LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099440.D
Acq On : 13 Oct 2017 15:32
Operator : SJ/JU
Sample : I5713-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

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-BF092317.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	2.128	3	7	23	rVB	178348	250295	7.90%	1.006%
2	5.069	503	507	517	rBV	155658	189057	5.97%	0.760%
3	5.475	572	576	595	rBV	1463237	1455354	45.94%	5.849%
4	6.487	744	748	761	rBV	935491	926583	29.25%	3.724%
5	6.628	767	772	775	rBV	2399921	2380706	75.15%	9.567%
6	6.851	807	810	814	rBV	696463	558415	17.63%	2.244%
7	7.010	832	837	840	rBV	2551841	2277844	71.90%	9.154%
8	7.422	901	907	910	rBV	1687492	1782790	56.28%	7.164%
9	8.133	1024	1028	1031	rBV	949664	743349	23.46%	2.987%
10	9.210	1206	1211	1214	rBV	3445688	3167936	100.00%	12.731%
11	9.598	1274	1277	1281	rBV	144083	115036	3.63%	0.462%
12	9.686	1286	1292	1296	rBV5	20474	38079	1.20%	0.153%
13	9.886	1322	1326	1330	rBV2	920964	789350	24.92%	3.172%
14	10.086	1356	1360	1366	rBV6	29564	38917	1.23%	0.156%
15	10.680	1456	1461	1464	rBV	1647352	1577753	49.80%	6.340%
16	11.374	1575	1579	1583	rBV	856205	705519	22.27%	2.835%
17	11.586	1613	1615	1622	rVB4	38735	43500	1.37%	0.175%
18	11.686	1627	1632	1642	rBV	333317	563428	17.79%	2.264%
19	11.892	1664	1667	1671	rBV	141482	130346	4.11%	0.524%
20	12.610	1784	1789	1797	rBV	465842	687093	21.69%	2.761%
21	12.680	1798	1801	1809	rVB2	167834	215398	6.80%	0.866%
22	12.957	1844	1848	1852	rBV	2121580	2173827	68.62%	8.736%
23	13.480	1933	1937	1945	rVB3	88197	156043	4.93%	0.627%
24	13.827	1992	1996	1998	rBV2	106150	118018	3.73%	0.474%
25	13.963	2016	2019	2024	rVV	42617	40827	1.29%	0.164%
26	14.015	2024	2028	2036	rVB	509908	441543	13.94%	1.774%
27	14.145	2047	2050	2056	rVB	135258	132129	4.17%	0.531%
28	14.451	2099	2102	2106	rVB	194667	183848	5.80%	0.739%
29	14.745	2148	2152	2160	rBV2	1100232	1252023	39.52%	5.031%
30	14.833	2164	2167	2172	rVB	48555	66564	2.10%	0.267%
31	15.092	2207	2211	2217	rVB	193269	219546	6.93%	0.882%
32	15.486	2270	2278	2286	rBV3	369440	662057	20.90%	2.661%
33	15.898	2343	2348	2354	rBV	126861	197827	6.24%	0.795%
34	16.321	2417	2420	2427	rBV8	16577	34840	1.10%	0.140%

LSC Area Percent Report

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Data File : BF099440.D
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Operator : SJ/JU
Sample : I5713-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.398	2427	2433	2440	rVV	90098	170808	5.39%	0.686%
36	16.986	2526	2533	2541	rVB3	59912	146678	4.63%	0.589%
37	17.503	2613	2621	2626	rBV3	18402	44185	1.39%	0.178%
38	17.674	2644	2650	2660	rVB3	42041	118752	3.75%	0.477%
39	18.497	2782	2790	2801	rVB6	27389	87653	2.77%	0.352%

Sum of corrected areas: 24883916

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Misc :
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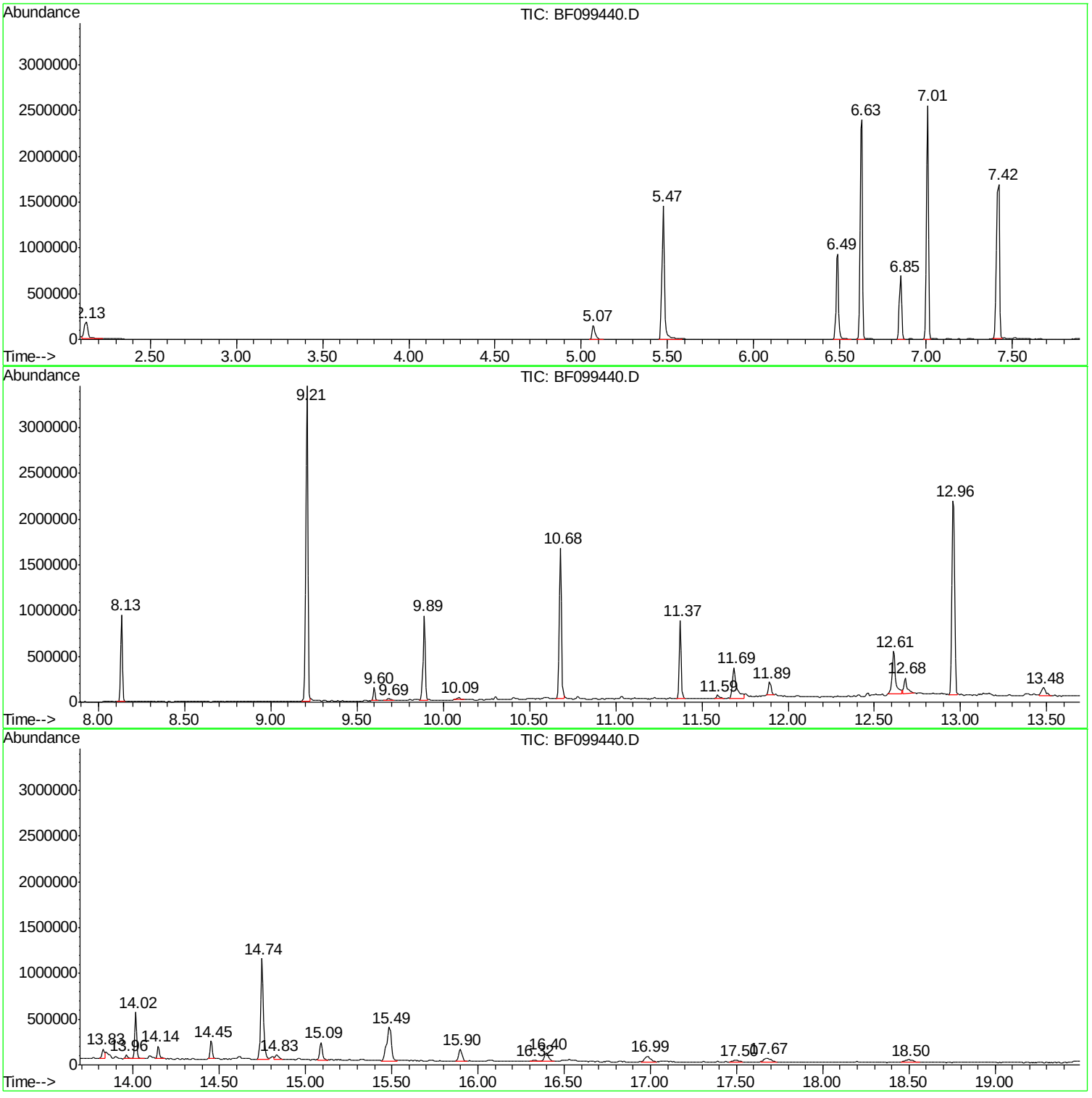
Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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Operator : SJ/JU
Sample : I5713-03
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ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

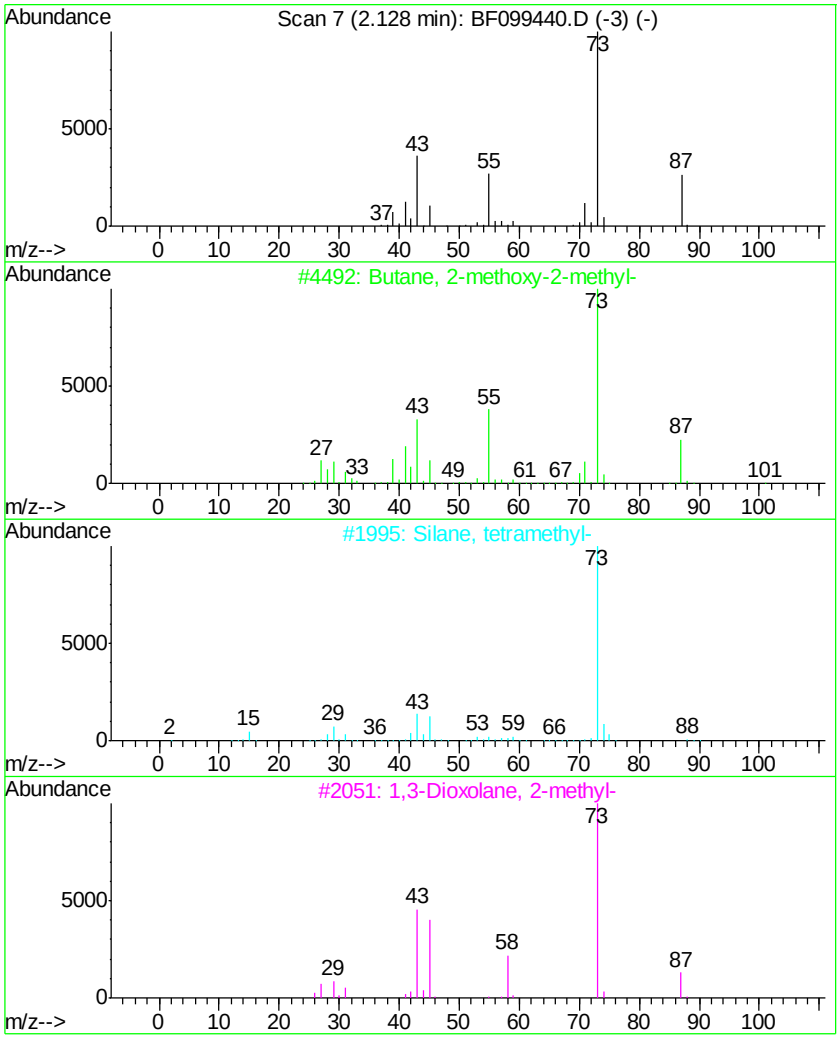
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

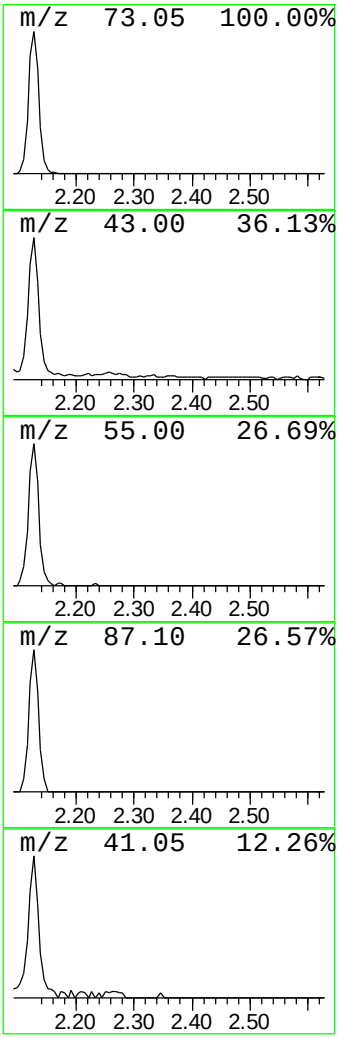
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	8.96 ng	250295	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	43
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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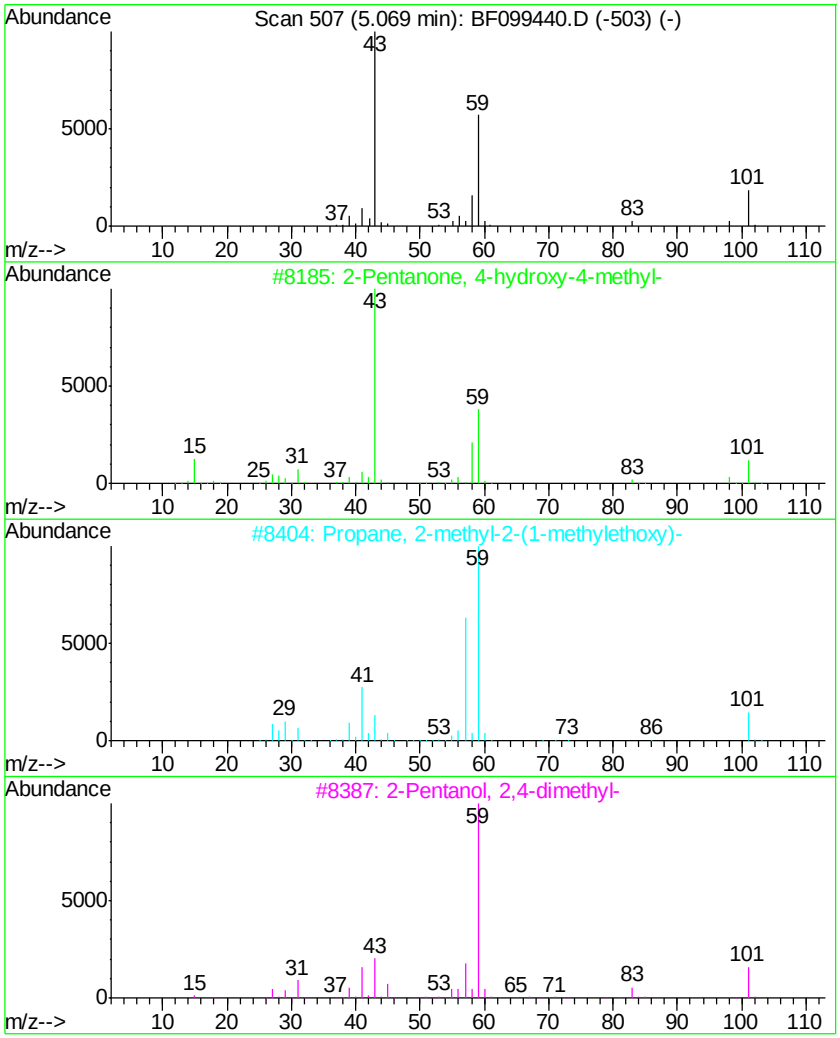
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

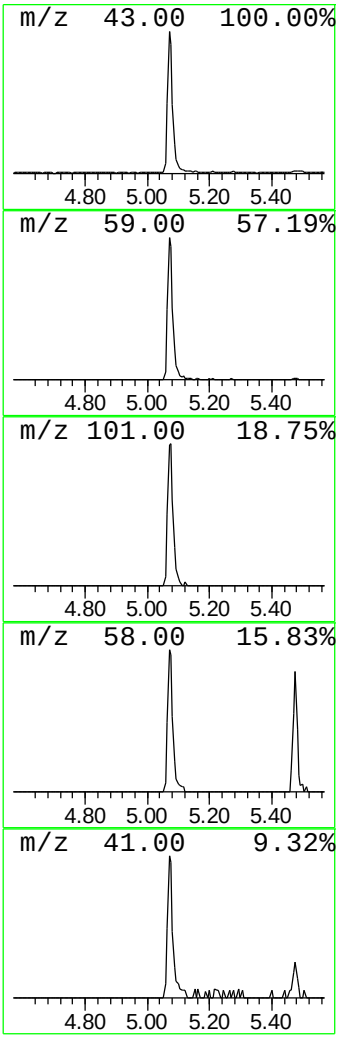
****

Peak Number 2 unknown5.07 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	6.77 ng	189057	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	28
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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Sample : I5713-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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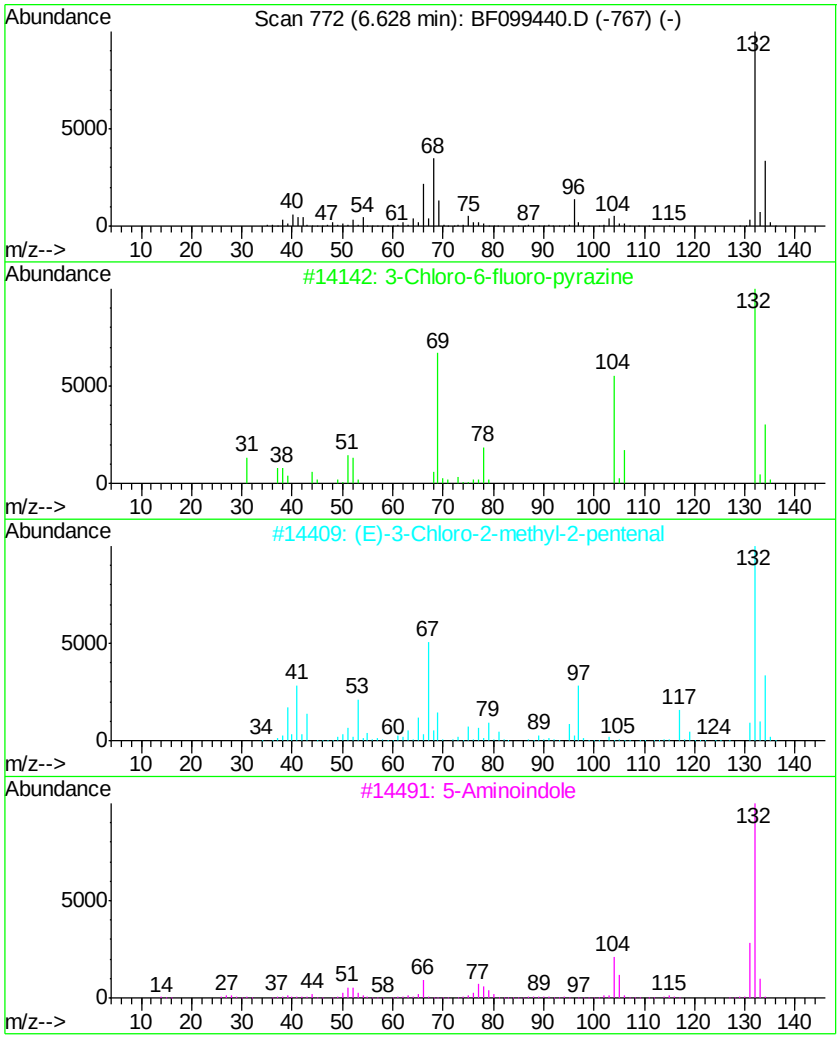
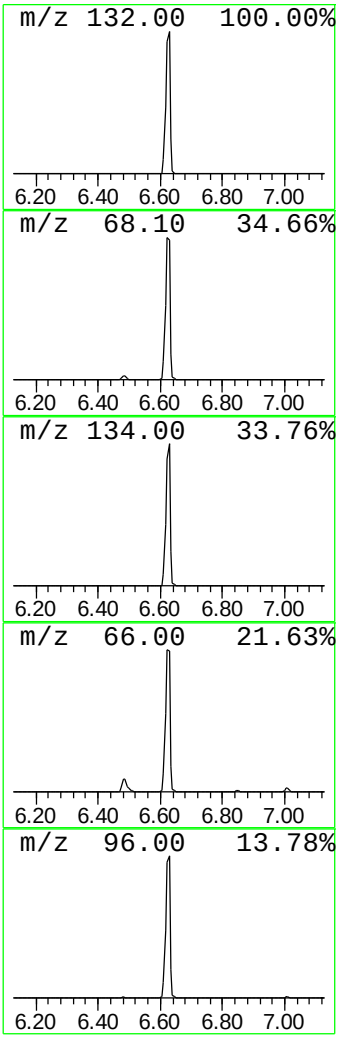
Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	85.27 ng	2380710	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	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Sample : I5713-03
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ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

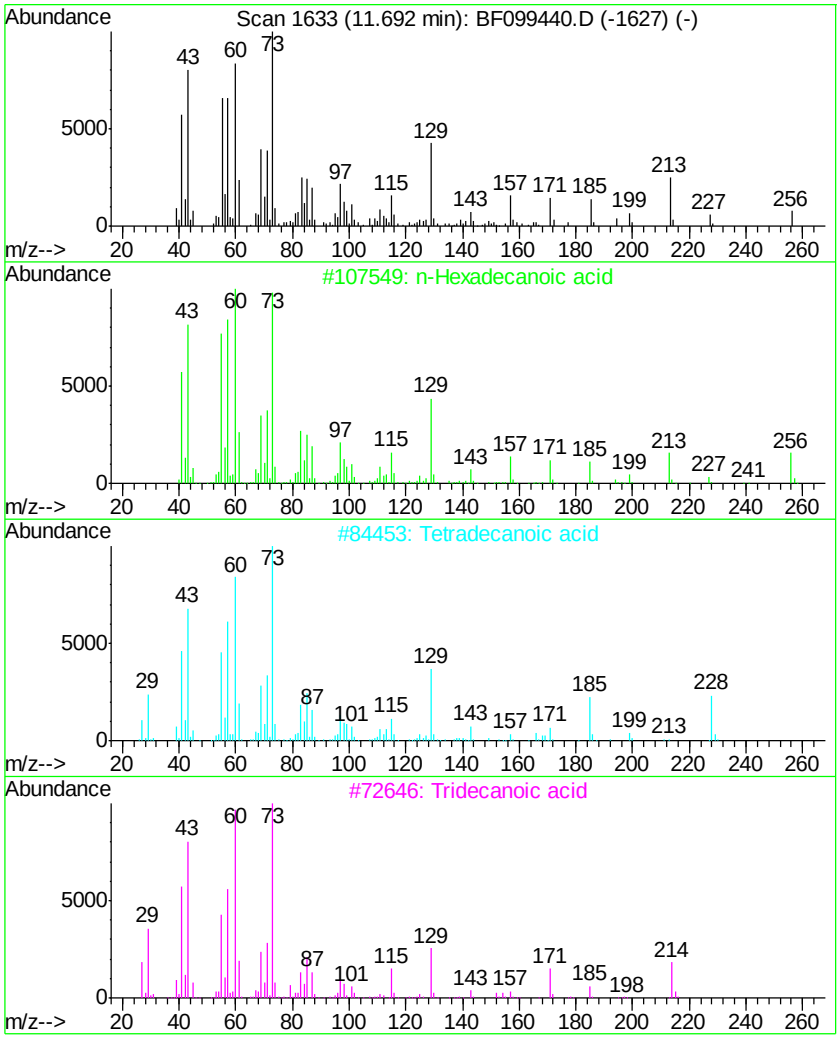
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

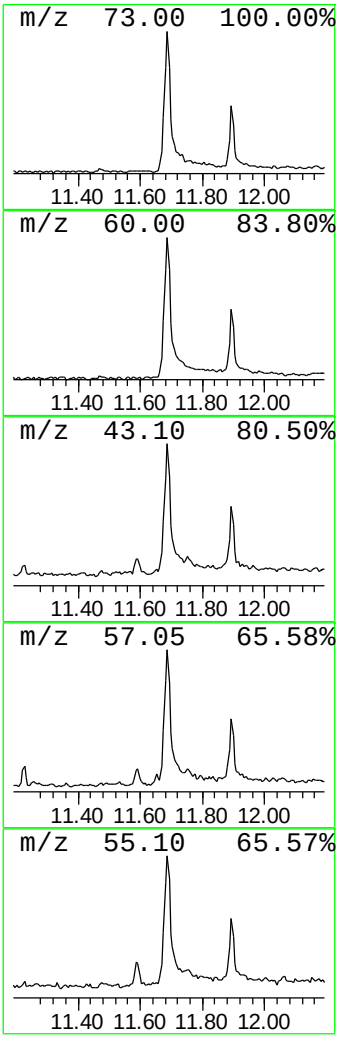
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	15.97 ng	563428	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





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Sample : I5713-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

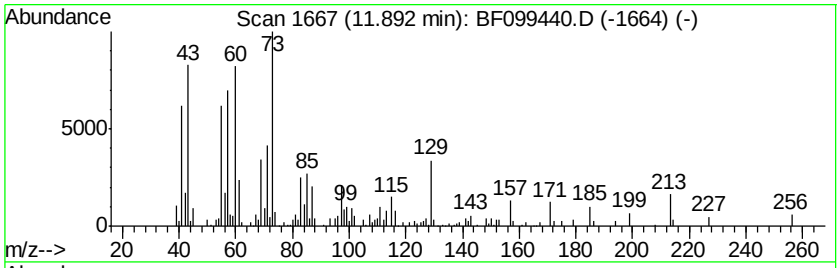
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

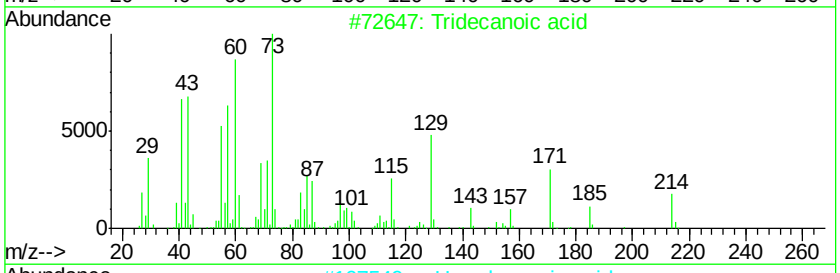
****

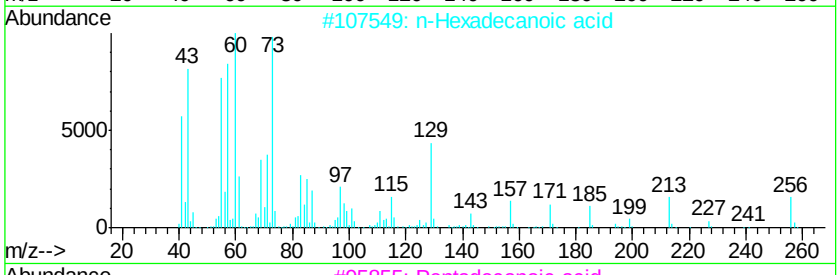
Peak Number 6 Tridecanoic acid Concentration Rank 17

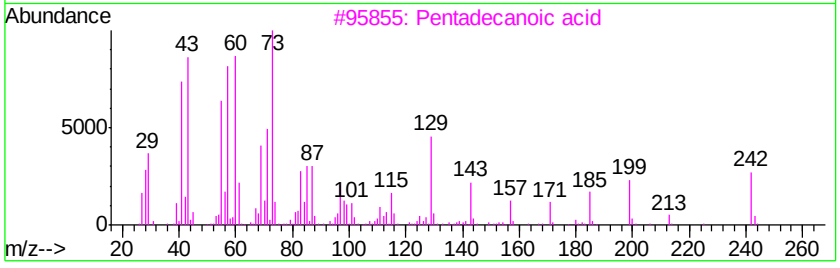
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	3.70 ng	130346	Phenanthrene-d10	11.37

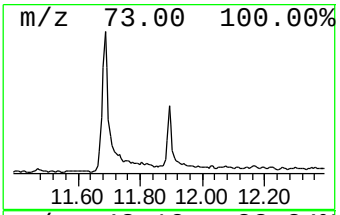
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	25
5	n-Decanoic acid	172	C10H20O2	000334-48-5	25

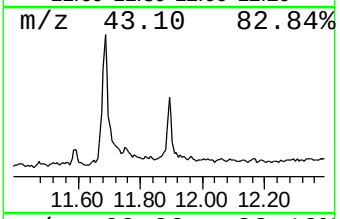


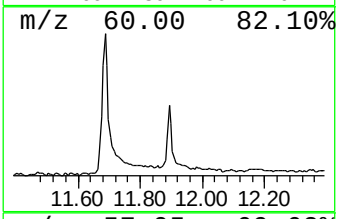


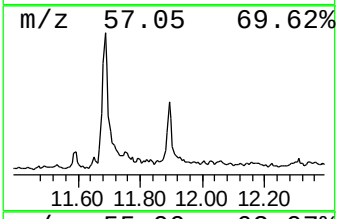


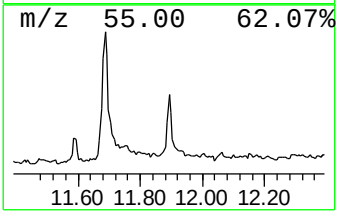












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Sample : I5713-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

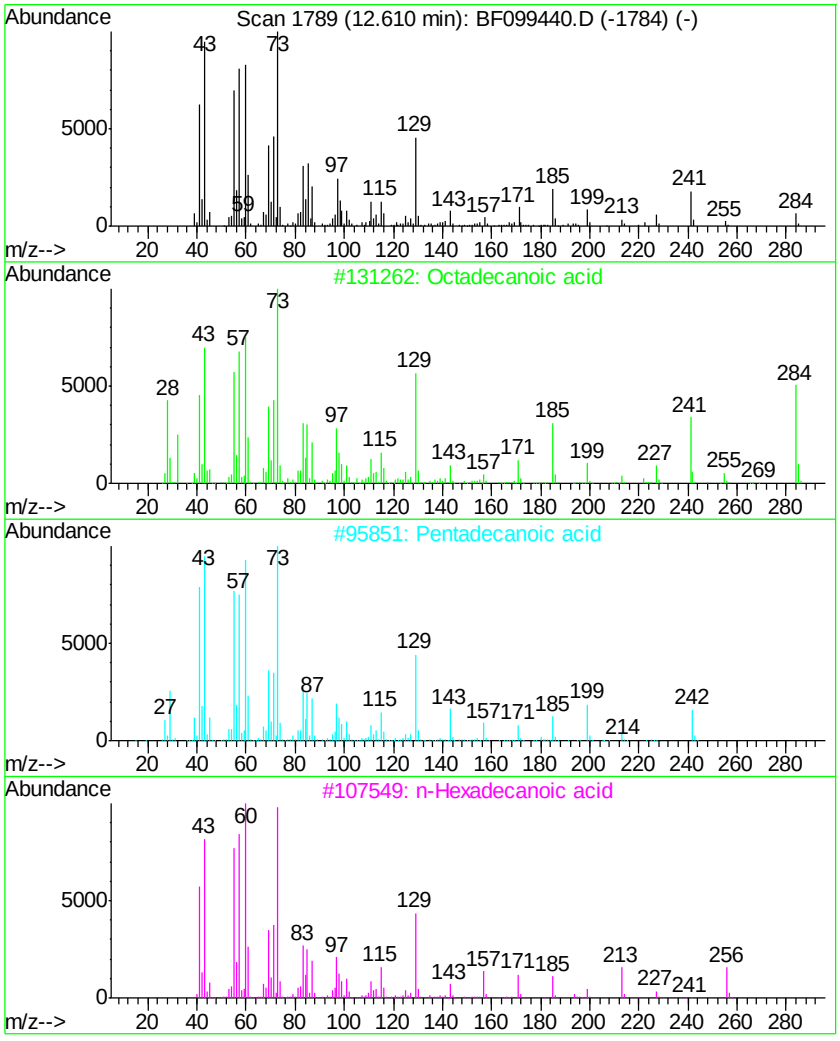
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

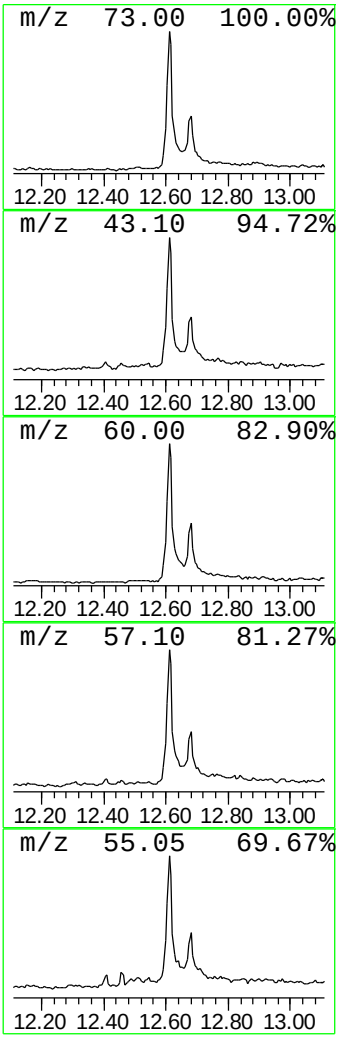
****

Peak Number 7 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.61	19.48 ng	687093	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





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Sample : I5713-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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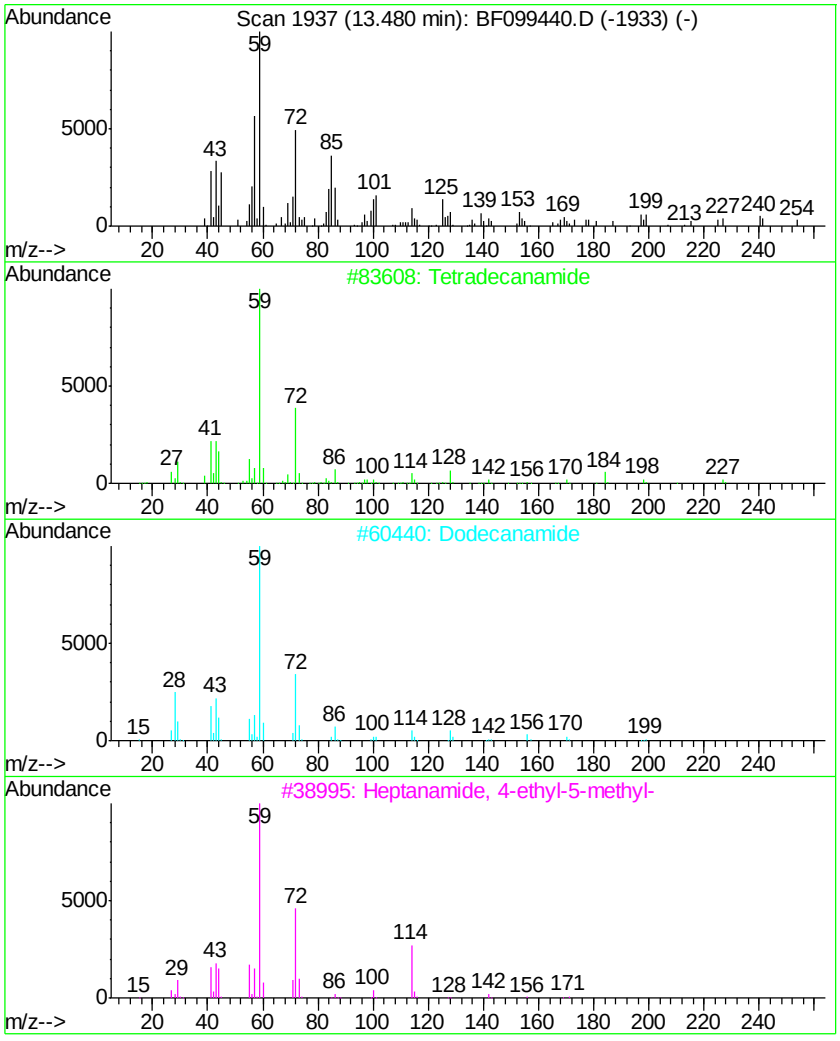
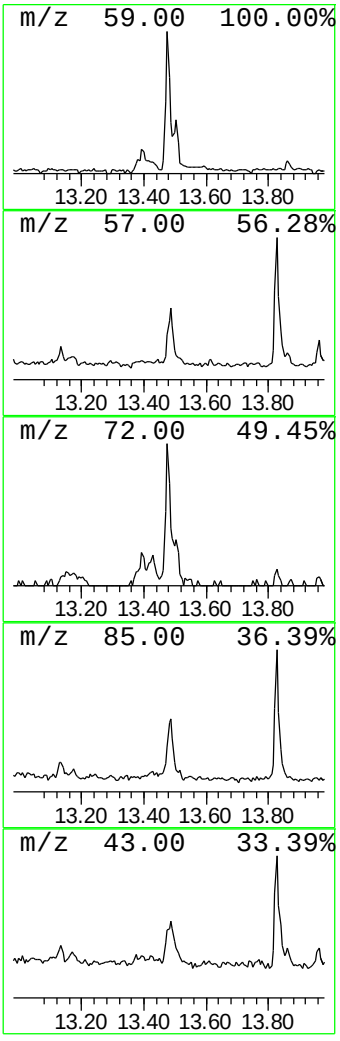
Peak Number 9 Tetradecanamide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	7.07 ng	156043	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanamide	227	C14H29NO	000638-58-4	58
2	Dodecanamide	199	C12H25NO	001120-16-7	50
3	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	47
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	43
5	.alpha.-L-Lyxo-Hexopyranoside, m...	203	C9H17NO4	032385-07-2	38





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Data File : BF099440.D
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Sample : I5713-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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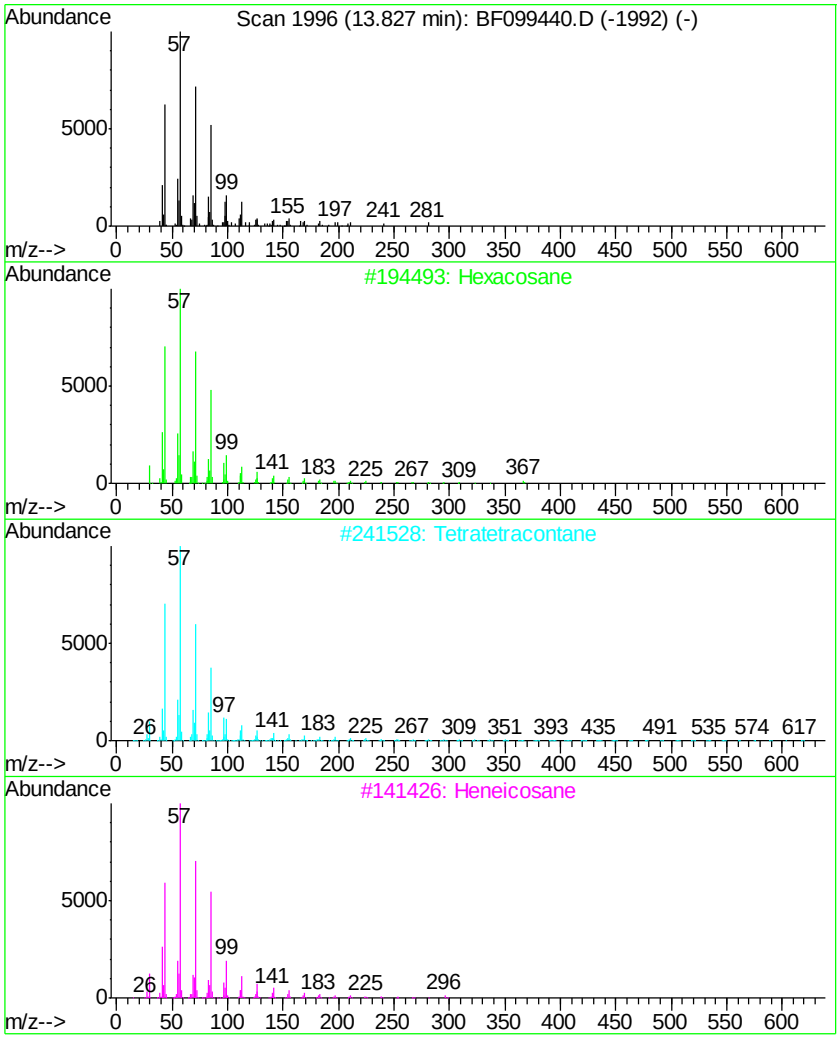
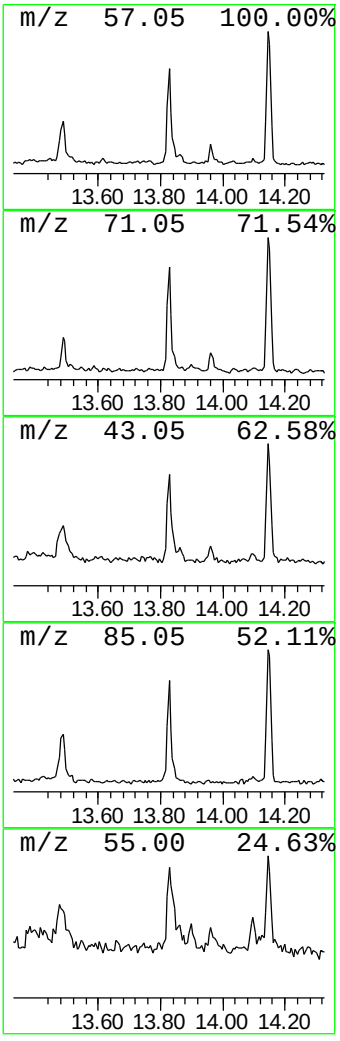
Peak Number 10 Hexacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	5.35 ng	118018	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Tetratetracontane	619	C44H90	007098-22-8	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Hentriacontane	437	C31H64	000630-04-6	87
5	Heptadecane	240	C17H36	000629-78-7	87





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Acq On : 13 Oct 2017 15:32
Operator : SJ/JU
Sample : I5713-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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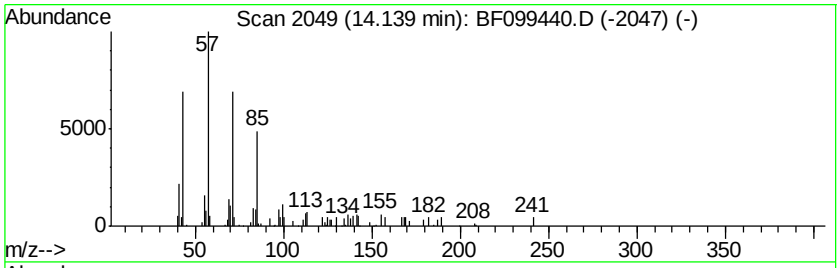
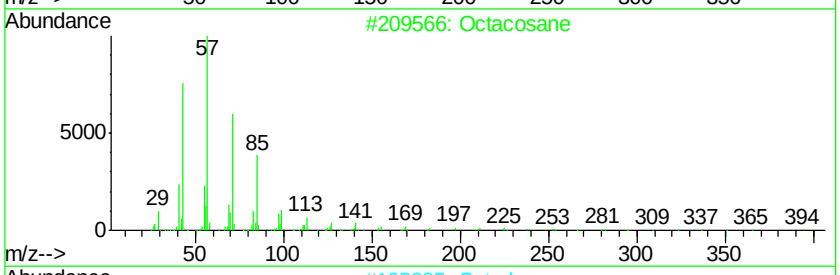
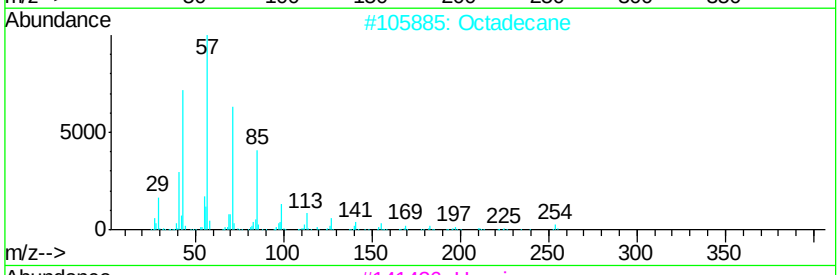
Peak Number 11 Octacosane Concentration Rank 12

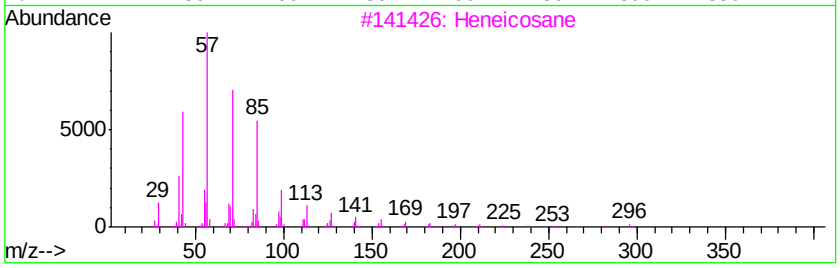
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	5.98 ng	132129	Chrysene-d12	14.02

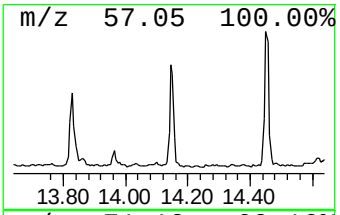
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Docosane	310	C22H46	000629-97-0	90
5	Eicosane	282	C20H42	000112-95-8	90

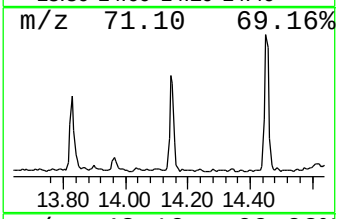


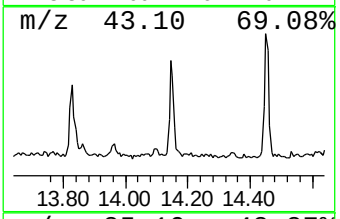


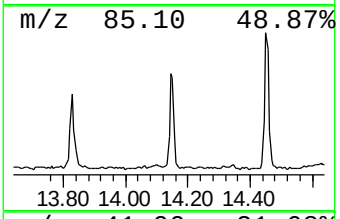


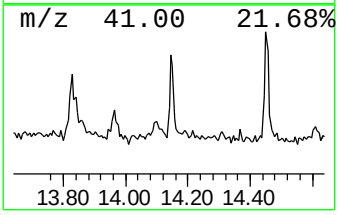












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Operator : SJ/JU
Sample : I5713-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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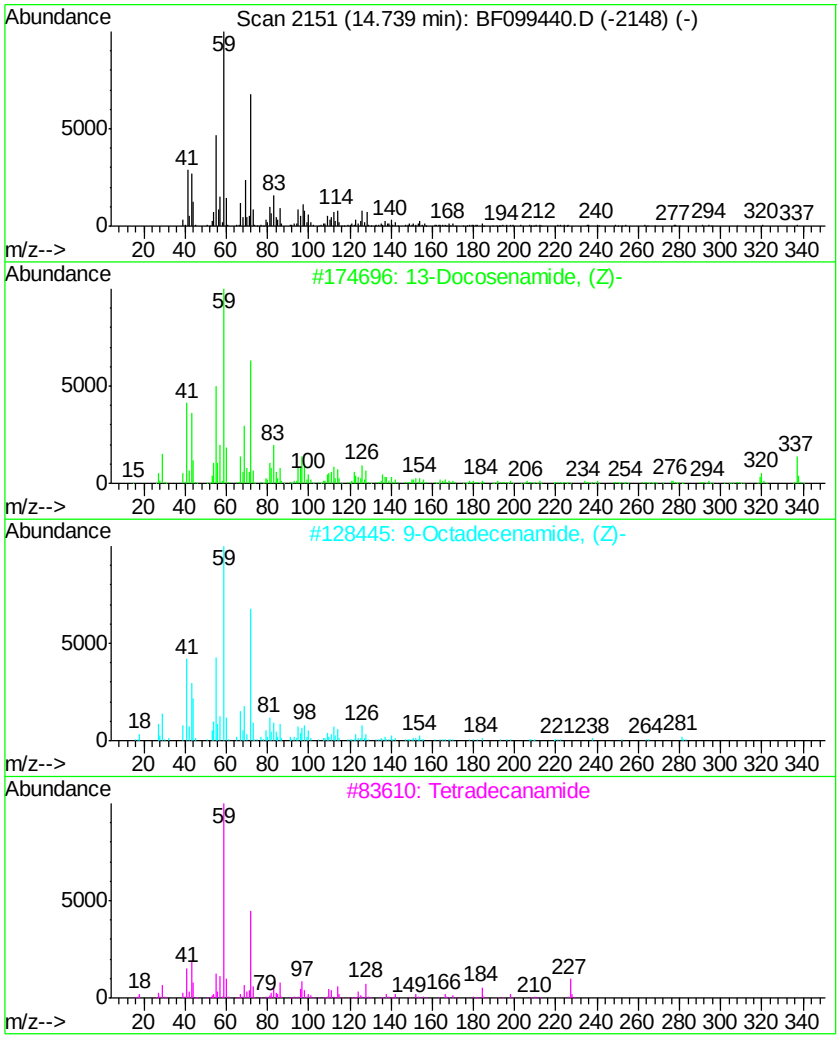
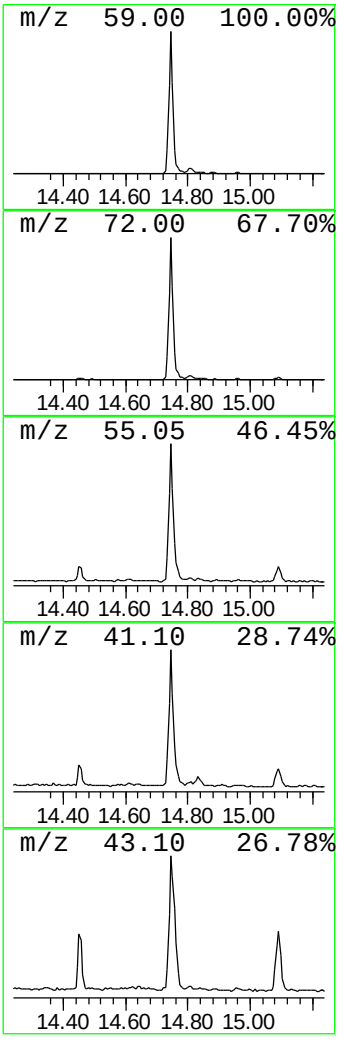
Peak Number 13 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	56.71 ng	1252020	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
3	Tetradecanamide	227	C14H29NO	000638-58-4	64
4	Decanamide-	171	C10H21NO	002319-29-1	59
5	2-Pentanol, 3-chloro-2-methyl-	136	C6H13ClO	074685-49-7	43





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Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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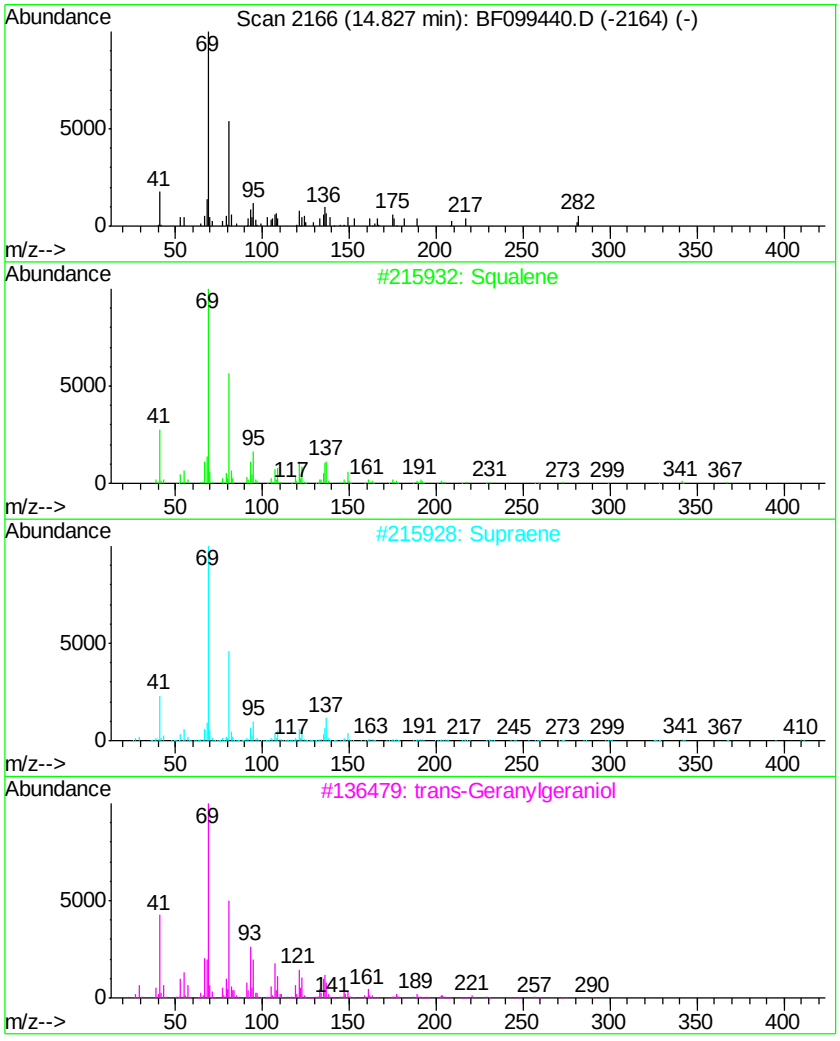
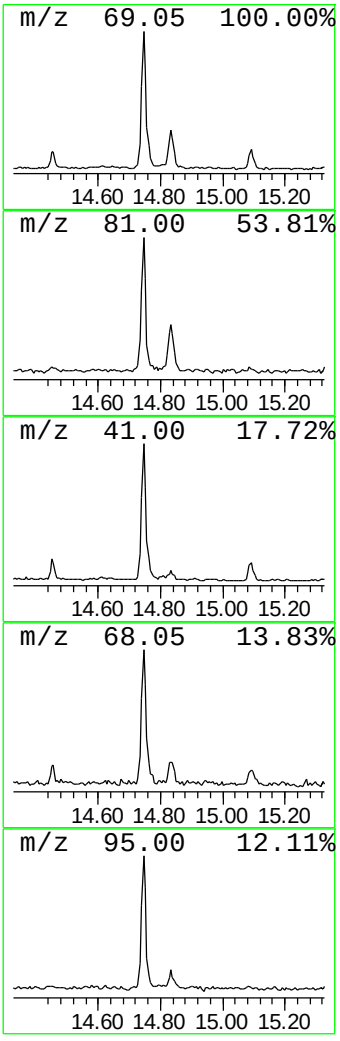
Peak Number 14 Squalene Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	2.01 ng	66564	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	86
2	Supraene	410	C30H50	007683-64-9	80
3	trans-Geranylgeraniol	290	C20H34O	024034-73-9	72
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59
5	Farnesol isomer a	222	C15H26O	1000108-92-4	50





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Sample : I5713-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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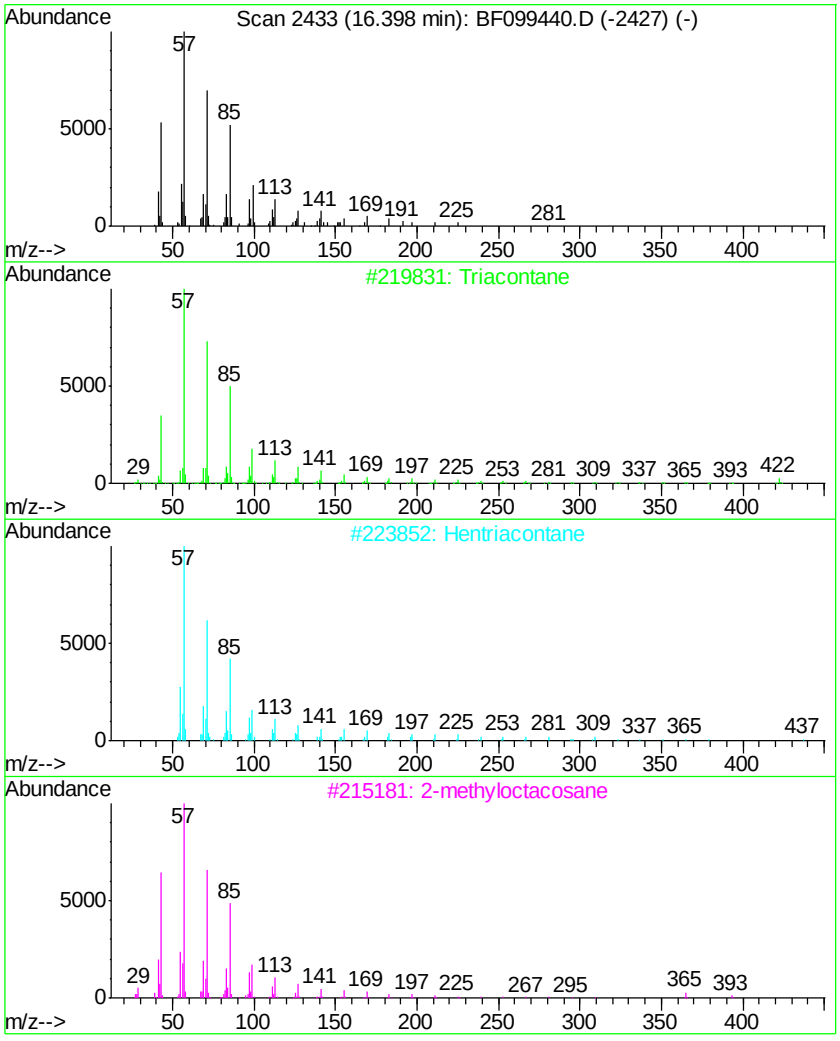
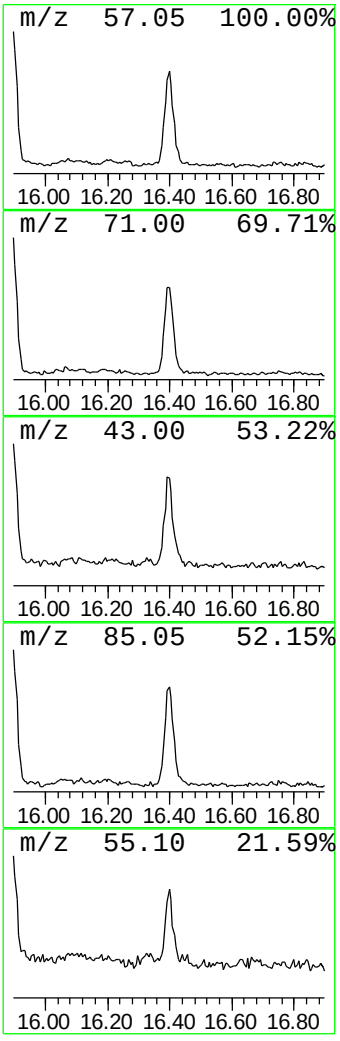
Peak Number 17 Triacontane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	5.16 ng	170808	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Octacosane	394	C28H58	000630-02-4	87





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Acq On : 13 Oct 2017 15:32
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ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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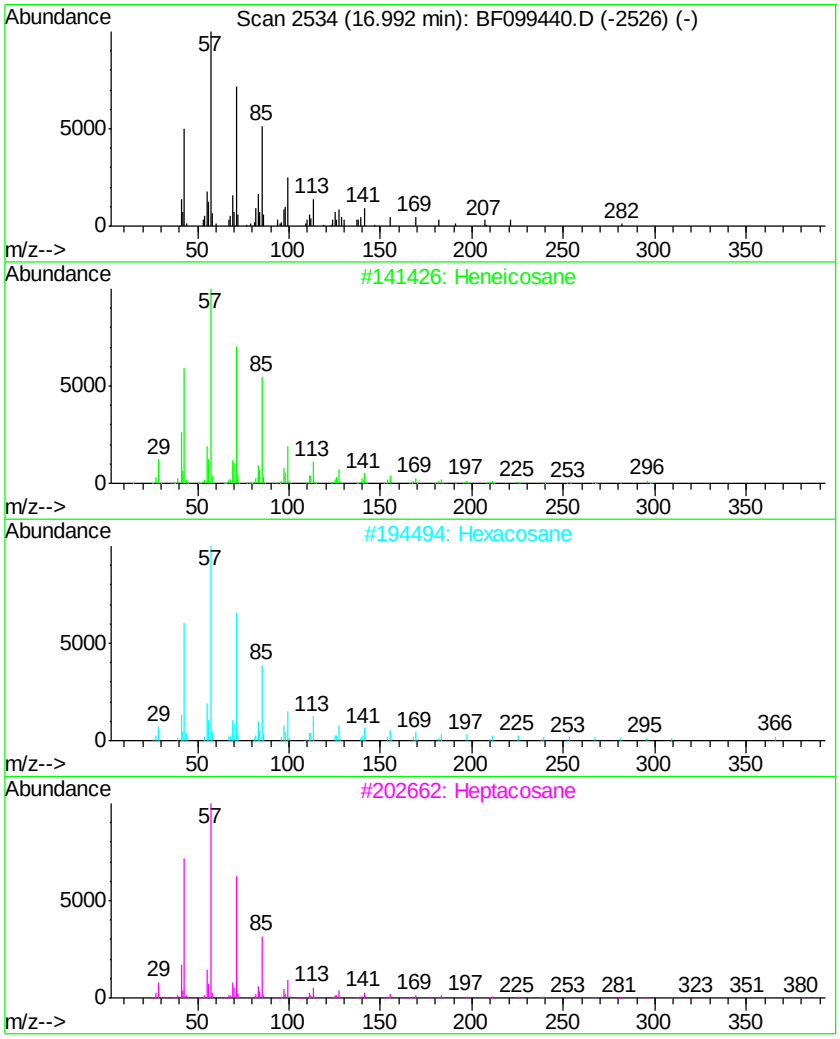
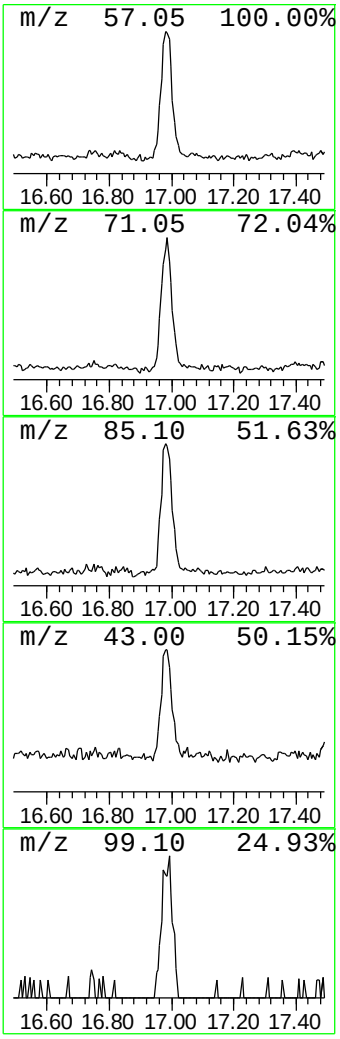
Peak Number 18 Heneicosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.99	4.43 ng	146678	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexacosane	366	C26H54	000630-01-3	87
3	Heptacosane	380	C27H56	000593-49-7	86
4	Tetracosane	338	C24H50	000646-31-1	86
5	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	86





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Acq On : 13 Oct 2017 15:32
Operator : SJ/JU
Sample : I5713-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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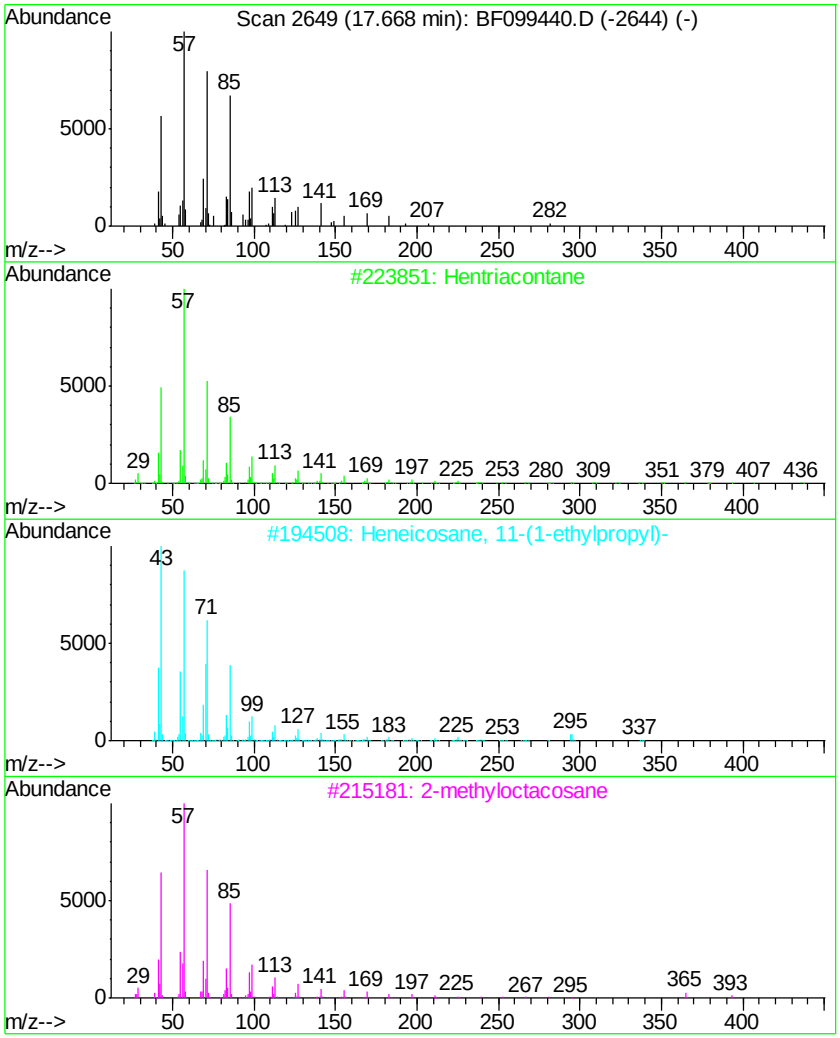
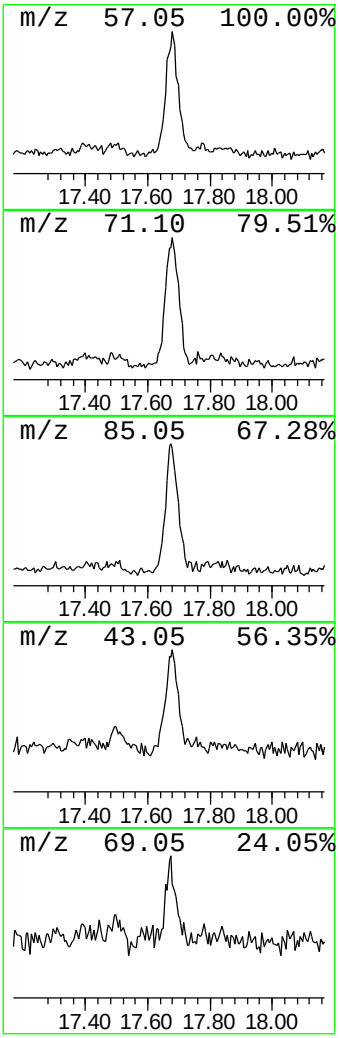
Peak Number 19 Hentriacontane Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.67	3.59 ng	118752	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Heptacosane	380	C27H56	000593-49-7	90





Tentatively Identified Compound (LSC) summary

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Data File : BF099440.D
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Operator : SJ/JU
Sample : I5713-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
Butane, 2-methoxy...	2.13	9.0	ng	250295	1	6.85	558415	20.0
unknown5.07	5.07	6.8	ng	189057	1	6.85	558415	20.0
unknown6.63	6.63	85.3	ng	2380710	1	6.85	558415	20.0
n-Hexadecanoic acid	11.69	16.0	ng	563428	4	11.37	705519	20.0
Tridecanoic acid	11.89	3.7	ng	130346	4	11.37	705519	20.0
Octadecanoic acid	12.61	19.5	ng	687093	4	11.37	705519	20.0
Tetradecanamide	13.48	7.1	ng	156043	5	14.02	441543	20.0
Hexacosane	13.83	5.3	ng	118018	5	14.02	441543	20.0
Octacosane	14.14	6.0	ng	132129	5	14.02	441543	20.0
13-Docosenamide, ...	14.74	56.7	ng	1252020	5	14.02	441543	20.0
Squalene	14.83	2.0	ng	66564	6	15.49	662057	20.0
Triacontane	16.40	5.2	ng	170808	6	15.49	662057	20.0
Heneicosane	16.99	4.4	ng	146678	6	15.49	662057	20.0
Hentriacontane	17.67	3.6	ng	118752	6	15.49	662057	20.0