LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100804.D
Acq On : 22 Nov 2017 2:53
Operator : SJ/JU
Sample : I6466-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-2-E(4-5)

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-BF110817.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	5.098	508	512	523	rBV	237290	300985	15.97%	1.868%
2	5.492	574	579	583	rBV	1581189	1645428	87.33%	10.214%
3	6.504	745	751	759	rBV	1634346	1752605	93.02%	10.880%
4	6.645	770	775	778	rBV	1810706	1719061	91.24%	10.671%
5	6.875	810	814	817	rBV	541349	465809	24.72%	2.892%
6	7.028	836	840	843	rBV	1548374	1333482	70.78%	8.278%
7	7.433	904	909	912	rBV	1062976	1057014	56.10%	6.562%
8	8.151	1027	1031	1035	rBV	659444	596506	31.66%	3.703%
9	8.704	1122	1125	1129	rBV	96227	77499	4.11%	0.481%
10	9.227	1209	1214	1217	rBV	2091032	1884106	100.00%	11.696%
11	9.616	1277	1280	1284	rBV	51479	43667	2.32%	0.271%
12	9.910	1326	1330	1334	rBV	758332	627938	33.33%	3.898%
13	10.621	1447	1451	1454	rBV	376138	295161	15.67%	1.832%
14	10.698	1460	1464	1467	rBV	1094317	938254	49.80%	5.824%
15	11.398	1579	1583	1585	rBV	565435	532330	28.25%	3.305%
16	11.416	1585	1586	1589	rVB	39345	28846	1.53%	0.179%
17	11.910	1665	1670	1676	rVB4	25263	36009	1.91%	0.224%
18	12.604	1785	1788	1792	rBV	53427	49411	2.62%	0.307%
19	12.833	1822	1827	1831	rBV	52540	62104	3.30%	0.386%
20	12.980	1847	1852	1855	rBV	1365500	1210305	64.24%	7.513%
21	13.862	1999	2002	2010	rBV2	49270	56969	3.02%	0.354%
22	14.033	2025	2031	2034	rBV	544582	495372	26.29%	3.075%
23	14.057	2034	2035	2040	rVB	37589	27548	1.46%	0.171%
24	14.492	2106	2109	2115	rBV7	17689	30892	1.64%	0.192%
25	15.074	2204	2208	2215	rBV	25531	46829	2.49%	0.291%
26	15.133	2215	2218	2221	rVB2	20667	21940	1.16%	0.136%
27	15.380	2257	2260	2265	rVB	16892	20368	1.08%	0.126%
28	15.445	2268	2271	2277	rVB	20091	24655	1.31%	0.153%
29	15.509	2277	2282	2293	rBV	328547	444521	23.59%	2.759%
30	15.956	2354	2358	2363	rVB	40069	54674	2.90%	0.339%
31	16.462	2439	2444	2452	rVB2	45032	73516	3.90%	0.456%
32	17.062	2541	2546	2553	rVB2	36242	70994	3.77%	0.441%
33	17.768	2660	2666	2675	rVB5	22827	57121	3.03%	0.355%
34	18.603	2805	2808	2817	rVB8	12772	27076	1.44%	0.168%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100804.D
Acq On : 22 Nov 2017 2:53
Operator : SJ/JU
Sample : I6466-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-2-E(4-5)

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-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 16108995

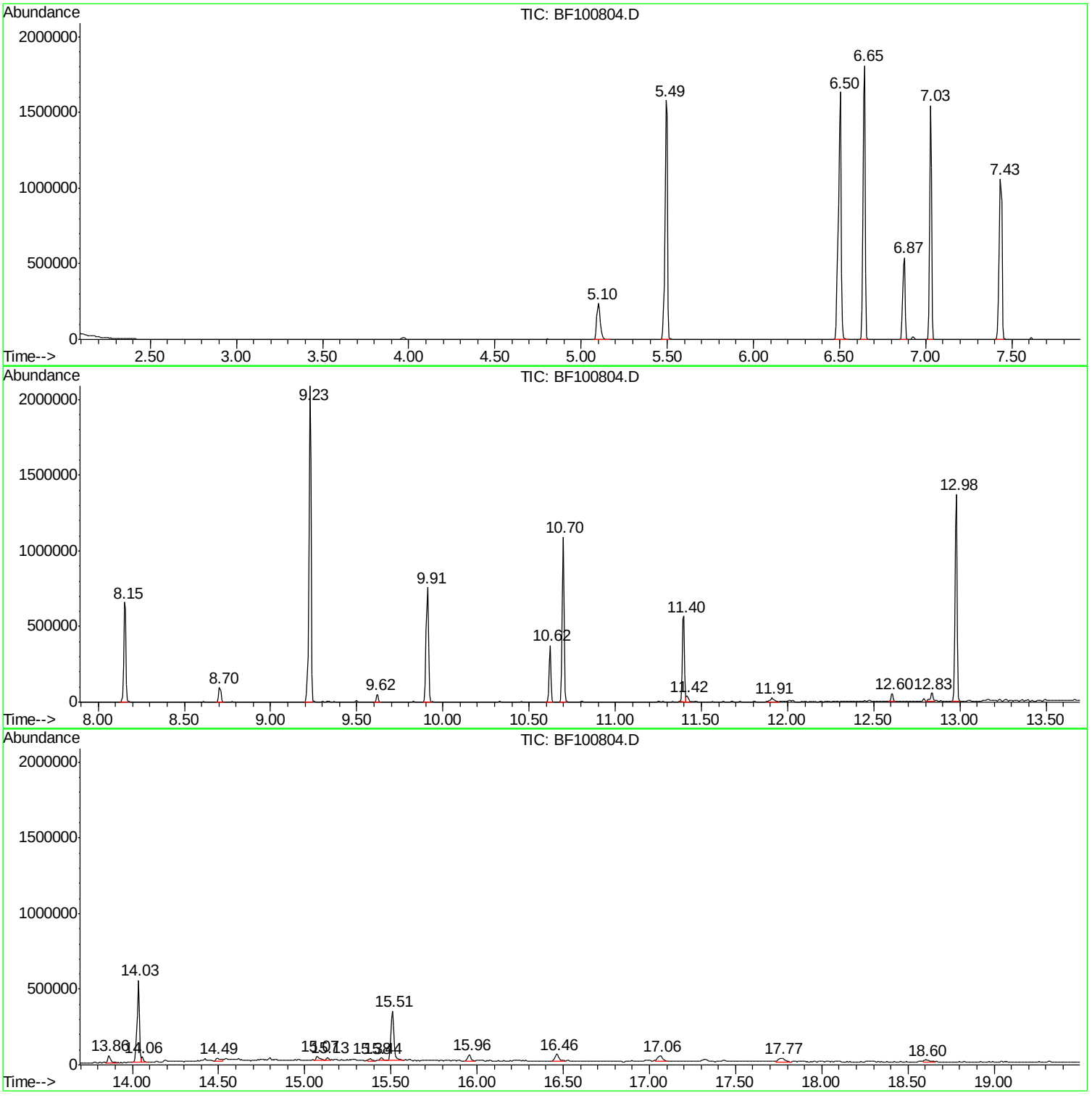
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100804.D
Acq On : 22 Nov 2017 2:53
Operator : SJ/JU
Sample : I6466-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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\BF112117\
Data File : BF100804.D
Acq On : 22 Nov 2017 2:53
Operator : SJ/JU
Sample : I6466-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

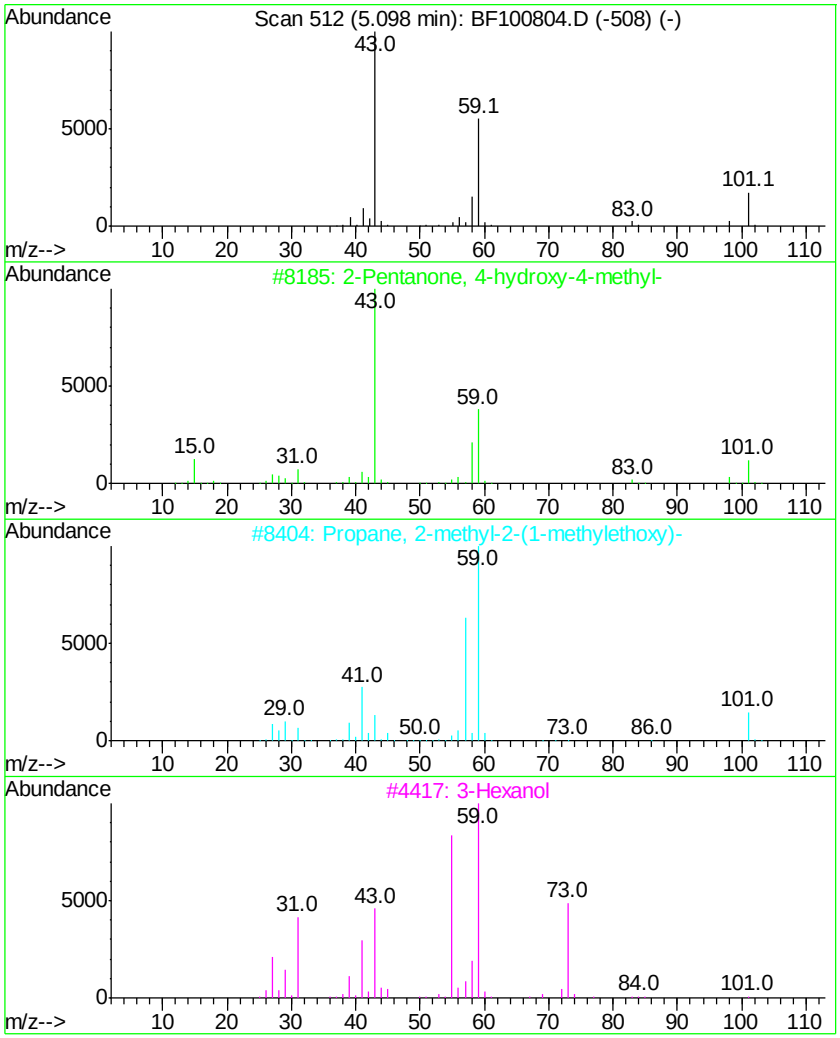
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

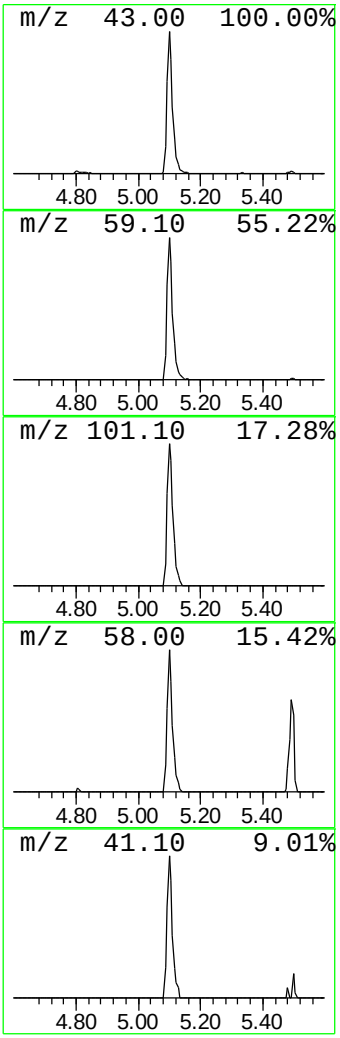
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	12.92 ng	300985	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol	102	C6H14O	000623-37-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100804.D
Acq On : 22 Nov 2017 2:53
Operator : SJ/JU
Sample : I6466-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

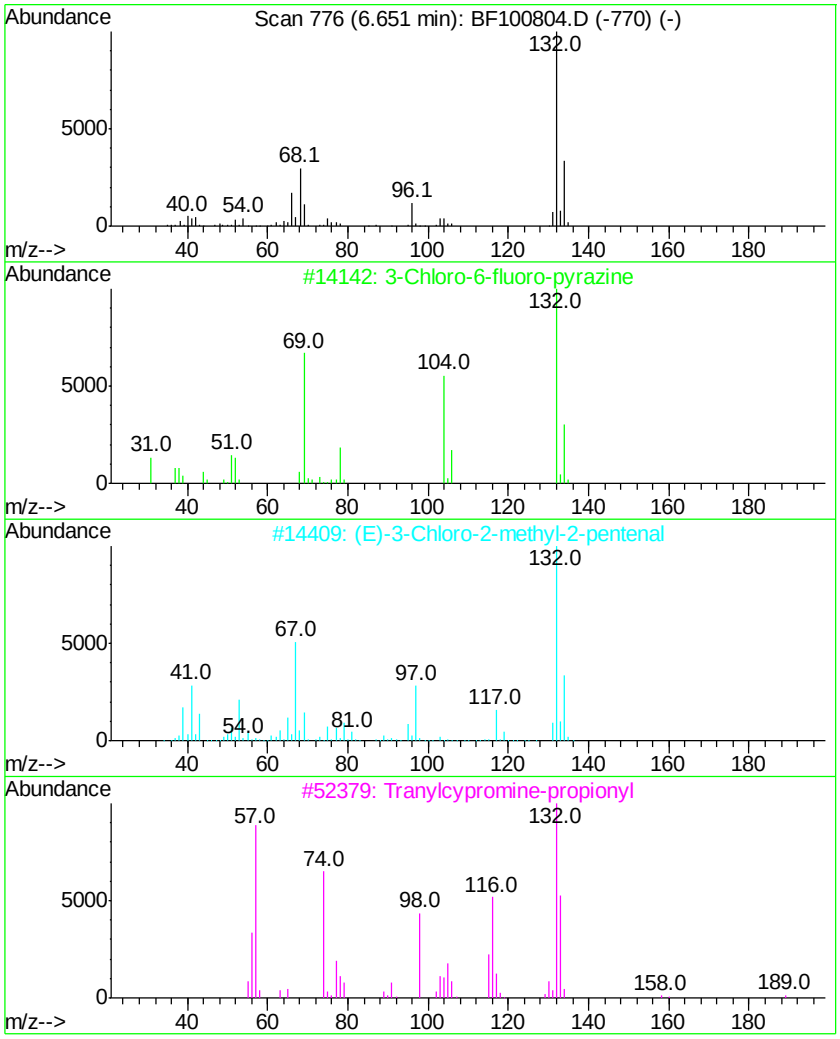
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

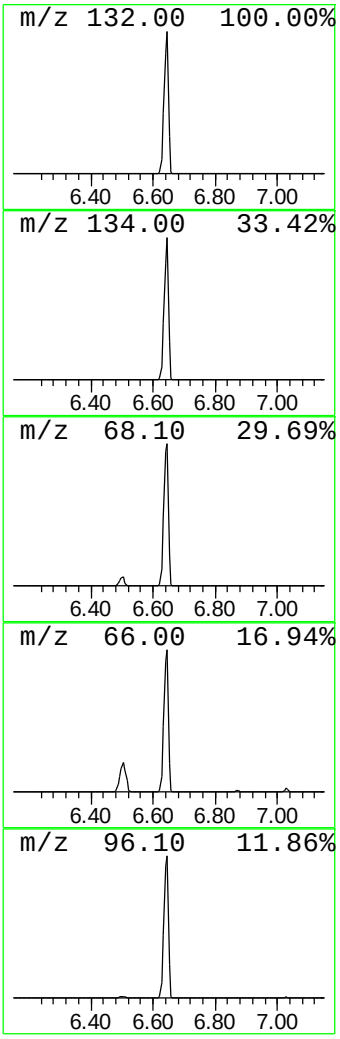
****

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	73.81 ng	1719060	1,4-Dichlorobenzene-d4	6.87

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	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Xenon	132	Xe	007440-63-3	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100804.D
Acq On : 22 Nov 2017 2:53
Operator : SJ/JU
Sample : I6466-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

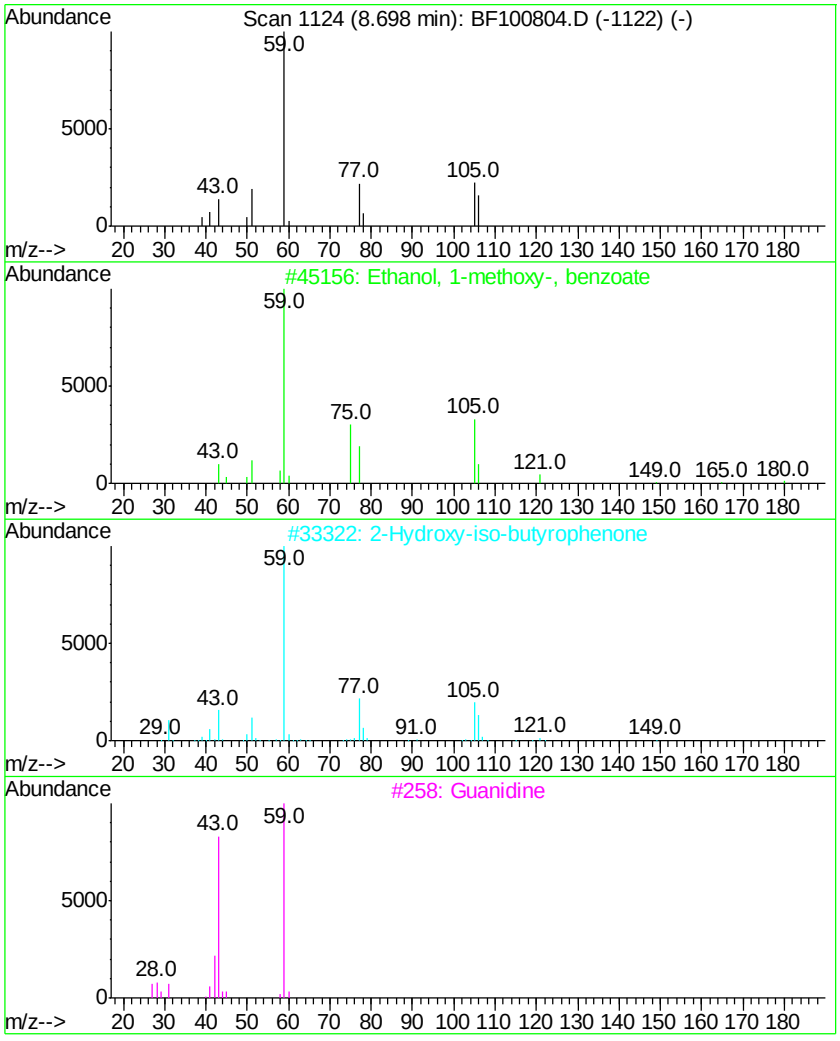
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

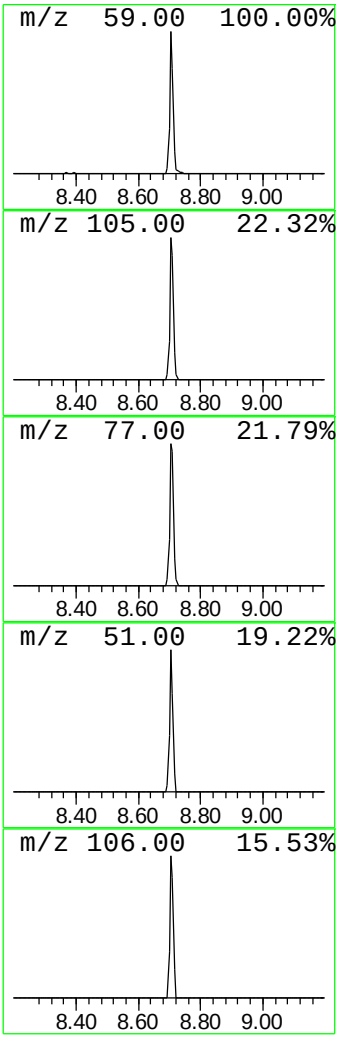
****

Peak Number 4 Ethanol, 1-methoxy-, benzoate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.70	2.60 ng	77499	Naphthalene-d8	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	64
2	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	47
3	Guanidine	59	CH5N3	000113-00-8	7
4	Formamide, N-methyl-	59	C2H5NO	000123-39-7	5
5	Acetamide	59	C2H5NO	000060-35-5	5





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100804.D
Acq On : 22 Nov 2017 2:53
Operator : SJ/JU
Sample : I6466-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

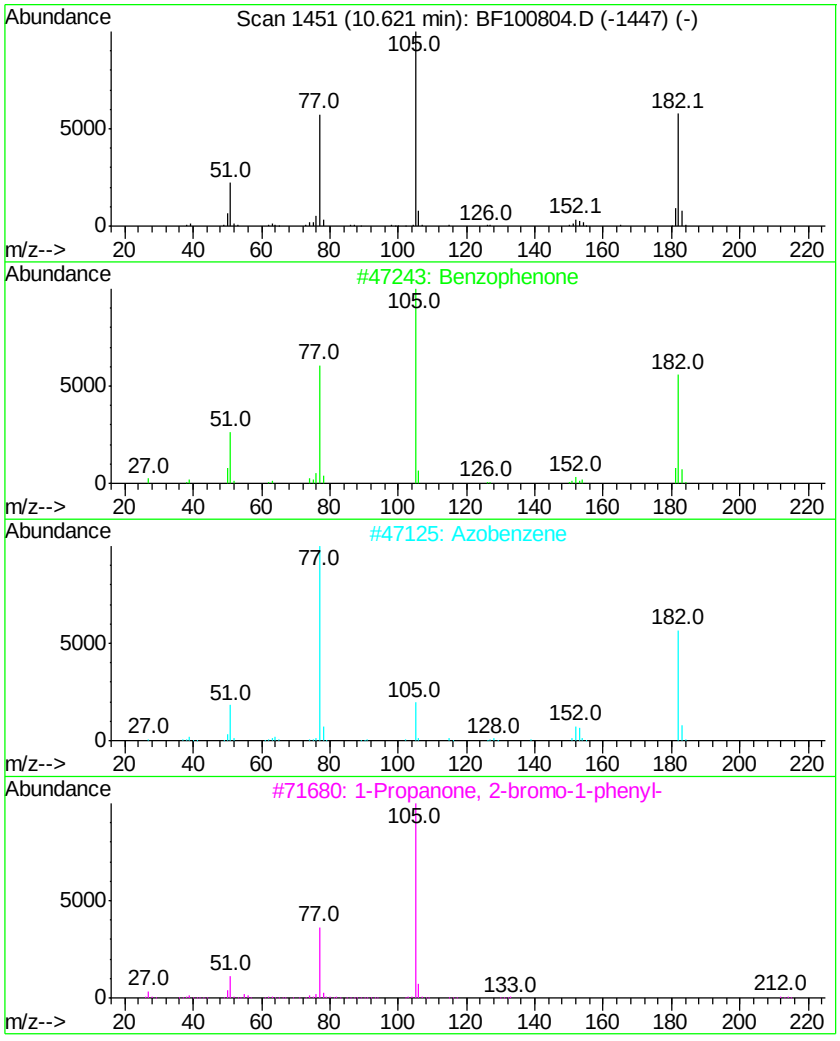
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

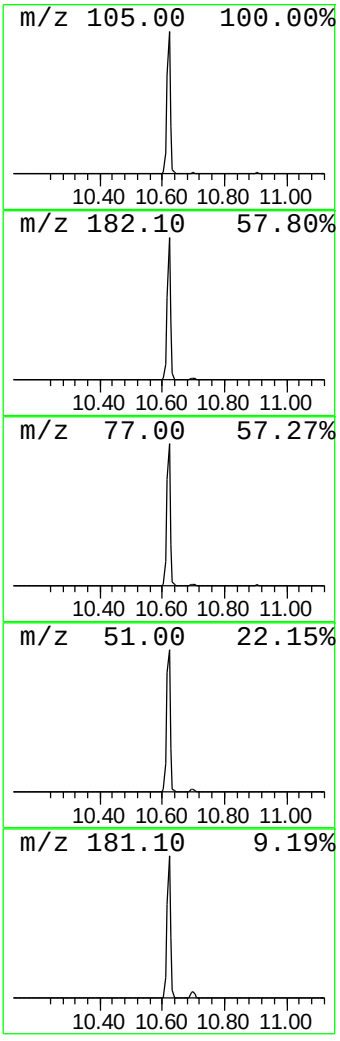
****

Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	9.40 ng	295161	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	53
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100804.D
Acq On : 22 Nov 2017 2:53
Operator : SJ/JU
Sample : I6466-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

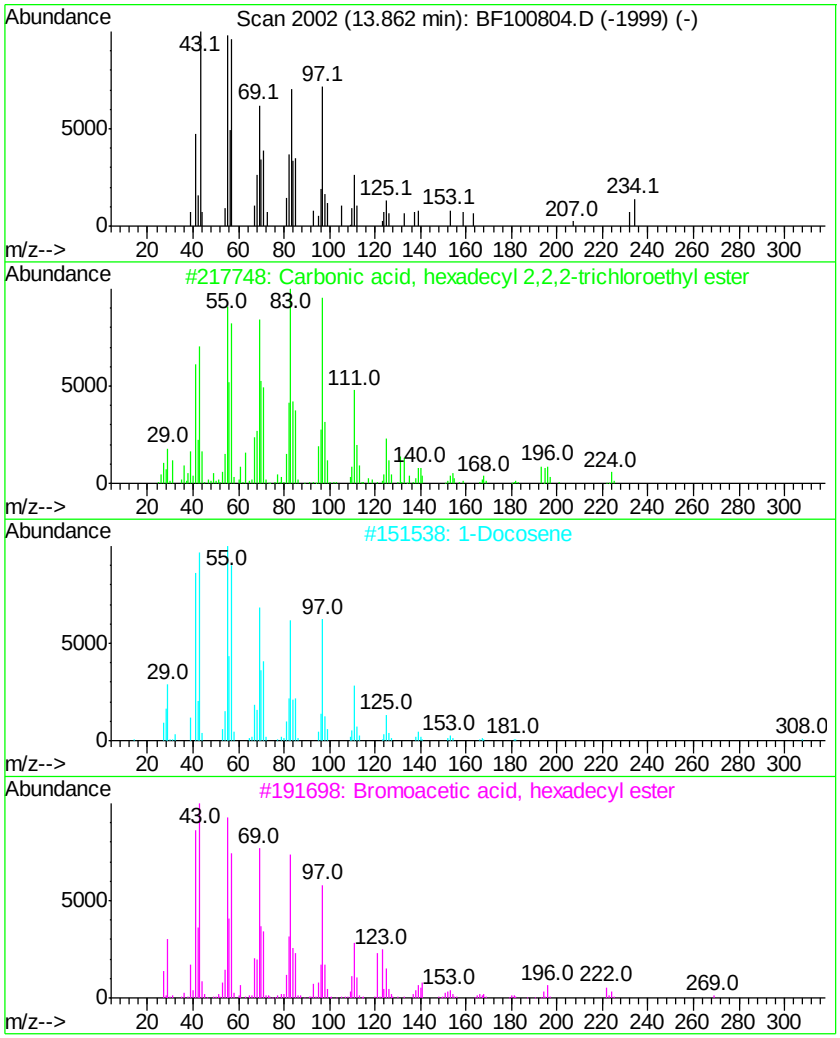
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

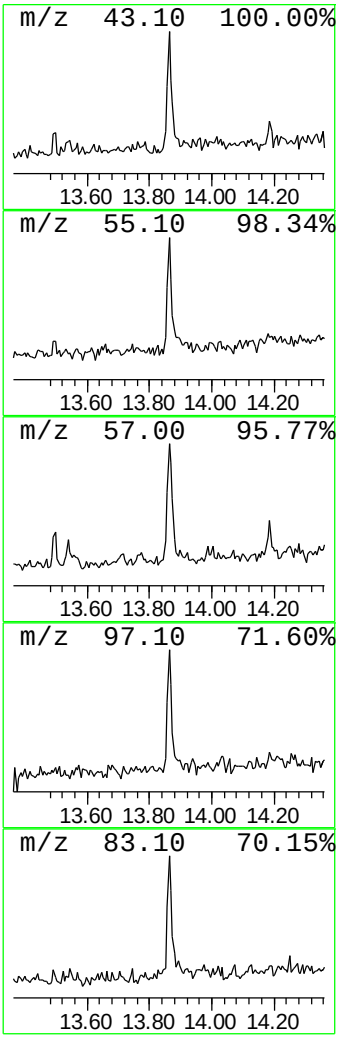
****

Peak Number 7 Carbonic acid, hexadecyl 2,... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	2.30 ng	56969	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	91
2	1-Docosene	308	C22H44	001599-67-3	91
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
4	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	90
5	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	90





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Acq On : 22 Nov 2017 2:53
Operator : SJ/JU
Sample : I6466-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

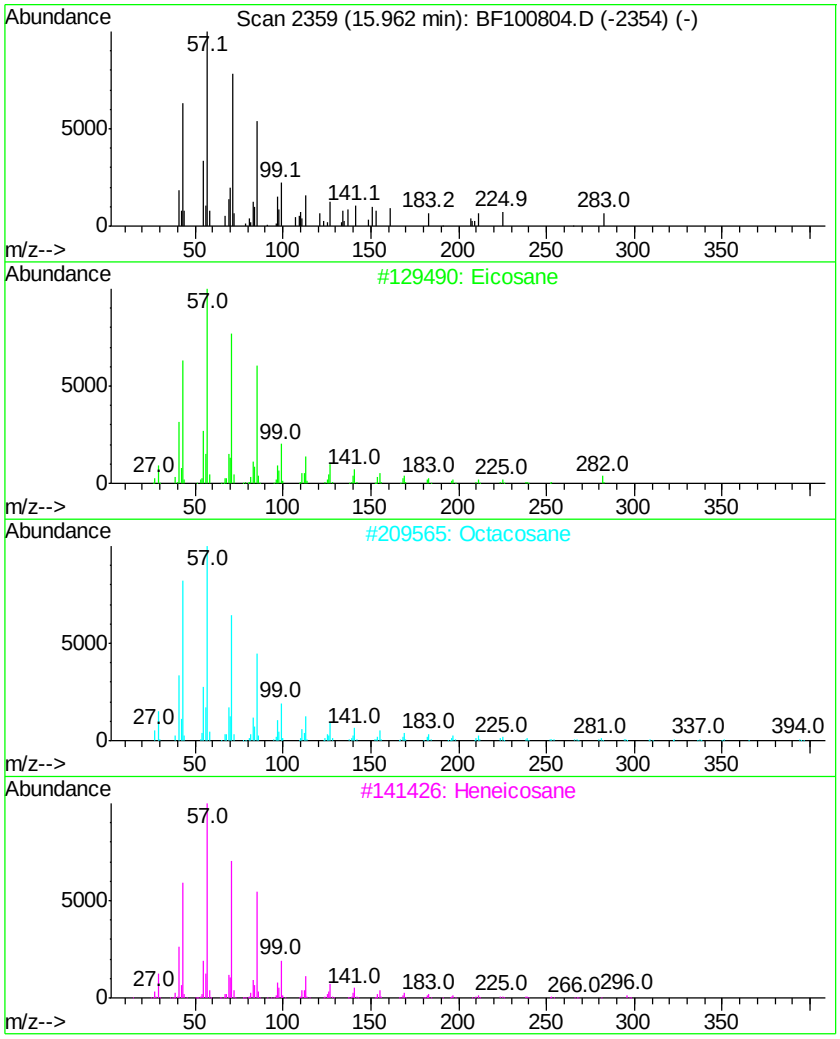
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

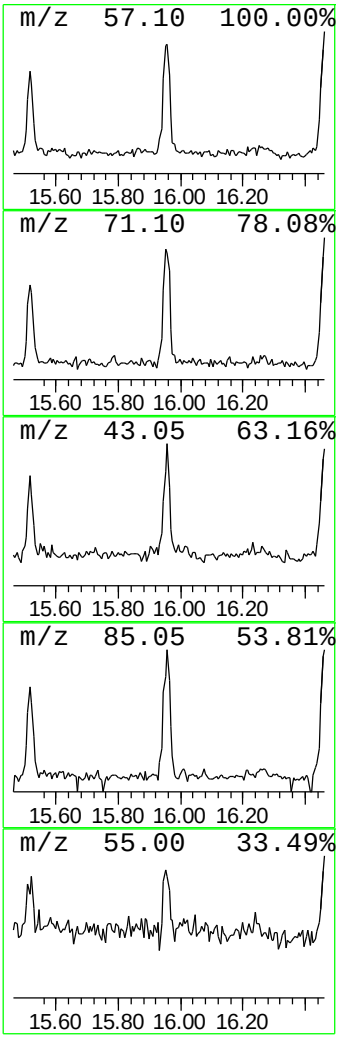
****

Peak Number 9 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	2.46 ng	54674	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Octacosane	394	C28H58	000630-02-4	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Pentacosane	352	C25H52	000629-99-2	87
5	Heptacosane	380	C27H56	000593-49-7	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100804.D
Acq On : 22 Nov 2017 2:53
Operator : SJ/JU
Sample : I6466-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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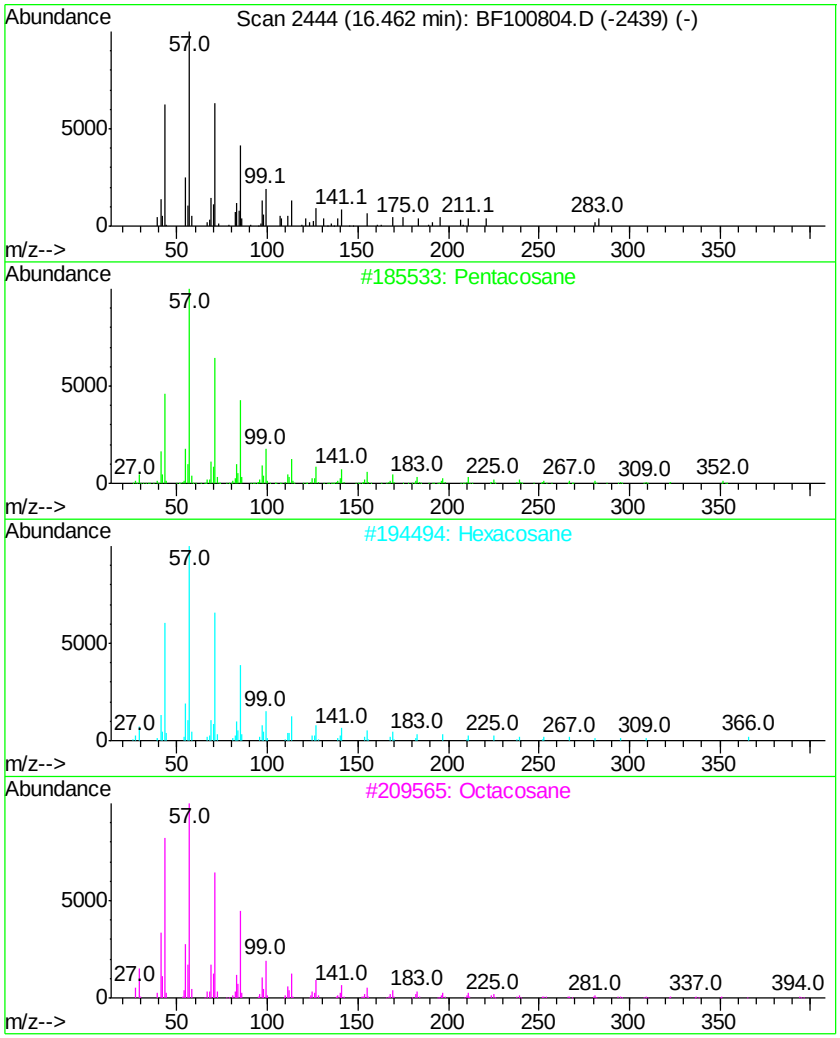
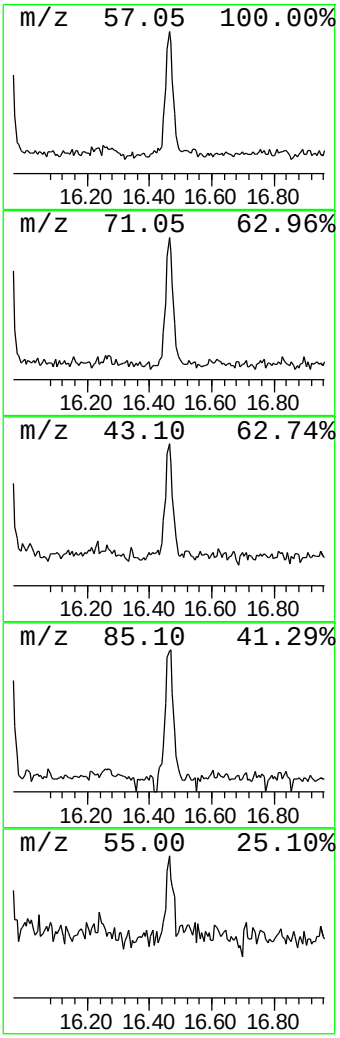
Peak Number 10 Pentacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	3.31 ng	73516	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Heptacosane	380	C27H56	000593-49-7	87
5	Tetratetracontane	619	C44H90	007098-22-8	87





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Acq On : 22 Nov 2017 2:53
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Sample : I6466-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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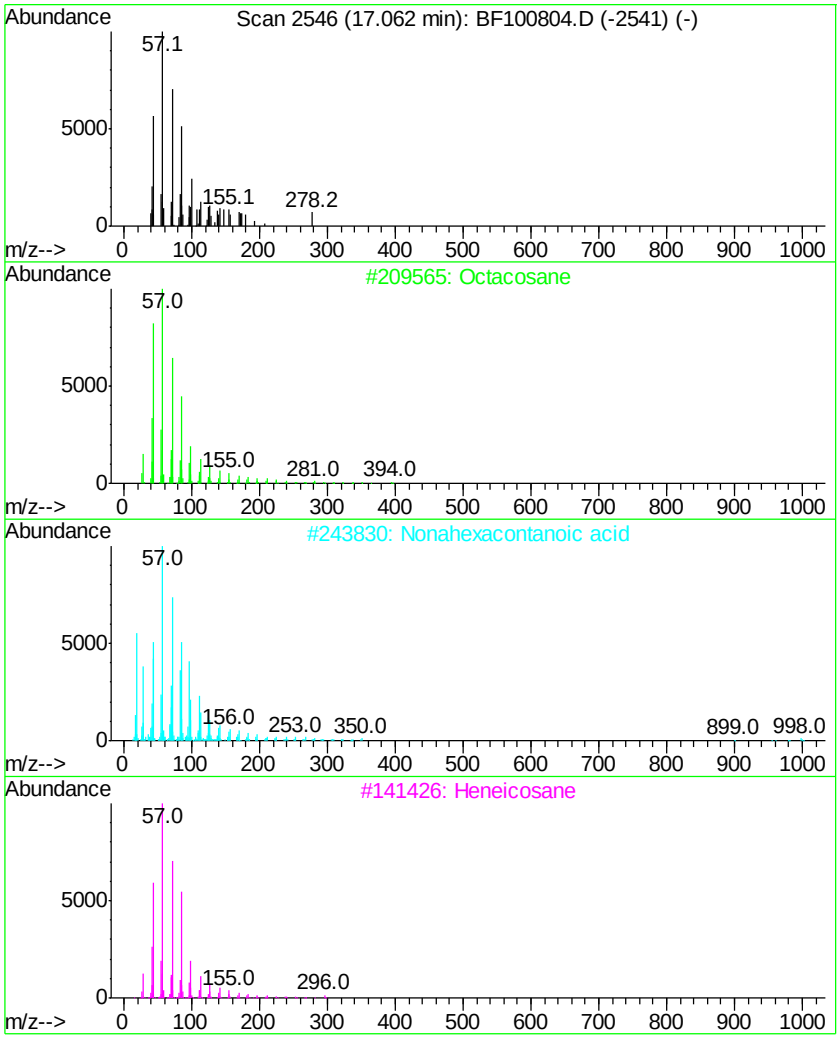
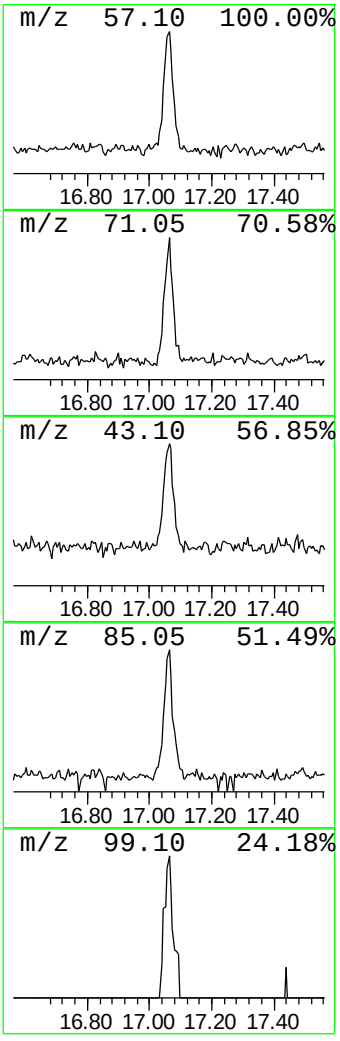
Peak Number 11 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.06	3.19 ng	70994	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Nonahexacontanoic acid	999	C69H138O2	040710-32-5	86
3	Heneicosane	296	C21H44	000629-94-7	86
4	Pentacosane	352	C25H52	000629-99-2	83
5	Hexacosane	366	C26H54	000630-01-3	83





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100804.D
Acq On : 22 Nov 2017 2:53
Operator : SJ/JU
Sample : I6466-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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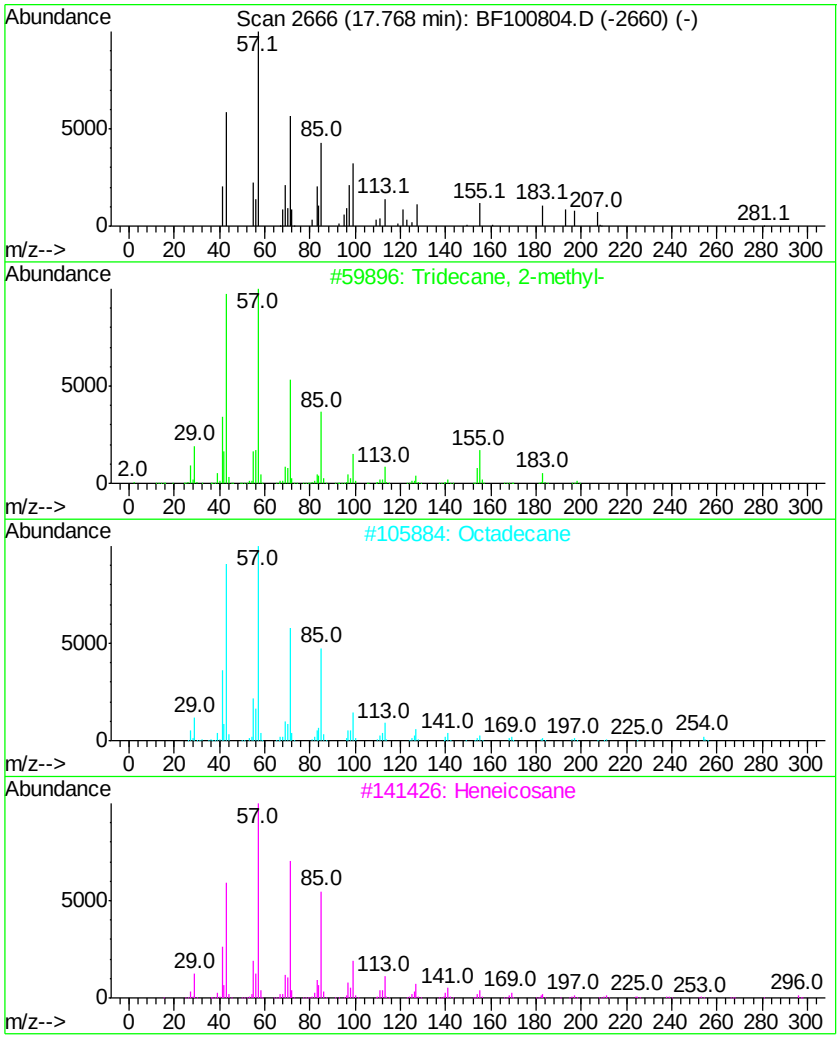
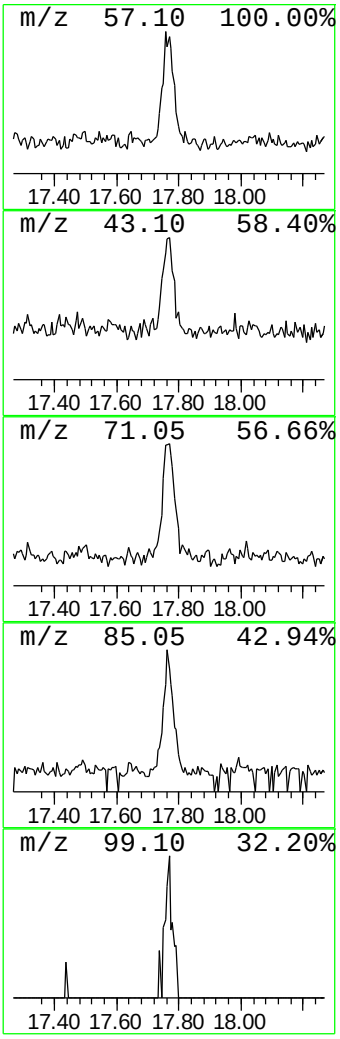
Peak Number 12 Tridecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.77	2.57 ng	57121	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 2-methyl-	198	C14H30	001560-96-9	53
2	Octadecane	254	C18H38	000593-45-3	53
3	Heneicosane	296	C21H44	000629-94-7	53
4	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	53
5	Heptadecane	240	C17H36	000629-78-7	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112117\
Data File : BF100804.D
Acq On : 22 Nov 2017 2:53
Operator : SJ/JU
Sample : I6466-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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
2-Pentanone, 4-hy...	5.10	12.9	ng	300985	1	6.87	465809	20.0
unknown6.65	6.65	73.8	ng	1719060	1	6.87	465809	20.0
Ethanol, 1-methox...	8.70	2.6	ng	77499	2	8.15	596506	20.0
Benzophenone	10.62	9.4	ng	295161	3	9.91	627938	20.0
Carbonic acid, he...	13.86	2.3	ng	56969	5	14.03	495372	20.0
Eicosane	15.96	2.5	ng	54674	6	15.51	444521	20.0
Pentacosane	16.46	3.3	ng	73516	6	15.51	444521	20.0
Octacosane	17.06	3.2	ng	70994	6	15.51	444521	20.0
Tridecane, 2-methyl-	17.77	2.6	ng	57121	6	15.51	444521	20.0