Supporting Information

Novel Xanomeline-Containing Bitopic Ligands of Muscarinic Acetylcholine Receptors: Design, Synthesis and FRET Investigation

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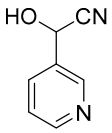
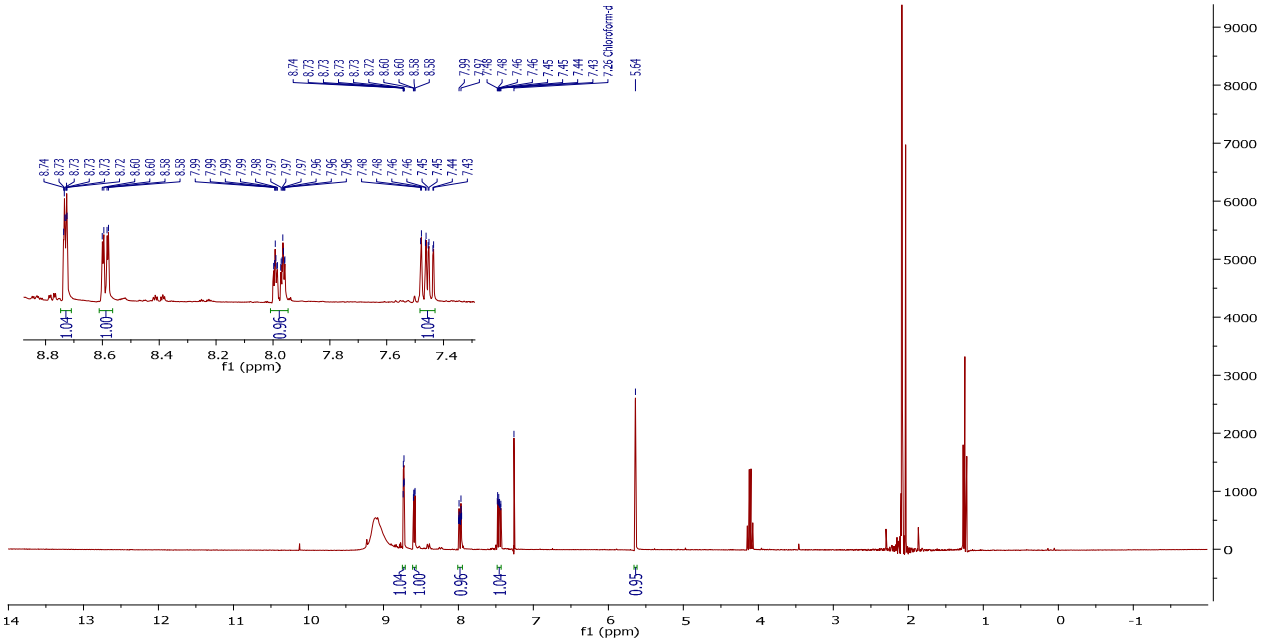
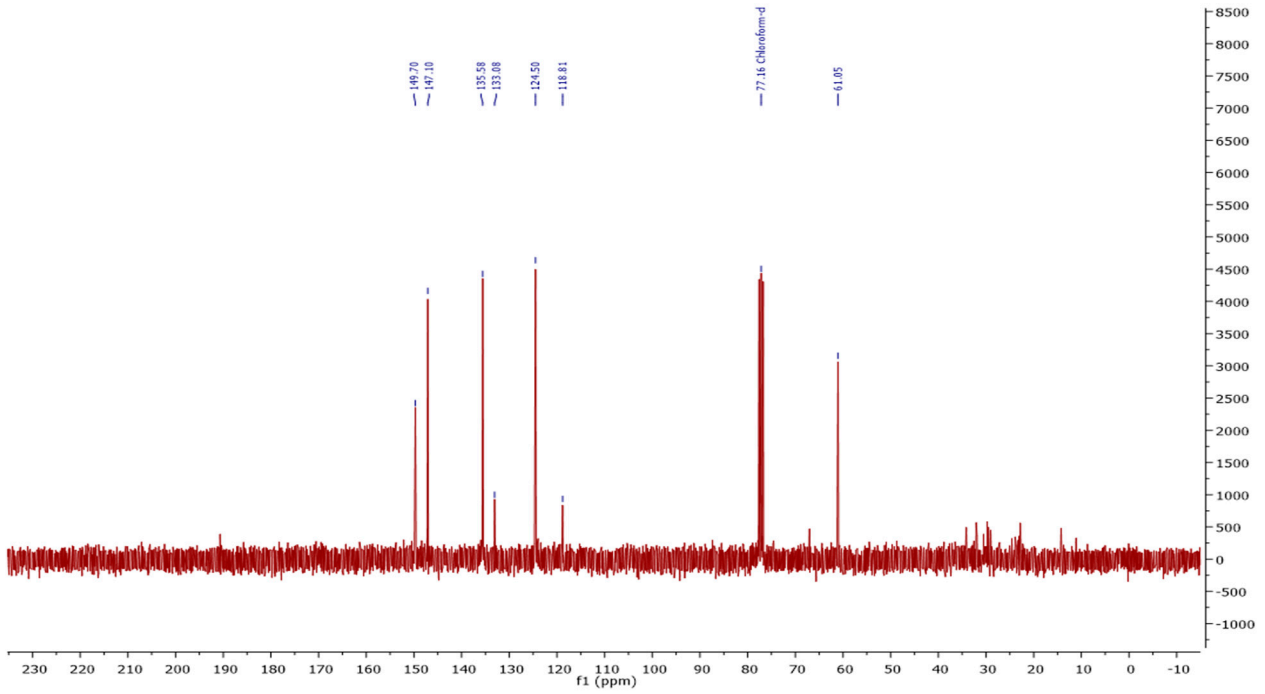
Compound 15



^{1}H NMR spectrum



^{13}C NMR spectrum



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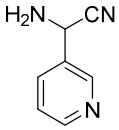

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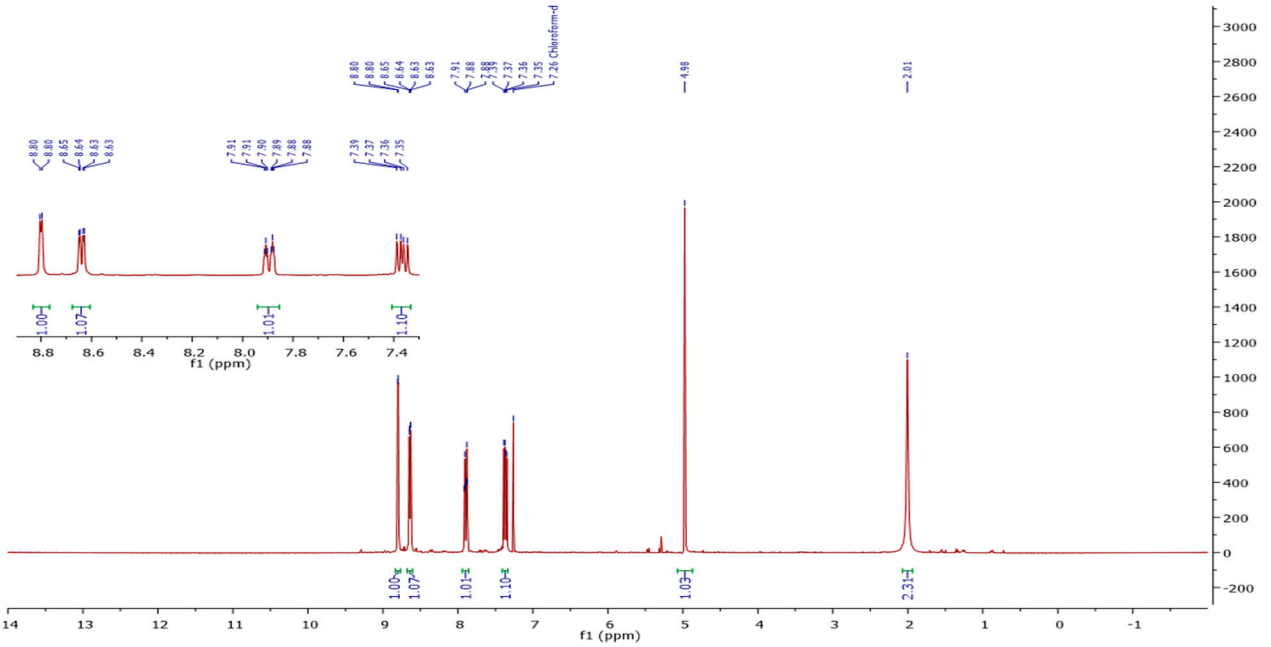

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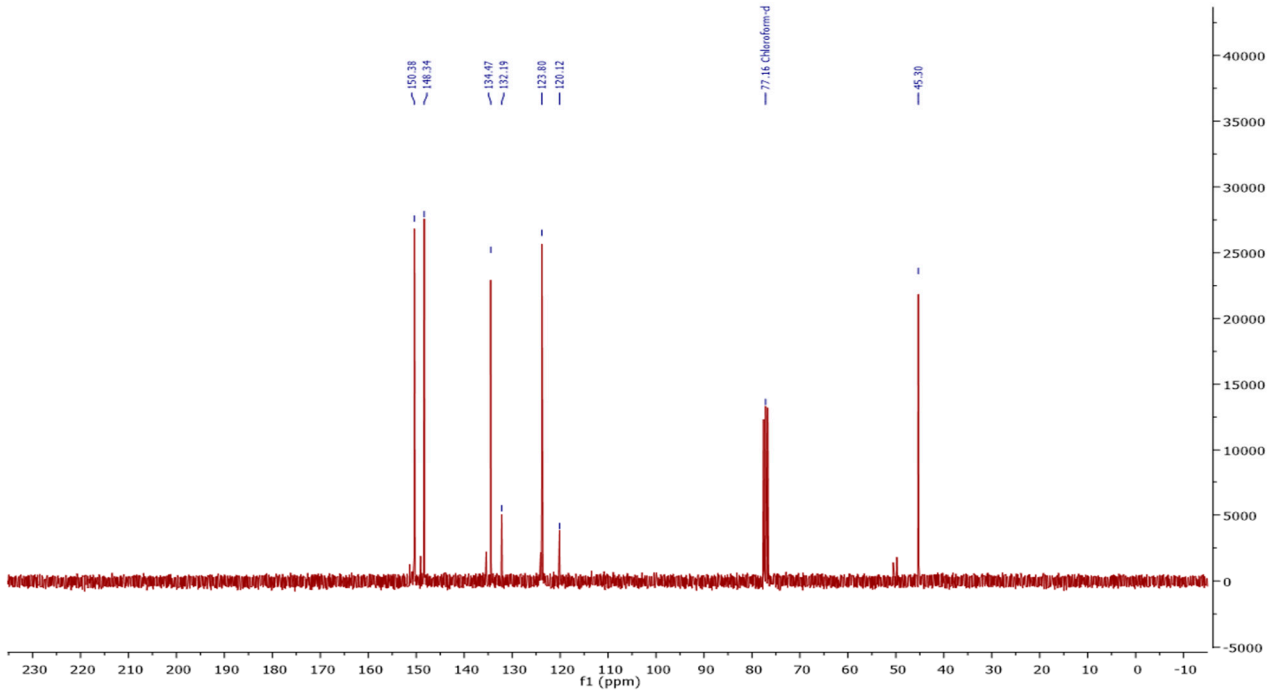

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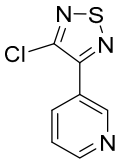

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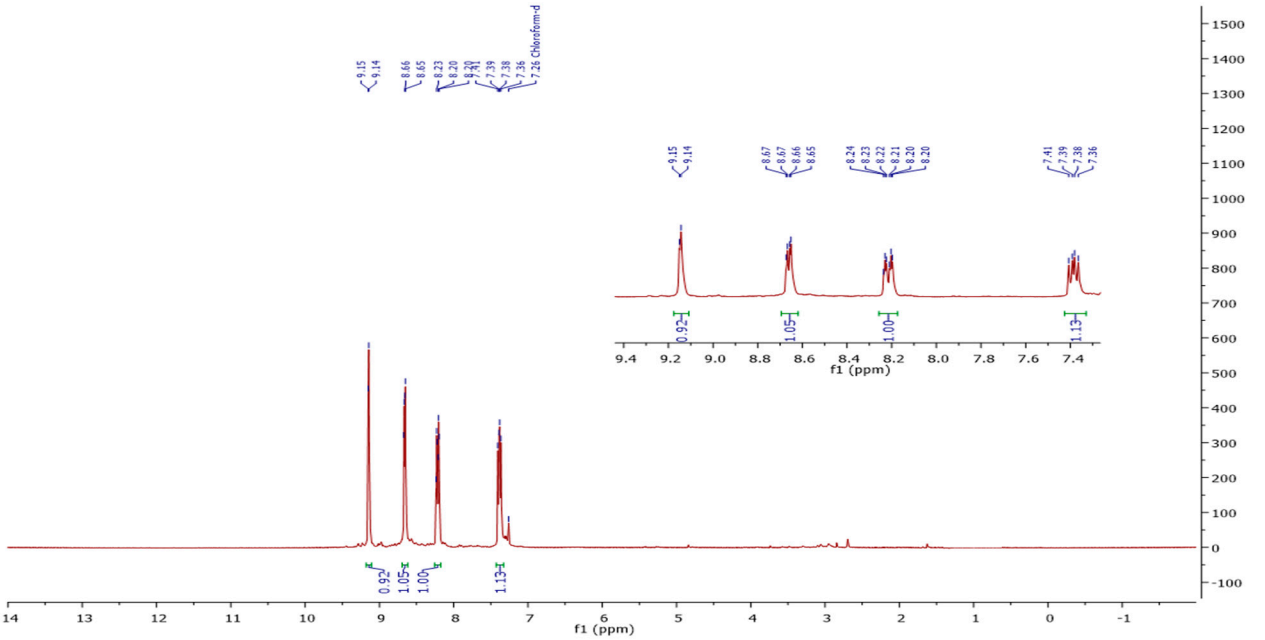

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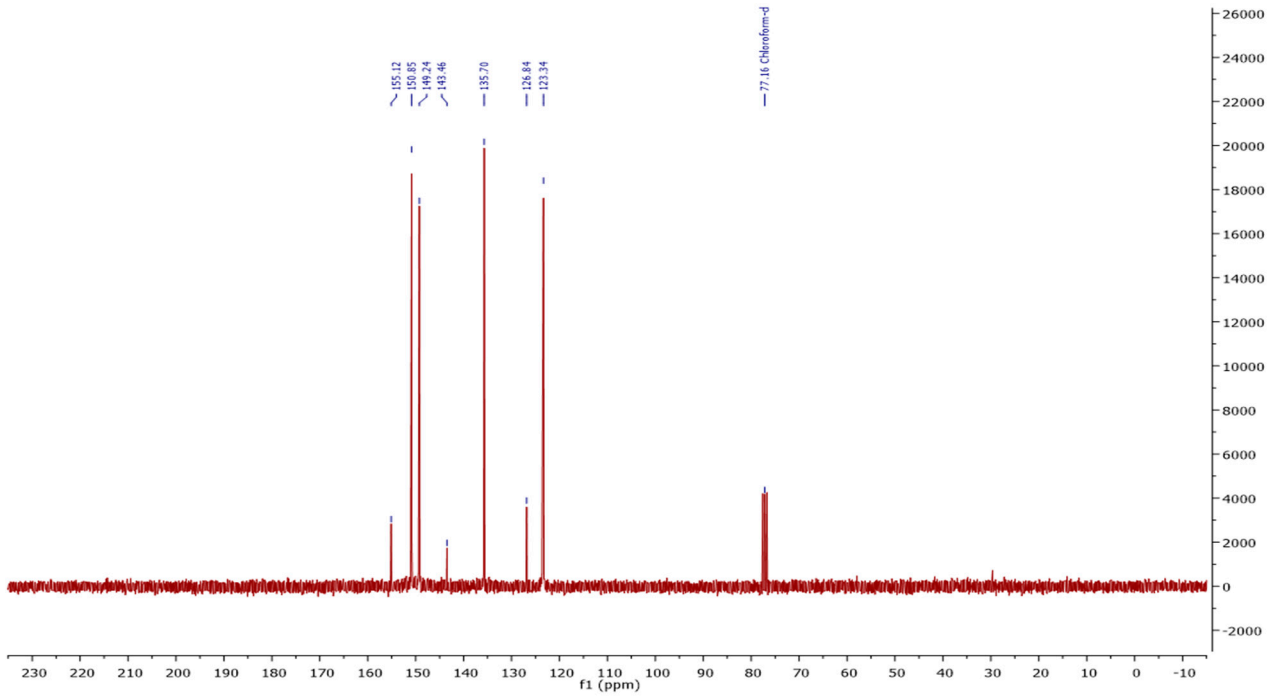

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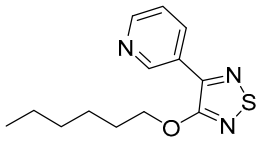

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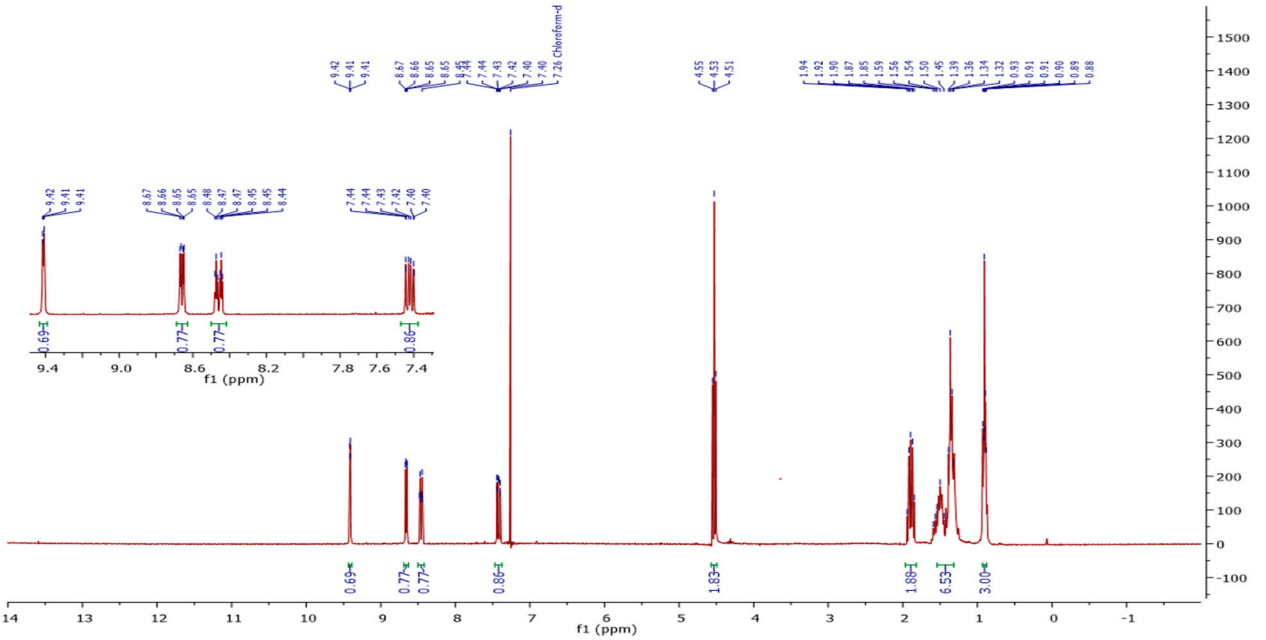

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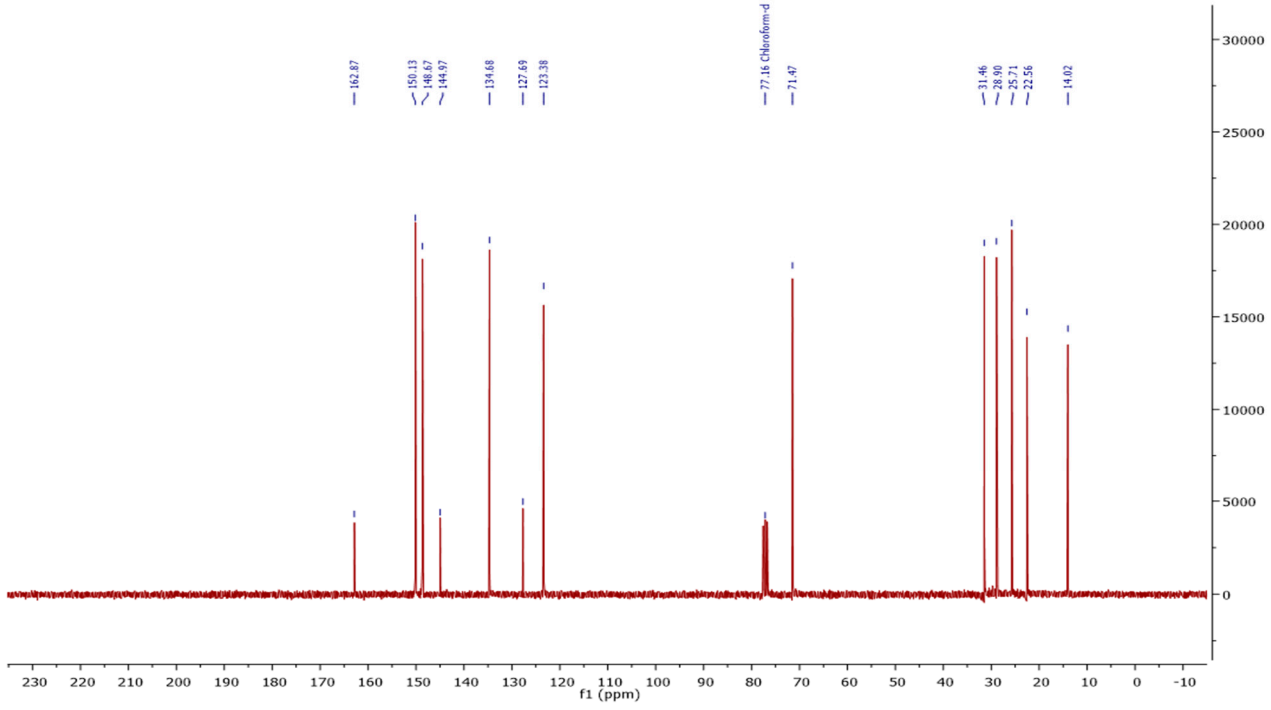

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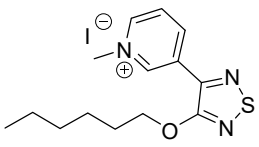

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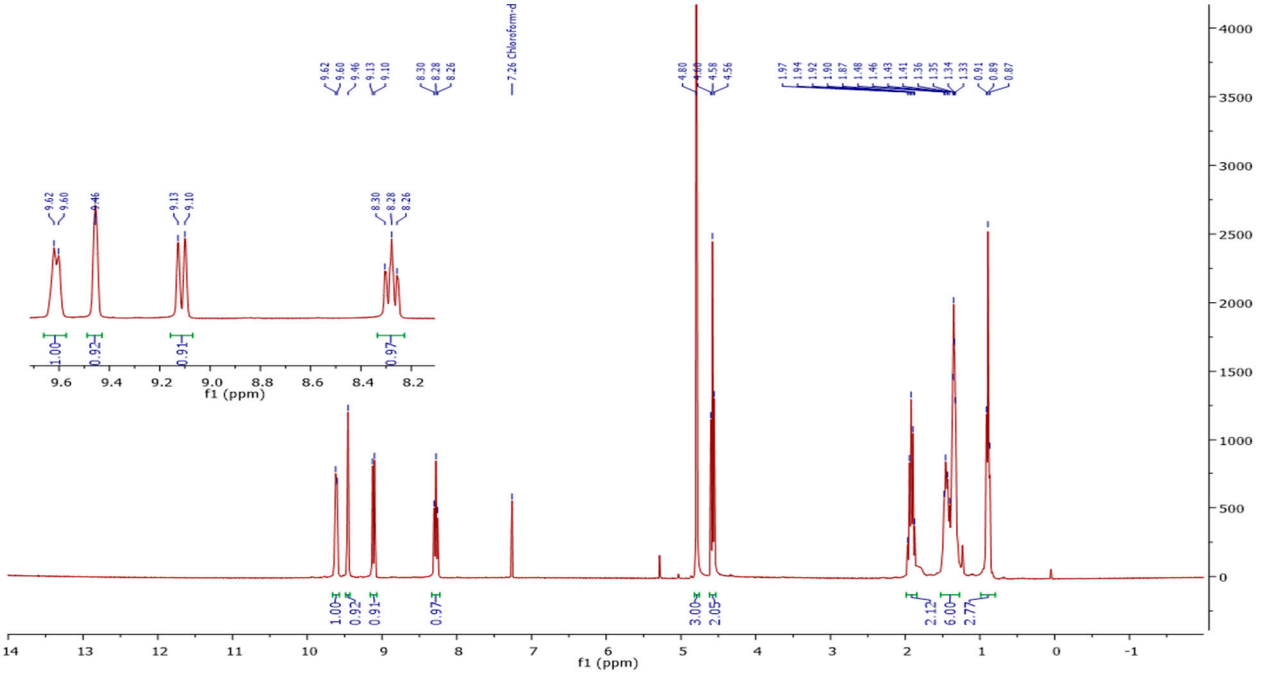

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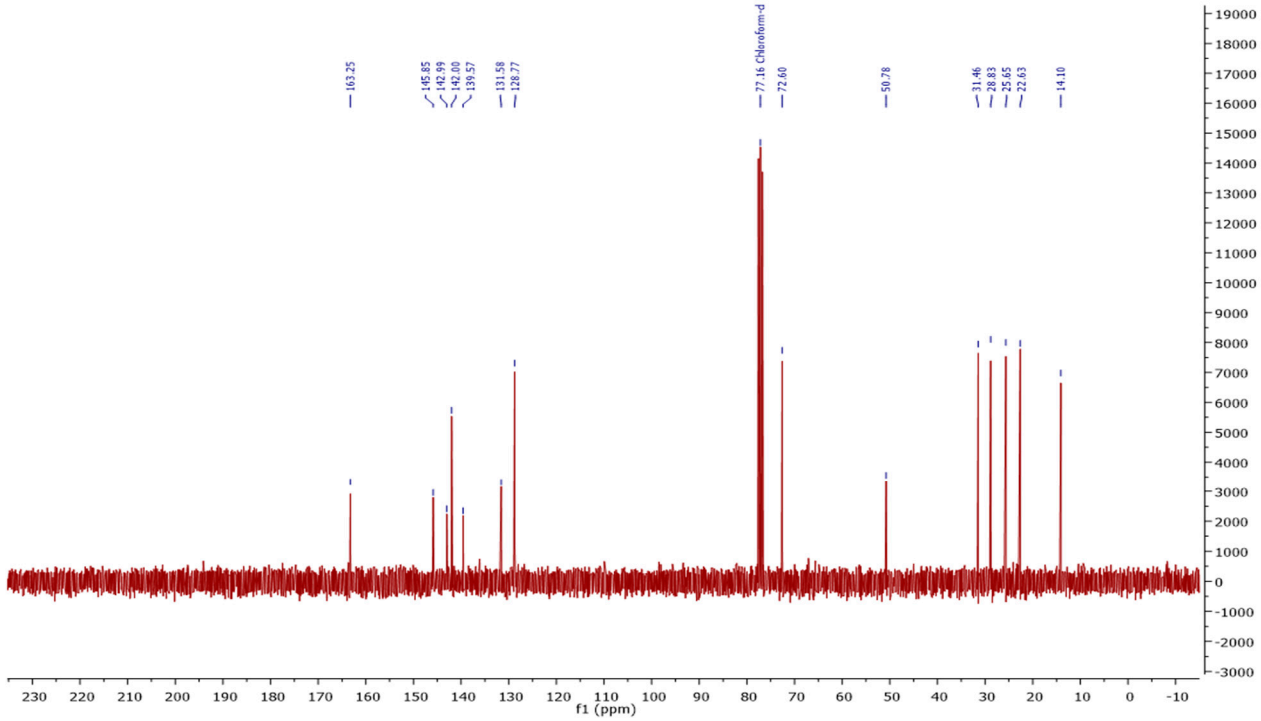

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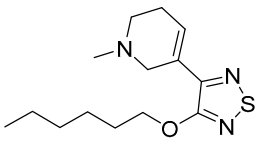

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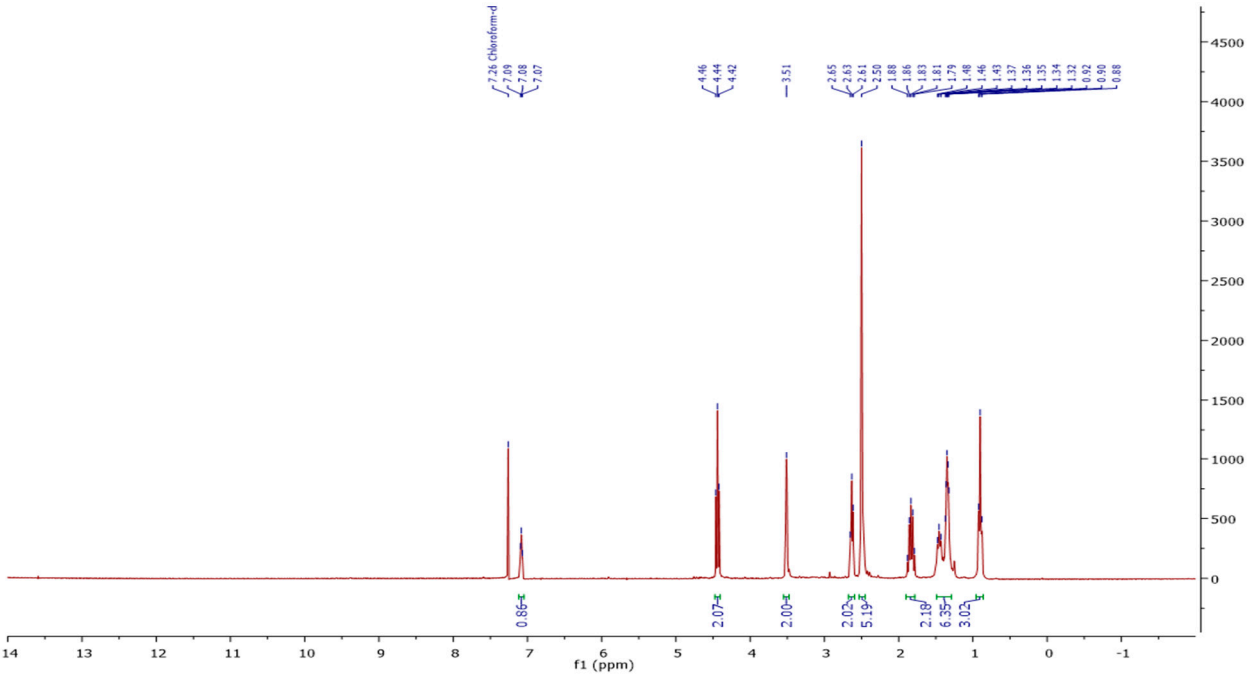

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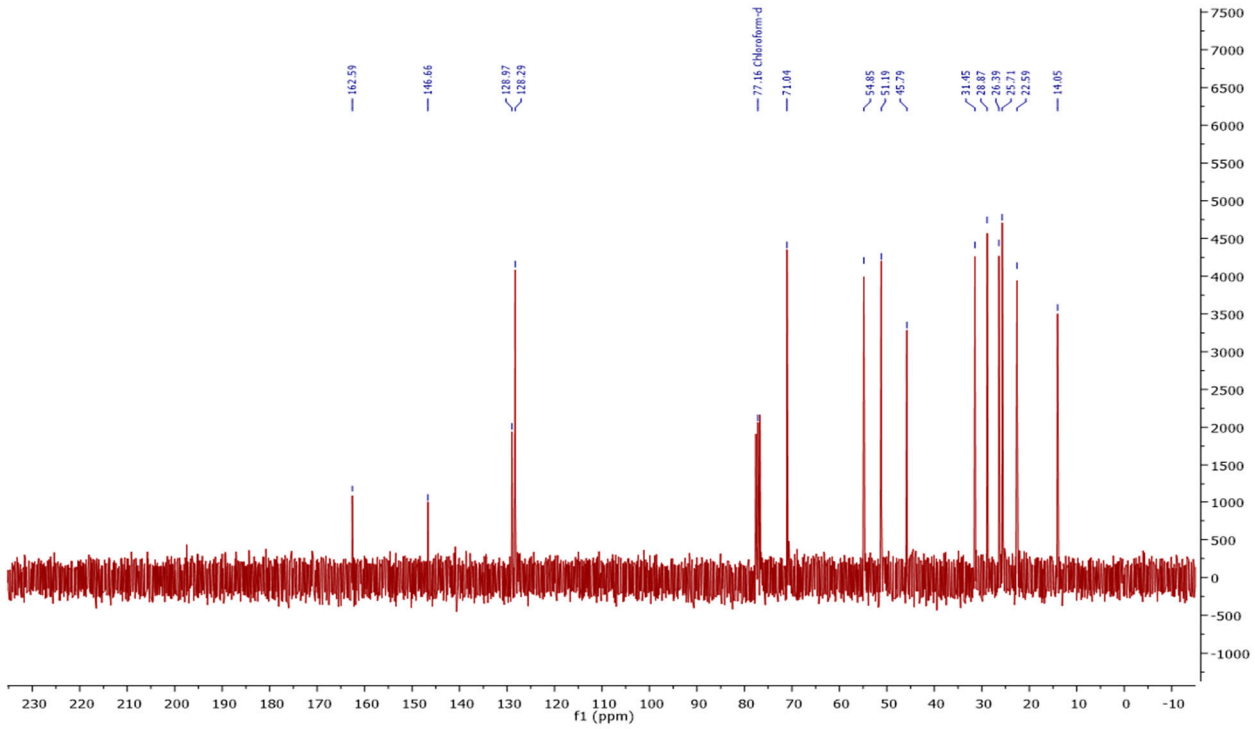

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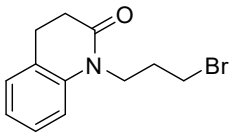

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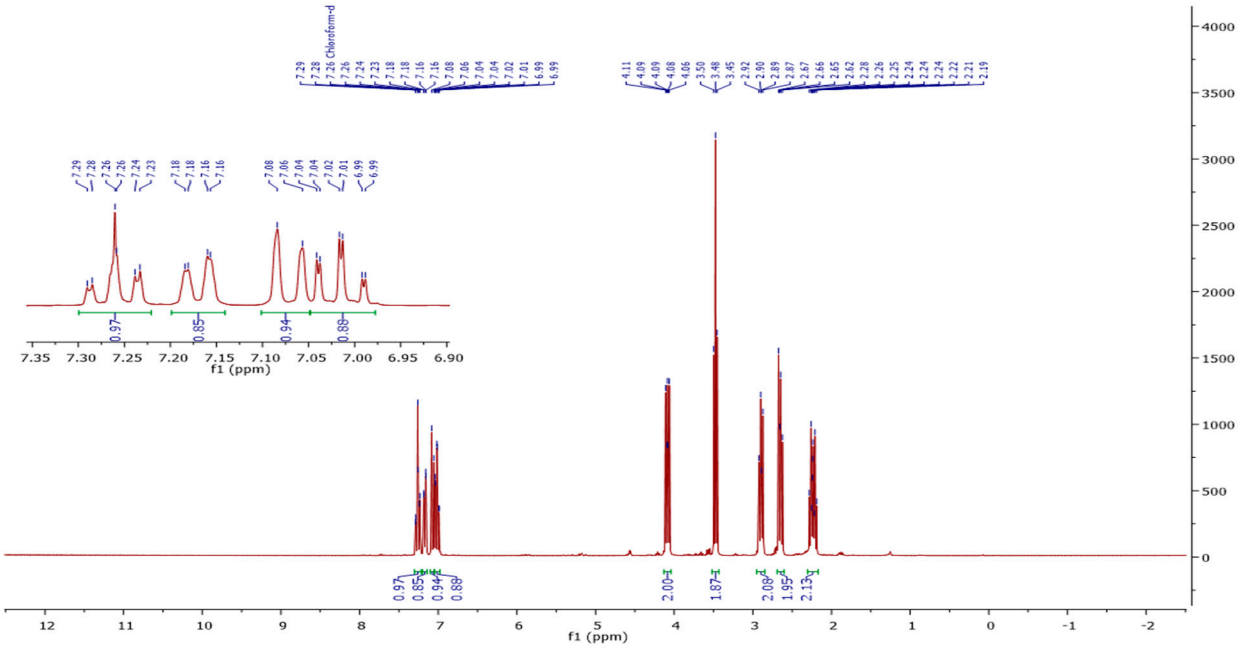

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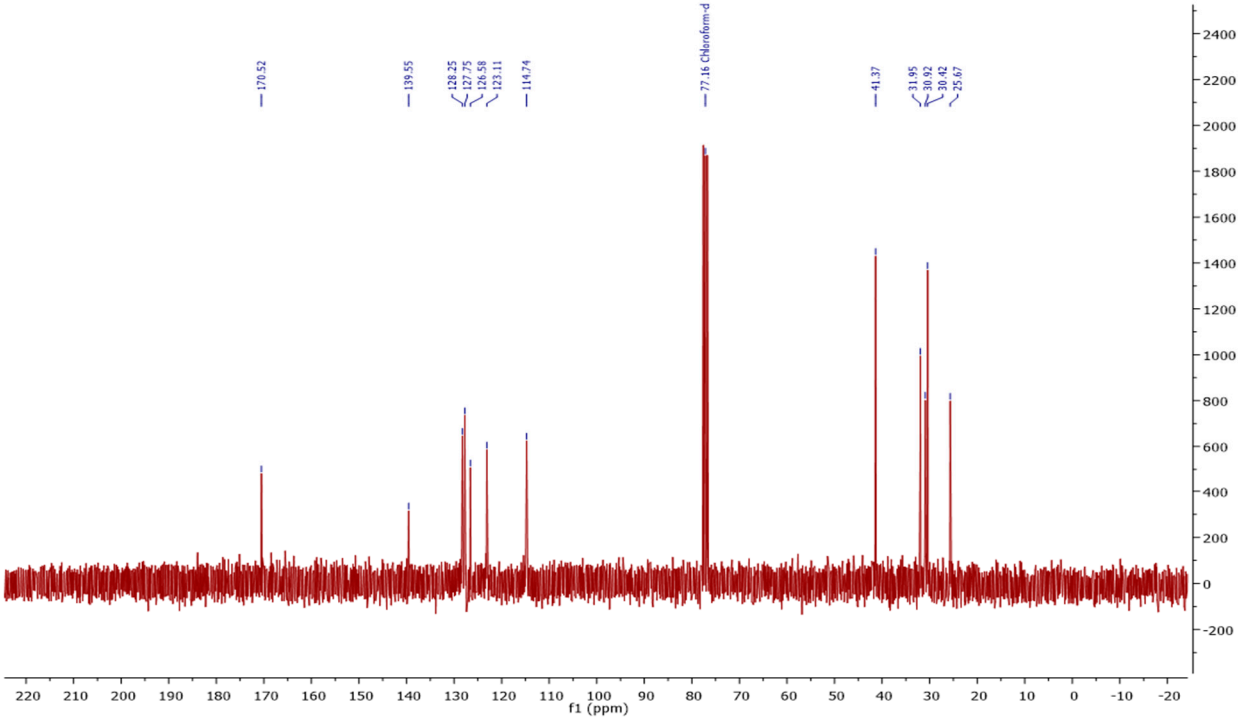

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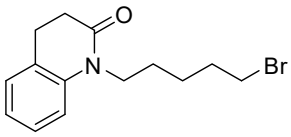

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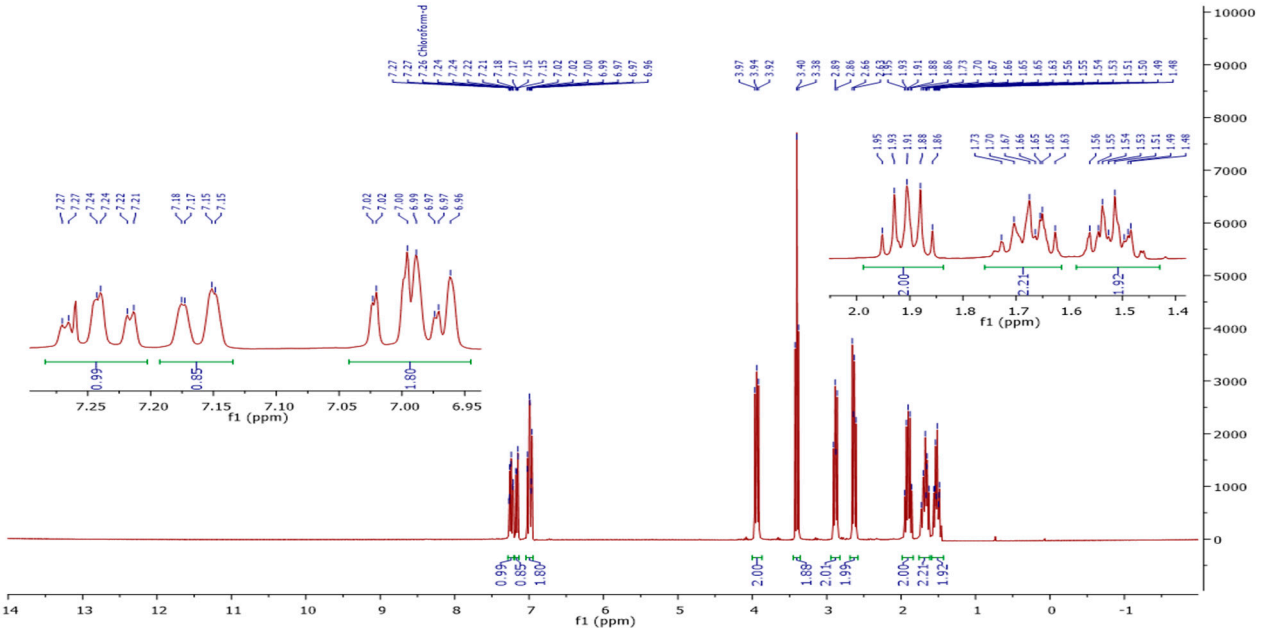

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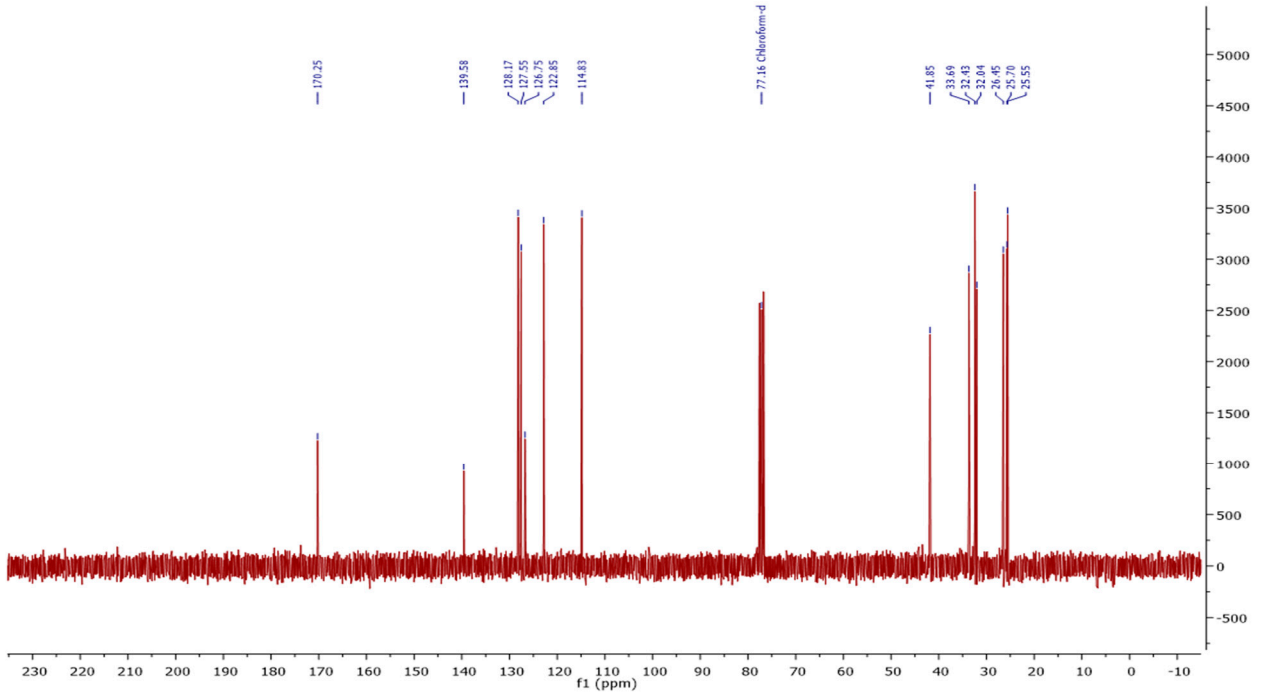

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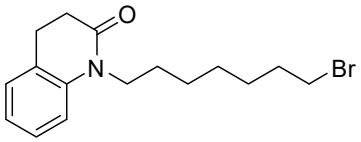

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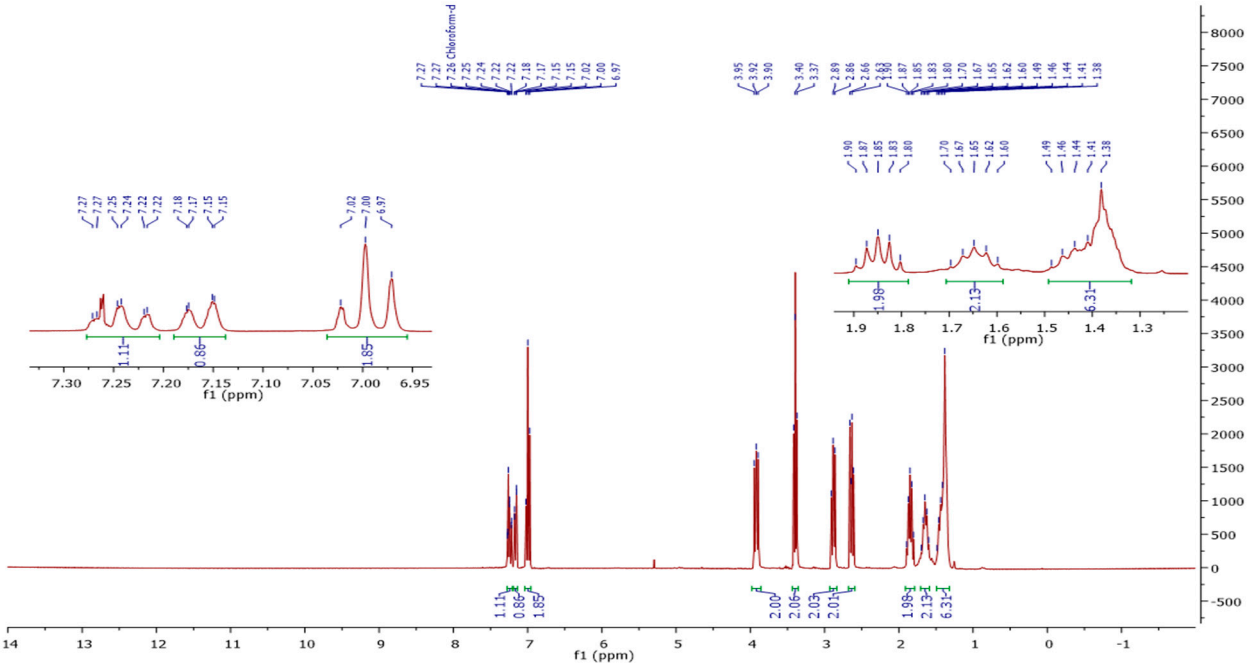

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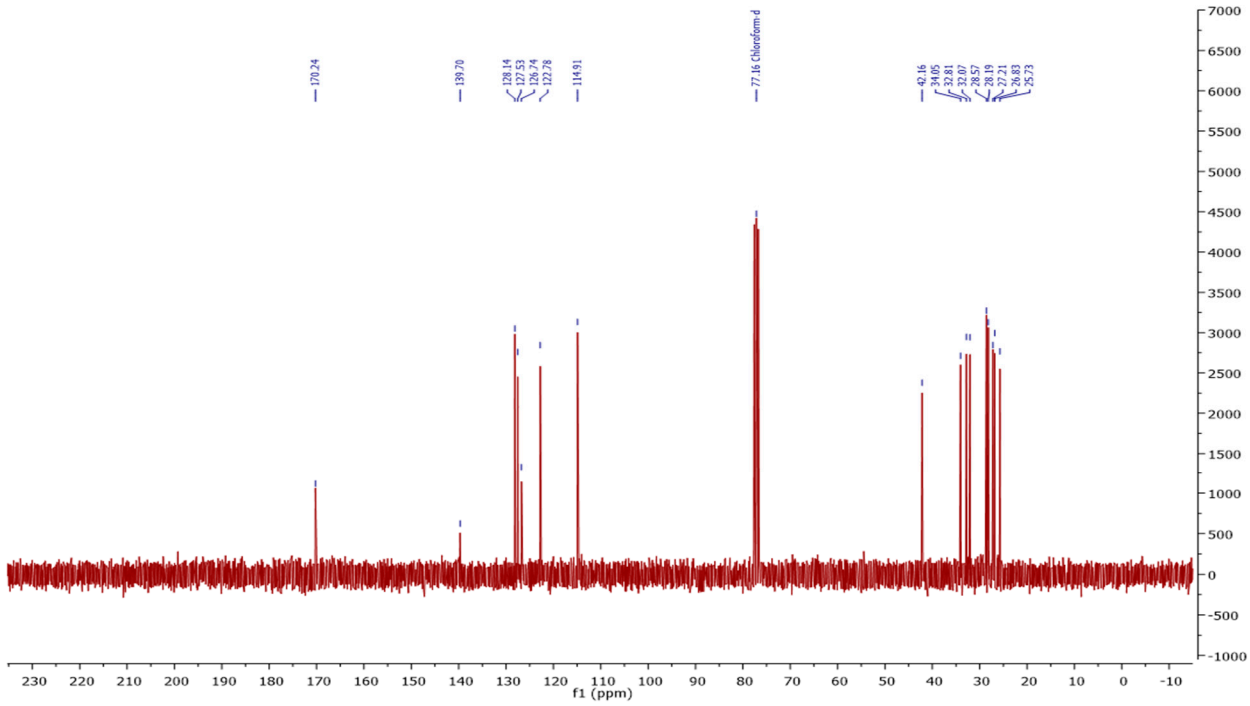

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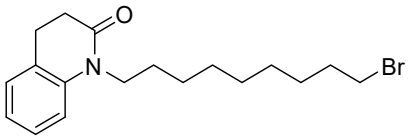

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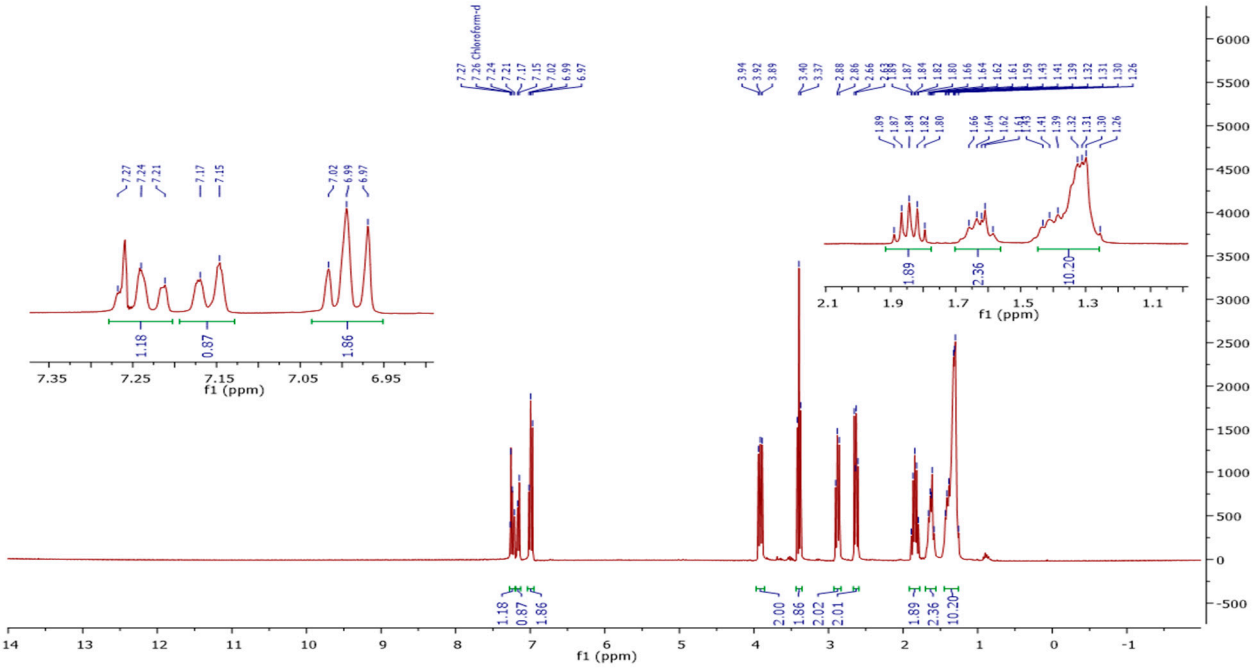

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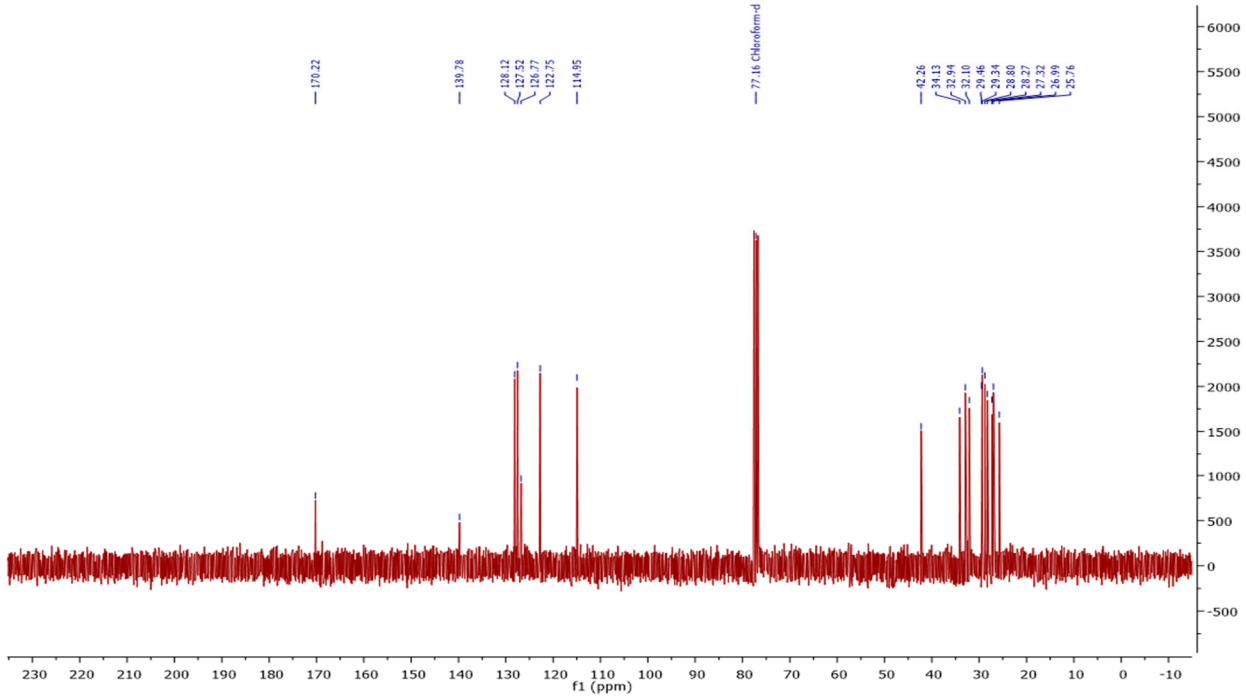

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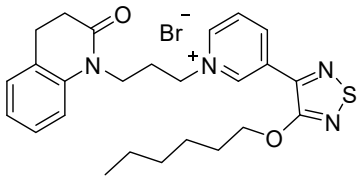

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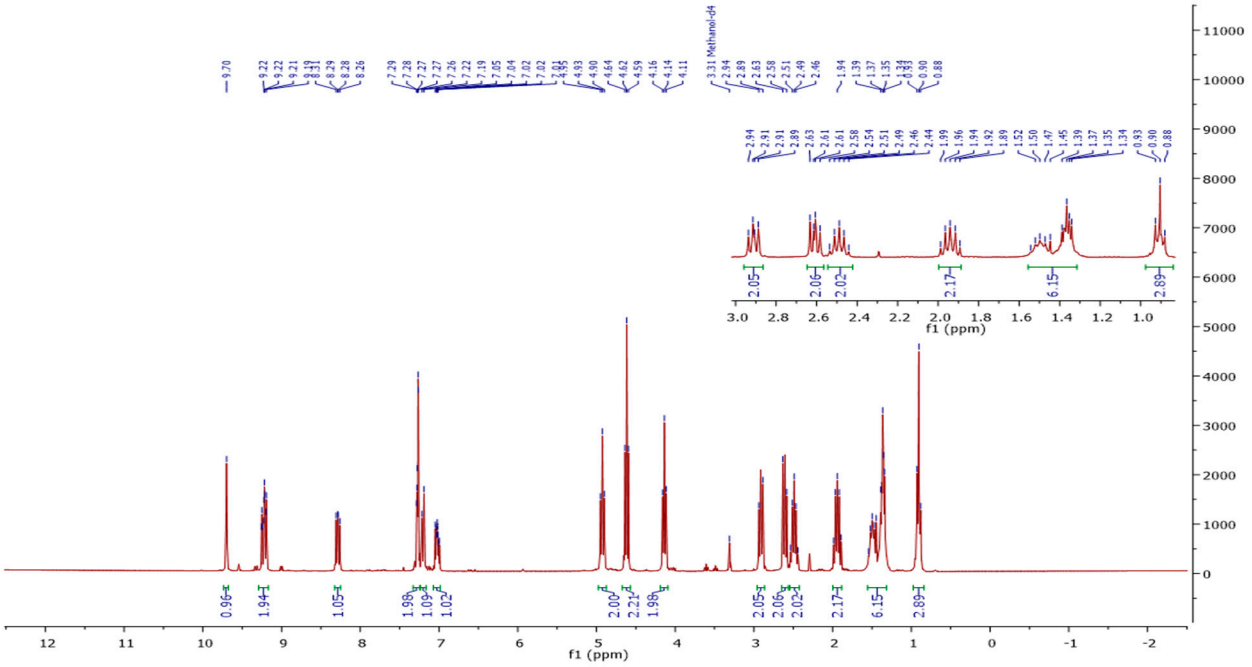

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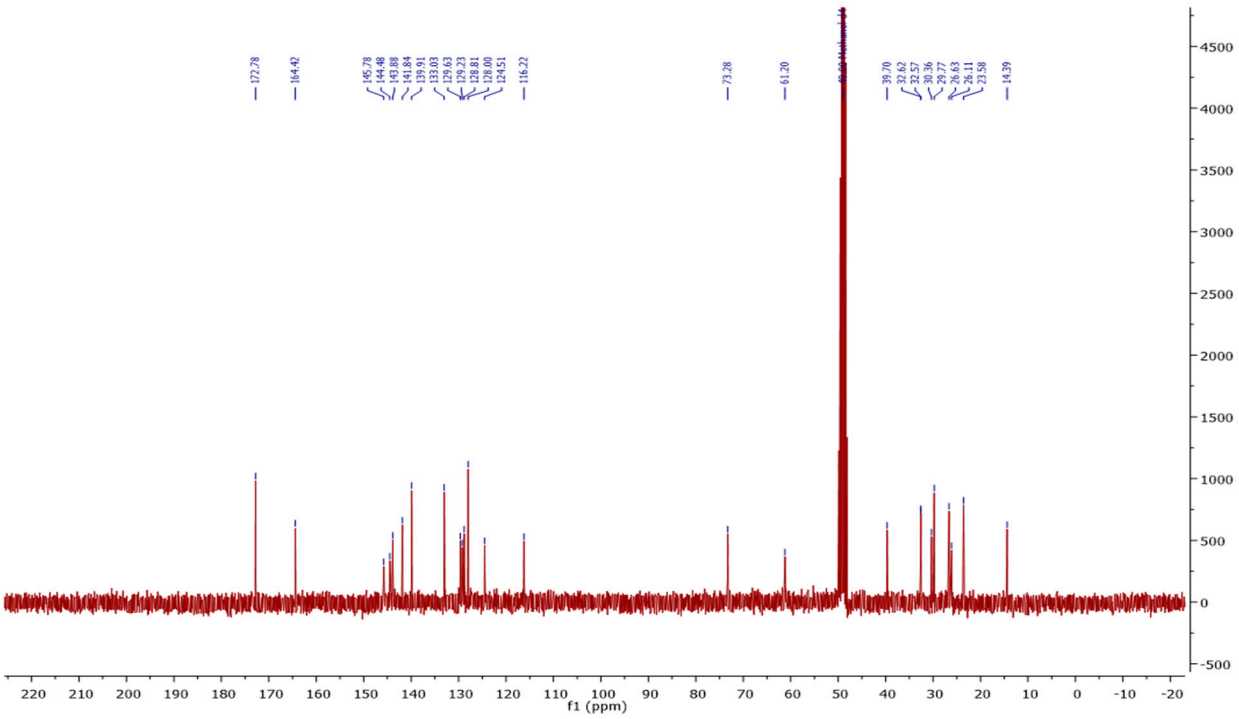

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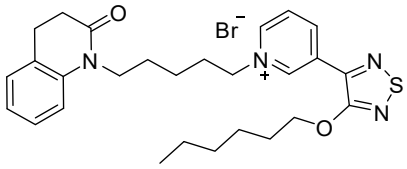

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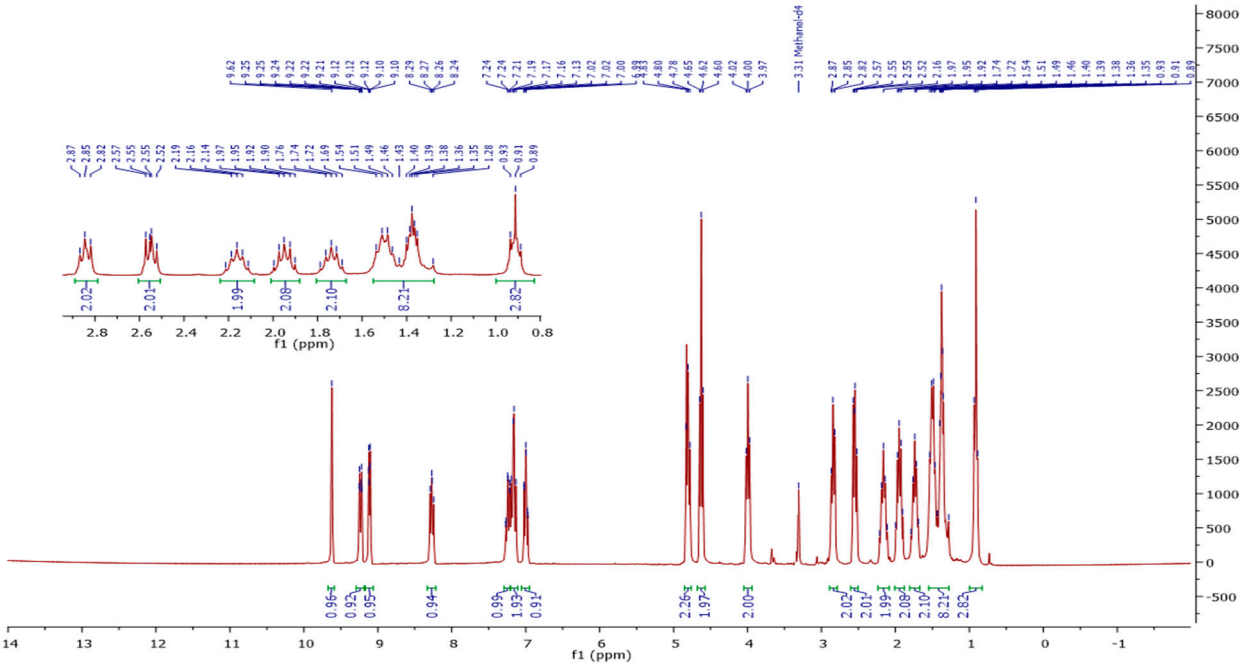

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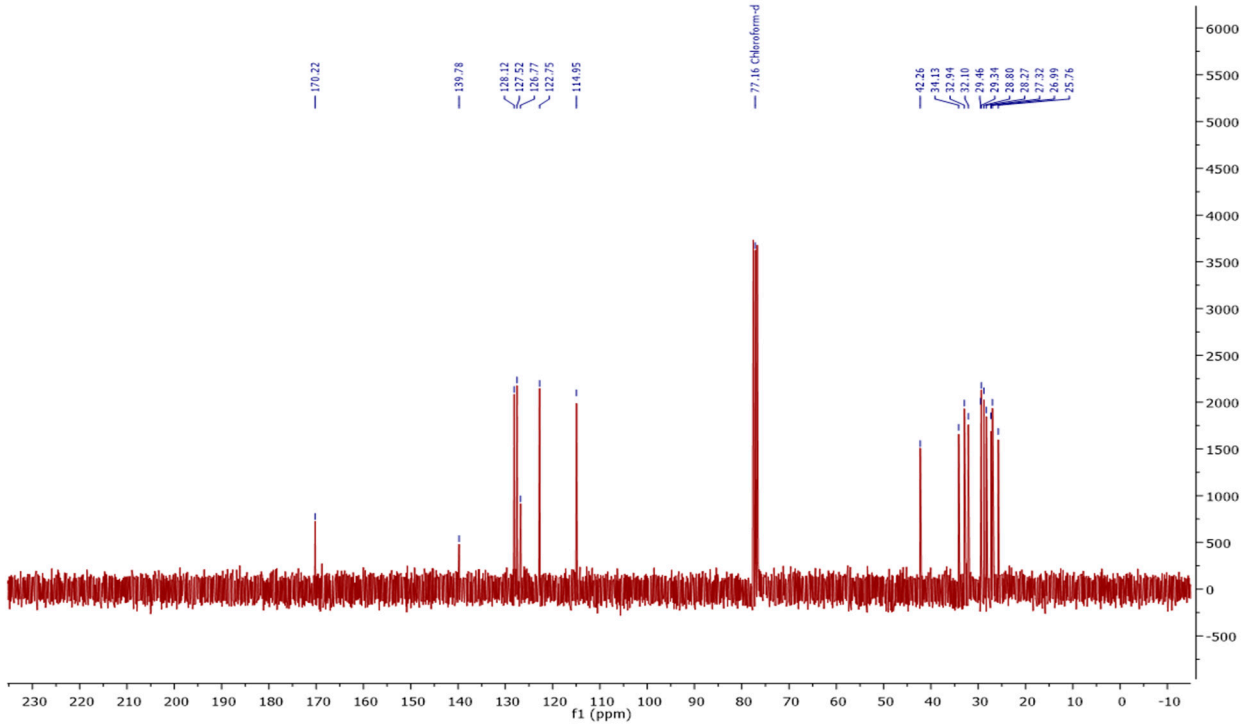

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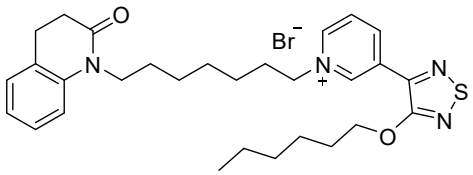

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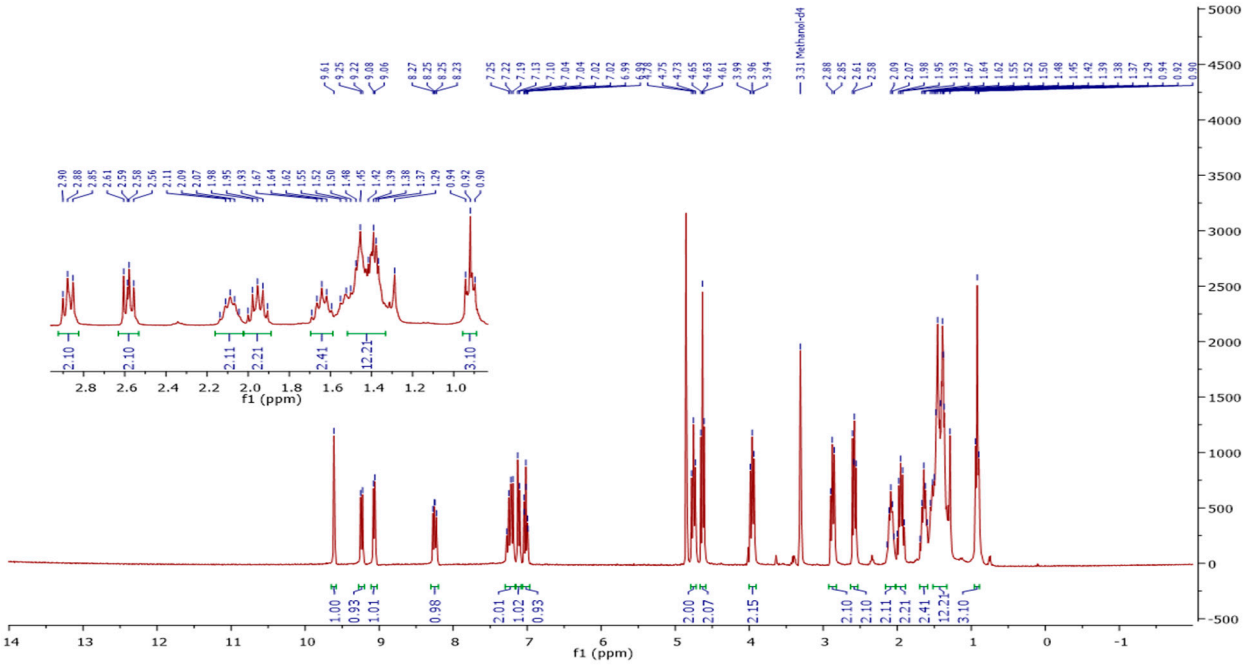

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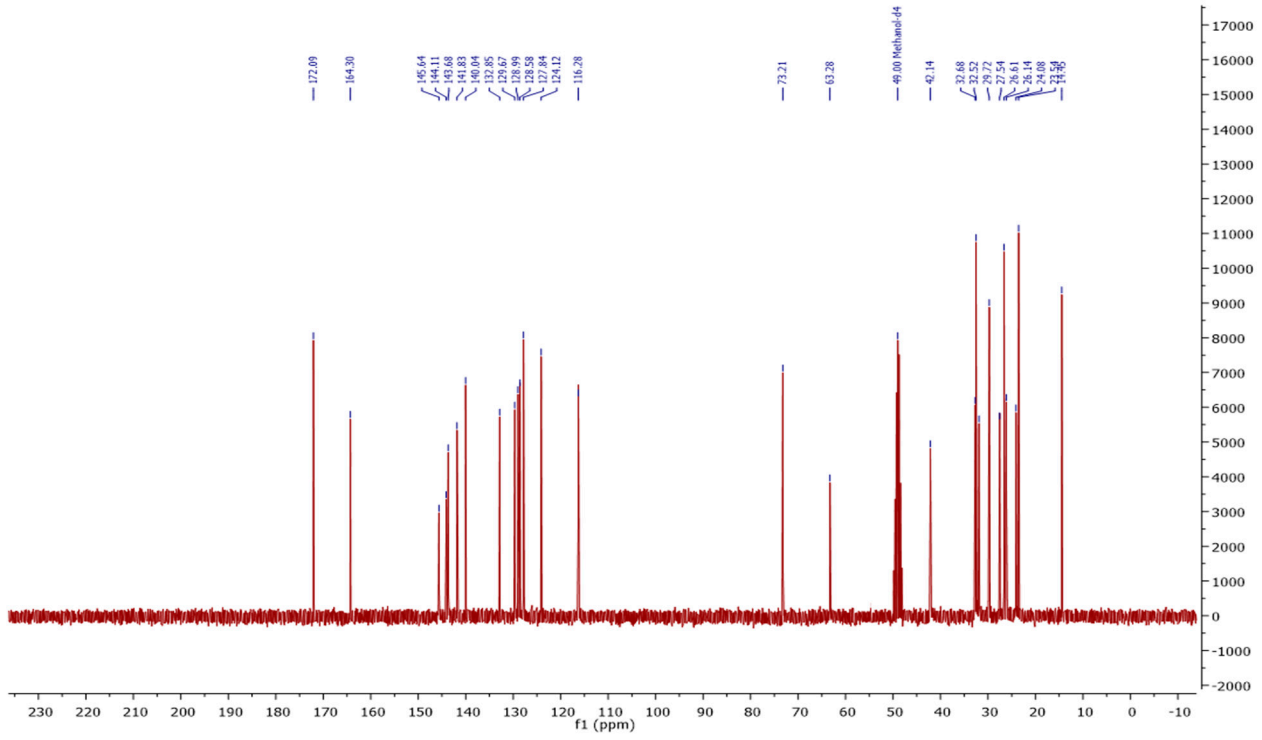

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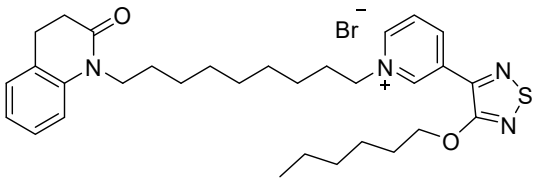

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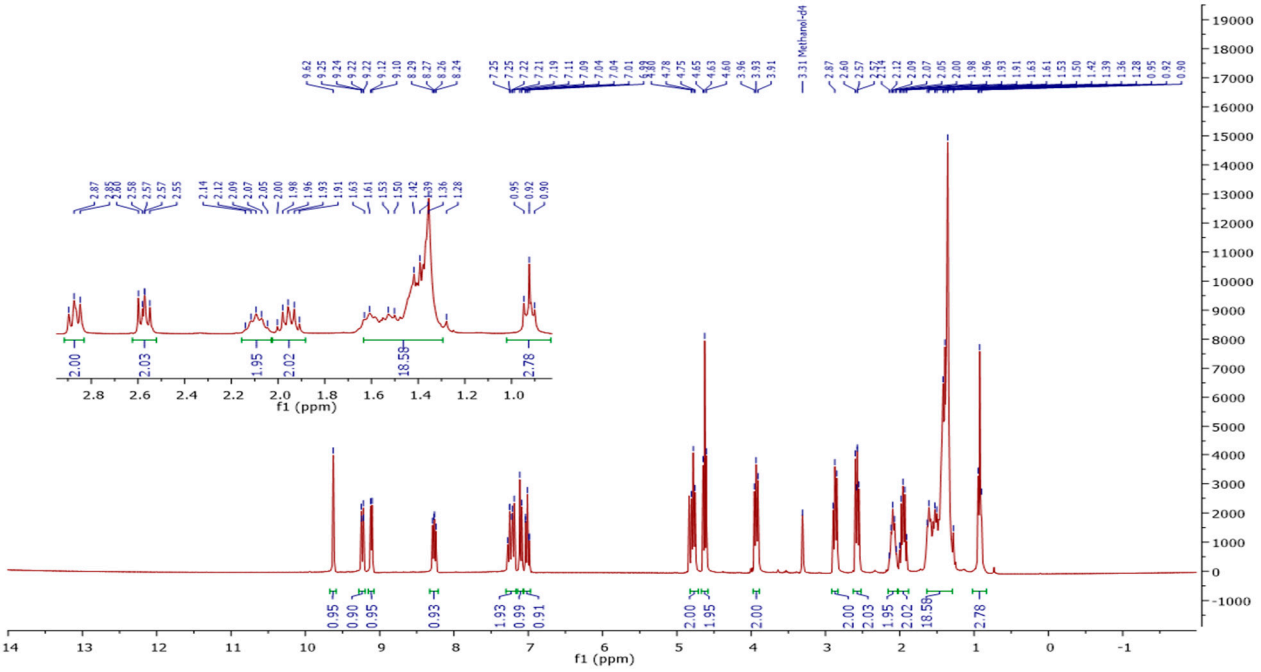

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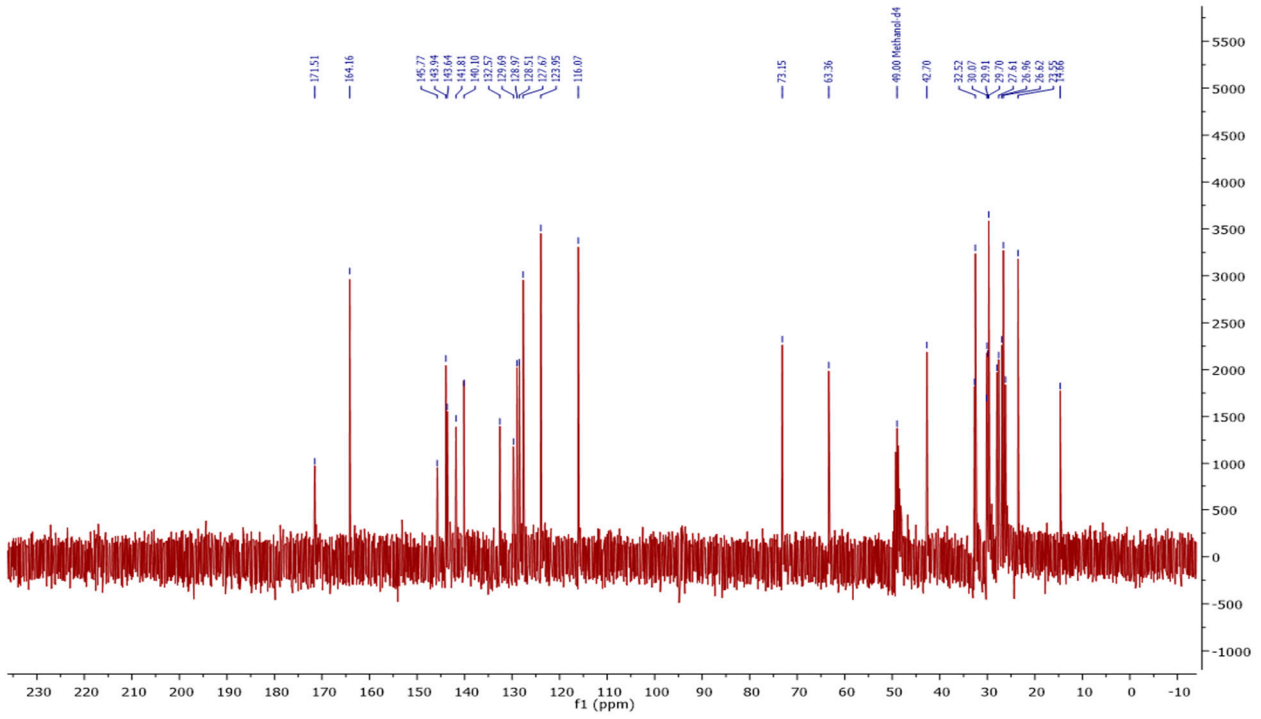

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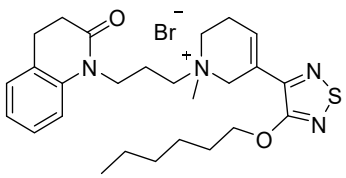

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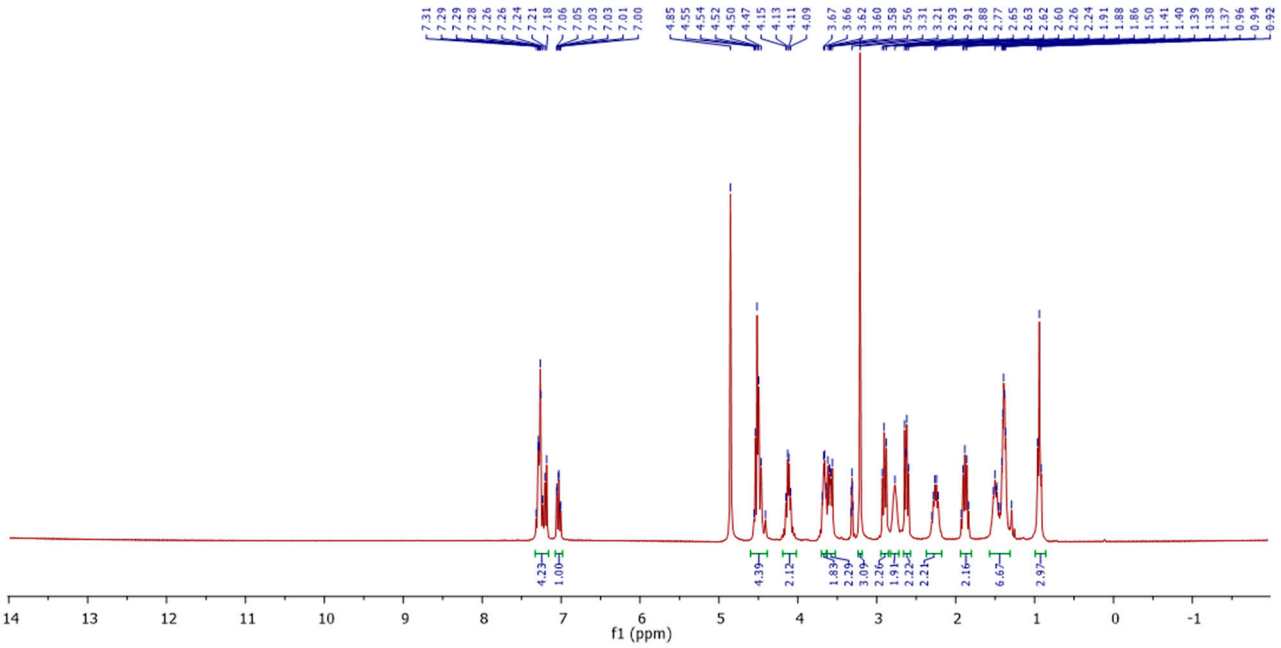

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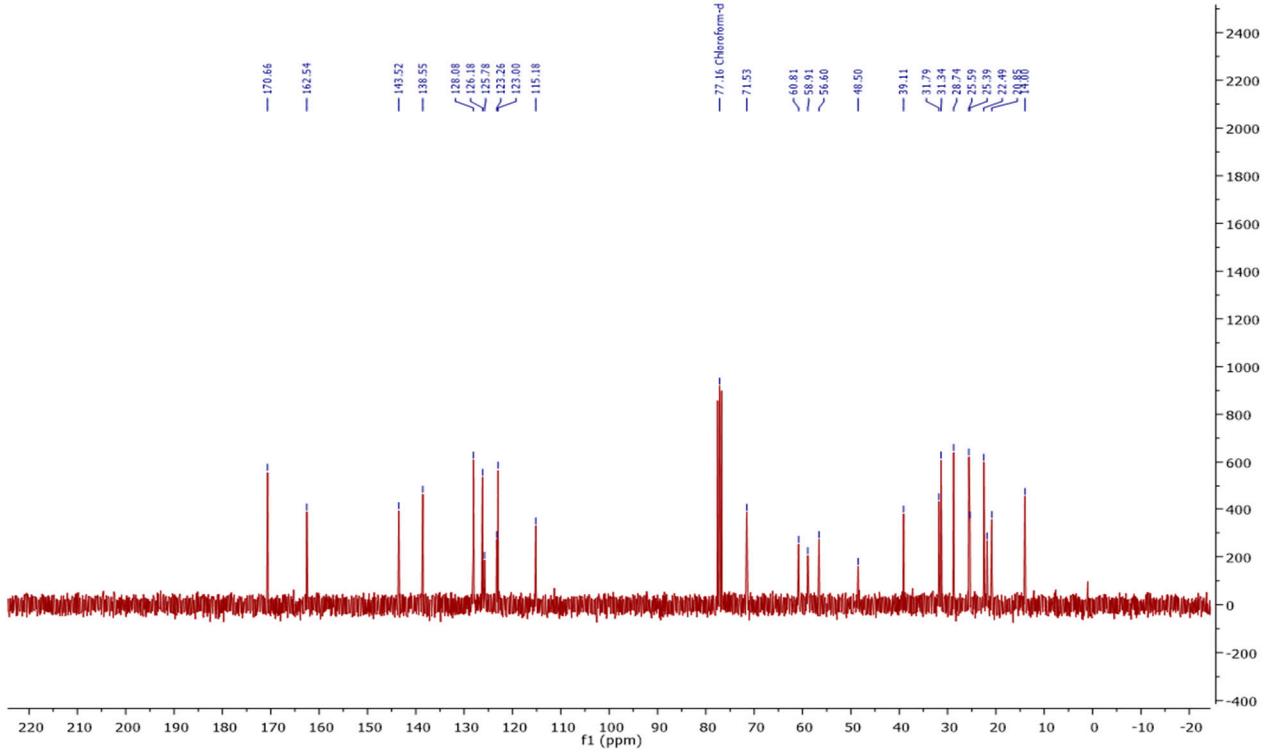

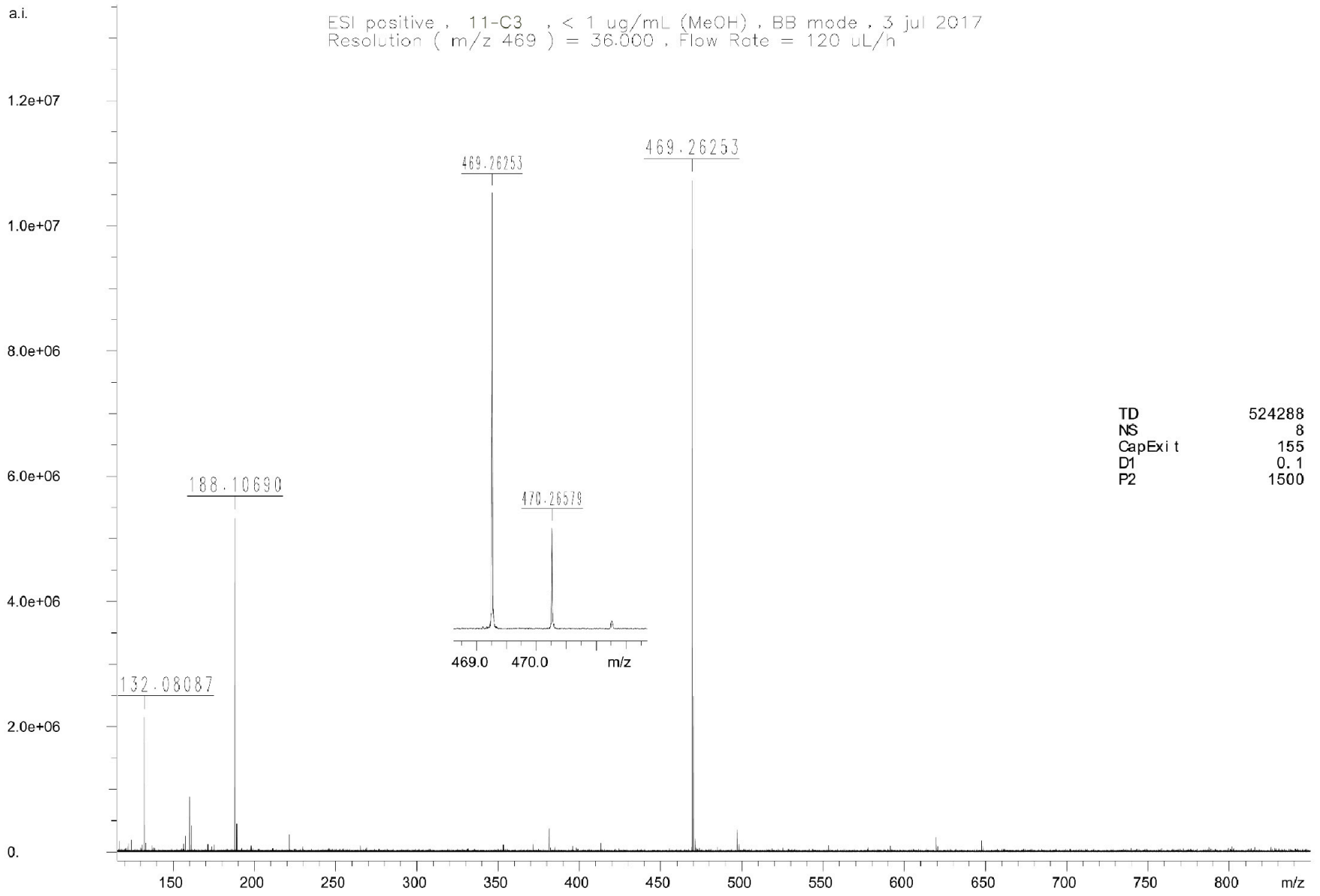
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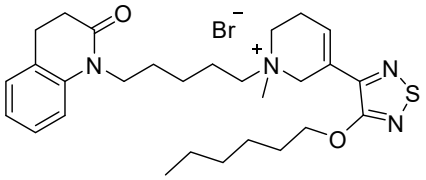
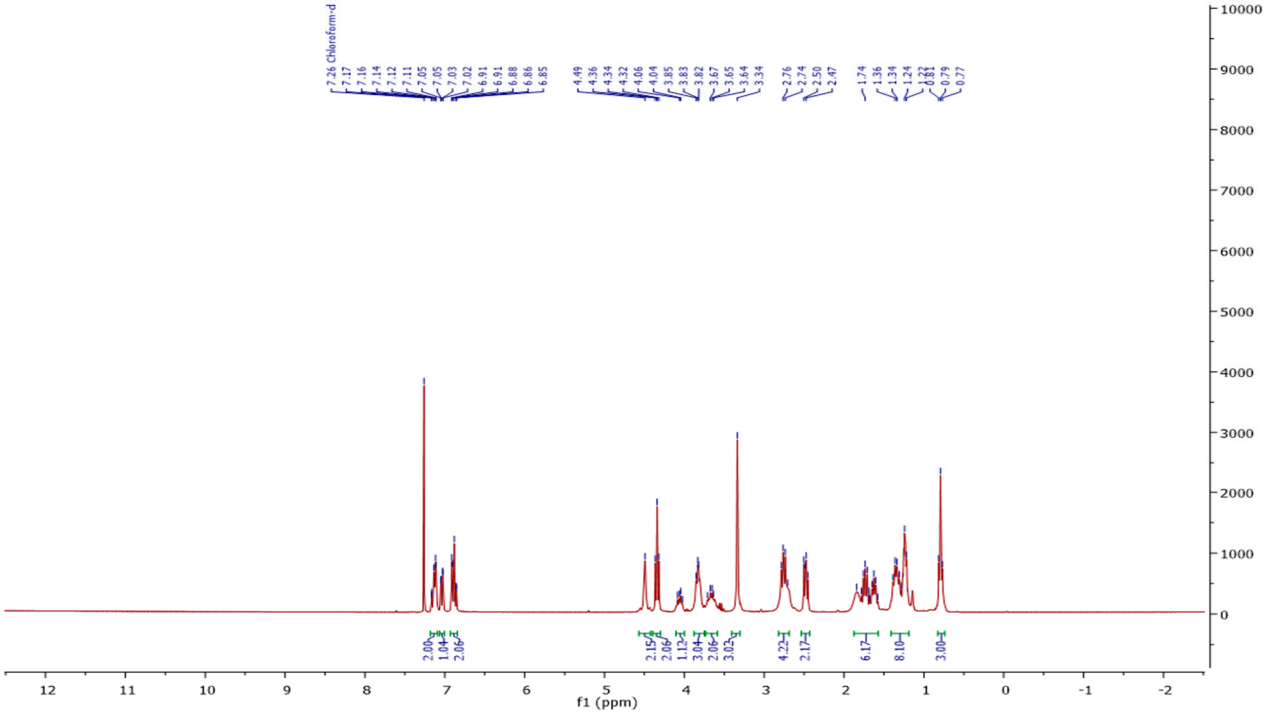
ESI positive , 11-C3 , < 1 ug/mL (MeOH) , BB mode , 3 jul 2017
Resolution (m/z 469) = 36.000 , Flow Rate = 120 uL/h
1.2e+07
1.0e+07
8.0e+06
6.0e+06
4.0e+06
2.0e+06
0.
469.26253
469.26253
188.10690
470.26579
132.08087
469.0
470.0
m/z
150
200
250
300
350
400
450
500
550
600
650
700
750
800
m/z
TD 524288
NS 8
CapExit 155
D1 0.1
P2 1500

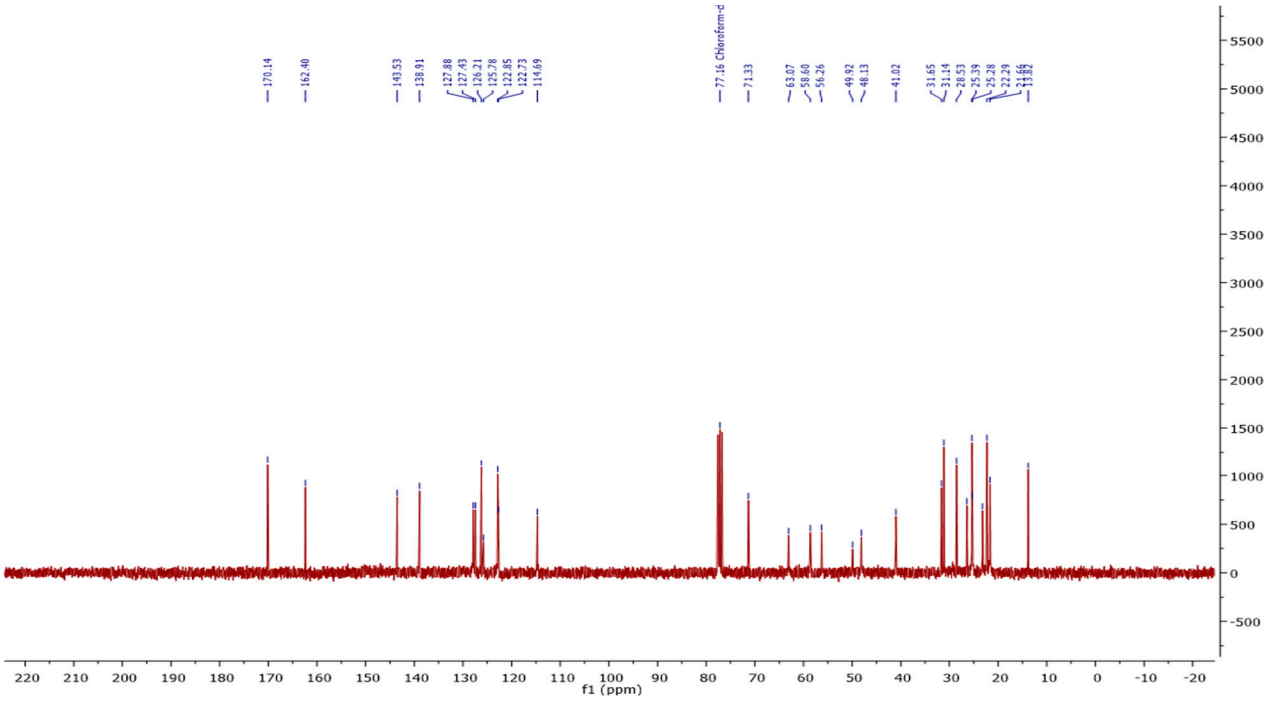
13-C5

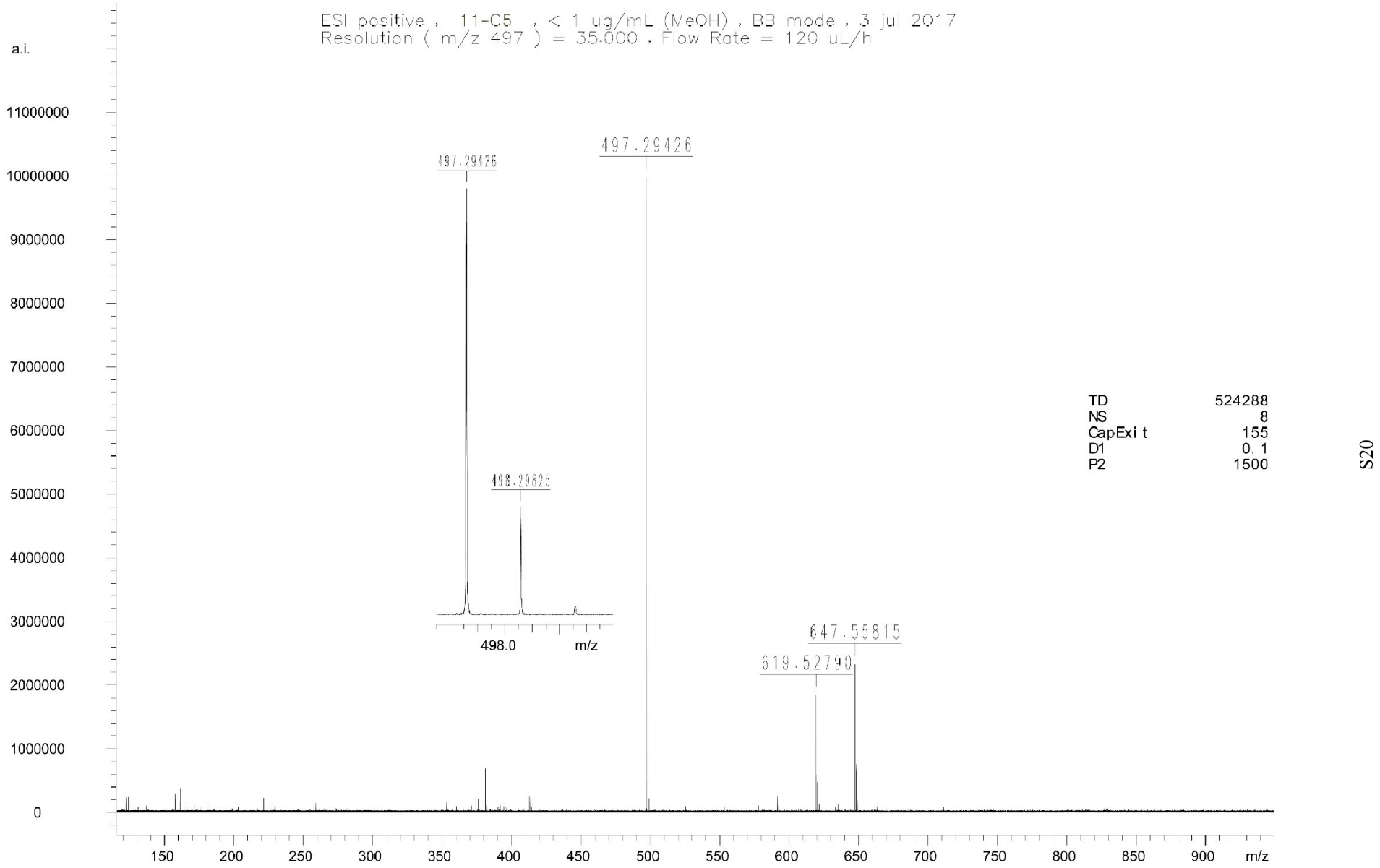


^{1}H NMR spectrum

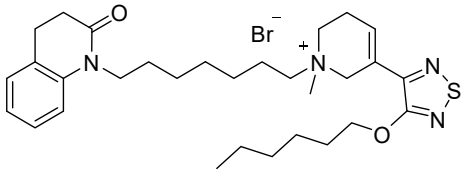


^{13}C NMR spectrum




ESI positive , 11-C5 , < 1 ug/mL (MeOH) , BB mode , 3 jul 2017
Resolution (m/z 497) = 35.000 , Flow Rate = 120 uL/h
a.i.
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
497.29426
497.29426
498.29825
498.0
m/z
647.55815
619.52790
TD 524288
NS 8
CapExit 155
D1 0.1
P2 1500
150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 m/z

13-C7



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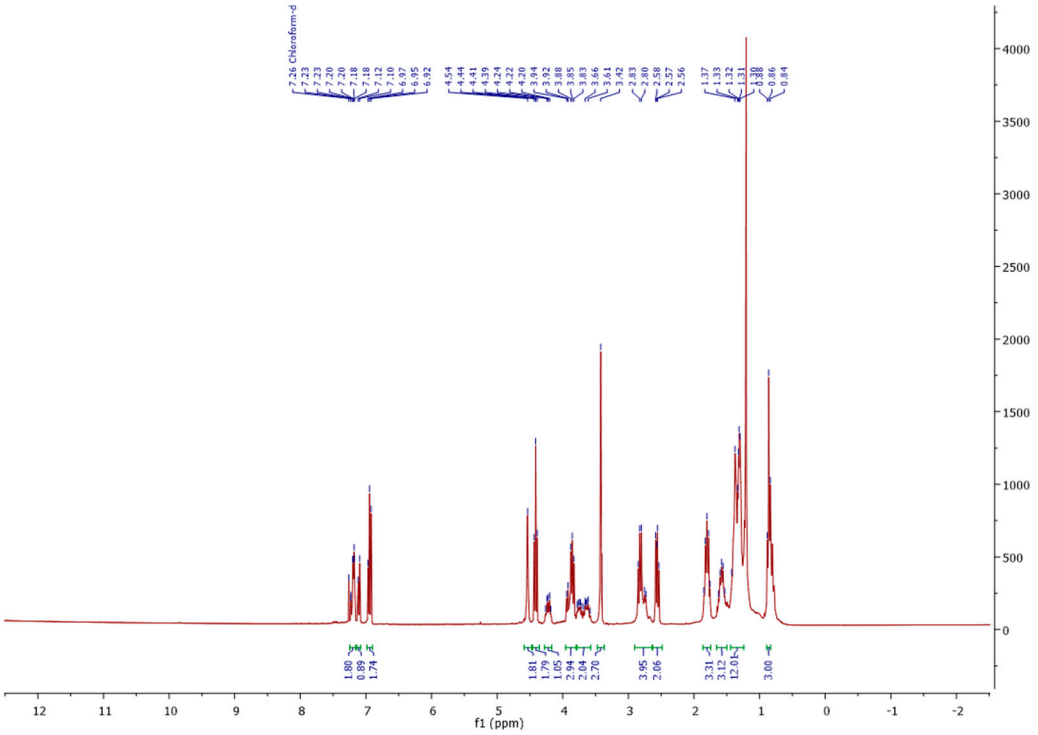
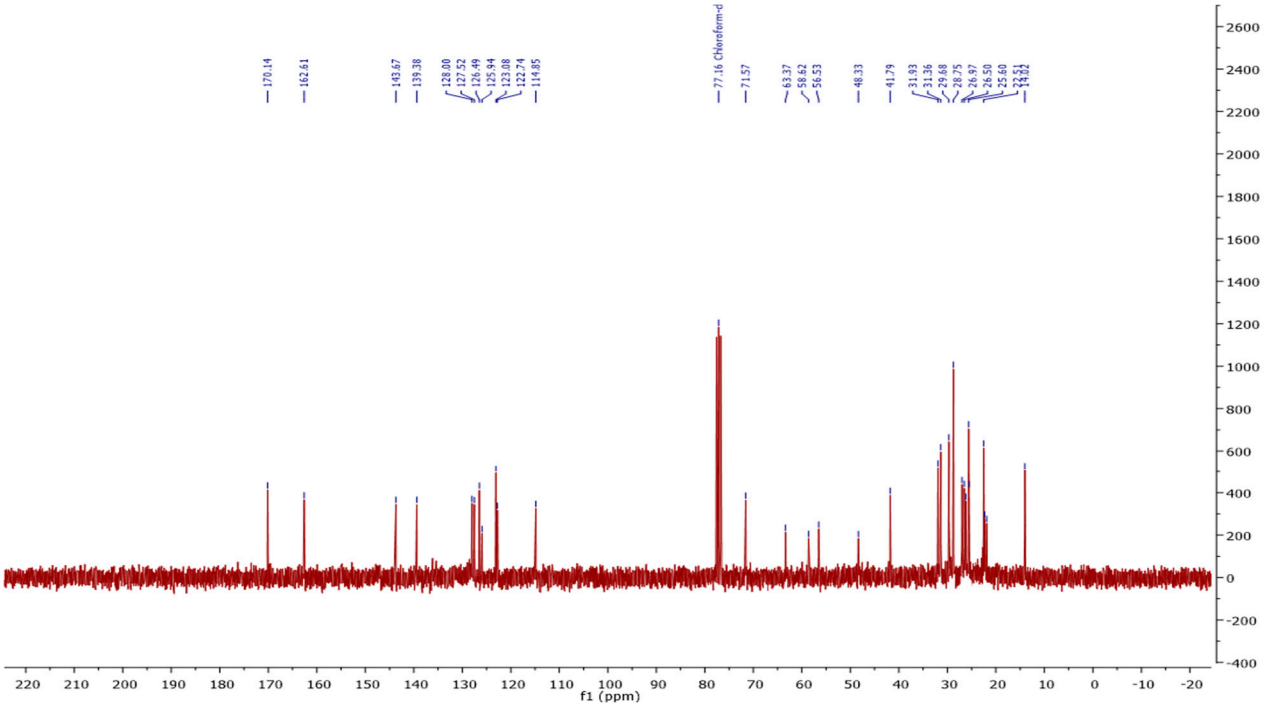
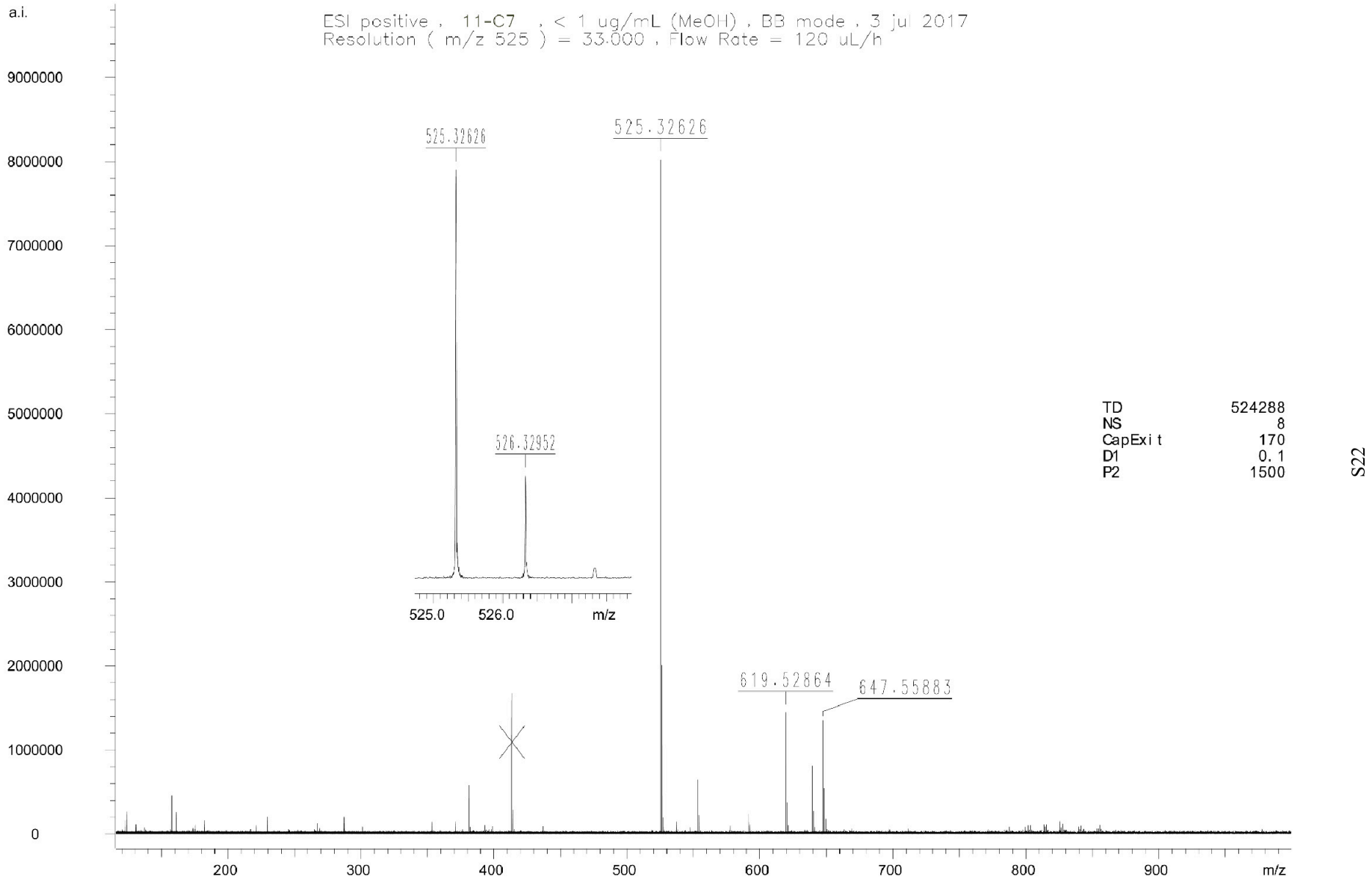
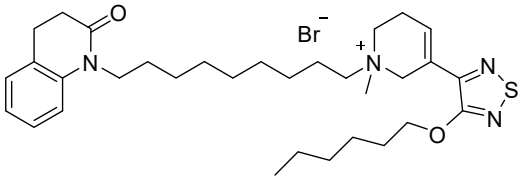


^{13}C NMR spectrum

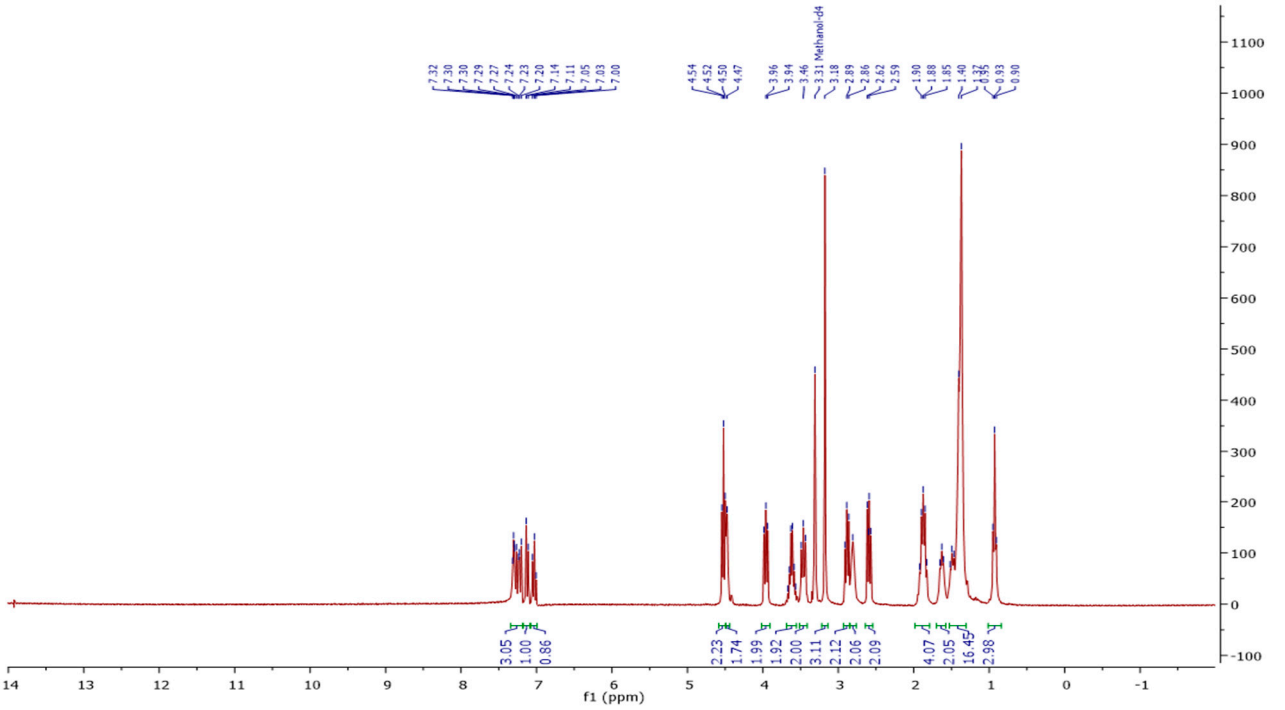



a.i.
ESI positive , 11-C7 , < 1 ug/mL (MeOH) , BB mode , 3 jul 2017
Resolution (m/z 525) = 33.000 , Flow Rate = 120 uL/h
525.32626
525.32626
526.32952
525.0
526.0
m/z
619.52864
647.55883
TD 524288
NS 8
CapExit 170
D1 0.1
P2 1500
S22
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
200
300
400
500
600
700
800
900
m/z

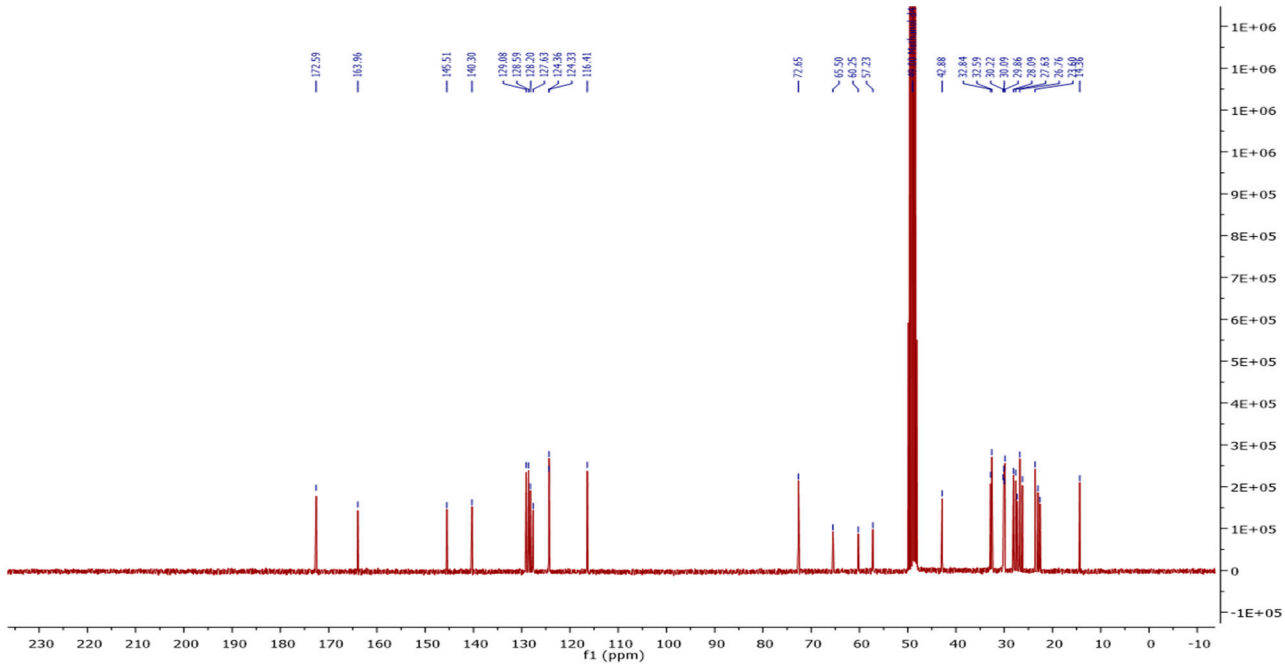
13-C9

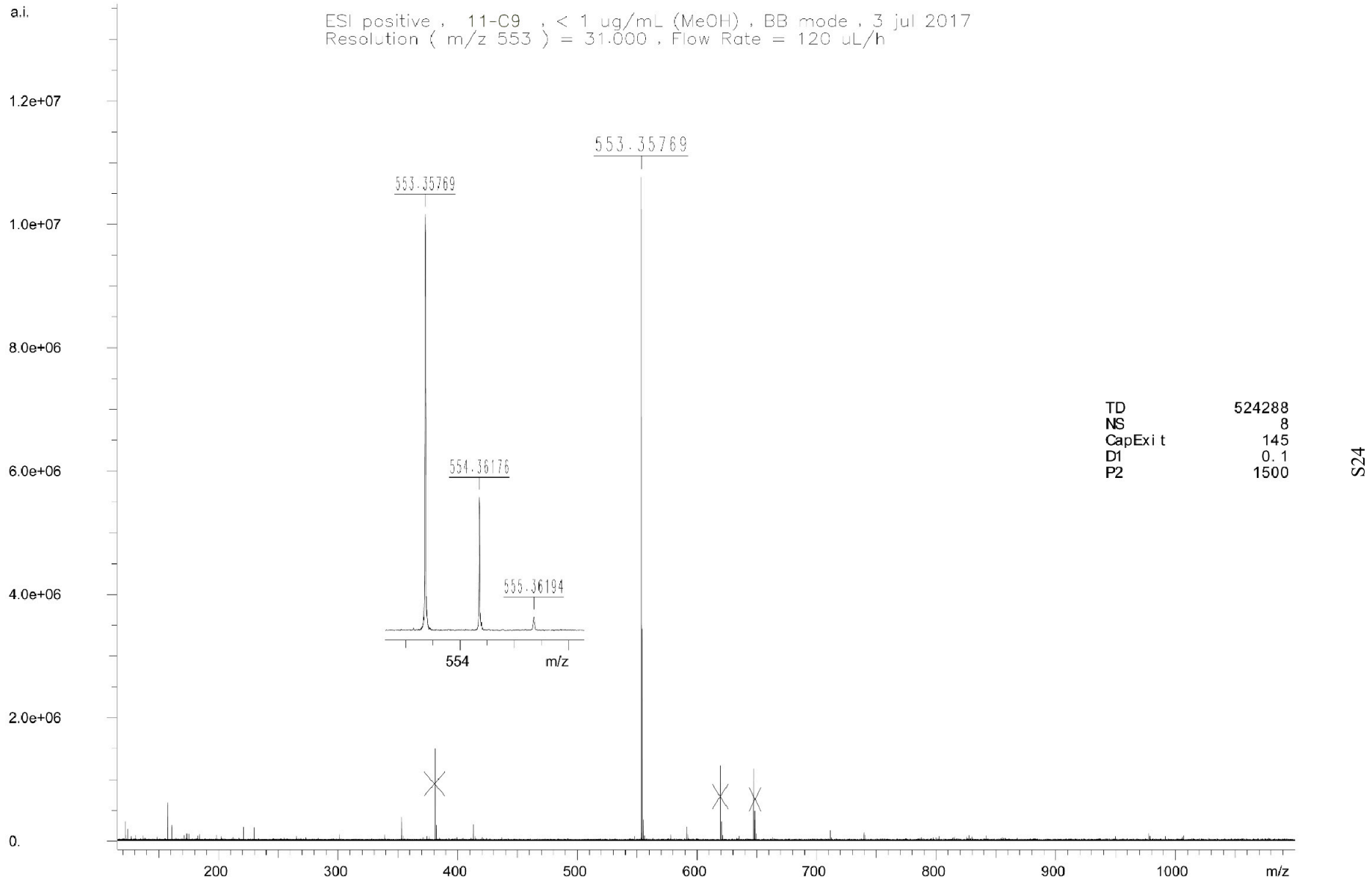


^{1}H NMR spectrum

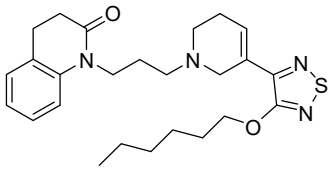


^{13}C NMR spectrum

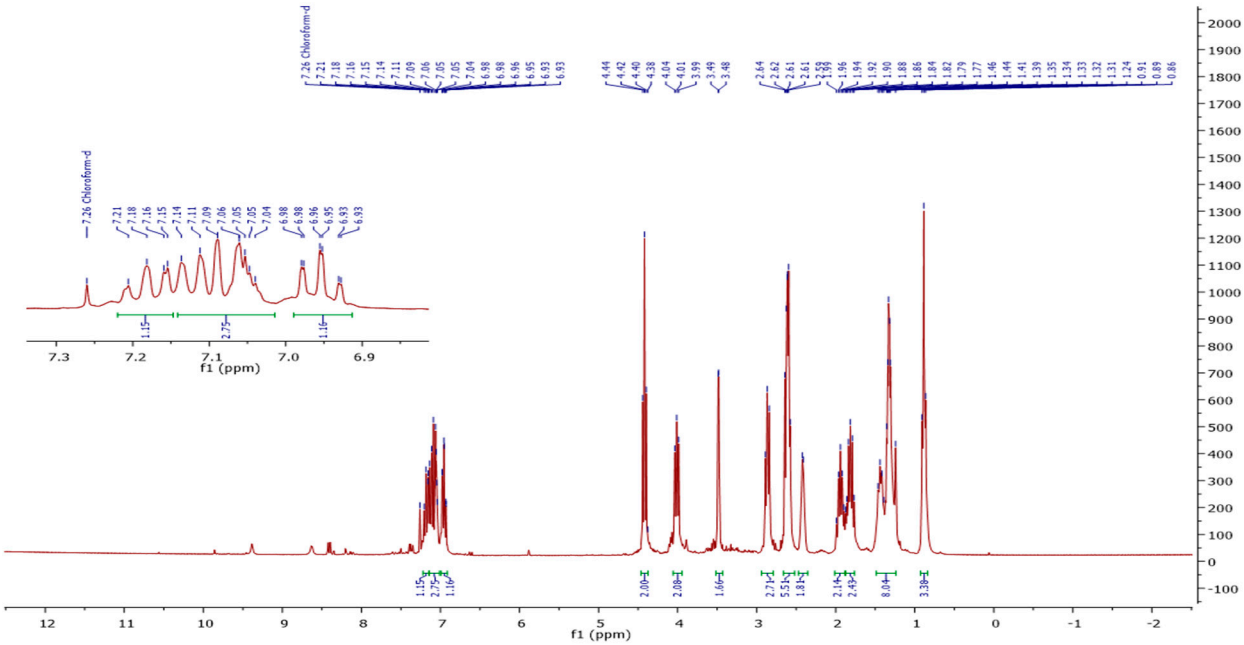



a.i.
ESI positive , 11-C9 , < 1 ug/mL (MeOH) , BB mode , 3 jul 2017
Resolution (m/z 553) = 31.000 , Flow Rate = 120 uL/h
1.2e+07
1.0e+07
8.0e+06
6.0e+06
4.0e+06
2.0e+06
0.
553.35769
553.35769
554.36176
555.36194
554
m/z
TD 524288
NS 8
CapExit 145
D1 0.1
P2 1500
200
300
400
500
600
700
800
900
1000
m/z

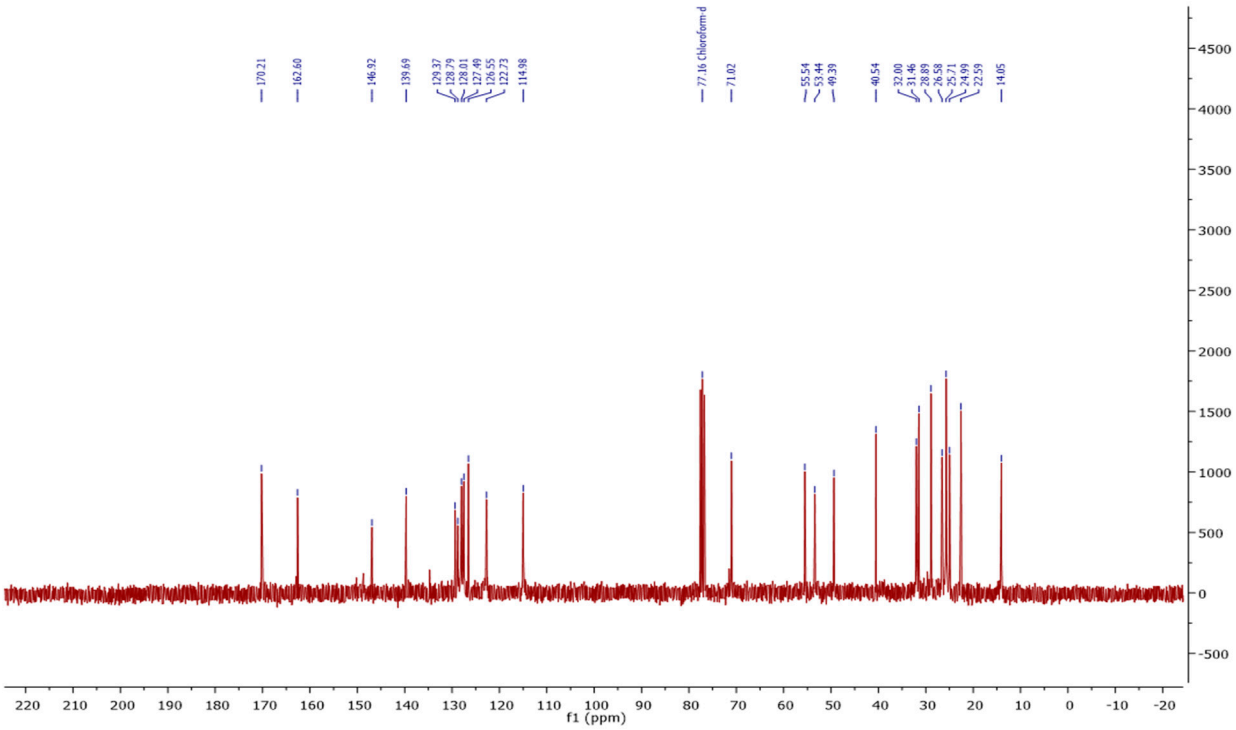
12-C3



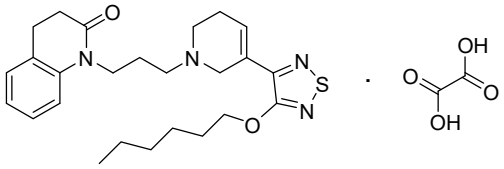
^{1}H NMR spectrum



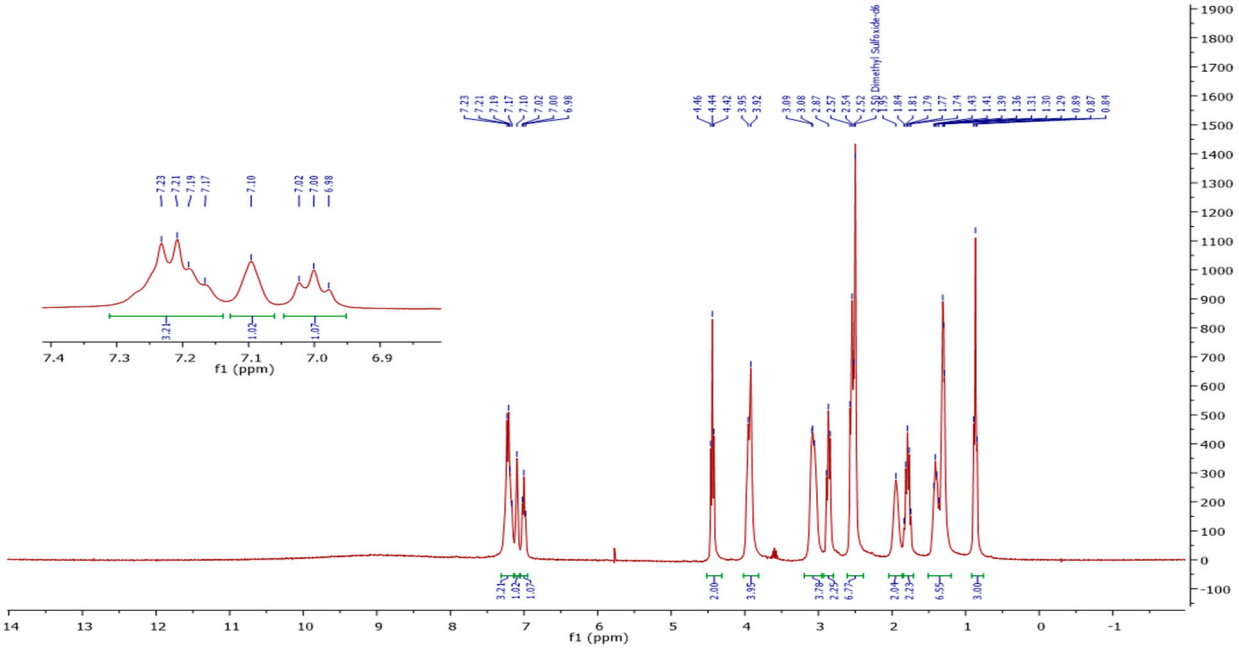
^{13}C NMR spectrum



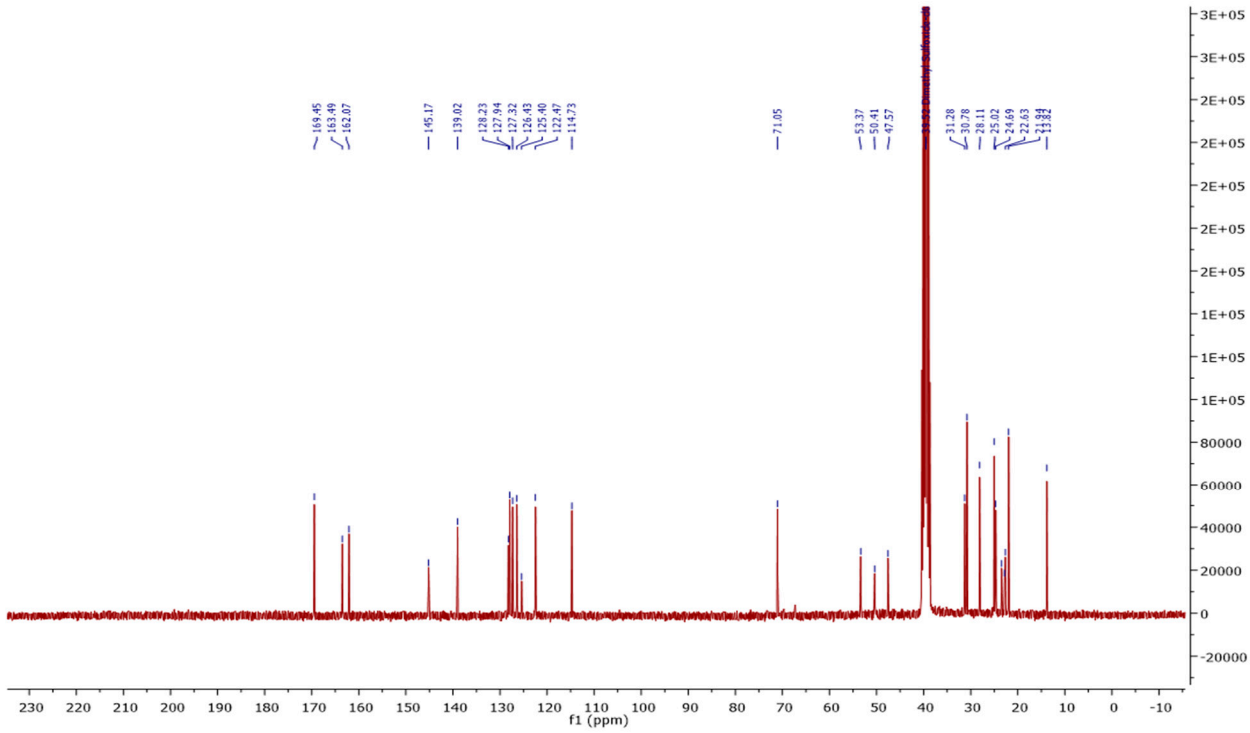
12-C3 Oxalate



^{1}H NMR spectrum



^{13}C NMR spectrum



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e-mail: info@labredox.com

Codice Fiscale 08709300153
Partita IVA 00834700965
R.E.A. MB 1114865
Reg. Imp. Monza Brianza 08709300153

Analytical Chemistry & Process Safety Testing

Certificato di Analisi
Certificate of Analysis

N°Campione/ Sample N°: 2016001294/LAB

Data apertura/ Registration date: 19/02/16

Richiedente/ Requested by:
Dallanoce

Committente/ Company:
UNIVERSITA' DI MILANO-Dip.Scienze Farm."Pietro Pratesi"

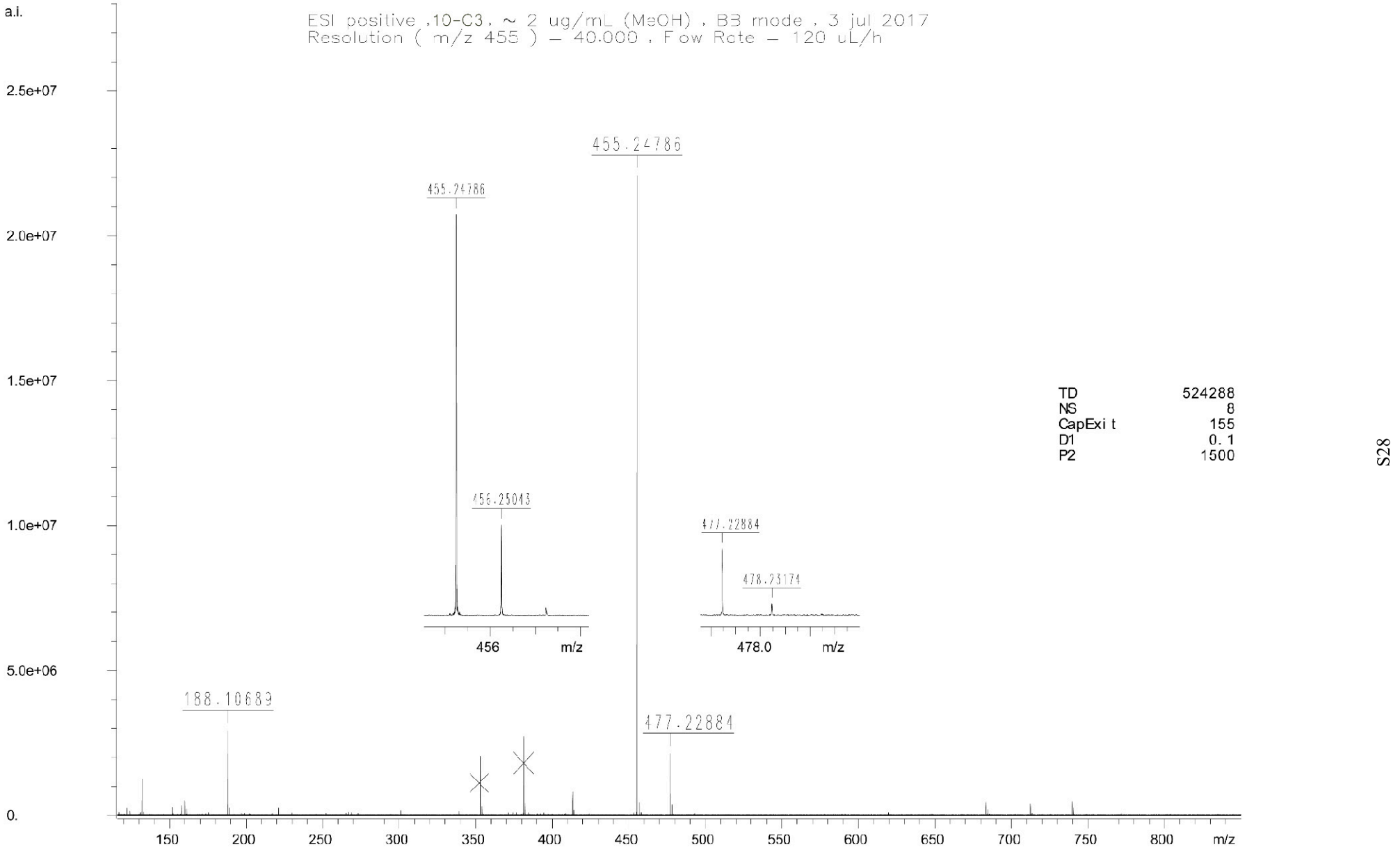
Campione/ Sample:
Q3X

Lotto/ Batch:

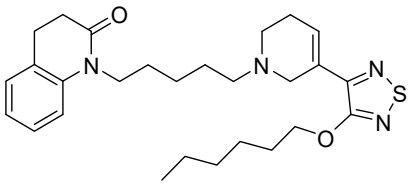
Analisi - Analysis Metodo Analitico - Analytical method	Risultati Results	Specifiche Specifications
CHN SOP - MET 019		
Carbonio	58.23%	
Idrogeno	6.57%	
Azoto	9.88%	

Note Chiusura/ Notes:

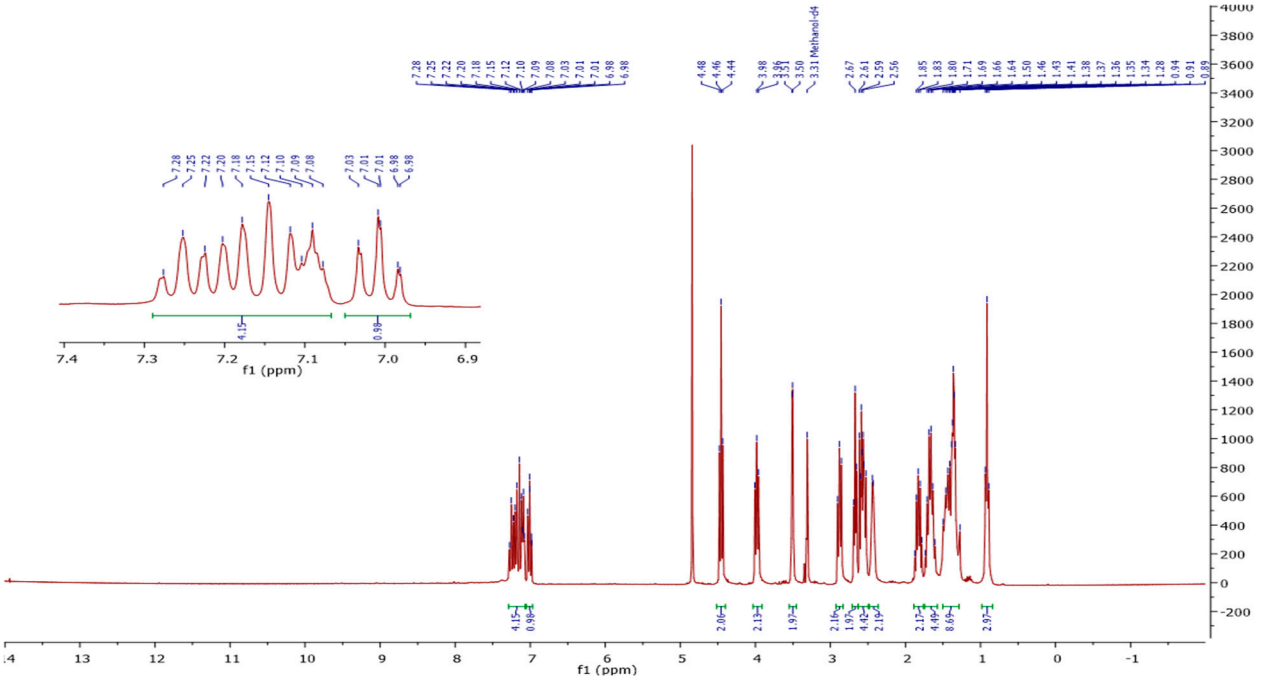
Calculated Elementary analysis for stoichiometry for 1:1
Anal. calcd for $C_{27}H_{36}N_4O_6S$: C, 59.54; H, 6.66; N, 10.29; found: C, 58,23; H, 6,57; N, 9.88.


ESI positive ,10-C3, ~ 2 ug/mL (MeOH) , BB mode , 3 jul 2017
Resolution (m/z 455) = 40.000 , Flow Rate = 120 uL/h
a.i.
2.5e+07
2.0e+07
1.5e+07
1.0e+07
5.0e+06
0.
455.24786
455.24786
456.25043
456
m/z
477.22884
478.23174
478.0
m/z
188.10689
477.22884
150
200
250
300
350
400
450
500
550
600
650
700
750
800
m/z
TD 524288
NS 8
CapExit 155
D1 0.1
P2 1500

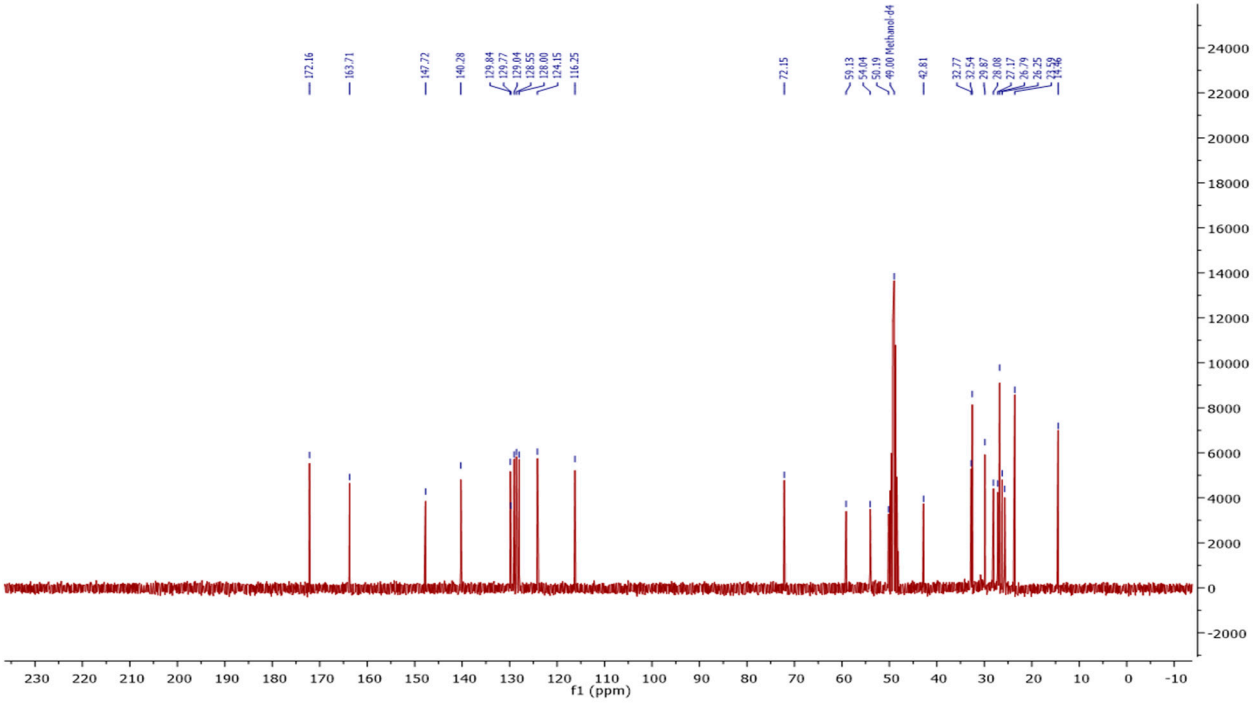
12-C5

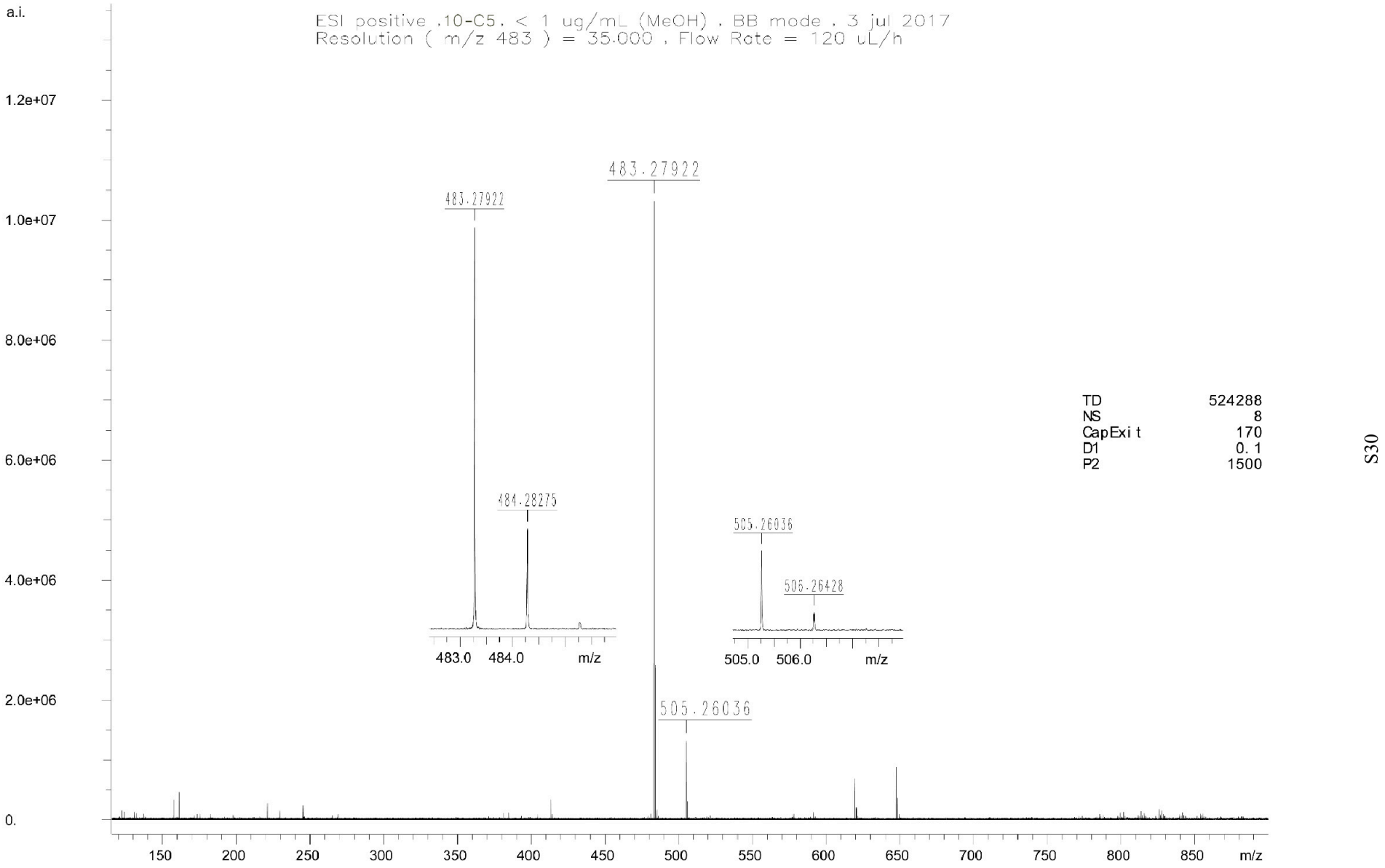


^{1}H NMR spectrum



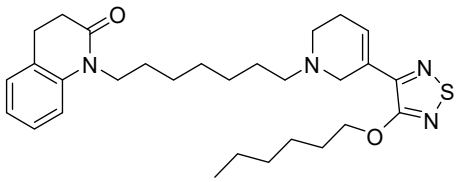
^{13}C NMR spectrum



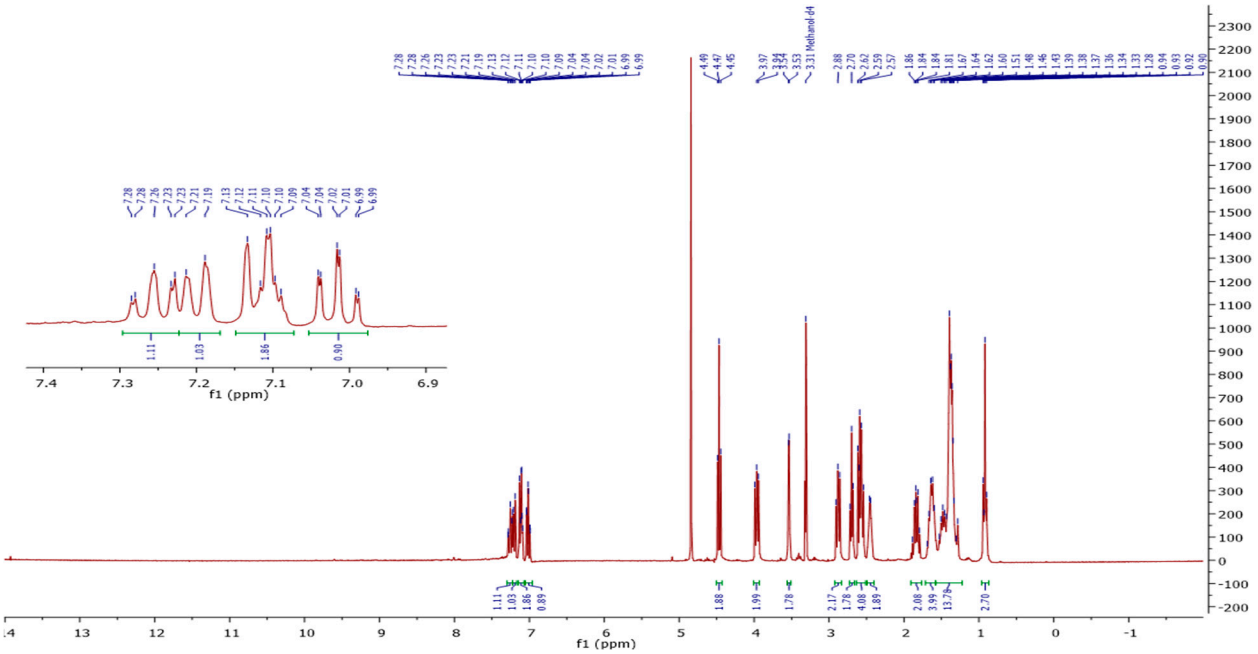

a.i.
ESI positive ,10-C5, < 1 ug/mL (MeOH) , BB mode , 3 jul 2017
Resolution (m/z 483) = 35.000 , Flow Rate = 120 uL/h
1.2e+07
1.0e+07
8.0e+06
6.0e+06
4.0e+06
2.0e+06
0.
483.27922
483.27922
484.28275
505.26036
505.26036
506.26428
483.0
484.0
m/z
505.0
506.0
m/z
TD 524288
NS 8
CapExit 170
D1 0.1
P2 1500
150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 m/z

S30

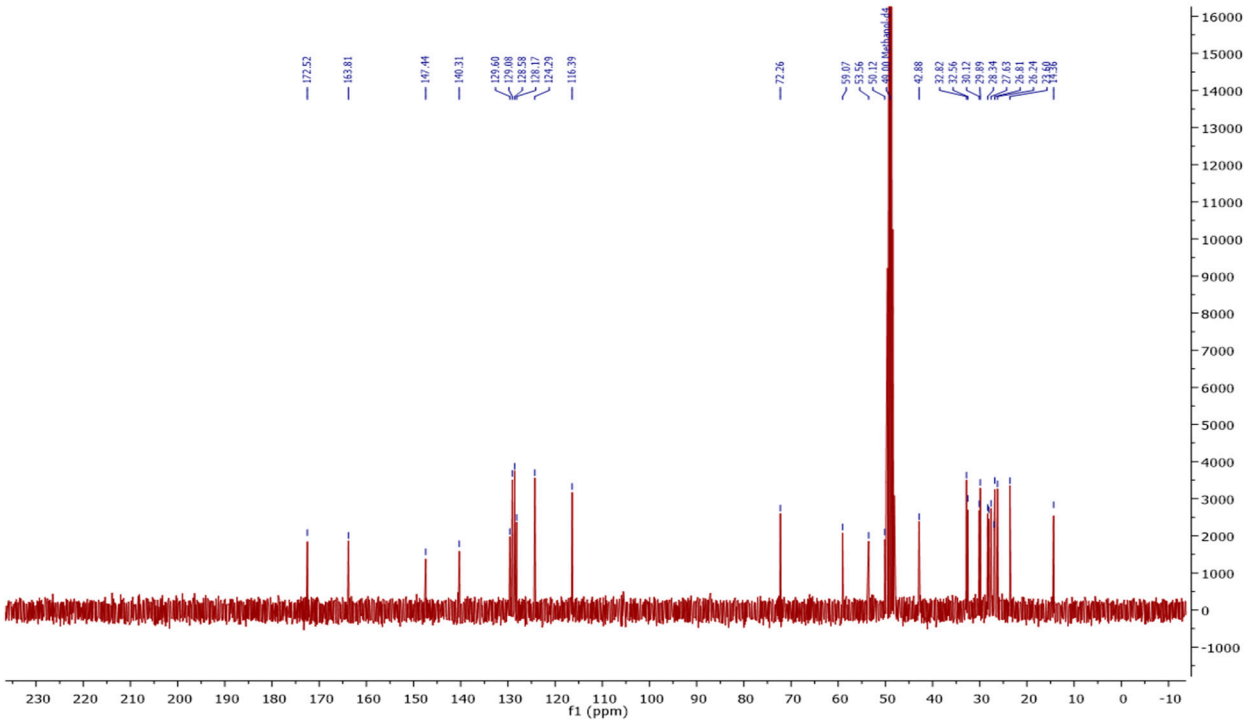
12-C7

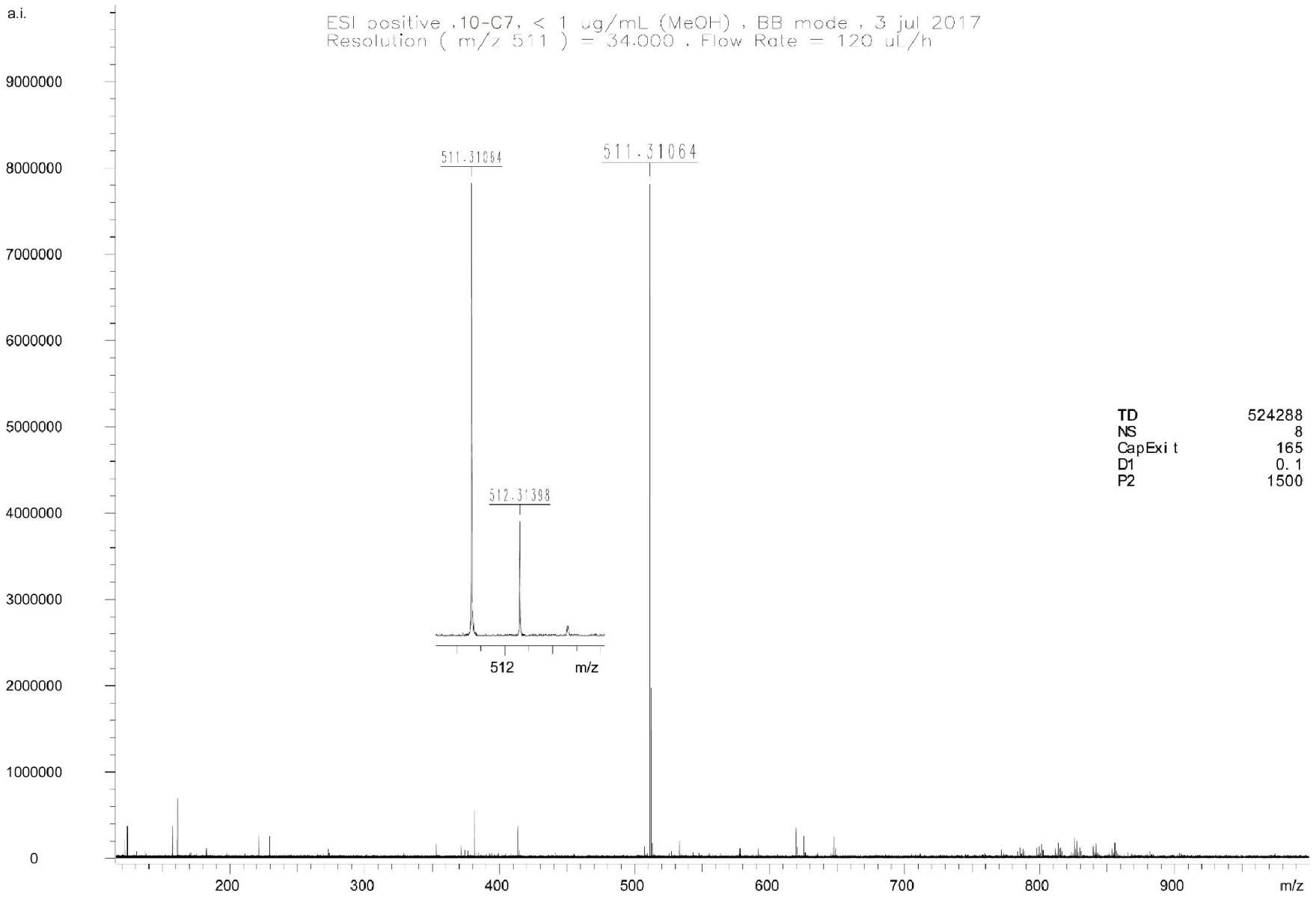


^{1}H NMR spectrum



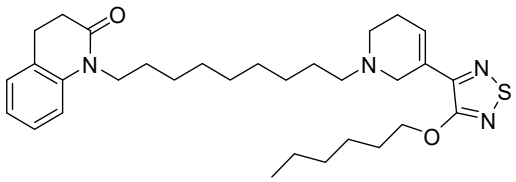
^{13}C NMR spectrum



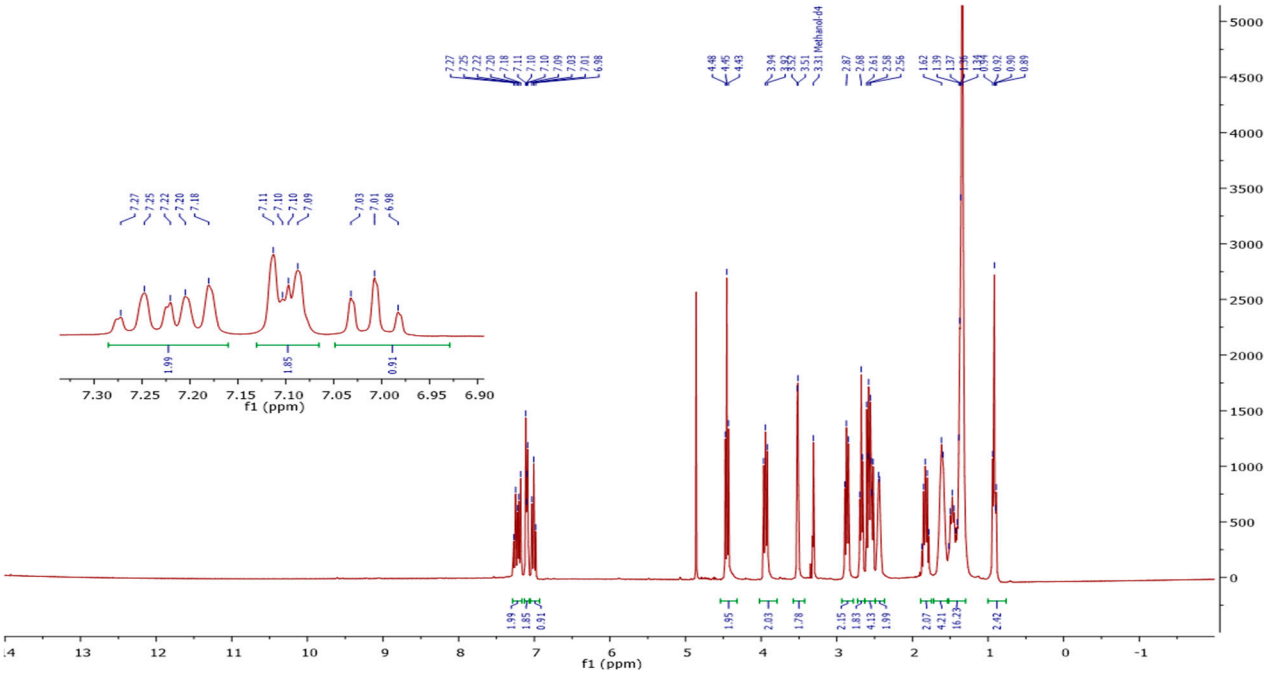

a.i.
ESI positive ,10-C7, < 1 ug/mL (MeOH) , BB mode , 3 jul 2017
Resolution (m/z 511) = 34.000 , Flow Rate = 120 ul/h
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
511.31064
511.31064
512.31398
512
m/z
TD 524288
NS 8
CapExit 165
D1 0.1
P2 1500
200
300
400
500
600
700
800
900
m/z

S32

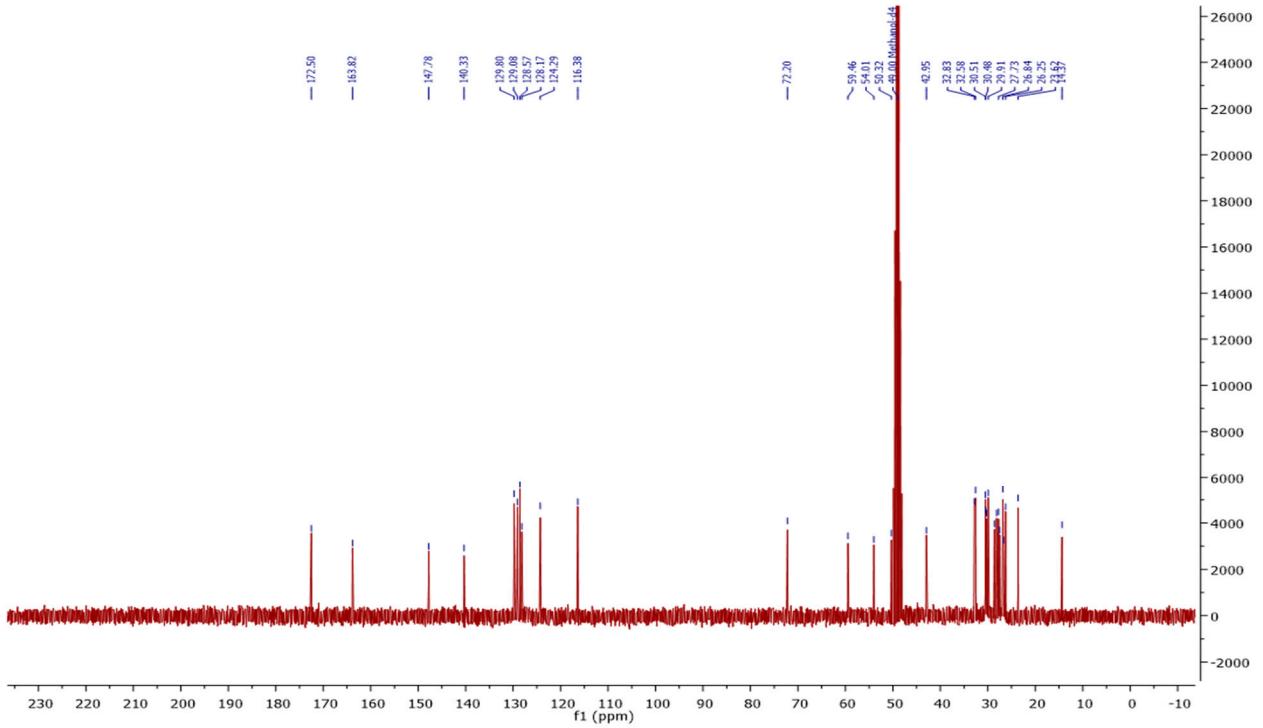
12-C9

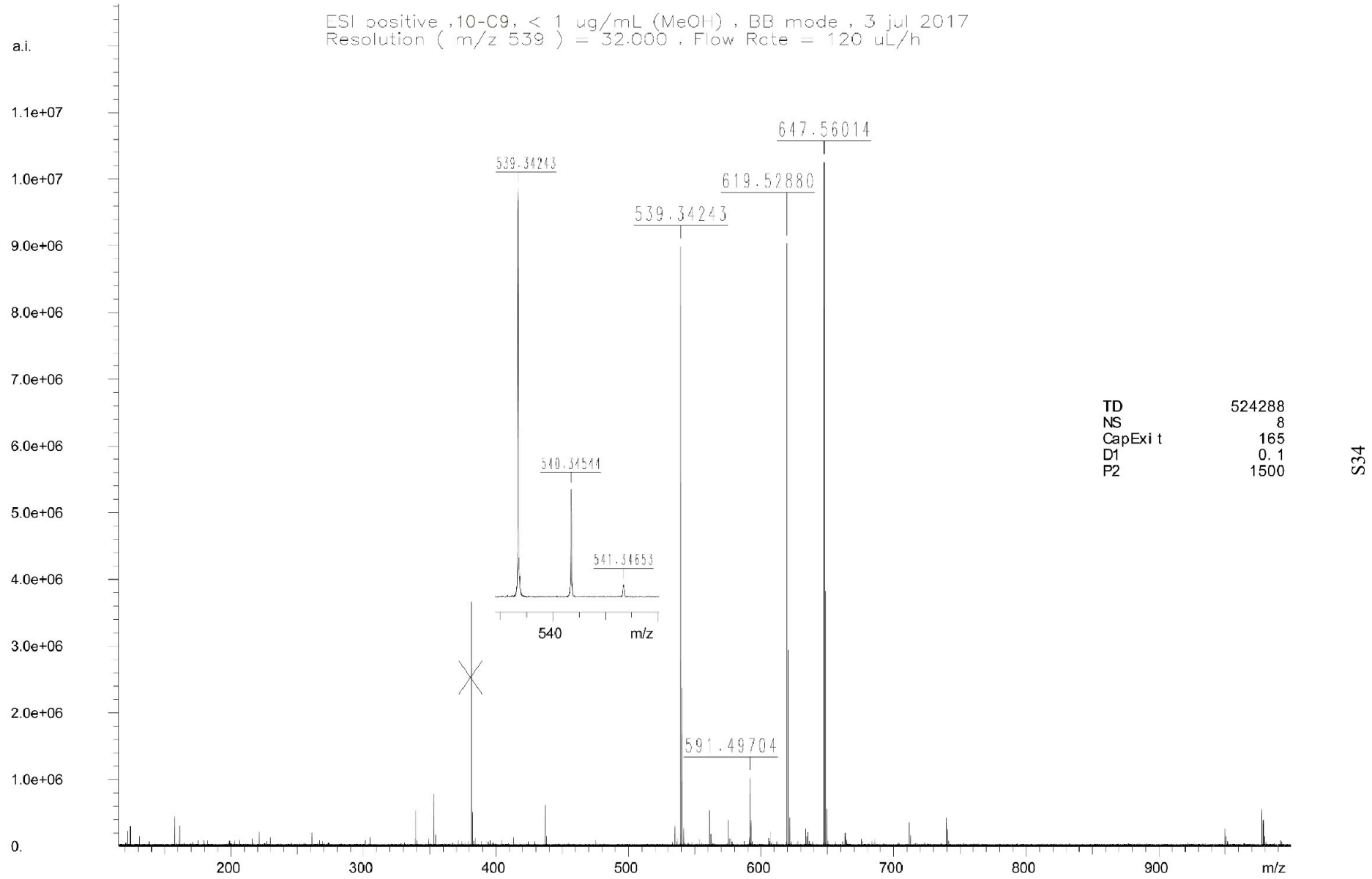


^{1}H NMR spectrum



^{13}C NMR spectrum




ESI positive ,10-C9, < 1 ug/mL (MeOH) , BB mode , 3 jul 2017
Resolution (m/z 539) = 32.000 , Flow Rate = 120 uL/h
a.i.
1.1e+07
1.0e+07
9.0e+06
8.0e+06
7.0e+06
6.0e+06
5.0e+06
4.0e+06
3.0e+06
2.0e+06
1.0e+06
0.
647.56014
619.52880
539.34243
539.34243
540.34544
541.34653
540
m/z
591.49704
200
300
400
500
600
700
800
900
m/z
TD 524288
NS 8
CapExit 165
D1 0.1
P2 1500
S34