LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\Data\BF042017\
Data File : BF094543.D
Acq On : 20 Apr 2017 14:33
Operator : SJ/MA
Sample : I2744-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1(5-7)20170418

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:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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	3.919	333	337	348	rVB	407880	458849	14.96%	1.727%
2	4.319	400	405	420	rVB	2561992	2538561	82.79%	9.553%
3	4.701	467	470	474	rBV	30757	30872	1.01%	0.116%
4	5.389	582	587	590	rBV	2338102	2634127	85.91%	9.913%
5	5.519	604	609	612	rBV	2837919	2695884	87.92%	10.145%
6	5.766	647	651	655	rBV	698735	634161	20.68%	2.386%
7	5.942	676	681	684	rBV	2286640	2094390	68.30%	7.882%
8	6.413	756	761	764	rBV	1688785	1689147	55.09%	6.357%
9	7.254	900	904	908	rBV	932087	874423	28.52%	3.291%
10	8.578	1125	1129	1133	rBV	2978548	3066234	100.00%	11.539%
11	9.077	1210	1214	1218	rBV	805573	700428	22.84%	2.636%
12	9.389	1261	1267	1276	rVB2	1016586	976352	31.84%	3.674%
13	9.989	1364	1369	1373	rVB	62782	58763	1.92%	0.221%
14	10.366	1428	1433	1438	rBV	1729645	1834685	59.84%	6.904%
15	10.572	1464	1468	1476	rBV	77741	100824	3.29%	0.379%
16	11.124	1558	1562	1565	rBV	57681	51336	1.67%	0.193%
17	11.207	1572	1576	1580	rBV	990403	1023346	33.37%	3.851%
18	11.942	1697	1701	1708	rBV2	43859	49266	1.61%	0.185%
19	13.189	1907	1913	1917	rBV	2550252	3004731	97.99%	11.307%
20	14.354	2107	2111	2121	rBV3	53463	98610	3.22%	0.371%
21	14.454	2124	2128	2133	rBV	893635	961716	31.36%	3.619%
22	15.571	2314	2318	2323	rBV	106698	110068	3.59%	0.414%
23	15.854	2361	2366	2370	rBV	26576	34415	1.12%	0.130%
24	16.077	2400	2404	2413	rBV	635961	721286	23.52%	2.714%
25	16.201	2421	2425	2430	rVB	30579	37794	1.23%	0.142%
26	16.577	2485	2489	2494	rBV3	31224	42633	1.39%	0.160%
27	17.006	2558	2562	2572	rVB4	30801	50593	1.65%	0.190%

Sum of corrected areas: 26573494

LSC Report - Integrated Chromatogram

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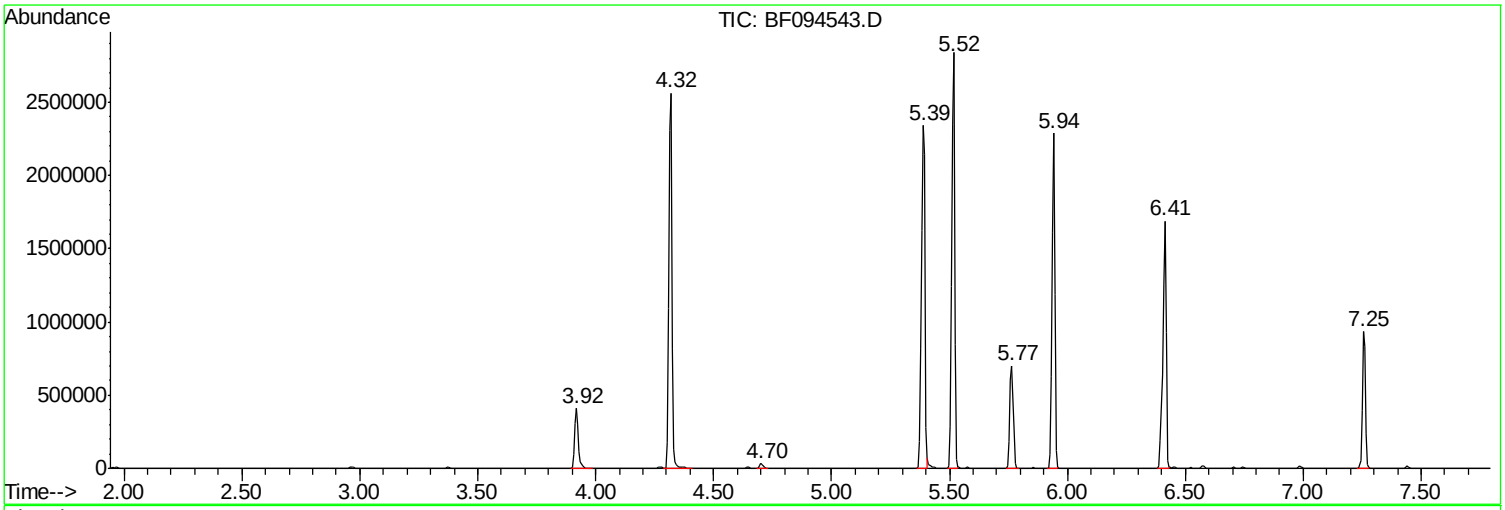
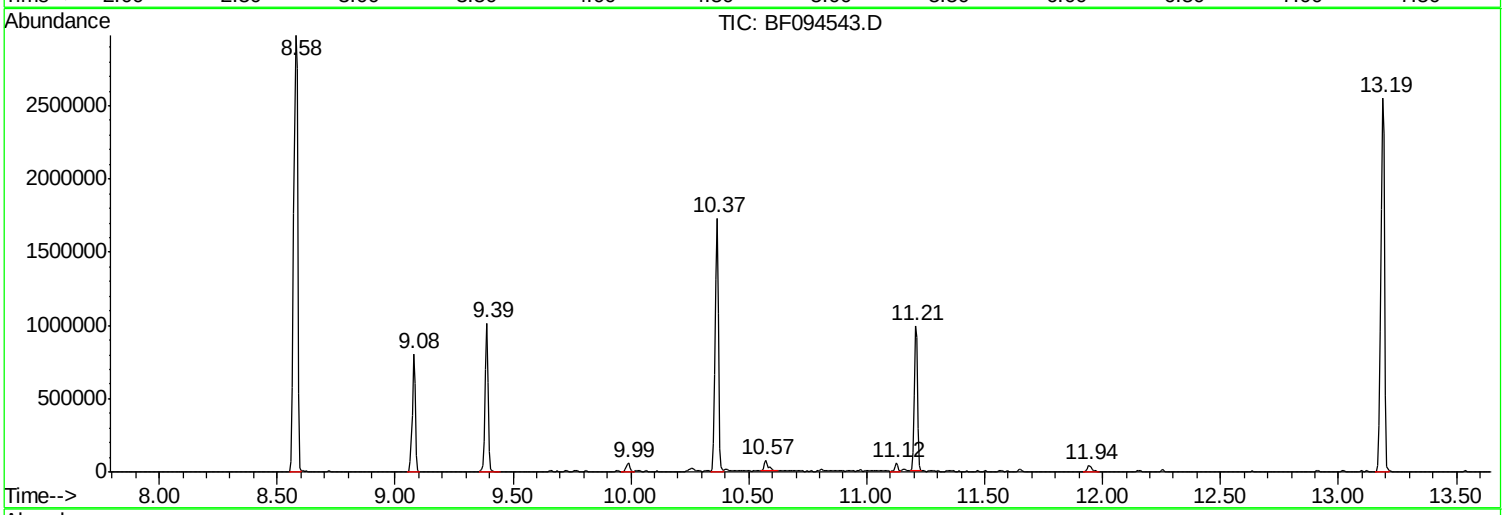
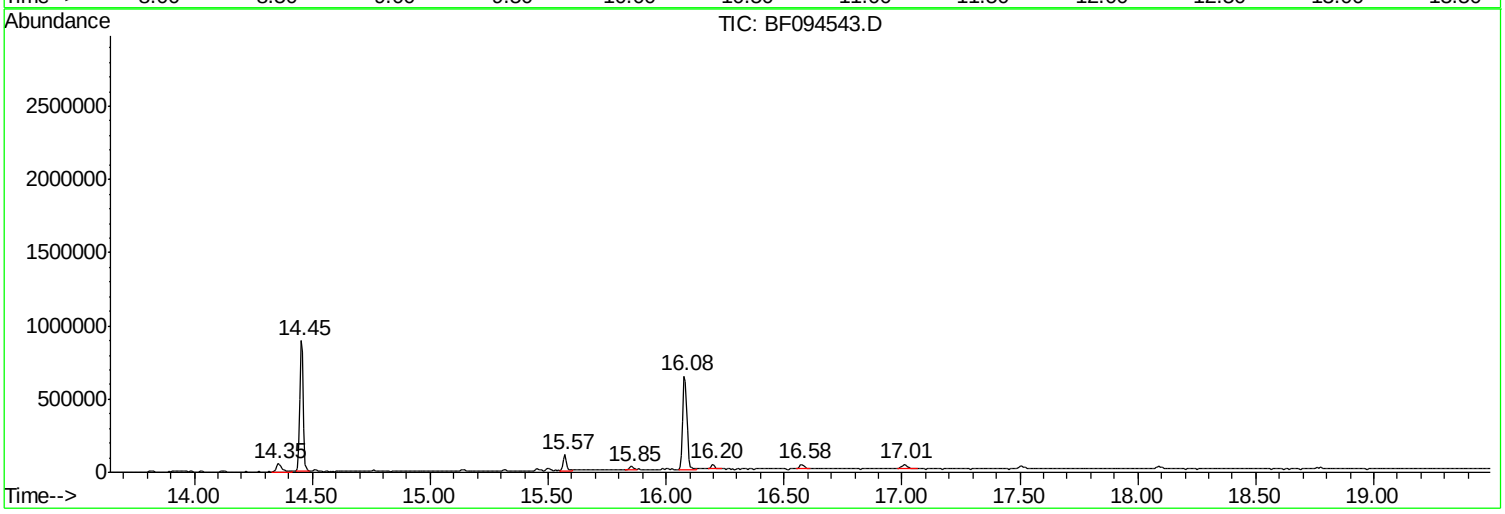
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Library Search Compound Report

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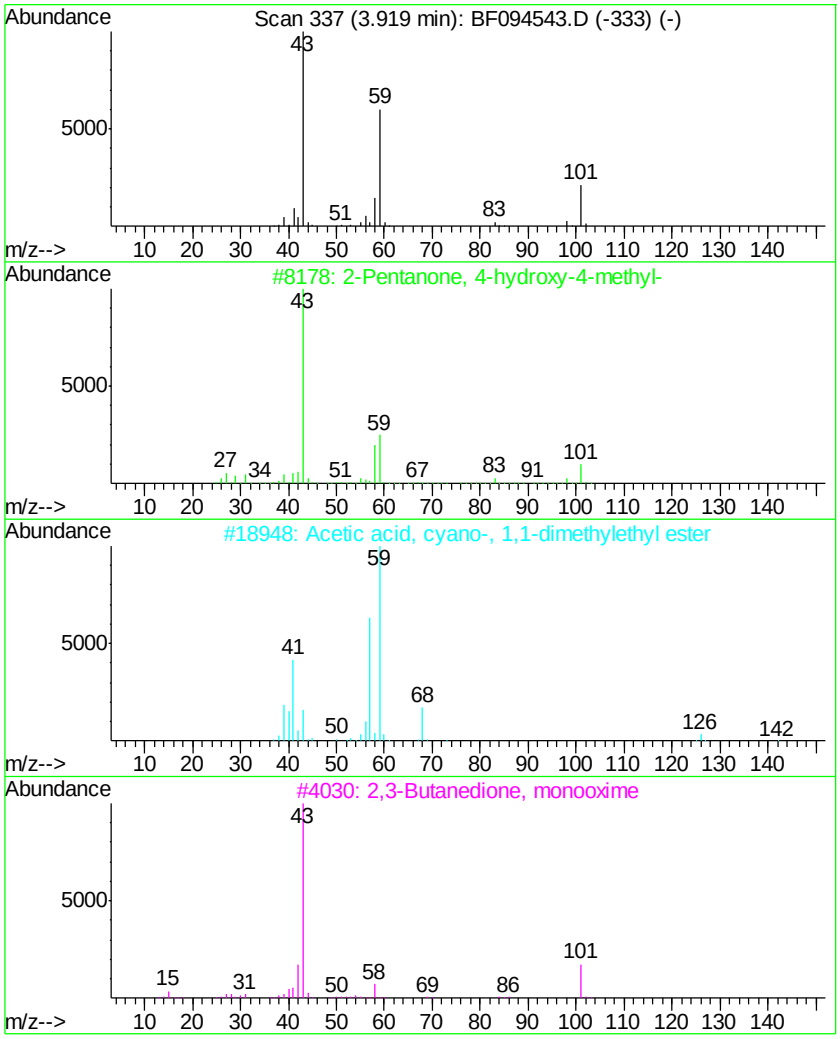
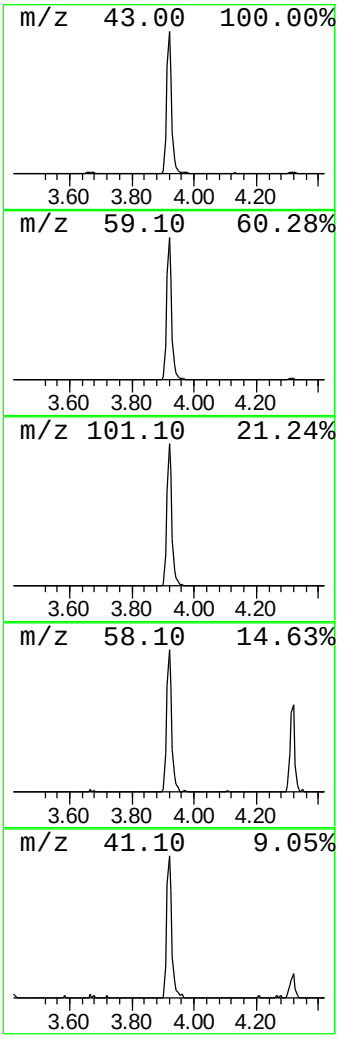
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.92	14.47 ng	458849	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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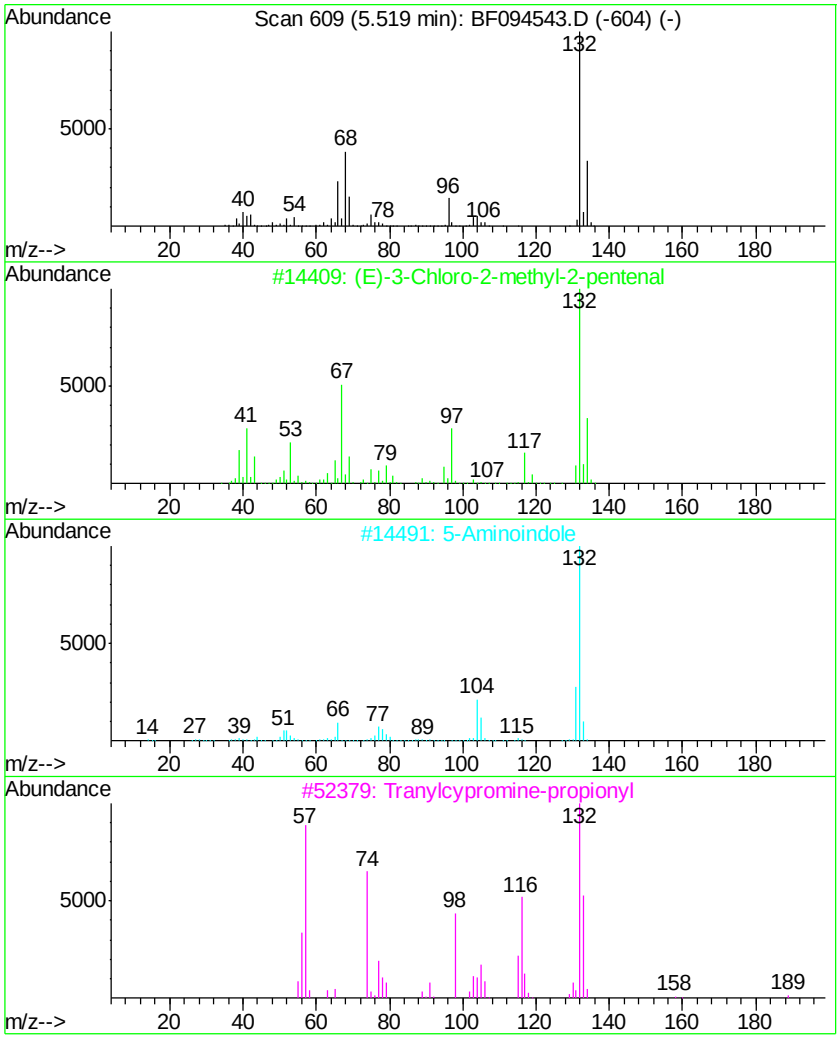
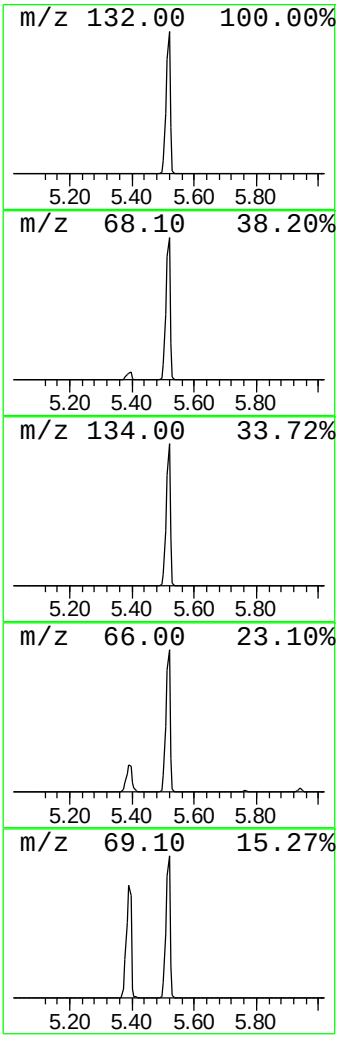
Peak Number 2 unknown5.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.52	85.02 ng	2695880	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Xenon	132	Xe	007440-63-3	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Instrument :
BNA_F
ClientSampleId :
SB-1(5-7)20170418

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

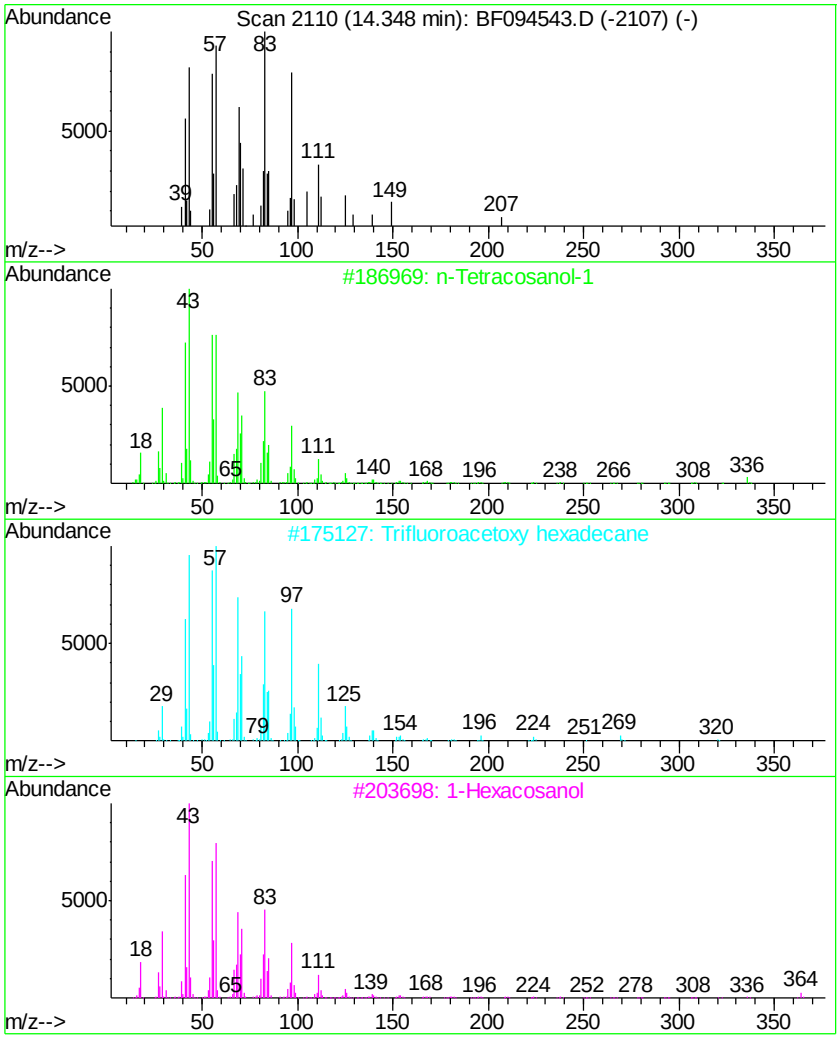
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

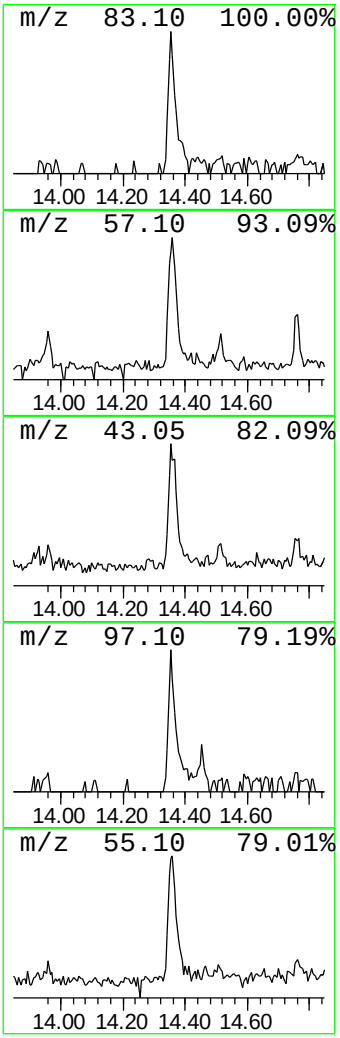
****

Peak Number 4 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	2.05 ng	98610	Chrysene-d12	14.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
3	1-Hexacosanol	382	C26H54O	000506-52-5	83
4	1-Hexadecanol	242	C16H34O	036653-82-4	83
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	80





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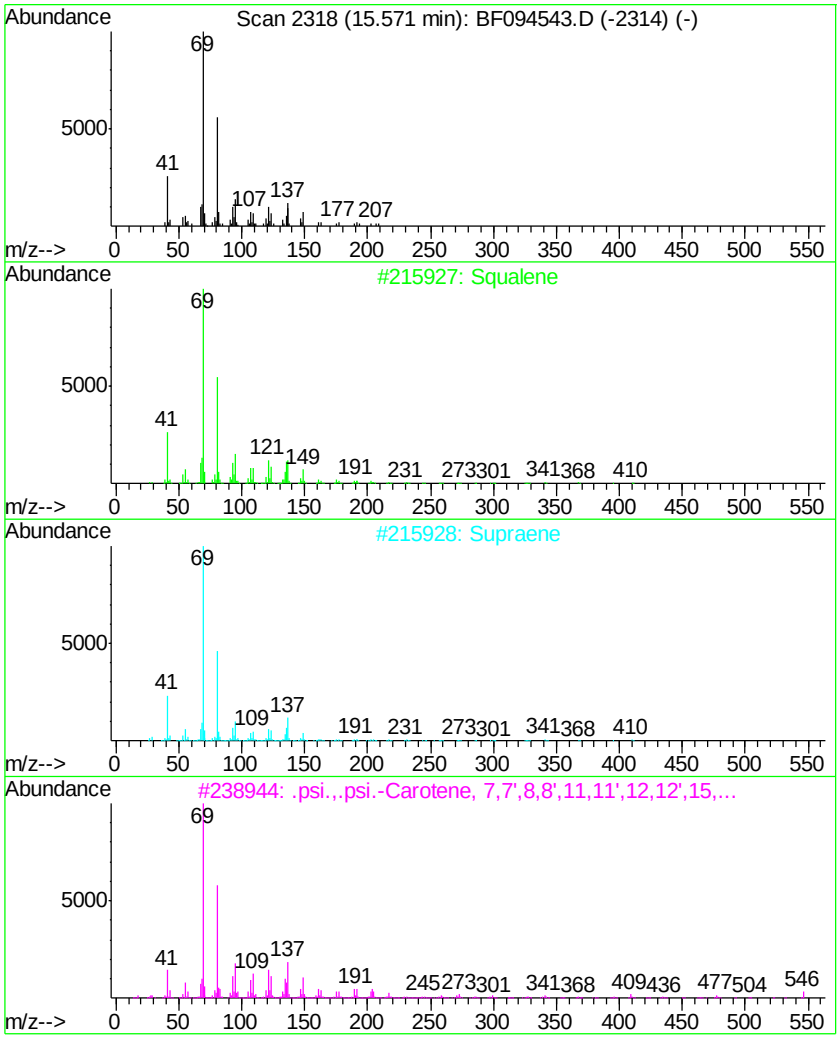
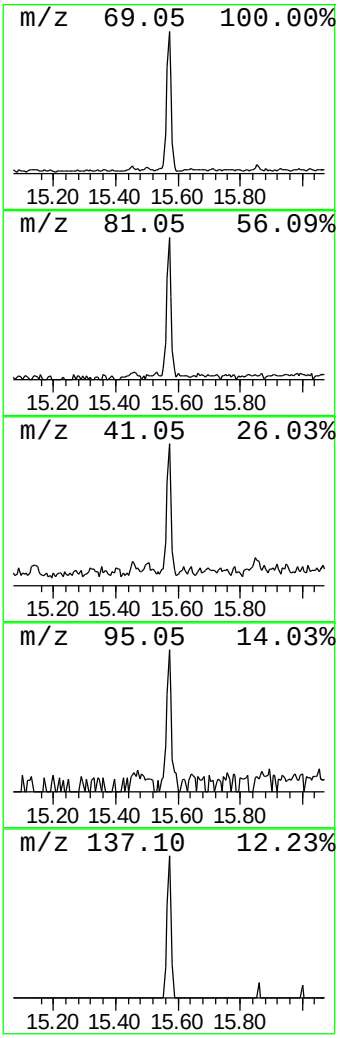
****

Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.57	3.05 ng	110068	Perylene-d12	16.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	90
2	Supraene	410	C30H50	007683-64-9	87
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	78
4	trans-Farnesol	222	C15H26O	000106-28-5	59
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	47





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	3.92	14.5	ng	458849	1	5.77	634161	20.0
unknown5.52	5.52	85.0	ng	2695880	1	5.77	634161	20.0
n-Tetracosanol-1	14.35	2.0	ng	98610	5	14.45	961716	20.0
Squalene	15.57	3.0	ng	110068	6	16.08	721286	20.0