

Appendix IV: Reference library

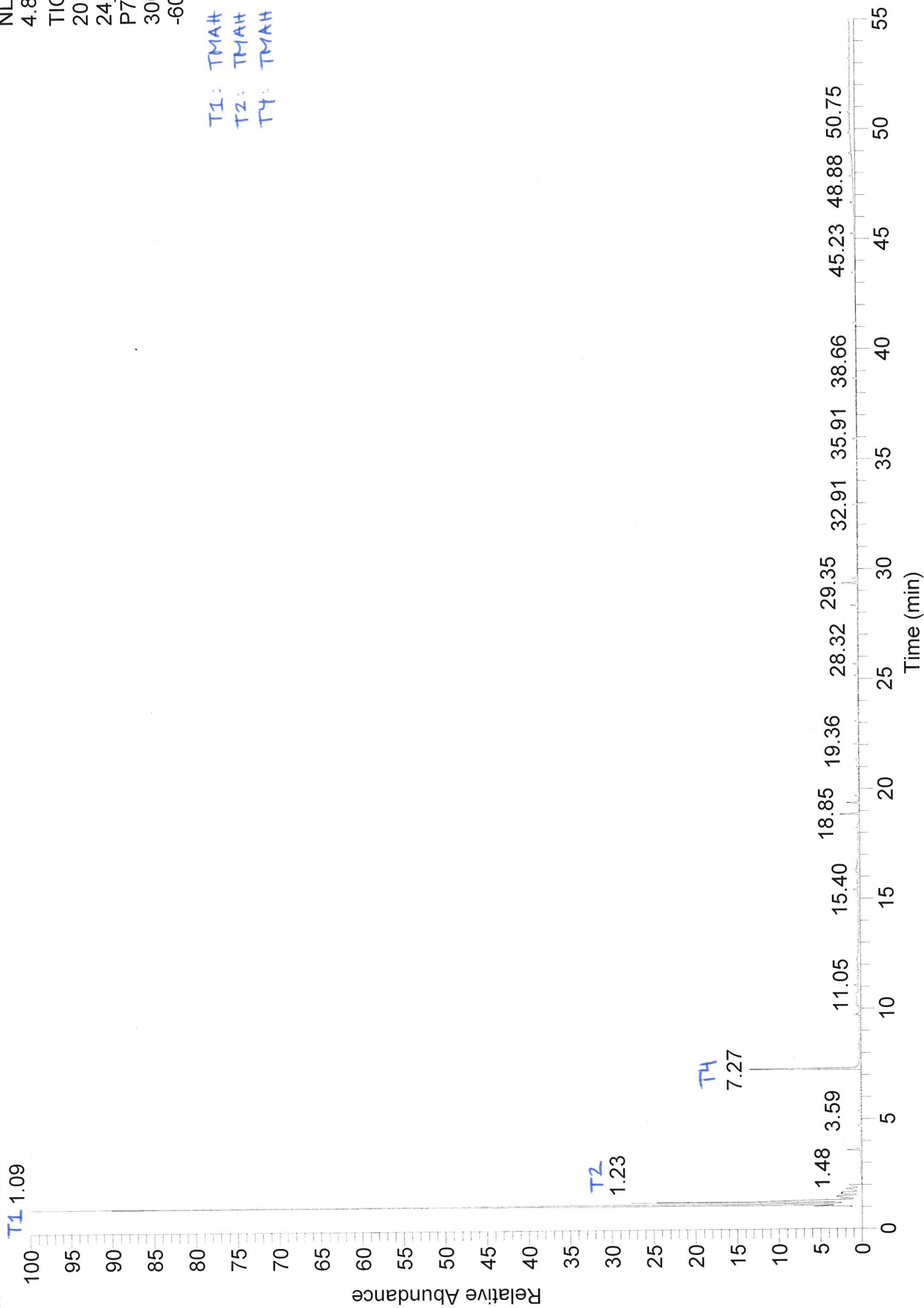
Listed approximately according to occurrence in pyrogram ($\sim t_R$) in temperature programme 1 (TP1)

TMAH (ScA)	pp. 1-2
TMAH (ScB)	pp. 3-4
Pyrrole (g)	pp. 5-6
Pyrrole+TMAH	pp. 7-8
Toluene (g)	p. 9
Toluene + TMAH	p. 9
Indole (g)	pp. 10-11
Dimethylated diacids (Su, Az, Se)	pp. 12-15
Fatty acids (La, Pe, P, S) + TMAH	pp. 16-17
Methylated fatty acids (M, P, O, Li)	pp. 18-19
Methylated oleic acid (O)	pp. 20-21
Alkyl nitriles (C17, C18)	pp. 22-25
Proline-Glycine (dipeptide) +TMAH	pp. 26-28
Cholesterol +TMAH	pp. 29-31

RT: 0.00 - 55.02
T1 1.09

NL:
4.84E7
TIC MS
2018-09-
24_blankTMAH_
P700_GC40-
300_MS_(45)60
-600_MTM_a

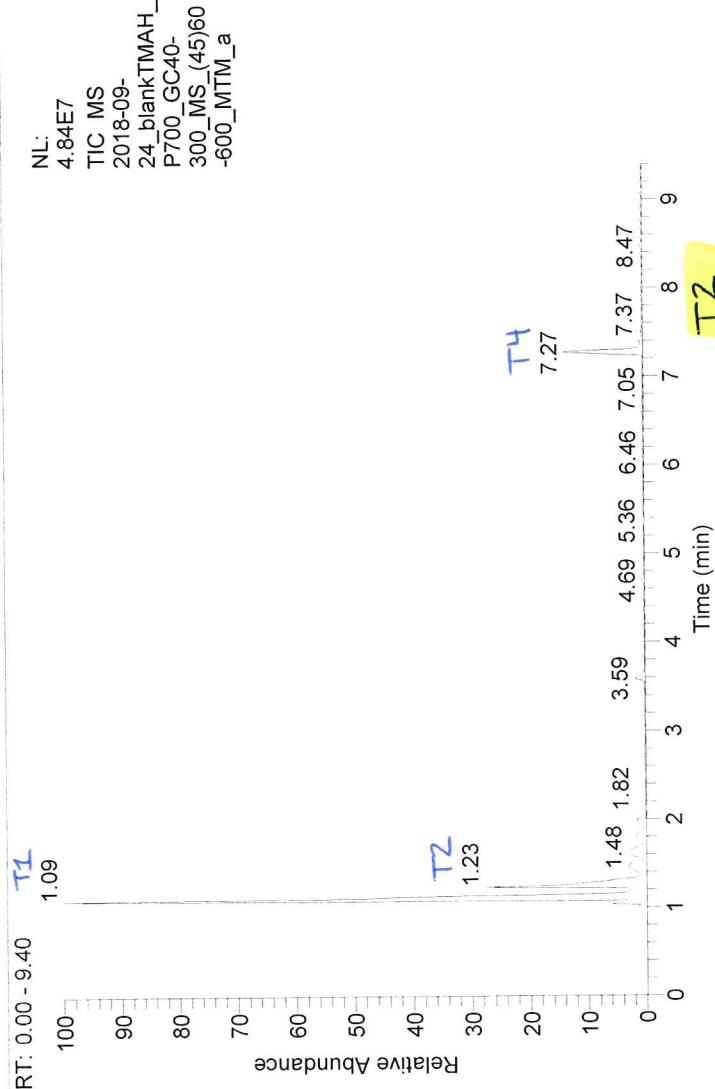
T1: TMAH fragment 1
T2: TMAH fragment 2
T4: TMAH fragment 4



T1

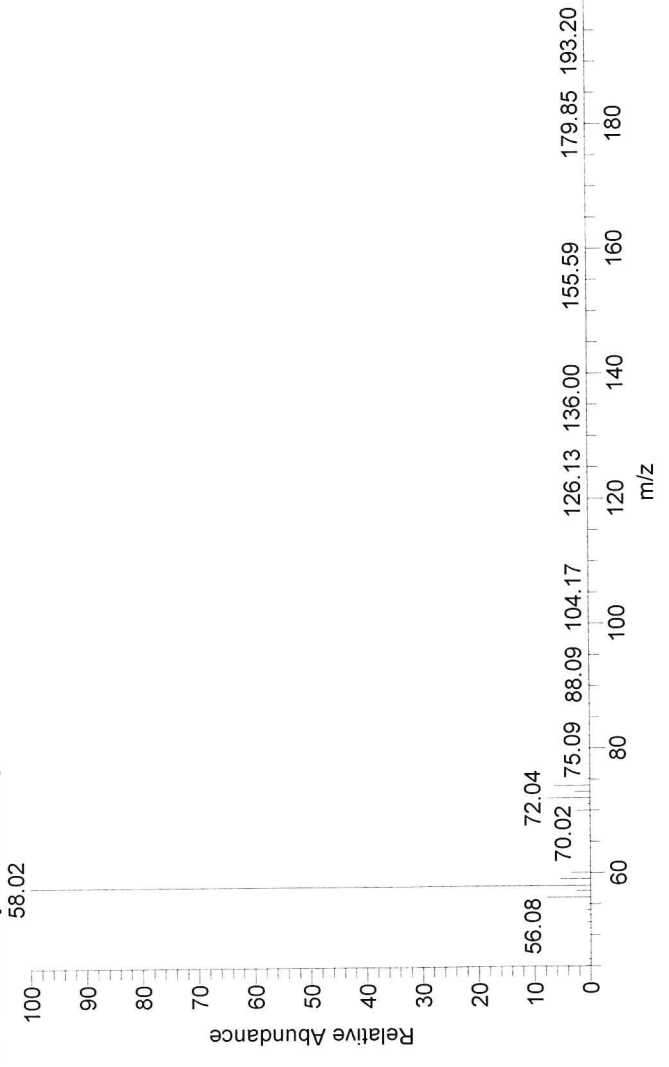
RT: 0.00 - 9.40

NL: 4.84E7
TIC MS
2018-09-24_blankTMAH_P700_GC40-300_MS_(45)60-600_MTM_a #12



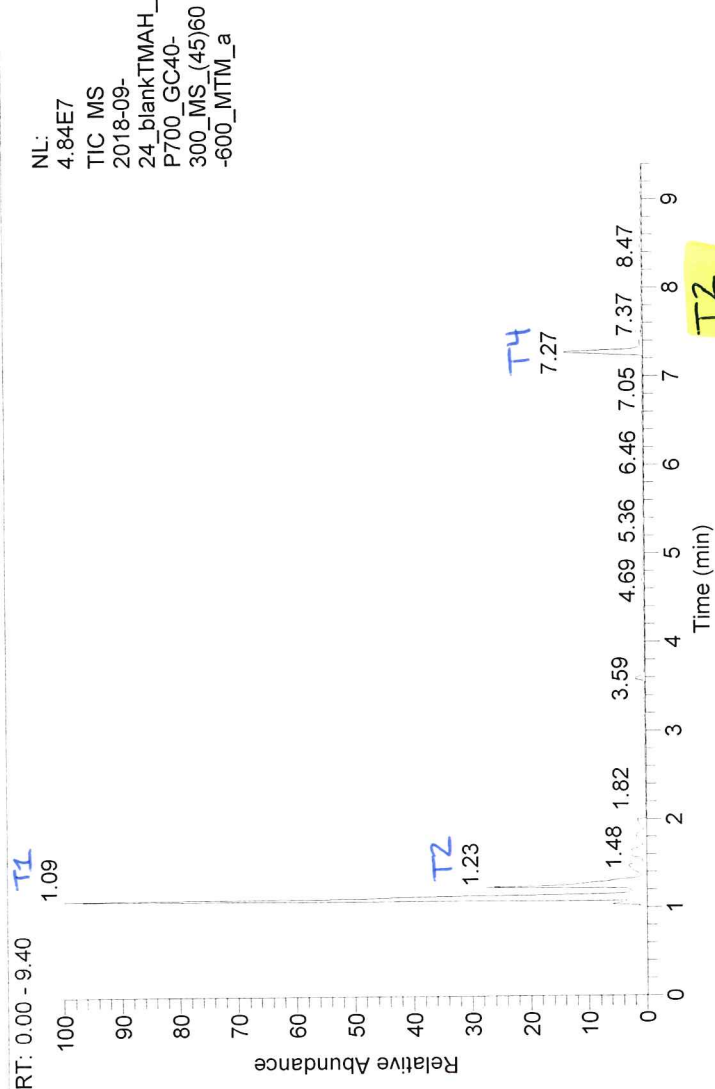
2018-09-24_blankTMAH_P700_GC40-300_MS_(45)60-600_MTM_a #29

T: + c Full ms [45.00-600.00]



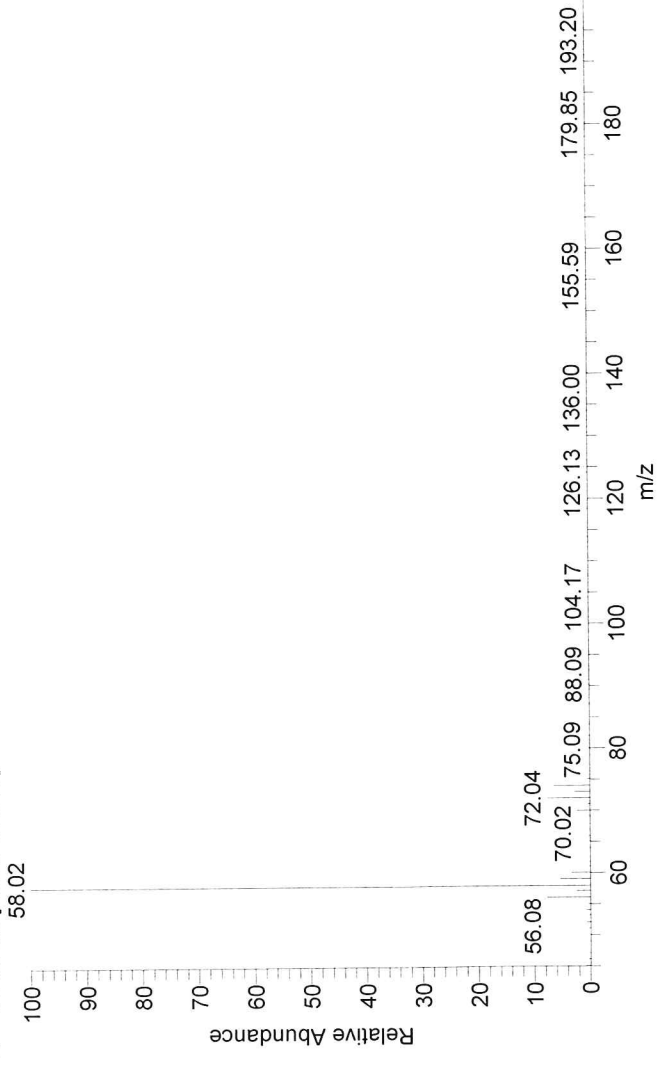
T1

RT: 1.09 AV: 1 NL: 3.07E7



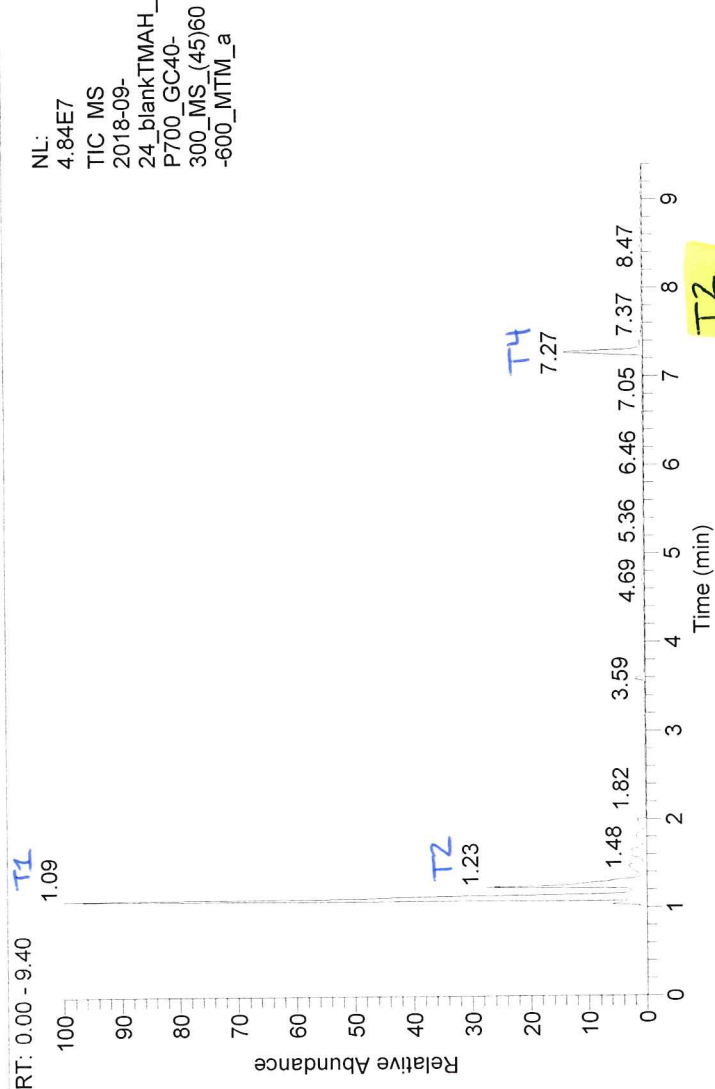
2018-09-24_blankTMAH_P700_GC40-300_MS_(45)60-600_MTM_a #757

T: + c Full ms [60.00-600.00]



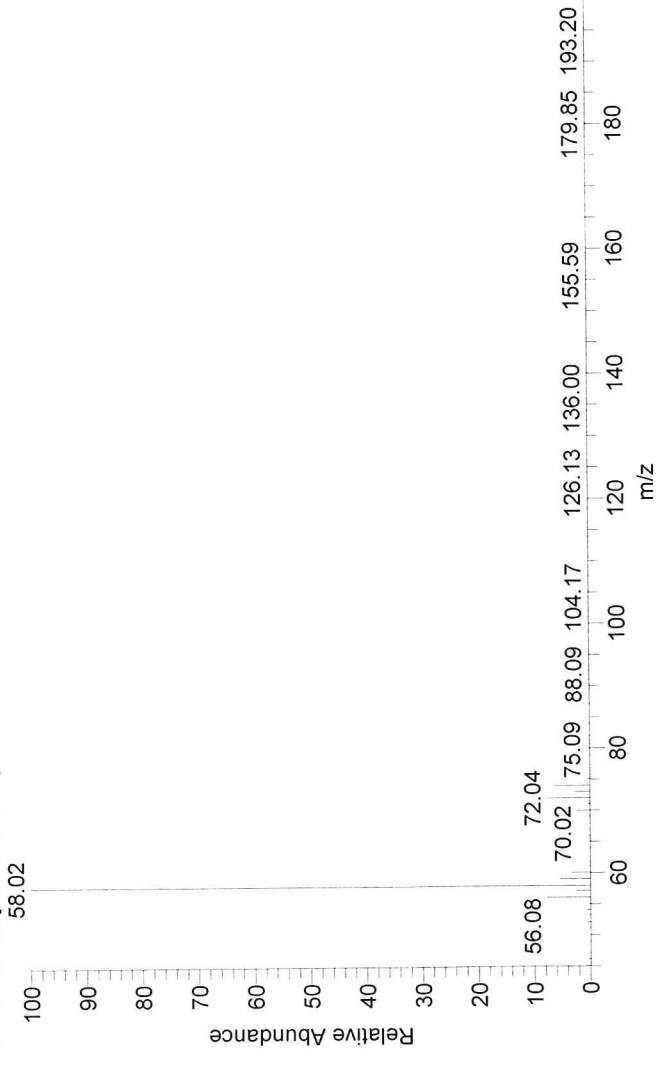
T4

RT: 7.27 AV: 1 NL: 5.04E6



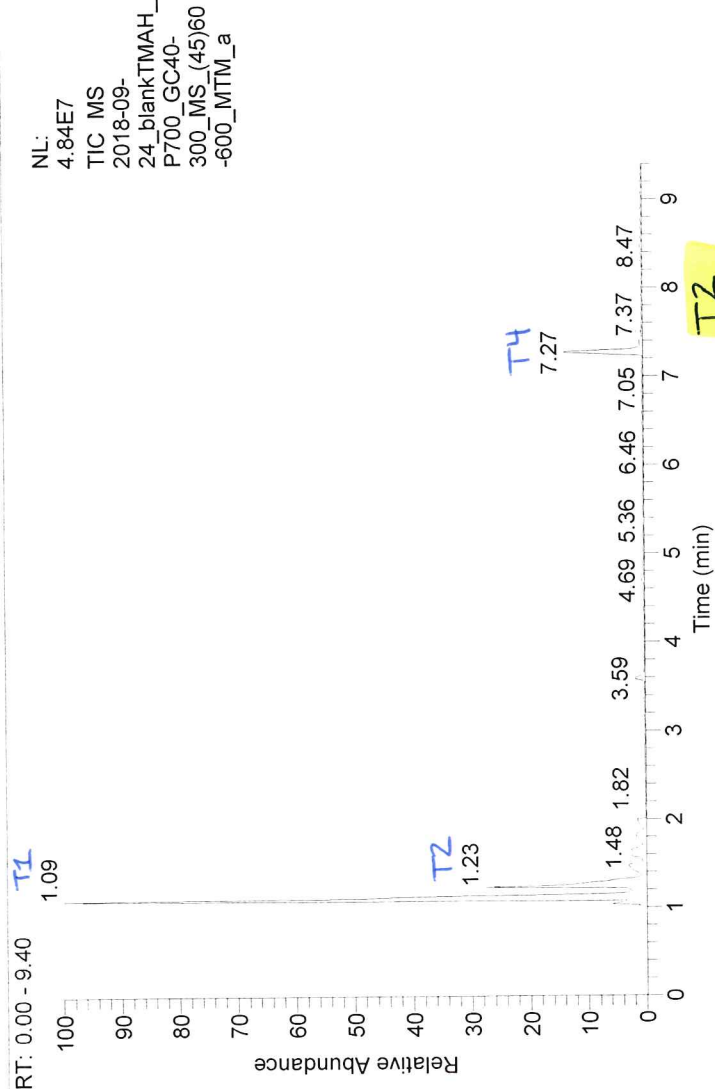
2018-09-24_blankTMAH_P700_GC40-300_MS_(45)60-600_MTM_a #757

T: + c Full ms [60.00-600.00]



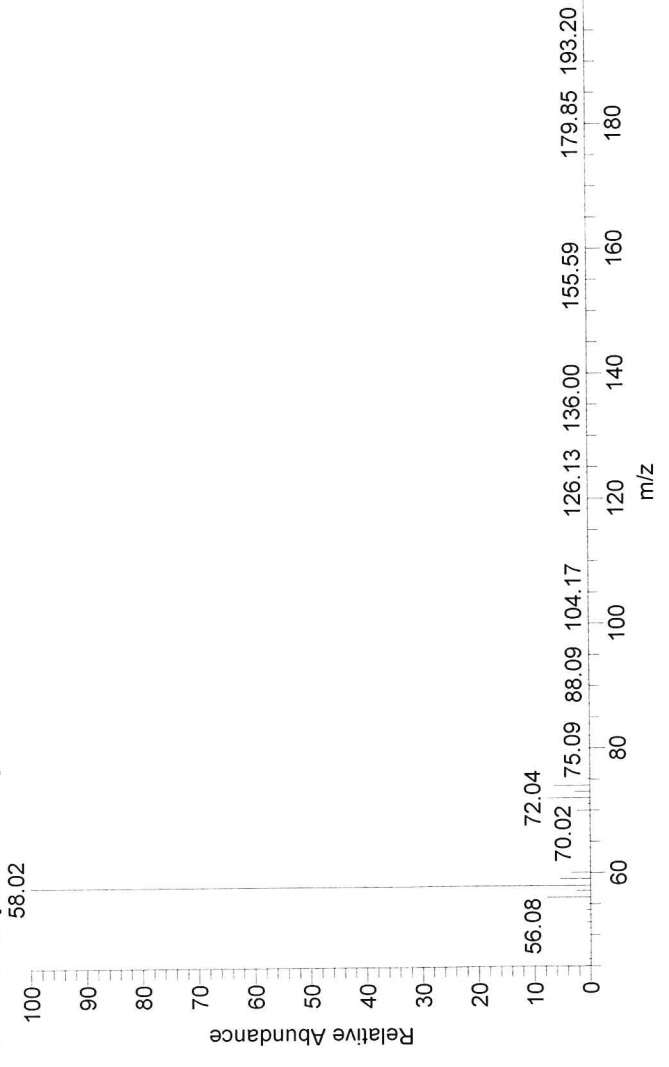
T4

RT: 7.27 AV: 1 NL: 5.04E6



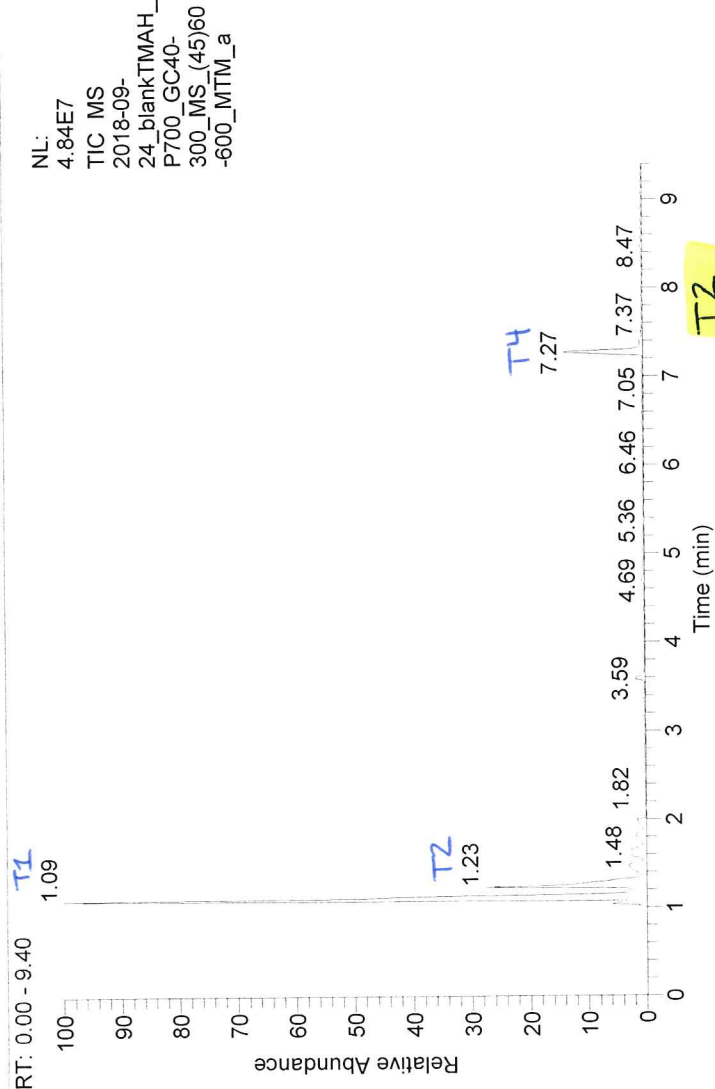
2018-09-24_blankTMAH_P700_GC40-300_MS_(45)60-600_MTM_a #757

T: + c Full ms [60.00-600.00]



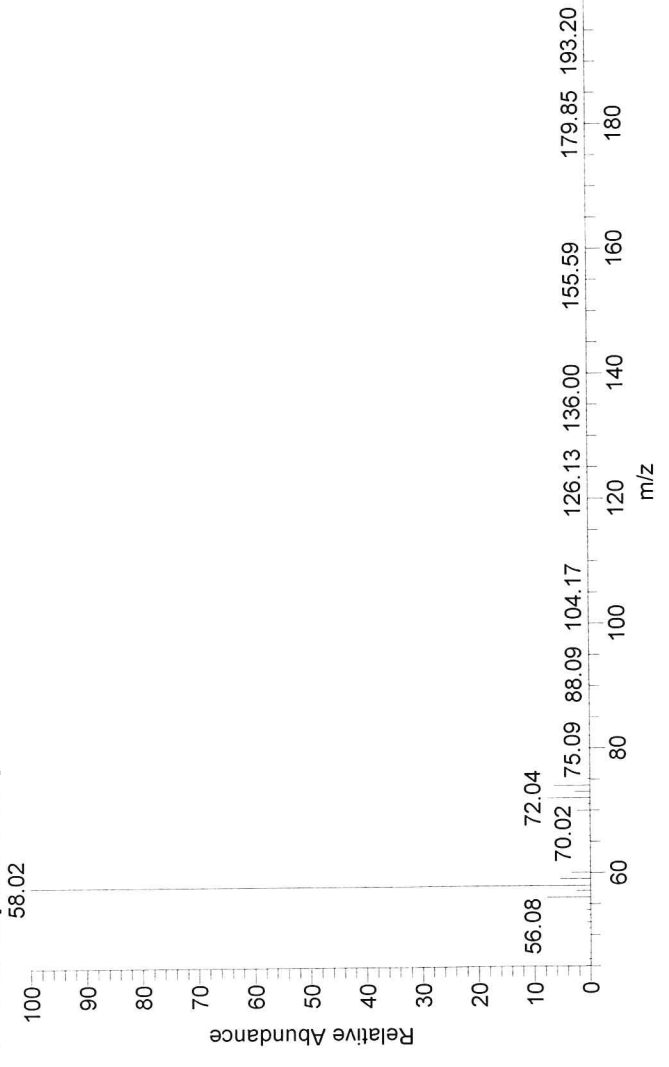
T4

RT: 7.27 AV: 1 NL: 5.04E6



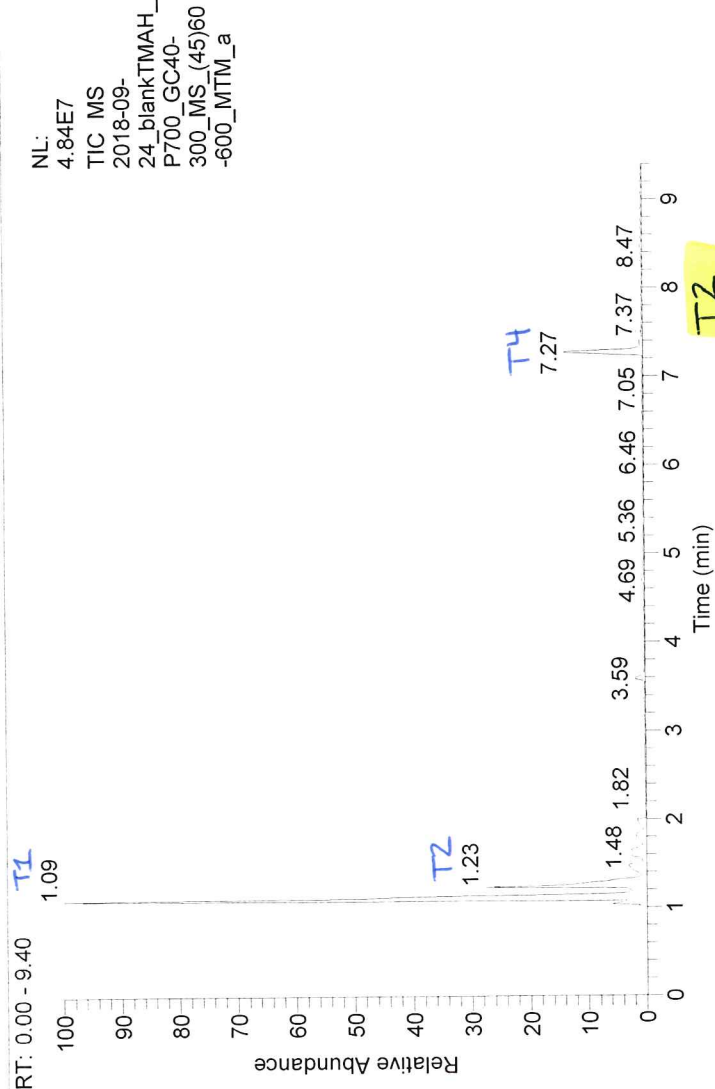
2018-09-24_blankTMAH_P700_GC40-300_MS_(45)60-600_MTM_a #757

T: + c Full ms [60.00-600.00]



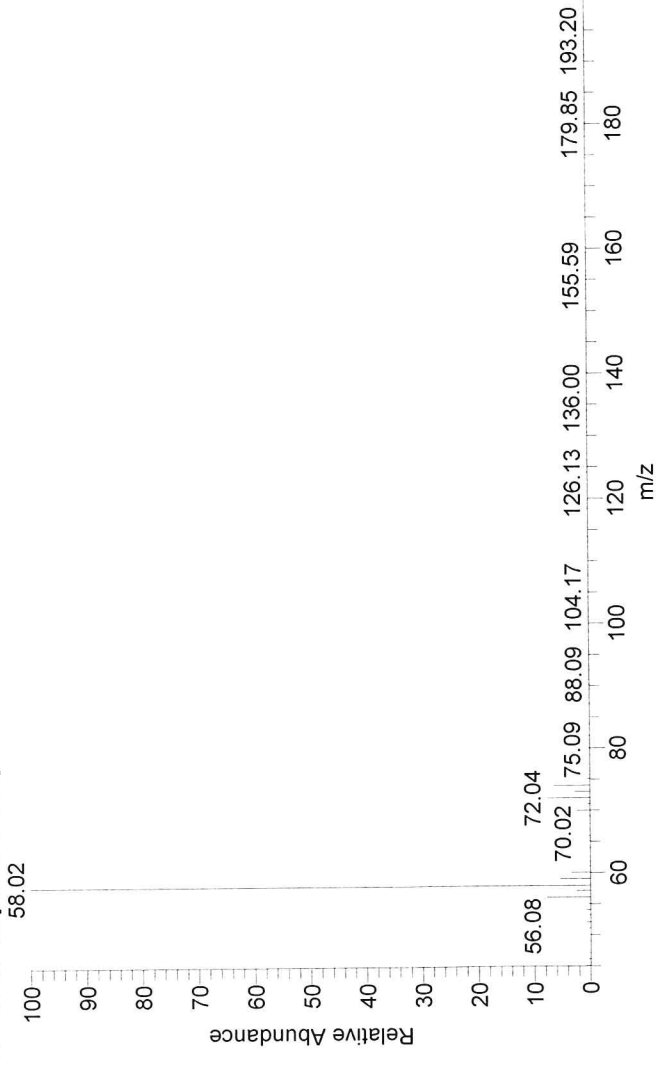
T4

RT: 7.27 AV: 1 NL: 5.04E6



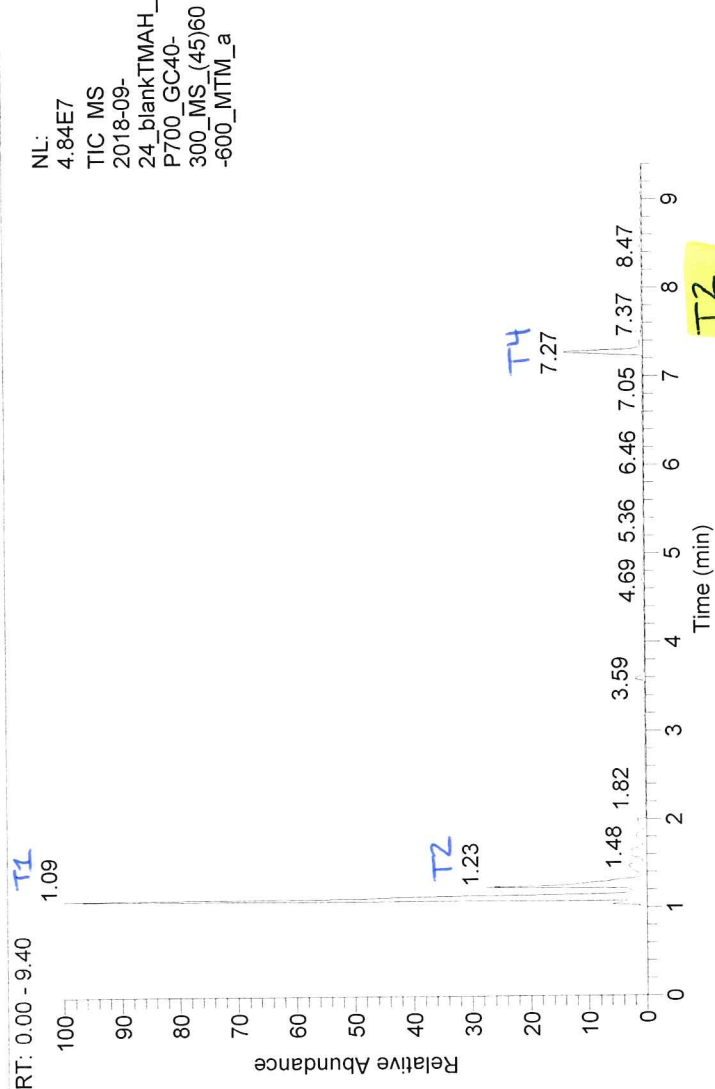
2018-09-24_blankTMAH_P700_GC40-300_MS_(45)60-600_MTM_a #757

T: + c Full ms [60.00-600.00]



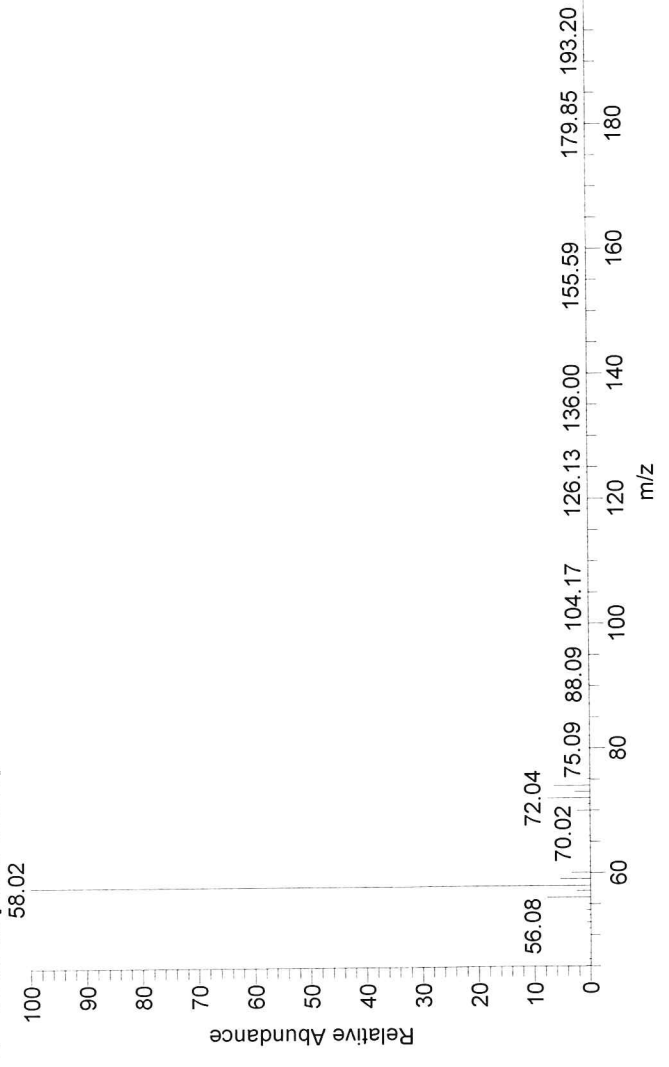
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RT: 7.27 AV: 1 NL: 5.04E6



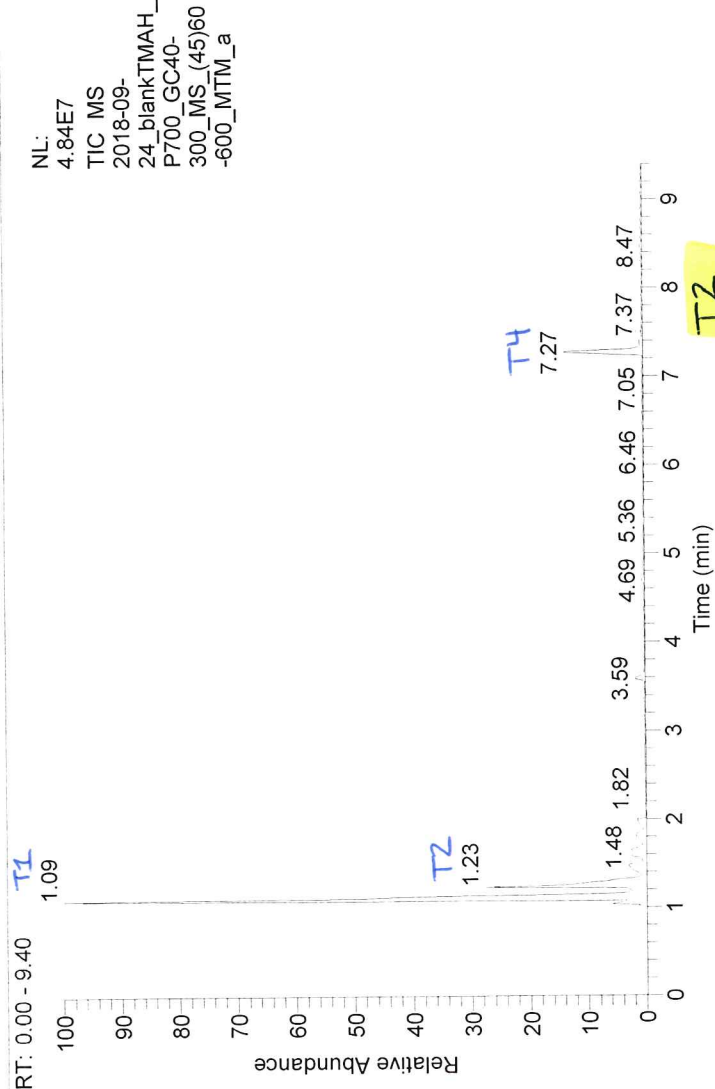
2018-09-24_blankTMAH_P700_GC40-300_MS_(45)60-600_MTM_a #757

T: + c Full ms [60.00-600.00]



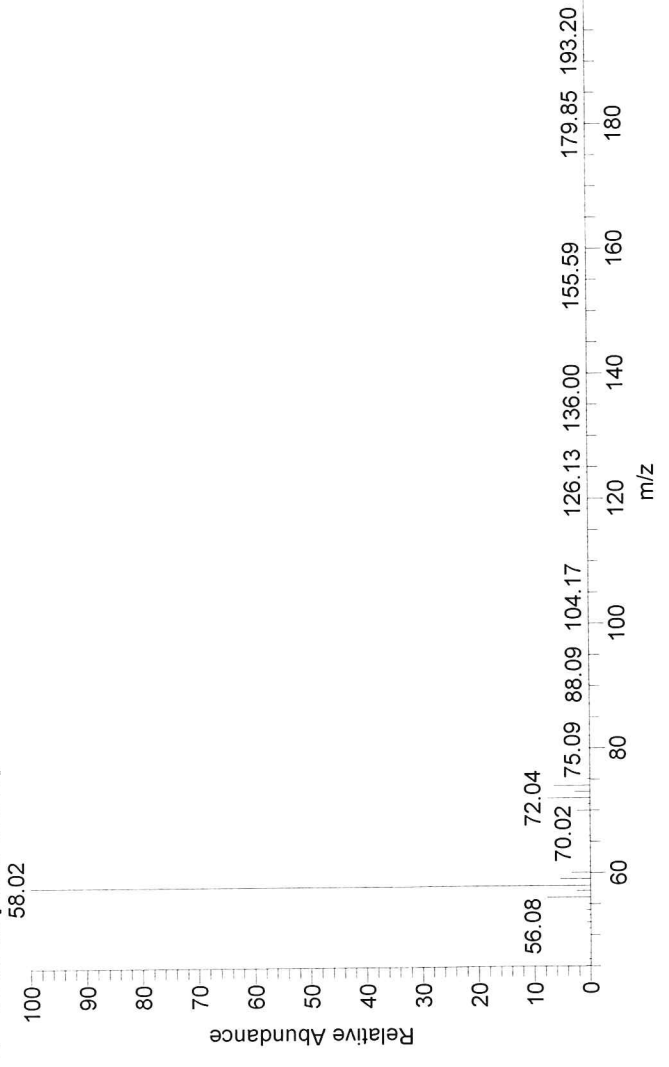
T4

RT: 7.27 AV: 1 NL: 5.04E6



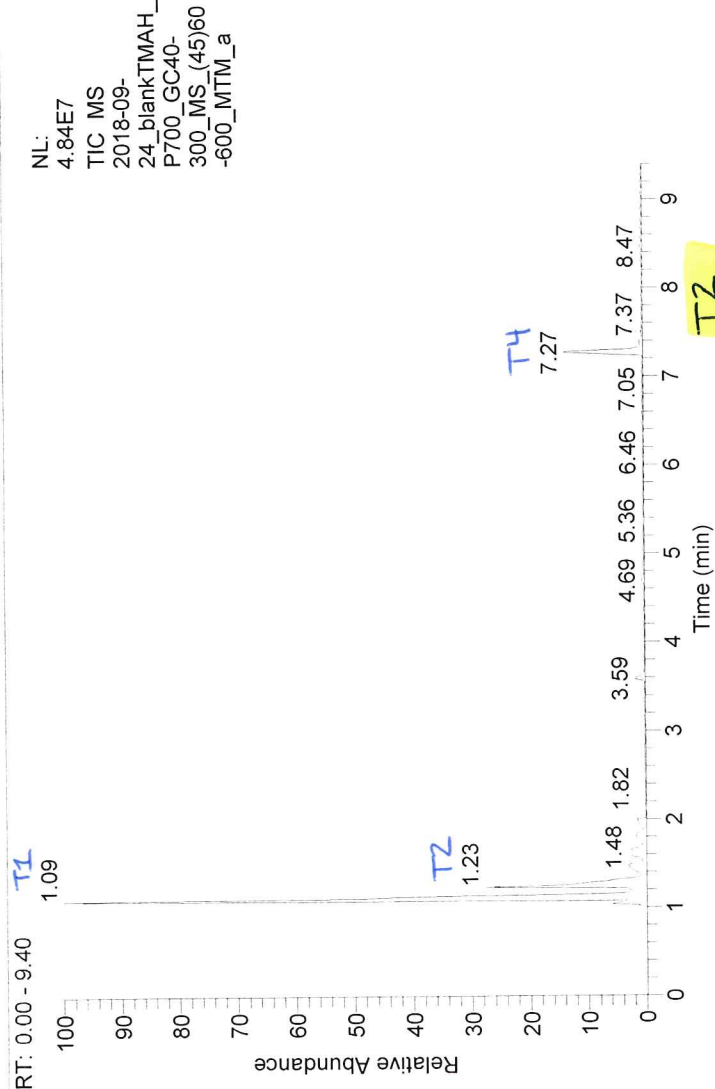
2018-09-24_blankTMAH_P700_GC40-300_MS_(45)60-600_MTM_a #757

T: + c Full ms [60.00-600.00]



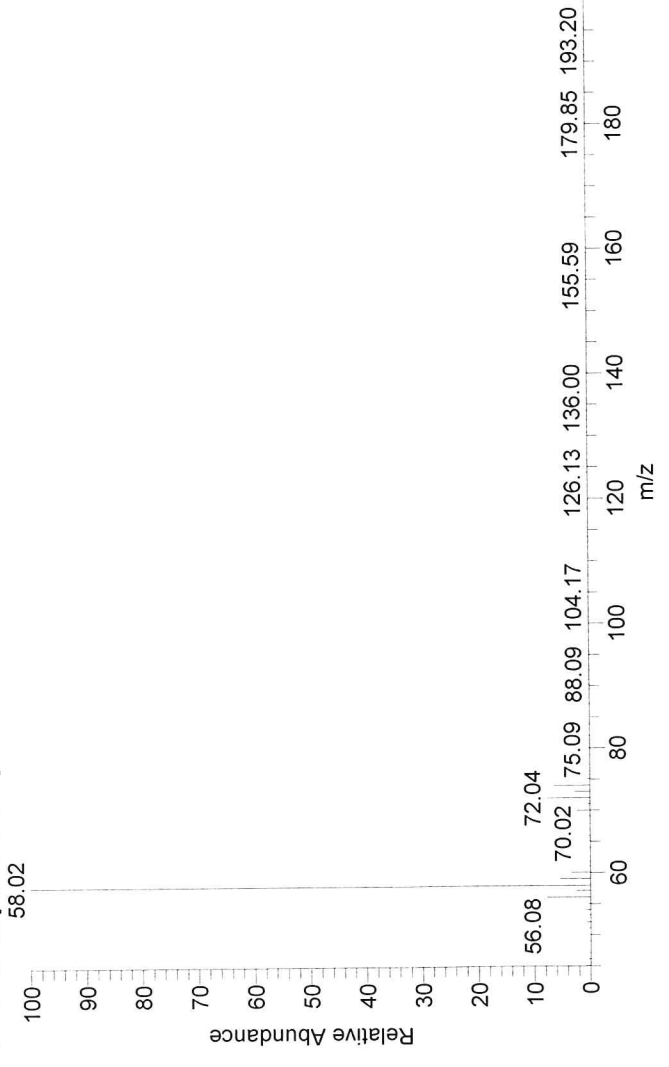
T4

RT: 7.27 AV: 1 NL: 5.04E6



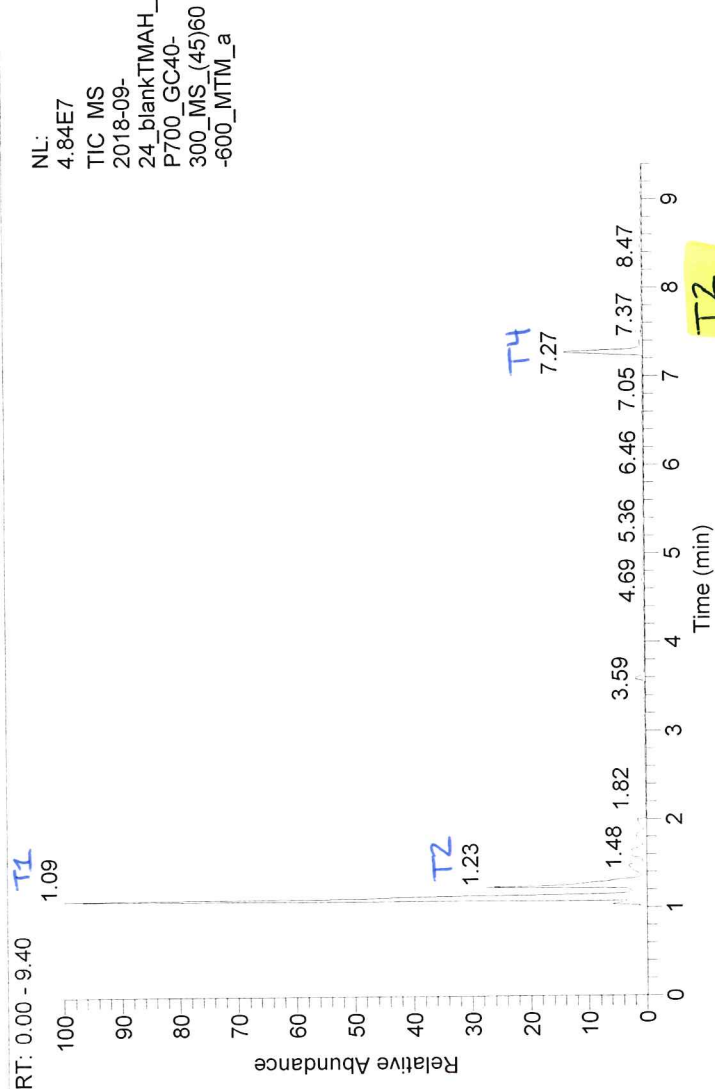
2018-09-24_blankTMAH_P700_GC40-300_MS_(45)60-600_MTM_a #757

T: + c Full ms [60.00-600.00]



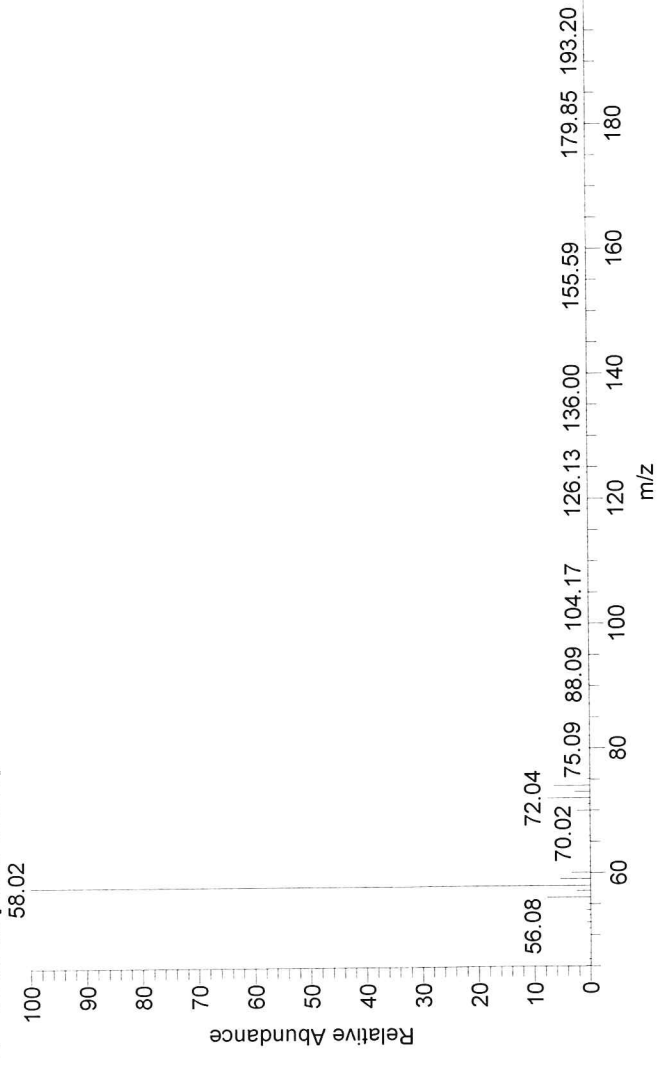
T4

RT: 7.27 AV: 1 NL: 5.04E6



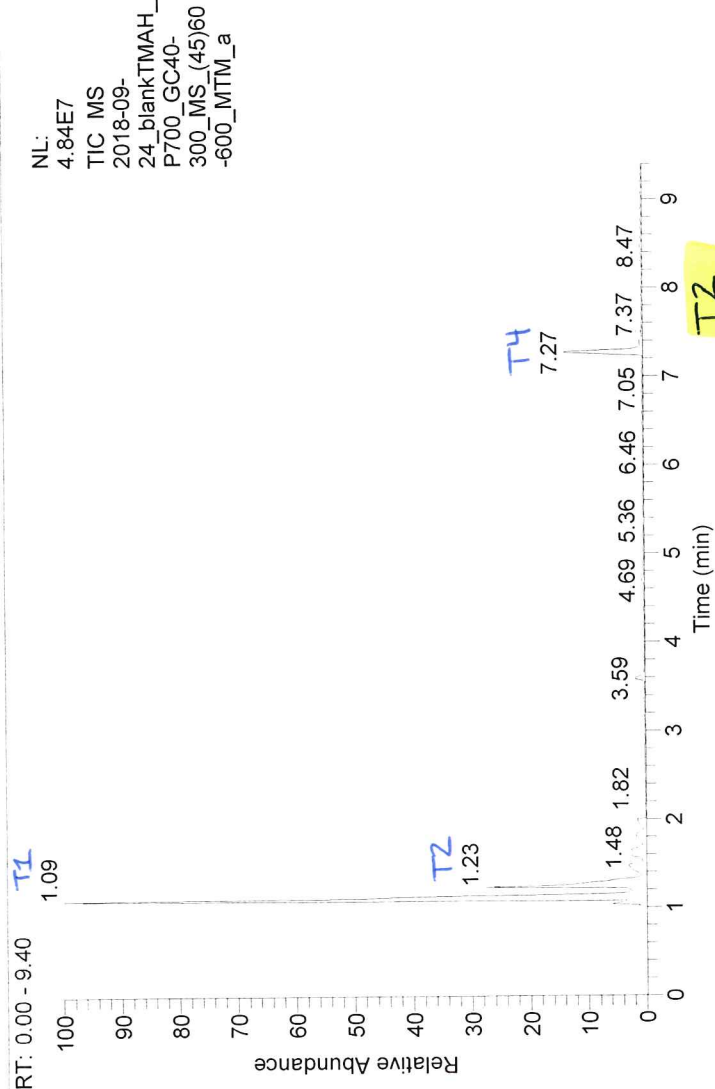
2018-09-24_blankTMAH_P700_GC40-300_MS_(45)60-600_MTM_a #757

T: + c Full ms [60.00-600.00]



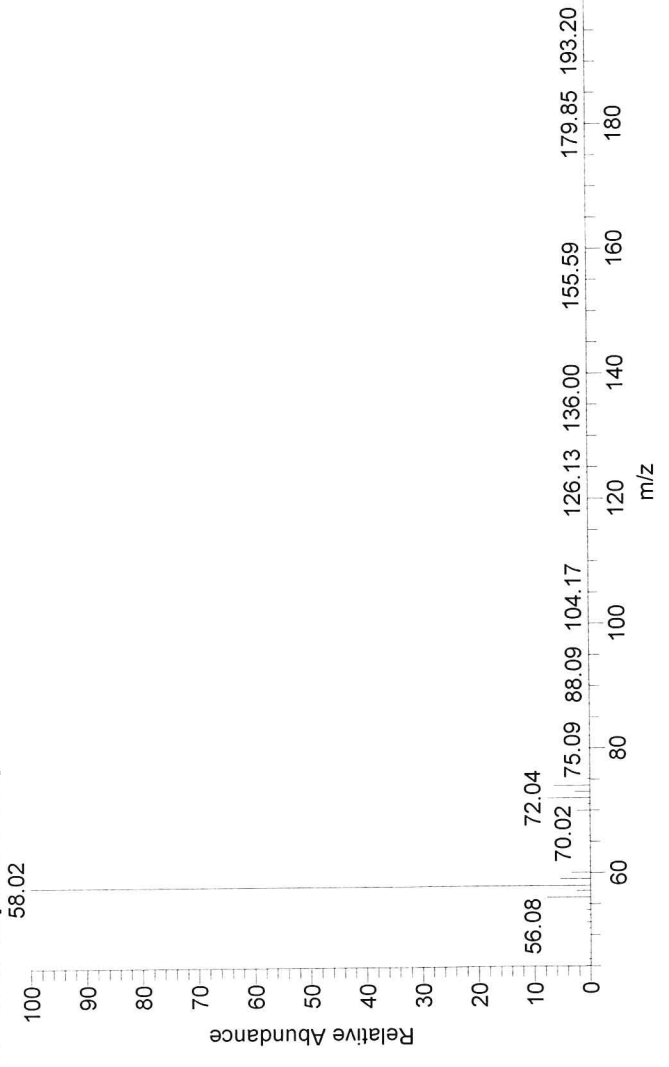
T4

RT: 7.27 AV: 1 NL: 5.04E6



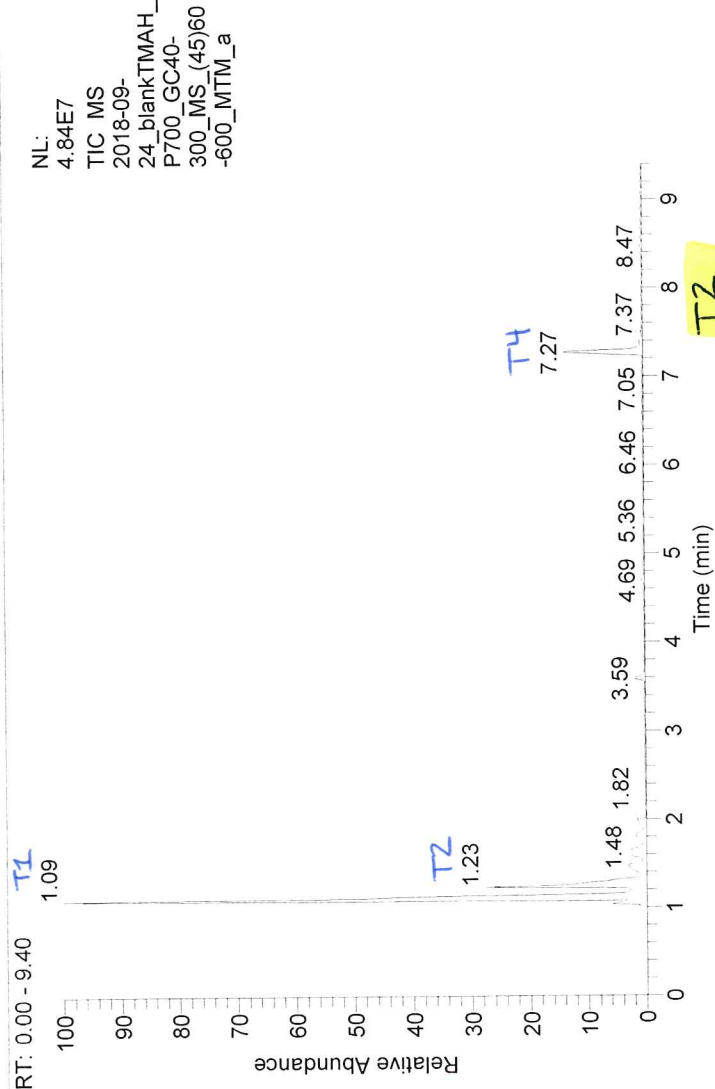
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T: + c Full ms [60.00-600.00]



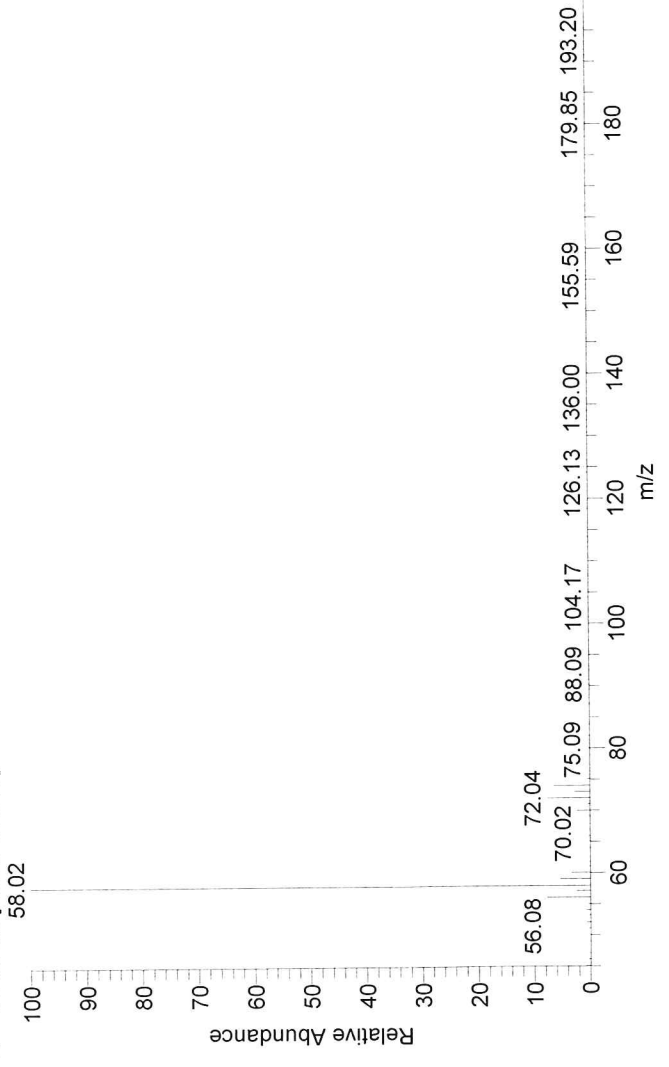
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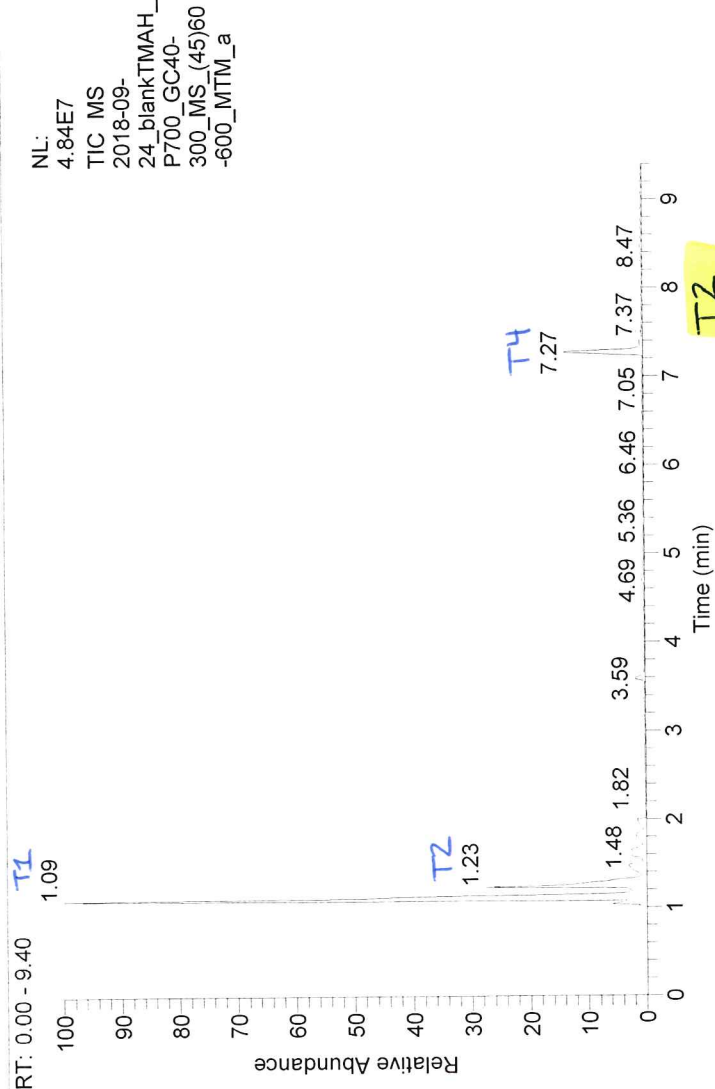
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T: + c Full ms [60.00-600.00]



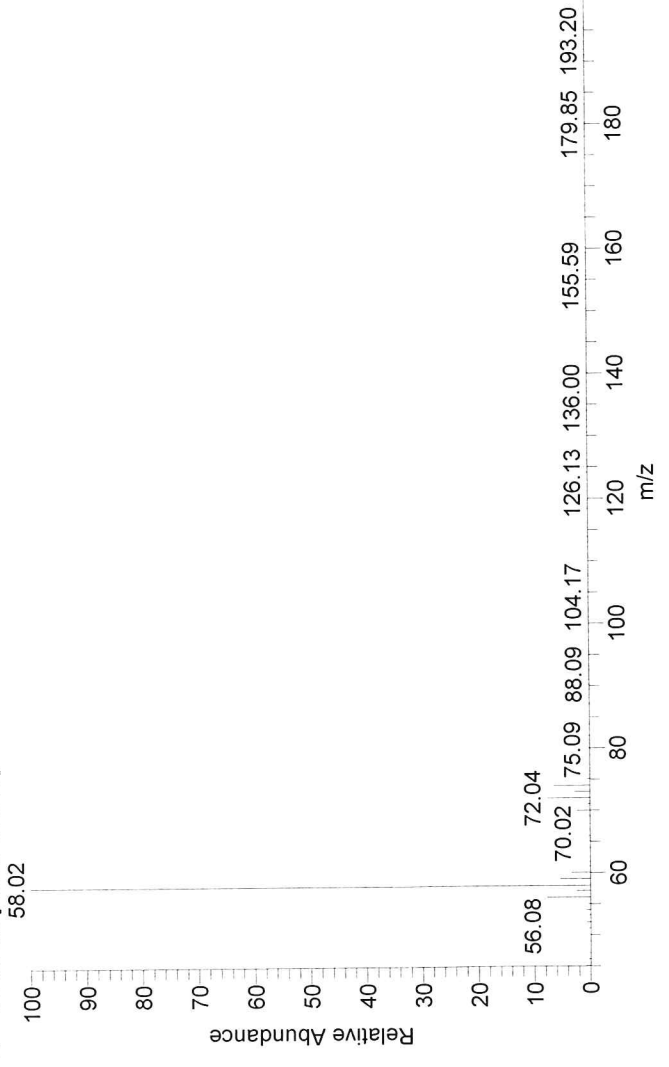
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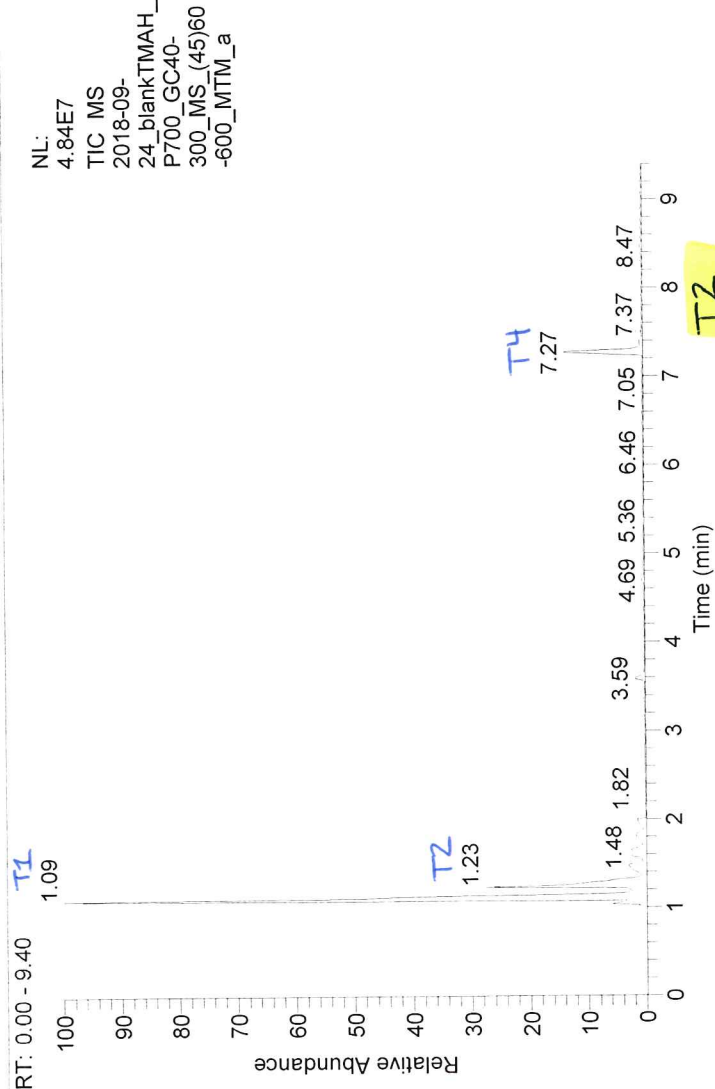
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T: + c Full ms [60.00-600.00]



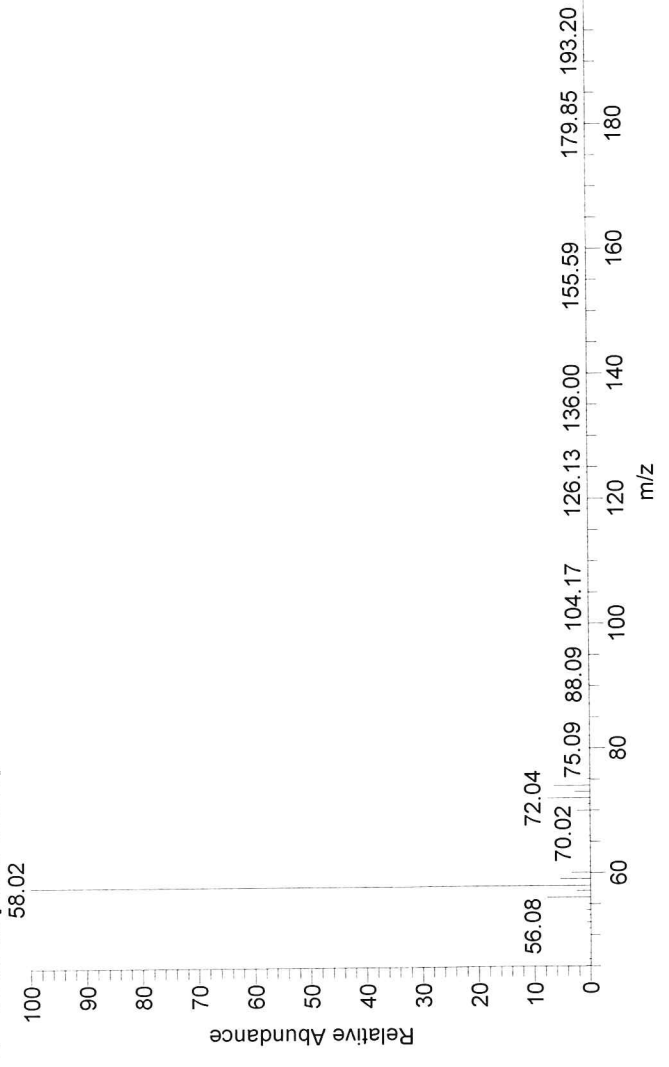
T4

RT: 7.27 AV: 1 NL: 5.04E6



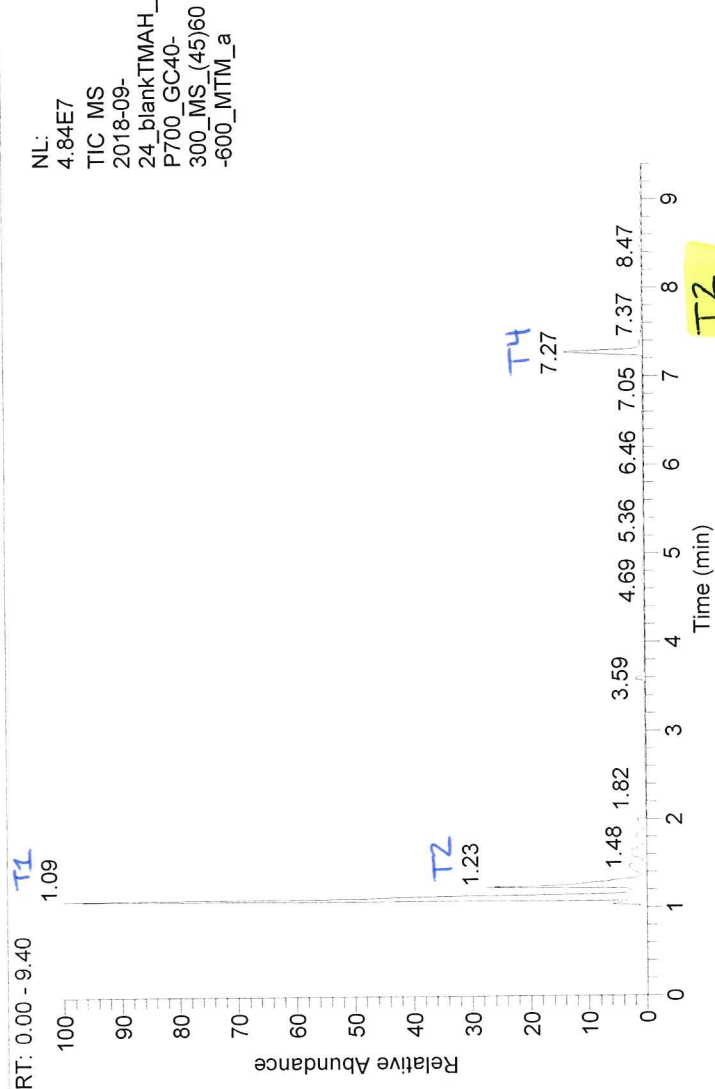
2018-09-24_blankTMAH_P700_GC40-300_MS_(45)60-600_MTM_a #757

T: + c Full ms [60.00-600.00]



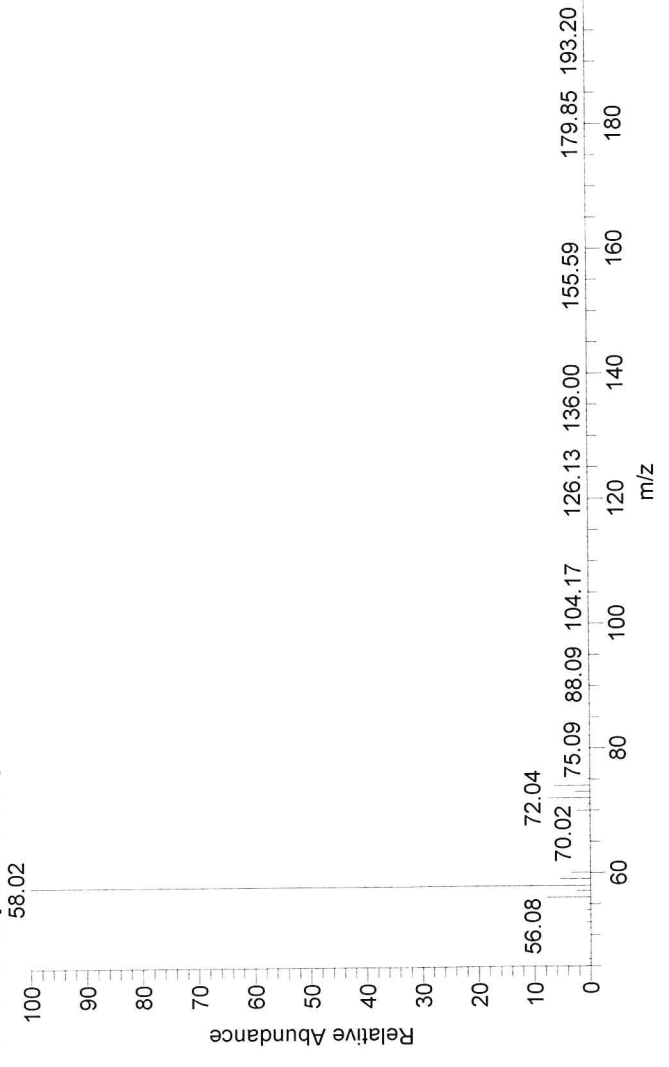
T4

RT: 7.27 AV: 1 NL: 5.04E6



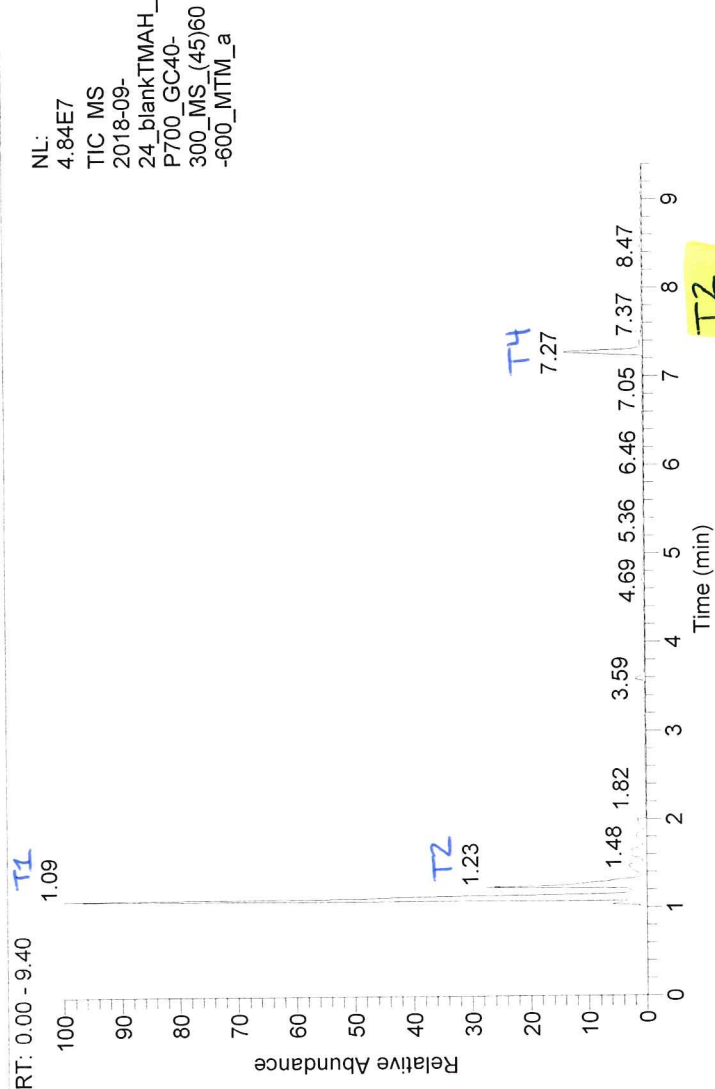
2018-09-24_blankTMAH_P700_GC40-300_MS_(45)60-600_MTM_a #757

T: + c Full ms [60.00-600.00]



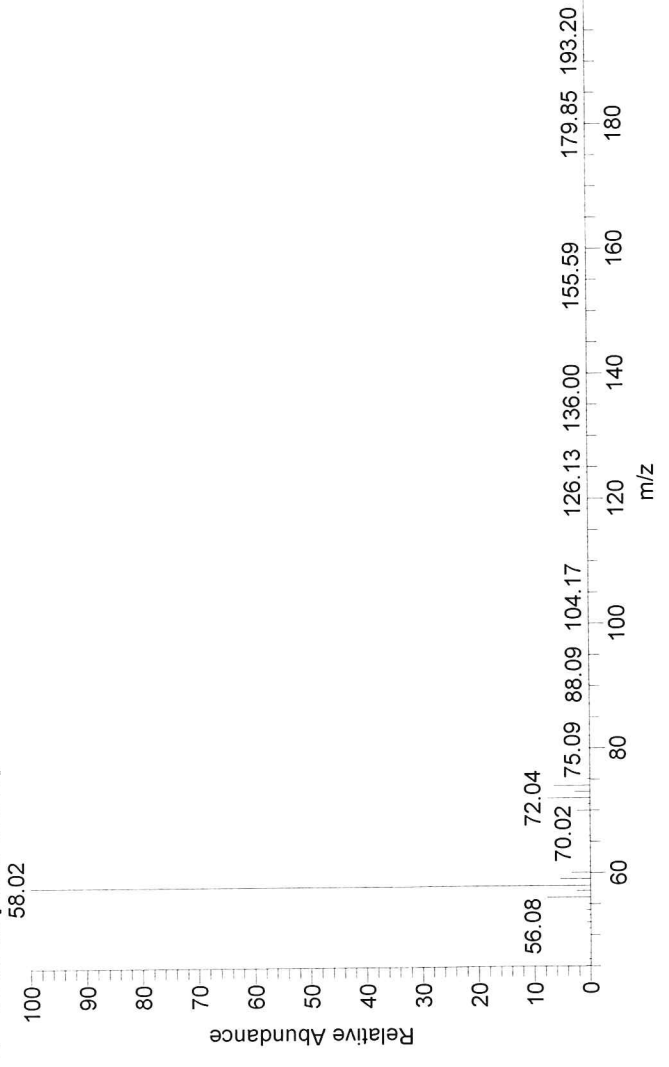
T4

RT: 7.27 AV: 1 NL: 5.04E6



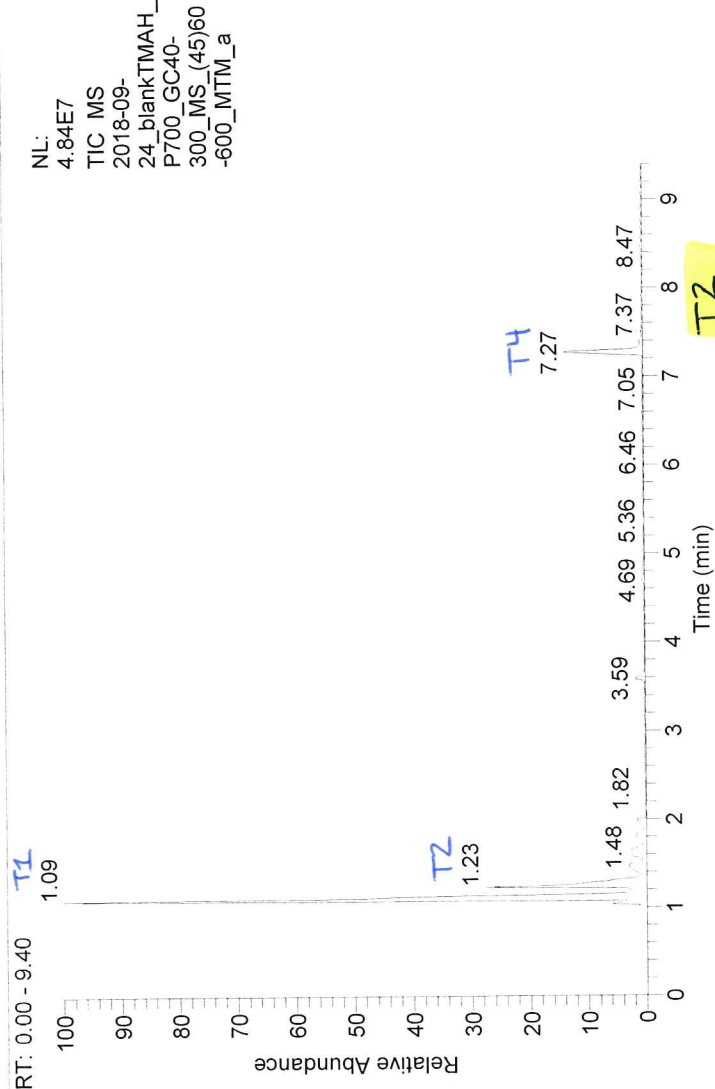
2018-09-24_blankTMAH_P700_GC40-300_MS_(45)60-600_MTM_a #757

T: + c Full ms [60.00-600.00]



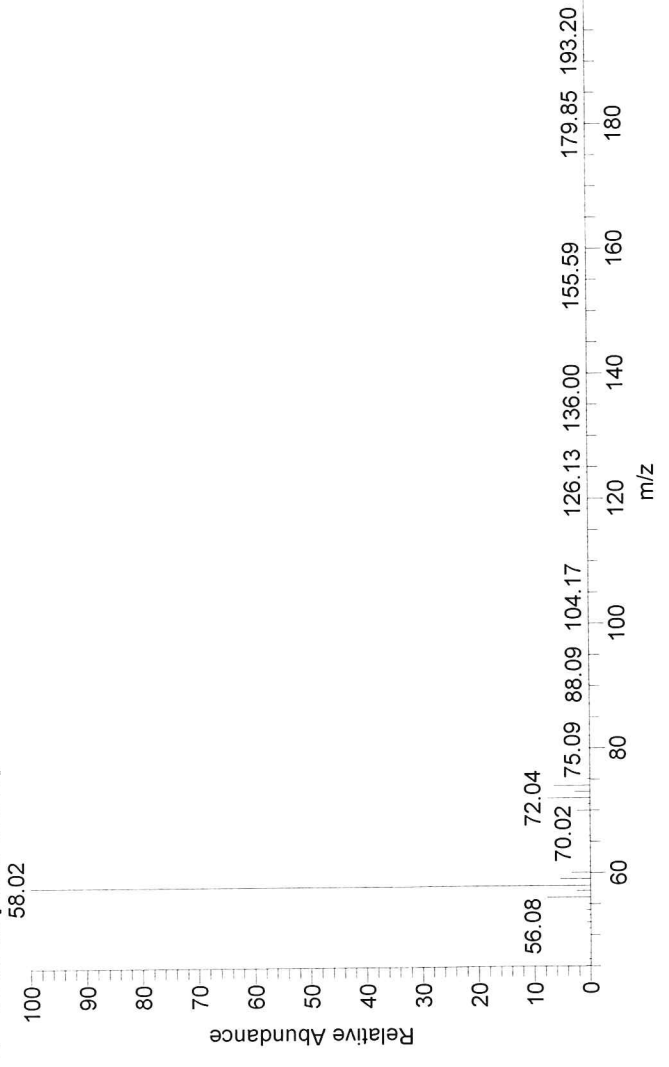
T4

RT: 7.27 AV: 1 NL: 5.04E6



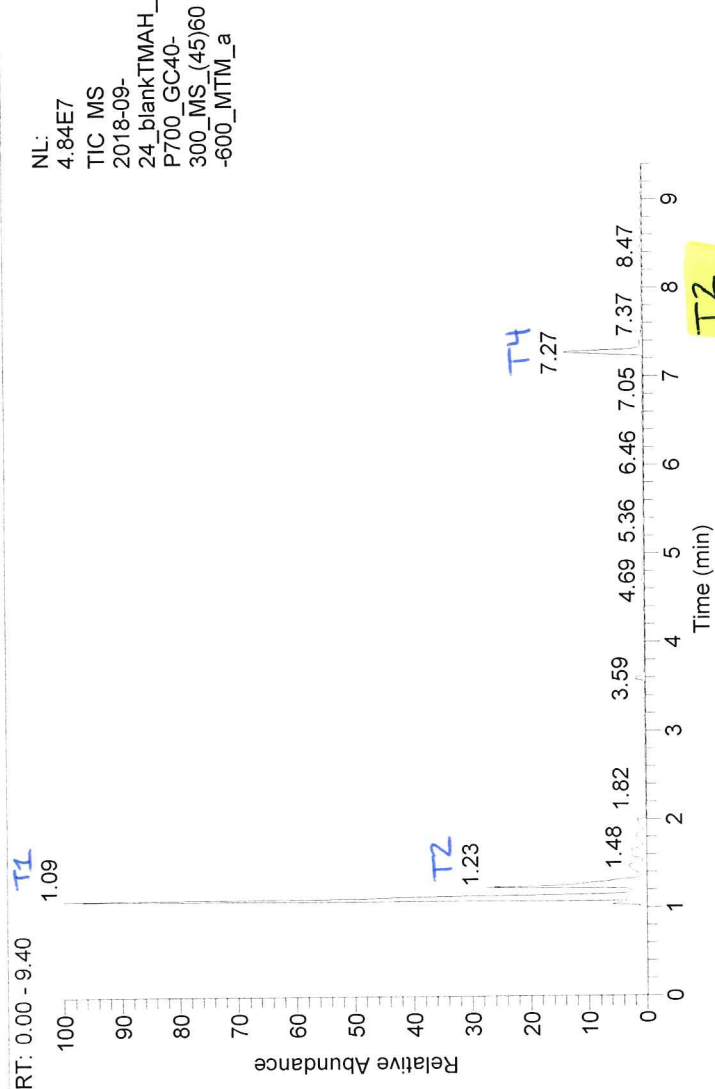
2018-09-24_blankTMAH_P700_GC40-300_MS_(45)60-600_MTM_a #757

T: + c Full ms [60.00-600.00]



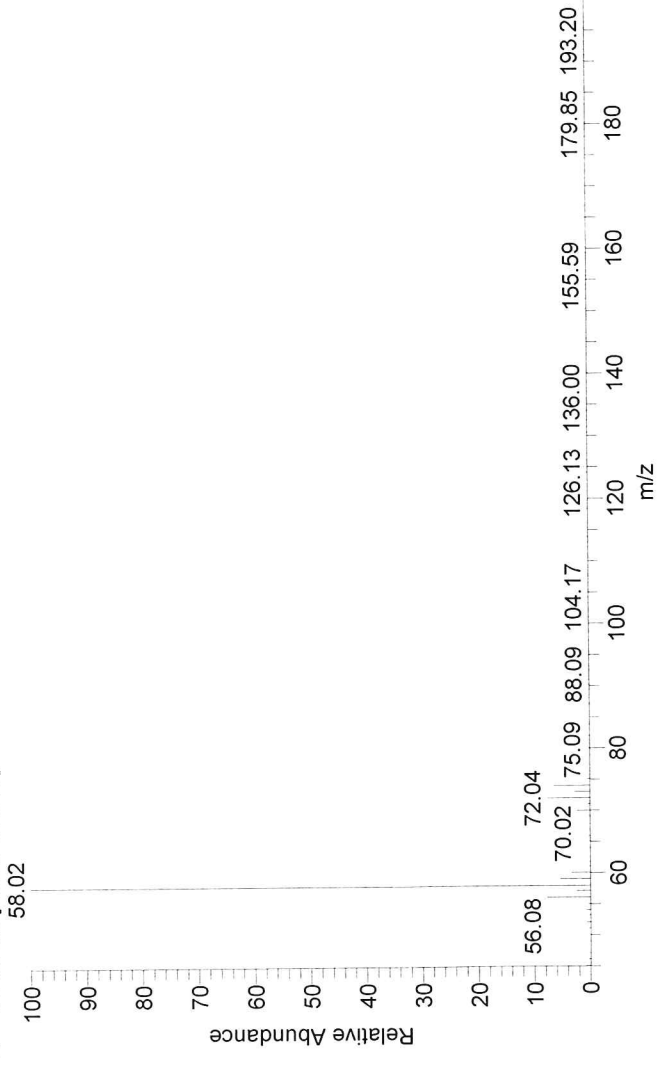
T4

RT: 7.27 AV: 1 NL: 5.04E6



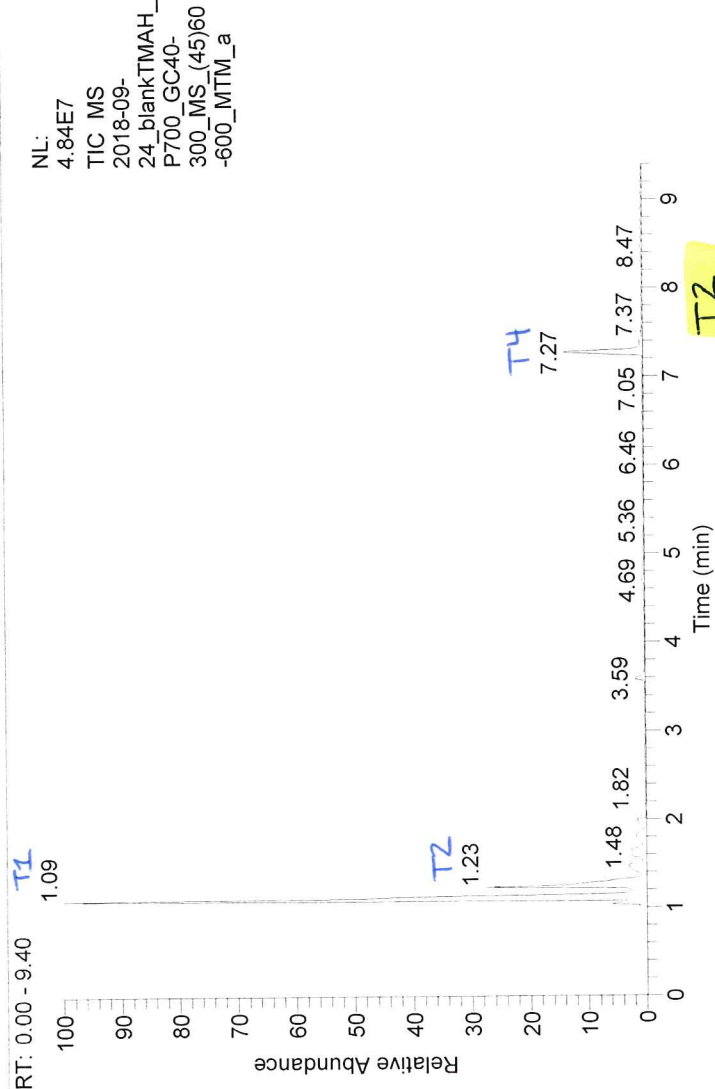
2018-09-24_blankTMAH_P700_GC40-300_MS_(45)60-600_MTM_a #757

T: + c Full ms [60.00-600.00]



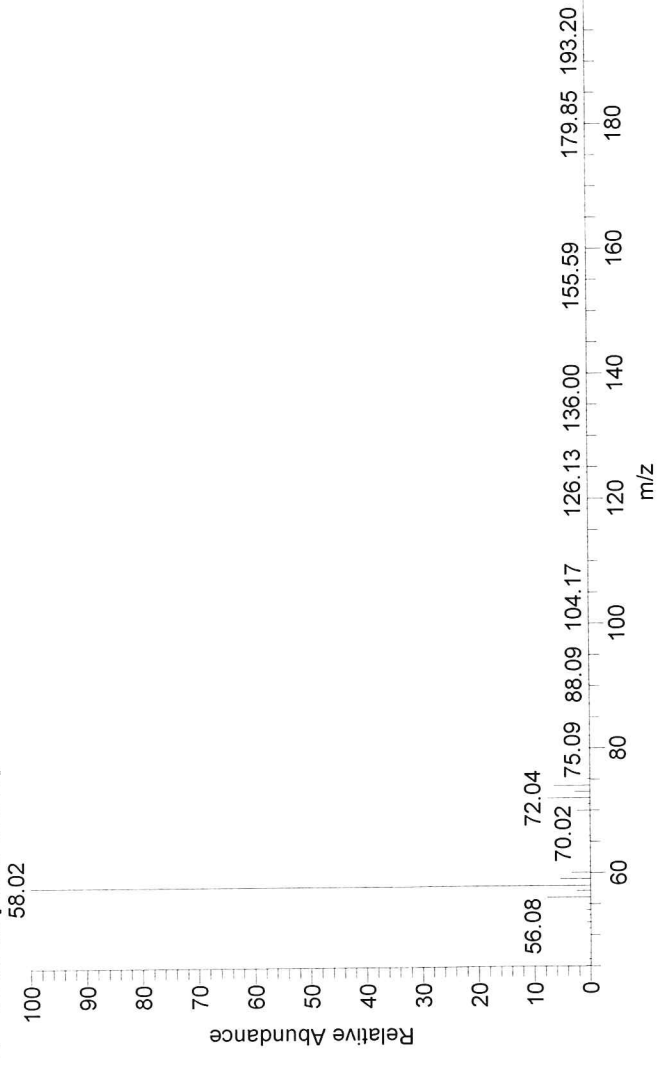
T4

RT: 7.27 AV: 1 NL: 5.04E6



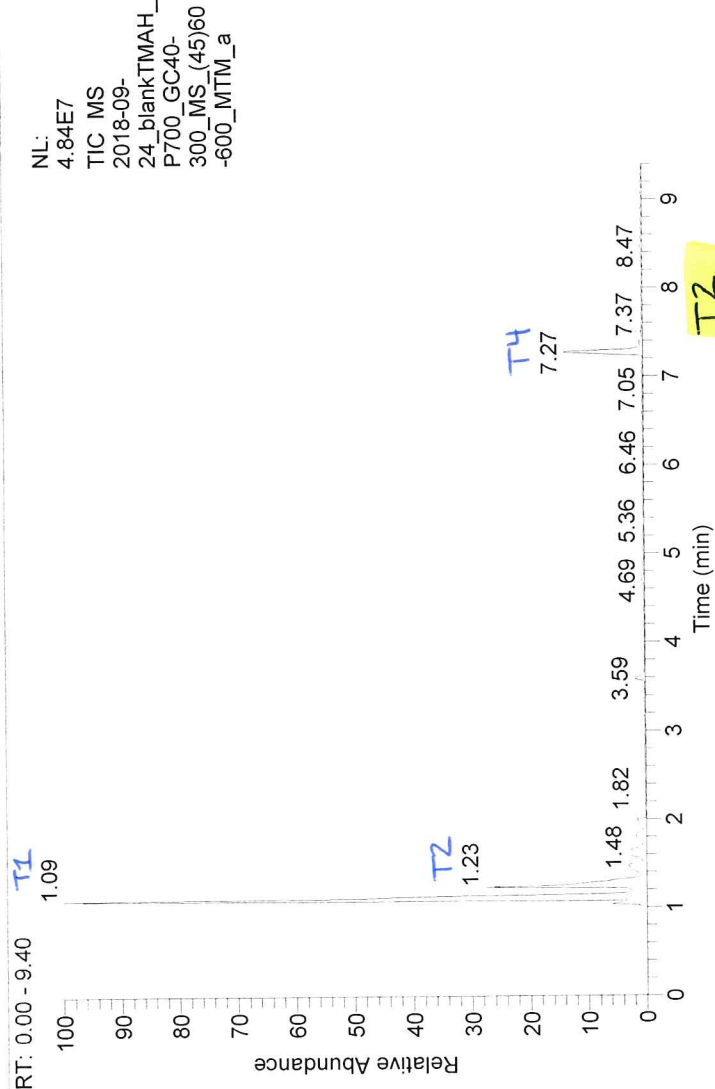
2018-09-24_blankTMAH_P700_GC40-300_MS_(45)60-600_MTM_a #757

T: + c Full ms [60.00-600.00]



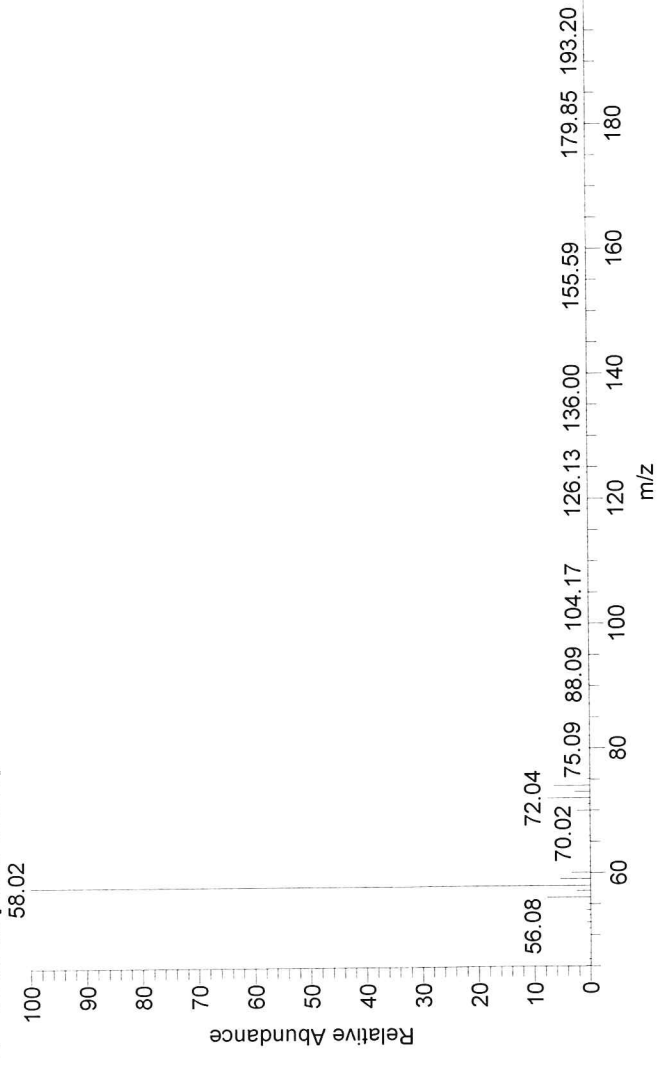
T4

RT: 7.27 AV: 1 NL: 5.04E6



2018-09-24_blankTMAH_P700_GC40-300_MS_(45)60-600_MTM_a #757

T: + c Full ms [60.00-600.00]



TMAH (ScB) Pyrogram

2018-10-09_blank_TMAH_manu_P700_GC40-...

2018-10-09_d

10/10/18 11:53:15

TMAH manu flask

RT: 0.00 - 55.03

T1 1.13

NL:

3.70E6

TIC MS

2018-10-

09_blank_TMAH_

manu_P700_GC4

0-300_MS(45)60-

600_MTM_d

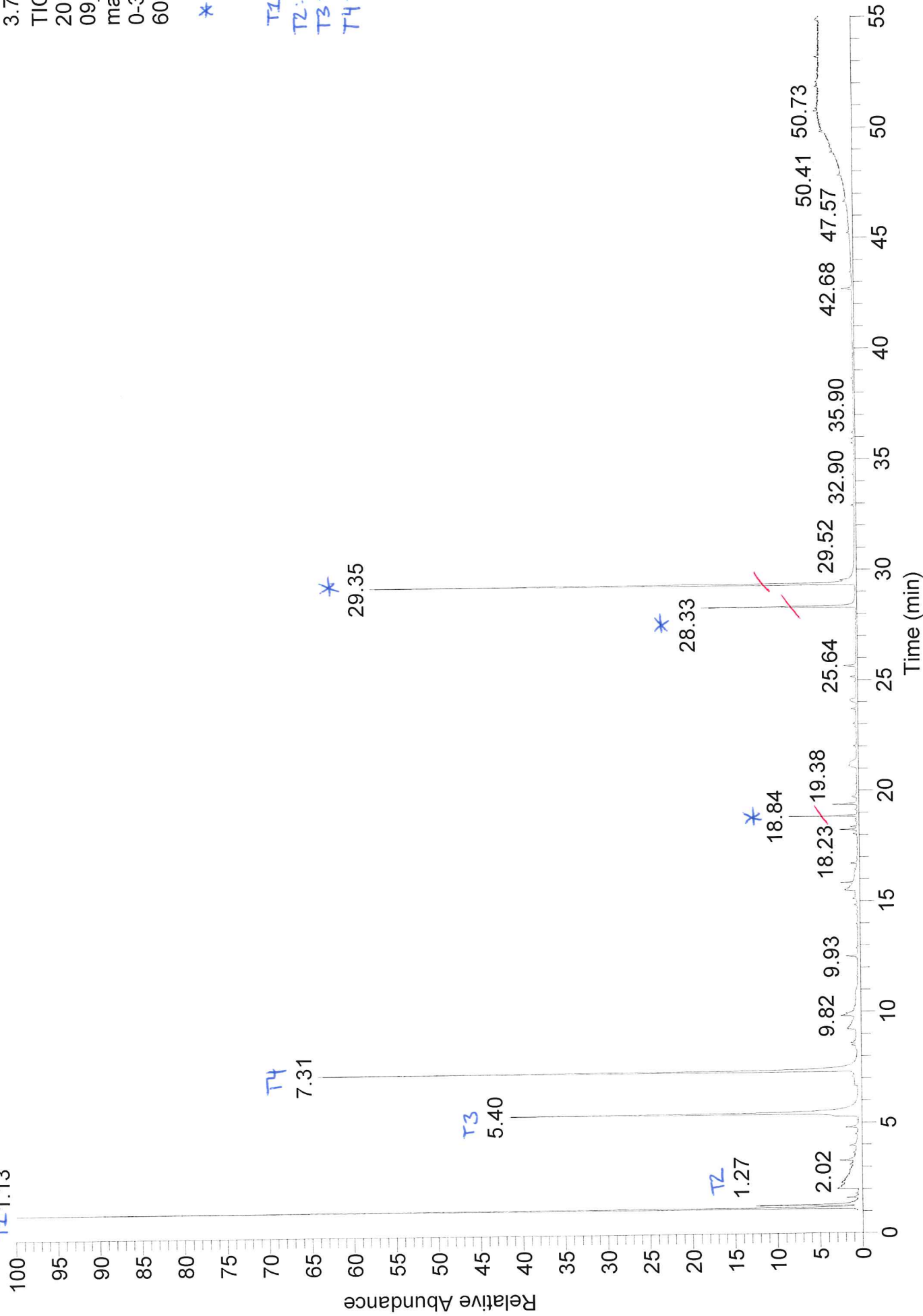
* Contamination/
interference

T1: TMAH fragment 1

T2: TMAH fragment 2

T3: TMAH fragment 3

T4: TMAH fragment 4



air- (3)

TMAH (scB) Mass spectra

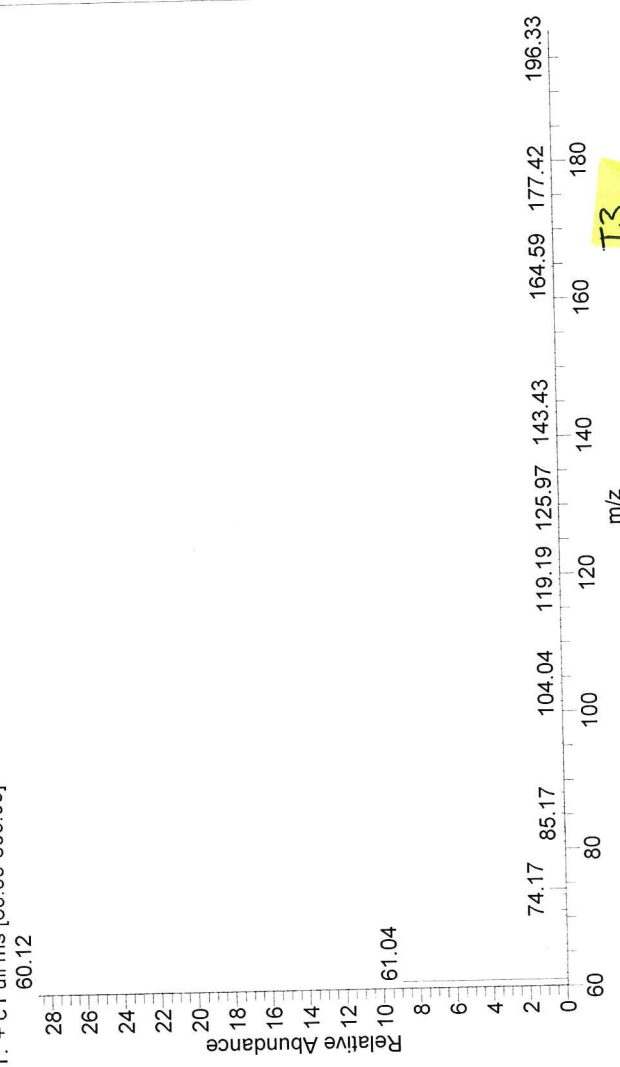
10/10/18 11:53:15 TMAH manu flask

T1

T2

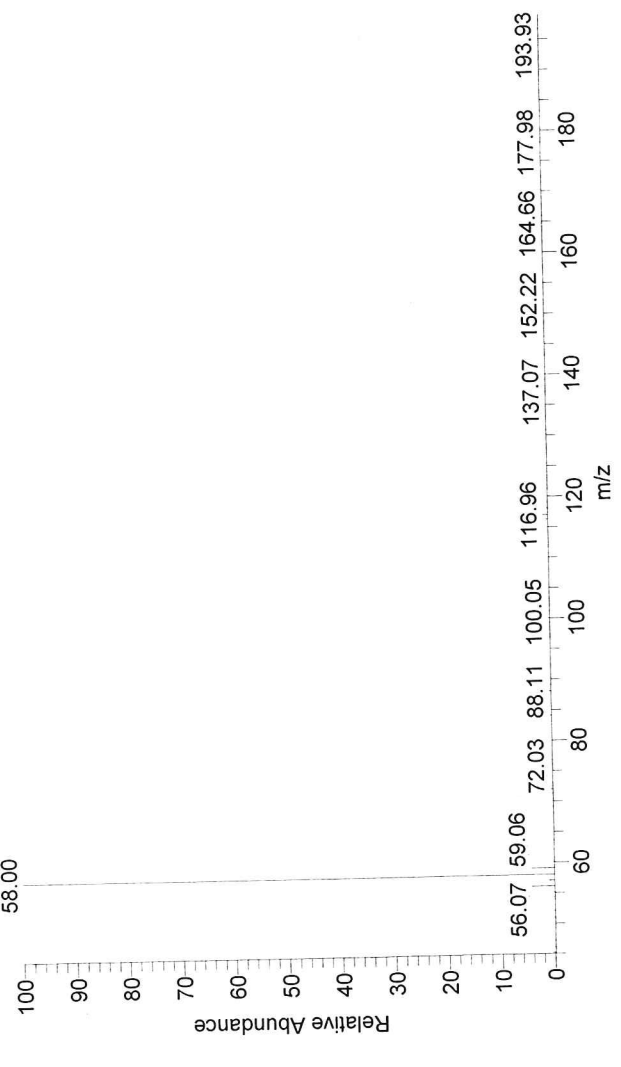
2018-10-09_blank_TMAH_manu_P700_GC40-...
2018-10-09_d
2018-10-09_blank_TMAH_manu_P700_GC40-300_MS(45)60-600_MTM_d #16
T: + c Full ms [60.00-600.00] RT: 1.13 AV: 1 NL:

2018-10-09_blank_TMAH_manu_P700_GC40-300_MS(45)60-600_MTM_d #35
T: + c Full ms [60.00-600.00] RT: 1.28 AV: 1 NL:



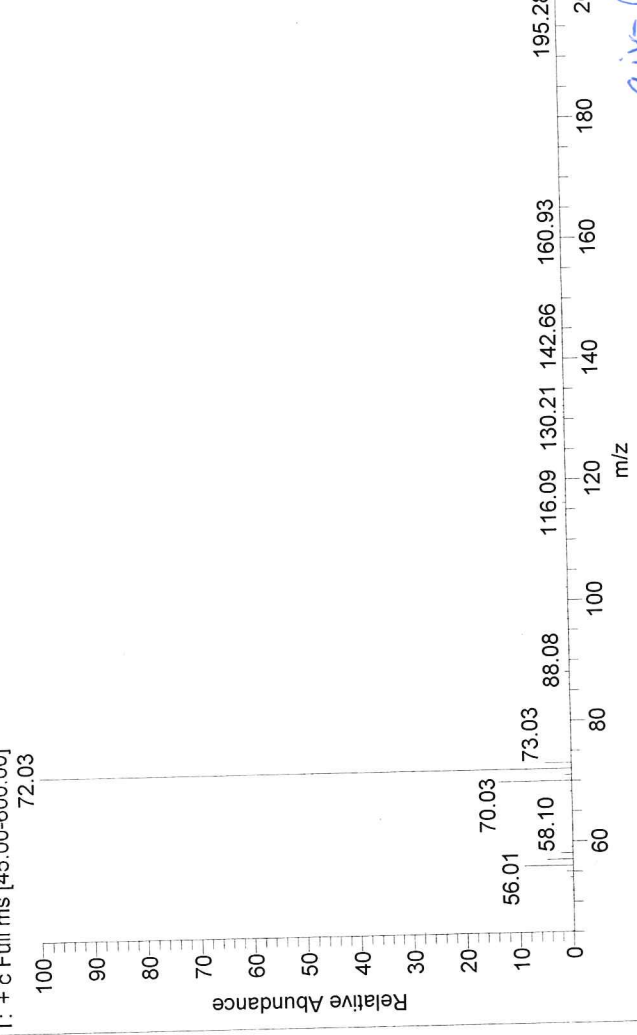
T3

2018-10-09_blank_TMAH_manu_P700_GC40-300_MS(45)60-600_MTM_d #509
T: + c Full ms [45.00-600.00] RT: 5.40 AV: 1 NL:



T4

2018-10-09_blank_TMAH_manu_P700_GC40-300_MS(45)60-600_MTM_d #720
T: + c Full ms [45.00-600.00] RT: 7.31 AV: 1 NL:



air-4

gas injected,
No Pyrolysis

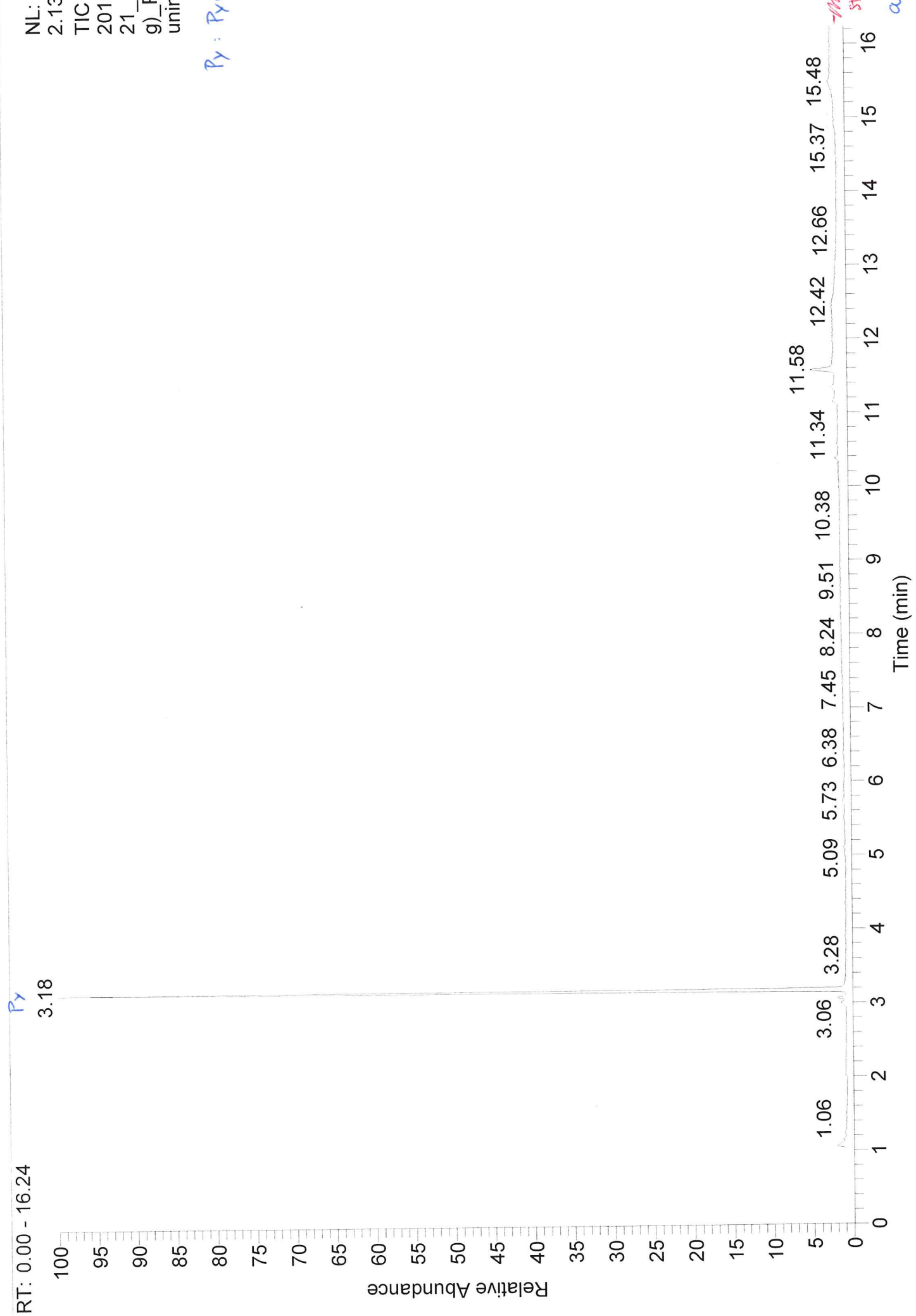
01/21/19 15:19:32

Pyrolyse (g) Pyrogram
2019-01-21_Pyrrole(g)_Py-uninst

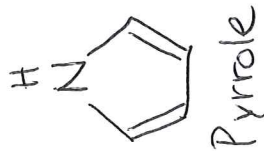
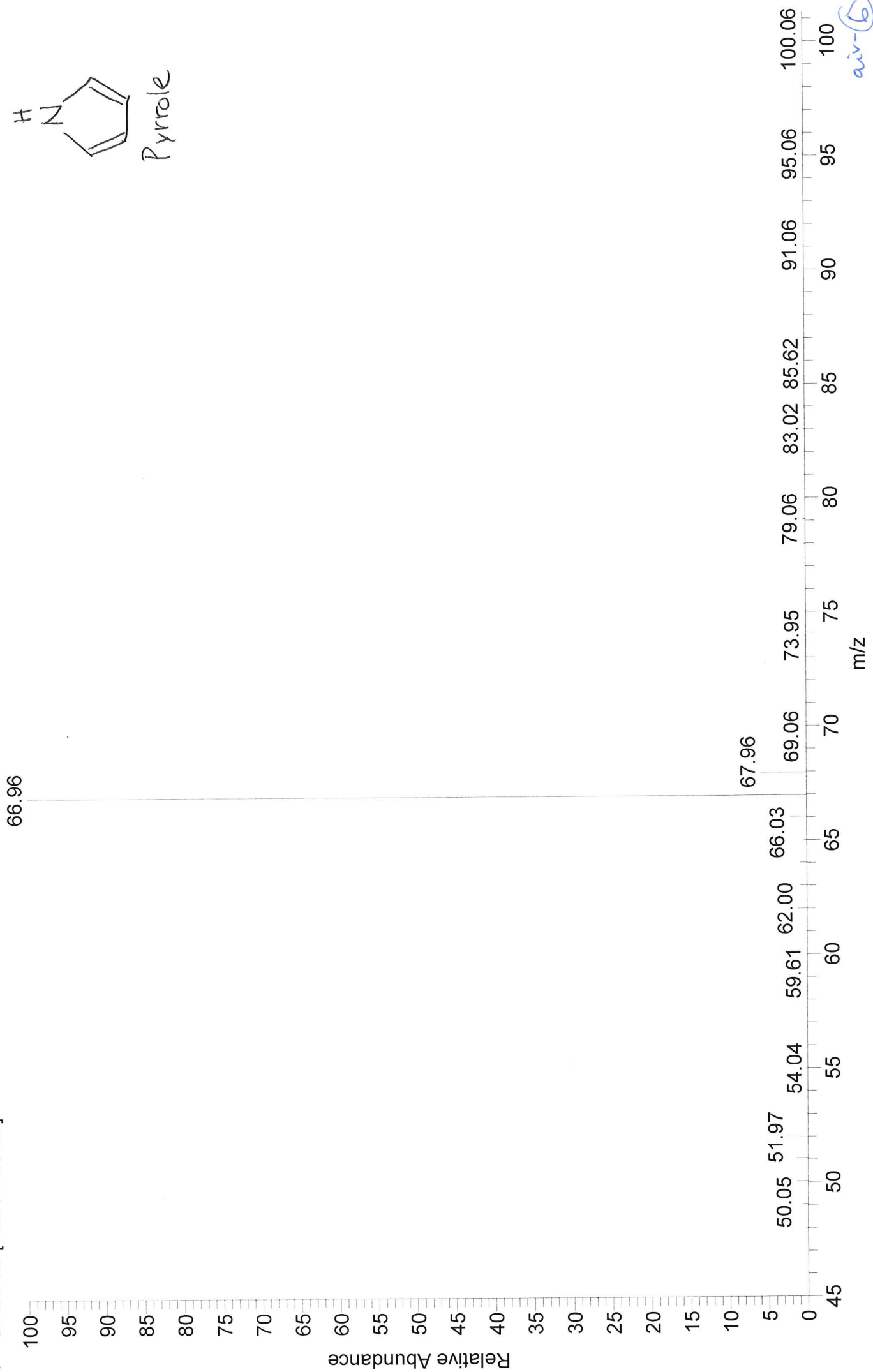
RT: 0.00 - 16.24

NL:
2.13E6
TIC MS
2019-01-
21_Pyrrole(
g)_Py-
uninst

Py: Pyrrole



Py
2019-01-21_Pyrrole(g)_Py-uninst #226 RT: 3.16 AV: 1 NL: 6.18E5
T: + c Full ms [45.00-600.00]



air-6

Pyrolysis + TMAH Pyrogram

2018-10-09_pyrrole_P700_GC40-300_MS(4...

2018-10-09_b

10/09/18 12:43:02

Pyrrole, ref

RT: 0.00 - 55.02

NL:

7.08E6

TIC MS

2018-10-

09_pyrrole_P70

0_GC40-

300_MS(45)60-

600_MTM_c

Me-Py: Methylated

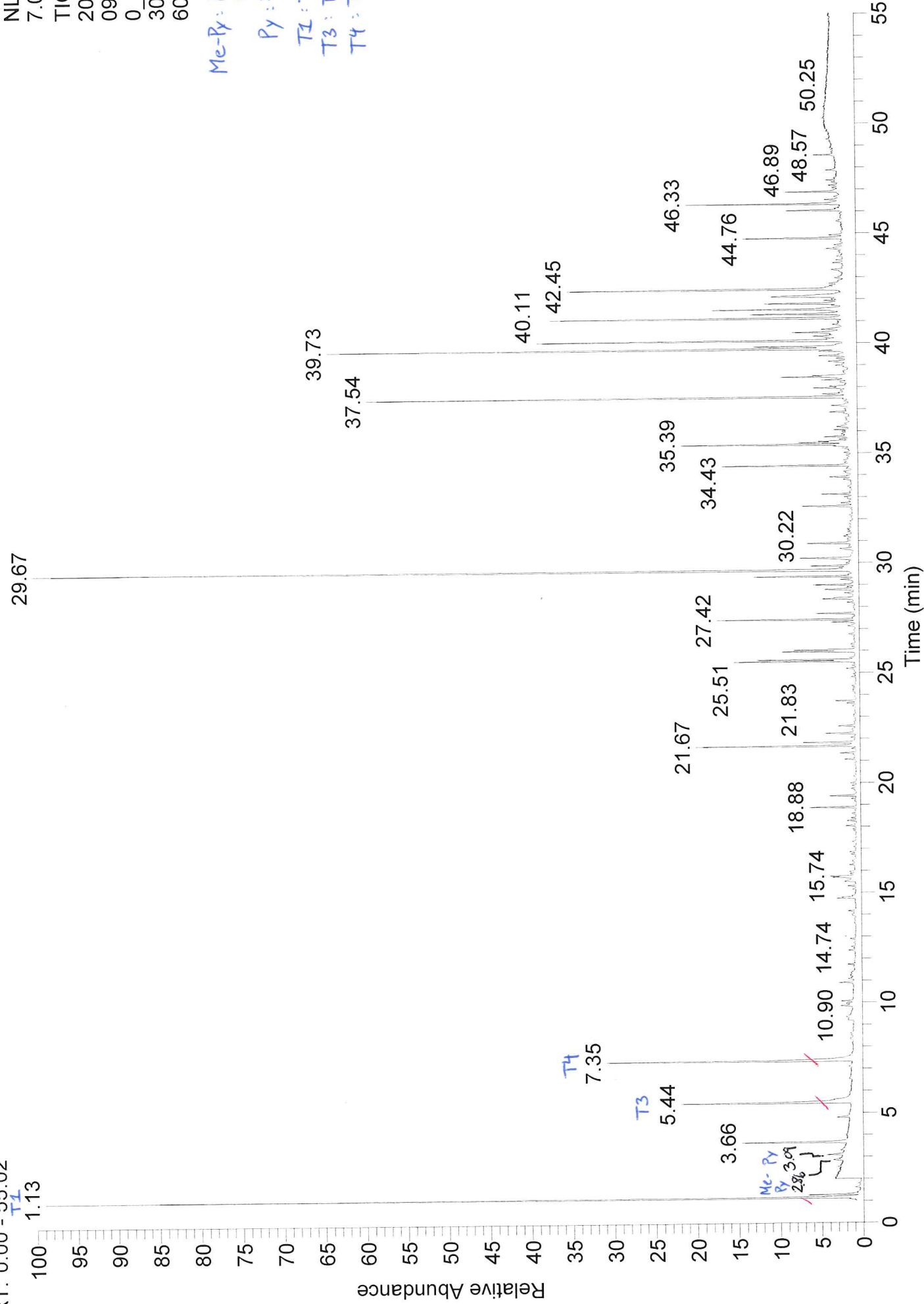
Pyrrole

Py: Pyrrole

T1: TMAH fragment 1

T3: TMAH fragment 3

T4: TMAH fragment 4



air-7

Pyrrole + TMAH Pyrogram (Zoom)

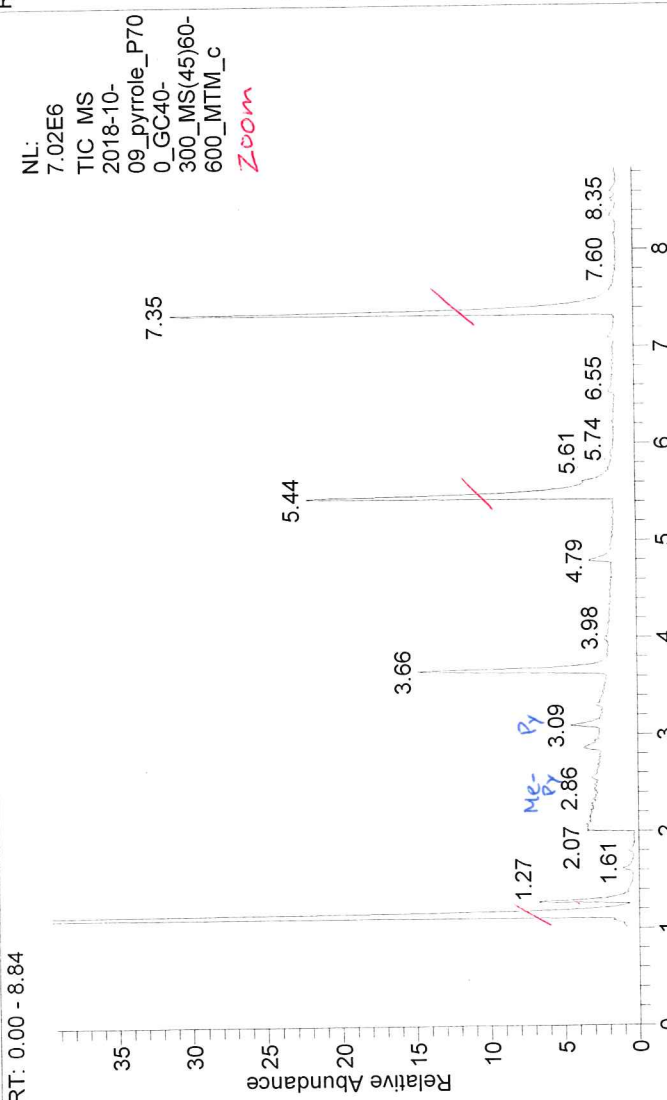
2018-10-09_pyrrole_P700_GC40-300_MS(4...

2018-10-09_b

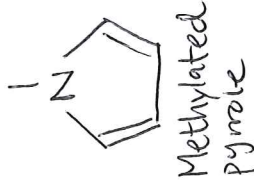
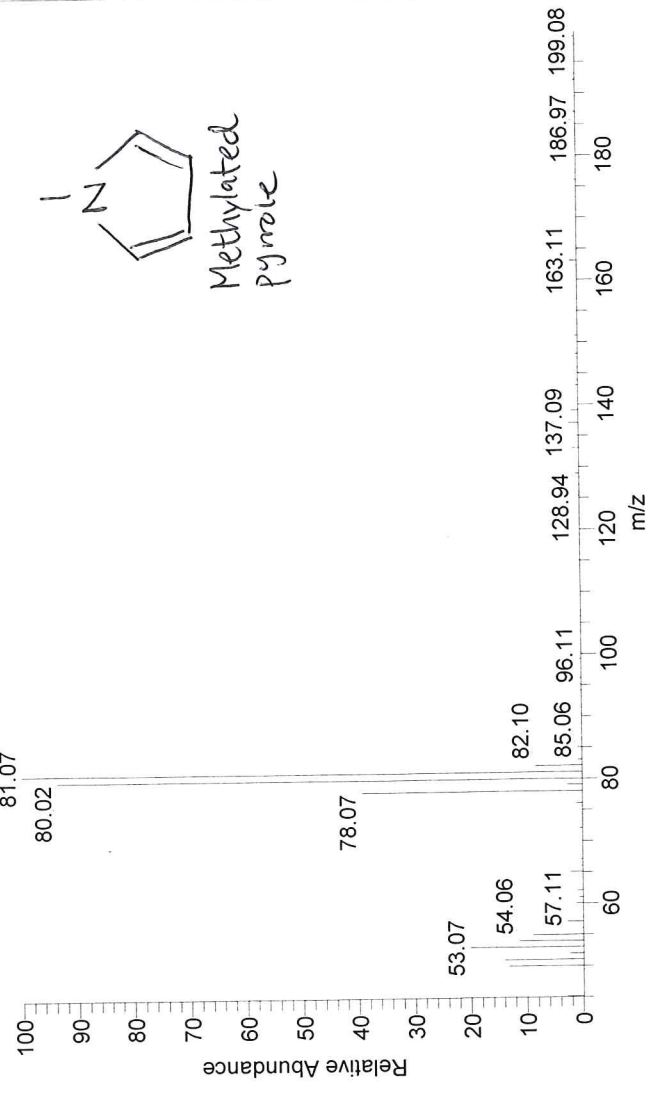
RT: 0.00 - 8.84

10/09/18 12:43:02

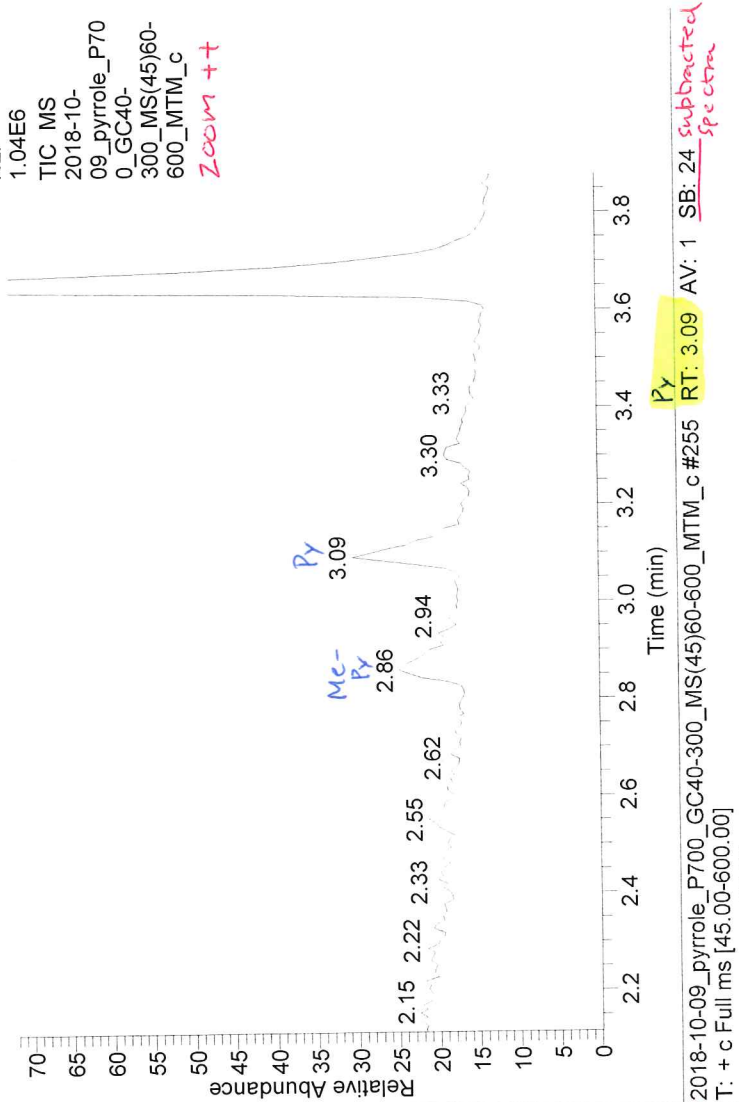
Pyrrole, ref



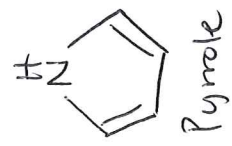
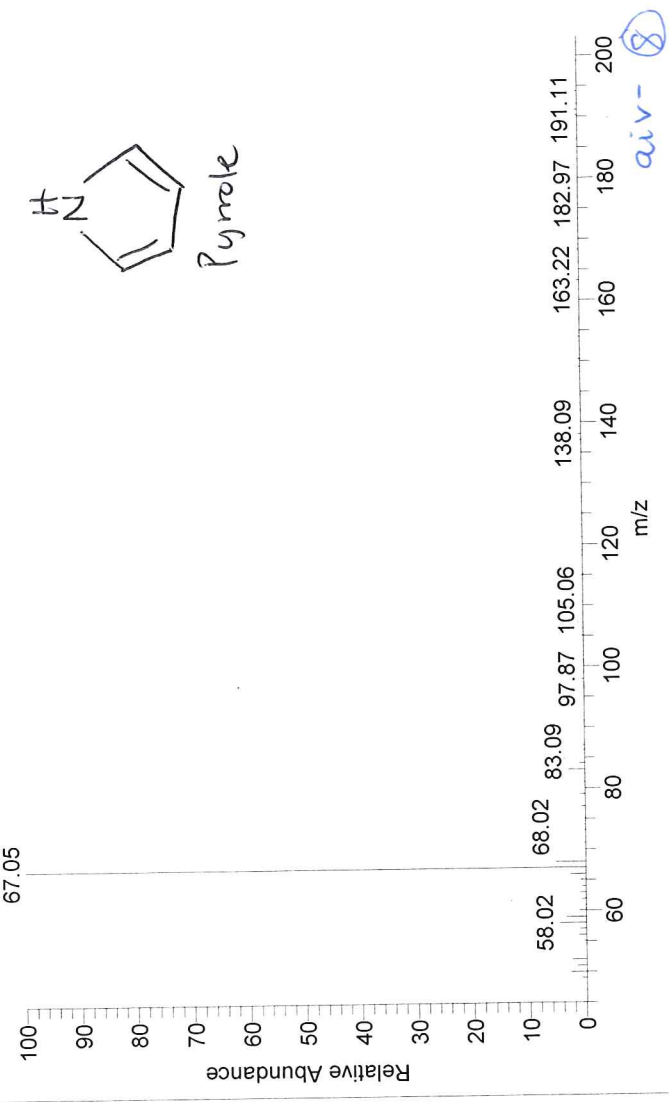
Pyrrole + TMAH, Mass Spectra
2018-10-09_pyrrole_P700_GC40-300_MS(45)60-600_MTM_c #227
T: + c Full ms [45.00-600.00]



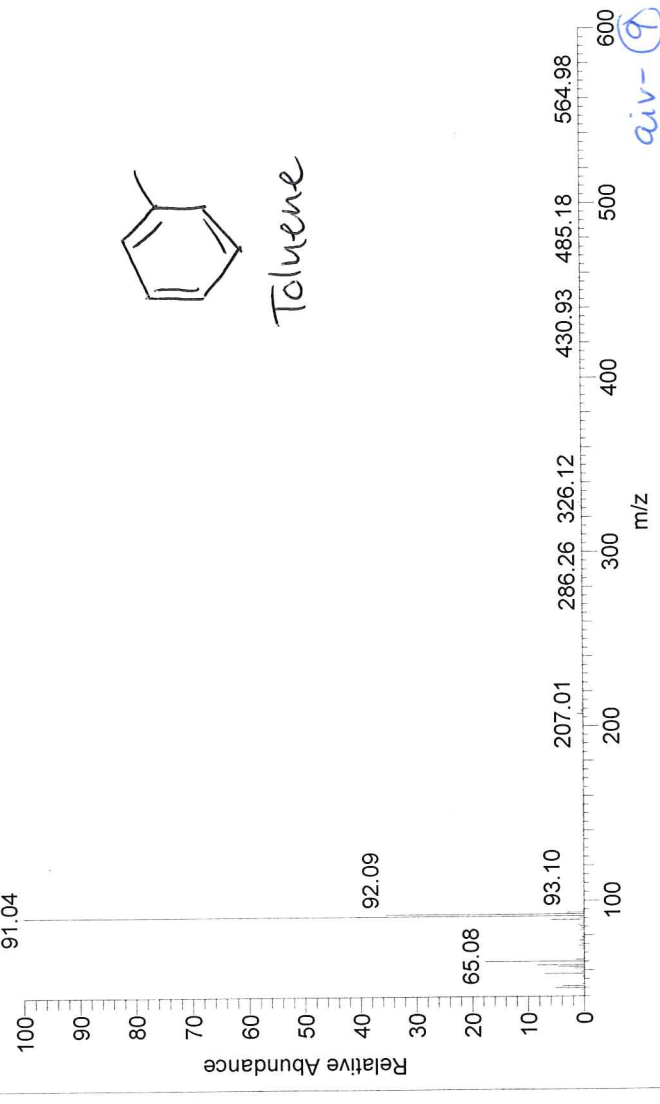
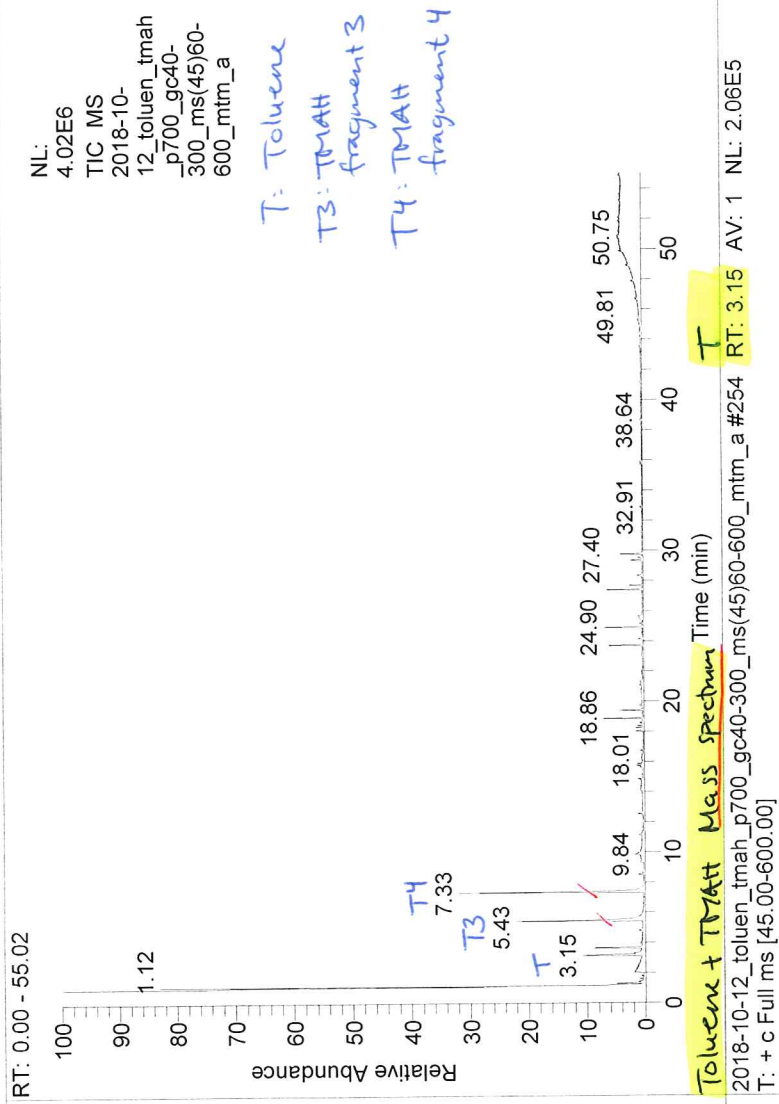
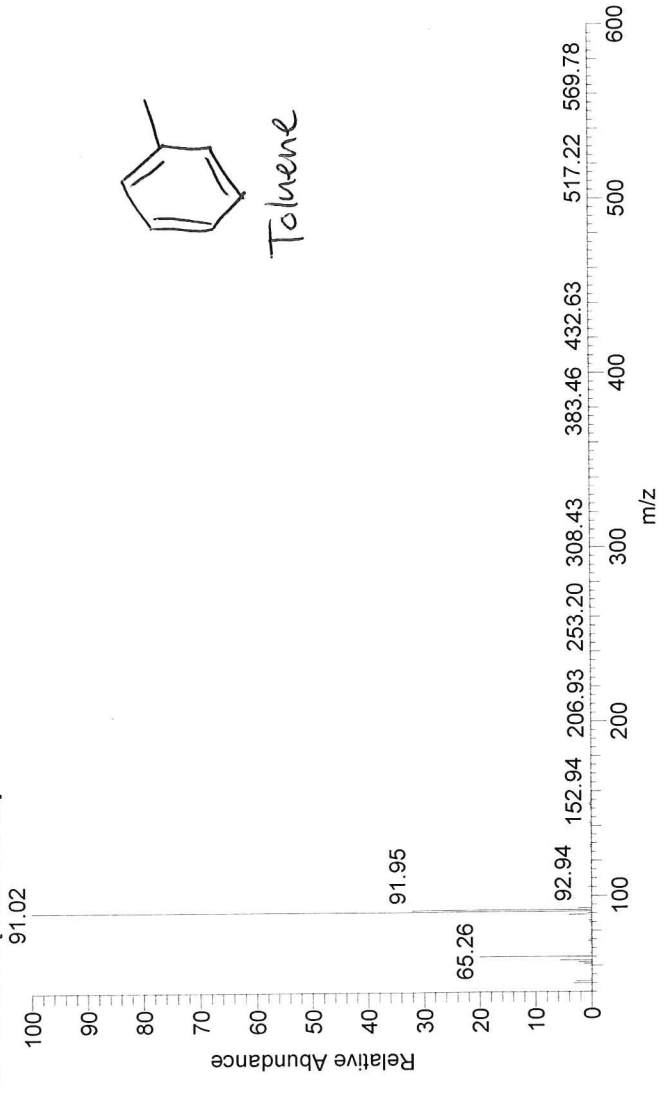
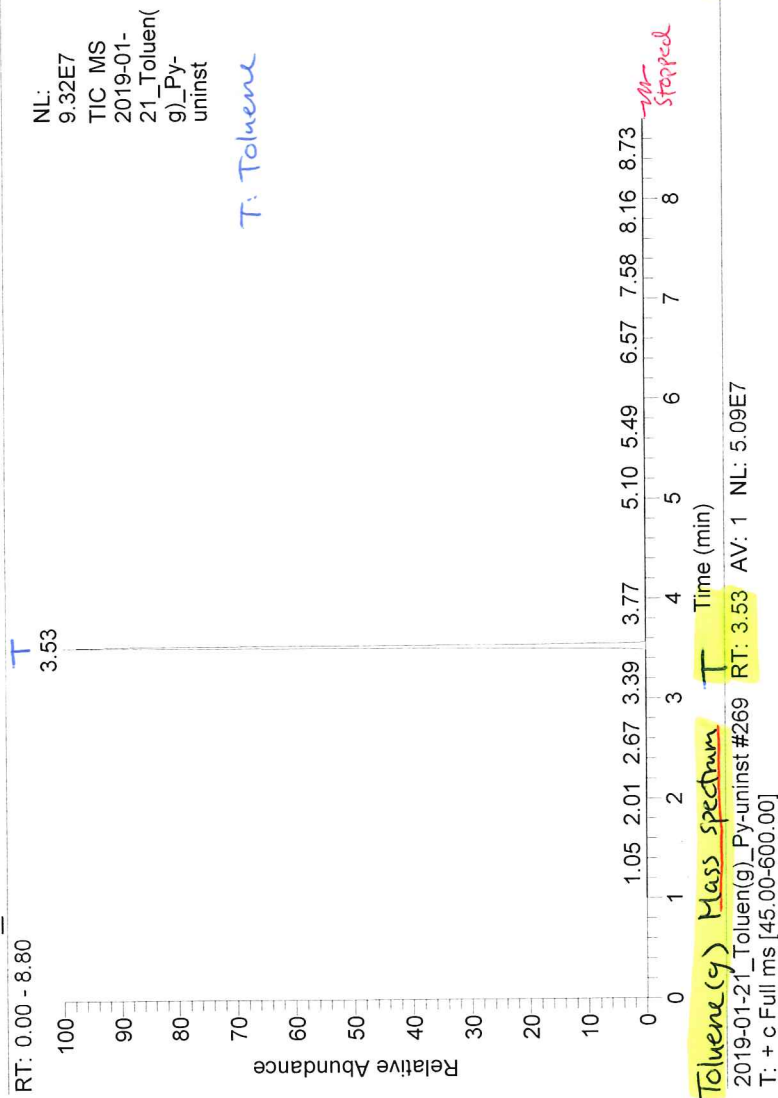
RT: 2.12 - 3.88



Pyrrole, ref
2018-10-09_pyrrole_P700_GC40-300_MS(45)60-600_MTM_c #255
T: + c Full ms [45.00-600.00]



Toluene (g)	Pyrogram	Toluene + TMAH	Pyrogram
2018-10-12	toluen tmah p700 ac40-300		toluen + TMAH
		gas injected	
		no pyrolysis	
		10/12/18	12:43:42



Indole (g) Pyrogram
2019-01-22_Indole(g)_Py-uninst_2_1901...

01/22/19 15:19:33

gas injected
no pyrolysis

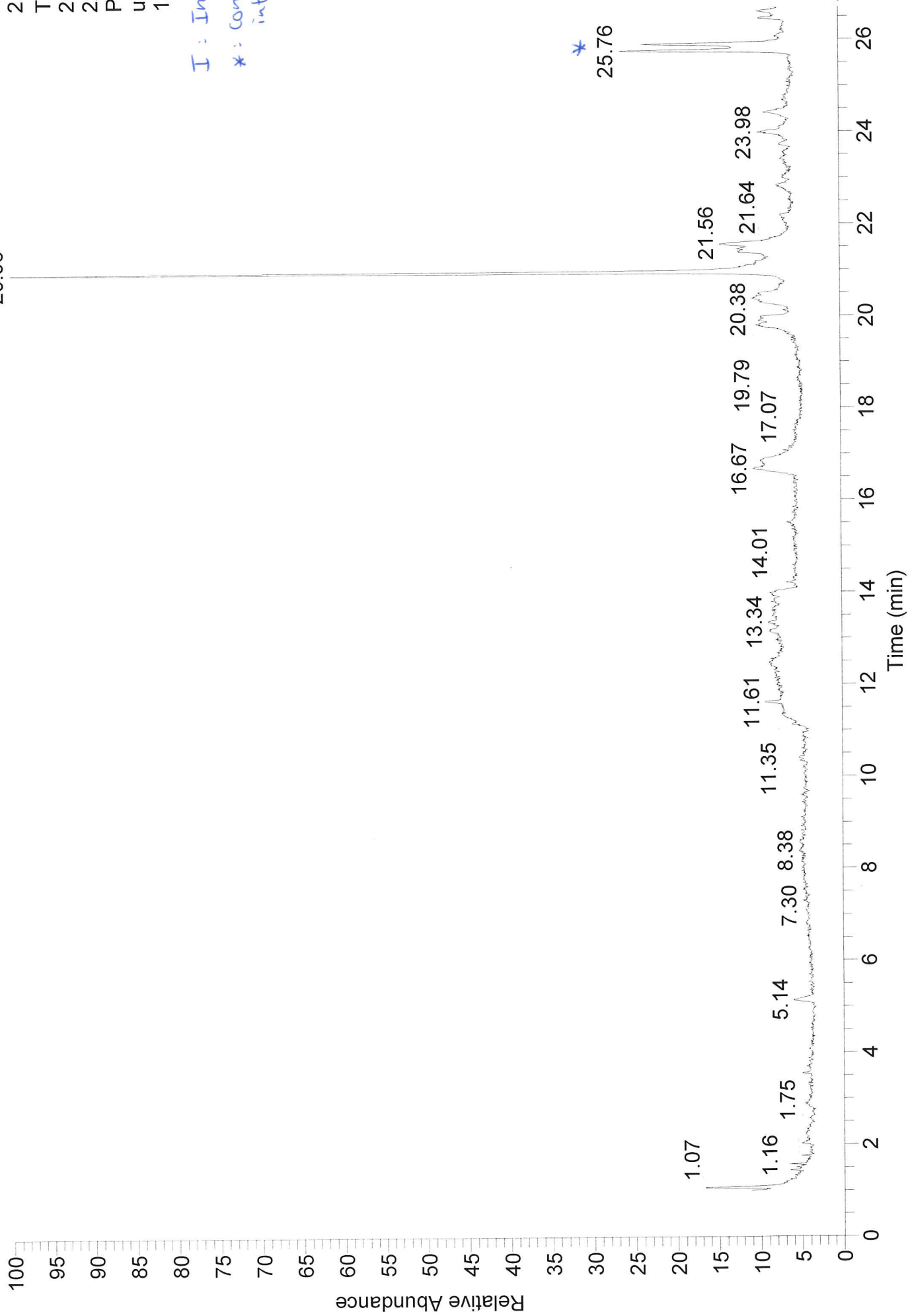
I

RT: 0.00 - 26.70

NL:
2.81E5
TIC MS
2019-01-
22_Indole(g)_
Py-
uninst_2_190
122151933

I: Indole

*: Contamination/
interference



MM-
Stopped
air- (15)

01/22/19 15:19:33

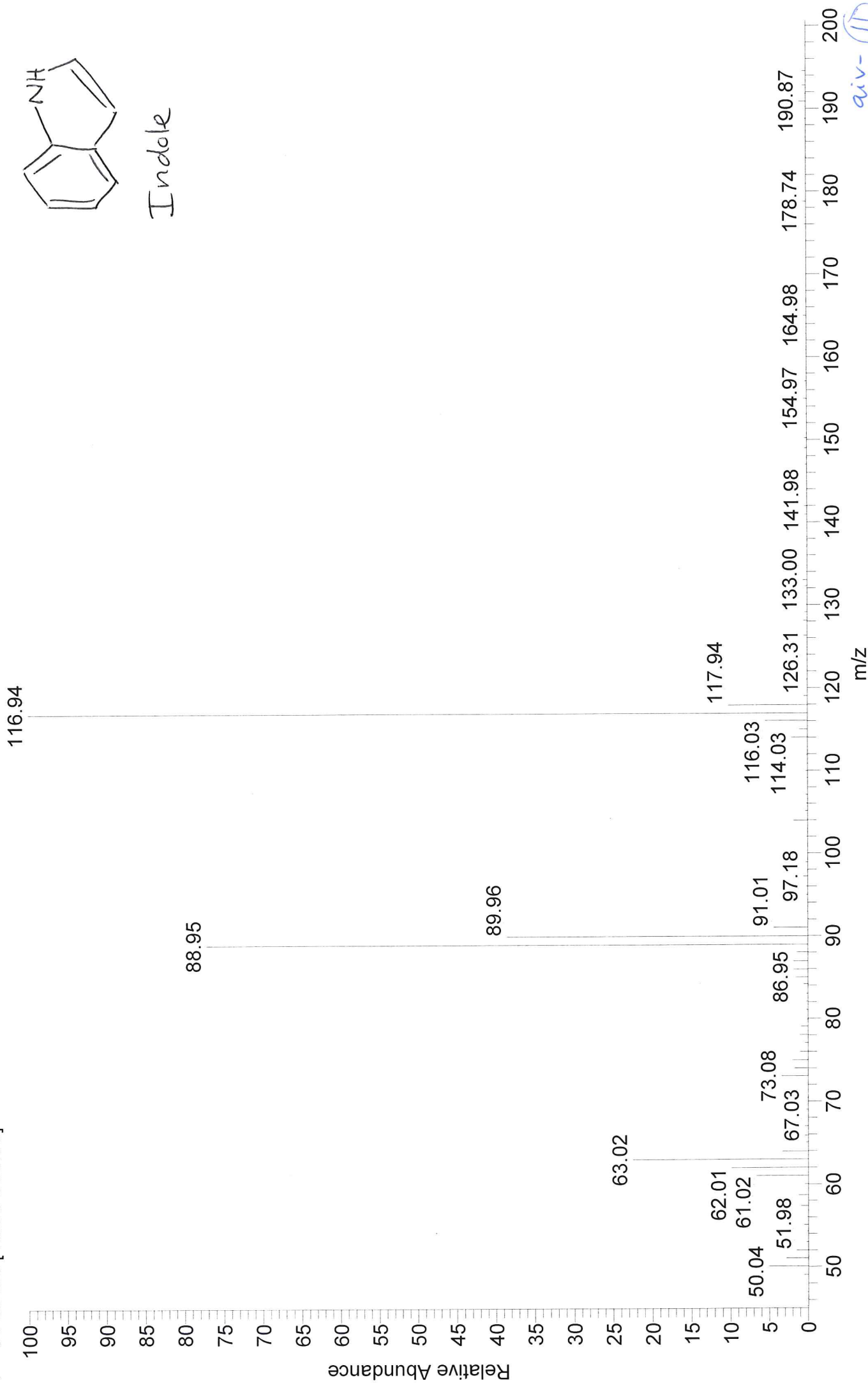
Gas injected
No pyrolysis

I

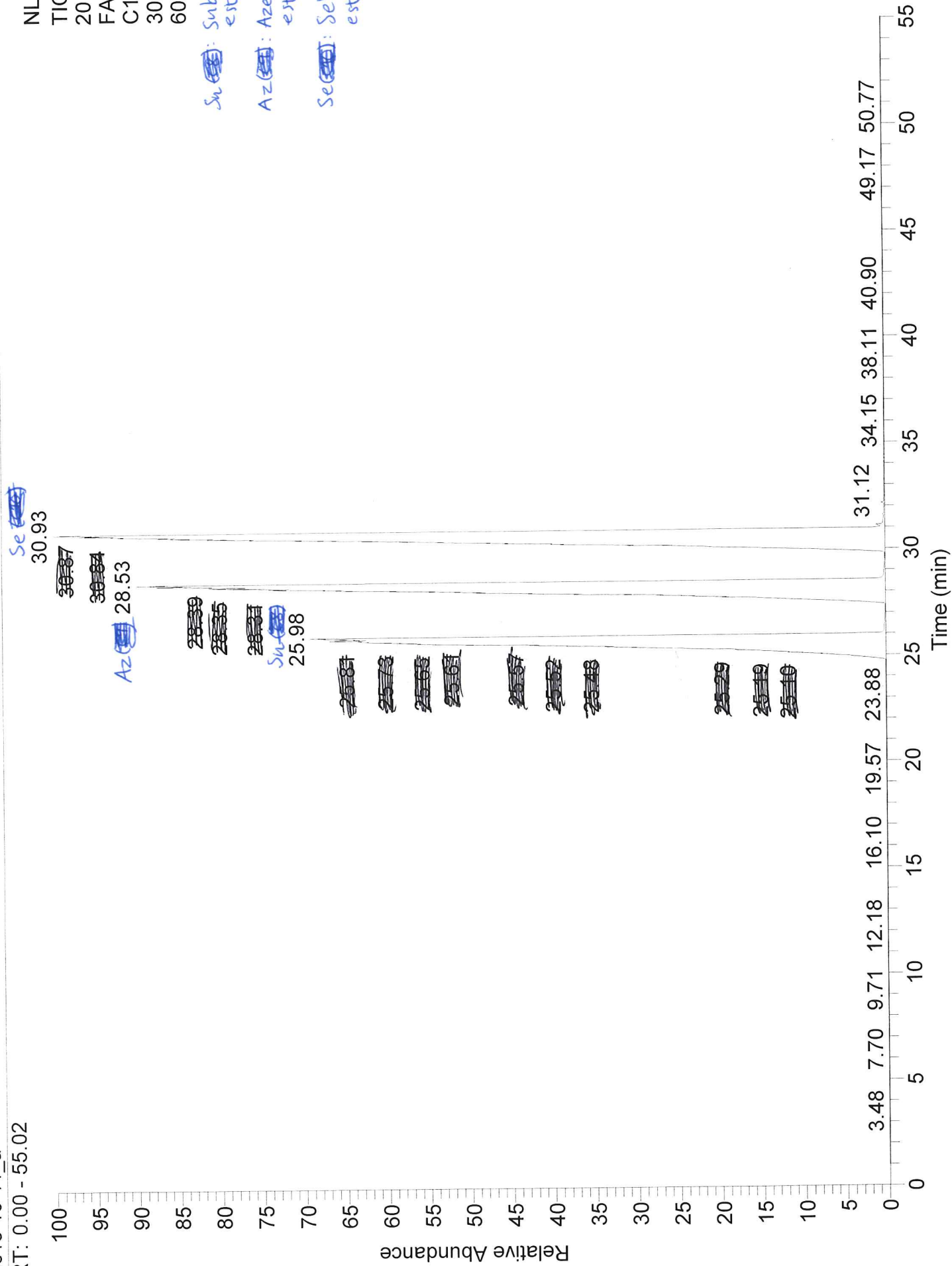
RT: 20.95 AV: 1 NL: 7.36E4

2019-01-22_Indole(g)_Py-uninst_2_190122151933 #2090

T: + c Full ms [45.00-600.00]



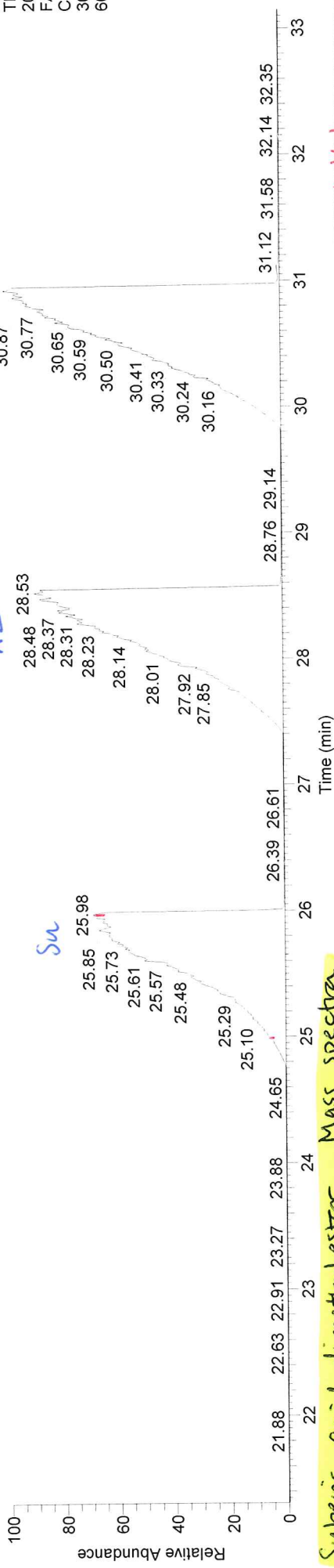
av- (11)



2018-10-11_a

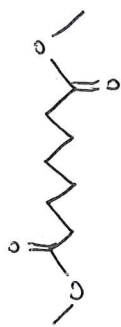
RT: 21.31 - 33.15

NL: 1.18E9
TIC MS
2018-10-11_diMe-
FAdiesters(C8-C9-
C10)_P700_GC40-
300_MS(45)60-
600_MTM_a

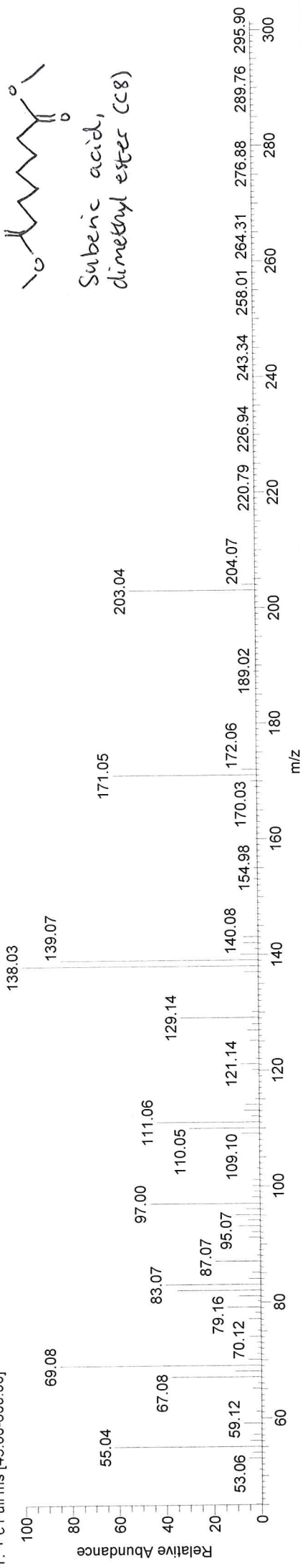


Subenic acid, dimethyl ester Mass spectra

2018-10-11_diMe-FAdiesters(C8-C9-C10)_P700_GC40-300_MS(45)60-600_MTM_a #2545 RT: 24.99 AV: 1 NL: 6.52E6 (beginning of peak, more representative)

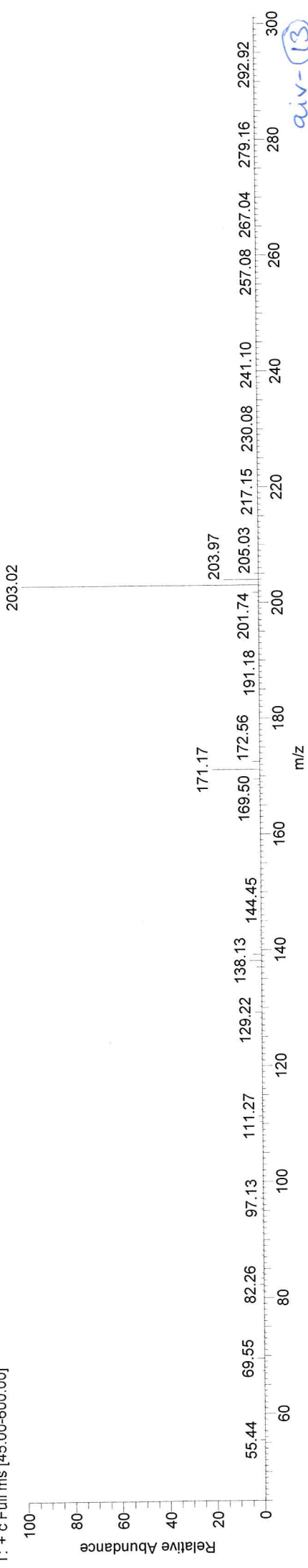


Subenic acid,
dimethyl ester (C8)



Subenic acid, dimethyl ester Mass spectra

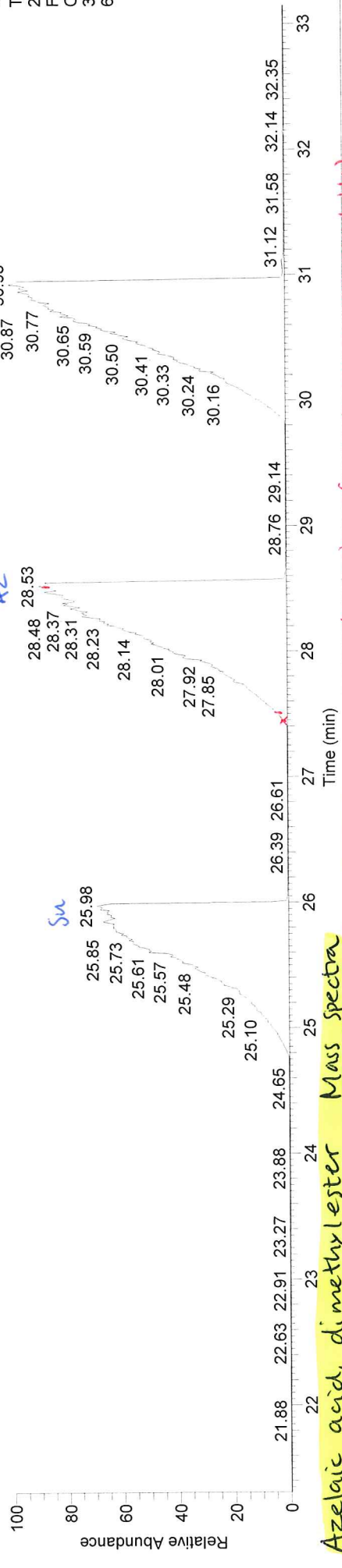
2018-10-11_diMe-FAdiesters(C8-C9-C10)_P700_GC40-300_MS(45)60-600_MTM_a #2660 RT: 25.98 AV: 1 NL: 4.11E8 (top of peak)



div-13

2018-10-11_a

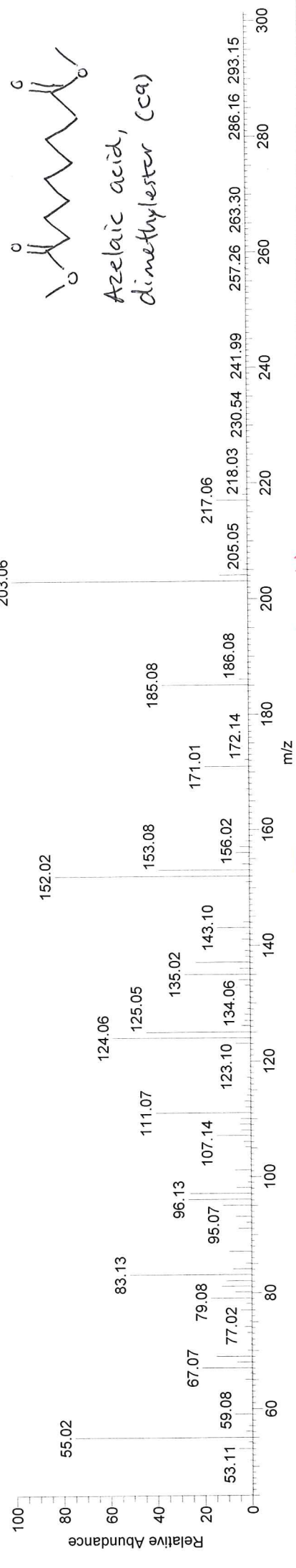
RT: 21.31 - 33.15



Azelaic acid, dimethylester Mass Spectra

2018-10-11_diMe-FAdiesters(C8-C9-C10)_P700_GC40-300_MS(45)60-600_MTM_a #2844 RT: 27.51 NL: 4.85E6 AV: 1

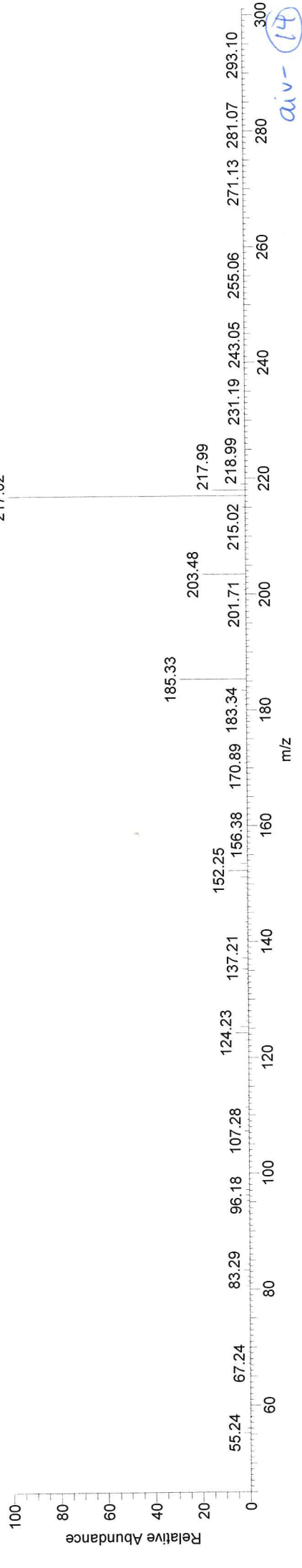
(Beginning of peak, more representative)



Azelaic acid, dimethylester Mass Spectra

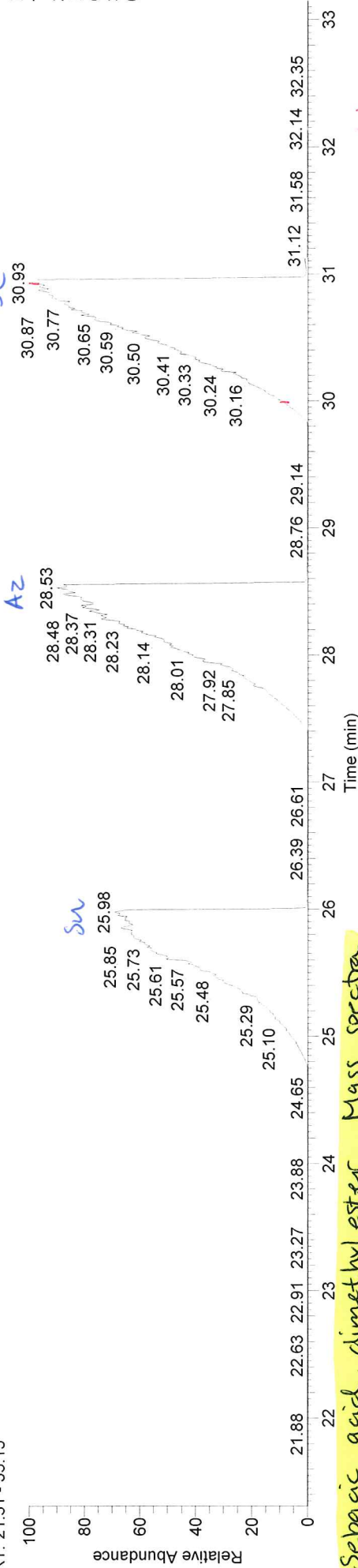
2018-10-11_diMe-FAdiesters(C8-C9-C10)_P700_GC40-300_MS(45)60-600_MTM_a #2959 RT: 28.51 NL: 4.06E8 AV: 1

(Top of peak)



div-14

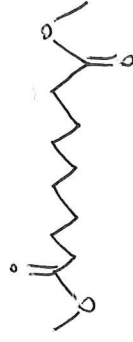
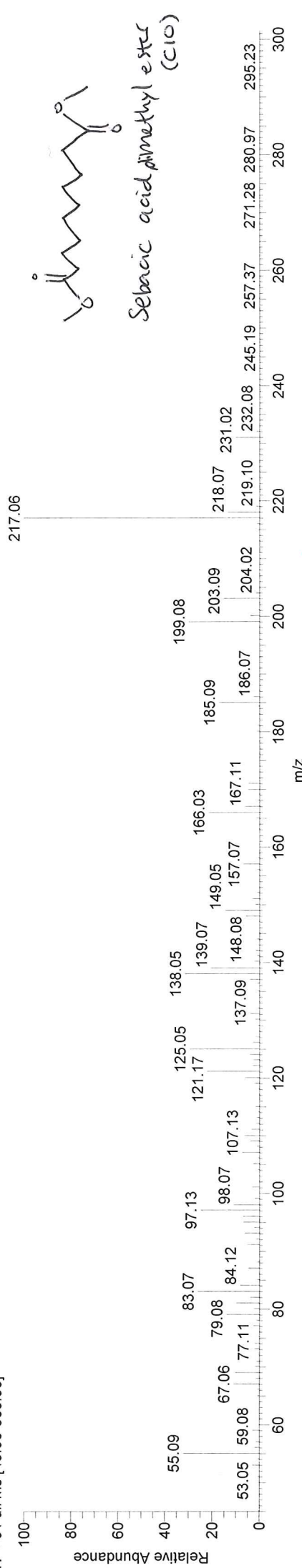
RT: 21.31 - 33.15



Sebacic acid, dimethyl ester Mass spectra

2018-10-11_diMe-FAdiesters(C8-C9-C10)_P700_GC40-300_MS(45)60-600_MTM_a #3128 RT: 29.93 AV: 1 NL: 8.53E6 (Beginning of peak, more representative)

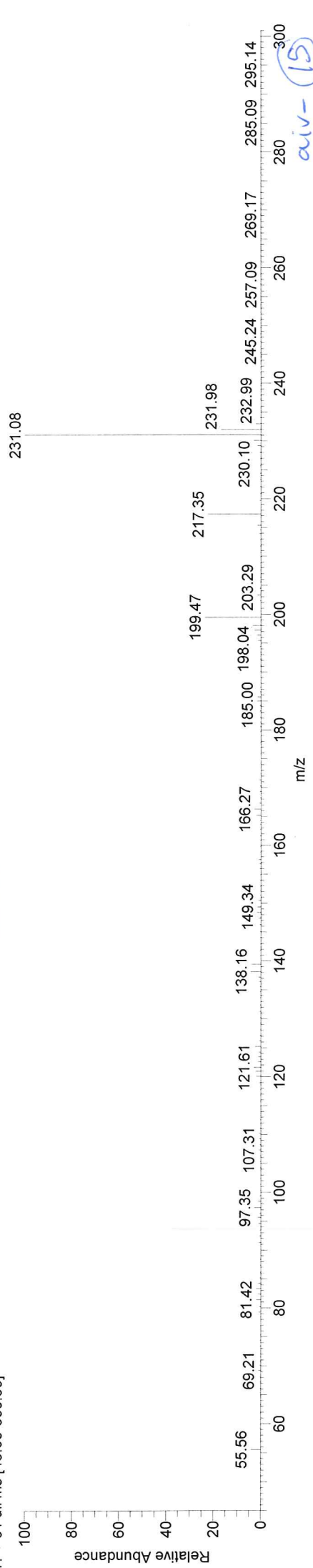
T: + c Full ms [45.00-600.00]



Sebacic acid dimethyl ester (C10)

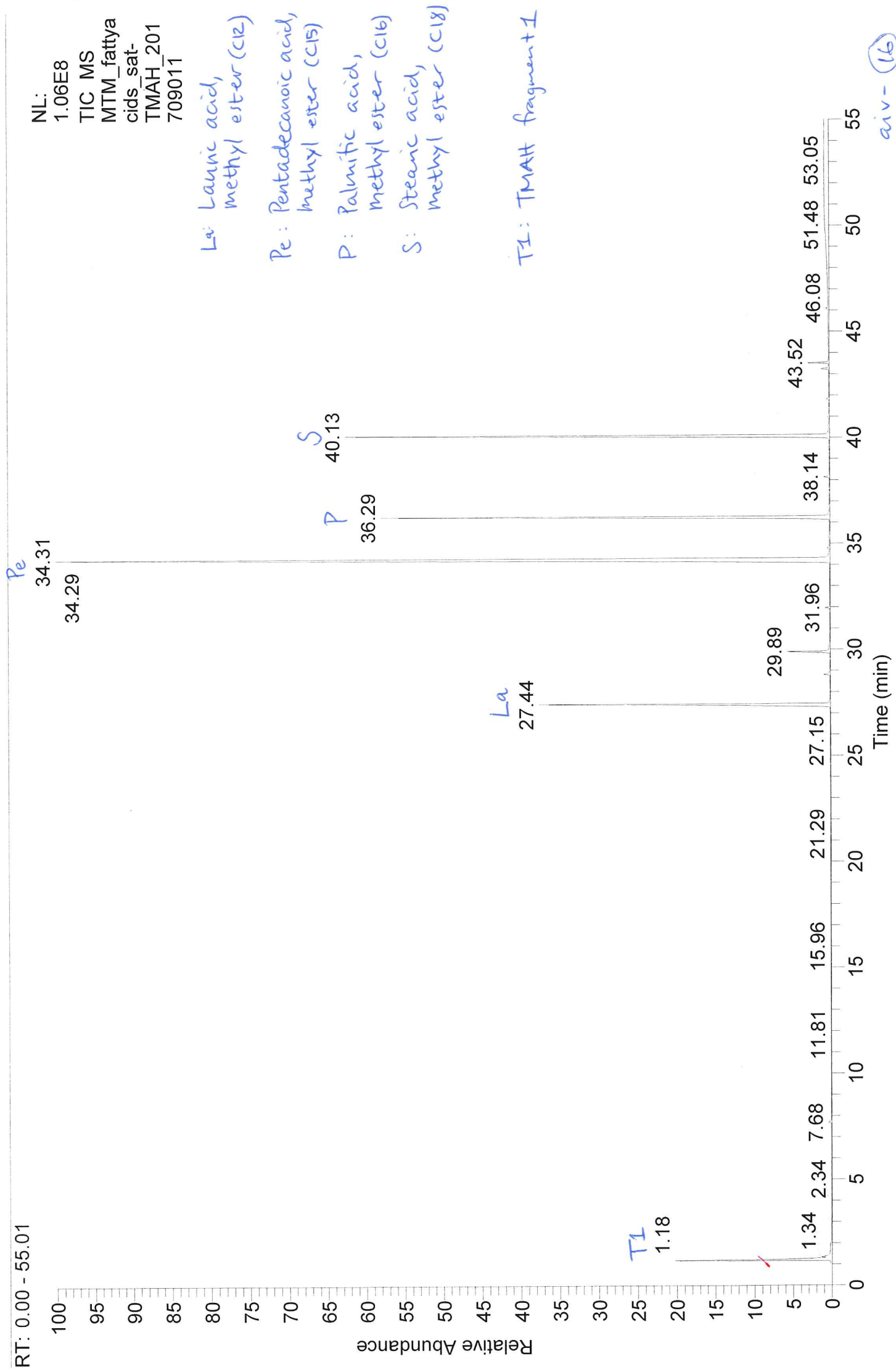
2018-10-11_diMe-FAdiesters(C8-C9-C10)_P700_GC40-300_MS(45)60-600_MTM_a #3242 RT: 30.93 AV: 1 NL: 4.24E8 (Top of peak)

T: + c Full ms [45.00-600.00]



av-15

RT: 0.00 - 55.01

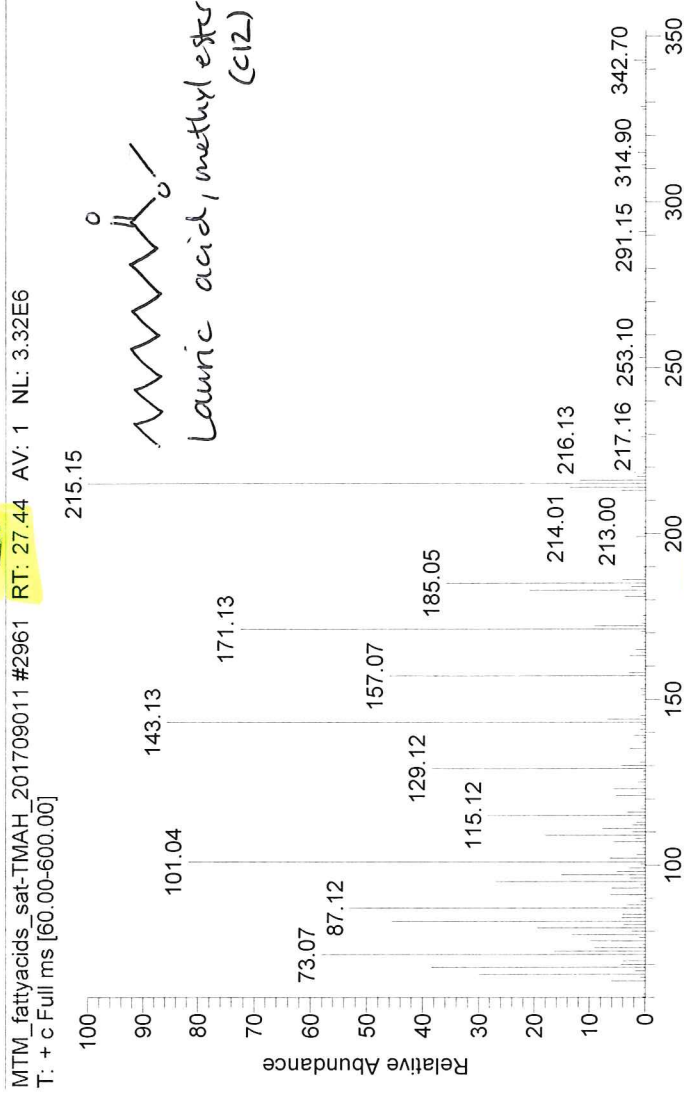


Fatty acids (C12, C15, C16, C18) + TMAH Mass Spectra

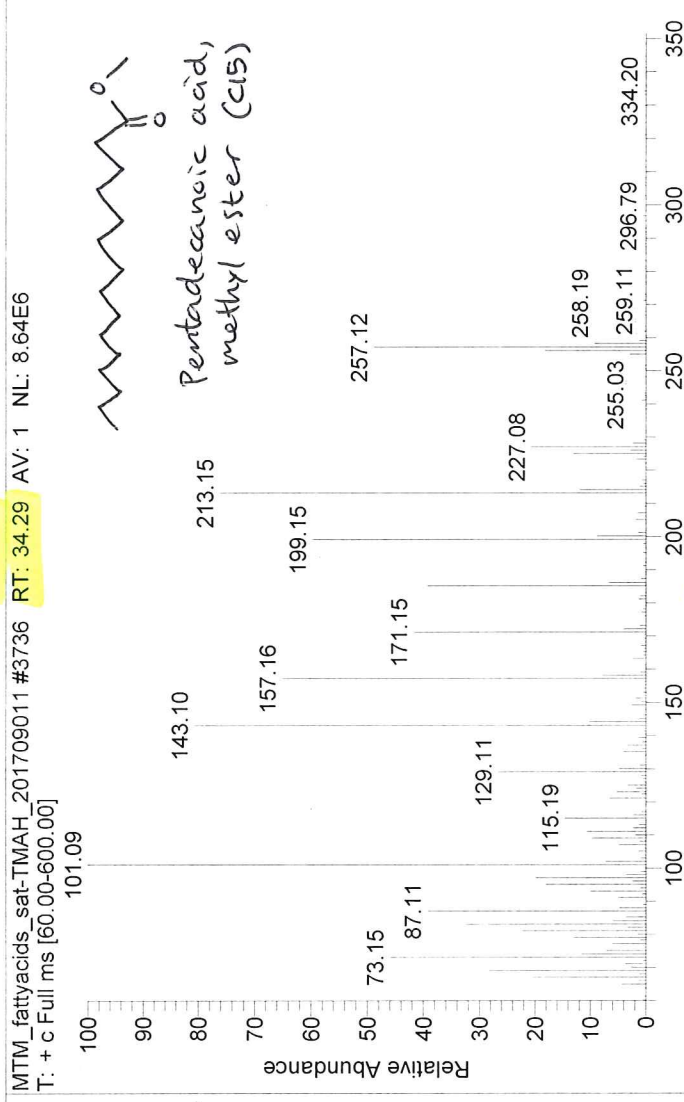
09/11/17 14:33:06

MTM_fattyacids_sat-TMAH_201709011

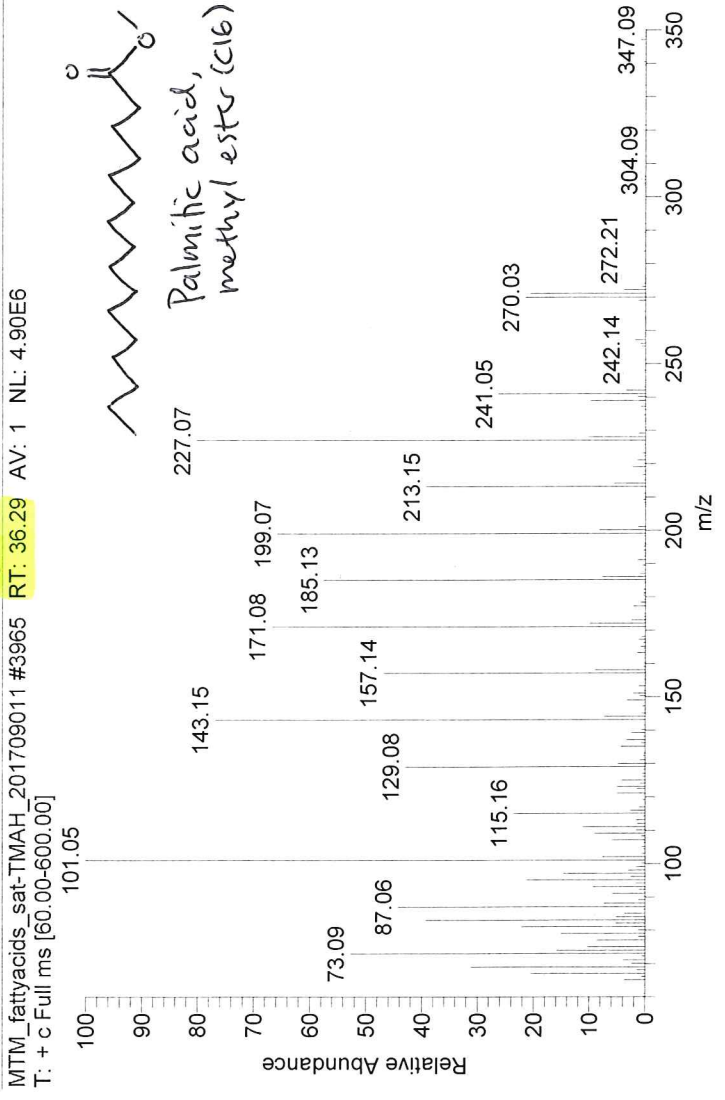
La



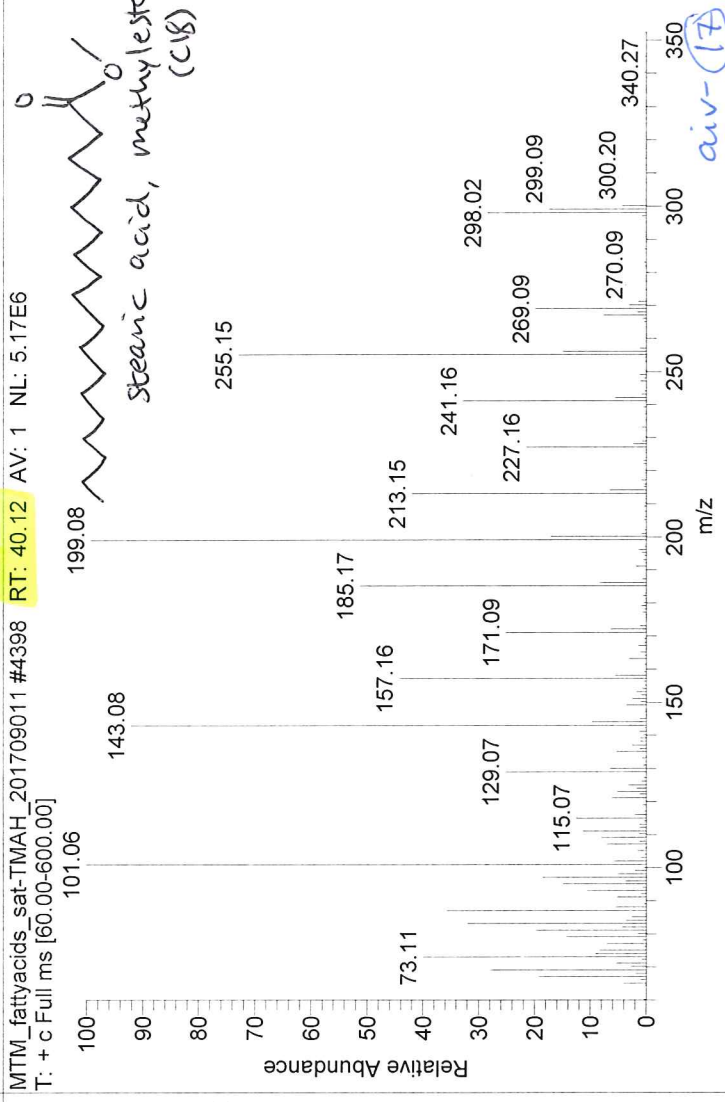
Pe



P



S

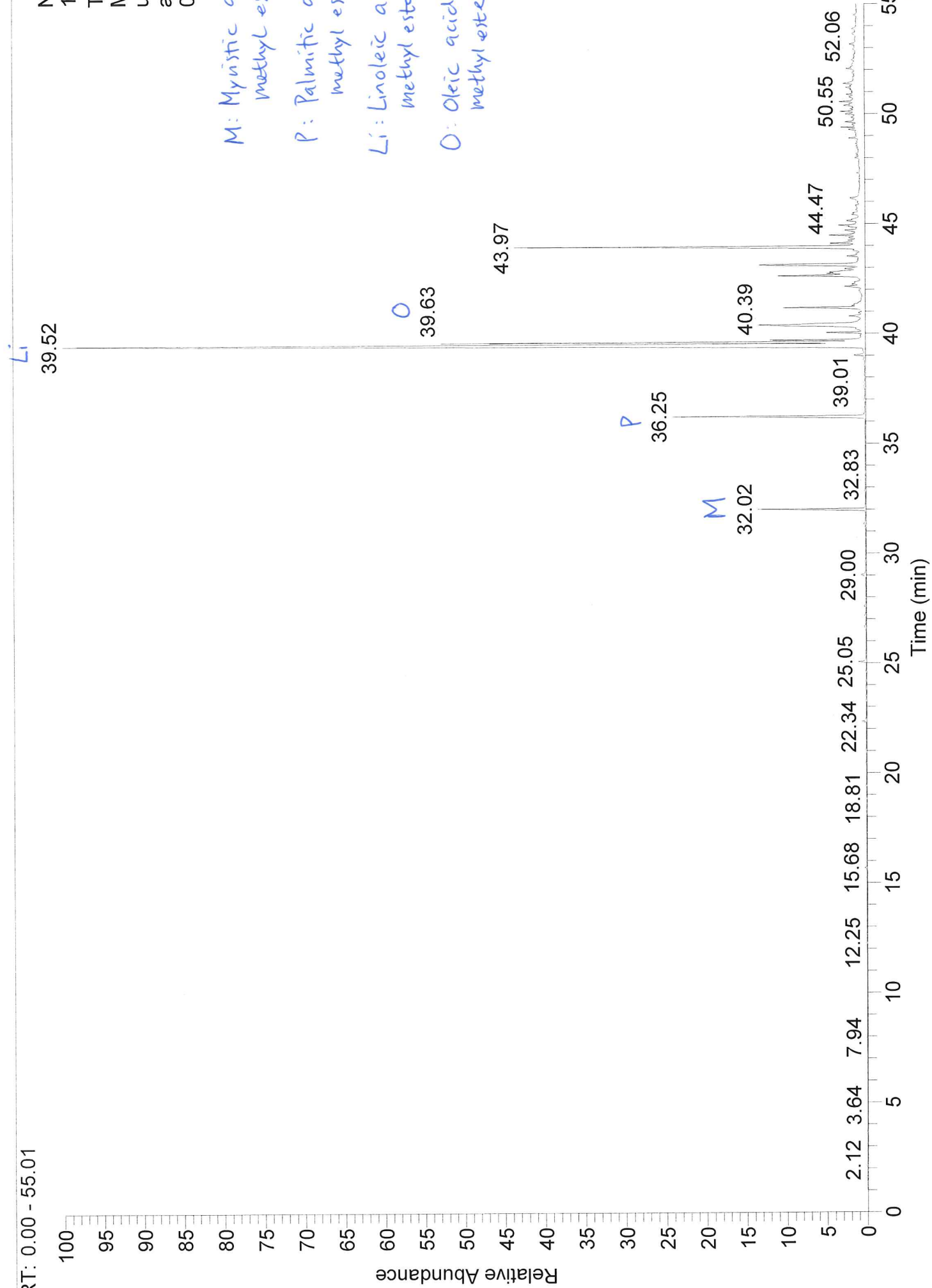


div-17

RT: 0.00 - 55.01

NL:
1.36E8
TIC MS
MTM_met
unsat_fatty
acids_2017
09013

M: Myristic acid,
methyl ester (C14:0)
P: Palmitic acid,
methyl ester (C16:0)
Li: Linoleic acid,
methyl ester (C18:2)
O: Oleic acid,
methyl ester (C18:1)



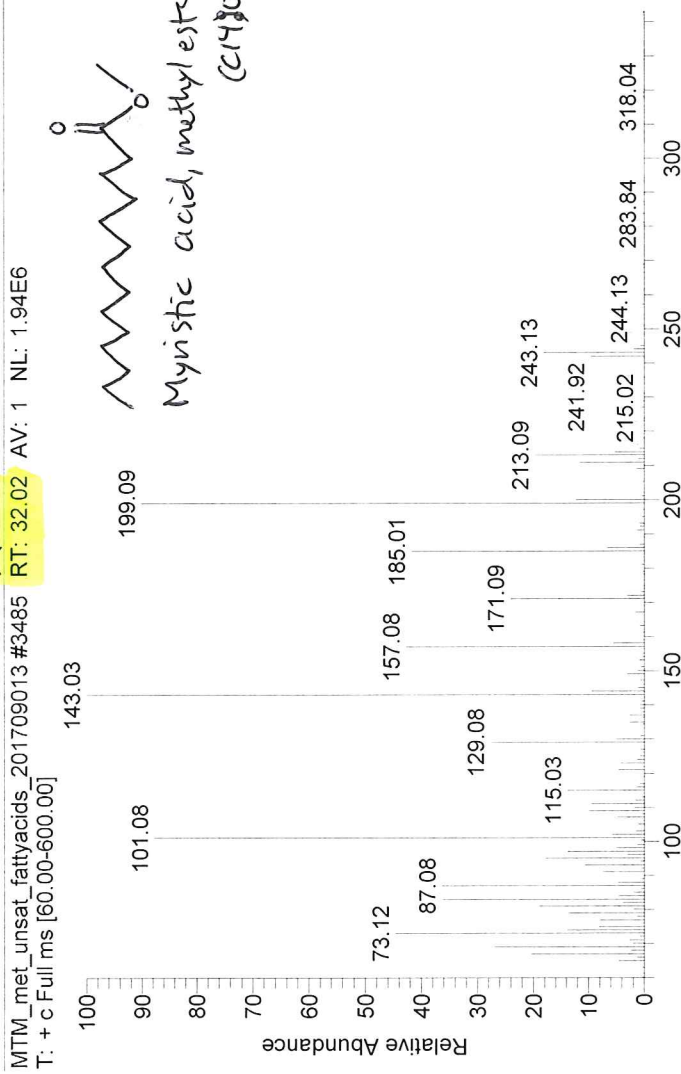
Methylated fatty acids (C14:0, C16:0, C18:1, C18:2) in toluene Mass Spectra

MTM_met_unsat_fattyacids_201709013

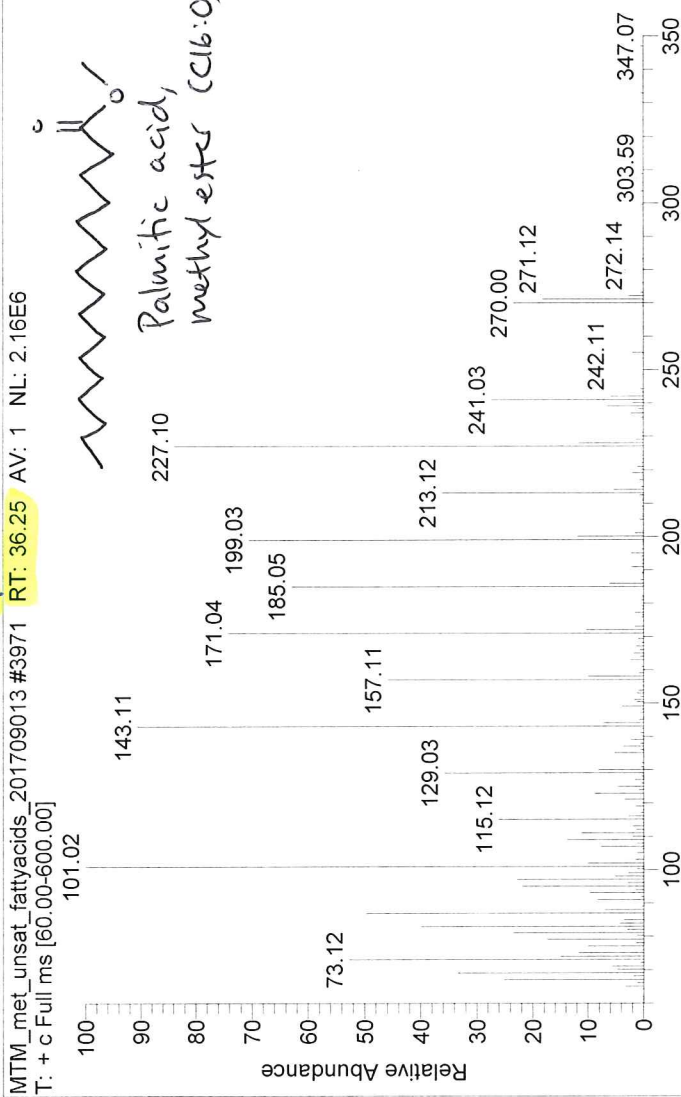
09/13/17 13:51:06

met unsat fatty acids

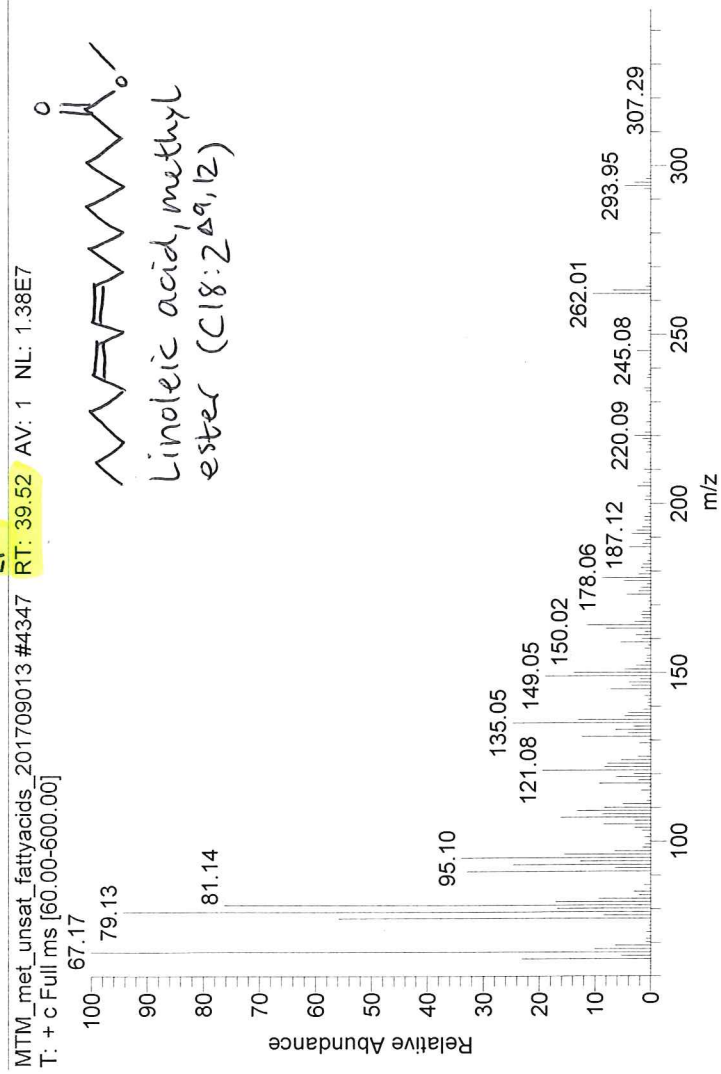
M



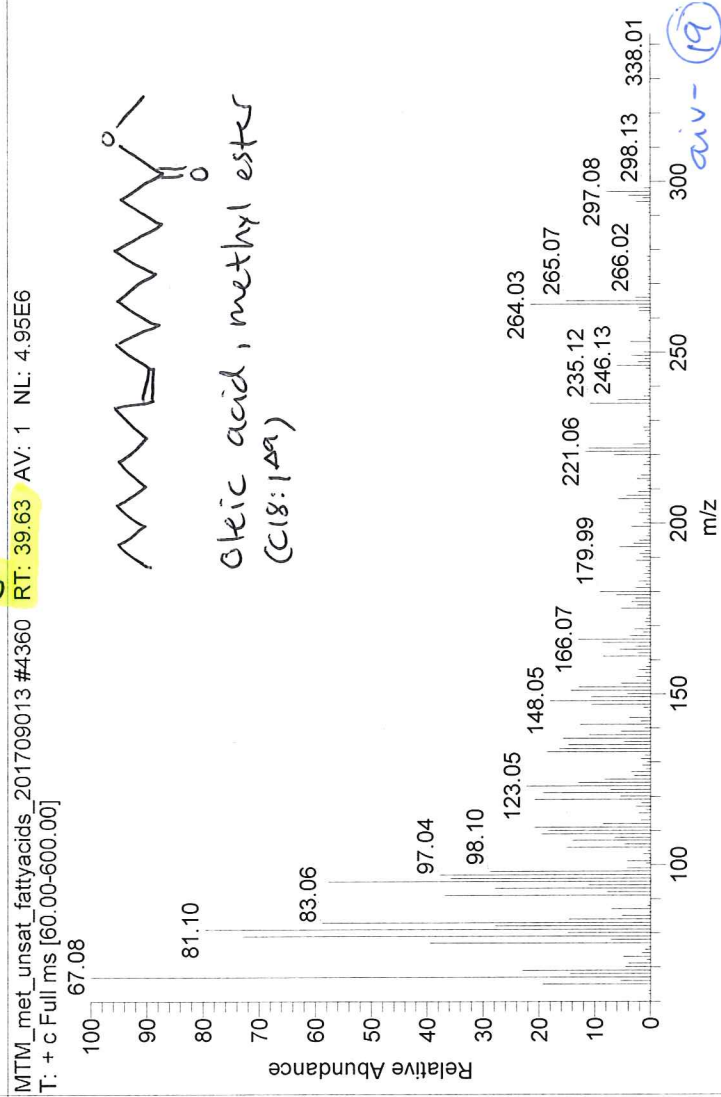
P



L



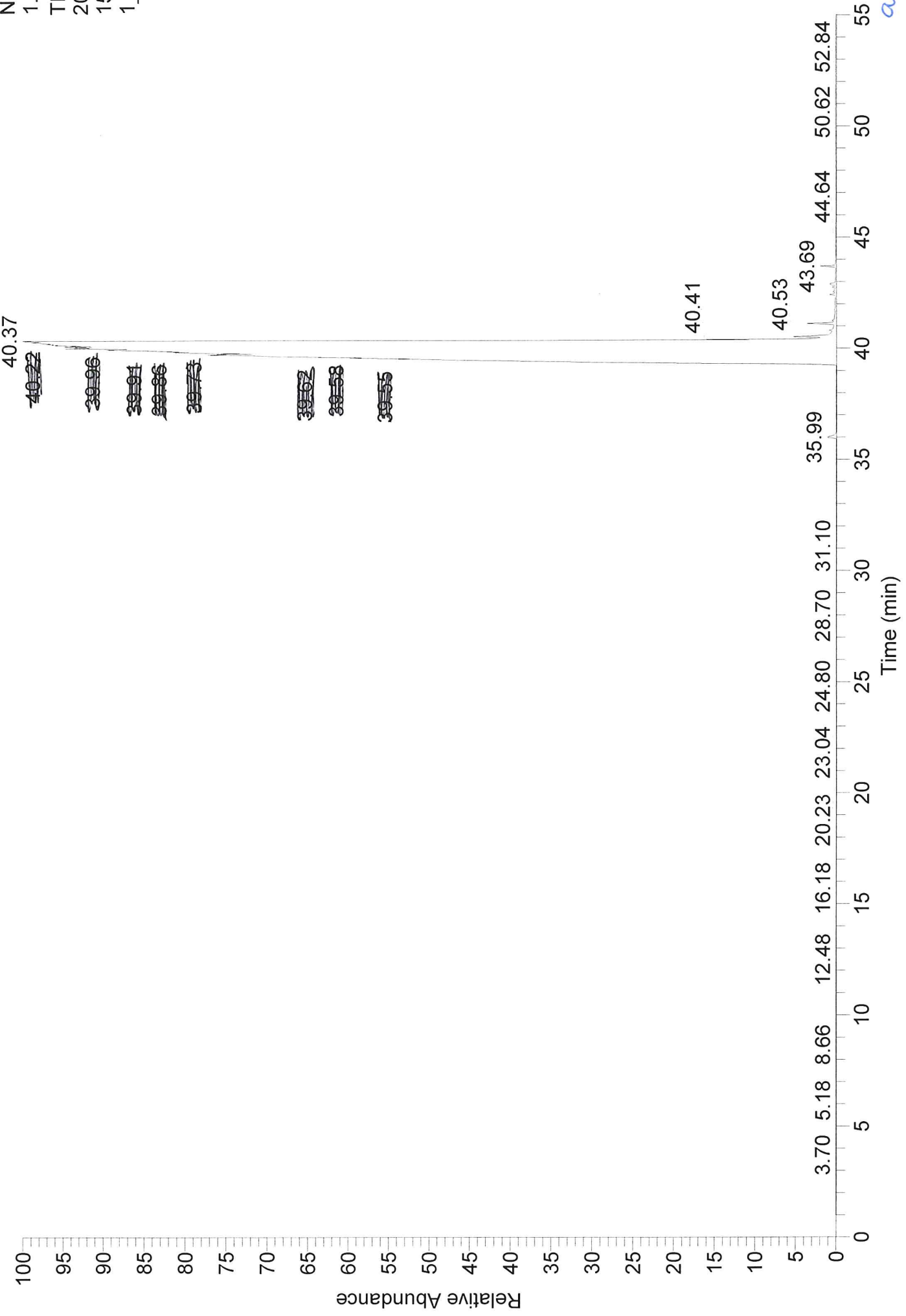
O



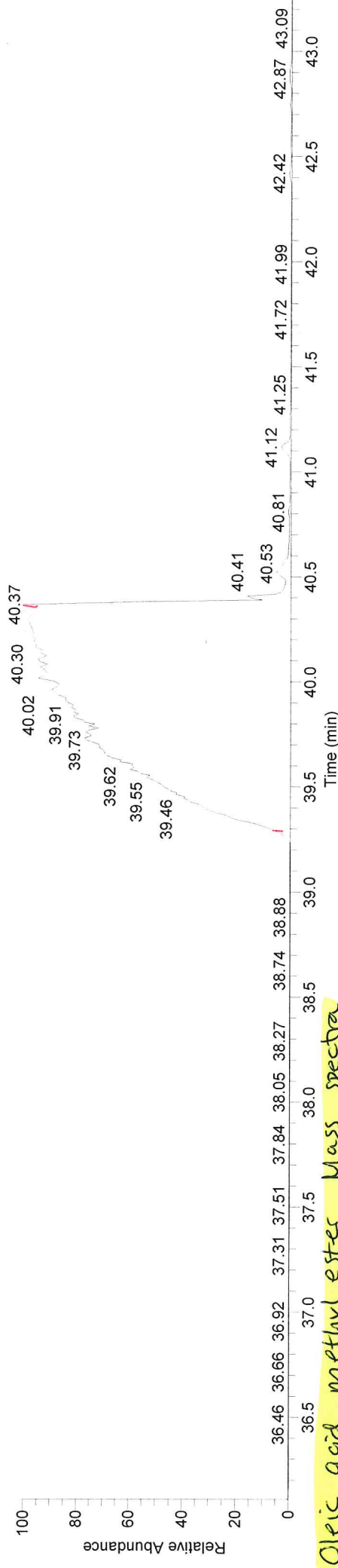
av-19

RT: 0.00 - 55.03

NL:
1.12E9
TIC MS
2019-02-
15_MeC18-
1_P700

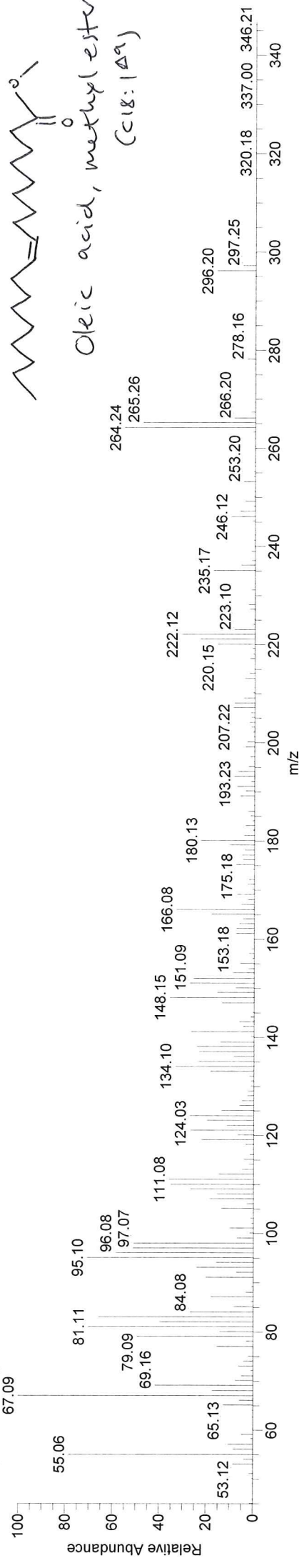


RT: 36.11 - 43.25

Oleic acid, methyl ester Mass spectra

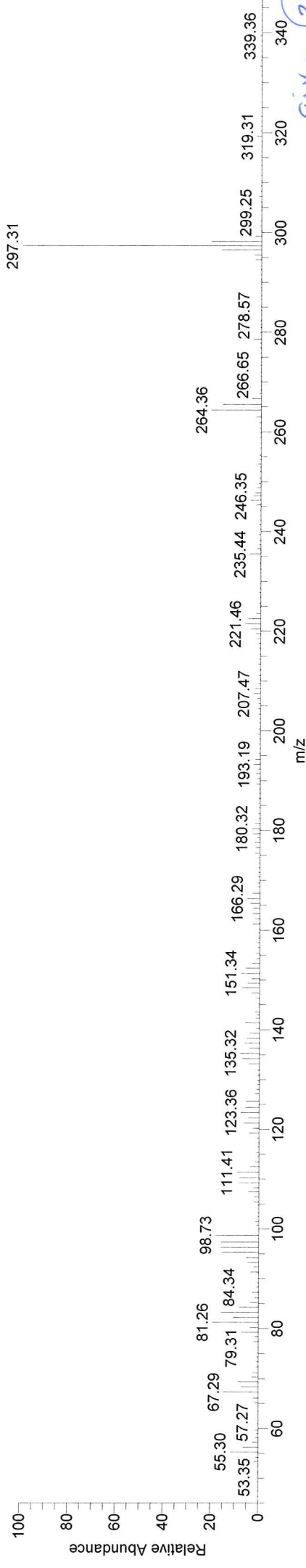
2019-02-15_MeC18-1_P700 #4053 RT: 39.30 AV: 1 NL: 3.44E6

T: + c Full ms [45.00-600.00]



2019-02-15_MeC18-1_P700 #4153 RT: 40.37 AV: 1 NL: 1.41E8

T: + c Full ms [45.00-600.00]



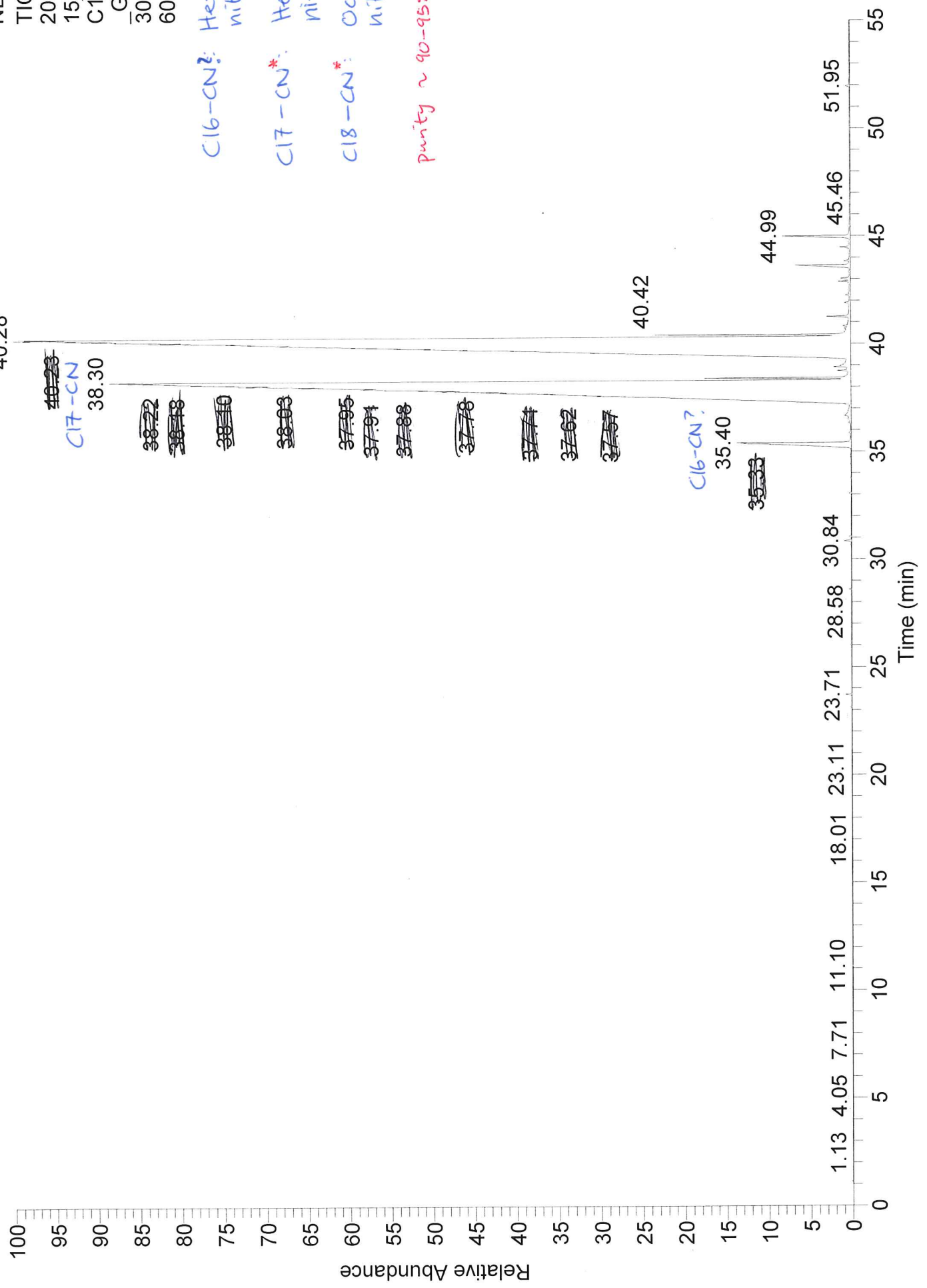
Alkyl nitriles (C17, C18) + TMAH Pyrogram

10/15/18 11:09:20

Nitriles (C17-C18)

NL: 7.36E8
TIC MS
2018-10-
15_nitriles(C17-
C18)_TMAH_P700
GC40-
300_MS(45)60-
600_MTM_a

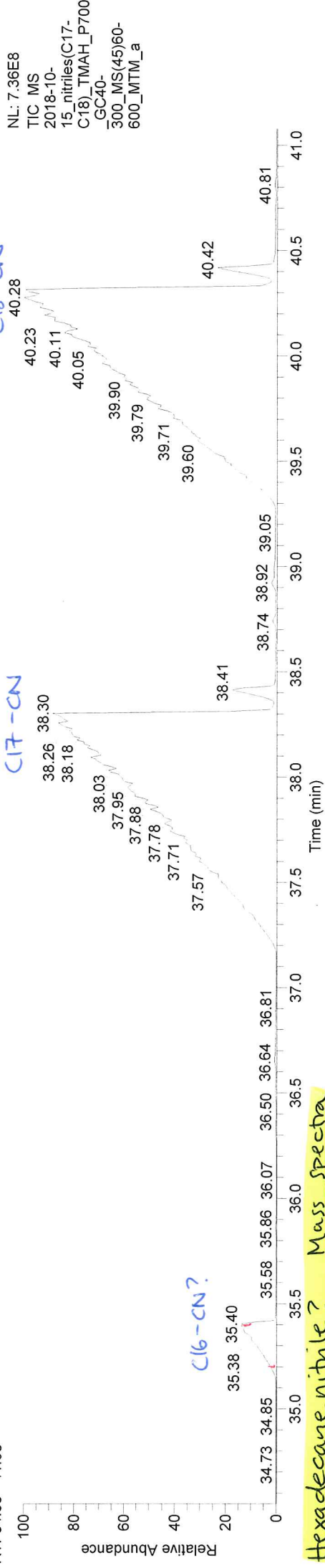
RT: 0.00 - 55.01



C16-CN? Hexadecane nitrile
C17-CN? Heptadecane nitrile
C18-CN? Octadecane nitrile

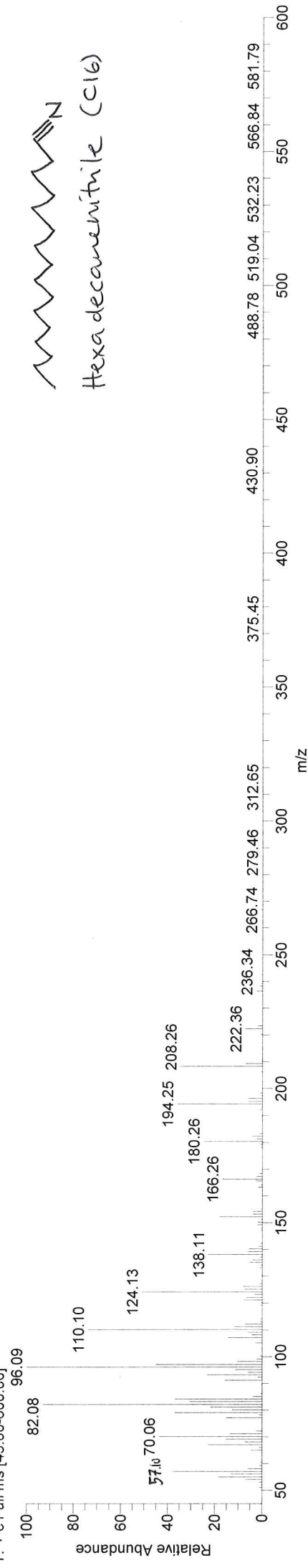
purity ~ 90-95%

RT: 34.55 - 41.08

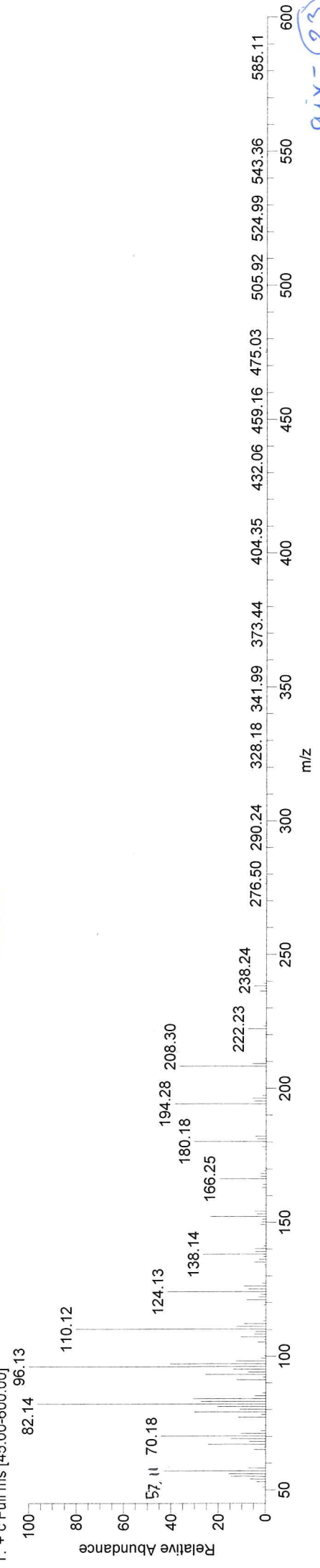


Hexadecanenitrile? Mass Spectra

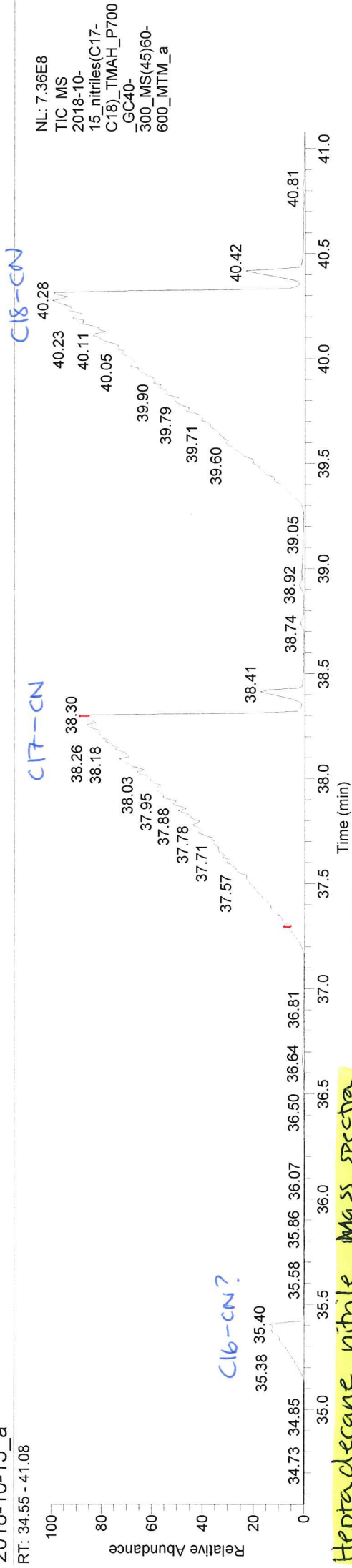
2018-10-15_nitriles(C17-C18)_TMAH_P700_GC40-300_MS(45)60-600_MTM_a #3696 RT: 35.20 AV: 1 NL: 1.39E6
T: + c Full ms [45.00-600.00]



2018-10-15_nitriles(C17-C18)_TMAH_P700_GC40-300_MS(45)60-600_MTM_a #3721 RT: 35.40 AV: 1 NL: 8.92E6
T: + c Full ms [45.00-600.00]



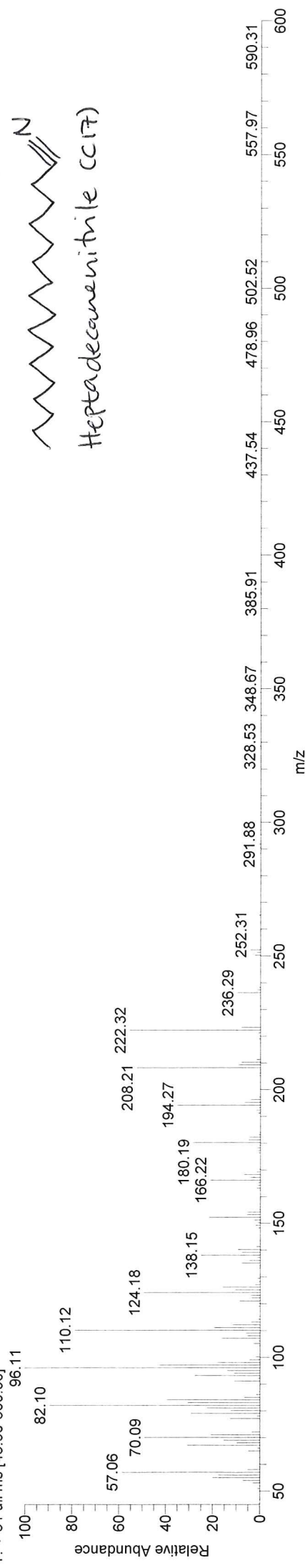
air-23



2018-10-15_nitriles(C17-C18)_TMAH_P700_GC40-300_MS(45)60-600_MTM_a #3947 RT: 37.29 AV: 1 NL: 3.49E6

T: + c Full ms [45.00-600.00]

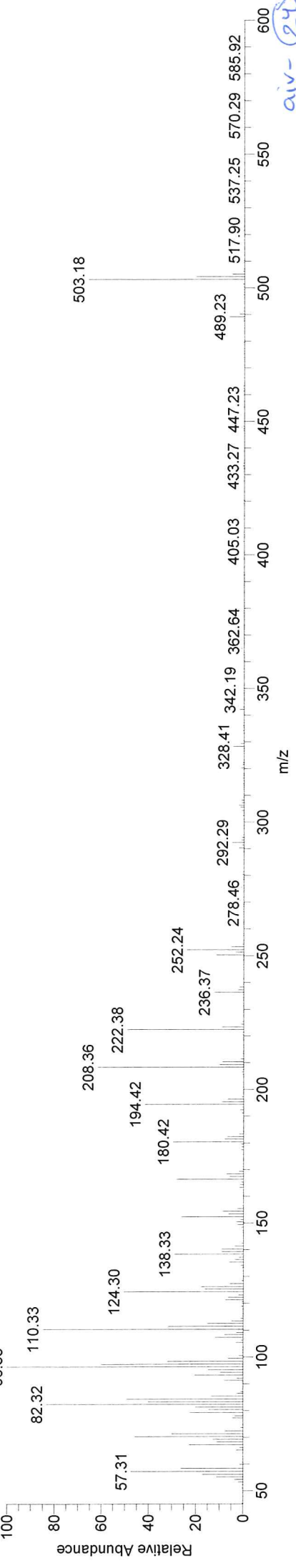
96.11



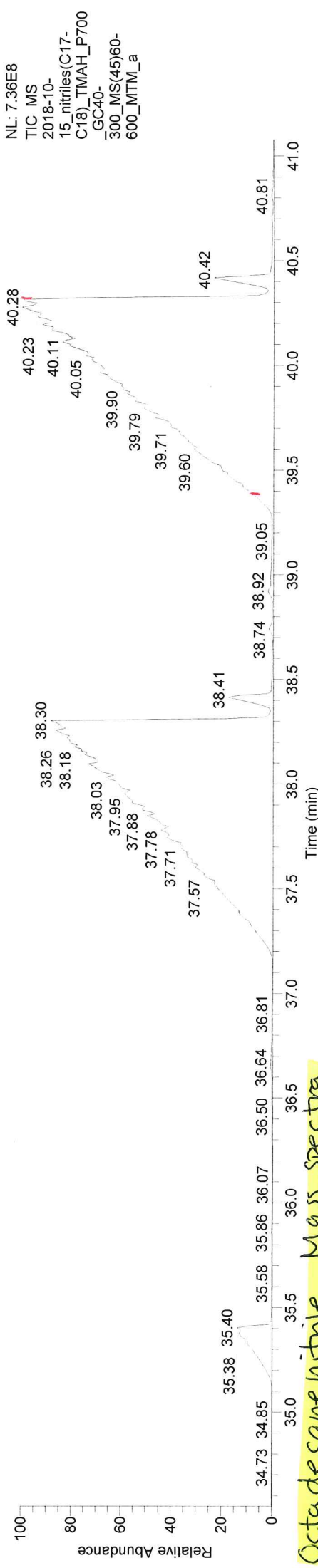
2018-10-15_nitriles(C17-C18)_TMAH_P700_GC40-300_MS(45)60-600_MTM_a #4064 RT: 38.30 AV: 1 NL: 3.94E7

T: + c Full ms [45.00-600.00]

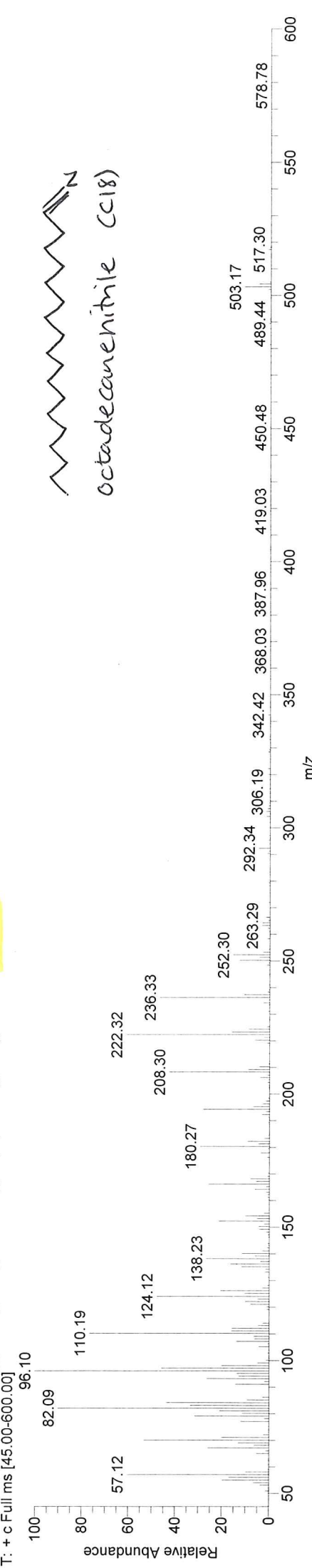
96.33



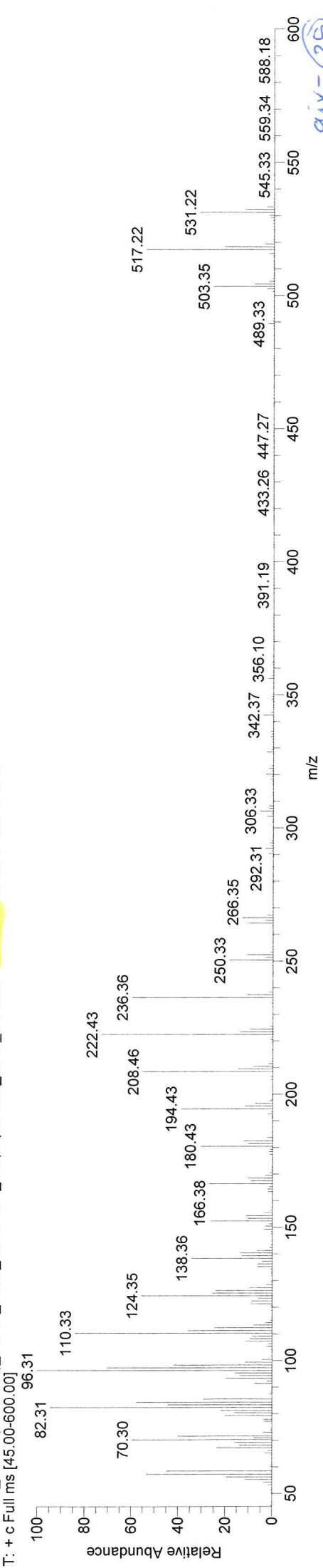
RT: 34.55 - 41.08



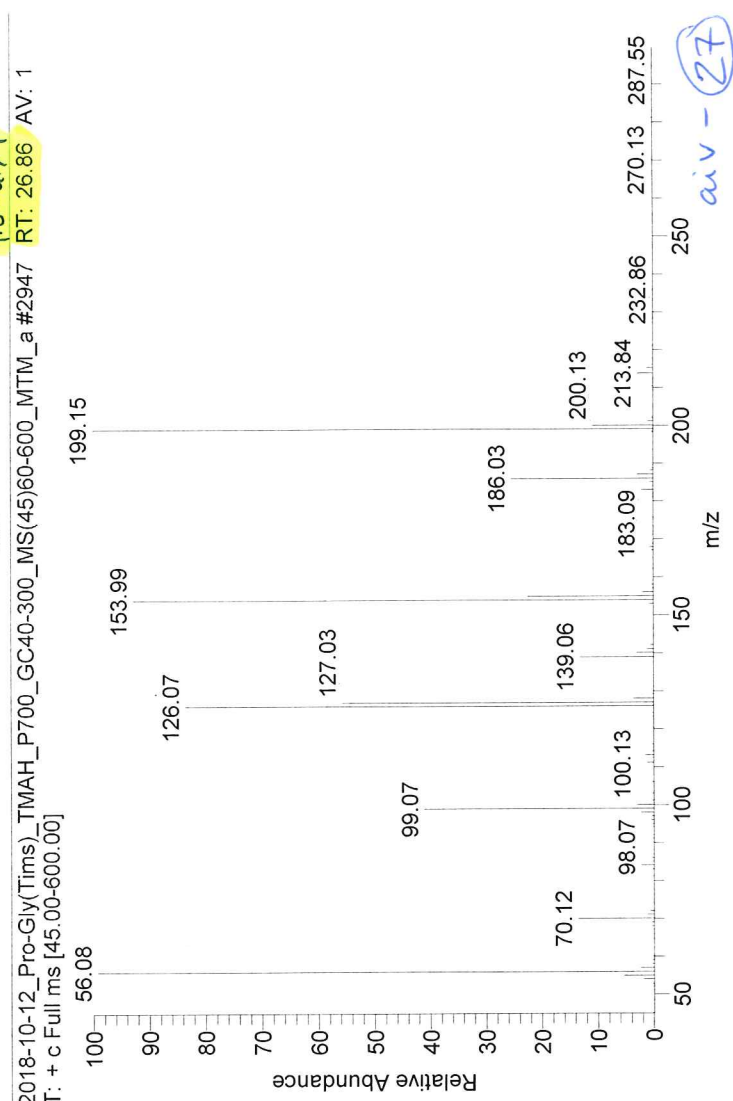
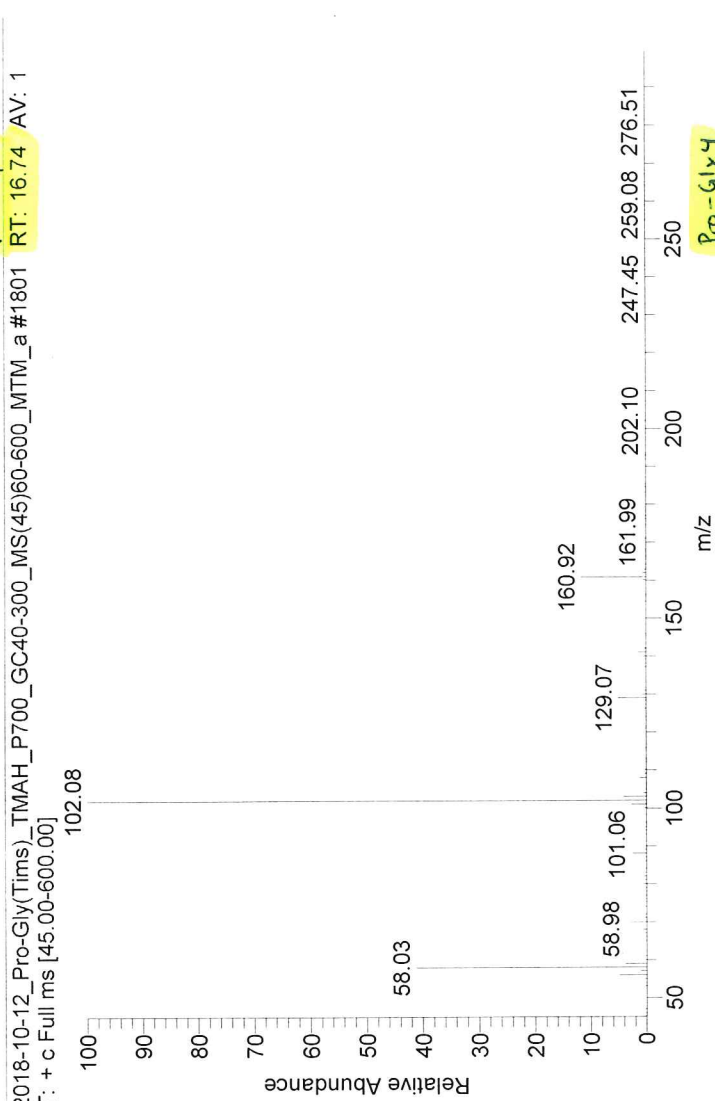
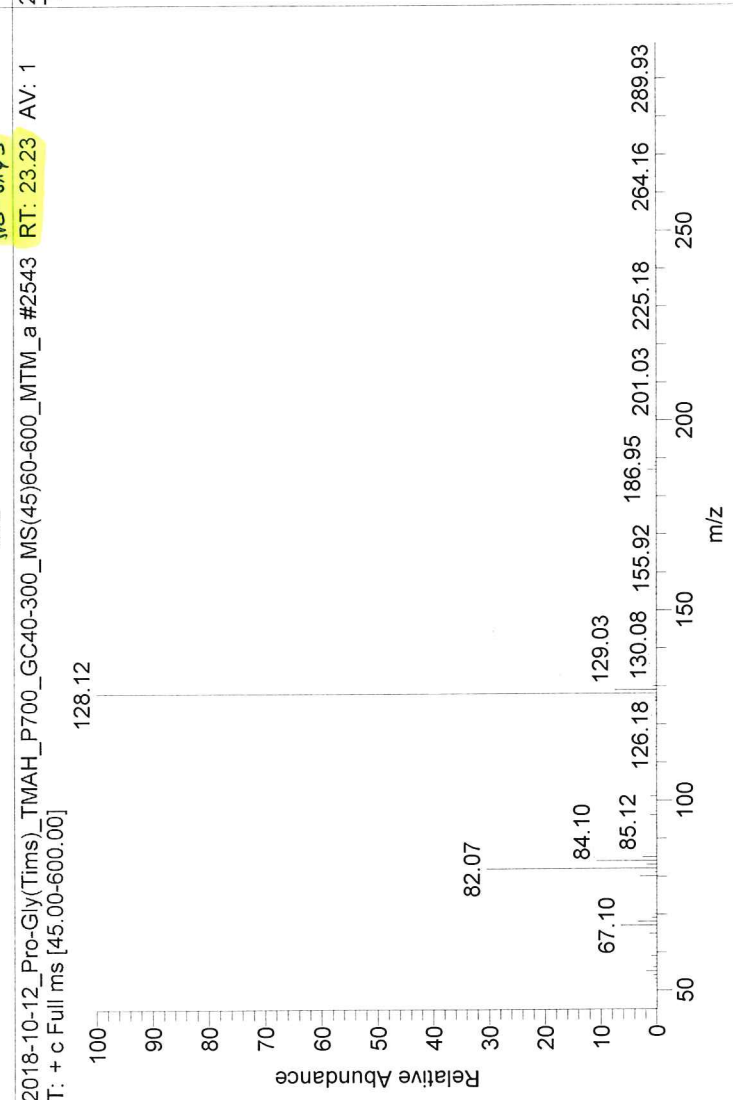
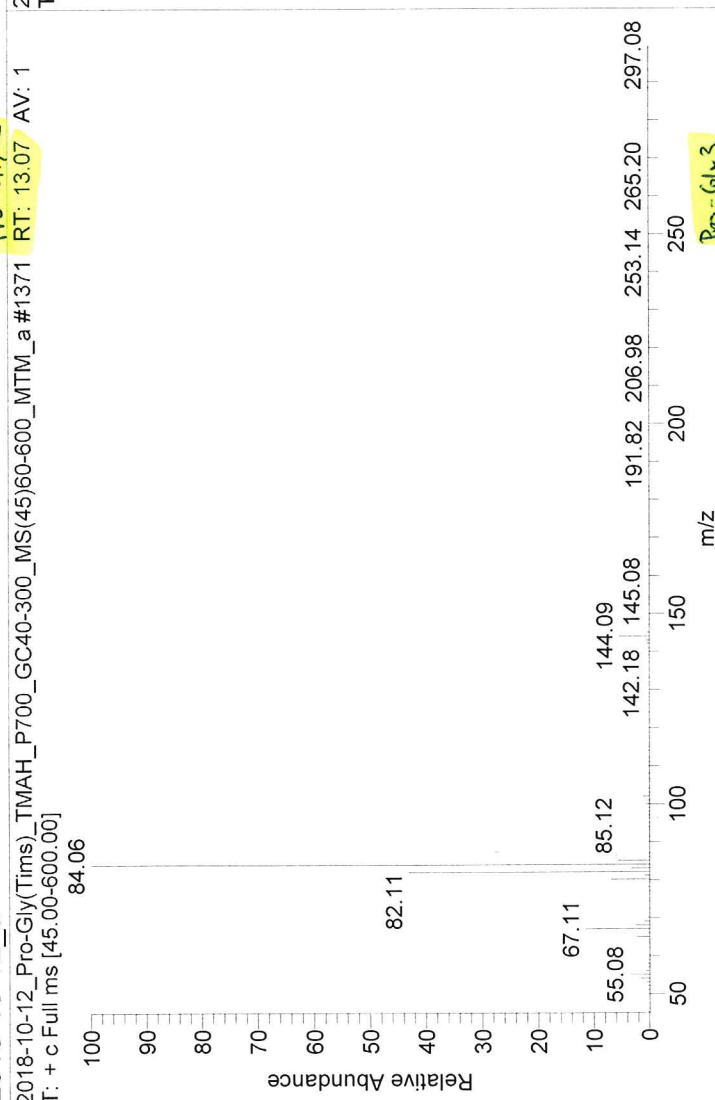
Octadecanenitrile Mass spectra



2018-10-15_nitriles(C17-C18)_TMAH_P700_GC40-300_MS(45)60-600_MTM_a #4296 RT: 40.31 AV: 1 NL: 3.47E7



div-25



Proline-glycine (dipeptide) + TMAH Mass spectra part 2

10/12/18 15:24:55

Pro-Gly(Tims) TMAH

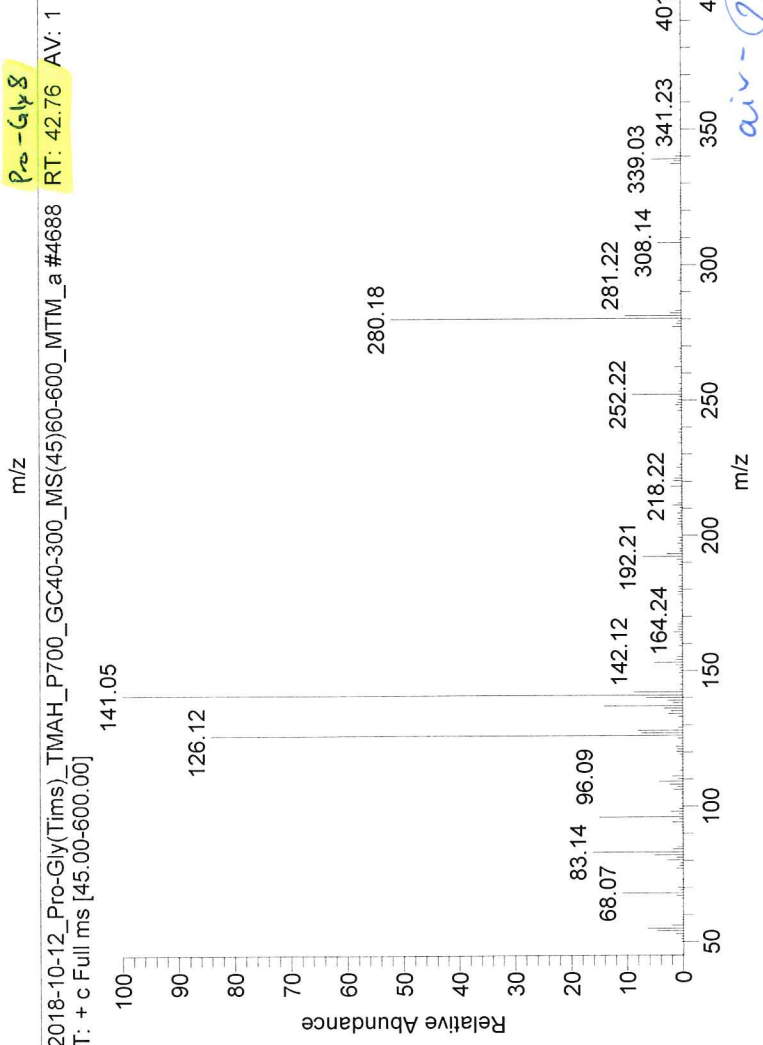
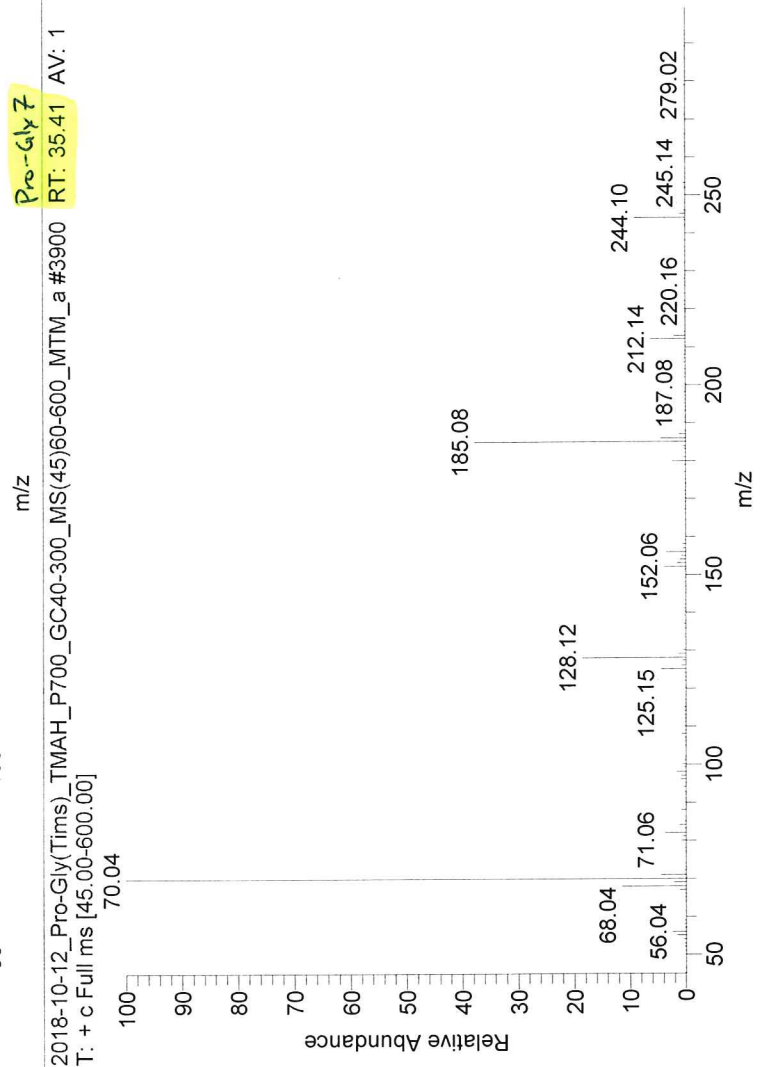
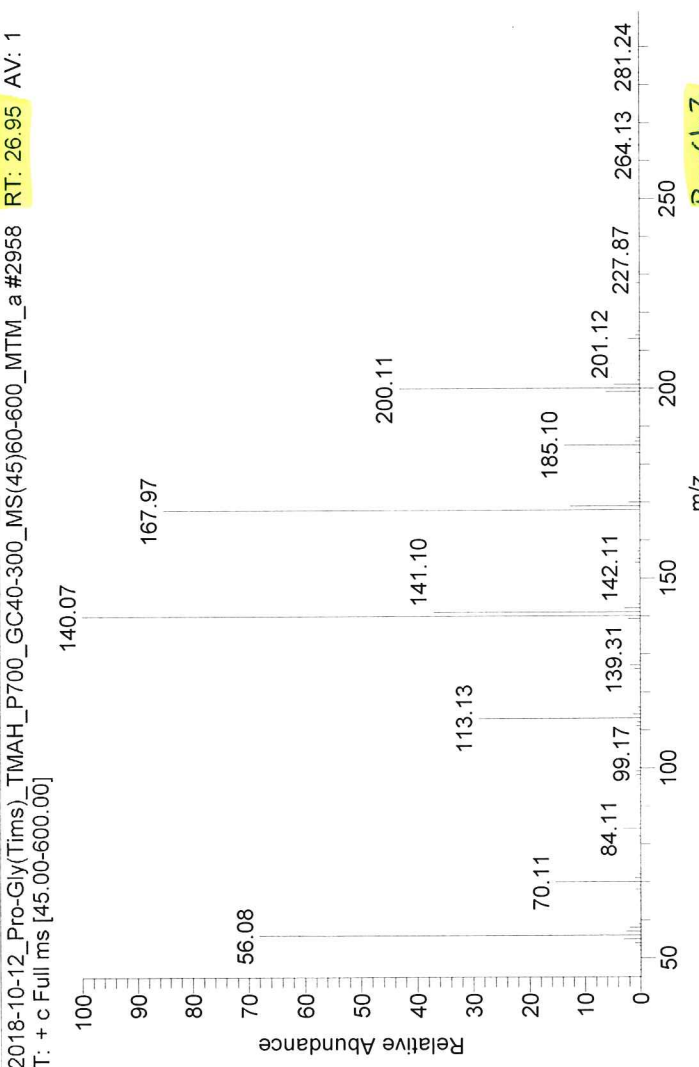
2018-10-12 Pro-Gly(Tims) TMAH_P700_GC...

Pro-Gly 5

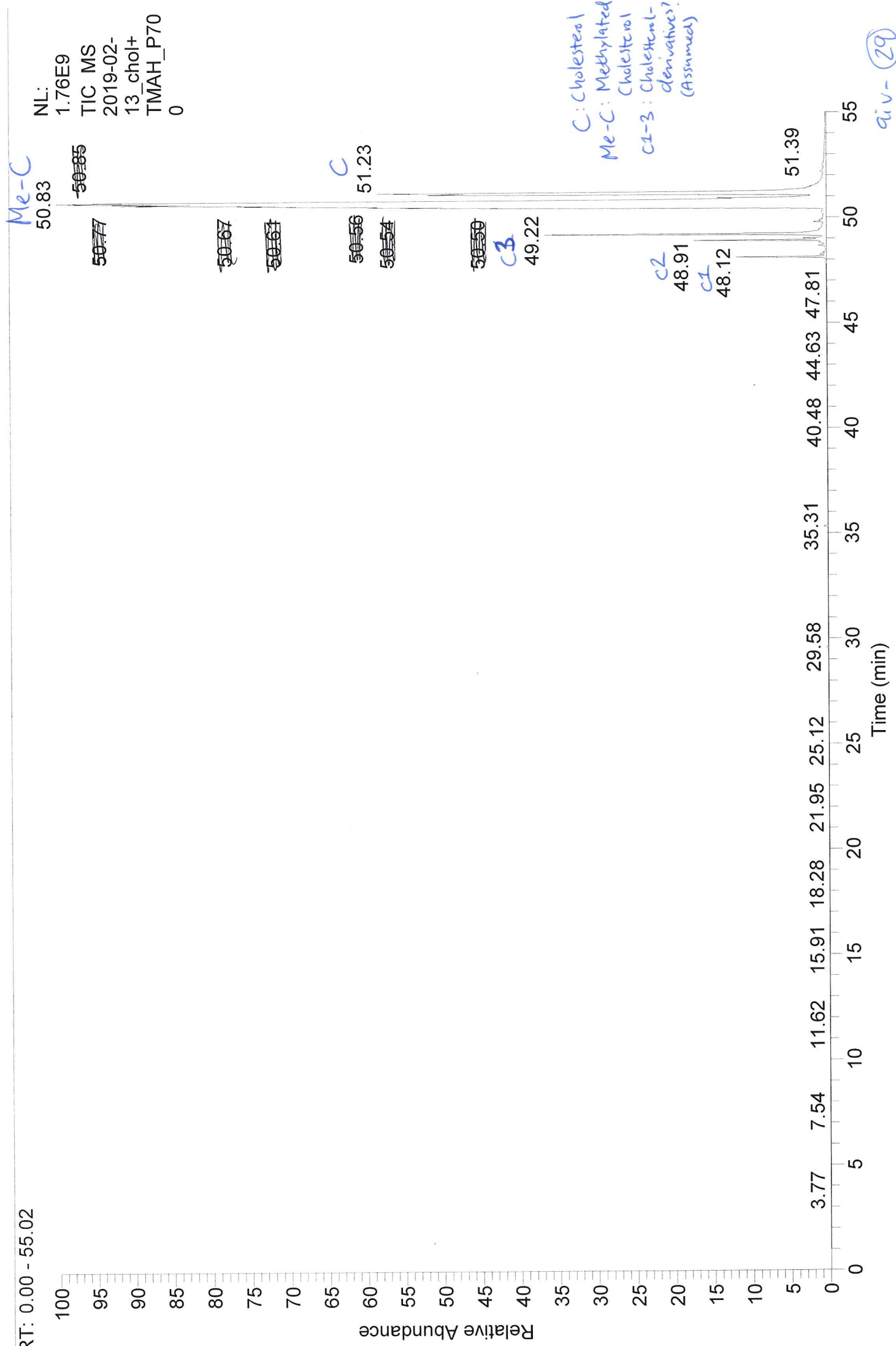
2018-10-12 Pro-Gly(Tims) TMAH_P700_GC40-300_MS(45)60-600_MTM_a #2958 RT: 26.95 AV: 1

Pro-Gly 6

2018-10-12 Pro-Gly(Tims) TMAH_P700_GC40-300_MS(45)60-600_MTM_a #3413 RT: 30.97 AV: 1



air-28



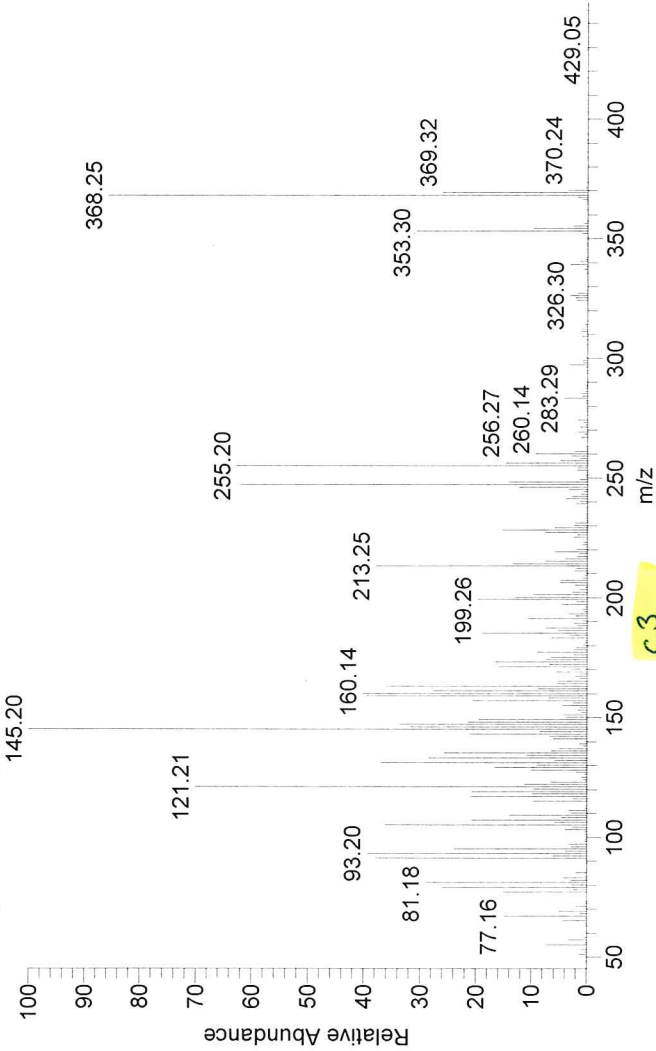
Cholesterol + TMAH Mass spectra part 1

02/13/19 15:38:14

2019-02-13_chol+TMAH_P700

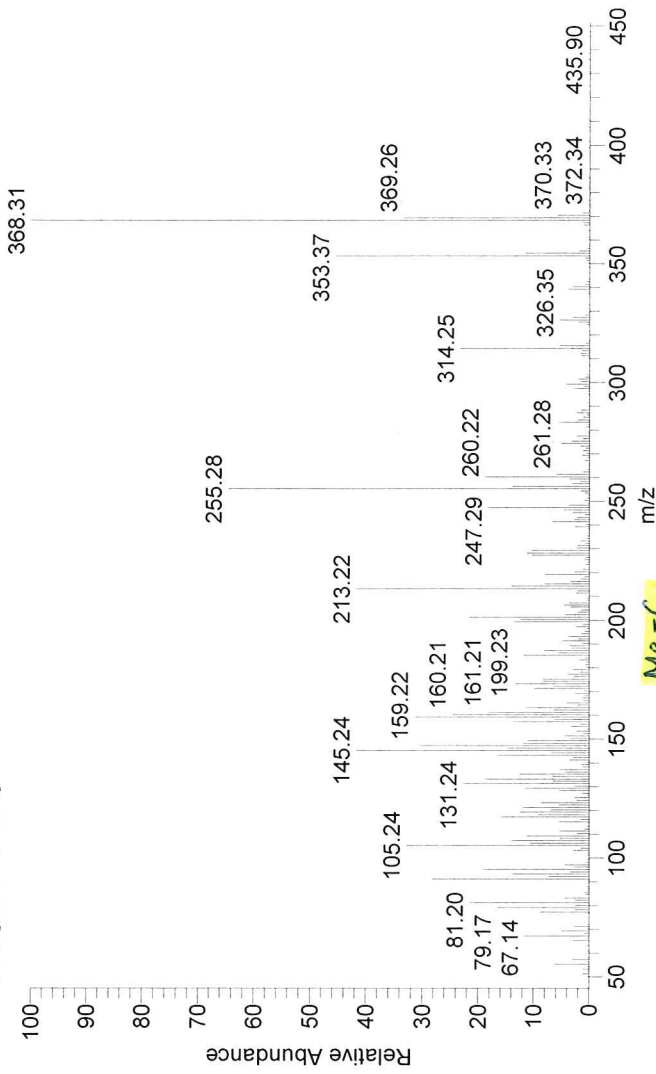
C1

2019-02-13_chol+TMAH_P700 #5114 RT: 48.12 AV: 1 NL: 1.11E7
T: + c Full ms [45.00-600.00]



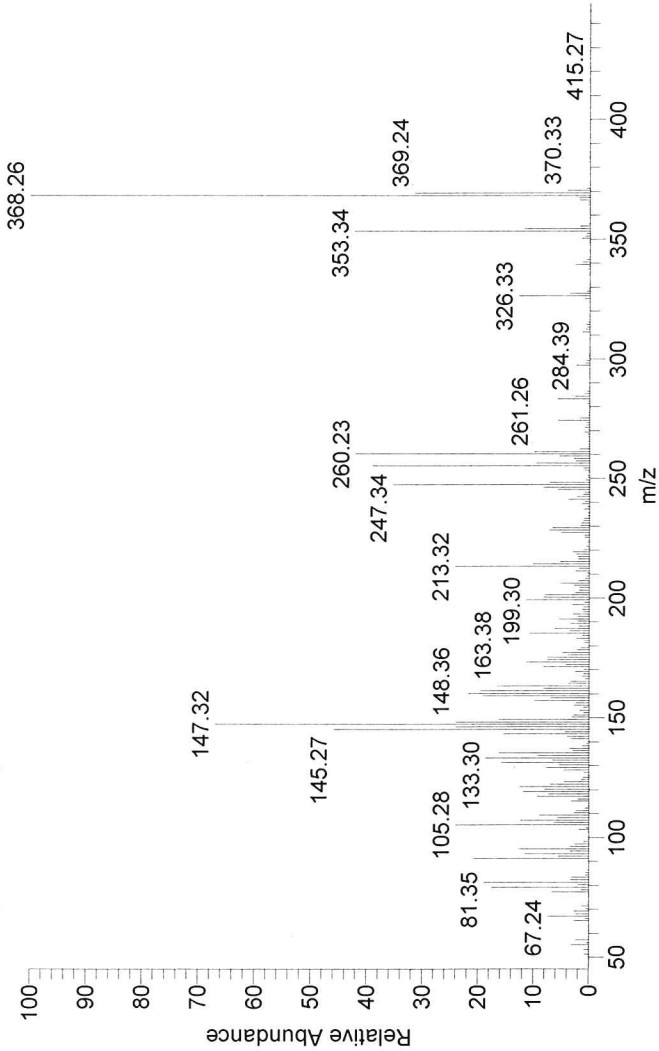
C2

2019-02-13_chol+TMAH_P700 #5204 RT: 48.91 AV: 1 NL: 2.03E7
T: + c Full ms [45.00-600.00]



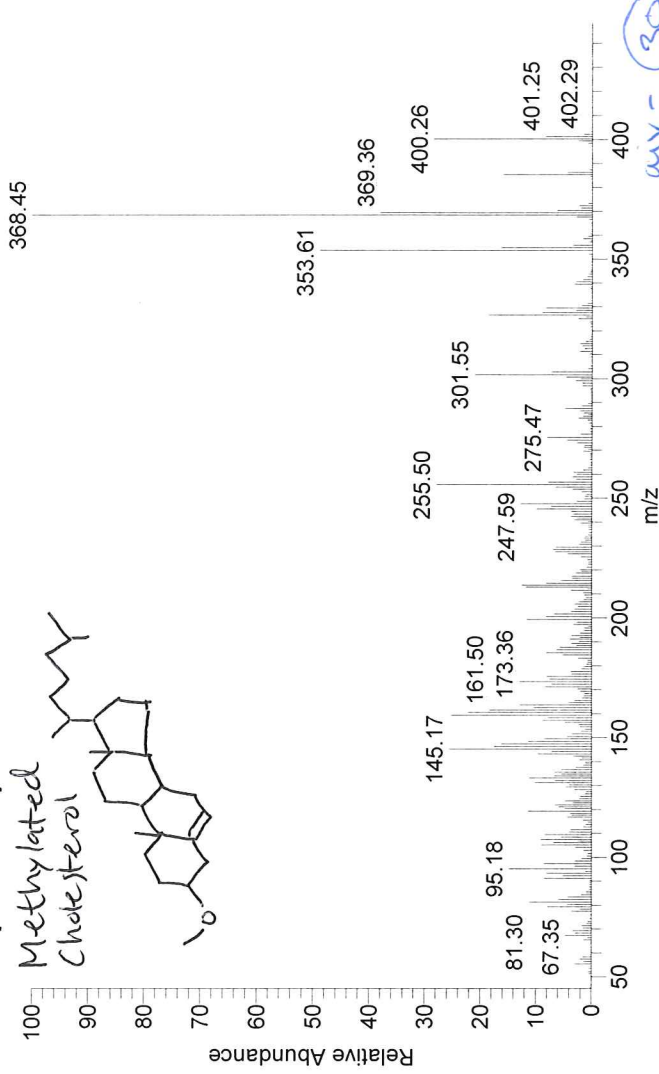
C3

2019-02-13_chol+TMAH_P700 #5239 RT: 49.22 AV: 1 NL: 4.72E7
T: + c Full ms [45.00-600.00]



Me-C

2019-02-13_chol+TMAH_P700 #5415 RT: 50.83 AV: 1 NL: 1.29E8
T: + c Full ms [45.00-600.00]

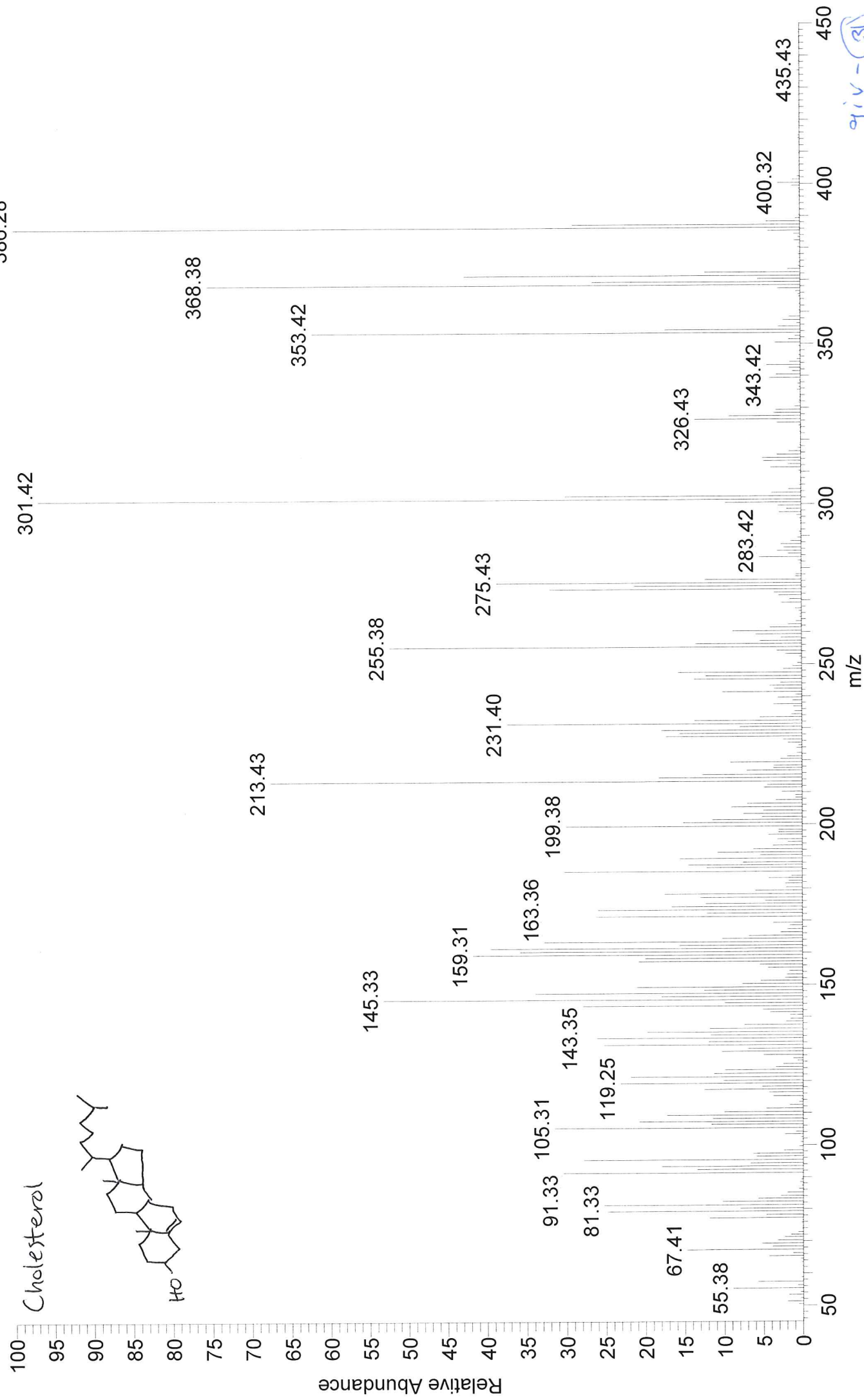


uv - 30

C

2019-02-13_chol+TMAH_P700 #5458 RT: 51.23 AV: 1 NL: 3.88E7

T: + c Full ms [45.00-600.00]



qiv-31