LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030718\
Data File : BF103501.D
Acq On : 7 Mar 2018 15:21
Operator : SJ/JU
Sample : J1699-65
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B19

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-BF022218.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	2.140	4	9	19	rVB	196404	299984	9.74%	1.102%
2	5.104	509	513	525	rBV	61202	107910	3.50%	0.396%
3	5.492	575	579	604	rBV	2001805	2990361	97.07%	10.983%
4	6.498	747	750	770	rBV	2069270	3047385	98.92%	11.193%
5	6.633	770	773	798	rVB	2633794	3070020	99.65%	11.276%
6	6.863	809	812	828	rBV	689623	840705	27.29%	3.088%
7	7.016	835	838	864	rVB	1990547	2234794	72.54%	8.208%
8	7.433	905	909	933	rBV	1408911	2082843	67.61%	7.650%
9	8.151	1027	1031	1055	rBV	757988	1198945	38.92%	4.404%
10	9.222	1209	1213	1223	rBV	2836106	3080656	100.00%	11.315%
11	9.292	1223	1225	1230	rVB	32304	37308	1.21%	0.137%
12	9.622	1275	1281	1286	rBV	116428	140810	4.57%	0.517%
13	9.822	1311	1315	1319	rBV	78990	68172	2.21%	0.250%
14	9.904	1325	1329	1343	rBV	1041483	1163133	37.76%	4.272%
15	10.316	1396	1399	1402	rVB	100904	80441	2.61%	0.295%
16	10.539	1432	1437	1439	rBV	26913	35740	1.16%	0.131%
17	10.704	1461	1465	1477	rBV	1204964	1594848	51.77%	5.858%
18	10.792	1477	1480	1485	rVB	90739	94991	3.08%	0.349%
19	11.239	1553	1556	1559	rBV	39261	35545	1.15%	0.131%
20	11.404	1580	1584	1597	rBV	857967	993529	32.25%	3.649%
21	11.768	1643	1646	1650	rBV	179267	141169	4.58%	0.519%
22	12.457	1760	1763	1765	rBV	178774	170133	5.52%	0.625%
23	12.480	1765	1767	1775	rVV	330530	320808	10.41%	1.178%
24	12.563	1778	1781	1785	rVB	88154	74020	2.40%	0.272%
25	12.986	1848	1853	1864	rBV	2020905	1992925	64.69%	7.320%
26	13.862	1999	2002	2010	rBV	89132	128453	4.17%	0.472%
27	14.057	2031	2035	2044	rBV	605544	654531	21.25%	2.404%
28	15.562	2287	2291	2301	rVB2	334005	545976	17.72%	2.005%

Sum of corrected areas: 27226135

LSC Report - Integrated Chromatogram

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Data File : BF103501.D
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Operator : SJ/JU
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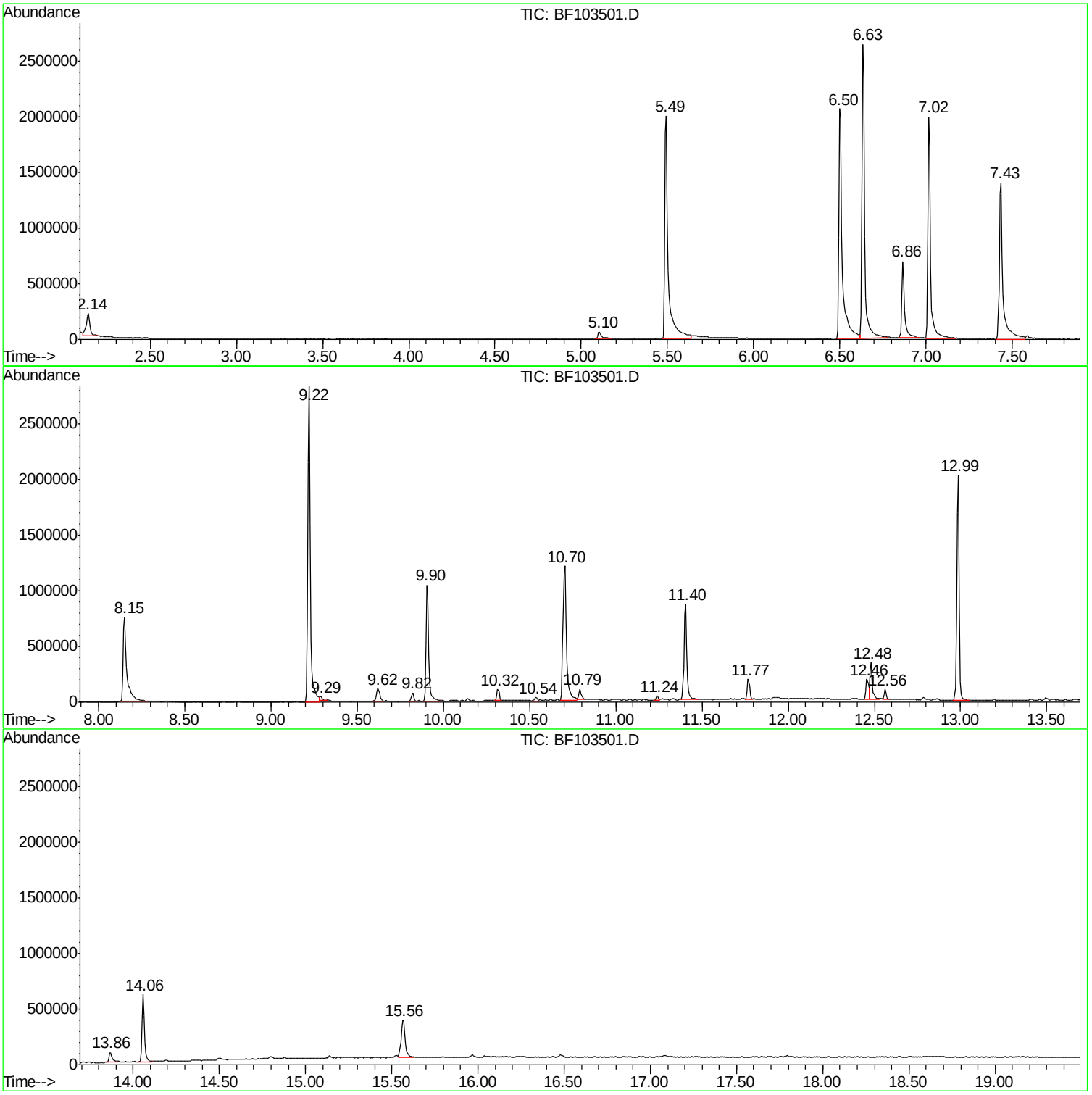
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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\BF030718\
Data File : BF103501.D
Acq On : 7 Mar 2018 15:21
Operator : SJ/JU
Sample : J1699-65
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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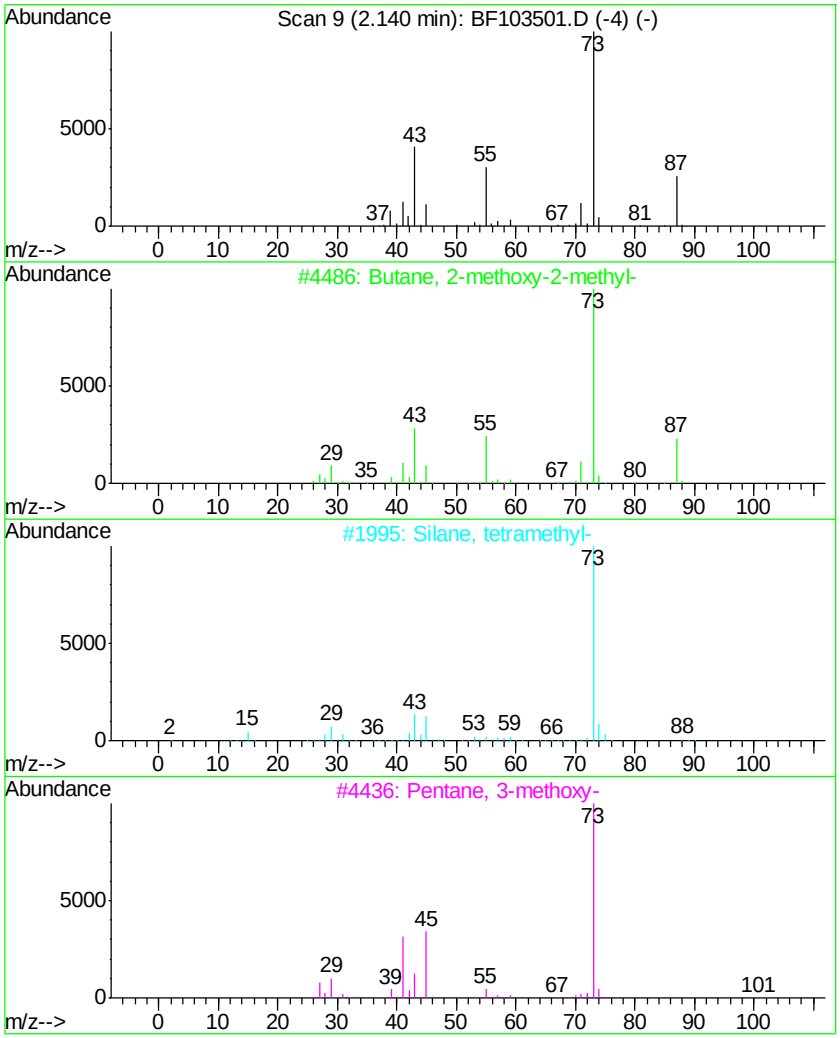
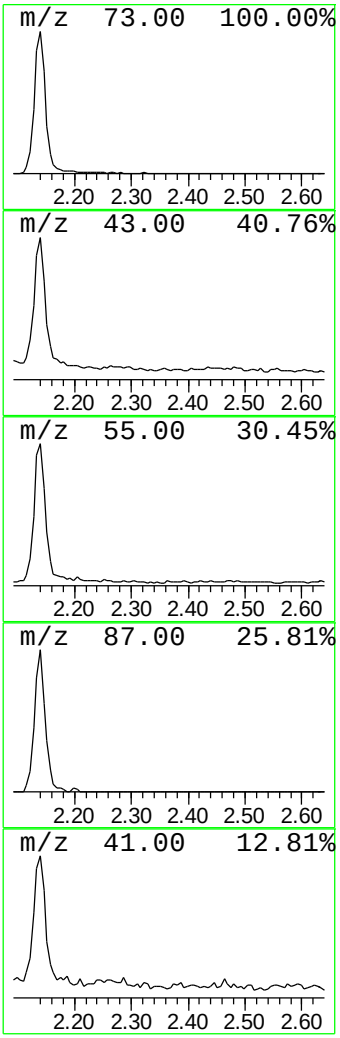
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	7.14 ng	299984	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BF103501.D
Acq On : 7 Mar 2018 15:21
Operator : SJ/JU
Sample : J1699-65
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

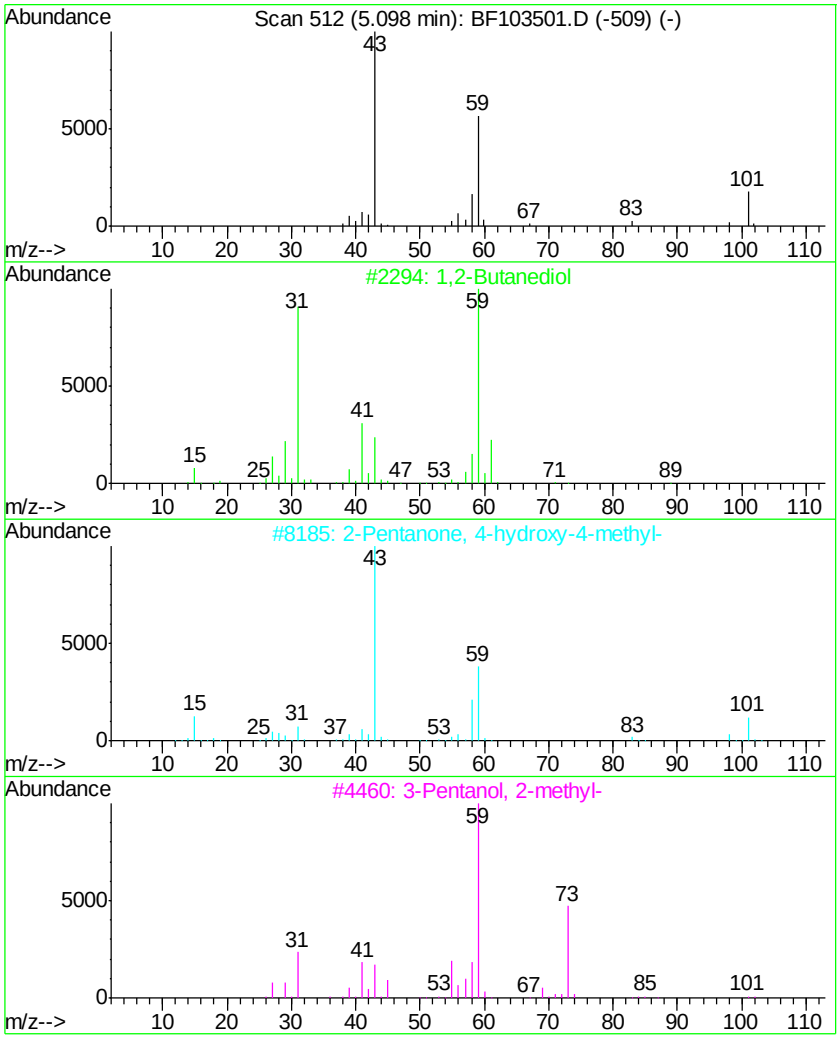
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

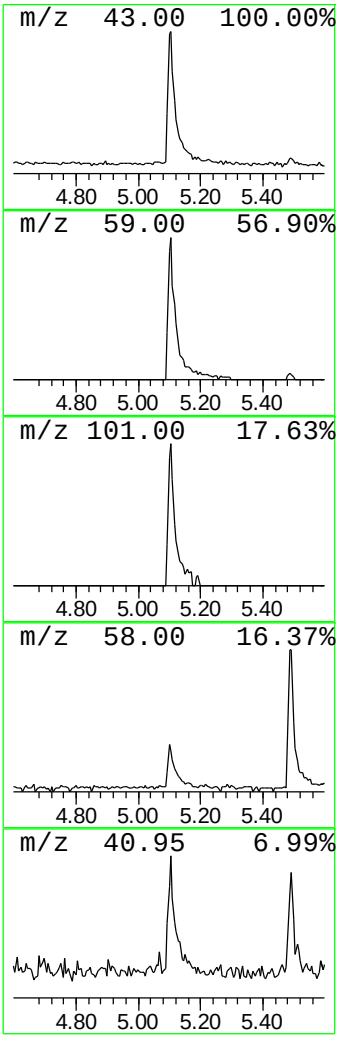
****

Peak Number 2 unknown5.10 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	2.57 ng	107910	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Butanediol	90	C4H10O2	000584-03-2	37
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	33
3	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9
4	2-Pentanol, 2,3-dimethyl-	116	C7H16O	004911-70-0	9
5	3-Pentanol	88	C5H12O	000584-02-1	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030718\
Data File : BF103501.D
Acq On : 7 Mar 2018 15:21
Operator : SJ/JU
Sample : J1699-65
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

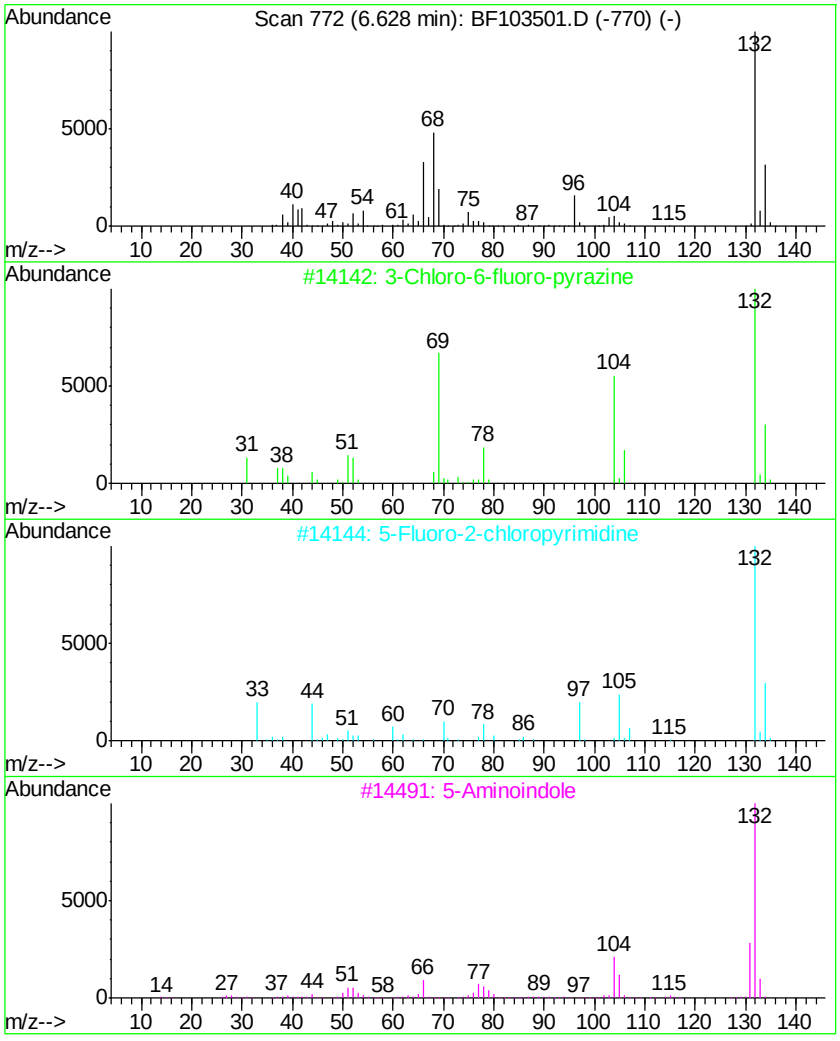
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

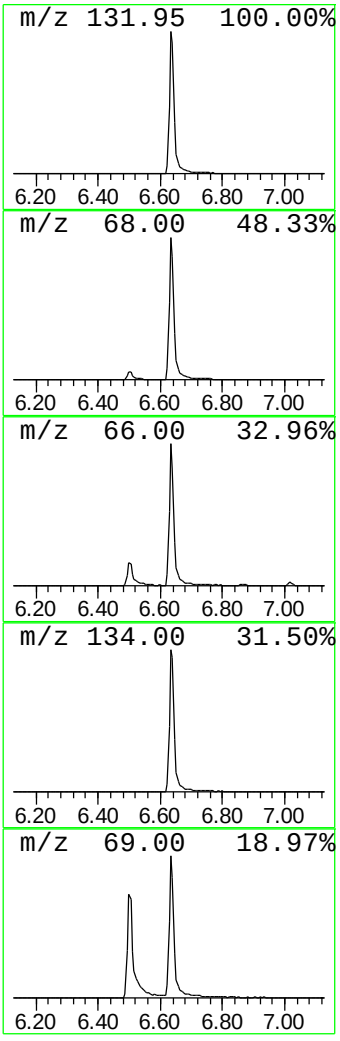
****

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	73.03 ng	3070020	1,4-Dichlorobenzene-d4	6.86

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	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030718\
Data File : BF103501.D
Acq On : 7 Mar 2018 15:21
Operator : SJ/JU
Sample : J1699-65
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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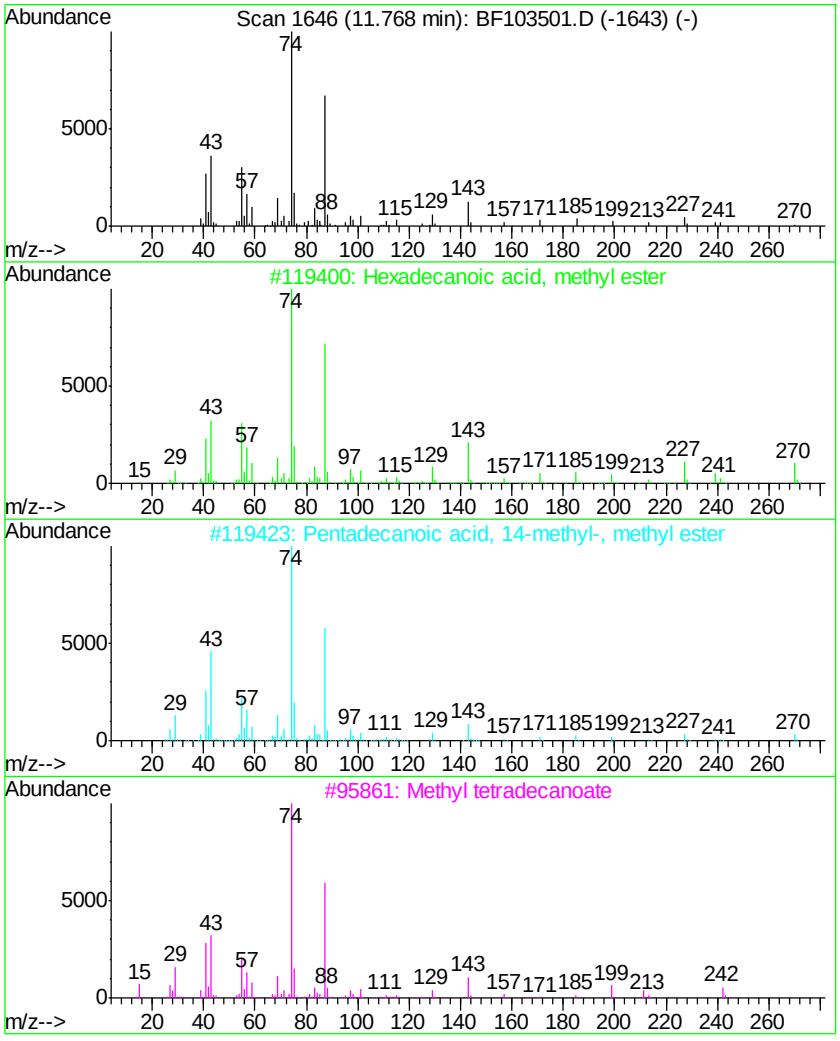
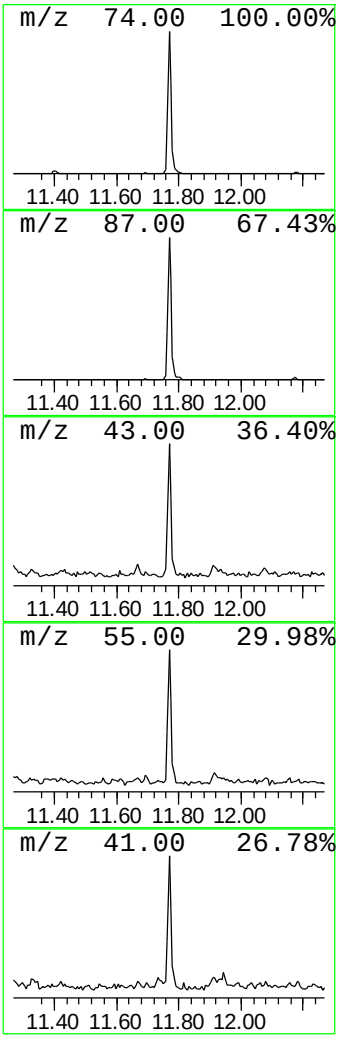
Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	2.84 ng	141169	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	90
4	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	90
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030718\
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Operator : SJ/JU
Sample : J1699-65
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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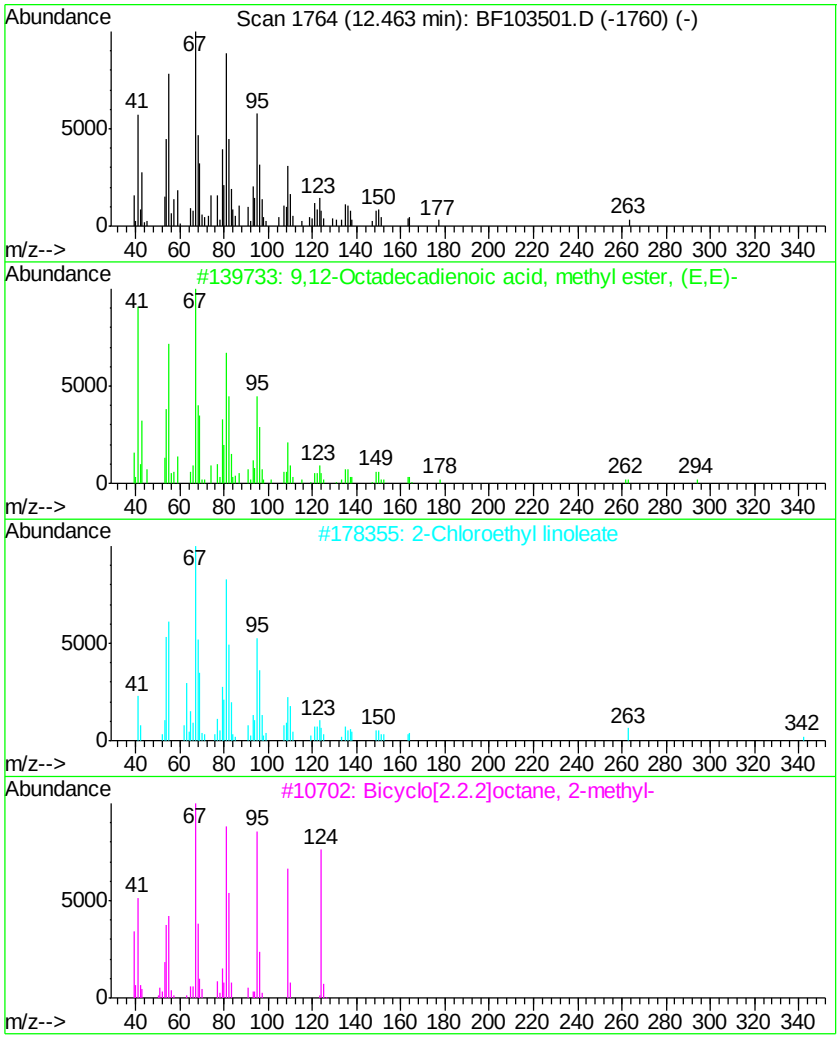
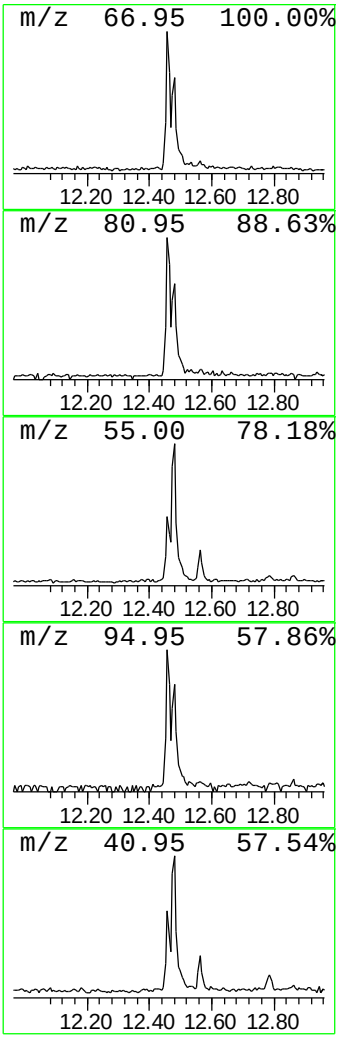
Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	3.42 ng	170133	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	93
2	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	90
3	Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	87
4	11,14-Eicosadienoic acid, methyl...	322	C21H38O2	002463-02-7	76
5	7-Hexadecyne	222	C16H30	074685-28-2	72





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Sample : J1699-65
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

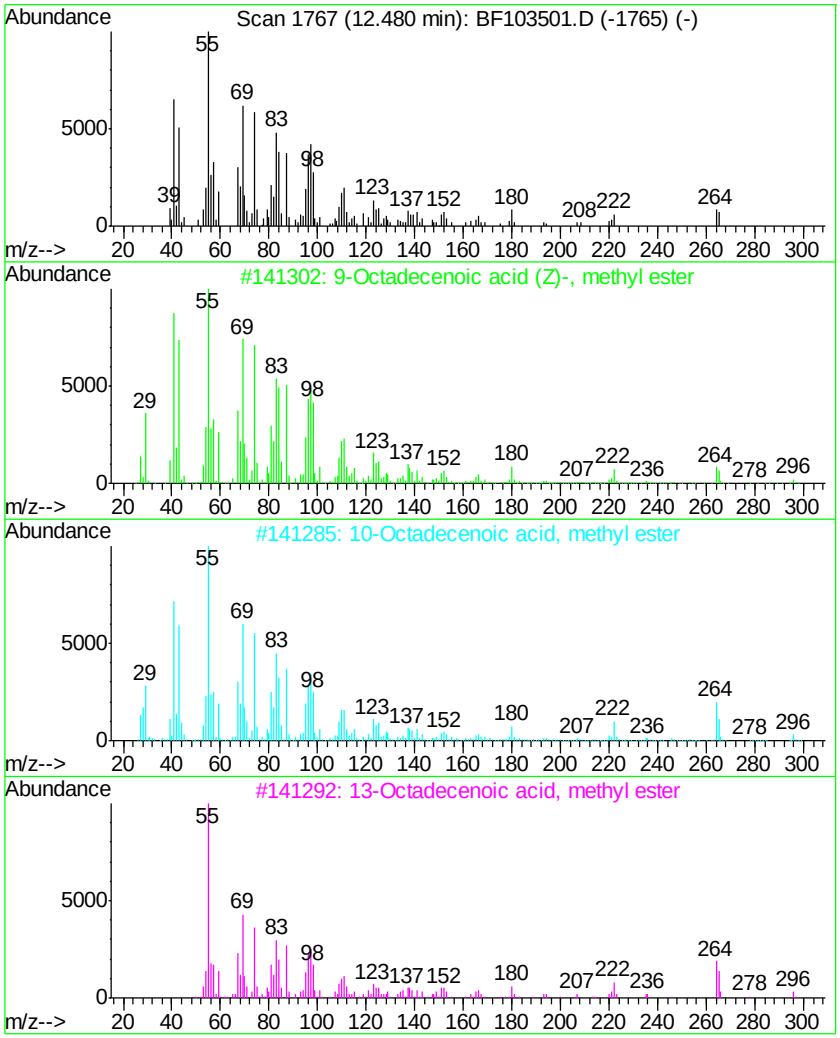
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

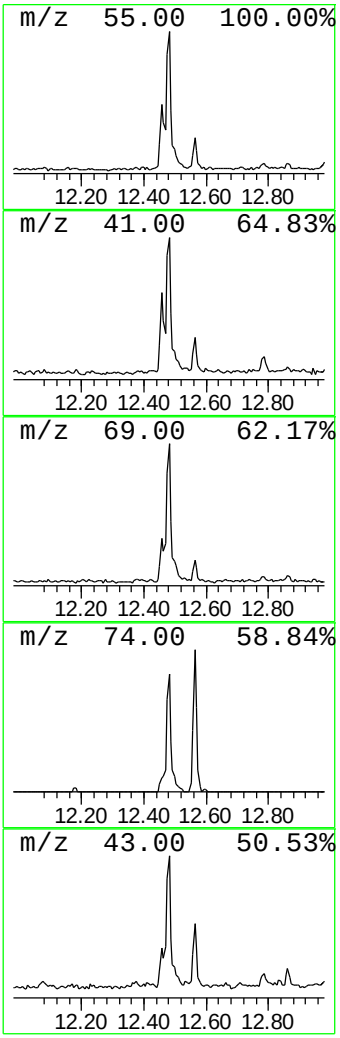
****

Peak Number 7 9-Octadecenoic acid (Z)-, m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	6.46 ng	320808	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
5	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	87





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Sample : J1699-65
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Instrument : BNA_F
ClientSampleId : B19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

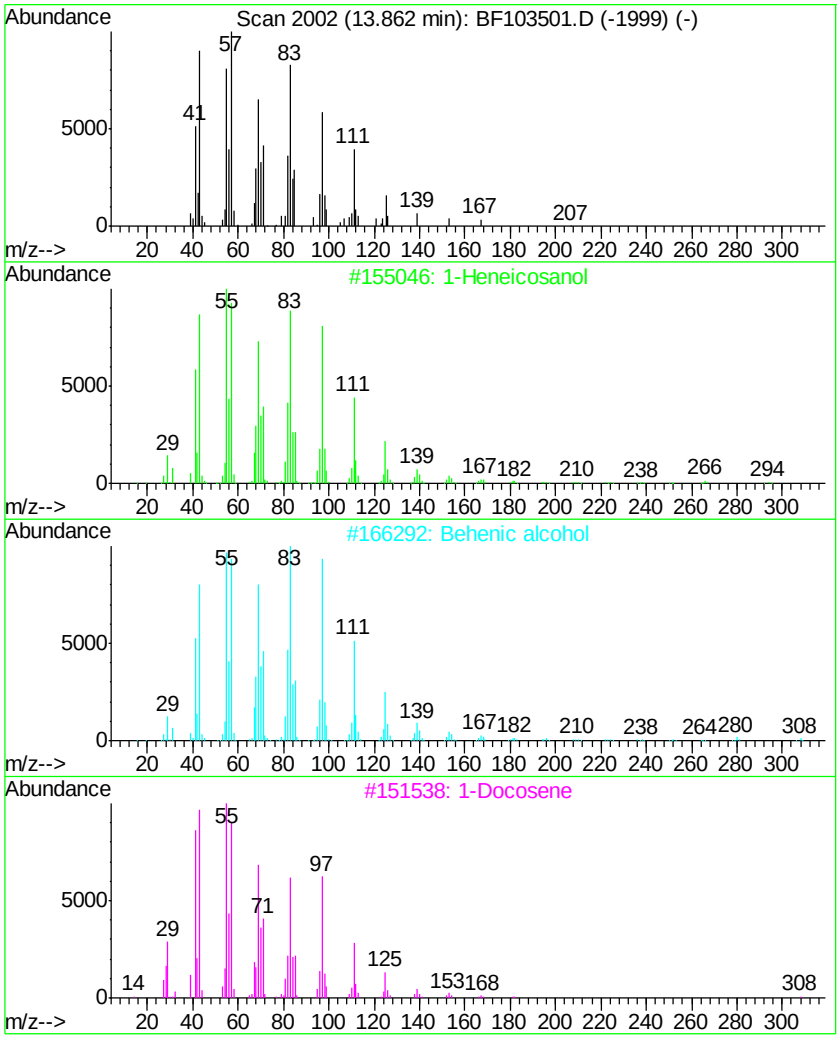
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

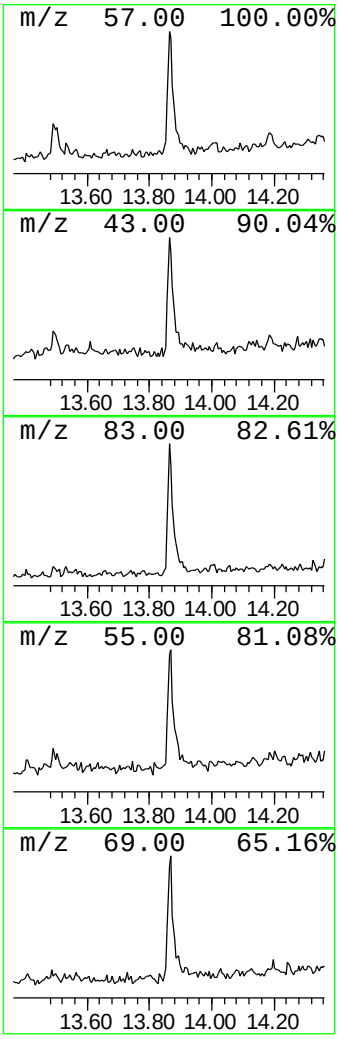
****

Peak Number 8 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	3.93 ng	128453	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	1-Docosene	308	C22H44	001599-67-3	91
4	Octacosanol	410	C28H58O	000557-61-9	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





Tentatively Identified Compound (LSC) summary

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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
Butane, 2-methoxy...	2.14	7.1	ng	299984	1	6.86	840705	20.0
unknown5.10	5.10	2.6	ng	107910	1	6.86	840705	20.0
unknown6.63	6.63	73.0	ng	3070020	1	6.86	840705	20.0
Hexadecanoic acid...	11.77	2.8	ng	141169	4	11.40	993529	20.0
9,12-Octadecadien...	12.46	3.4	ng	170133	4	11.40	993529	20.0
9-Octadecenoic ac...	12.48	6.5	ng	320808	4	11.40	993529	20.0
1-Heneicosanol	13.86	3.9	ng	128453	5	14.06	654531	20.0