LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109053.D
Acq On : 17 Sep 2018 17:29
Operator : JU/SJ
Sample : J4935-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHASE-1

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-BF091418.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	4.913	435	438	446	rVB	83562	100113	4.13%	0.445%
2	5.331	504	509	512	rBV	2583197	2388914	98.61%	10.630%
3	6.354	678	683	686	rBV	2534659	2390280	98.66%	10.636%
4	6.490	701	706	709	rBV	2802329	2422699	100.00%	10.780%
5	6.719	742	745	749	rBV	836738	718481	29.66%	3.197%
6	6.878	768	772	775	rBV	2315676	1888362	77.94%	8.402%
7	7.278	836	840	843	rBV	1634603	1449222	59.82%	6.448%
8	8.001	959	963	966	rBV	1028790	794290	32.79%	3.534%
9	9.078	1142	1146	1149	rBV	2787327	2211540	91.28%	9.840%
10	9.466	1209	1212	1216	rBV	174108	153712	6.34%	0.684%
11	9.748	1257	1260	1264	rBV	881944	801329	33.08%	3.566%
12	10.536	1390	1394	1409	rBV	1495221	1432109	59.11%	6.372%
13	11.225	1508	1511	1515	rBV	988884	855726	35.32%	3.808%
14	11.766	1599	1603	1607	rBV3	45071	47005	1.94%	0.209%
15	12.813	1776	1781	1784	rBV	2378099	2265237	93.50%	10.079%
16	13.724	1932	1936	1945	rBV	81304	141019	5.82%	0.627%
17	13.854	1954	1958	1961	rBV	1061321	993526	41.01%	4.421%
18	14.342	2038	2041	2045	rBV	33330	31171	1.29%	0.139%
19	14.636	2089	2091	2096	rVB	49512	55793	2.30%	0.248%
20	14.707	2099	2103	2108	rVB	310132	300599	12.41%	1.338%
21	14.954	2143	2145	2152	rVB	60587	62283	2.57%	0.277%
22	15.254	2192	2196	2201	rBV	606470	731081	30.18%	3.253%
23	15.313	2202	2206	2211	rVB	61955	78786	3.25%	0.351%
24	15.713	2271	2274	2280	rVB	49419	66635	2.75%	0.296%
25	16.189	2350	2355	2367	rVB5	40813	93991	3.88%	0.418%

Sum of corrected areas: 22473903

LSC Report - Integrated Chromatogram

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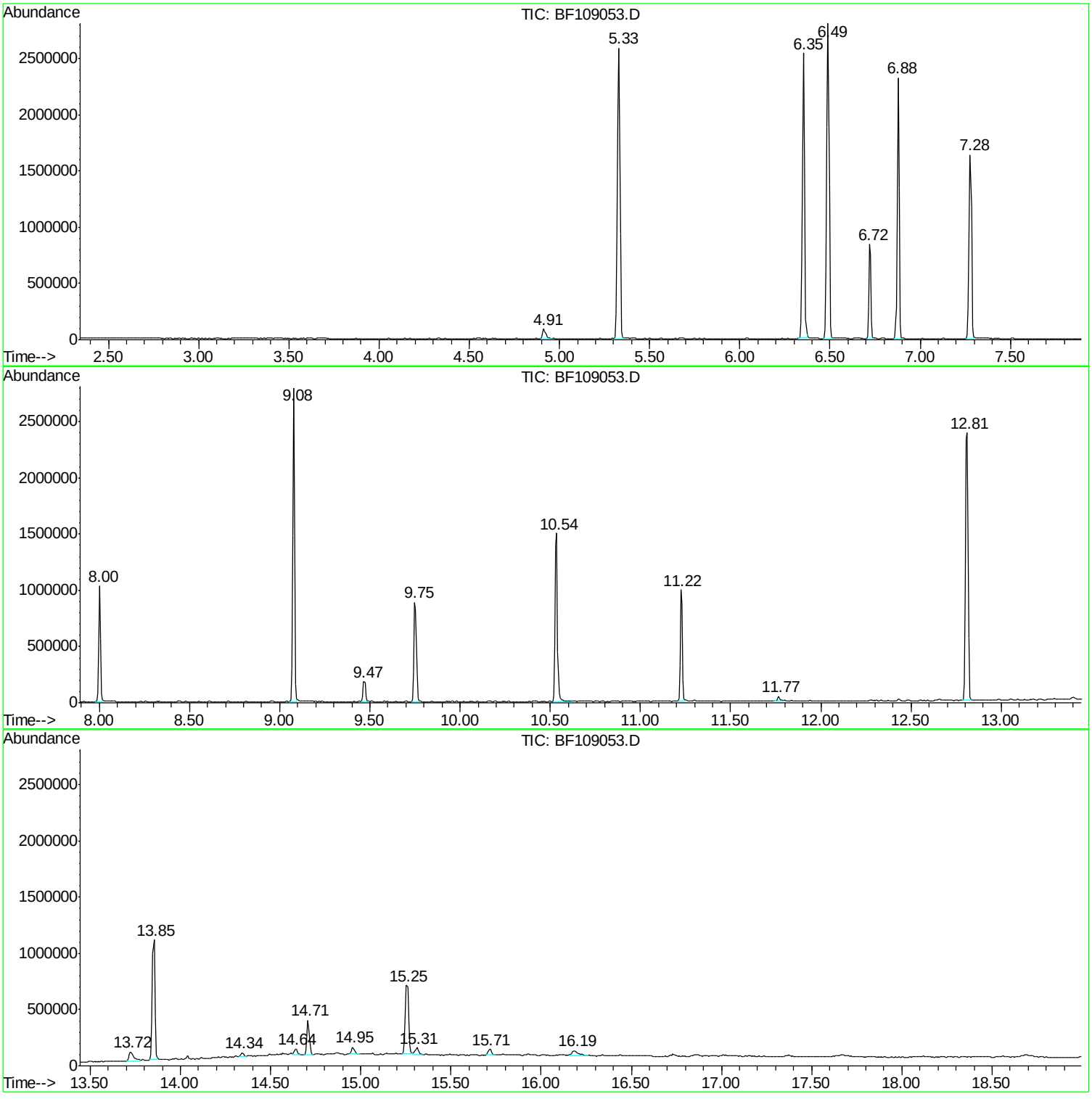
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHASE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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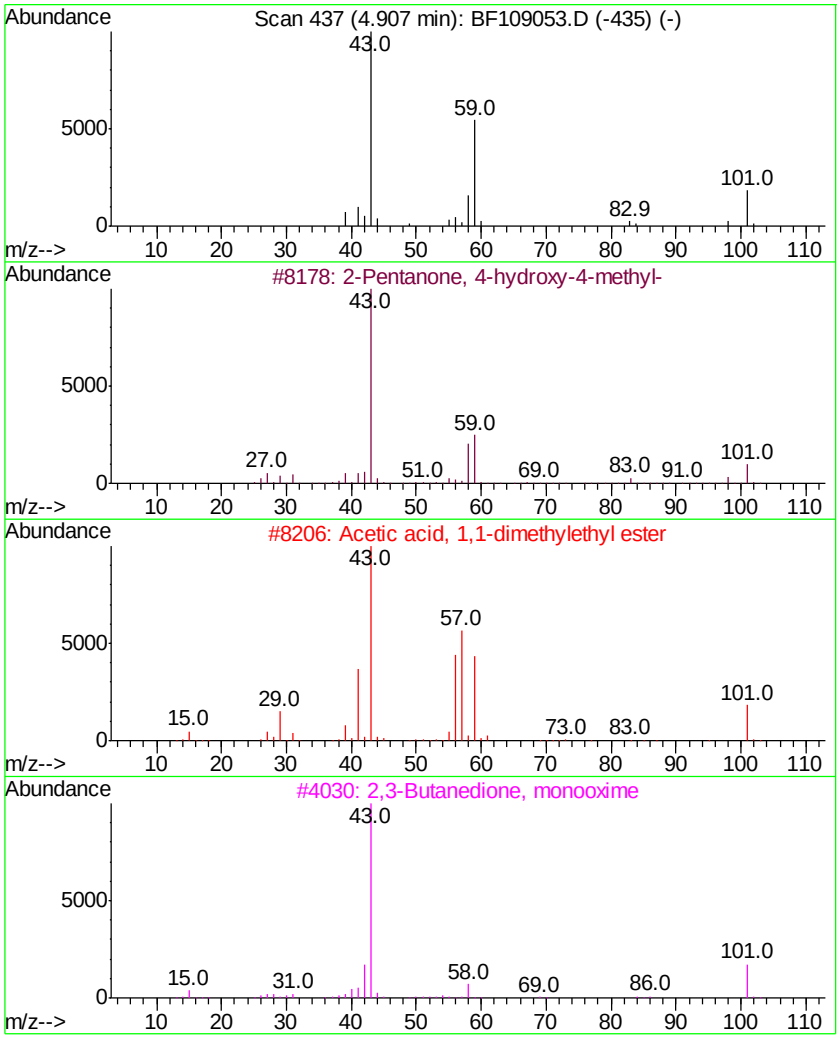
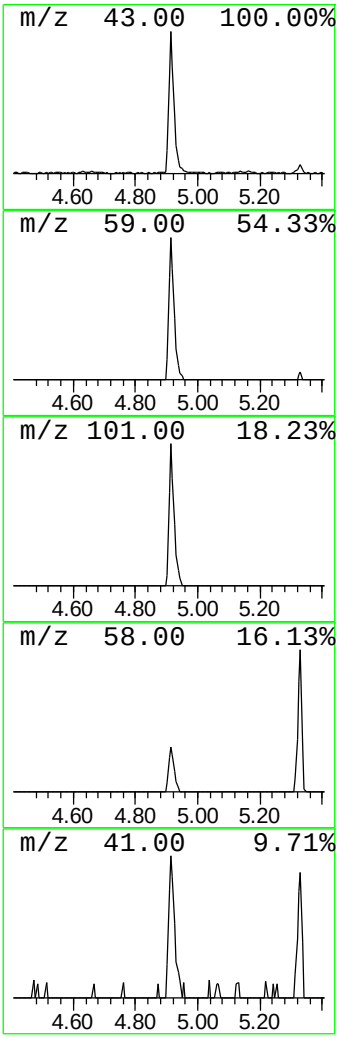
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	2.79 ng	100113	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	23
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17





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Sample : J4935-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHASE-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

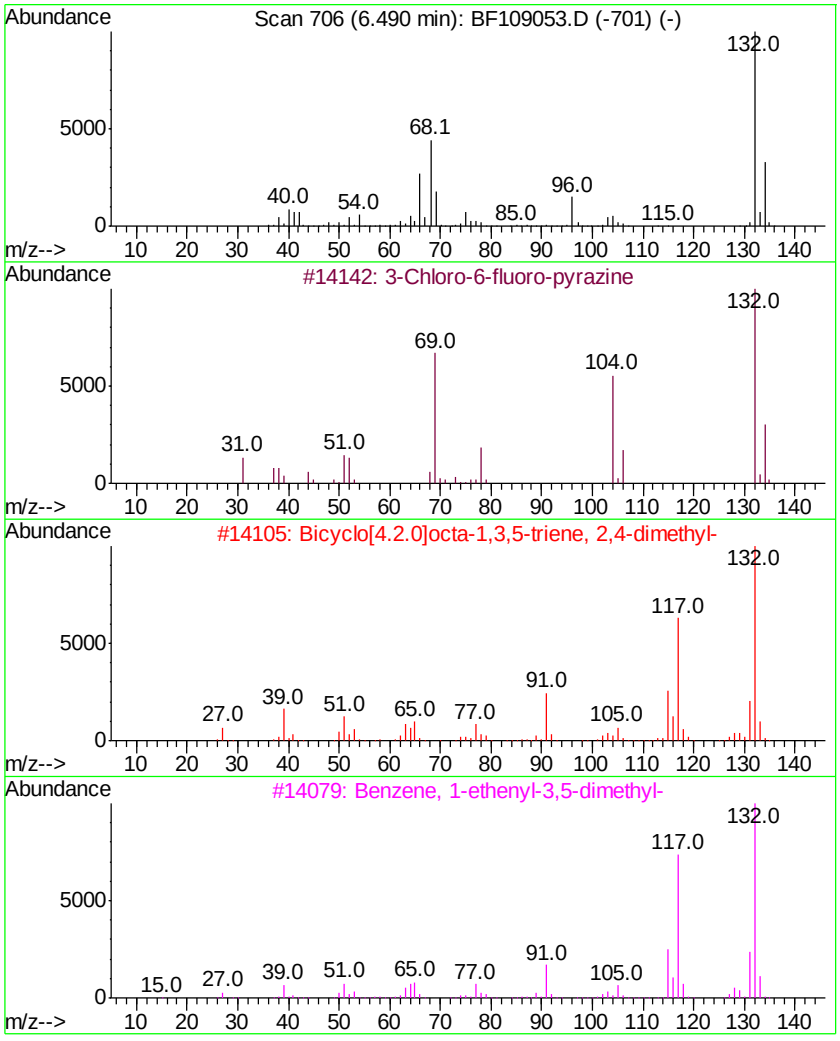
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

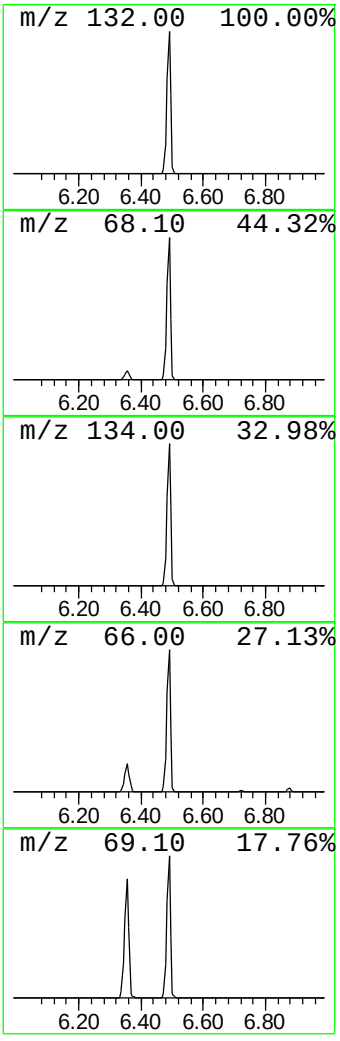
****

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	67.44 ng	2422700	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Library Search Compound Report

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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHASE-1

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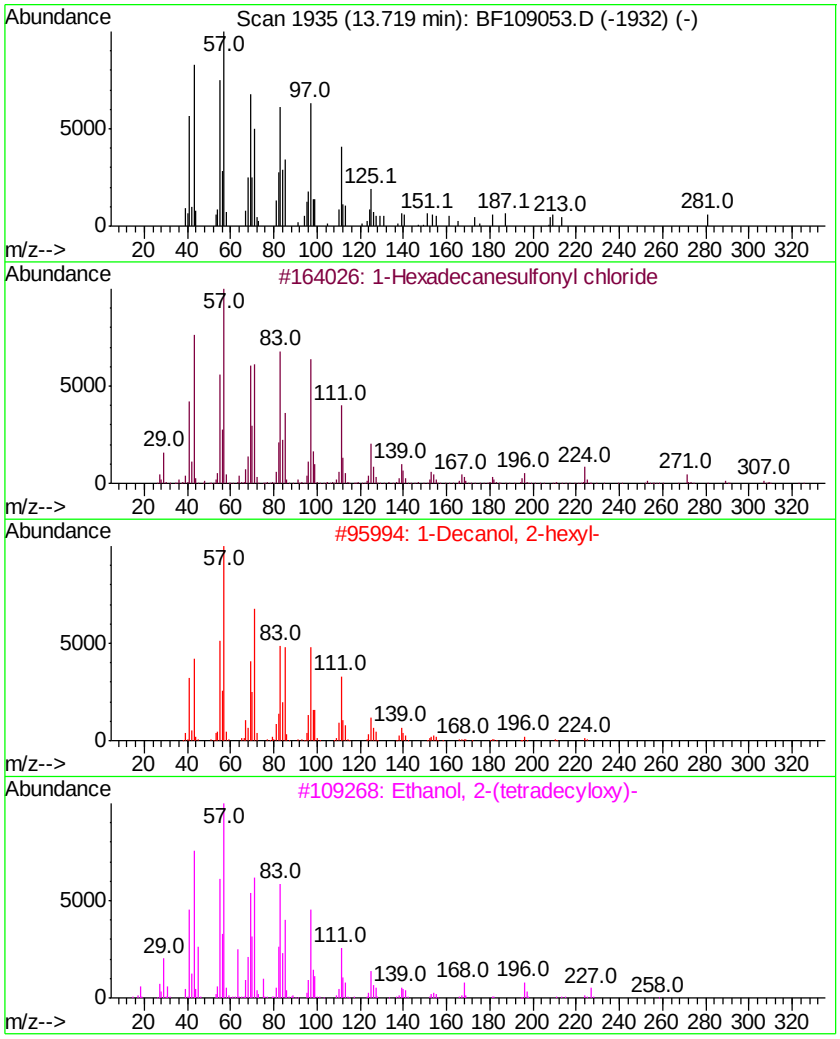
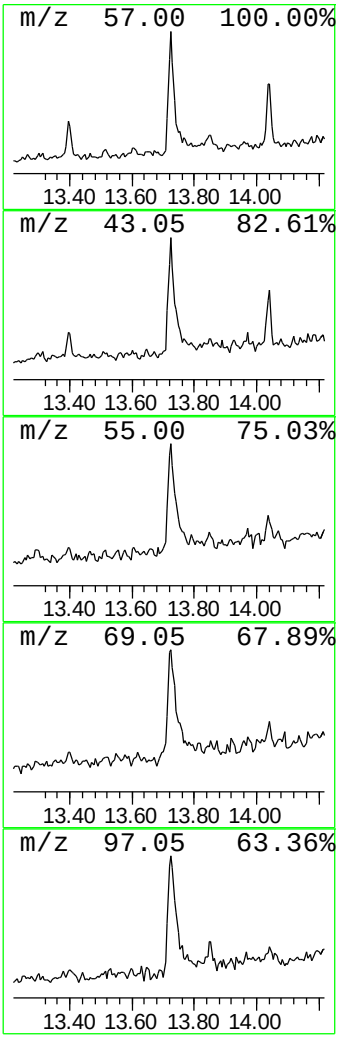
Peak Number 4 1-Hexadecanesulfonyl chloride Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	2.84 ng	141019	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	90
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	90
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	83
5	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	81





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHASE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
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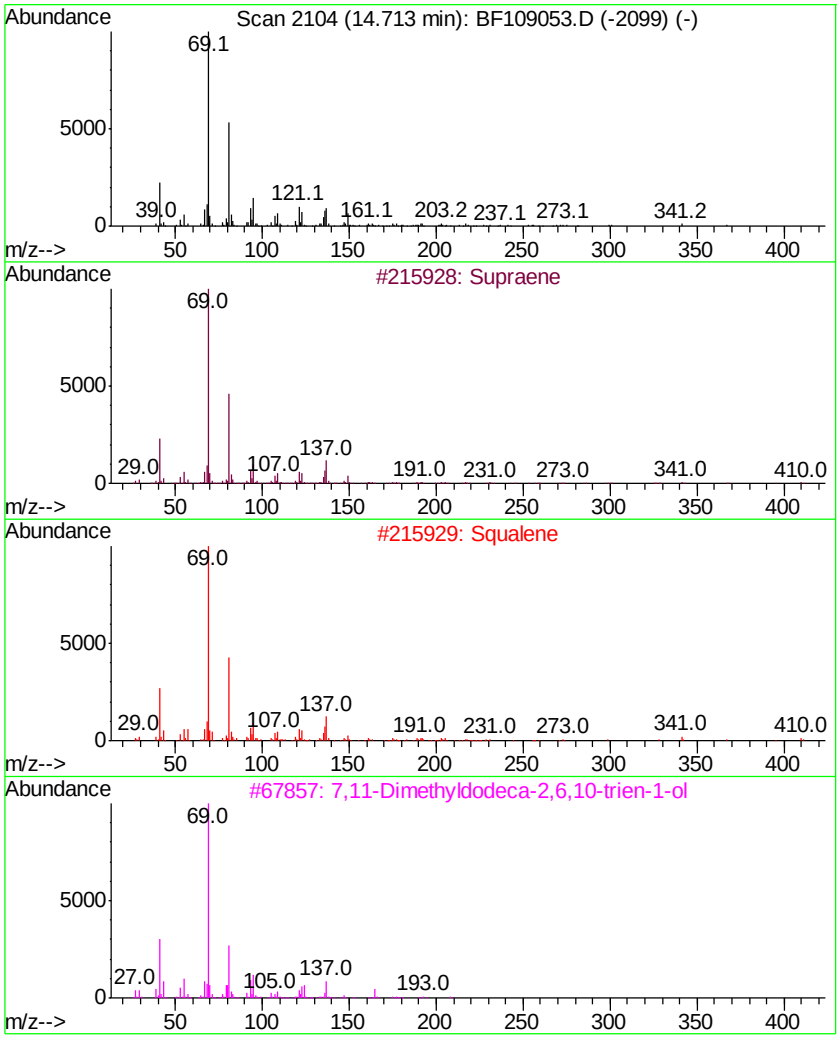
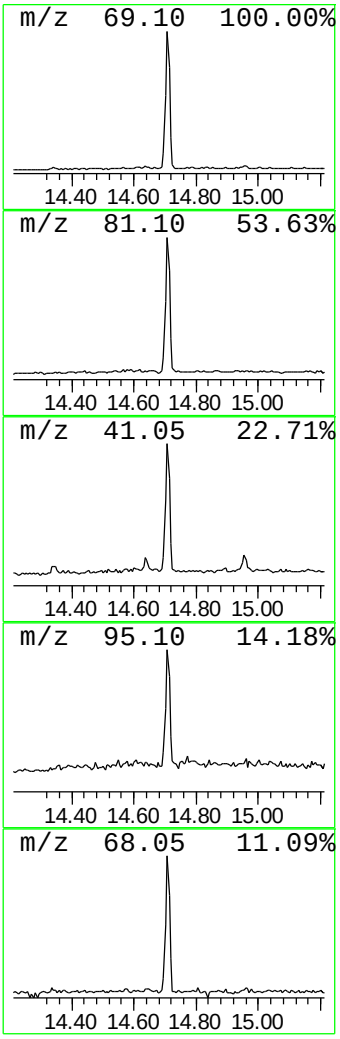
Peak Number 5 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	8.22 ng	300599	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	72
5	1,5-Heptadiene, 3,3-dimethyl-, (E)-	124	C9H16	067682-47-7	50





Library Search Compound Report

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Instrument : BNA_F
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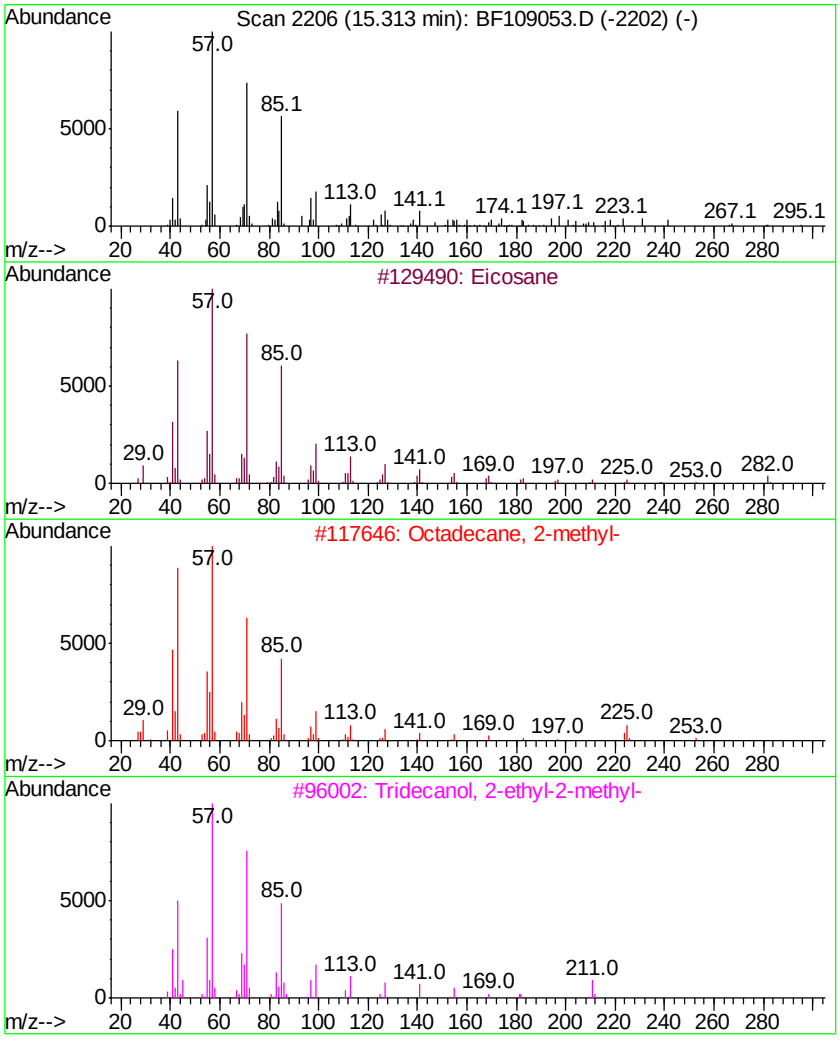
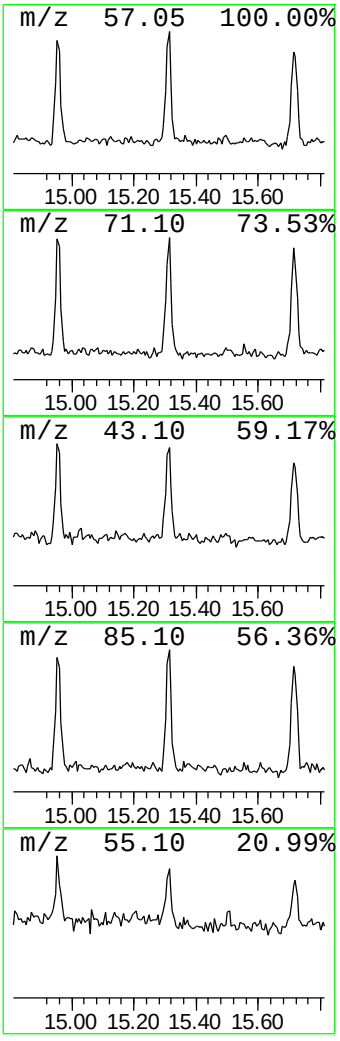
****

Peak Number 6 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	2.16 ng	78786	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	86
3	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	86
4	Triacontane	422	C30H62	000638-68-6	86
5	Heneicosane	296	C21H44	000629-94-7	83





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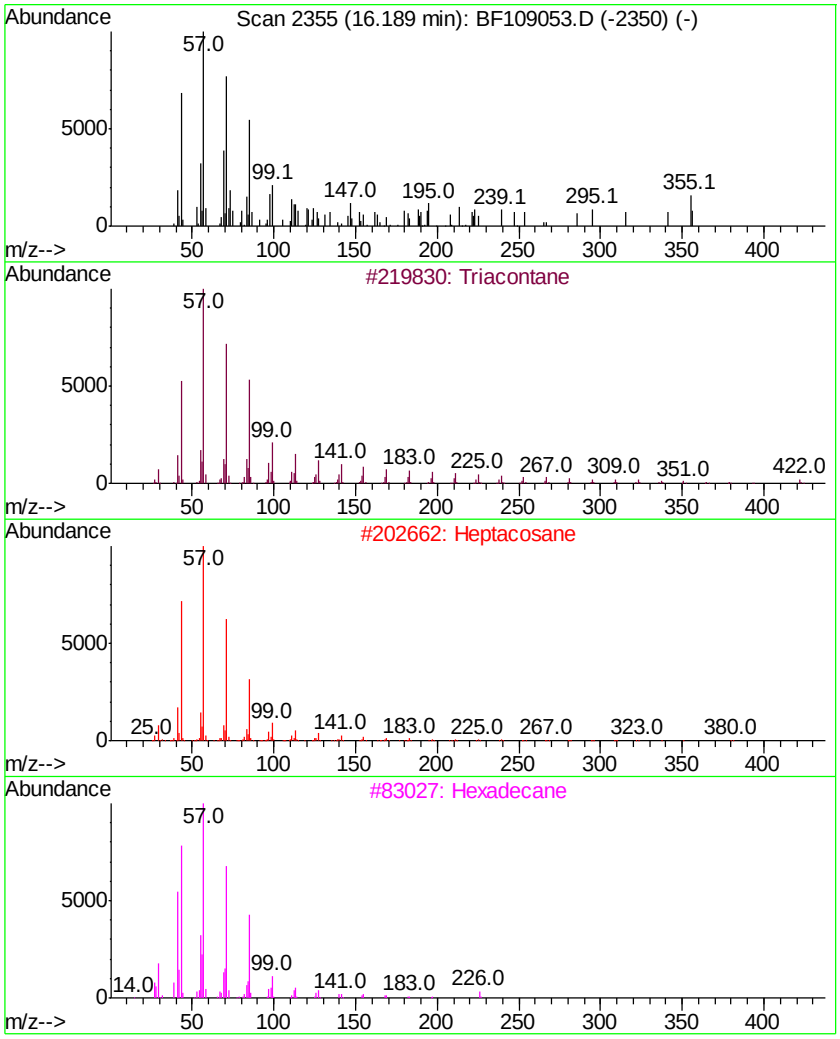
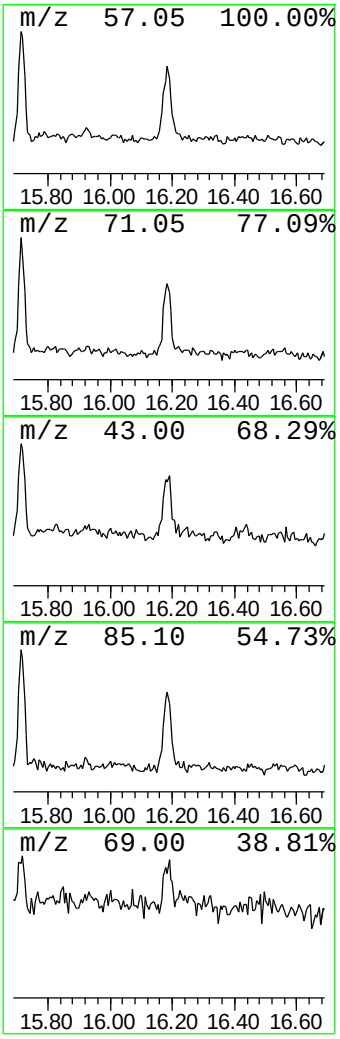
Peak Number 7 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.57 ng	93991	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	64
2	Heptacosane	380	C27H56	000593-49-7	59
3	Hexadecane	226	C16H34	000544-76-3	59
4	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	59
5	Tetracosane	338	C24H50	000646-31-1	59





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...	4.91	2.8	ng	100113	1	6.72	718481	20.0
unknown6.49	6.49	67.4	ng	2422700	1	6.72	718481	20.0
1-Hexadecanesulfo...	13.72	2.8	ng	141019	5	13.85	993526	20.0
Supraene	14.71	8.2	ng	300599	6	15.25	731081	20.0
Eicosane	15.31	2.2	ng	78786	6	15.25	731081	20.0
Triacontane	16.19	2.6	ng	93991	6	15.25	731081	20.0