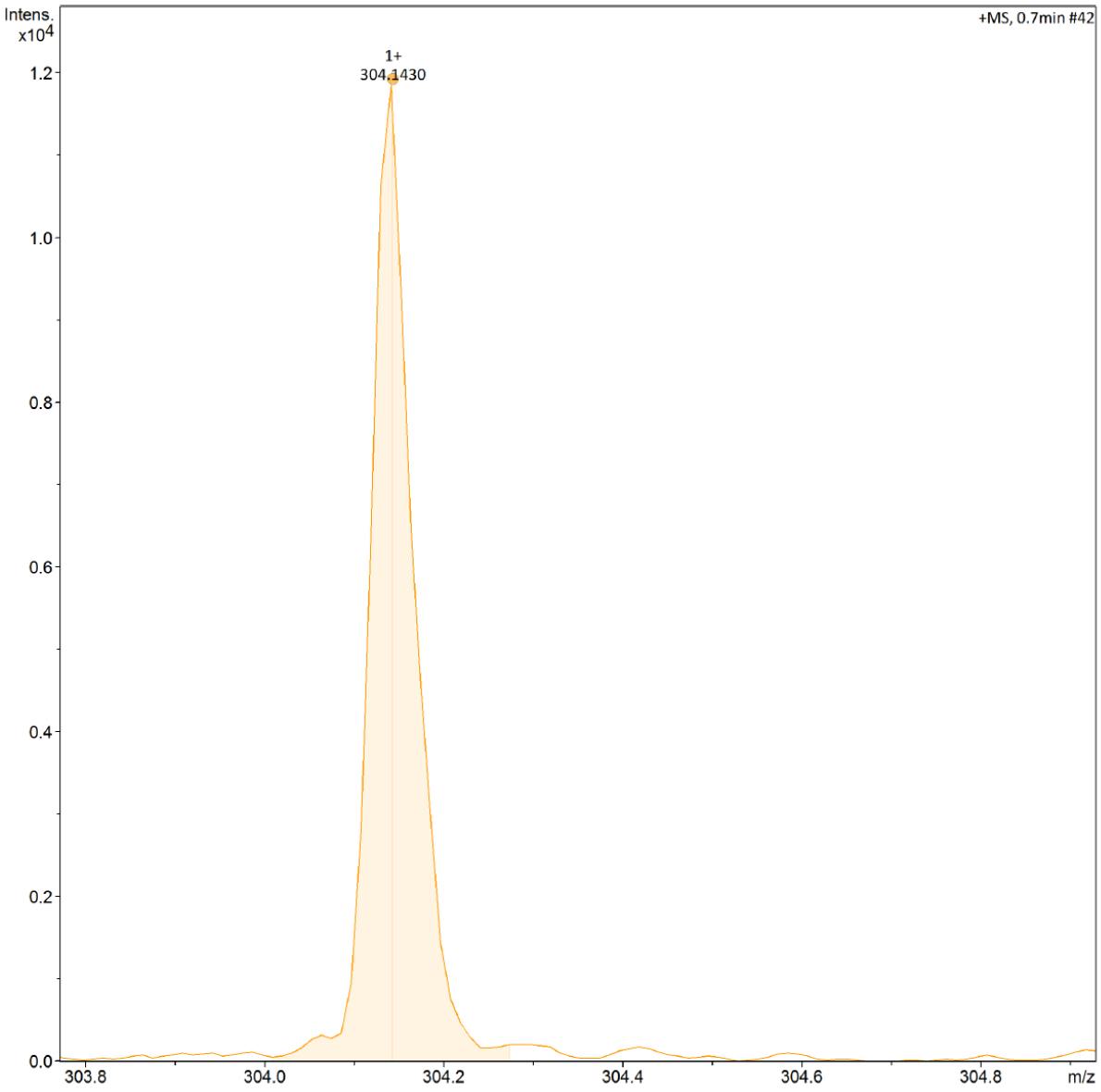

7.451
7.432
7.412
7.321
7.303
7.283
7.175
7.154
N3
N
N
Cl
N
O
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
2.00
0.97
2.04


173.36
172.23
171.74
151.19
129.78
126.69
121.15
N3
N
N
Cl
N
O
200 180 160 140 120 100 80 60 40 20 0 ppm

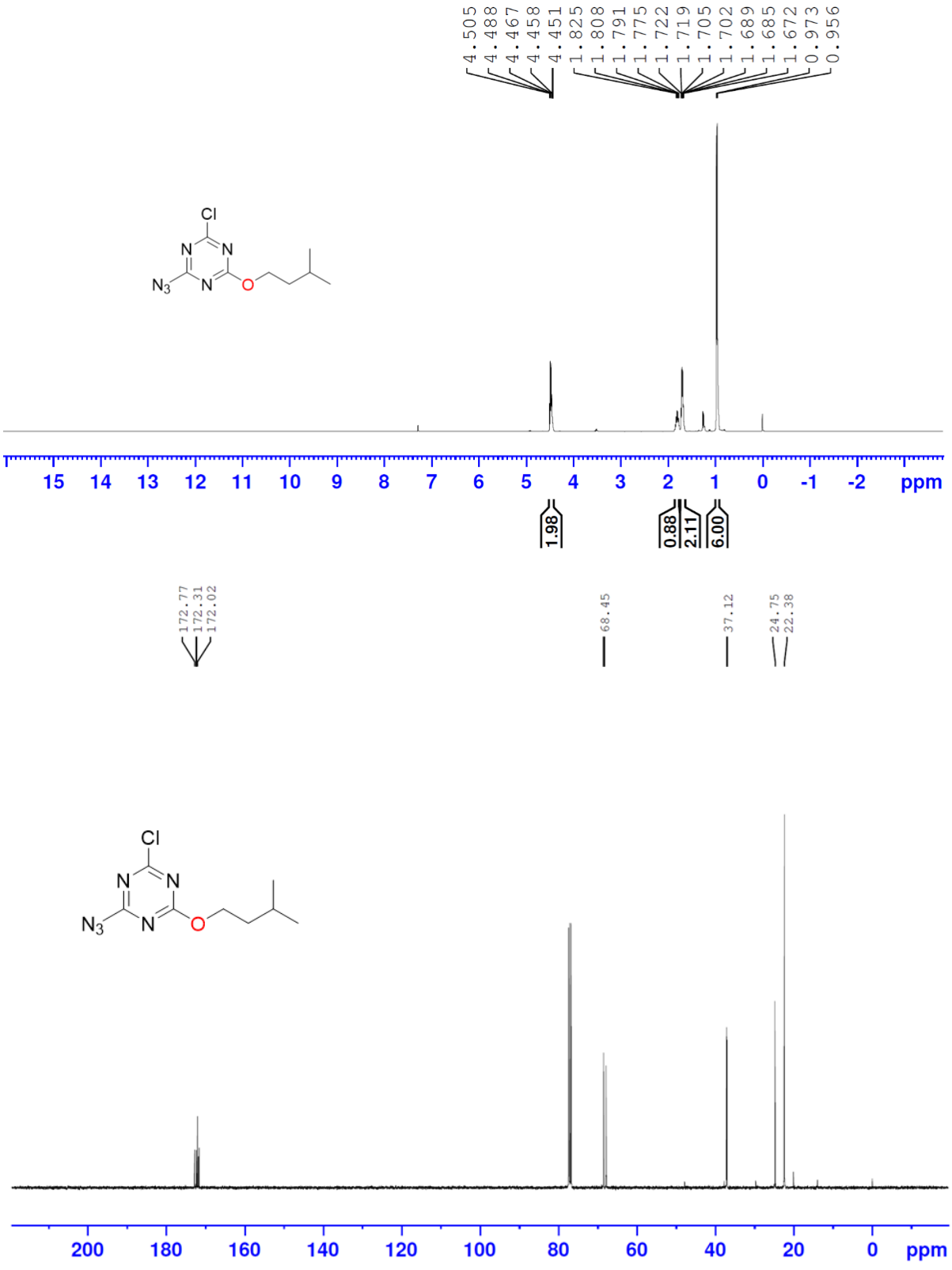


5.7. Characterization of *2-chloro-4-(isopentyloxy)-6-(isopentylthio)-1,3,5-triazine* (8)

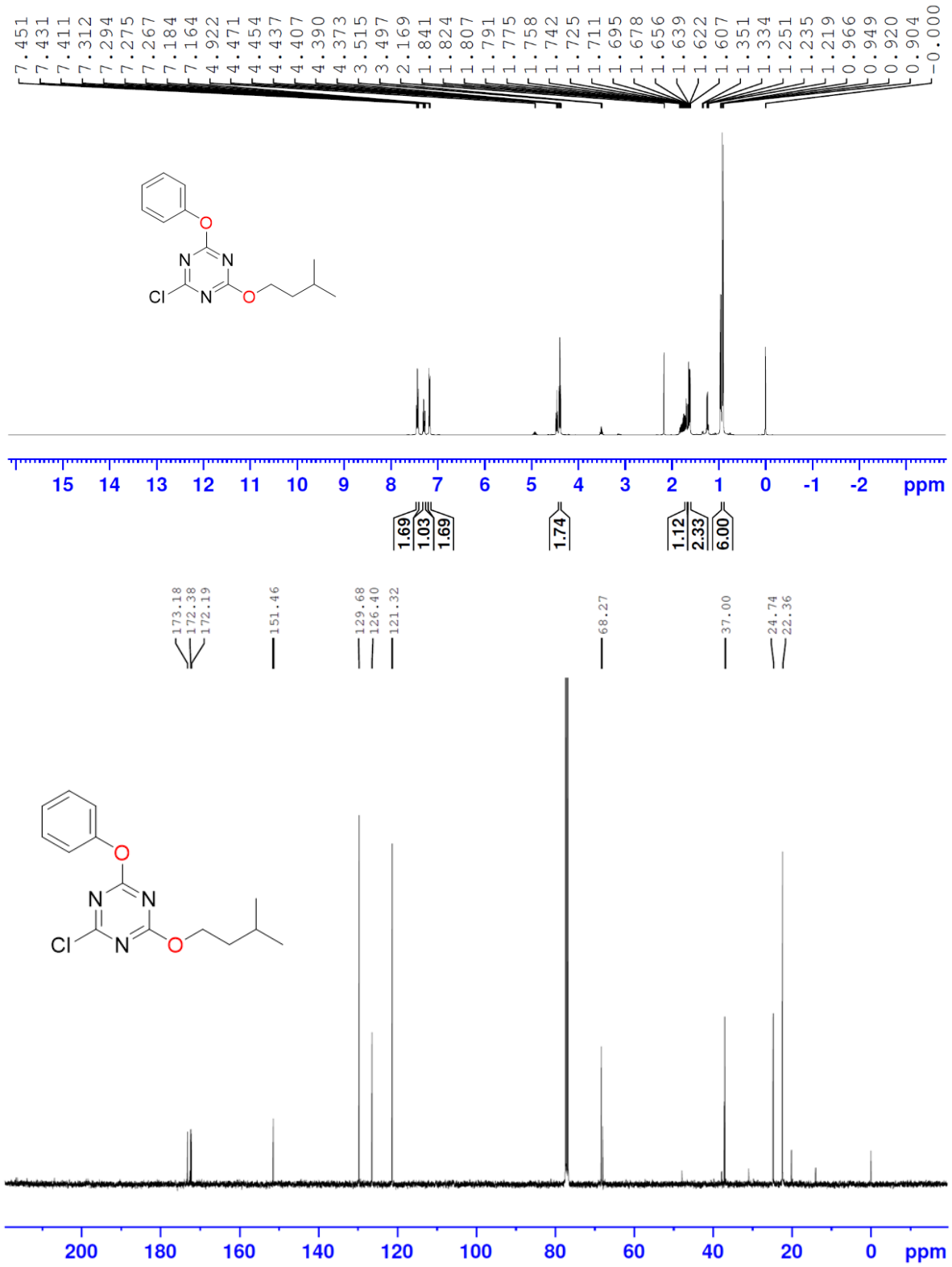

7.268
4.444
4.437
4.427
4.411
4.394
3.159
3.143
3.140
3.120
3.104
1.779
1.744
1.728
1.711
1.701
1.693
1.684
1.672
1.667
1.655
1.650
1.643
1.638
1.624
1.611
1.605
1.597
1.589
1.504
1.487
1.256
1.213
0.960
0.957
0.952
0.944
0.940
0.935
0.906
0.866
0.850
0.832
-0.000
O
N
N
N3
N
S
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.87
1.95
2.19
4.26
12.00
185.52
182.54
170.07
67.27
37.92
37.26
28.66
24.84
22.45
22.28
22.24
O
N
N
N3
N
S
200 180 160 140 120 100 80 60 40 20 0 ppm

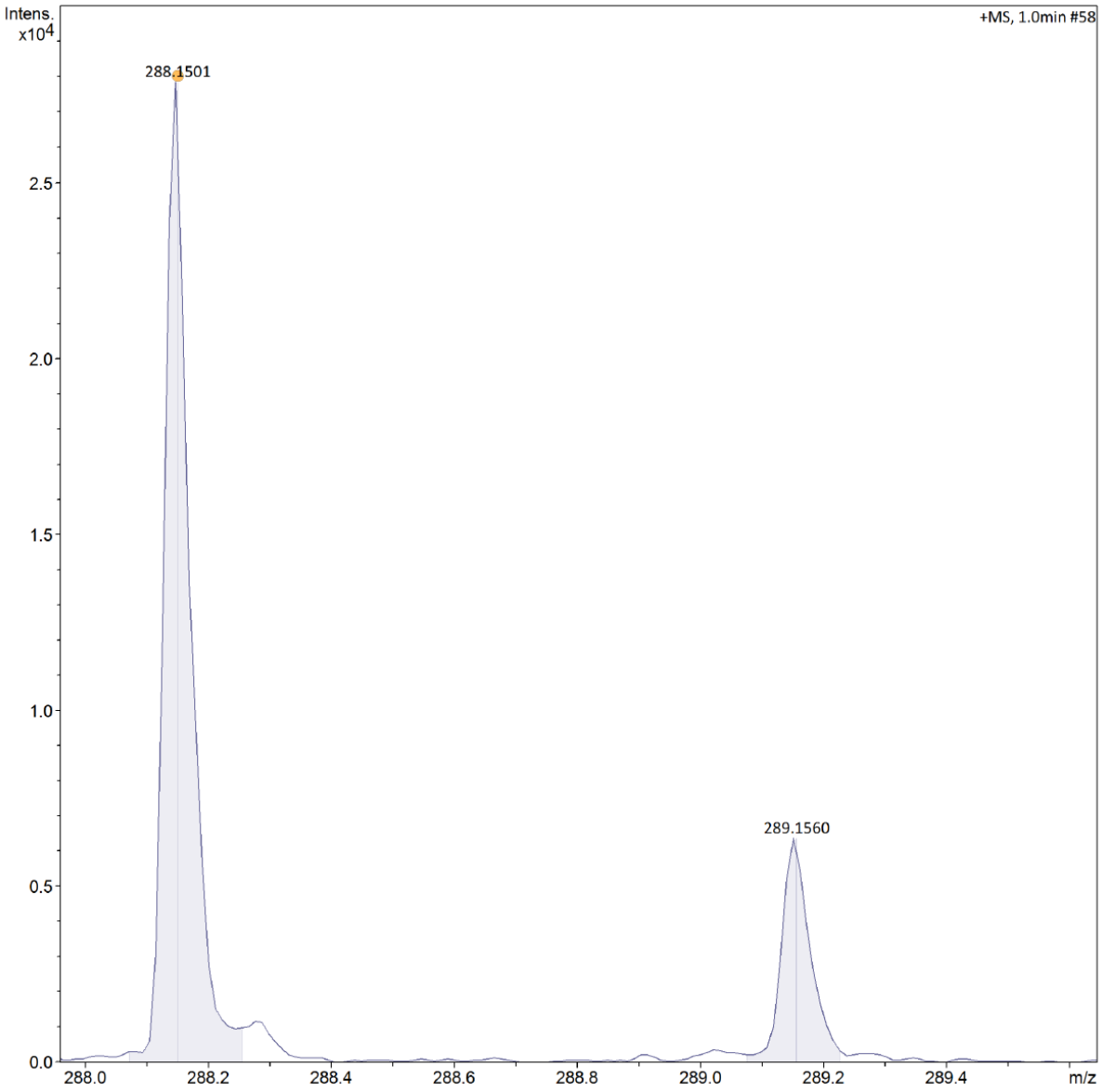


5.8. Characterization of *2-azido-4-chloro-6-(isopentyloxy)-1,3,5-triazine (*9)

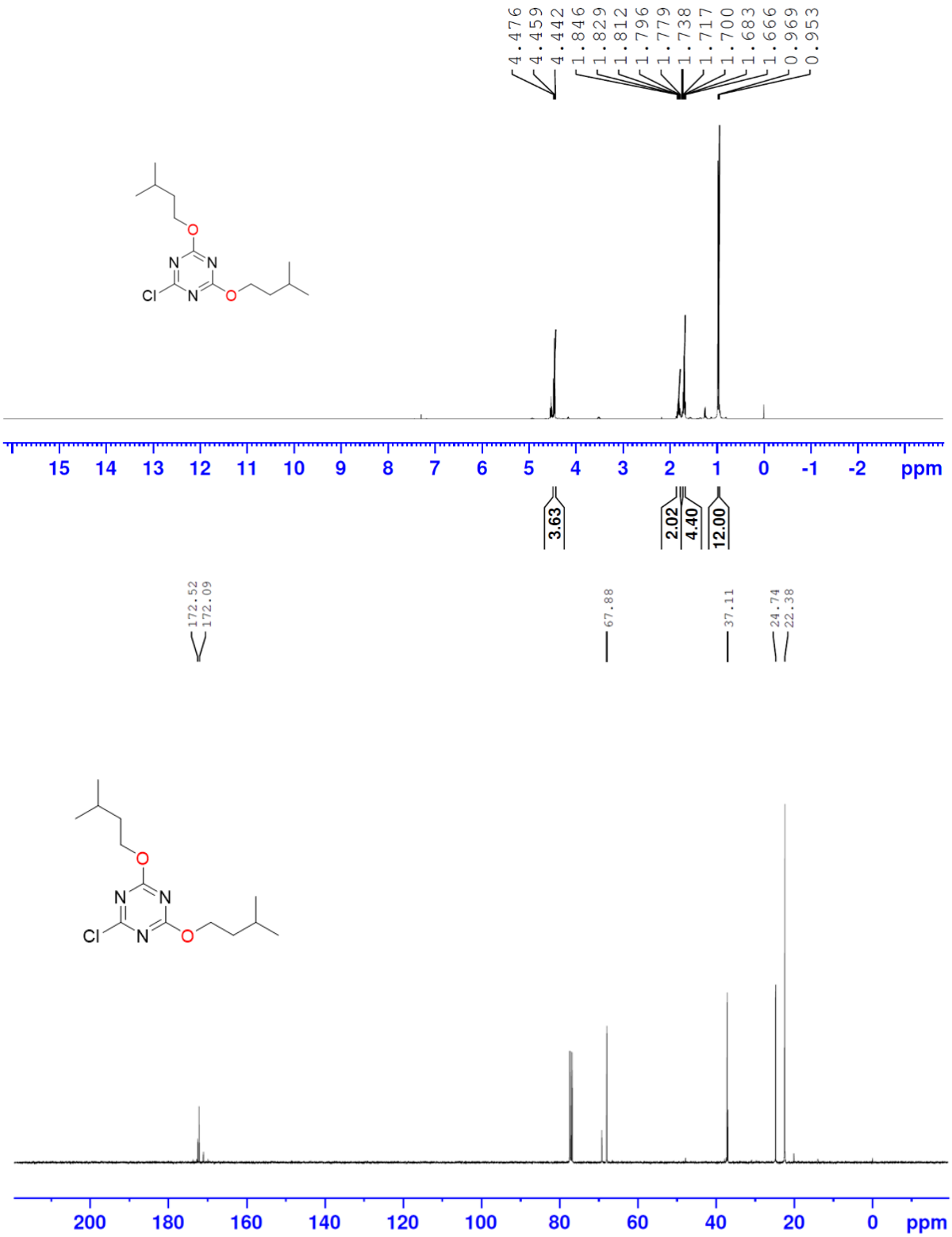


5.9. Characterization of *2-chloro-4-(isopentyloxy)-6-phenoxy-1,3,5-triazine* (10)

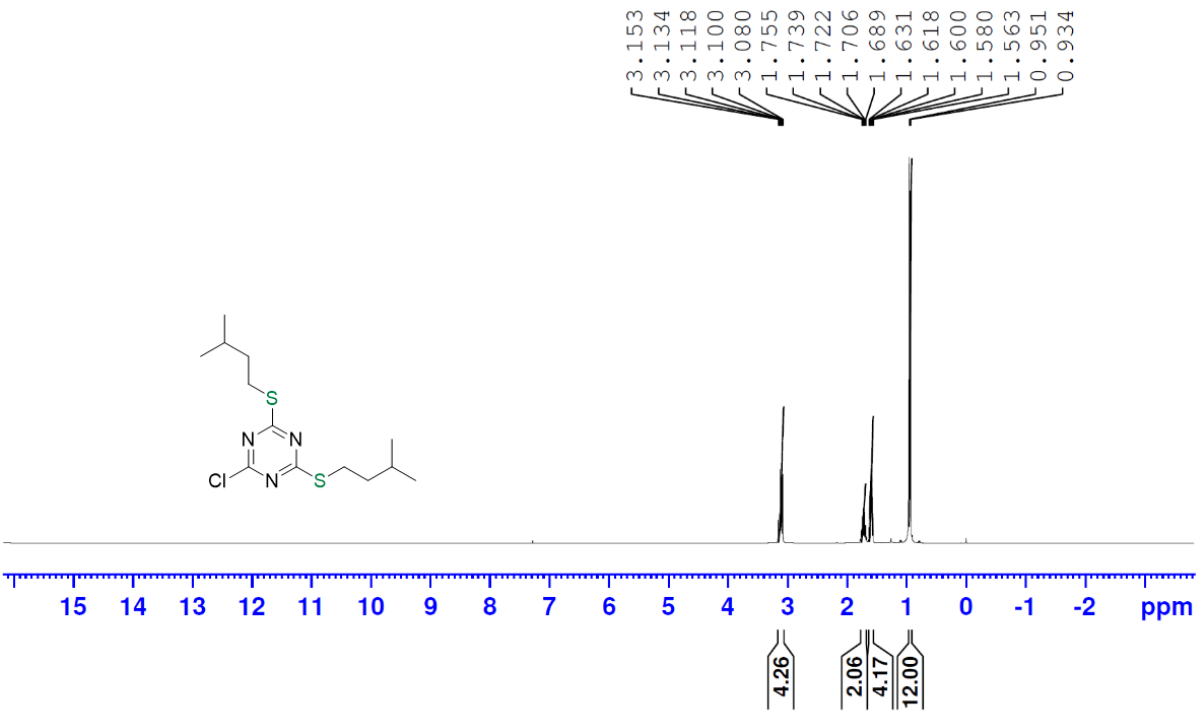

7.451
7.431
7.411
7.312
7.294
7.275
7.267
7.184
7.164
4.922
4.471
4.454
4.437
4.407
4.390
4.373
3.515
3.497
2.169
1.841
1.824
1.807
1.791
1.775
1.758
1.742
1.725
1.711
1.695
1.678
1.656
1.639
1.622
1.607
1.351
1.334
1.251
1.235
1.219
0.966
0.949
0.920
0.904
-0.000
O
N
N
Cl
N
O
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.69
1.03
1.69
1.74
1.12
2.33
6.00
173.18
172.38
172.19
151.46
129.68
126.40
121.32
68.27
37.00
24.74
22.36
O
N
N
Cl
N
O
200 180 160 140 120 100 80 60 40 20 0 ppm

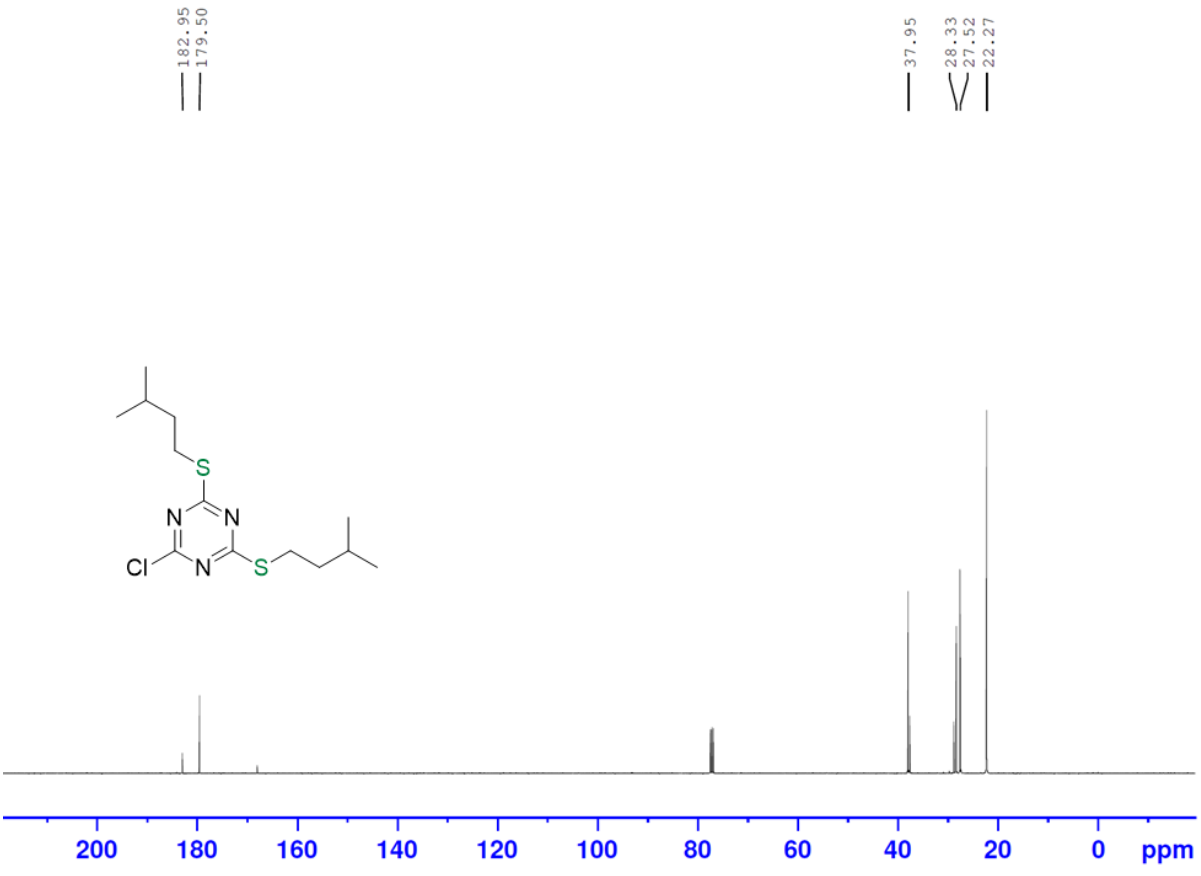


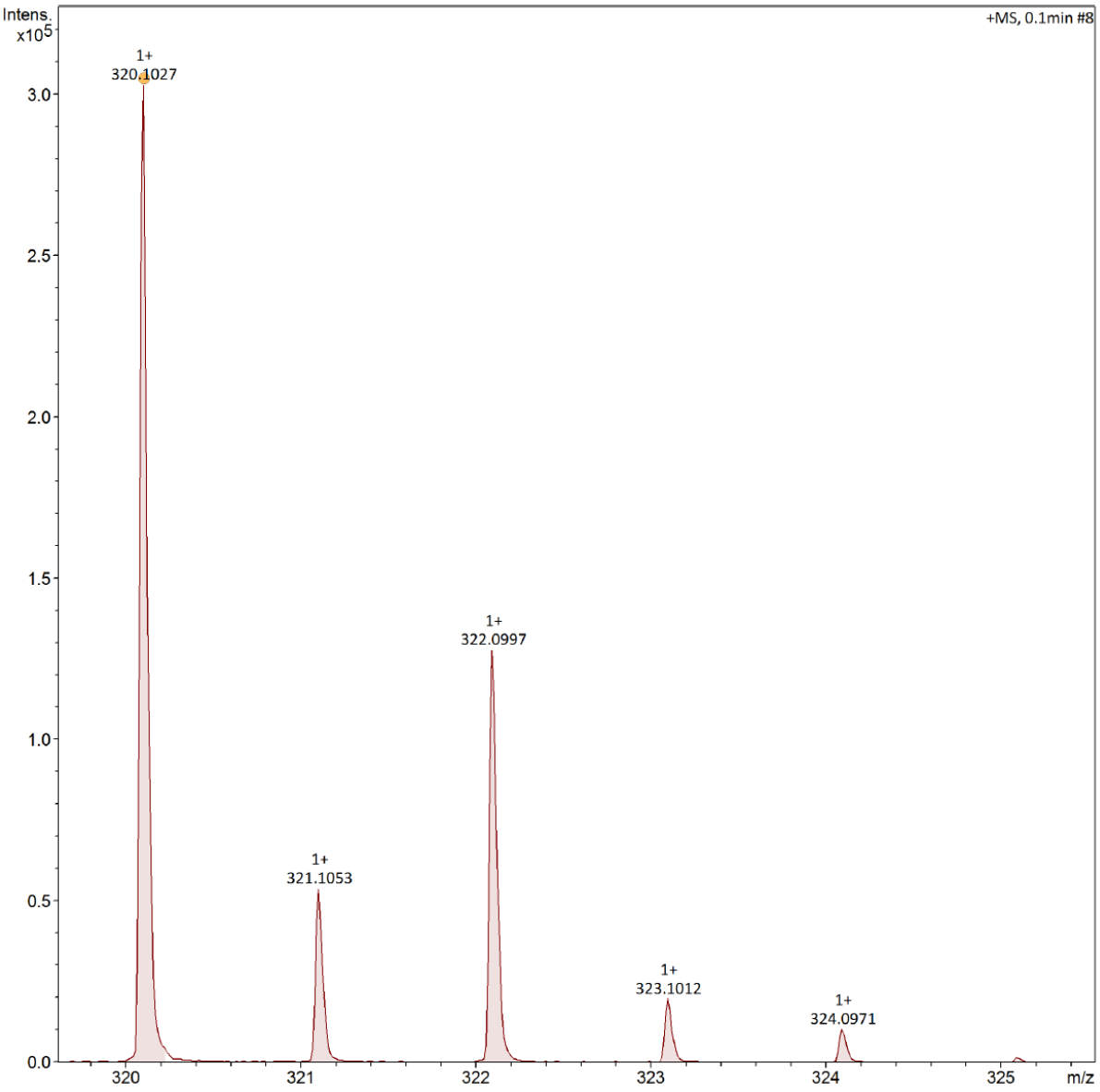
5.10. Characterization of *2-chloro-4,6-bis(isopentyloxy)-1,3,5-triazine* (11)



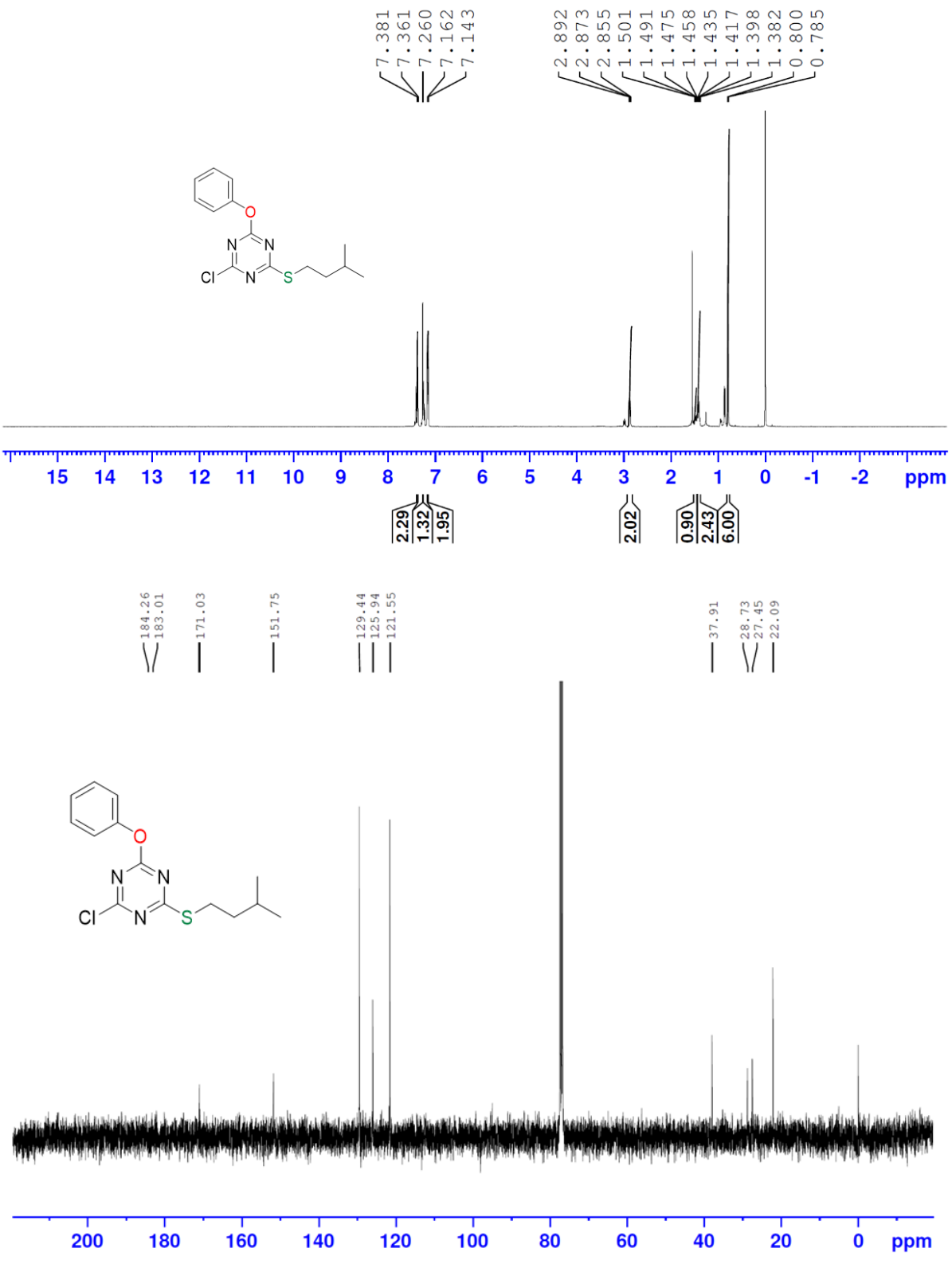
5.11. Characterization of *2-chloro-4,6-bis(isopentylthio)-1,3,5-triazine* (12)

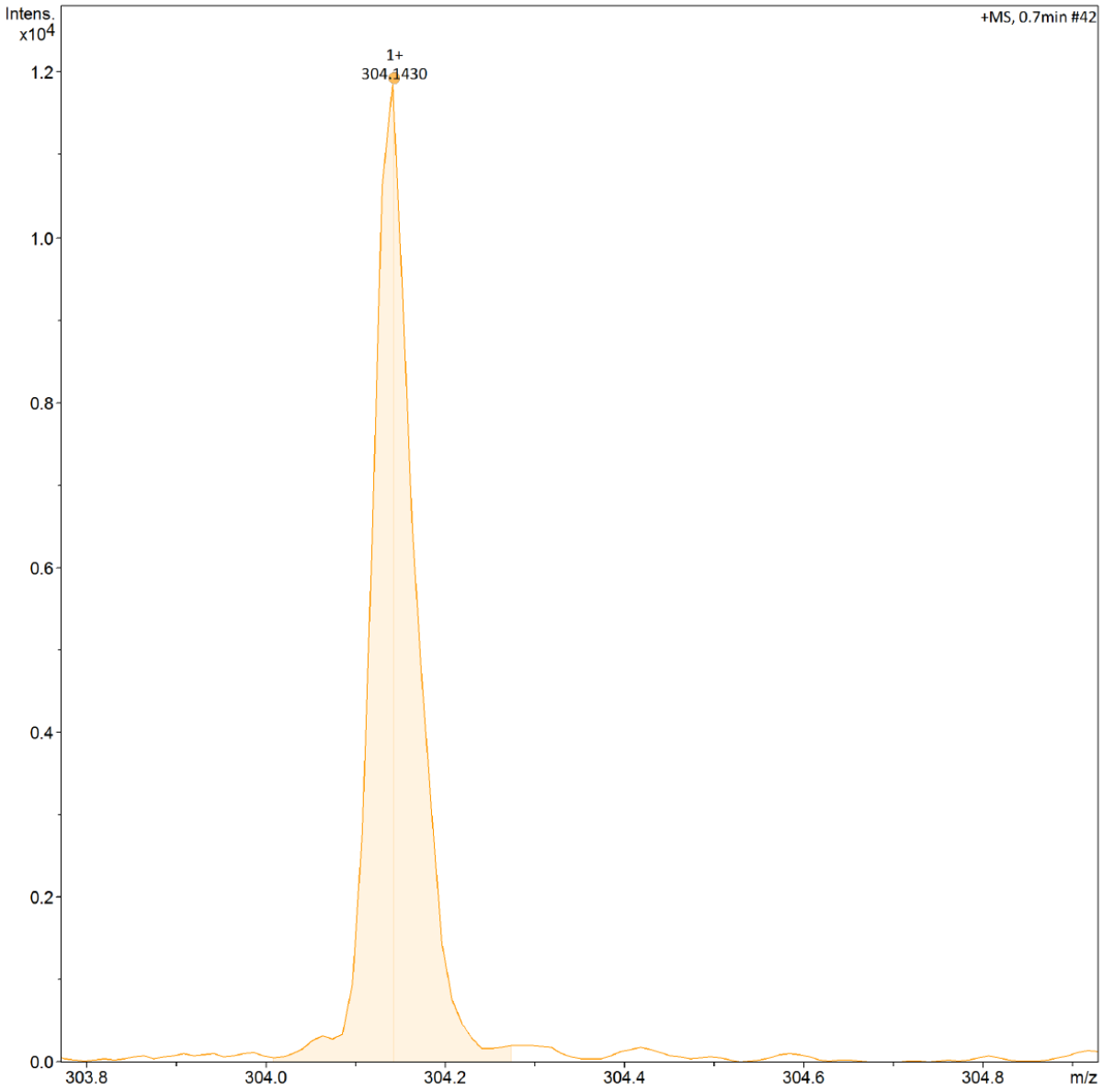

3.153
3.134
3.118
3.100
3.080
1.755
1.739
1.722
1.706
1.689
1.631
1.618
1.600
1.580
1.563
0.951
0.934
S
N
N
Cl
N
S
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
4.26
2.06
4.17
12.00


182.95
179.50
37.95
28.33
27.52
22.27
S
N
N
Cl
N
S
200 180 160 140 120 100 80 60 40 20 0 ppm

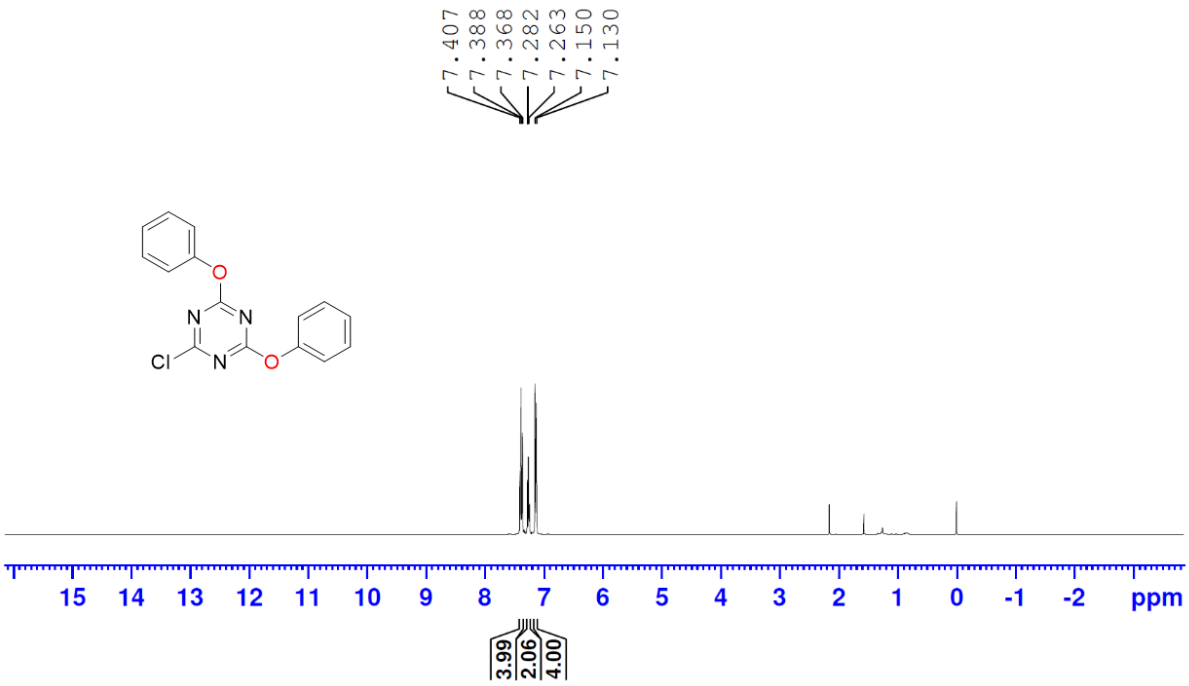


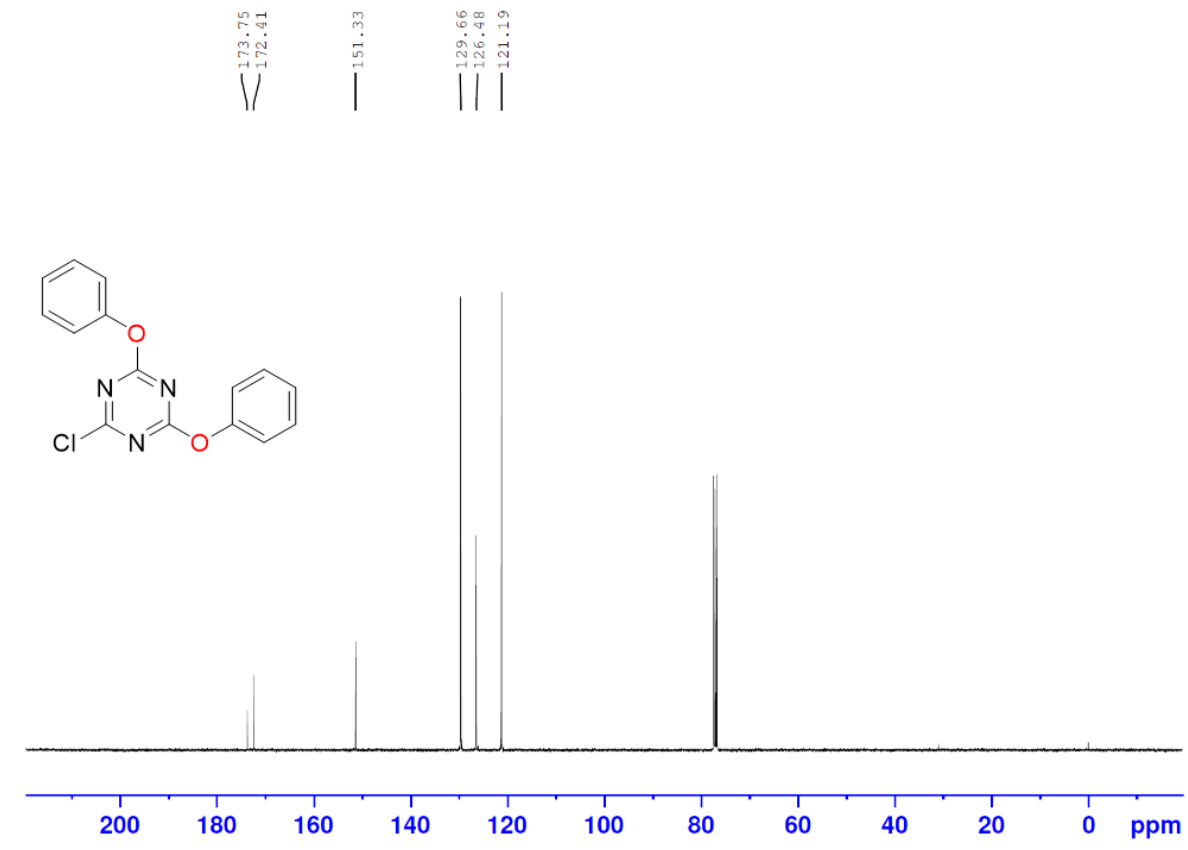
5.12. Characterization of *2-chloro-4-(isopentylthio)-6-phenoxy-1,3,5-triazine* (13)

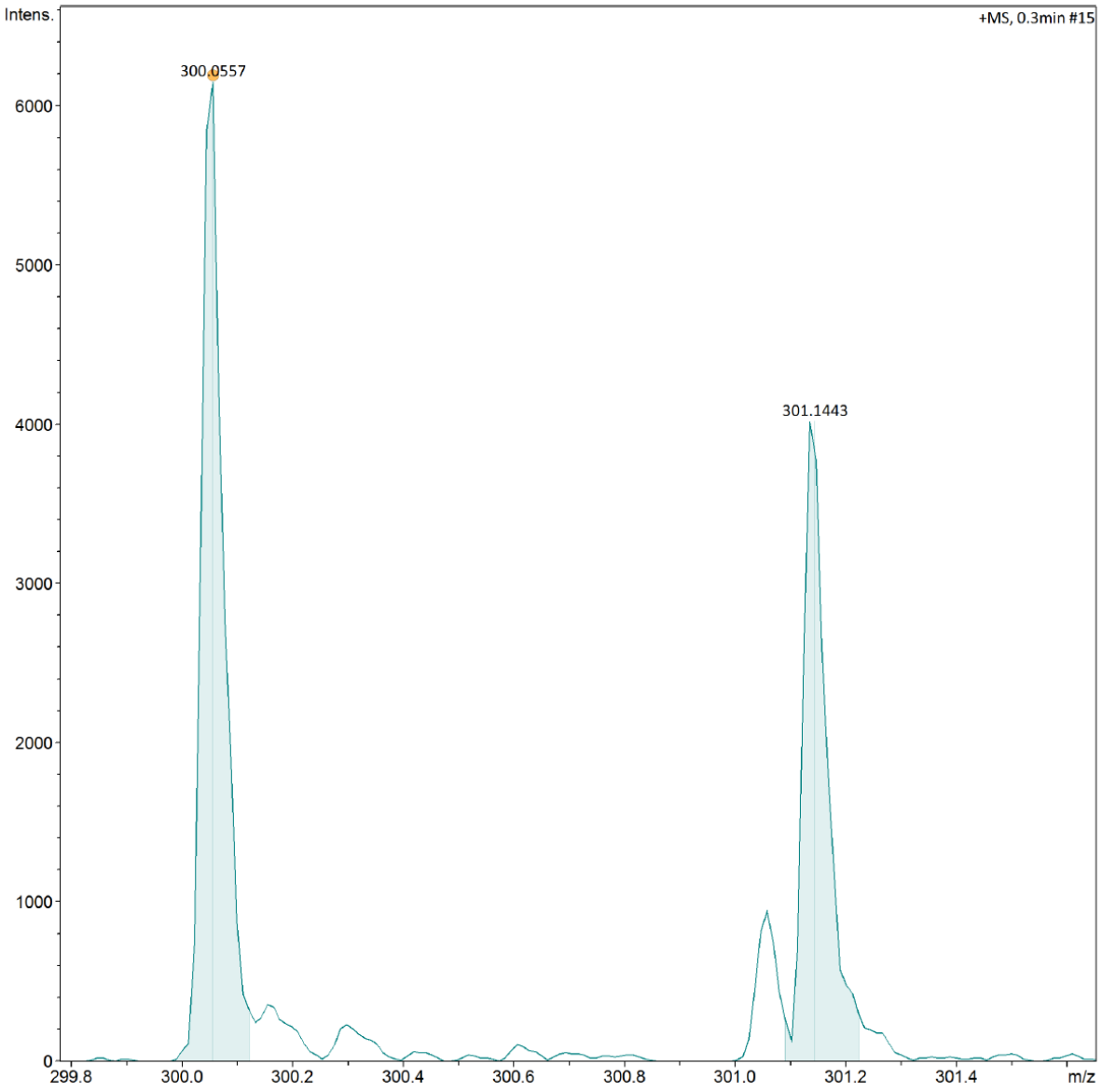

7.381
7.361
7.260
7.162
7.143
2.892
2.873
2.855
1.501
1.491
1.475
1.458
1.435
1.417
1.398
1.382
0.800
0.785
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
2.29
1.32
1.95
2.02
0.90
2.43
6.00
184.26
183.01
171.03
151.75
129.44
125.94
121.55
37.91
28.73
27.45
22.09
200 180 160 140 120 100 80 60 40 20 0 ppm



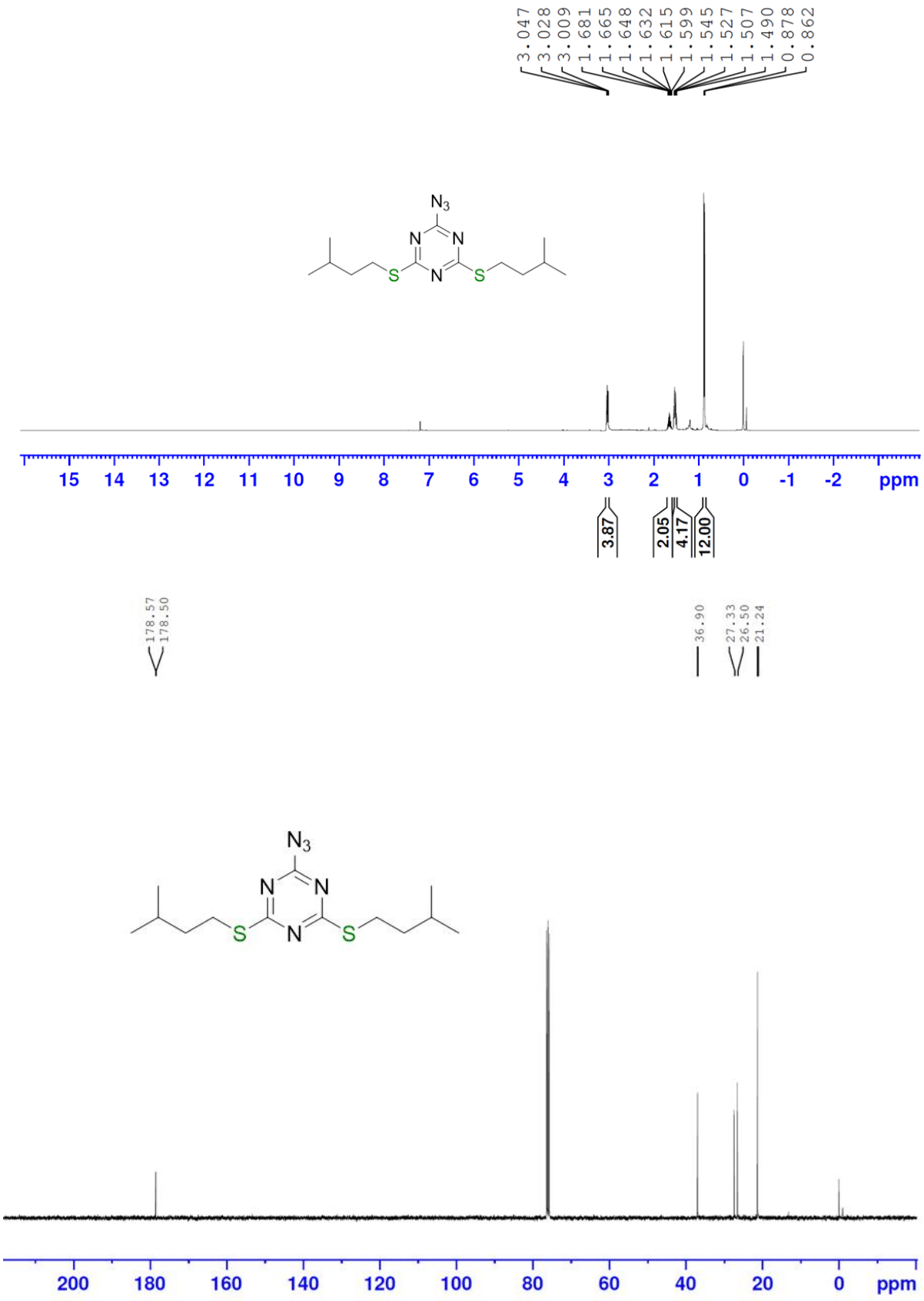
5.13. Characterization of *2-chloro-4,6-diphenoxy-1,3,5-triazine* (14)


7.407
7.388
7.368
7.282
7.263
7.150
7.130
Cl
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
3.99
2.06
4.00

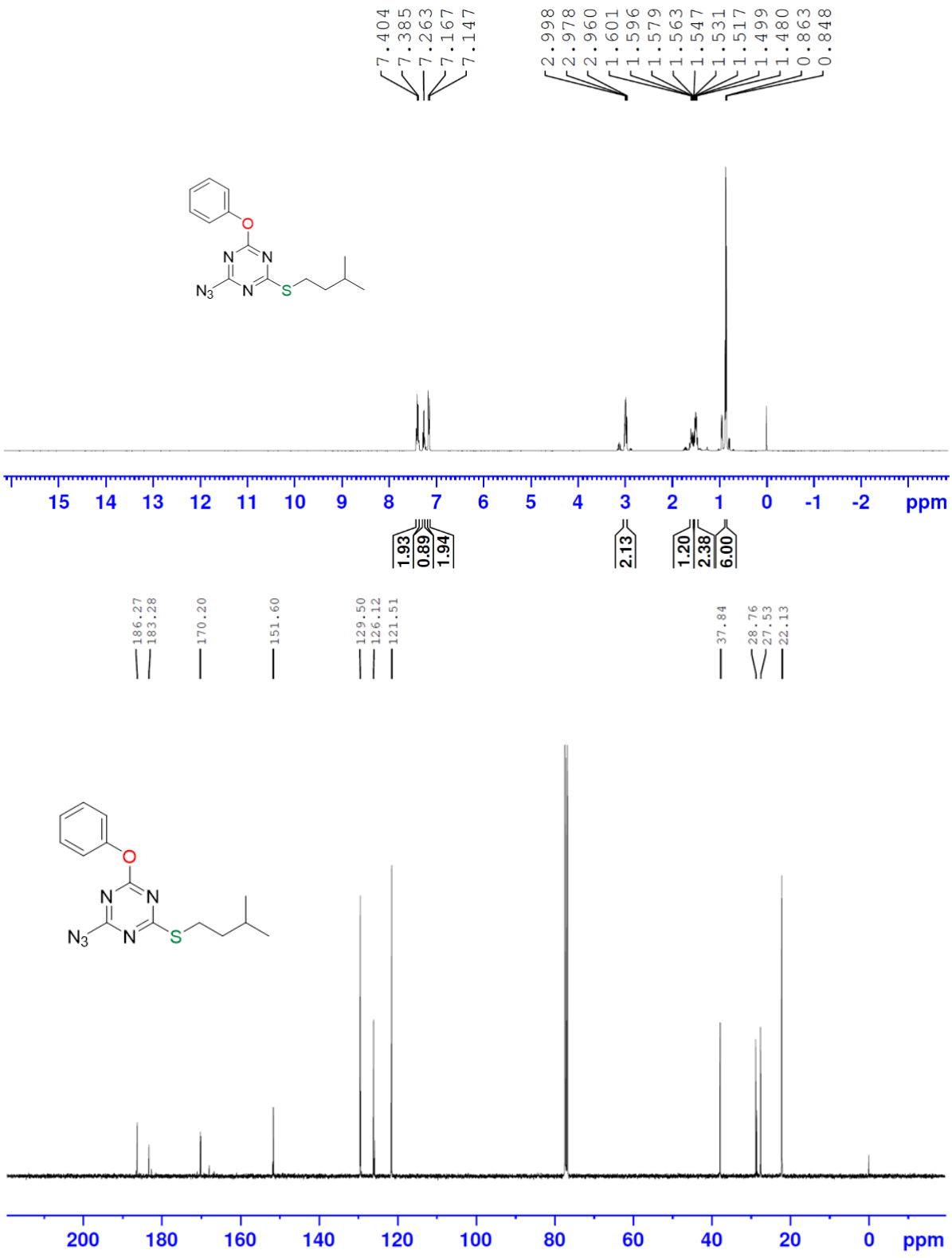

173.75
172.41
151.33
129.66
126.48
121.19
Cl
200 180 160 140 120 100 80 60 40 20 0 ppm

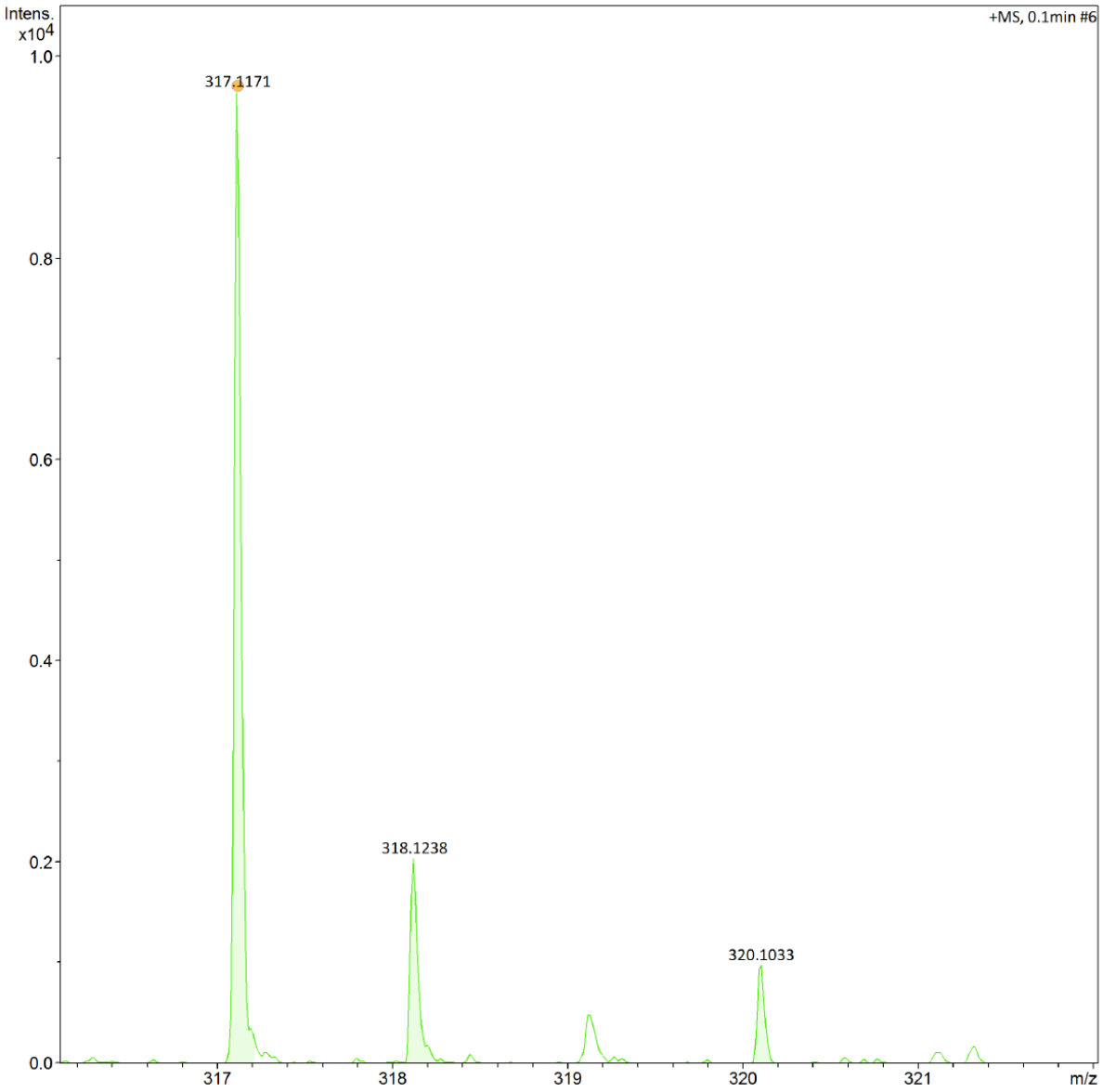


5.14. Characterization of *2-azido-4,6-bis(isopentylthio)-1,3,5-triazine* (15)

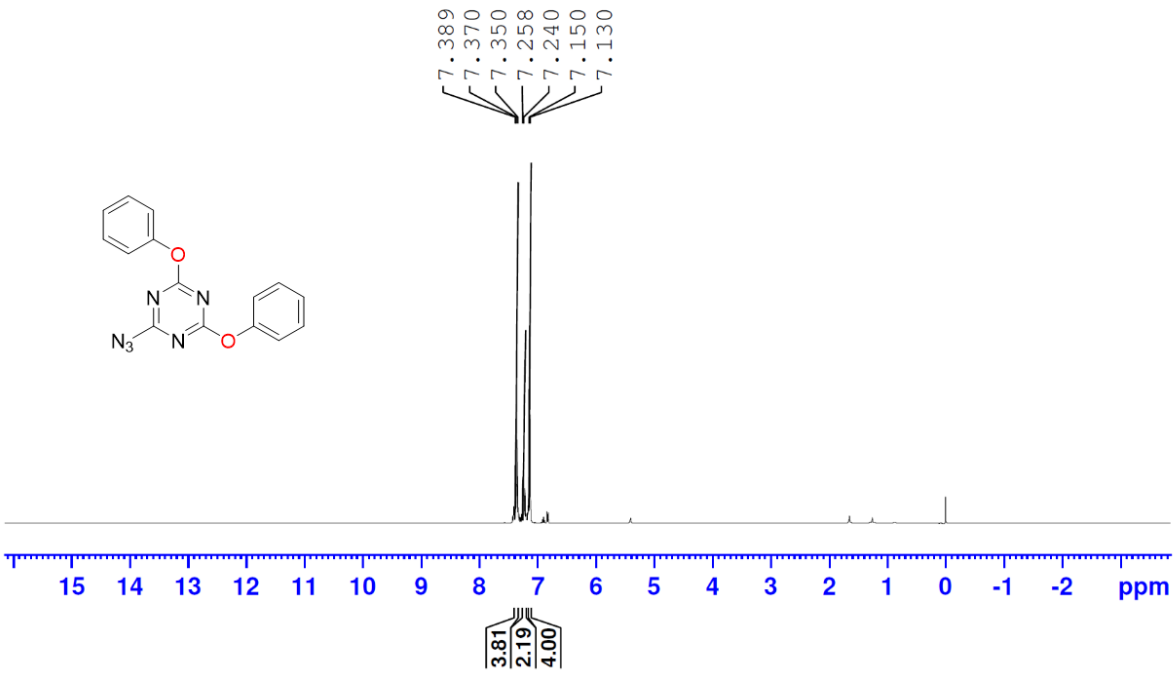


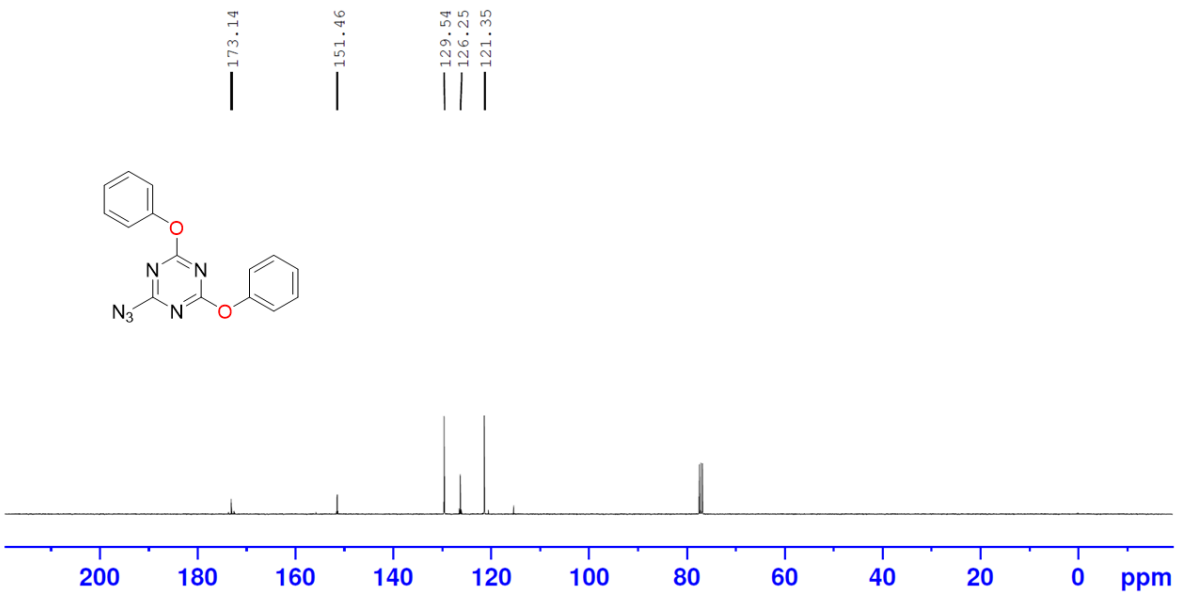
5.15. Characterization of *2-azido-4-(isopentylthio)-6-phenoxy-1,3,5-triazine* (16)

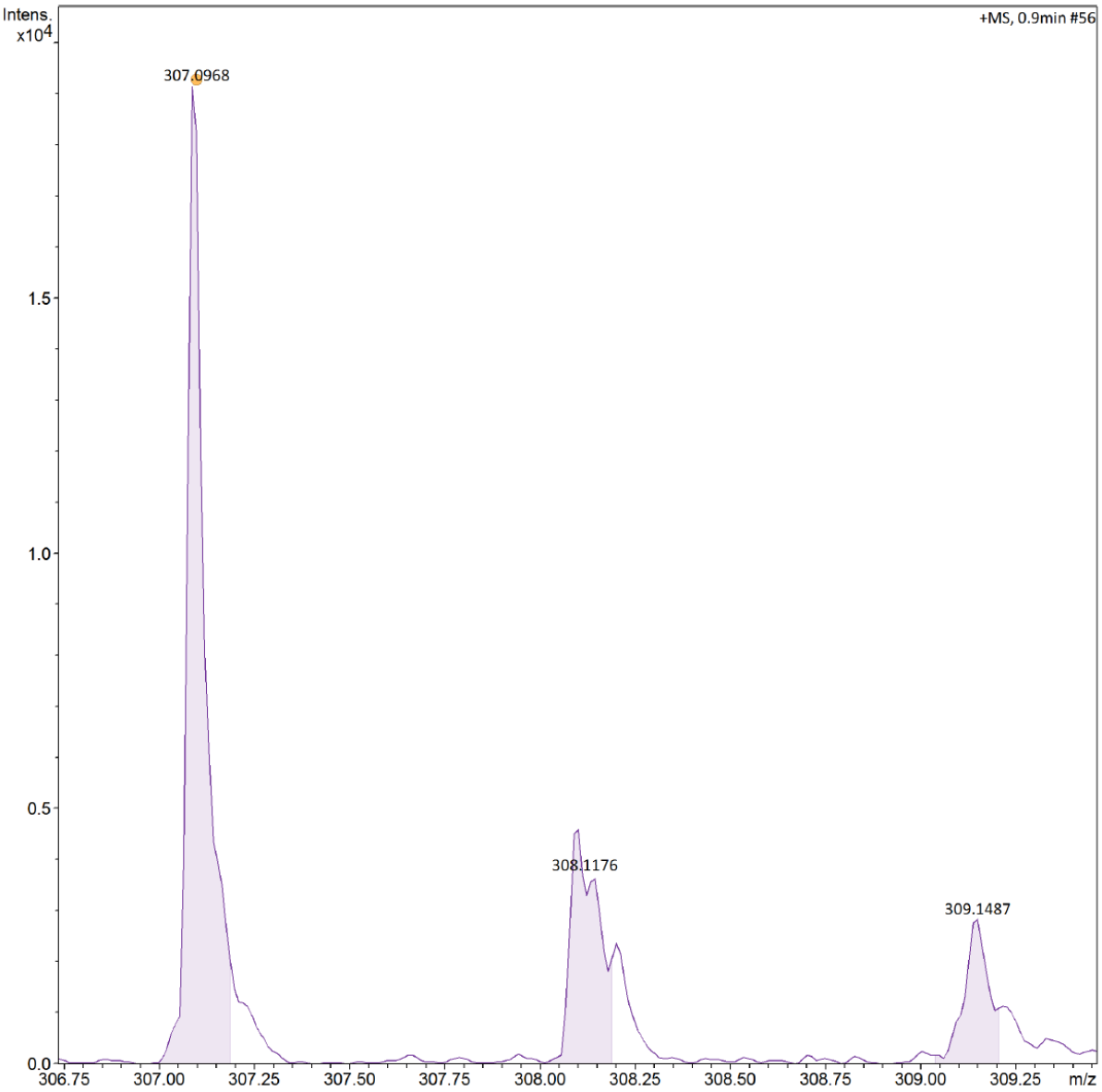

7.404
7.385
7.263
7.167
7.147
2.998
2.978
2.960
1.601
1.596
1.579
1.563
1.547
1.531
1.517
1.499
1.480
0.863
0.848
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.93
0.89
1.94
2.13
1.20
2.38
6.00
186.27
183.28
170.20
151.60
129.50
126.12
121.51
37.84
28.76
27.53
22.13
200 180 160 140 120 100 80 60 40 20 0 ppm



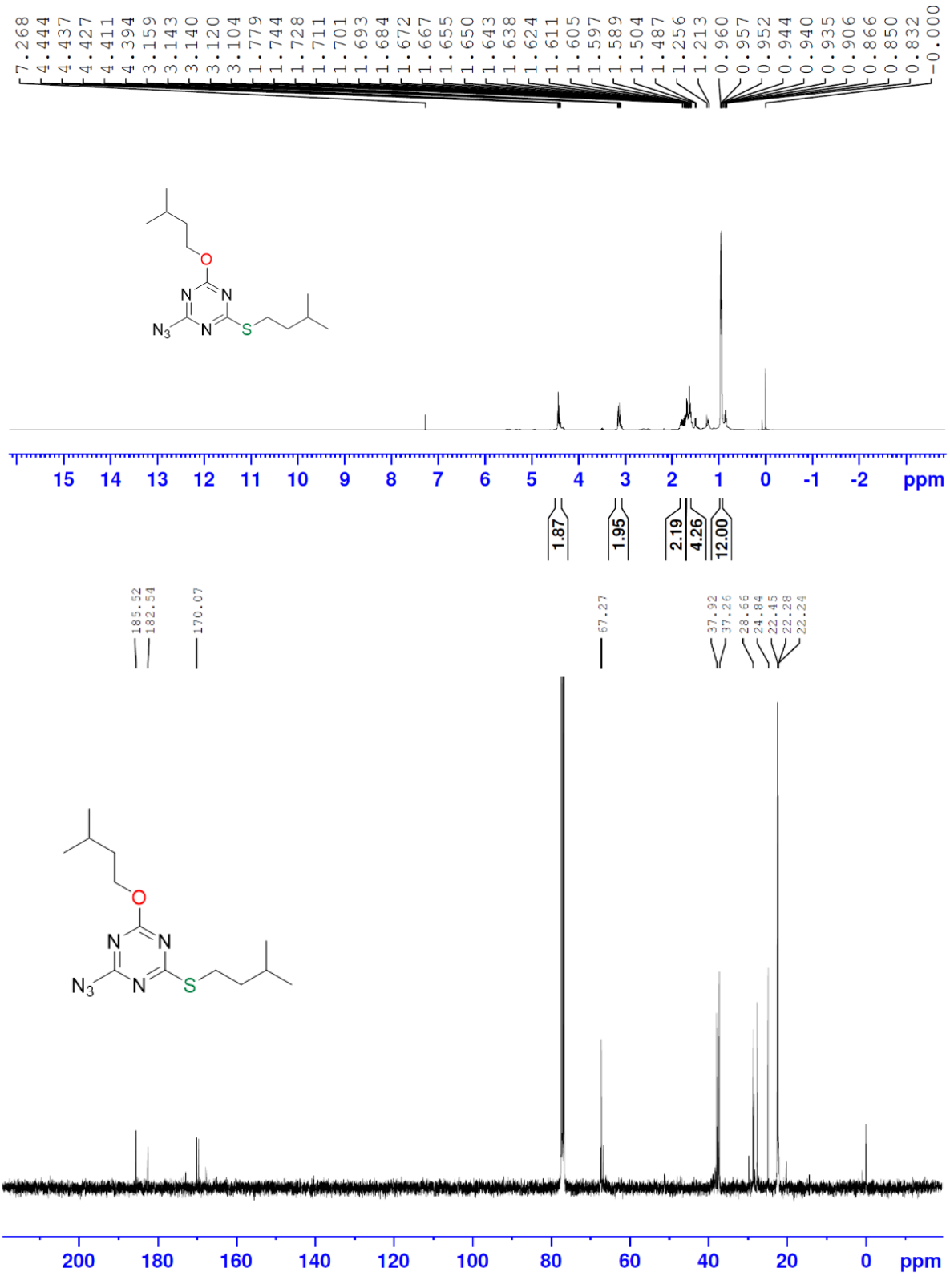
5.16. Characterization of *2-azido-4,6-diphenoxy-1,3,5-triazine* (17)

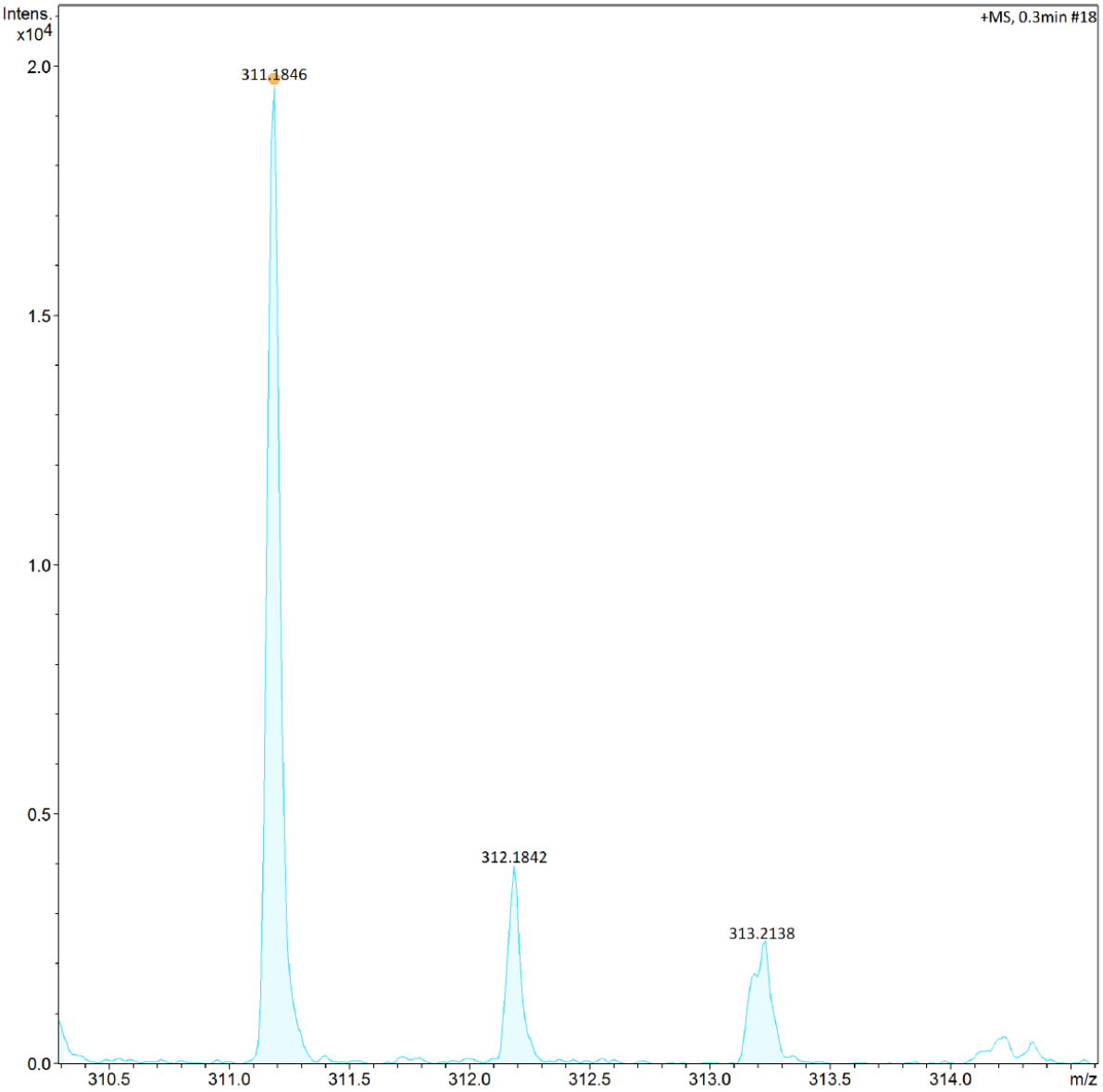

7.389
7.370
7.350
7.258
7.240
7.150
7.130
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
3.81
2.19
4.00


173.14
151.46
129.54
126.25
121.35
200 180 160 140 120 100 80 60 40 20 0 ppm

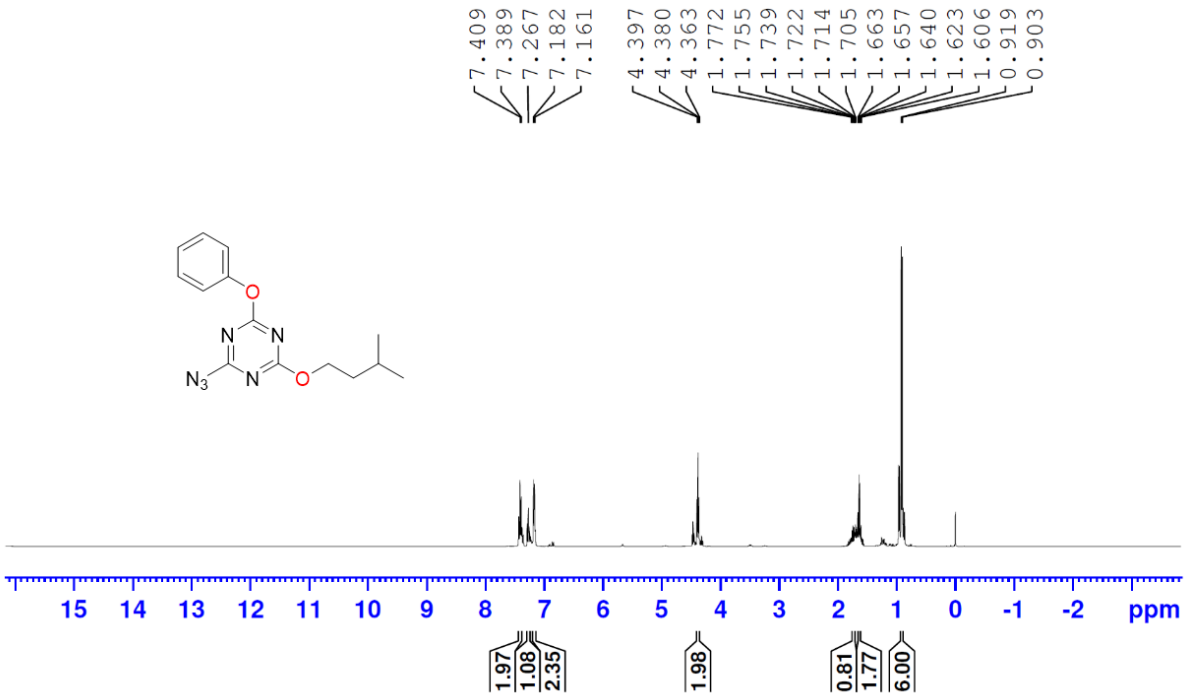


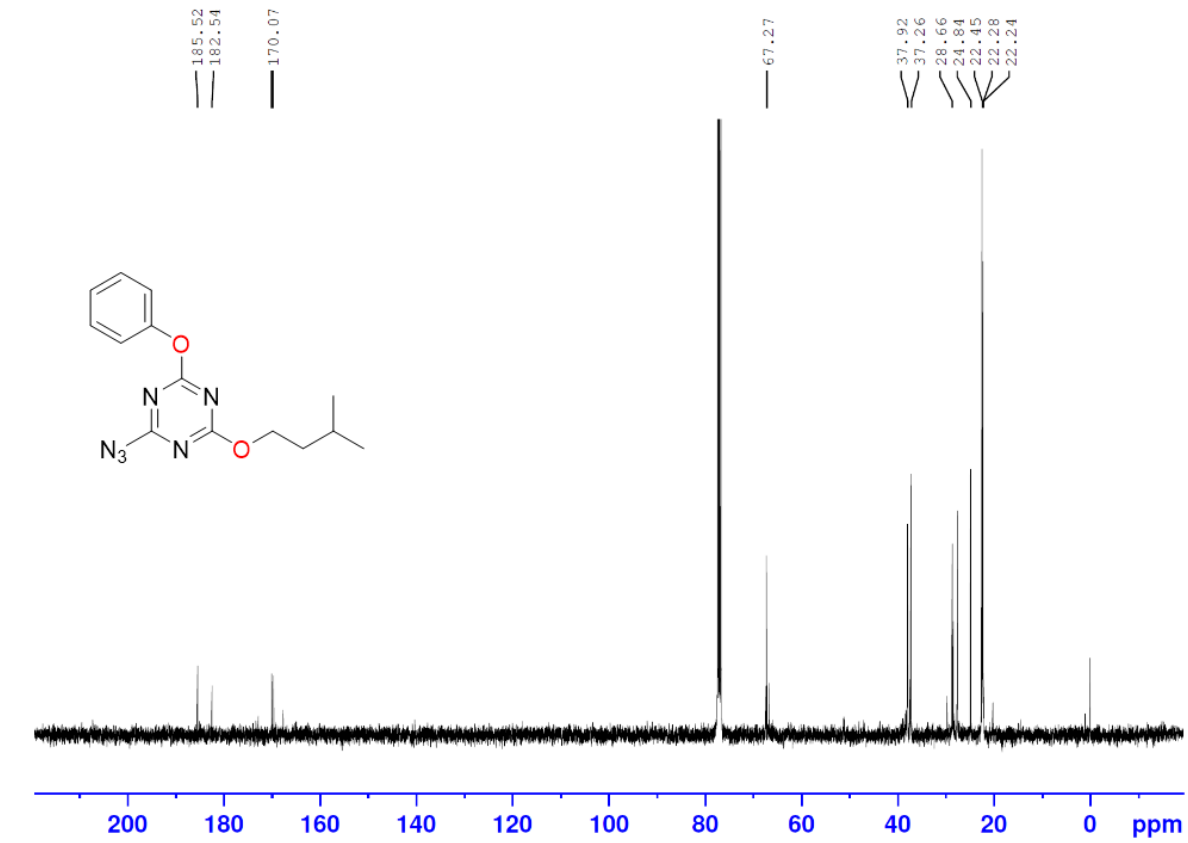
5.17. Characterization of *2-azido-4-(isopentyloxy)-6-(isopentylthio)-1,3,5-triazine* (18)

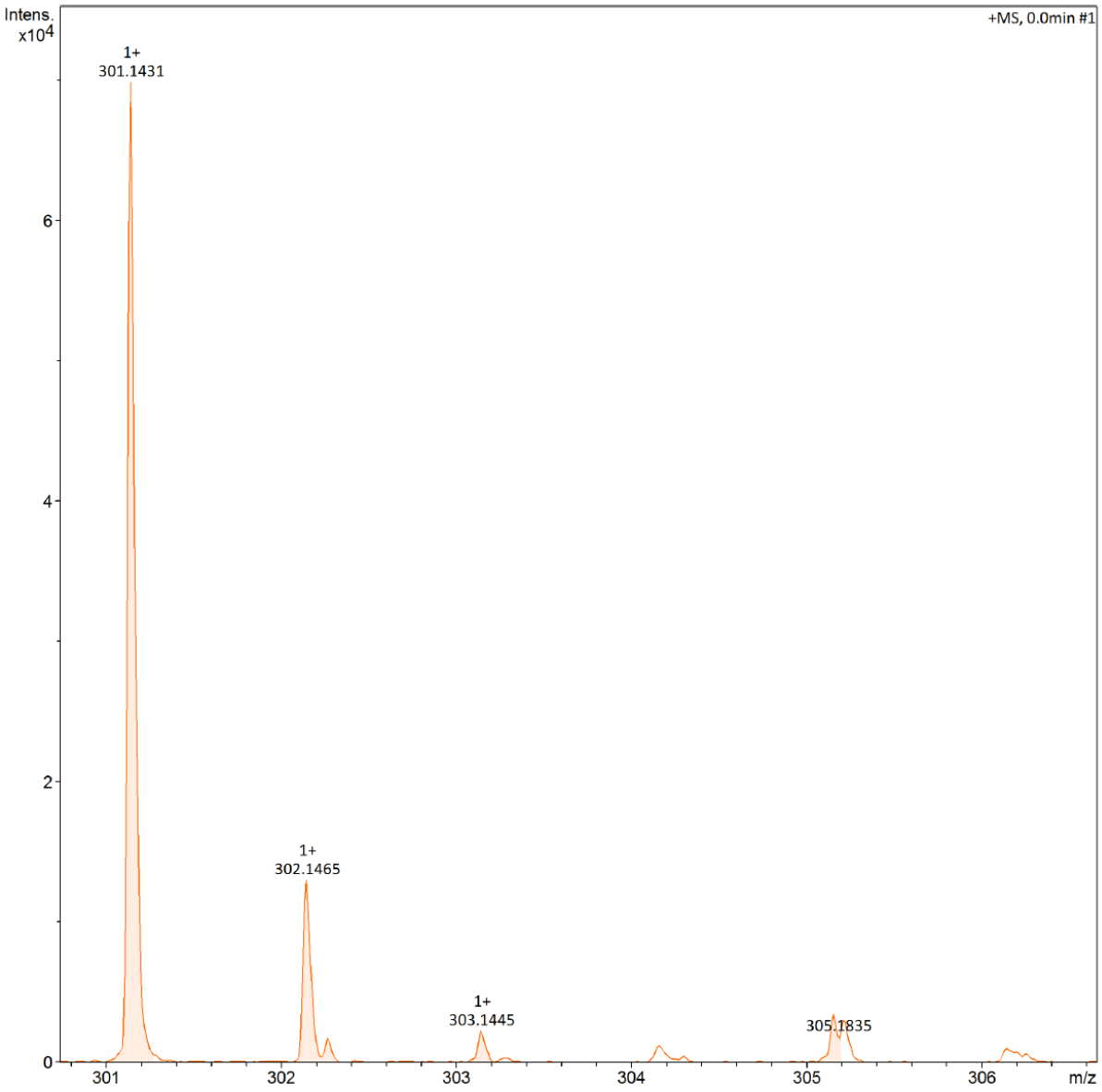

7.268
4.444
4.437
4.427
4.411
4.394
3.159
3.143
3.140
3.120
3.104
1.779
1.744
1.728
1.711
1.701
1.693
1.684
1.672
1.667
1.655
1.650
1.643
1.638
1.624
1.611
1.605
1.597
1.589
1.504
1.487
1.256
1.213
0.960
0.957
0.952
0.944
0.940
0.935
0.906
0.866
0.850
0.832
0.000
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.87
1.95
2.19
4.26
12.00
185.52
182.54
170.07
67.27
37.92
37.26
28.66
24.84
22.45
22.28
22.24
200 180 160 140 120 100 80 60 40 20 0 ppm

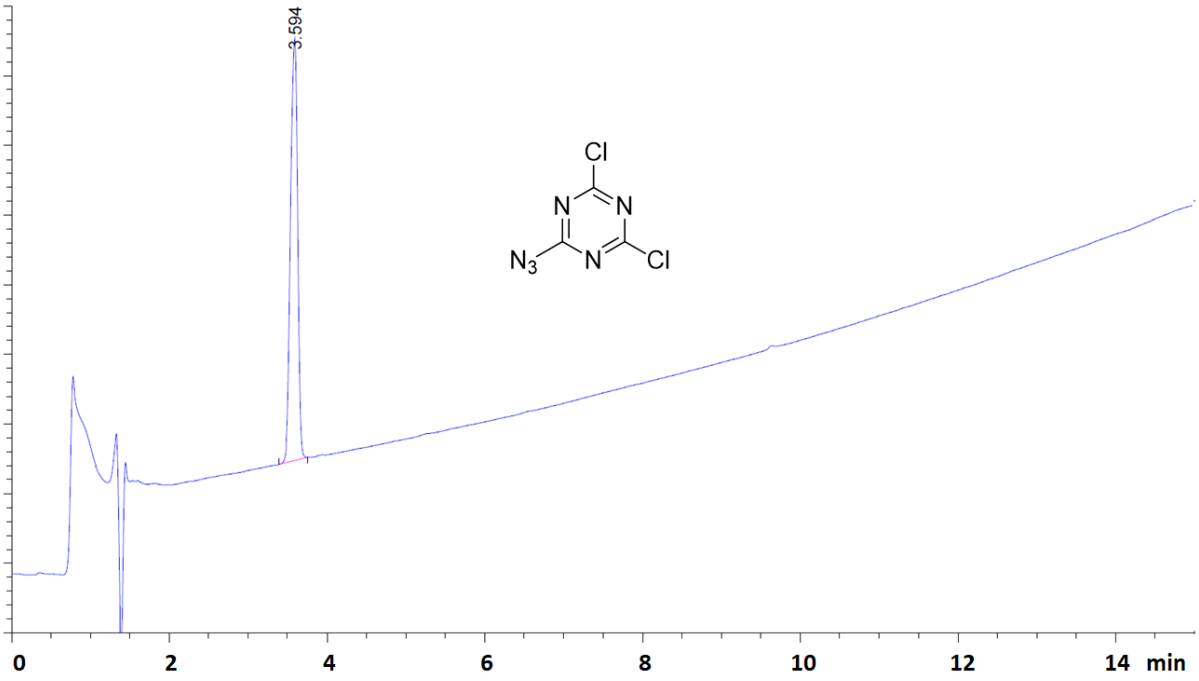


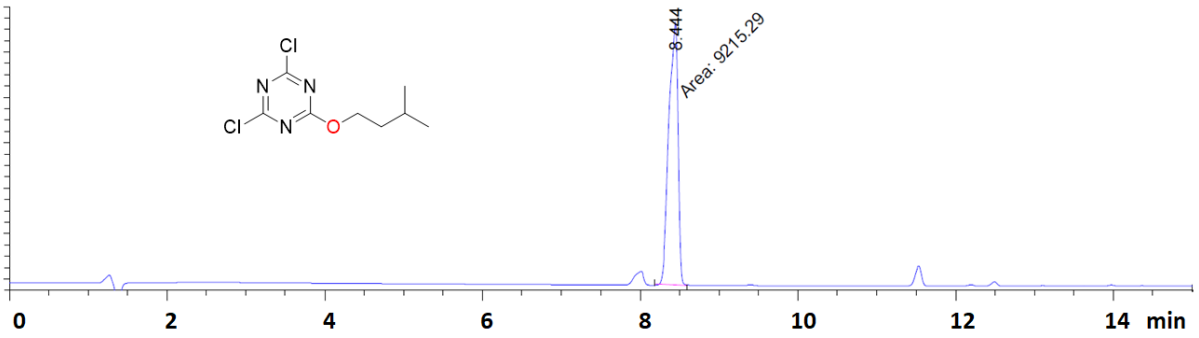
5.18. Characterization of *2-azido-4-(isopentyloxy)-6-phenoxy-1,3,5-triazine* (19)

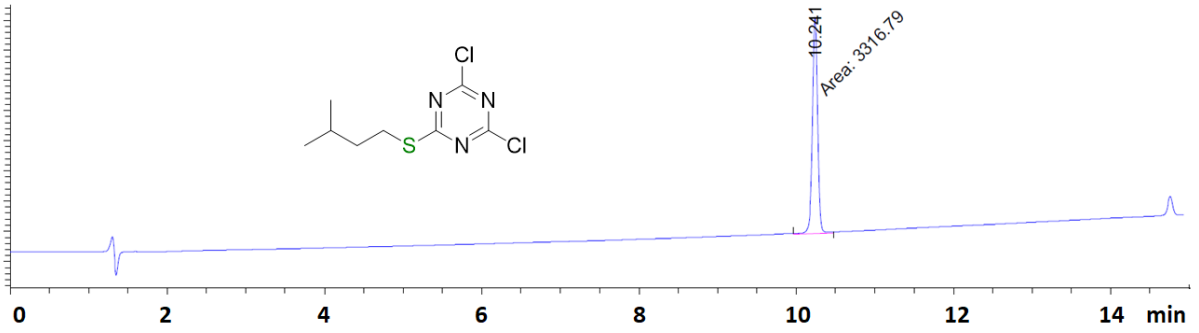

7.409
7.389
7.267
7.182
7.161
4.397
4.380
4.363
1.772
1.755
1.739
1.722
1.714
1.705
1.663
1.657
1.640
1.623
1.606
0.919
0.903
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.97
1.08
2.35
1.98
0.81
1.77
6.00

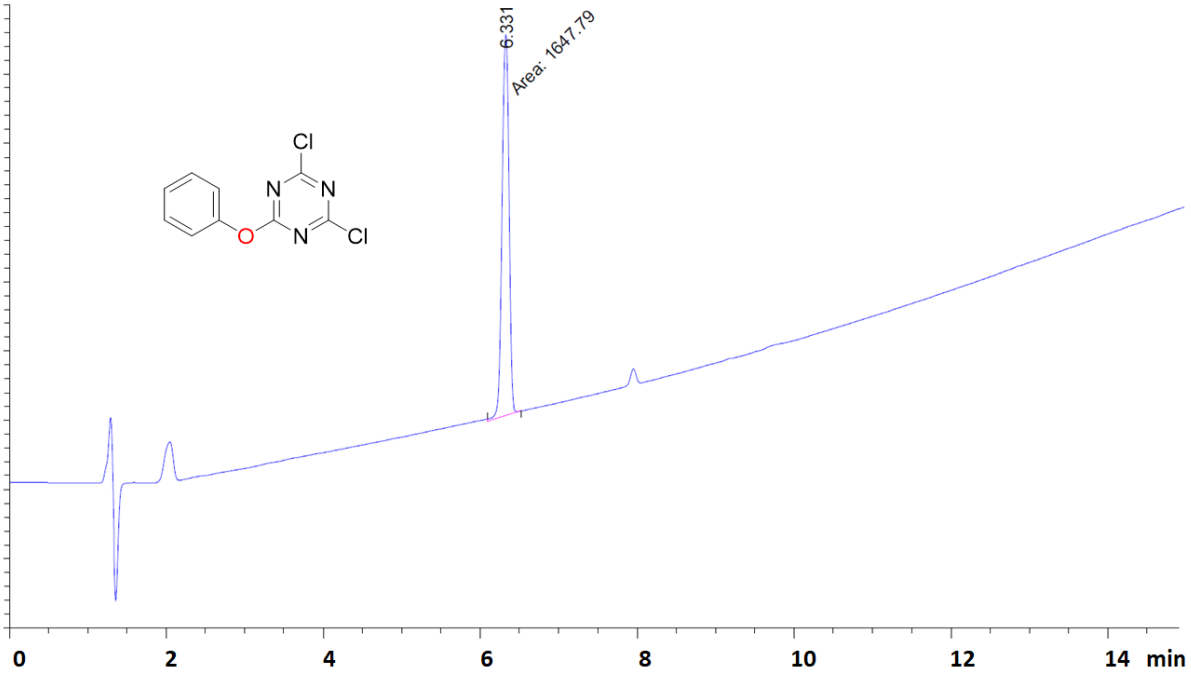

185.52
182.54
170.07
67.27
37.92
37.26
28.66
24.84
22.45
22.28
22.24
200 180 160 140 120 100 80 60 40 20 0 ppm

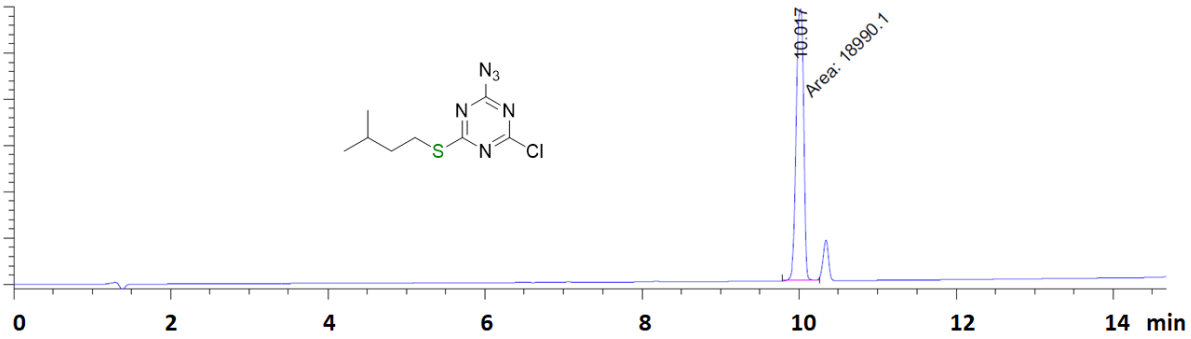

Intens.
x10^4
+MS, 0.0min #1
1+
301.1431
1+
302.1465
1+
303.1445
305.1835
6
4
2
0
301
302
303
304
305
306
m/z

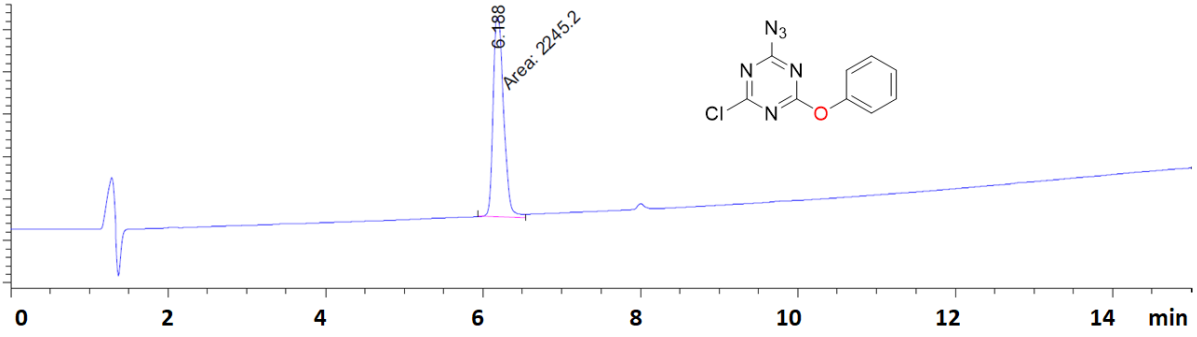

3.594
Cl
N
N
N3
N
Cl
0
2
4
6
8
10
12
14
min

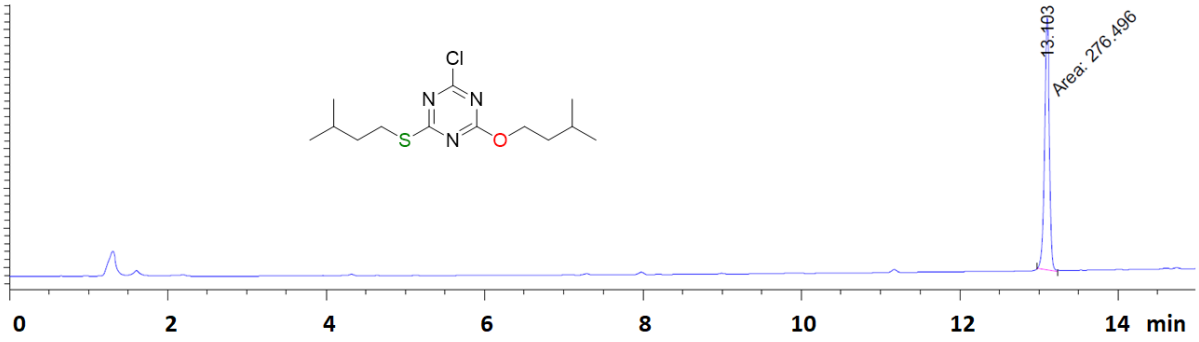

Cl
N
N
Cl
N
O
8.444
Area: 9215.29
0
2
4
6
8
10
12
14
min

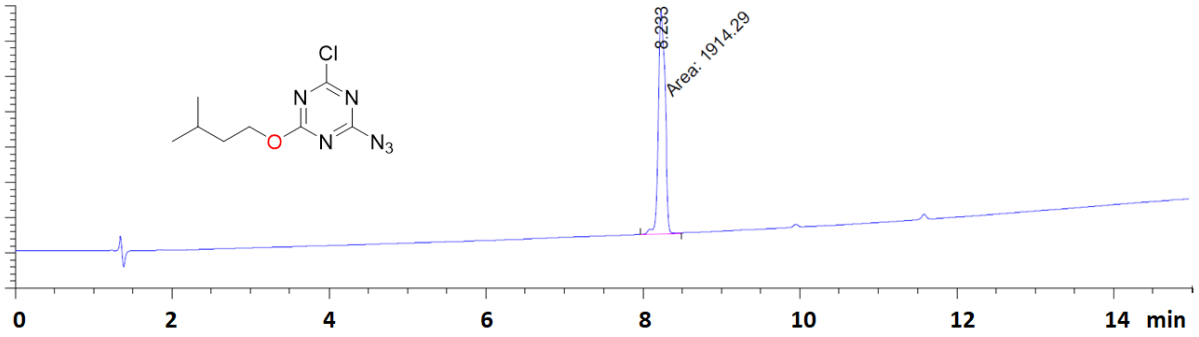

Cl
N
N
S
N
Cl
10.241
Area: 3316.79
0
2
4
6
8
10
12
14
min

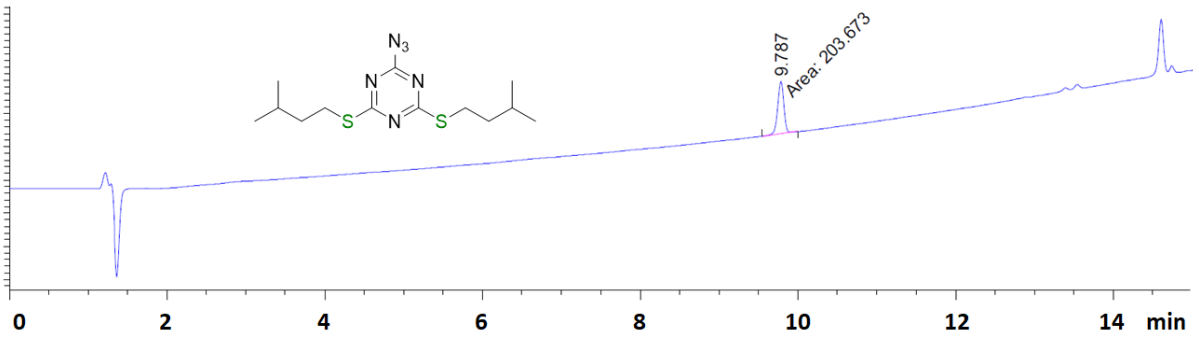

6.331
Area: 1647.79
Cl
N
N
O
N
Cl
0
2
4
6
8
10
12
14
min

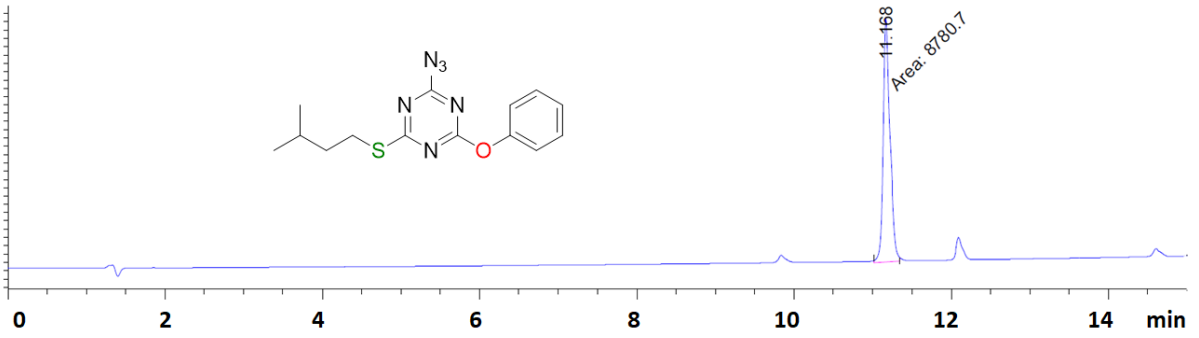

10.017
Area: 18990.1
N3
N
N
S
N
Cl
0
2
4
6
8
10
12
14
min

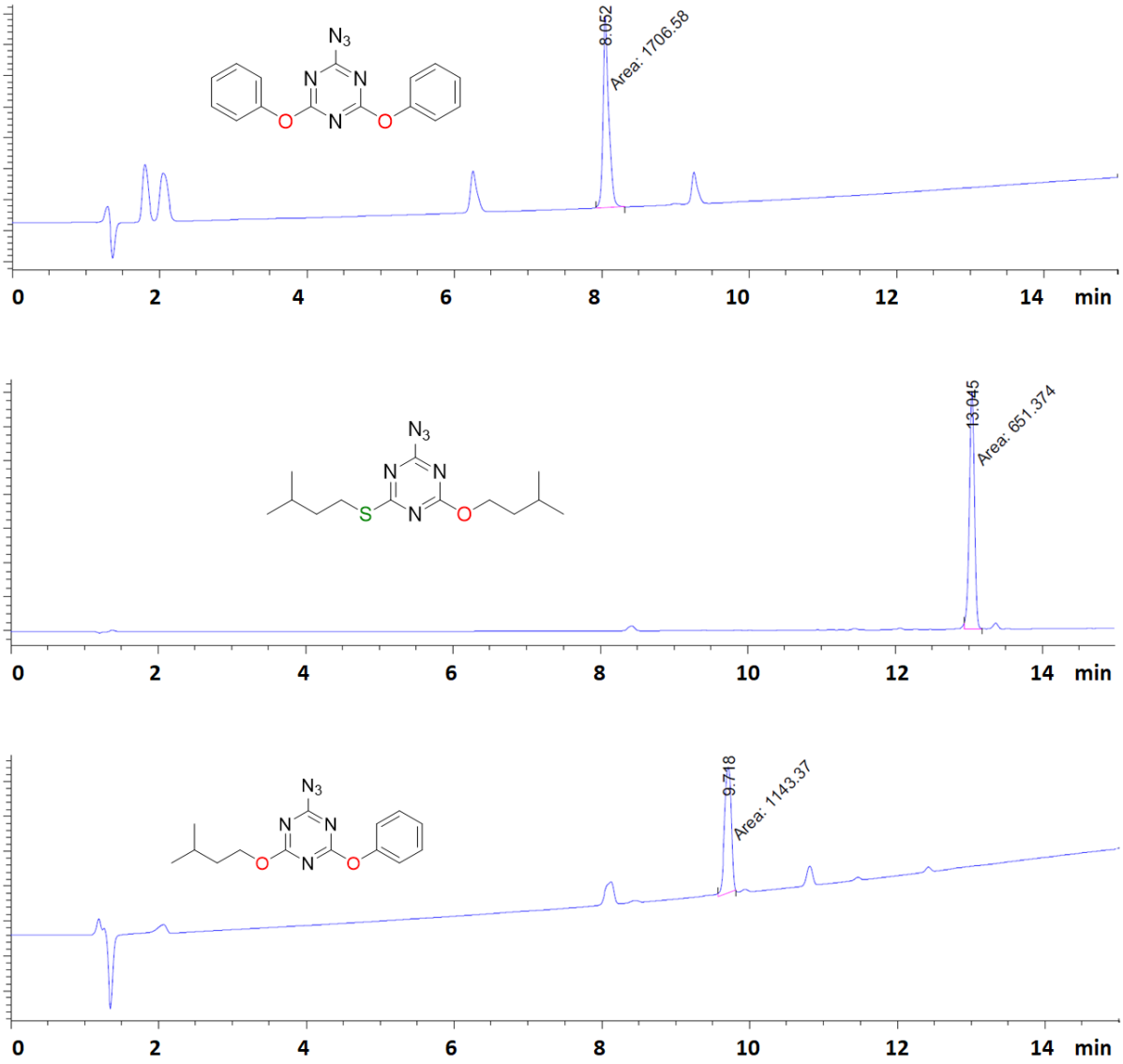

6.188
Area: 2245.2
N3
N
N
Cl
N
O
0
2
4
6
8
10
12
14
min


Cl
N
N
S
N
O
13.103
Area: 276.496
0
2
4
6
8
10
12
14
min


Cl
N
N
O
N
N3
8.233
Area: 1914.29
0
2
4
6
8
10
12
14
min


N3
N
N
S
N
S
9.787
Area: 203.673
0
2
4
6
8
10
12
14
min


N3
N
N
S
N
O
11.168
Area: 8780.7
0
2
4
6
8
10
12
14
min



6. **Theoretical calculations:** Cartesian Coordinates of molecules for NBO calculations

1. TA

0 1

C	1.27012700	-0.16535400	-0.00003900
C	-0.77814500	-1.01726200	0.00001100
C	-0.49180600	1.18253700	0.00006400
Cl	-1.15664700	2.78037700	-0.00007600
Cl	-1.82980500	-2.39171400	0.00000200
Cl	2.98629300	-0.38858700	0.00005600
N	0.83176700	1.08718400	0.00000400
N	-1.35730100	0.17665000	0.00001300
N	0.52577000	-1.26395100	-0.00000500

1 6 1.0 7 1.5 9 1.5
2 5 1.0 8 1.5 9 1.5
3 4 1.0 7 1.5 8 1.5
4
5
6
7
8
9

2. TA-N_3

0 1

C	-0.76237900	-0.82579500	-0.00000200
C	1.44699800	-0.58946300	0.00000100
C	0.15044100	1.20945600	0.00000000
N	0.42944500	-1.43038800	-0.00000100
N	-0.96527600	0.49958200	-0.00000100
N	1.39089500	0.74011600	0.00000100
Cl	-0.02562300	2.93580700	0.00000000
Cl	3.03430900	-1.28912700	0.00000000
N	-1.85236800	-1.68409300	-0.00000100
N	-2.97621100	-1.13882600	0.00000000
N	-4.04906000	-0.80906700	0.00000200

1 4 1.5 5 1.5 9 1.0
2 4 2.0 6 1.5 8 1.0
3 5 2.0 6 1.5 7 1.0
4
5
6
7
8
9 10 2.0
10 11 3.0
11

3. TA-SH

0 1

C	2.03884400	1.05837700	0.75750500
H	1.75712200	0.28435700	1.47200900
H	2.69099500	1.77264900	1.26335500
C	2.69872500	0.46433700	-0.48736100
H	2.97432700	1.27231300	-1.17549400
H	1.96596400	-0.15976900	-1.00597800
C	3.94444700	-0.39188000	-0.17923600
H	3.64213000	-1.17275300	0.53123100
C	4.43023100	-1.08613400	-1.45928200
H	4.73649300	-0.35003100	-2.21057500
H	5.29052900	-1.72986500	-1.25547200
H	3.64431500	-1.70608700	-1.89988100

C	5.07922300	0.42148900	0.46026000
H	5.39173900	1.24007200	-0.19789300
H	4.79078000	0.85568400	1.42120400
H	5.95403200	-0.20958700	0.64006100
C	-0.70340000	0.83288800	0.22189900
C	-2.85177100	0.38308700	-0.19446800
C	-1.45034900	-1.27192300	0.24823100
N	-1.92411100	1.31012300	-0.07990400
N	-0.41390200	-0.46493700	0.39682200
N	-2.69662100	-0.93174900	-0.04653100
Cl	-1.14631300	-2.97323200	0.46116800
Cl	-4.45797400	0.92332000	-0.58318200
S	0.53507400	2.05600000	0.39960400

1 2 1.0 3 1.0 4 1.0 25 1.0
2
3
4 5 1.0 6 1.0 7 1.0
5
6
7 8 1.0 9 1.0 13 1.0
8
9 10 1.0 11 1.0 12 1.0
10
11
12
13 14 1.0 15 1.0 16 1.0
14
15
16
17 20 1.5 21 1.5 25 1.0
18 20 2.0 22 1.5 24 1.0
19 21 2.0 22 1.5 23 1.0
20
21
22
23
24
25

4. TA-OH

0 1

C	1.87398500	0.85705300	0.89190900
H	1.69890100	-0.02743000	1.50487500
H	2.39283500	1.61278100	1.47878300
C	2.61918200	0.51226400	-0.39074000
H	2.75926700	1.42690800	-0.97855200
H	1.99266900	-0.16097700	-0.98334500
C	3.98413400	-0.16265100	-0.14889700

H	3.81170800	-1.05035400	0.47428100
C	4.57724100	-0.63767000	-1.48264100
H	4.76720000	0.20992400	-2.14982900
H	5.52695000	-1.15684800	-1.32678200
H	3.90035800	-1.32441800	-1.99861700
C	4.97351900	0.75282100	0.58843100
H	5.14184000	1.67759100	0.02568500
H	4.62502200	1.02793300	1.58744100
H	5.94122400	0.25808000	0.70863500
C	-0.46684400	0.74865900	0.36152200
C	-2.63292300	0.67188000	-0.14379400
C	-1.51770700	-1.21048700	0.17171900
N	-1.58564200	1.43451900	0.08031800
N	-0.37883800	-0.58712200	0.41871600
N	-2.68591100	-0.66018200	-0.11823500
Cl	-1.47634800	-2.95012700	0.23073300
Cl	-4.12515000	1.48344700	-0.51775100
O	0.59459000	1.49233000	0.59826000

1 2 1.0 3 1.0 4 1.0 25 1.0
2
3
4 5 1.0 6 1.0 7 1.0
5
6
7 8 1.0 9 1.0 13 1.0
8
9 10 1.0 11 1.0 12 1.0
10
11
12
13 14 1.0 15 1.0 16 1.0
14
15
16
17 20 1.5 21 1.5 25 1.5
18 20 2.0 22 1.5 24 1.0
19 21 2.0 22 1.5 23 1.0
20
21
22
23
24
25

5. TA-pOH

0 1

C	-0.29789400	-0.70903800	0.00004700
C	-1.36530100	1.24195700	0.00006700

C	-2.51752800	-0.64699800	-0.00003600
N	-0.19765400	0.62134000	0.00010600
N	-1.43977700	-1.40511700	-0.00002100
N	-2.56708300	0.68346600	-0.00000300
Cl	-4.04887000	-1.46796000	-0.00009700
Cl	-1.32062600	2.97940400	0.00016100
O	0.80285700	-1.45634000	0.00005600
C	2.07222300	-0.84326300	0.00000900
C	2.69650500	-0.59774300	1.21385500
C	2.69618700	-0.59722600	-1.21392200
C	3.98616600	-0.06975700	1.20722400
H	2.18199300	-0.81850900	2.14098700
C	3.98583100	-0.06927300	-1.20741100
H	2.18139500	-0.81762300	-2.14098700
C	4.63043800	0.19619800	-0.00011500
H	4.48675000	0.12981300	2.14745100
H	4.48620200	0.13067400	-2.14767200
H	5.63407400	0.60486200	-0.00018500

1 4 1.5 5 1.5 9 1.5
2 4 2.0 6 1.5 8 1.0
3 5 2.0 6 1.5 7 1.0
4
5
6
7
8
9 10 1.0
10 11 1.5 12 1.5
11 13 1.5 14 1.0
12 15 1.5 16 1.0
13 17 1.5 18 1.0
14
15 17 1.5 19 1.0
16
17 20 1.0
18
19
20

6. TA-N_3-OH

0 1

C	2.37843800	-0.92694900	0.04010400
C	0.19188000	-0.50078000	-0.03909400
C	1.66152200	1.17615200	-0.07911600
N	1.15221700	-1.42633800	0.03044300
N	2.70960400	0.37827000	-0.01296700
N	0.38709100	0.82658800	-0.09683100
Cl	1.99419200	2.88744000	-0.15203100

N	3.40145900	-1.87151000	0.11315800
N	4.56286300	-1.41867400	0.12438300
N	5.65968100	-1.17494200	0.14398900
O	-1.04055900	-0.97371000	-0.04946700
C	-2.15324900	-0.03839100	-0.11522900
H	-2.07432300	0.64790900	0.72839600
H	-2.06559400	0.54245400	-1.03674900
C	-3.42519100	-0.86785900	-0.08598000
H	-3.46472300	-1.43111200	0.85355500
H	-3.37020300	-1.60552300	-0.89296900
C	-4.71166700	-0.03427100	-0.24451900
H	-4.62455300	0.54450600	-1.17424200
C	-4.92123200	0.95509300	0.91193400
H	-4.97218500	0.42697600	1.87052800
H	-4.11927600	1.69473700	0.97939800
H	-5.85886900	1.50358500	0.78623600
C	-5.92483900	-0.96404500	-0.38657700
H	-6.84275800	-0.39076200	-0.54371600
H	-5.80778400	-1.64878500	-1.23139700
H	-6.06091600	-1.56823300	0.51686100

1 4 1.5 5 1.5 8 1.0
2 4 1.5 6 1.5 11 1.5
3 5 2.0 6 2.0 7 1.0
4
5
6
7
8 9 2.0
9 10 3.0
10
11 12 1.0
12 13 1.0 14 1.0 15 1.0
13
14
15 16 1.0 17 1.0 18 1.0
16
17
18 19 1.0 20 1.0 24 1.0
19
20 21 1.0 22 1.0 23 1.0
21
22
23
24 25 1.0 26 1.0 27 1.0
25
26
27

7. TA-N_3-SH

0 1

C	2.71691500	-0.79606200	0.04211000
C	0.48171300	-0.69508600	-0.00771100
C	1.69359200	1.17842200	-0.08009200
N	1.57326700	-1.46677200	0.05473200
N	2.84943500	0.54180700	-0.02440400
N	0.48313600	0.64805100	-0.07769100
Cl	1.77627700	2.91966400	-0.16645500
N	3.86616100	-1.58185500	0.10457200
N	4.95004700	-0.96583100	0.09300500
N	5.99981800	-0.56498500	0.09185100
C	-2.27352000	-0.20752100	-0.09631300
H	-2.09136600	0.47126400	0.73497200
H	-2.10359200	0.33598100	-1.02664000
C	-3.67696200	-0.81610300	-0.05370900
H	-3.82877700	-1.33044300	0.90299700
H	-3.76265400	-1.57843100	-0.83602800
C	-4.80329300	0.21855700	-0.25455000
H	-4.61151800	0.73738600	-1.20344000
C	-4.84344000	1.27100800	0.86295900
H	-4.99517100	0.79630700	1.83879900
H	-3.92312900	1.85803700	0.91514600
H	-5.66782600	1.97185100	0.70450600
C	-6.15650100	-0.49578500	-0.37584800
H	-6.96271700	0.21921700	-0.56191000
H	-6.15484000	-1.21959500	-1.19597400
H	-6.39788000	-1.03577600	0.54613200
S	-1.03633200	-1.56734800	0.00597700

1 4 1.5 5 1.5 8 1.0
2 4 1.5 6 1.5 27 1.0
3 5 2.0 6 2.0 7 1.0
4
5
6
7
8 9 2.0
9 10 3.0
10
11 12 1.0 13 1.0 14 1.0 27 1.0
12
13
14 15 1.0 16 1.0 17 1.0
15
16
17 18 1.0 19 1.0 23 1.0
18
19 20 1.0 21 1.0 22 1.0
20
21

22
23 24 1.0 25 1.0 26 1.0
24
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8. TA-N_3-pOH

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C	-2.25312900	-0.81190600	0.00007500
C	-0.02842500	-0.79116900	0.00006500
C	-1.15610100	1.12520700	-0.00011700
O	1.10366200	-1.49559700	0.00010700
N	-3.43060300	-1.55601300	0.00012800
N	-1.13639700	-1.52857400	0.00014000
N	0.03130800	0.54504900	-0.00006200
N	-2.33564200	0.53107600	-0.00005500
N	-4.49086100	-0.89927600	0.00006500
N	-5.52513900	-0.46067700	-0.00001100
Cl	-1.16706800	2.86741200	-0.00026600
C	2.34688800	-0.83515500	0.00008000
C	2.96251600	-0.56521600	1.21353500
C	2.96287200	-0.56614000	-1.21339500
C	4.23241200	0.00864500	1.20720500
H	2.45600600	-0.80368600	2.14070500
C	4.23276900	0.00772600	-1.20713000
H	2.45663100	-0.80531800	-2.14053000
C	4.86737100	0.29686100	0.00002000
H	4.72508000	0.22694500	2.14751400
H	4.72571300	0.22531200	-2.14746000
H	5.85572300	0.74131100	-0.00000500

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9. TA-SH-SH

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C	-3.45466800	-0.36305400	-0.93230900
H	-2.59093000	-0.75889500	-1.46730900
H	-4.32307400	-0.41843500	-1.59152400
C	-3.68704900	-1.10812000	0.38301700
H	-4.56324000	-0.68823300	0.89135600
H	-2.82744300	-0.93502300	1.03612700
C	-3.87739700	-2.62871200	0.20788800
H	-3.00899700	-3.00989700	-0.34605900
C	-3.89606100	-3.31786600	1.57957900
H	-4.74120800	-2.96705900	2.18198800
H	-3.99163000	-4.40247300	1.47453200
H	-2.97922800	-3.11477400	2.14030400
C	-5.14215000	-2.97805500	-0.59010100
H	-6.03690200	-2.59061200	-0.09003600
H	-5.12119200	-2.56847900	-1.60345800
H	-5.25717700	-4.06192800	-0.68048700
C	-1.49501000	1.54493100	-0.30890300
C	0.22180300	2.87247700	0.20344300
C	0.54253200	0.67054400	0.07034000
N	-1.05799700	2.80306400	-0.09120700
N	-0.74277000	0.44991900	-0.23808200
N	1.08743500	1.87158800	0.30368500
Cl	0.86586100	4.47070700	0.50066800
C	3.18812400	-0.07661400	0.59352900
H	3.06242700	0.52090400	1.49555200
H	3.49459500	0.59251600	-0.20950700
C	4.19747600	-1.20390500	0.82553400
H	5.12608800	-0.72885700	1.16768500
H	3.85232700	-1.82899800	1.65678900
C	4.52314700	-2.10497200	-0.38234100
H	3.59479300	-2.59277100	-0.70571100
C	5.50390700	-3.20784600	0.03941300
H	5.10658400	-3.80099200	0.86836400
H	5.71064900	-3.88915500	-0.79054600
H	6.45915200	-2.77963100	0.36274200
C	5.07524000	-1.31011000	-1.57362800
H	4.35394300	-0.58358900	-1.95611300
H	5.98511400	-0.76723200	-1.29363000
H	5.33037000	-1.97941000	-2.39995600
S	1.53673000	-0.77415700	0.15903300
S	-3.19677500	1.44583300	-0.73190800

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10. TA-OH-SH

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C	-3.41859300	-0.16169600	-0.99954300
H	-2.66115800	-0.74876200	-1.52030500
H	-4.26438300	0.01359200	-1.66250400
C	-3.84209300	-0.82847700	0.30342200

H	-4.58682900	-0.19609900	0.80106800
H	-2.97004400	-0.88102100	0.96152600
C	-4.41145300	-2.24863300	0.11499300
H	-3.66457600	-2.83805200	-0.43371200
C	-4.61996100	-2.91662000	1.48121900
H	-5.35328300	-2.36345100	2.07797400
H	-4.98941500	-3.93964800	1.36649000
H	-3.68788700	-2.95849500	2.05169400
C	-5.71652600	-2.26016800	-0.69567900
H	-6.48381200	-1.65036700	-0.20605200
H	-5.58252700	-1.87685200	-1.71059800
H	-6.10855000	-3.27731000	-0.78339600
C	-1.63143000	1.33398600	-0.42519400
C	-0.00834000	2.74937400	0.12147100
C	0.43910600	0.57178100	0.00255500
N	-1.27323600	2.61275000	-0.20506400
N	-0.82345300	0.28096500	-0.33530300
N	0.91127600	1.79961400	0.24787500
Cl	0.53957500	4.38189000	0.43039800
C	3.10054100	-0.03508900	0.62175000
H	2.90650900	0.54869400	1.52061900
H	3.40361200	0.65472600	-0.16465600
C	4.15723200	-1.10969300	0.89106800
H	5.04437800	-0.58991000	1.27560900
H	3.80952000	-1.75815700	1.70315300
C	4.58103100	-1.98357200	-0.30629900
H	3.69224700	-2.50866600	-0.67864600
C	5.58867700	-3.04613200	0.15381300
H	5.17751400	-3.66687600	0.95539600
H	5.86789100	-3.70714800	-0.67134800
H	6.50581800	-2.57921900	0.52975000
C	5.15437800	-1.15295800	-1.46266600
H	4.42131600	-0.45451100	-1.87399100
H	6.02469500	-0.57373300	-1.13386500
H	5.47888000	-1.80162700	-2.28111900
S	1.50788700	-0.81727000	0.11806200
O	-2.90205100	1.17639400	-0.76085600

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11. TA-pOH-SH

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C	1.11021000	-0.16652600	0.12736700
C	1.00020800	2.04014300	-0.09167300
C	-0.87213200	0.86571900	0.19368300
N	1.78356800	0.96941800	-0.04952400
N	-0.21100600	-0.28832000	0.25456400
N	-0.30932800	2.07996900	0.01942500
Cl	1.81085600	3.56949800	-0.32165900
C	-3.01630700	-0.88426200	0.57681700
H	-2.42785800	-1.24235200	1.42083200
H	-2.68800900	-1.42456900	-0.31036000
C	-4.51315300	-1.06307900	0.84472400
H	-4.66942500	-2.12737000	1.06391400
H	-4.77964300	-0.52249500	1.75991100
C	-5.47631000	-0.64704500	-0.28504700
H	-5.32033100	0.41923100	-0.49216200
C	-6.92920000	-0.82266700	0.17788000
H	-7.13172300	-0.24845400	1.08680200

H	-7.63060800	-0.48888300	-0.59179600
H	-7.14712900	-1.87497600	0.39172900
C	-5.22179800	-1.42012600	-1.58618900
H	-4.22181400	-1.23657200	-1.98695100
H	-5.32976700	-2.49914900	-1.42759000
H	-5.93935900	-1.12548300	-2.35695800
S	-2.61849300	0.90100400	0.34339500
O	1.77887000	-1.32383700	0.18917400
C	3.18034700	-1.33084000	0.07333100
C	3.74807700	-1.53492800	-1.17602500
C	3.95184800	-1.23442700	1.22260300
C	5.13483400	-1.63019300	-1.27584200
H	3.11271800	-1.61767800	-2.04927600
C	5.33748800	-1.33088400	1.11097000
H	3.47271600	-1.08706400	2.18272400
C	5.93020400	-1.52675200	-0.13562200
H	5.59166000	-1.78730900	-2.24605700
H	5.95220400	-1.25429400	2.00031900
H	7.00821400	-1.60169400	-0.21771400

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12. TA-OH-OH

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C	-2.98859700	-0.06783500	-1.02243600
H	-2.21658100	-0.72545600	-1.42336200
H	-3.76611100	0.08234500	-1.76996700
C	-3.55118900	-0.60485000	0.28771300
H	-4.30889800	0.09331500	0.66278300
H	-2.74210500	-0.63054500	1.02342800
C	-4.16091000	-2.01553800	0.16720600
H	-3.39052100	-2.67729400	-0.25107400
C	-4.52826700	-2.54978400	1.55860500
H	-5.29377800	-1.92245900	2.02810100
H	-4.92469200	-3.56735600	1.49777600
H	-3.65852500	-2.56797500	2.22144900
C	-5.38065700	-2.05555200	-0.76612900
H	-6.16551600	-1.37926000	-0.40979900
H	-5.13219400	-1.76868200	-1.79125700
H	-5.80472100	-3.06283200	-0.80549500
C	-1.18187900	1.40271200	-0.44303000
C	0.46043400	2.79970400	0.08474900
C	0.81897000	0.60657600	0.16891200
N	-0.78697200	2.68361000	-0.30526500
N	-0.42960900	0.33115000	-0.21815300
N	1.32989700	1.82975500	0.34244000
Cl	1.06051500	4.42925300	0.29367600
C	2.95735600	-0.25183400	0.81226900
H	2.95240300	0.27836900	1.76678900
H	3.45740400	0.38328900	0.07986300
C	3.60001100	-1.62167300	0.94124800
H	4.60687900	-1.46793300	1.35108500
H	3.04373900	-2.19459900	1.69105400
C	3.69747100	-2.44279100	-0.35915600
H	2.68555900	-2.52895700	-0.77108200
C	4.20301800	-3.85835500	-0.04884500
H	3.55247600	-4.36589300	0.66954300
H	4.24223900	-4.47032700	-0.95443500
H	5.21275500	-3.83075400	0.37622500
C	4.58761600	-1.76867400	-1.41295500
H	4.21386200	-0.78400200	-1.70561100
H	5.61020700	-1.64202300	-1.03953800
H	4.64045200	-2.37716600	-2.32011900
O	1.58049200	-0.45442900	0.38997200

O -2.43506300 1.26501200 -0.84758500

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13. TA-pOH-OH

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C 1.02676100 -0.48809700 -0.18477700
C 0.43531100 1.64452500 -0.03570400

C	-1.12048900	0.08215400	-0.34039100
N	1.43109500	0.77979000	-0.02408000
N	-0.22162900	-0.90149300	-0.34563100
N	-0.85182500	1.38973700	-0.18526200
Cl	0.86880200	3.32475500	0.17100500
C	-3.42402600	0.70570200	-0.51956300
H	-3.20256100	1.42892600	-1.30660900
H	-3.40918700	1.23450000	0.43495500
C	-4.73806500	-0.00931100	-0.77912000
H	-5.51013000	0.76460600	-0.88161100
H	-4.66937800	-0.51007100	-1.75086600
C	-5.17510900	-1.02953400	0.28975900
H	-4.36001000	-1.75224600	0.40888400
C	-6.41597100	-1.79346200	-0.19232500
H	-6.22726000	-2.30106200	-1.14280100
H	-6.71933300	-2.55081400	0.53595700
H	-7.26428300	-1.11502100	-0.33800100
C	-5.43781100	-0.37451600	1.65305100
H	-4.54964500	0.11987300	2.05518400
H	-6.23558500	0.37370900	1.58214700
H	-5.75071000	-1.12259000	2.38679800
O	1.94262400	-1.46319400	-0.19134700
C	3.30356800	-1.15291300	-0.02919600
C	4.09466200	-1.01567100	-1.16077400
C	3.83807000	-1.09329700	1.25017000
C	5.46182300	-0.79580500	-1.00252200
H	3.64363000	-1.08280900	-2.14323400
C	5.20595900	-0.87259500	1.39662400
H	3.19218500	-1.21796100	2.11058900
C	6.01832100	-0.72197200	0.27342300
H	6.09059900	-0.68481300	-1.87833400
H	5.63588600	-0.82106900	2.39023500
H	7.08195500	-0.55157900	0.39239600
O	-2.37479200	-0.30179300	-0.50738900

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14. TA-pOH-pOH

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C	-1.11138800	-0.76792300	0.00070300
C	-0.00002300	1.15290900	-0.00580600
C	1.11138500	-0.76790200	0.00090300
N	-1.18435300	0.56861500	-0.00387400
N	0.00000300	-1.49435900	0.00328500
N	1.18431600	0.56863800	-0.00367500
Cl	-0.00003900	2.89784400	-0.01188300
O	-2.24108100	-1.48128200	0.00274100
C	-3.48669400	-0.82871900	0.00257400
C	-4.10989900	-0.57284700	-1.21034800
C	-4.10066400	-0.55220600	1.21571800
C	-5.38330000	-0.00685300	-1.20427600
H	-3.60506000	-0.81576100	-2.13728600
C	-5.37403200	0.01374300	1.20969500
H	-3.58890100	-0.77914600	2.14291100
C	-6.01551100	0.28820900	0.00270100
H	-5.88092800	0.20021200	-2.14458000
H	-5.86444000	0.23695900	2.15009500
H	-7.00656500	0.72669200	0.00276200
O	2.24108300	-1.48123600	0.00326900
C	3.48671800	-0.82868500	0.00268500
C	4.10869000	-0.57085900	-1.21045500
C	4.10191900	-0.55418700	1.21565800
C	5.38210000	-0.00488100	-1.20474600
H	3.60293100	-0.81222100	-2.13729600

C	5.37529400	0.01175600	1.20926700
H	3.59106600	-0.78267400	2.14297000
C	6.01553200	0.28821900	0.00207000
H	5.87876700	0.20372200	-2.14521700
H	5.86667700	0.23340900	2.14952700
H	7.00658700	0.72670000	0.00184600

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