LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120617\
Data File : BF101175.D
Acq On : 6 Dec 2017 18:39
Operator : SJ/JU
Sample : I6685-03 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-120517-B

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-BF113017.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	5.057	503	505	511	rBV	6662	6943	2.43%	0.204%
2	5.457	570	573	586	rBV	136680	141526	49.54%	4.154%
3	6.475	742	746	757	rBV	138749	145951	51.09%	4.284%
4	6.616	767	770	778	rBB	194479	160516	56.19%	4.712%
5	6.845	806	809	817	rBB	275595	219975	77.00%	6.457%
6	6.998	832	835	843	rBB	140792	125990	44.10%	3.698%
7	7.410	902	905	913	rBV	97801	87731	30.71%	2.575%
8	8.128	1024	1027	1034	rBV	337375	272196	95.28%	7.990%
9	9.198	1206	1209	1217	rBV	182875	164587	57.61%	4.831%
10	9.598	1274	1277	1282	rVB2	10666	8800	3.08%	0.258%
11	9.804	1310	1312	1317	rBV2	8908	8443	2.96%	0.248%
12	9.886	1322	1326	1333	rBV	329563	285683	100.00%	8.386%
13	10.304	1394	1397	1399	rBV	9639	7158	2.51%	0.210%
14	10.528	1432	1435	1438	rBV	3350	3281	1.15%	0.096%
15	10.675	1457	1460	1468	rVB	81555	72343	25.32%	2.124%
16	10.780	1475	1478	1482	rBV	6358	7848	2.75%	0.230%
17	11.104	1529	1533	1536	rBV	74162	58769	20.57%	1.725%
18	11.227	1550	1554	1555	rBV	4816	4012	1.40%	0.118%
19	11.374	1575	1579	1584	rBV	313943	258844	90.61%	7.598%
20	11.433	1588	1589	1595	rVB	2375	3821	1.34%	0.112%
21	11.716	1634	1637	1641	rBV3	1967	3532	1.24%	0.104%
22	11.757	1641	1644	1647	rBV	104464	90478	31.67%	2.656%
23	11.886	1663	1666	1670	rBV4	6913	7004	2.45%	0.206%
24	11.951	1674	1677	1680	rBV	35599	27040	9.47%	0.794%
25	12.439	1757	1760	1762	rBV	278294	235721	82.51%	6.919%
26	12.463	1762	1764	1767	rVB	281214	208517	72.99%	6.121%
27	12.545	1775	1778	1781	rBV2	58347	45621	15.97%	1.339%
28	12.598	1783	1787	1791	rBV6	6400	12045	4.22%	0.354%
29	12.727	1805	1809	1811	rBV	8733	6858	2.40%	0.201%
30	12.786	1814	1819	1821	rBV5	6299	9968	3.49%	0.293%
31	12.821	1822	1825	1827	rBV4	4955	4750	1.66%	0.139%
32	12.904	1836	1839	1841	rBV4	3006	3512	1.23%	0.103%
33	12.957	1844	1848	1851	rVV	161684	140365	49.13%	4.120%
34	13.033	1856	1861	1864	rBV6	5660	9631	3.37%	0.283%

LSC Area Percent Report

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Data File : BF101175.D
Acq On : 6 Dec 2017 18:39
Operator : SJ/JU
Sample : I6685-03 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-120517-B

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-BF113017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.145	1875	1880	1883	rBV7	9109	18385	6.44%	0.540%
36	13.180	1883	1886	1890	rVV3	5417	7110	2.49%	0.209%
37	13.274	1899	1902	1904	rVB4	4896	5408	1.89%	0.159%
38	13.398	1921	1923	1924	rVB2	5686	3280	1.15%	0.096%
39	13.604	1957	1958	1961	rBV3	4744	4309	1.51%	0.126%
40	13.839	1996	1998	2003	rBV4	14802	19930	6.98%	0.585%
41	13.874	2003	2004	2007	rVB3	7007	4918	1.72%	0.144%
42	13.945	2013	2016	2017	rBV3	9677	7077	2.48%	0.208%
43	14.021	2025	2029	2032	rBV	260397	241996	84.71%	7.104%
44	14.898	2176	2178	2179	rBV2	8414	7296	2.55%	0.214%
45	15.110	2213	2214	2217	rVB3	16224	9078	3.18%	0.266%
46	15.498	2275	2280	2286	rVB	168377	213389	74.69%	6.264%
47	15.621	2297	2301	2305	rBV7	10796	15075	5.28%	0.443%

Sum of corrected areas: 3406710

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Misc :
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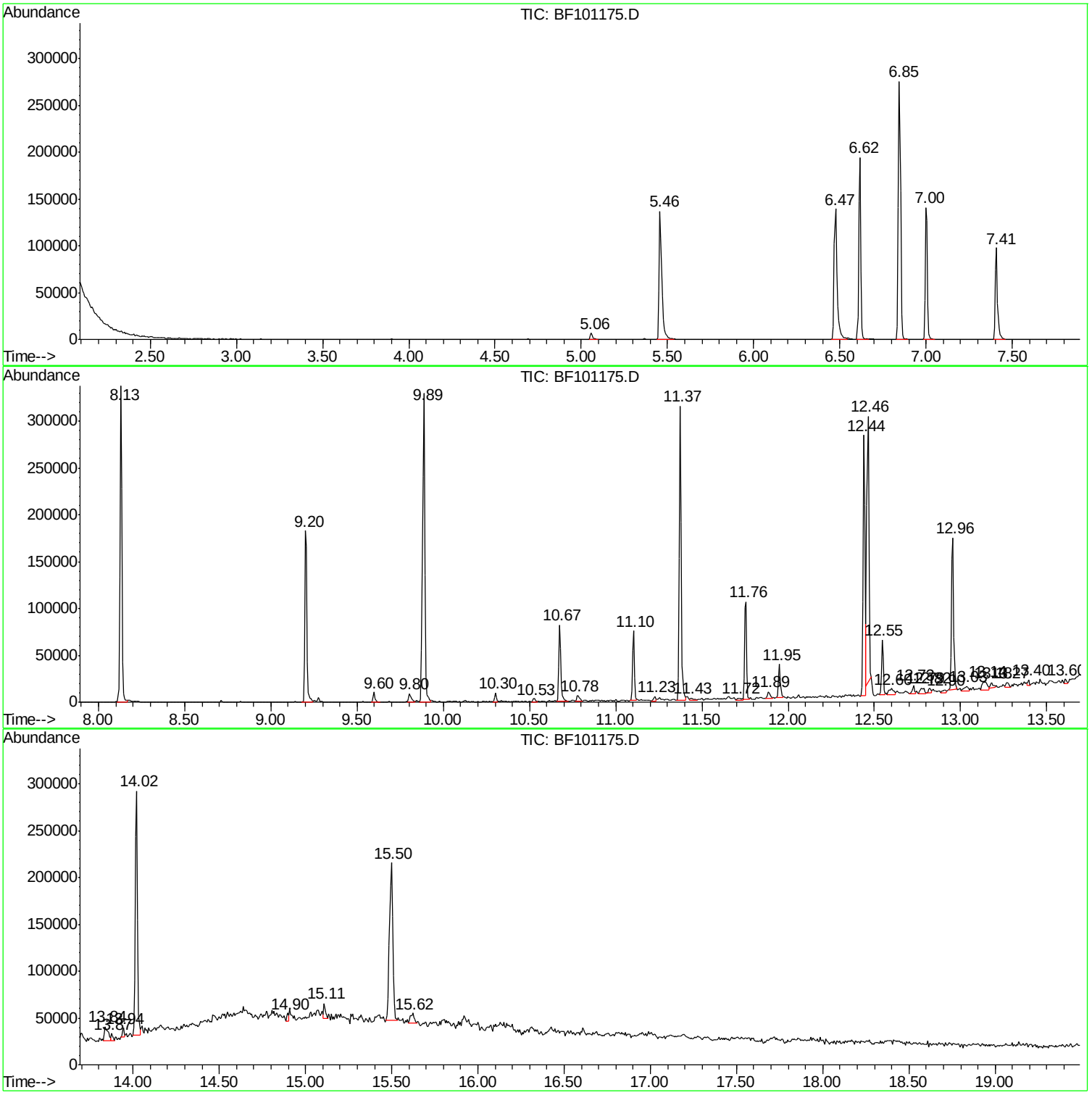
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120617\
Data File : BF101175.D
Acq On : 6 Dec 2017 18:39
Operator : SJ/JU
Sample : I6685-03 5X
Misc :
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Instrument : BNA_F
ClientSampleId : AU-06-120517-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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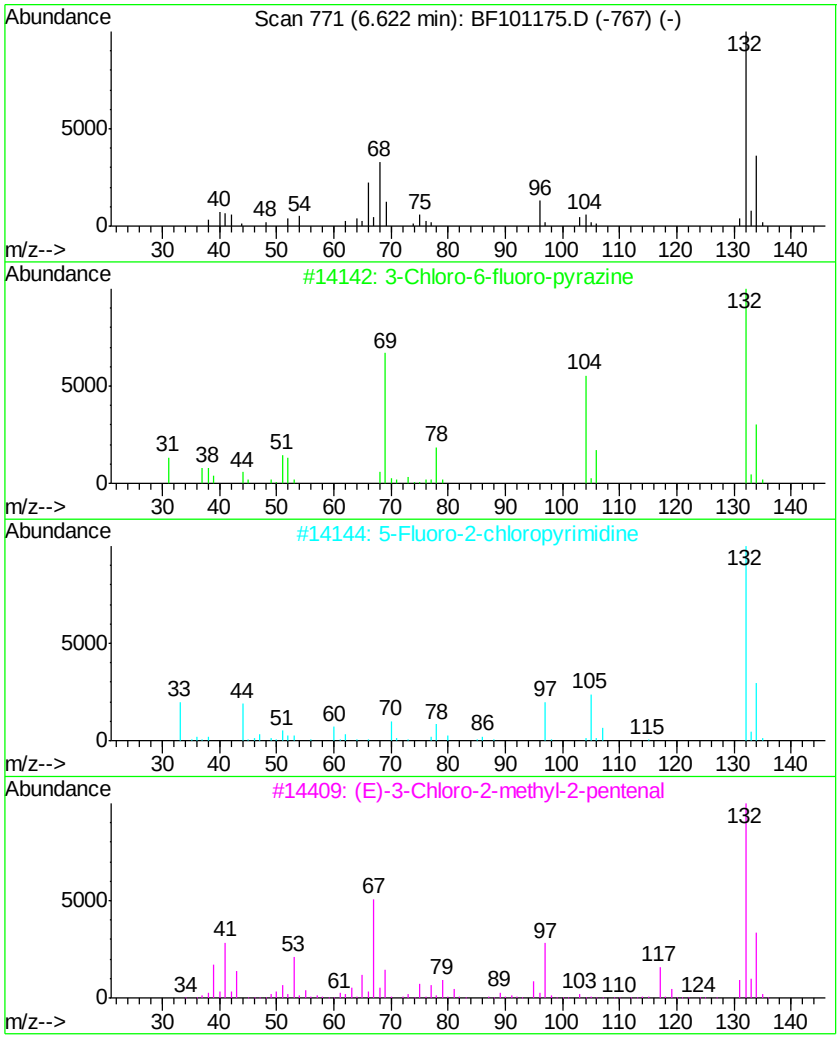
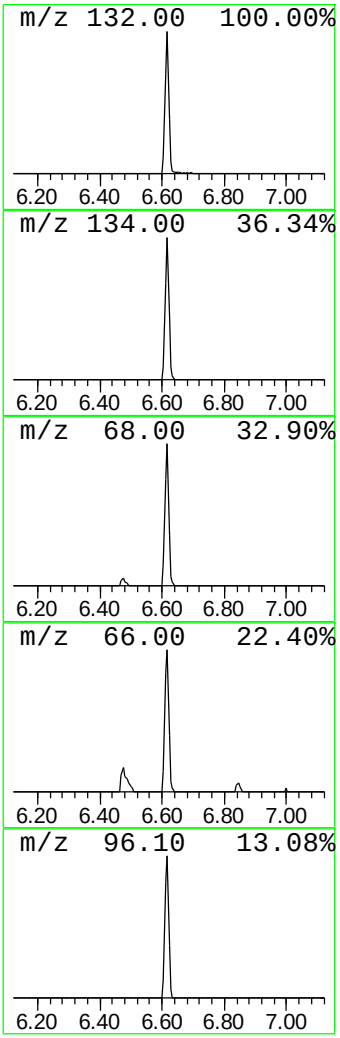
Peak Number 1 unknown6.62 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	14.59 ng	160516	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-120517-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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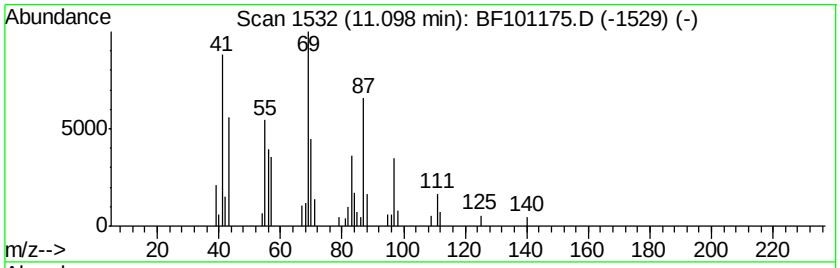
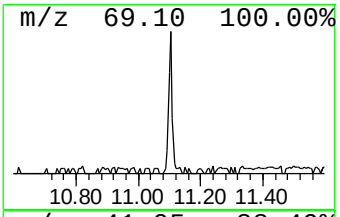
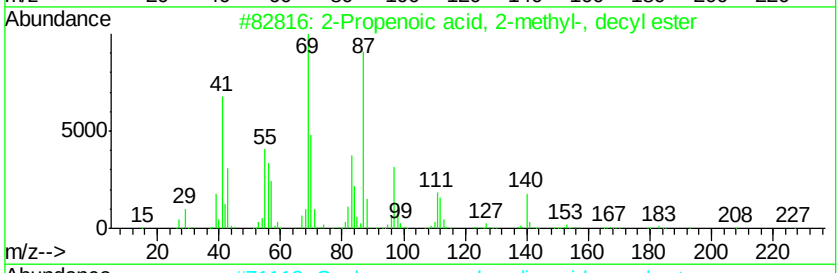
Peak Number 3 2-Propenoic acid, 2-methyl-... Concentration Rank 6

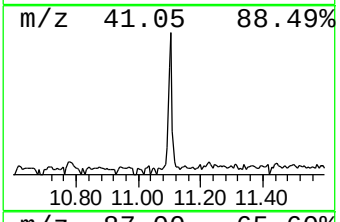
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.10	4.54 ng	58769	Phenanthrene-d10	11.37

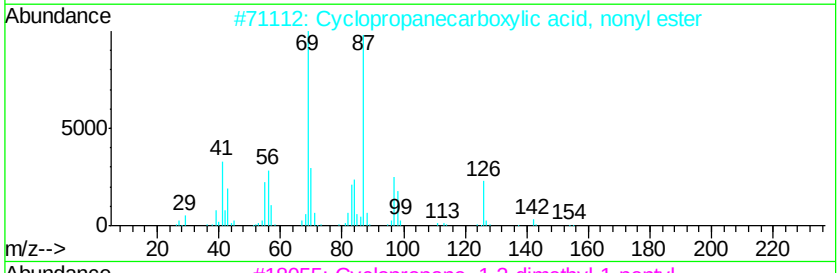
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, 2-methyl-, dec...	226	C14H26O2	003179-47-3	91
2	Cyclopropanecarboxylic acid, non...	212	C13H24O2	060128-06-5	64
3	Cyclopropane, 1,2-dimethyl-1-pen...	140	C10H20	062238-04-4	46
4	1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	43
5	Cyclopentane, pentyl-	140	C10H20	003741-00-2	38

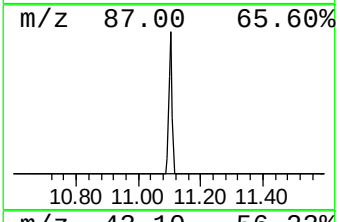


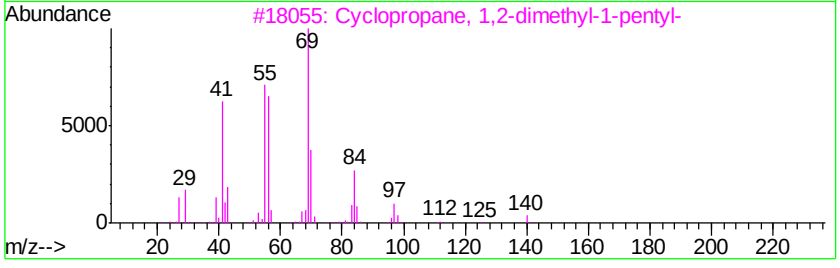


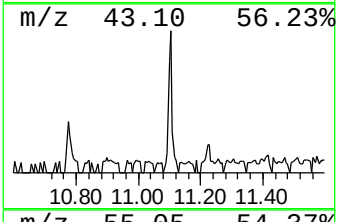


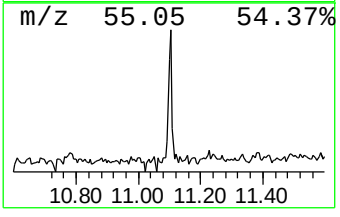












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Sample : I6685-03 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-120517-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

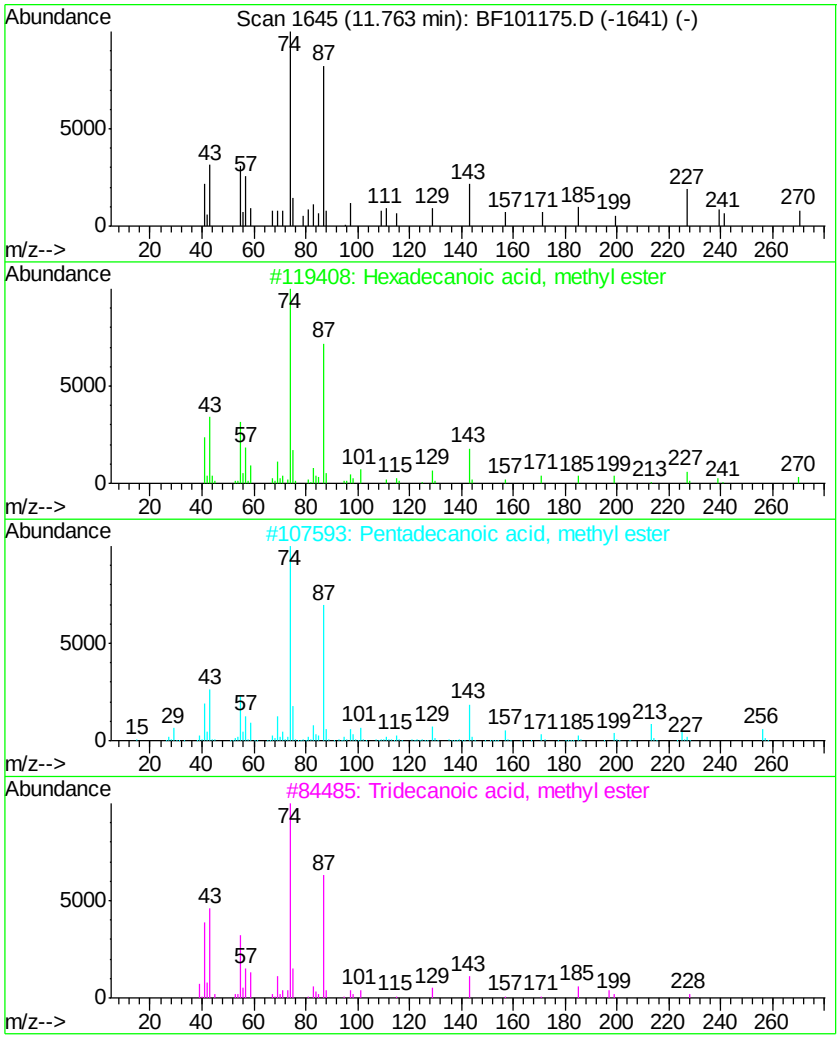
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

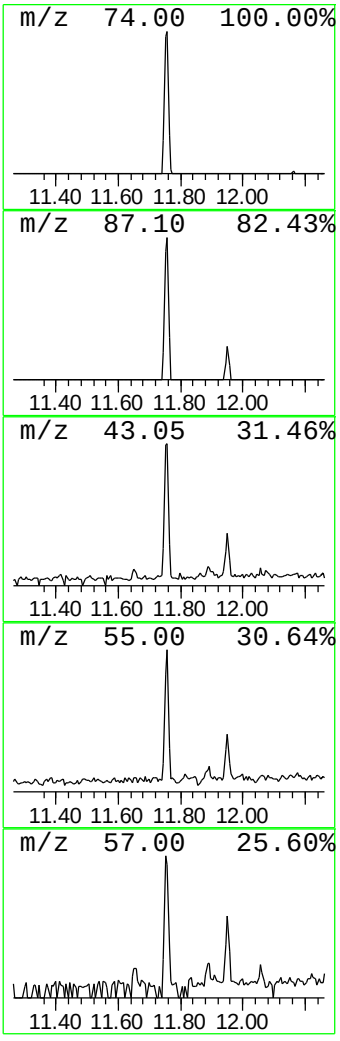
****

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	6.99 ng	90478	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	81
4	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	81
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80





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Operator : SJ/JU
Sample : I6685-03 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-120517-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
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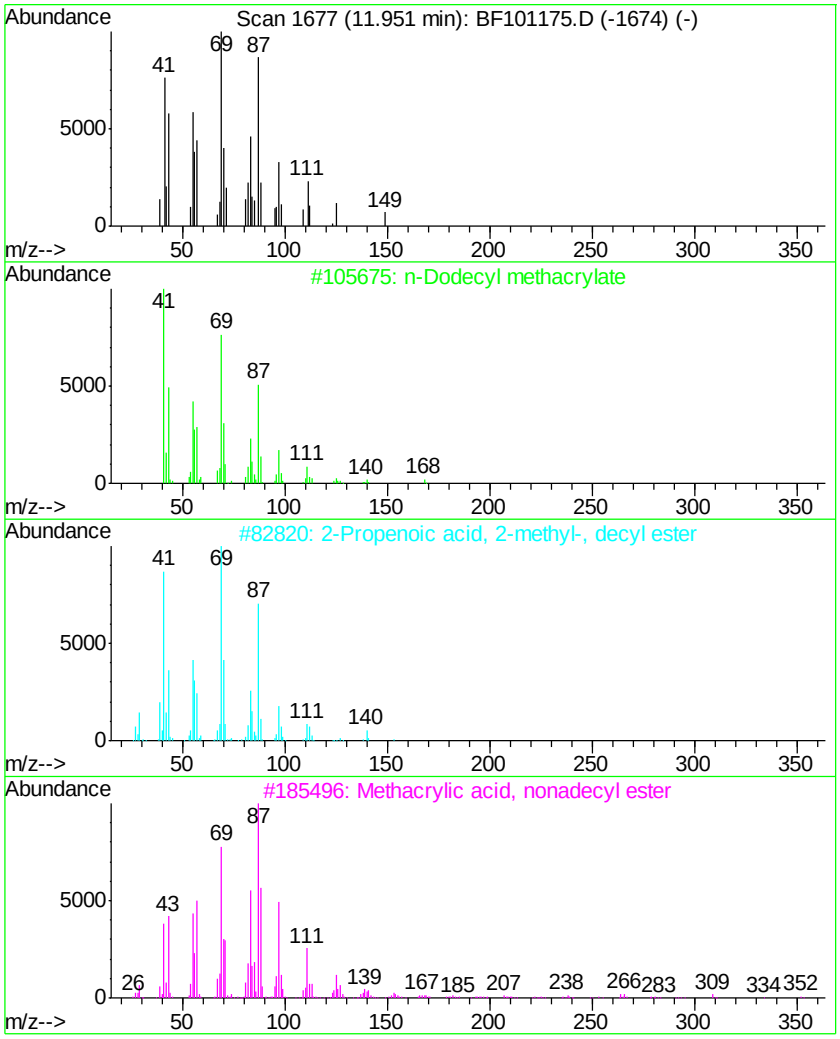
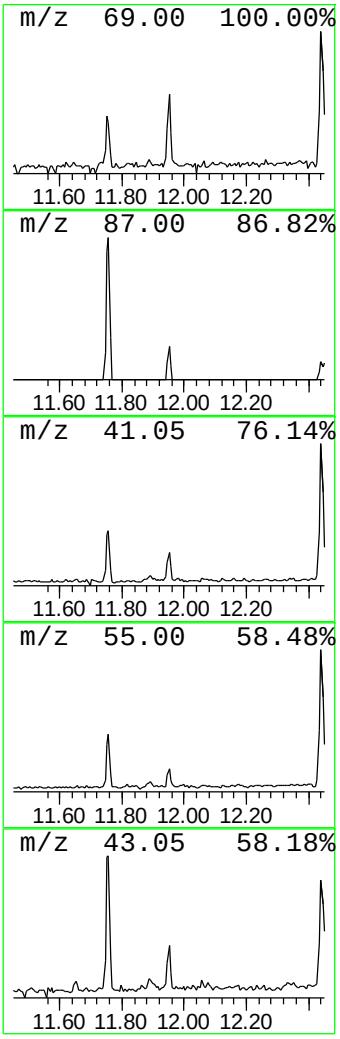
****

Peak Number 5 n-Dodecyl methacrylate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	2.09 ng	27040	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	80
2	2-Propenoic acid, 2-methyl-, dec...	226	C14H26O2	003179-47-3	64
3	Methacrylic acid, nonadecyl ester	352	C23H44O2	1000340-29-5	47
4	1-Octadecanol	270	C18H38O	000112-92-5	30
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	30





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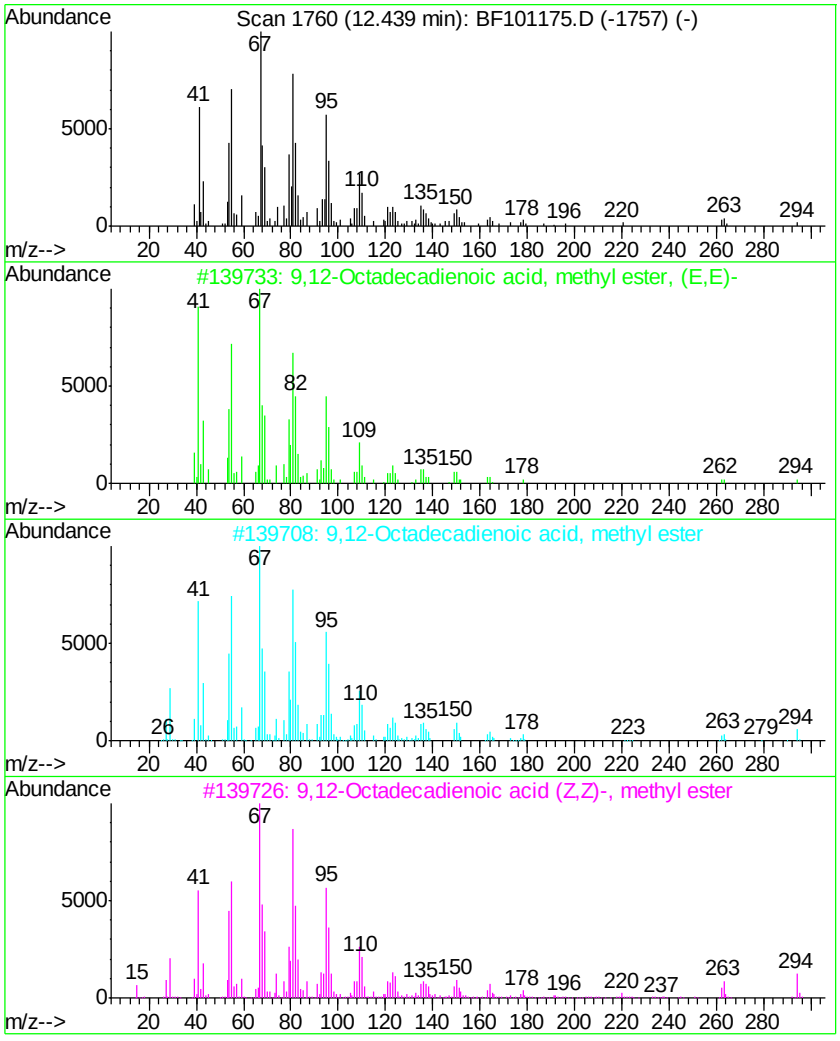
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

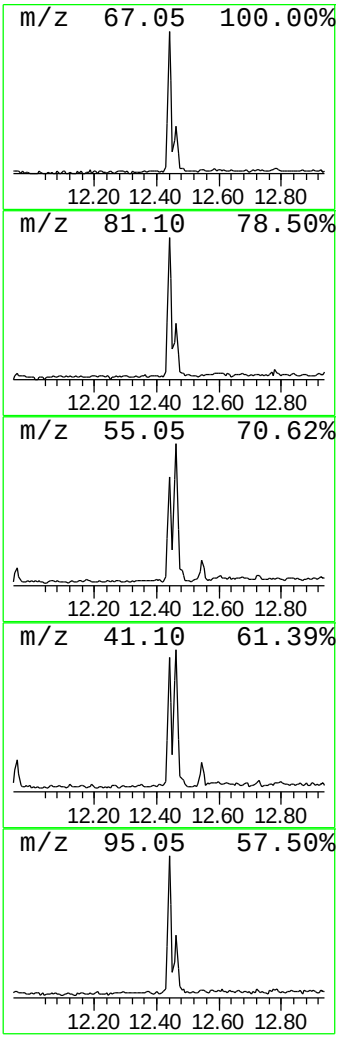
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.44	18.21 ng	235721	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	97
4	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	97
5	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95





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

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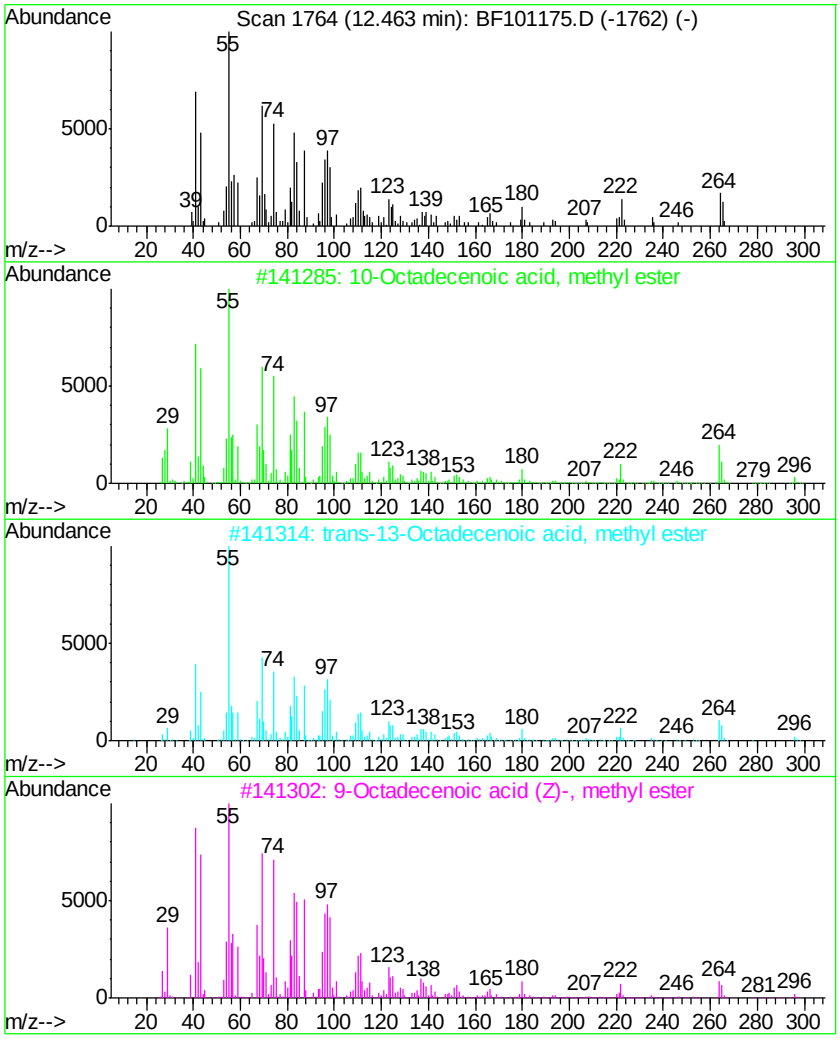
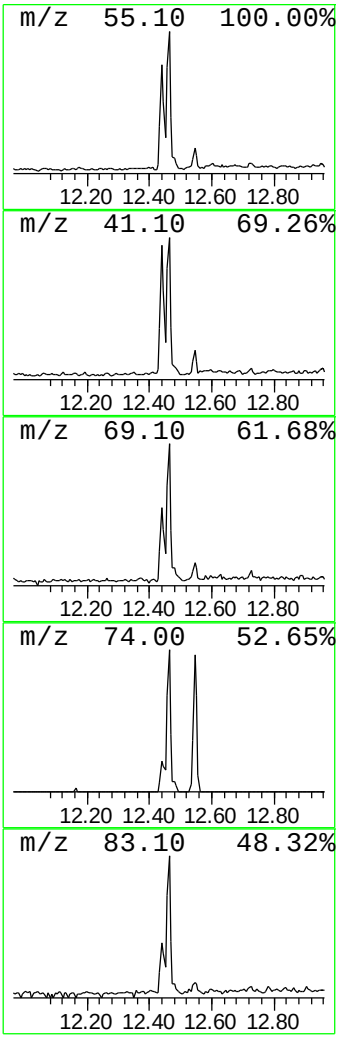
Peak Number 7 10-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	16.11 ng	208517	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	95
2	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	94
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91





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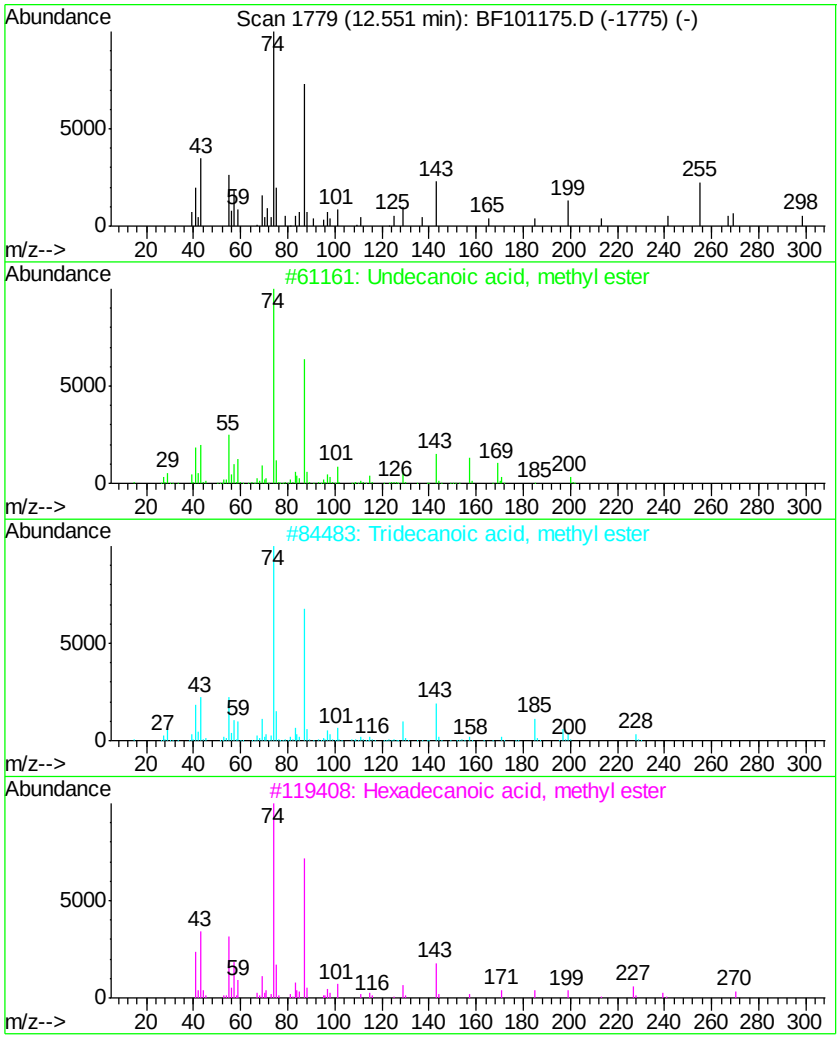
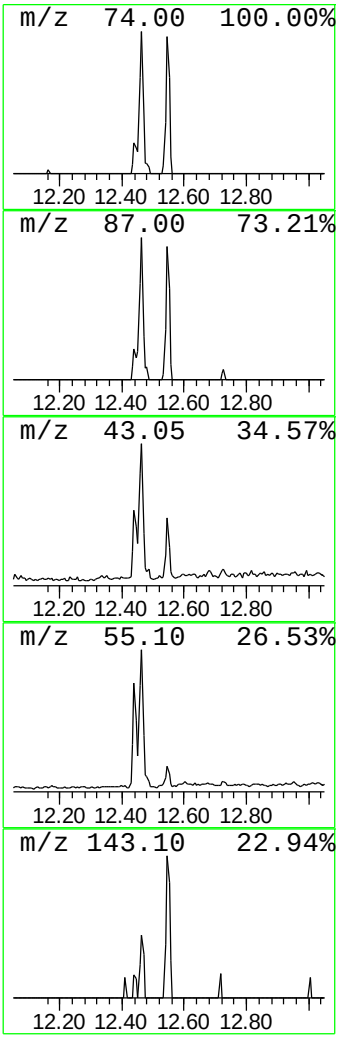
Peak Number 8 Undecanoic acid, methyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	3.52 ng	45621	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid, methyl ester	200	C12H24O2	001731-86-8	87
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	86
3	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	86
5	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120617\
Data File : BF101175.D
Acq On : 6 Dec 2017 18:39
Operator : SJ/JU
Sample : I6685-03 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-120517-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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
unknown6.62	6.62	14.6	ng	160516	1	6.85	219975	20.0
2-Propenoic acid,...	11.10	4.5	ng	58769	4	11.37	258844	20.0
Hexadecanoic acid...	11.76	7.0	ng	90478	4	11.37	258844	20.0
n-Dodecyl methacr...	11.95	2.1	ng	27040	4	11.37	258844	20.0
9,12-Octadecadien...	12.44	18.2	ng	235721	4	11.37	258844	20.0
10-Octadecenoic a...	12.46	16.1	ng	208517	4	11.37	258844	20.0
Undecanoic acid, ...	12.55	3.5	ng	45621	4	11.37	258844	20.0