LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050517\
Data File : BF094933.D
Acq On : 5 May 2017 23:56
Operator : SJ/MA
Sample : I2950-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-8(13-15)20170502

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-BF050217.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	5.043	523	528	545	rBV	203004	420633	12.85%	1.671%
2	5.666	630	634	661	rBV	1659299	2524809	77.14%	10.033%
3	7.266	900	906	921	rBV	1890929	2661374	81.31%	10.576%
4	7.384	921	926	934	rVB	2210584	2851985	87.14%	11.333%
5	7.719	979	983	993	rBV	418862	510927	15.61%	2.030%
6	7.960	1019	1024	1035	rBV	1828587	2134846	65.23%	8.483%
7	8.619	1131	1136	1161	rBV	1231695	1730022	52.86%	6.875%
8	9.742	1322	1327	1340	rBV	482847	649596	19.85%	2.581%
9	11.519	1623	1629	1650	rBV	2588891	3272988	100.00%	13.006%
10	12.207	1742	1746	1760	rBV	193011	247605	7.57%	0.984%
11	12.572	1803	1808	1821	rBV2	547103	726500	22.20%	2.887%
12	13.866	2022	2028	2043	rBV	1260543	1893971	57.87%	7.526%
13	14.189	2079	2083	2086	rBV	40735	51387	1.57%	0.204%
14	14.971	2211	2216	2231	rVV	522364	752428	22.99%	2.990%
15	15.942	2376	2381	2390	rBV	168183	214694	6.56%	0.853%
16	17.024	2562	2565	2574	rBV2	34750	52955	1.62%	0.210%
17	17.301	2606	2612	2616	rBV	2429439	2940937	89.85%	11.686%
18	18.577	2819	2829	2835	rBV6	26629	78641	2.40%	0.312%
19	18.636	2835	2839	2855	rVB	503669	724979	22.15%	2.881%
20	19.771	3028	3032	3037	rVB	69027	73814	2.26%	0.293%
21	20.300	3114	3122	3135	rBV	316229	484586	14.81%	1.926%
22	20.400	3135	3139	3144	rVB2	24895	34756	1.06%	0.138%
23	20.771	3197	3202	3211	rVB2	26579	44603	1.36%	0.177%
24	21.200	3269	3275	3282	rBV2	27027	47251	1.44%	0.188%
25	21.694	3352	3359	3366	rBV6	18862	39127	1.20%	0.155%

Sum of corrected areas: 25165414

LSC Report - Integrated Chromatogram

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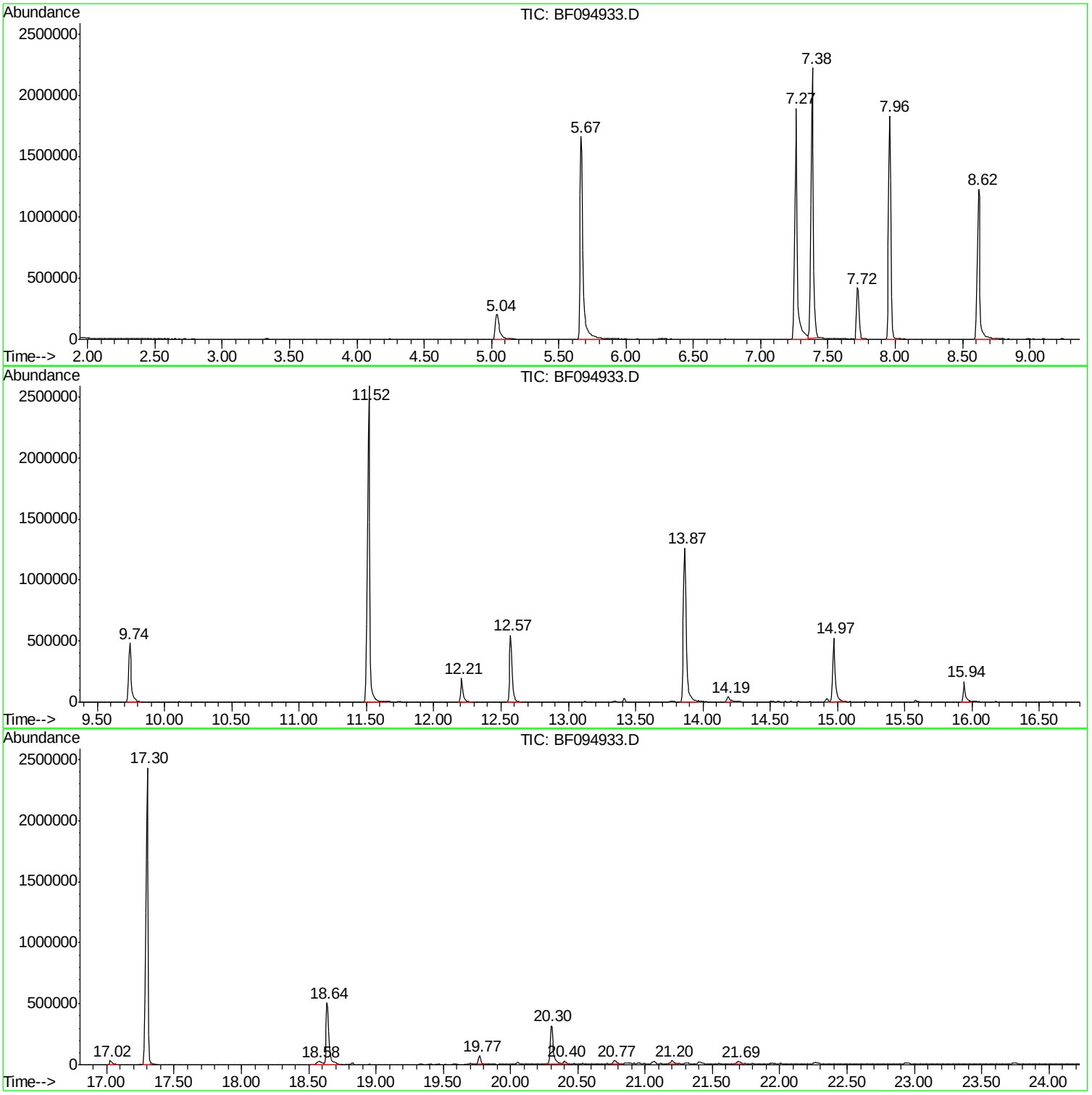
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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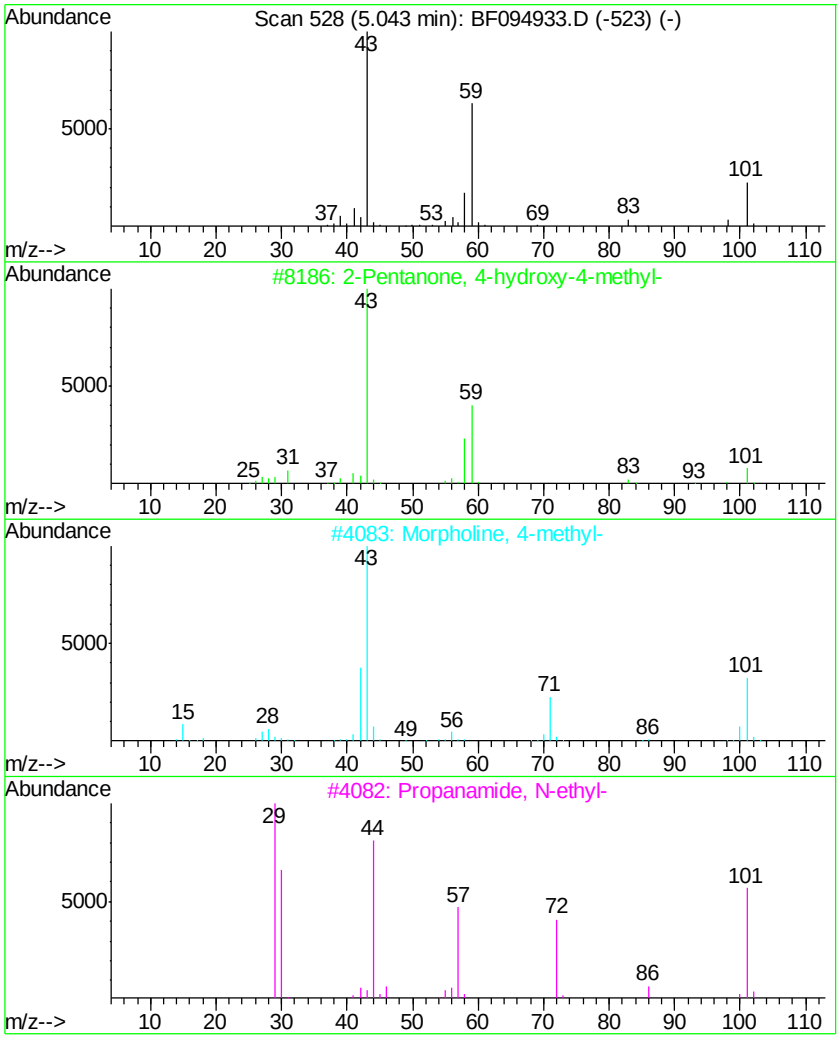
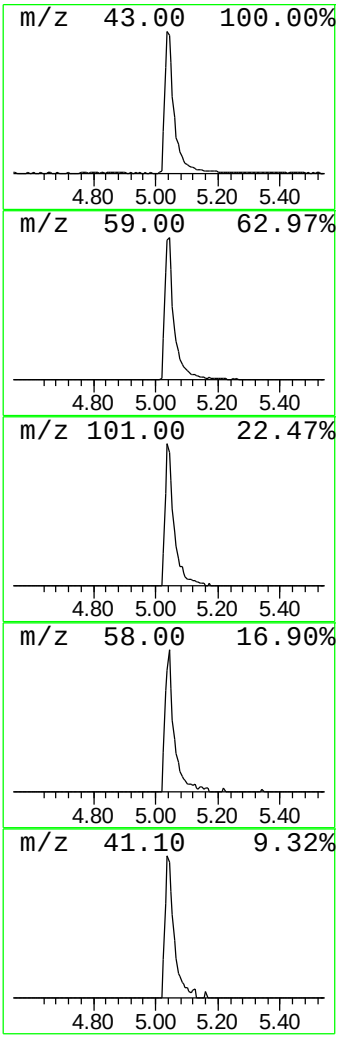
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	16.47 ng	420633	1,4-Dichlorobenzene-d4	7.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3	Propanamide, N-ethyl-	101	C5H11NO	005129-72-6	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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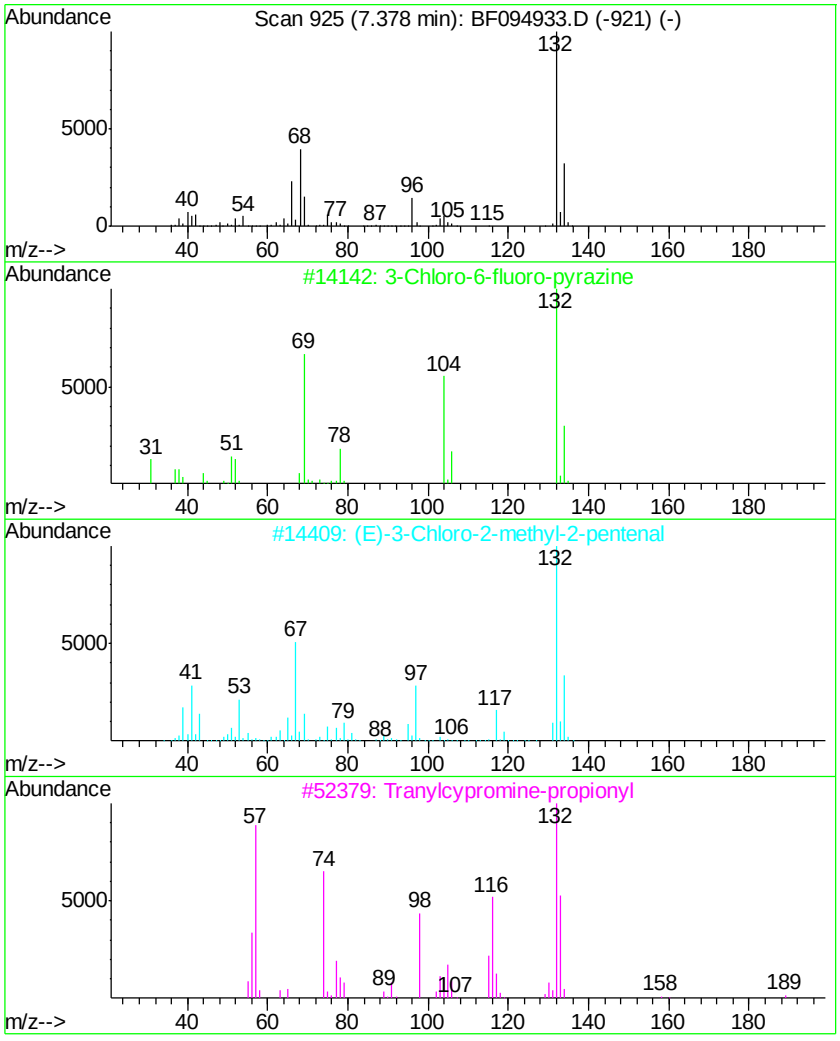
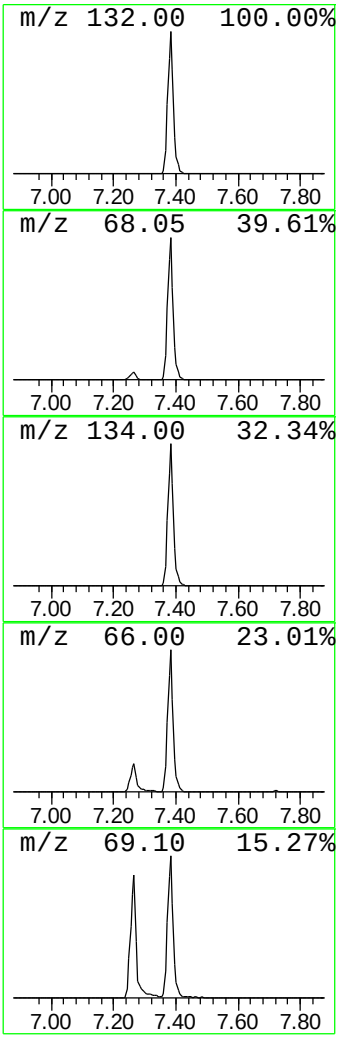
Peak Number 2 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	111.64 ng	2851990	1,4-Dichlorobenzene-d4	7.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





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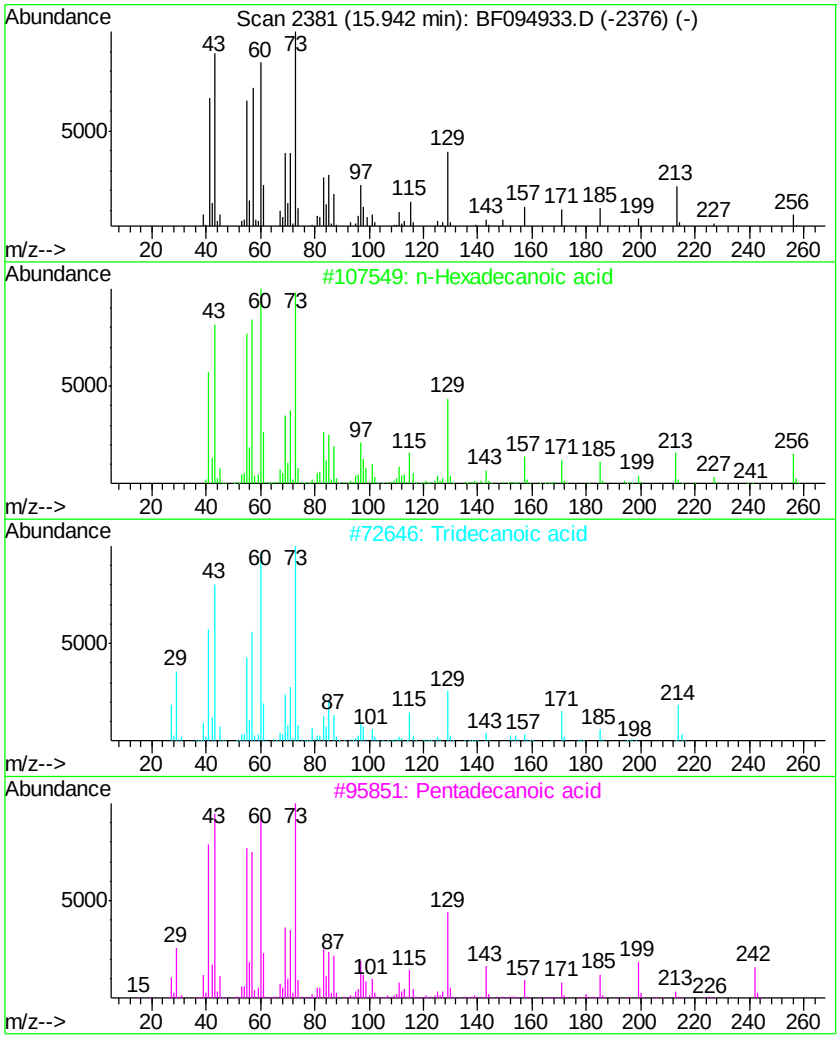
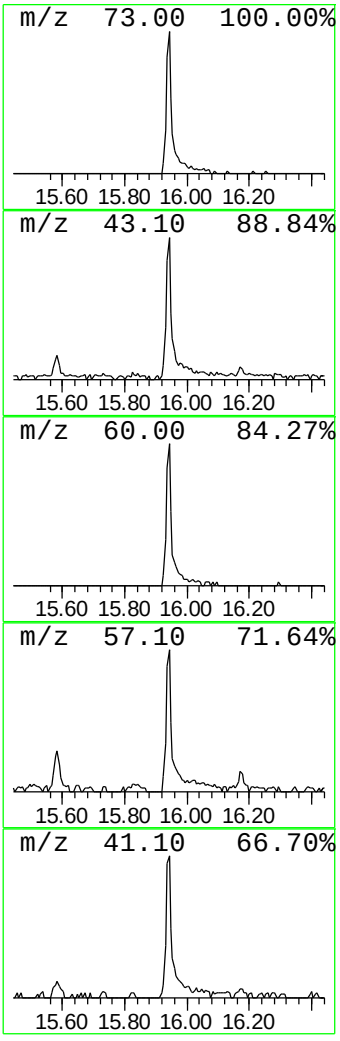
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	5.71 ng	214694	Phenanthrene-d10	14.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Instrument :
BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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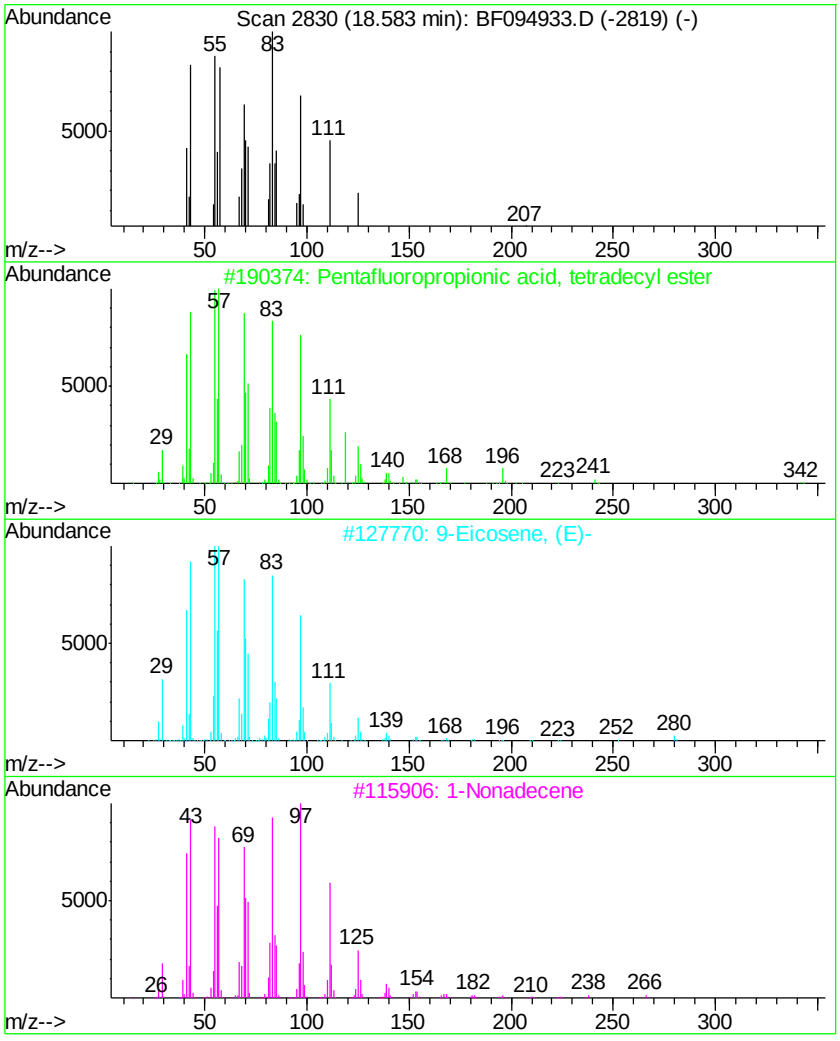
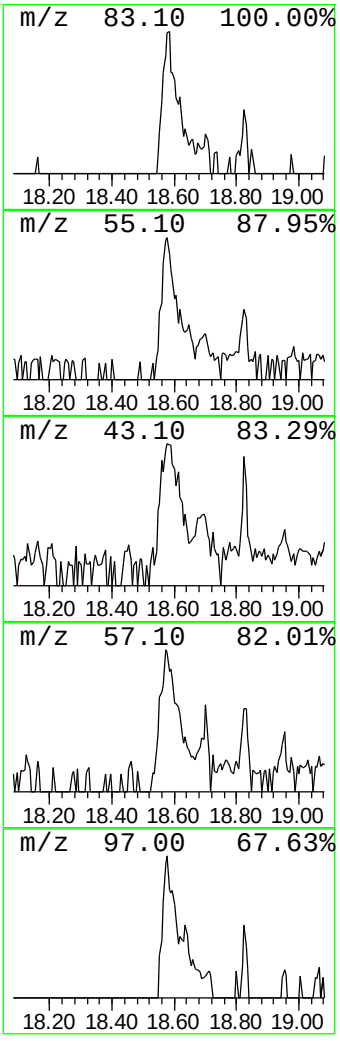
Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.58	2.17 ng	78641	Chrysene-d12	18.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
3	1-Nonadecene	266	C19H38	018435-45-5	87
4	1-Hexadecanol	242	C16H34O	036653-82-4	87
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	86





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Instrument :
BNA_F
ClientSampleId :
SB-8(13-15)20170502

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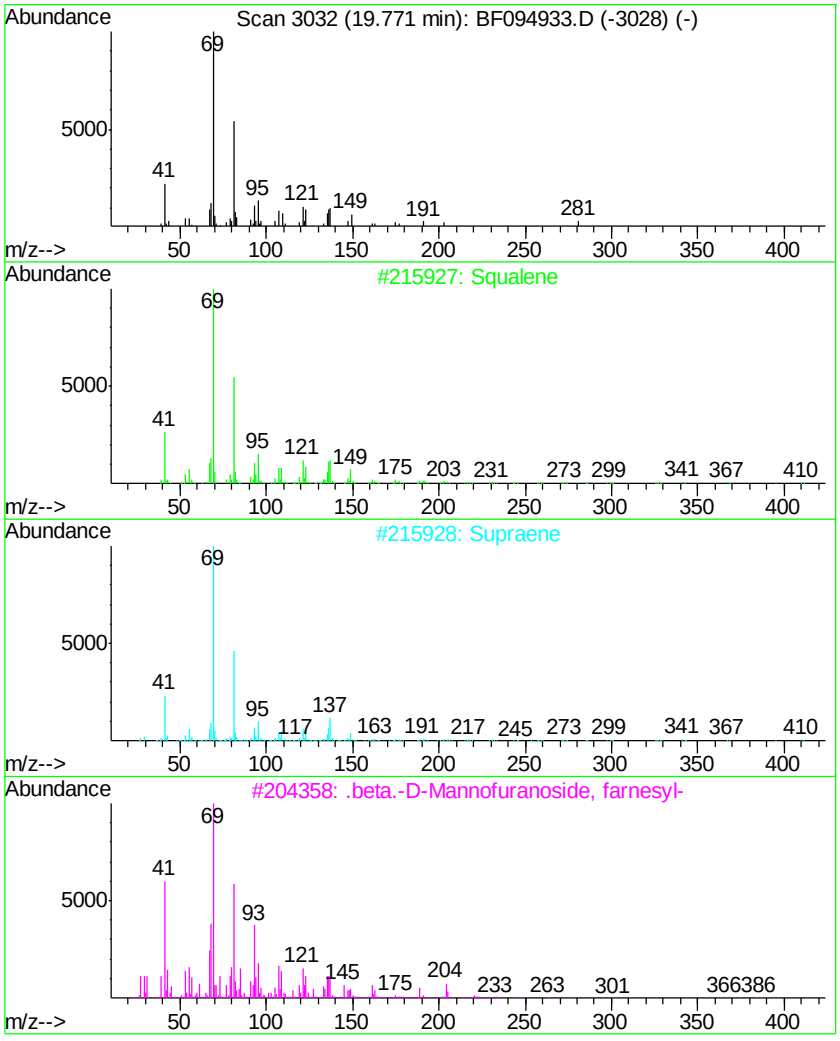
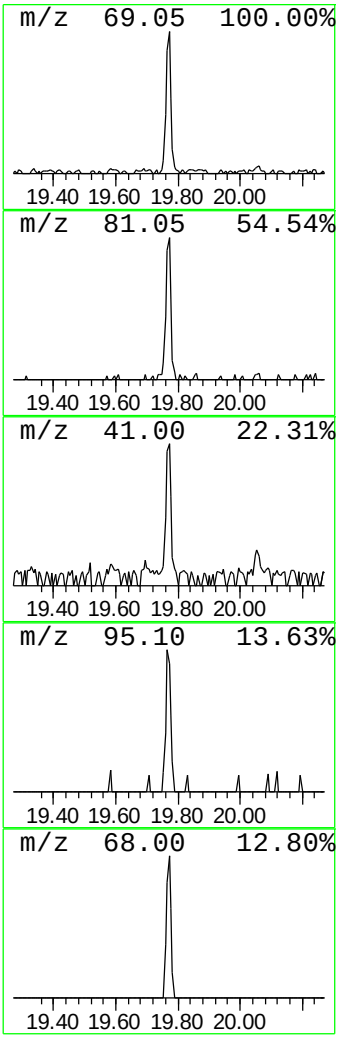
Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.77	3.05 ng	73814	Perylene-d12	20.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	86
3	.beta.-D-Mannofuranoside, farnesyl-	384	C21H36O6	1000155-15-5	78
4	4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	64
5	2,6-Octadiene, 4,5-dimethyl-	138	C10H18	018476-57-8	43





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	16.5	ng	420633	1	7.72	510927	20.0
unknown7.38	7.38	111.6	ng	2851990	1	7.72	510927	20.0
n-Hexadecanoic acid	15.94	5.7	ng	214694	4	14.97	752428	20.0
Pentafluoropropio...	18.58	2.2	ng	78641	5	18.64	724979	20.0
Squalene	19.77	3.0	ng	73814	6	20.30	484586	20.0