LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102246.D
Acq On : 20 Jan 2018 4:39
Operator : SJ/JU
Sample : J1113-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-15-2.5-3.0

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-BF010918.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	4.928	477	483	491	rVB	170975	263684	7.16%	0.819%
2	5.334	547	552	555	rBV	3395745	3468738	94.19%	10.775%
3	6.363	721	727	730	rBV	3188062	3577340	97.14%	11.112%
4	6.493	744	749	752	rBV	3685215	3543053	96.21%	11.006%
5	6.716	784	787	791	rBV	964267	841825	22.86%	2.615%
6	6.875	810	814	817	rBV	3110450	2756913	74.86%	8.564%
7	7.287	878	884	887	rBV	2299955	2271716	61.69%	7.057%
8	7.469	912	915	918	rVB	51700	41120	1.12%	0.128%
9	7.998	1001	1005	1009	rBV	1268261	1130254	30.69%	3.511%
10	9.081	1184	1189	1192	rBV	4064155	3682614	100.00%	11.439%
11	9.157	1198	1202	1204	rBV	55790	44601	1.21%	0.139%
12	9.475	1251	1256	1258	rBV	345739	309088	8.39%	0.960%
13	9.686	1288	1292	1295	rBV	190592	147826	4.01%	0.459%
14	9.751	1300	1303	1307	rVB	1273402	1179104	32.02%	3.663%
15	10.004	1343	1346	1350	rBV2	40697	38786	1.05%	0.120%
16	10.186	1373	1377	1379	rVB	218986	179280	4.87%	0.557%
17	10.404	1409	1414	1416	rBV	53945	62483	1.70%	0.194%
18	10.545	1431	1438	1441	rBV	2229193	2090336	56.76%	6.493%
19	10.657	1454	1457	1465	rBV	188474	183686	4.99%	0.571%
20	11.104	1530	1533	1536	rBV	65010	52088	1.41%	0.162%
21	11.239	1552	1556	1559	rBV	1149490	1058513	28.74%	3.288%
22	12.645	1792	1795	1798	rBV	240841	186562	5.07%	0.580%
23	12.722	1805	1808	1812	rVB	116254	91078	2.47%	0.283%
24	12.822	1821	1825	1829	rBV	2537207	2521286	68.46%	7.832%
25	13.304	1901	1907	1911	rBV2	64179	87400	2.37%	0.271%
26	13.351	1911	1915	1917	rBV	139190	123812	3.36%	0.385%
27	13.716	1973	1977	1984	rBV	343305	357945	9.72%	1.112%
28	13.868	1999	2003	2007	rBV	832528	765536	20.79%	2.378%
29	14.039	2029	2032	2034	rBV	43278	41789	1.13%	0.130%
30	14.345	2081	2084	2088	rBV	96577	110074	2.99%	0.342%
31	14.639	2132	2134	2139	rBV	35780	47979	1.30%	0.149%
32	15.292	2240	2245	2249	rBV	629850	762401	20.70%	2.368%
33	15.727	2316	2319	2323	rBV	32197	45301	1.23%	0.141%
34	17.209	2567	2571	2579	rVB9	61626	128005	3.48%	0.398%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102246.D
Acq On : 20 Jan 2018 4:39
Operator : SJ/JU
Sample : J1113-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-15-2.5-3.0

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-BF010918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 32192216

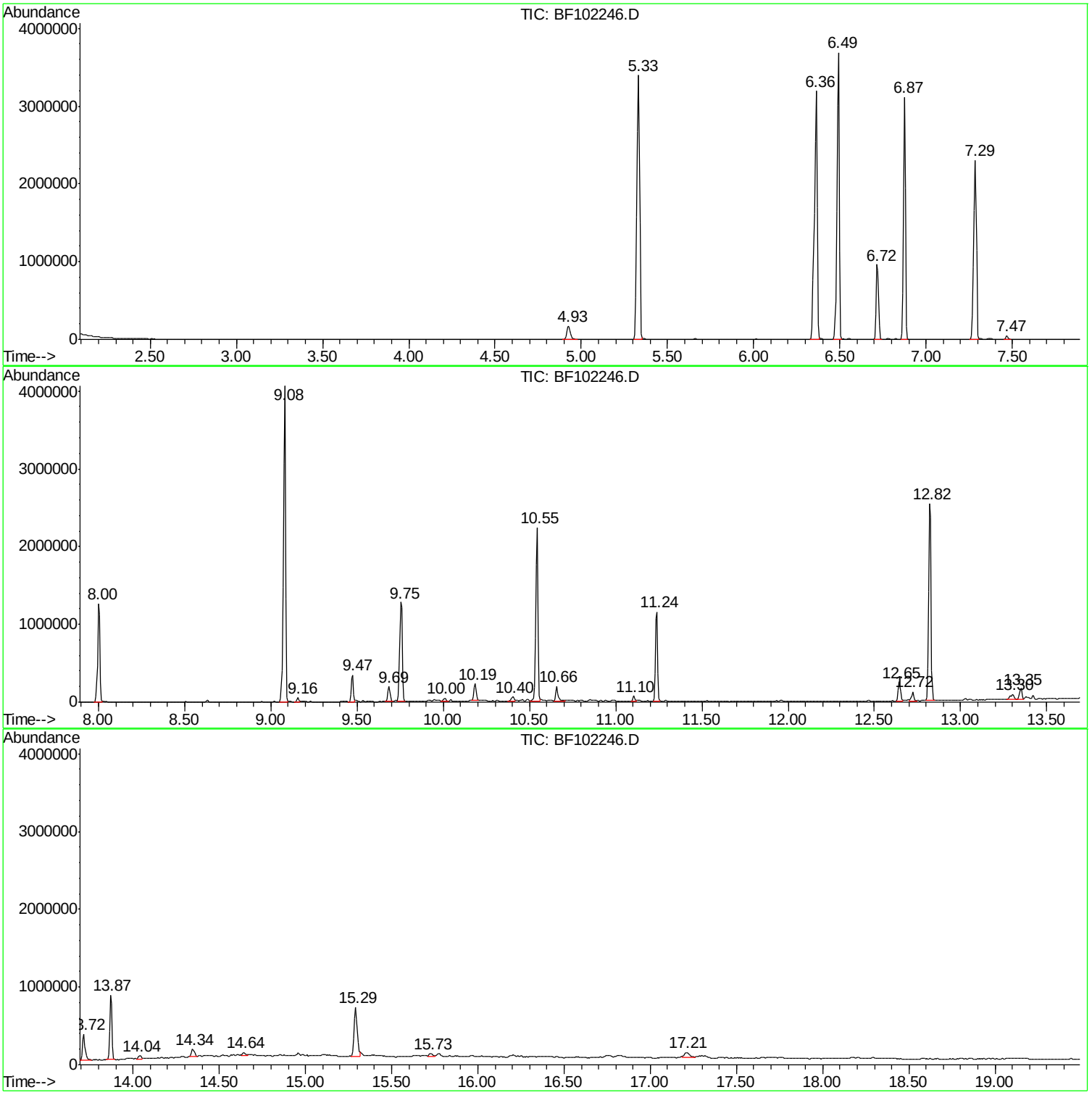
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102246.D
Acq On : 20 Jan 2018 4:39
Operator : SJ/JU
Sample : J1113-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-15-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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\BF011918\
Data File : BF102246.D
Acq On : 20 Jan 2018 4:39
Operator : SJ/JU
Sample : J1113-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-15-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

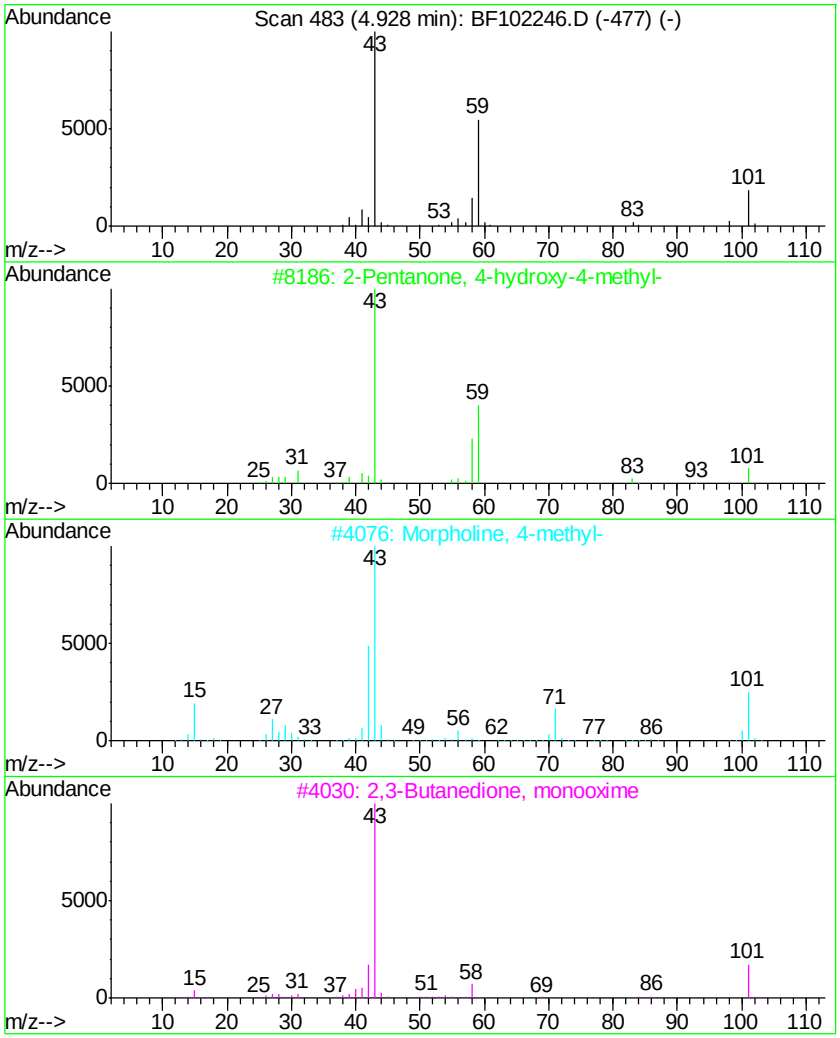
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

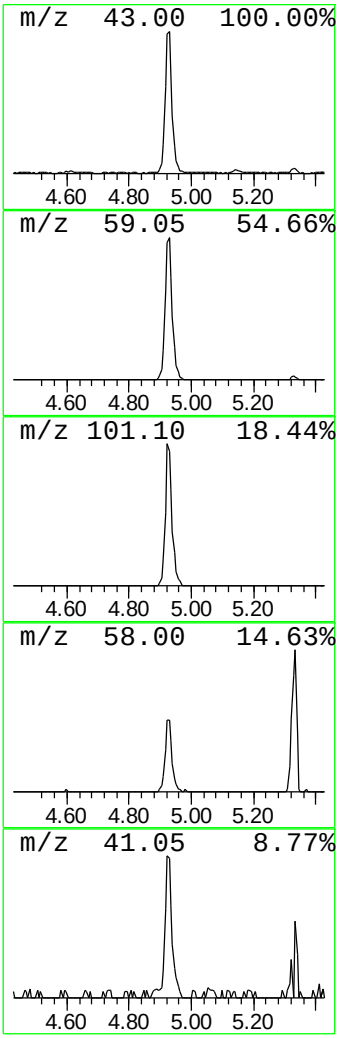
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	6.26 ng	263684	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	56
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
5	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102246.D
Acq On : 20 Jan 2018 4:39
Operator : SJ/JU
Sample : J1113-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-15-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

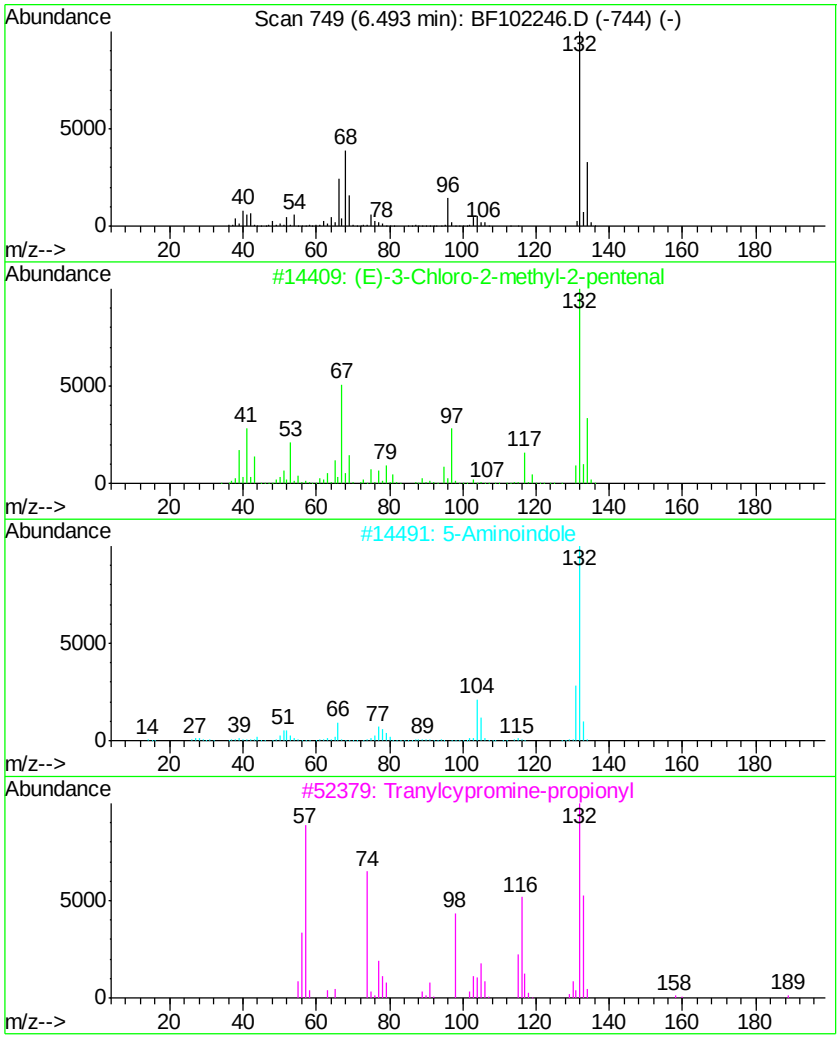
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

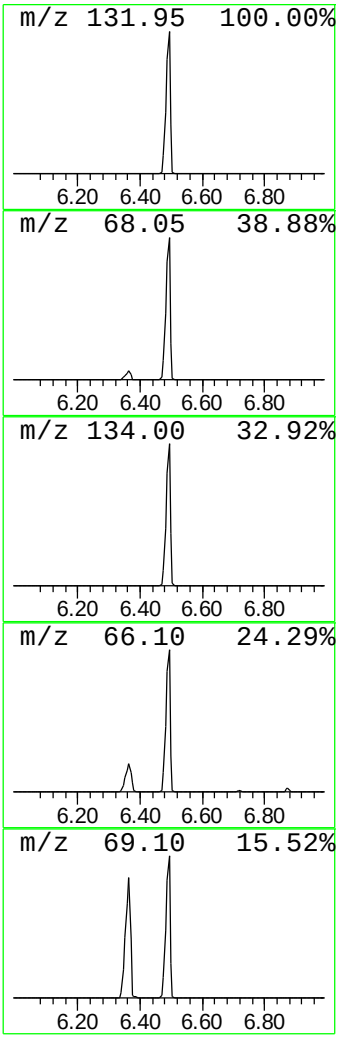
****

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	84.18 ng	3543050	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102246.D
Acq On : 20 Jan 2018 4:39
Operator : SJ/JU
Sample : J1113-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-15-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

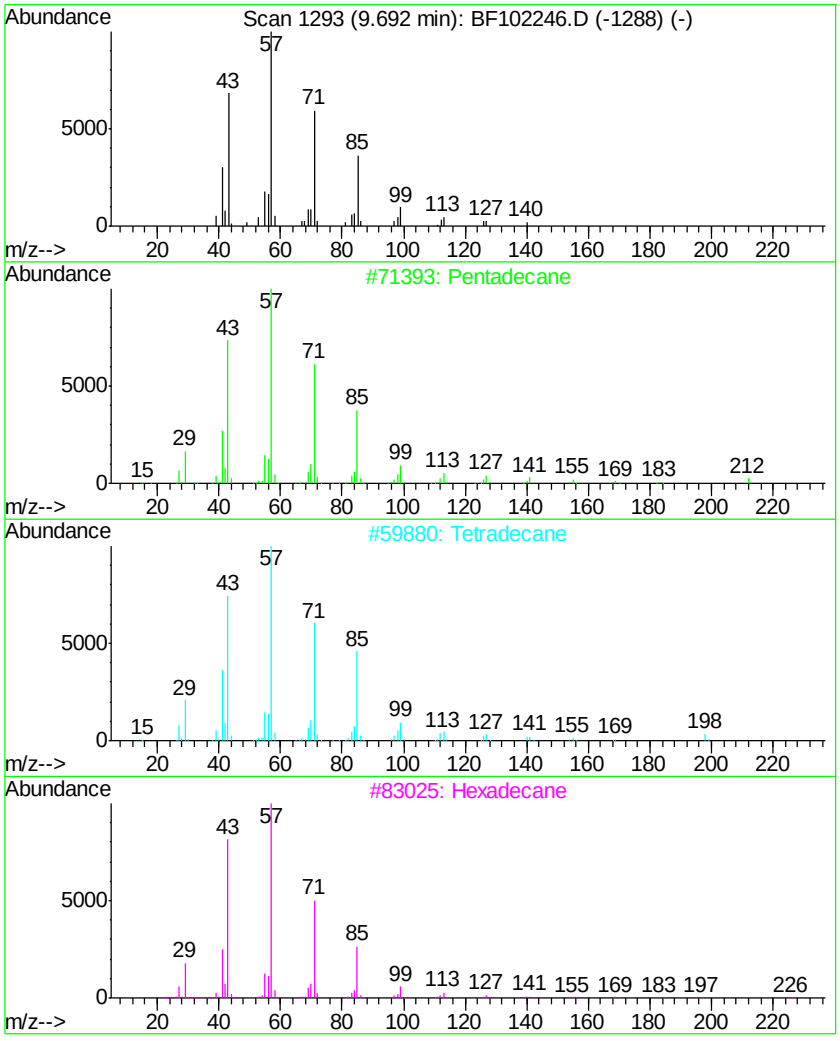
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

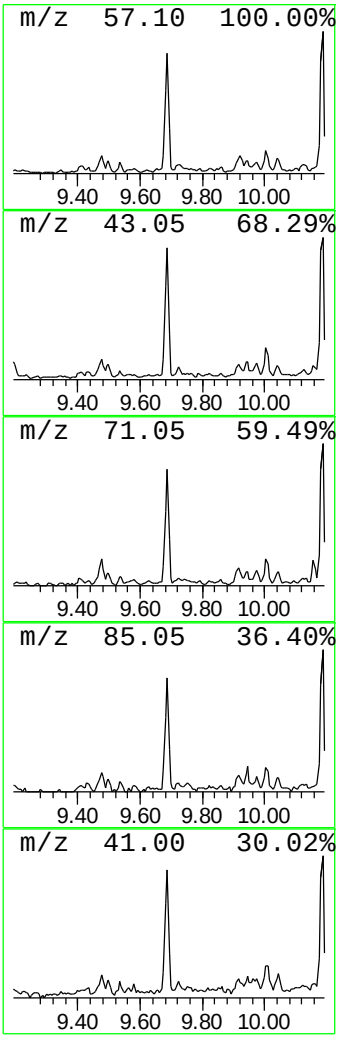
****

Peak Number 4 Pentadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.69	2.51 ng	147826	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	97
2	Tetradecane	198	C14H30	000629-59-4	91
3	Hexadecane	226	C16H34	000544-76-3	91
4	Tridecane	184	C13H28	000629-50-5	90
5	Tridecane, 4,8-dimethyl-	212	C15H32	055030-62-1	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102246.D
Acq On : 20 Jan 2018 4:39
Operator : SJ/JU
Sample : J1113-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-15-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

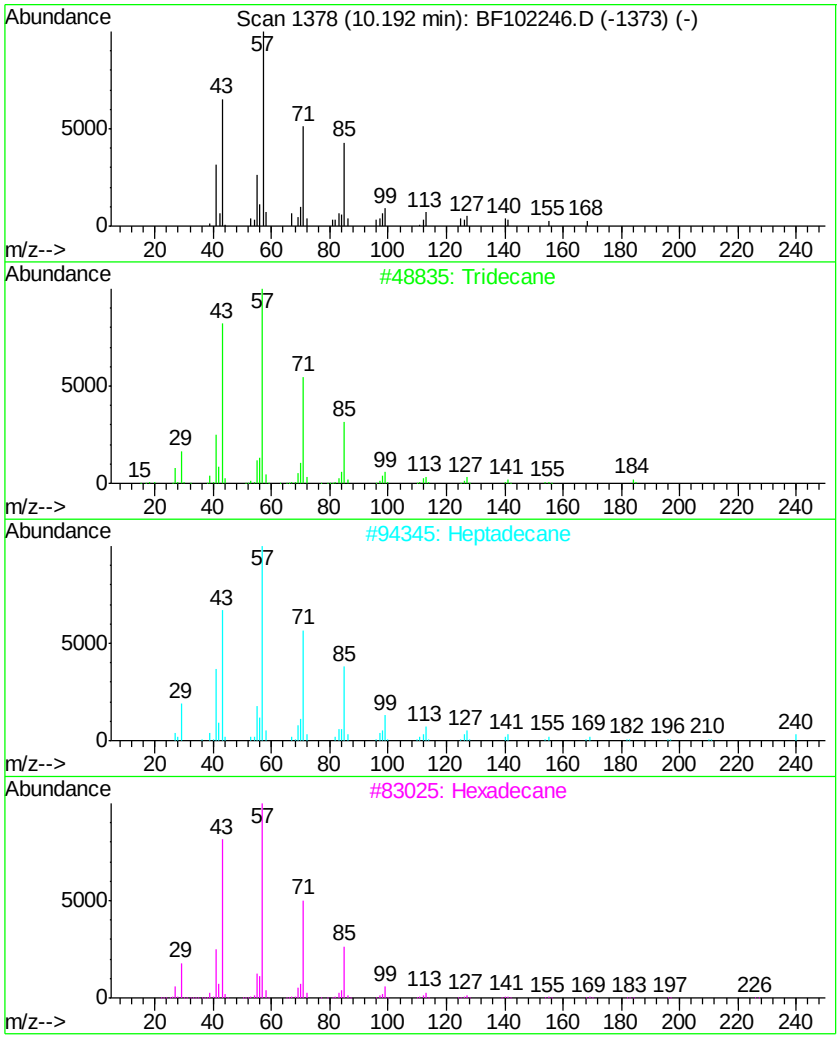
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

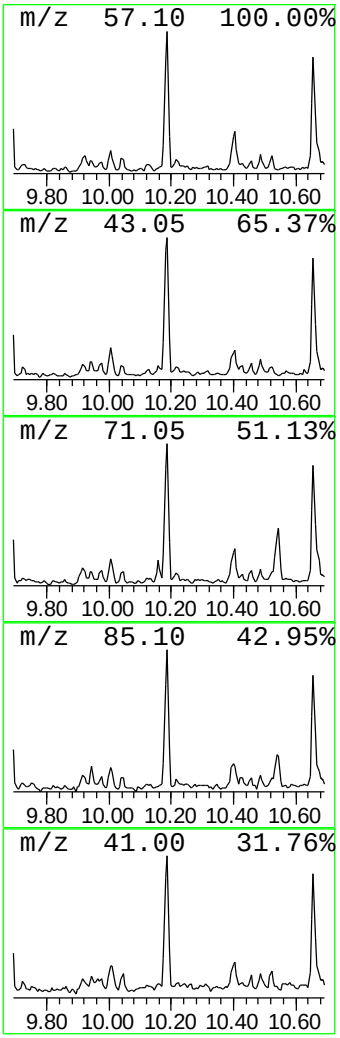
****

Peak Number 5 Tridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.19	3.04 ng	179280	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Heptadecane	240	C17H36	000629-78-7	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Tetradecane	198	C14H30	000629-59-4	87
5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102246.D
Acq On : 20 Jan 2018 4:39
Operator : SJ/JU
Sample : J1113-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-15-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

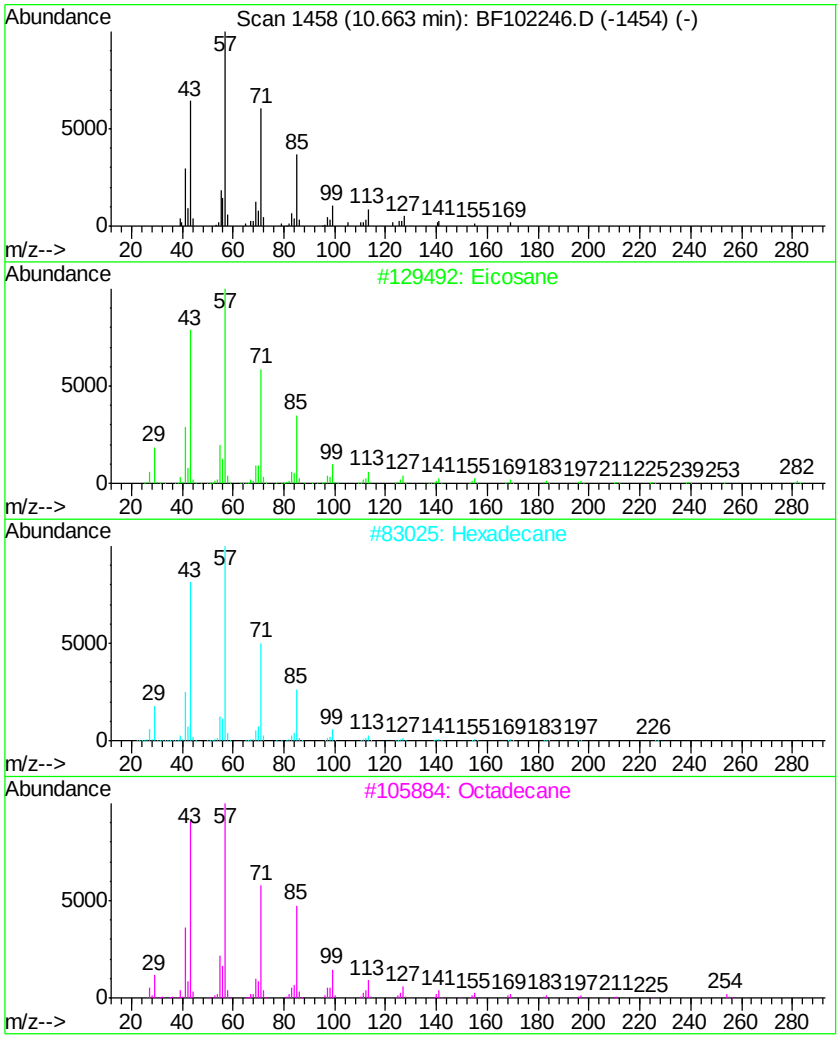
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

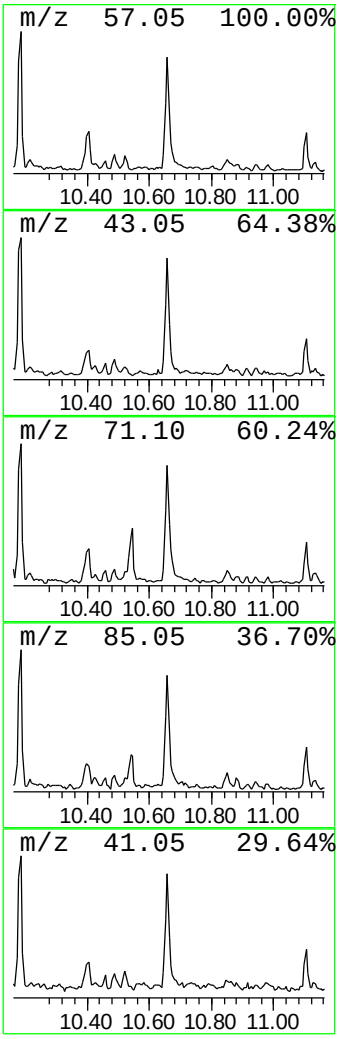
****

Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	3.47 ng	183686	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Octadecane	254	C18H38	000593-45-3	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Heptacosane	380	C27H56	000593-49-7	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102246.D
Acq On : 20 Jan 2018 4:39
Operator : SJ/JU
Sample : J1113-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-15-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

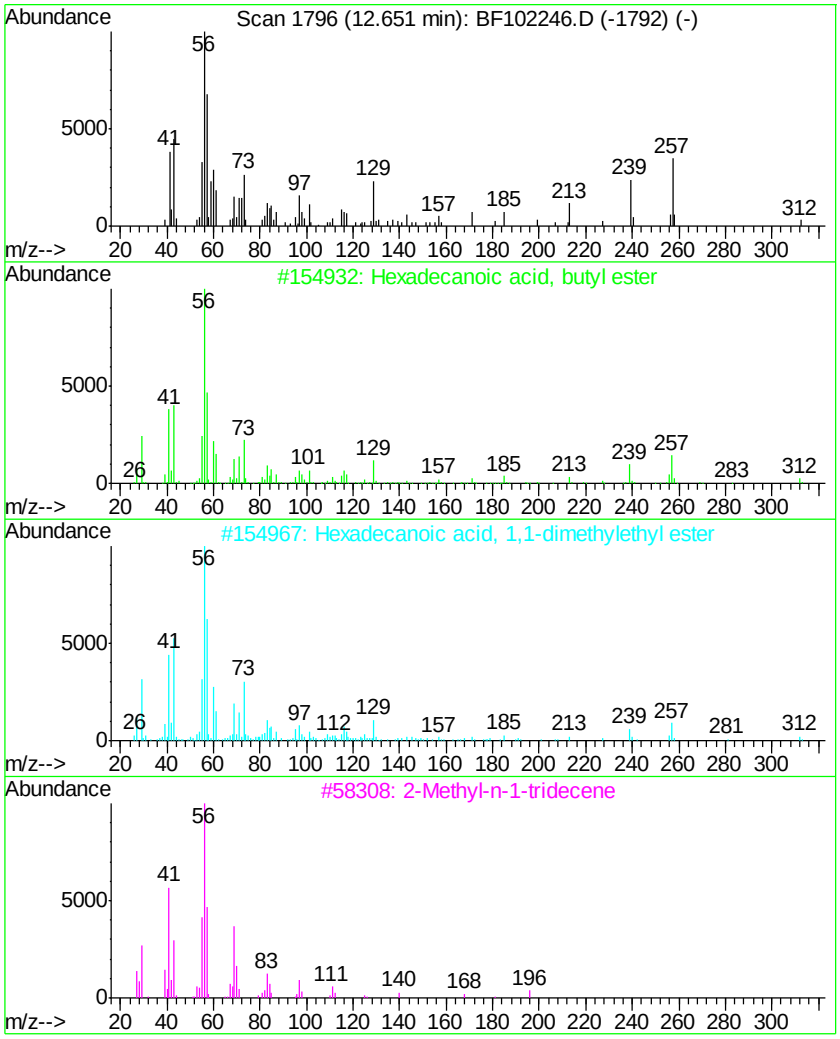
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

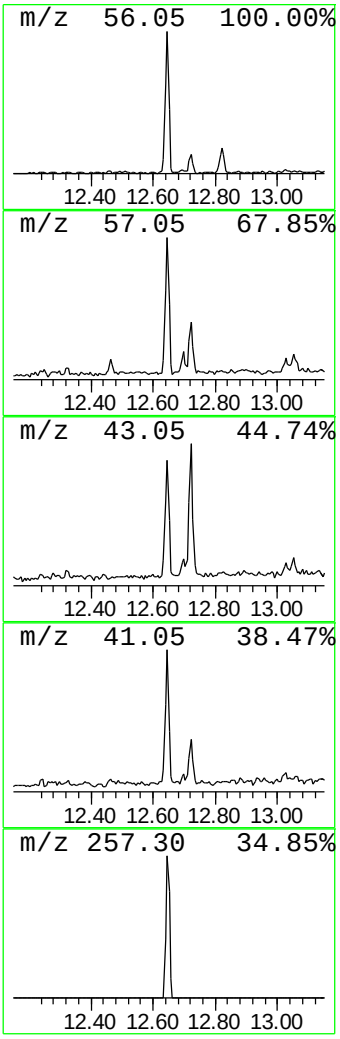
****

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	4.87 ng	186562	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	96
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	93
3	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	27
4	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	27
5	Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102246.D
Acq On : 20 Jan 2018 4:39
Operator : SJ/JU
Sample : J1113-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-15-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

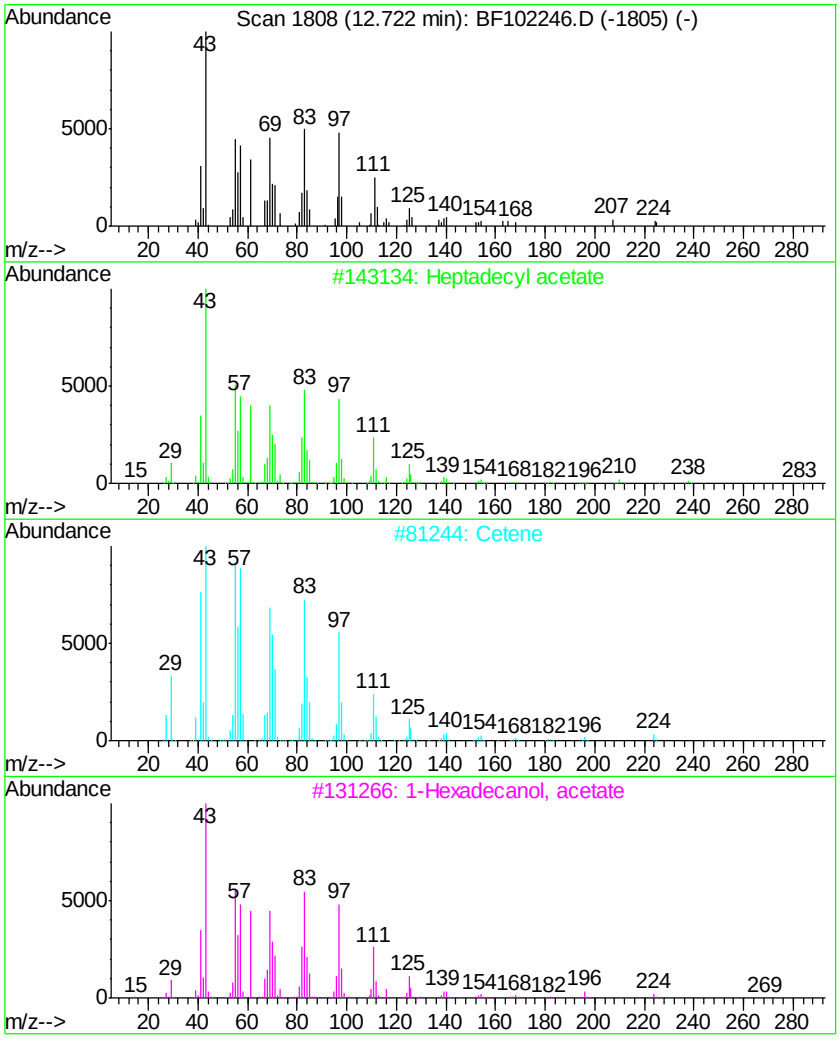
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

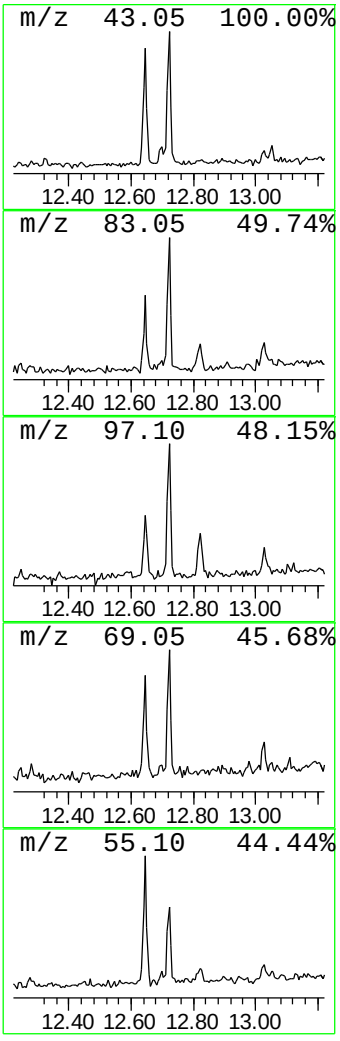
****

Peak Number 8 Heptadecyl acetate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	2.38 ng	91078	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl acetate	298	C19H38O2	000822-20-8	90
2	Cetene	224	C16H32	000629-73-2	87
3	1-Hexadecanol, acetate	284	C18H36O2	000629-70-9	87
4	1-Tetradecyl acetate	256	C16H32O2	000638-59-5	80
5	1-Pentadecanol acetate	270	C17H34O2	000629-58-3	68





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Data File : BF102246.D
Acq On : 20 Jan 2018 4:39
Operator : SJ/JU
Sample : J1113-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-15-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

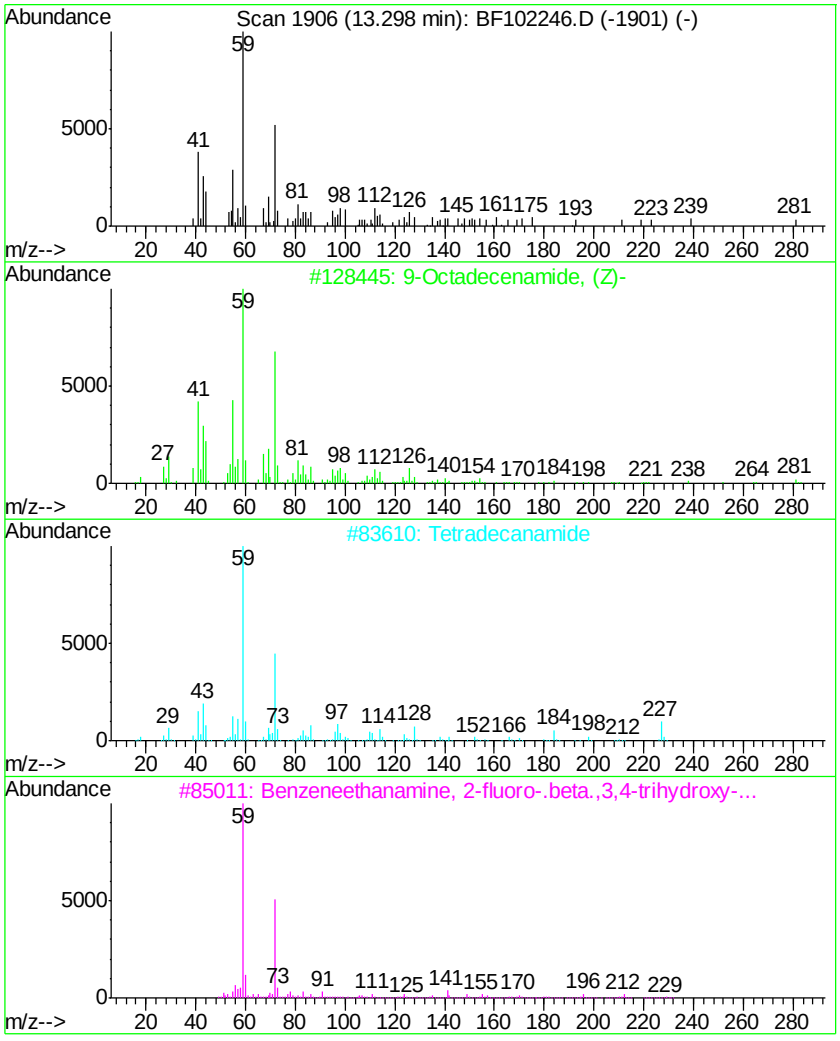
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

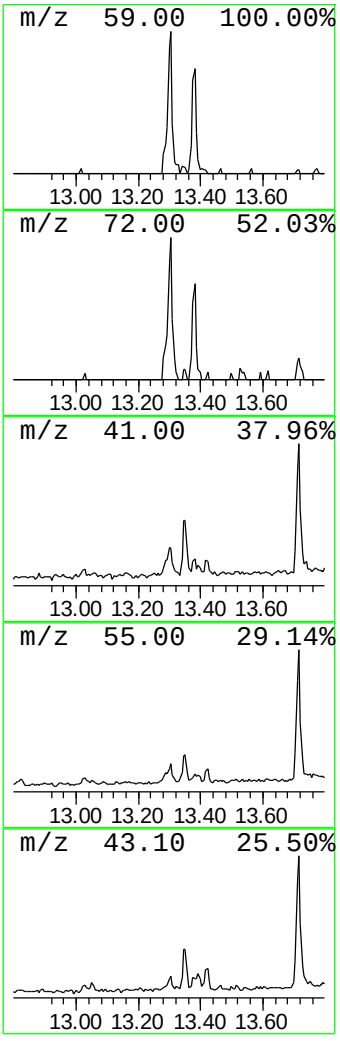
****

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.30	2.28 ng	87400	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2	Tetradecanamide	227	C14H29NO	000638-58-4	64
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	53
4	7-Nonenamide	155	C9H17NO	090949-53-4	50
5	Nonanamide	157	C9H19NO	001120-07-6	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102246.D
Acq On : 20 Jan 2018 4:39
Operator : SJ/JU
Sample : J1113-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-15-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

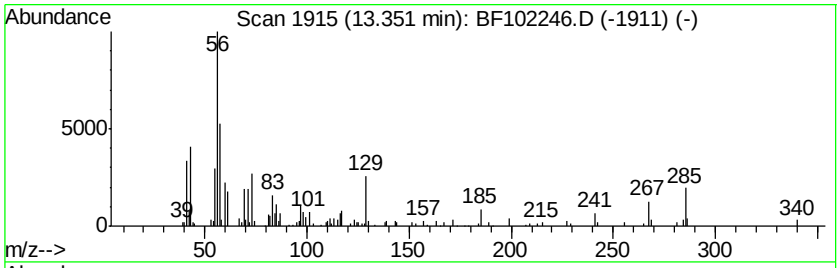
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

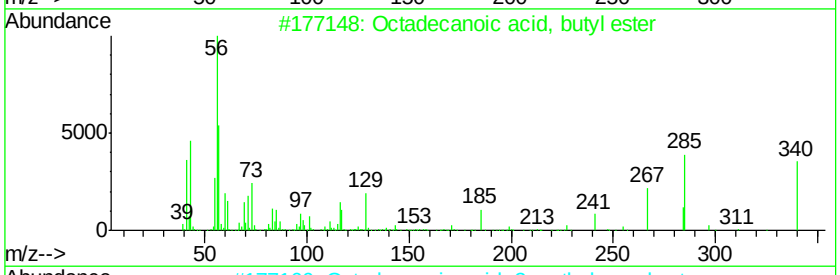
****

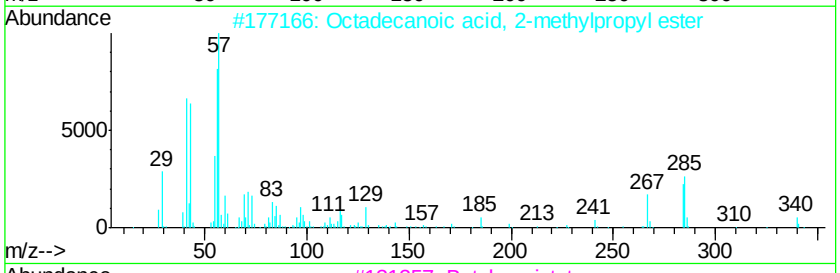
Peak Number 10 Octadecanoic acid, butyl ester Concentration Rank 8

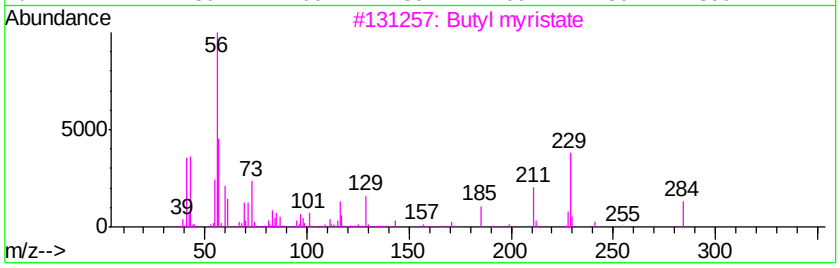
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	3.23 ng	123812	Chrysene-d12	13.87

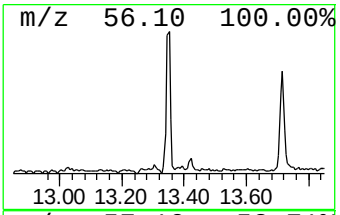
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	64
3	Butyl myristate	284	C18H36O2	000110-36-1	58
4	1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	37
5	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	35

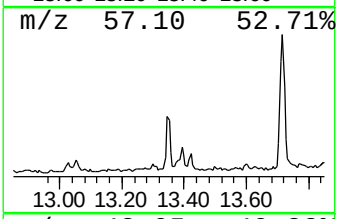


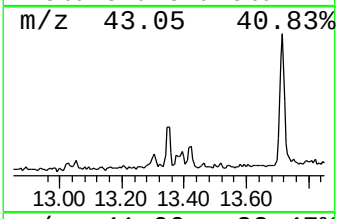


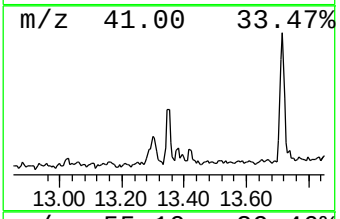


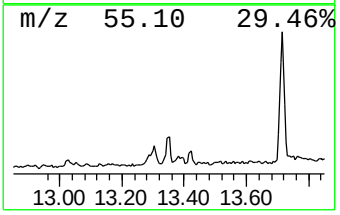












Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102246.D
Acq On : 20 Jan 2018 4:39
Operator : SJ/JU
Sample : J1113-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-15-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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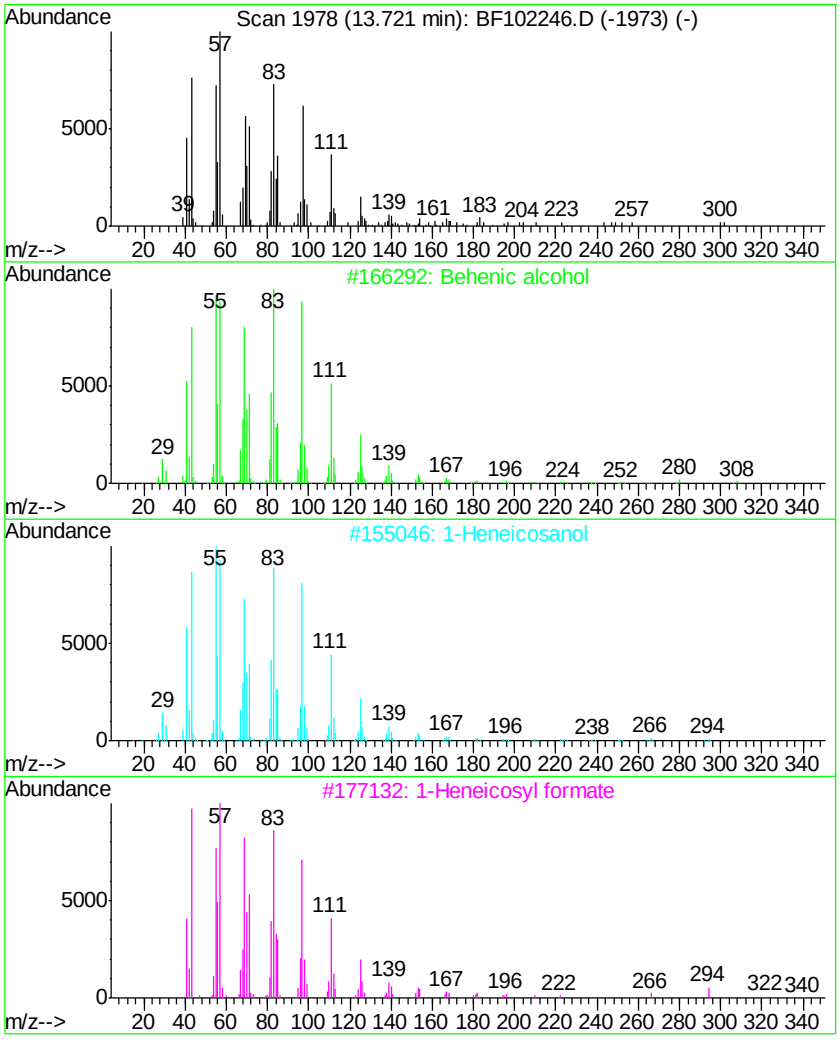
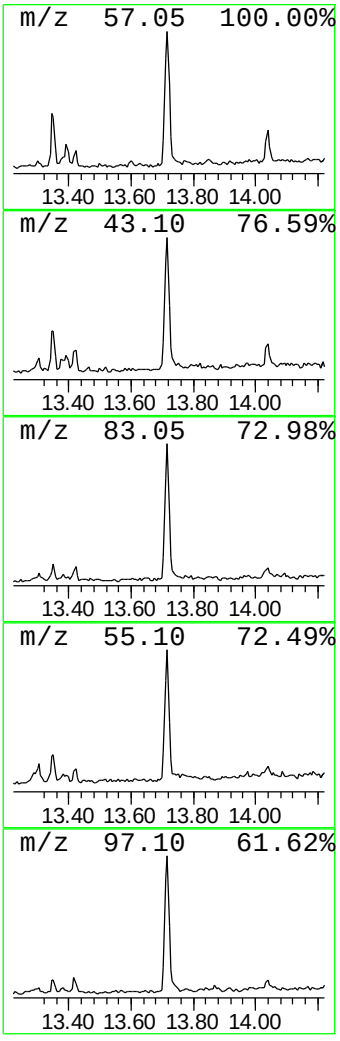
Peak Number 11 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	9.35 ng	357945	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94





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Data File : BF102246.D
Acq On : 20 Jan 2018 4:39
Operator : SJ/JU
Sample : J1113-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-15-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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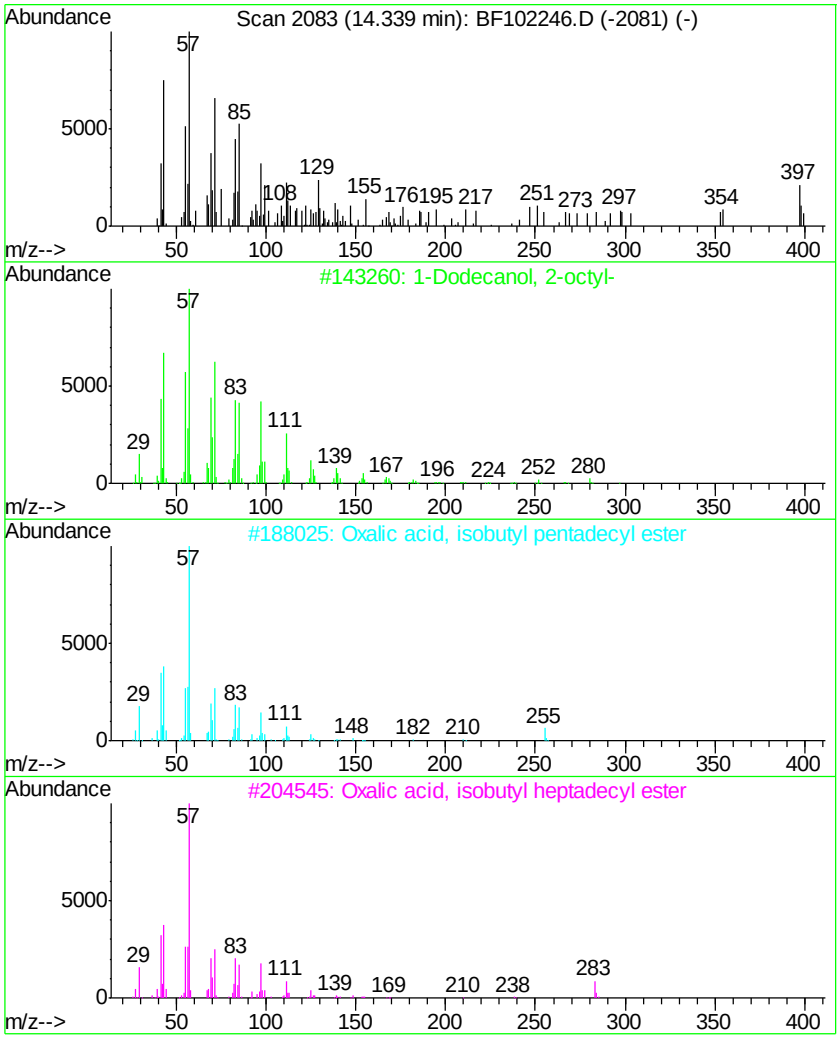
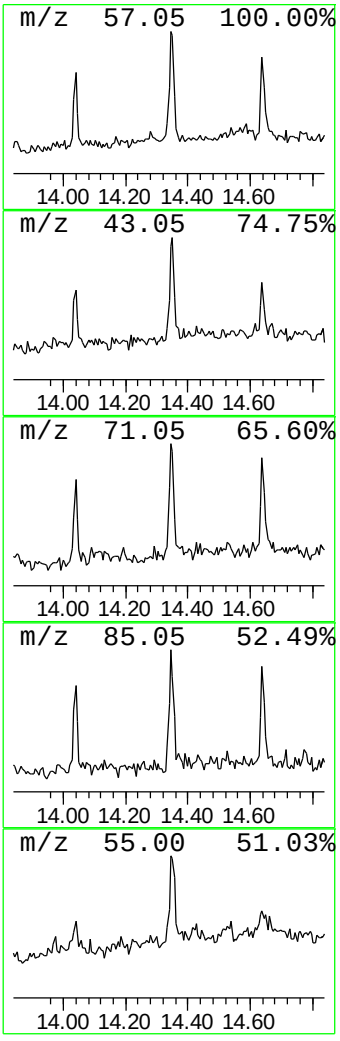
Peak Number 12 1-Dodecanol, 2-octyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	2.88 ng	110074	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	83
2	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	83
3	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	83
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	83
5	Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102246.D
Acq On : 20 Jan 2018 4:39
Operator : SJ/JU
Sample : J1113-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-15-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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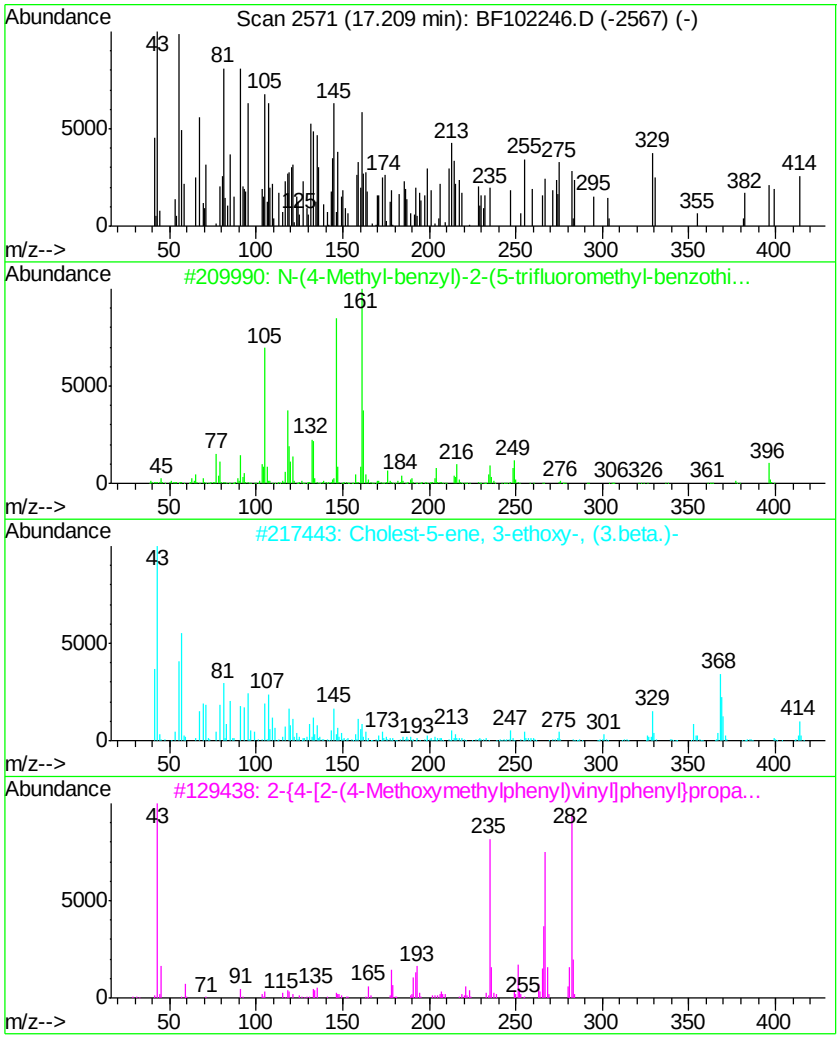
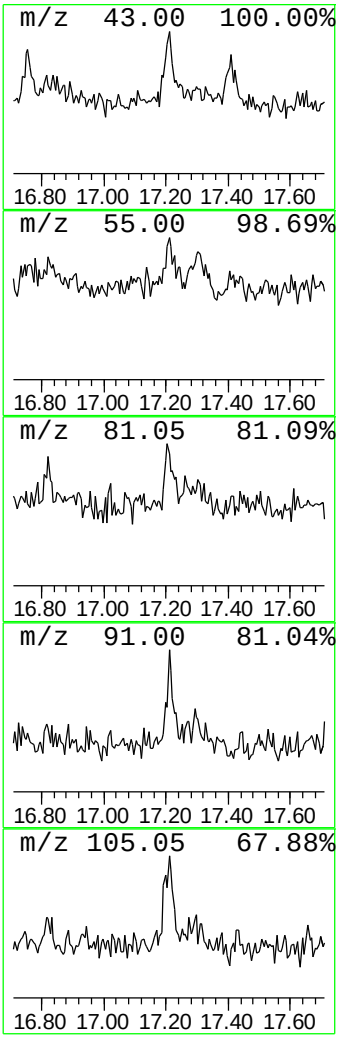
Peak Number 13 unknown17.21 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.21	3.36 ng	128005	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-(4-Methyl-benzyl)-2-(5-trifluo...	396	C18H15F3N2OS2	1000275-06-6	11
2	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	10
3	2-{4-[2-(4-Methoxymethylphenyl)v...	282	C19H22O2	1000202-17-4	10
4	5.alpha.-Stigmast-9(11)-en-3.bet...	414	C29H50O	077794-81-1	9
5	Stigmastan-3-en-6-ol	414	C29H50O	1000214-19-7	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
Data File : BF102246.D
Acq On : 20 Jan 2018 4:39
Operator : SJ/JU
Sample : J1113-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-15-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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...	4.93	6.3	ng	263684	1	6.72	841825	20.0
unknown6.49	6.49	84.2	ng	3543050	1	6.72	841825	20.0
Pentadecane	9.69	2.5	ng	147826	3	9.75	1179100	20.0
Tridecane	10.19	3.0	ng	179280	3	9.75	1179100	20.0
Eicosane	10.66	3.5	ng	183686	4	11.24	1058510	20.0
Hexadecanoic acid...	12.65	4.9	ng	186562	5	13.87	765536	20.0
Heptadecyl acetate	12.72	2.4	ng	91078	5	13.87	765536	20.0
9-Octadecenamide,...	13.30	2.3	ng	87400	5	13.87	765536	20.0
Octadecanoic acid...	13.35	3.2	ng	123812	5	13.87	765536	20.0
Behenic alcohol	13.72	9.3	ng	357945	5	13.87	765536	20.0
1-Dodecanol, 2-oc...	14.34	2.9	ng	110074	5	13.87	765536	20.0
unknown17.21	17.21	3.4	ng	128005	6	15.29	762401	20.0