LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
Data File : BF096169.D
Acq On : 23 Jun 2017 20:25
Operator : SJ/MA
Sample : I3784-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P.56-B-COMP

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-BF060517.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	1.540	7	9	59	rVB	1042149	2301338	100.00%	11.161%
2	4.428	496	500	528	rBV2	73393	258177	11.22%	1.252%
3	5.145	618	622	660	rBV	741104	1748010	75.96%	8.477%
4	6.839	906	910	920	rBV	996948	1591860	69.17%	7.720%
5	6.922	920	924	939	rVB	1194702	2073507	90.10%	10.056%
6	7.257	977	981	994	rBV	266446	384211	16.70%	1.863%
7	7.492	1017	1021	1046	rBV	838435	1196507	51.99%	5.803%
8	8.186	1134	1139	1162	rBV	642558	1053413	45.77%	5.109%
9	9.292	1323	1327	1341	rBV	362669	551646	23.97%	2.675%
10	11.074	1624	1630	1647	rVB	1326239	1712180	74.40%	8.303%
11	11.774	1744	1749	1760	rBV	210716	293451	12.75%	1.423%
12	12.110	1802	1806	1812	rBV2	456344	599235	26.04%	2.906%
13	12.163	1812	1815	1823	rVB2	26480	44528	1.93%	0.216%
14	12.968	1946	1952	1957	rVB	22749	30894	1.34%	0.150%
15	13.021	1957	1961	1969	rBV	16760	28620	1.24%	0.139%
16	13.415	2022	2028	2044	rBV	728852	1142662	49.65%	5.541%
17	13.739	2078	2083	2092	rBV4	22753	39011	1.70%	0.189%
18	14.504	2209	2213	2217	rVV	437073	566252	24.61%	2.746%
19	14.545	2217	2220	2229	rVB	109664	184374	8.01%	0.894%
20	14.651	2234	2238	2245	rBV	23670	35222	1.53%	0.171%
21	15.327	2350	2353	2356	rBV	26584	29850	1.30%	0.145%
22	15.374	2357	2361	2365	rVV2	21465	28537	1.24%	0.138%
23	15.474	2375	2378	2382	rBV4	19728	26151	1.14%	0.127%
24	15.539	2385	2389	2395	rVB2	91715	124531	5.41%	0.604%
25	15.986	2461	2465	2471	rVB4	16468	23455	1.02%	0.114%
26	16.345	2518	2526	2532	rBV	169429	240178	10.44%	1.165%
27	16.645	2573	2577	2584	rBV	221979	293150	12.74%	1.422%
28	16.898	2615	2620	2628	rVB	1155798	1358236	59.02%	6.587%
29	16.980	2628	2634	2637	rBV7	14265	27321	1.19%	0.132%
30	17.127	2656	2659	2664	rVB	27667	35432	1.54%	0.172%
31	17.262	2679	2682	2686	rBV4	29061	40322	1.75%	0.196%
32	17.892	2785	2789	2795	rBV2	178147	207855	9.03%	1.008%
33	18.150	2829	2833	2842	rBV	178352	266694	11.59%	1.293%
34	18.245	2842	2849	2854	rBV2	402454	605566	26.31%	2.937%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
Data File : BF096169.D
Acq On : 23 Jun 2017 20:25
Operator : SJ/MA
Sample : I3784-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P.56-B-COMP

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-BF060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	18.380	2869	2872	2878	rVB5	15749	29926	1.30%	0.145%
36	18.515	2891	2895	2901	rBV8	23676	33932	1.47%	0.165%
37	18.721	2926	2930	2933	rBV	72655	78257	3.40%	0.380%
38	18.956	2967	2970	2977	rVV2	96843	150488	6.54%	0.730%
39	19.021	2978	2981	2986	rVB	86525	102656	4.46%	0.498%
40	19.527	3063	3067	3070	rBV	72559	91681	3.98%	0.445%
41	19.703	3091	3097	3101	rVV8	20719	43473	1.89%	0.211%
42	19.815	3113	3116	3122	rBV	51037	60997	2.65%	0.296%
43	19.874	3123	3126	3130	rBV	72034	81133	3.53%	0.393%
44	19.921	3130	3134	3143	rVV	303347	405907	17.64%	1.968%
45	20.350	3204	3207	3210	rBV4	18636	25408	1.10%	0.123%
46	20.391	3211	3214	3219	rVV4	18150	37235	1.62%	0.181%
47	20.733	3269	3272	3277	rVB2	23935	35034	1.52%	0.170%
48	21.103	3331	3335	3341	rBV5	27350	55632	2.42%	0.270%
49	21.433	3385	3391	3399	rBV2	54658	102560	4.46%	0.497%
50	21.609	3415	3421	3430	rVB2	32274	77524	3.37%	0.376%
51	22.797	3617	3623	3635	rVB2	24015	66077	2.87%	0.320%

Sum of corrected areas: 20620296

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Sample : I3784-03
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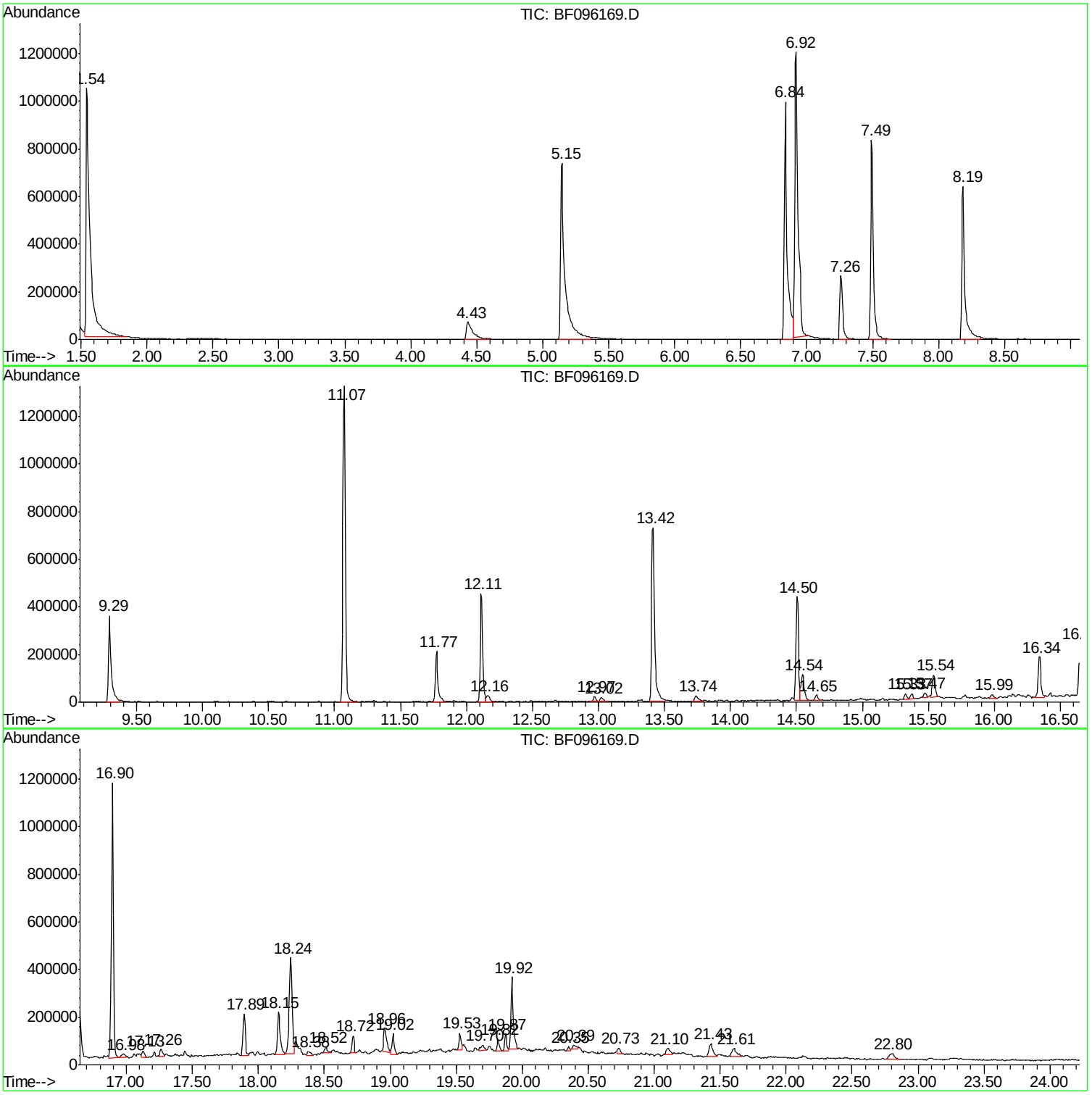
Instrument : BNA_F
ClientSampleId : P.56-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
Data File : BF096169.D
Acq On : 23 Jun 2017 20:25
Operator : SJ/MA
Sample : I3784-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P.56-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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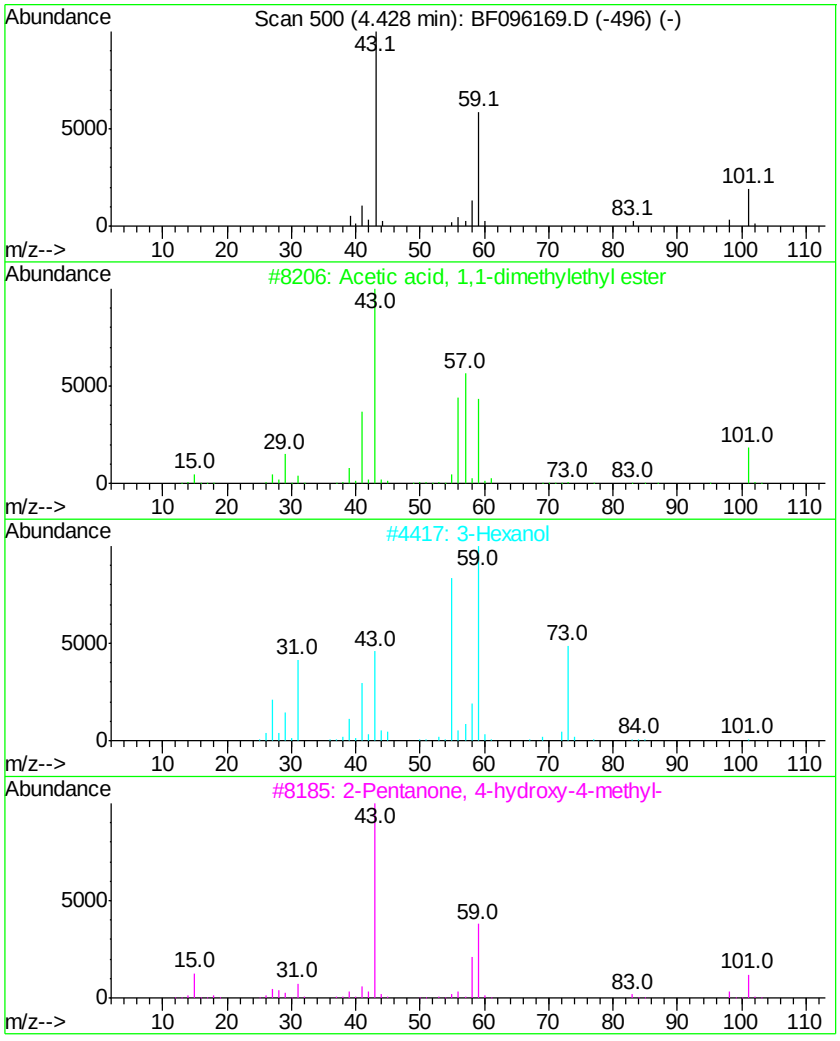
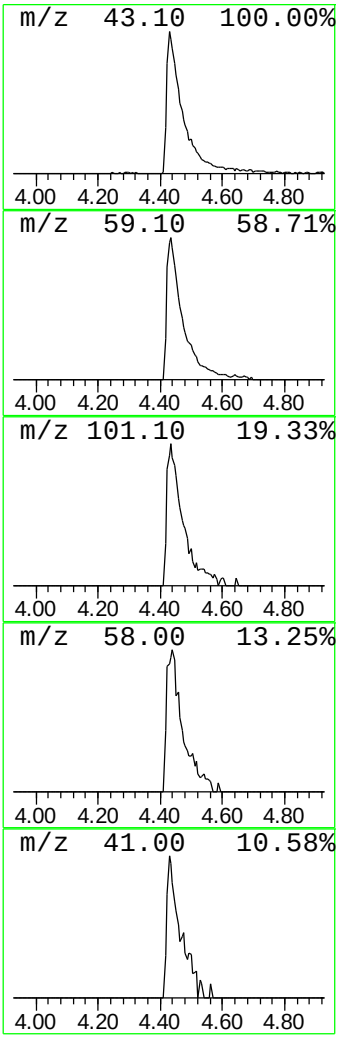
Peak Number 2 unknown4.43 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.43	13.44 ng	258177	1,4-Dichlorobenzene-d4	7.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
2	3-Hexanol	102	C6H14O	000623-37-0	28
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
Data File : BF096169.D
Acq On : 23 Jun 2017 20:25
Operator : SJ/MA
Sample : I3784-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P.56-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

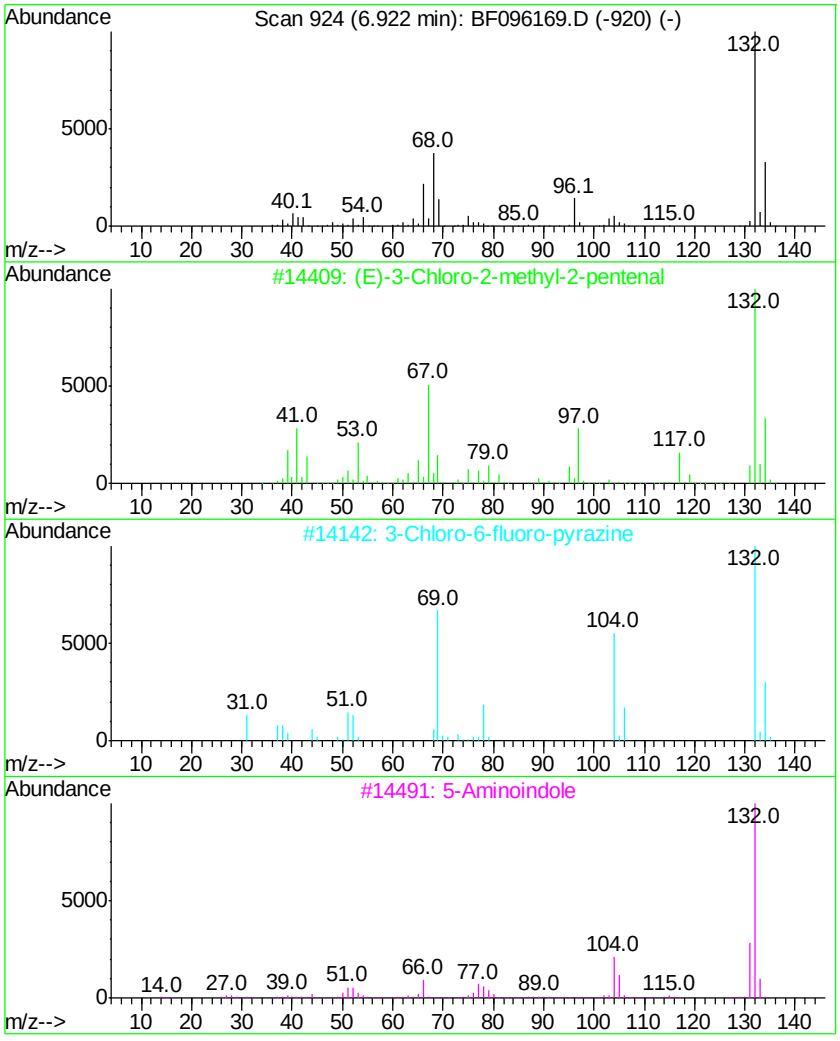
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

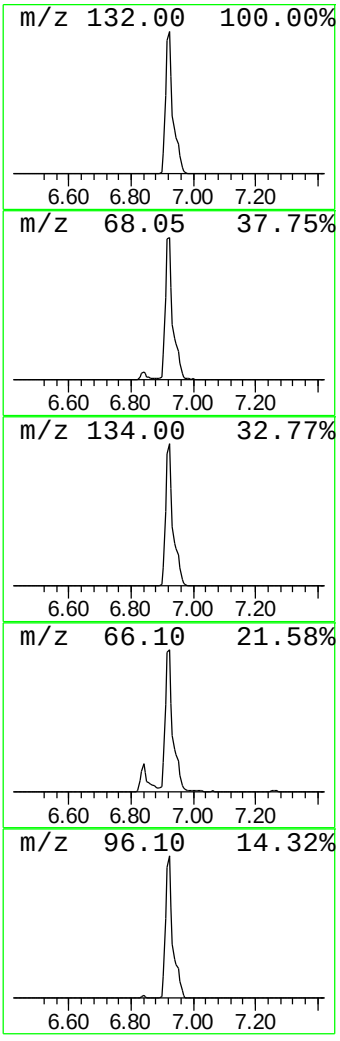
****

Peak Number 3 unknown6.92 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.92	107.94 ng	2073510	1,4-Dichlorobenzene-d4	7.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
Data File : BF096169.D
Acq On : 23 Jun 2017 20:25
Operator : SJ/MA
Sample : I3784-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P.56-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

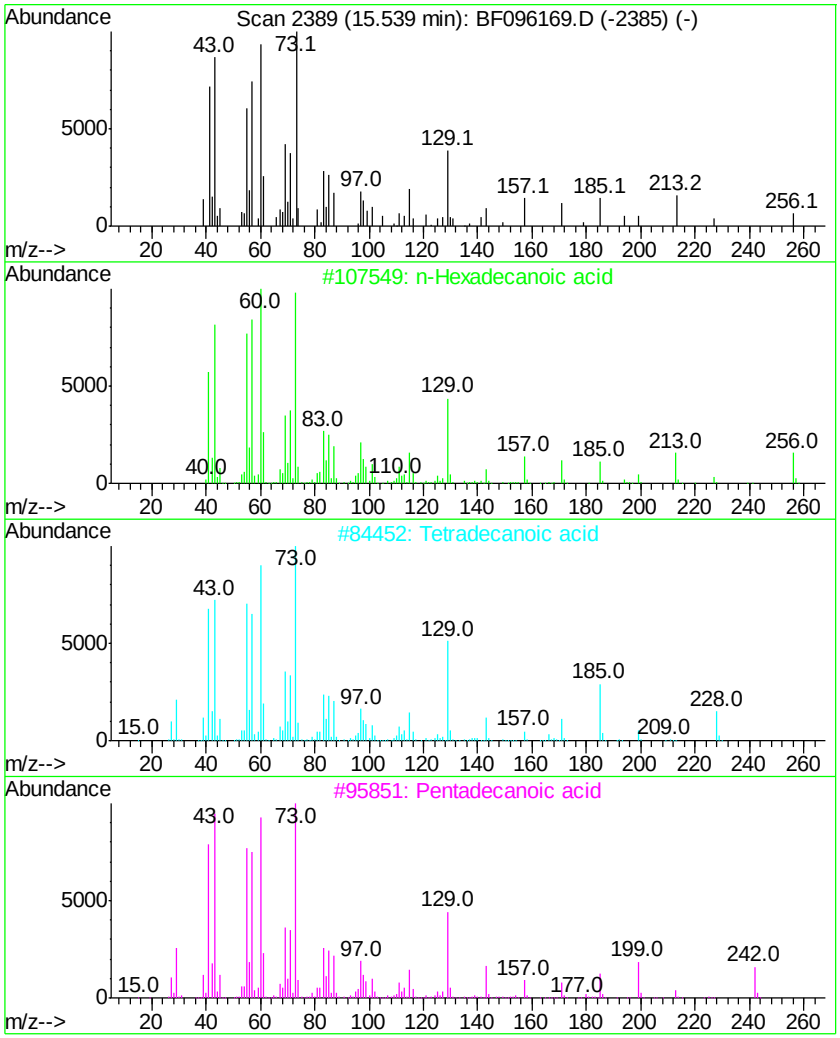
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

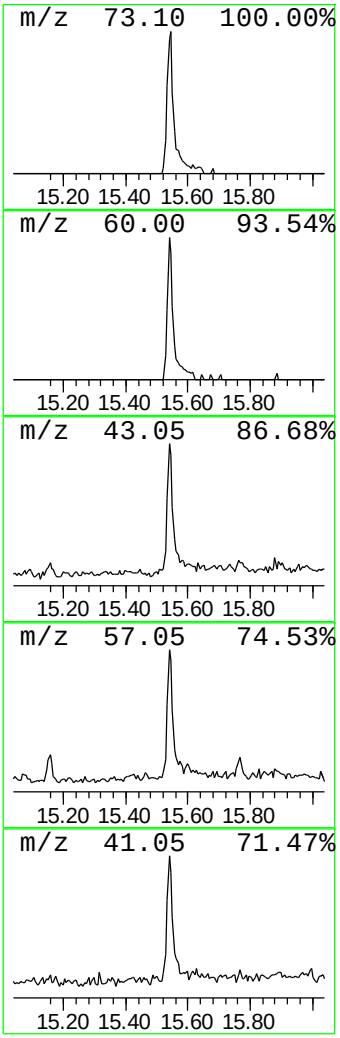
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.54	4.40 ng	124531	Phenanthrene-d10	14.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Data File : BF096169.D
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Operator : SJ/MA
Sample : I3784-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P.56-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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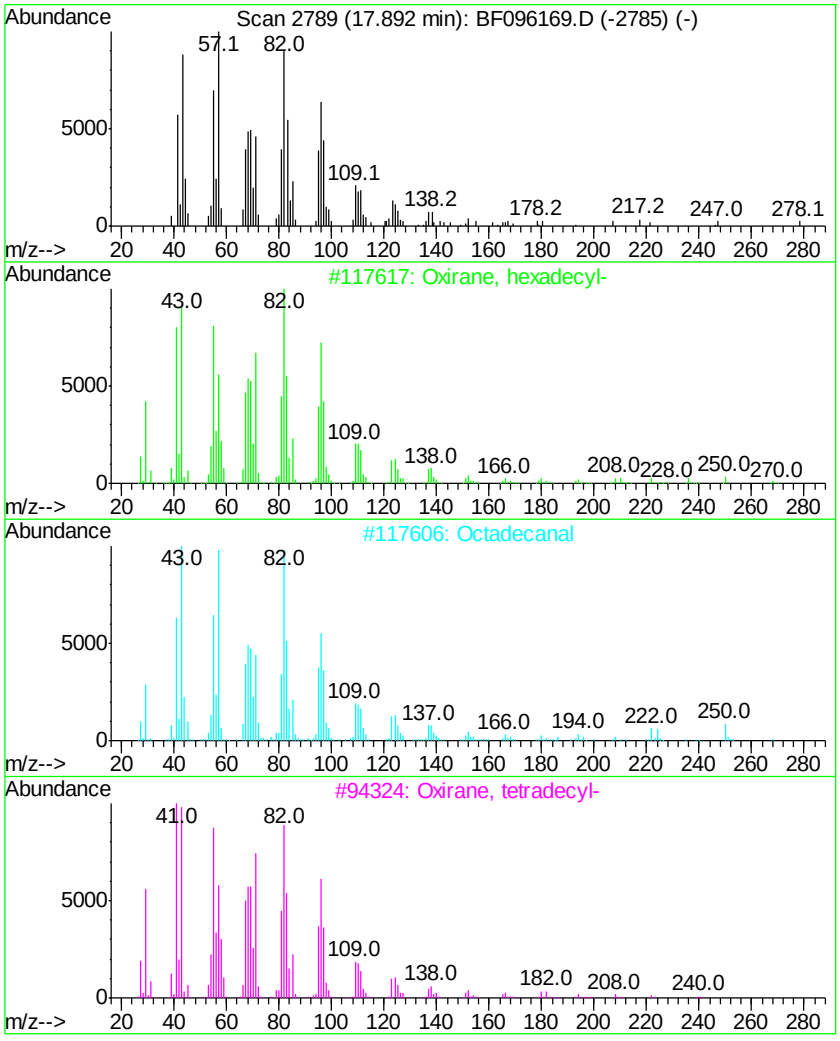
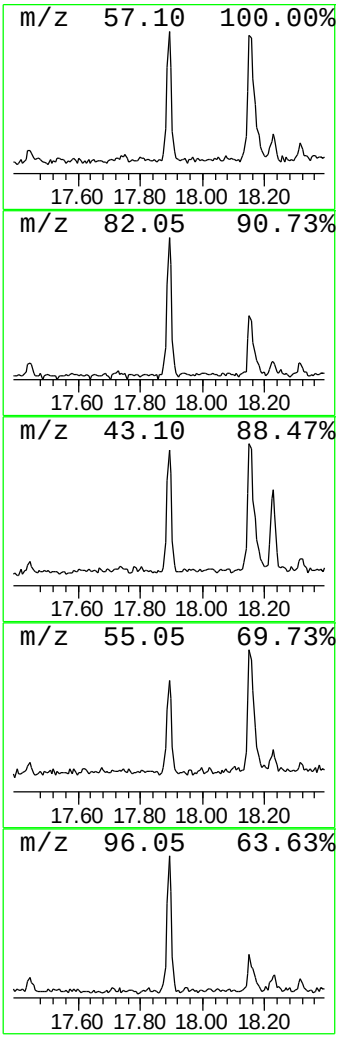
Peak Number 6 Oxirane, hexadecyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.89	6.86 ng	207855	Chrysene-d12	18.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	93
2	Octadecanal	268	C18H36O	000638-66-4	91
3	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	91
4	Hexadecanal	240	C16H32O	000629-80-1	91
5	Heptadecanal	254	C17H34O	1000376-70-0	91





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Sample : I3784-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P.56-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

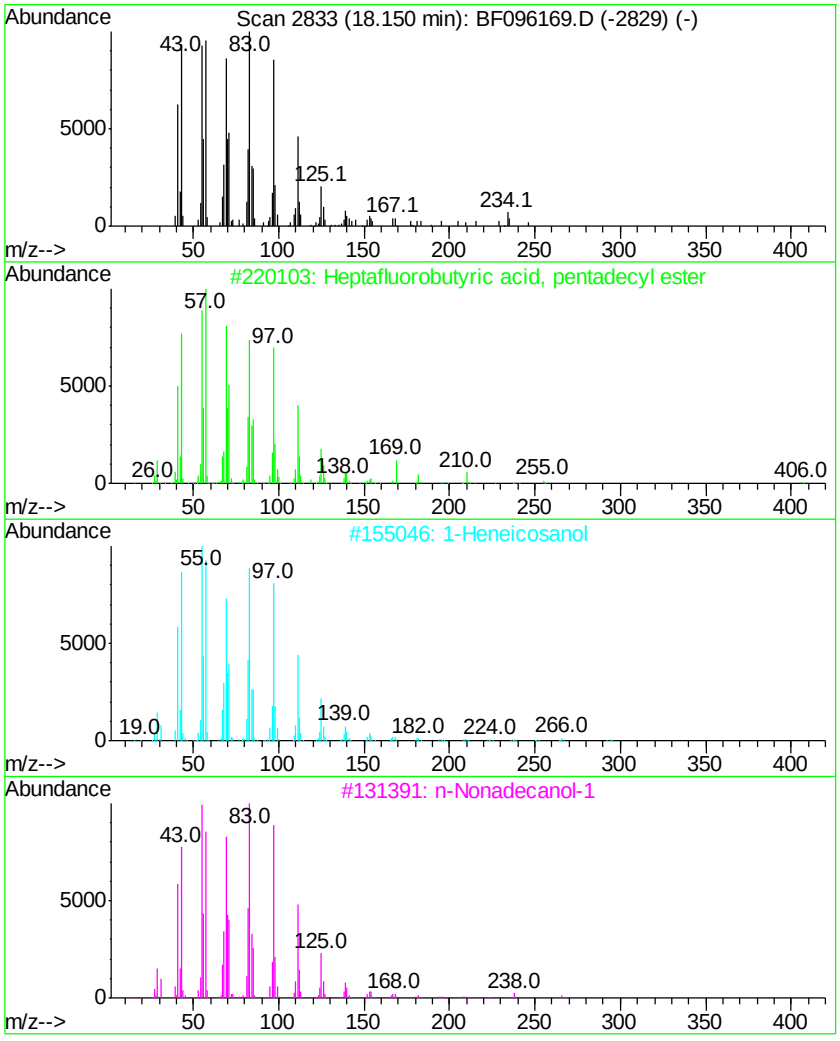
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

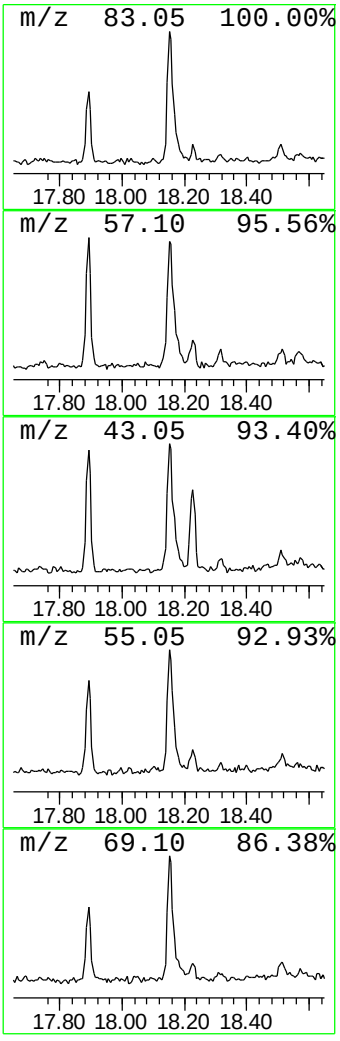
****

Peak Number 7 Heptafluorobutyric acid, pe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.15	8.81 ng	266694	Chrysene-d12	18.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
5	Behenic alcohol	326	C22H46O	000661-19-8	95





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ClientSampleId : P.56-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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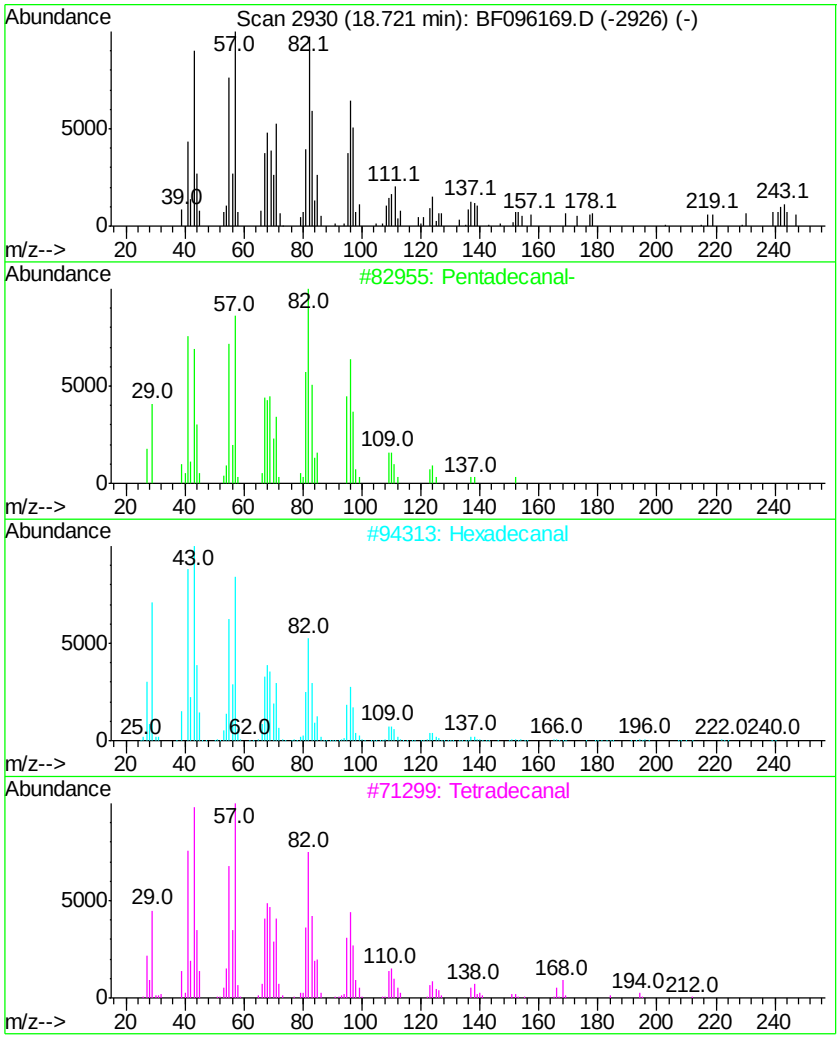
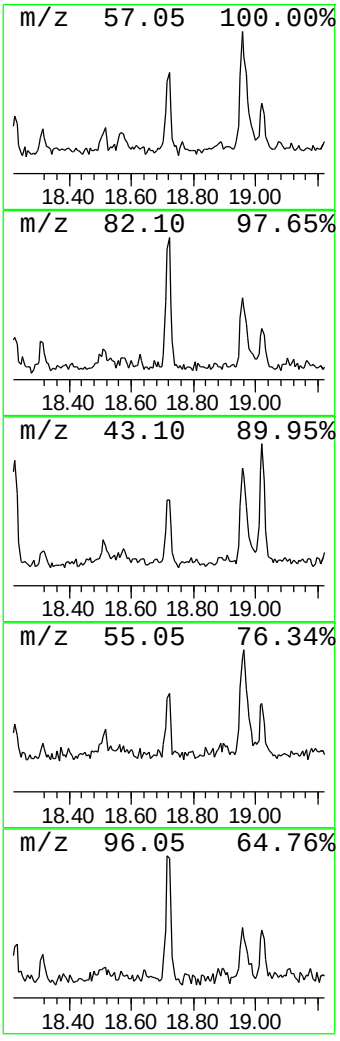
Peak Number 8 Pentadecanal- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.72	2.58 ng	78257	Chrysene-d12	18.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanal-	226	C15H30O	002765-11-9	81
2	Hexadecanal	240	C16H32O	000629-80-1	80
3	Tetradecanal	212	C14H28O	000124-25-4	80
4	1,19-Eicosadiene	278	C20H38	014811-95-1	74
5	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	62





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Sample : I3784-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P.56-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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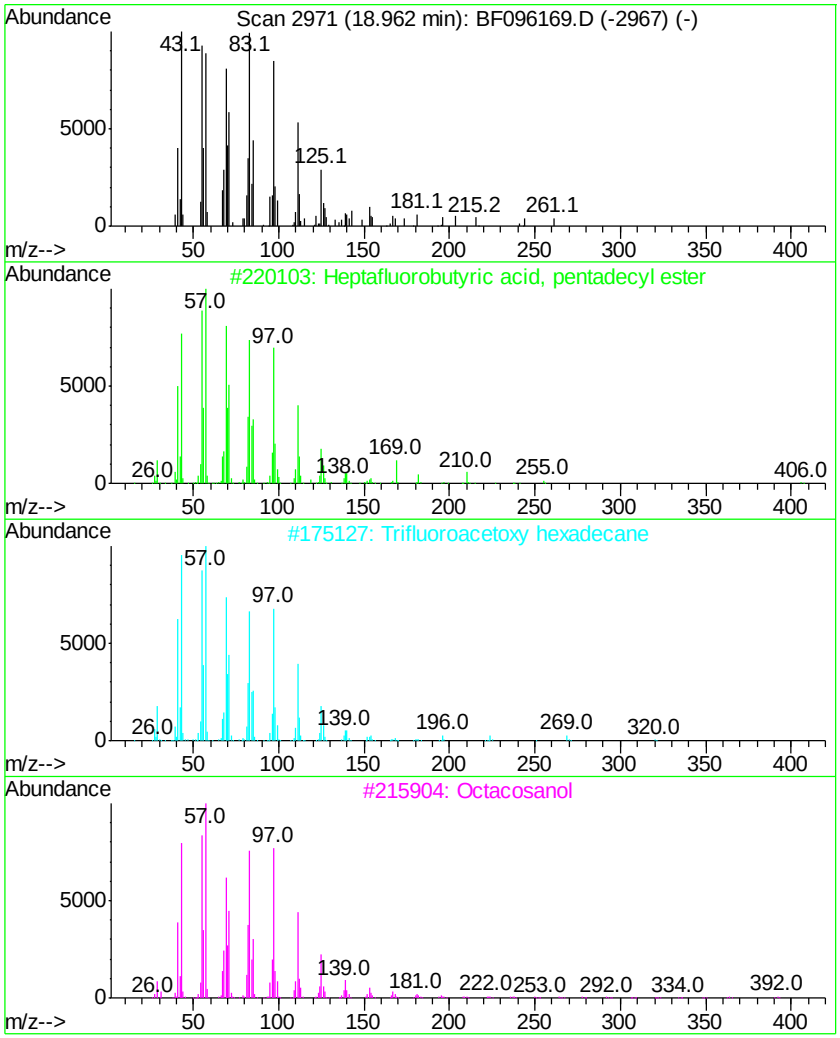
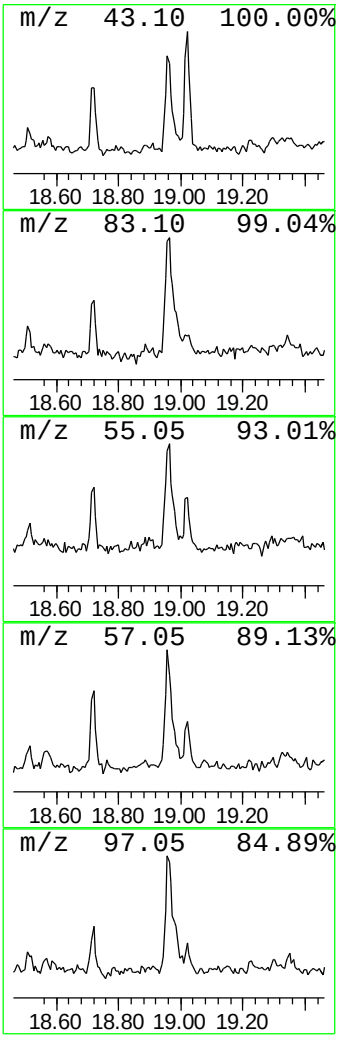
Peak Number 9 Octadecyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.96	4.97 ng	150488	Chrysene-d12	18.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3	Octacosanol	410	C28H58O	000557-61-9	90
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
Data File : BF096169.D
Acq On : 23 Jun 2017 20:25
Operator : SJ/MA
Sample : I3784-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P.56-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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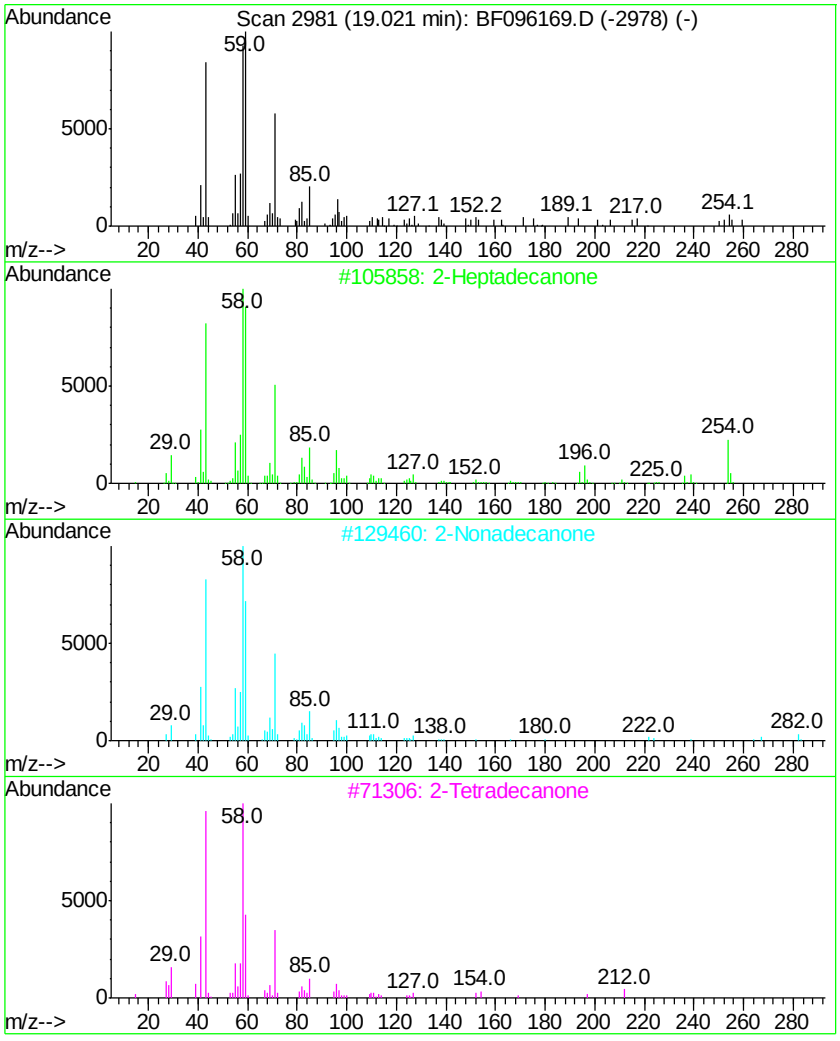
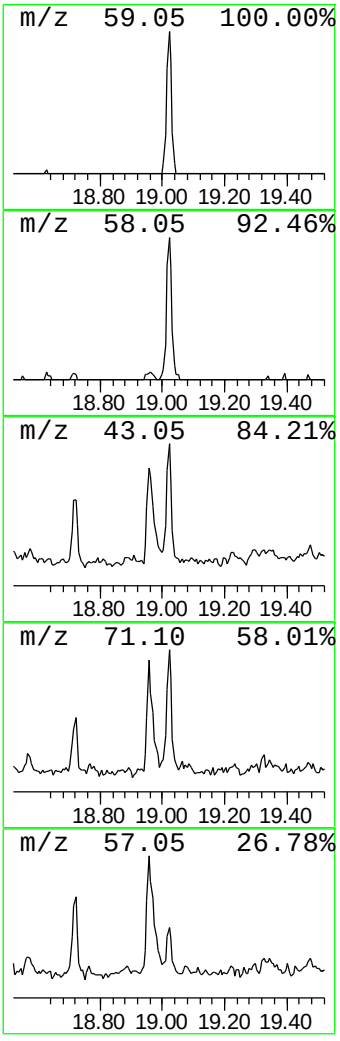
Peak Number 10 2-Heptadecanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.02	3.39 ng	102656	Chrysene-d12	18.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptadecanone	254	C17H34O	002922-51-2	95
2	2-Nonadecanone	282	C19H38O	000629-66-3	64
3	2-Tetradecanone	212	C14H28O	002345-27-9	53
4	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	50
5	2-Pentadecanone	226	C15H30O	002345-28-0	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
Data File : BF096169.D
Acq On : 23 Jun 2017 20:25
Operator : SJ/MA
Sample : I3784-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P.56-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

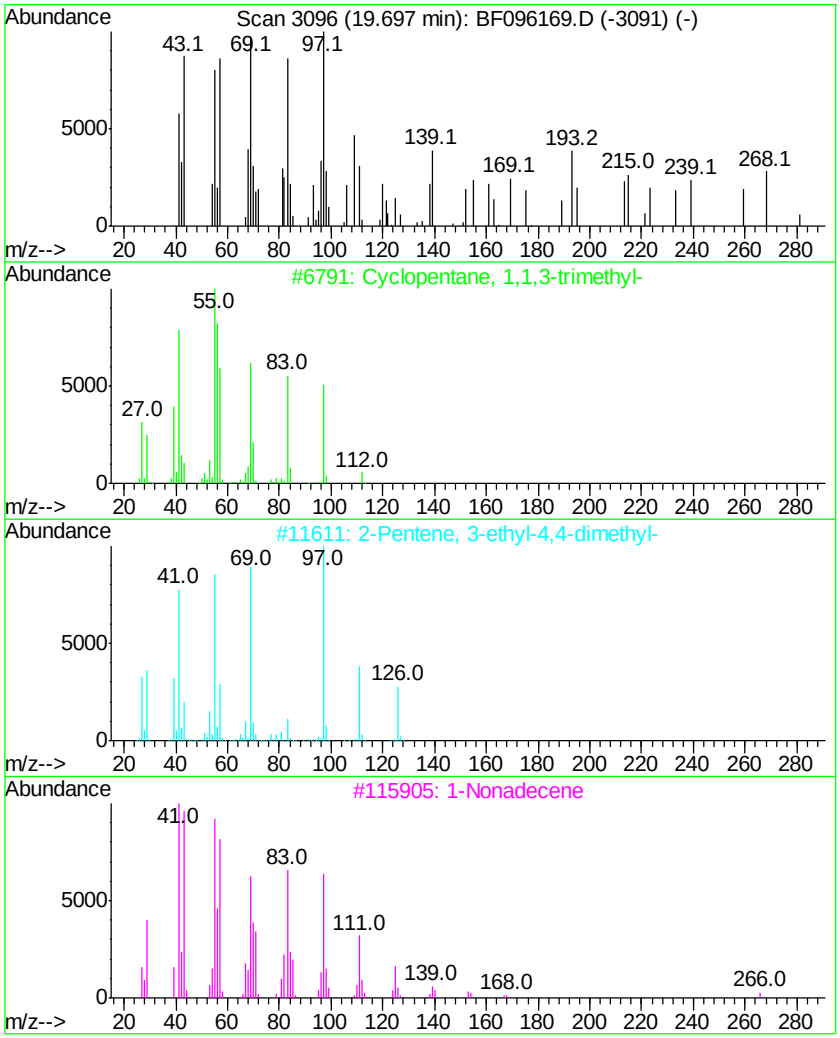
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

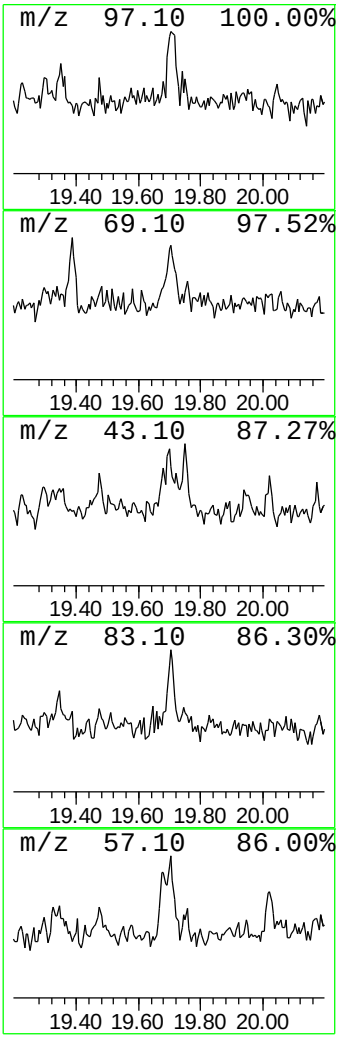
****

Peak Number 11 Cyclopentane, 1,1,3-trimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.70	2.14 ng	43473	Perylene-d12	19.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	53
2	2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	053907-59-8	43
3	1-Nonadecene	266	C19H38	018435-45-5	38
4	1-Docosene	308	C22H44	001599-67-3	38
5	Cyclohexanone, 3-ethyl-	126	C8H14O	022461-89-8	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
Data File : BF096169.D
Acq On : 23 Jun 2017 20:25
Operator : SJ/MA
Sample : I3784-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P.56-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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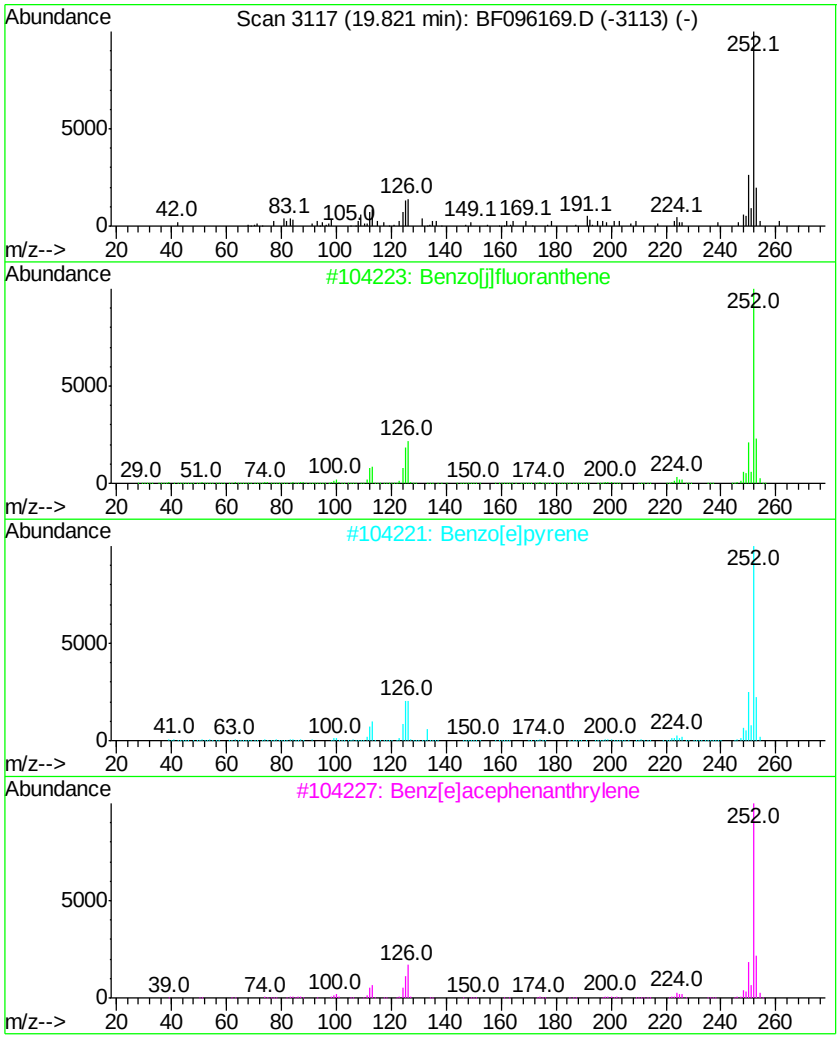
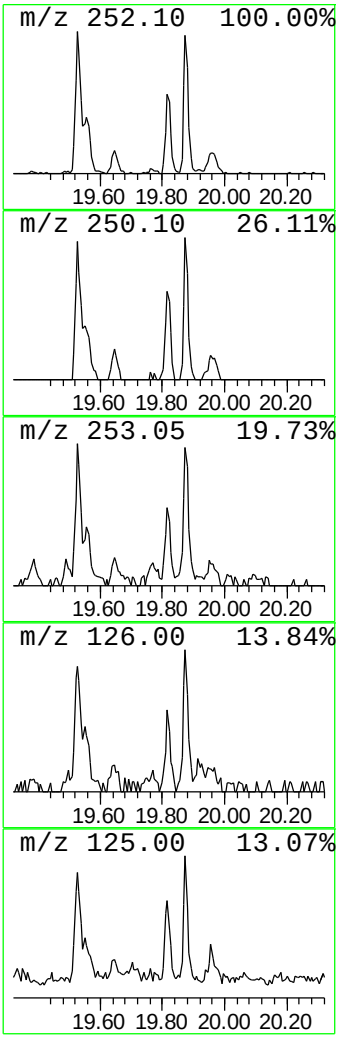
Peak Number 12 Benzo[j]fluoranthene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.82	3.01 ng	60997	Perylene-d12	19.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
2	Benzo[e]pyrene	252	C20H12	000192-97-2	94
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
4	Perylene	252	C20H12	000198-55-0	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
Data File : BF096169.D
Acq On : 23 Jun 2017 20:25
Operator : SJ/MA
Sample : I3784-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P.56-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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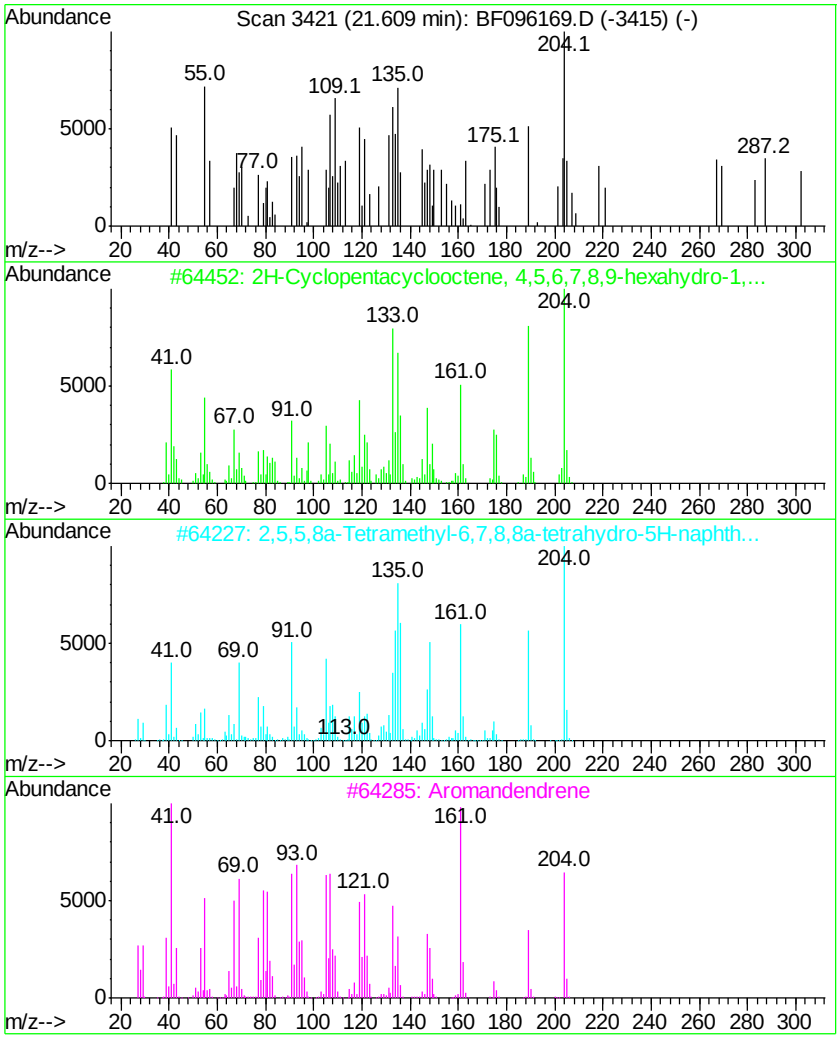
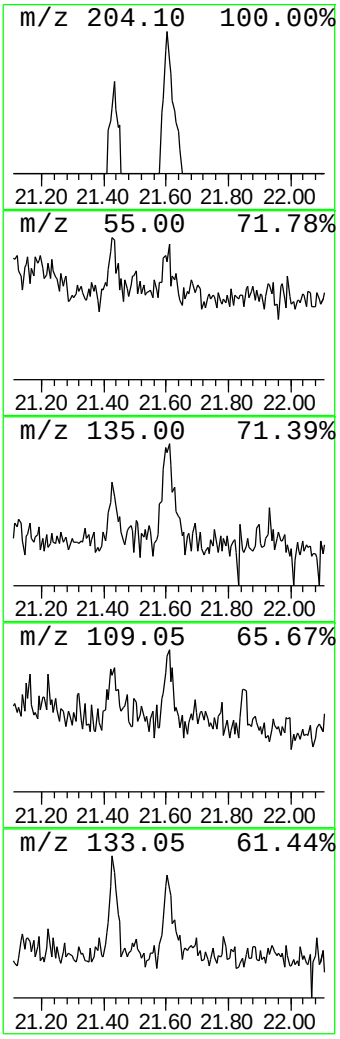
Peak Number 13 2H-Cyclopentacyclooctene, 4... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.61	3.82 ng	77524	Perylene-d12	19.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Cyclopentacyclooctene, 4,5,6,...	204	C15H24	1000221-85-8	55
2	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	46
3	Aromandendrene	204	C15H24	000489-39-4	46
4	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	45
5	1H-Cycloprop[e]azulene, decahydr...	204	C15H24	072747-25-2	38





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
Data File : BF096169.D
Acq On : 23 Jun 2017 20:25
Operator : SJ/MA
Sample : I3784-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P.56-B-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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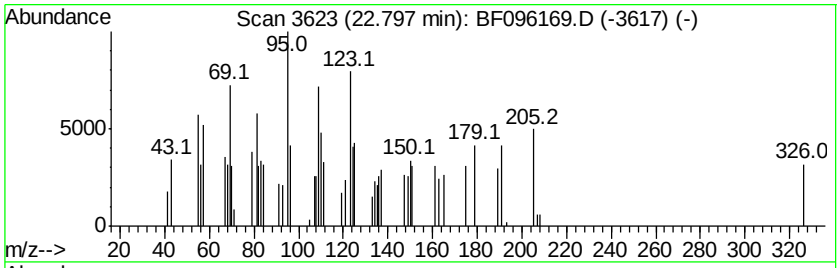
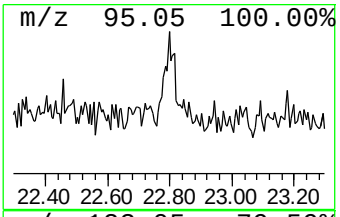
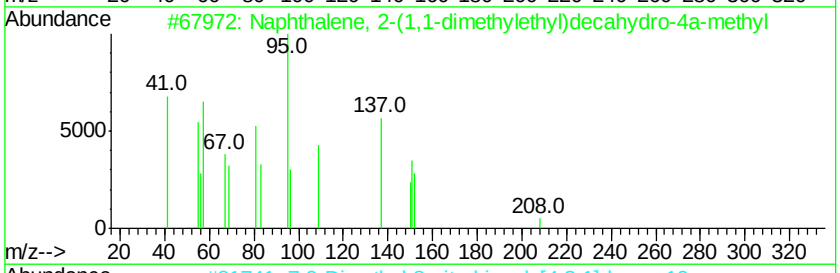
Peak Number 14 unknown22.80 Concentration Rank 11

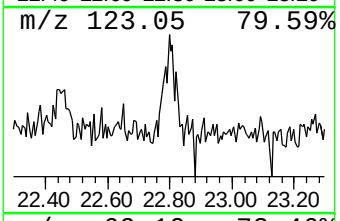
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.80	3.26 ng	66077	Perylene-d12	19.92

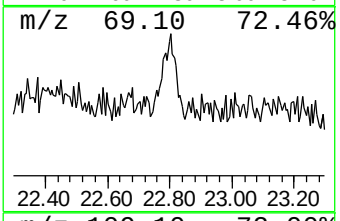
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-(1,1-dimethylethy...	208	C15H28	054934-96-2	25
2	7,9-Dimethyl-8-nitrobicyclo[4.3....	225	C12H19NO3	129967-66-4	22
3	Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	22
4	1-Cyclohexyl-1-(4-methylcyclohex...	208	C15H28	002027-12-5	15
5	7-Heptadecyne, 17-chloro-	270	C17H31Cl	056554-75-7	14

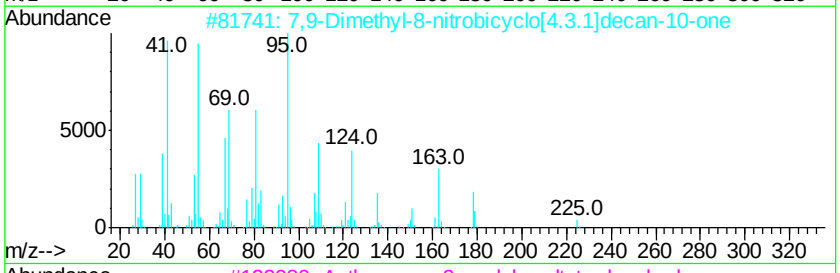


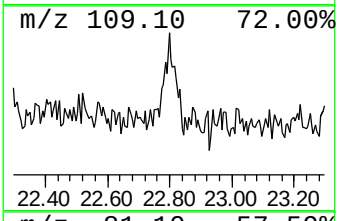


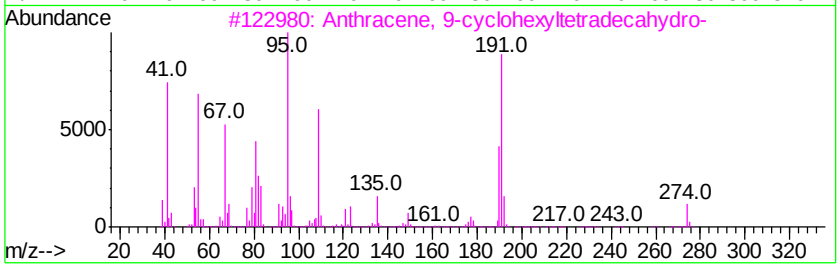


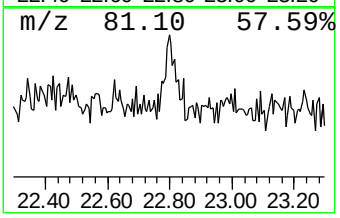












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062317\
Data File : BF096169.D
Acq On : 23 Jun 2017 20:25
Operator : SJ/MA
Sample : I3784-03
Misc :
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ClientSampleId : P.56-B-COMP

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown4.43	4.43	13.4	ng	258177	1	7.26	384211	20.0
unknown6.92	6.92	107.9	ng	2073510	1	7.26	384211	20.0
n-Hexadecanoic acid	15.54	4.4	ng	124531	4	14.50	566252	20.0
Oxirane, hexadecyl-	17.89	6.9	ng	207855	5	18.24	605566	20.0
Heptafluorobutyri...	18.15	8.8	ng	266694	5	18.24	605566	20.0
Pentadecanal-	18.72	2.6	ng	78257	5	18.24	605566	20.0
Octadecyl trifluo...	18.96	5.0	ng	150488	5	18.24	605566	20.0
2-Heptadecanone	19.02	3.4	ng	102656	5	18.24	605566	20.0
Cyclopentane, 1,1...	19.70	2.1	ng	43473	6	19.92	405907	20.0
Benzo[j]fluoranthene	19.82	3.0	ng	60997	6	19.92	405907	20.0
2H-Cyclopentacycl...	21.61	3.8	ng	77524	6	19.92	405907	20.0
unknown22.80	22.80	3.3	ng	66077	6	19.92	405907	20.0