LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090618\
Data File : BF108840.D
Acq On : 6 Sep 2018 22:58
Operator : JU/SJ
Sample : J4803-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q2-I5

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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	4.931	437	441	447	rVB	122487	146670	3.64%	0.394%
2	5.342	506	511	514	rBV	3627328	3399382	84.44%	9.131%
3	6.366	680	685	688	rBV	3864900	3523206	87.52%	9.463%
4	6.501	704	708	711	rBV	3989414	3580228	88.94%	9.617%
5	6.566	716	719	722	rBV	111795	88049	2.19%	0.237%
6	6.736	744	748	751	rBV	1787365	1414829	35.15%	3.800%
7	6.889	770	774	778	rVB	3238429	2858548	71.01%	7.678%
8	7.289	837	842	845	rBV	2390376	2257014	56.07%	6.062%
9	8.013	961	965	969	rBV	1943806	1749639	43.46%	4.700%
10	9.089	1144	1148	1152	rBV	4483667	4025567	100.00%	10.813%
11	9.219	1167	1170	1173	rVB	57238	54519	1.35%	0.146%
12	9.483	1211	1215	1218	rBV	1456506	1067753	26.52%	2.868%
13	9.766	1259	1263	1267	rBV	2184182	1791316	44.50%	4.812%
14	10.548	1392	1396	1399	rBV	1977442	1890561	46.96%	5.078%
15	10.648	1410	1413	1416	rBV	90862	84223	2.09%	0.226%
16	11.242	1510	1514	1517	rBV	1744498	1444548	35.88%	3.880%
17	11.783	1603	1606	1615	rVB	389497	377190	9.37%	1.013%
18	12.442	1716	1718	1721	rBV	63623	63801	1.58%	0.171%
19	12.565	1736	1739	1745	rBV3	110646	133456	3.32%	0.358%
20	12.824	1779	1783	1786	rBV	3198099	2821217	70.08%	7.578%
21	13.736	1935	1938	1946	rVB	242933	272436	6.77%	0.732%
22	13.865	1956	1960	1963	rBV	1805784	1520987	37.78%	4.085%
23	14.624	2086	2089	2092	rBV	238896	259486	6.45%	0.697%
24	14.724	2103	2106	2110	rVB	842066	754823	18.75%	2.027%
25	15.271	2194	2199	2204	rBV	1415017	1650412	41.00%	4.433%

Sum of corrected areas: 37229860

LSC Report - Integrated Chromatogram

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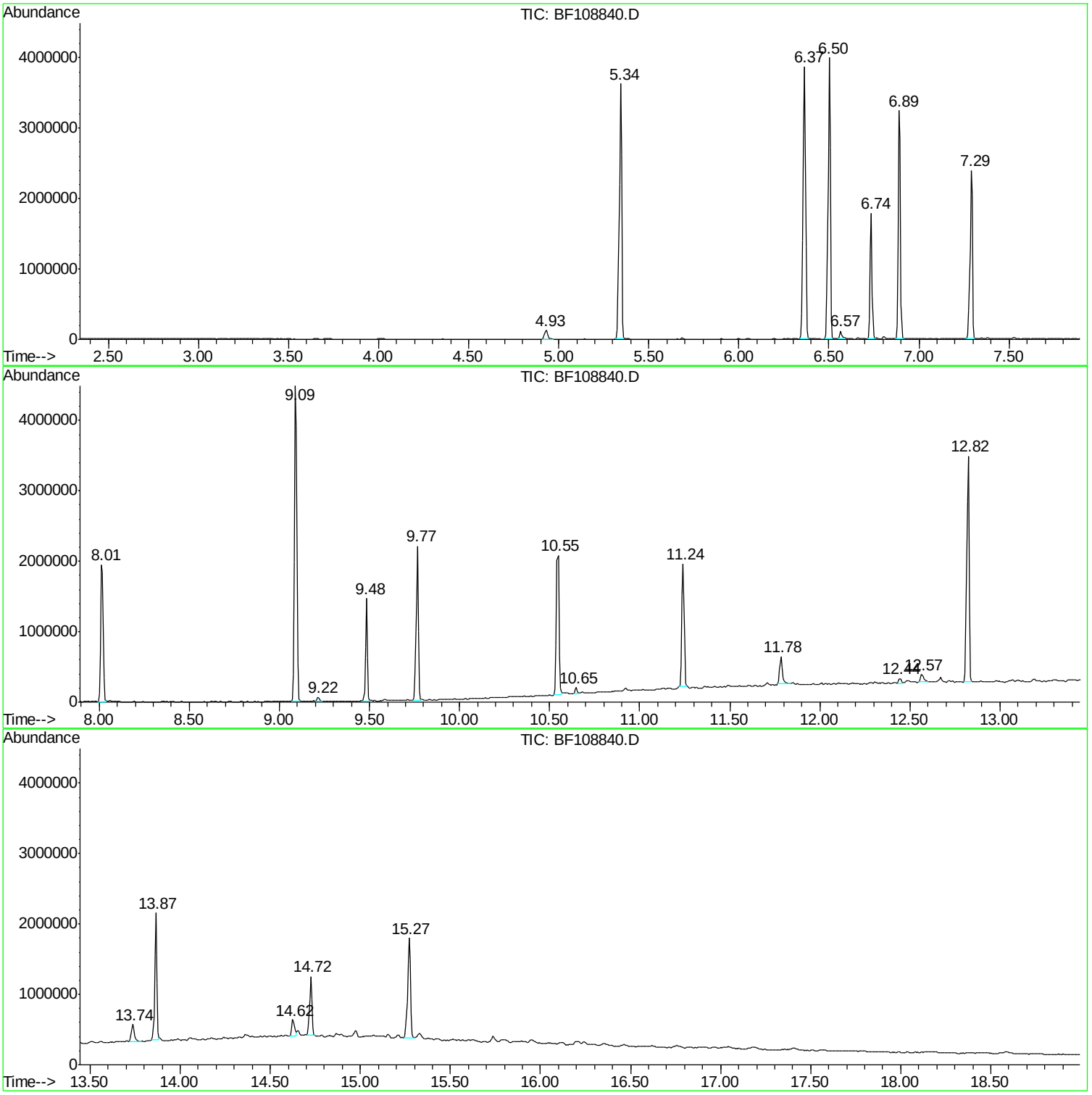
Operator : JU/SJ
Sample : J4803-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q2-I5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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

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Data File : BF108840.D
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Operator : JU/SJ
Sample : J4803-13
Misc :
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Instrument : BNA_F
ClientSampleId : EP1-Q2-I5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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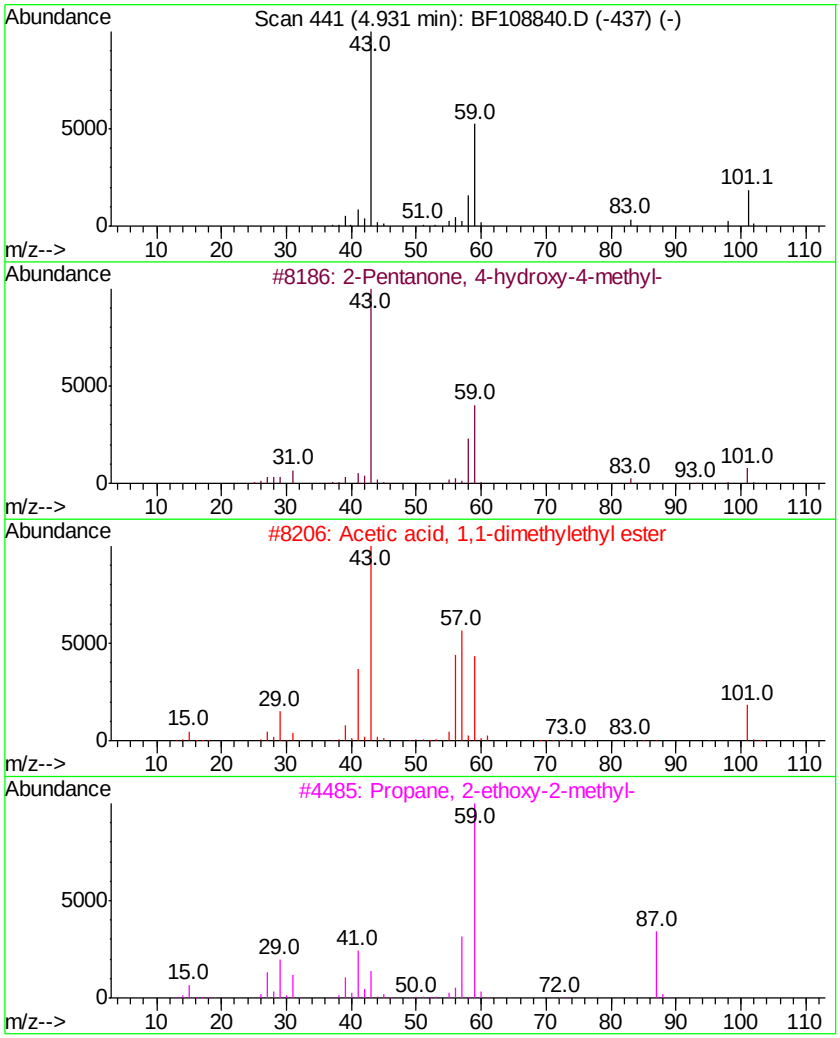
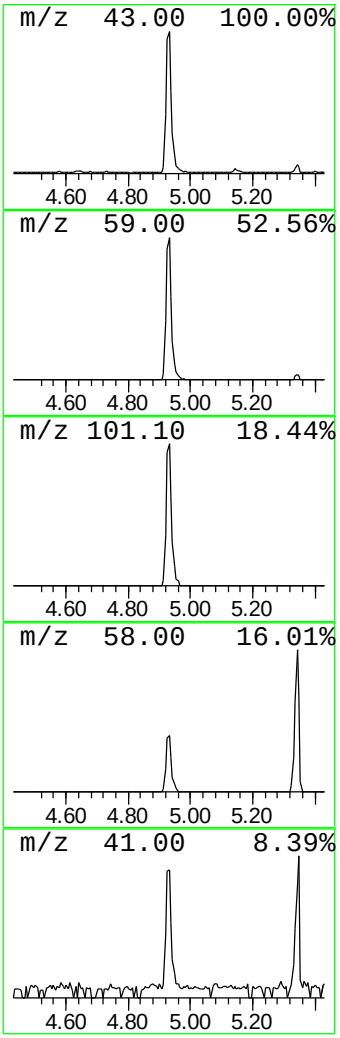
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	2.07 ng	146670	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

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Operator : JU/SJ
Sample : J4803-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q2-I5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

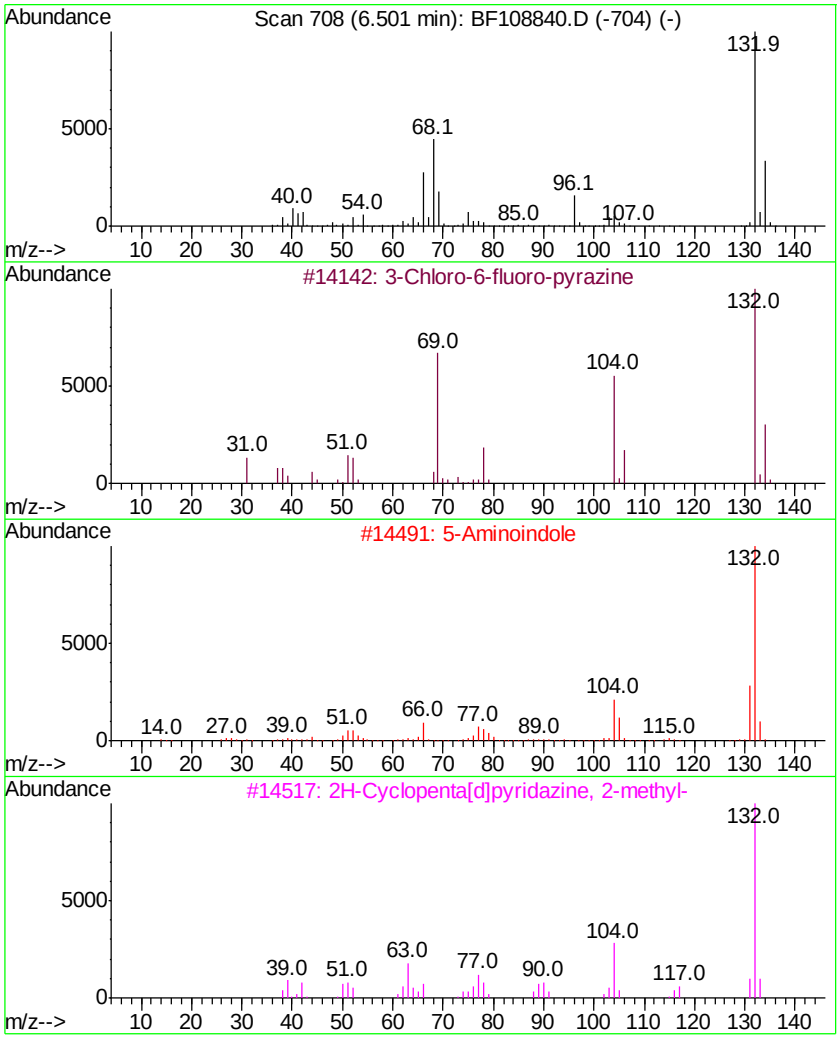
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

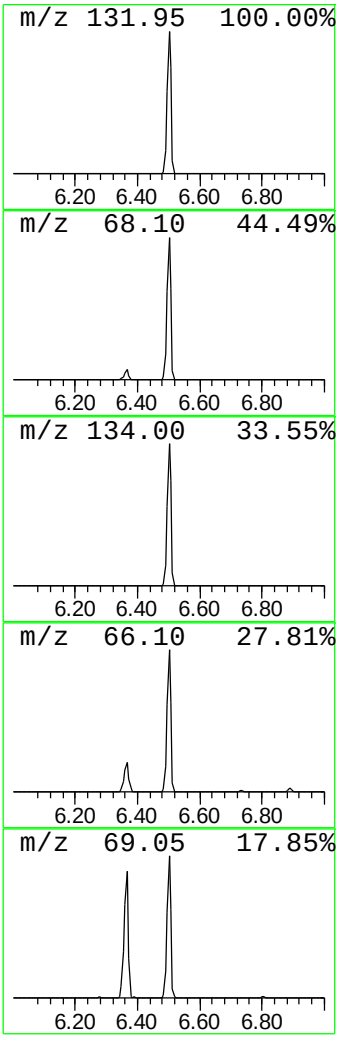
****

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	50.61 ng	3580230	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090618\
Data File : BF108840.D
Acq On : 6 Sep 2018 22:58
Operator : JU/SJ
Sample : J4803-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q2-I5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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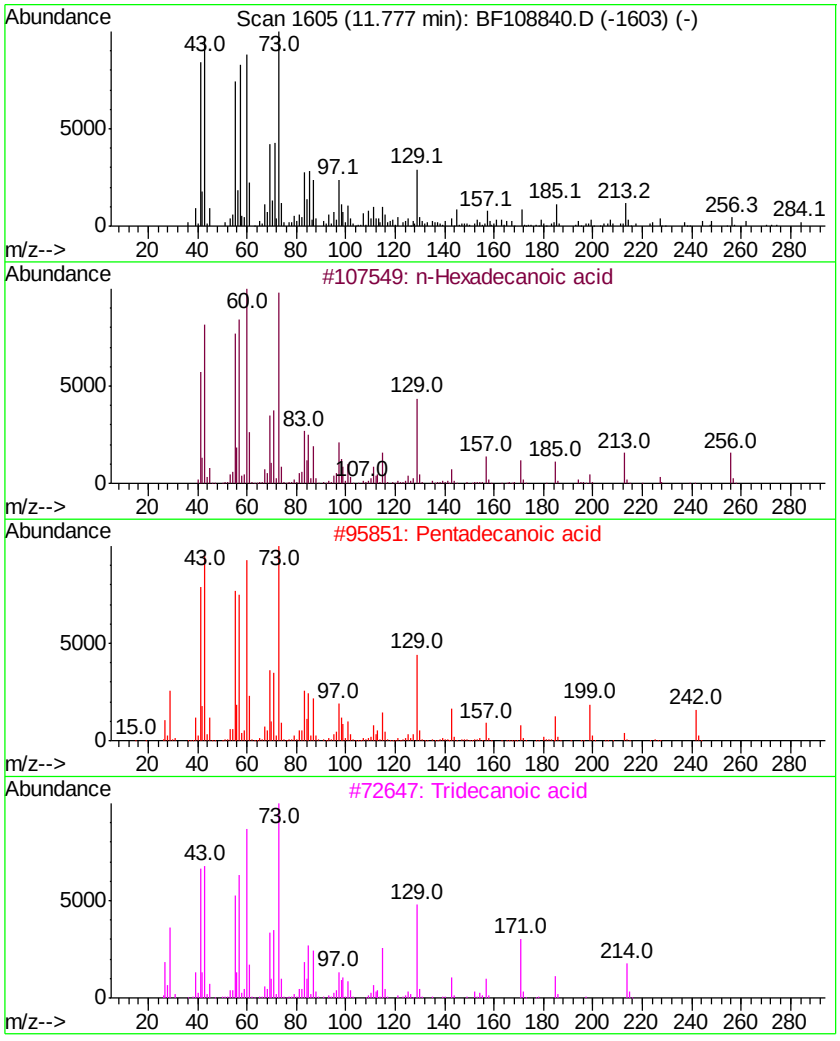
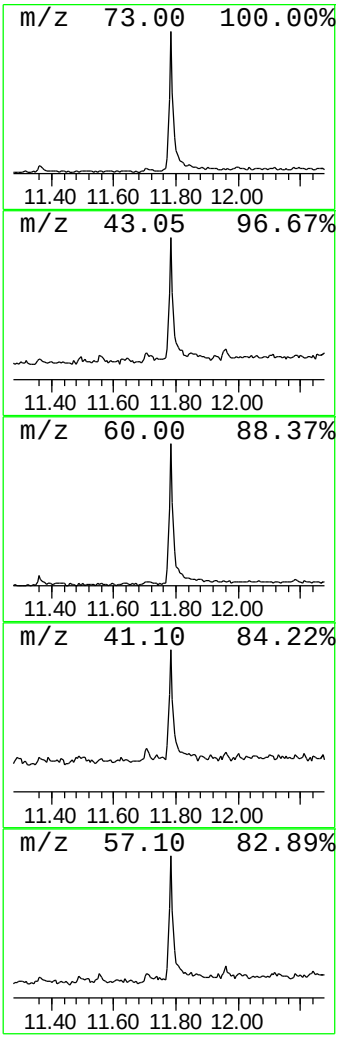
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	5.22 ng	377190	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Octadecanoic acid	284	C18H36O2	000057-11-4	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	81





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090618\
Data File : BF108840.D
Acq On : 6 Sep 2018 22:58
Operator : JU/SJ
Sample : J4803-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q2-I5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

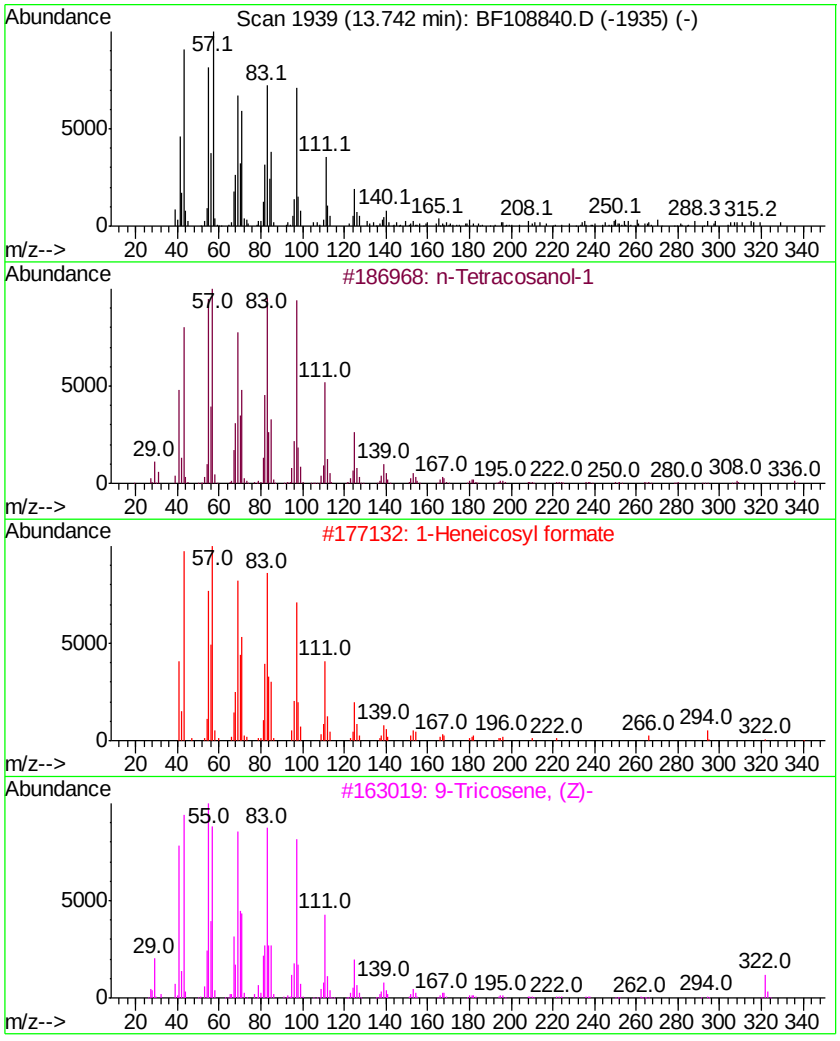
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

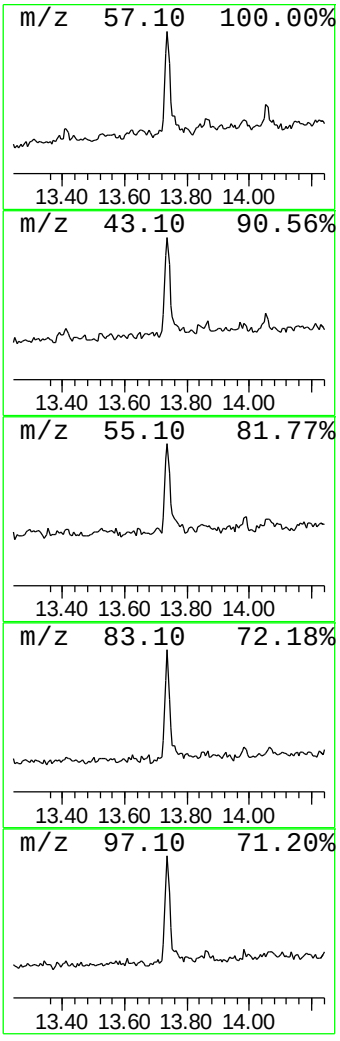
****

Peak Number 5 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	3.58 ng	272436	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	9-Tricosene, (Z)-	322	C23H46	027519-02-4	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090618\
Data File : BF108840.D
Acq On : 6 Sep 2018 22:58
Operator : JU/SJ
Sample : J4803-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP1-Q2-I5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

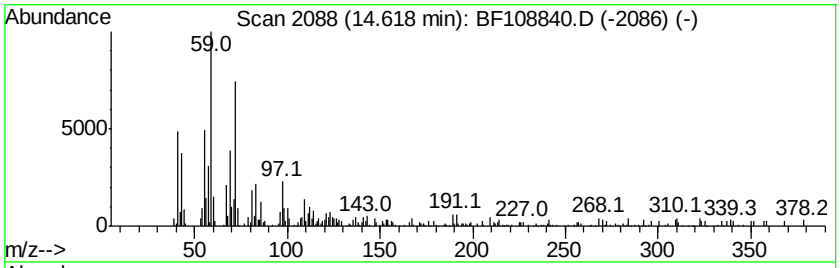
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

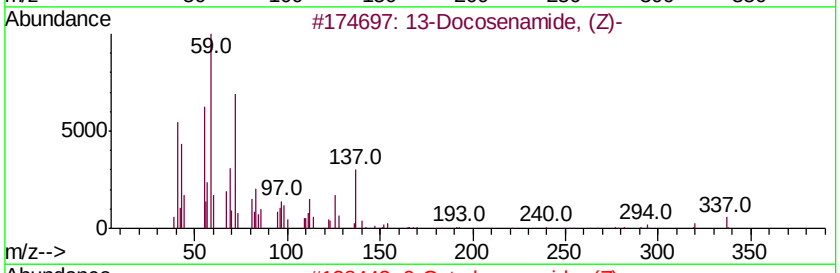
****

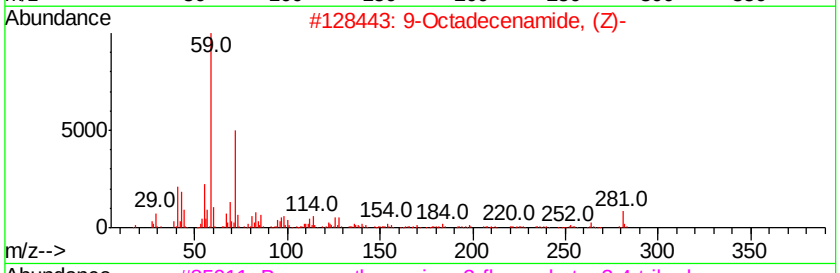
Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 6

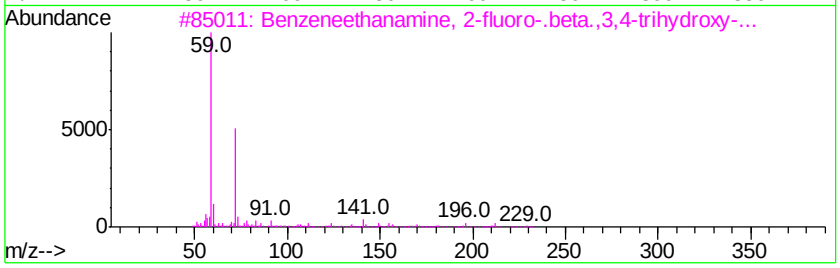
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	3.14 ng	259486	Perylene-d12	15.27

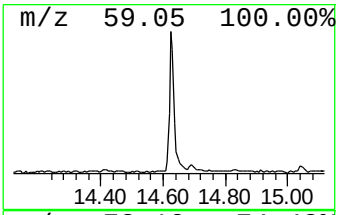
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	83
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	59
4	Dodecanamide	199	C12H25NO	001120-16-7	43
5	Tetradecanamide	227	C14H29NO	000638-58-4	43

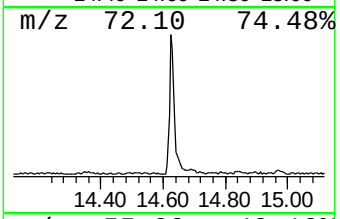


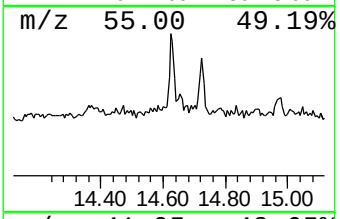


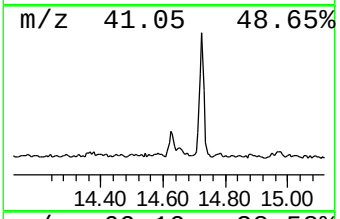


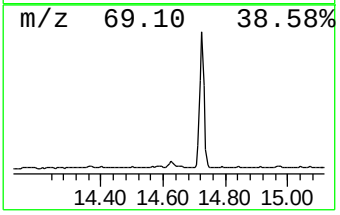












Library Search Compound Report

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

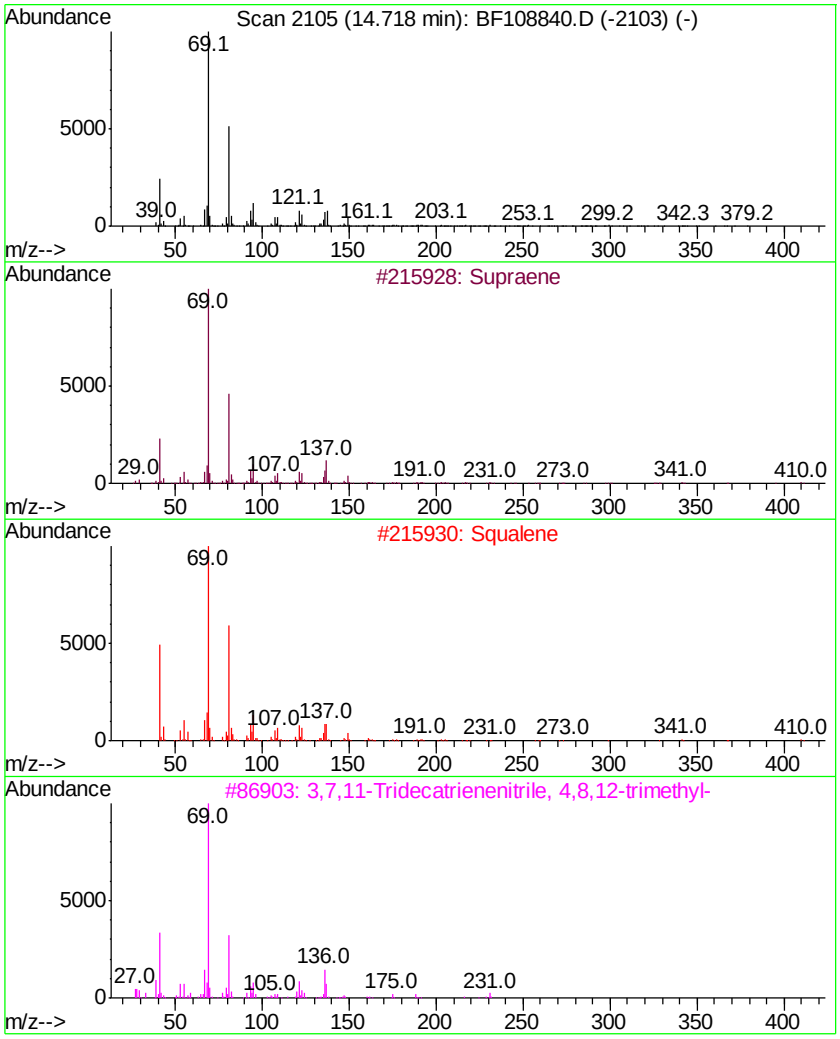
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

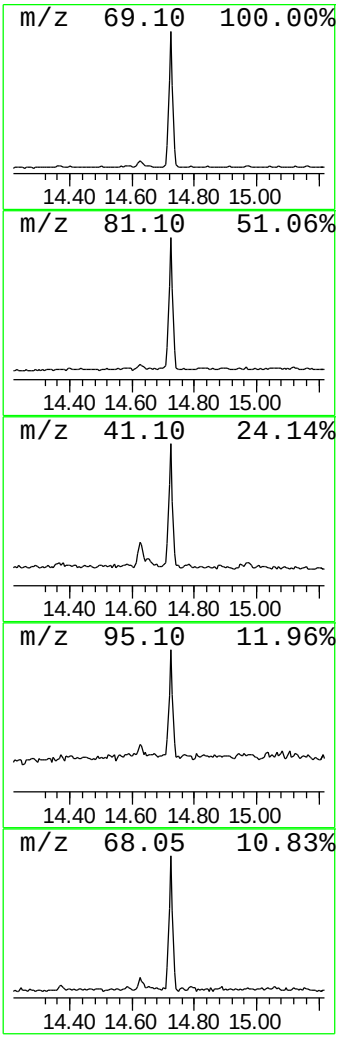
****

Peak Number 7 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	9.15 ng	754823	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	72
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.93	2.1	ng	146670	1	6.74	1414830	20.0
unknown6.50	6.50	50.6	ng	3580230	1	6.74	1414830	20.0
n-Hexadecanoic acid	11.78	5.2	ng	377190	4	11.24	1444550	20.0
n-Tetracosanol-1	13.74	3.6	ng	272436	5	13.87	1520990	20.0
13-Docosenamide, ...	14.62	3.1	ng	259486	6	15.27	1650410	20.0
Supraene	14.72	9.2	ng	754823	6	15.27	1650410	20.0