LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100417\
Data File : BF099088.D
Acq On : 5 Oct 2017 1:12
Operator : SJ/JU
Sample : I5588-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-EPE-115-4B(10-12)

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	2.140	5	9	28	rVB	144522	235550	6.18%	0.697%
2	5.092	507	511	524	rVB	515642	736874	19.34%	2.181%
3	5.487	573	578	582	rBV	2985606	3263816	85.67%	9.660%
4	6.498	741	750	758	rBV	2749347	3490019	91.61%	10.329%
5	6.639	769	774	777	rBV	3325379	3375984	88.62%	9.992%
6	6.863	808	812	816	rBV	1017602	824208	21.63%	2.439%
7	7.022	832	839	842	rBV	2886685	2680078	70.35%	7.932%
8	7.434	902	909	911	rBV	1932181	2193697	57.58%	6.493%
9	7.510	917	922	931	rVB	34794	45915	1.21%	0.136%
10	8.145	1026	1030	1033	rBV	1337897	1071301	28.12%	3.171%
11	8.539	1094	1097	1106	rVB2	45774	51642	1.36%	0.153%
12	9.222	1207	1213	1216	rBV	3943643	3809667	100.00%	11.275%
13	9.610	1275	1279	1282	rBV	655453	504129	13.23%	1.492%
14	9.898	1324	1328	1332	rBV	1261977	1153207	30.27%	3.413%
15	10.322	1398	1400	1403	rVB	60697	41230	1.08%	0.122%
16	10.692	1458	1463	1466	rBV	2088015	2021767	53.07%	5.984%
17	10.792	1477	1480	1489	rBV	71944	77082	2.02%	0.228%
18	11.386	1577	1581	1584	rBV	1295022	1103583	28.97%	3.266%
19	11.769	1643	1646	1649	rVB	340543	244024	6.41%	0.722%
20	11.904	1663	1669	1674	rBV2	225575	225740	5.93%	0.668%
21	12.457	1759	1763	1764	rBV	410643	342848	9.00%	1.015%
22	12.474	1764	1766	1769	rVB	737927	569922	14.96%	1.687%
23	12.563	1778	1781	1784	rBV	150405	120246	3.16%	0.356%
24	12.598	1784	1787	1794	rVV	96551	95316	2.50%	0.282%
25	12.692	1798	1803	1812	rBV	63920	108187	2.84%	0.320%
26	12.774	1814	1817	1820	rVV	67484	52702	1.38%	0.156%
27	12.827	1823	1826	1829	rVB	74445	64999	1.71%	0.192%
28	12.974	1844	1851	1854	rBV	3158671	3222145	84.58%	9.536%
29	13.498	1937	1940	1942	rBV	50363	38979	1.02%	0.115%
30	13.857	1997	2001	2004	rBV	120508	132505	3.48%	0.392%
31	14.021	2026	2029	2033	rBV	728091	678842	17.82%	2.009%
32	14.480	2104	2107	2114	rBV4	45293	50621	1.33%	0.150%
33	14.639	2131	2134	2138	rBV	44515	42668	1.12%	0.126%
34	14.786	2156	2159	2163	rVB	46383	41603	1.09%	0.123%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I5588-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-EPE-115-4B(10-12)

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	15.121	2213	2216	2220	rVB	41311	48274	1.27%	0.143%
36	15.498	2275	2280	2291	rVB	554643	693921	18.21%	2.054%
37	15.939	2351	2355	2360	rVB2	38921	56125	1.47%	0.166%
38	16.445	2436	2441	2449	rVB2	39233	70988	1.86%	0.210%
39	17.039	2534	2542	2553	rBV3	32653	77059	2.02%	0.228%
40	17.739	2655	2661	2671	rVB4	28244	69311	1.82%	0.205%
41	18.574	2795	2803	2811	rBV4	23039	61069	1.60%	0.181%

Sum of corrected areas: 33787843

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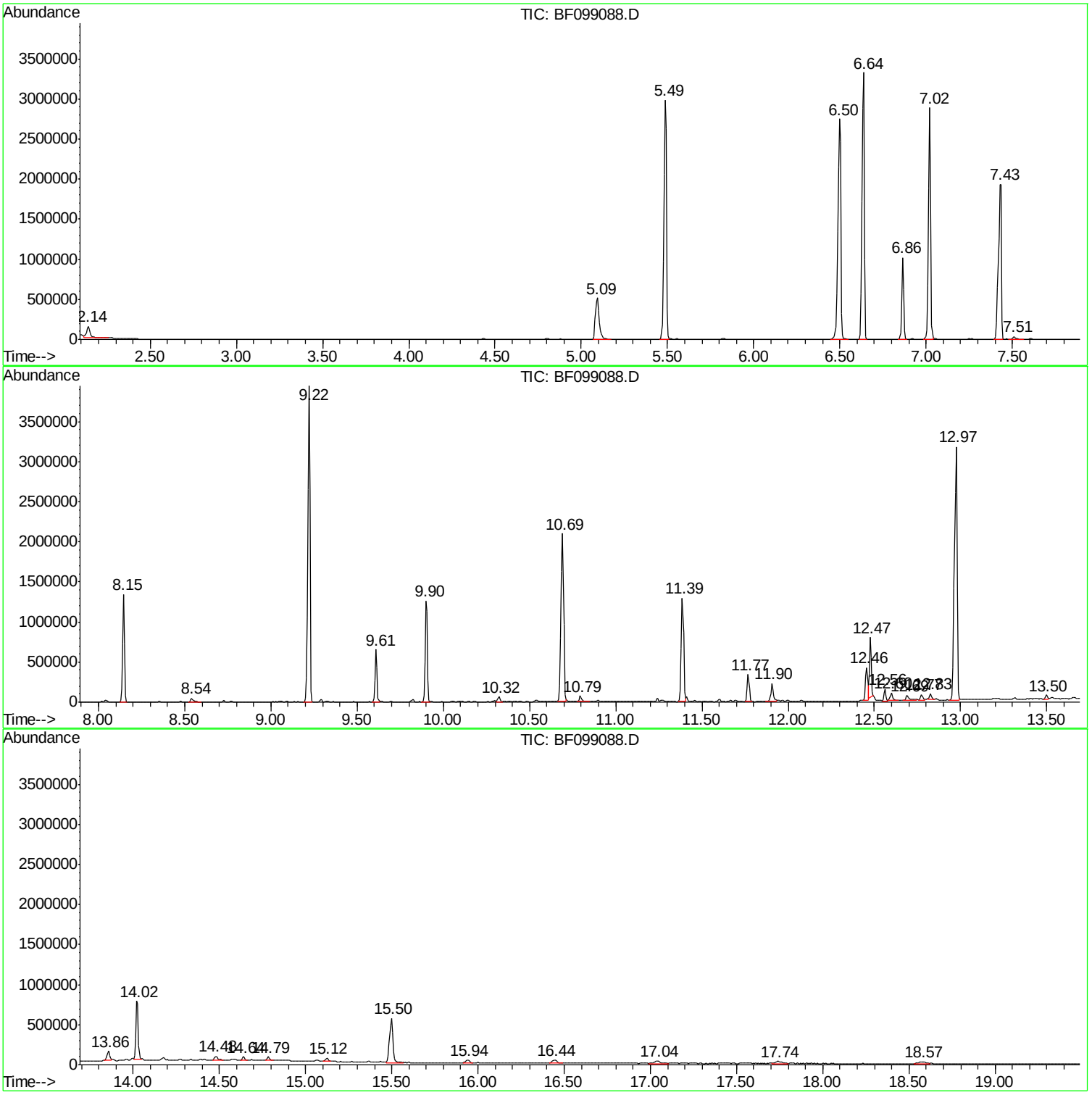
Instrument :
BNA_F
ClientSampleId :
SASP2P-EPE-115-4B(10-12)

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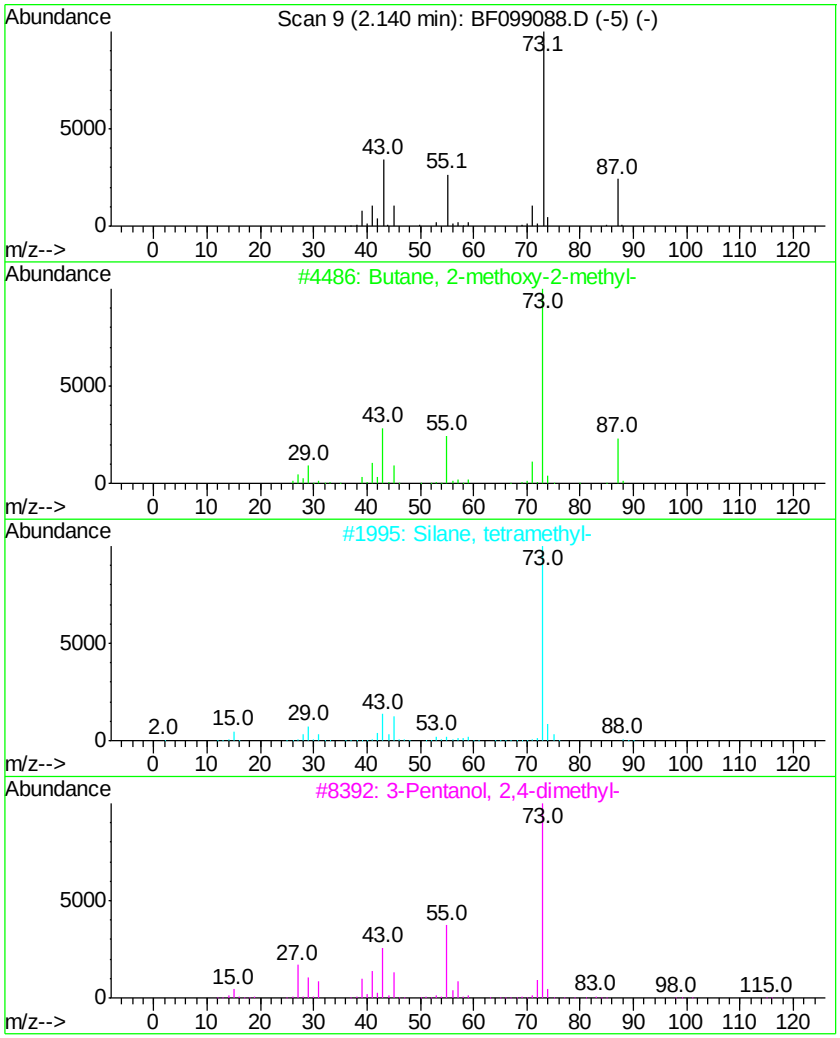
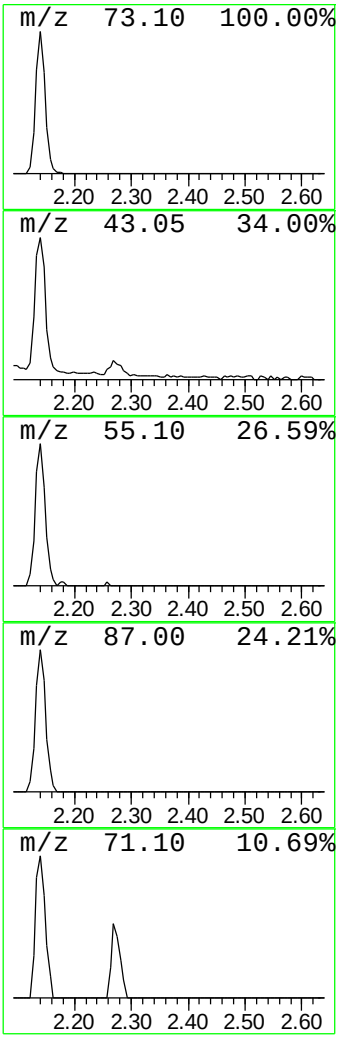
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	5.72 ng	235550	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	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	43
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	25





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Instrument : BNA_F
ClientSampleId : SASP2P-EPE-115-4B(10-12)

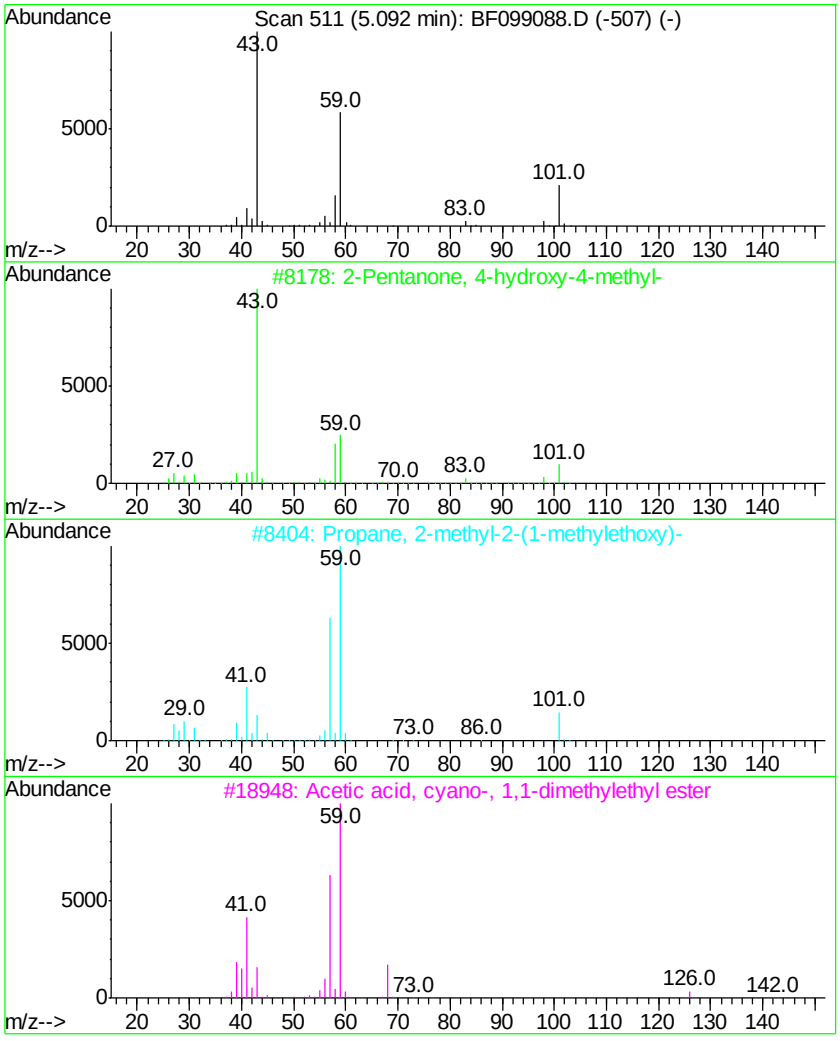
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

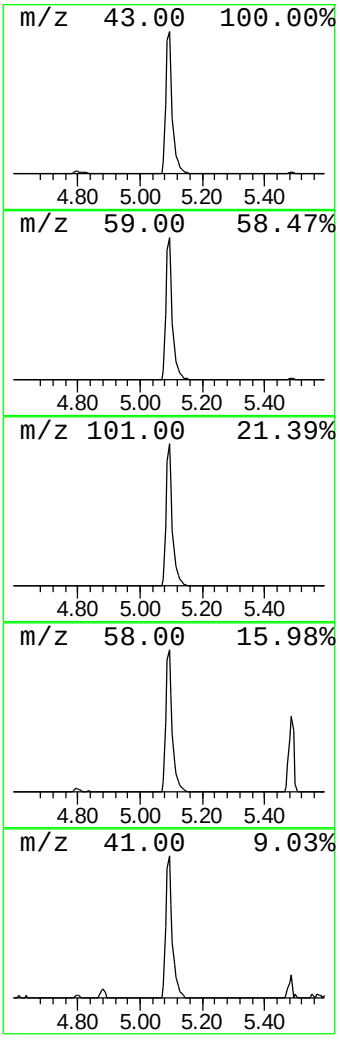
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	17.88 ng	736874	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9





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Sample : I5588-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-EPE-115-4B(10-12)

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
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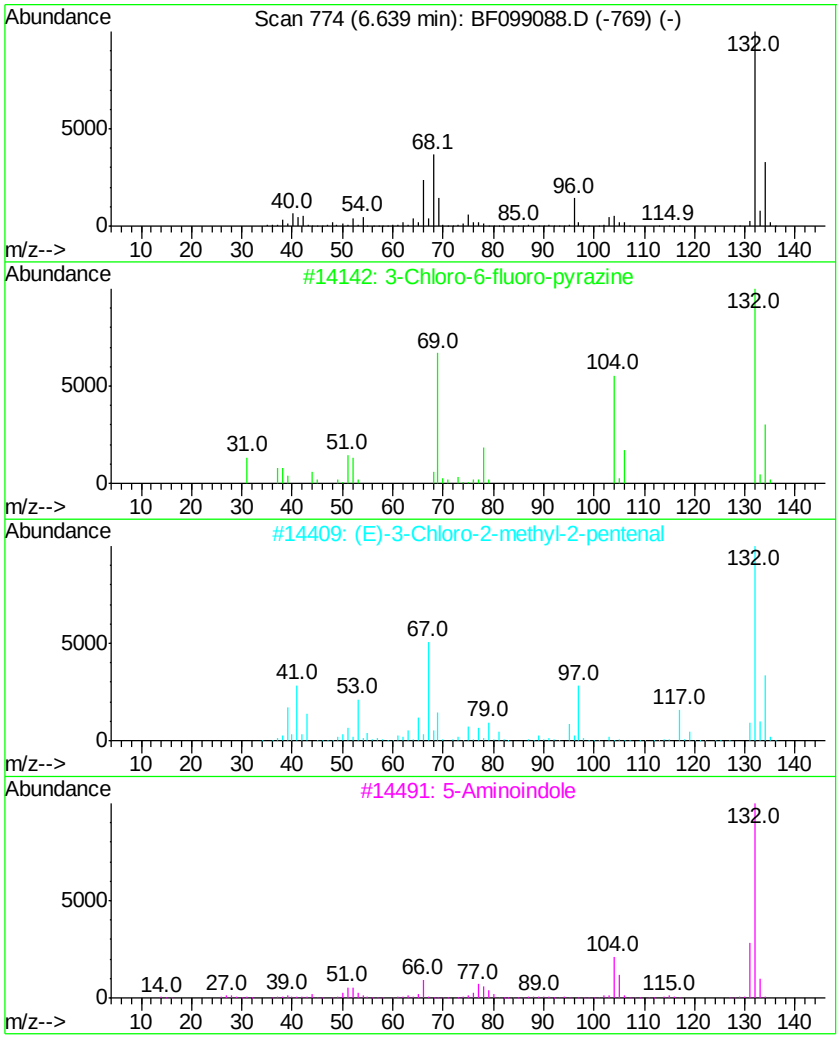
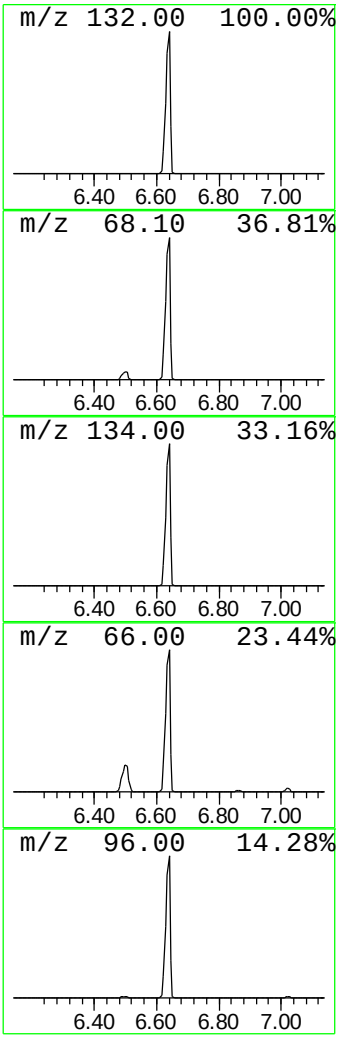
****

Peak Number 3 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	81.92 ng	3375980	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	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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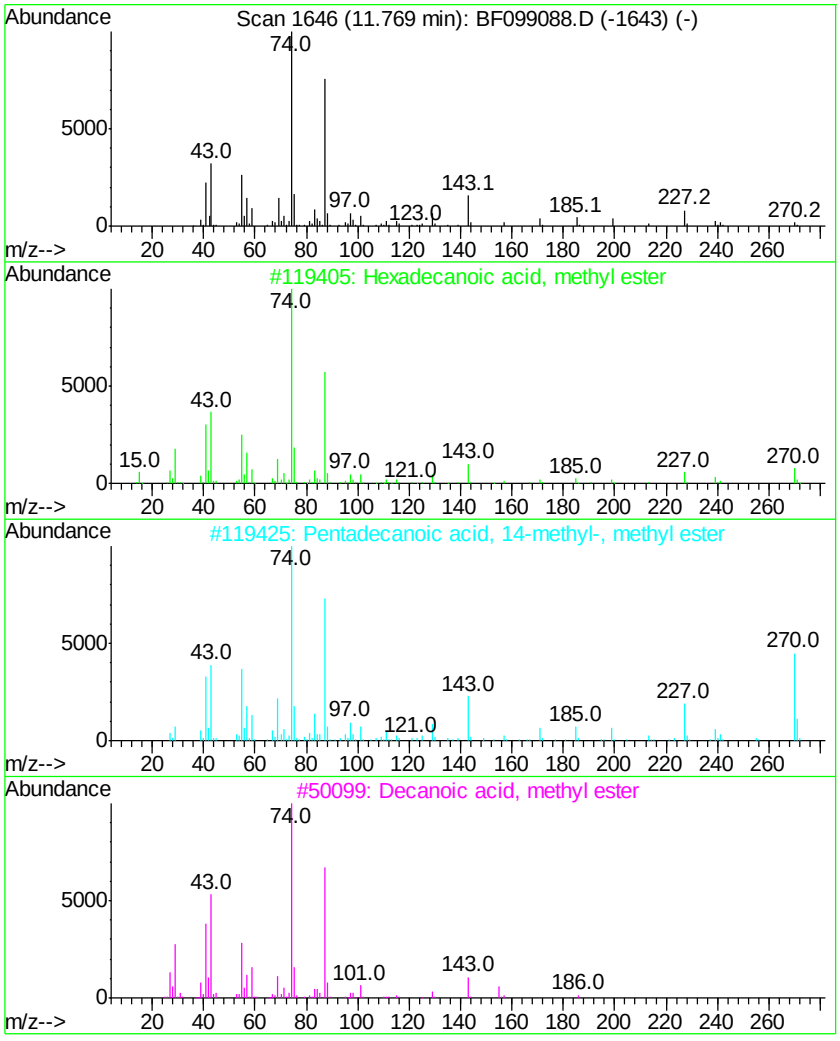
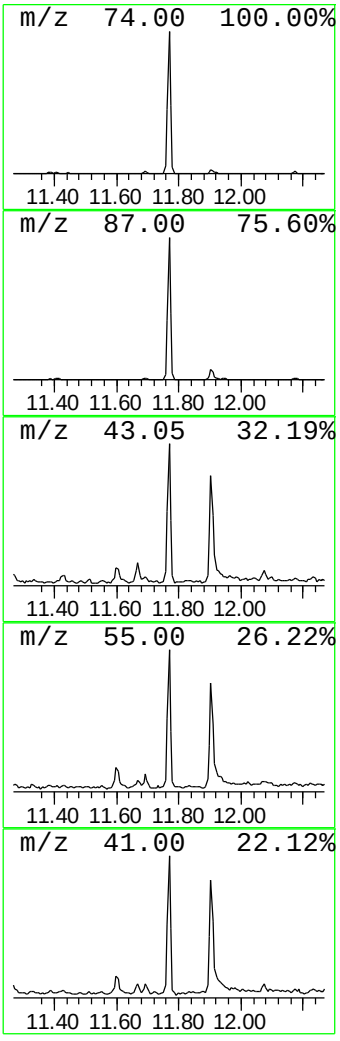
Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	4.42 ng	244024	Phenanthrene-d10	11.39

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	95
3	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	90
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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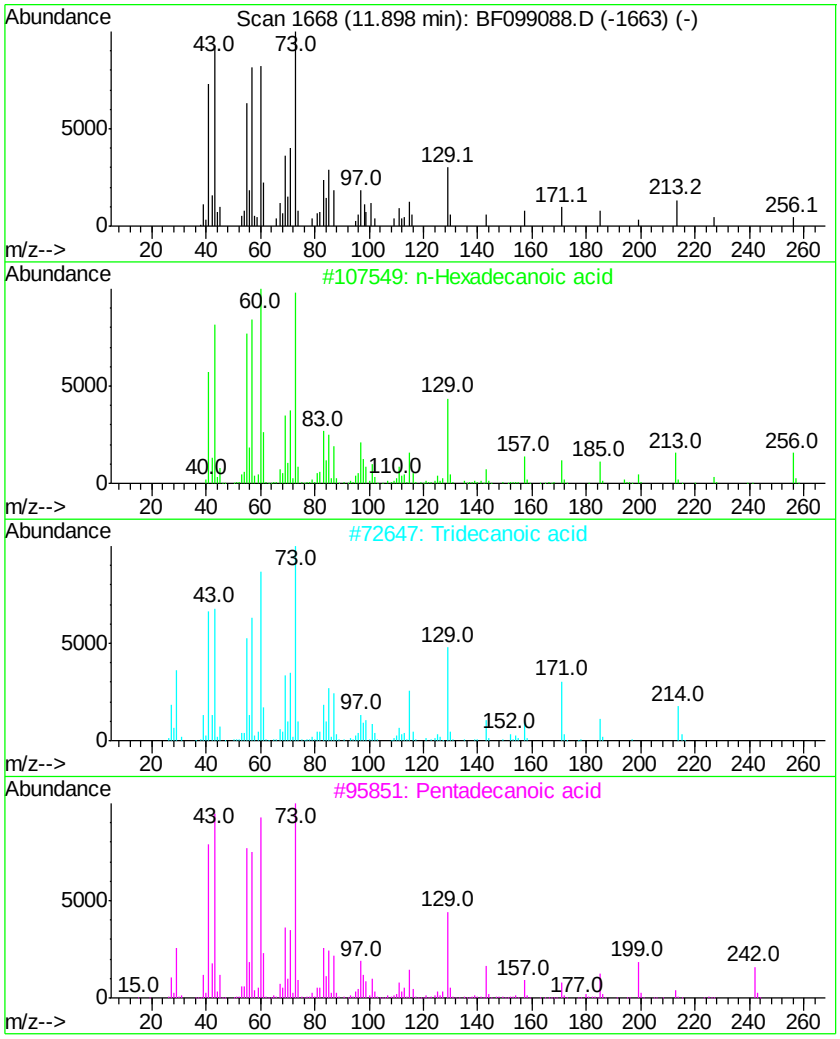
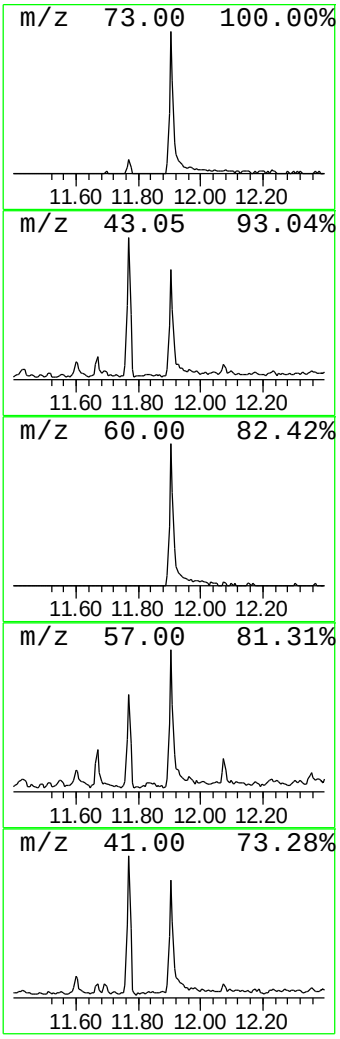
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	4.09 ng	225740	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	25





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ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-EPE-115-4B(10-12)

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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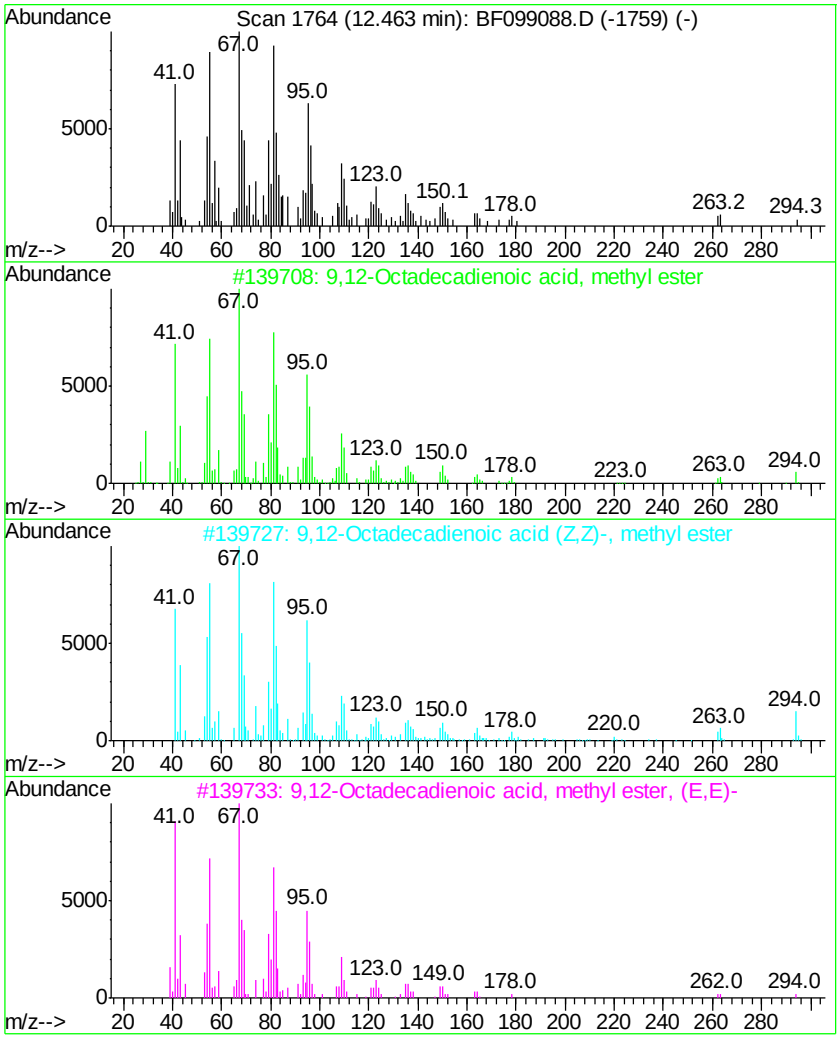
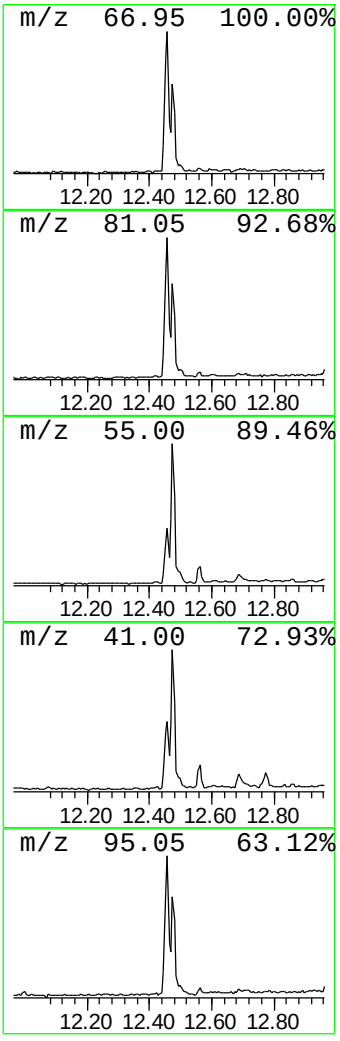
Peak Number 7 9,12-Octadecadienoic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	6.21 ng	342848	Phenanthrene-d10	11.39

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





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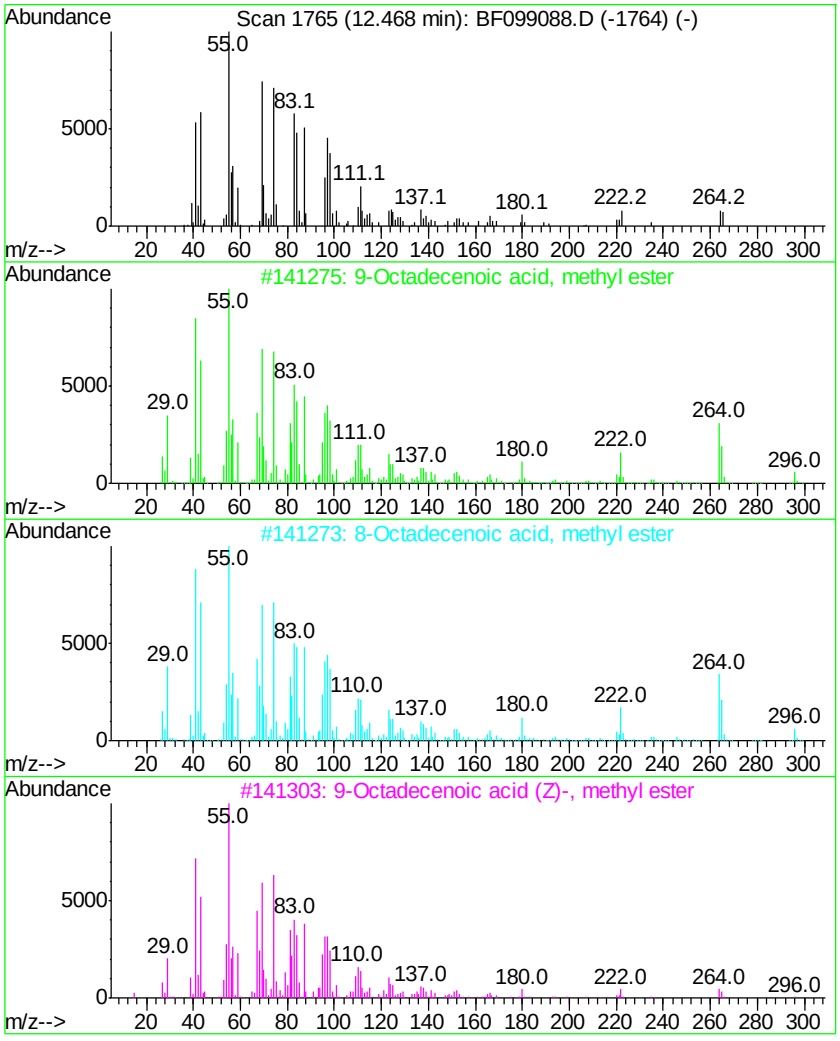
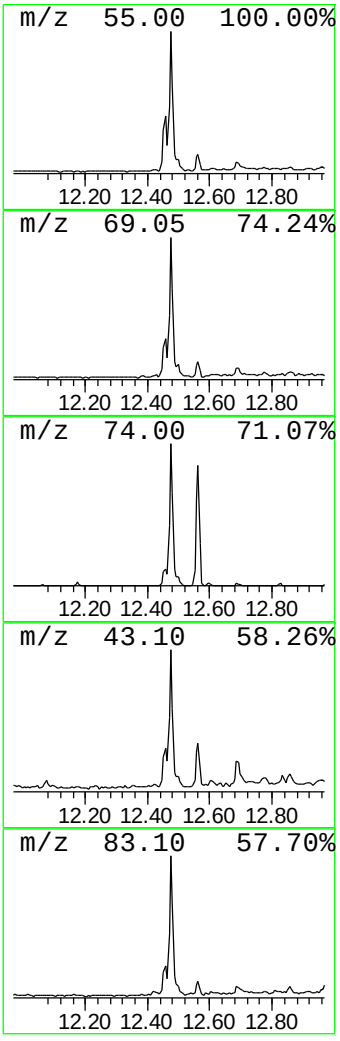
Peak Number 8 9-Octadecenoic acid, methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.47	10.33 ng	569922	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	96
2	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	94
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	94
4	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	91
5	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	91





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Operator : SJ/JU
Sample : I5588-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-EPE-115-4B(10-12)

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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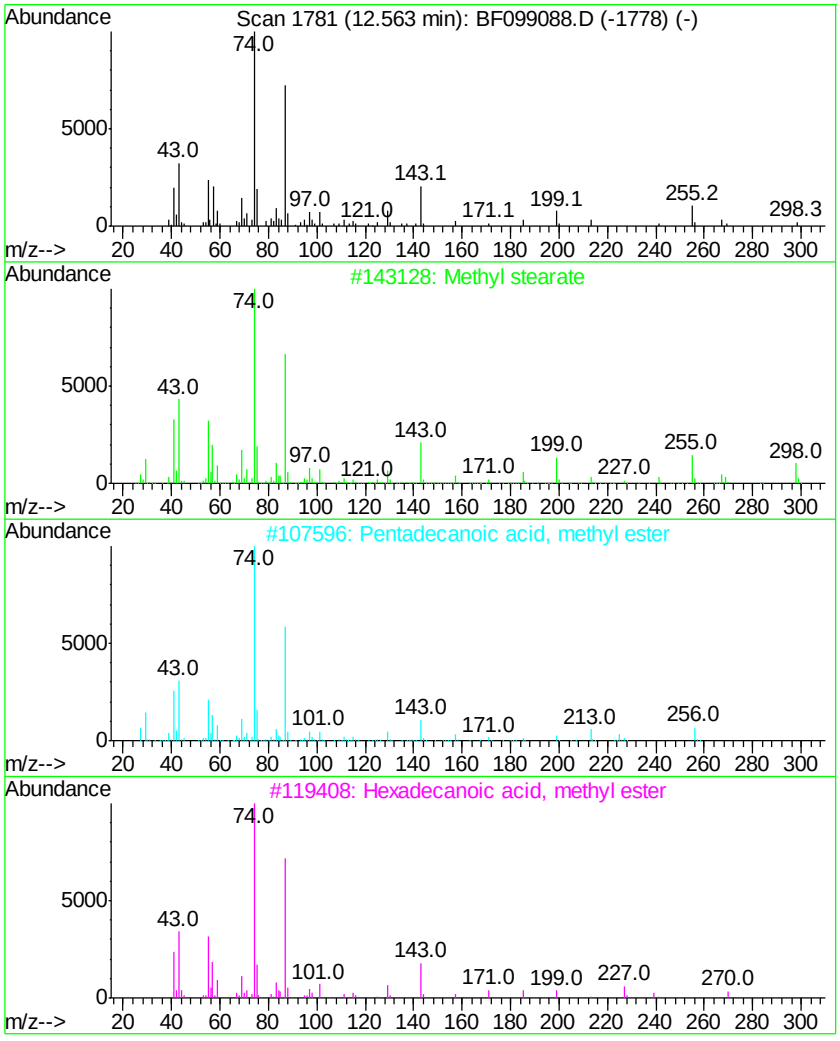
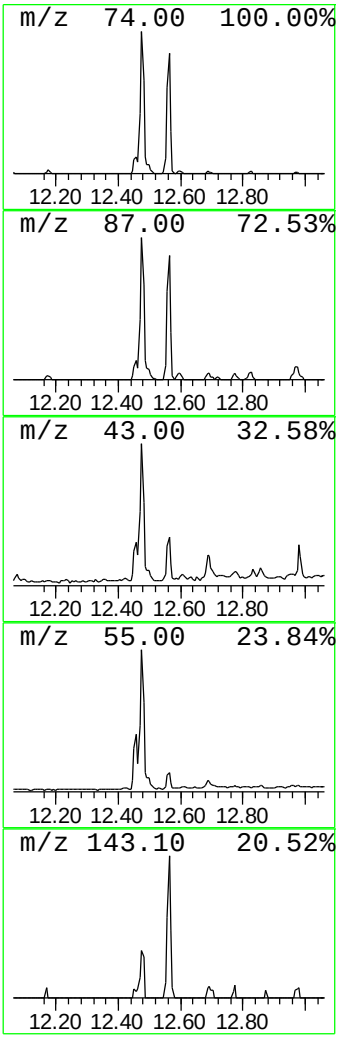
Peak Number 9 Methyl stearate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	2.18 ng	120246	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
3	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	87
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	80
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80





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ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-EPE-115-4B(10-12)

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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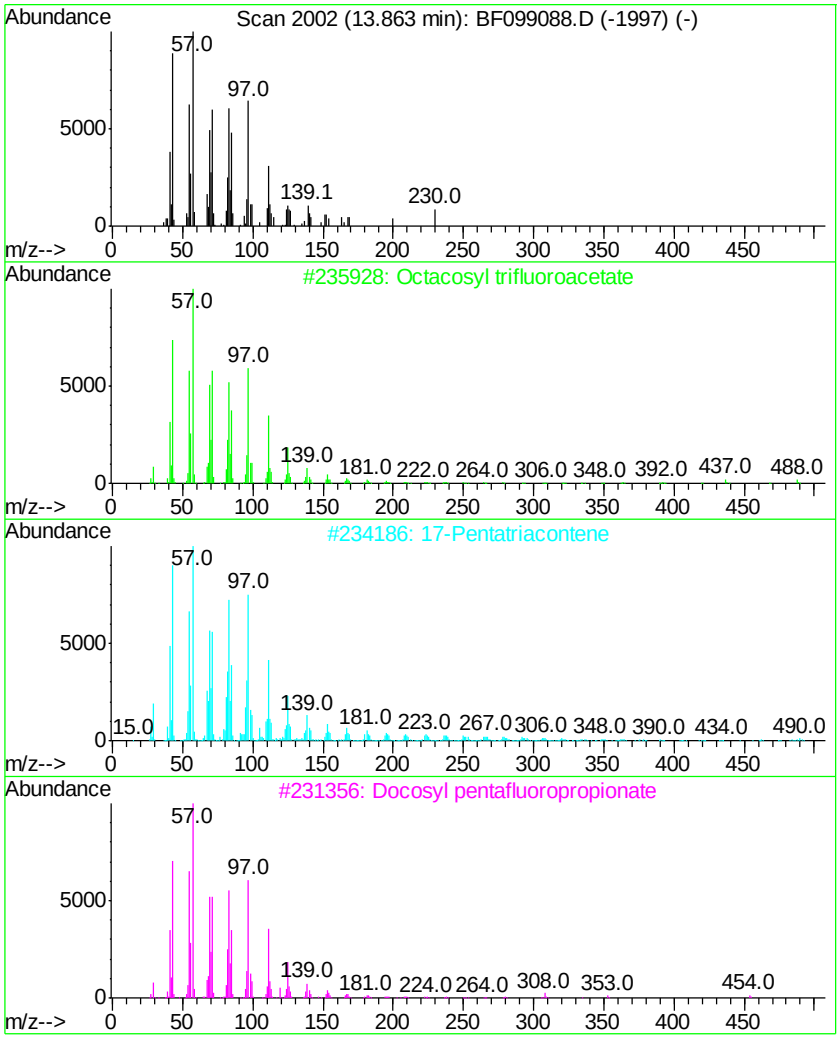
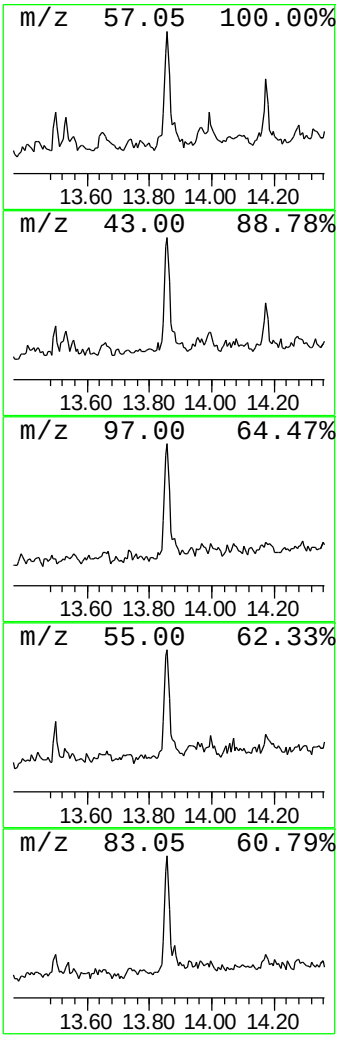
Peak Number 10 Octacosyl trifluoroacetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	3.90 ng	132505	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87
4	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	87
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100417\
Data File : BF099088.D
Acq On : 5 Oct 2017 1:12
Operator : SJ/JU
Sample : I5588-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-EPE-115-4B(10-12)

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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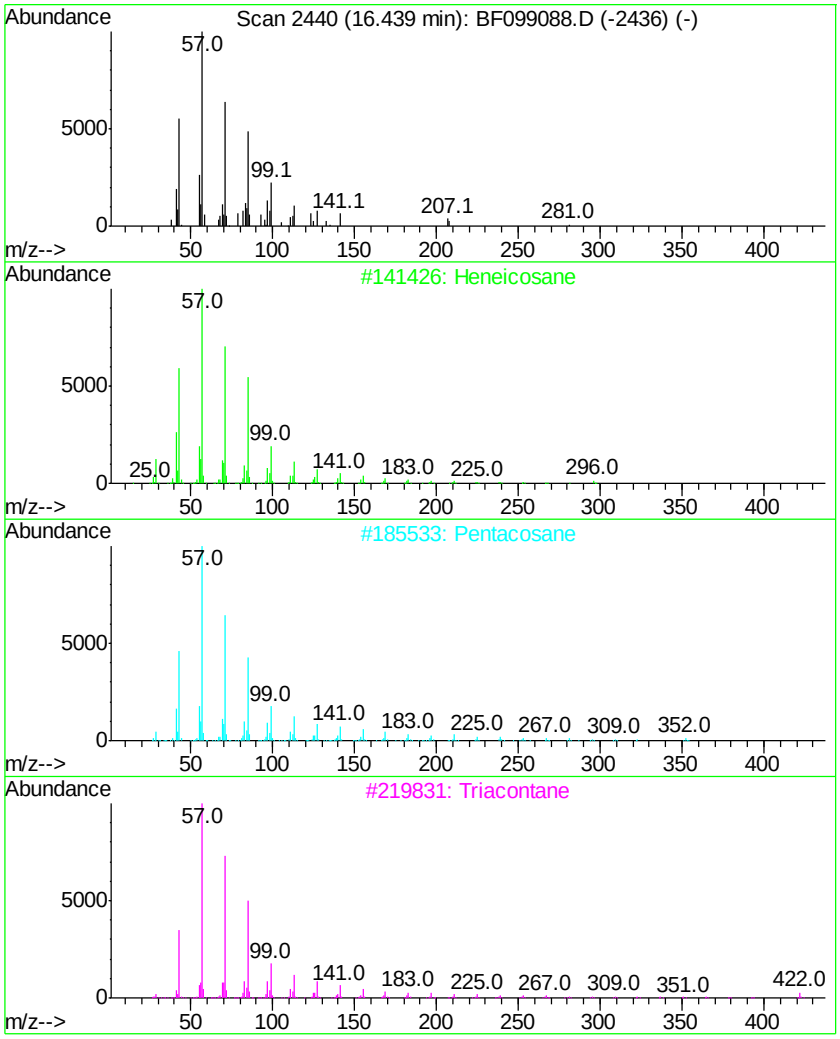
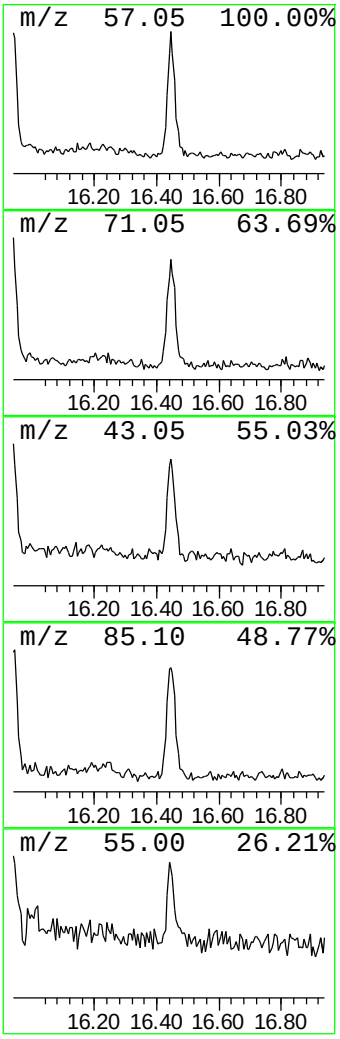
Peak Number 11 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.44	2.05 ng	70988	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Triacontane	422	C30H62	000638-68-6	90
4	Hexacosane	366	C26H54	000630-01-3	87
5	Octadecane	254	C18H38	000593-45-3	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100417\
Data File : BF099088.D
Acq On : 5 Oct 2017 1:12
Operator : SJ/JU
Sample : I5588-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-EPE-115-4B(10-12)

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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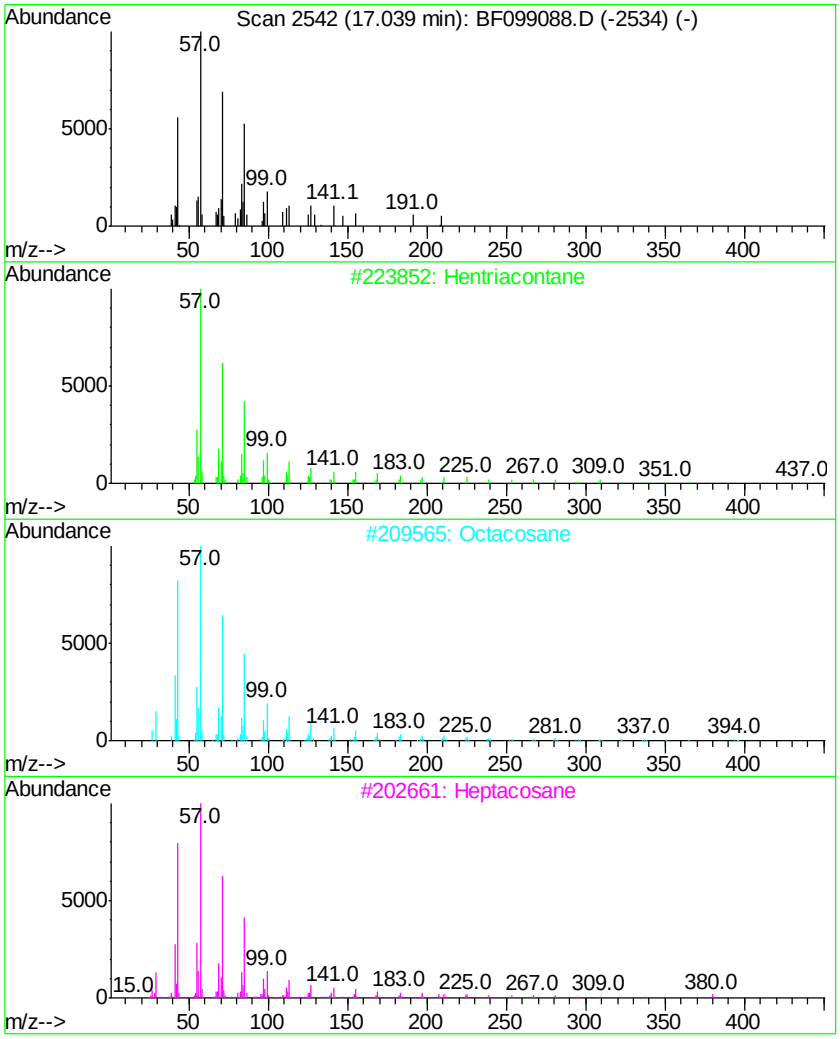
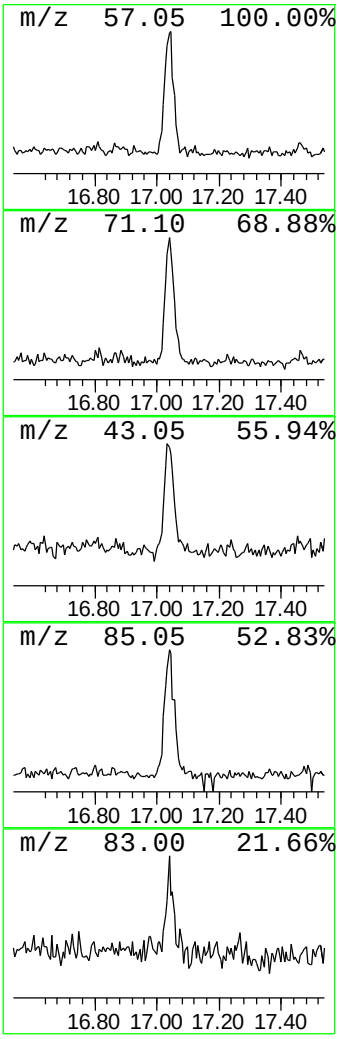
Peak Number 12 Hentriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.04	2.22 ng	77059	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	Hexacosane	366	C26H54	000630-01-3	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
Data File : BF099088.D
Acq On : 5 Oct 2017 1:12
Operator : SJ/JU
Sample : I5588-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-EPE-115-4B(10-12)

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...	2.14	5.7	ng	235550	1	6.86	824208	20.0
2-Pentanone, 4-hy...	5.09	17.9	ng	736874	1	6.86	824208	20.0
unknown6.64	6.64	81.9	ng	3375980	1	6.86	824208	20.0
Hexadecanoic acid...	11.77	4.4	ng	244024	4	11.39	1103580	20.0
n-Hexadecanoic acid	11.90	4.1	ng	225740	4	11.39	1103580	20.0
9,12-Octadecadien...	12.46	6.2	ng	342848	4	11.39	1103580	20.0
9-Octadecenoic ac...	12.47	10.3	ng	569922	4	11.39	1103580	20.0
Methyl stearate	12.56	2.2	ng	120246	4	11.39	1103580	20.0
Octacosyl trifluo...	13.86	3.9	ng	132505	5	14.03	678842	20.0
Heneicosane	16.44	2.0	ng	70988	6	15.50	693921	20.0
Hentriacontane	17.04	2.2	ng	77059	6	15.50	693921	20.0