LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083018\
Data File : BF108662.D
Acq On : 31 Aug 2018 1:16
Operator : JU/SJ
Sample : J4700-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082818-SIDI-F-D-S

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.672	560	567	568	rBV2	48824	91292	2.55%	0.497%
2	6.660	730	735	751	rBV	83813	317410	8.86%	1.728%
3	6.772	751	754	782	rVV	631728	1367402	38.19%	7.444%
4	7.001	790	793	815	rVB	218994	508911	14.21%	2.770%
5	7.154	815	819	843	rBV	1688225	2201744	61.49%	11.985%
6	7.566	885	889	912	rBV	1028568	1830737	51.13%	9.966%
7	8.284	1007	1011	1040	rBV	333246	647670	18.09%	3.526%
8	9.354	1189	1193	1218	rBV	3122296	3580869	100.00%	19.493%
9	9.742	1256	1259	1275	rBV	155606	223208	6.23%	1.215%
10	10.042	1306	1310	1326	rBV	547680	684715	19.12%	3.727%
11	10.695	1418	1421	1427	rBV	75846	68859	1.92%	0.375%
12	10.836	1441	1445	1470	rBV	830630	1283032	35.83%	6.984%
13	11.536	1561	1564	1581	rBV	474128	678487	18.95%	3.693%
14	13.119	1829	1833	1849	rBV	2806319	2960869	82.69%	16.118%
15	14.030	1983	1988	2002	rBV3	49671	128249	3.58%	0.698%
16	14.189	2012	2015	2026	rBV	680635	792565	22.13%	4.314%
17	15.019	2152	2156	2160	rVB	81343	84340	2.36%	0.459%
18	15.295	2199	2203	2207	rBV	33956	36586	1.02%	0.199%
19	15.707	2268	2273	2275	rBV	38821	51989	1.45%	0.283%
20	15.748	2275	2280	2293	rVB	382863	612013	17.09%	3.332%
21	16.171	2347	2352	2357	rVB	47289	80158	2.24%	0.436%
22	16.718	2440	2445	2451	rVB3	41517	73810	2.06%	0.402%
23	17.365	2549	2555	2563	rVB3	29531	65454	1.83%	0.356%

Sum of corrected areas: 18370369

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083018\
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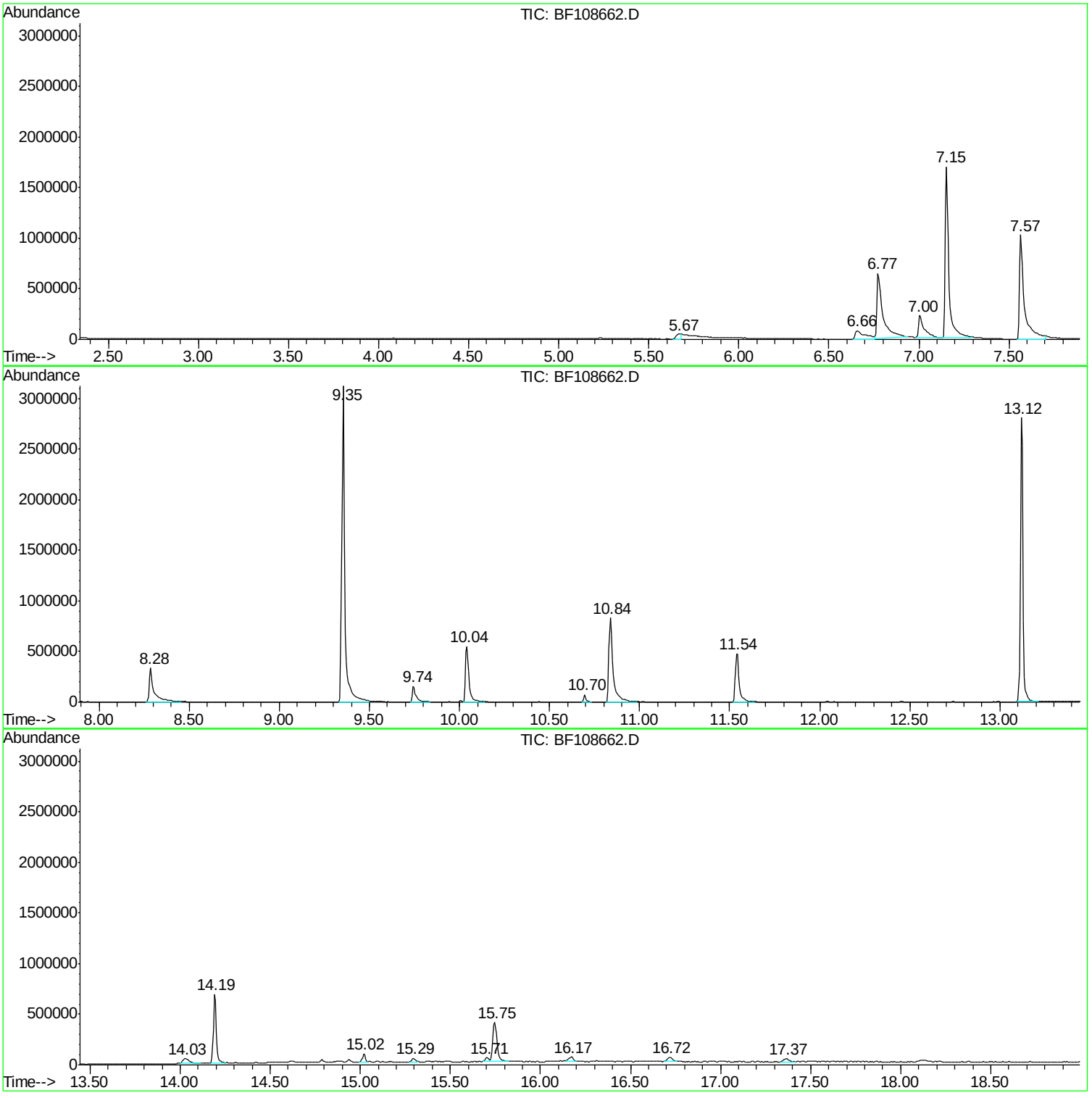
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
082818-SIDI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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Data File : BF108662.D
Acq On : 31 Aug 2018 1:16
Operator : JU/SJ
Sample : J4700-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082818-SIDI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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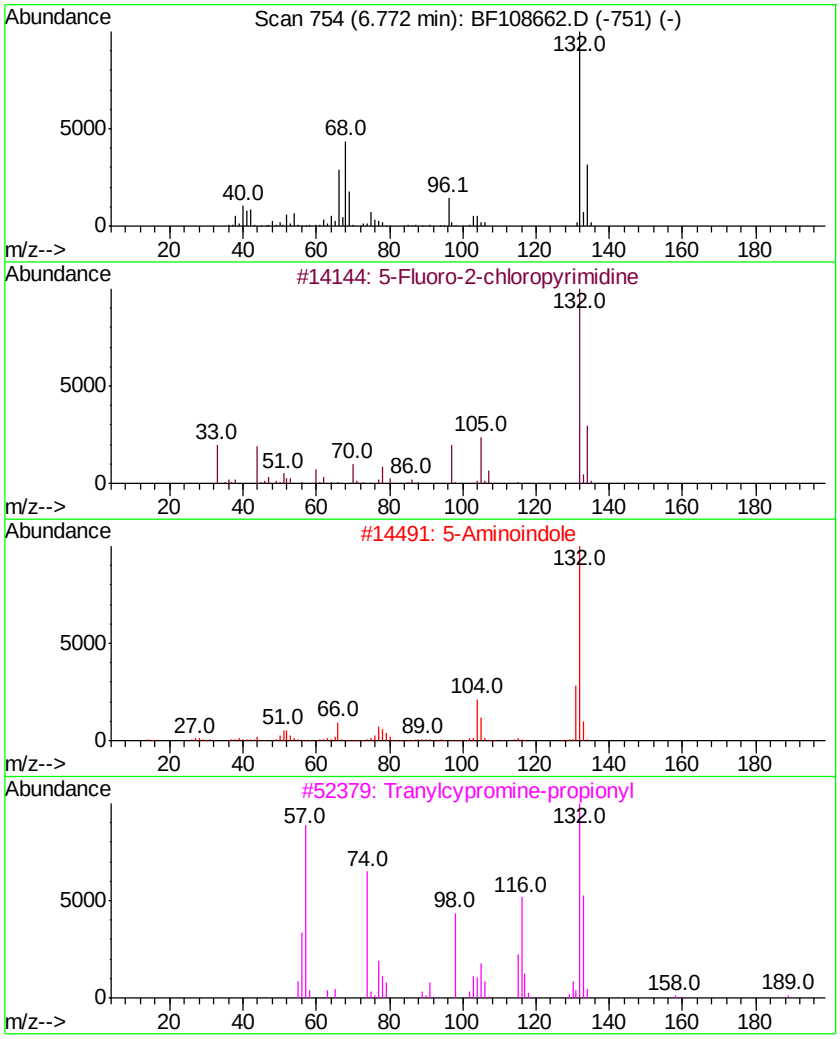
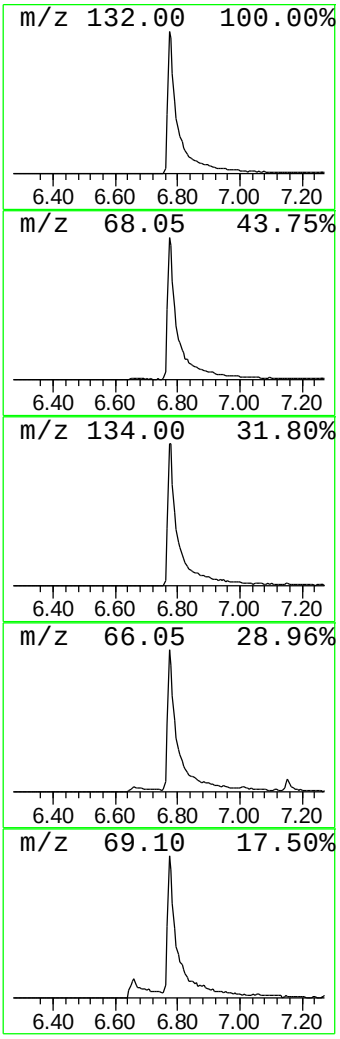
Peak Number 1 unknown6.77 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	53.74 ng	1367400	1,4-Dichlorobenzene-d4	7.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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Data File : BF108662.D
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Operator : JU/SJ
Sample : J4700-02
Misc :
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Instrument : BNA_F
ClientSampleId : 082818-SIDI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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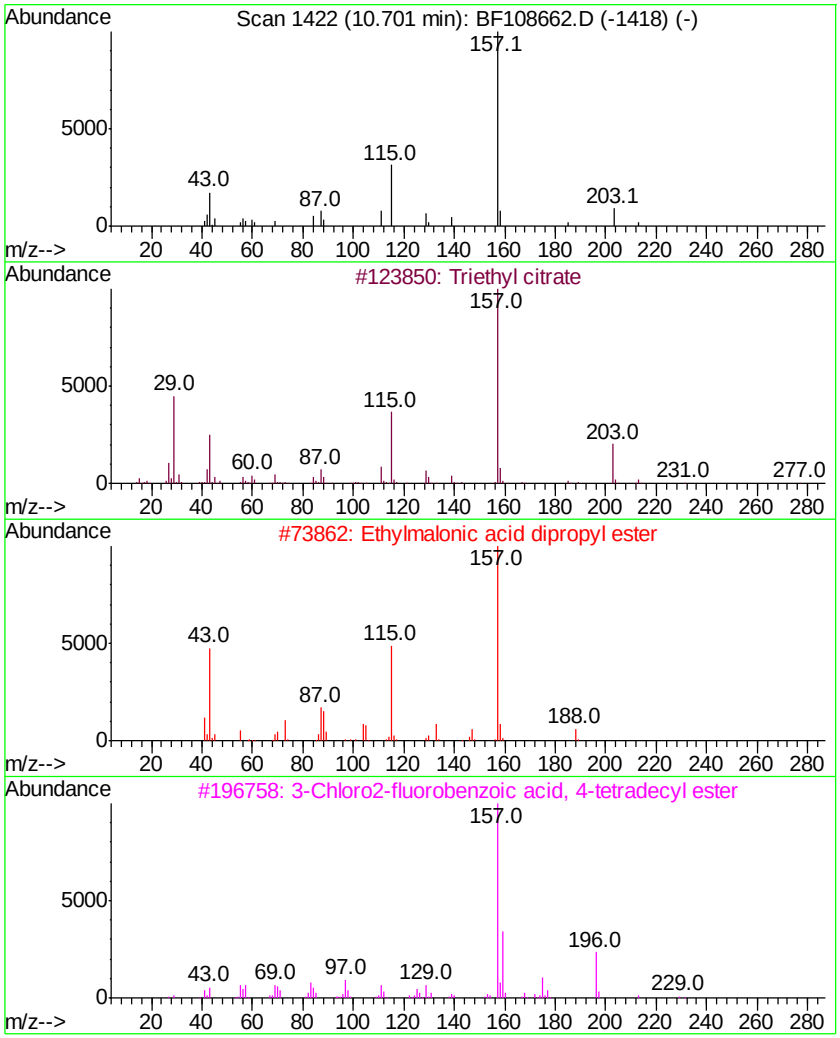
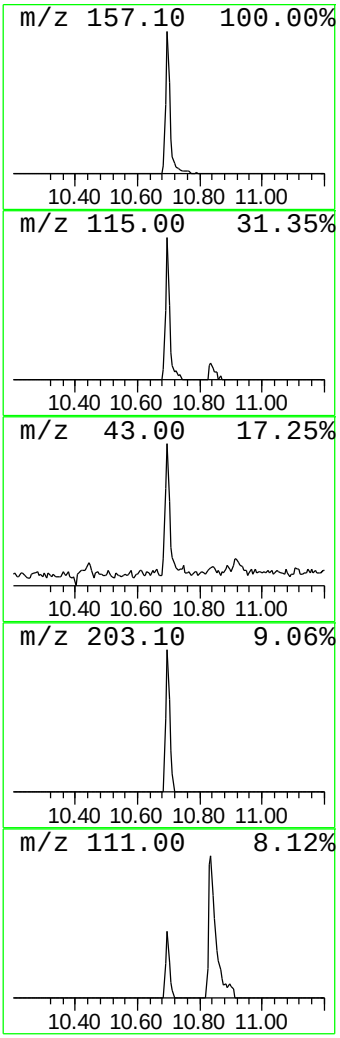
Peak Number 3 Triethyl citrate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	2.01 ng	68859	Acenaphthene-d10	10.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	91
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	64
3	3-Chloro2-fluorobenzoic acid, 4-...	370	C21H32ClFO2	1000338-64-7	40
4	3-Chloro2-fluorobenzoic acid, 6-...	370	C21H32ClFO2	1000338-64-9	40
5	3-Chloro2-fluorobenzoic acid, 5-...	384	C22H34ClFO2	1000338-65-2	33





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Data File : BF108662.D
Acq On : 31 Aug 2018 1:16
Operator : JU/SJ
Sample : J4700-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082818-SIDI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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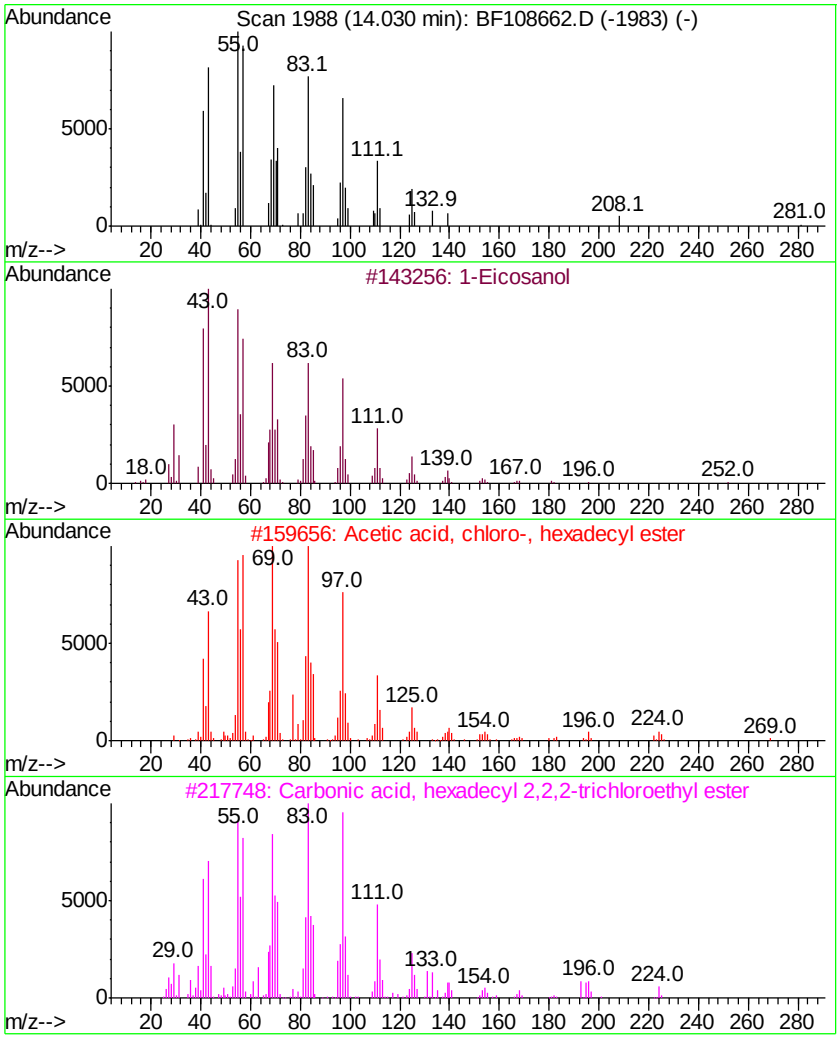
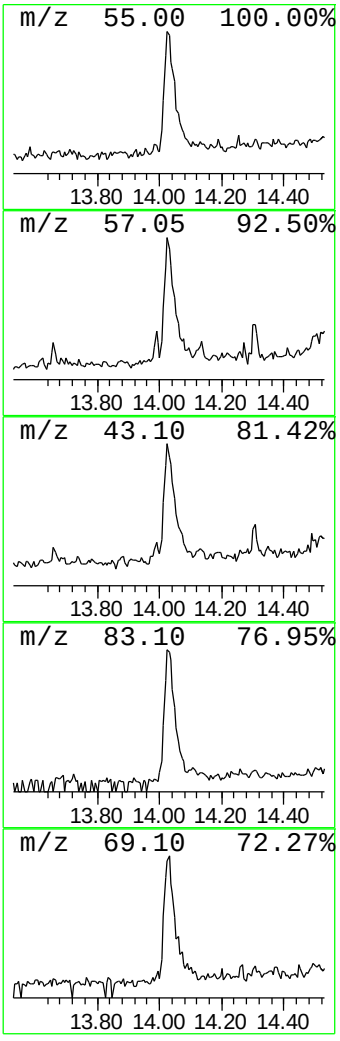
Peak Number 4 1-Eicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.03	3.24 ng	128249	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosanol	298	C20H42O	000629-96-9	91
2	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	91
3	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	91
4	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





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Instrument : BNA_F
ClientSampleId : 082818-SIDI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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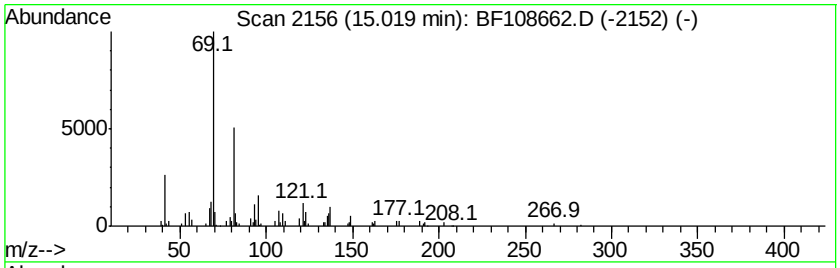
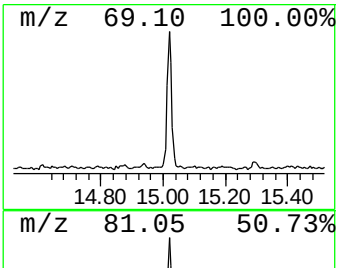
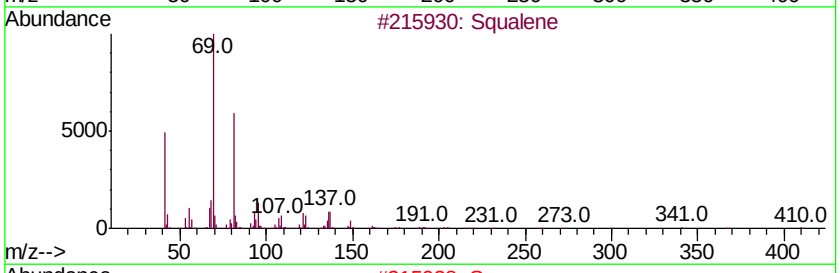
Peak Number 5 Squalene Concentration Rank 4

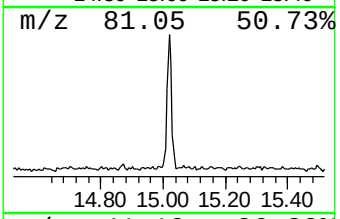
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	2.76 ng	84340	Perylene-d12	15.75

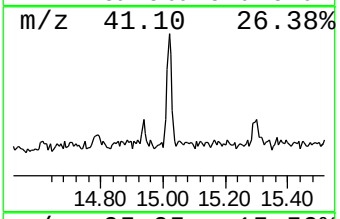
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	87
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	59
5	Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	47

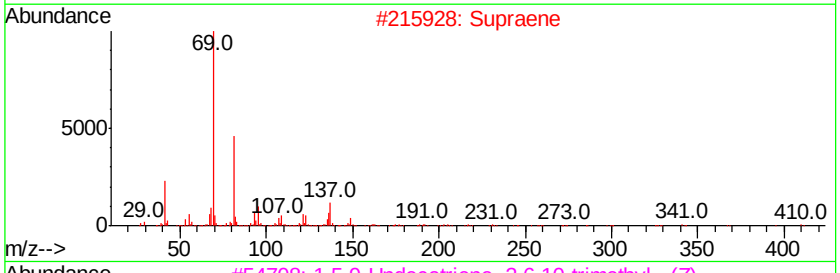


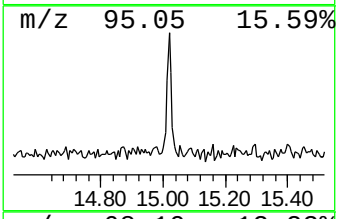


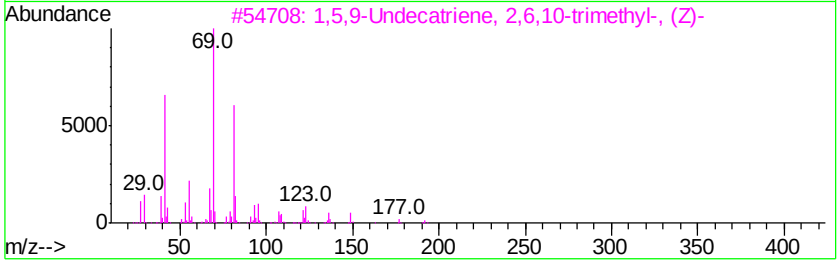


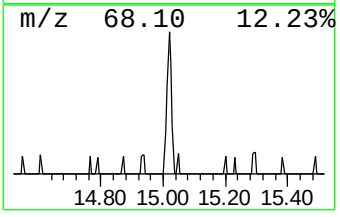












Library Search Compound Report

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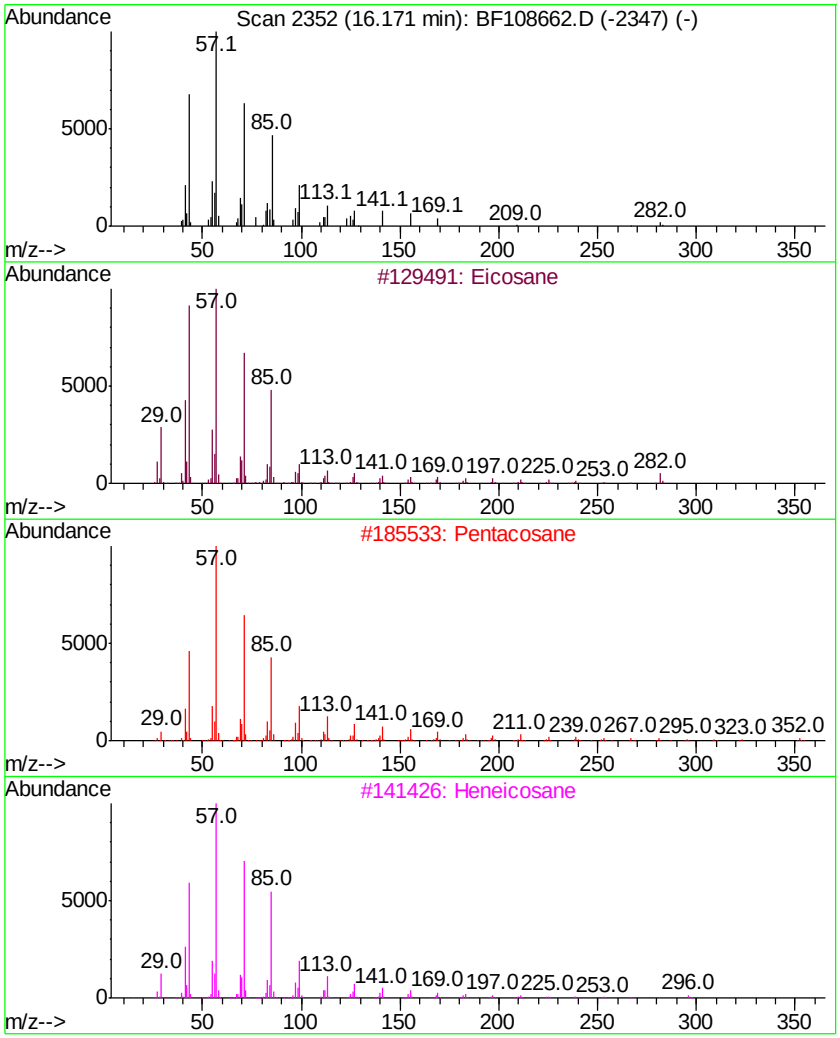
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

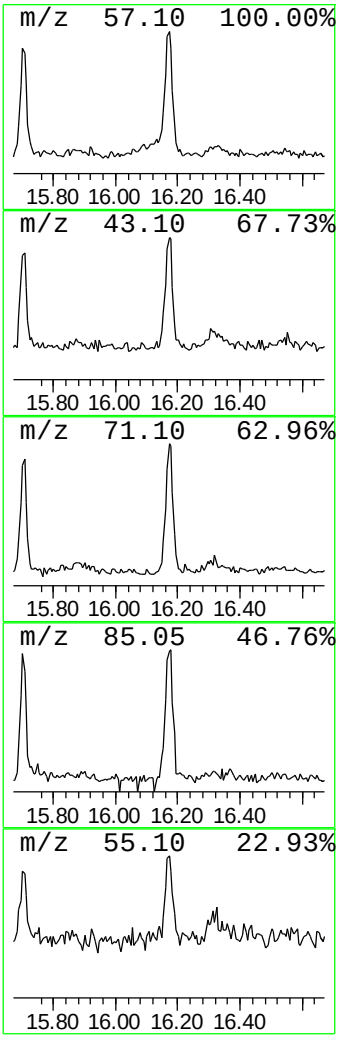
****

Peak Number 6 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	2.62 ng	80158	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Pentacosane	352	C25H52	000629-99-2	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Triacontane	422	C30H62	000638-68-6	90





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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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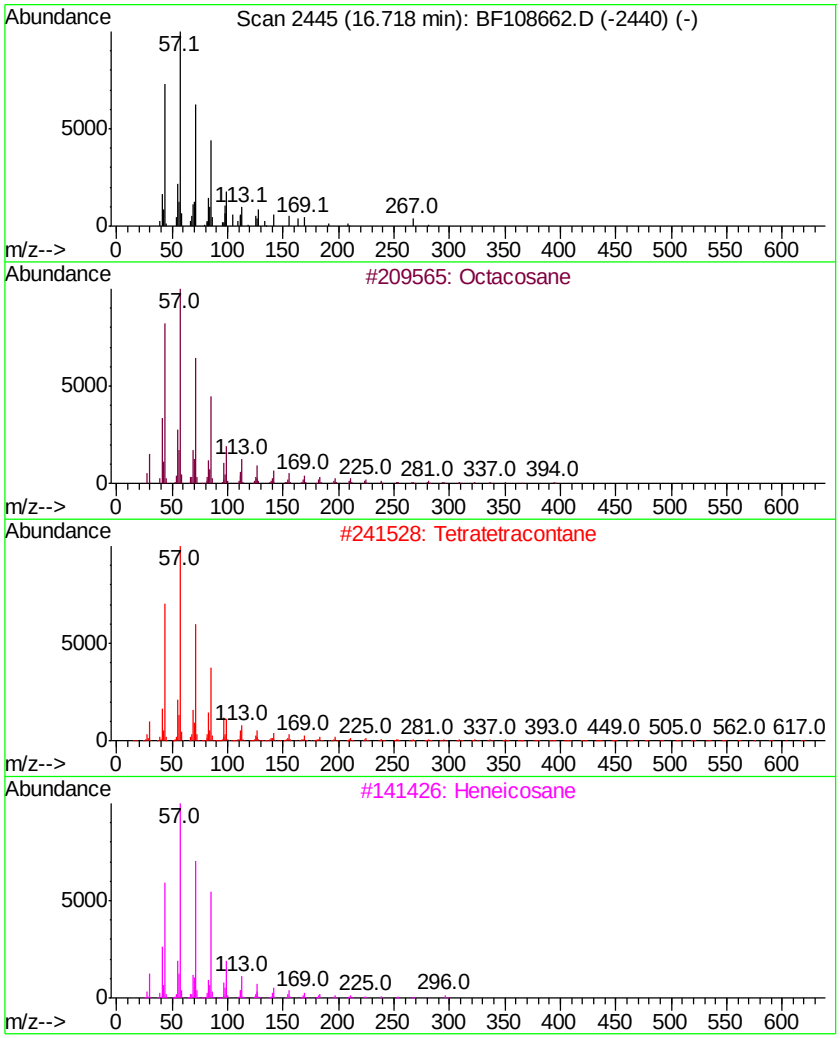
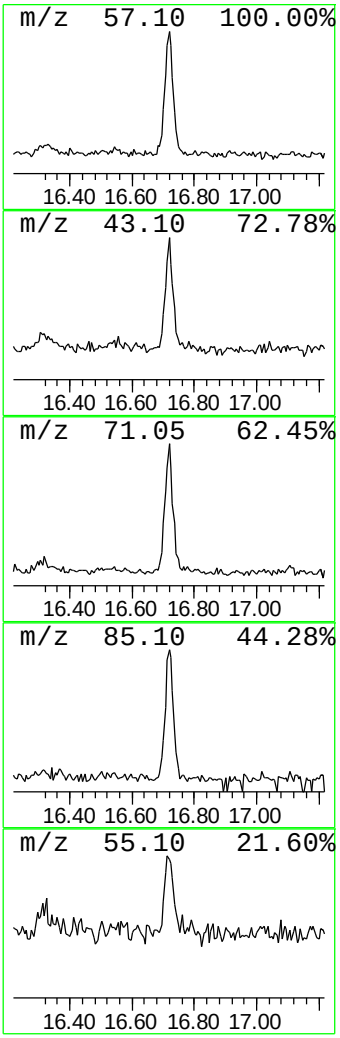
Peak Number 7 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	2.41 ng	73810	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Docosane	310	C22H46	000629-97-0	90
5	Hexatriacontane	507	C36H74	000630-06-8	87





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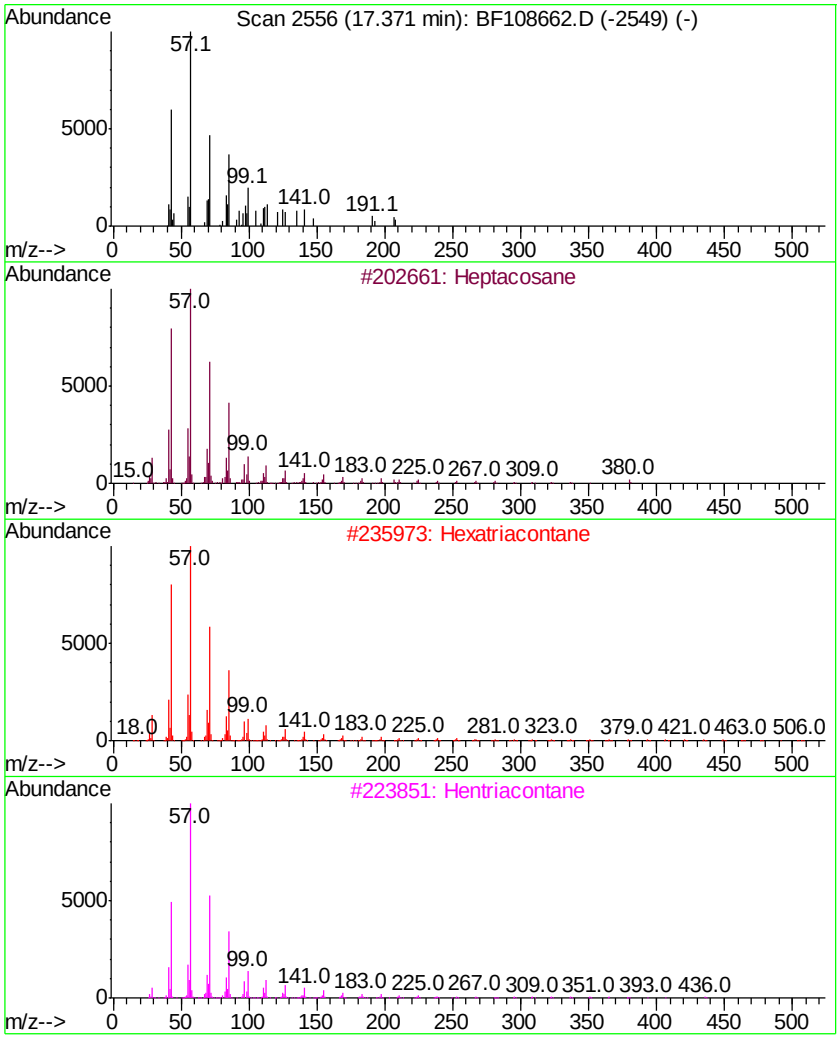
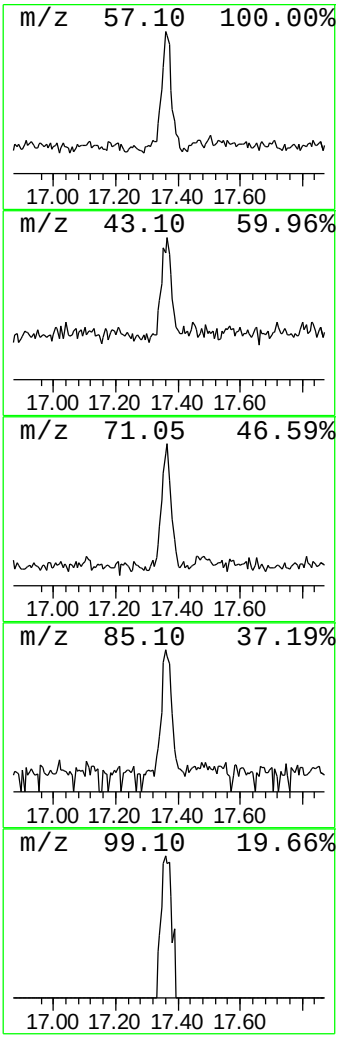
Peak Number 8 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.37	2.14 ng	65454	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	74
2	Hexatriacontane	507	C36H74	000630-06-8	72
3	Hentriacontane	437	C31H64	000630-04-6	72
4	Hexacosane	366	C26H54	000630-01-3	72
5	Pentacosane	352	C25H52	000629-99-2	72





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.77	6.77	53.7	ng	1367400	1	7.01	508911	20.0
Triethyl citrate	10.70	2.0	ng	68859	3	10.04	684715	20.0
1-Eicosanol	14.03	3.2	ng	128249	5	14.19	792565	20.0
Squalene	15.02	2.8	ng	84340	6	15.75	612013	20.0
Eicosane	16.17	2.6	ng	80158	6	15.75	612013	20.0
Octacosane	16.72	2.4	ng	73810	6	15.75	612013	20.0
Heptacosane	17.37	2.1	ng	65454	6	15.75	612013	20.0