LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098423.D
Acq On : 12 Sep 2017 1:02
Operator : SJ/JU
Sample : I5138-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-UTS-TS006-01

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-BF091117.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	3.622	254	261	269	rBV	73896	111944	1.45%	0.185%
2	4.204	357	360	369	rBV	105676	158525	2.05%	0.262%
3	4.869	469	473	493	rVB	672873	1171151	15.12%	1.935%
4	5.287	539	544	547	rBV	6357577	7183502	92.74%	11.870%
5	6.322	715	720	736	rBV	5699158	7745875	100.00%	12.799%
6	6.445	736	741	744	rBV	6680343	6873138	88.73%	11.357%
7	6.669	775	779	787	rBV	1752247	1592772	20.56%	2.632%
8	6.822	801	805	809	rBV	4866238	4803631	62.02%	7.937%
9	7.240	870	876	879	rBV	4423369	4697291	60.64%	7.762%
10	7.951	992	997	1000	rBV	2465047	2118000	27.34%	3.500%
11	9.028	1174	1180	1183	rBV	6073997	5621880	72.58%	9.289%
12	9.110	1189	1194	1198	rBV3	83605	97384	1.26%	0.161%
13	9.422	1239	1247	1251	rBV	1372456	1193117	15.40%	1.971%
14	9.698	1288	1294	1298	rBV	2251924	2220233	28.66%	3.669%
15	10.416	1412	1416	1421	rBV	115666	122362	1.58%	0.202%
16	10.492	1421	1429	1432	rBV	3768239	3614336	46.66%	5.972%
17	10.604	1444	1448	1456	rVB3	94187	150990	1.95%	0.249%
18	10.739	1468	1471	1473	rBV2	79564	82721	1.07%	0.137%
19	10.763	1473	1475	1477	rVB2	120343	87044	1.12%	0.144%
20	10.839	1486	1488	1493	rVB4	73411	112448	1.45%	0.186%
21	10.886	1493	1496	1499	rBV	152877	140578	1.81%	0.232%
22	10.957	1505	1508	1518	rVB3	77143	122786	1.59%	0.203%
23	11.069	1522	1527	1533	rVB3	62072	94791	1.22%	0.157%
24	11.180	1541	1546	1553	rBV	2307939	2011156	25.96%	3.323%
25	11.251	1553	1558	1561	rVB3	79322	120544	1.56%	0.199%
26	11.580	1611	1614	1619	rVB2	89828	105681	1.36%	0.175%
27	12.263	1726	1730	1732	rBV	241035	238695	3.08%	0.394%
28	12.280	1732	1733	1737	rVB3	155804	120957	1.56%	0.200%
29	12.651	1793	1796	1806	rVB2	92076	146212	1.89%	0.242%
30	12.763	1811	1815	1819	rBV	3816526	3719335	48.02%	6.146%
31	13.327	1908	1911	1916	rBV3	55708	85269	1.10%	0.141%
32	13.657	1964	1967	1980	rBV	469124	540781	6.98%	0.894%
33	13.810	1988	1993	1997	rBV	1265499	1252373	16.17%	2.069%
34	14.292	2071	2075	2079	rBV3	79067	104484	1.35%	0.173%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098423.D
Acq On : 12 Sep 2017 1:02
Operator : SJ/JU
Sample : I5138-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-UTS-TS006-01

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-BF091117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.563	2118	2121	2126	rBV2	111268	142400	1.84%	0.235%
36	15.210	2227	2231	2239	rVB	1003197	1162397	15.01%	1.921%
37	15.627	2299	2302	2306	rBV2	69381	87972	1.14%	0.145%
38	15.674	2308	2310	2317	rVB3	71951	105395	1.36%	0.174%
39	17.057	2538	2545	2555	rBV10	130778	458526	5.92%	0.758%

Sum of corrected areas: 60518676

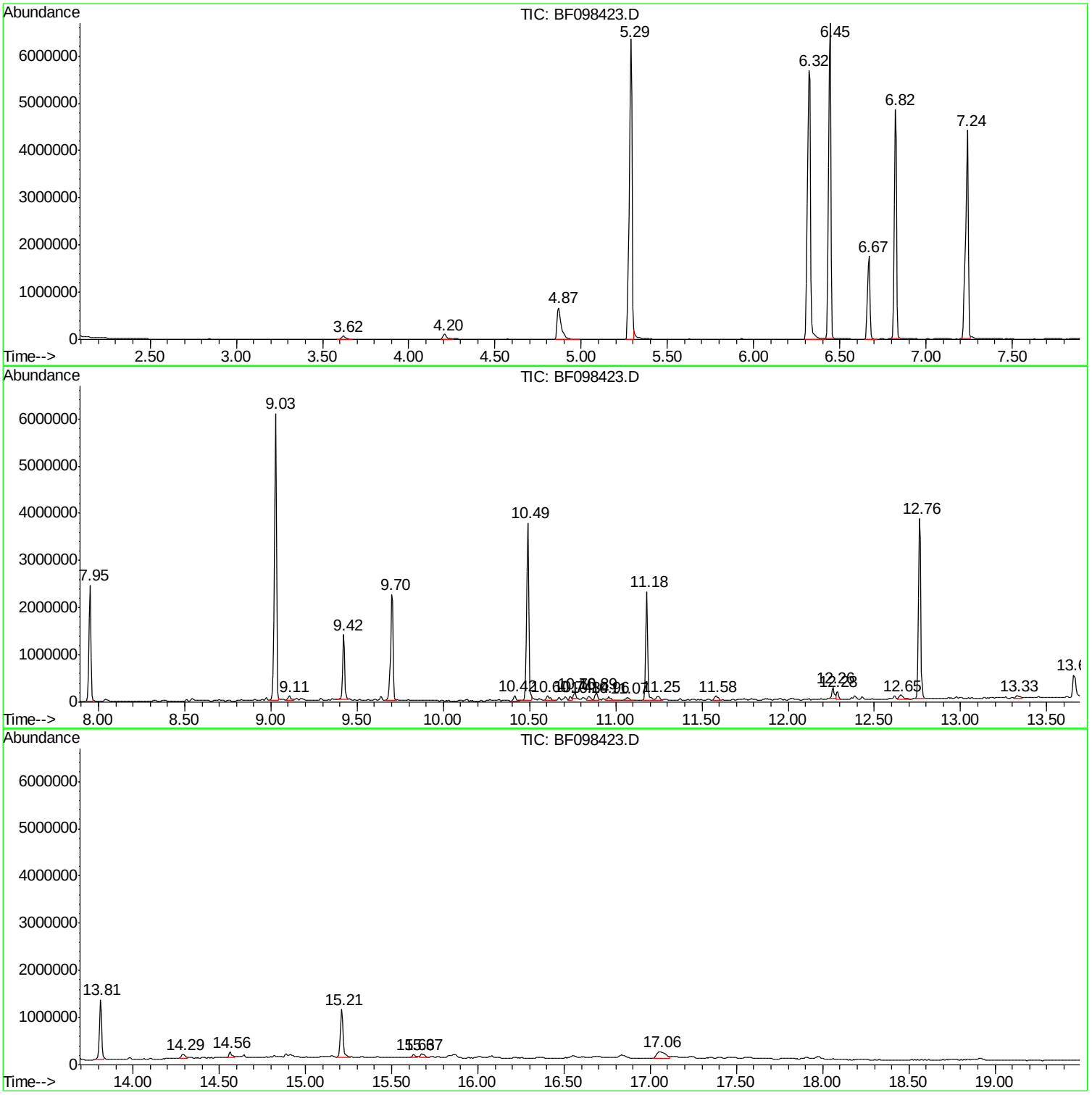
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098423.D
Acq On : 12 Sep 2017 1:02
Operator : SJ/JU
Sample : I5138-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-UTS-TS006-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098423.D
Acq On : 12 Sep 2017 1:02
Operator : SJ/JU
Sample : I5138-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-UTS-TS006-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

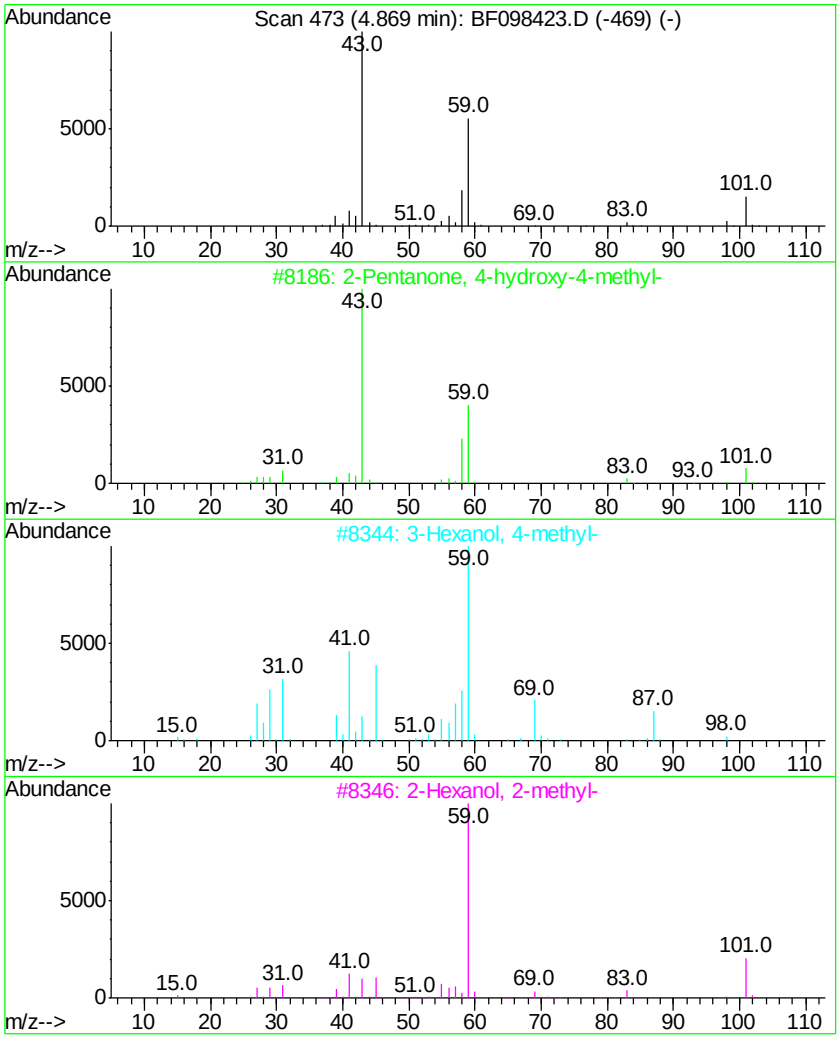
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

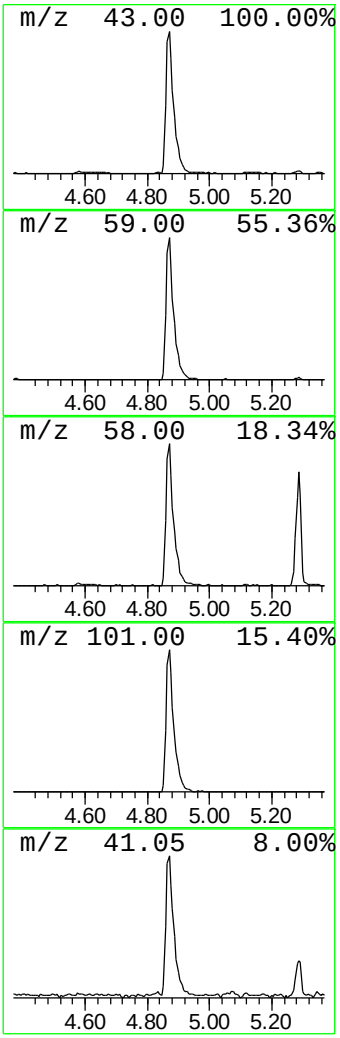
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	14.71 ng	1171150	1,4-Dichlorobenzene-d4	6.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Octanol	130	C8H18O	000589-98-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098423.D
Acq On : 12 Sep 2017 1:02
Operator : SJ/JU
Sample : I5138-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-UTS-TS006-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

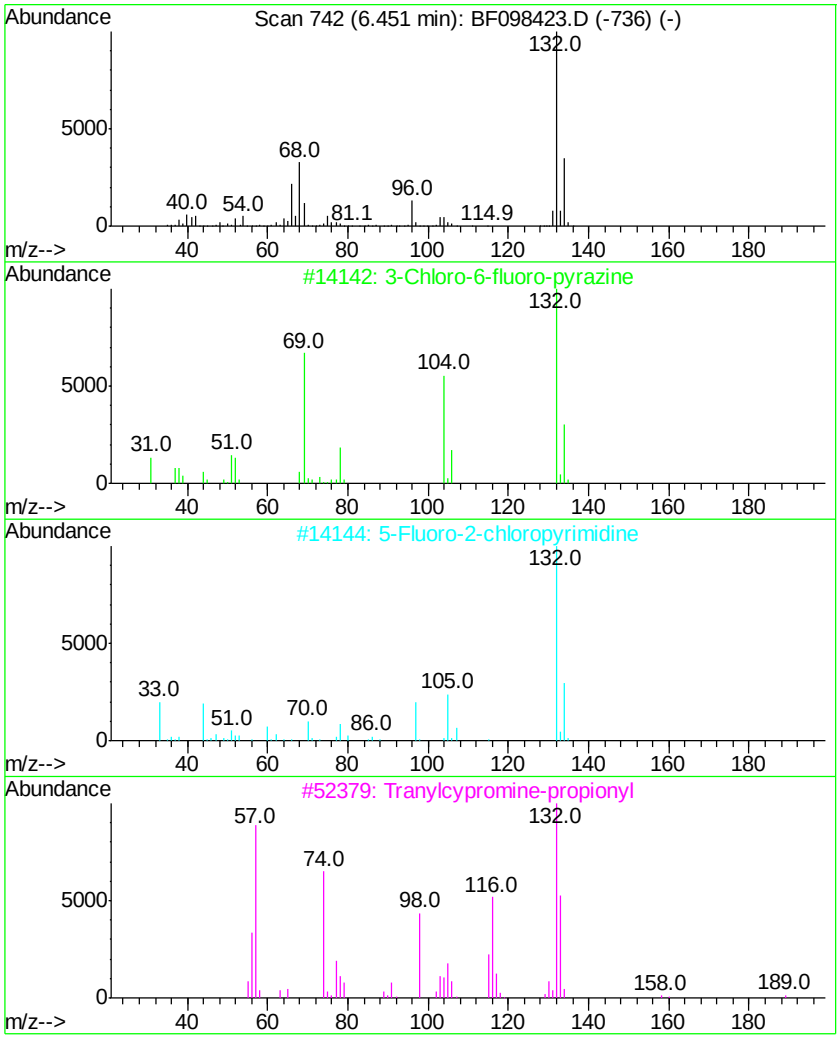
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

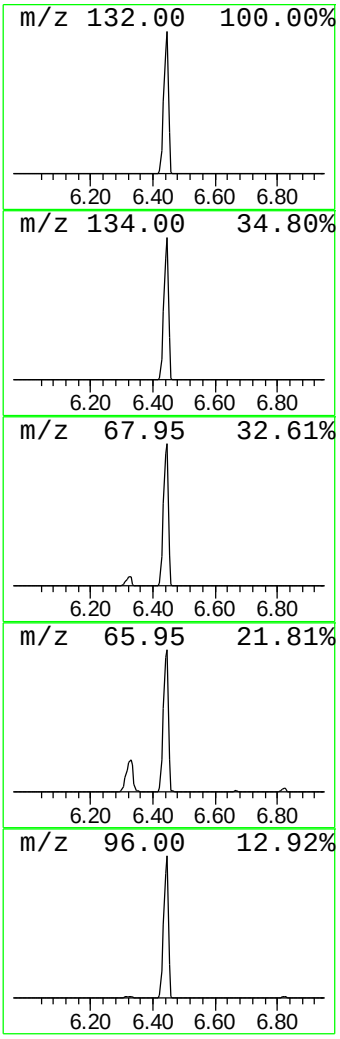
****

Peak Number 2 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	86.30 ng	6873140	1,4-Dichlorobenzene-d4	6.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098423.D
Acq On : 12 Sep 2017 1:02
Operator : SJ/JU
Sample : I5138-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-UTS-TS006-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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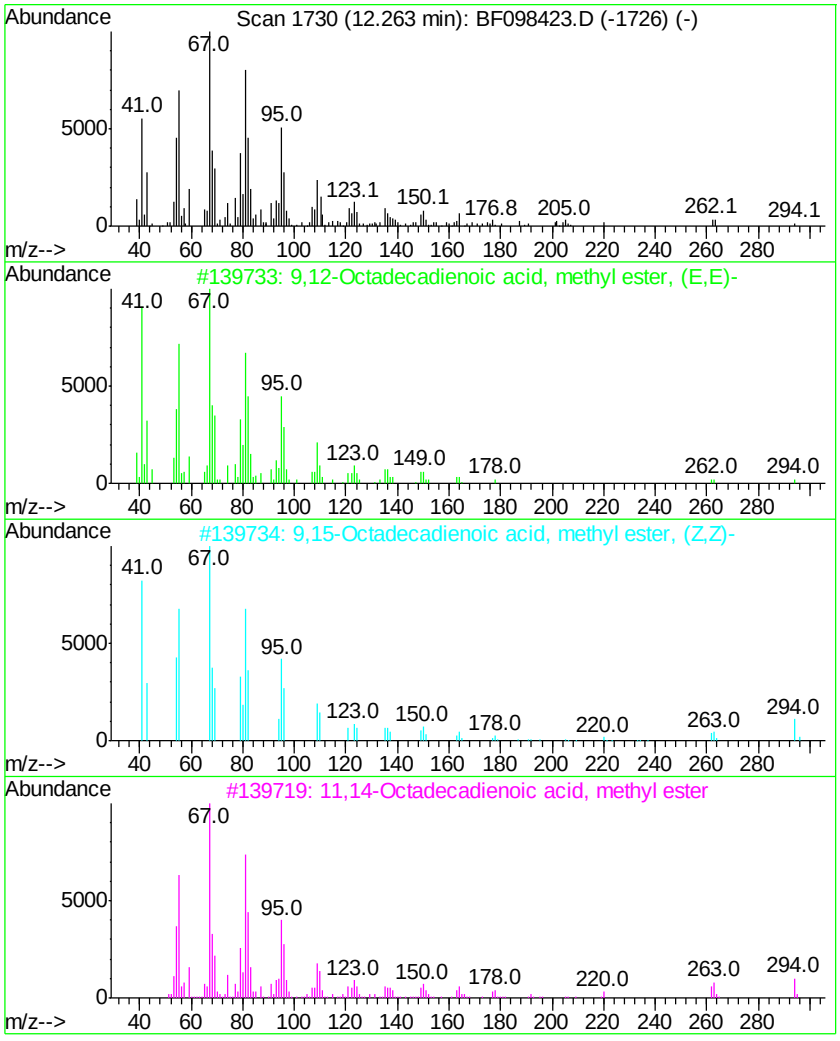
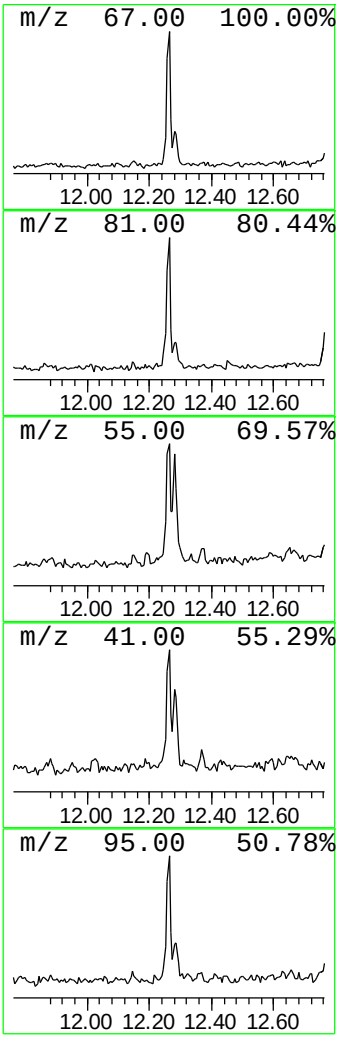
Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	2.37 ng	238695	Phenanthrene-d10	11.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98
3	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	94
4	11-Octadecynoic acid, methyl ester	294	C19H34O2	026543-37-3	92
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	90





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098423.D
Acq On : 12 Sep 2017 1:02
Operator : SJ/JU
Sample : I5138-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-UTS-TS006-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

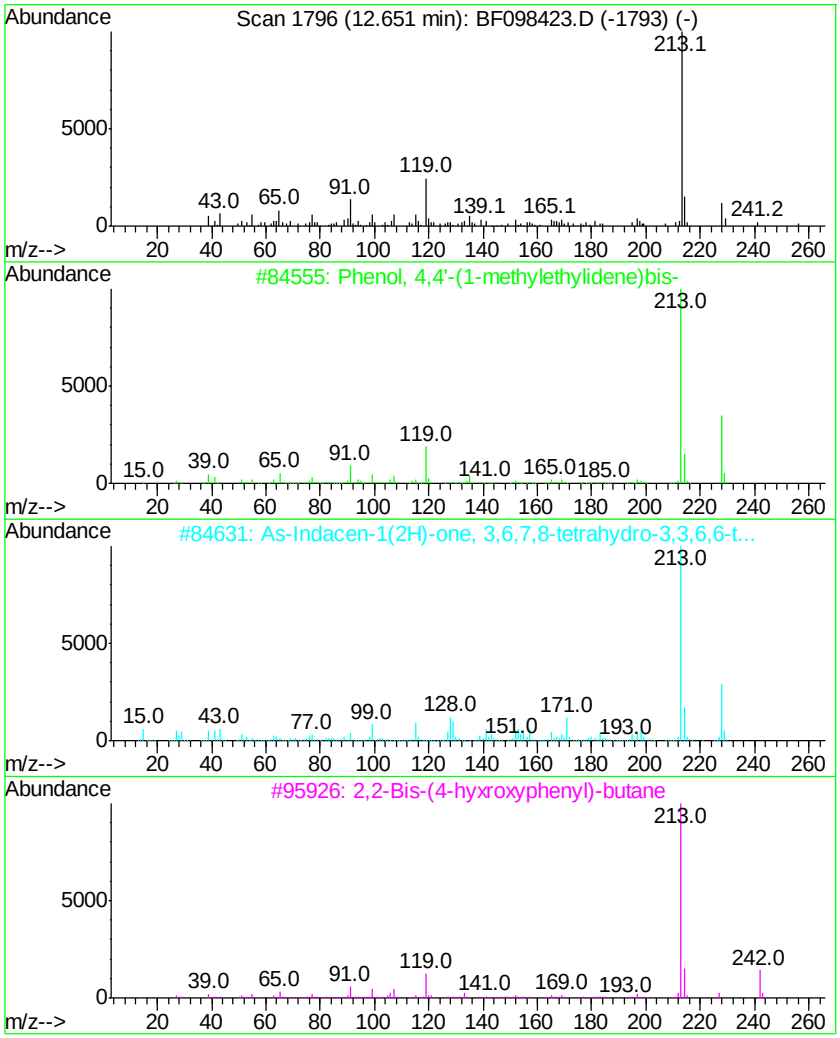
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

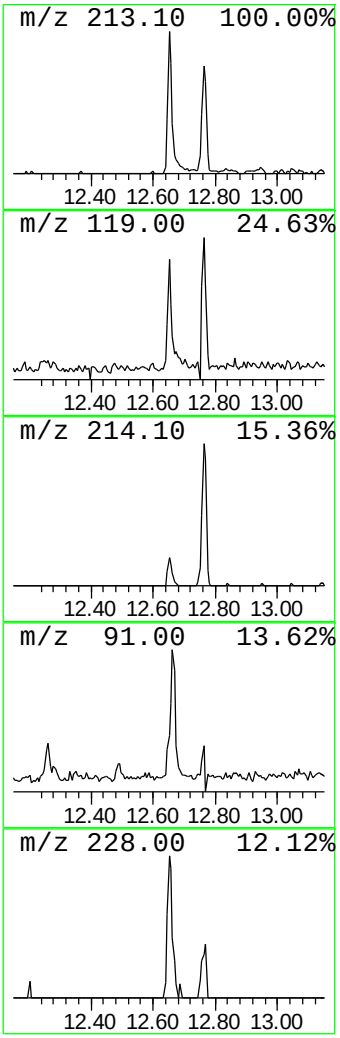
****

Peak Number 5 Phenol, 4,4'-(1-methylethyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.33 ng	146212	Chrysene-d12	13.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	94
2	As-Indacen-1(2H)-one, 3,6,7,8-te...	228	C16H20O	055591-18-9	59
3	2,2-Bis-(4-hyxroxyphenyl)-butane	242	C16H18O2	000077-40-7	59
4	Carbamic acid, [1,1'-biphenyl]-3...	213	C13H11NO2	055030-29-0	52
5	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	52





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098423.D
Acq On : 12 Sep 2017 1:02
Operator : SJ/JU
Sample : I5138-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-UTS-TS006-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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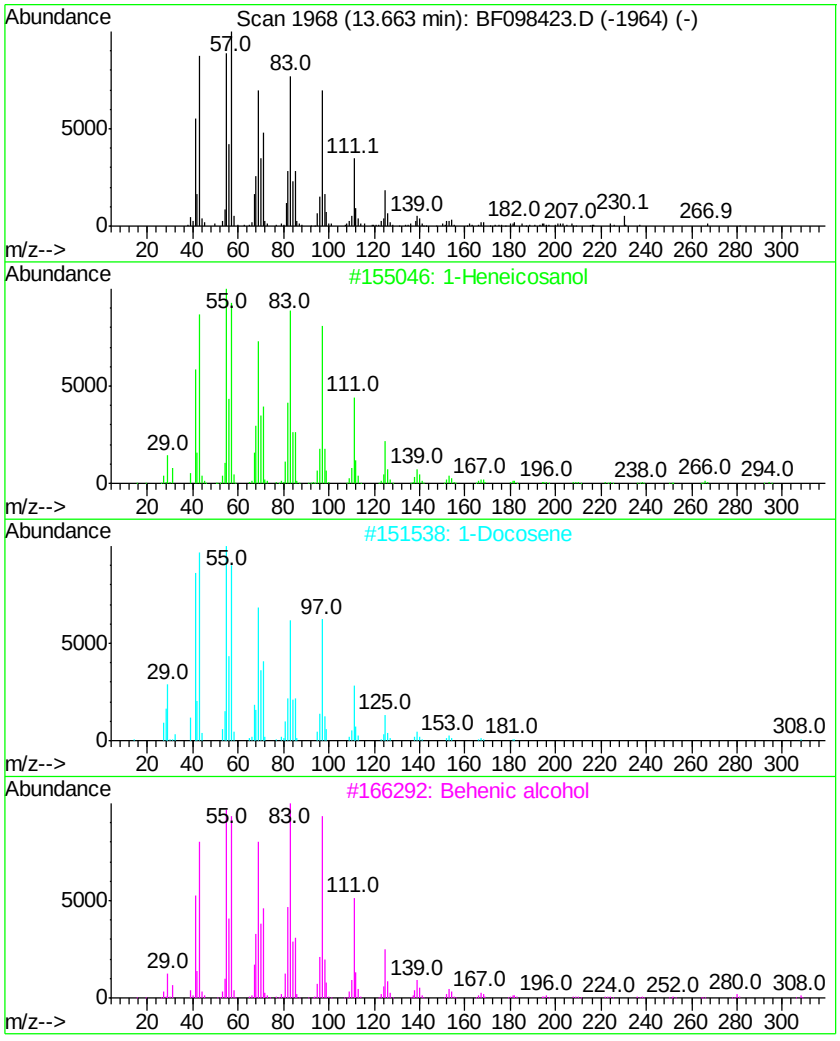
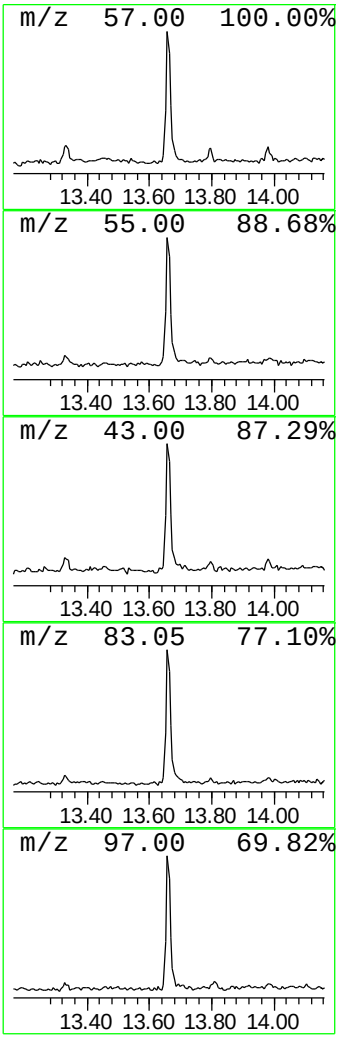
****

Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	8.64 ng	540781	Chrysene-d12	13.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	1-Docosene	308	C22H44	001599-67-3	94
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91





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Data File : BF098423.D
Acq On : 12 Sep 2017 1:02
Operator : SJ/JU
Sample : I5138-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-UTS-TS006-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

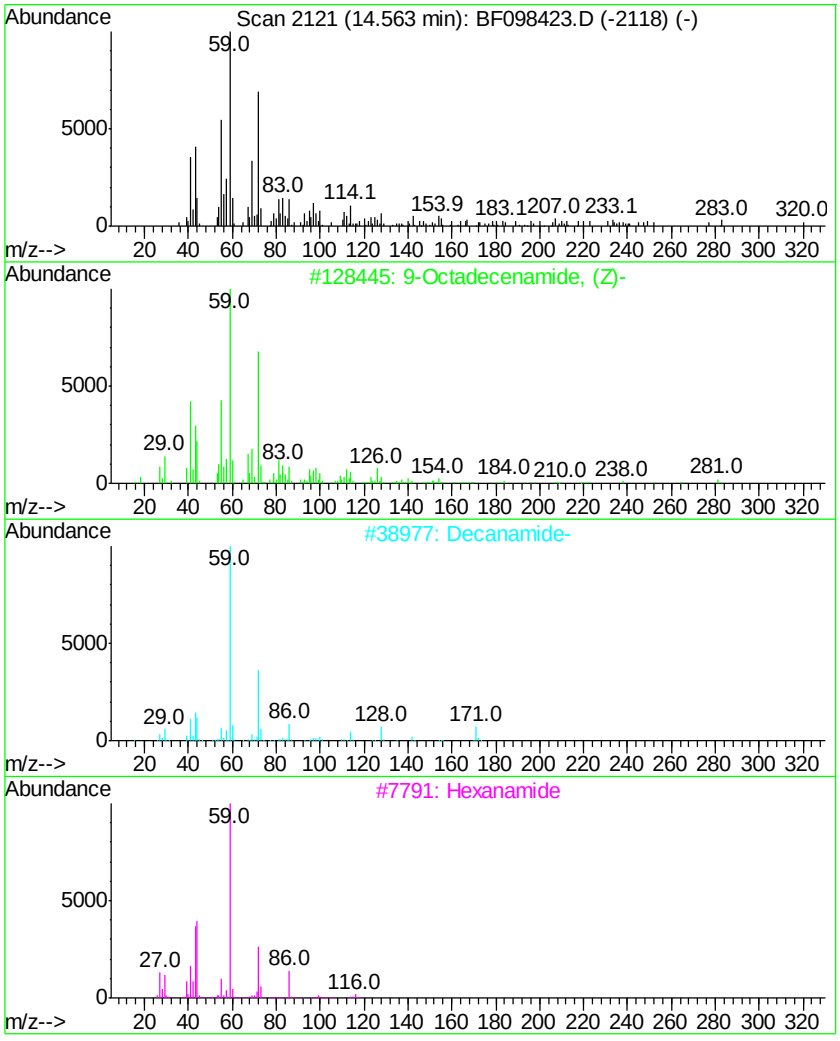
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

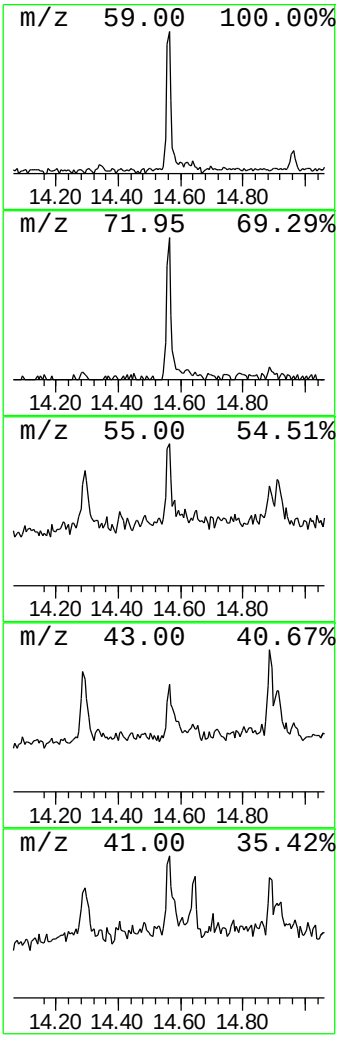
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	2.45 ng	142400	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
2	Decanamide-	171	C10H21NO	002319-29-1	80
3	Hexanamide	115	C6H13NO	000628-02-4	53
4	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50
5	Silane, hexyl-	116	C6H16Si	001072-14-6	50





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Data File : BF098423.D
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

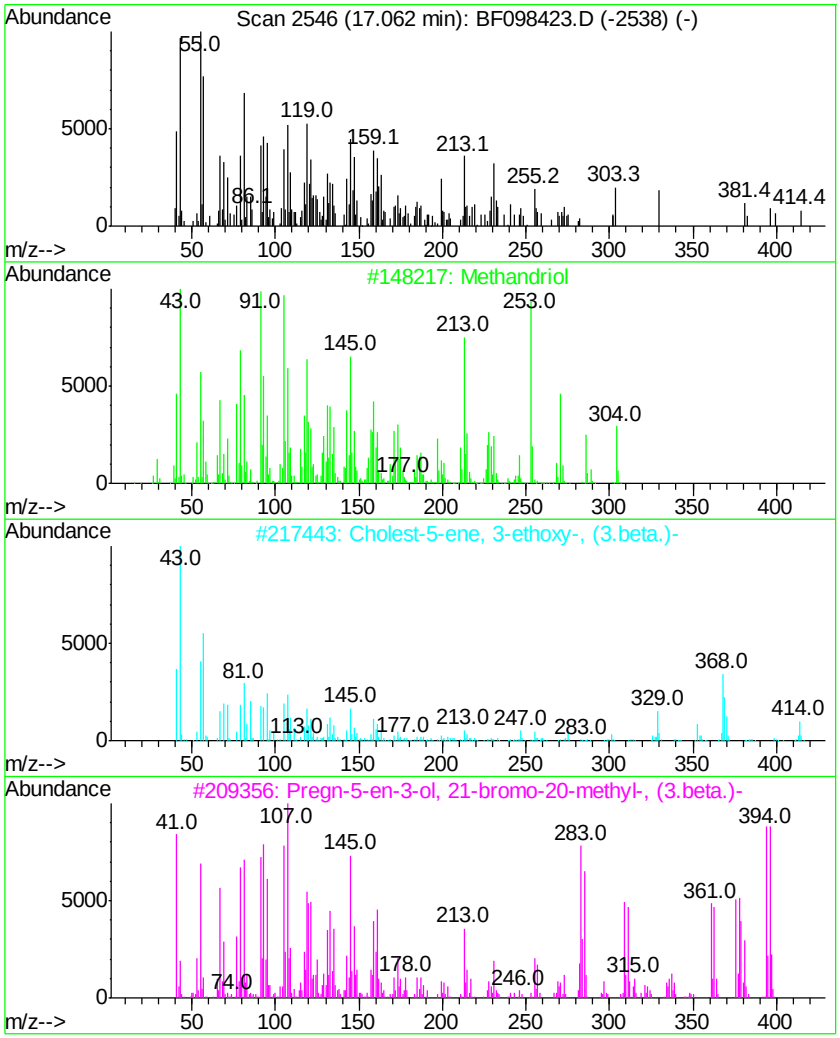
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

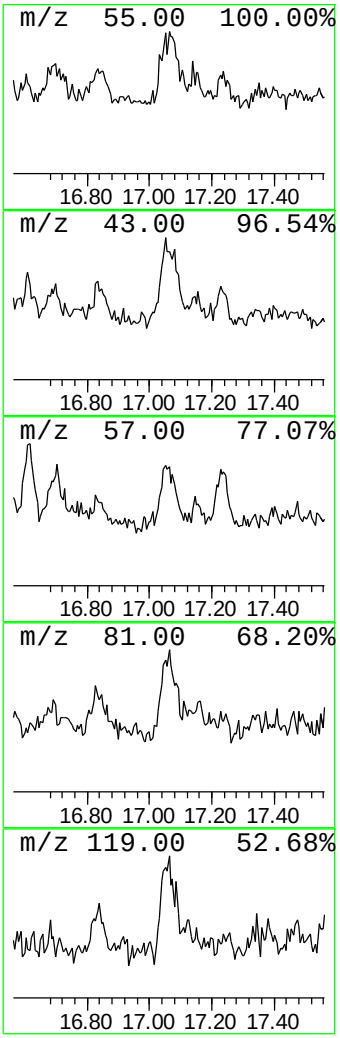
****

Peak Number 8 unknown17.06 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.06	7.89 ng	458526	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methandriol	304	C20H32O2	000521-10-8	37
2	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	28
3	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	25
4	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	17
5	Benzeneethanol, .alpha.-methyl-3...	178	C12H18O	054518-11-5	14





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF091117\
Data File : BF098423.D
Acq On : 12 Sep 2017 1:02
Operator : SJ/JU
Sample : I5138-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-UTS-TS006-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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...	4.87	14.7	ng	1171150	1	6.67	1592770	20.0
unknown6.45	6.45	86.3	ng	6873140	1	6.67	1592770	20.0
9,12-Octadecadien...	12.26	2.4	ng	238695	4	11.18	2011160	20.0
Phenol, 4,4'-(1-m...	12.65	2.3	ng	146212	5	13.81	1252370	20.0
1-Heneicosanol	13.66	8.6	ng	540781	5	13.81	1252370	20.0
9-Octadecenamide,...	14.56	2.5	ng	142400	6	15.21	1162400	20.0
unknown17.06	17.06	7.9	ng	458526	6	15.21	1162400	20.0