Electronic Supplementary Material (ESI) for Dalton Transactions.

Highly luminescent lanthanide complexes sensitised by tertiary amide-linked carbostyril antennae

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X-ray diffraction data. Measurements were performed using graphite-monochromatized Mo K_α radiation at 150 K using a Bruker D8 APEX-II equipped with a CCD camera. The structure was solved by direct methods (SHELXS-2014) and refined by full-matrix least-squares techniques against F^2 (SHELXL-2018). The non-hydrogen atoms were refined with anisotropic displacement parameters. The H atoms of the CH_2 / CH groups were refined with common isotropic displacement parameters for the H atoms of the same group and idealized geometry. The H atoms of the methyl groups were refined with common isotropic displacement parameters for the H atoms of the same group and idealized staggered geometry; one methyl group is modelled as a disordered staggered configuration.

Specific for **5a**:
NH protons are located on the difference map or placed at idealized positions. The cyclen ring shows a positional disorder which is modelled with an occupancy of 0.59 and 0.41 of the two different orientations, respectively.

Specific for **Dy9d**:
Solvent accessible voids were treated using the squeeze algorithm accounting for a 189 electrons in a 531 $Å^3$ large void. The final output of squeeze is appended to the cif file. In addition a refine prior to applying squeeze is attached.

CCDC 1832851 and 1833918 contain the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

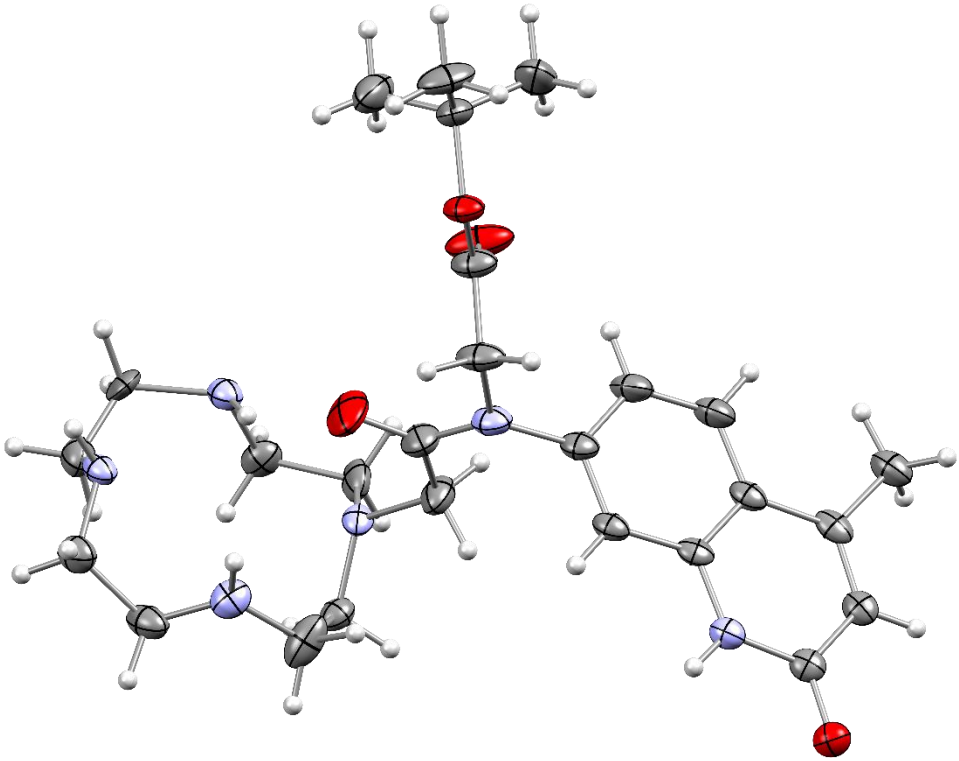


Figure S1. ORTEP plot of **5a**. Ellipsoids are drawn at a 30% probability level. For clarity, only one of the disordered cyclen parts is shown.

Table S1. Crystal data and structure refinement for **ao_dks_57_059a_1_0m_a**.

CCDC-No	1832851	
Empirical formula	$C_{26}H_{40}N_6O_4$	
Formula weight	500.64	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	α = 12.6859(9) Å	α = 90°.
	β = 14.9050(11) Å	β = 94.431(2)°.
	γ = 14.1864(11) Å	γ = 90°.
Volume	2674.4(3) $Å^3$	
Z	4	
Density (calculated)	1.243 Mg/m^3	
Absorption coefficient	0.085 mm^{-1}	
F(000)	1080	
Crystal size	0.2 x 0.12 x 0.1 mm^3	
Theta range for data collection	2.075 to 26.398°.	
Index ranges	–15<=h<=15, –18<=k<=18, –17<=l<=17	
Reflections collected	30611	
Independent reflections	5479 [R(int) = 0.0494]	
Completeness to theta = 25.242°	100.0%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.7088	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5479 / 0 / 450	
Goodness-of-fit on F^2	1.025	
Final R indices [I>2σ(I)]	R1 = 0.0618, wR2 = 0.1482	
R indices (all data)	R1 = 0.1098, wR2 = 0.1759	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.254 and -0.227 e.$Å^{-3}$	

Table S2. Bond lengths [Å] and angles [°] for ao_dks_57_059a_1_0m_a.

C(1)-O(0)	1.246(3)
C(1)-N(1)	1.364(3)
C(1)-C(2)	1.434(4)
C(2)-C(3)	1.349(4)
C(3)-C(4)	1.448(4)
C(3)-C(10)	1.496(4)
C(4)-C(5)	1.398(4)
C(4)-C(9)	1.402(3)
C(5)-C(6)	1.368(4)
C(6)-C(7)	1.395(4)
C(7)-C(8)	1.368(4)
C(7)-N(2)	1.438(4)
C(8)-C(9)	1.398(4)
C(9)-N(1)	1.378(3)
C(12)-N(2)	1.460(3)
C(12)-C(13)	1.517(4)
C(13)-O(3)	1.194(3)
C(13)-O(4)	1.330(3)
C(14)-O(4)	1.484(3)
C(14)-C(16)	1.496(4)
C(14)-C(15)	1.501(4)
C(14)-C(17)	1.507(4)
C(18)-O(2)	1.215(4)
C(18)-N(2)	1.370(4)
C(18)-C(19)	1.521(4)
C(19)-N(10B)	1.365(11)
C(19)-N(10A)	1.537(7)
O(0)-C(1)-N(1)	120.2(2)
O(0)-C(1)-C(2)	124.1(2)
N(1)-C(1)-C(2)	115.8(2)
C(3)-C(2)-C(1)	123.0(3)
C(2)-C(3)-C(4)	119.1(2)
C(2)-C(3)-C(10)	121.4(3)
C(4)-C(3)-C(10)	119.5(3)
C(5)-C(4)-C(9)	117.6(3)
C(5)-C(4)-C(3)	124.0(2)
C(9)-C(4)-C(3)	118.4(2)
C(6)-C(5)-C(4)	121.4(3)
C(5)-C(6)-C(7)	120.0(3)
C(8)-C(7)-C(6)	120.5(3)
C(8)-C(7)-N(2)	119.6(2)
C(6)-C(7)-N(2)	119.9(2)
C(7)-C(8)-C(9)	119.3(2)
N(1)-C(9)-C(8)	119.6(2)
N(1)-C(9)-C(4)	119.2(2)
C(8)-C(9)-C(4)	121.2(2)
N(2)-C(12)-C(13)	112.3(2)
O(3)-C(13)-O(4)	125.5(3)
O(3)-C(13)-C(12)	125.2(3)
O(4)-C(13)-C(12)	109.3(2)
O(4)-C(14)-C(16)	109.8(2)
O(4)-C(14)-C(15)	110.2(2)
C(16)-C(14)-C(15)	112.5(3)
O(4)-C(14)-C(17)	101.9(2)

C(16)-C(14)-C(17)	111.2(3)
C(15)-C(14)-C(17)	110.8(3)
O(2)-C(18)-N(2)	120.6(3)
O(2)-C(18)-C(19)	123.2(3)
N(2)-C(18)-C(19)	116.1(3)
N(10B)-C(19)-C(18)	102.1(5)
C(18)-C(19)-N(10A)	116.6(3)

Symmetry transformations used to generate equivalent atoms:

Table S3. Crystal data and structure refinement for **ao_keb_dk_dy_glyme_1_0m_a**.

CCDC-No	1833918	
Empirical formula	$C_{30}H_{40}DyN_6O_{12}$	
Formula weight	824.19 [+ solvent]	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	α = 8.7962(2) Å	α = 100.199(1)°.
	β = 14.4010(4) Å	β = 98.078(1)°.
	γ = 17.6620(5) Å	γ = 107.476(1)°.
Volume	2055.13(9) $Å^3$	
Z	2	
Density (calculated)	1.332 Mg/m^3	
Absorption coefficient	1.873 mm^{-1}	
F(000)	834	
Crystal size	0.12 x 0.10 x 0.04 mm^3	
Theta range for data collection (2Θ)	3.412 to 61.754°.	
Index ranges	–12<=h<=12, –20<=k<=20, –25<=l<=24	
Reflections collected	46688	
Independent reflections	12686 [R(int) = 0.0474]	
Completeness to theta = 25.242°	99.9%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6008	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12686/2/451	
Goodness-of-fit on F^2	0.998	
Final R indices [I>2σ(I)]	R1 = 0.0318, wR2 = 0.0686	
R indices (all data)	R1 = 0.0396, wR2 = 0.0708	
Largest diff. peak and hole	1.63 and –1.25 $e.Å^{-3}$	

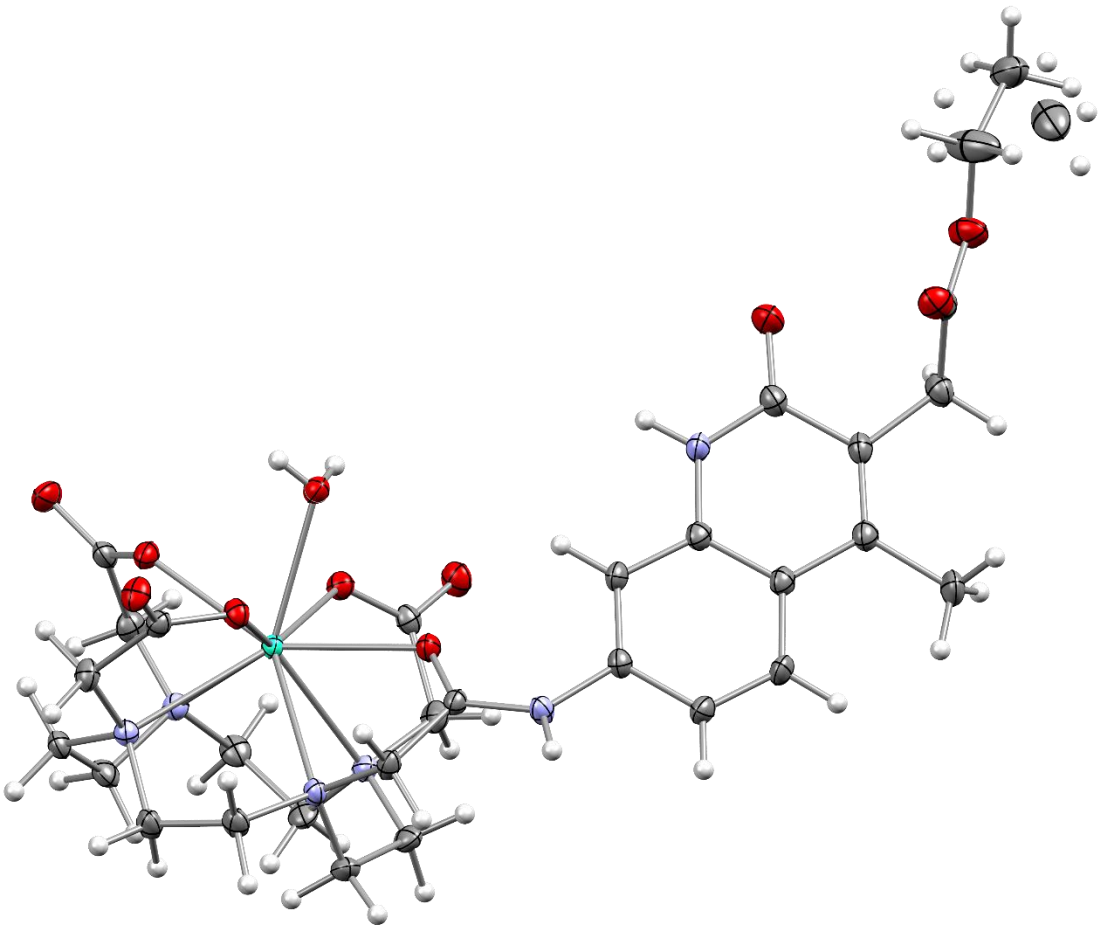


Figure S2. ORTEP plot of **Dy9d**. Ellipsoids are drawn at a 50% probability level.

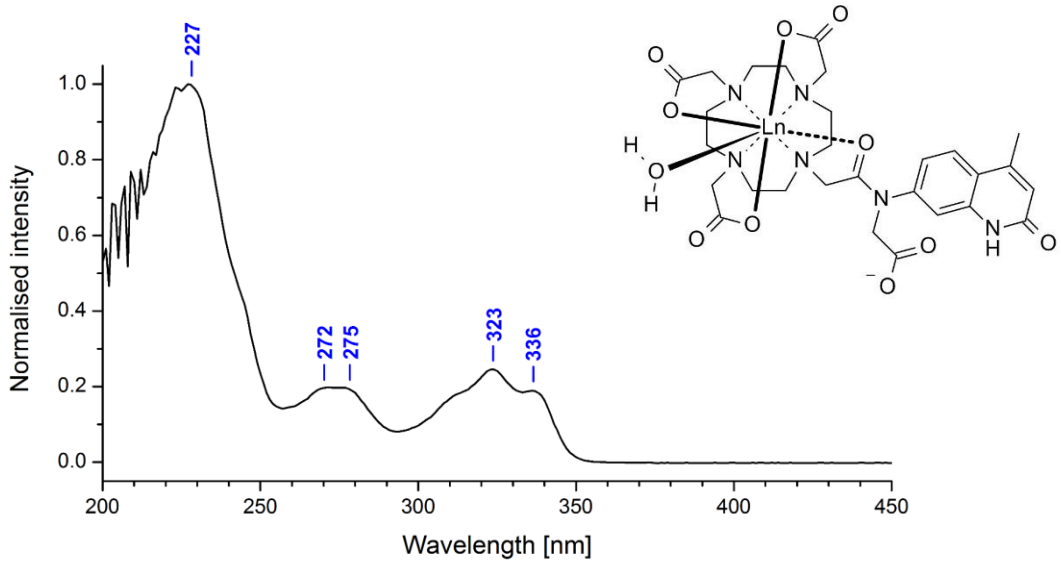


Figure S3. Normalised absorption spectrum of **Gd1a** in 0.01 M PIPES-buffered aqueous solution, pH 6.5. Blue numbers show local maxima of the spectra.

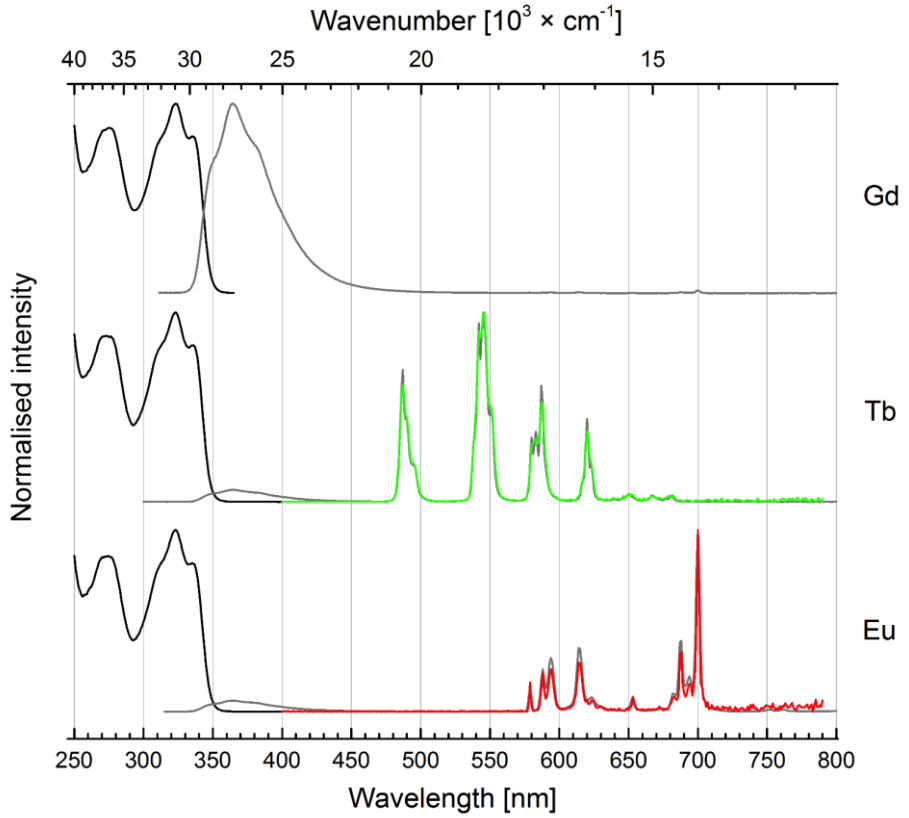


Figure S4. Excitation spectra of the Ln-centered emissions (Tb 545 nm, Eu 700 nm) and of the ligand centered emission (**Gd1a** 364 nm) at 298 K (black lines, left). Steady-state emission spectra of **Ln1a** at 298 K (grey lines, right) and time-resolved emission spectra showing the Ln-centered emissions (Tb (green), Eu (red), 298 K, coloured lines, right). Excitation at λ_{ex} = 336 nm; [**Ln1a**] = nominally 3.0×10^{-5} M, PIPES-buffered aqueous solutions 0.01 M, pH 6.5.

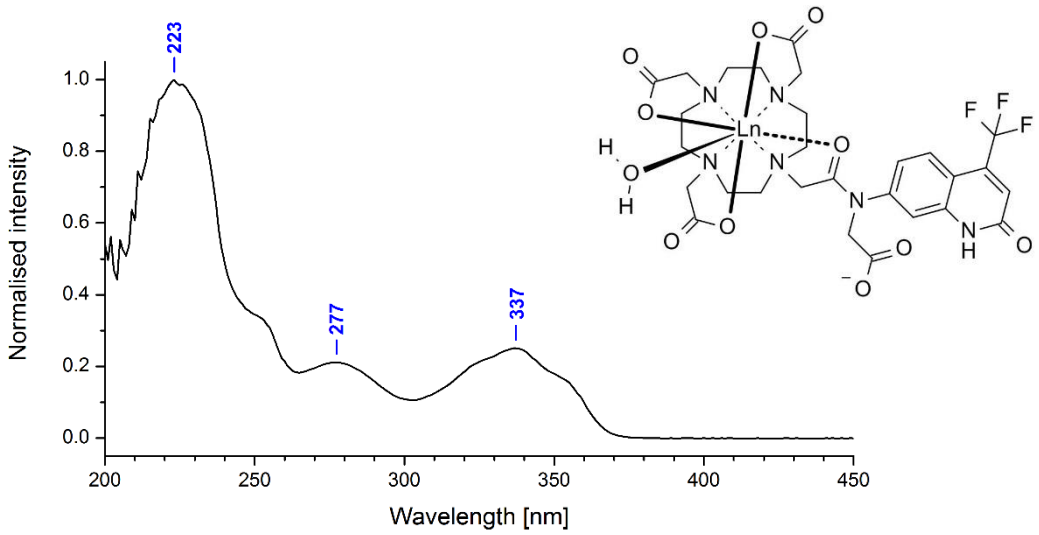


Figure S5. Normalised absorption spectrum of **Gd1b** in 0.01 M PIPES-buffered aqueous solution, pH 6.5. Blue numbers show local maxima of the spectra.

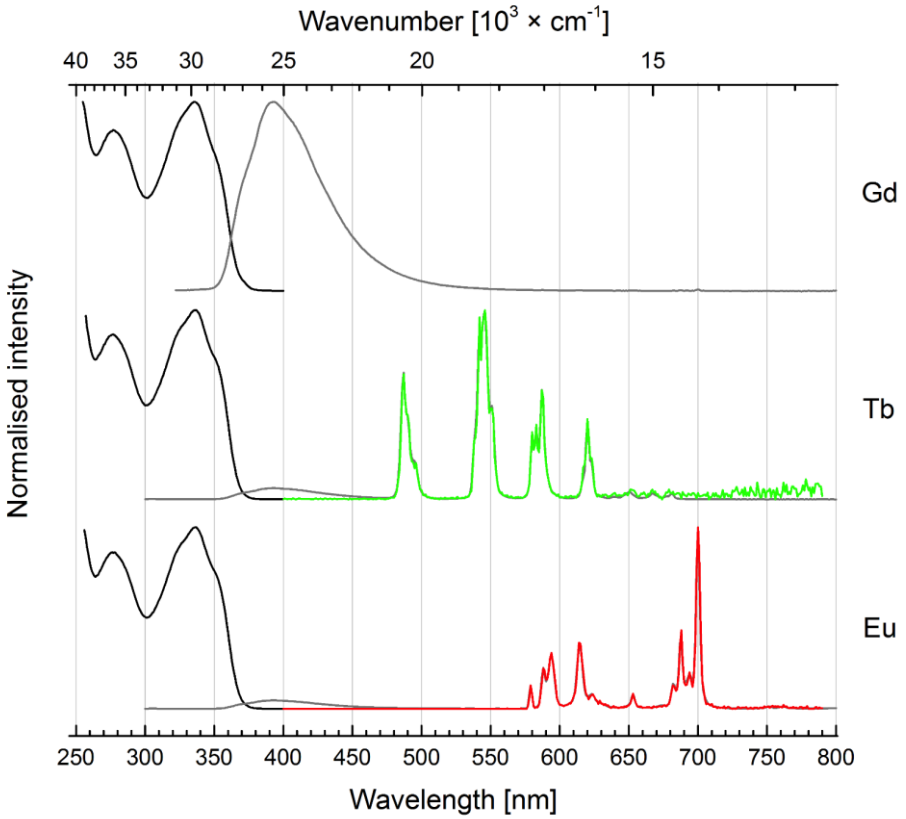


Figure S6. Excitation spectra of the Ln-centered emissions (Tb 545 nm, Eu 700 nm) and of the ligand centered emission (**Gd1b** 393 nm) at 298 K (black lines, left). Steady-state emission spectra of **Ln1b** at 298 K (grey lines, right) and time-resolved emission spectra showing the Ln-centered emissions (Tb (green), Eu (red), 298 K, coloured lines, right). Excitation at λ_{ex} = 336 nm; [**Ln1b**] = nominally 3.0×10^{-5} M, PIPES-buffered aqueous solutions 0.01 M, pH 6.5.

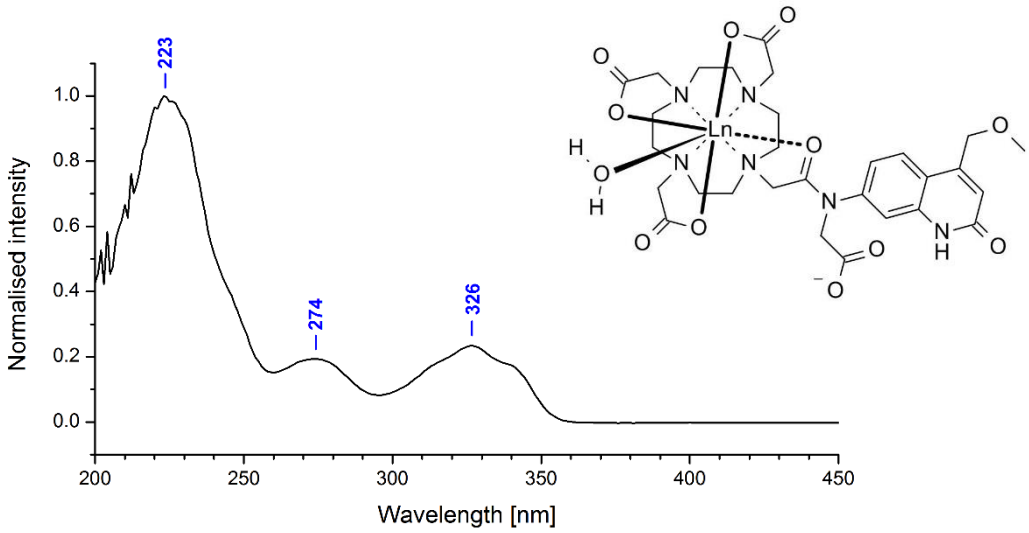


Figure S7. Normalised absorption spectrum of **Gd1c** in 0.01 M PIPES-buffered aqueous solution, pH 6.5. Blue numbers show local maxima of the spectra.

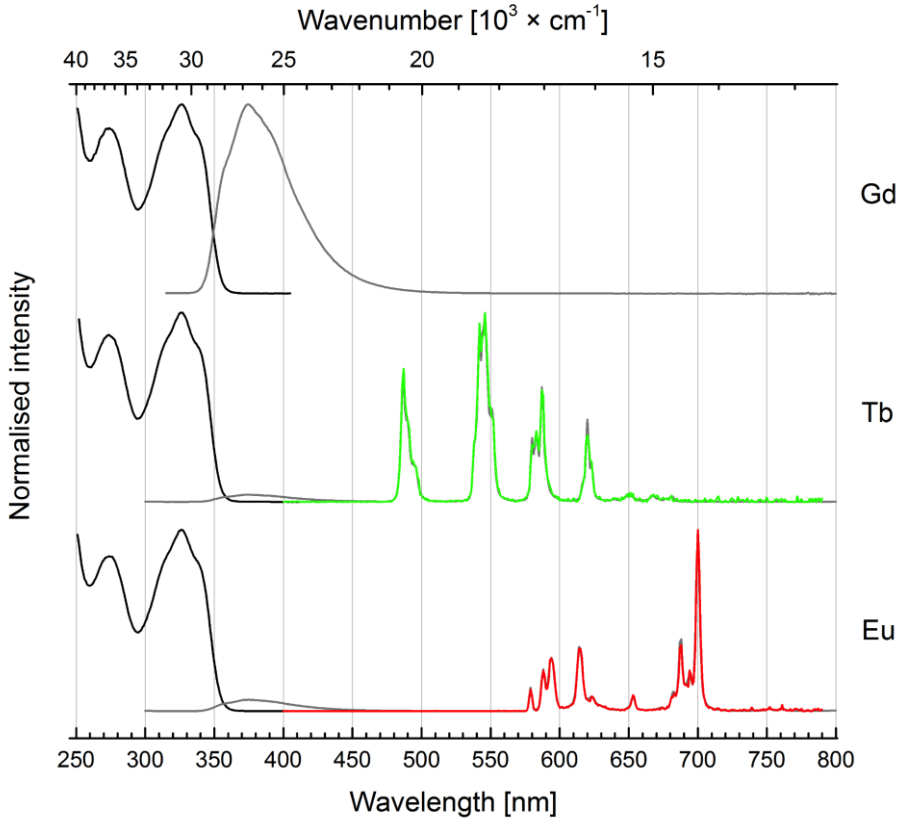


Figure S8. Excitation spectra of the Ln-centered emissions (Tb 545 nm, Eu 700 nm) and of the ligand centered emission (**Gd1c** 374 nm) at 298 K (black lines, left). Steady-state emission spectra of **Ln1c** at 298 K (grey lines, right) and time-resolved emission spectra showing the Ln-centered emissions (Tb (green), Eu (red), 298 K, coloured lines, right). Excitation at λ_{ex} = 336 nm; [**Ln1c**] = nominally 3.0×10^{-5} M, PIPES-buffered aqueous solutions 0.01 M, pH 6.5.

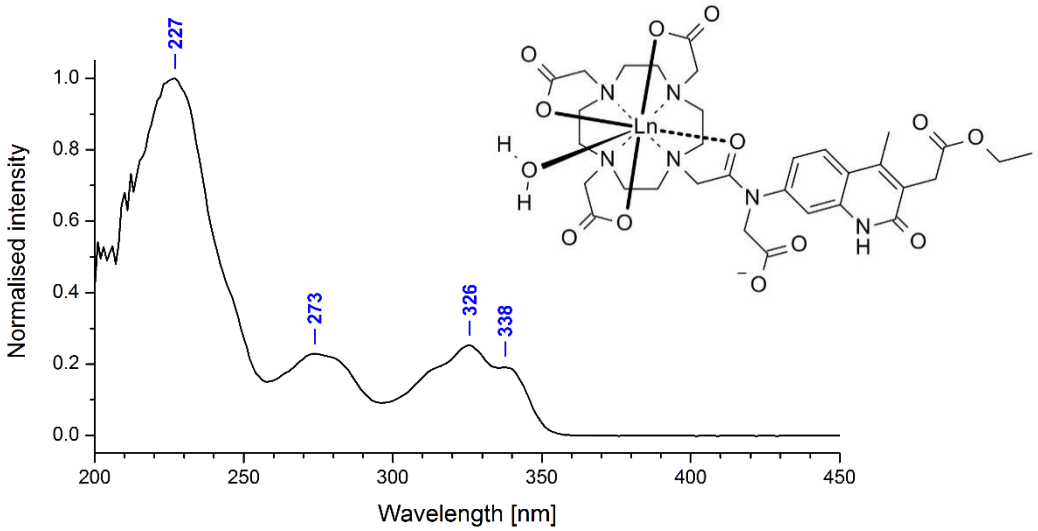


Figure S9. Normalised absorption spectrum of **Gd1d** in 0.01 M PIPES-buffered aqueous solution, pH 6.5. Blue numbers show local maxima of the spectra.

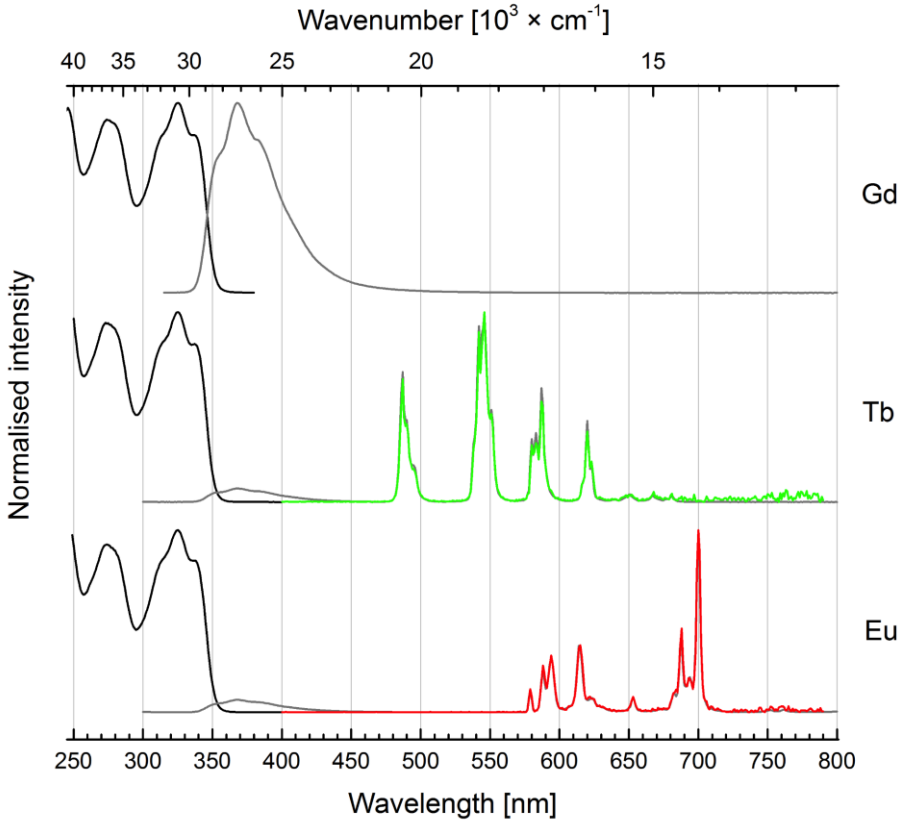


Figure S10. Excitation spectra of the Ln-centered emissions (Tb 545 nm, Eu 700 nm) and of the ligand centered emission (**Gd1d** 374 nm) at 298 K (black lines, left). Steady-state emission spectra of **Ln1d** at 298 K (grey lines, right) and time-resolved emission spectra showing the Ln-centered emissions (Tb (green), Eu (red), 298 K, coloured lines, right). Excitation at λ_{ex} = 336 nm; [**Ln1d**] = nominally 3.0×10^{-5} M, PIPES-buffered aqueous solutions 0.01 M, pH 6.5.

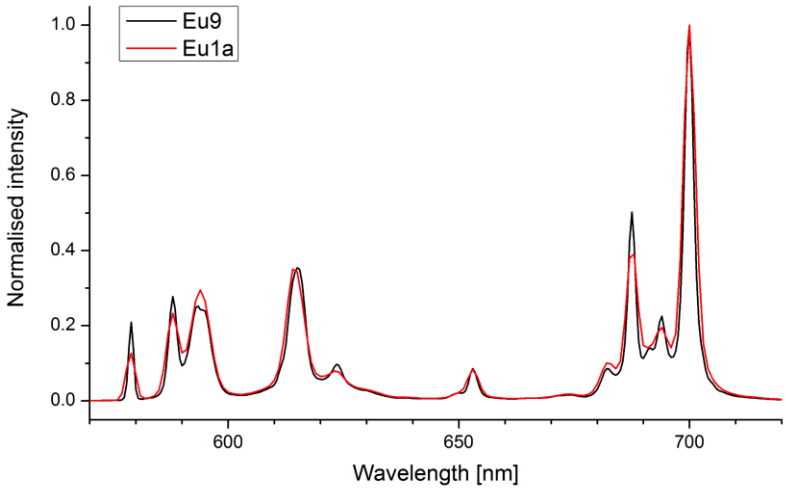


Figure S11. Overlaid emission spectra (normalised at 700 nm) of **Eu1a** and **Eu9**.

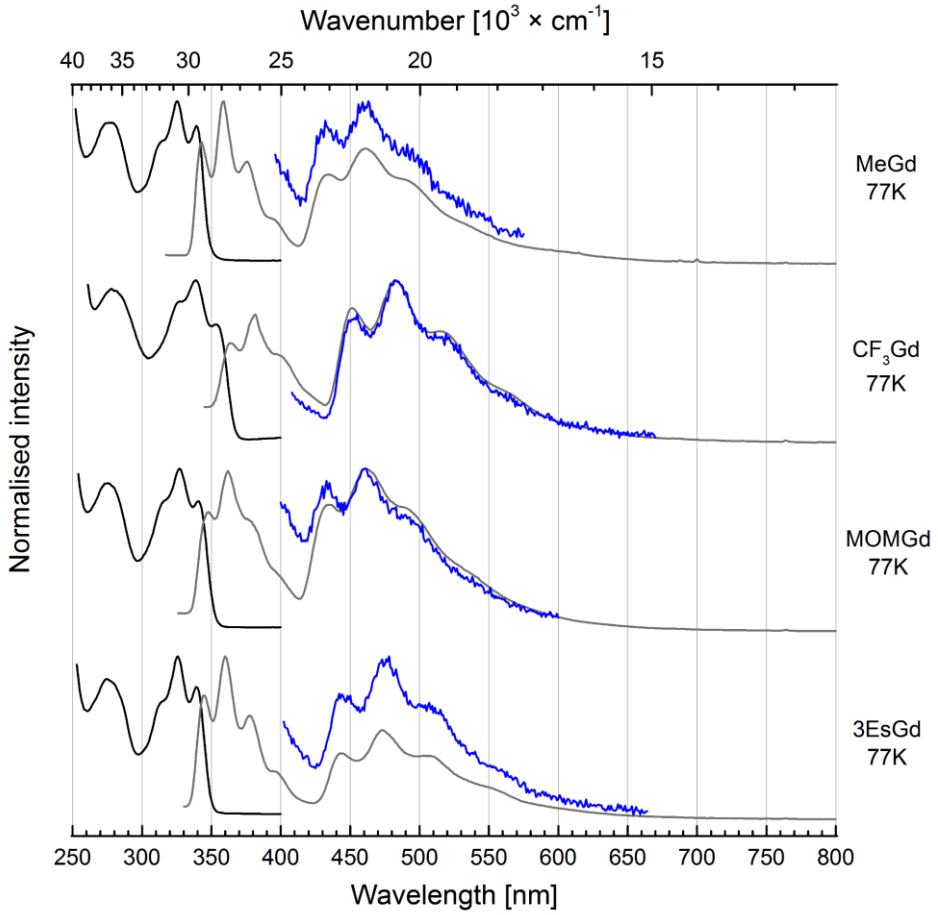


Figure S12. Excitation spectra of the ligand-centered phosphorescence (triplet state) emissions (**Gd1a** 461 nm, **Gd1b** 482 nm, **Gd1c** 461 nm, **Gd1d** 473 nm) at 77 K (black lines, left). Steady-state emission spectra (grey lines, right) and time-resolved emission spectra (blue lines, right) 40 ms delay after pulsed excitation at λ_{max} (lowest in energy) of the Gd complexes at 77 K with 10% glycerol added to 30 μM, PIPES-buffered aqueous solutions 0.01 M, pH 6.5.

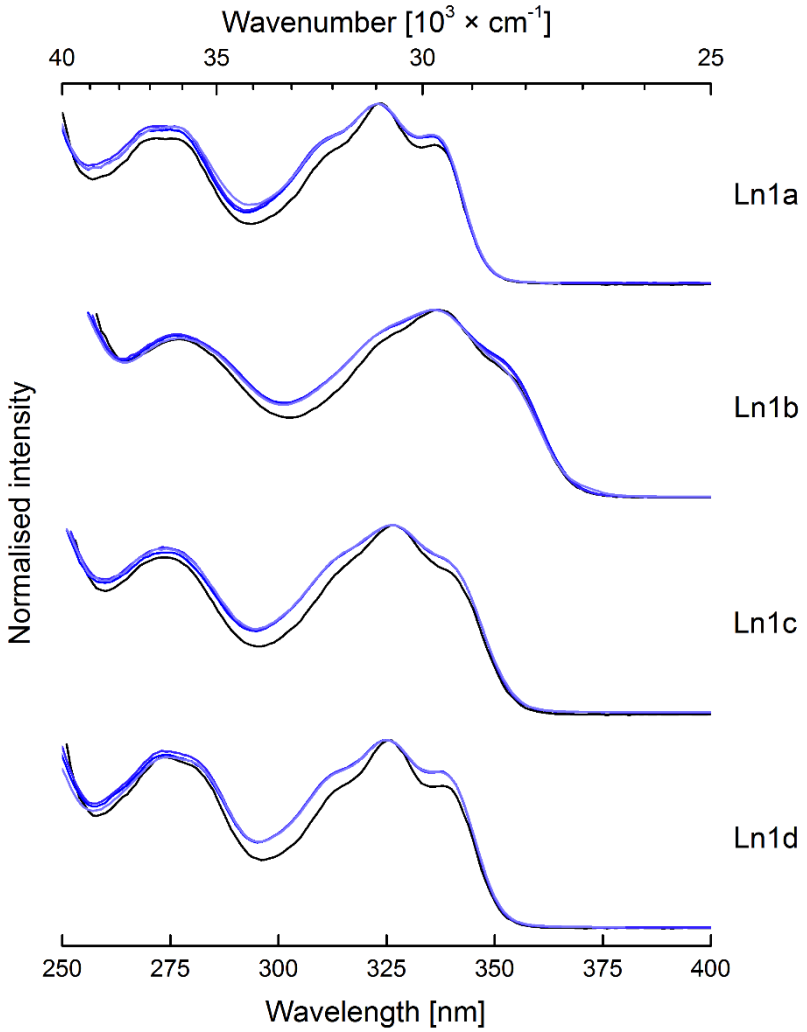
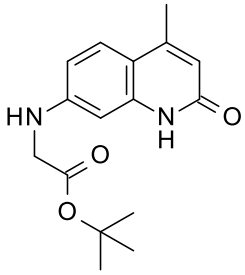


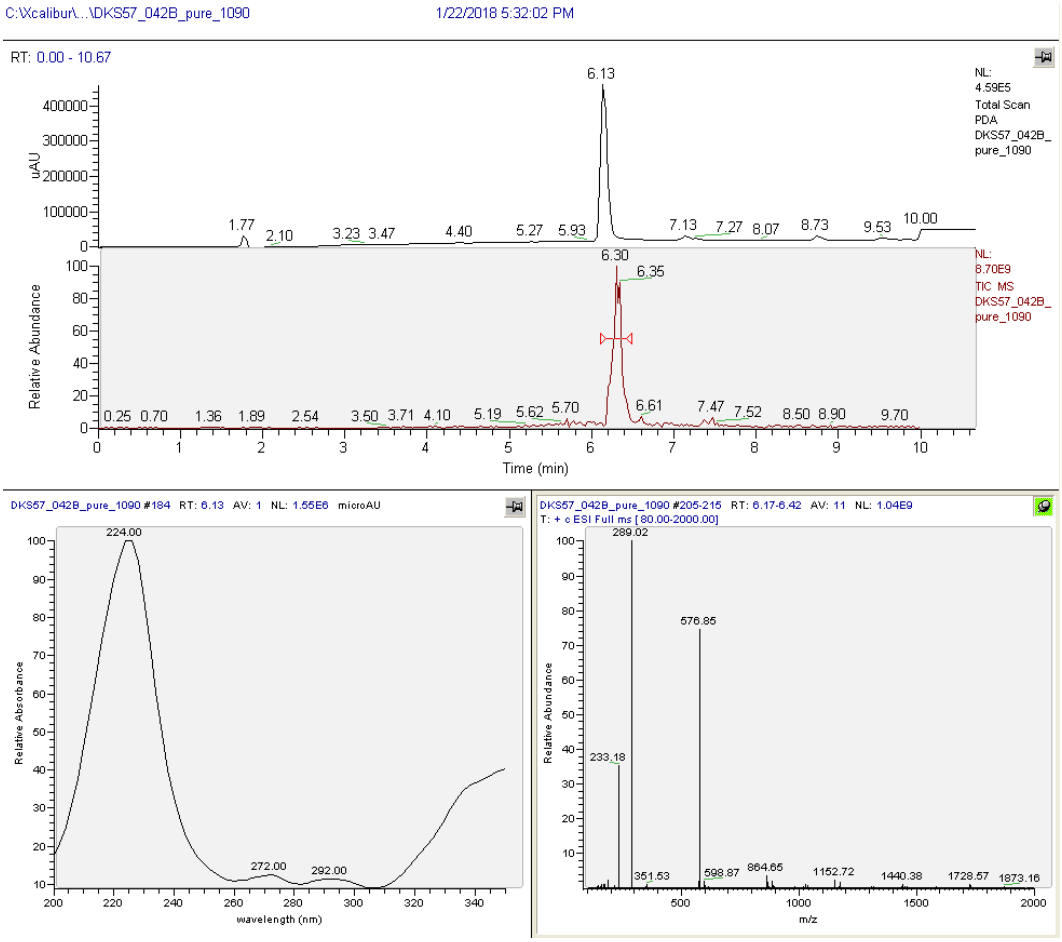
Figure S13. Overlaid absorption (black) and excitation spectra of all **Ln1a-d** complexes. Excitation spectra of the Ln-centered emissions (Tb 545 nm, Eu 700 nm) and of the ligand centered emission (380, 400, 425 and 395 nm for Gd1a-d, respectively), are shown in blue, [**Ln1a-d**] = nominally 3.0×10^{-5} M, PIPES-buffered aqueous solutions 0.01 M, pH 6.5.

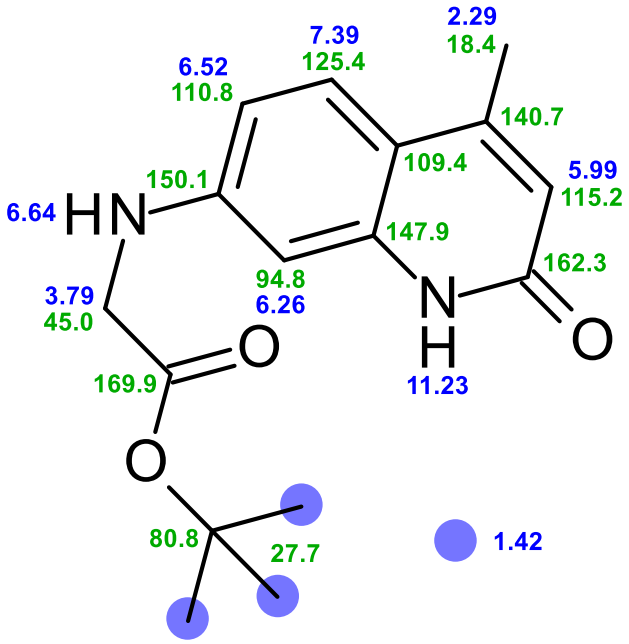
Synthetic procedures and characterization data

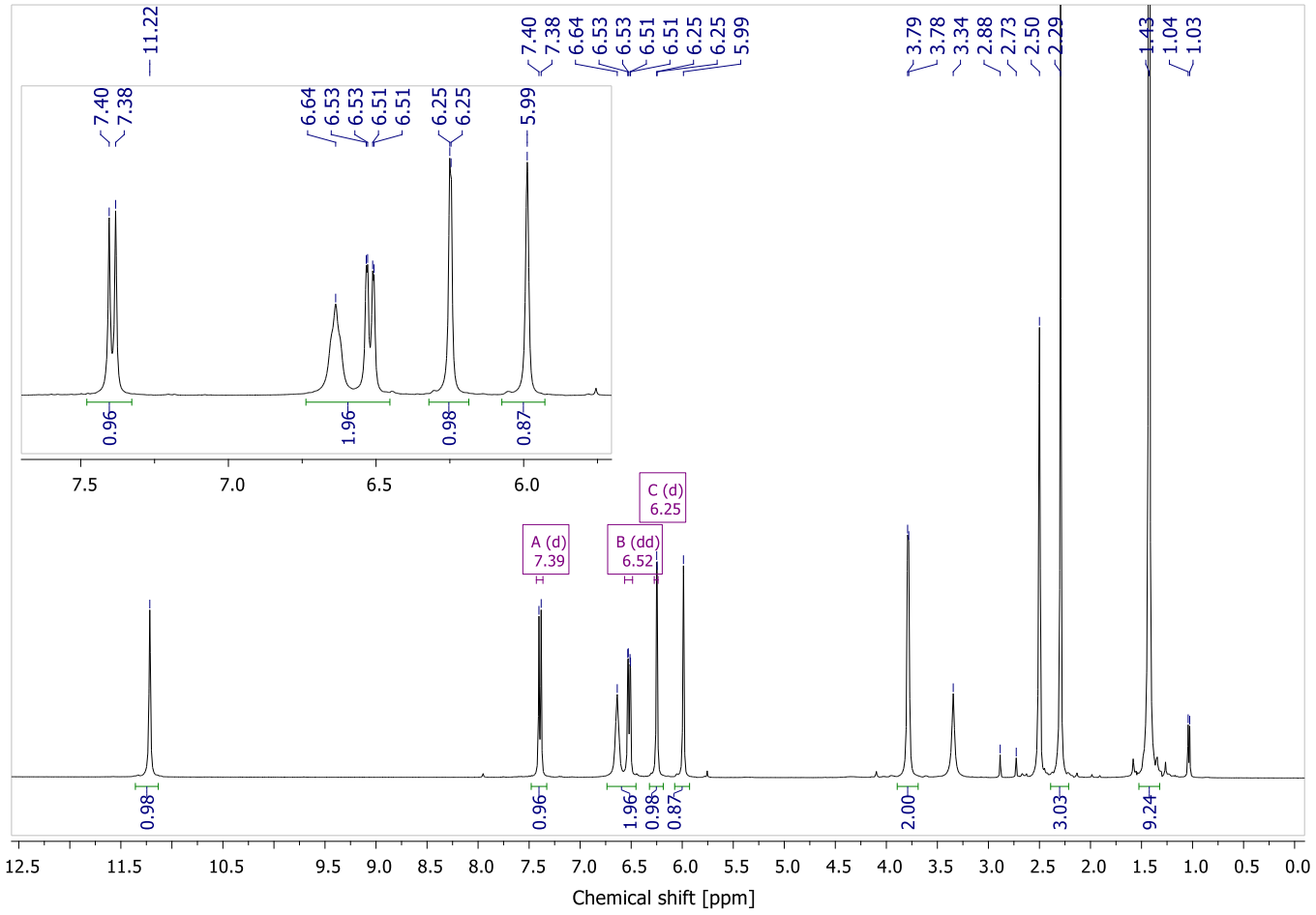
DKS57_042B

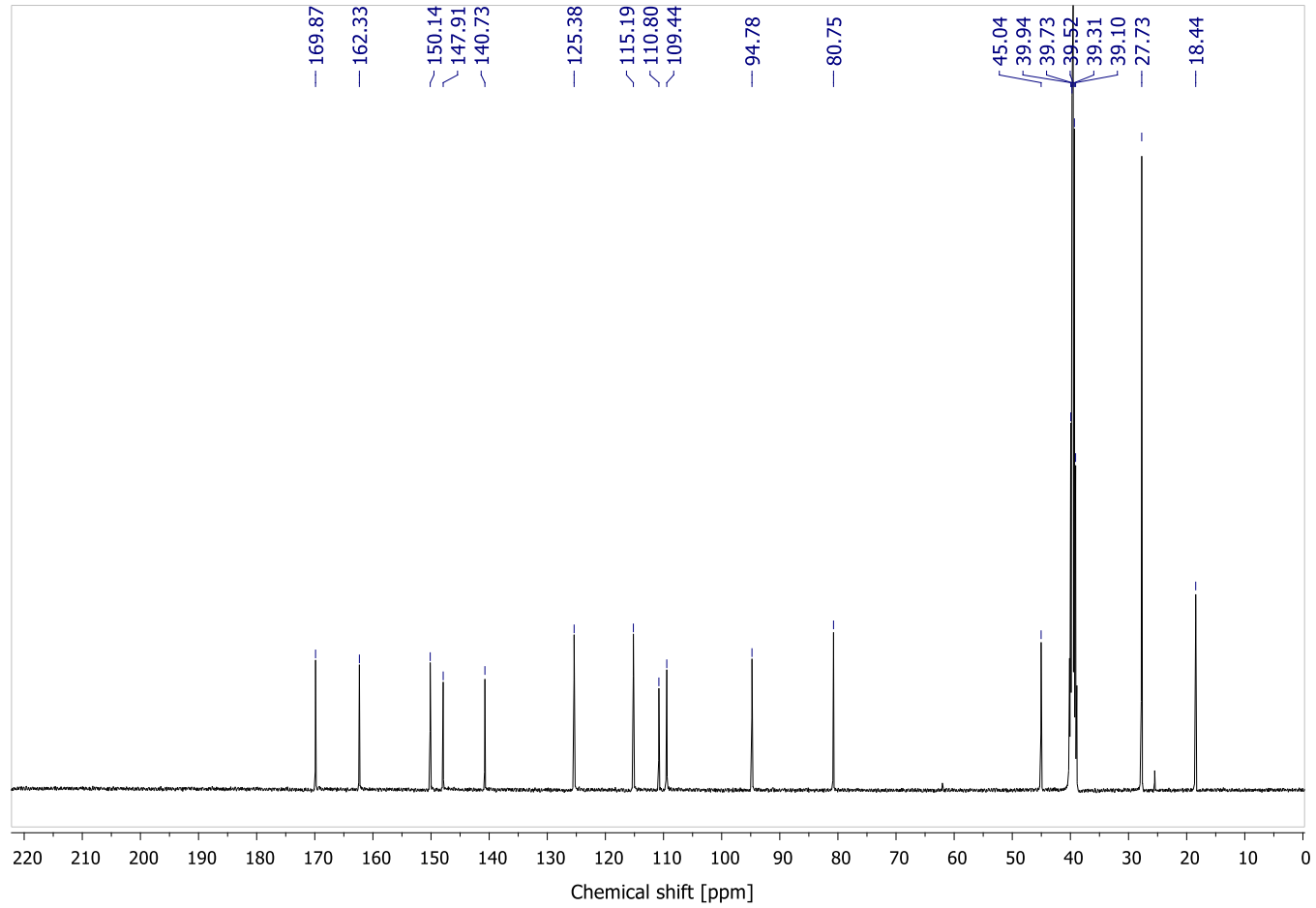


Formula Weight : 288,34(1)
Exact Mass : 288,14739
Formula : $C_{16}H_{20}N_2O_3$
Composition : C 66,65% H 6,99% N 9,72% O 16,65%

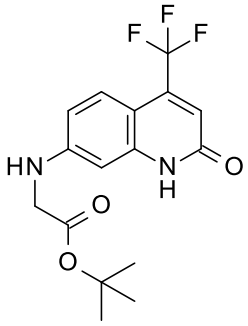





11.22
7.40
7.38
6.64
6.53
6.53
6.51
6.51
6.25
6.25
5.99
3.79
3.78
3.34
2.88
2.73
2.50
2.29
1.43
1.04
1.03
A (d)
7.39
B (dd)
6.52
C (d)
6.25
0.98
0.96
1.96
0.98
0.87
2.00
3.03
9.24
Chemical shift [ppm]

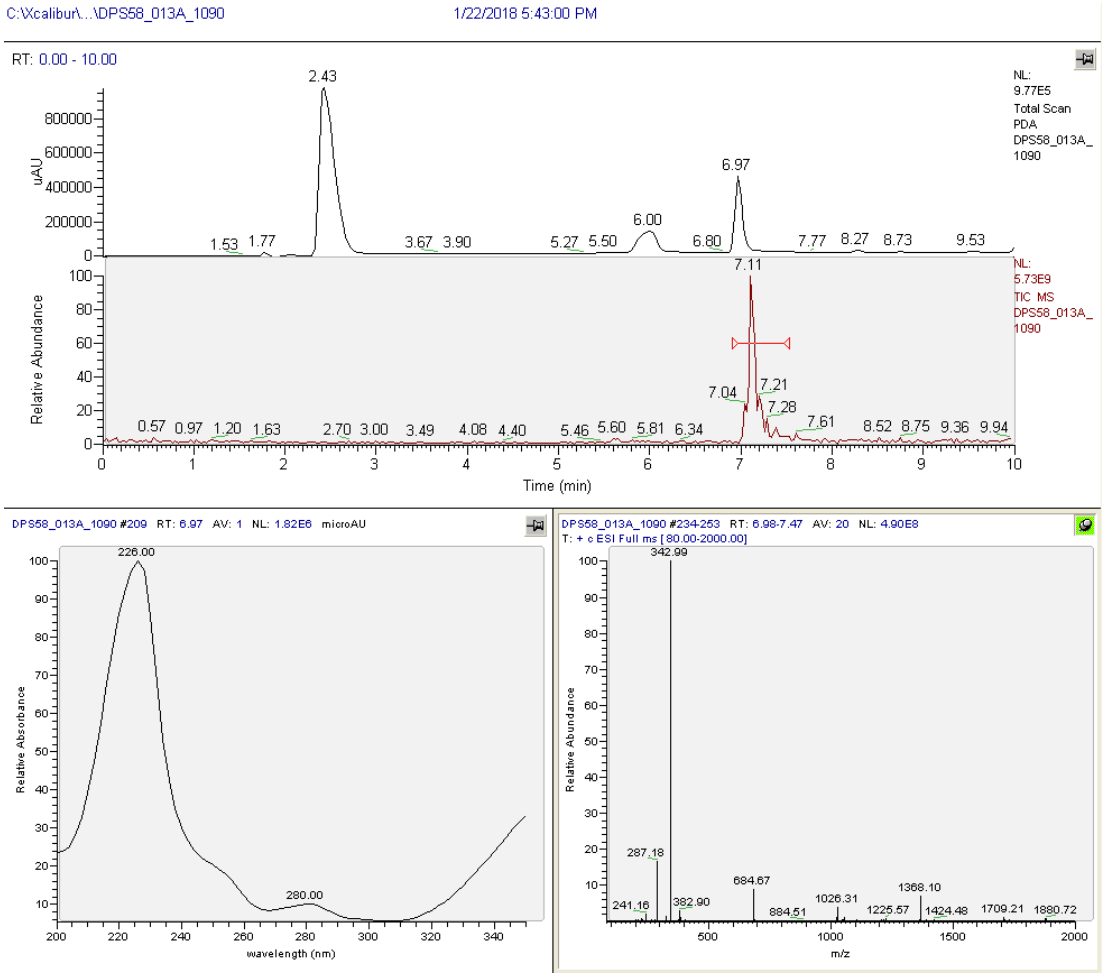

169.87
162.33
150.14
147.91
140.73
125.38
115.19
110.80
109.44
94.78
80.75
45.04
39.94
39.73
39.52
39.31
39.10
27.73
18.44
Chemical shift [ppm]

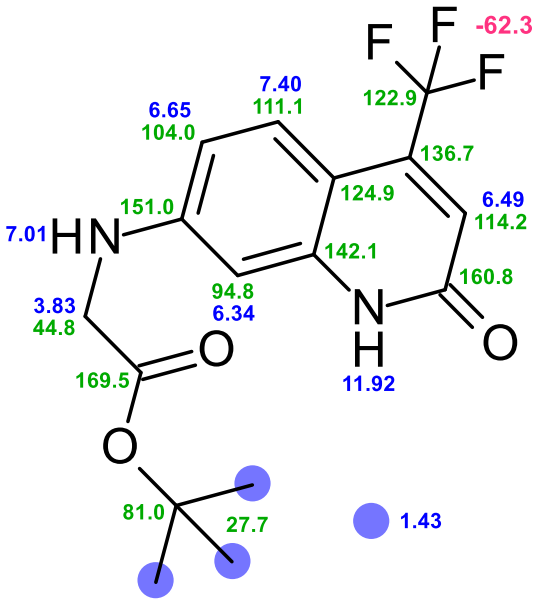
DKS57_028A

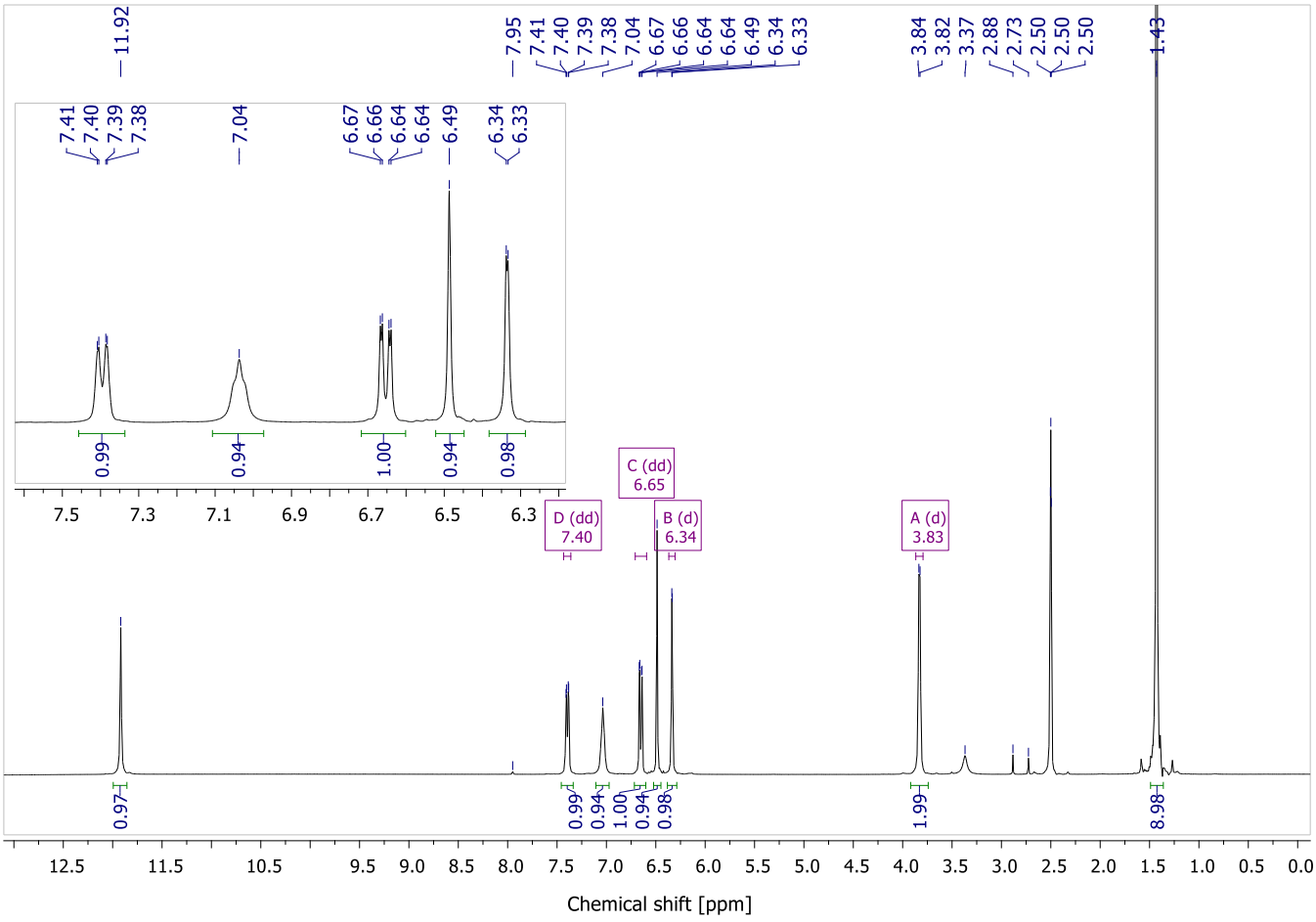


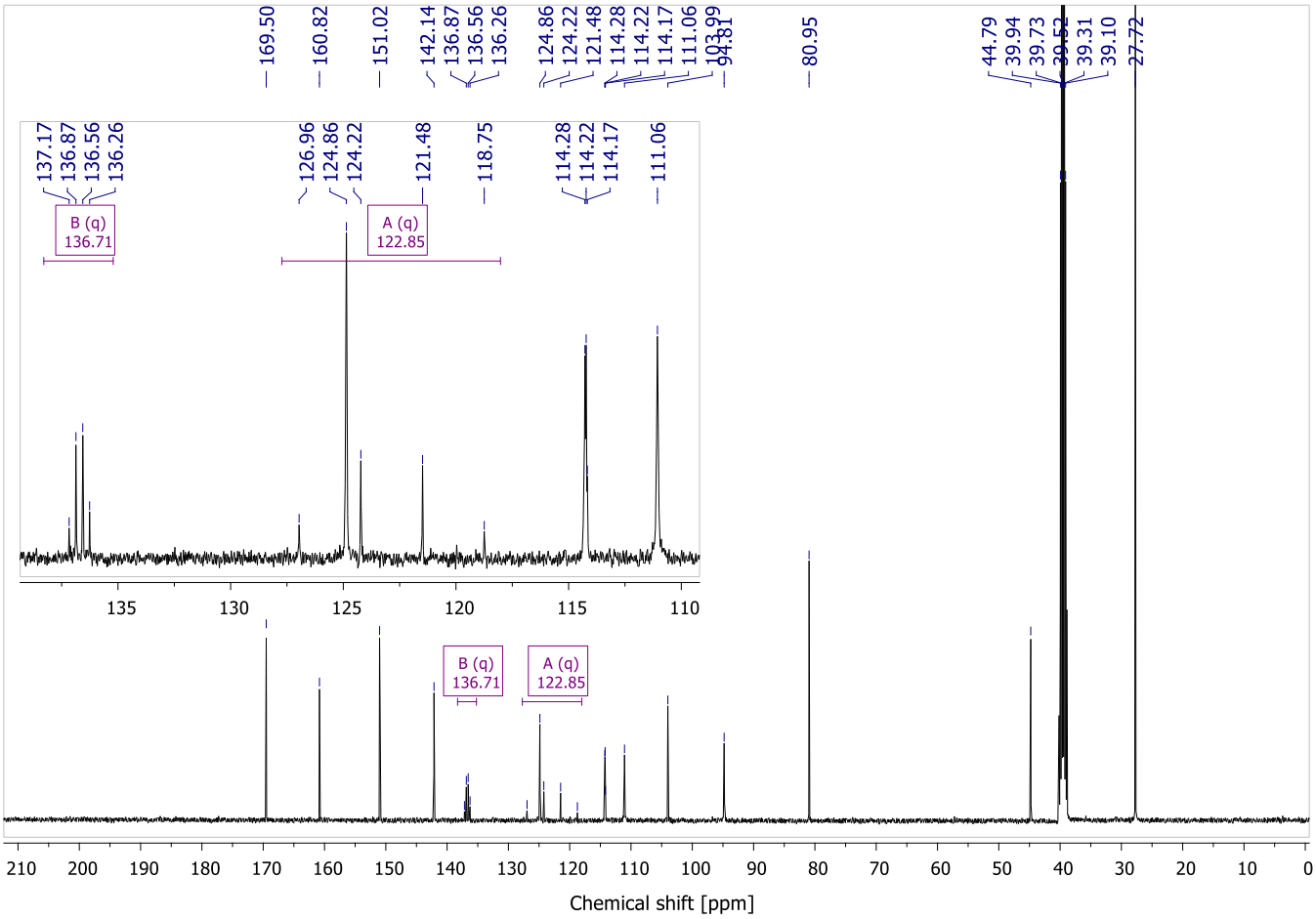
Formula Weight : 342,31(1)
Exact Mass : 342,11913
Formula : $C_{16}H_{17}F_3N_2O_3$
Composition : C 56,14% H 5,01% N 8,18% O 14,02% F 16,65%

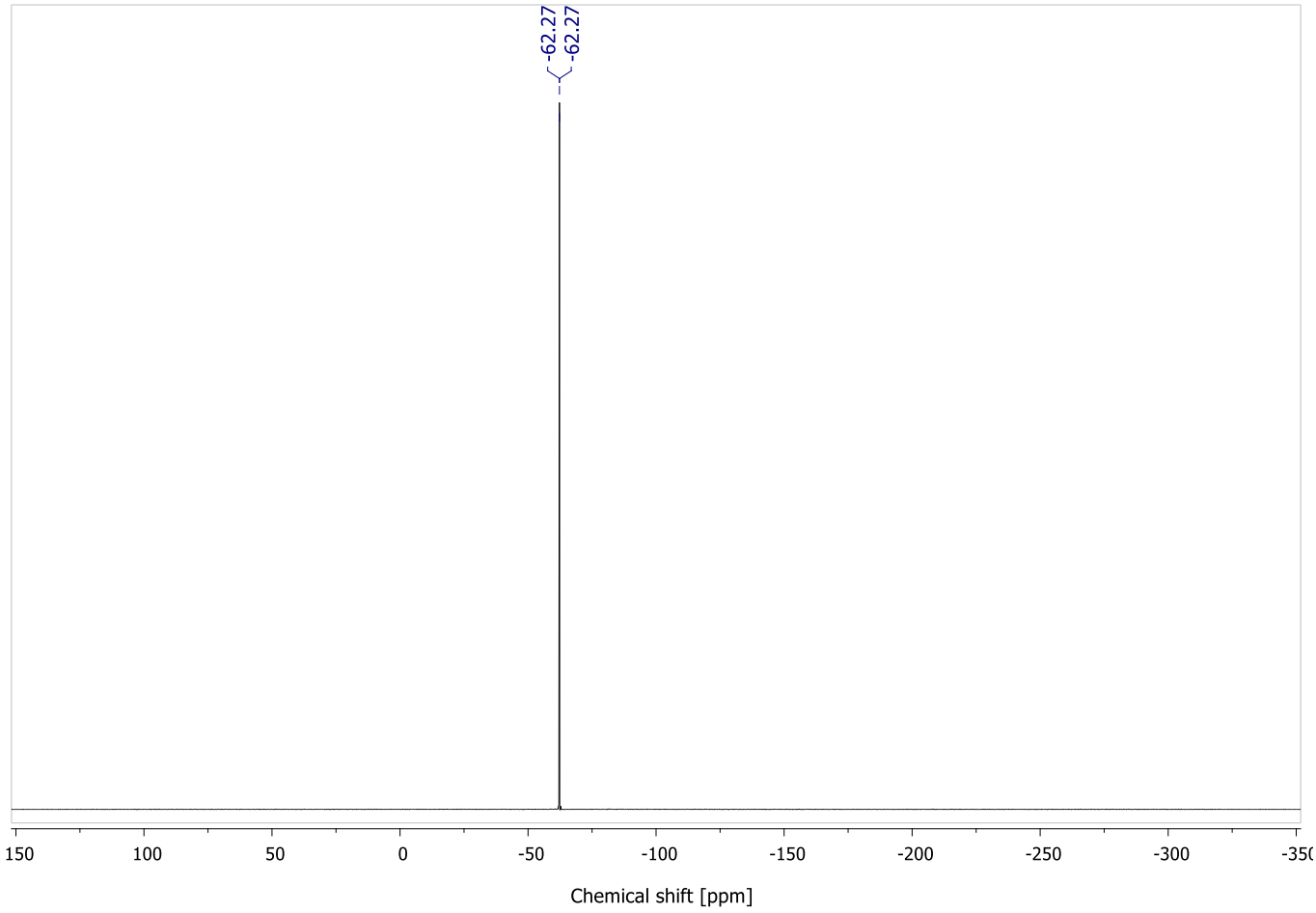
(**Note:** t_R: 5.90 min is some sort of solvent absorbtion below 240 nm)



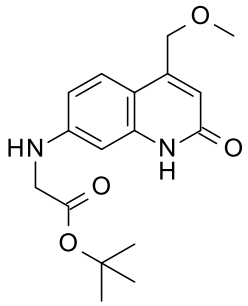



11.92
7.95
7.41
7.40
7.39
7.38
7.04
6.67
6.66
6.64
6.64
6.49
6.34
6.33
3.84
3.82
3.37
2.88
2.73
2.50
2.50
2.50
1.43
C (dd)
6.65
D (dd)
7.40
B (d)
6.34
A (d)
3.83
0.97
0.99
0.94
1.00
0.94
0.98
1.99
8.98
Chemical shift [ppm]

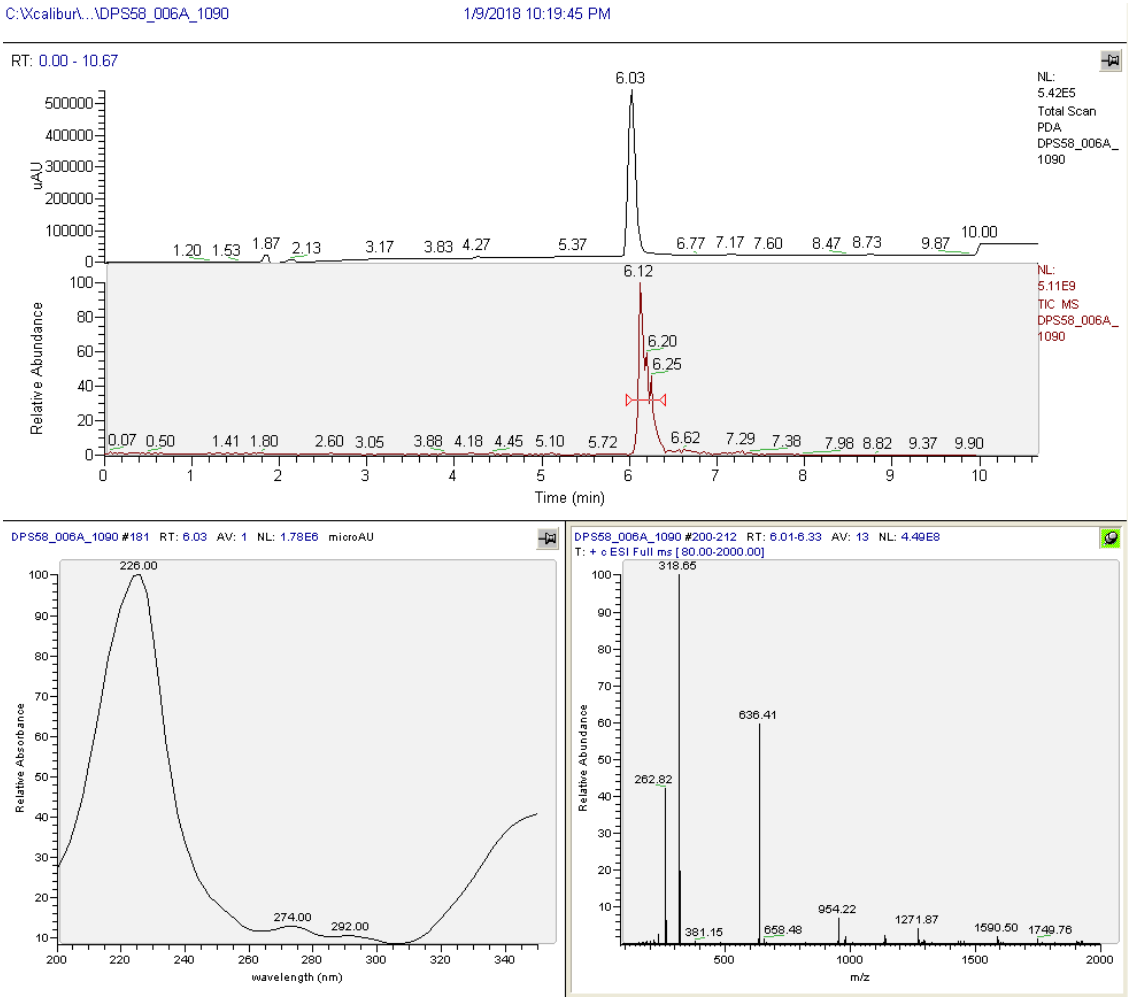

169.50
160.82
151.02
142.14
136.87
136.56
136.26
124.86
124.22
121.48
114.28
114.22
114.17
111.06
103.99
94.81
80.95
44.79
39.94
39.73
39.52
39.31
39.10
27.72
B (q)
136.71
A (q)
122.85
Chemical shift [ppm]

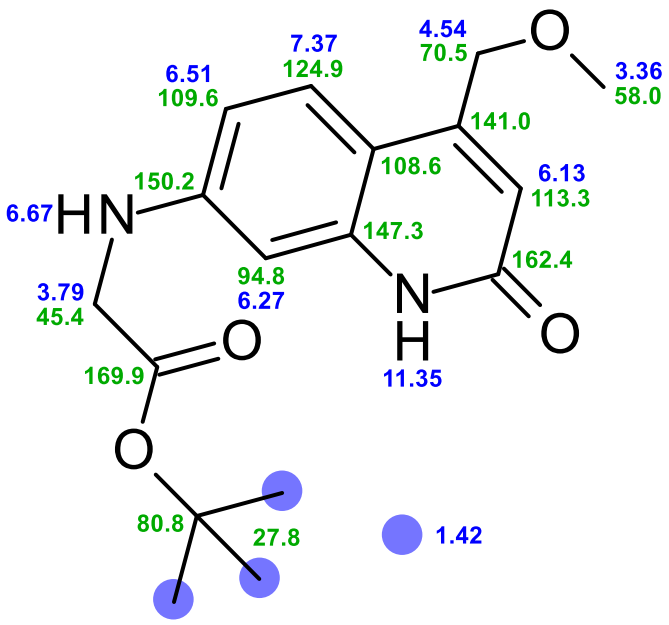

-62.27
-62.27
150
100
50
0
-50
-100
-150
-200
-250
-300
Chemical shift [ppm]

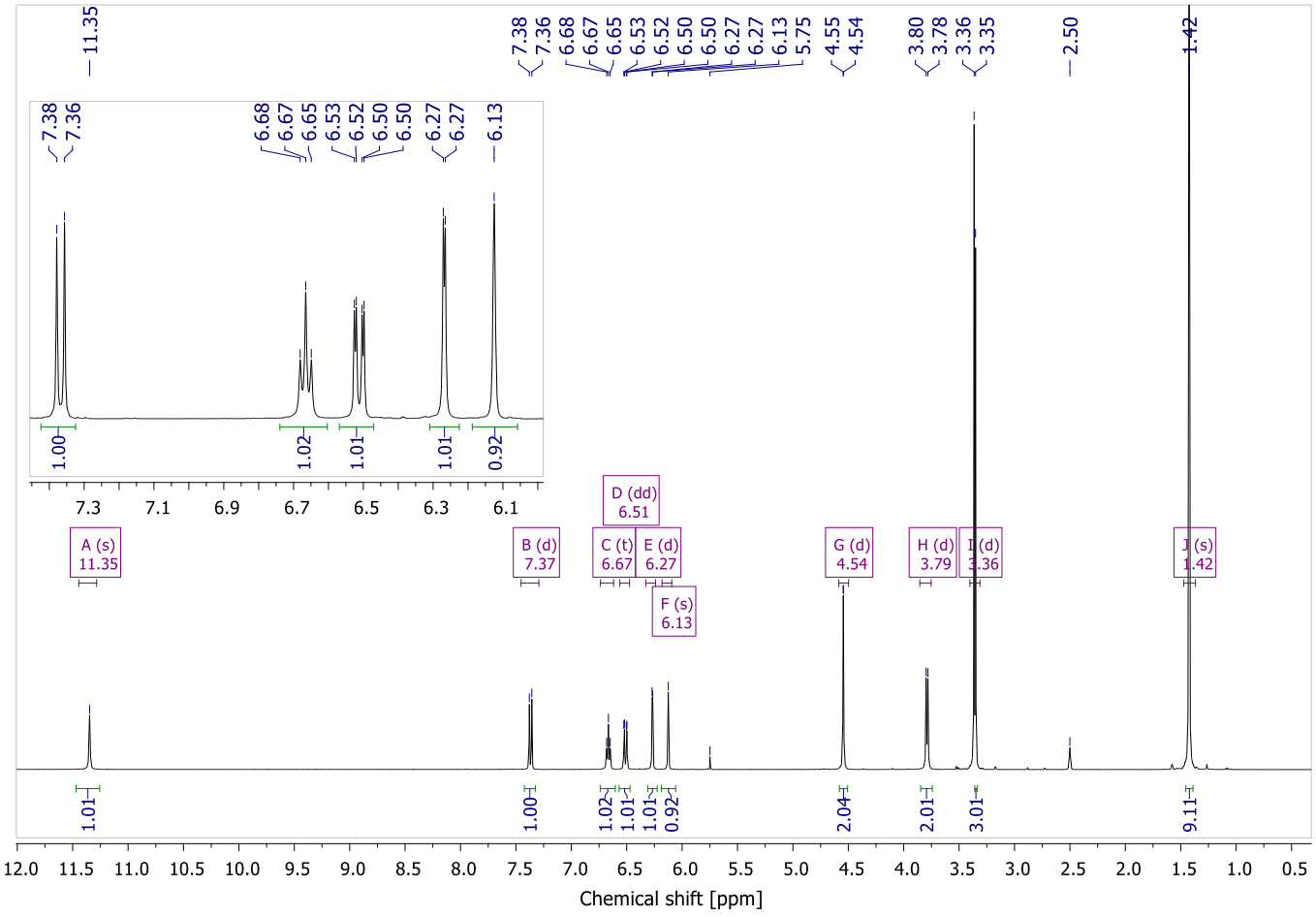
DPS58_006A

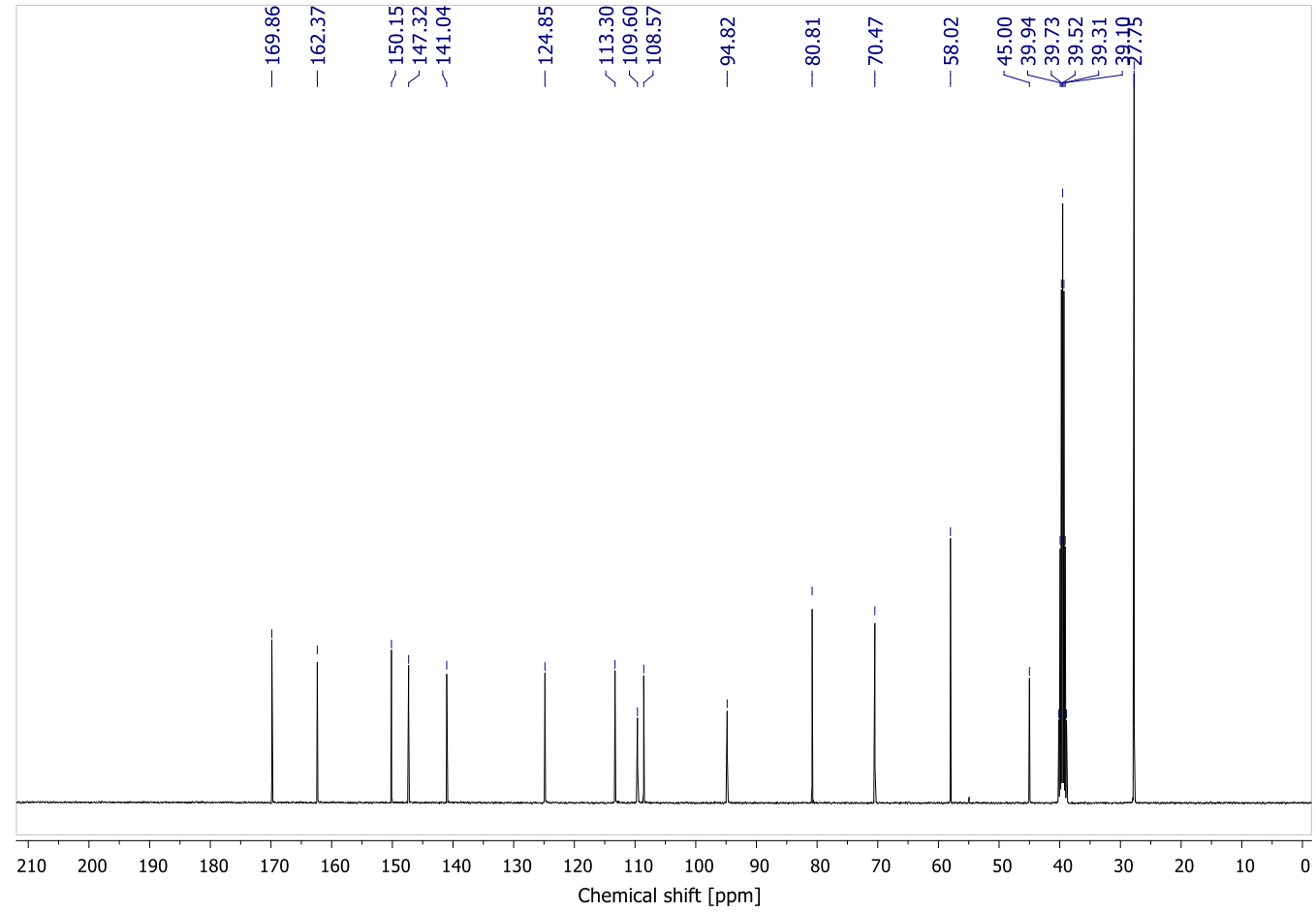


Formula Weight : 318,37(1)
Exact Mass : 318,15796
Formula : $C_{17}H_{22}N_2O_4$
Composition : C 64,13% H 6,97% N 8,80% O 20,10%

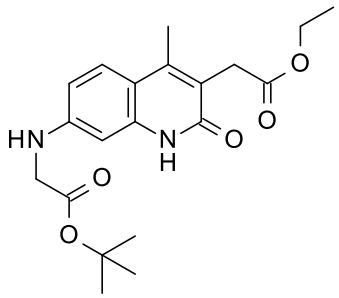




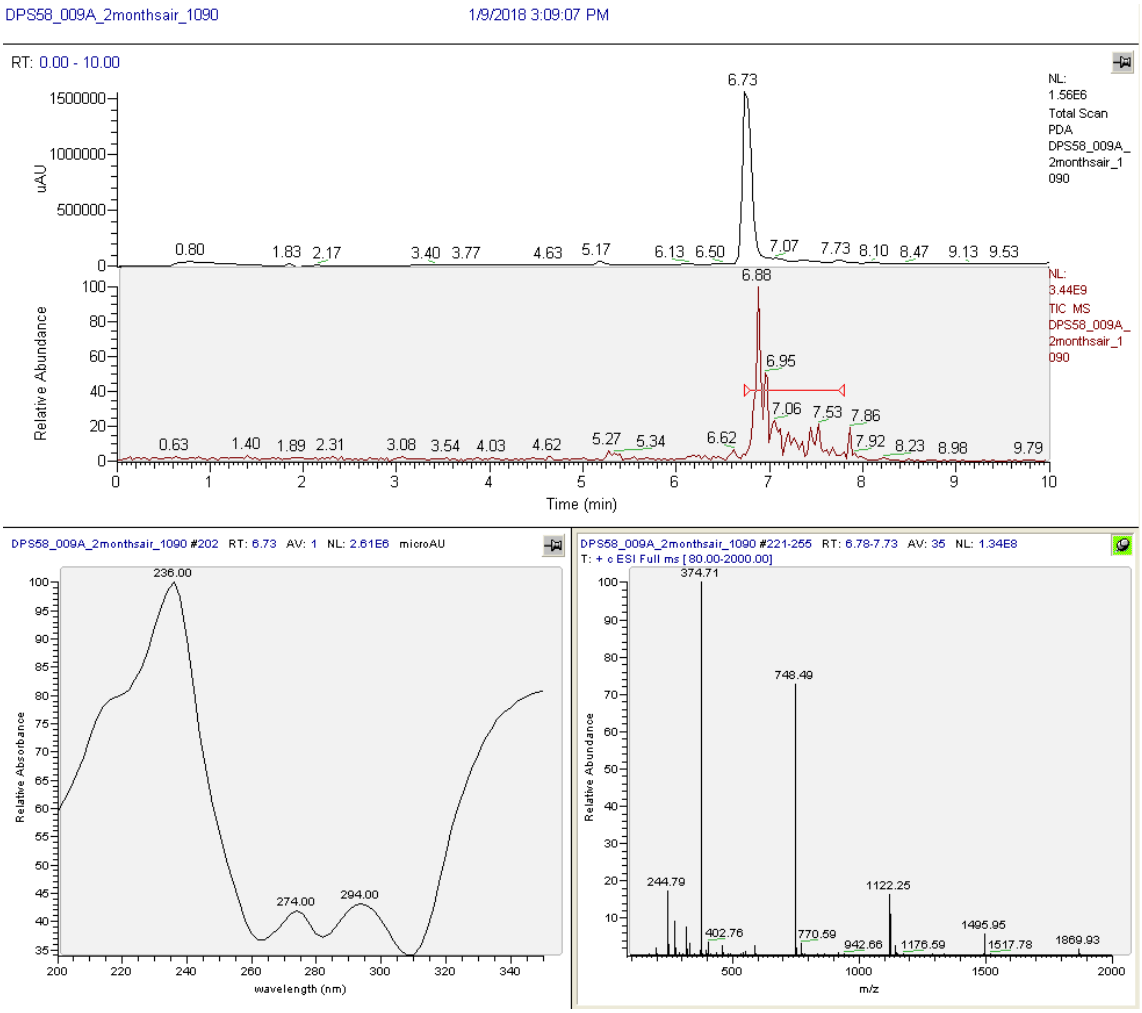

11.35
7.38
7.36
6.68
6.67
6.65
6.53
6.52
6.50
6.50
6.27
6.27
6.13
5.75
4.55
4.54
3.80
3.78
3.36
3.35
2.50
1.42
A (s) 11.35
B (d) 7.37
C (t) 6.67
D (dd) 6.51
E (d) 6.27
F (s) 6.13
G (d) 4.54
H (d) 3.79
I (d) 3.36
J (s) 1.42
1.01
1.00
1.02
1.01
1.01
0.92
2.04
2.01
3.01
9.11
Chemical shift [ppm]

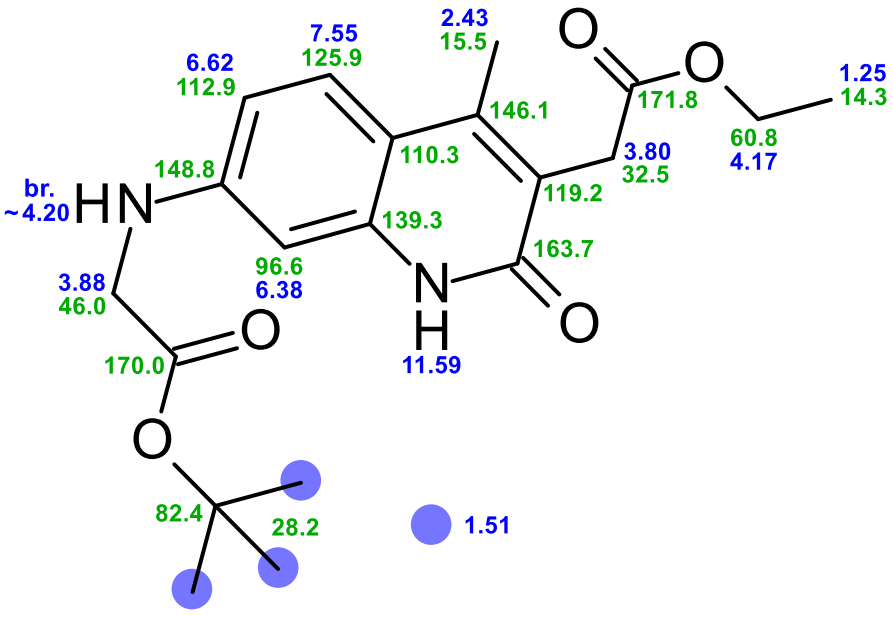

169.86
162.37
150.15
147.32
141.04
124.85
113.30
109.60
108.57
94.82
80.81
70.47
58.02
45.00
39.94
39.73
39.52
39.31
39.10
27.75
Chemical shift [ppm]

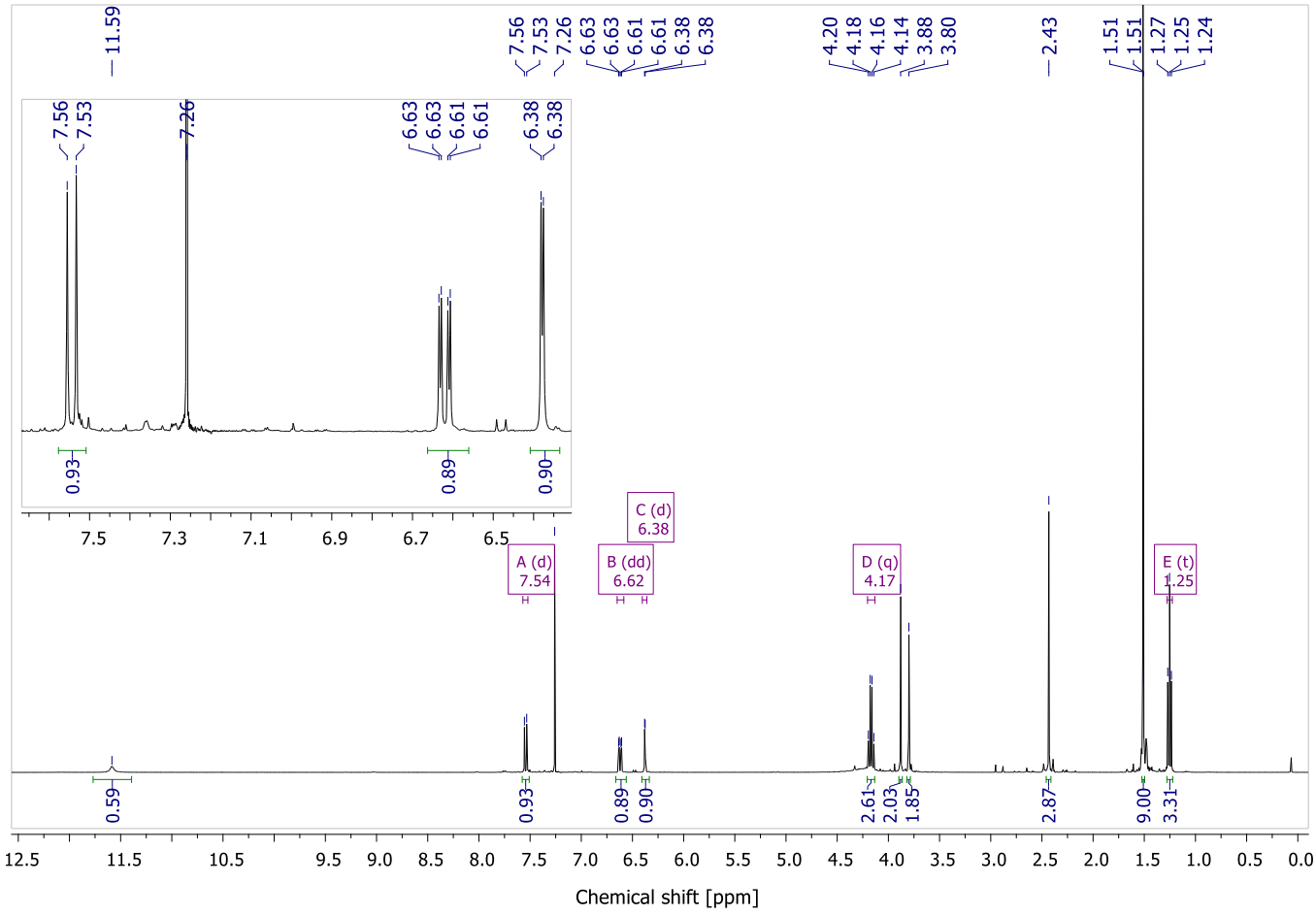
DPS58_009A

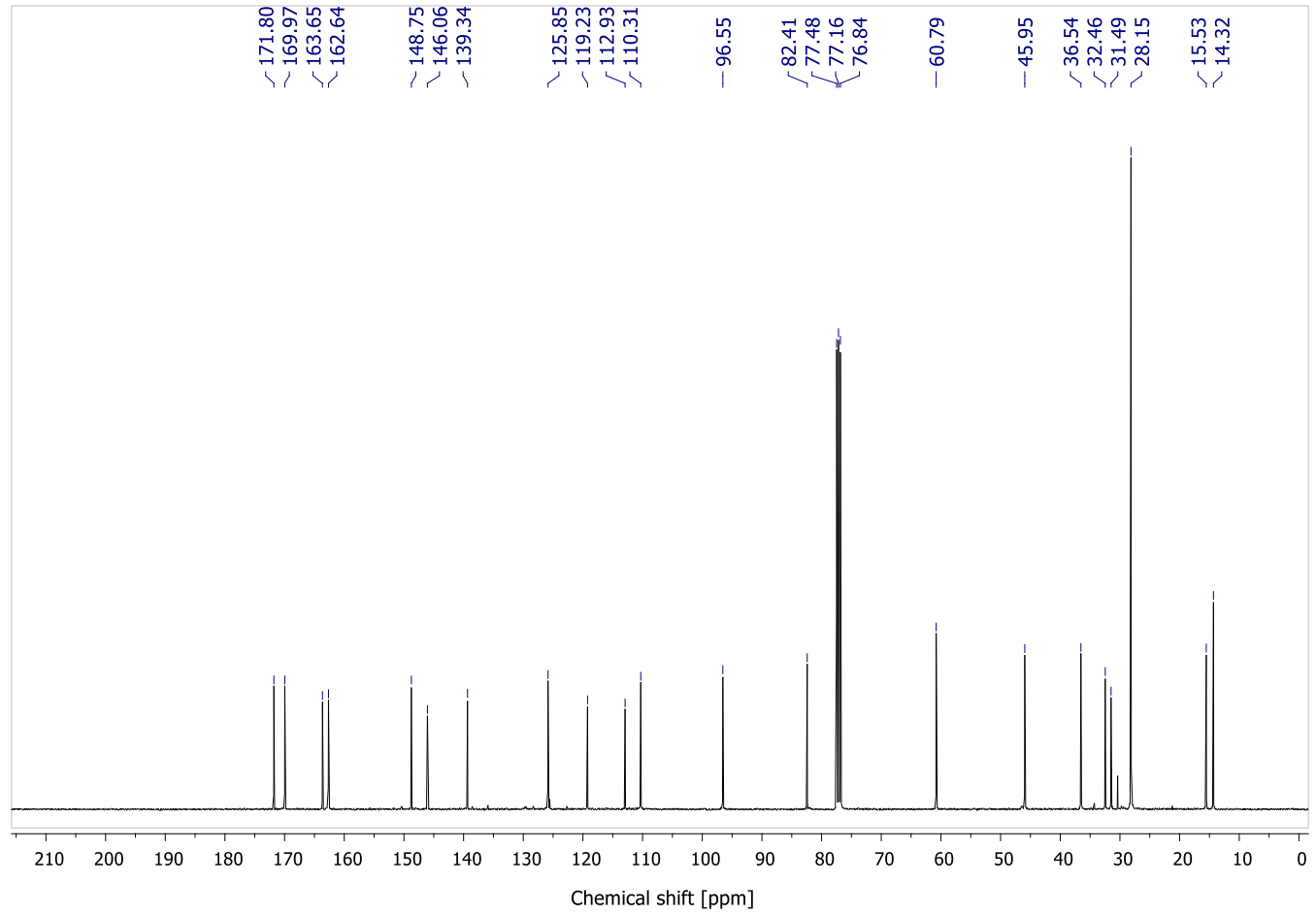


Formula Weight : 374,43(2)
Exact Mass : 374,18417
Formula : $C_{20}H_{26}N_2O_5$
Composition : C 64,15% H 7,00% N 7,48% O 21,36%

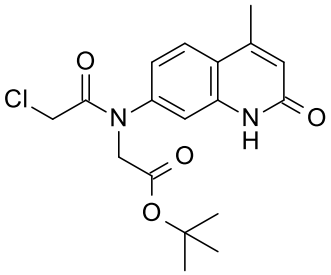




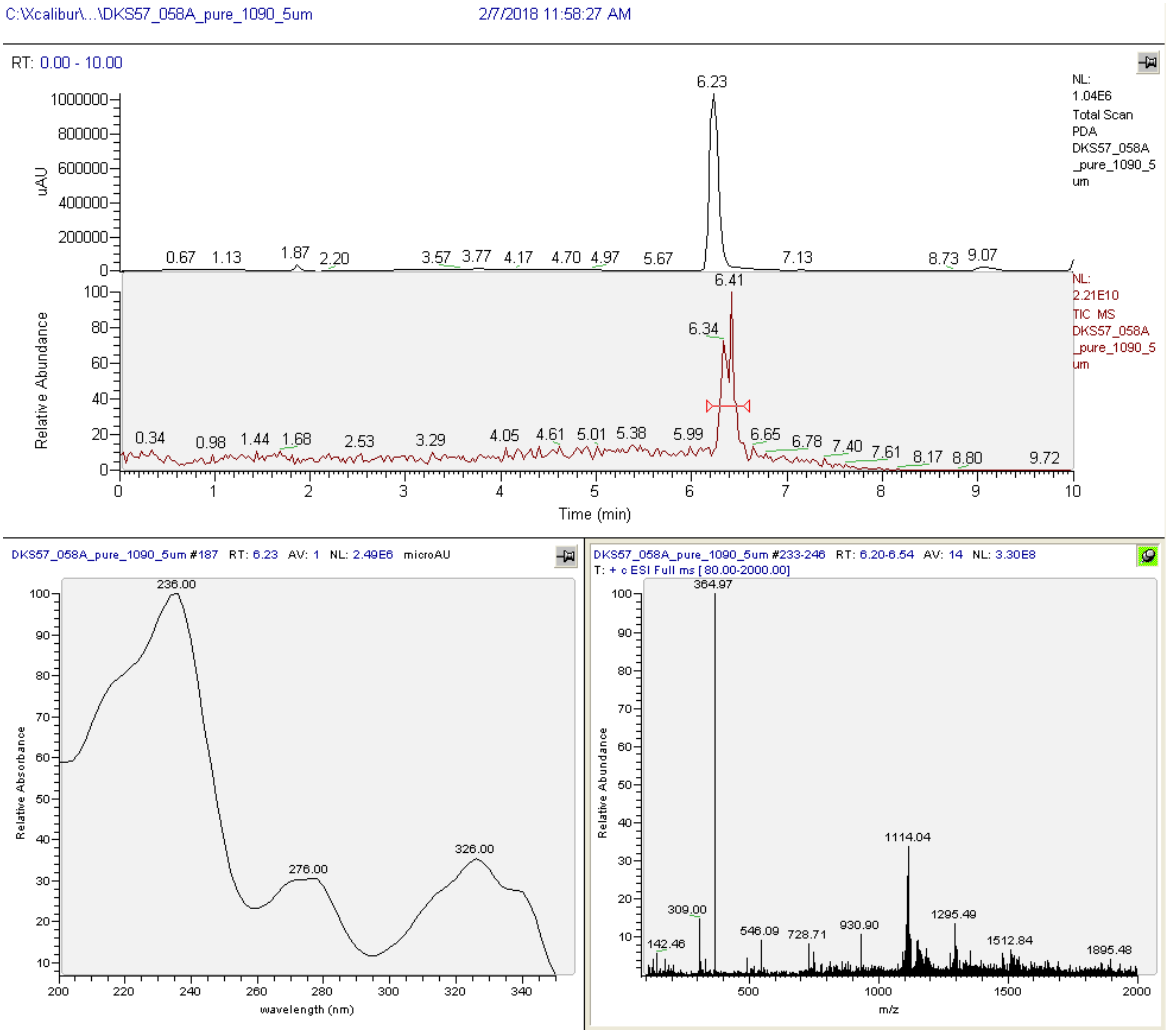

11.59
7.56
7.53
7.26
6.63
6.63
6.61
6.61
6.38
6.38
4.20
4.18
4.16
4.14
3.88
3.80
2.43
1.51
1.51
1.27
1.25
1.24
A (d) 7.54
B (dd) 6.62
C (d) 6.38
D (q) 4.17
E (t) 1.25
Chemical shift [ppm]

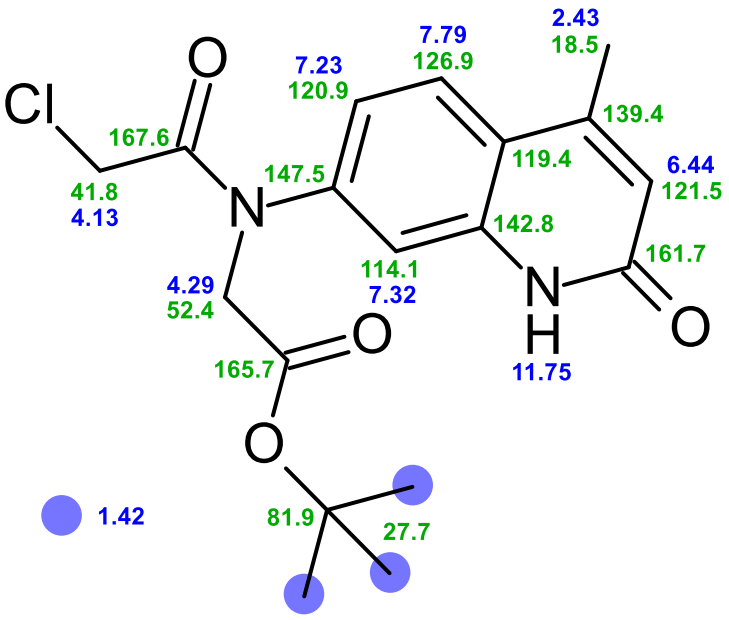

171.80
169.97
163.65
162.64
148.75
146.06
139.34
125.85
119.23
112.93
110.31
96.55
82.41
77.48
77.16
76.84
60.79
45.95
36.54
32.46
31.49
28.15
15.53
14.32
Chemical shift [ppm]

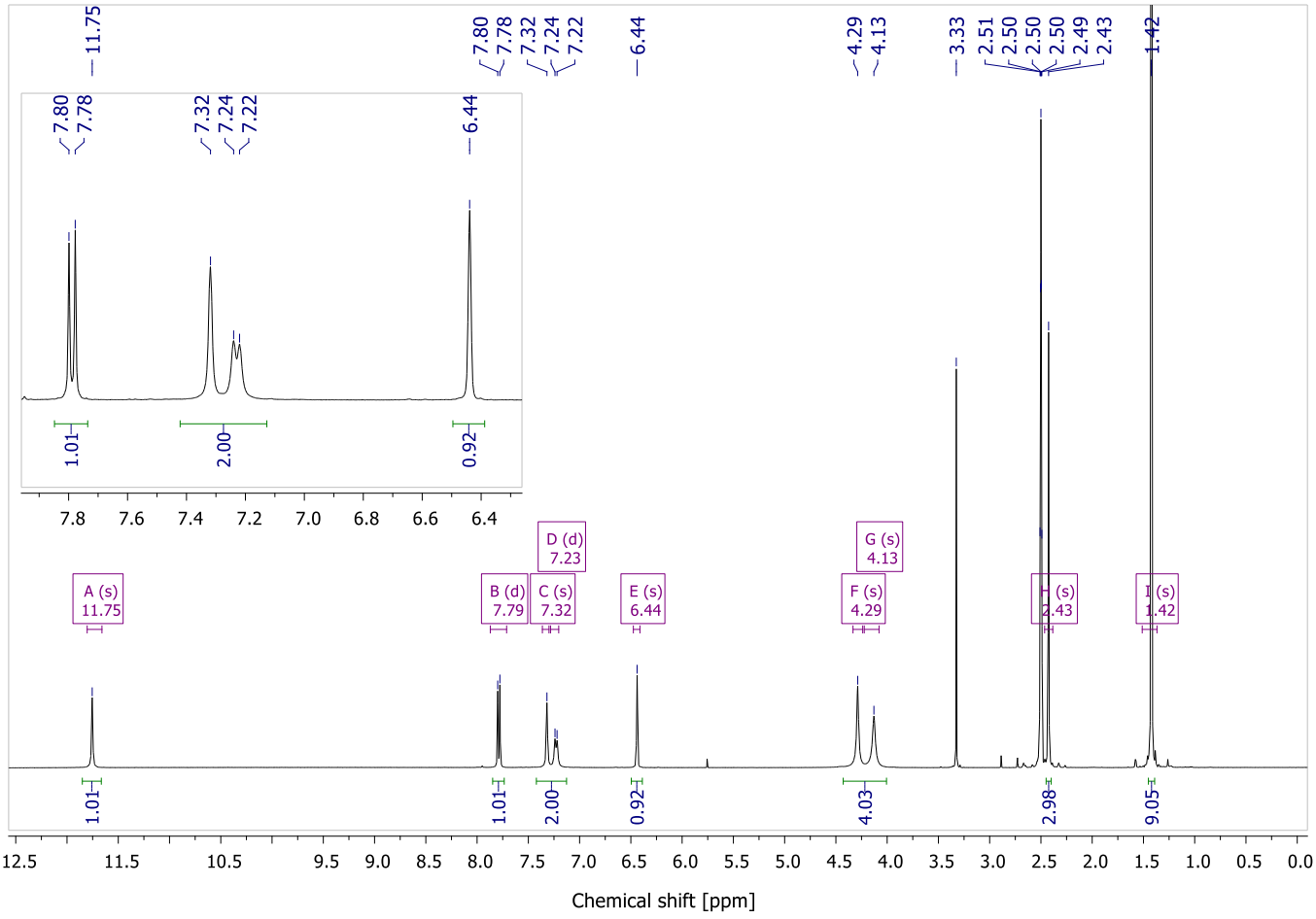
DKS57_058A

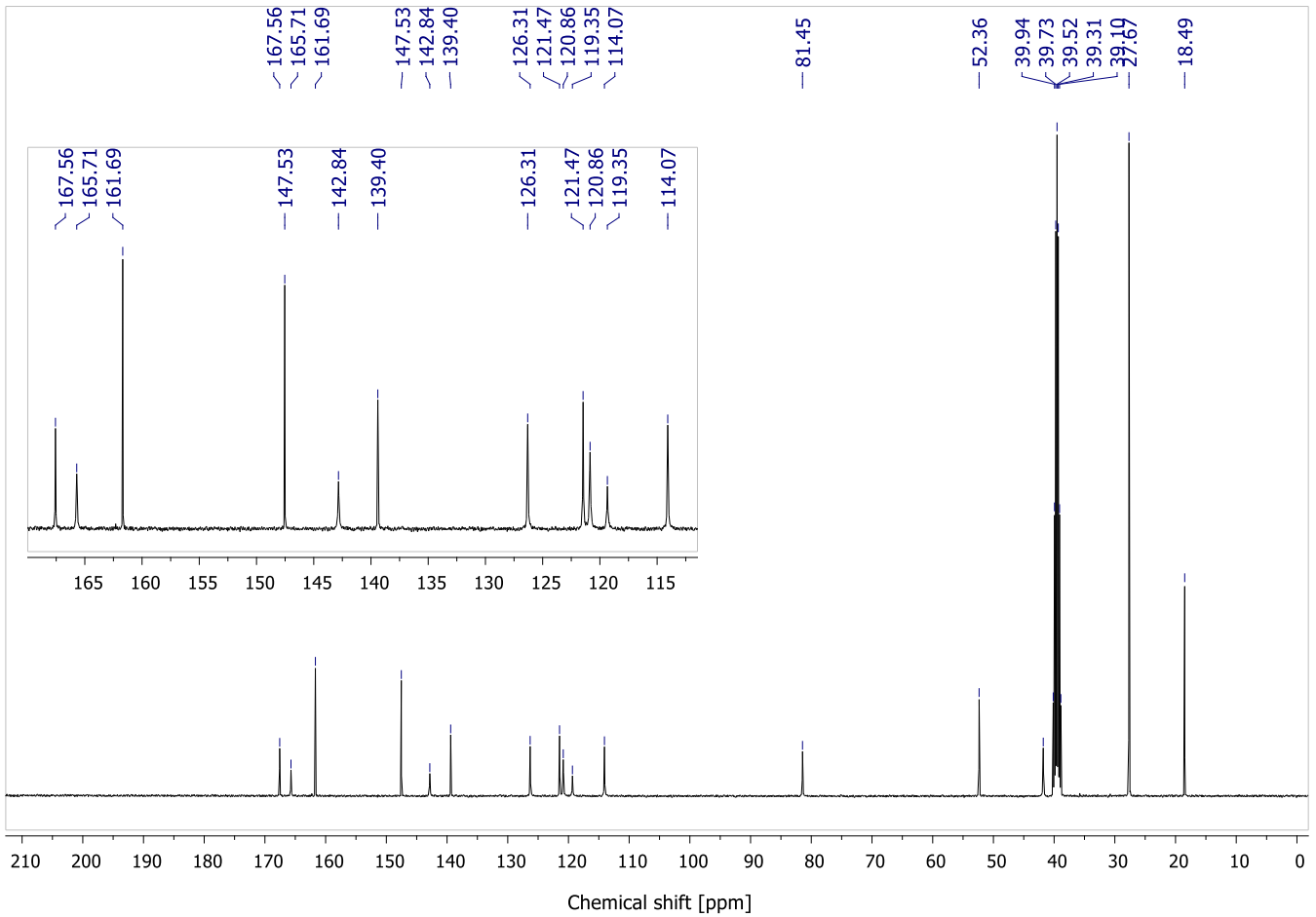


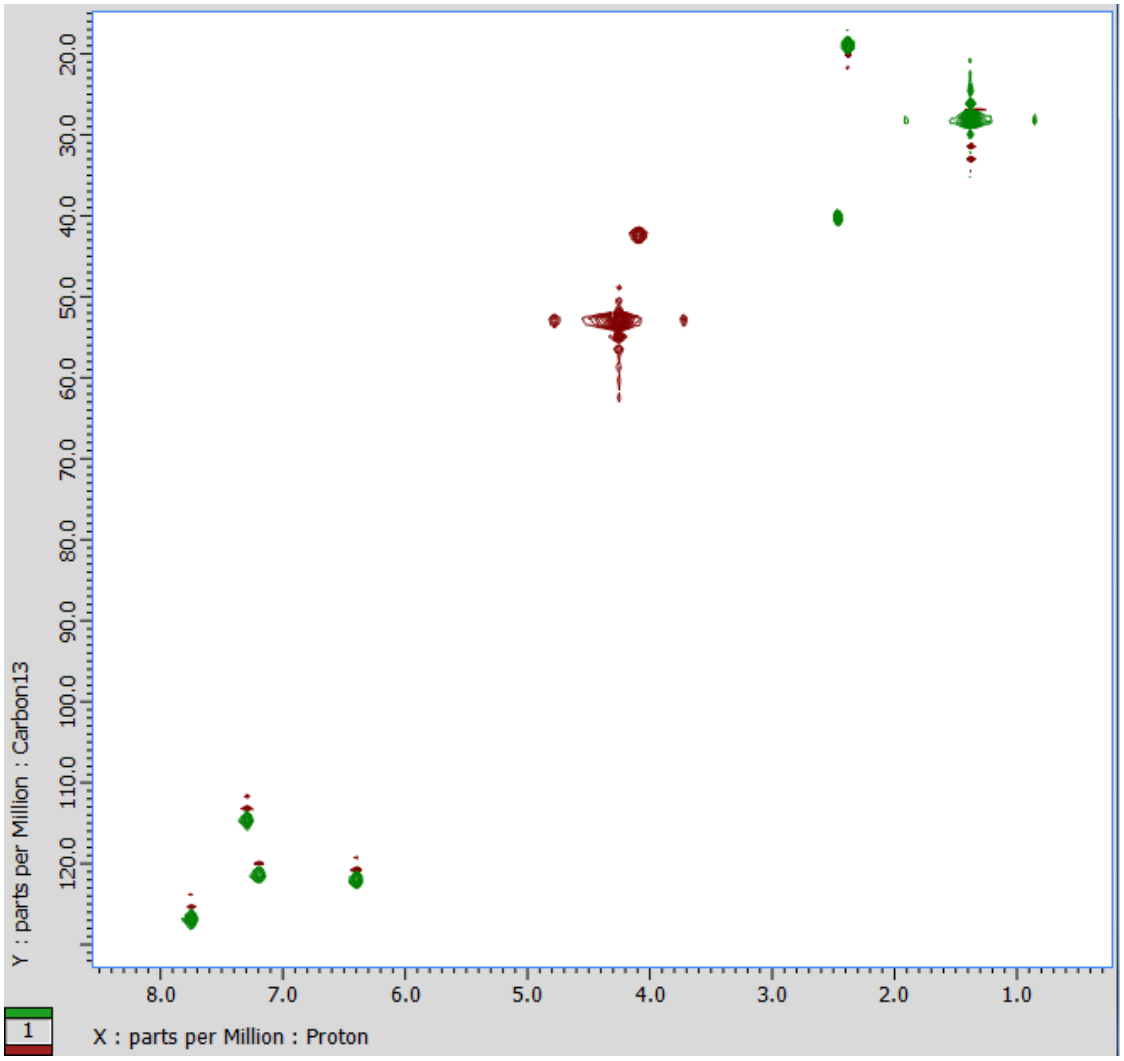
Formula Weight : 364,82(1)
Exact Mass : 364,11898
Formula : $C_{18}H_{21}ClN_2O_4$
Composition : C 59,26% H 5,80% N 7,68% O 17,54% Cl 9,72%

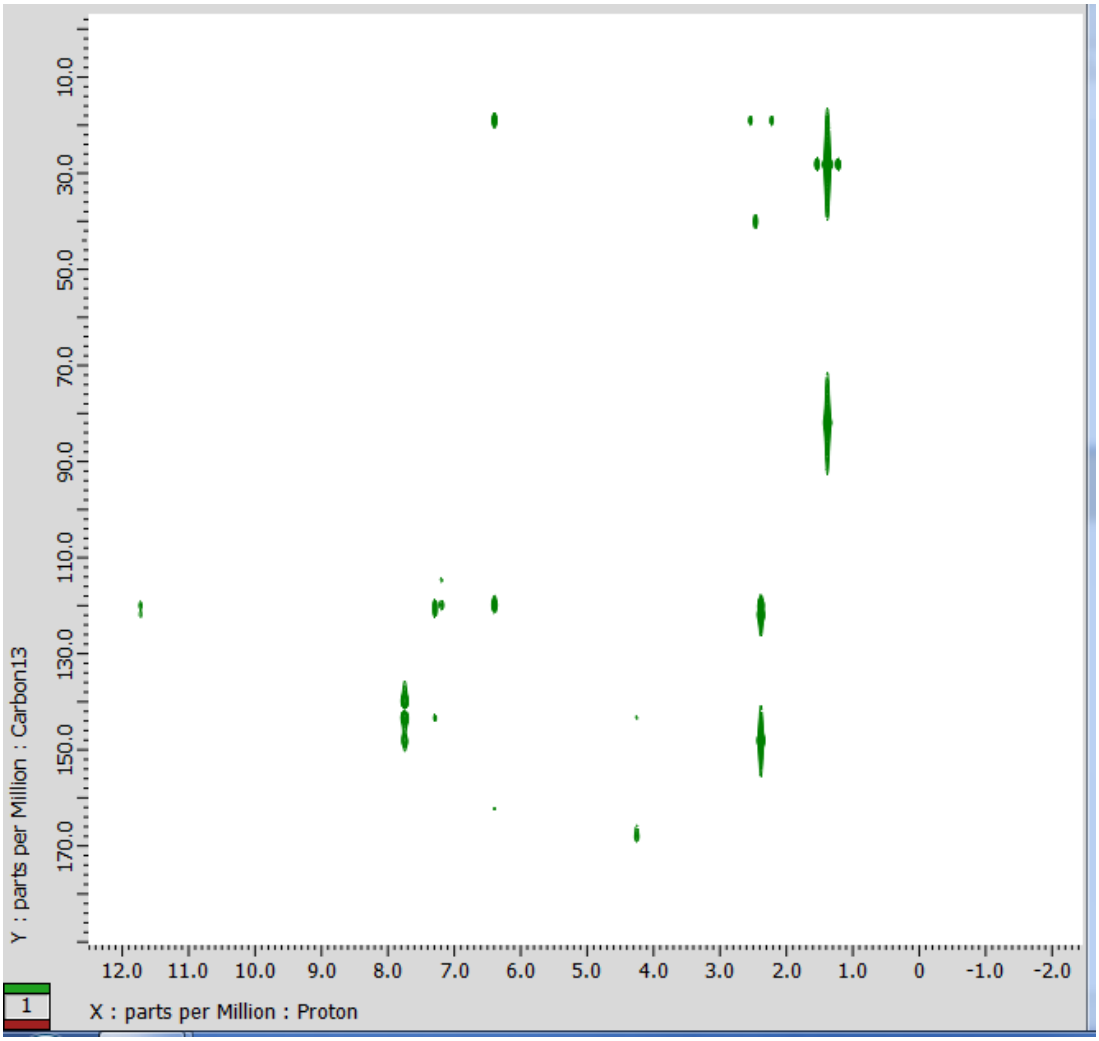




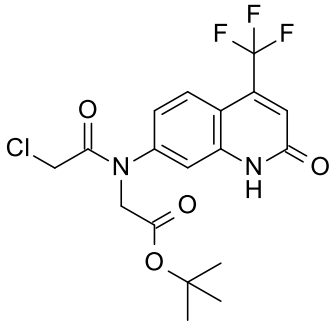

11.75
7.80
7.78
7.32
7.24
7.22
6.44
4.29
4.13
3.33
2.51
2.50
2.50
2.50
2.49
2.43
1.42
A (s) 11.75
B (d) 7.79
C (s) 7.32
D (d) 7.23
E (s) 6.44
F (s) 4.29
G (s) 4.13
H (s) 2.43
I (s) 1.42
1.01
1.01
2.00
0.92
4.03
2.98
9.05
Chemical shift [ppm]


167.56
165.71
161.69
147.53
142.84
139.40
126.31
121.47
120.86
119.35
114.07
81.45
52.36
39.94
39.73
39.52
39.31
18.49
Chemical shift [ppm]

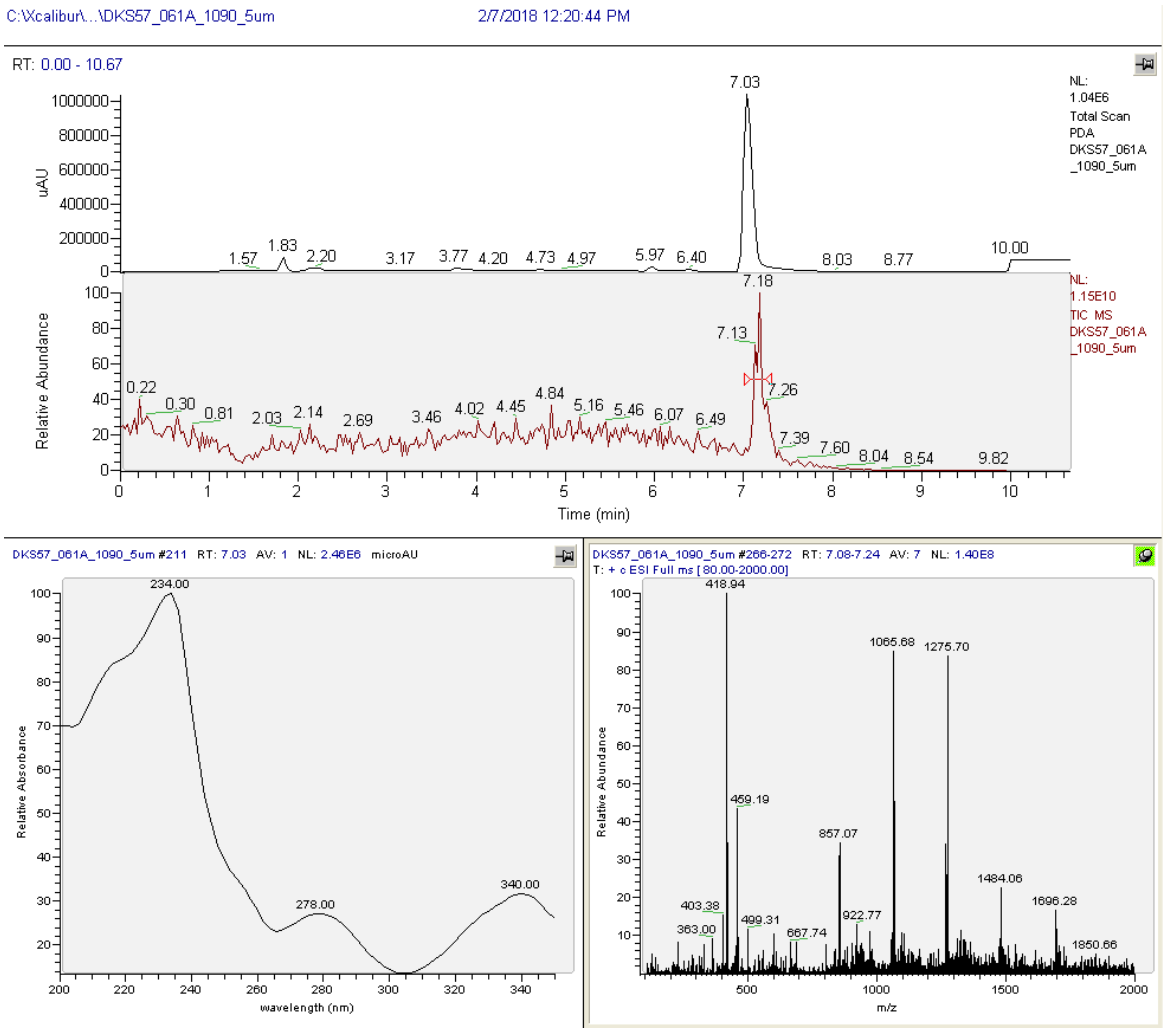

Y : parts per Million : Carbon13
20.0
30.0
40.0
50.0
60.0
70.0
80.0
90.0
100.0
110.0
120.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
1
X : parts per Million : Proton

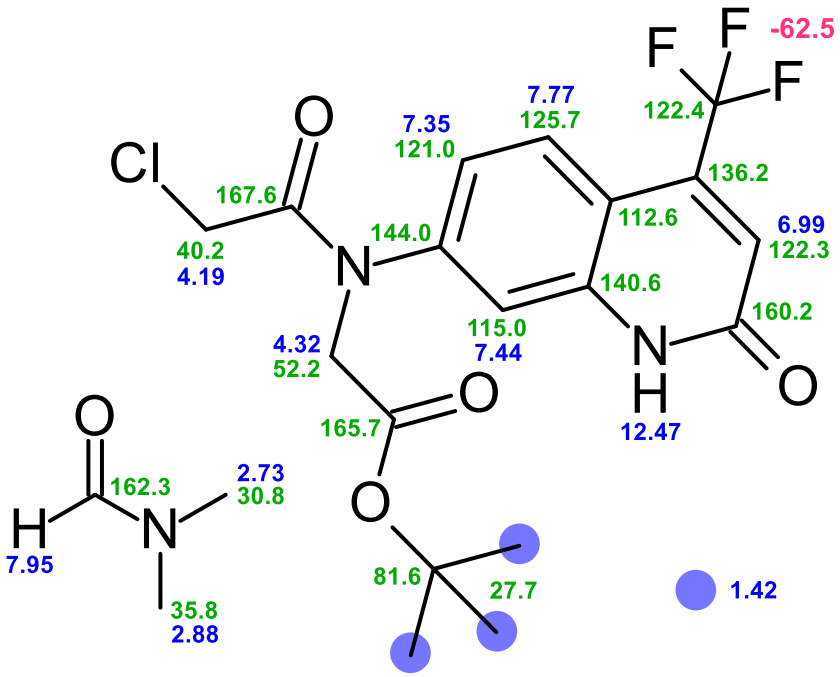

Y : parts per Million : Carbon13
10.0
30.0
50.0
70.0
90.0
110.0
130.0
150.0
170.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
1
X : parts per Million : Proton

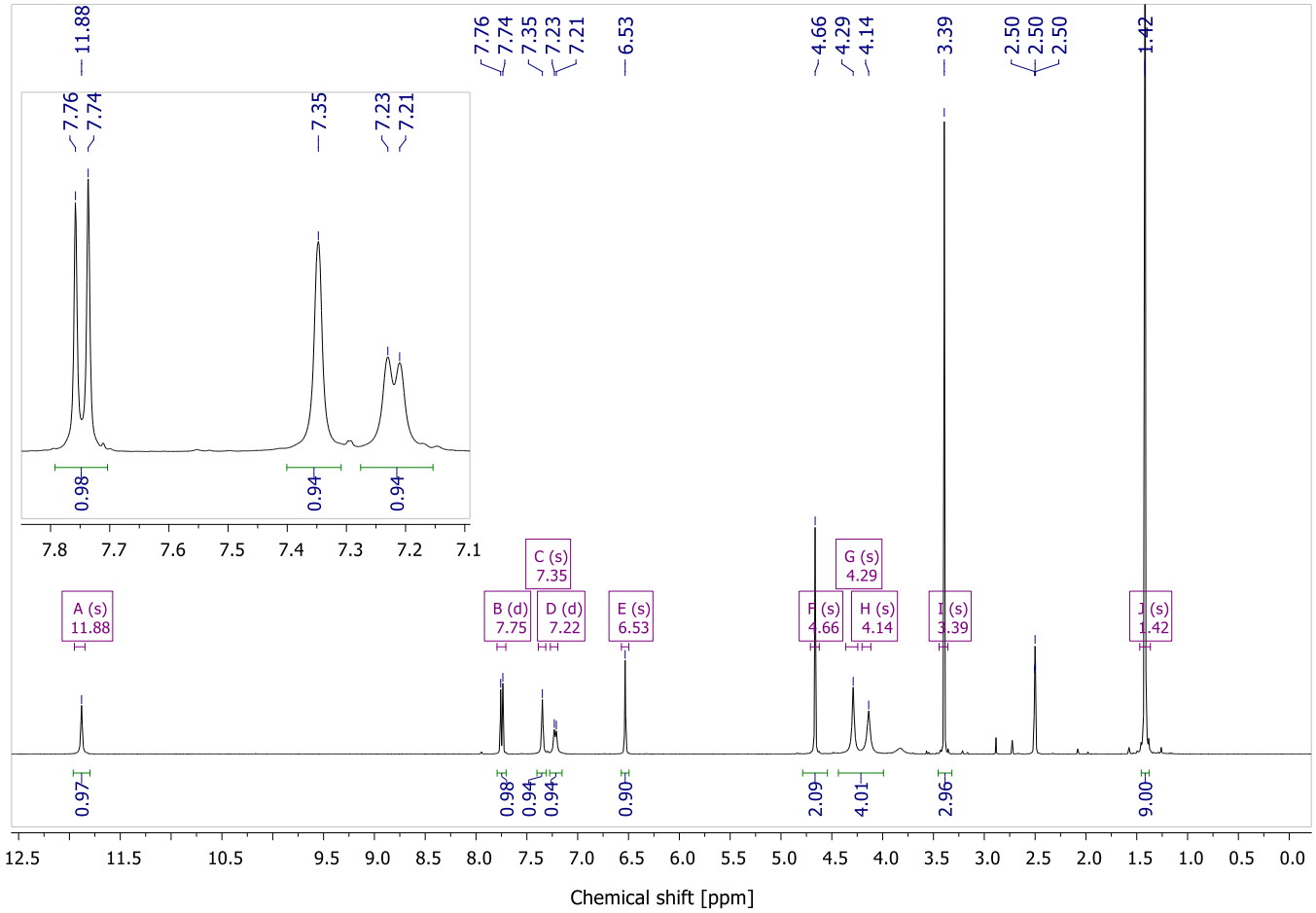
DKS57_061A

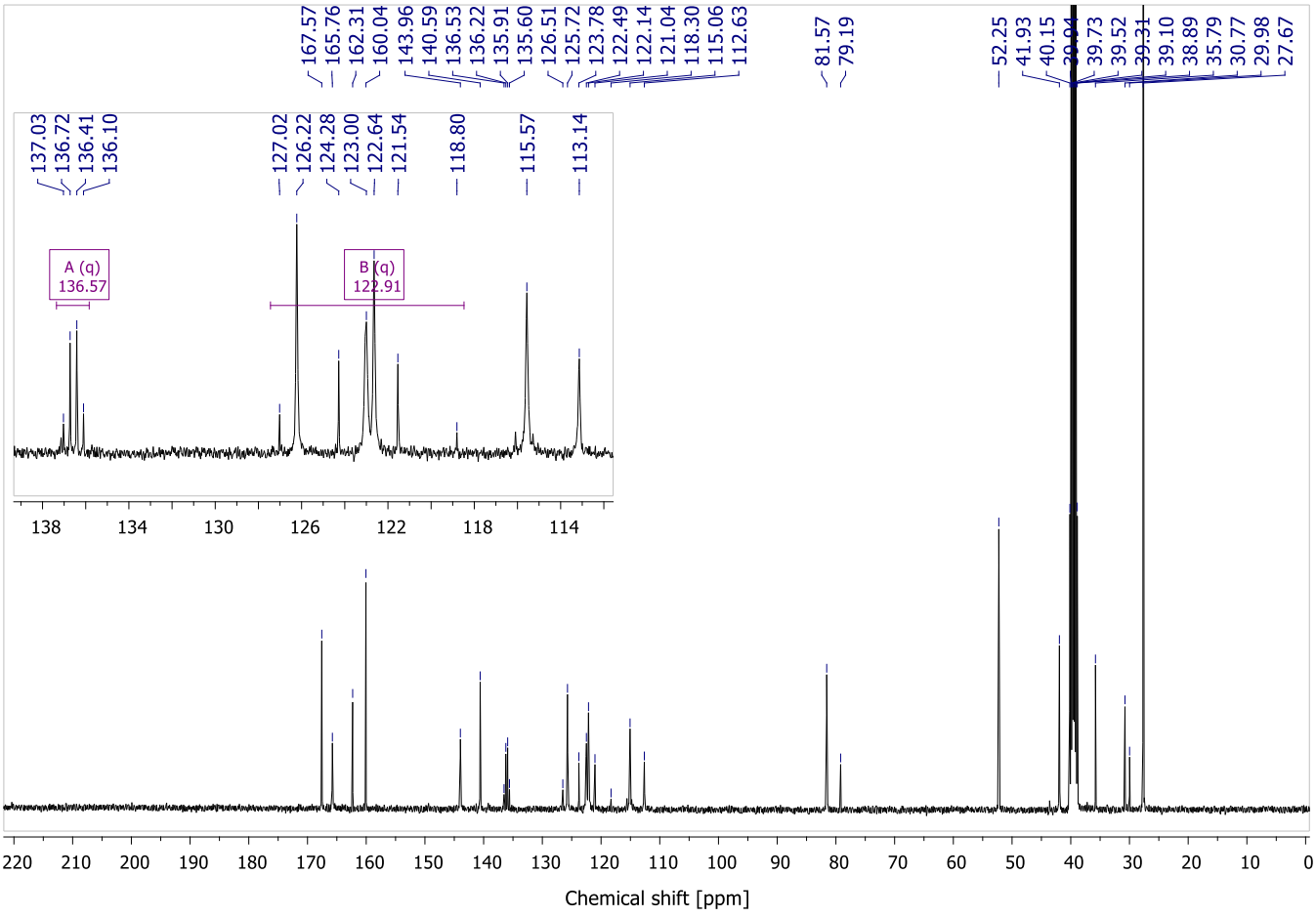


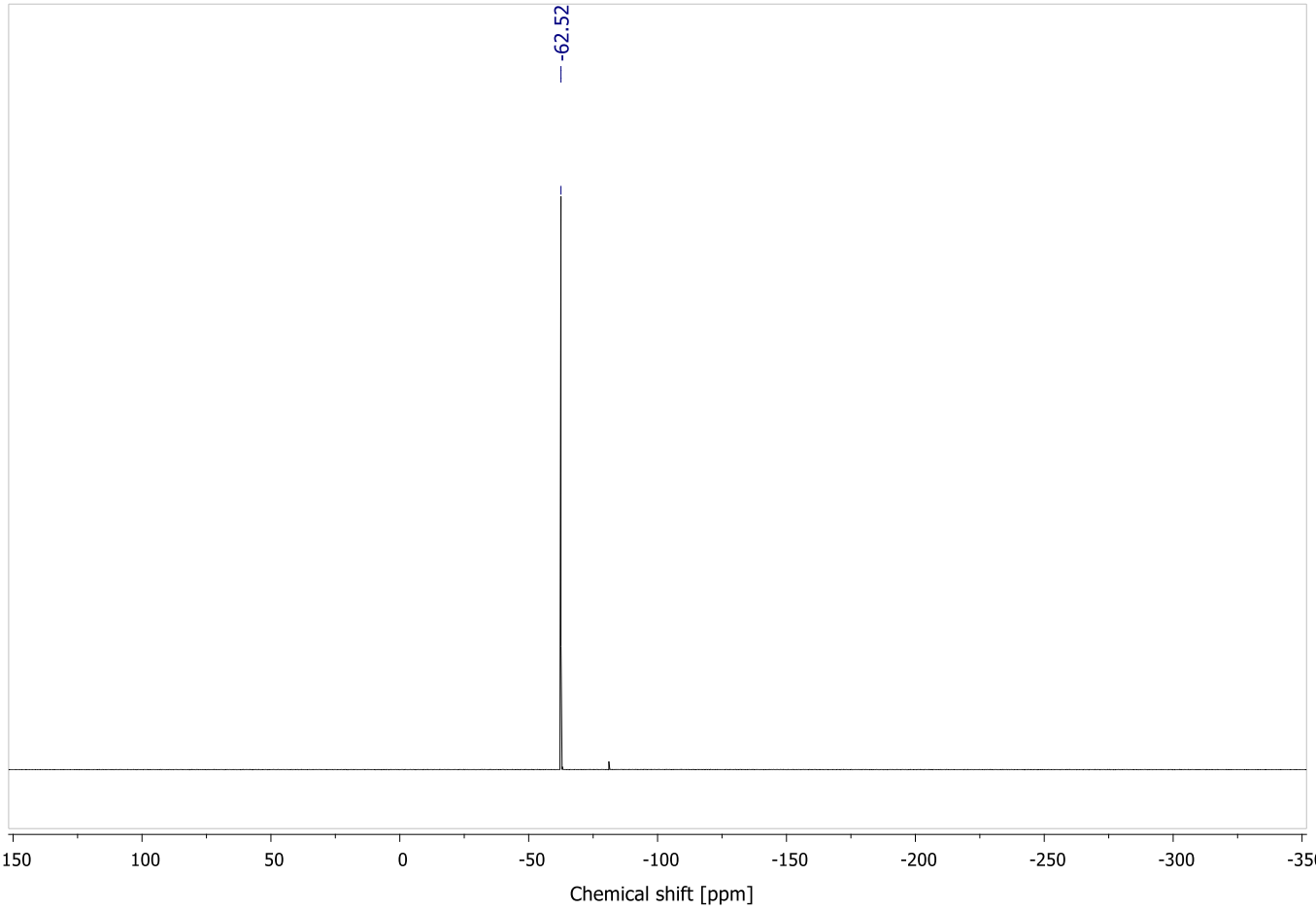
Formula Weight : 418,79(1)
Exact Mass : 418,09072
Formula : $C_{18}H_{18}ClF_3N_2O_4$
Composition : C 51,62% H 4,33% N 6,69% O 15,28%
Cl 8,47% F 13,61%

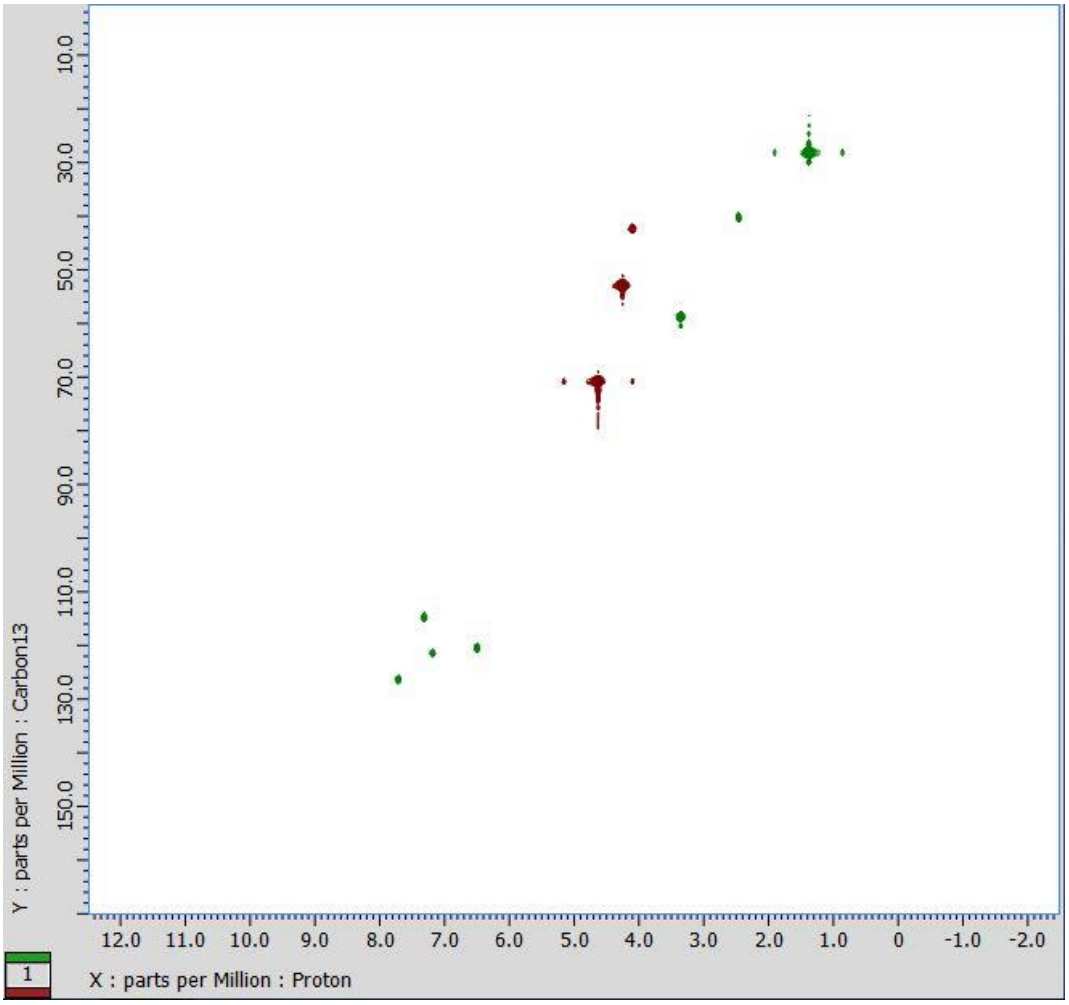


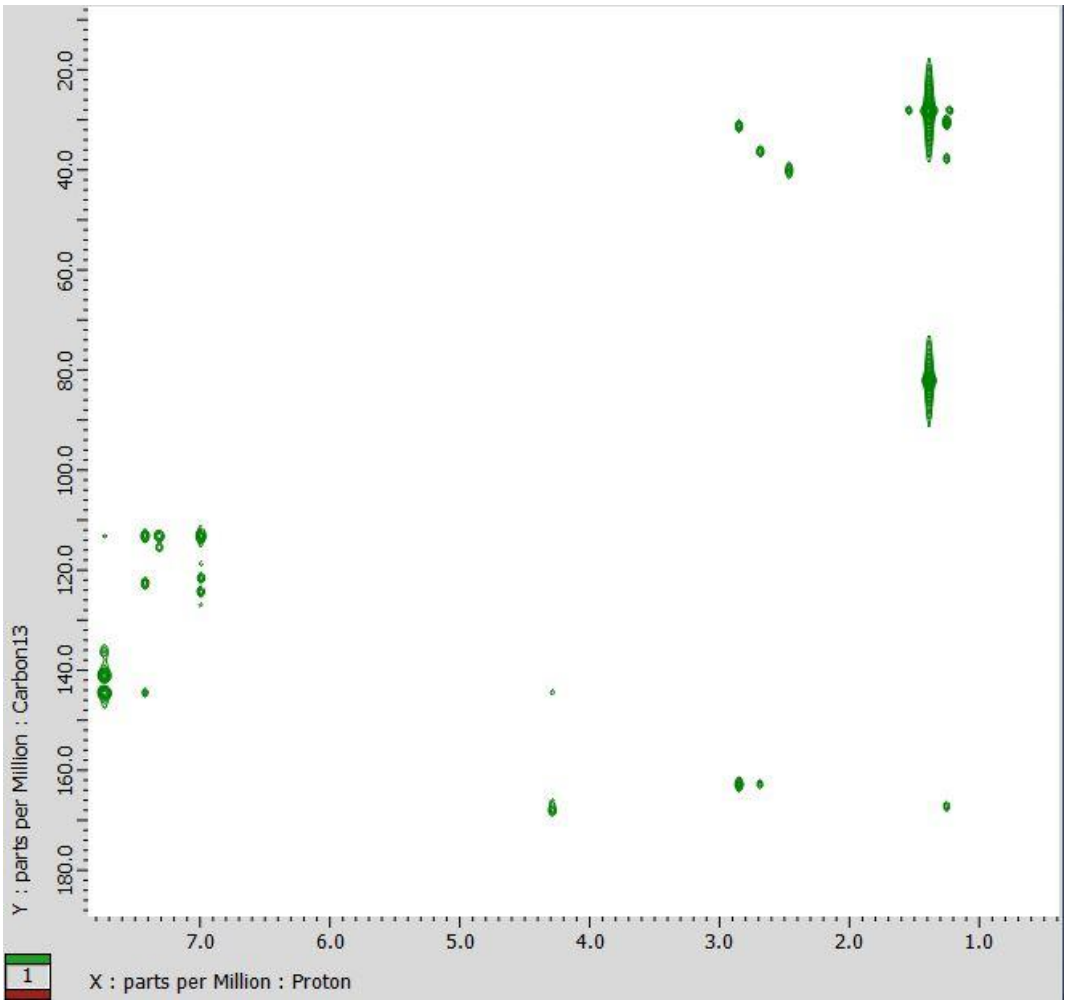

-62.5
F
F
F
122.4
7.77
125.7
7.35
121.0
136.2
6.99
122.3
112.6
144.0
140.6
160.2
115.0
7.44
4.32
52.2
12.47
O
Cl
167.6
40.2
4.19
N
H
O
165.7
O
O
162.3
2.73
30.8
H
N
7.95
35.8
2.88
81.6
27.7
1.42


11.88
7.76
7.74
7.35
7.23
7.21
6.53
4.66
4.29
4.14
3.39
2.50
2.50
2.50
1.42
A (s) 11.88
B (d) 7.75
C (s) 7.35
D (d) 7.22
E (s) 6.53
F (s) 4.66
G (s) 4.29
H (s) 4.14
I (s) 3.39
J (s) 1.42
0.98
0.94
0.94
0.97
0.98
0.94
0.94
0.90
2.09
4.01
2.96
9.00
Chemical shift [ppm]

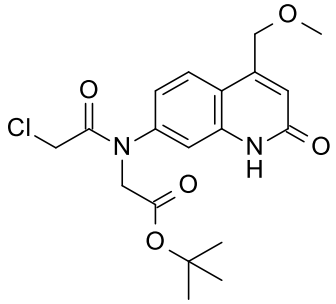

167.57
165.76
162.31
160.04
143.96
140.59
136.53
136.22
135.91
135.60
126.51
125.72
123.78
122.49
122.14
121.04
118.30
115.06
112.63
81.57
79.19
52.25
41.93
40.15
39.73
39.52
39.31
39.10
38.89
35.79
30.77
29.98
27.67
137.03
136.72
136.41
136.10
127.02
126.22
124.28
123.00
122.64
121.54
118.80
115.57
113.14
A (q)
136.57
B (q)
122.91
138
134
130
126
122
118
114
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical shift [ppm]


-62.52
150
100
50
0
-50
-100
-150
-200
-250
-300
-350
Chemical shift [ppm]

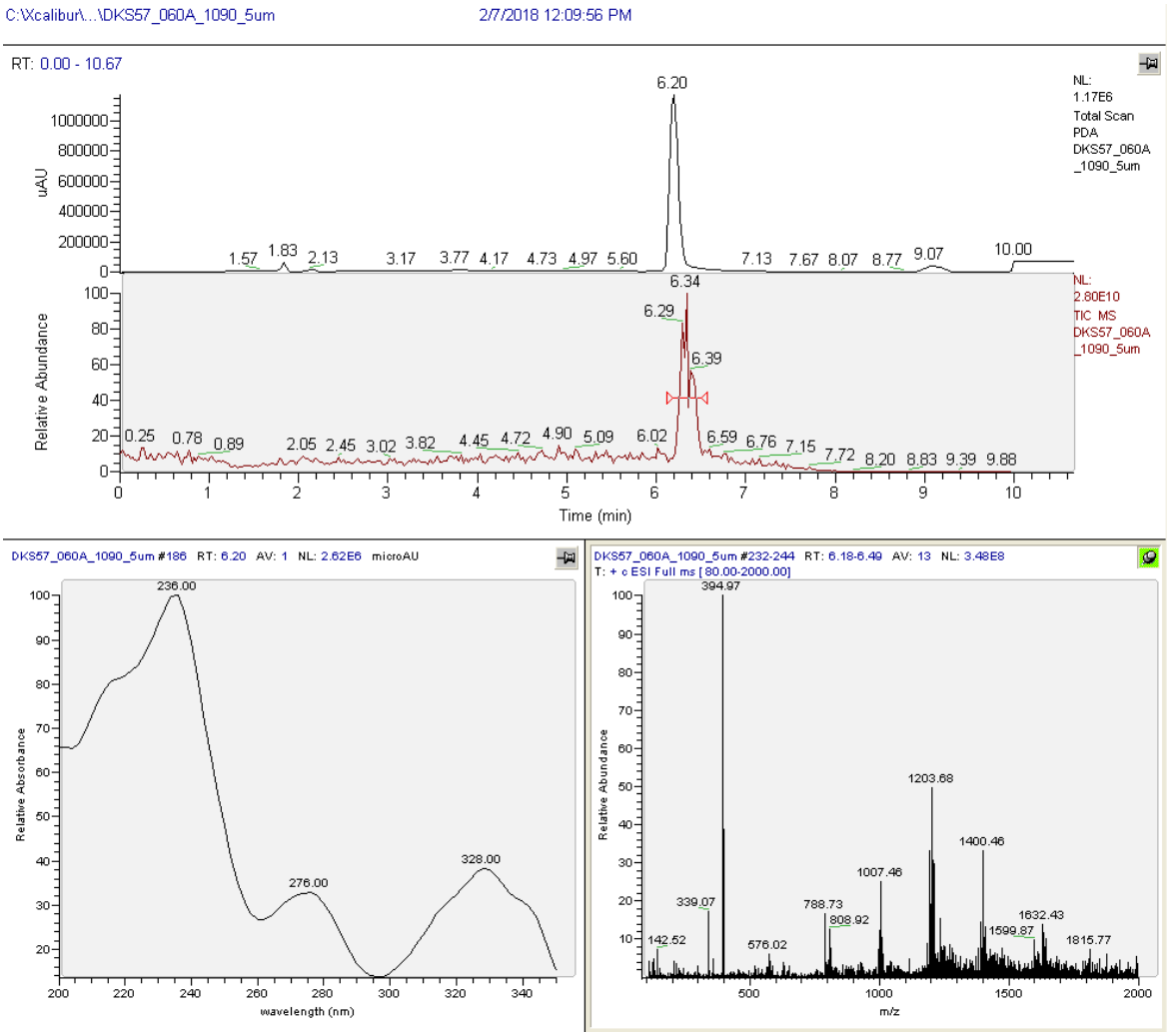

10.0
30.0
50.0
70.0
90.0
110.0
130.0
150.0
Y : parts per Million : Carbon13
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
1
X : parts per Million : Proton

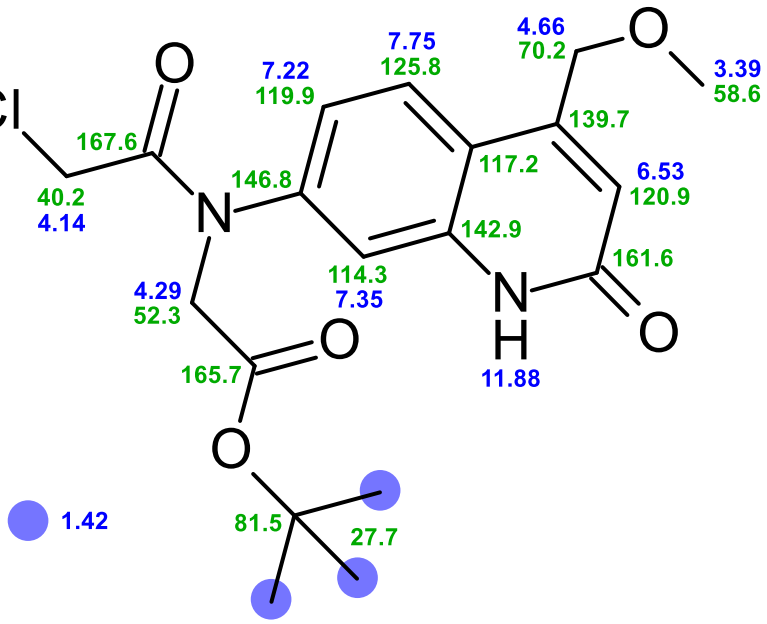

20.0
40.0
60.0
80.0
100.0
120.0
140.0
160.0
180.0
Y : parts per Million : Carbon13
7.0
6.0
5.0
4.0
3.0
2.0
1.0
1
X : parts per Million : Proton

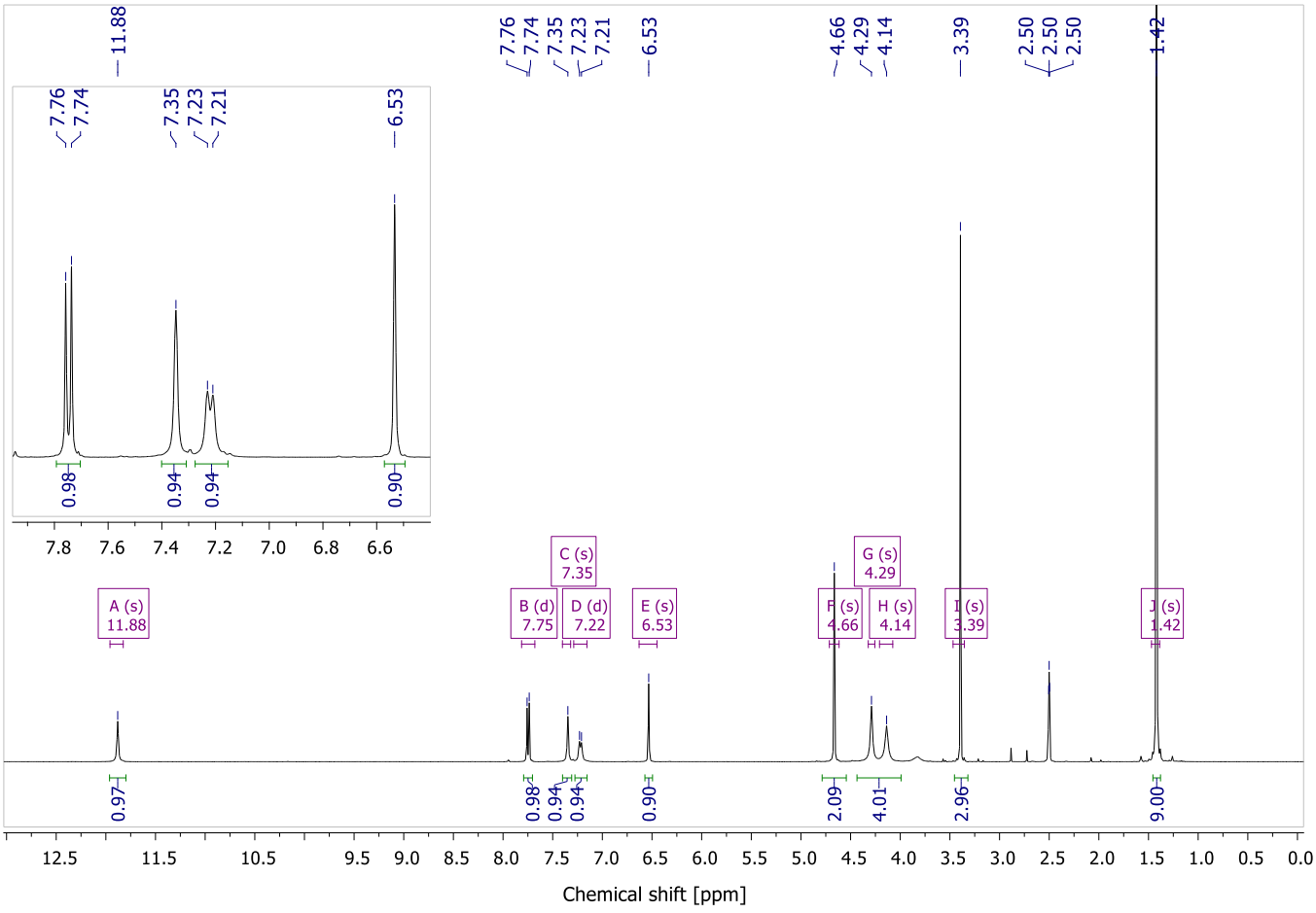
DKS57_060A

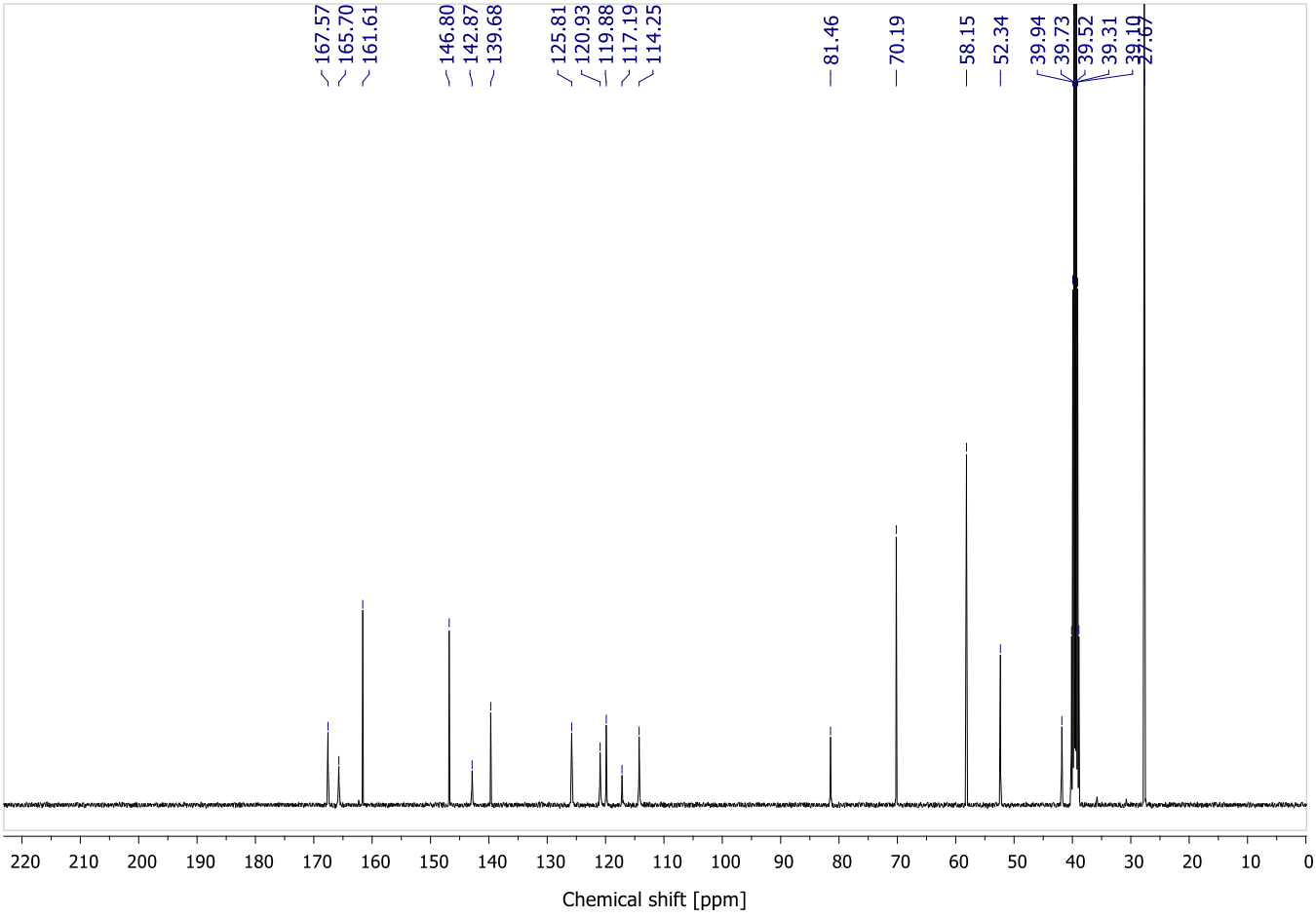


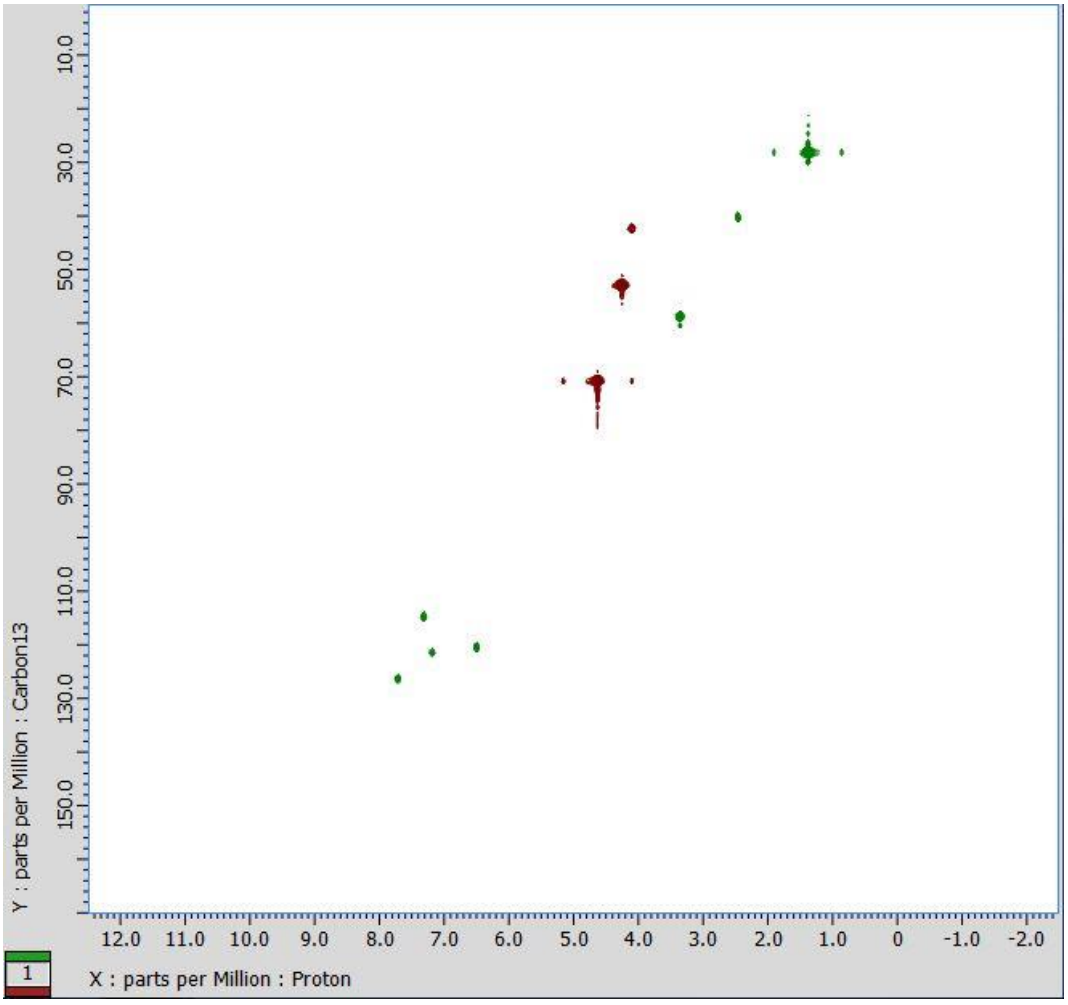
Formula Weight : 394,85(2)
Exact Mass : 394,12955
Formula : $C_{19}H_{23}ClN_2O_5$
Composition : C 57,80% H 5,87% N 7,09% O 20,26% Cl 8,98%

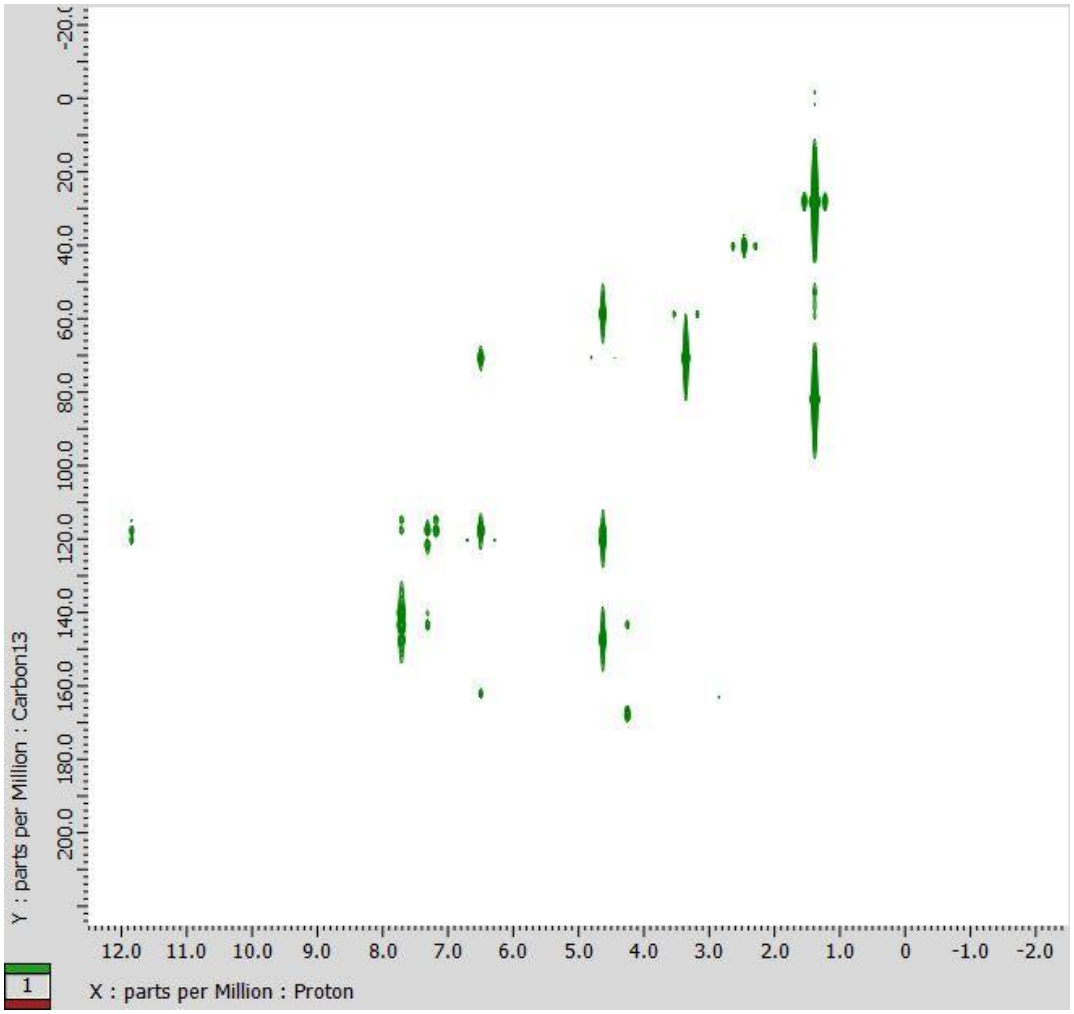




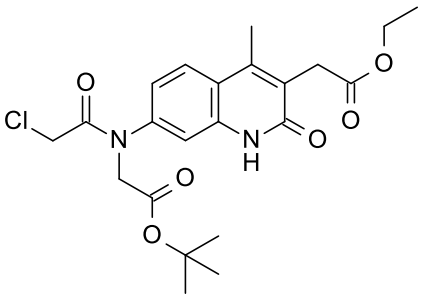

11.88
7.76
7.74
7.35
7.23
7.21
6.53
4.66
4.29
4.14
3.39
2.50
2.50
2.50
1.42
A (s) 11.88
B (d) 7.75
C (s) 7.35
D (d) 7.22
E (s) 6.53
F (s) 4.66
G (s) 4.29
H (s) 4.14
I (s) 3.39
J (s) 1.42
0.97
0.98
0.94
0.94
0.90
2.09
4.01
2.96
9.00
Chemical shift [ppm]


167.57
165.70
161.61
146.80
142.87
139.68
125.81
120.93
119.88
117.19
114.25
81.46
70.19
58.15
52.34
39.94
39.73
39.52
39.31
39.10
27.67
Chemical shift [ppm]

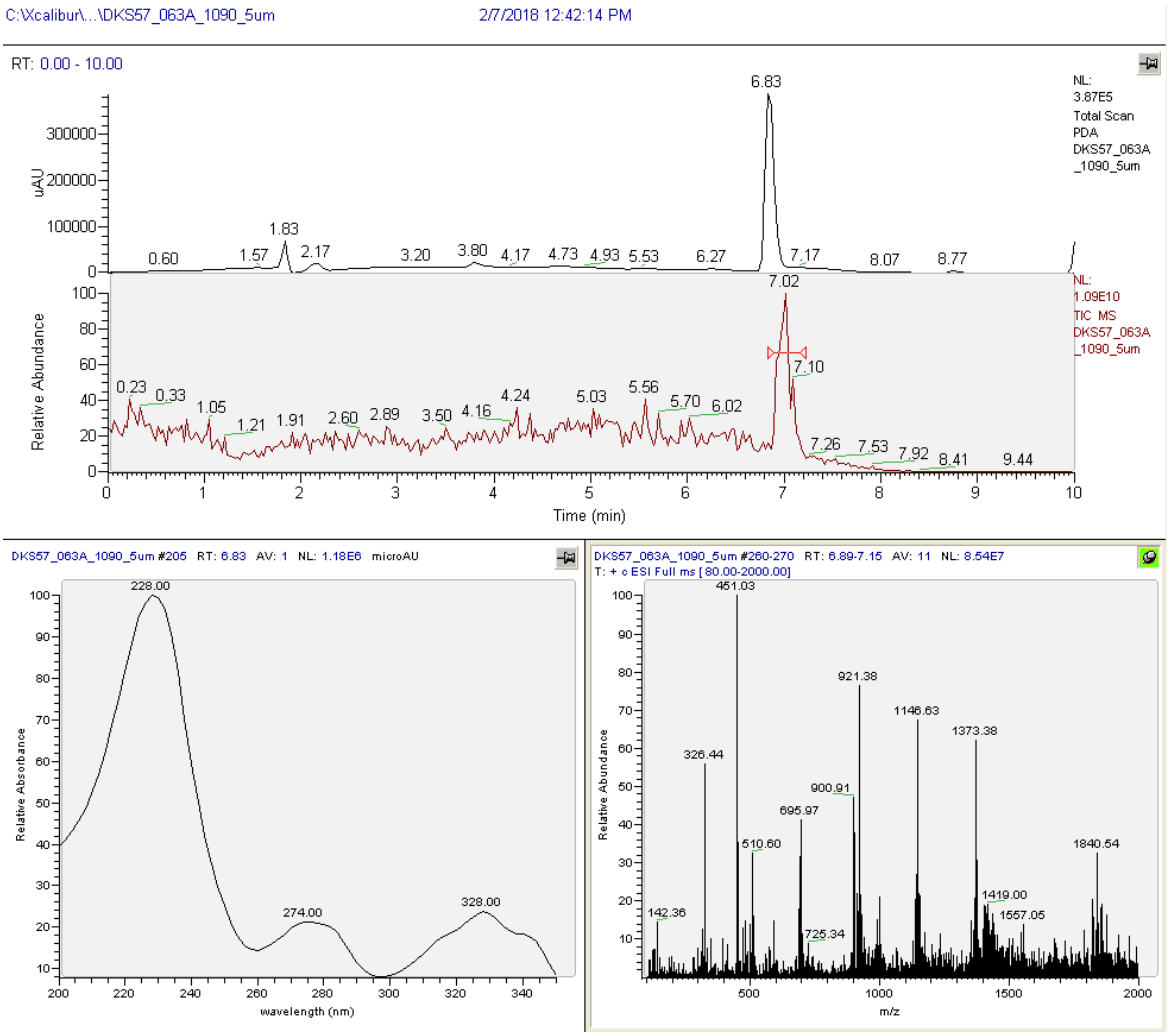

Y : parts per Million : Carbon13
10.0
30.0
50.0
70.0
90.0
110.0
130.0
150.0
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 -1.0 -2.0
1
X : parts per Million : Proton

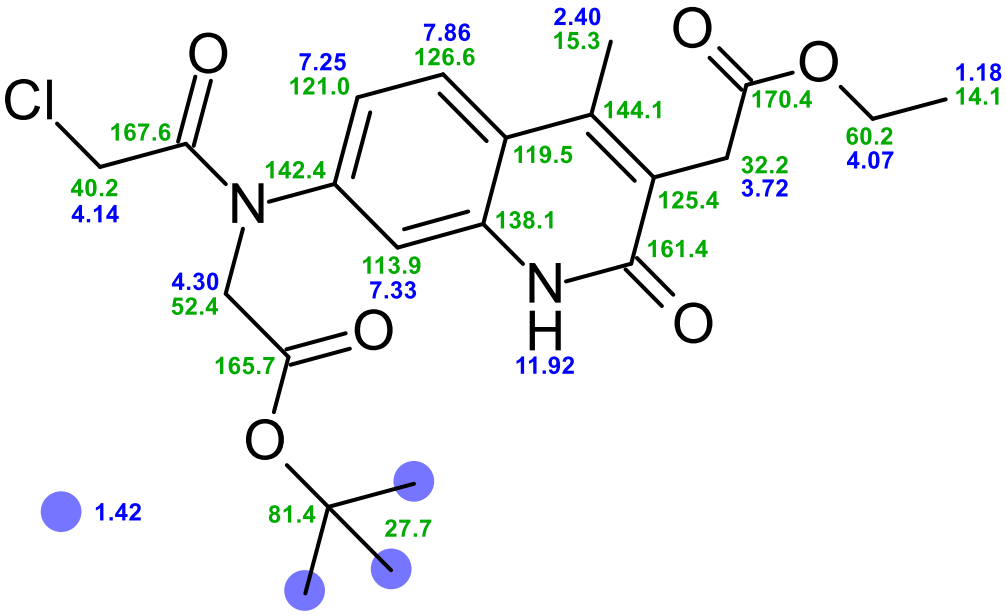

Y : parts per Million : Carbon13
0
20.0
40.0
60.0
80.0
100.0
120.0
140.0
160.0
180.0
200.0
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 -1.0 -2.0
1
X : parts per Million : Proton

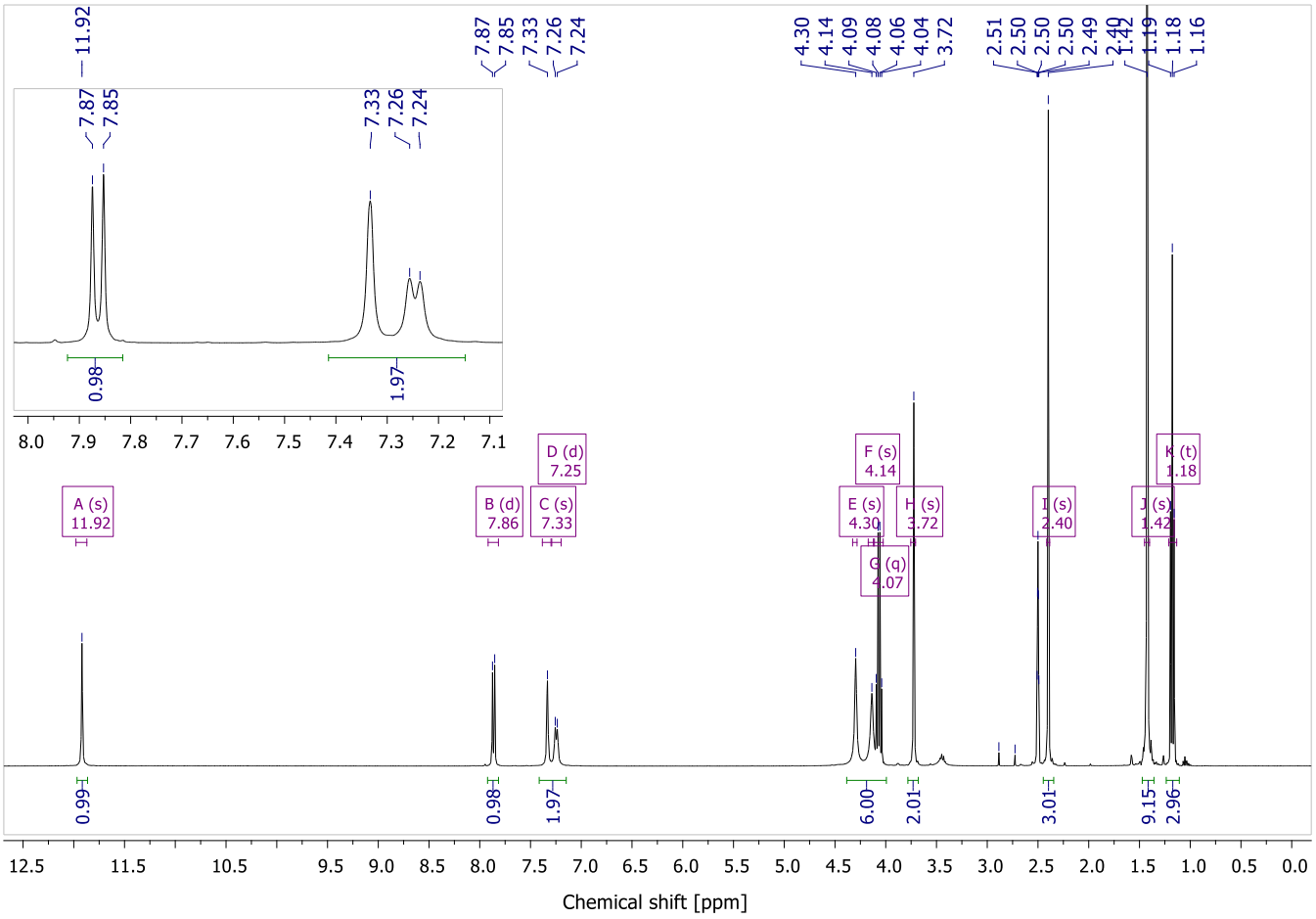
DKS57_063A

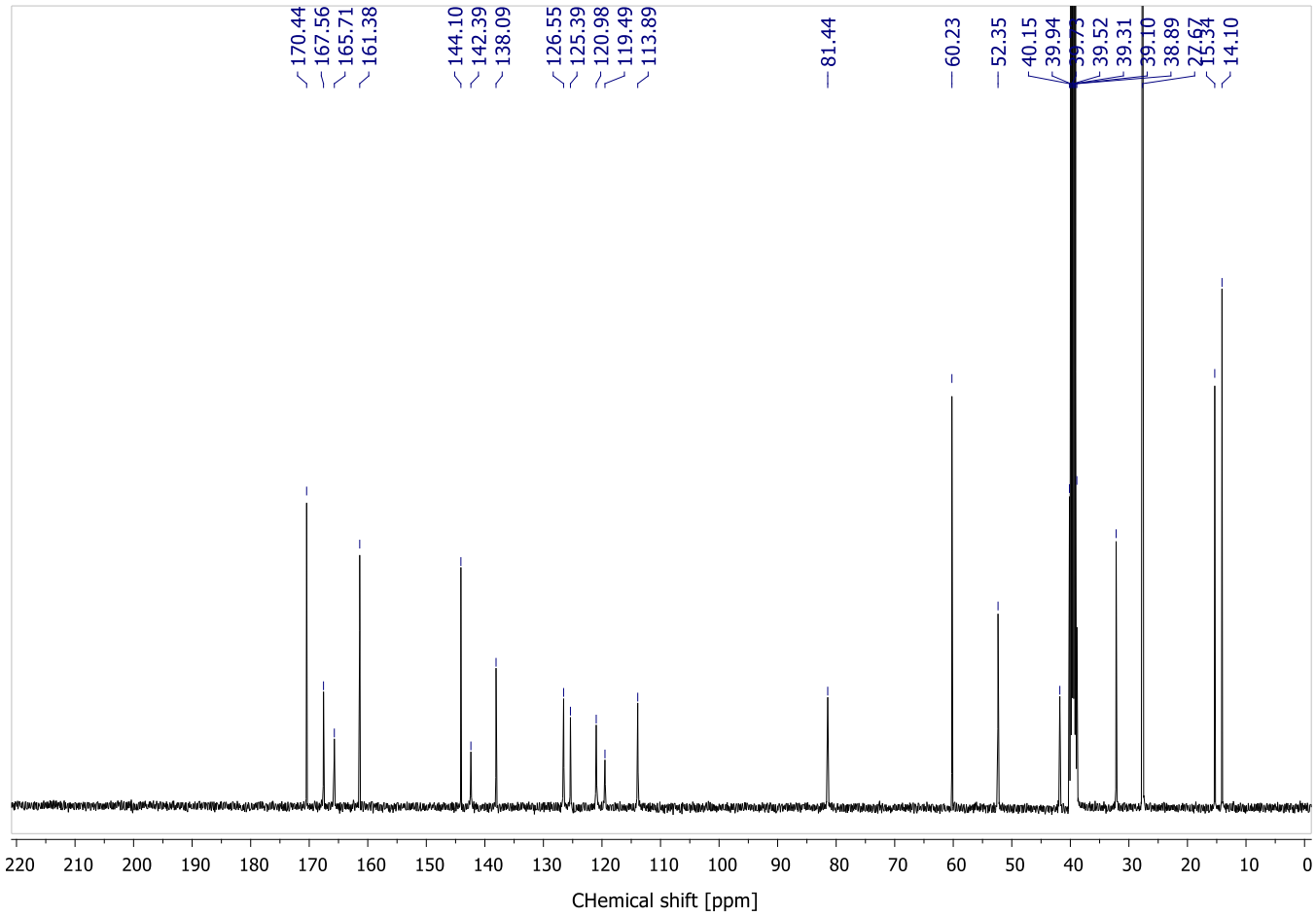


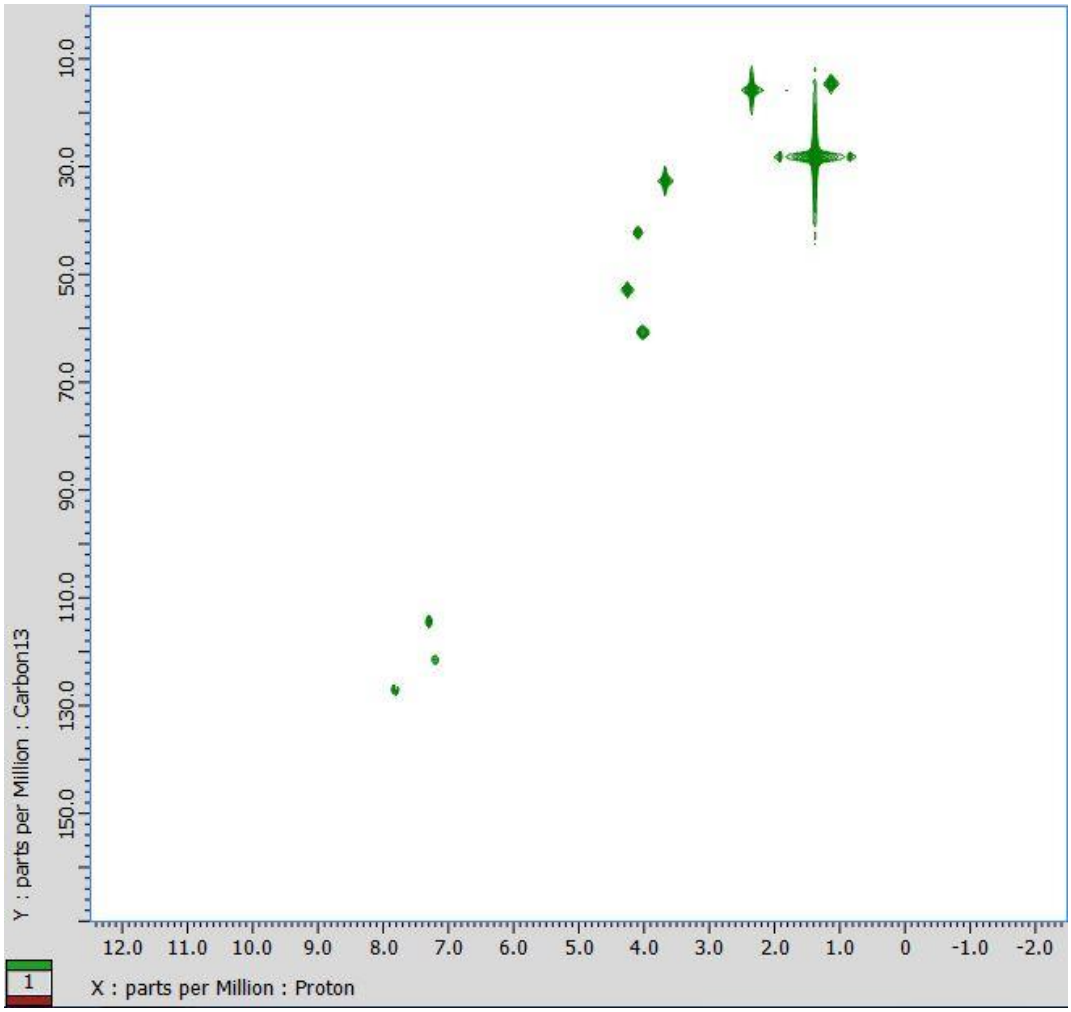
Formula Weight : 450,91(2)
Exact Mass : 450,15576
Formula : $C_{22}H_{27}ClN_2O_6$
Composition : C 58,60% H 6,04% N 6,21% O 21,29% Cl 7,86%

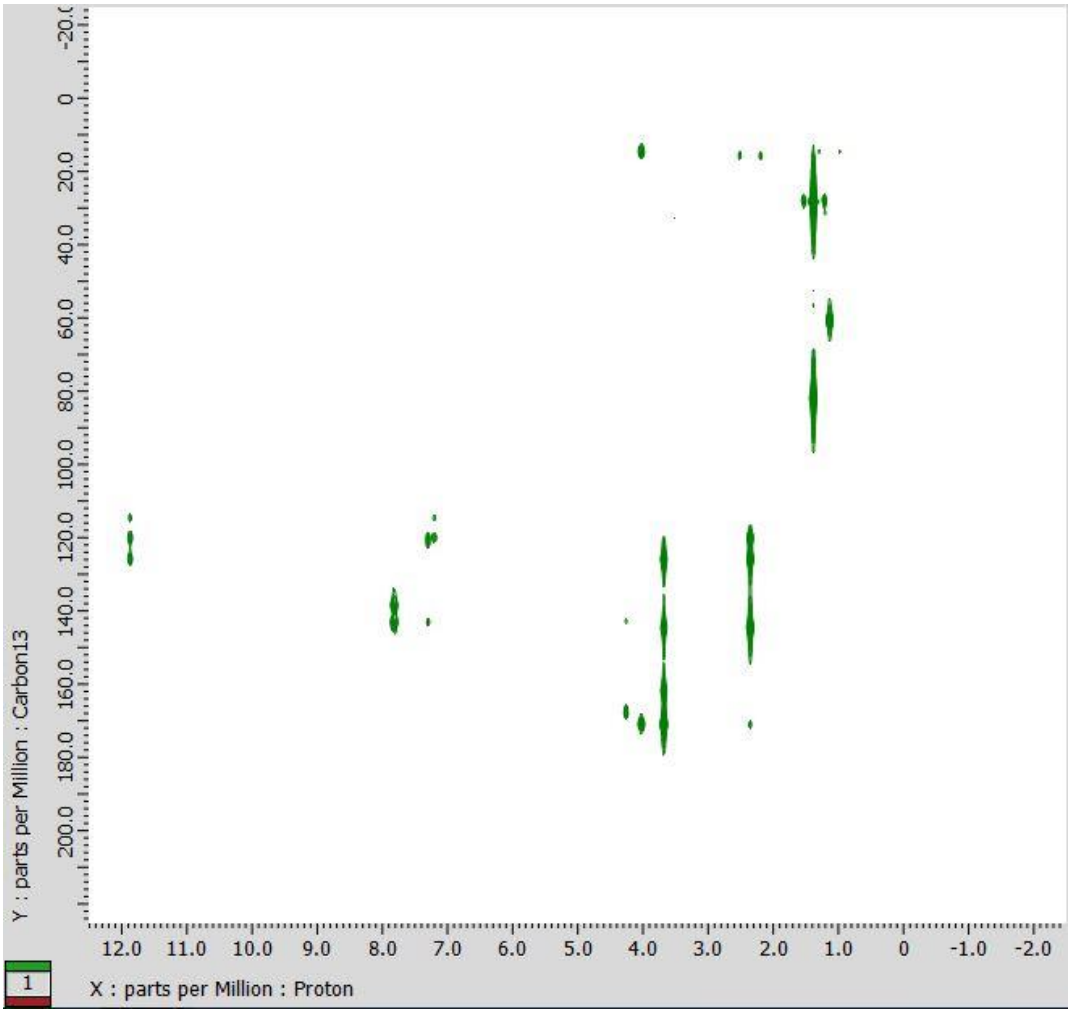




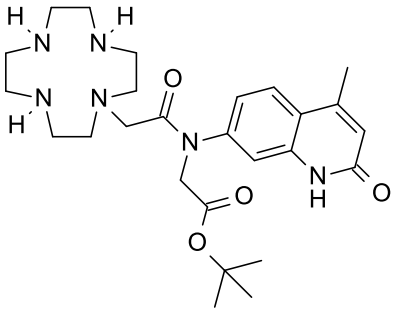

11.92
7.87
7.85
7.33
7.26
7.24
4.30
4.14
4.09
4.08
4.06
4.04
3.72
2.51
2.50
2.50
2.49
2.40
1.42
1.19
1.18
1.16
A (s) 11.92
B (d) 7.86
C (s) 7.33
D (d) 7.25
E (s) 4.30
F (s) 4.14
G (q) 4.07
H (s) 3.72
I (s) 2.40
J (s) 1.42
K (t) 1.18
0.98
1.97
0.99
0.98
1.97
6.00
2.01
3.01
9.15
2.96
Chemical shift [ppm]


170.44
167.56
165.71
161.38
144.10
142.39
138.09
126.55
125.39
120.98
119.49
113.89
81.44
60.23
52.35
40.15
39.94
39.73
39.52
39.31
39.10
38.89
27.67
15.34
14.10
CHemical shift [ppm]

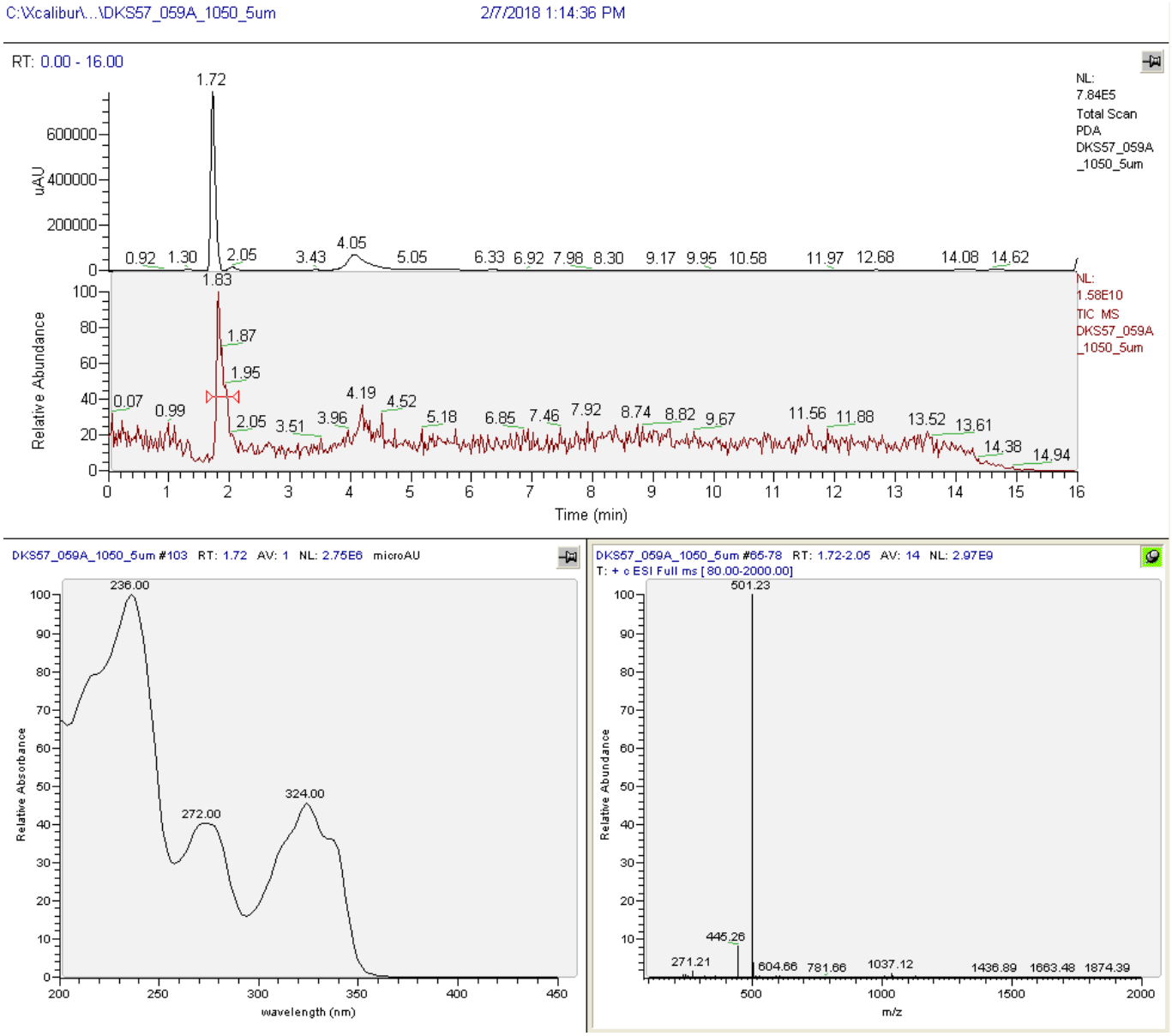

Y : parts per Million : Carbon13
10.0
30.0
50.0
70.0
90.0
110.0
130.0
150.0
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 -1.0 -2.0
1
X : parts per Million : Proton

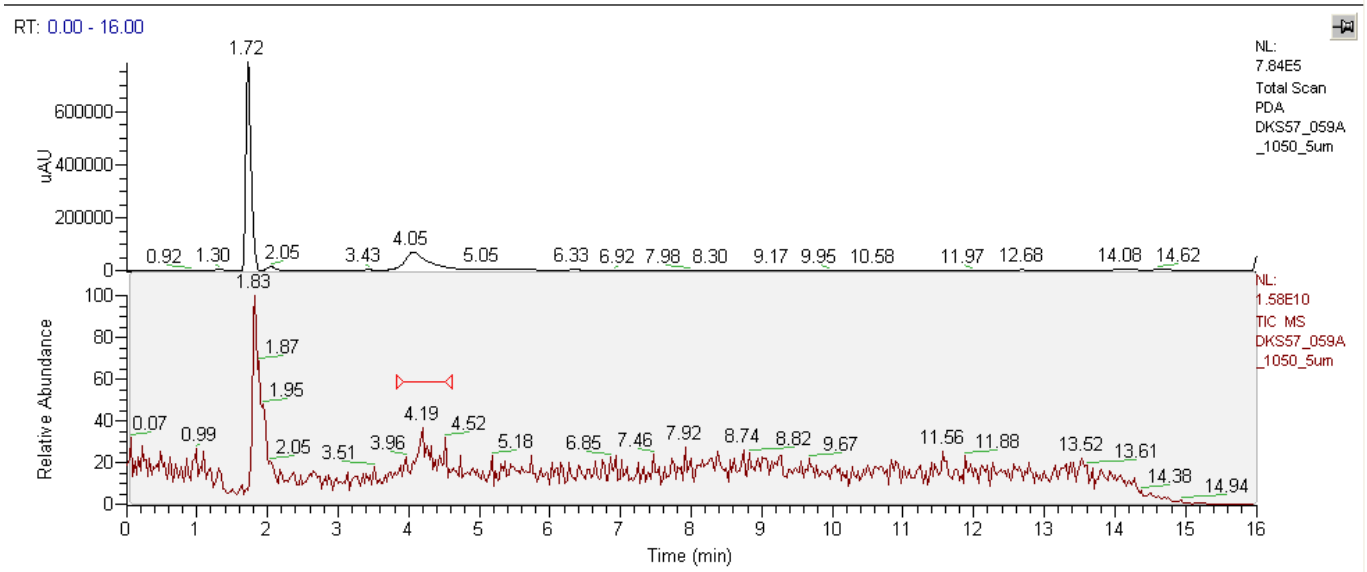

Y : parts per Million : Carbon13
0
20.0
40.0
60.0
80.0
100.0
120.0
140.0
160.0
180.0
200.0
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 -1.0 -2.0
1
X : parts per Million : Proton

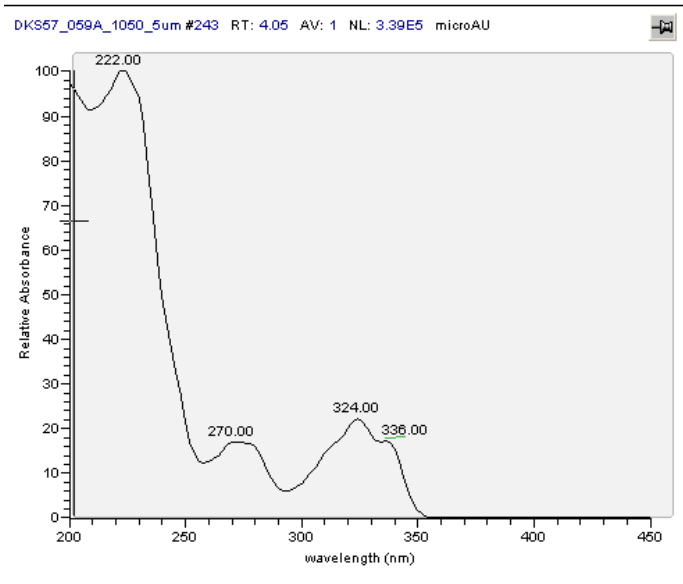
DKS57_059A

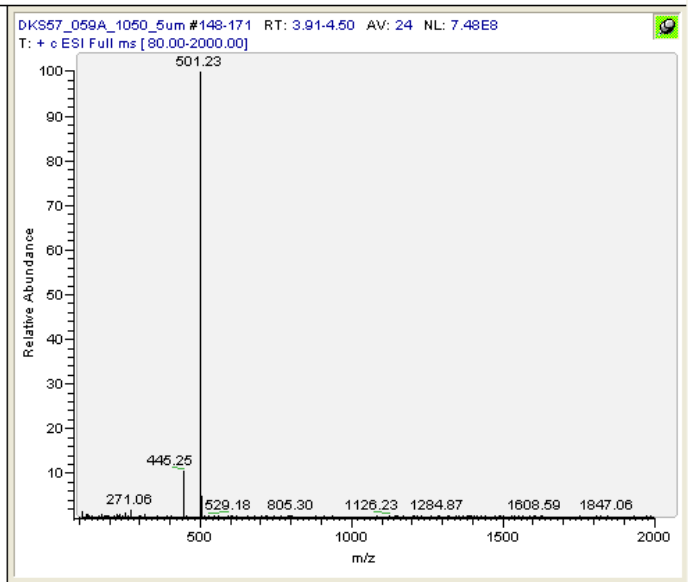


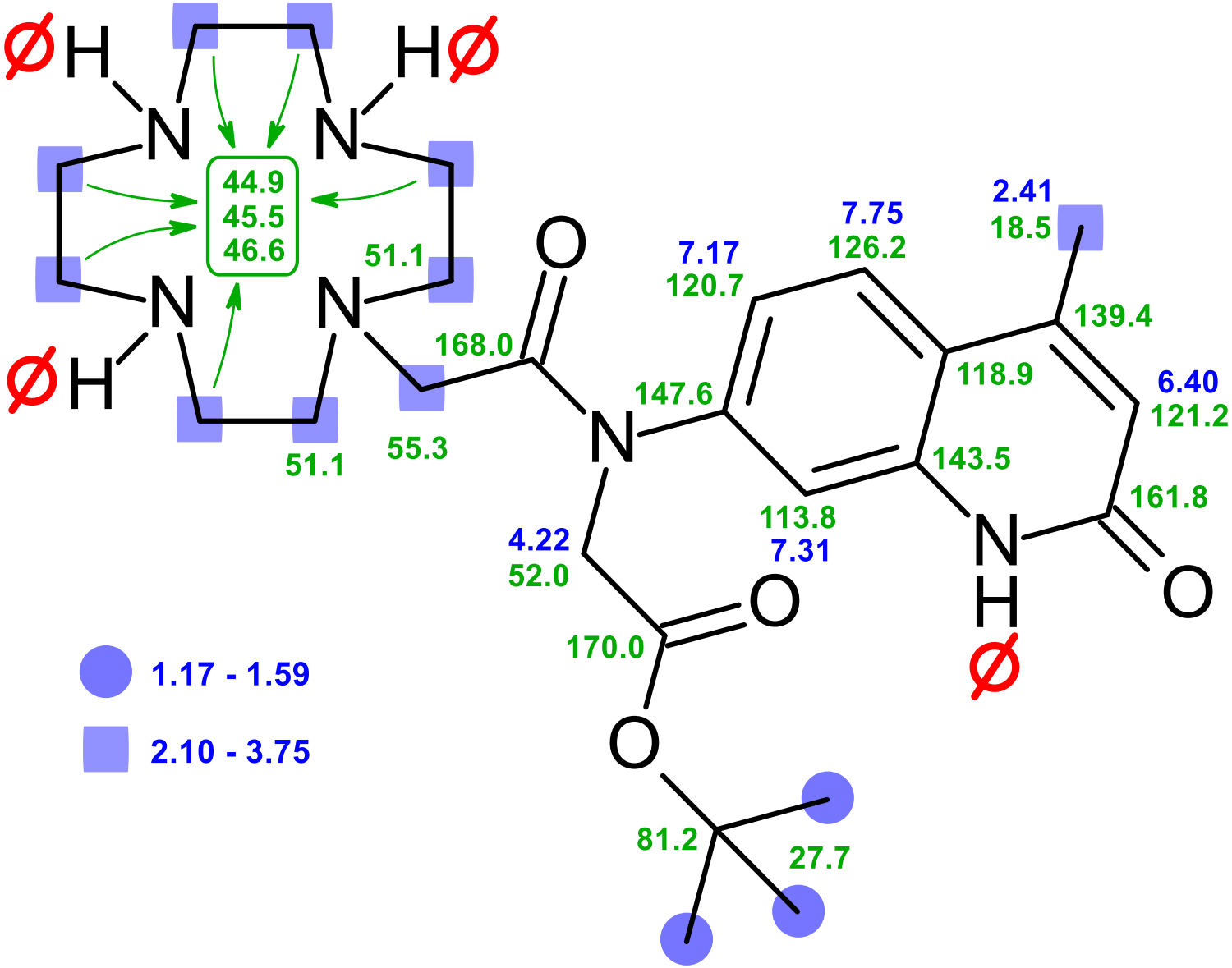
Formula Weight : 500,63(2)
Exact Mass : 500,31110
Formula : $C_{26}H_{40}N_6O_4$
Composition : C 62,38% H 8,05% N 16,79% O 12,78%

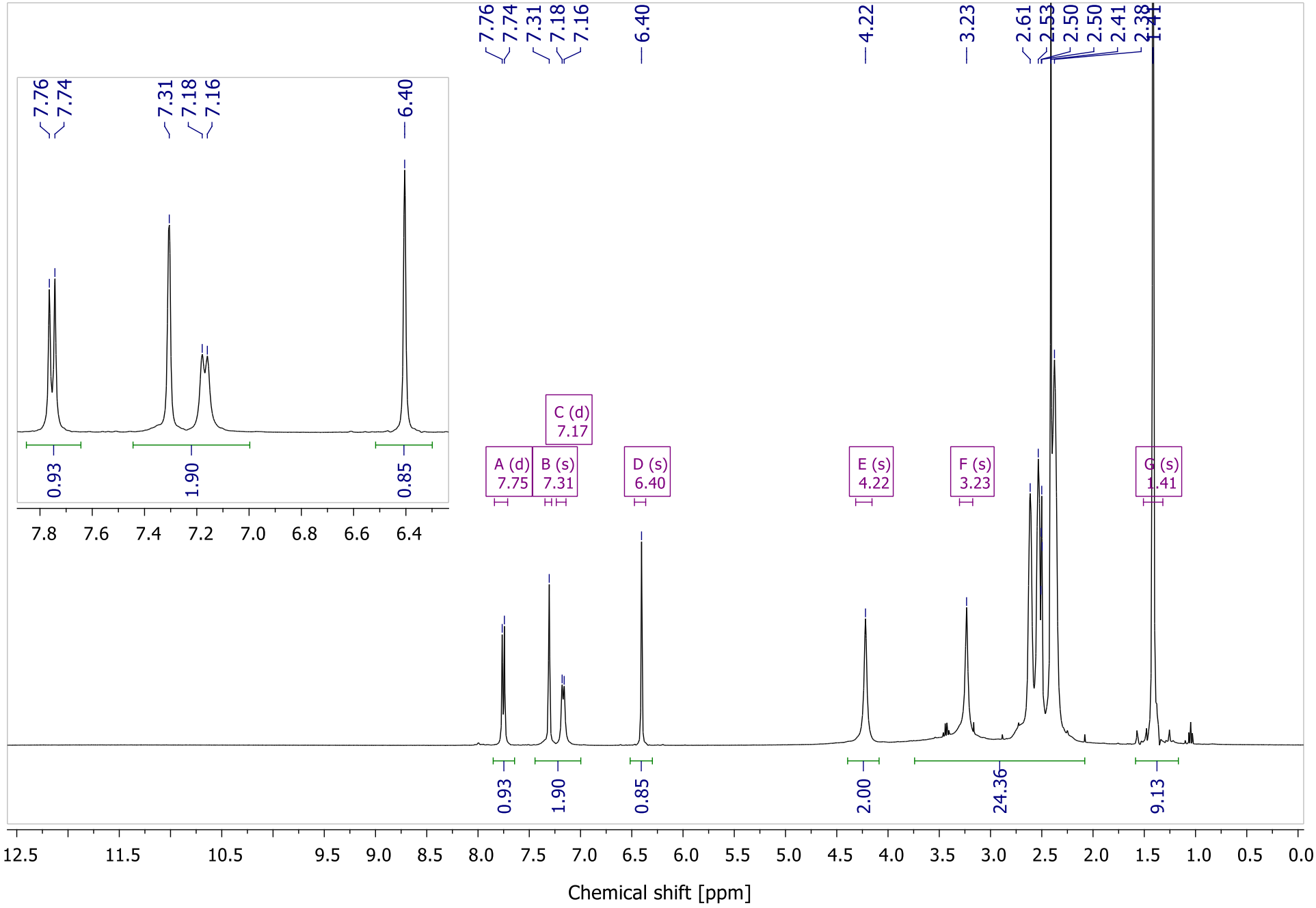


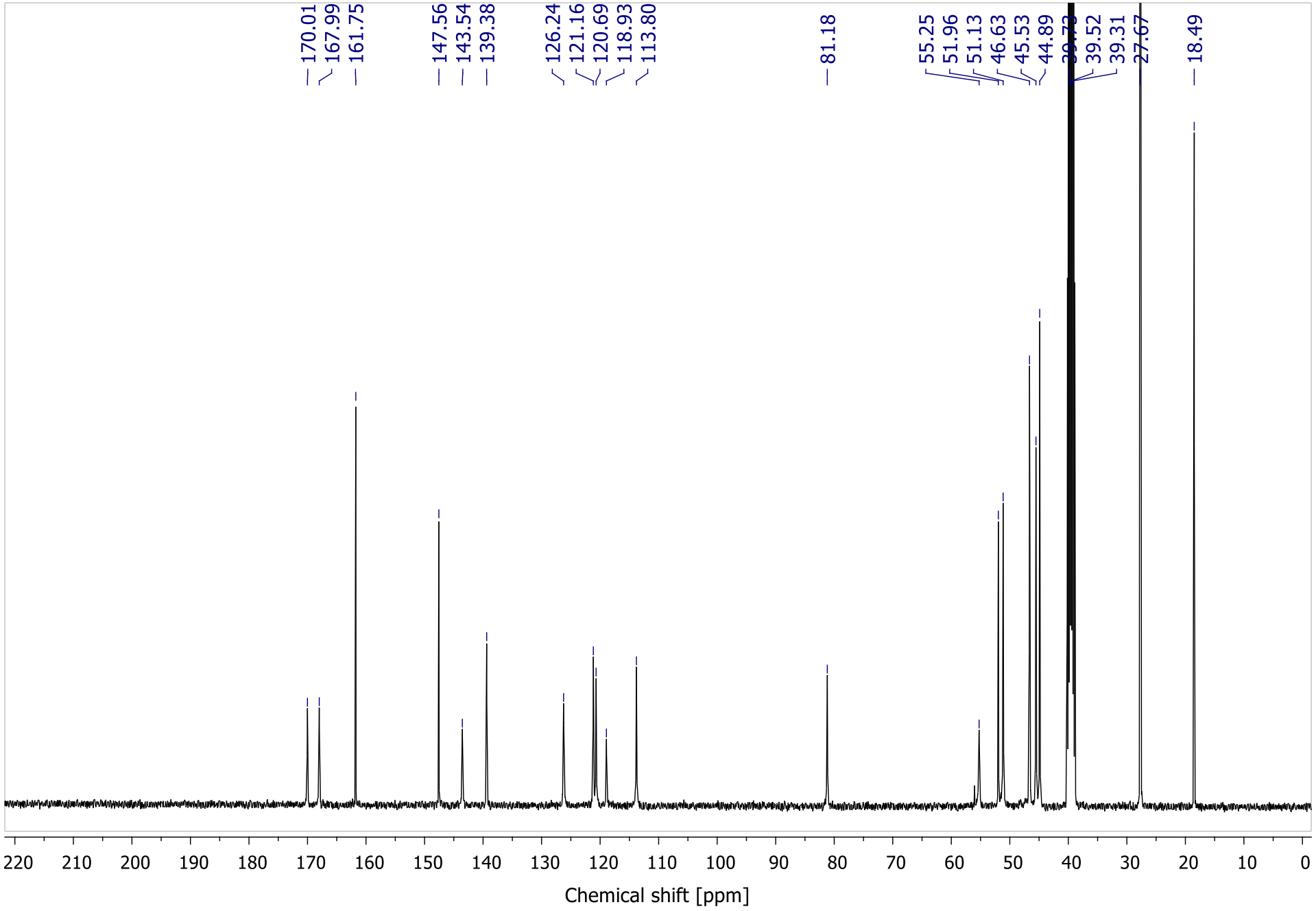

RT: 0.00 - 16.00
NL:
7.84E5
Total Scan
PDA
DKS57_059A
_1050_5um
uAU
1.72
0.92 1.30 2.05 3.43 4.05 5.05 6.33 6.92 7.98 8.30 9.17 9.95 10.58 11.97 12.68 14.08 14.62
NL:
1.58E10
TIC MS
DKS57_059A
_1050_5um
Relative Abundance
1.83
1.87
1.95
0.07 0.99 2.05 3.51 3.96 4.19 4.52 5.18 6.85 7.46 7.92 8.74 8.82 9.67 11.56 11.88 13.52 13.61 14.38 14.94
Time (min)


DKS57_059A_1050_5um #243 RT: 4.05 AV: 1 NL: 3.39E5 microAU
222.00
270.00
324.00
336.00
Relative Absorbance
wavelength (nm)

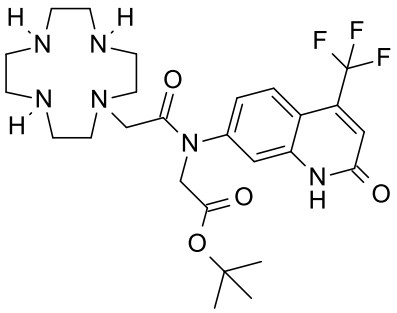

DKS57_059A_1050_5um #148-171 RT: 3.91-4.50 AV: 24 NL: 7.48E8
T: + c ESI Full ms [80.00-2000.00]
501.23
445.25
271.06
529.18 805.30 1126.23 1284.87 1608.59 1847.06
Relative Abundance
m/z


Ø H
H Ø
N
N
N
N
Ø H
44.9
45.5
46.6
51.1
51.1
55.3
168.0
O
147.6
N
7.17
120.7
7.75
126.2
2.41
18.5
139.4
118.9
6.40
121.2
143.5
161.8
113.8
7.31
N
H
Ø
O
4.22
52.0
O
170.0
O
81.2
27.7
1.17 - 1.59
2.10 - 3.75

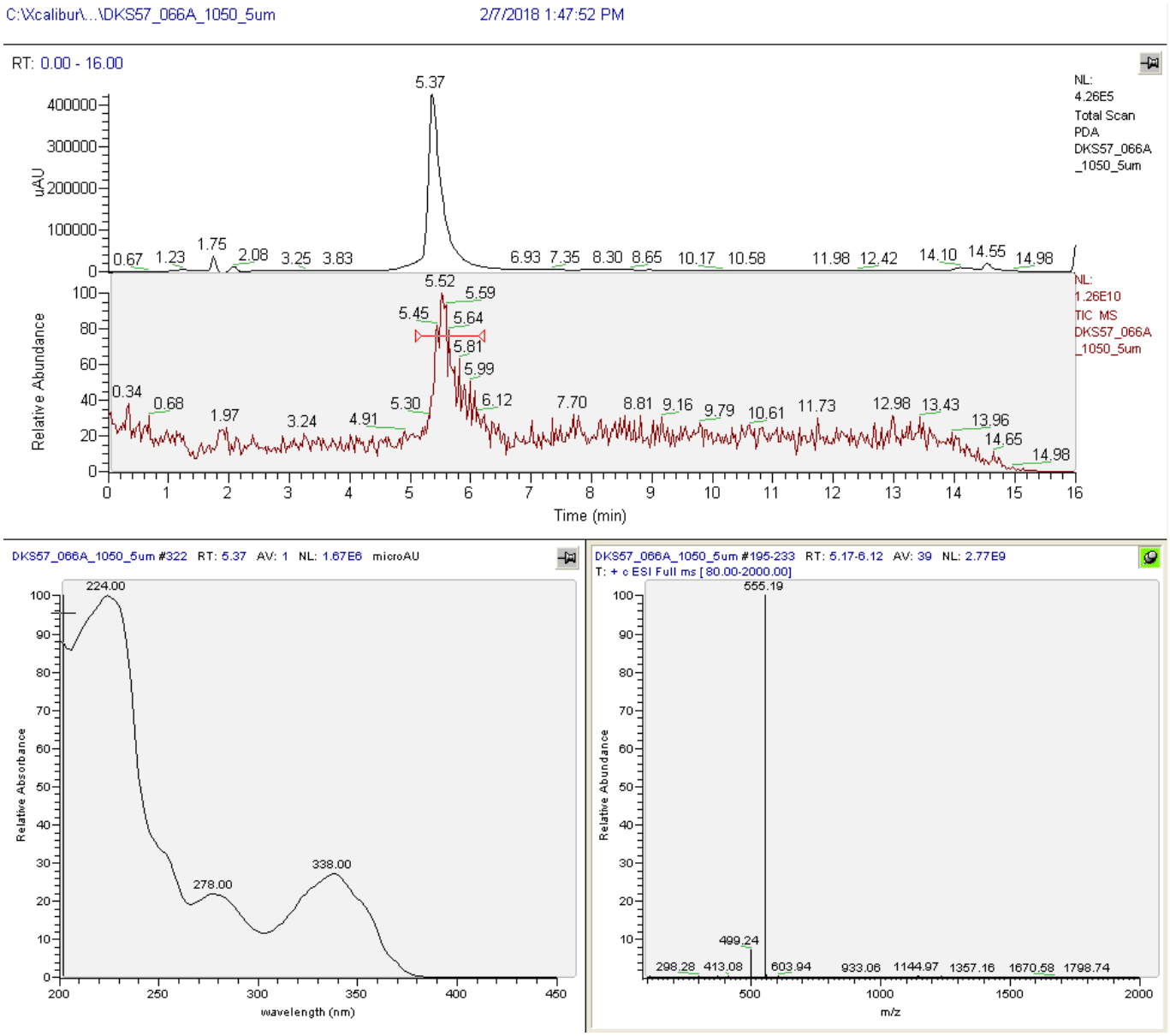

7.76
7.74
7.31
7.18
7.16
6.40
4.22
3.23
2.61
2.53
2.50
2.50
2.41
2.38
1.41
A (d)
7.75
B (s)
7.31
C (d)
7.17
D (s)
6.40
E (s)
4.22
F (s)
3.23
G (s)
1.41
0.93
1.90
0.85
2.00
24.36
9.13
Chemical shift [ppm]

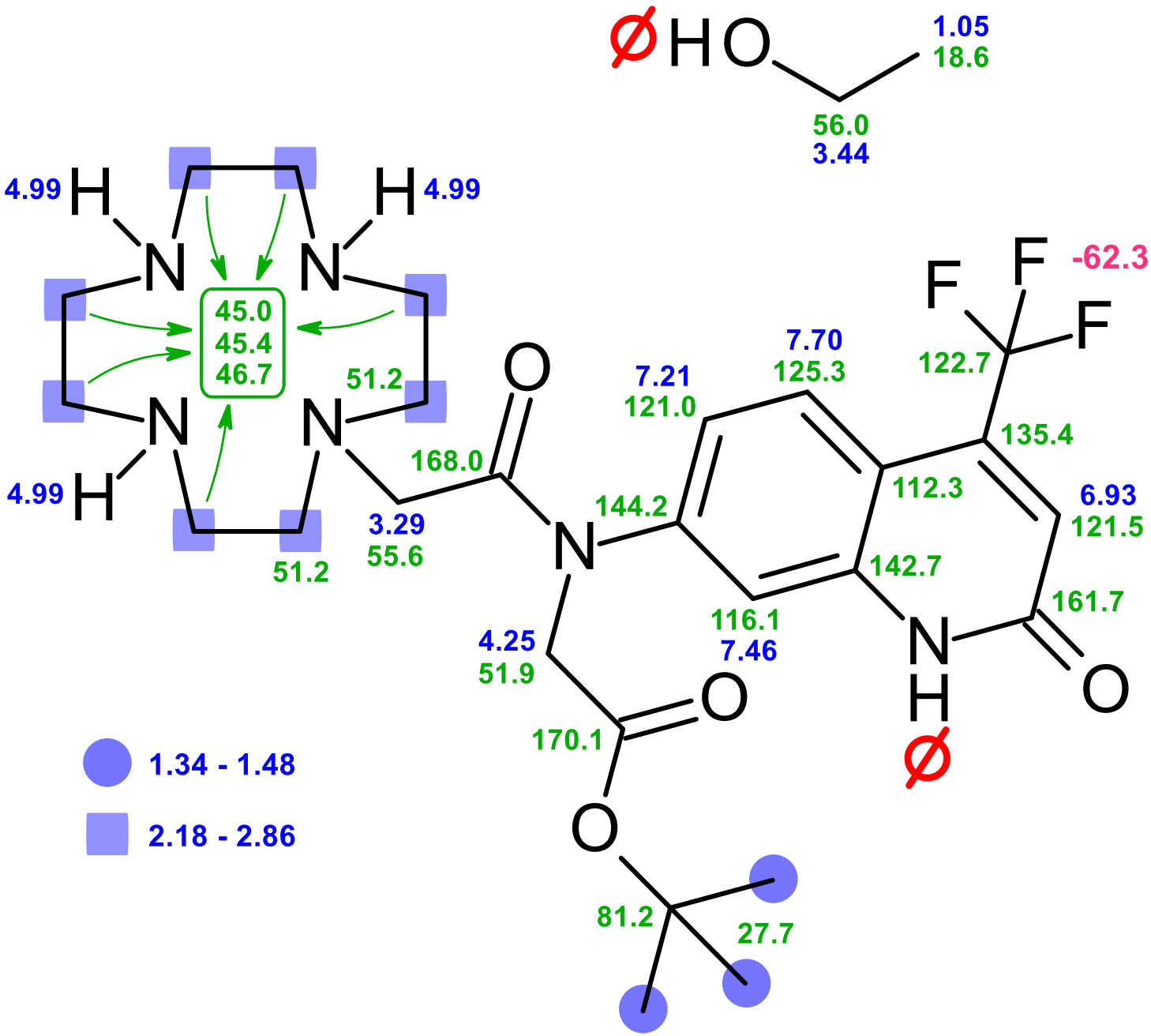

170.01
167.99
161.75
147.56
143.54
139.38
126.24
121.16
120.69
118.93
113.80
81.18
55.25
51.96
51.13
46.63
45.53
44.89
39.52
39.31
27.67
18.49
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical shift [ppm]

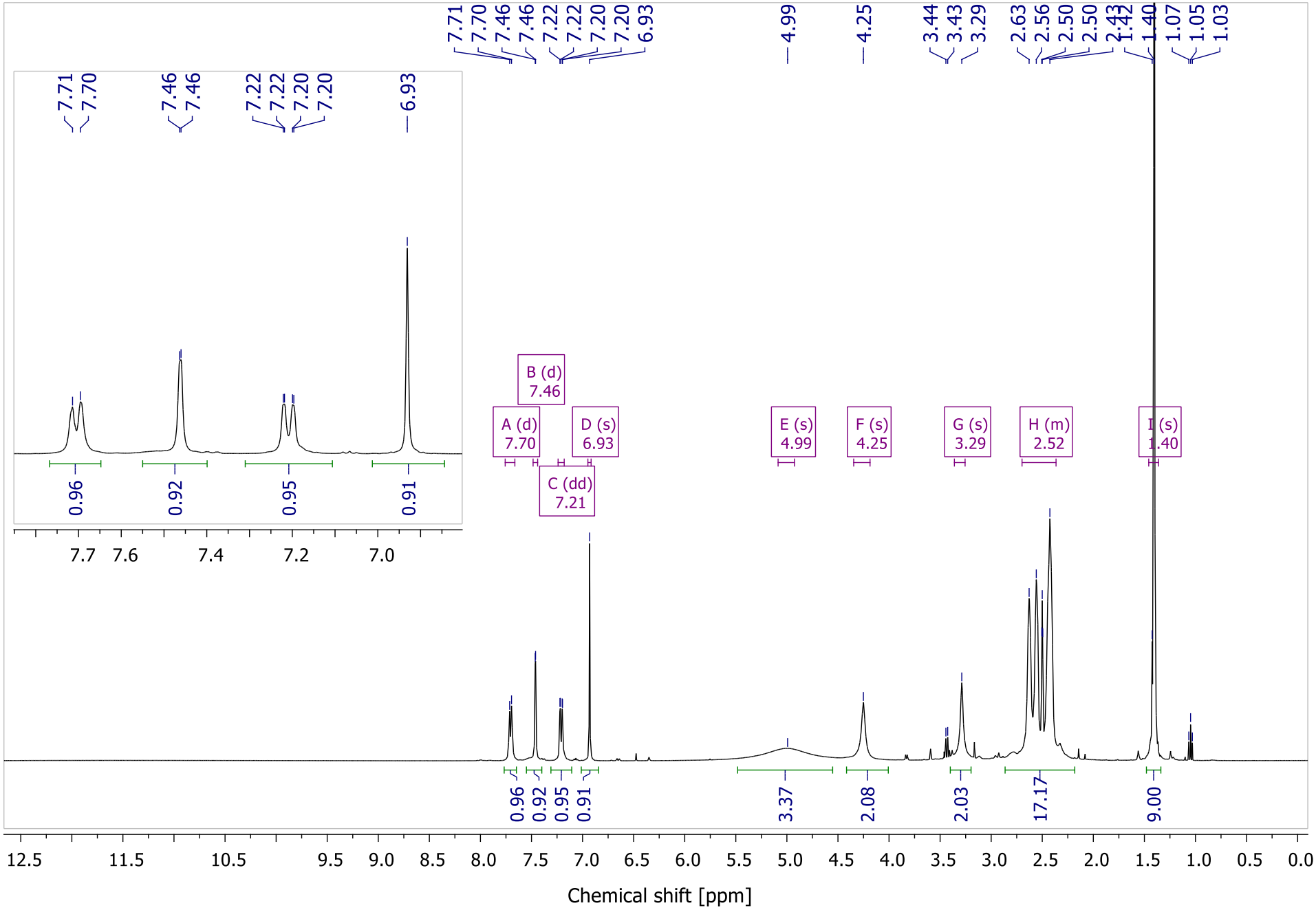
DKS57_066A

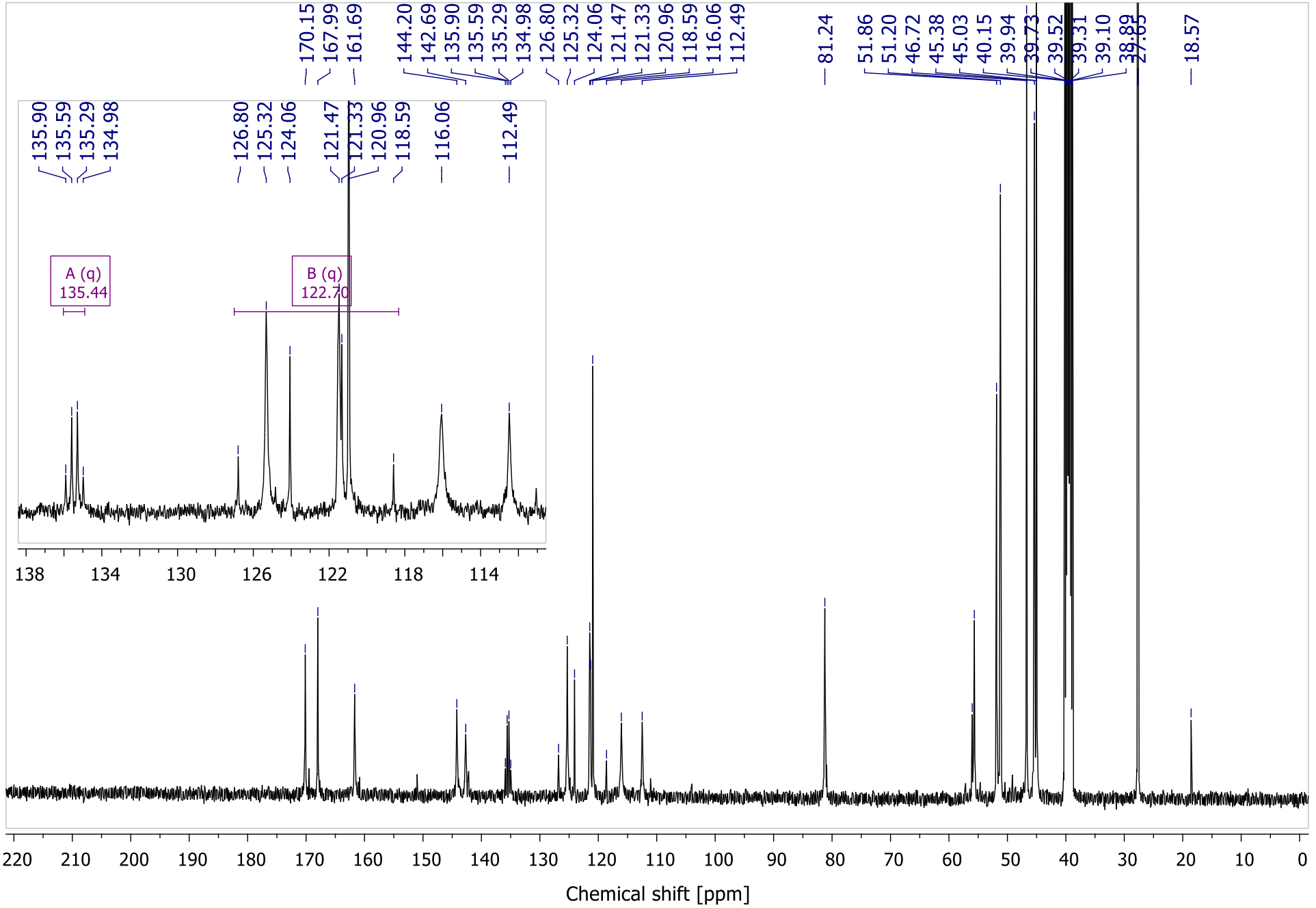


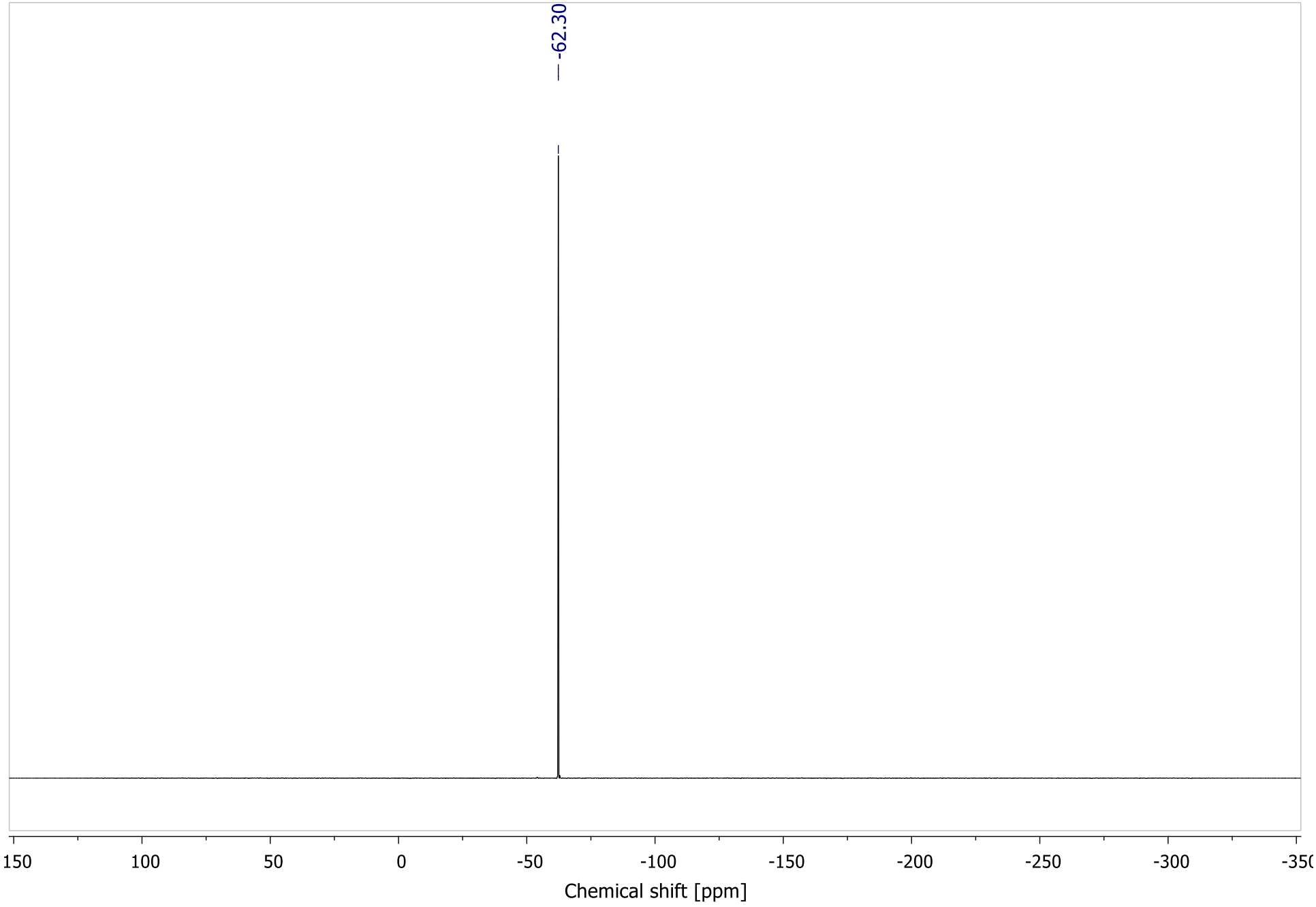
Formula Weight : 554,60(2)
Exact Mass : 554,28284
Formula : $C_{26}H_{37}F_3N_6O_4$
Composition : C 56,31% H 6,72% N 15,15% O 11,54% F 10,28%



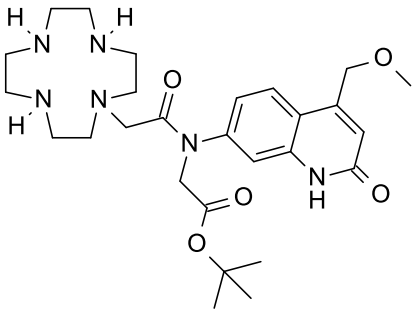

Ø
HO
1.05
18.6
56.0
3.44
4.99
H
N
N
H
4.99
45.0
45.4
46.7
51.2
N
N
4.99
H
51.2
168.0
O
3.29
55.6
144.2
N
7.21
121.0
7.70
125.3
F
F
F
-62.3
122.7
135.4
112.3
6.93
121.5
142.7
161.7
116.1
7.46
N
H
Ø
O
4.25
51.9
O
170.1
O
81.2
27.7
1.34 - 1.48
2.18 - 2.86


7.71
7.70
7.46
7.46
7.22
7.22
7.20
7.20
6.93
4.99
4.25
3.44
3.43
3.29
2.63
2.56
2.50
2.50
2.43
1.42
1.40
1.07
1.05
1.03
B (d)
7.46
A (d)
7.70
D (s)
6.93
C (dd)
7.21
E (s)
4.99
F (s)
4.25
G (s)
3.29
H (m)
2.52
I (s)
1.40
0.96
0.92
0.95
0.91
3.37
2.08
2.03
17.17
9.00
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Chemical shift [ppm]

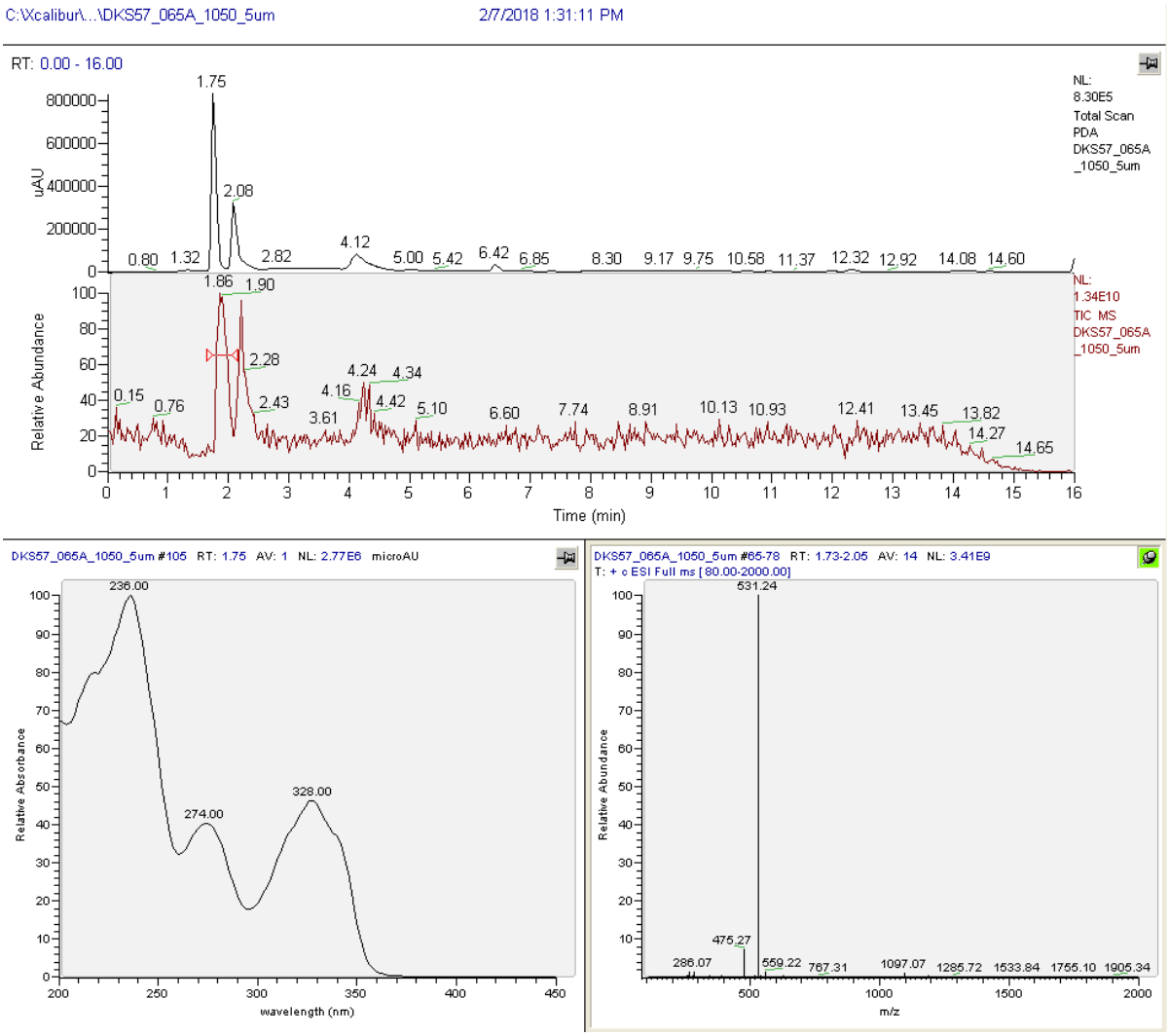

170.15
167.99
161.69
144.20
142.69
135.90
135.59
135.29
134.98
126.80
125.32
124.06
121.47
121.33
120.96
118.59
116.06
112.49
81.24
51.86
51.20
46.72
45.38
45.03
40.15
39.94
39.73
39.52
39.31
39.10
38.89
27.85
18.57
A (q)
135.44
B (q)
122.70
138
134
130
126
122
118
114
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical shift [ppm]

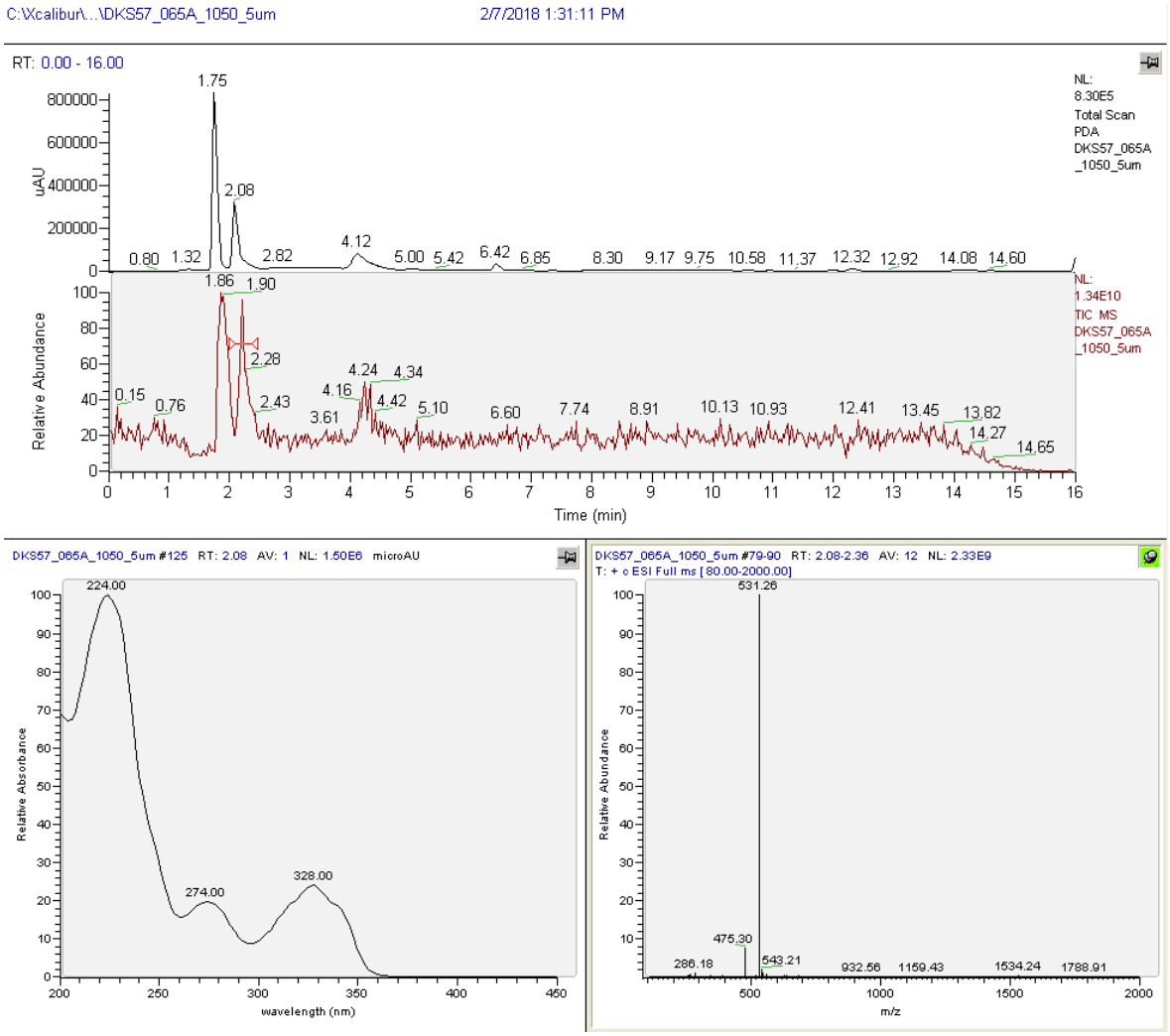

-62.30
150
100
50
0
-50
-100
-150
-200
-250
-300
-350
Chemical shift [ppm]

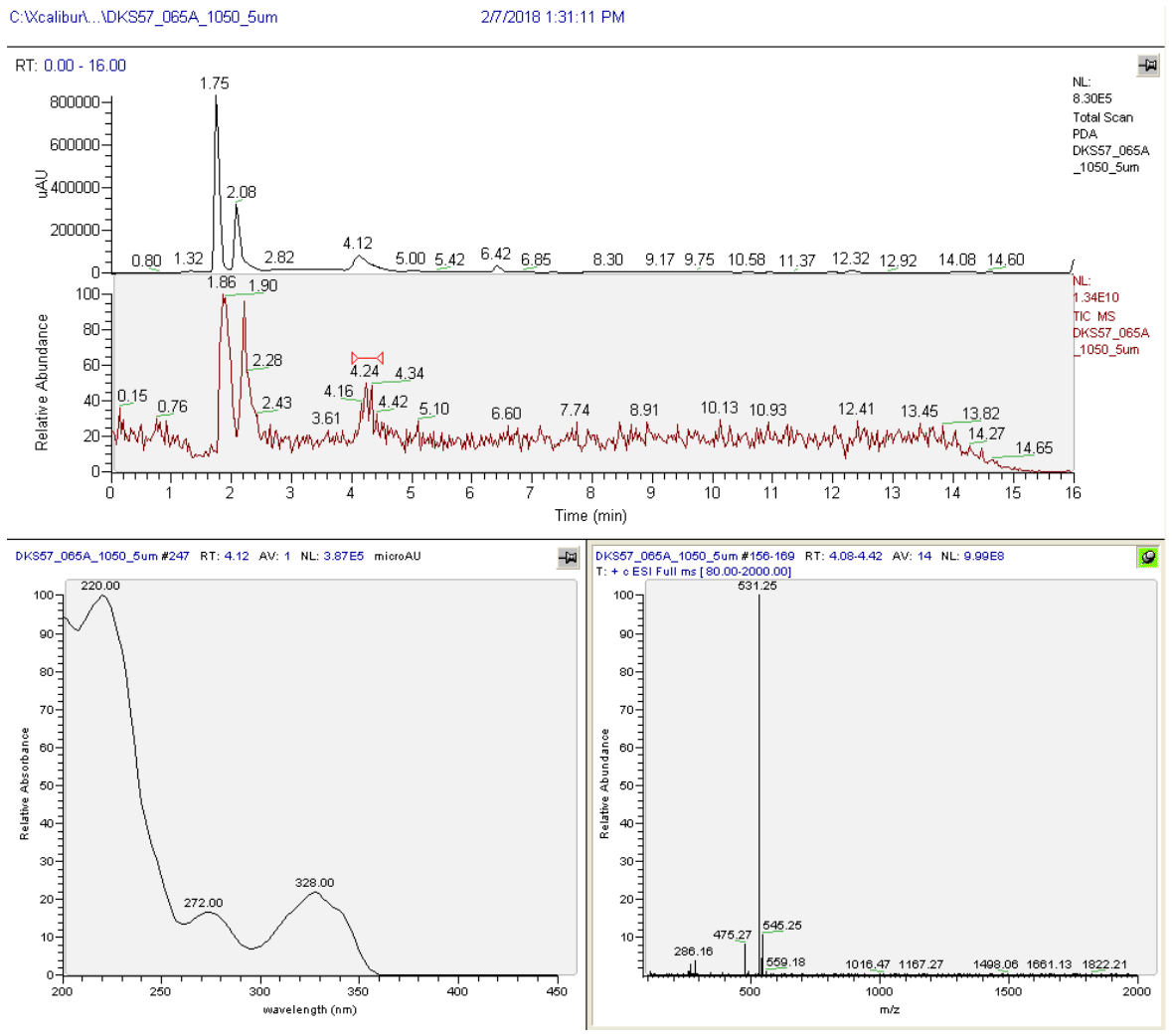
DKS57_065A

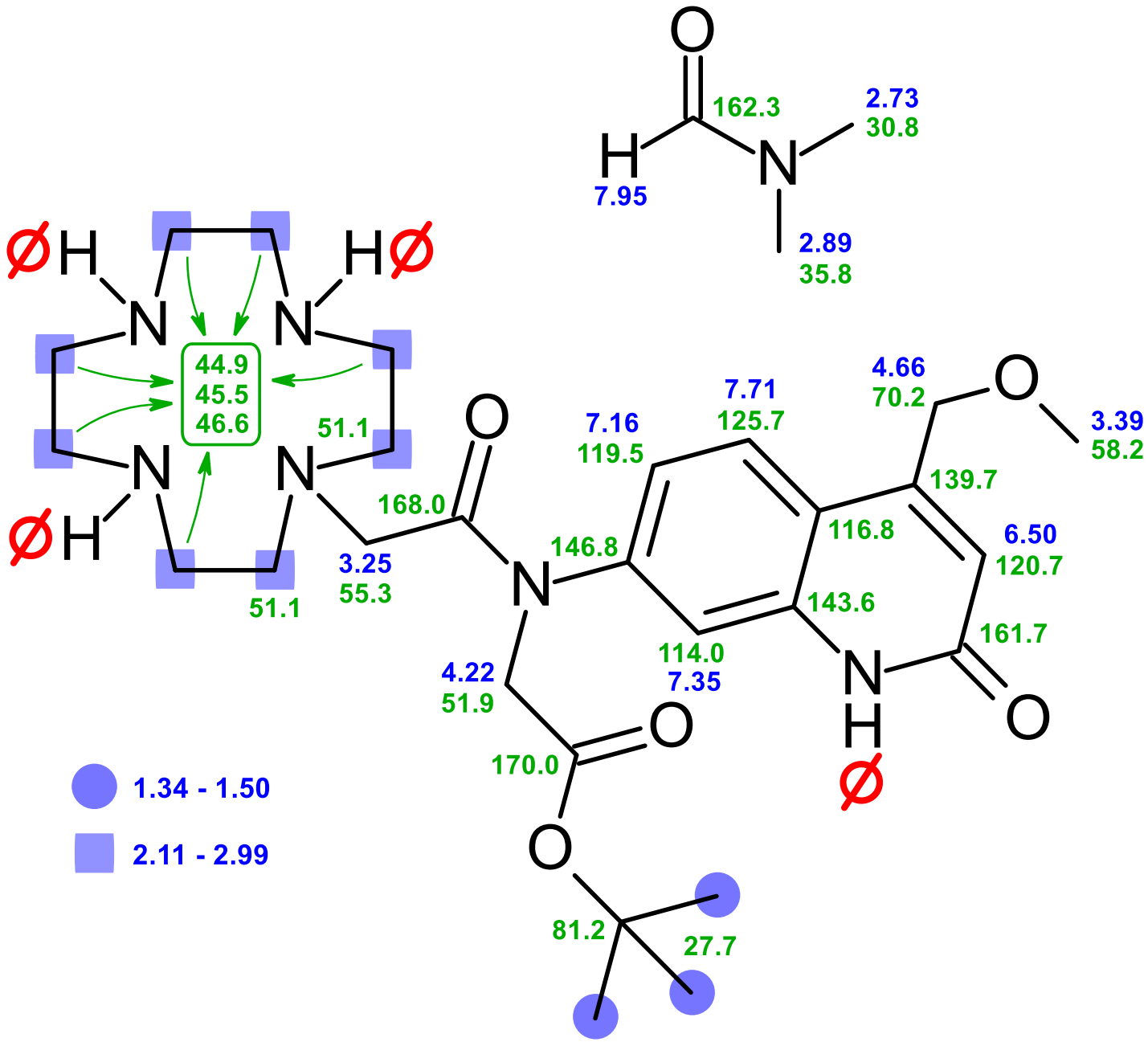


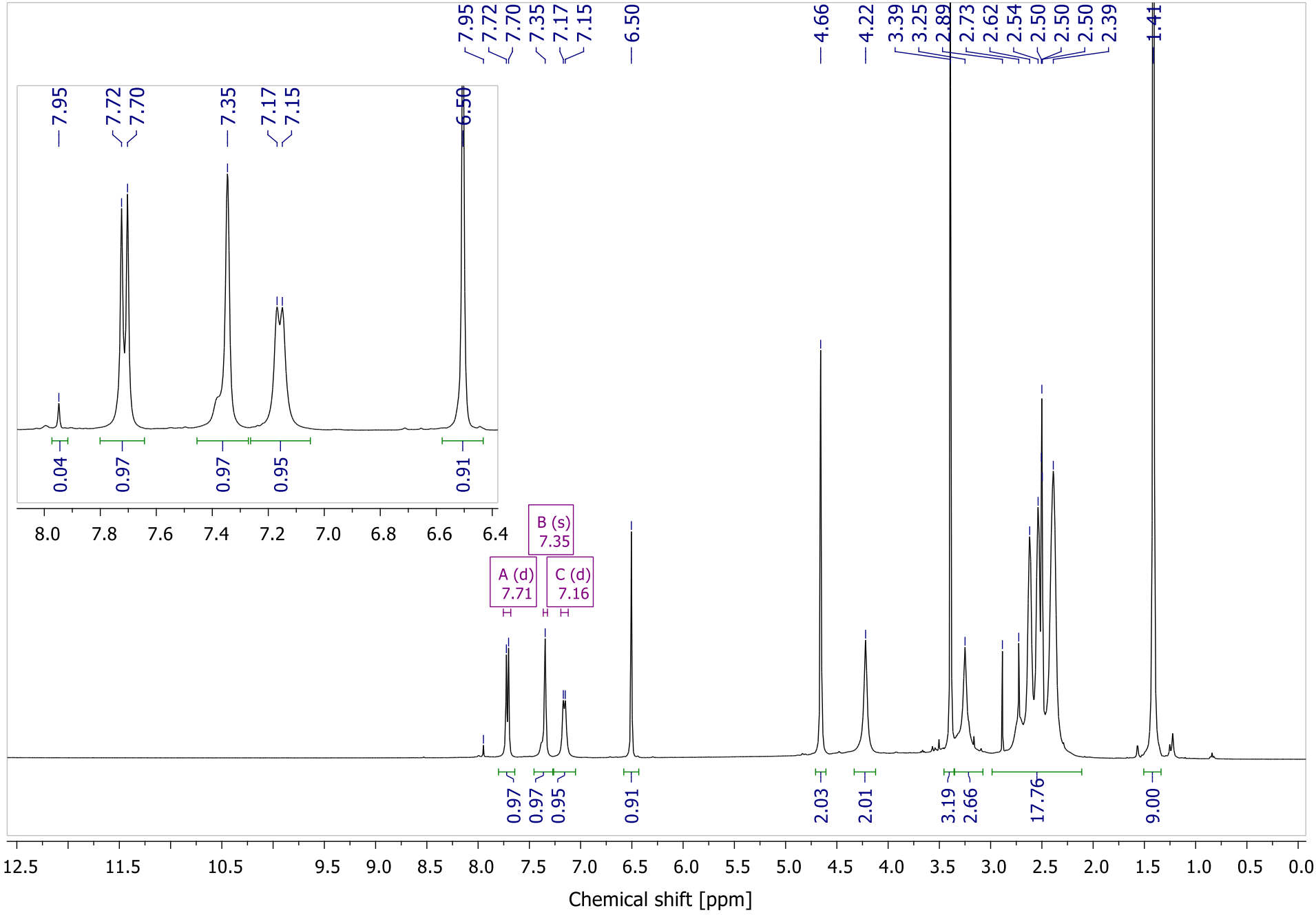
Formula Weight : 530.66(2)
Exact Mass : 530.32167
Formula : $C_{27}H_{42}N_6O_5$
Composition : C 61.11% H 7.98% N 15.84% O 15.08%

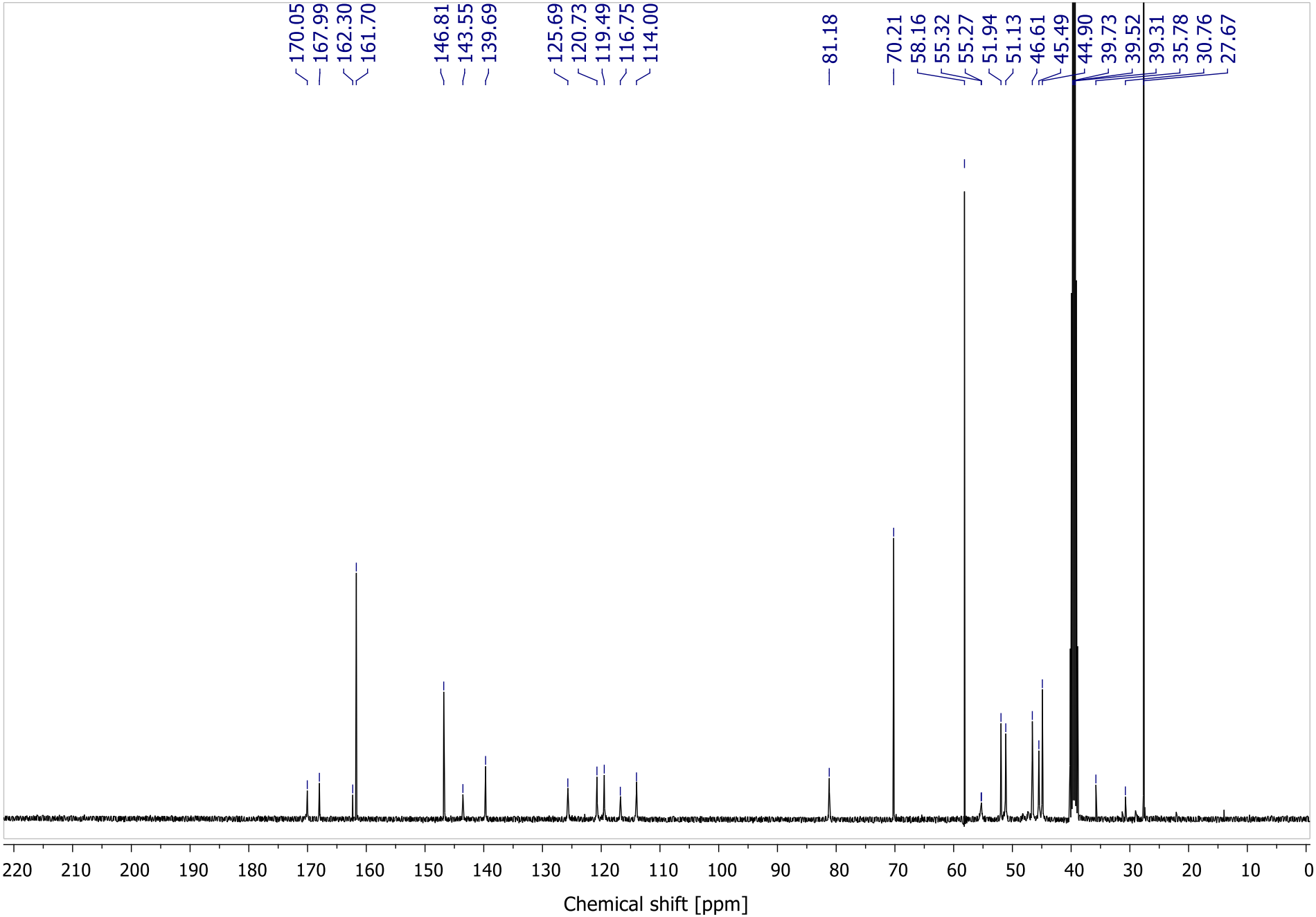



C:\Xcalibur\...\DKS57_065A_1050_5um 2/7/2018 1:31:11 PM
RT: 0.00 - 16.00
NL: 8.30E5 Total Scan PDA DKS57_065A _1050_5um
uAU
Relative Abundance
NL: 1.34E10 TIC MS DKS57_065A _1050_5um
Time (min)
DKS57_065A_1050_5um #125 RT: 2.08 AV: 1 NL: 1.50E6 microAU
Relative Absorbance
wavelength (nm)
DKS57_065A_1050_5um #79-90 RT: 2.08-2.36 AV: 12 NL: 2.33E9
T: + c ESI Full ms [80.00-2000.00]
Relative Abundance
m/z

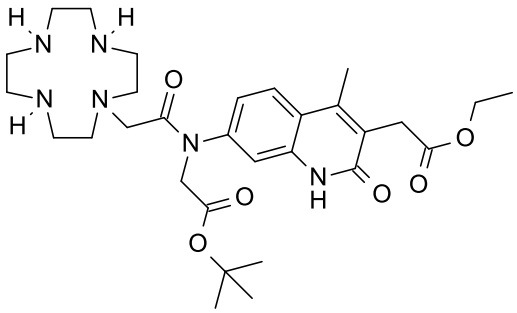

C:\Xcalibur\...\DKS57_065A_1050_5um 2/7/2018 1:31:11 PM
RT: 0.00 - 16.00
NL: 8.30E5 Total Scan PDA DKS57_065A _1050_5um
uAU
Relative Abundance
NL: 1.34E10 TIC MS DKS57_065A _1050_5um
Time (min)
DKS57_065A_1050_5um #247 RT: 4.12 AV: 1 NL: 3.87E5 microAU
Relative Absorbance
wavelength (nm)
DKS57_065A_1050_5um #156-169 RT: 4.08-4.42 AV: 14 NL: 9.99E8
T: + c ESI Full ms [80.00-2000.00]
Relative Abundance
m/z


O
162.3
2.73
30.8
H
7.95
N
2.89
35.8
Ø H
H Ø
N
N
44.9
45.5
46.6
51.1
N
N
Ø H
51.1
168.0
O
3.25
55.3
N
146.8
7.16
119.5
7.71
125.7
4.66
70.2
O
3.39
58.2
139.7
116.8
6.50
120.7
143.6
161.7
114.0
7.35
N
H
Ø
O
4.22
51.9
O
170.0
O
81.2
27.7
1.34 - 1.50
2.11 - 2.99

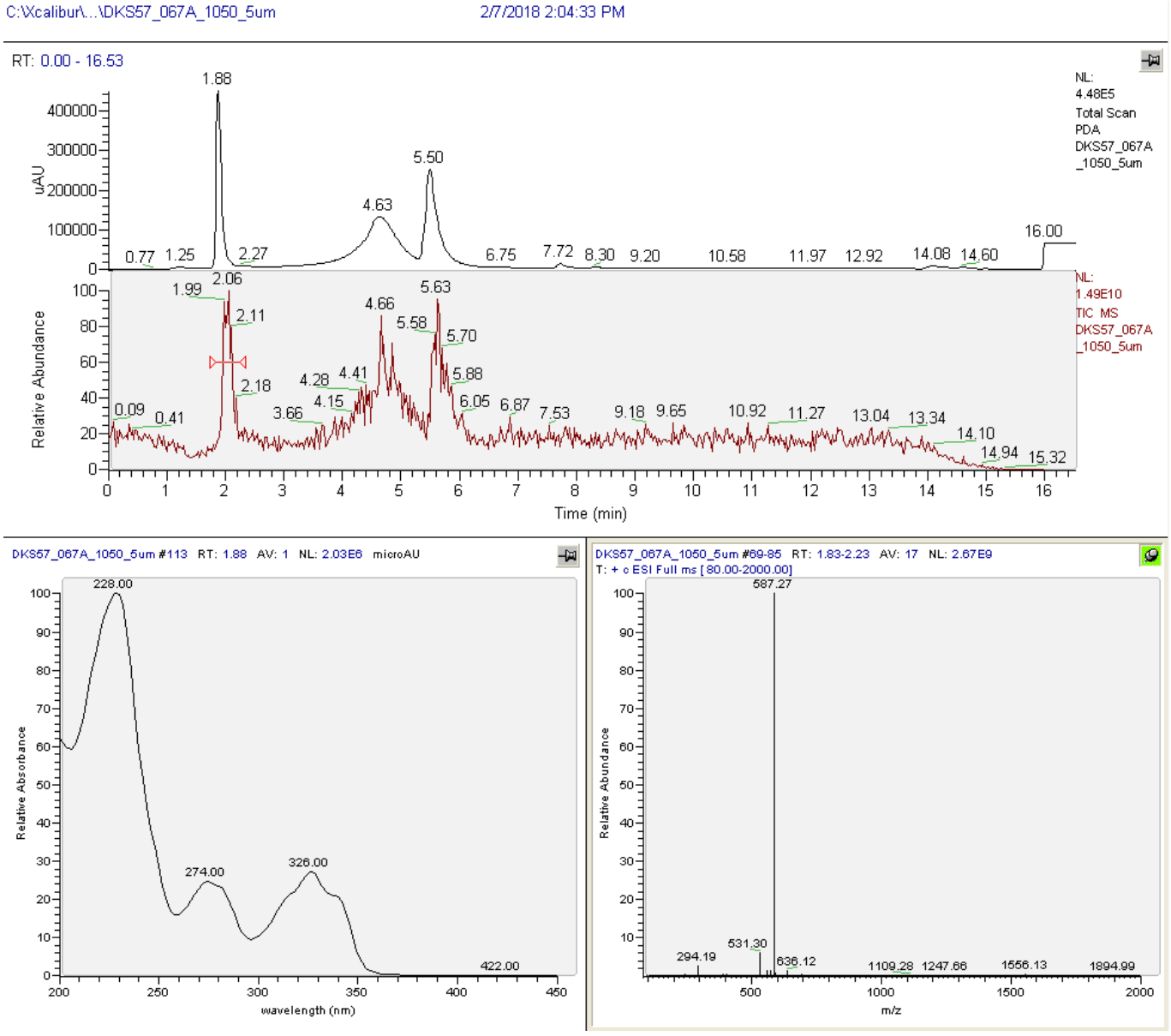

7.95
7.72
7.70
7.35
7.17
7.15
6.50
4.66
4.22
3.39
3.25
2.89
2.73
2.62
2.54
2.50
2.50
2.50
2.39
1.41
A (d)
7.71
B (s)
7.35
C (d)
7.16
0.97
0.97
0.95
0.91
2.03
2.01
3.19
2.66
17.76
9.00
Chemical shift [ppm]

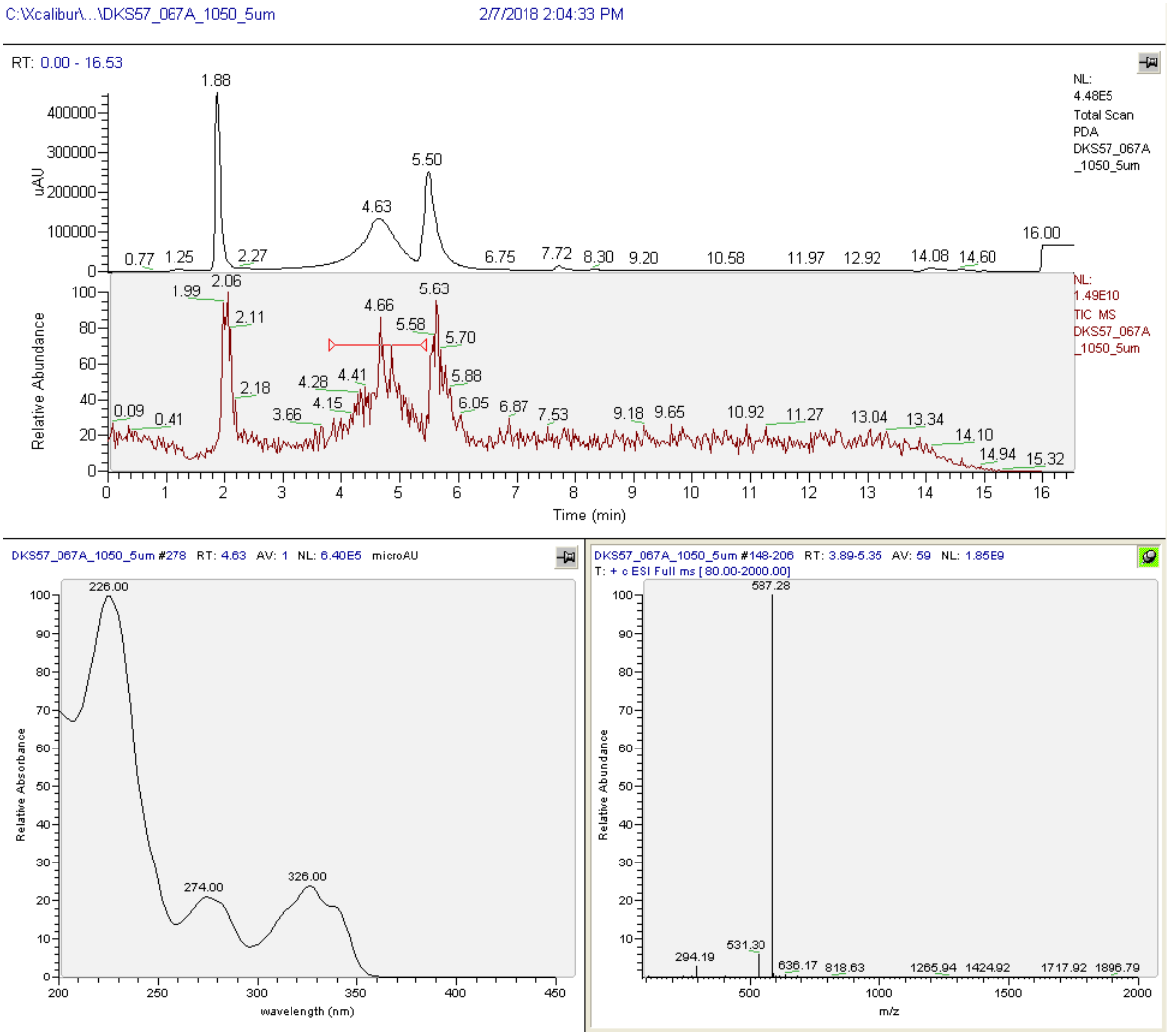

170.05
167.99
162.30
161.70
146.81
143.55
139.69
125.69
120.73
119.49
116.75
114.00
81.18
70.21
58.16
55.32
55.27
51.94
51.13
46.61
45.49
44.90
39.73
39.52
39.31
35.78
30.76
27.67
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical shift [ppm]

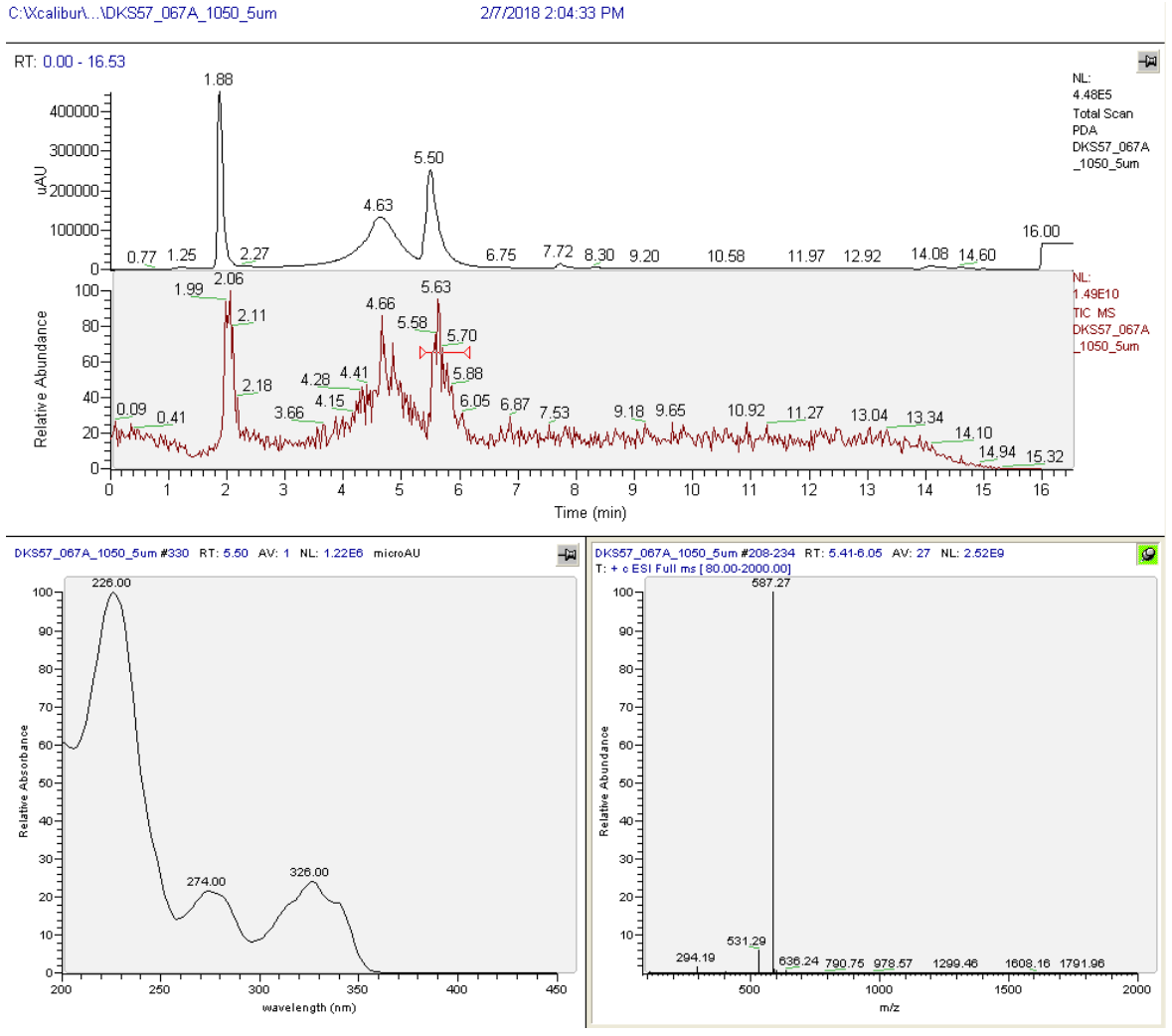
DKS57_067A

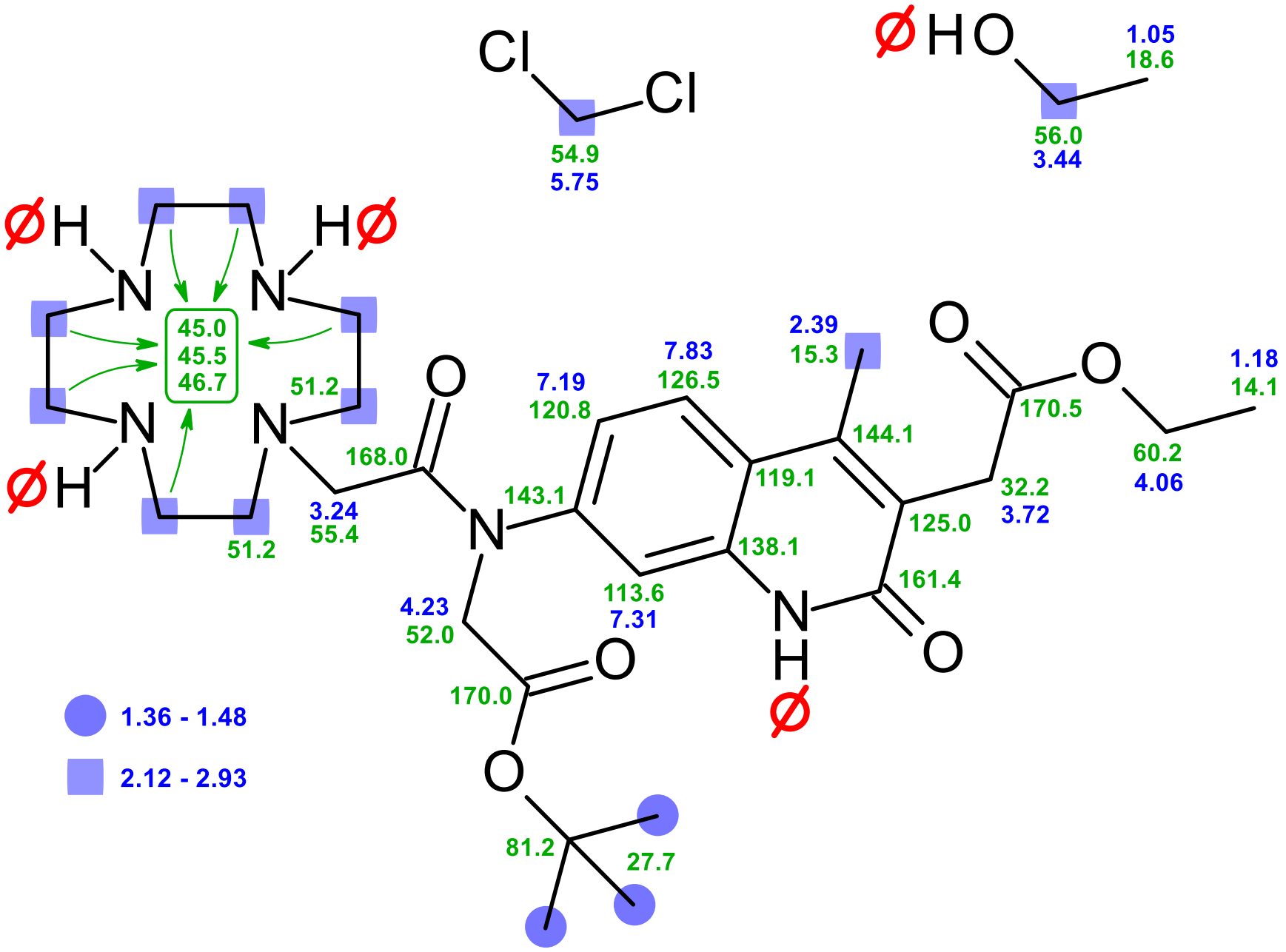


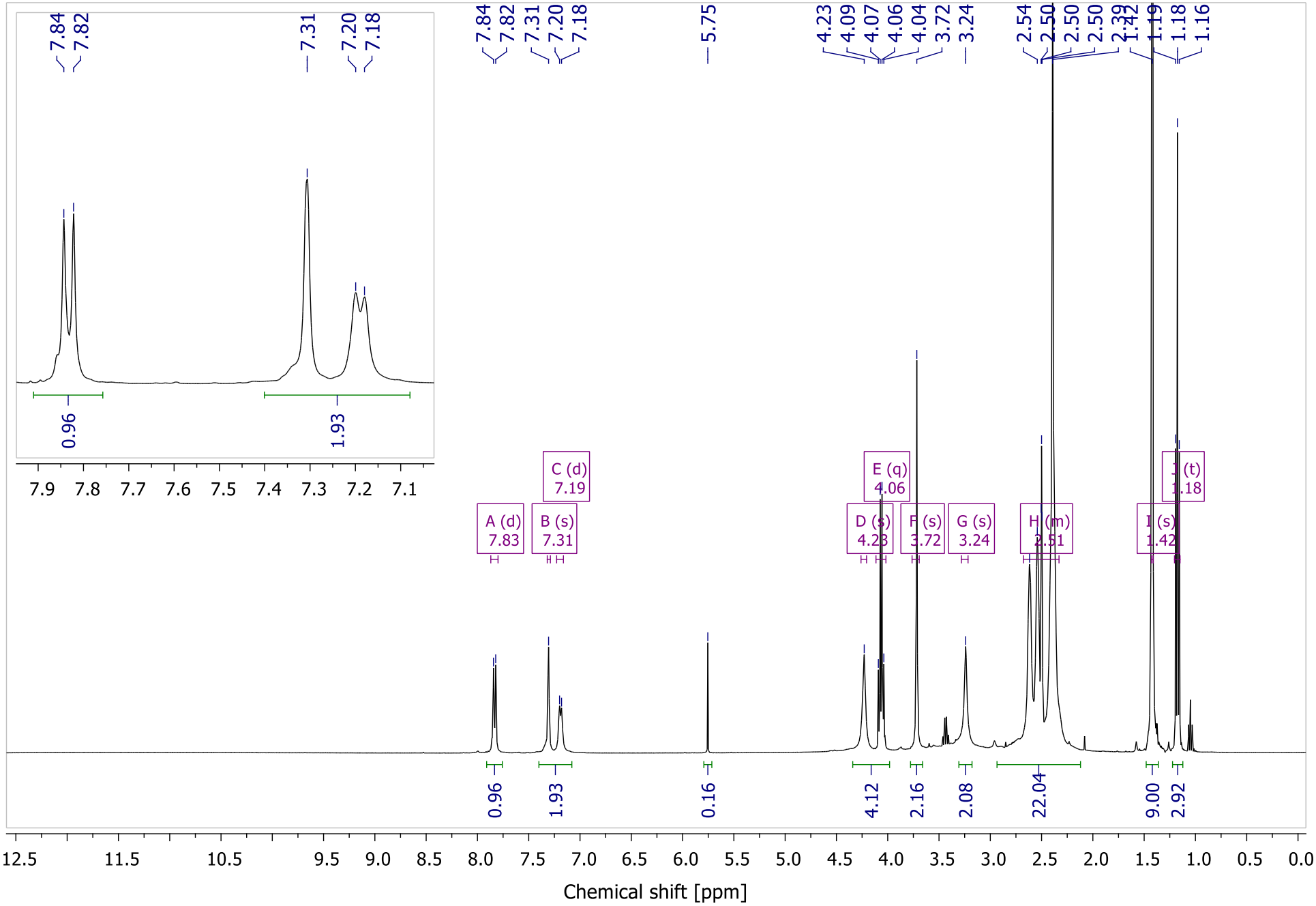
Formula Weight : 586.72(2)
Exact Mass : 586.34788
Formula : $C_{30}H_{46}N_6O_6$
Composition : C 61.41% H 7.90% N 14.32% O 16.36%

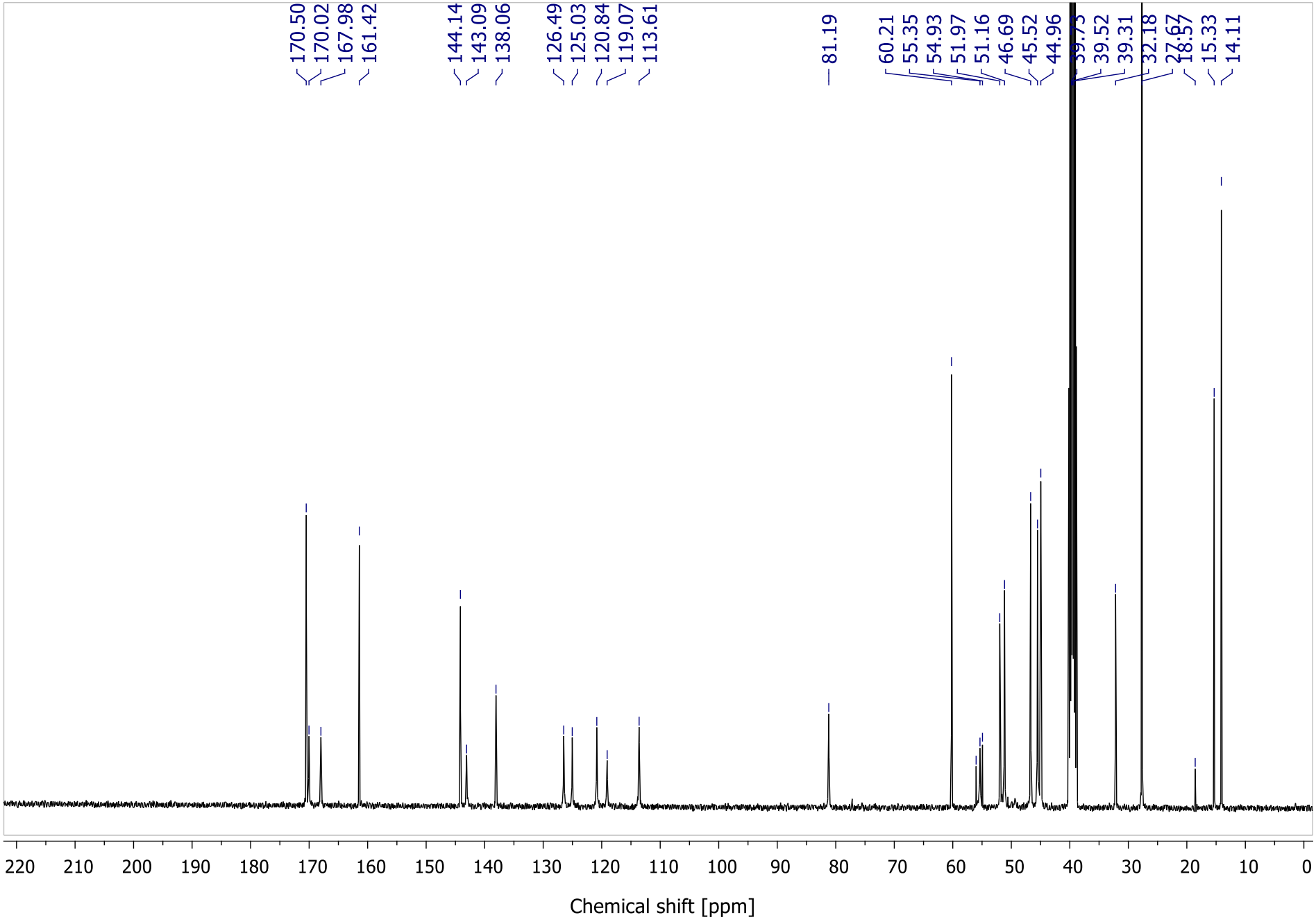



C:\Xcalibur\...\DKS57_067A_1050_5um 2/7/2018 2:04:33 PM
RT: 0.00 - 16.53
NL: 4.48E5 Total Scan PDA DKS57_067A _1050_5um
NL: 1.49E10 TIC MS DKS57_067A _1050_5um
uAU
Relative Abundance
Time (min)
DKS57_067A_1050_5um #278 RT: 4.63 AV: 1 NL: 6.40E5 microAU
Relative Absorbance
wavelength (nm)
DKS57_067A_1050_5um #148-206 RT: 3.89-5.35 AV: 59 NL: 1.85E9
T: + c ESI Full ms [80.00-2000.00]
Relative Abundance
m/z

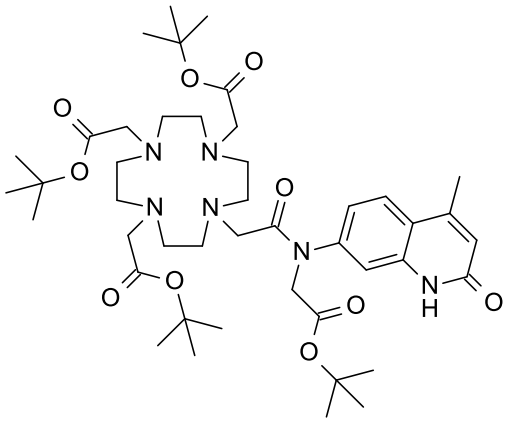

C:\Xcalibur\...\DKS57_067A_1050_5um 2/7/2018 2:04:33 PM
RT: 0.00 - 16.53
NL: 4.48E5 Total Scan PDA DKS57_067A _1050_5um
NL: 1.49E10 TIC MS DKS57_067A _1050_5um
uAU
Relative Abundance
Time (min)
DKS57_067A_1050_5um #330 RT: 5.50 AV: 1 NL: 1.22E6 microAU
Relative Absorbance
wavelength (nm)
DKS57_067A_1050_5um #208-234 RT: 5.41-6.05 AV: 27 NL: 2.52E9
T: + c ESI Full ms [80.00-2000.00]
Relative Abundance
m/z


Cl
Cl
54.9
5.75
Ø HO
1.05
18.6
56.0
3.44
Ø H
H Ø
N
N
N
N
Ø H
45.0
45.5
46.7
51.2
51.2
O
168.0
3.24
55.4
7.19
120.8
7.83
126.5
2.39
15.3
O
O
1.18
14.1
170.5
60.2
4.06
144.1
119.1
143.1
32.2
3.72
125.0
138.1
161.4
113.6
7.31
4.23
52.0
N
H
Ø
O
O
170.0
O
81.2
27.7
1.36 - 1.48
2.12 - 2.93

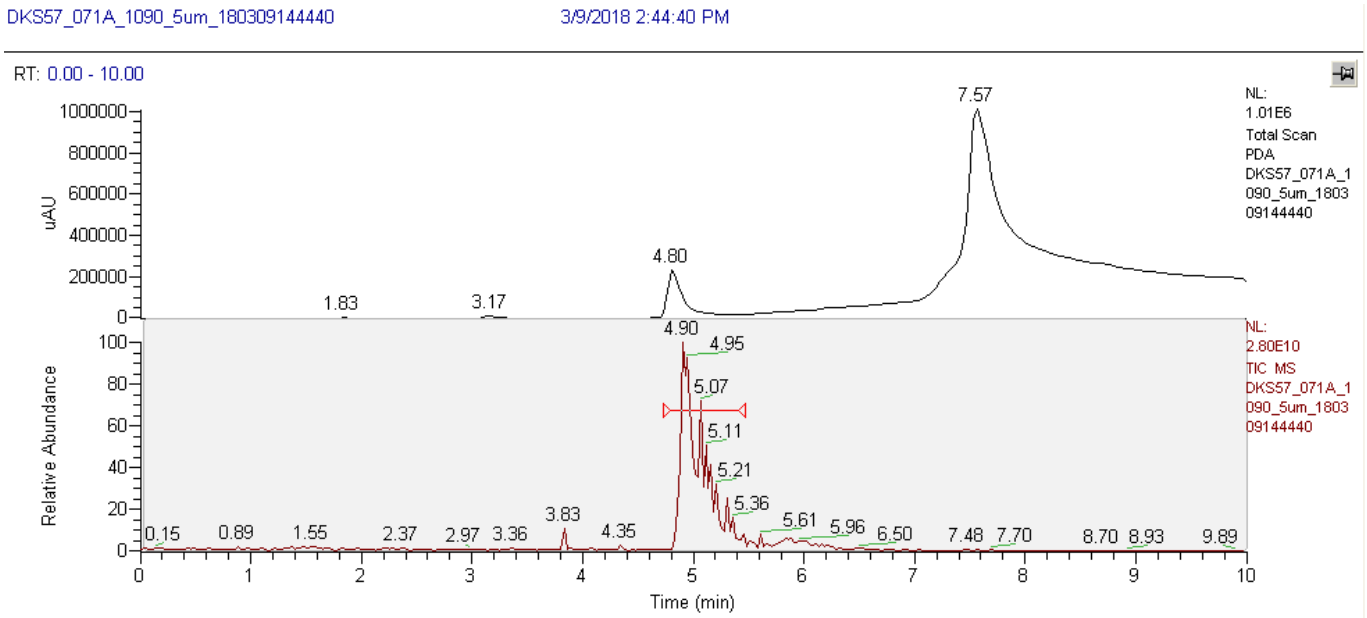

7.84
7.82
7.31
7.20
7.18
5.75
4.23
4.09
4.07
4.06
4.04
3.72
3.24
2.54
2.50
2.50
2.50
2.39
1.42
1.19
1.18
1.16
A (d) 7.83
B (s) 7.31
C (d) 7.19
D (s) 4.23
E (q) 4.06
F (s) 3.72
G (s) 3.24
H (m) 2.51
I (s) 1.42
J (t) 1.18
0.96
1.93
0.16
4.12
2.16
2.08
22.04
9.00
2.92
Chemical shift [ppm]

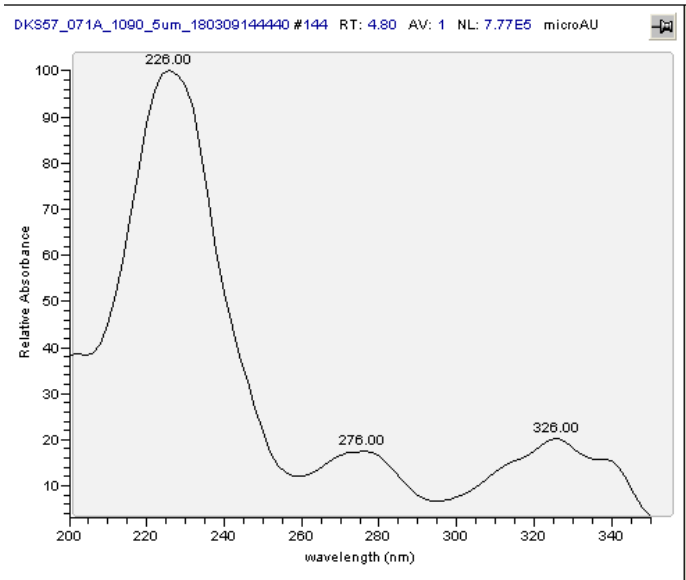

170.50
170.02
167.98
161.42
144.14
143.09
138.06
126.49
125.03
120.84
119.07
113.61
81.19
60.21
55.35
54.93
51.97
51.16
46.69
45.52
44.96
39.73
39.52
39.31
32.18
27.67
18.57
15.33
14.11
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical shift [ppm]

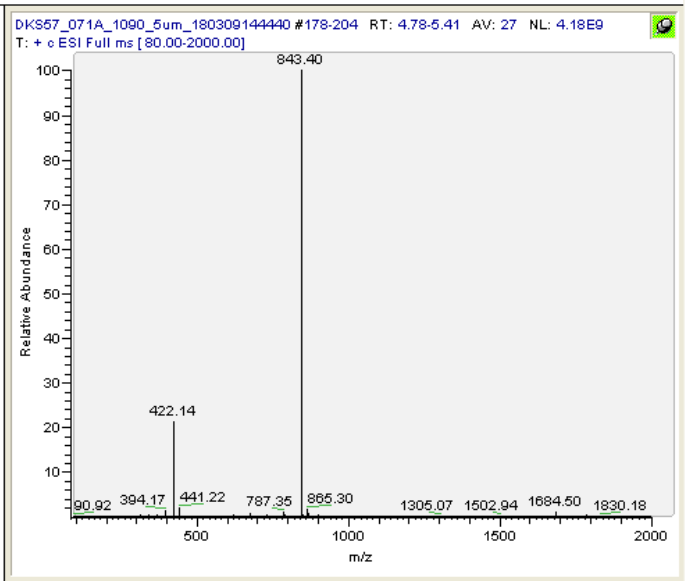
DKS57_071A

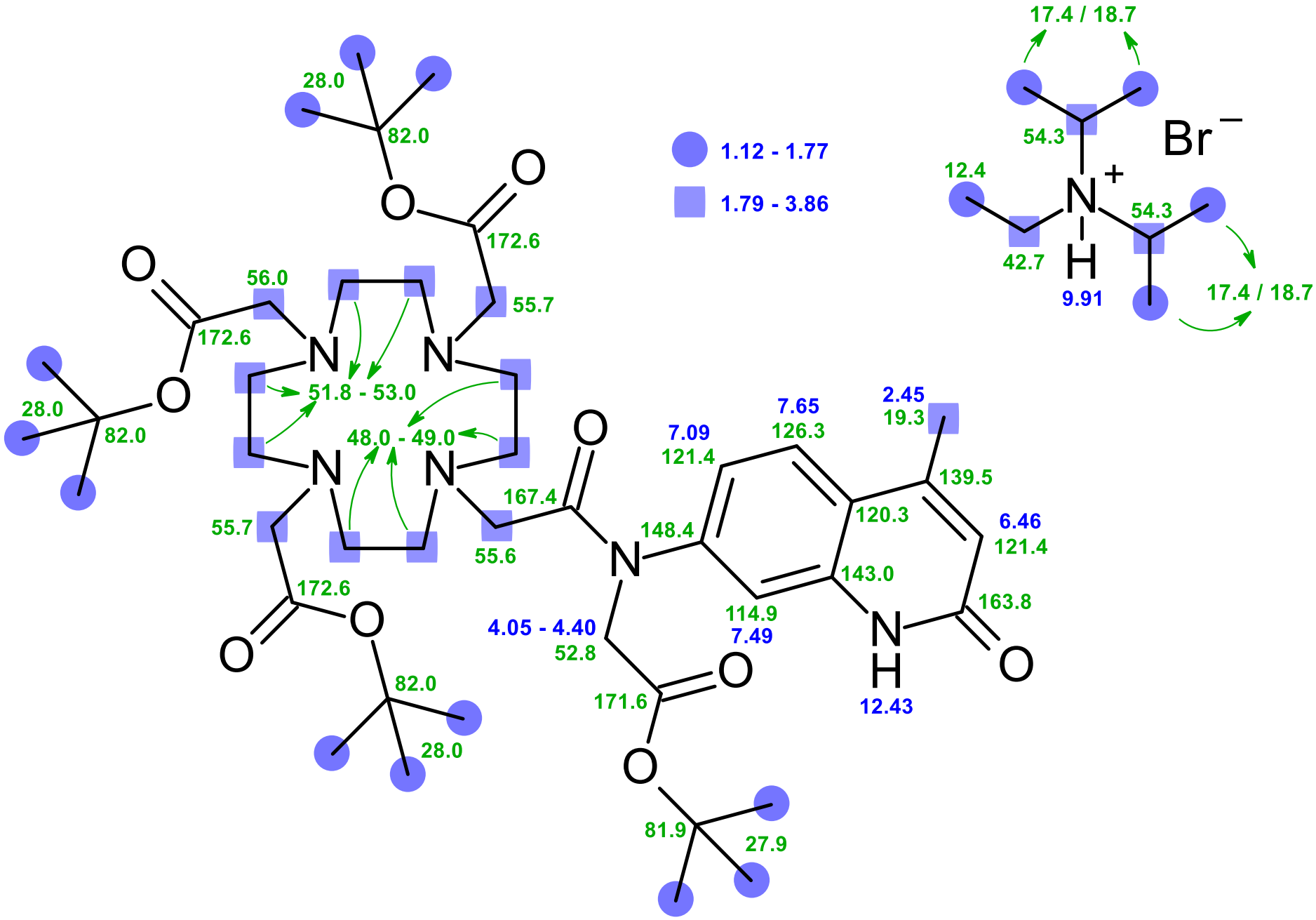


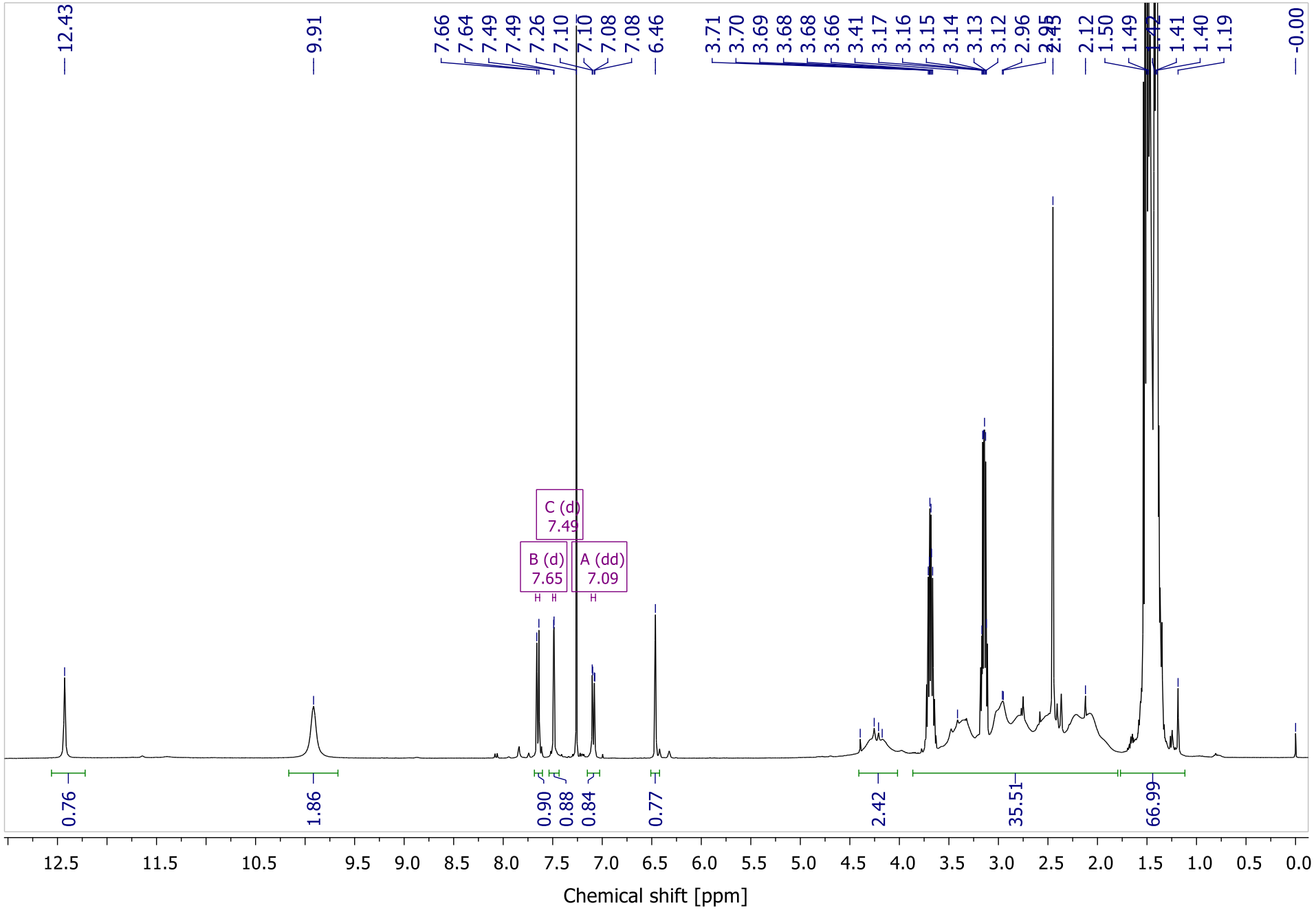
Formula Weight : 843.06(4)
Exact Mass : 842.51534
Formula : $C_{44}H_{70}N_6O_{10}$
Composition : C 62.68% H 8.37% N 9.97% O 18.98%

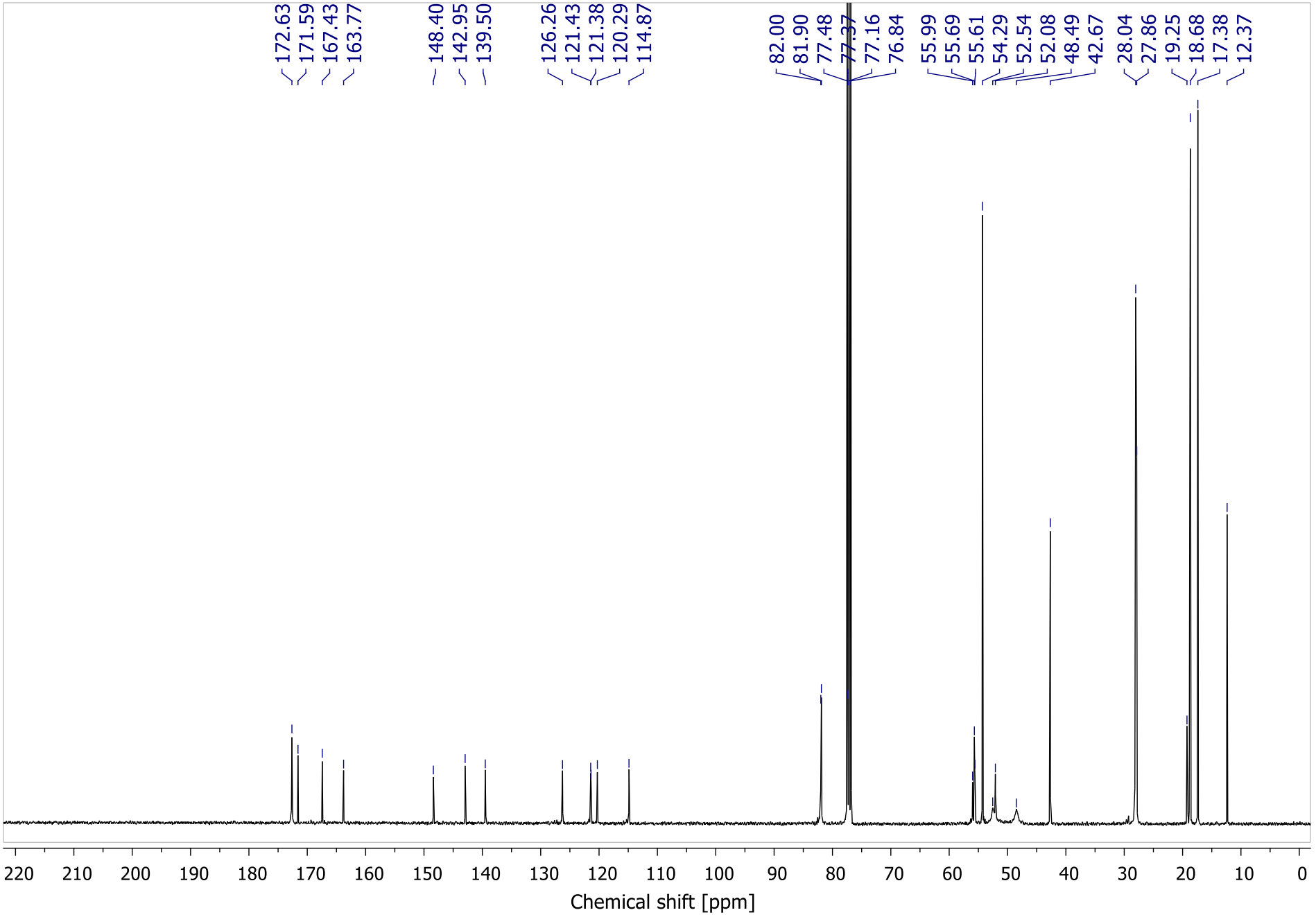




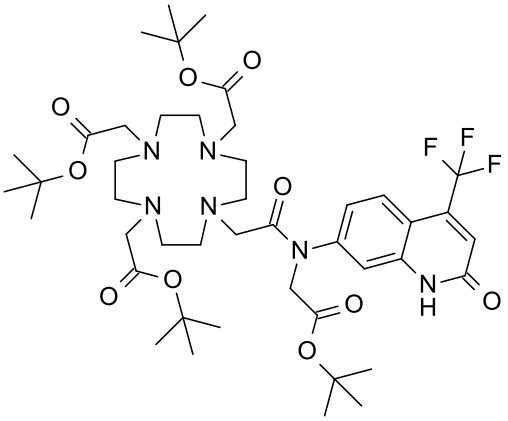



1.12 - 1.77
1.79 - 3.86
17.4 / 18.7
54.3
Br⁻
12.4
N
+
54.3
42.7
H
9.91
17.4 / 18.7
28.0
82.0
O
O
172.6
56.0
55.7
O
O
172.6
28.0
82.0
N
N
51.8 - 53.0
48.0 - 49.0
N
N
55.7
55.6
167.4
O
7.09
121.4
7.65
126.3
2.45
19.3
139.5
120.3
6.46
121.4
148.4
N
143.0
163.8
114.9
7.49
4.05 - 4.40
52.8
N
H
12.43
O
O
171.6
O
O
172.6
82.0
28.0
O
81.9
27.9

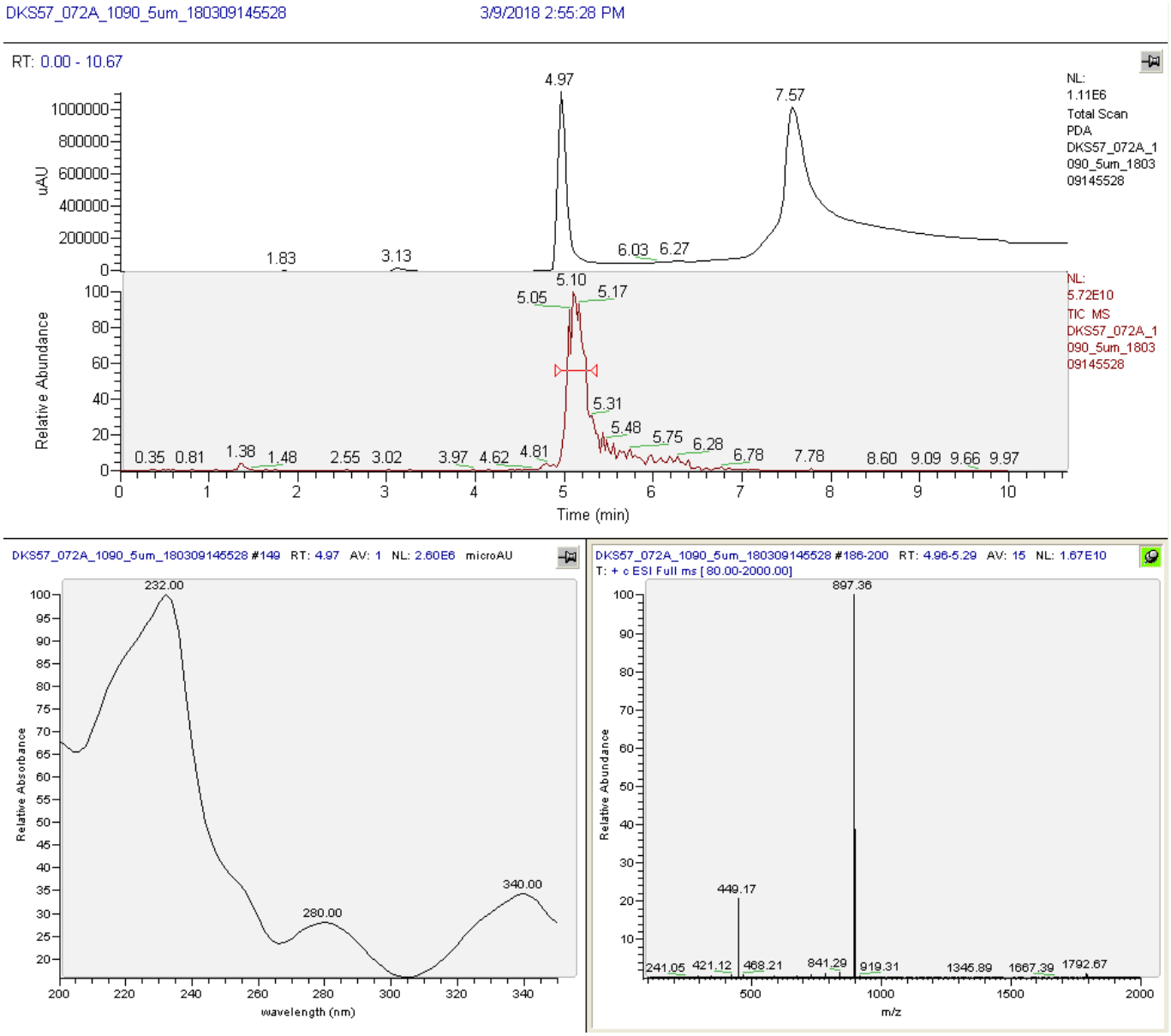

12.43
9.91
7.66
7.64
7.49
7.49
7.26
7.10
7.10
7.08
7.08
6.46
3.71
3.70
3.69
3.68
3.68
3.66
3.41
3.17
3.16
3.15
3.14
3.13
3.12
2.96
2.12
1.50
1.49
1.41
1.40
1.19
-0.00
C (d)
7.49
B (d)
7.65
A (dd)
7.09
0.76
1.86
0.90
0.88
0.84
0.77
2.42
35.51
66.99
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Chemical shift [ppm]

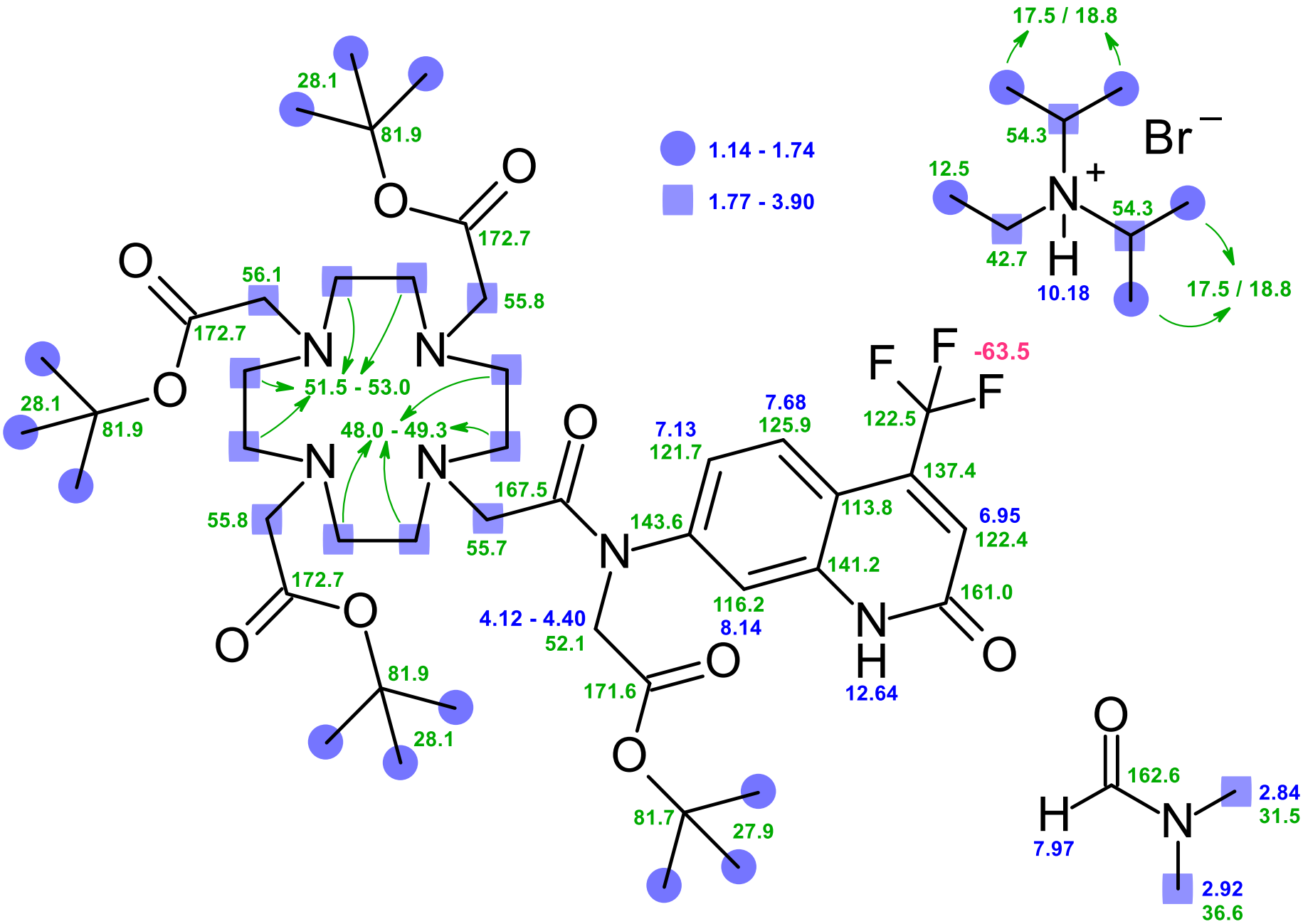

172.63
171.59
167.43
163.77
148.40
142.95
139.50
126.26
121.43
121.38
120.29
114.87
82.00
81.90
77.48
77.37
77.16
76.84
55.99
55.69
55.61
54.29
52.54
52.08
48.49
42.67
28.04
27.86
19.25
18.68
17.38
12.37
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical shift [ppm]

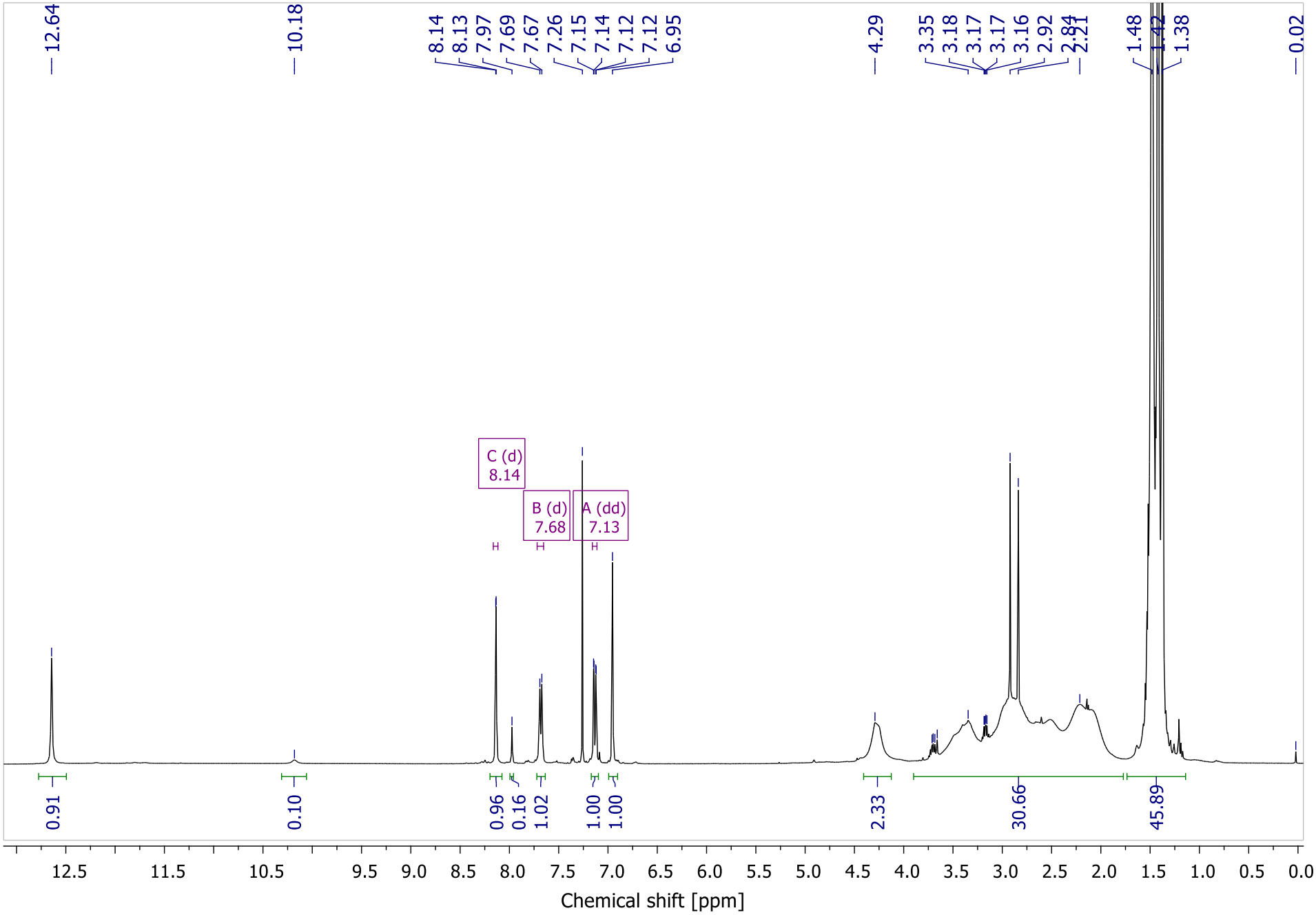
DKS57_072A

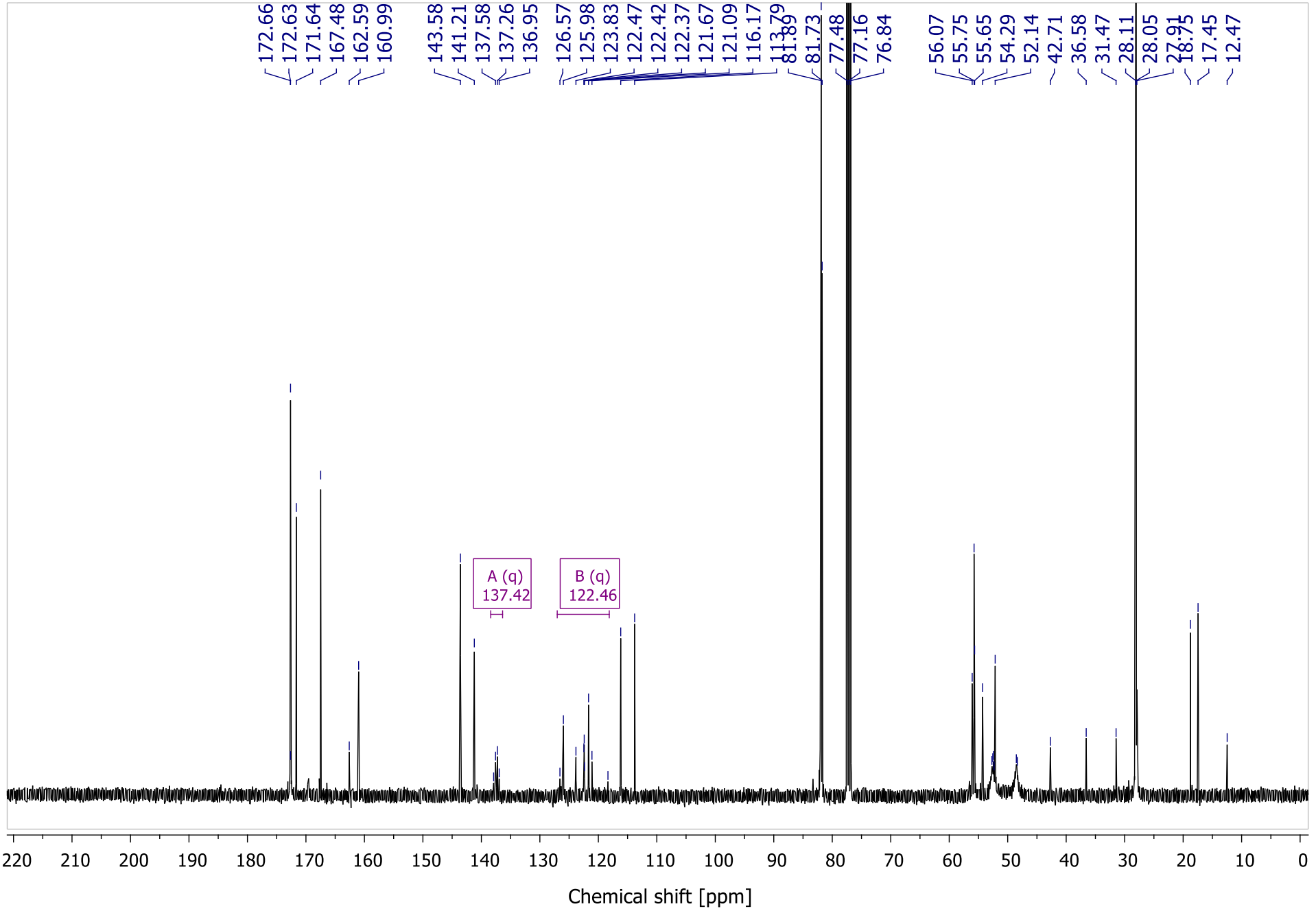


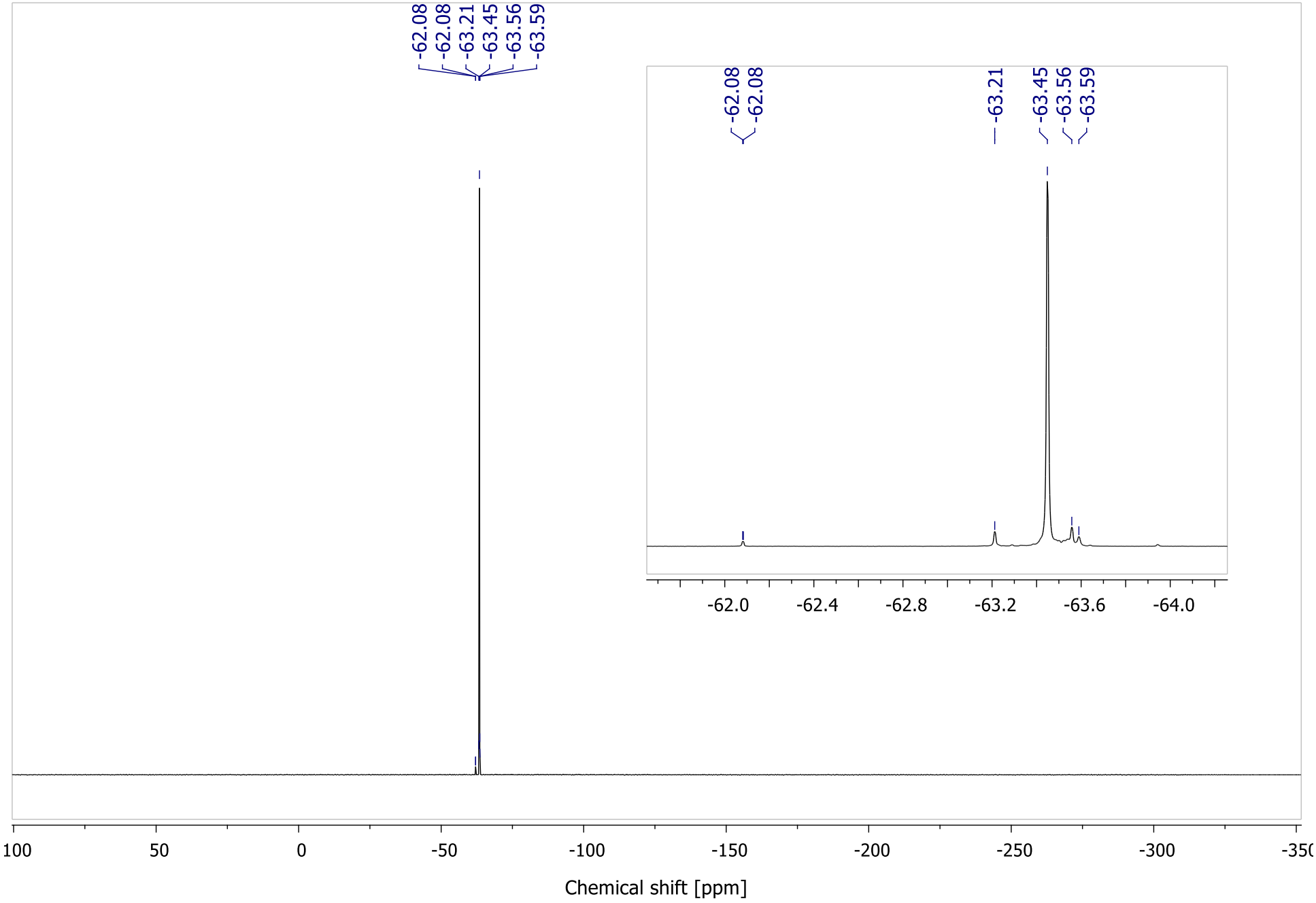
Formula Weight : 897.03(4)
Exact Mass : 896.48708
Formula : $C_{44}H_{67}F_3N_6O_{10}$
Composition : C 58.91% H 7.53% N 9.37%
O 17.84% F 6.35%



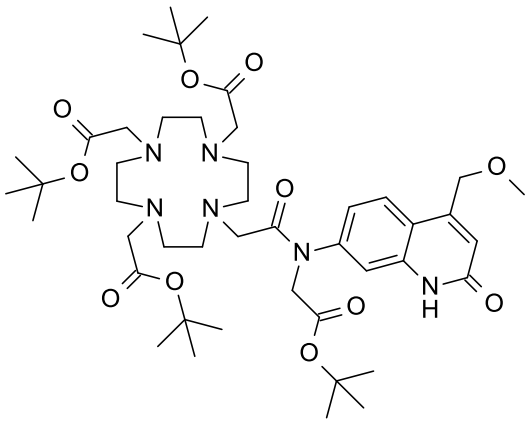

1.14 - 1.74
1.77 - 3.90
28.1
81.9
O
172.7
56.1
55.8
51.5 - 53.0
48.0 - 49.3
167.5
55.8
55.7
172.7
81.9
28.1
7.13
121.7
7.68
125.9
F
F
F
-63.5
122.5
137.4
113.8
6.95
122.4
143.6
141.2
161.0
116.2
8.14
4.12 - 4.40
52.1
171.6
81.7
27.9
12.64
17.5 / 18.8
54.3
Br
12.5
42.7
10.18
17.5 / 18.8
162.6
2.84
31.5
7.97
2.92
36.6


12.64
10.18
8.14
8.13
7.97
7.69
7.67
7.26
7.15
7.14
7.12
7.12
6.95
4.29
3.35
3.18
3.17
3.17
3.16
2.92
2.84
2.21
1.48
1.42
1.38
0.02
C (d)
8.14
B (d)
7.68
A (dd)
7.13
0.91
0.10
0.96
0.16
1.02
1.00
1.00
2.33
30.66
45.89
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Chemical shift [ppm]

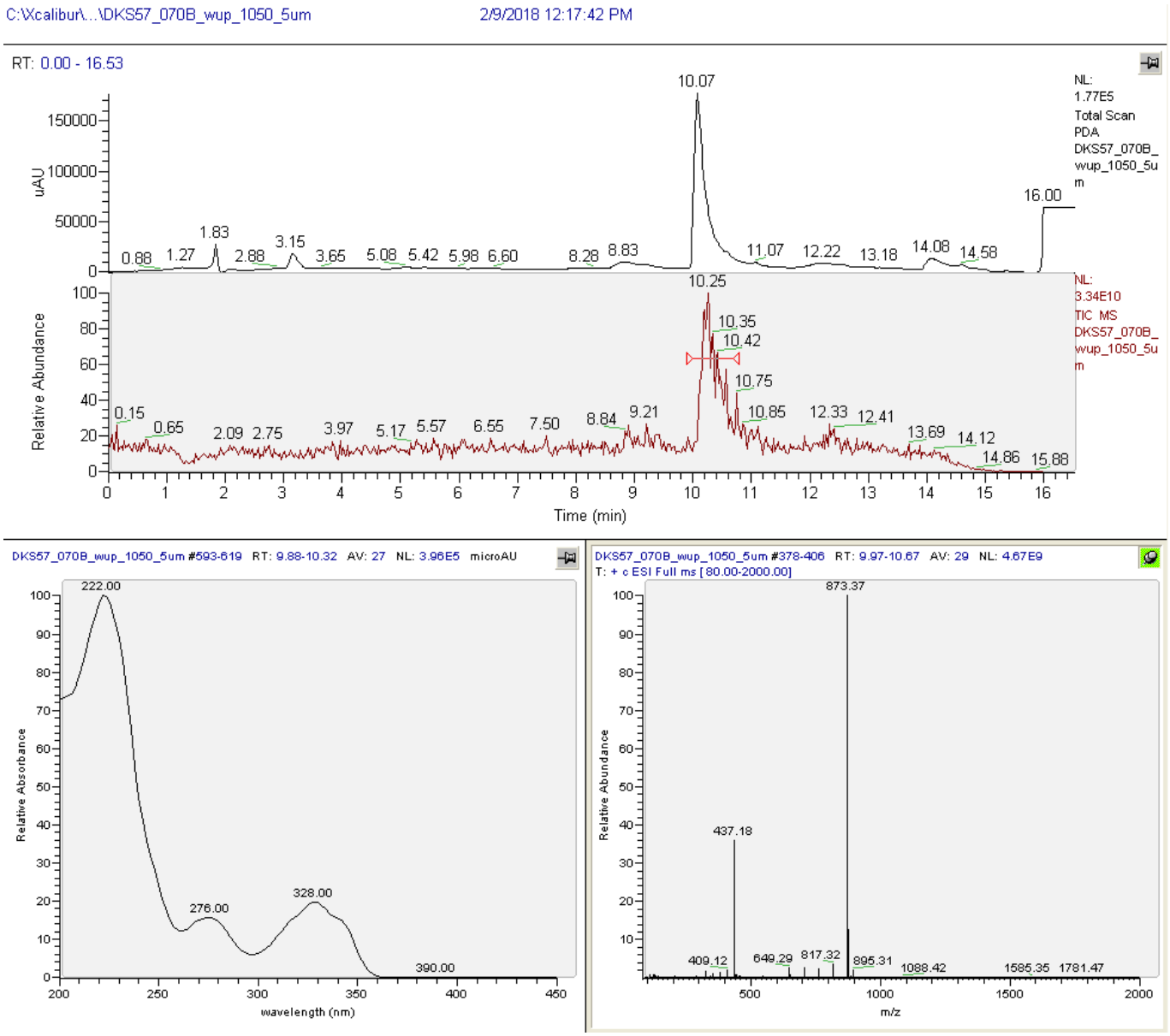

172.66
172.63
171.64
167.48
162.59
160.99
143.58
141.21
137.58
137.26
136.95
126.57
125.98
123.83
122.47
122.42
122.37
121.67
121.09
116.17
113.79
81.89
81.73
77.48
77.16
76.84
56.07
55.75
55.65
54.29
52.14
42.71
36.58
31.47
28.11
28.05
27.91
18.75
17.45
12.47
A (q)
137.42
B (q)
122.46
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical shift [ppm]

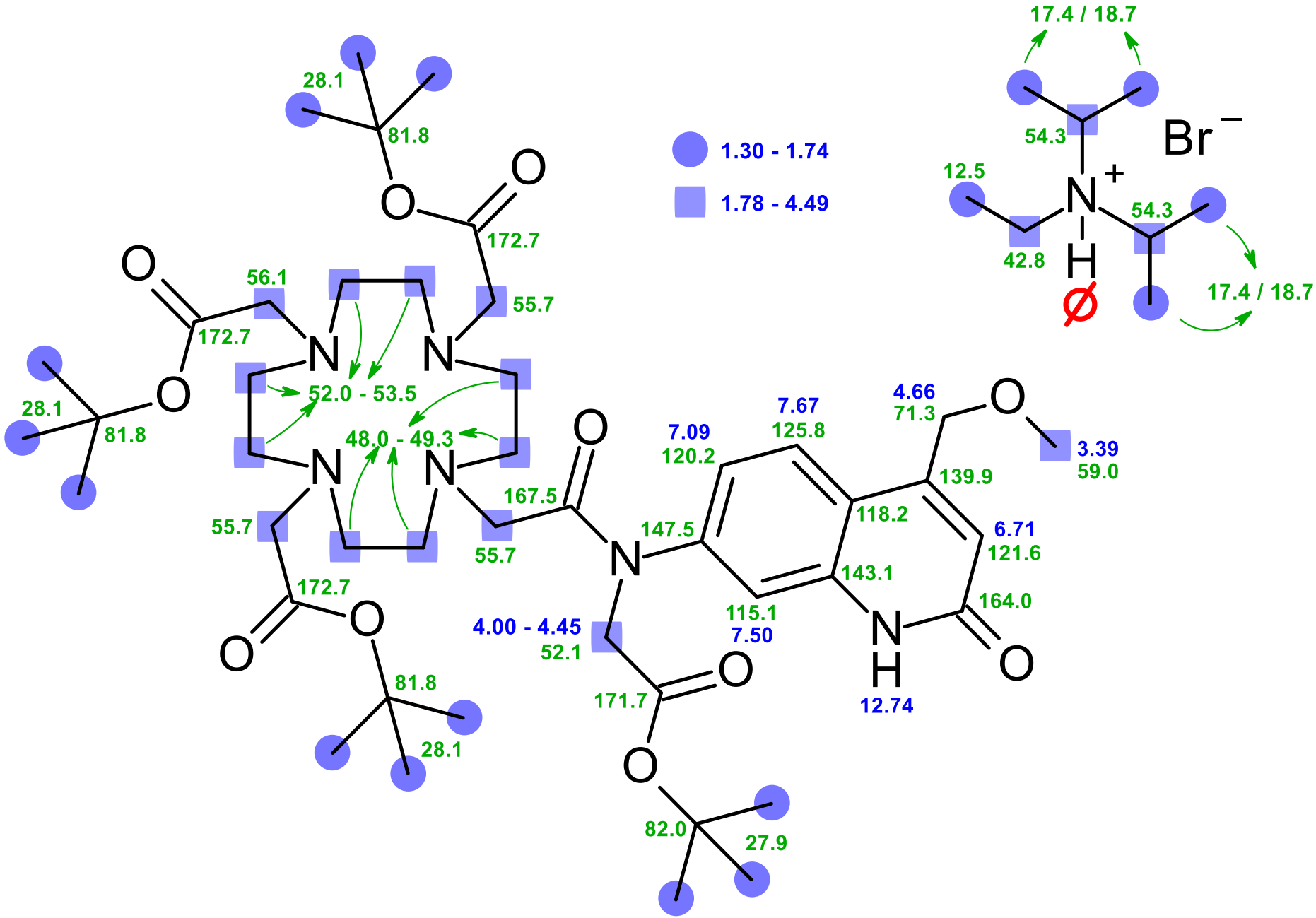

-62.08
-62.08
-63.21
-63.45
-63.56
-63.59
-62.08
-62.08
-63.21
-63.45
-63.56
-63.59
-62.0
-62.4
-62.8
-63.2
-63.6
-64.0
100
50
0
-50
-100
-150
-200
-250
-300
-350
Chemical shift [ppm]

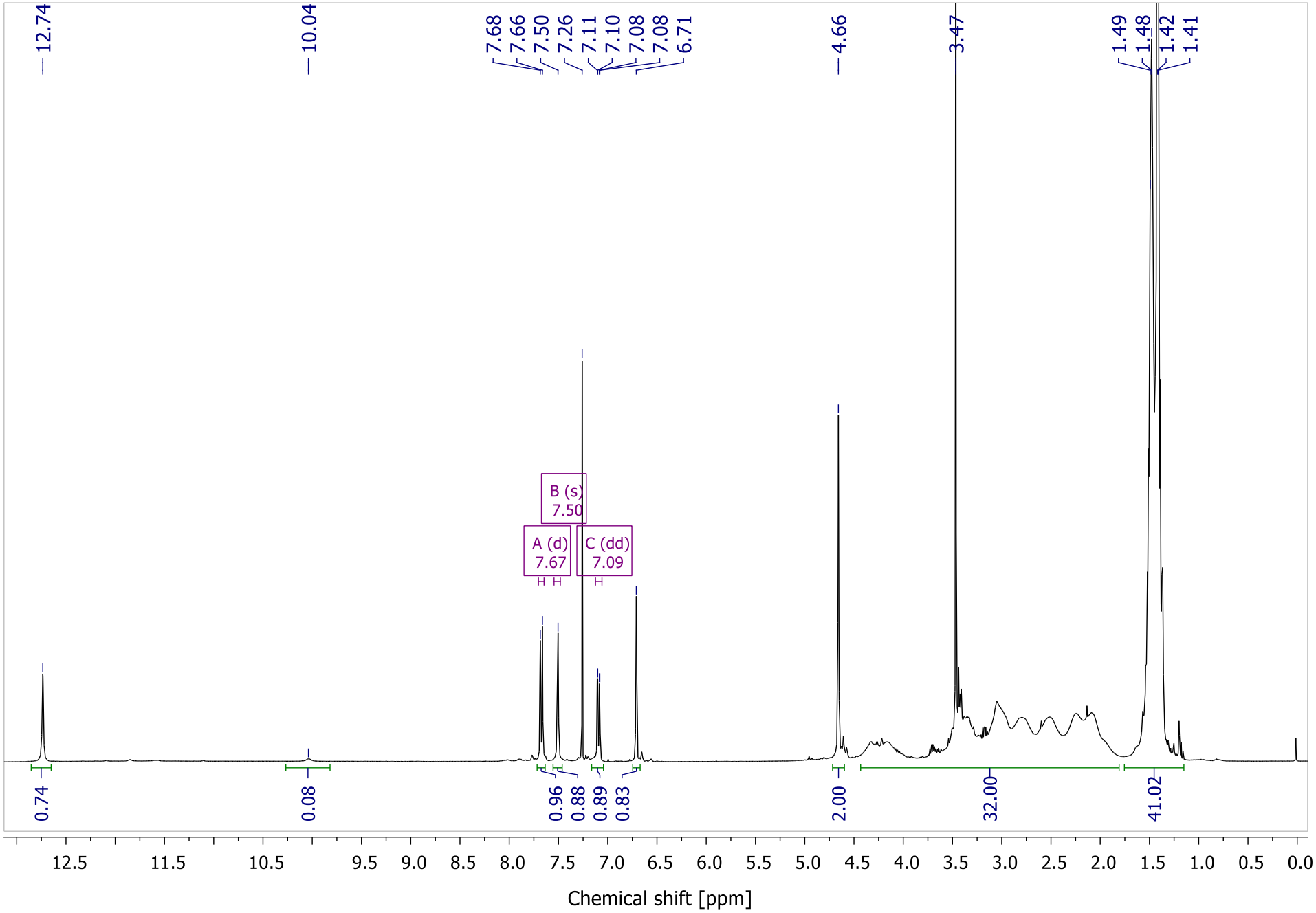
DKS57_070B

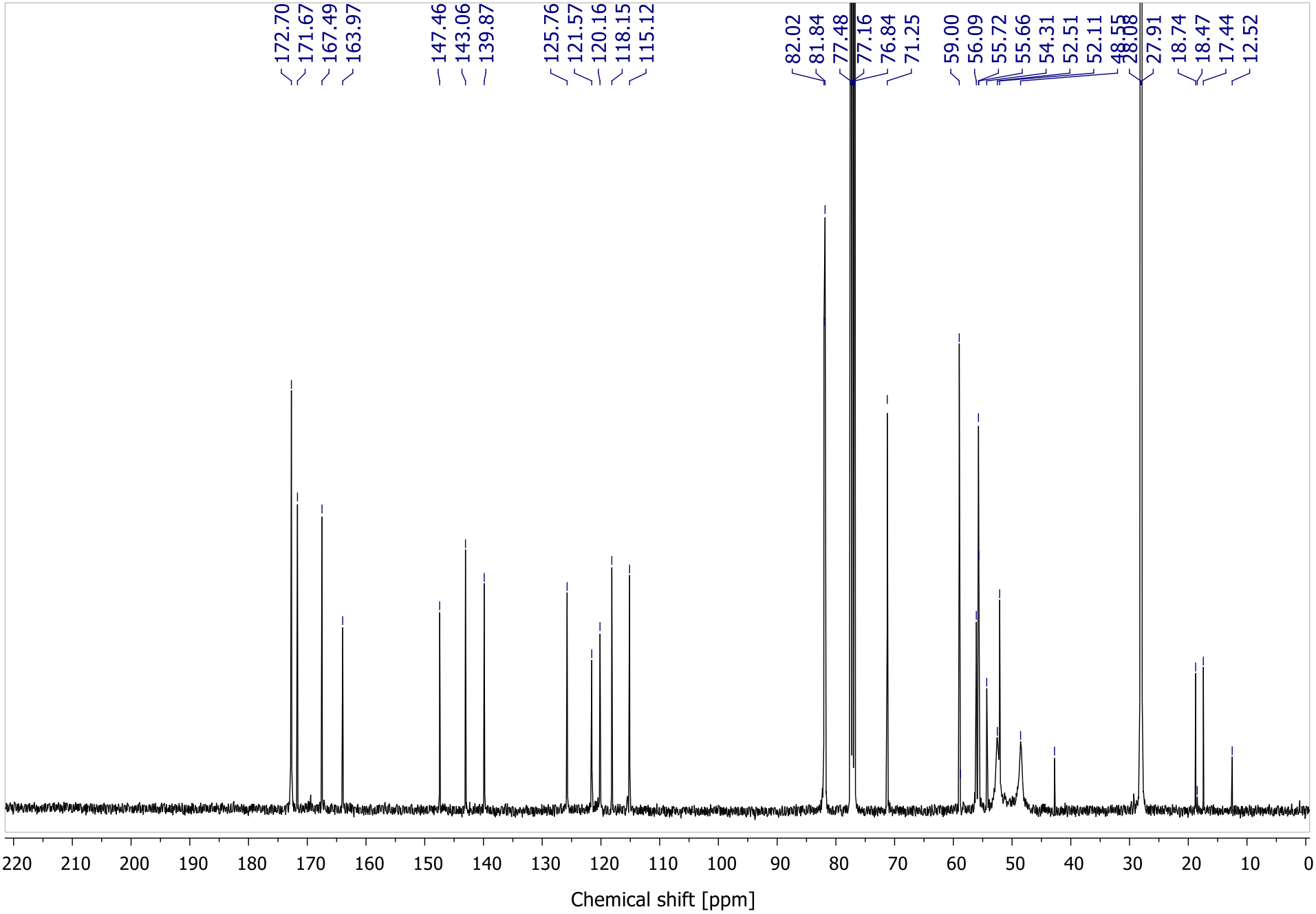


Formula Weight : 873.09(4)
Exact Mass : 872.52591
Formula : $C_{45}H_{72}N_6O_{11}$
Composition : C 61.90% H 8.31% N 9.63% O 20.16%

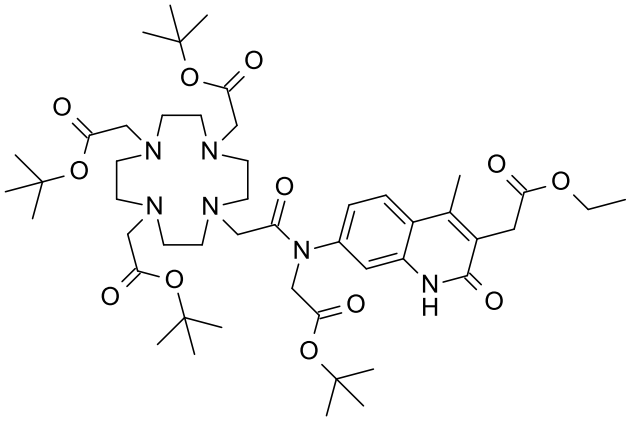



1.30 - 1.74
1.78 - 4.49
17.4 / 18.7
54.3
Br⁻
12.5
N⁺
54.3
42.8
H
Ø
17.4 / 18.7
28.1
81.8
O
172.7
56.1
55.7
O
172.7
O
28.1
81.8
N
N
52.0 - 53.5
48.0 - 49.3
N
N
55.7
55.7
167.5
O
7.09
120.2
7.67
125.8
4.66
71.3
O
3.39
59.0
139.9
147.5
118.2
6.71
121.6
N
143.1
164.0
115.1
7.50
4.00 - 4.45
52.1
O
O
N
H
12.74
O
171.7
172.7
O
O
81.8
28.1
O
82.0
27.9

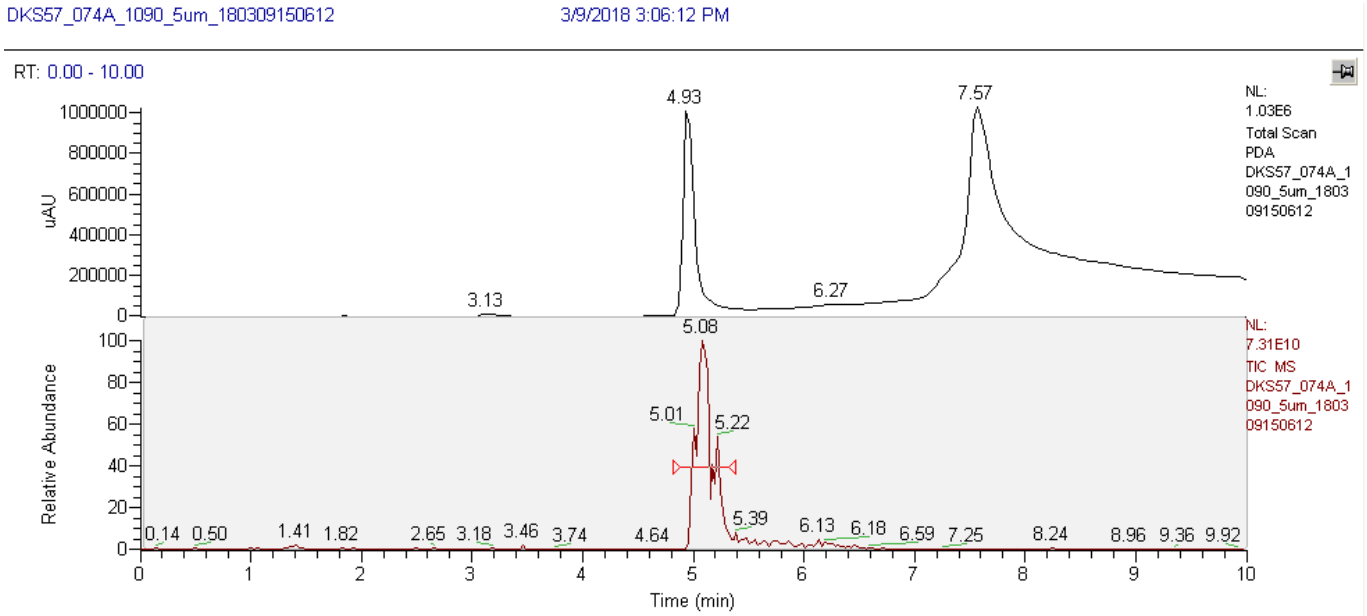

12.74
10.04
7.68
7.66
7.50
7.26
7.11
7.10
7.08
7.08
6.71
4.66
3.47
1.49
1.48
1.42
1.41
B (s)
7.50
A (d)
7.67
C (dd)
7.09
0.74
0.08
0.96
0.88
0.89
0.83
2.00
32.00
41.02
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Chemical shift [ppm]

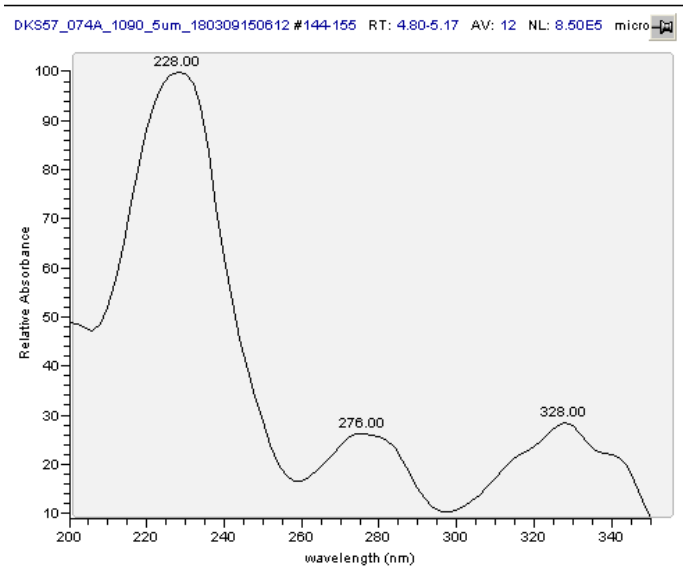

172.70
171.67
167.49
163.97
147.46
143.06
139.87
125.76
121.57
120.16
118.15
115.12
82.02
81.84
77.48
77.16
76.84
71.25
59.00
56.09
55.72
55.66
54.31
52.51
52.11
48.55
28.08
27.91
18.74
18.47
17.44
12.52
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical shift [ppm]

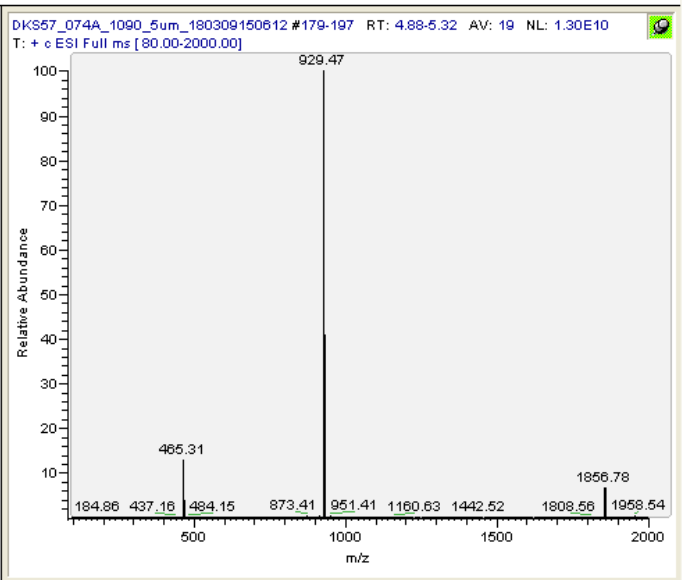
DKS57_074A

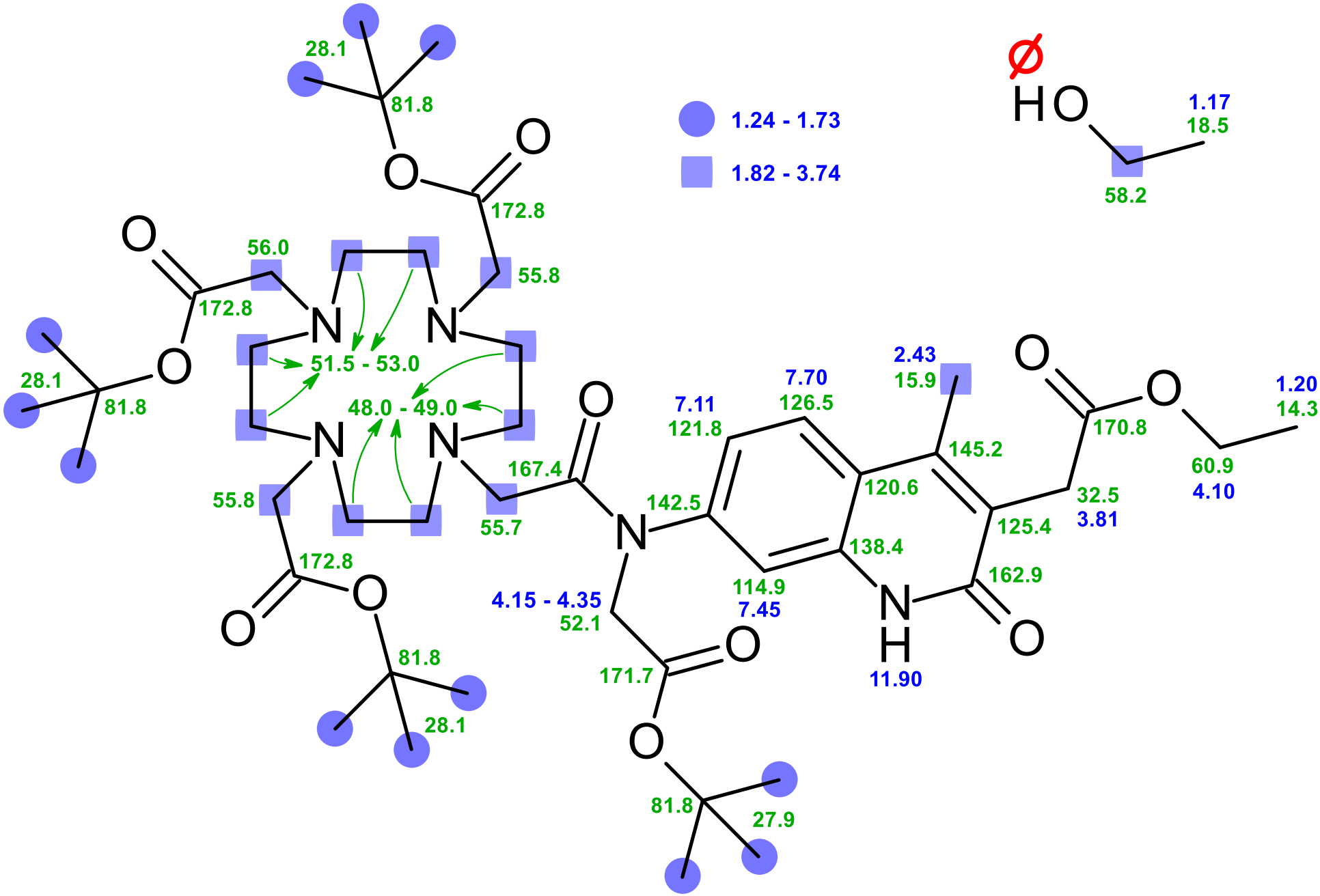


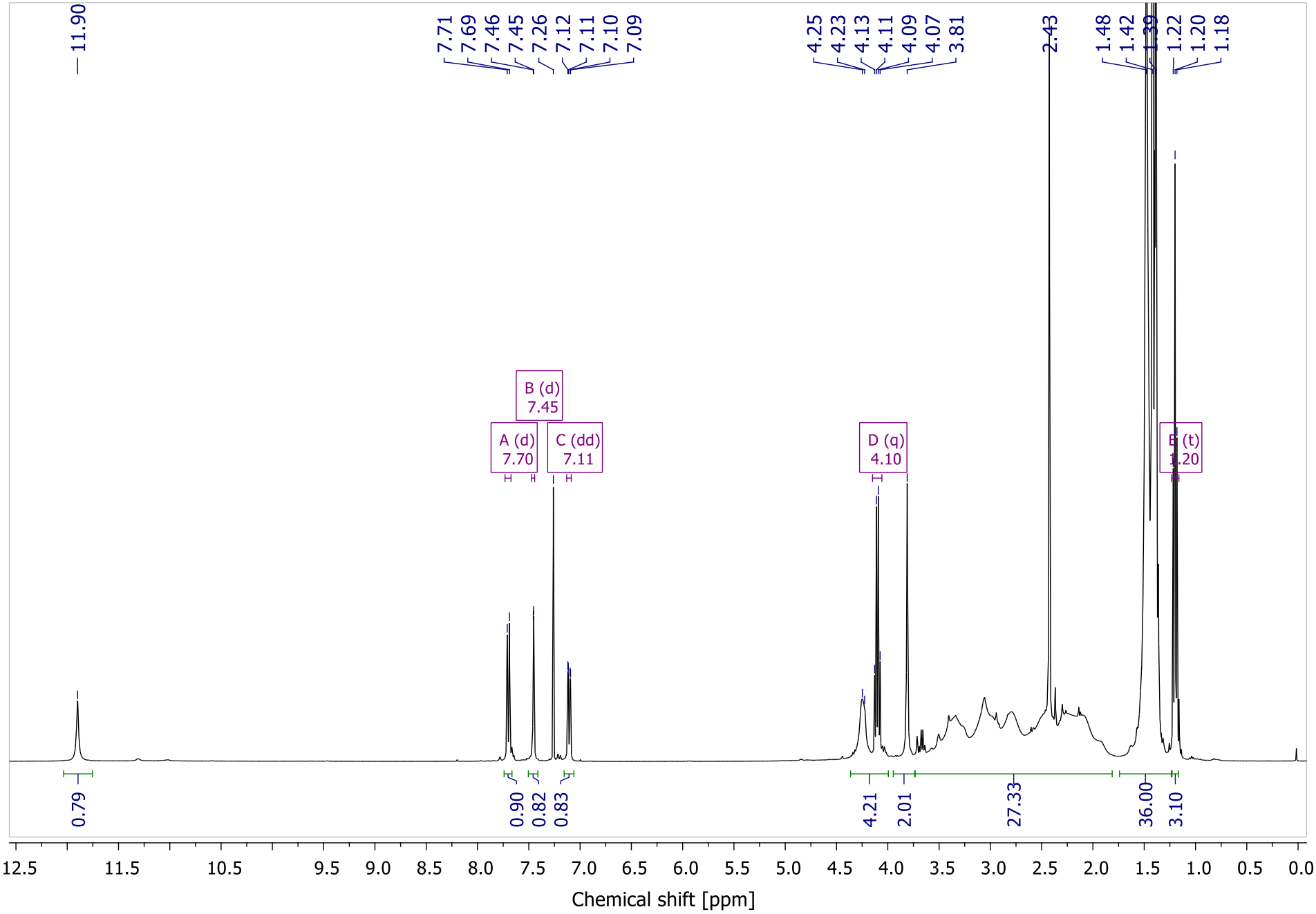
Formula Weight : 929.15(4)
Exact Mass : 928.55212
Formula : $C_{48}H_{76}N_6O_{12}$
Composition : C 62.05% H 8.24%
N 9.04% O 20.66%

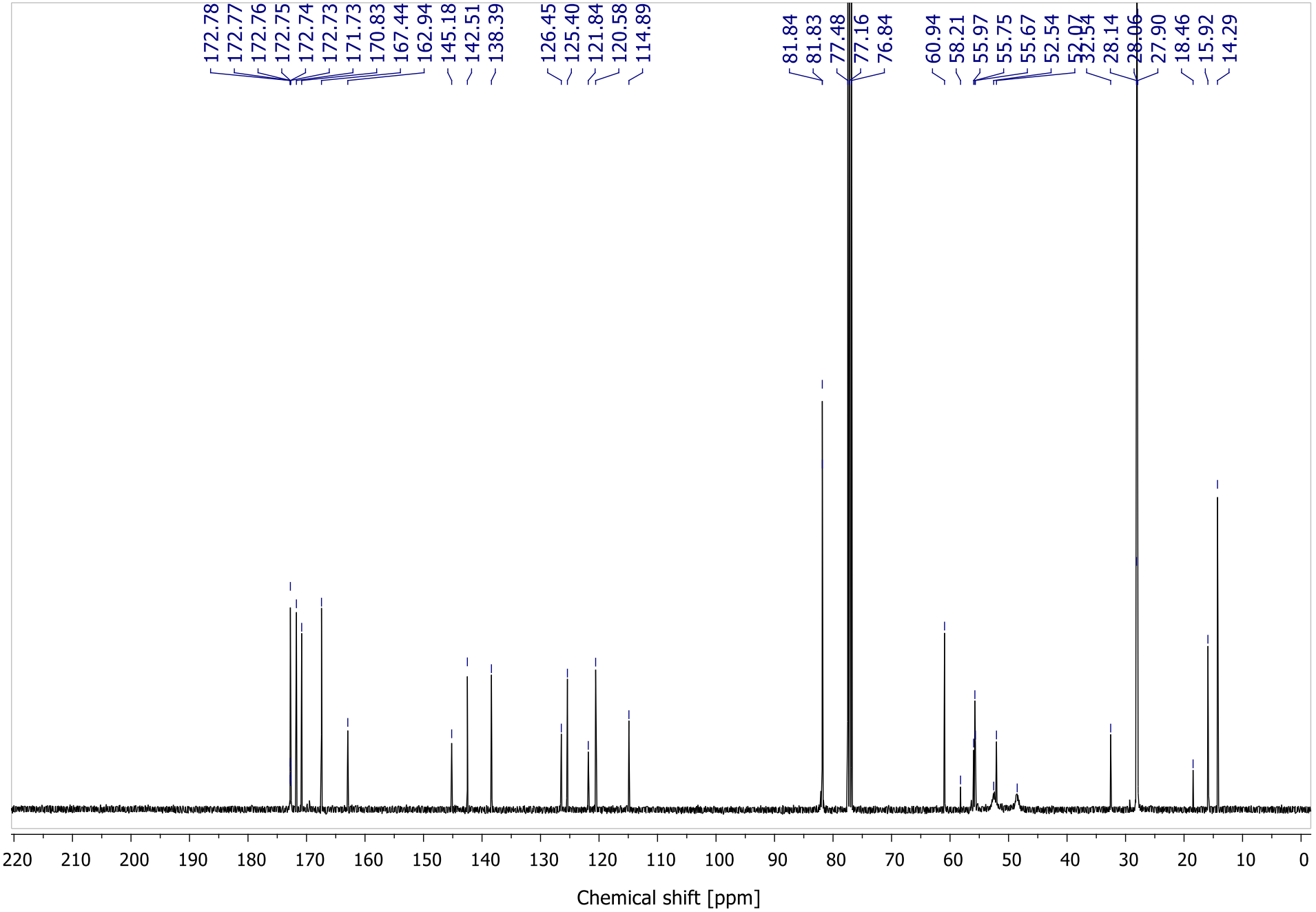




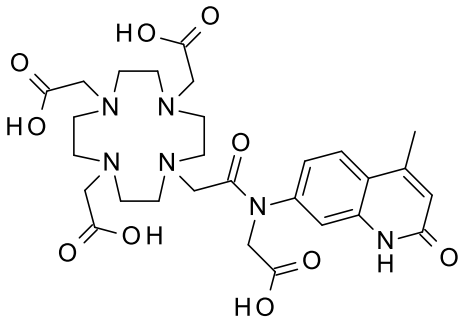



1.24 - 1.73
1.82 - 3.74
Ø
HO
1.17
18.5
58.2
28.1
81.8
O
O
172.8
55.8
56.0
O
172.8
N
N
51.5 - 53.0
48.0 - 49.0
N
N
28.1
81.8
O
55.8
55.7
167.4
O
N
142.5
7.11
121.8
7.70
126.5
2.43
15.9
120.6
145.2
O
O
170.8
1.20
14.3
60.9
4.10
32.5
3.81
125.4
138.4
162.9
114.9
7.45
N
H
11.90
O
4.15 - 4.35
52.1
O
171.7
O
81.8
27.9
O
172.8
O
O
81.8
28.1

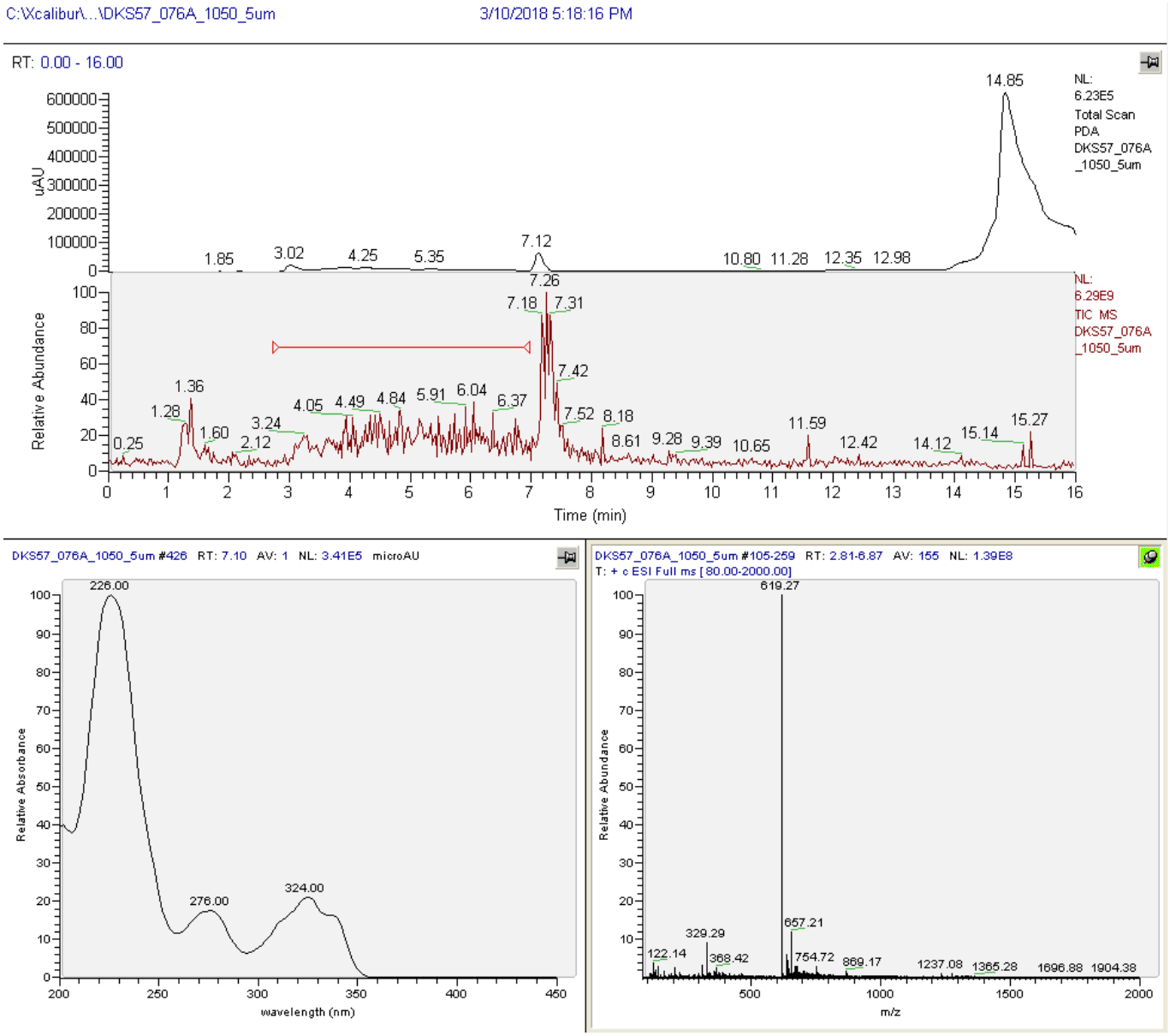

11.90
7.71
7.69
7.46
7.45
7.26
7.12
7.11
7.10
7.09
4.25
4.23
4.13
4.11
4.09
4.07
3.81
2.43
1.48
1.42
1.39
1.22
1.20
1.18
B (d)
7.45
A (d)
7.70
C (dd)
7.11
D (q)
4.10
E (t)
1.20
0.79
0.90
0.82
0.83
4.21
2.01
27.33
36.00
3.10
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Chemical shift [ppm]

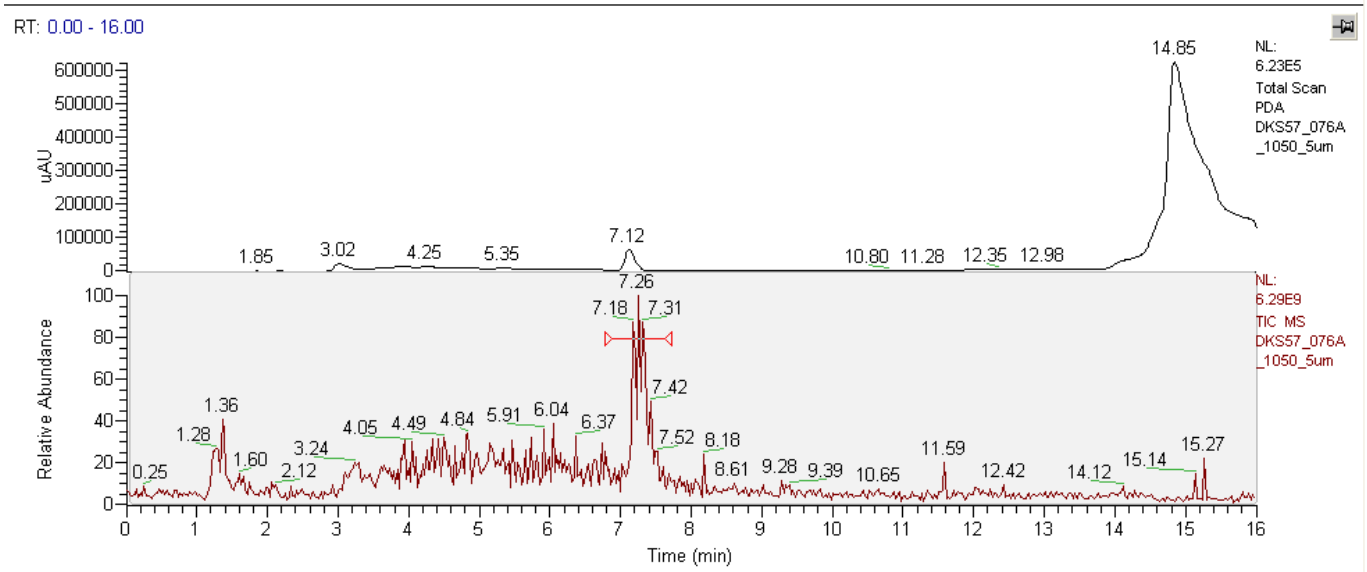

172.78
172.77
172.76
172.75
172.74
172.73
171.73
170.83
167.44
162.94
145.18
142.51
138.39
126.45
125.40
121.84
120.58
114.89
81.84
81.83
77.48
77.16
76.84
60.94
58.21
55.97
55.75
55.67
52.54
52.07
32.54
28.14
28.06
27.90
18.46
15.92
14.29
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical shift [ppm]

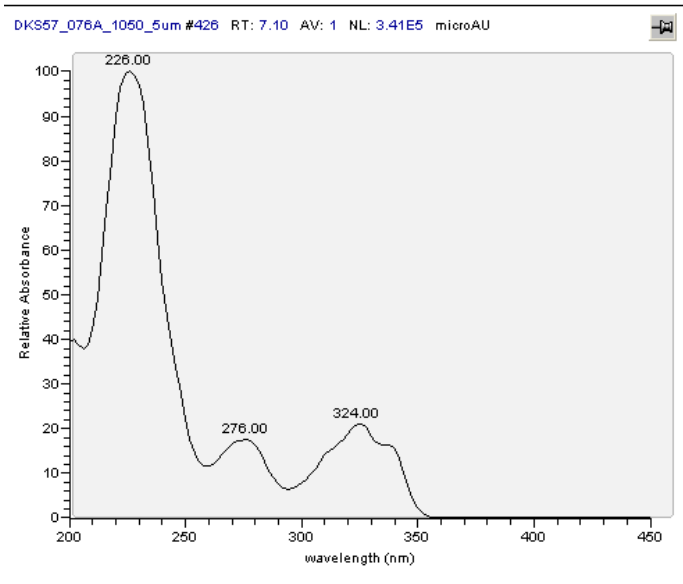
DKS57_076A

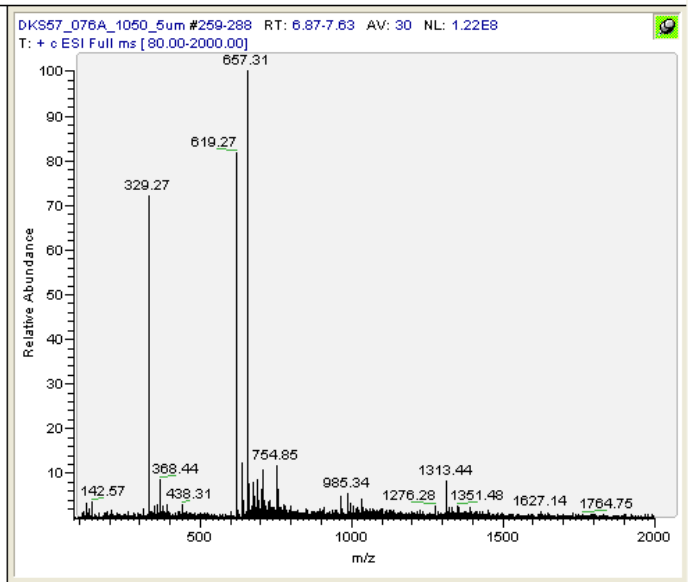


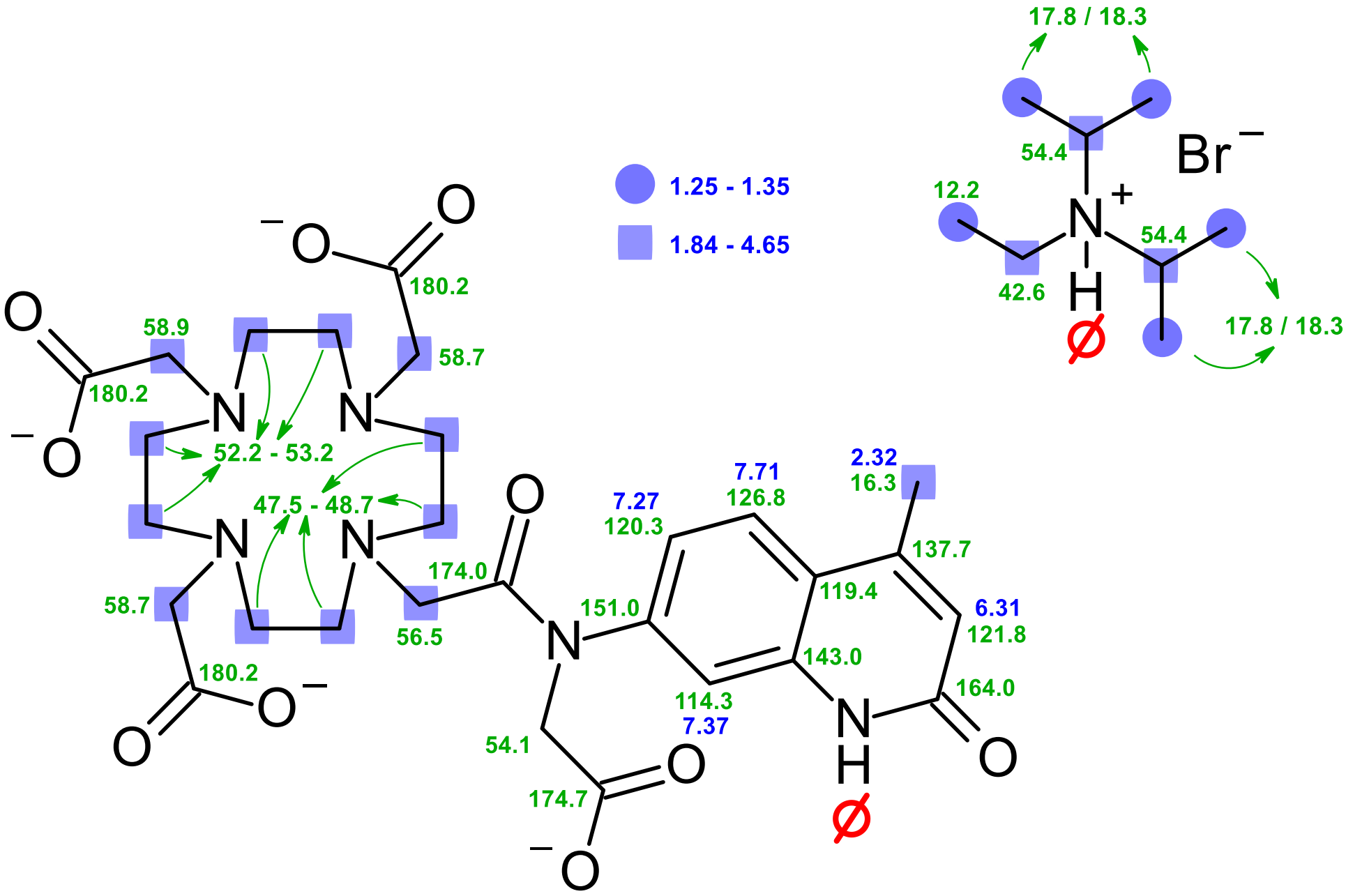
Formula Weight : 618.64(2)
Exact Mass : 618.26494
Formula : $C_{28}H_{38}N_6O_{10}$
Composition : C 54.36% H 6.19% N 13.58% O 25.86%

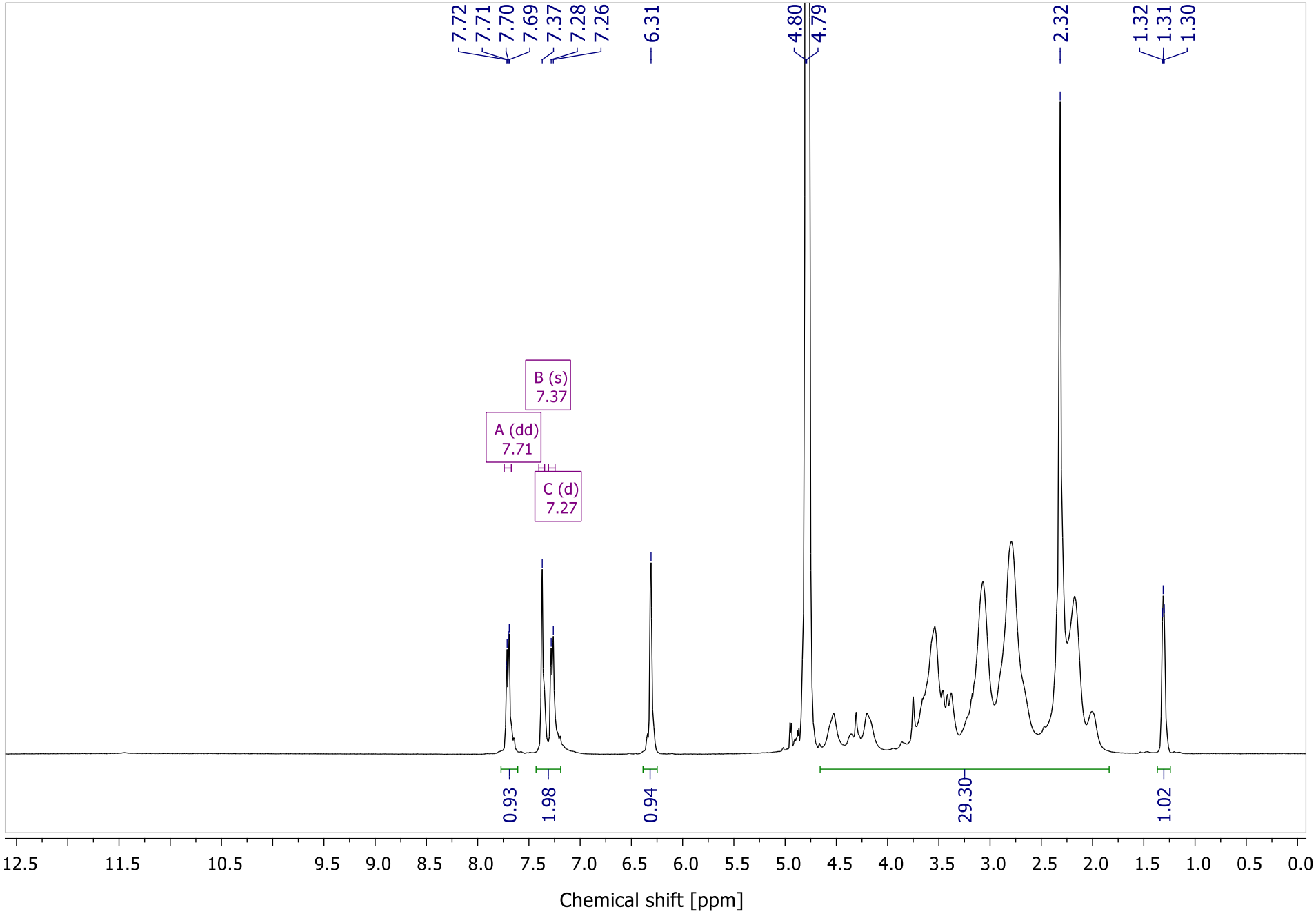


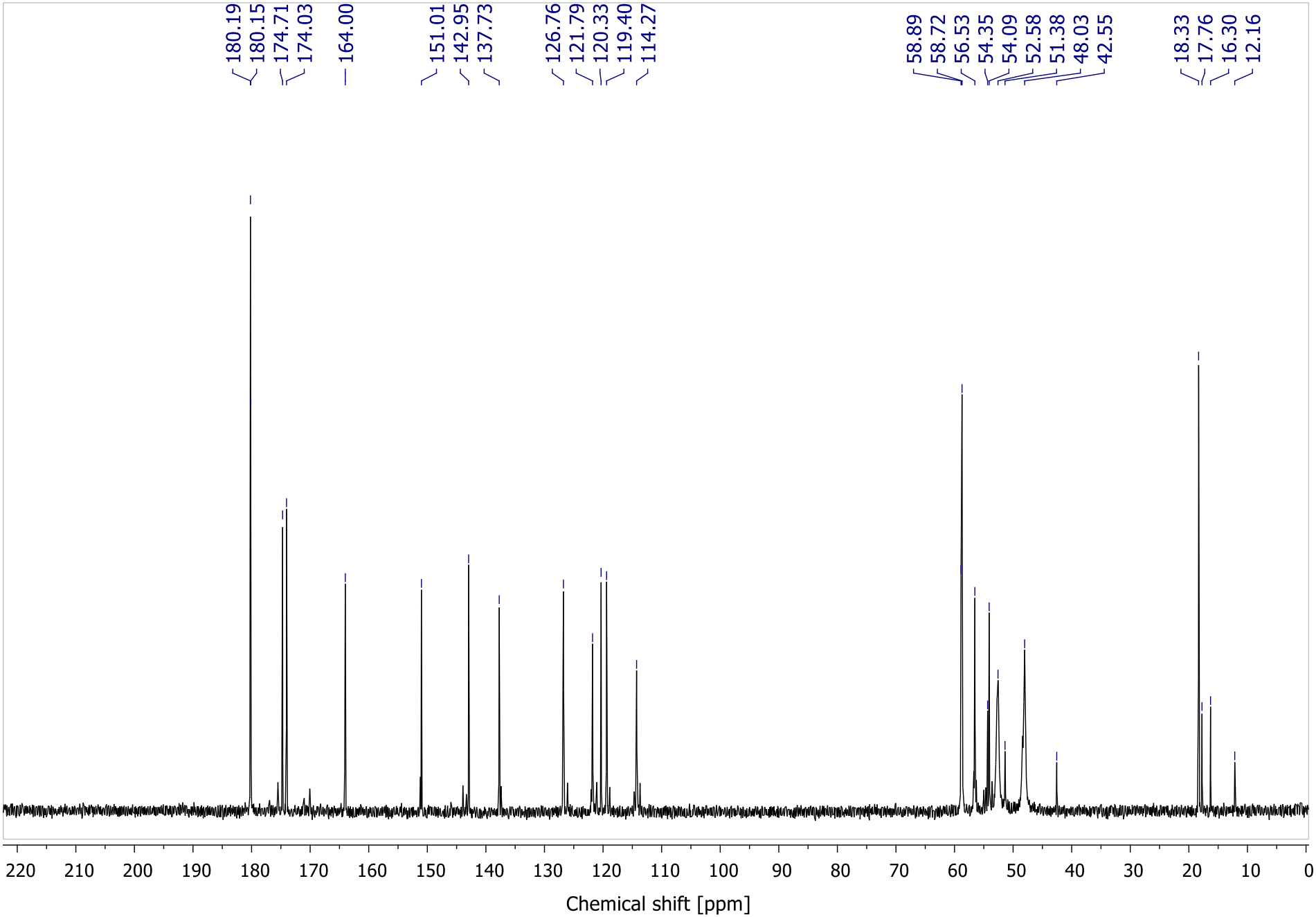

RT: 0.00 - 16.00
uAU
Relative Abundance
Time (min)
NL: 6.23E5 Total Scan PDA DKS57_076A_1050_5um
NL: 6.29E9 TIC MS DKS57_076A_1050_5um
14.85
7.12
7.26
7.18
7.31
7.42
1.36
1.28
1.60
3.24
2.12
0.25
4.05
4.49
4.84
5.91
6.04
6.37
7.52
8.18
8.61
9.28
9.39
10.65
11.59
12.42
14.12
15.14
15.27
1.85
3.02
4.25
5.35
10.80
11.28
12.35
12.98


DKS57_076A_1050_5um #426 RT: 7.10 AV: 1 NL: 3.41E5 microAU
Relative Absorbance
wavelength (nm)
226.00
276.00
324.00

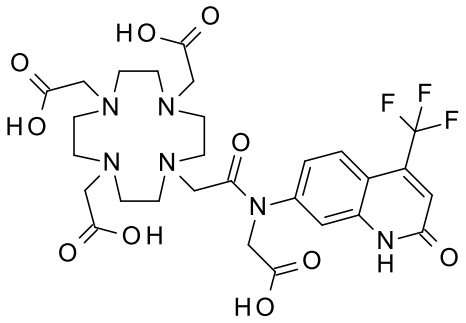

DKS57_076A_1050_5um #259-288 RT: 6.87-7.63 AV: 30 NL: 1.22E8
T: + c ESI Full ms [80.00-2000.00]
Relative Abundance
m/z
657.31
619.27
329.27
754.85
368.44
438.31
142.57
985.34
1313.44
1276.28
1351.48
1627.14
1764.75


1.25 - 1.35
1.84 - 4.65
17.8 / 18.3
54.4
Br⁻
12.2
N⁺
H
54.4
42.6
17.8 / 18.3
58.9
58.7
180.2
180.2
52.2 - 53.2
47.5 - 48.7
58.7
56.5
174.0
7.27
120.3
7.71
126.8
2.32
16.3
137.7
119.4
151.0
6.31
121.8
143.0
164.0
114.3
7.37
54.1
174.7
N
H
O

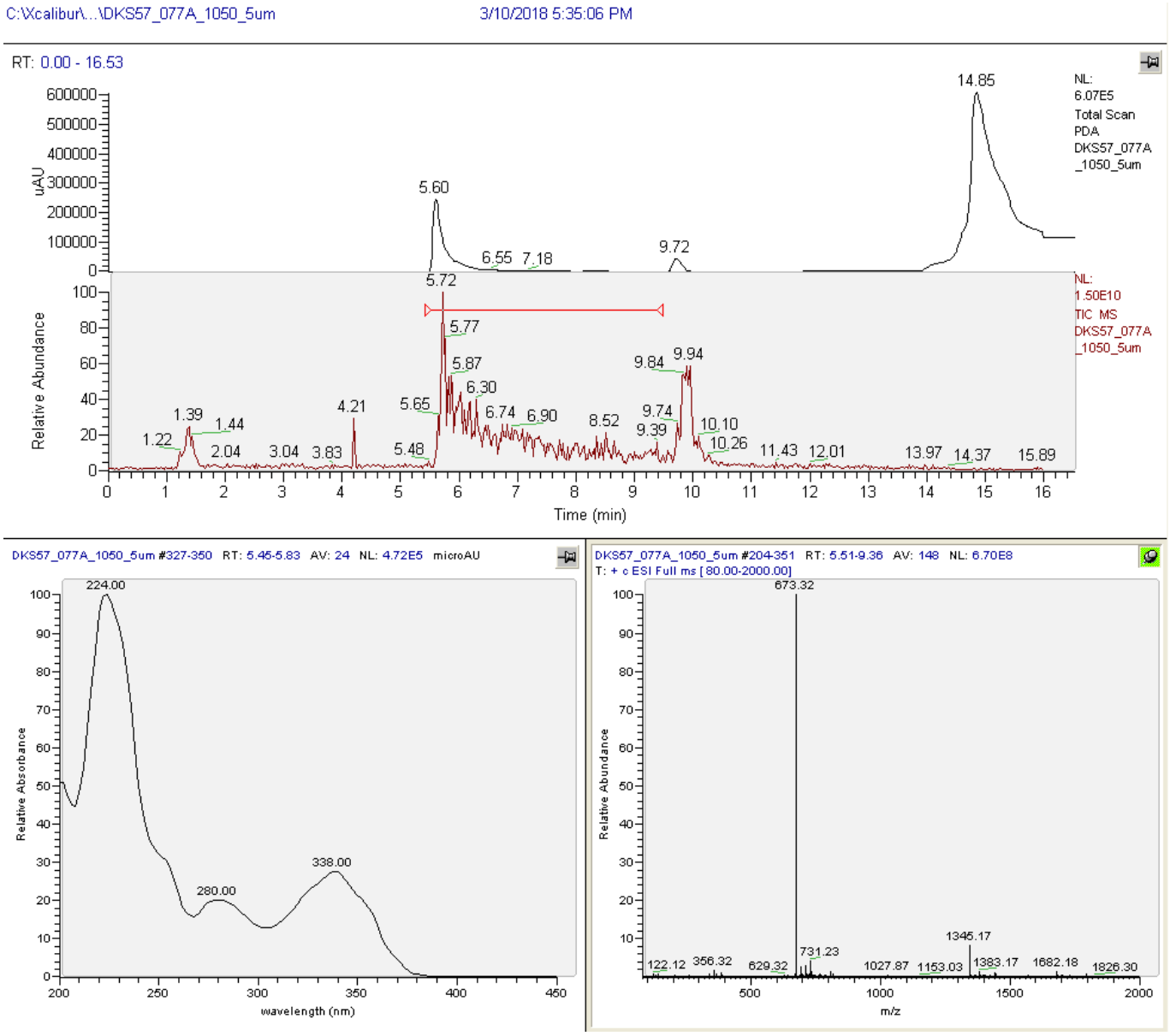

7.72
7.71
7.70
7.69
7.37
7.28
7.26
6.31
4.80
4.79
2.32
1.32
1.31
1.30
B (s)
7.37
A (dd)
7.71
C (d)
7.27
0.93
1.98
0.94
29.30
1.02
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Chemical shift [ppm]

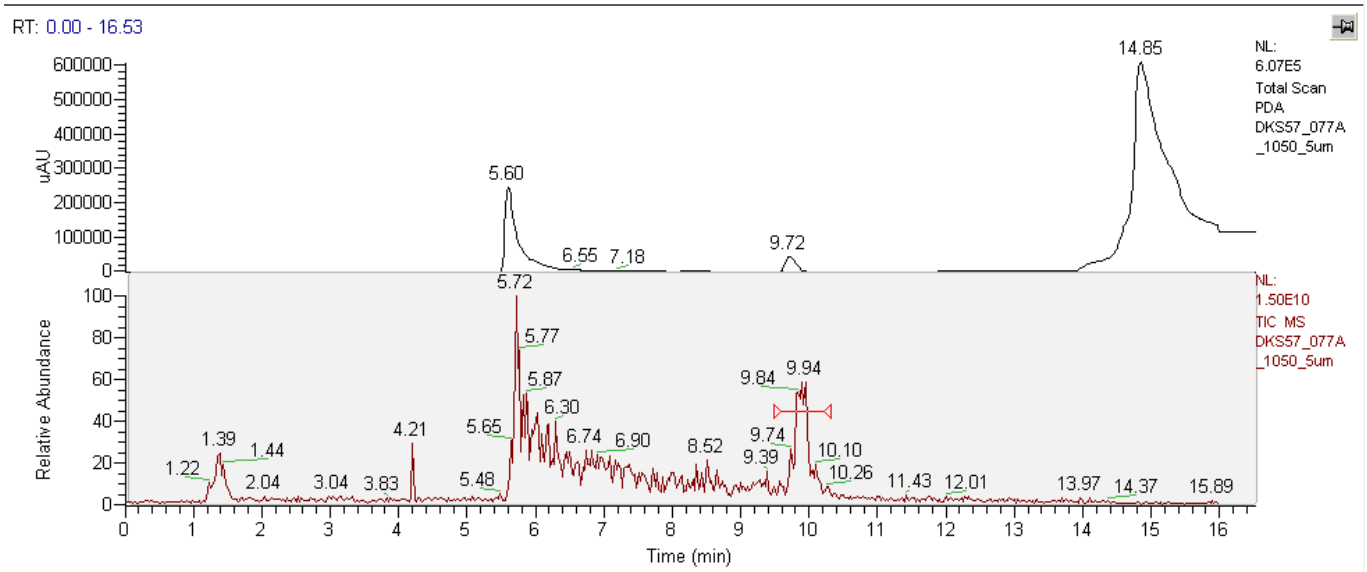

180.19
180.15
174.71
174.03
164.00
151.01
142.95
137.73
126.76
121.79
120.33
119.40
114.27
58.89
58.72
56.53
54.35
54.09
52.58
51.38
48.03
42.55
18.33
17.76
16.30
12.16
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical shift [ppm]

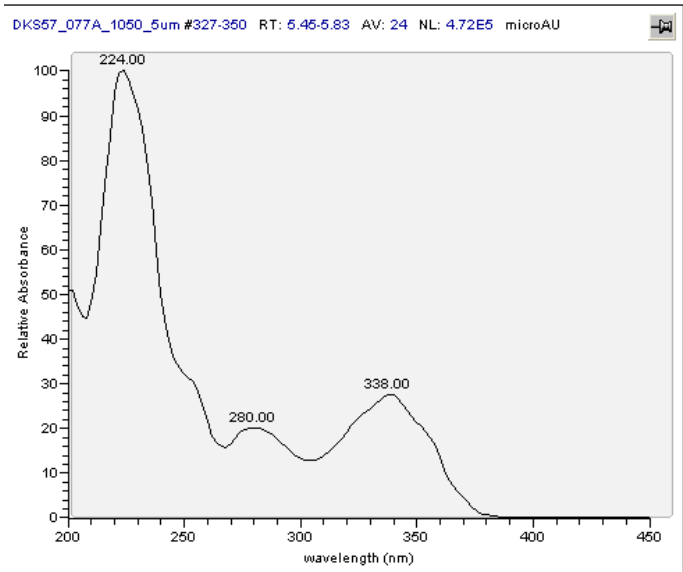
DKS57_077A

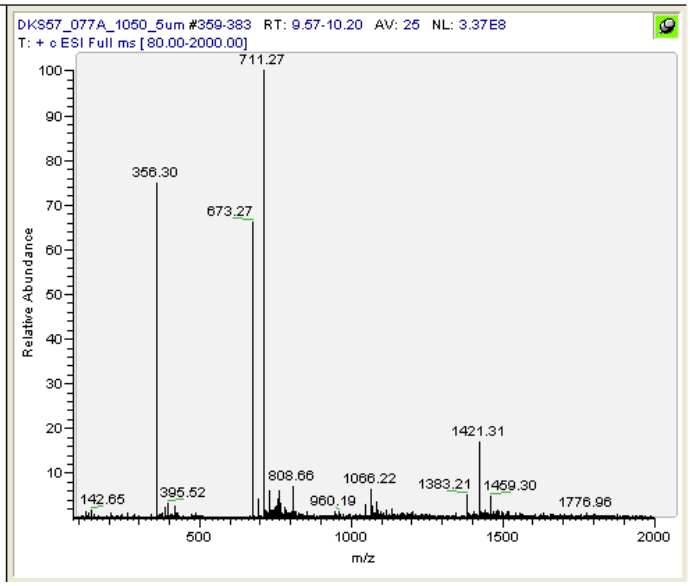


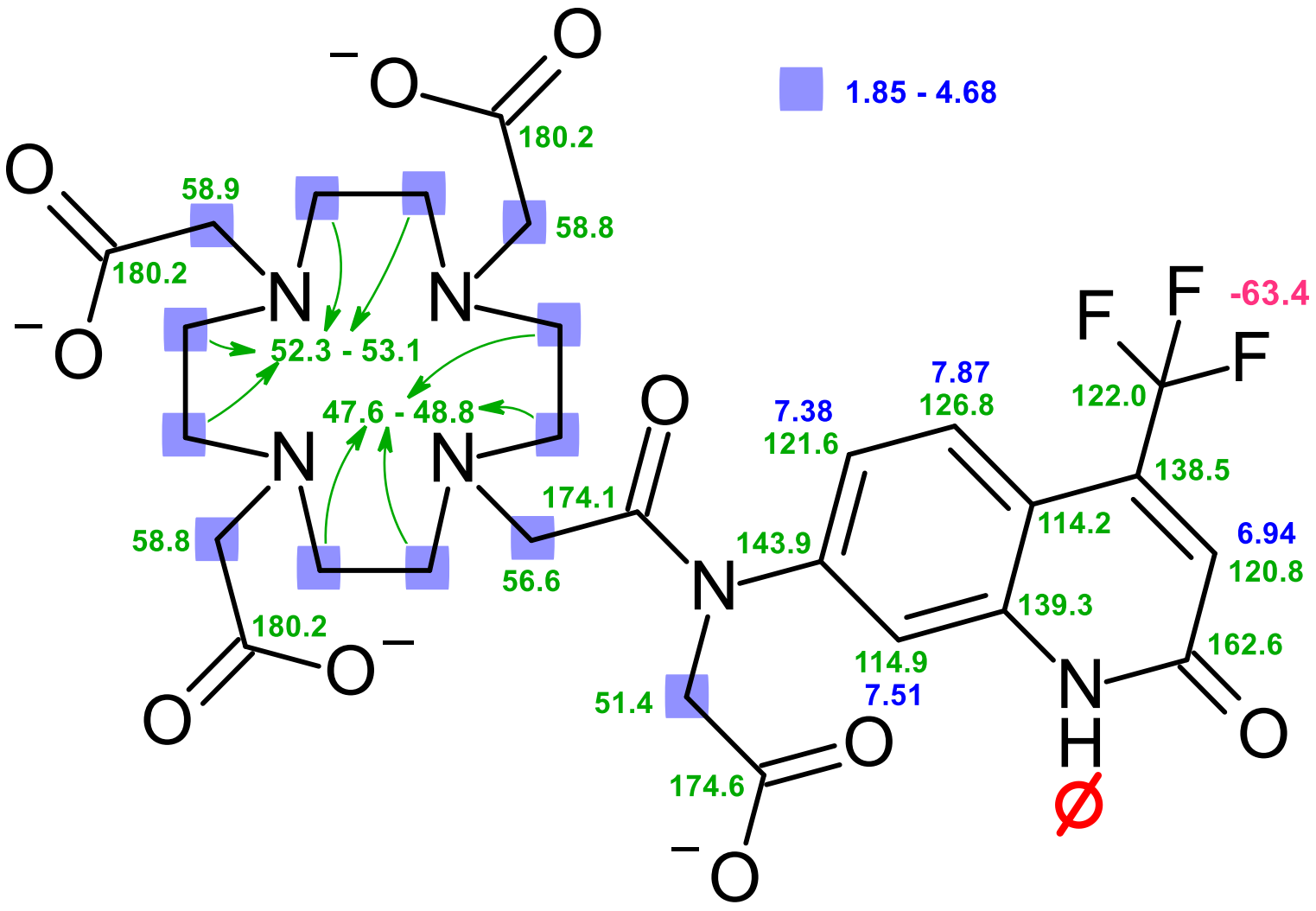
Formula Weight : 672.61(2)
Exact Mass : 672.23668
Formula : $C_{28}H_{35}F_3N_6O_{10}$
Composition : C 50.00% H 5.24% N 12.49%
O 23.79% F 8.47%

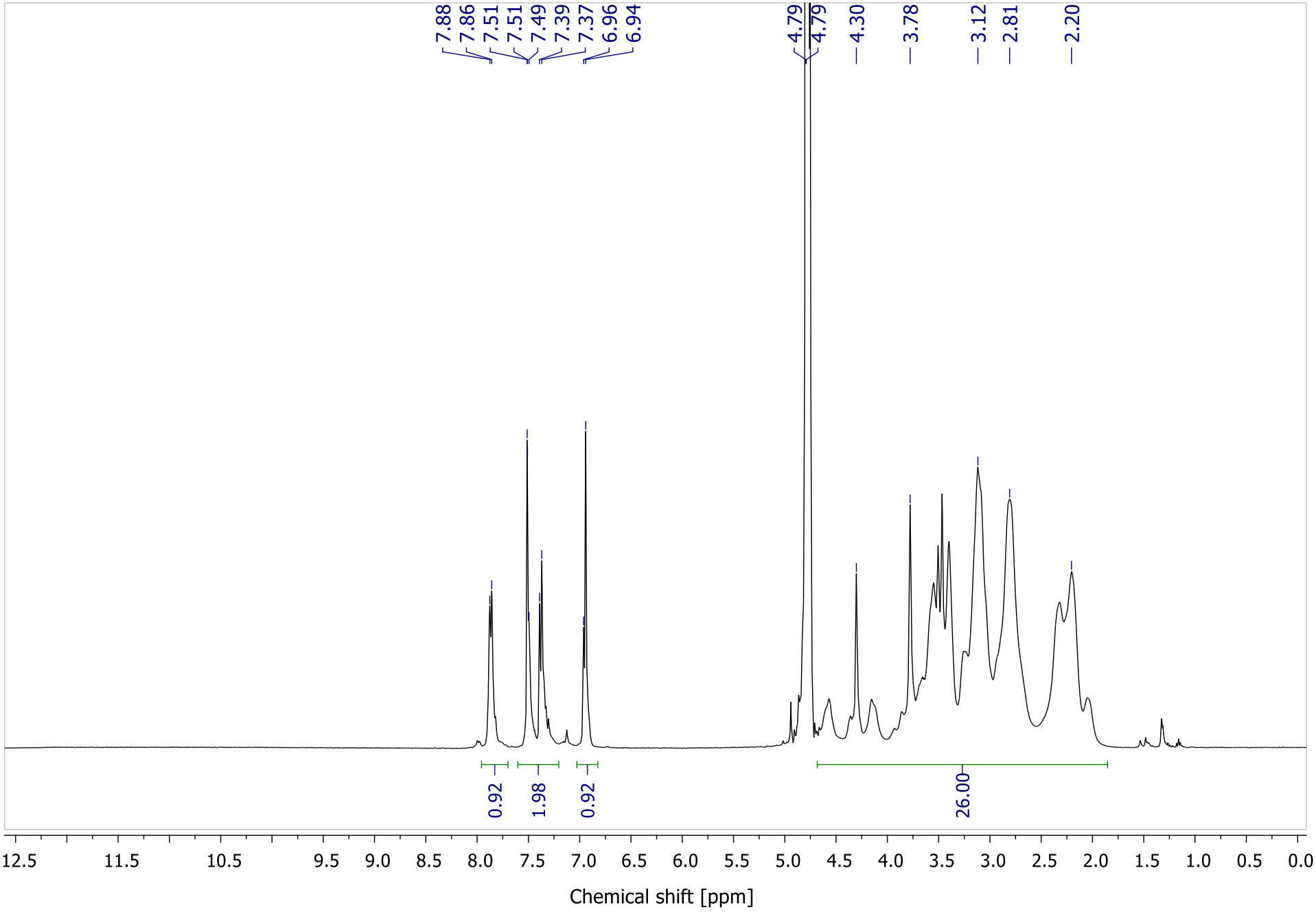


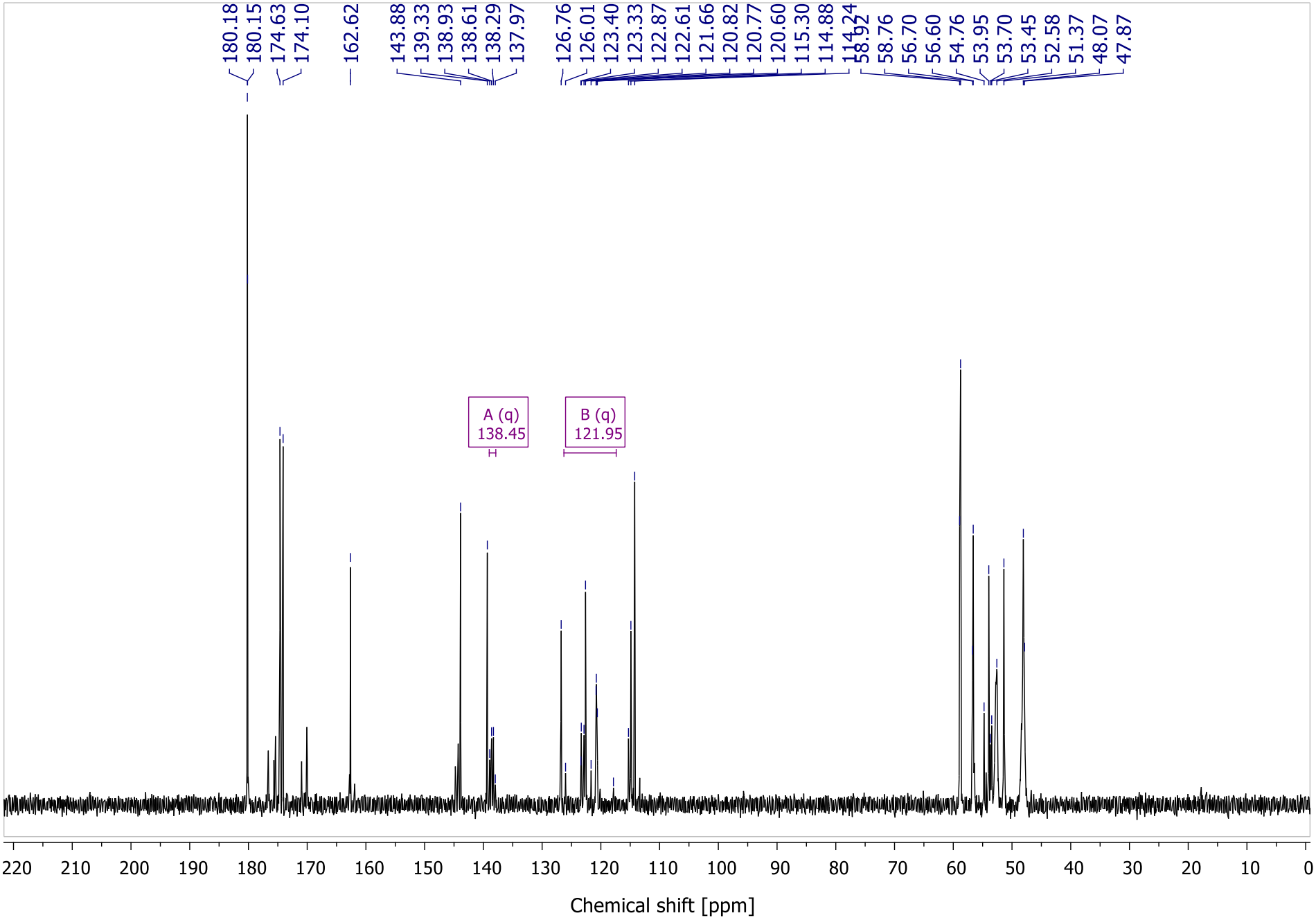

RT: 0.00 - 16.53
uAU
Relative Abundance
Time (min)
NL: 6.07E5 Total Scan PDA DKS57_077A _1050_5um
NL: 1.50E10 TIC MS DKS57_077A _1050_5um
14.85
5.60
6.55
7.18
9.72
5.72
5.77
5.87
6.30
6.74
6.90
8.52
9.84
9.94
9.74
9.39
10.10
10.26
11.43
12.01
13.97
14.37
15.89
1.22
1.39
1.44
2.04
3.04
3.83
4.21
5.48
5.65

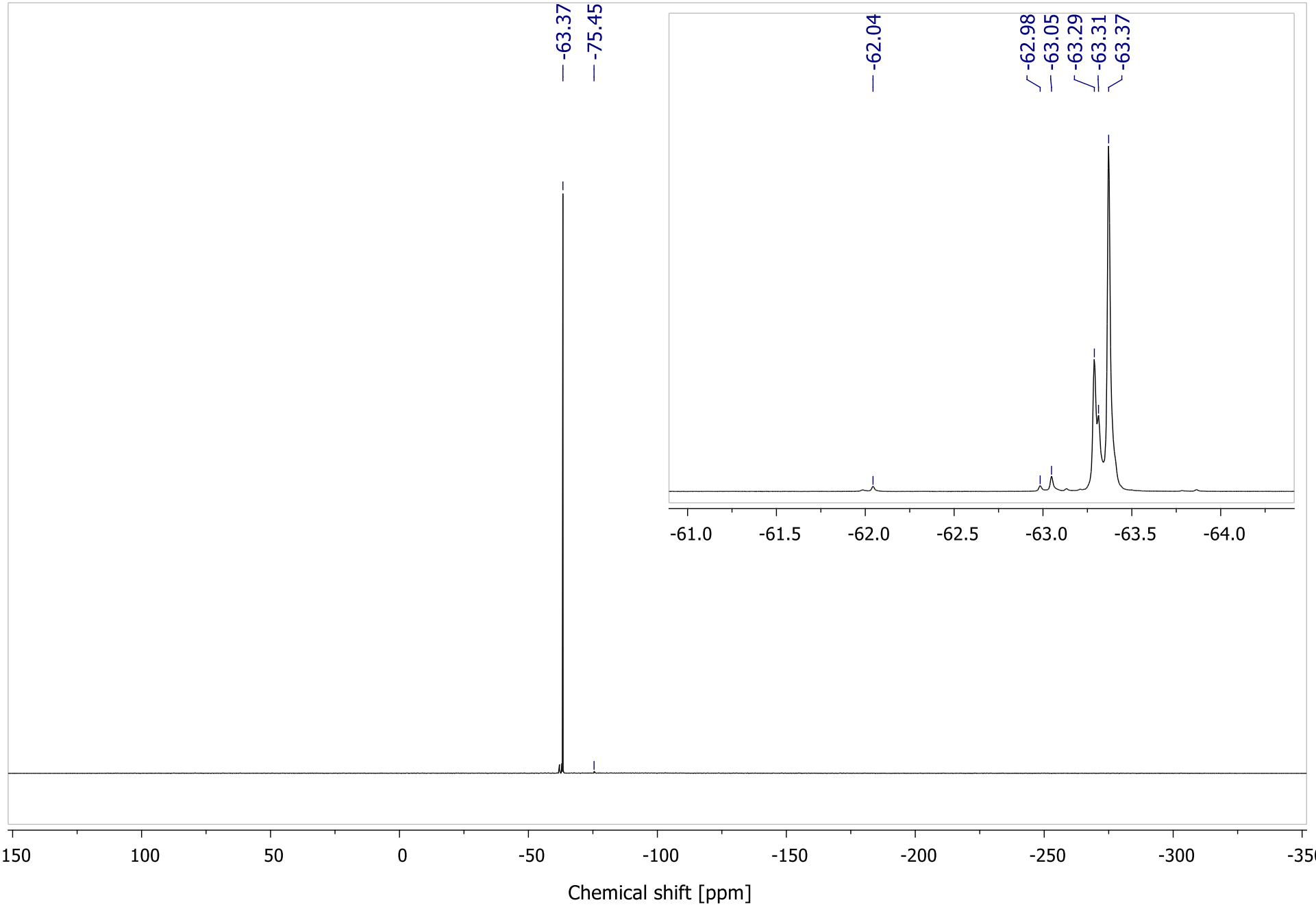

DKS57_077A_1050_5um #327-350 RT: 5.46-5.83 AV: 24 NL: 4.72E5 microAU
Relative Absorbance
wavelength (nm)
224.00
280.00
338.00


DKS57_077A_1050_5um #359-383 RT: 9.57-10.20 AV: 25 NL: 3.37E8
T: + c ESI Full ms [80.00-2000.00]
Relative Abundance
m/z
711.27
356.30
673.27
1421.31
808.66
1066.22
1383.21
1459.30
142.65
395.52
960.19
1776.96

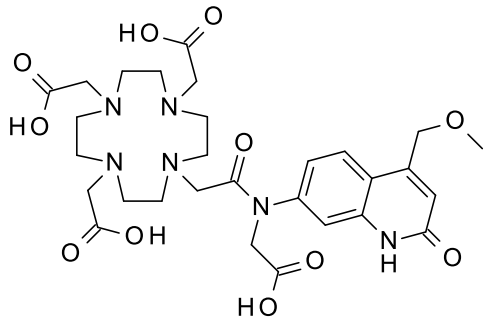

1.85 - 4.68
180.2
58.9
58.8
180.2
52.3 - 53.1
47.6 - 48.8
174.1
58.8
56.6
180.2
143.9
7.38
121.6
7.87
126.8
122.0
F
F
F
-63.4
138.5
114.2
6.94
120.8
139.3
162.6
114.9
7.51
51.4
174.6
N
H
O


7.88
7.86
7.51
7.51
7.49
7.39
7.37
6.96
6.94
4.79
4.79
4.30
3.78
3.12
2.81
2.20
0.92
1.98
0.92
26.00
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Chemical shift [ppm]

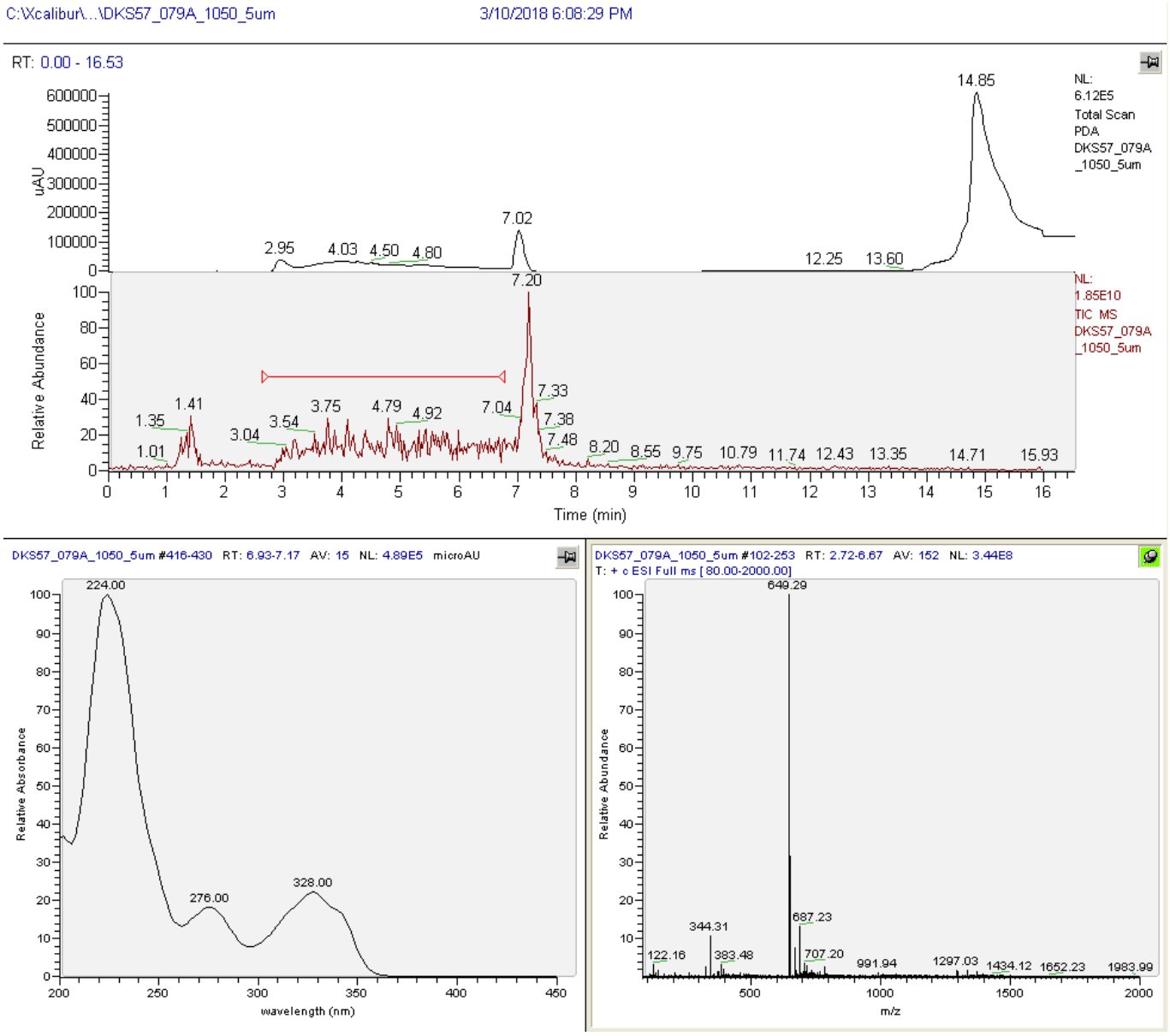

180.18
180.15
174.63
174.10
162.62
143.88
139.33
138.93
138.61
138.29
137.97
126.76
126.01
123.40
123.33
122.87
122.61
121.66
120.82
120.77
120.60
115.30
114.88
114.24
58.92
58.76
56.70
56.60
54.76
53.95
53.70
53.45
52.58
51.37
48.07
47.87
A (q)
138.45
B (q)
121.95
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical shift [ppm]


-63.37
-75.45
-62.04
-62.98
-63.05
-63.29
-63.31
-63.37
-61.0
-61.5
-62.0
-62.5
-63.0
-63.5
-64.0
150
100
50
0
-50
-100
-150
-200
-250
-300
Chemical shift [ppm]

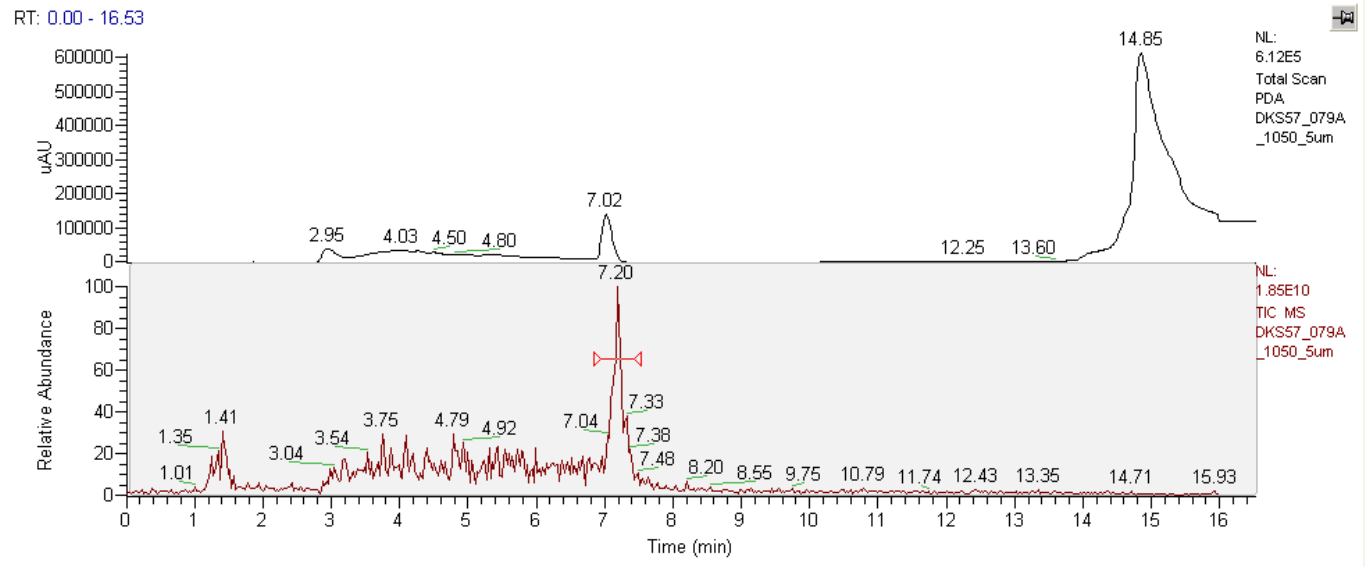
DKS57_079A

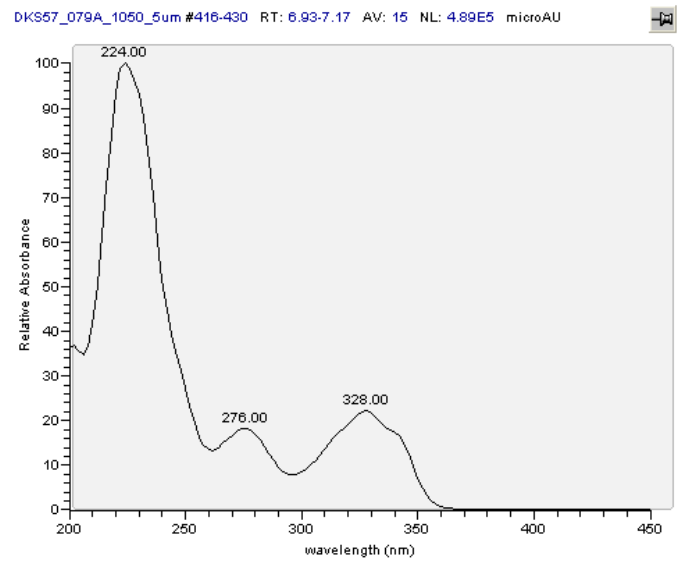


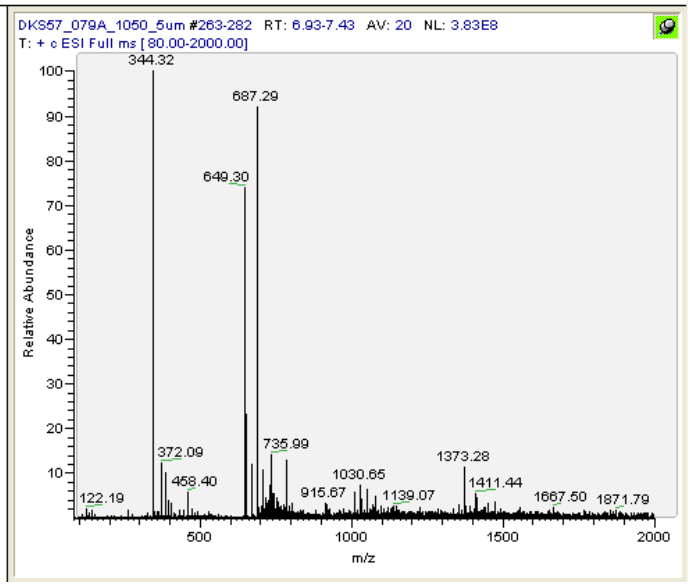
Formula Weight : 648.66(2)
Exact Mass : 648.27551
Formula : $C_{29}H_{40}N_6O_{11}$
Composition : C 53.70% H 6.22% N 12.96% O 27.13%

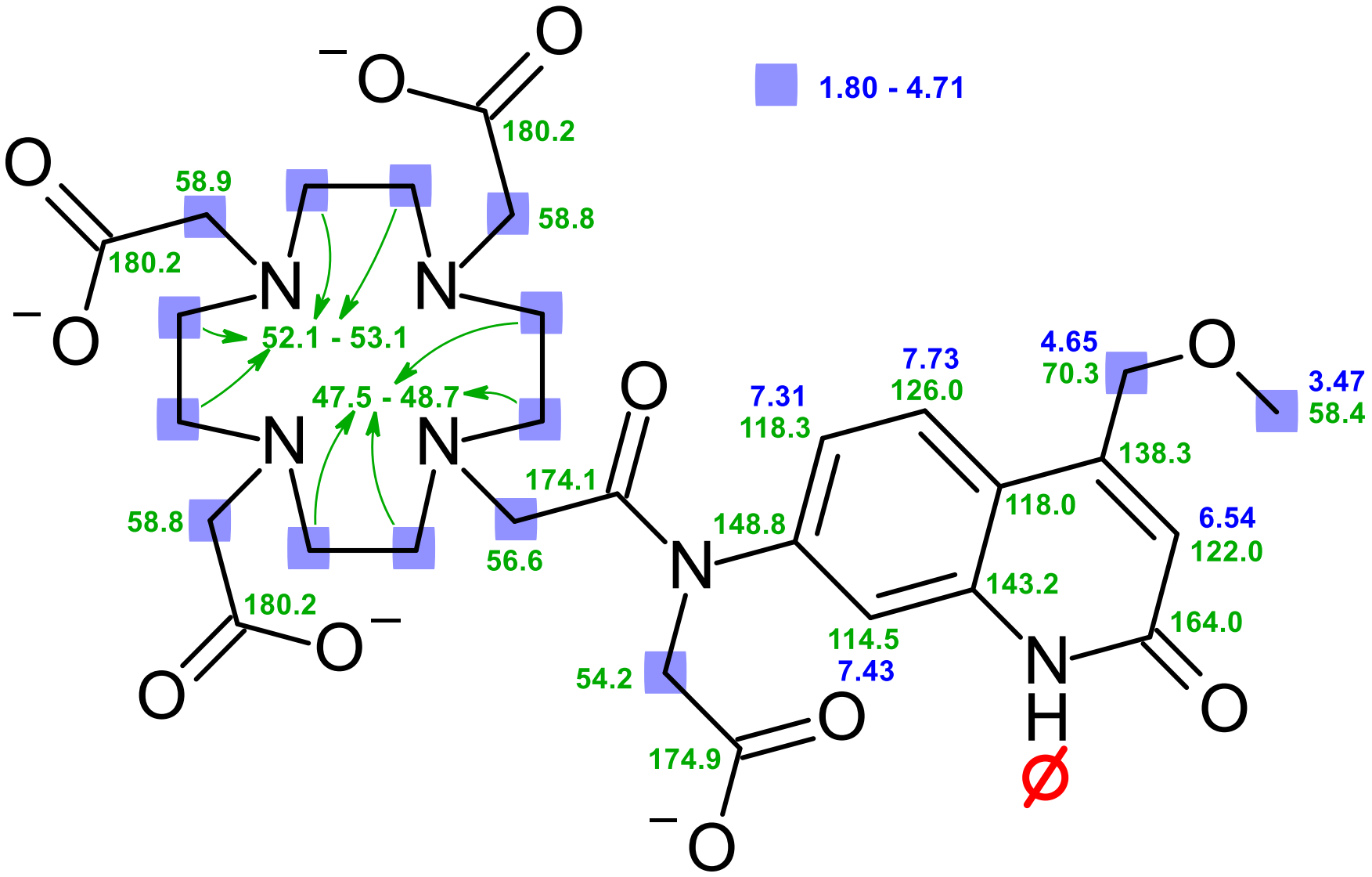


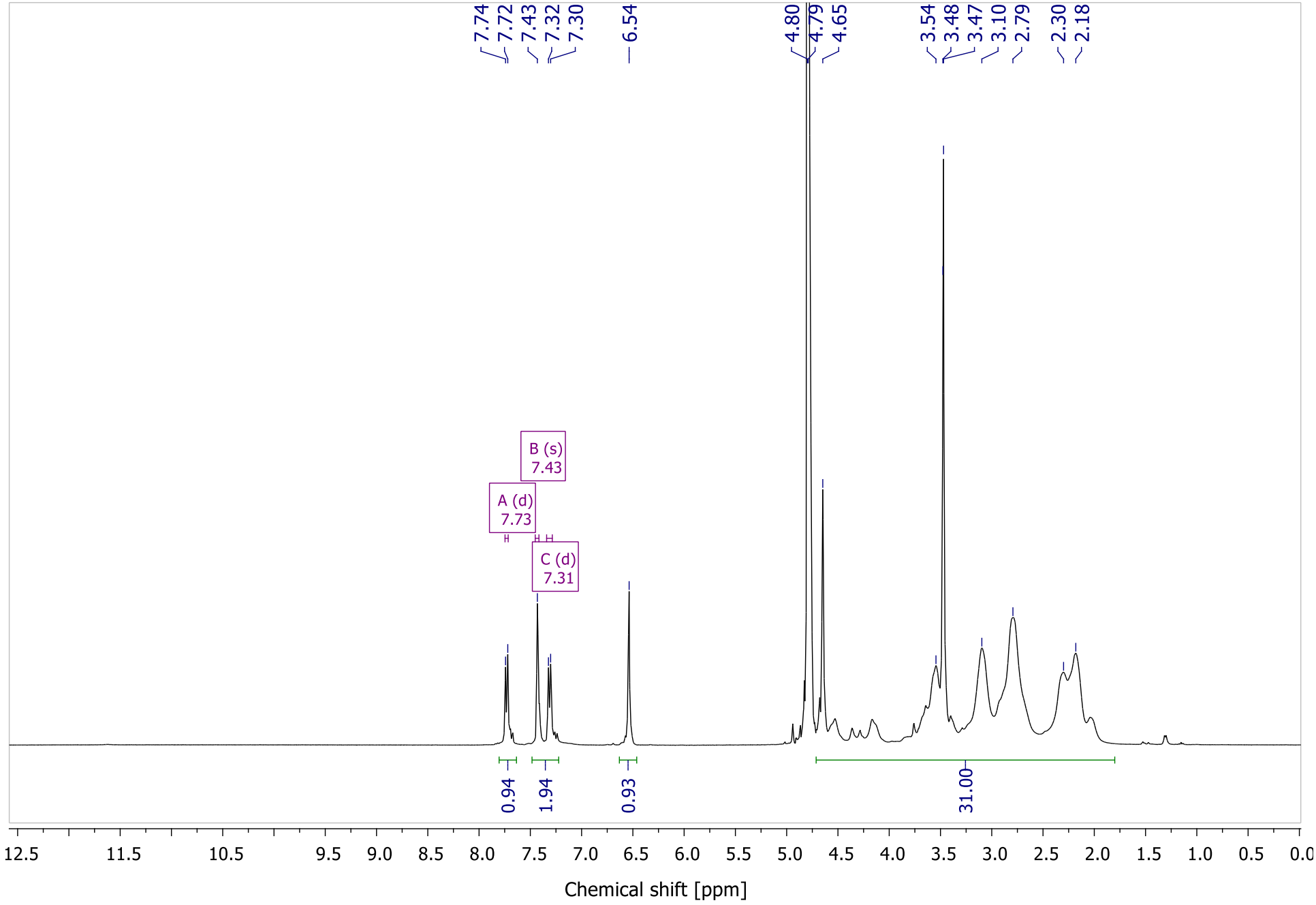
C:\Xcalibur\...\DKS57_079A_1050_5um 3/10/2018 6:08:29 PM

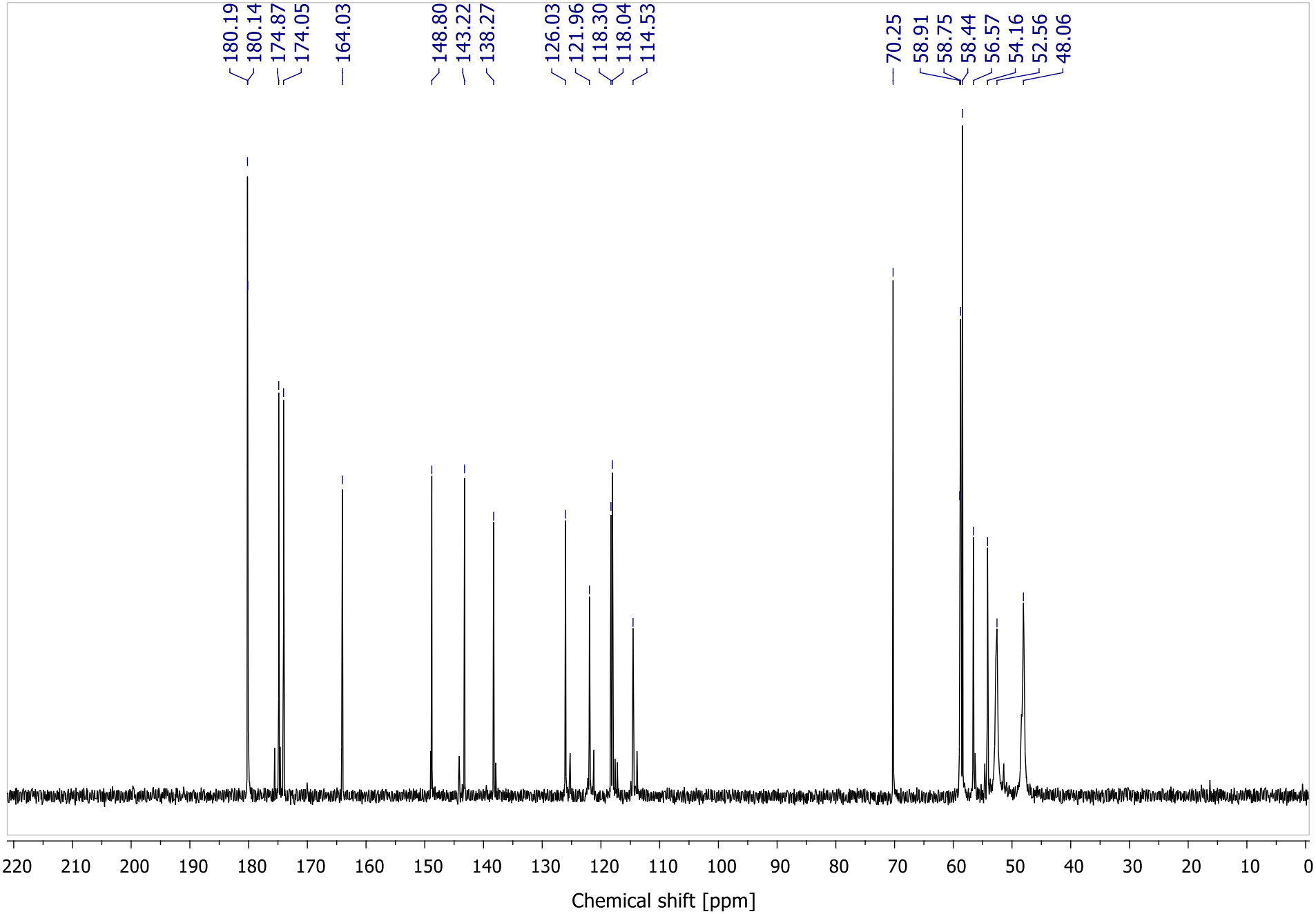




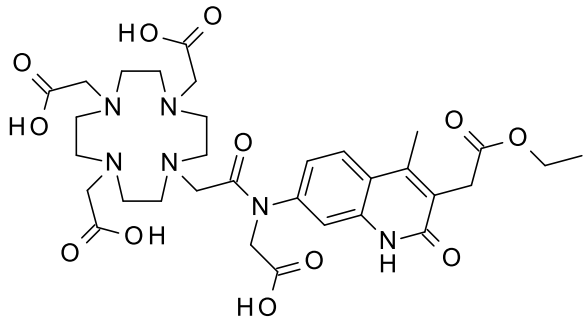



1.80 - 4.71
180.2
58.9
58.8
180.2
52.1 - 53.1
47.5 - 48.7
174.1
58.8
56.6
180.2
7.73
126.0
7.31
118.3
4.65
70.3
3.47
58.4
138.3
118.0
6.54
122.0
148.8
143.2
164.0
114.5
7.43
54.2
174.9
Ø

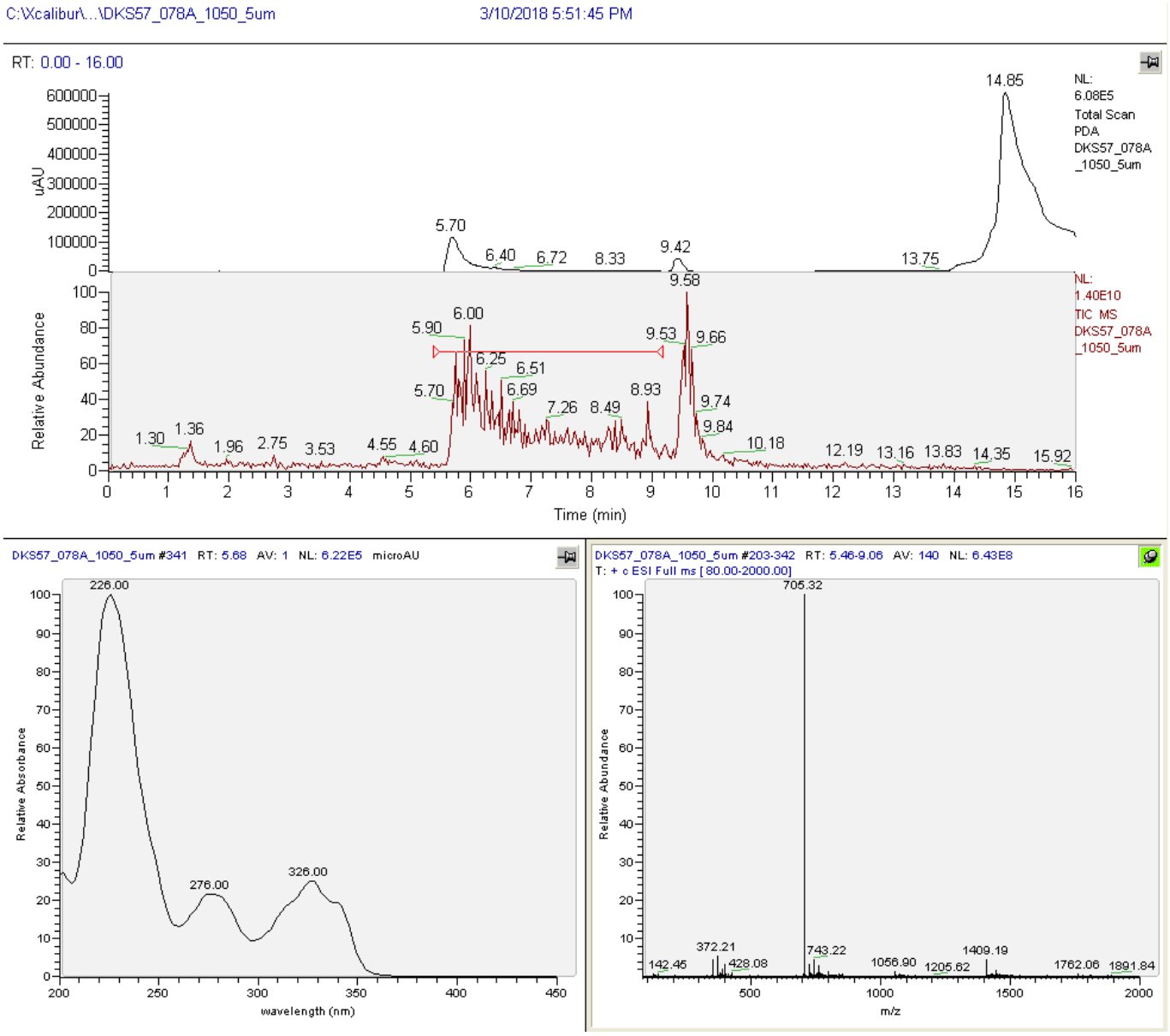

7.74
7.72
7.43
7.32
7.30
6.54
4.80
4.79
4.65
3.54
3.48
3.47
3.10
2.79
2.30
2.18
B (s)
7.43
A (d)
7.73
C (d)
7.31
0.94
1.94
0.93
31.00
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Chemical shift [ppm]

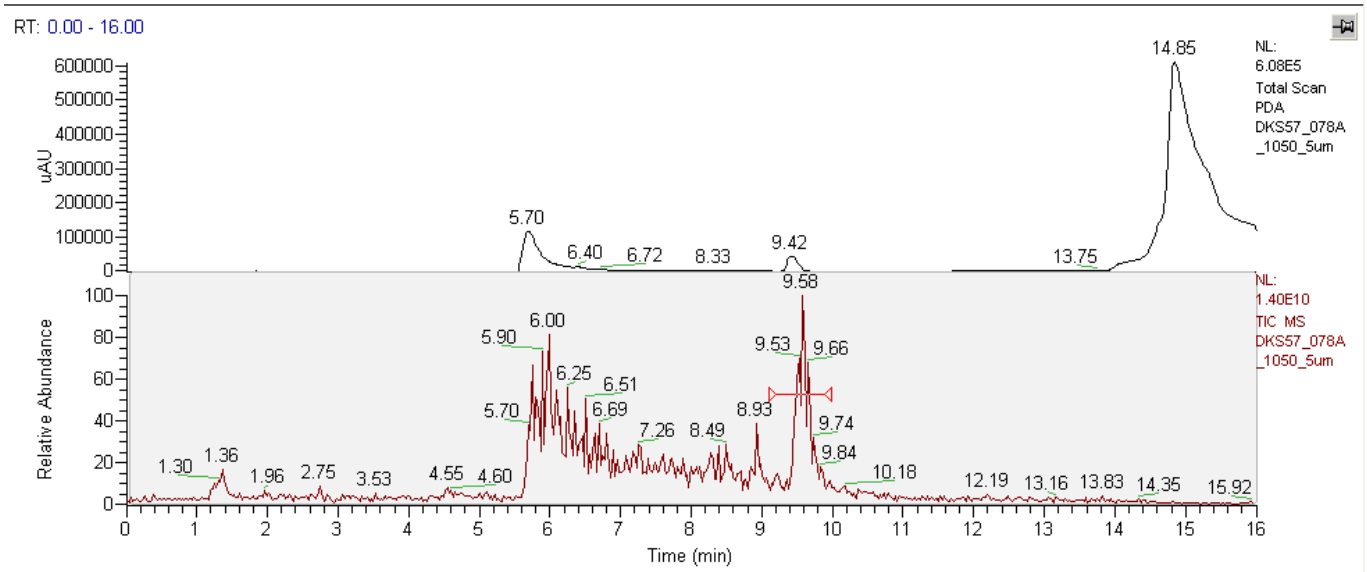

180.19
180.14
174.87
174.05
164.03
148.80
143.22
138.27
126.03
121.96
118.30
118.04
114.53
70.25
58.91
58.75
58.44
56.57
54.16
52.56
48.06
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical shift [ppm]

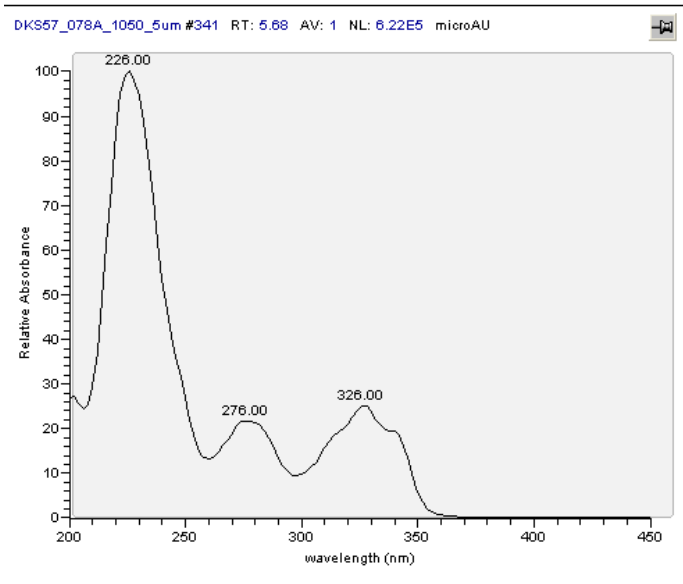
DKS57_078A

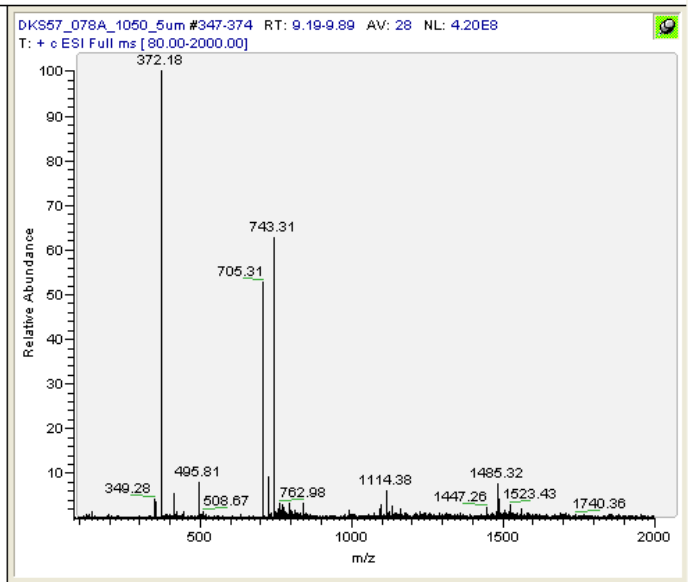


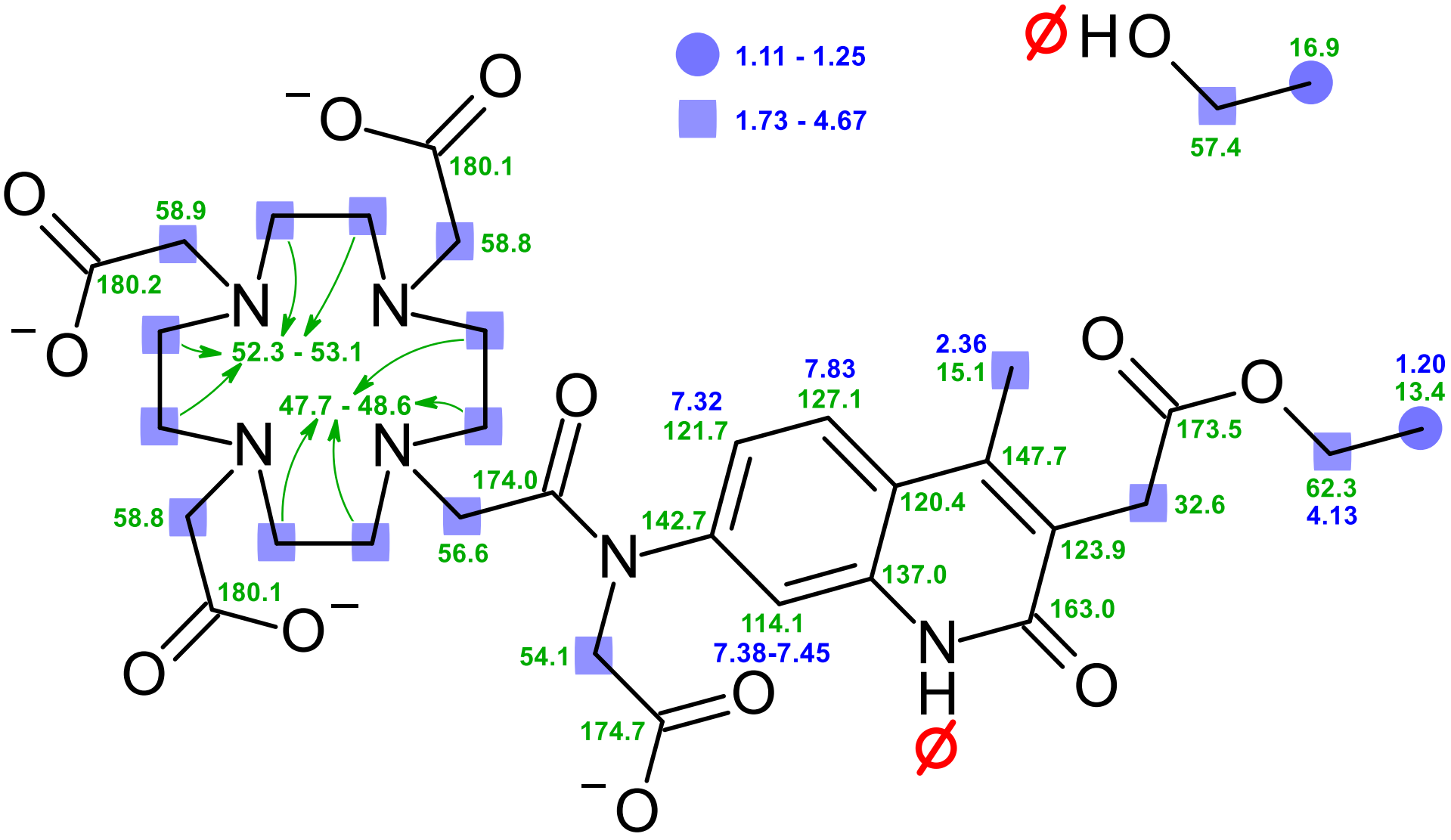
Formula Weight : 704.72(3)
Exact Mass : 704,30172
Formula : $C_{32}H_{44}N_6O_{12}$
Composition : C 54.54% H 6.29%
N 11.93% O 27.24%

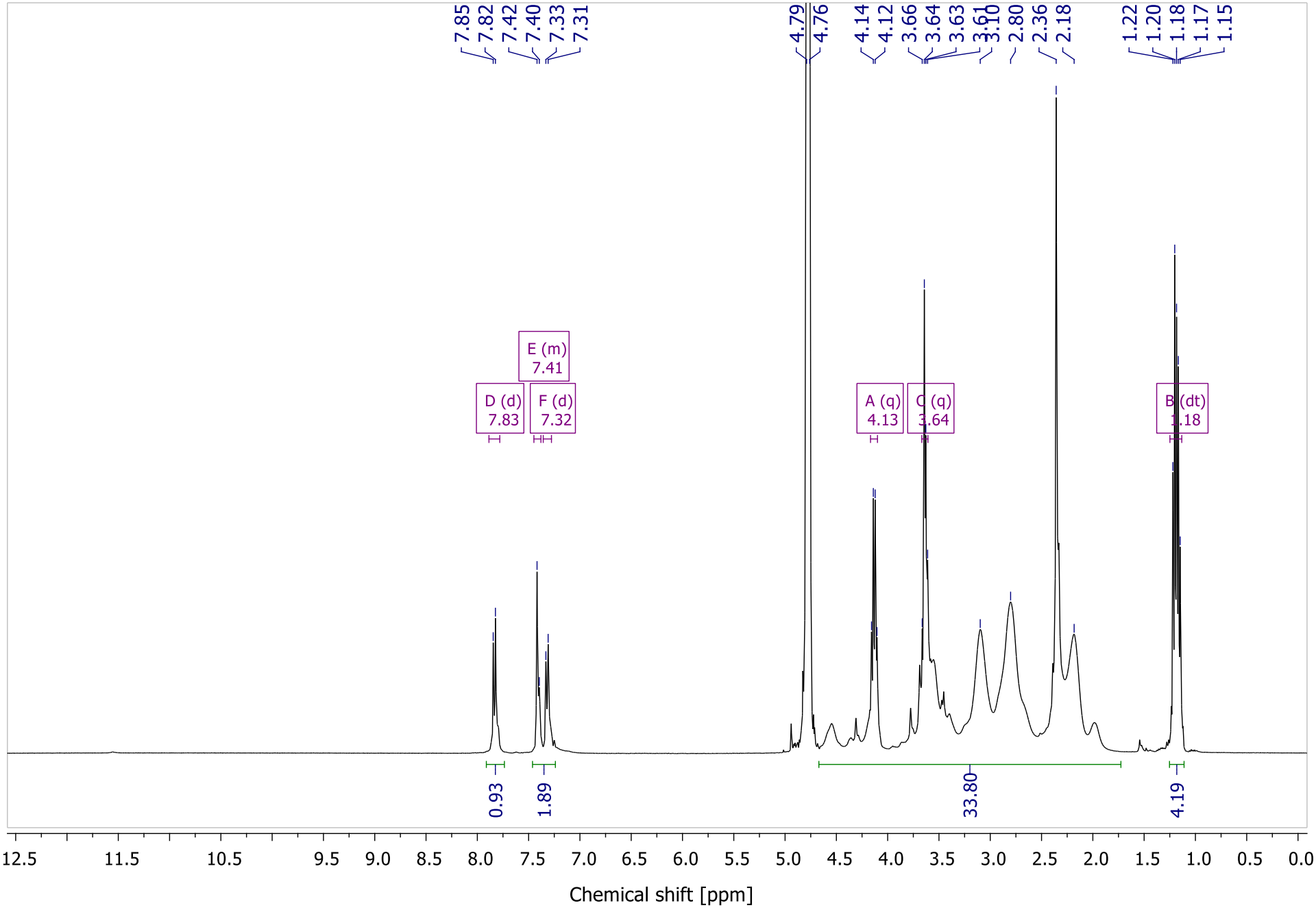


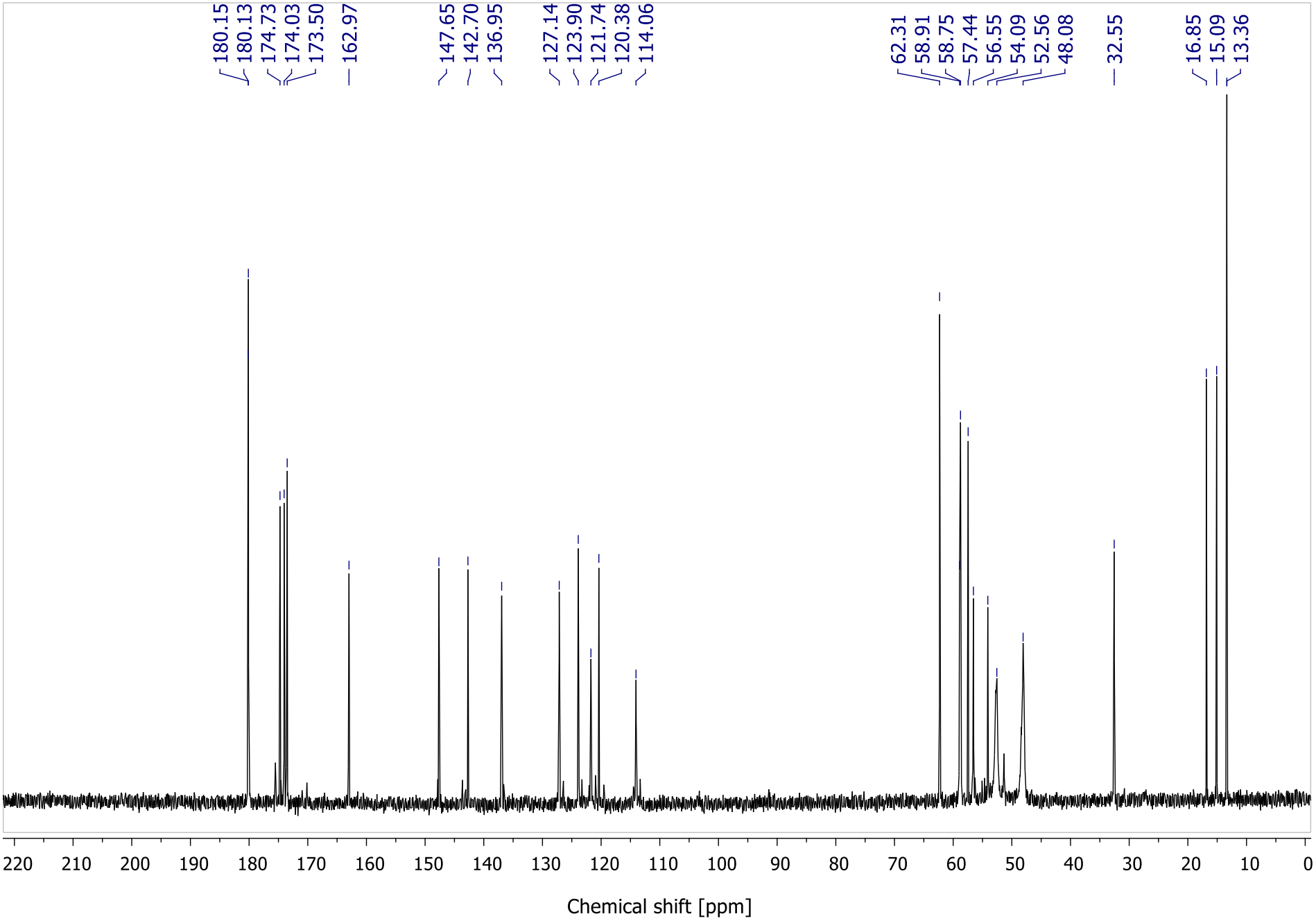

RT: 0.00 - 16.00
uAU
Relative Abundance
Time (min)
NL: 6.08E5 Total Scan PDA DKS57_078A_1050_5um
NL: 1.40E10 TIC MS DKS57_078A_1050_5um
14.85
5.70
6.40
6.72
8.33
9.42
13.75
9.58
6.00
5.90
9.53
9.66
6.25
6.51
5.70
6.69
8.93
9.74
7.26
8.49
9.84
1.30
1.36
1.96
2.75
3.53
4.55
4.60
10.18
12.19
13.16
13.83
14.35
15.92


DKS57_078A_1050_5um #341 RT: 5.68 AV: 1 NL: 6.22E5 microAU
Relative Absorbance
wavelength (nm)
226.00
276.00
326.00

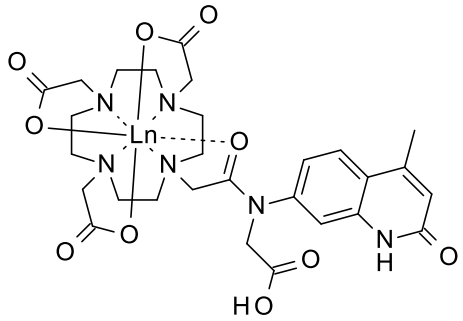

DKS57_078A_1050_5um #347-374 RT: 9.19-9.89 AV: 28 NL: 4.20E8
T: + c ESI Full ms [80.00-2000.00]
Relative Abundance
m/z
372.18
743.31
705.31
349.28
495.81
508.67
762.98
1114.38
1447.26
1485.32
1523.43
1740.36


1.11 - 1.25
1.73 - 4.67
HO
16.9
57.4
180.1
58.9
58.8
180.2
52.3 - 53.1
47.7 - 48.6
174.0
58.8
56.6
180.1
142.7
7.32
121.7
7.83
127.1
2.36
15.1
147.7
120.4
173.5
32.6
62.3
4.13
1.20
13.4
123.9
137.0
163.0
114.1
7.38-7.45
54.1
174.7


7.85
7.82
7.42
7.40
7.33
7.31
4.79
4.76
4.14
4.12
3.66
3.64
3.63
3.61
3.10
2.80
2.36
2.18
1.22
1.20
1.18
1.17
1.15
E (m)
7.41
D (d)
7.83
F (d)
7.32
A (q)
4.13
C (q)
3.64
B (dt)
1.18
0.93
1.89
33.80
4.19
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Chemical shift [ppm]


180.15
180.13
174.73
174.03
173.50
162.97
147.65
142.70
136.95
127.14
123.90
121.74
120.38
114.06
62.31
58.91
58.75
57.44
56.55
54.09
52.56
48.08
32.55
16.85
15.09
13.36
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical shift [ppm]

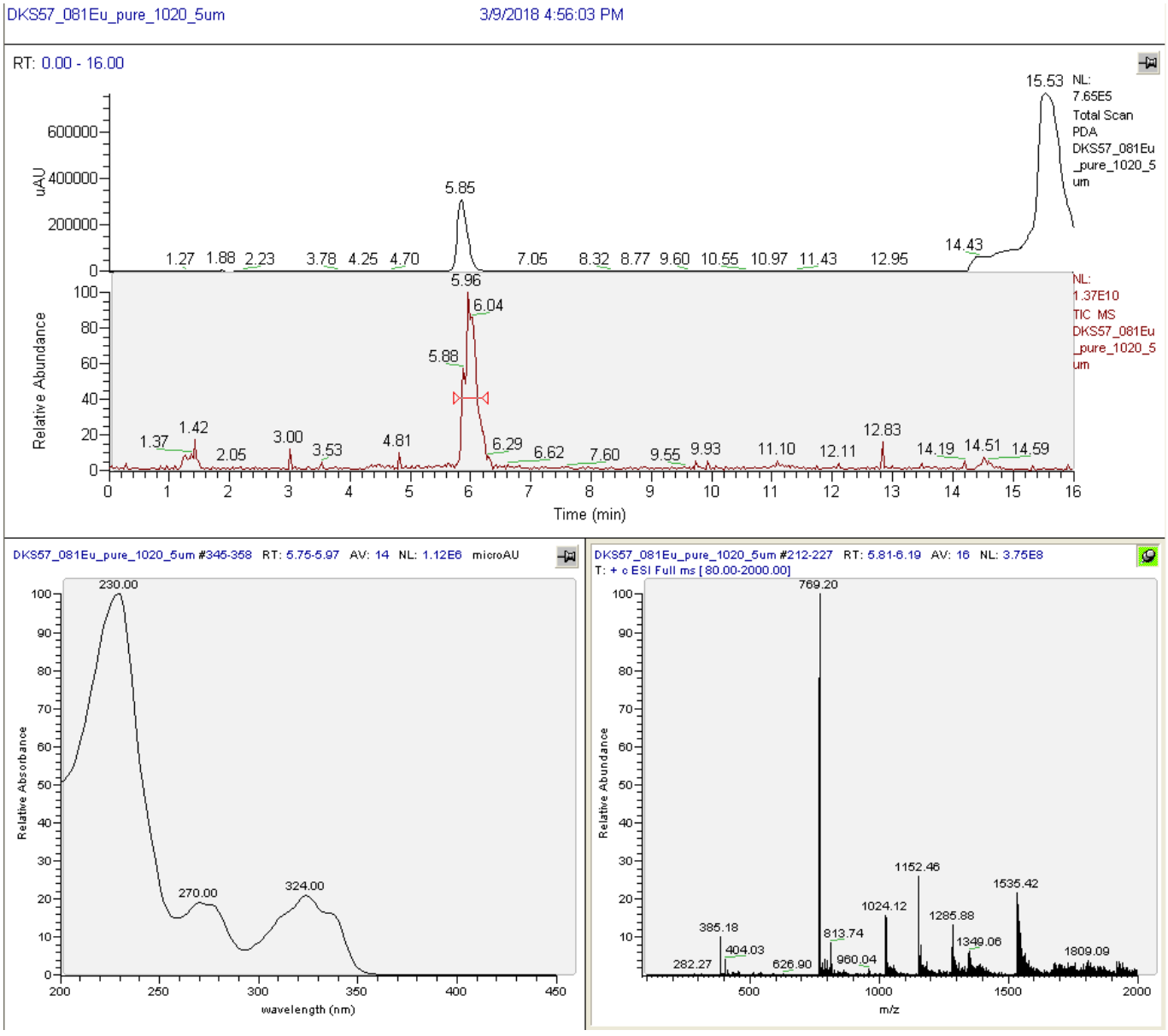
DKS57_081Ln (Eu, Tb, Gd)

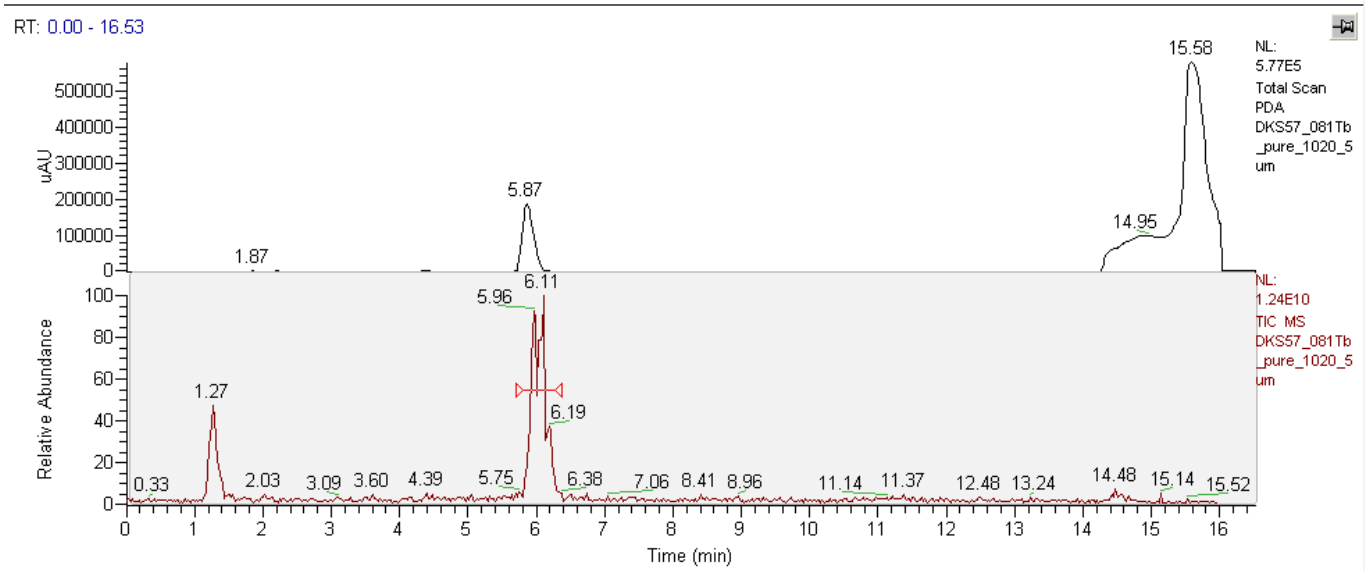


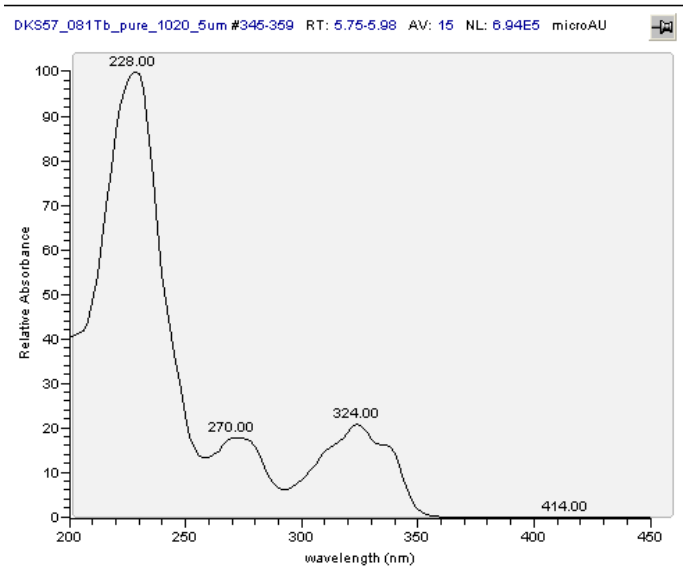
Formula Weight : 767.584
Exact Mass : 768.16269
Formula : $C_{28}H_{35}N_6O_{10}Eu$
Composition : C 43.81% H 4.60%
N 10.95% O 20.84% Eu 19.80%

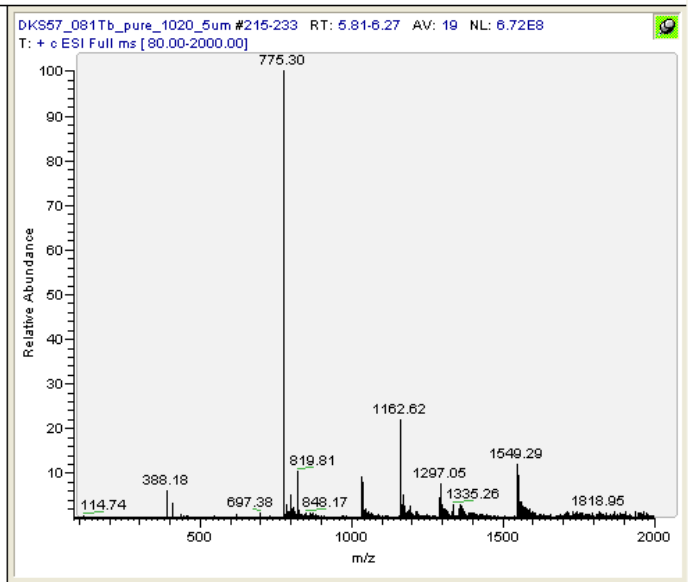
Formula Weight : 774.545
Exact Mass : 774.16681
Formula : $C_{28}H_{35}N_6O_{10}Tb$
Composition : C 43.42% H 4.55%
N 10.85% O 20.66% Tb 20.52%

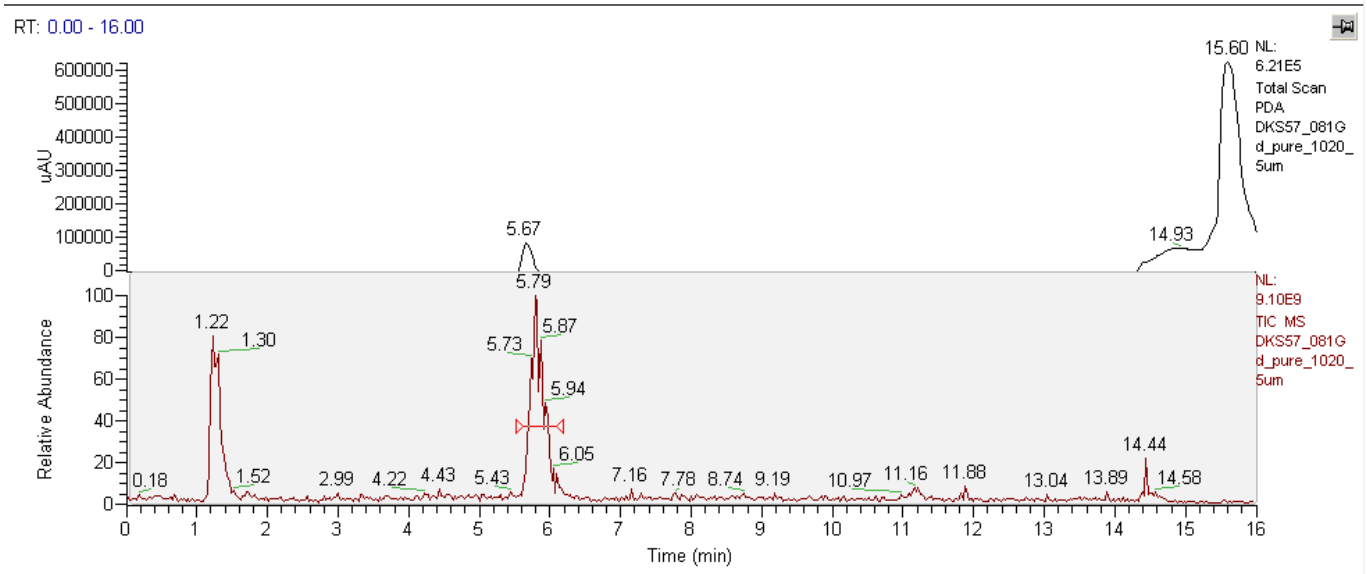
Formula Weight : 772.870
Exact Mass : 773.16557
Formula : $C_{28}H_{35}N_6O_{10}Gd$
Composition : C 43.51% H 4.56%
N 10.87% O 20.70% Gd 20.35%

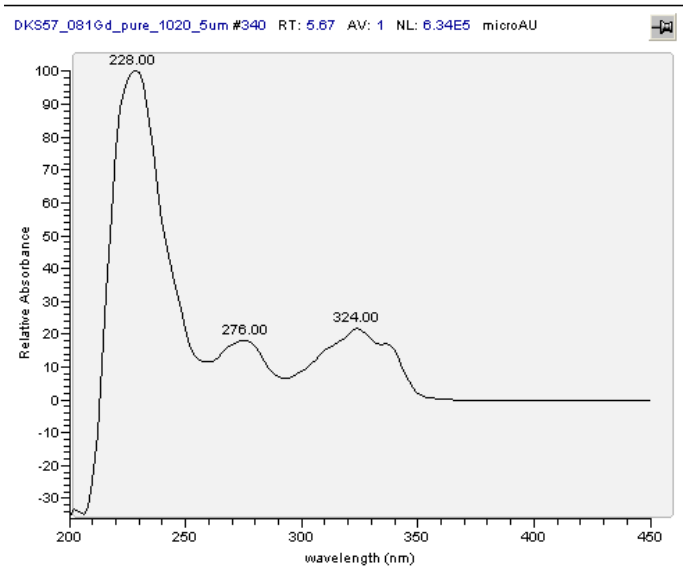


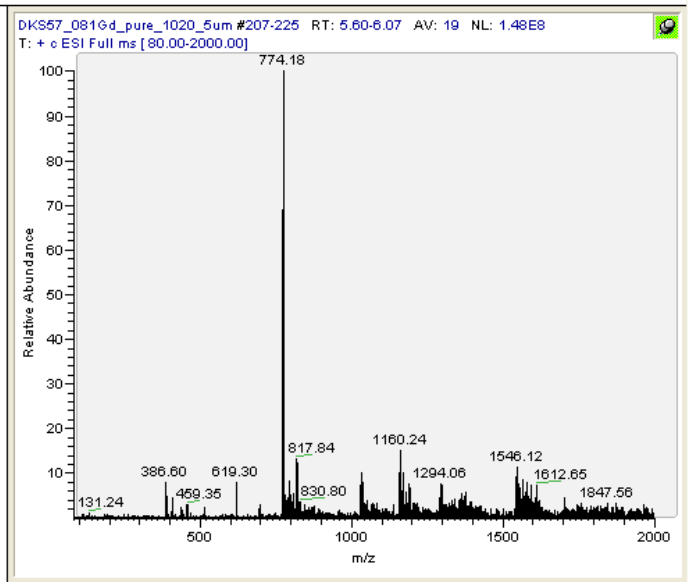

RT: 0.00 - 16.53
uAU
Relative Abundance
Time (min)
NL: 5.77E5 Total Scan PDA DKS57_081Tb _pure_1020_5 um
NL: 1.24E10 TIC MS DKS57_081Tb _pure_1020_5 um
15.58
14.95
5.87
1.87
6.11
5.96
1.27
6.19
0.33
2.03
3.09
3.60
4.39
5.75
6.38
7.06
8.41
8.96
11.14
11.37
12.48
13.24
14.48
15.14
15.52


DKS57_081Tb_pure_1020_5um #345-359 RT: 5.75-5.98 AV: 15 NL: 6.94E5 microAU
Relative Absorbance
wavelength (nm)
228.00
270.00
324.00
414.00

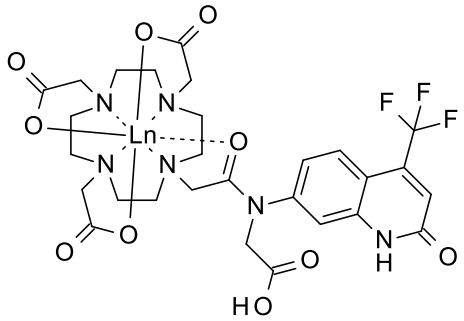

DKS57_081Tb_pure_1020_5um #215-233 RT: 5.81-6.27 AV: 19 NL: 6.72E8
T: + c ESI Full ms [80.00-2000.00]
Relative Abundance
m/z
775.30
1162.62
819.81
1549.29
388.18
1297.05
1335.26
1818.95
114.74
697.38
848.17


RT: 0.00 - 16.00
uAU
Relative Abundance
Time (min)
NL: 6.21E5 Total Scan PDA DKS57_081Gd_pure_1020_5um
NL: 9.10E9 TIC MS DKS57_081Gd_pure_1020_5um
15.60
14.93
5.67
5.79
5.87
5.73
5.94
6.05
1.22
1.30
1.52
0.18
2.99
4.22
4.43
5.43
7.16
7.78
8.74
9.19
10.97
11.16
11.88
13.04
13.89
14.44
14.58


DKS57_081Gd_pure_1020_5um #340 RT: 5.67 AV: 1 NL: 6.34E5 microAU
Relative Absorbance
wavelength (nm)
228.00
276.00
324.00


DKS57_081Gd_pure_1020_5um #207-225 RT: 5.60-6.07 AV: 19 NL: 1.48E8
T: + c ESI Full ms [80.00-2000.00]
Relative Abundance
m/z
774.18
817.84
1160.24
1546.12
1294.06
1612.65
1847.56
386.60
619.30
459.35
830.80
131.24

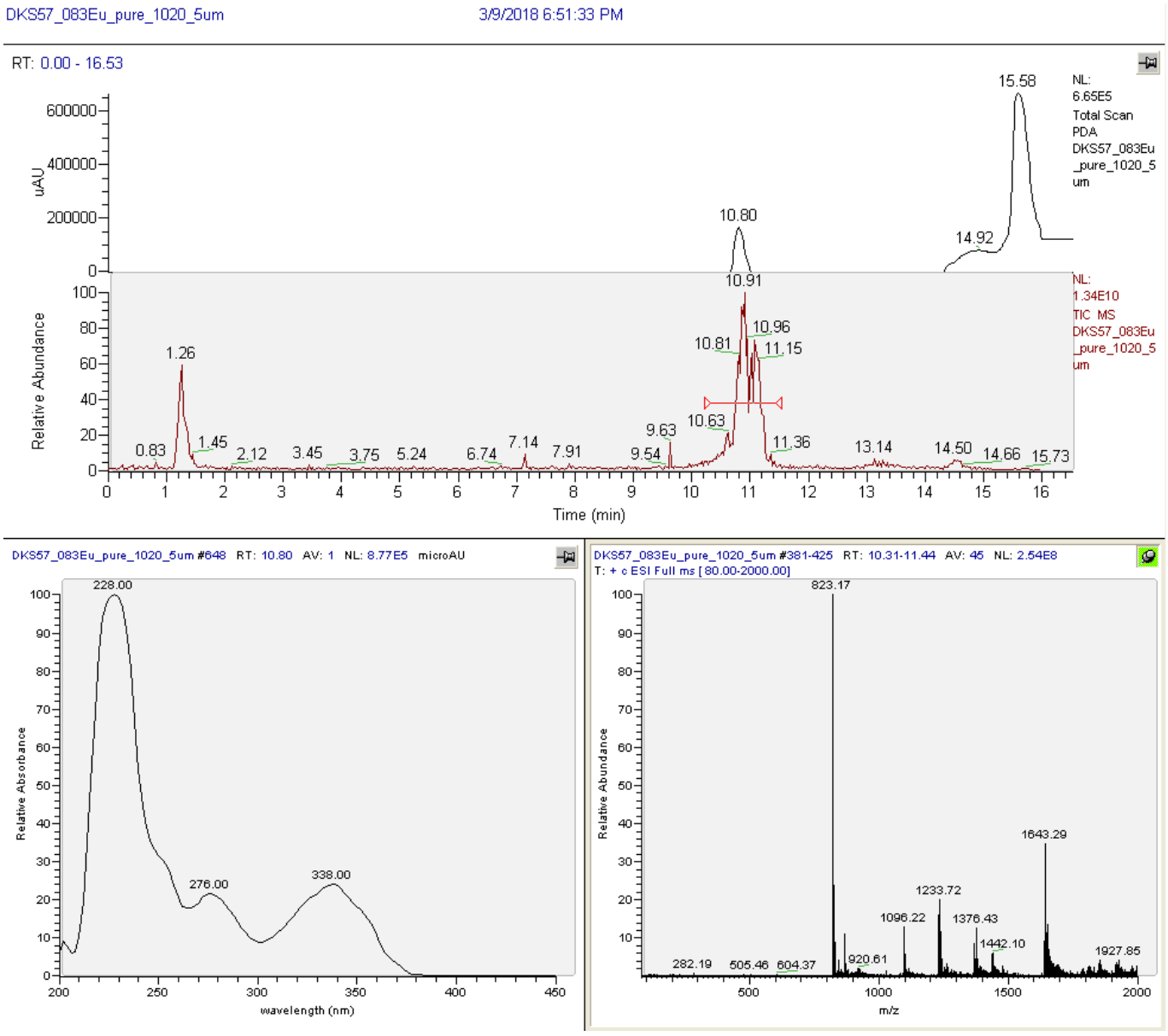
DKS57_083Ln (Eu, Tb, Gd)

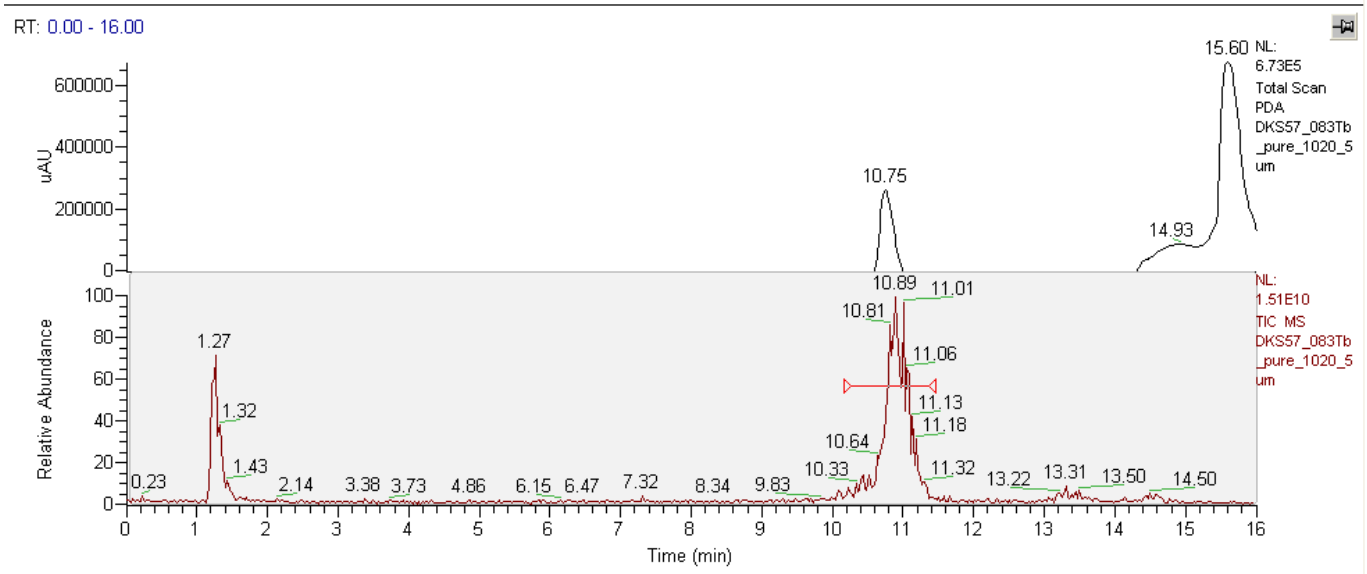


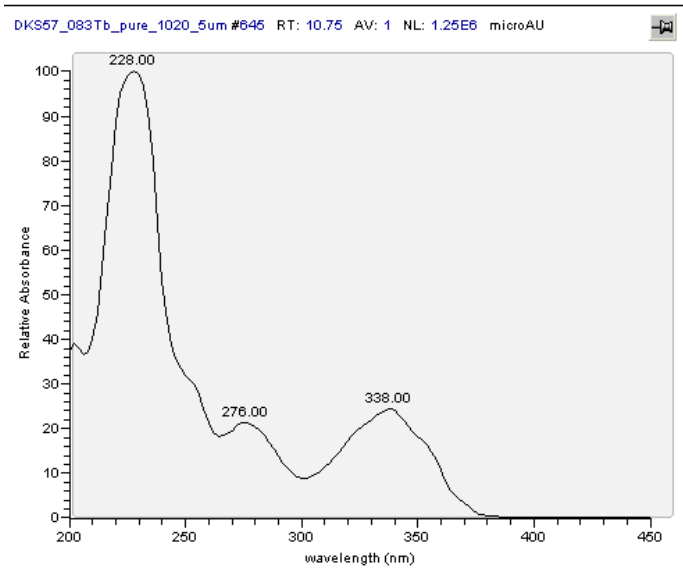
Formula Weight : 821.555
Exact Mass : 822.13443
Formula : $C_{28}H_{32}F_3N_6O_{10}Eu$
Composition : C 40.94% H 3.93% F 6.94%
N 10.23% O 19.47% Eu 18.50%

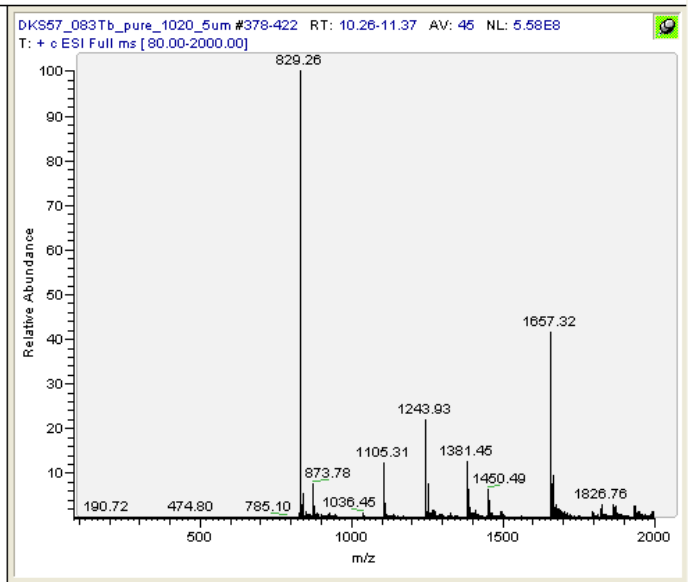
Formula Weight : 828.517
Exact Mass : 828.13854
Formula : $C_{28}H_{32}F_3N_6O_{10}Tb$
Composition : C 40.59% H 3.89% F 6.88%
N 10.14% O 19.31% Tb 19.18%

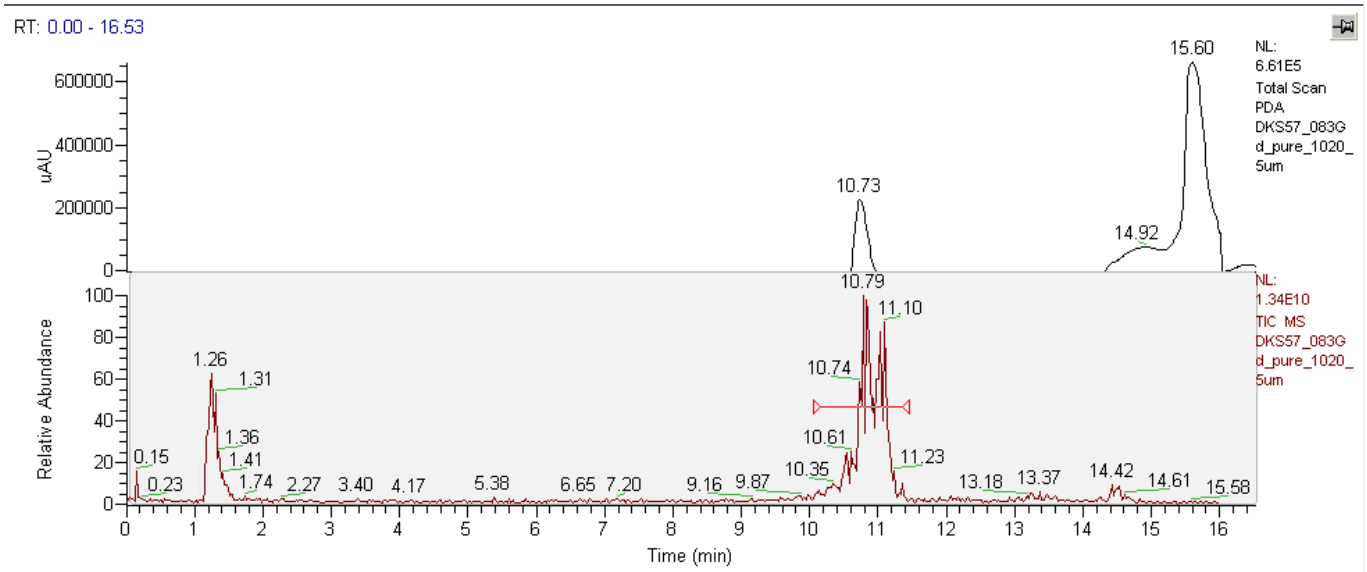
Formula Weight : 826.841
Exact Mass : 827.13730
Formula : $C_{28}H_{32}F_3N_6O_{10}Gd$
Composition : C 40.67% H 3.90% F 6.89%
N 10.16% O 19.35% Gd 19.35%

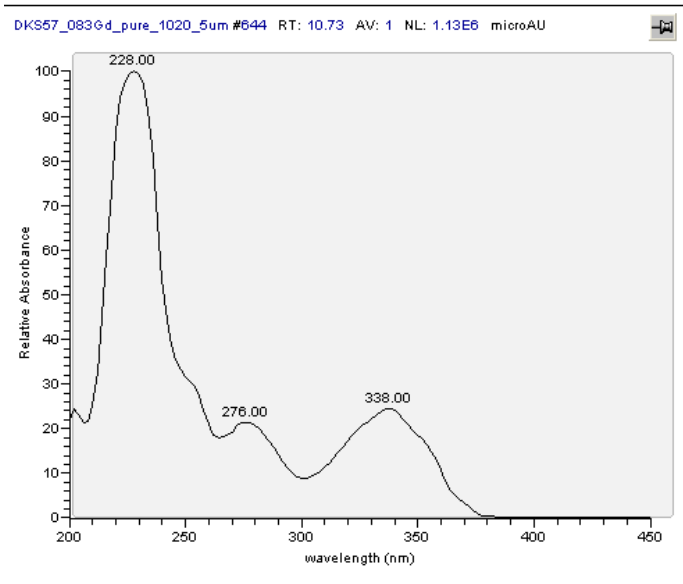


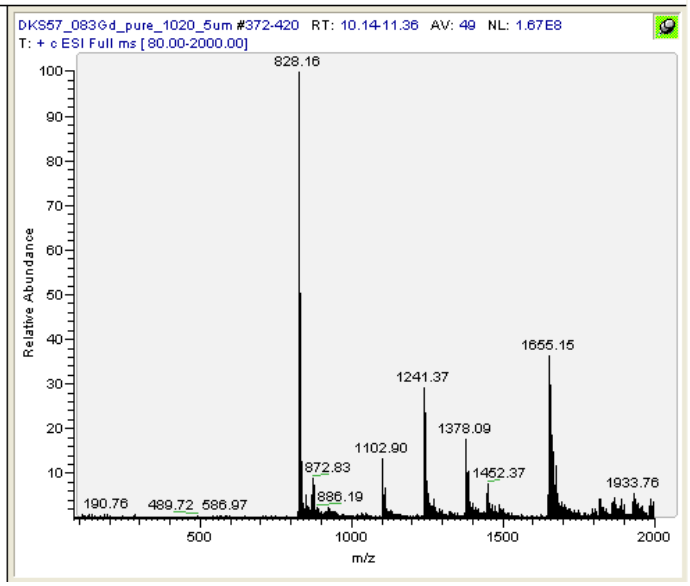

RT: 0.00 - 16.00
uAU
Relative Abundance
Time (min)
15.60
10.75
14.93
10.89
11.01
10.81
11.06
11.13
11.18
10.64
10.33
11.32
1.27
1.32
1.43
0.23
2.14
3.38
3.73
4.86
6.15
6.47
7.32
8.34
9.83
13.22
13.31
13.50
14.50
NL: 6.73E5 Total Scan PDA DKS57_083Tb _pure_1020_5 um
NL: 1.51E10 TIC MS DKS57_083Tb _pure_1020_5 um


DKS57_083Tb_pure_1020_5um #645 RT: 10.75 AV: 1 NL: 1.25E6 microAU
Relative Absorbance
wavelength (nm)
228.00
276.00
338.00

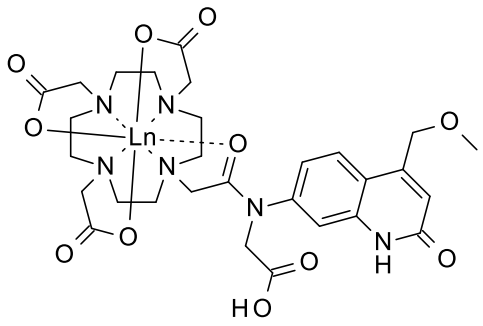

DKS57_083Tb_pure_1020_5um #378-422 RT: 10.26-11.37 AV: 45 NL: 5.58E8
T: + c ESI Full ms [80.00-2000.00]
Relative Abundance
m/z
829.26
1657.32
1243.93
1105.31
1381.45
873.78
1450.49
1826.76
1036.45
190.72
474.80
785.10


RT: 0.00 - 16.53
uAU
Relative Abundance
Time (min)
NL: 6.61E5 Total Scan PDA DKS57_083Gd_pure_1020_5um
NL: 1.34E10 TIC MS DKS57_083Gd_pure_1020_5um
15.60
14.92
10.73
10.79
11.10
10.74
10.61
10.35
11.23
1.26
1.31
1.36
1.41
1.74
0.15
0.23
2.27
3.40
4.17
5.38
6.65
7.20
9.16
9.87
13.18
13.37
14.42
14.61
15.58


DKS57_083Gd_pure_1020_5um #644 RT: 10.73 AV: 1 NL: 1.13E6 microAU
Relative Absorbance
wavelength (nm)
228.00
276.00
338.00


DKS57_083Gd_pure_1020_5um #372-420 RT: 10.14-11.36 AV: 49 NL: 1.67E8
T: + c ESI Full ms [80.00-2000.00]
Relative Abundance
m/z
828.16
1655.15
1241.37
1378.09
1102.90
872.83
1452.37
886.19
1933.76
190.76
489.72
586.97

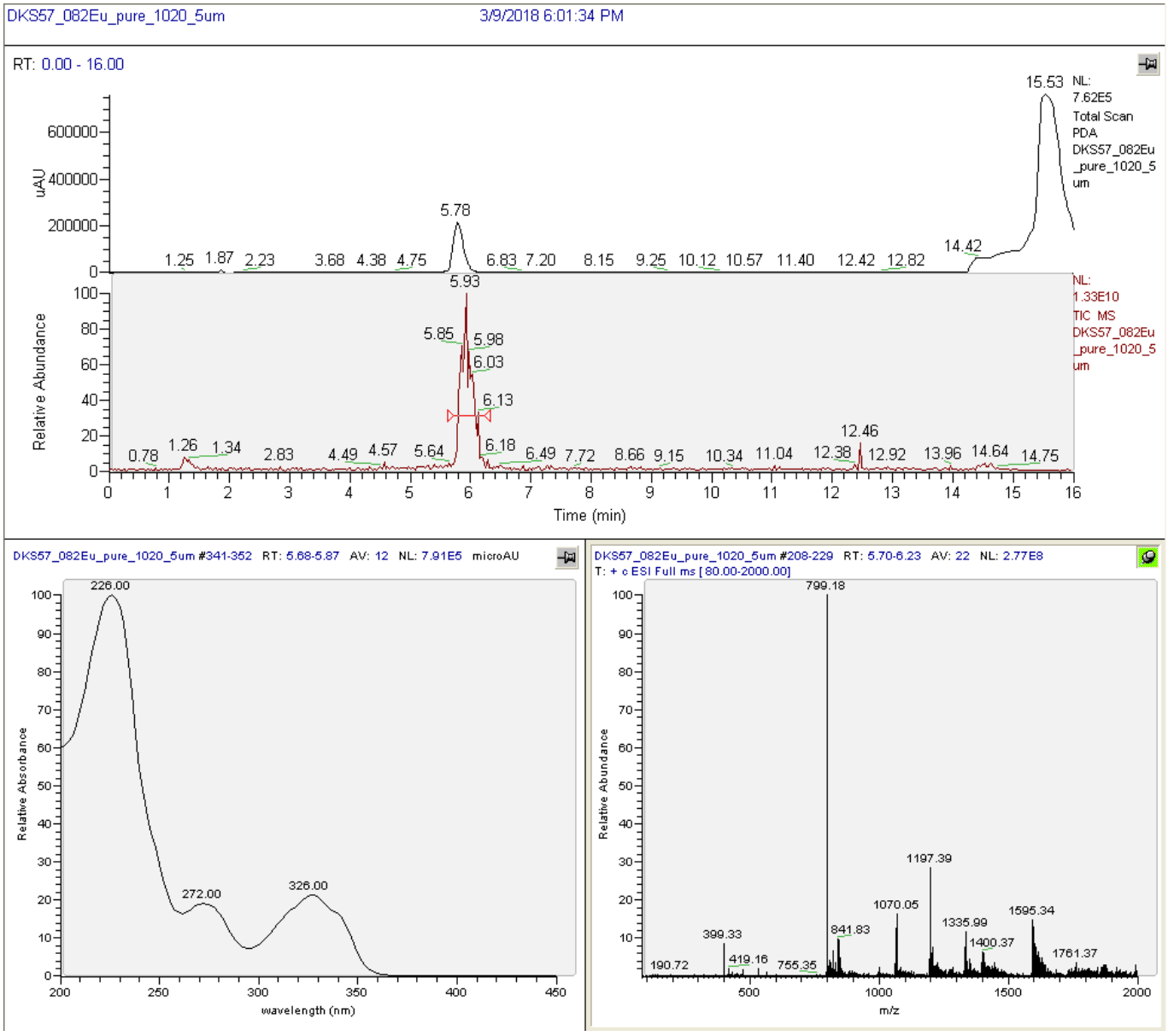
DKS57_082Ln (Eu, Tb, Gd)

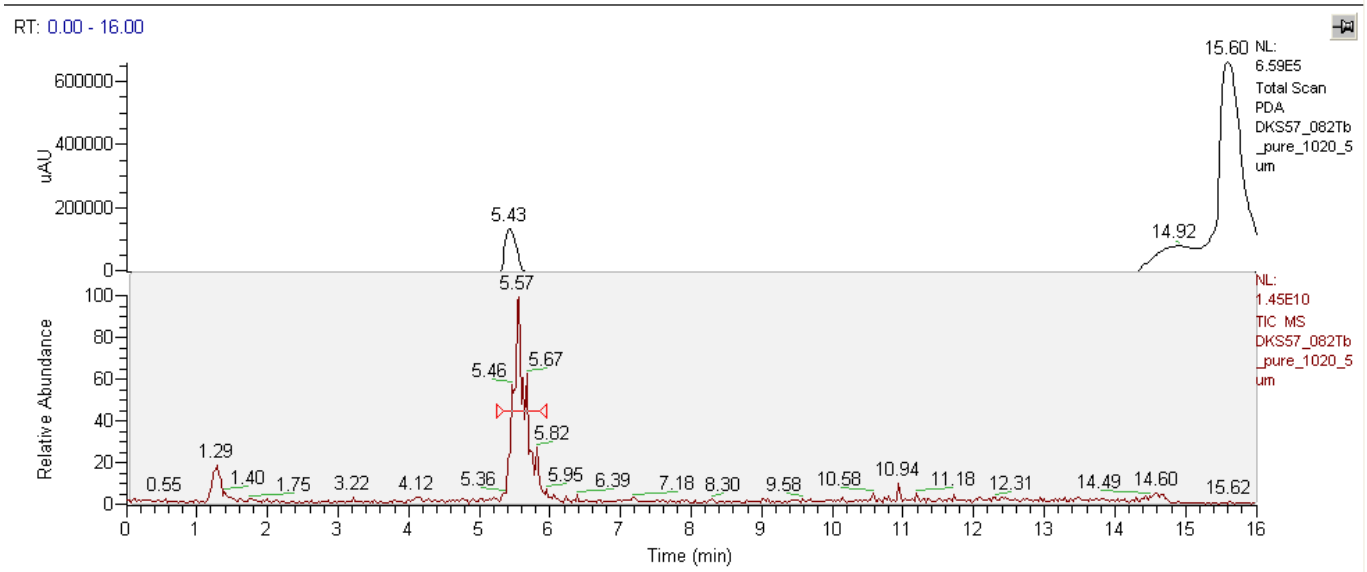


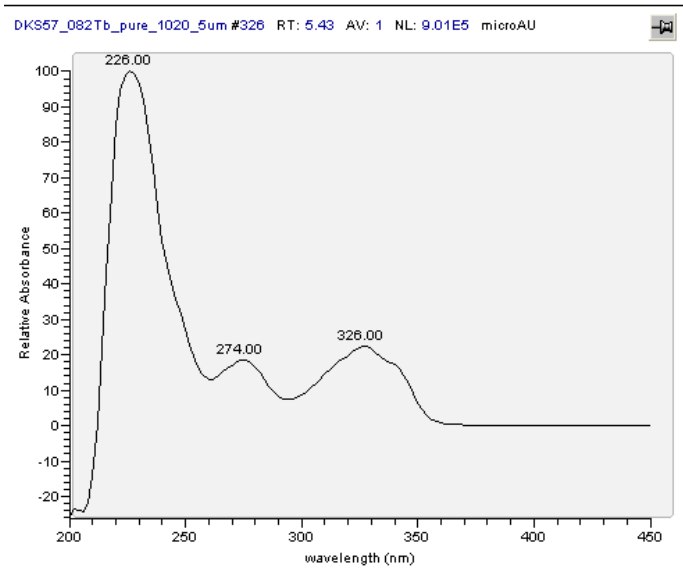
Formula Weight : 797.610
Exact Mass : 798.17326
Formula : $C_{29}H_{37}N_6O_{11}Eu$
Composition : C 43.67% H 4.68%
N 10.54% O 22.06% Eu 19.05%

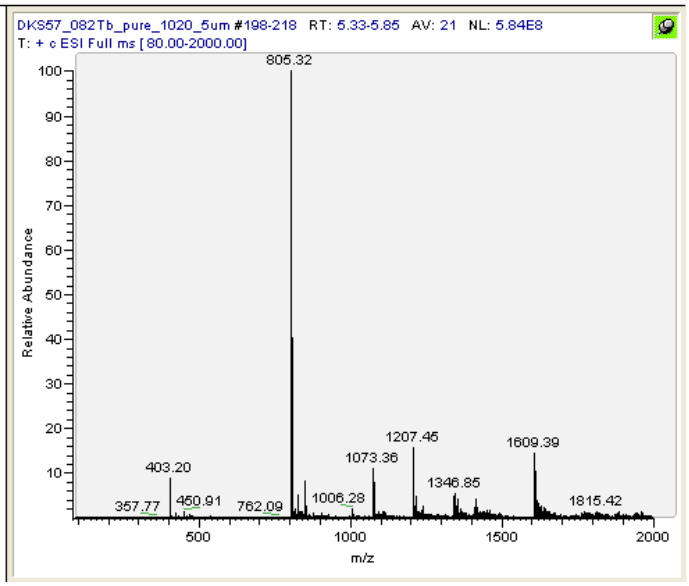
Formula Weight : 804.571
Exact Mass : 804.17737
Formula : $C_{29}H_{37}N_6O_{11}Tb$
Composition : C 43.29% H 4.64%
N 10.45% O 21.87% Tb 19.75%

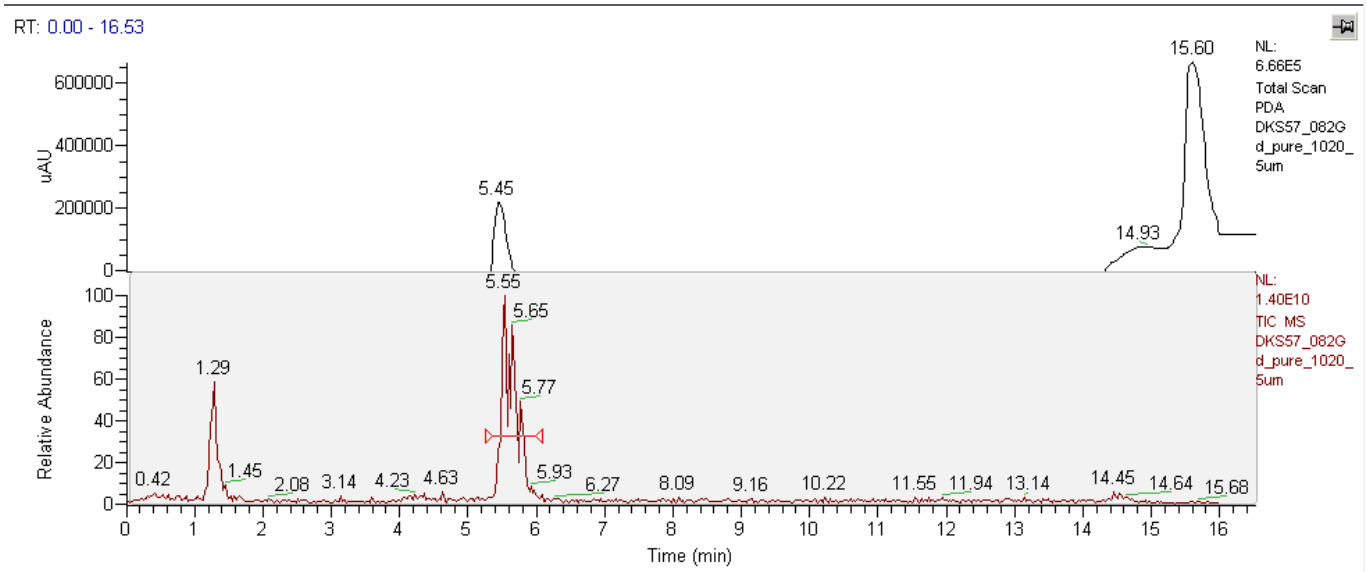
Formula Weight : 802.896
Exact Mass : 803.17613
Formula : $C_{29}H_{37}N_6O_{11}Gd$
Composition : C 43.38% H 4.65%
N 10.47% O 21.92% Gd 19.59%

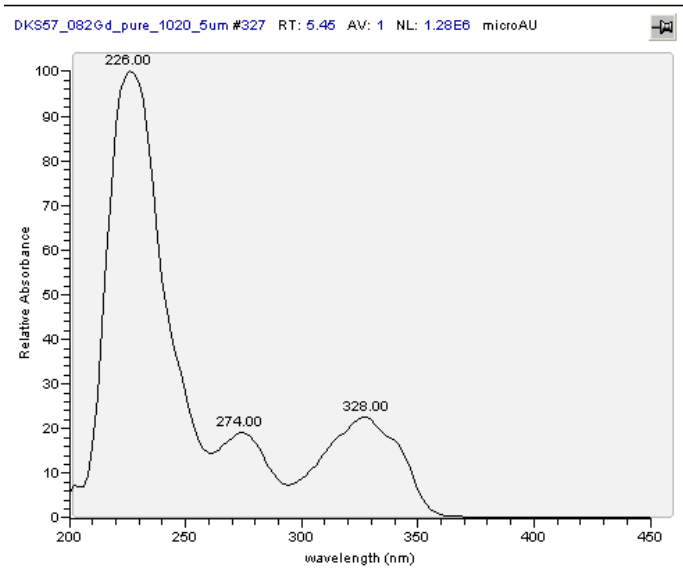


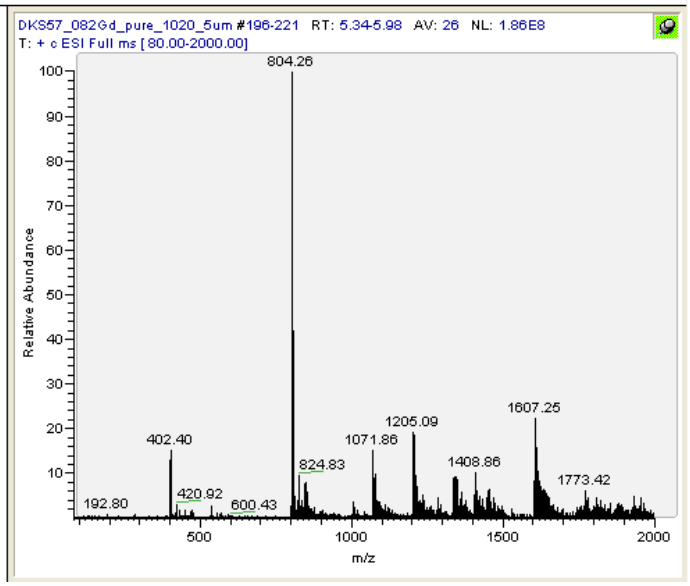

RT: 0.00 - 16.00
uAU
Relative Abundance
Time (min)
NL: 6.59E5 Total Scan PDA DKS57_082Tb _pure_1020_5 um
NL: 1.45E10 TIC MS DKS57_082Tb _pure_1020_5 um
15.60
14.92
5.43
5.57
5.46
5.67
5.82
1.29
1.40
1.75
3.22
4.12
5.36
5.95
6.39
7.18
8.30
9.58
10.58
10.94
11.18
12.31
14.49
14.60
15.62
0.55


DKS57_082Tb_pure_1020_5um #326 RT: 5.43 AV: 1 NL: 9.01E5 microAU
Relative Absorbance
wavelength (nm)
226.00
274.00
326.00

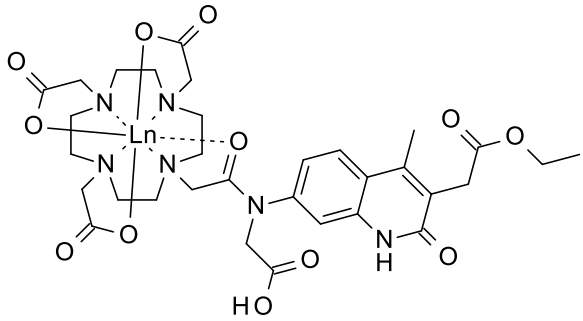

DKS57_082Tb_pure_1020_5um #198-218 RT: 5.33-5.85 AV: 21 NL: 5.84E8
T: + c ESI Full ms [80.00-2000.00]
Relative Abundance
m/z
805.32
1207.45
1609.39
1073.36
403.20
1346.85
357.77
450.91
762.09
1006.28
1815.42


RT: 0.00 - 16.53
uAU
600000
400000
200000
0
5.45
15.60
14.93
NL:
6.66E5
Total Scan
PDA
DKS57_082G
d_pure_1020_
5um
Relative Abundance
100
80
60
40
20
0
5.55
5.65
1.29
5.77
0.42
1.45
2.08
3.14
4.23
4.63
5.93
6.27
8.09
9.16
10.22
11.55
11.94
13.14
14.45
14.64
15.68
NL:
1.40E10
TIC MS
DKS57_082G
d_pure_1020_
5um
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16
Time (min)


DKS57_082Gd_pure_1020_5um #327 RT: 5.45 AV: 1 NL: 1.28E6 microAU
Relative Absorbance
100
90
80
70
60
50
40
30
20
10
0
226.00
274.00
328.00
200 250 300 350 400 450
wavelength (nm)


DKS57_082Gd_pure_1020_5um #196-221 RT: 5.34-5.98 AV: 26 NL: 1.86E8
T: + c ESI Full ms [80.00-2000.00]
Relative Abundance
100
90
80
70
60
50
40
30
20
10
804.26
1607.25
1205.09
402.40
1071.86
824.83
1408.86
1773.42
420.92
192.80
600.43
500 1000 1500 2000
m/z

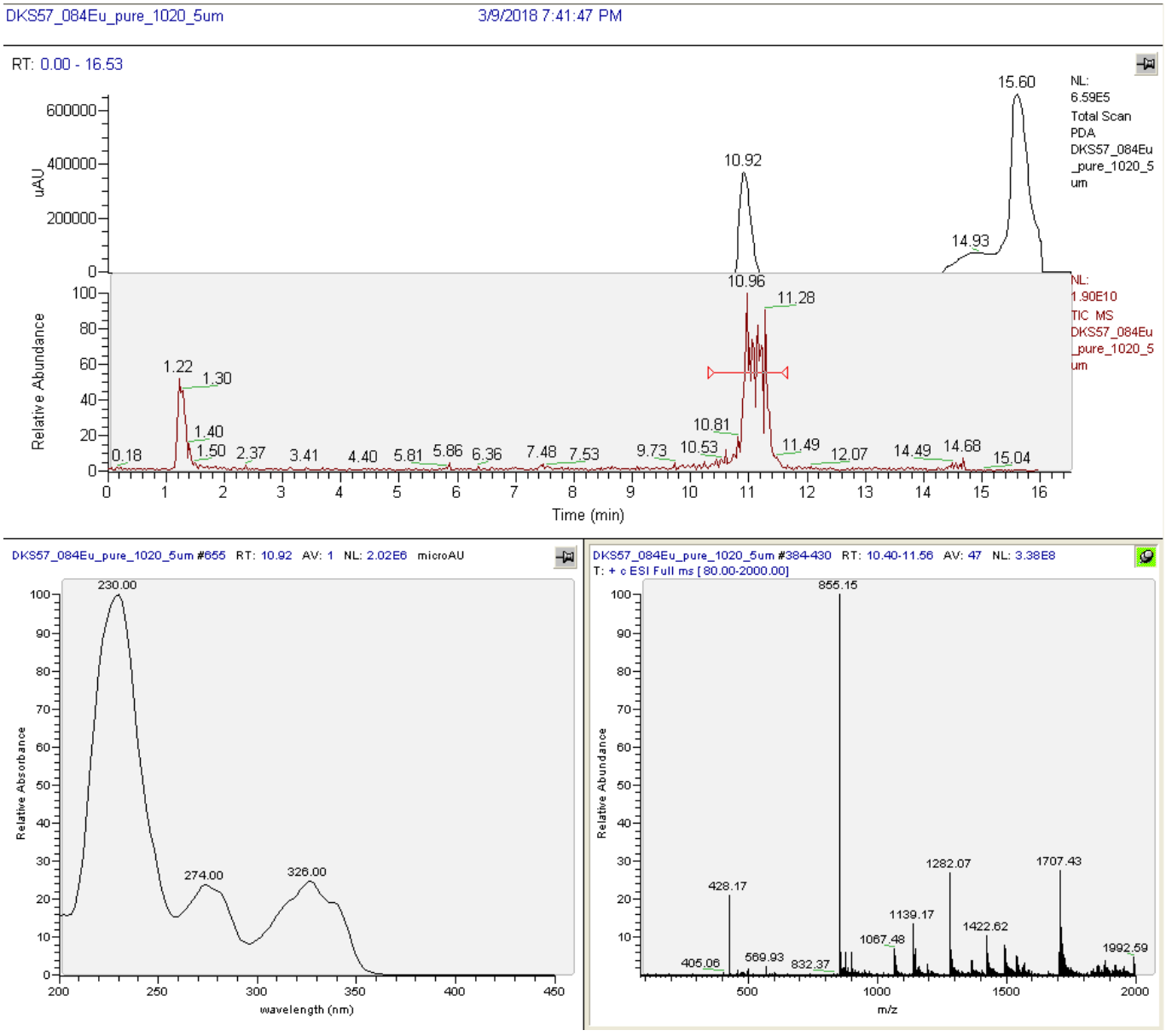
DKS57_084Ln (Eu, Tb, Gd)

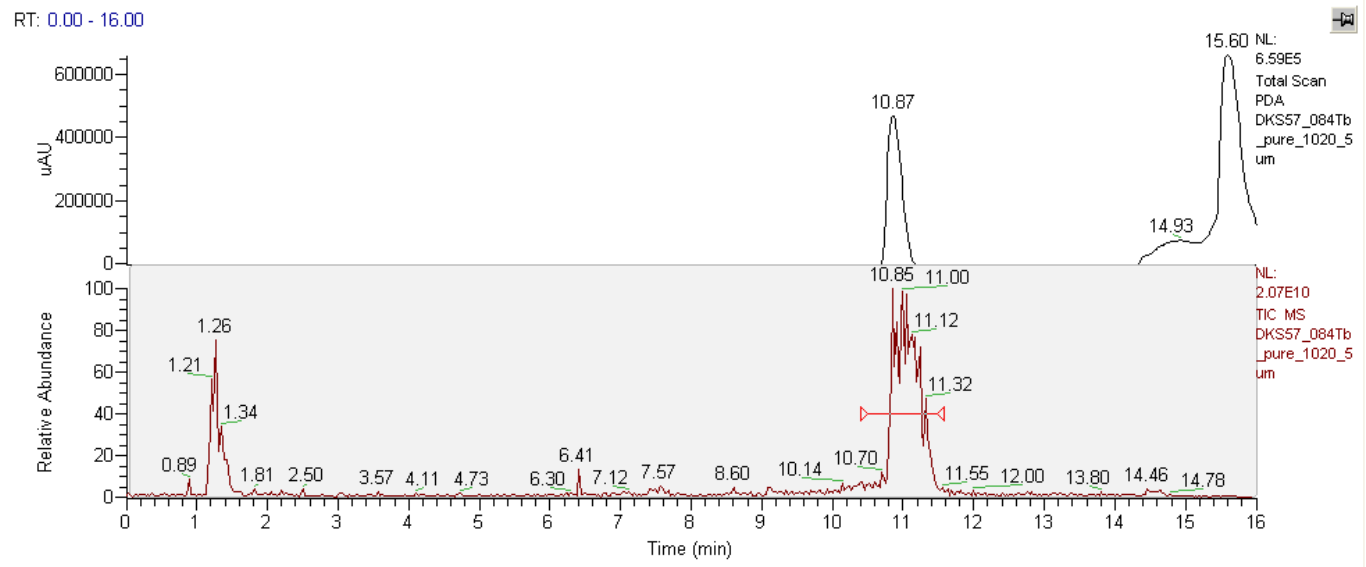


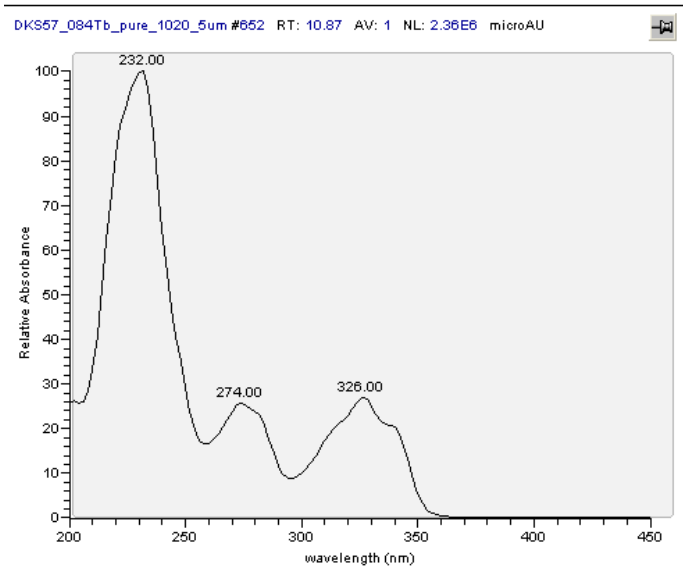
Formula Weight : 853.674
Exact Mass : 854.19947
Formula : $C_{32}H_{41}N_6O_{12}Eu$
Composition : C 45.02% H 4.84%
N 9.84% O 22.49% Eu 17.80%

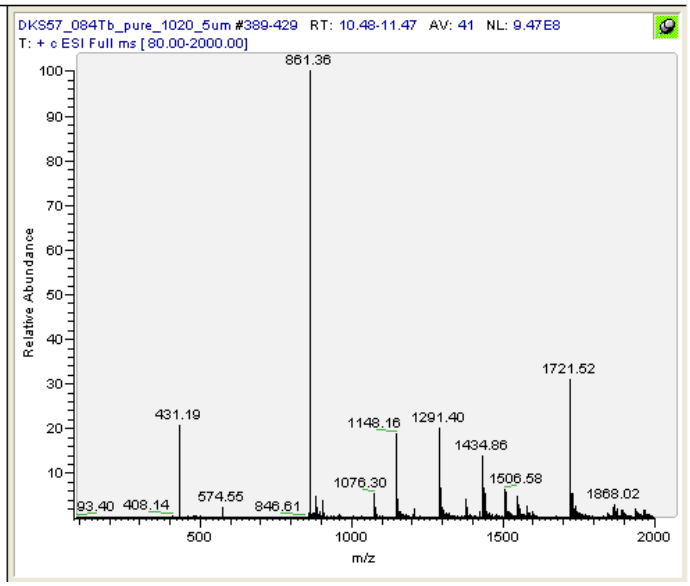
Formula Weight : 860.635
Exact Mass : 860.20359
Formula : $C_{32}H_{41}N_6O_{12}Tb$
Composition : C 44.66% H 4.80%
N 9.77% O 22.31% Tb 18.47%

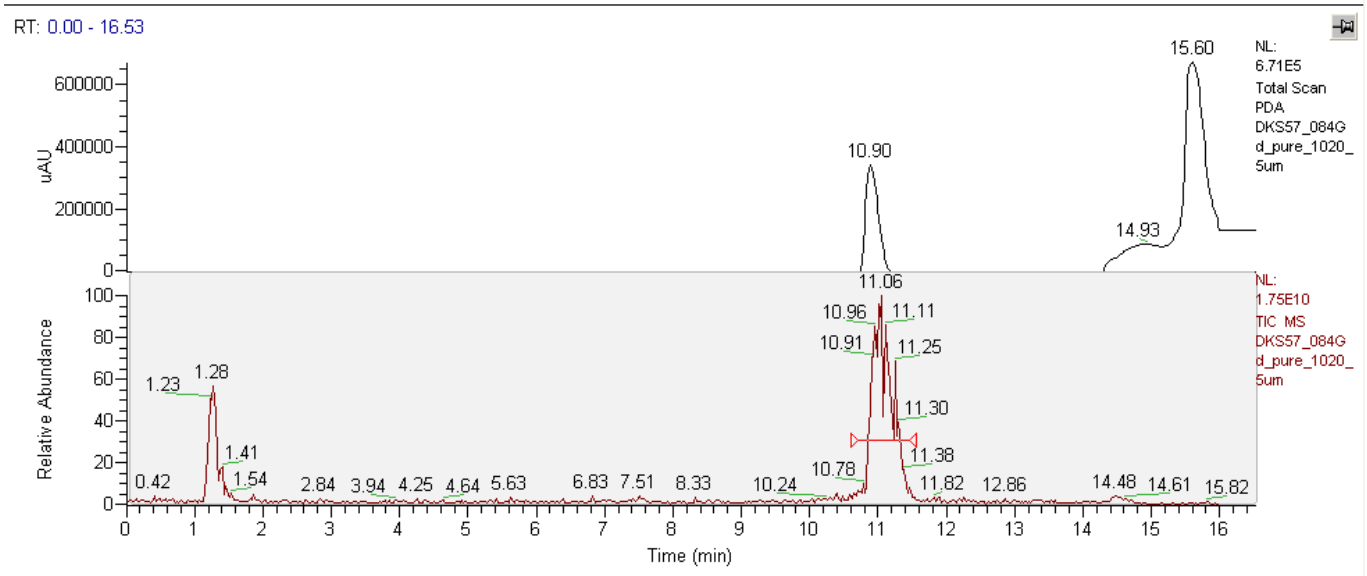
Formula Weight : 858.960
Exact Mass : 859.20235
Formula : $C_{32}H_{41}N_6O_{12}Gd$
Composition : C 44.75% H 4.81%
N 9.78% O 22.35% Gd 18.31%

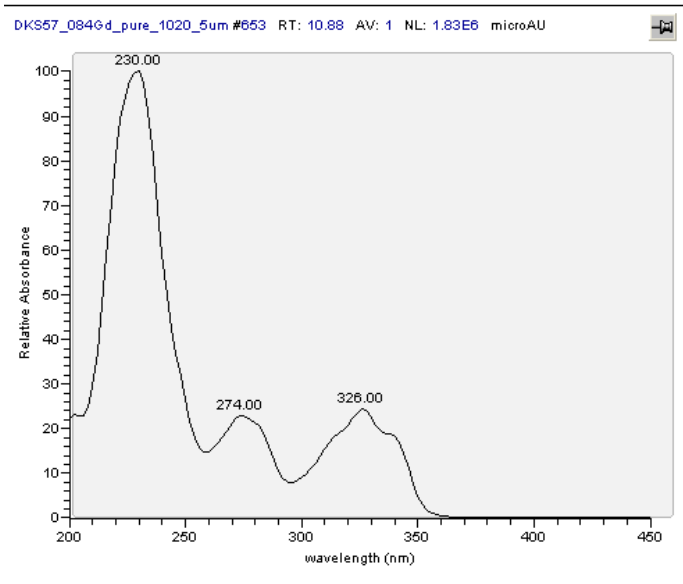


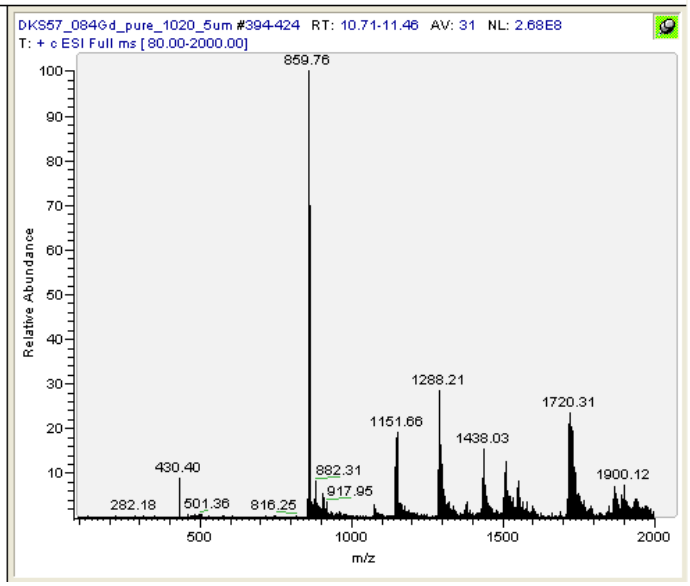

RT: 0.00 - 16.00
uAU
Relative Abundance
Time (min)
NL: 6.59E5 Total Scan PDA DKS57_084Tb _pure_1020_5 um
NL: 2.07E10 TIC MS DKS57_084Tb _pure_1020_5 um
10.87
15.60
14.93
10.85
11.00
11.12
11.32
1.26
1.21
1.34
0.89
1.81
2.50
3.57
4.11
4.73
6.30
6.41
7.12
7.57
8.60
10.14
10.70
11.55
12.00
13.80
14.46
14.78


DKS57_084Tb_pure_1020_5um #652 RT: 10.87 AV: 1 NL: 2.36E6 microAU
Relative Absorbance
wavelength (nm)
232.00
274.00
326.00


DKS57_084Tb_pure_1020_5um #389-429 RT: 10.48-11.47 AV: 41 NL: 9.47E8
T: + c ESI Full ms [80.00-2000.00]
Relative Abundance
m/z
861.36
1721.52
431.19
1148.16
1291.40
1434.86
1506.58
1076.30
1868.02
93.40
408.14
574.55
846.61


RT: 0.00 - 16.53
uAU
Relative Abundance
Time (min)
NL: 6.71E5 Total Scan PDA DKS57_084Gd_pure_1020_5um
NL: 1.75E10 TIC MS DKS57_084Gd_pure_1020_5um
15.60
14.93
10.90
11.06
10.96
11.11
10.91
11.25
11.30
11.38
10.78
1.23
1.28
1.41
1.54
0.42
2.84
3.94
4.25
4.64
5.63
6.83
7.51
8.33
10.24
11.82
12.86
14.48
14.61
15.82


DKS57_084Gd_pure_1020_5um #653 RT: 10.88 AV: 1 NL: 1.83E6 microAU
Relative Absorbance
wavelength (nm)
230.00
274.00
326.00


DKS57_084Gd_pure_1020_5um #394-424 RT: 10.71-11.46 AV: 31 NL: 2.68E8
T: + c ESI Full ms [80.00-2000.00]
Relative Abundance
m/z
859.76
1288.21
1720.31
1151.66
1438.03
430.40
882.31
917.95
1900.12
282.18
501.36
816.25