LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120717\
Data File : BF101218.D
Acq On : 7 Dec 2017 21:07
Operator : SJ/JU
Sample : I6717-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-3(10-20)

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-BF113017.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	5.081	505	509	521	rBB	55595	83796	5.69%	0.711%
2	5.469	570	575	578	rBV	1393205	1355790	92.13%	11.509%
3	6.487	742	748	759	rVB	1188387	1447655	98.37%	12.289%
4	6.616	765	770	773	rBV	1540493	1431201	97.25%	12.149%
5	6.839	805	808	813	rBV	308191	251312	17.08%	2.133%
6	6.998	831	835	838	rBV	1267352	1115291	75.79%	9.468%
7	7.410	900	905	908	rBV	814204	801932	54.49%	6.808%
8	8.122	1023	1026	1030	rBV	341172	301493	20.49%	2.559%
9	9.204	1204	1210	1213	rBV	1597618	1471633	100.00%	12.493%
10	9.592	1271	1276	1279	rBV	196865	149594	10.17%	1.270%
11	9.798	1306	1311	1316	rVB	21088	19908	1.35%	0.169%
12	9.880	1321	1325	1329	rVV2	348936	291220	19.79%	2.472%
13	10.304	1394	1397	1399	rVB	27503	22843	1.55%	0.194%
14	10.675	1456	1460	1464	rBV	817305	724735	49.25%	6.152%
15	10.774	1474	1477	1482	rBV	29455	31352	2.13%	0.266%
16	11.222	1550	1553	1556	rBV	26301	19982	1.36%	0.170%
17	11.374	1575	1579	1582	rBV	316097	265106	18.01%	2.250%
18	12.768	1812	1816	1819	rBV2	14823	18590	1.26%	0.158%
19	12.963	1844	1849	1852	rBV	1284190	1154013	78.42%	9.796%
20	13.433	1924	1929	1933	rBV	124085	169484	11.52%	1.439%
21	13.486	1936	1938	1940	rVV	65831	51964	3.53%	0.441%
22	13.504	1940	1941	1946	rVB4	15539	19183	1.30%	0.163%
23	13.633	1960	1963	1970	rVB5	9361	19002	1.29%	0.161%
24	13.839	1995	1998	2002	rBV2	36588	36269	2.46%	0.308%
25	14.021	2025	2029	2032	rBV	289204	237232	16.12%	2.014%
26	14.115	2042	2045	2048	rBV2	22108	25956	1.76%	0.220%
27	14.762	2152	2155	2159	rVB	65194	69353	4.71%	0.589%
28	15.498	2275	2280	2288	rBV	158026	194227	13.20%	1.649%

Sum of corrected areas: 11780116

LSC Report - Integrated Chromatogram

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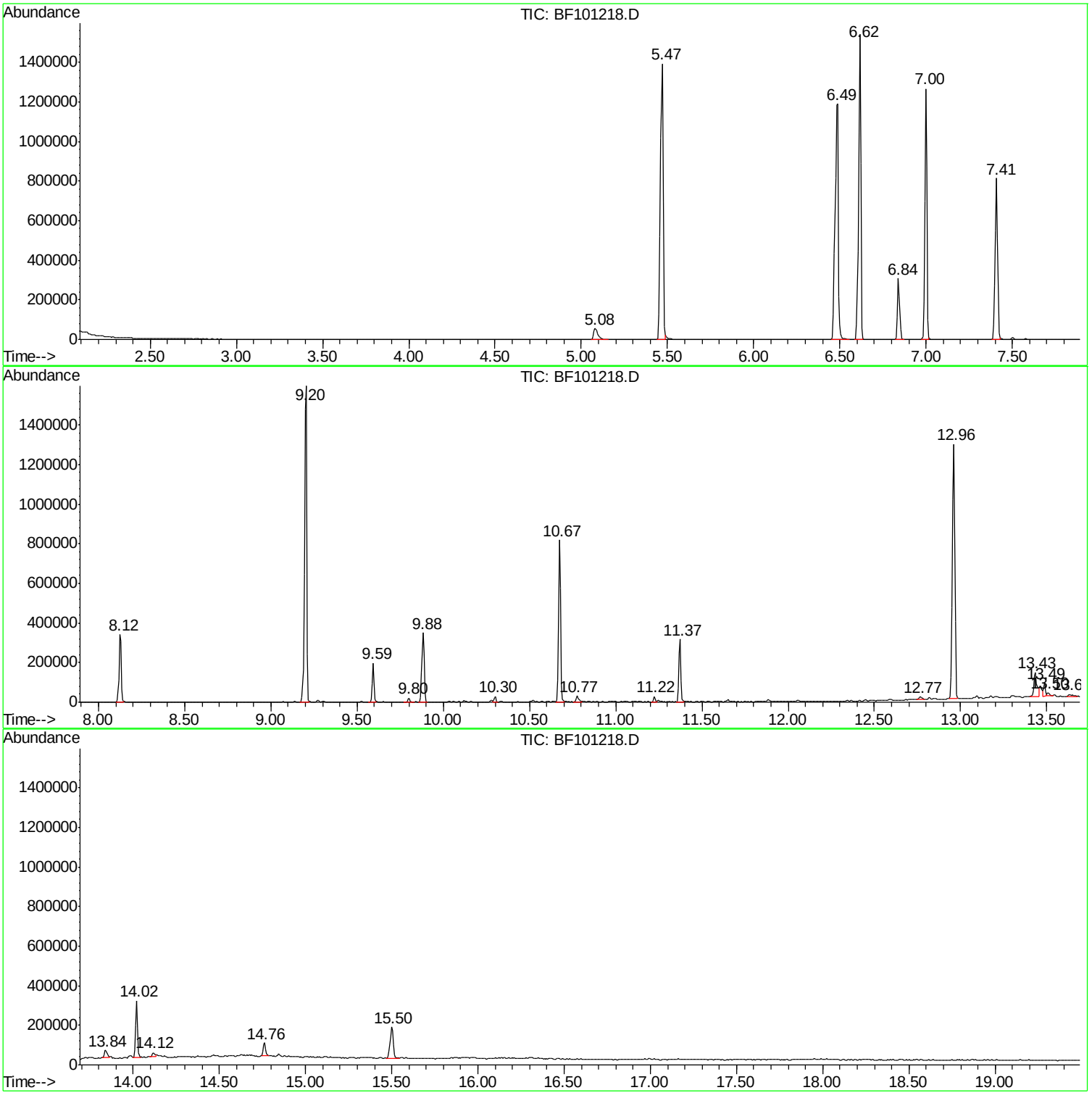
ClientSampleId : PB-3(10-20)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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Instrument : BNA_F
ClientSampleId : PB-3(10-20)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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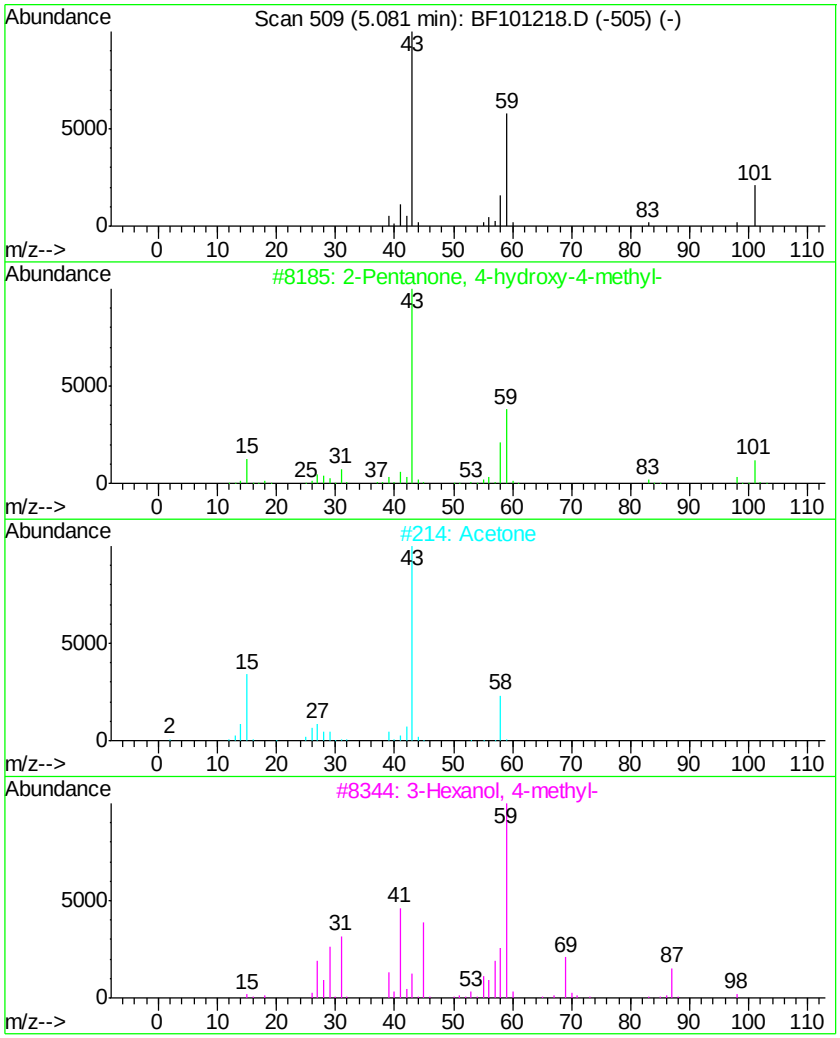
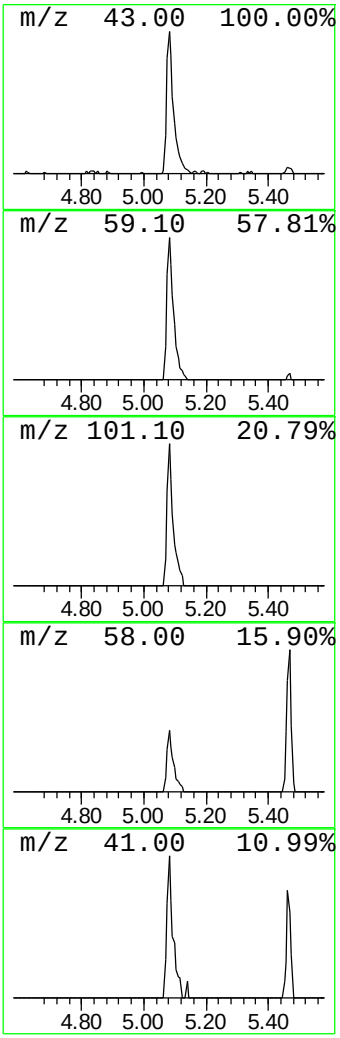
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	6.67 ng	83796	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetone	58	C3H6O	000067-64-1	9
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-3(10-20)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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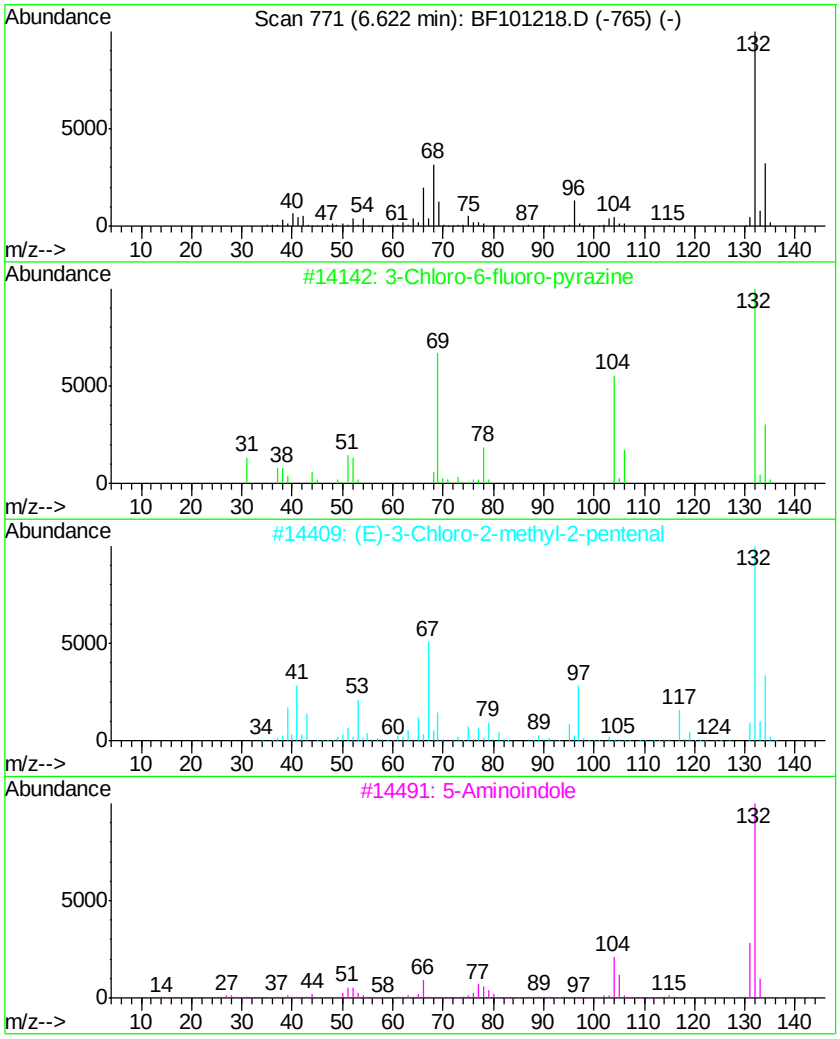
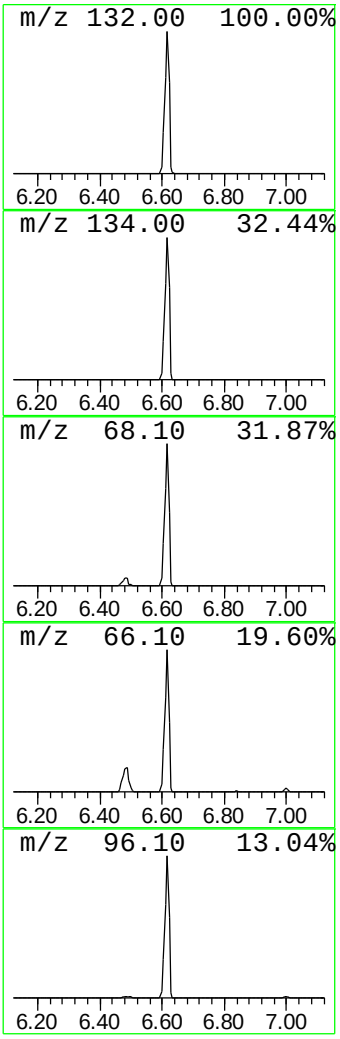
Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	113.90 ng	1431200	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120717\
Data File : BF101218.D
Acq On : 7 Dec 2017 21:07
Operator : SJ/JU
Sample : I6717-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-3(10-20)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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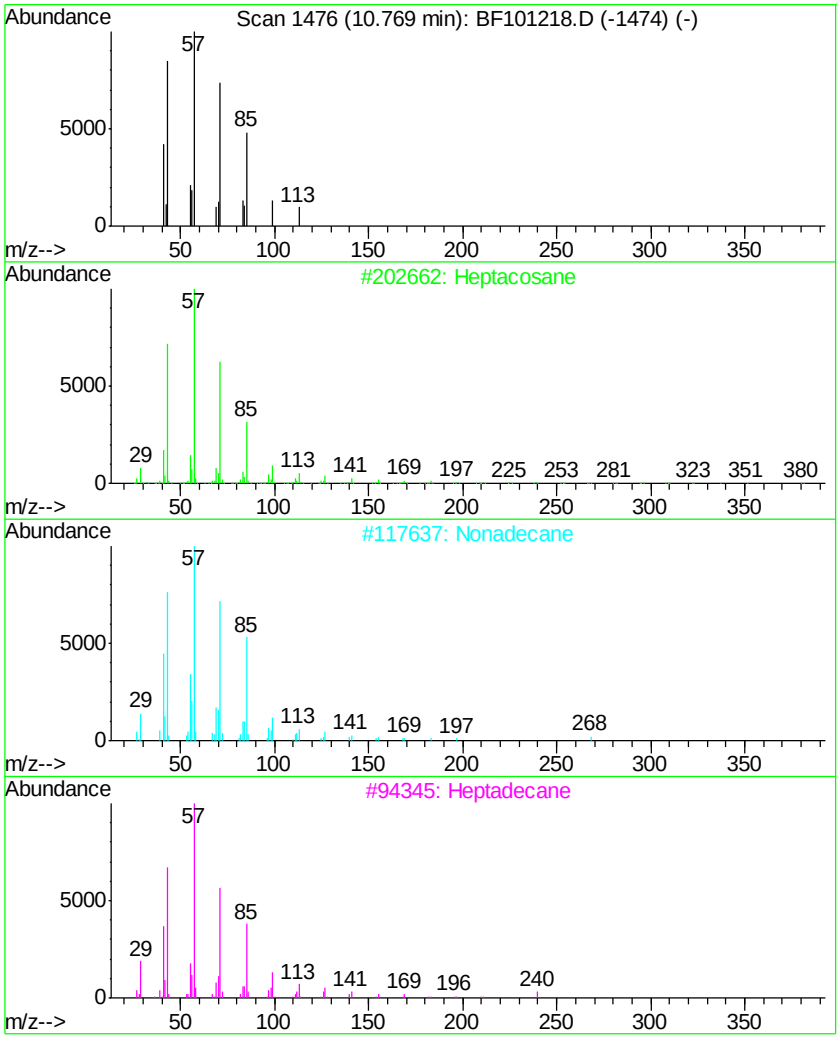
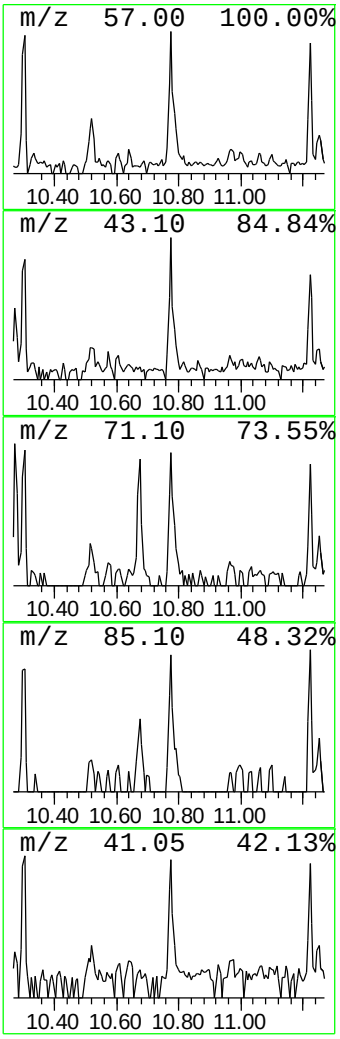
Peak Number 4 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	2.37 ng	31352	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	83
2	Nonadecane	268	C19H40	000629-92-5	78
3	Heptadecane	240	C17H36	000629-78-7	72
4	Tridecane	184	C13H28	000629-50-5	72
5	Pentadecane	212	C15H32	000629-62-9	72





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ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-3(10-20)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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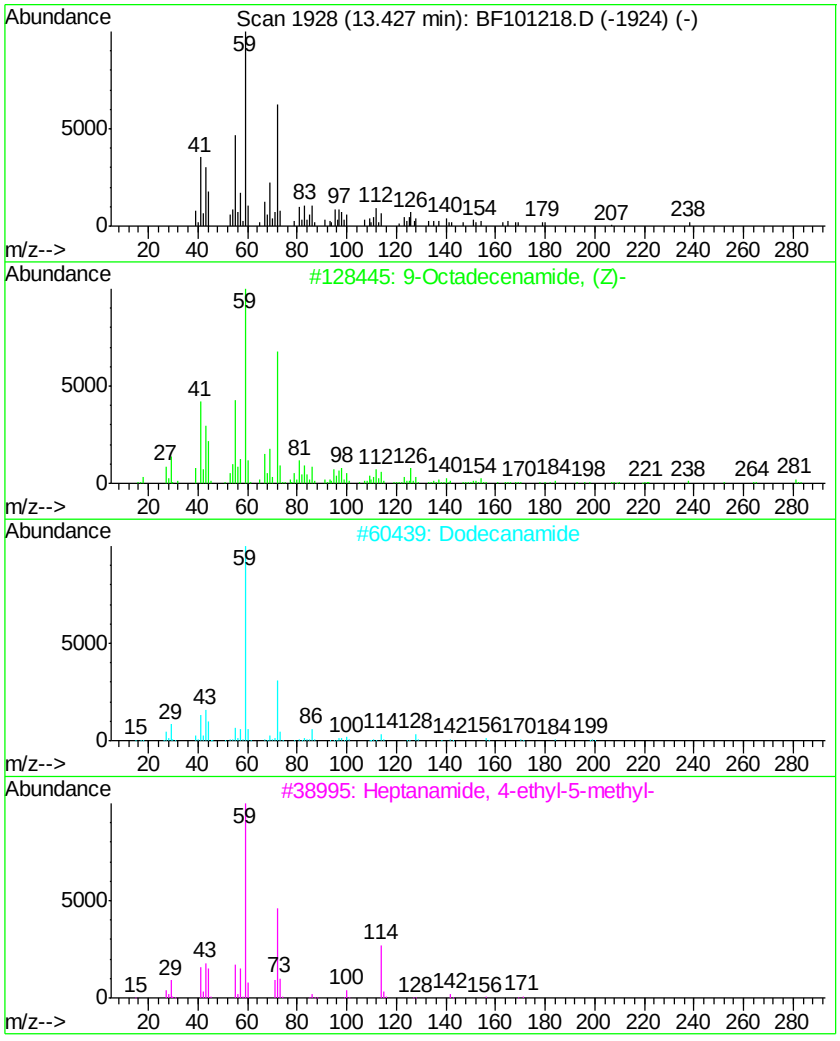
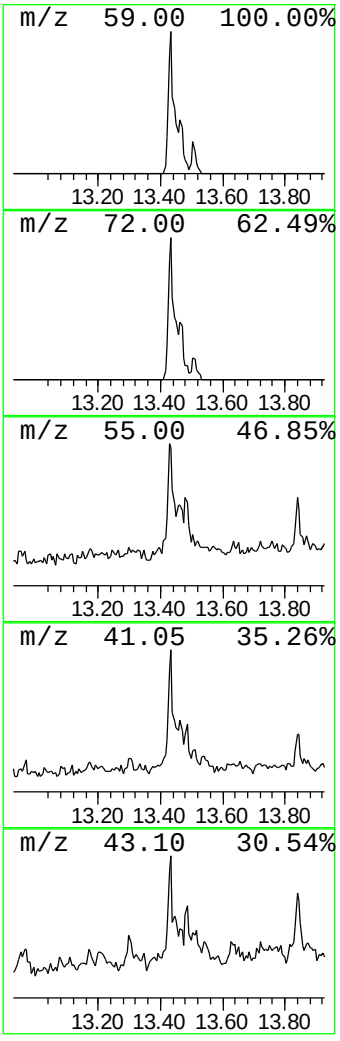
Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	14.29 ng	169484	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2	Dodecanamide	199	C12H25NO	001120-16-7	53
3	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	53
4	Octanamide	143	C8H17NO	000629-01-6	53
5	Hexadecanamide	255	C16H33NO	000629-54-9	53





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Sample : I6717-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-3(10-20)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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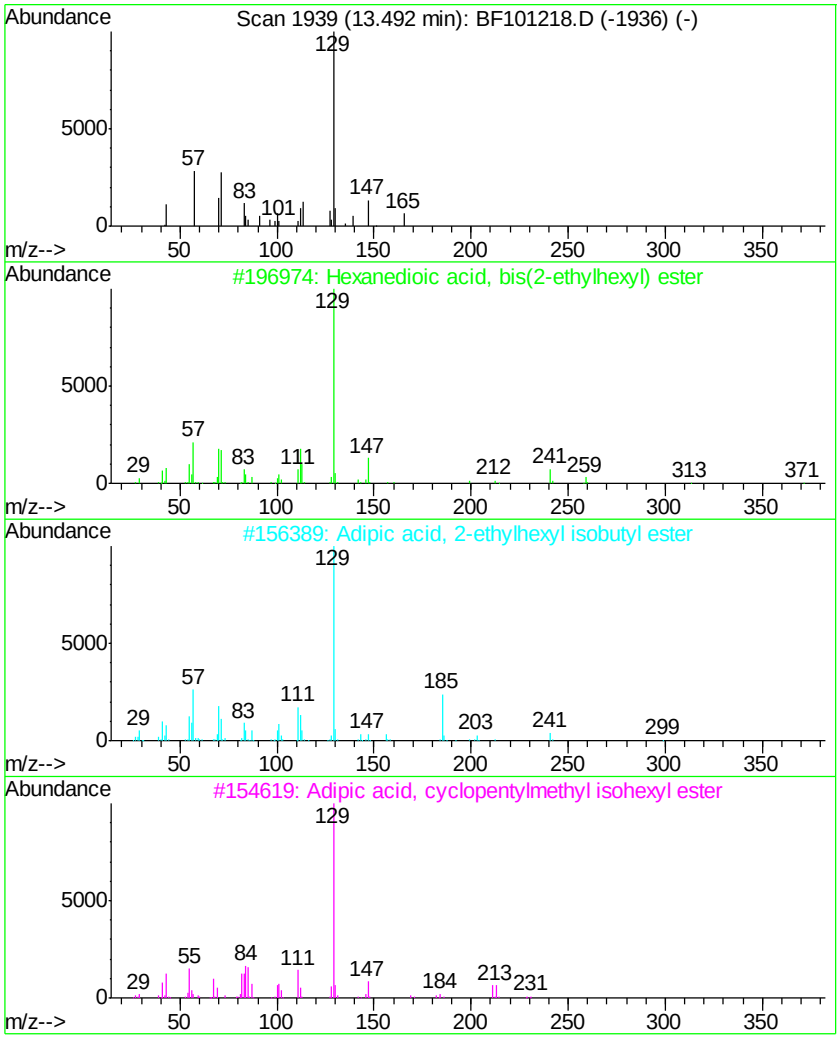
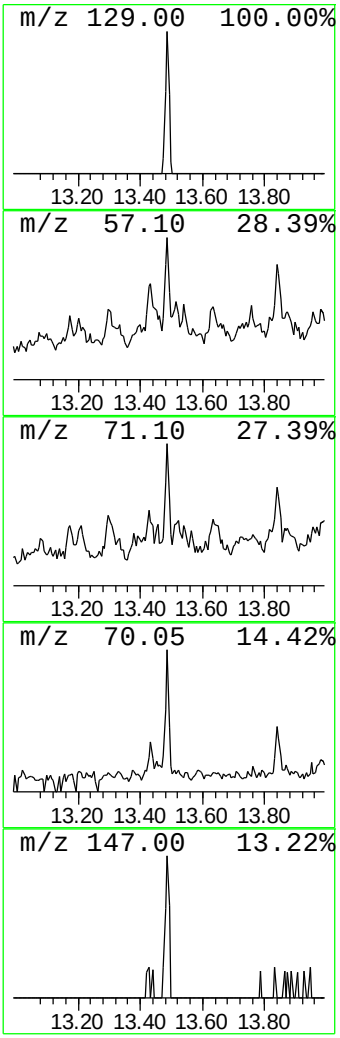
Peak Number 6 Hexanedioic acid, bis(2-eth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	4.38 ng	51964	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	83
2	Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1000324-48-0	64
3	Adipic acid, cyclopentylmethyl i...	312	C18H32O4	1000324-77-6	50
4	Cyclohexanecarboxylic acid, tetr...	324	C21H40O2	1000279-54-2	47
5	Adipic acid, isobutyl 2-octyl ester	314	C18H34O4	1000324-44-5	47





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Misc :
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Instrument : BNA_F
ClientSampleId : PB-3(10-20)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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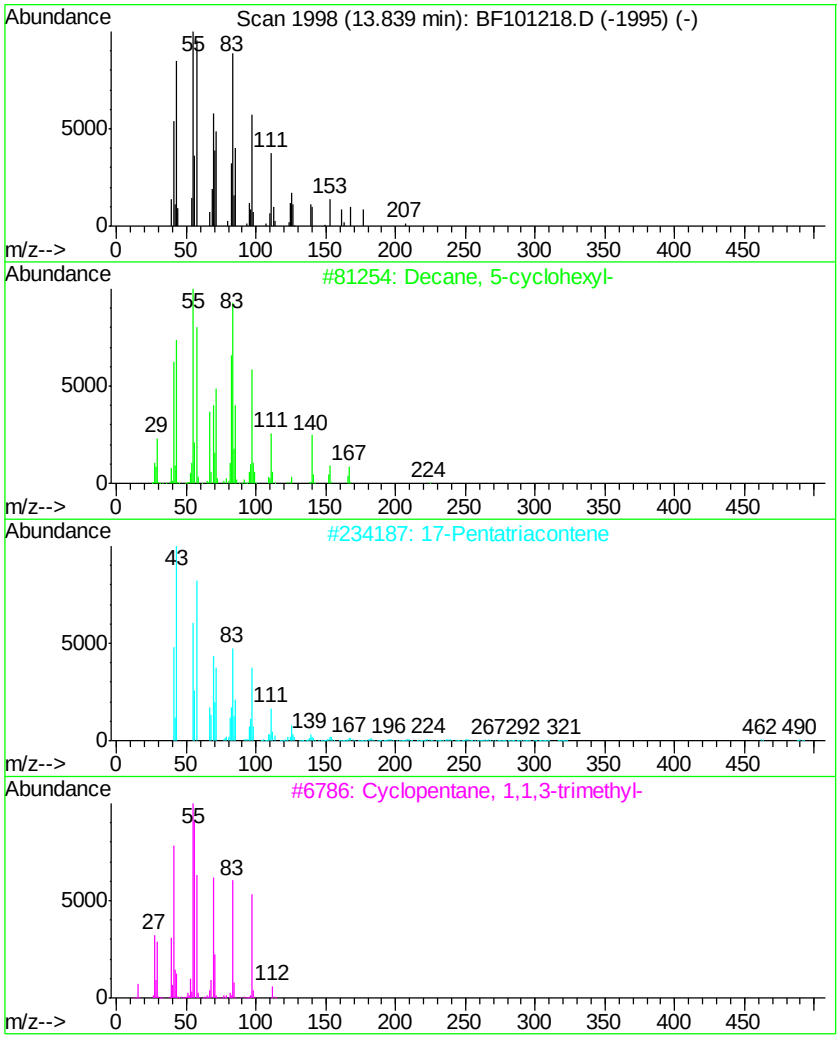
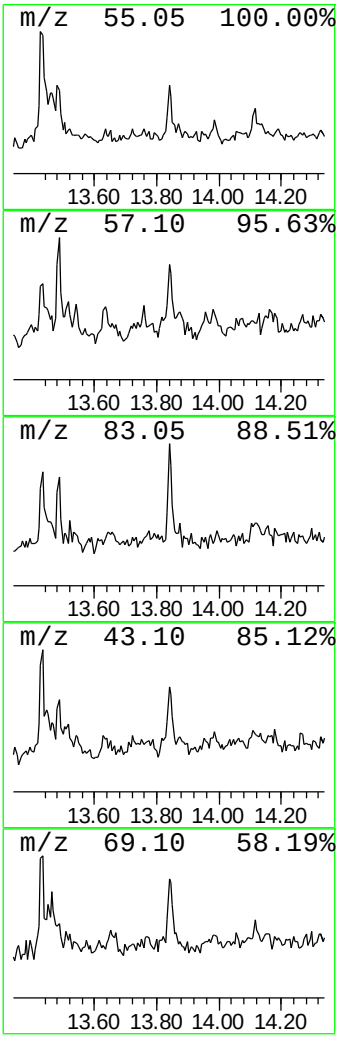
Peak Number 7 Decane, 5-cyclohexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	3.06 ng	36269	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 5-cyclohexyl-	224	C16H32	013151-76-3	72
2	17-Pentatriacontene	491	C35H70	006971-40-0	72
3	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	38
4	Cyclohexane, 1,2-dimethyl-, cis-	112	C8H16	002207-01-4	30
5	2,4-Pentadien-1-ol, 3-propyl-, (...	126	C8H14O	1000142-17-9	30





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
2-Pentanone, 4-hy...	5.08	6.7	ng	83796	1	6.84	251312	20.0
unknown6.62	6.62	113.9	ng	1431200	1	6.84	251312	20.0
Heptacosane	10.77	2.4	ng	31352	4	11.37	265106	20.0
9-Octadecenamide,...	13.43	14.3	ng	169484	5	14.02	237232	20.0
Hexanedioic acid,...	13.49	4.4	ng	51964	5	14.02	237232	20.0
Decane, 5-cyclohe...	13.84	3.1	ng	36269	5	14.02	237232	20.0