LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
Data File : BF099167.D
Acq On : 7 Oct 2017 00:27
Operator : SJ/JU
Sample : I5517-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-9

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	2.169	9	14	28	rVB	633132	803387	21.42%	2.908%
2	5.087	507	510	523	rVB	196457	219289	5.85%	0.794%
3	5.487	573	578	581	rBV	1738486	1658723	44.22%	6.004%
4	6.487	744	748	751	rBV	1289219	1015830	27.08%	3.677%
5	6.634	768	773	776	rBV	2967958	2801037	74.67%	10.139%
6	6.863	808	812	815	rBV	953428	778967	20.77%	2.820%
7	7.022	834	839	842	rBV	2772892	2604100	69.42%	9.426%
8	7.428	902	908	911	rBV	2052168	2151156	57.35%	7.786%
9	8.145	1025	1030	1033	rBV	1157246	1067927	28.47%	3.866%
10	8.551	1093	1099	1102	rBV	357766	411982	10.98%	1.491%
11	9.222	1207	1213	1216	rBV	3572800	3751058	100.00%	13.578%
12	9.898	1322	1328	1332	rBV	1349930	1176562	31.37%	4.259%
13	10.692	1457	1463	1466	rBV	2007650	2083829	55.55%	7.543%
14	11.245	1552	1557	1563	rBV6	28202	48233	1.29%	0.175%
15	11.386	1577	1581	1584	rBV	1369387	1178330	31.41%	4.265%
16	11.586	1611	1615	1624	rBV	181705	180731	4.82%	0.654%
17	12.739	1807	1811	1815	rBV	161189	148347	3.95%	0.537%
18	12.780	1815	1818	1821	rVB	109412	84791	2.26%	0.307%
19	12.974	1845	1851	1854	rBV	3144660	3412396	90.97%	12.352%
20	13.480	1935	1937	1941	rVB	73411	63728	1.70%	0.231%
21	13.745	1978	1982	1988	rVB2	45825	55765	1.49%	0.202%
22	14.021	2025	2029	2038	rVB	910328	821282	21.89%	2.973%
23	15.121	2212	2216	2221	rVB	42161	49311	1.31%	0.178%
24	15.492	2274	2279	2289	rBV	516666	700262	18.67%	2.535%
25	15.933	2349	2354	2360	rBV	57917	86526	2.31%	0.313%
26	16.439	2434	2440	2453	rVB2	59301	112666	3.00%	0.408%
27	17.033	2533	2541	2551	rBV2	40193	93483	2.49%	0.338%
28	17.727	2652	2659	2667	rVB3	28274	67043	1.79%	0.243%

Sum of corrected areas: 27626741

LSC Report - Integrated Chromatogram

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Misc :
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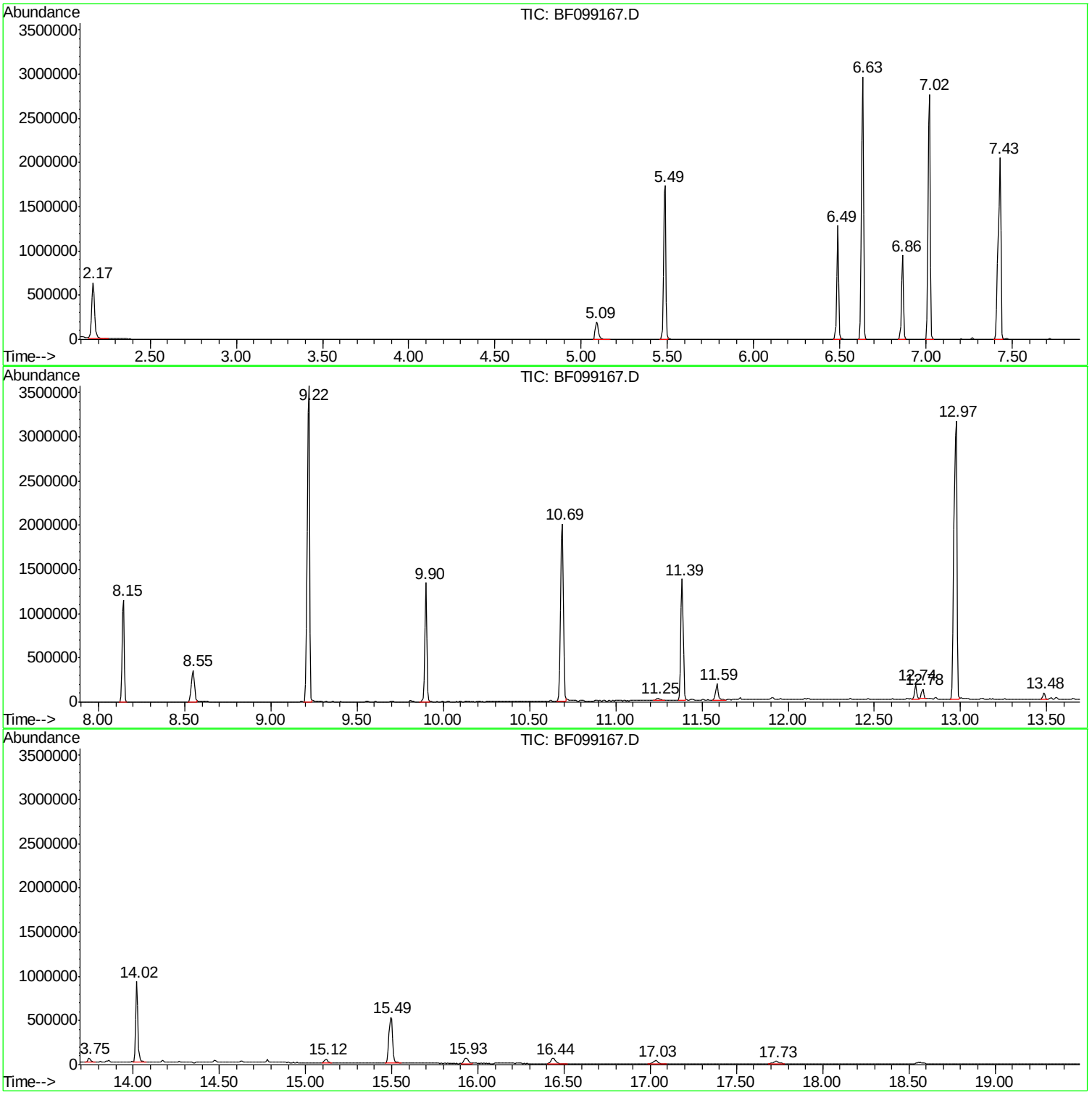
Instrument : BNA_F
ClientSampleId : MW-9

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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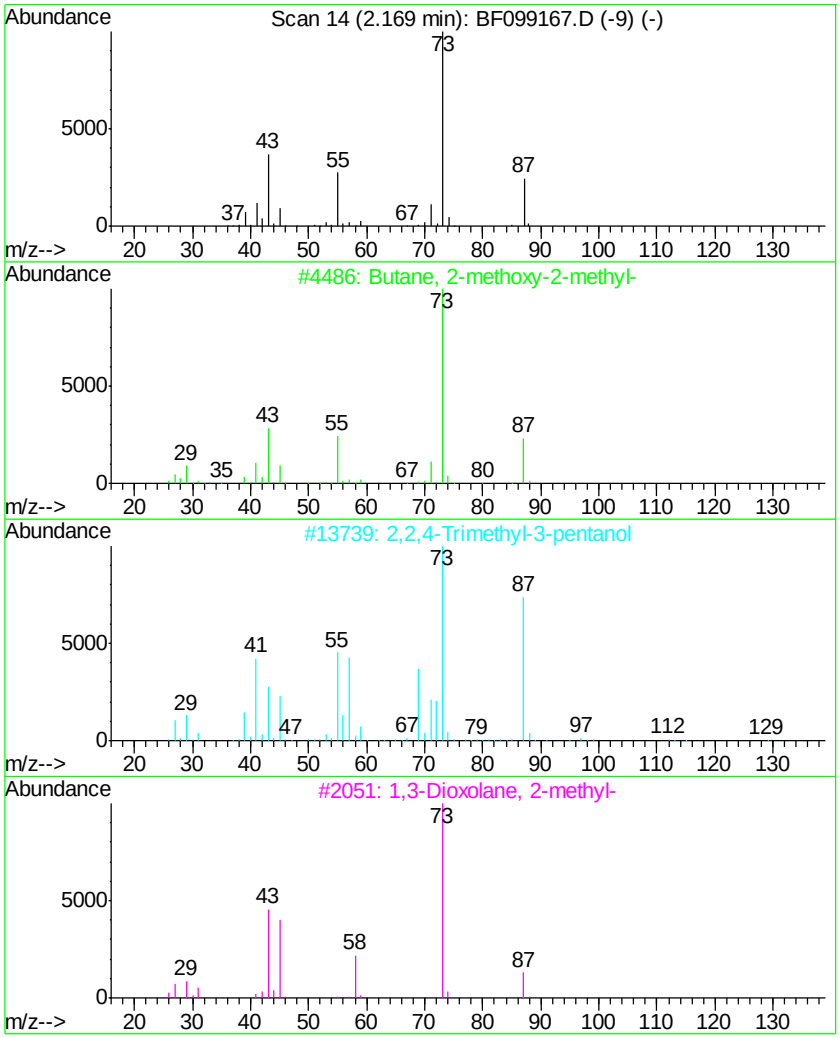
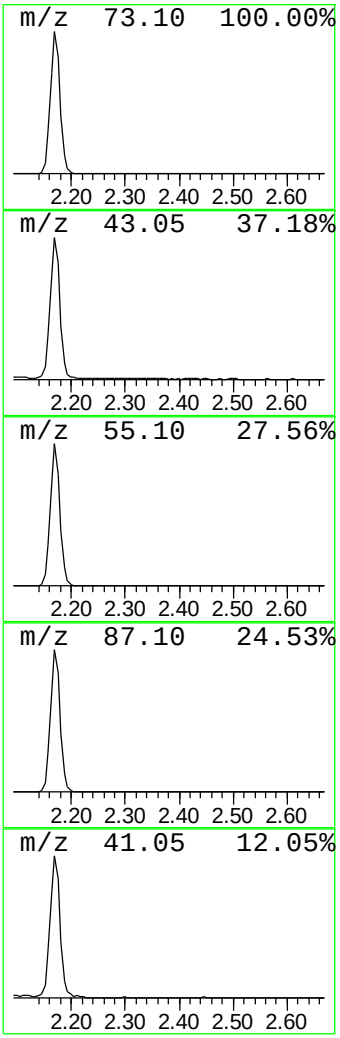
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	20.63 ng	803387	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	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Instrument : BNA_F
ClientSampleId : MW-9

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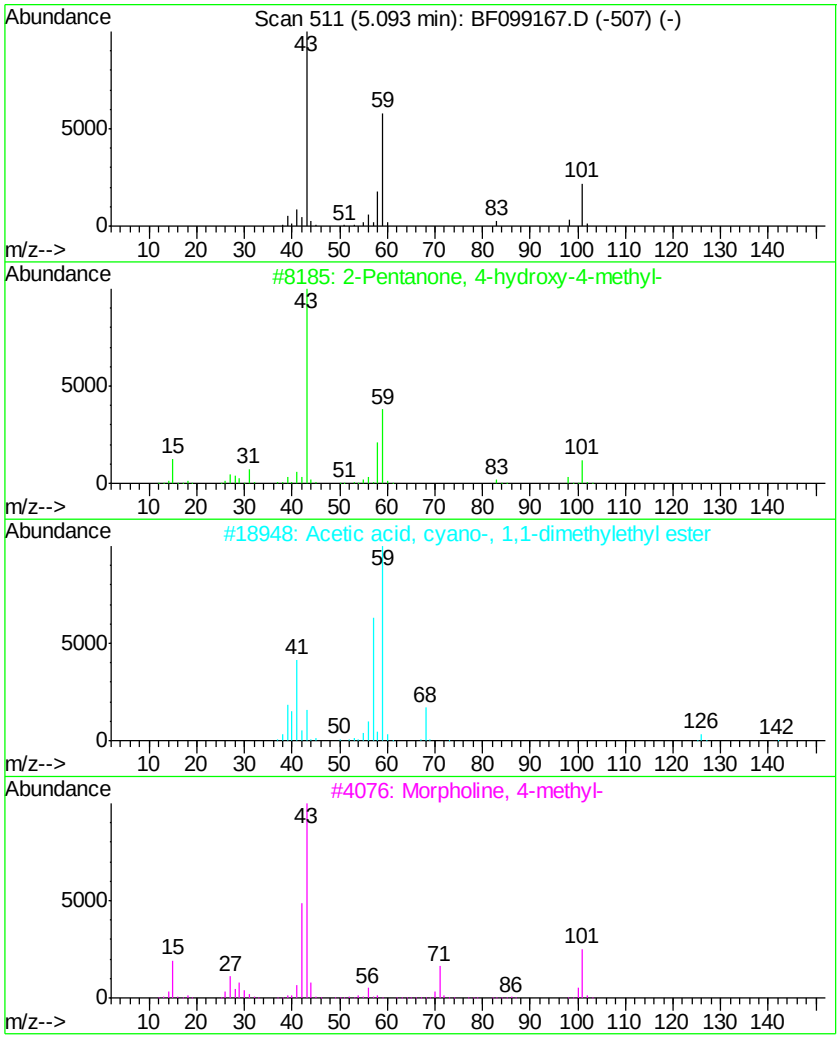
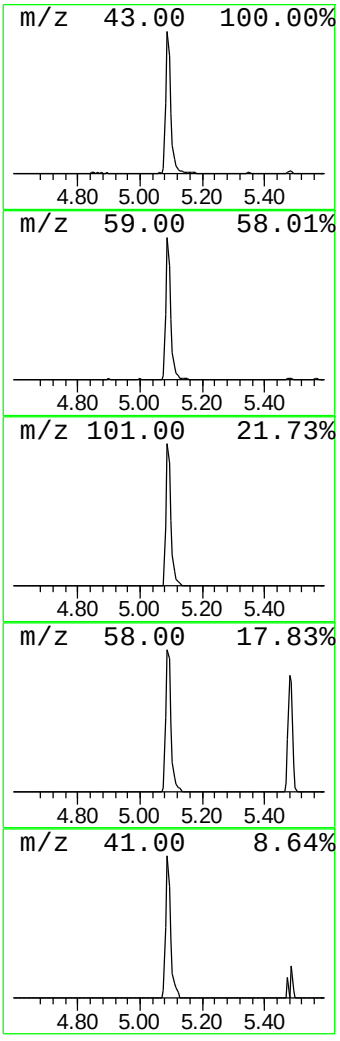
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	5.63 ng	219289	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	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Sample : I5517-05
Misc :
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Instrument : BNA_F
ClientSampleId : MW-9

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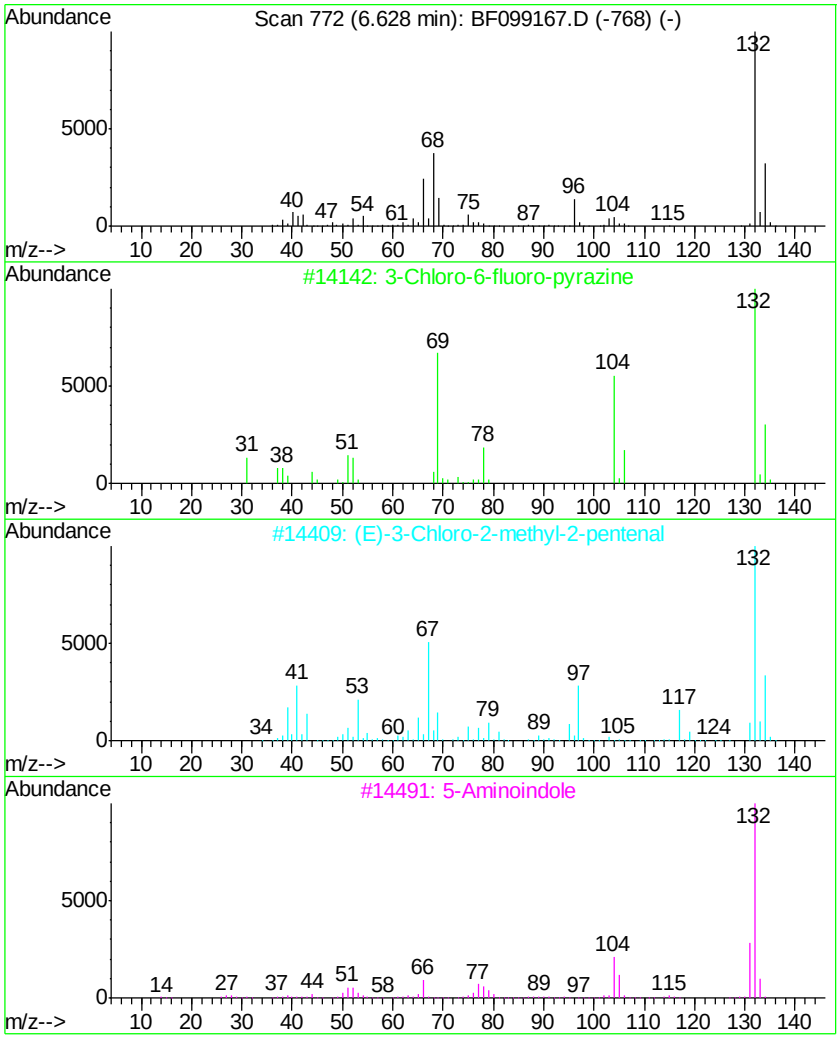
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

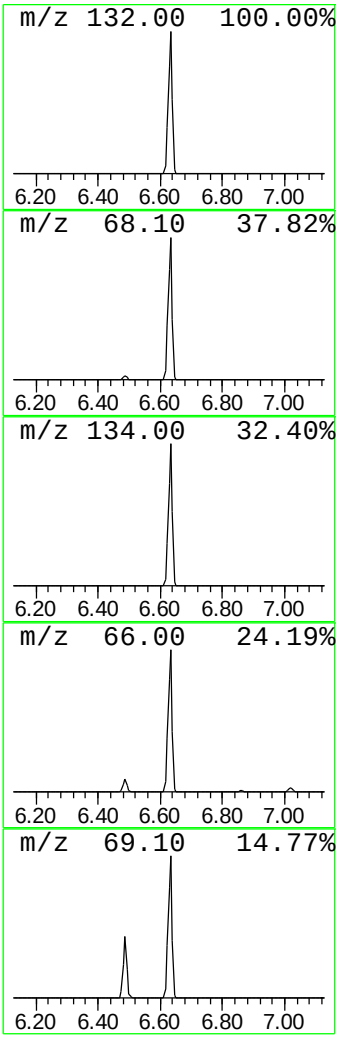
****

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	71.92 ng	2801040	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	Xenon	132	Xe	007440-63-3	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Instrument : BNA_F
ClientSampleId : MW-9

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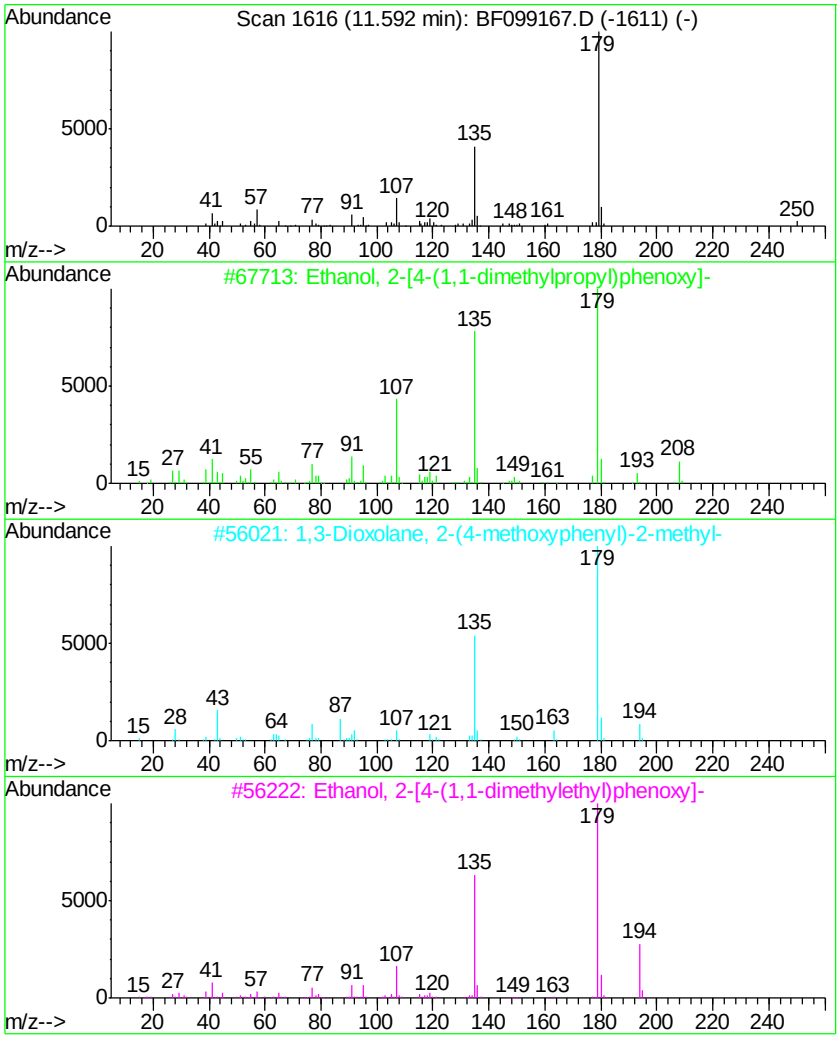
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

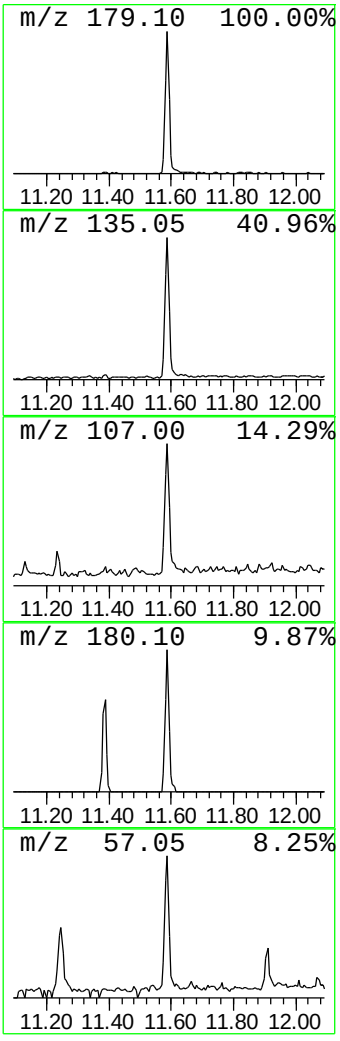
****

Peak Number 5 Ethanol, 2-[4-(1,1-dimethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.59	3.07 ng	180731	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[4-(1,1-dimethylpropy...	208	C13H20O2	006382-07-6	72
2	1,3-Dioxolane, 2-(4-methoxypheny...	194	C11H14O3	036881-00-2	72
3	Ethanol, 2-[4-(1,1-dimethylethyl...	194	C12H18O2	000713-46-2	50
4	Benzothiazole-6-carboxylic acid	179	C8H5NO2S	003622-35-3	47
5	Acetic acid, [2-[(2-propenylamin...	235	C12H13NO4	000119-45-9	37





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Instrument : BNA_F
ClientSampleId : MW-9

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

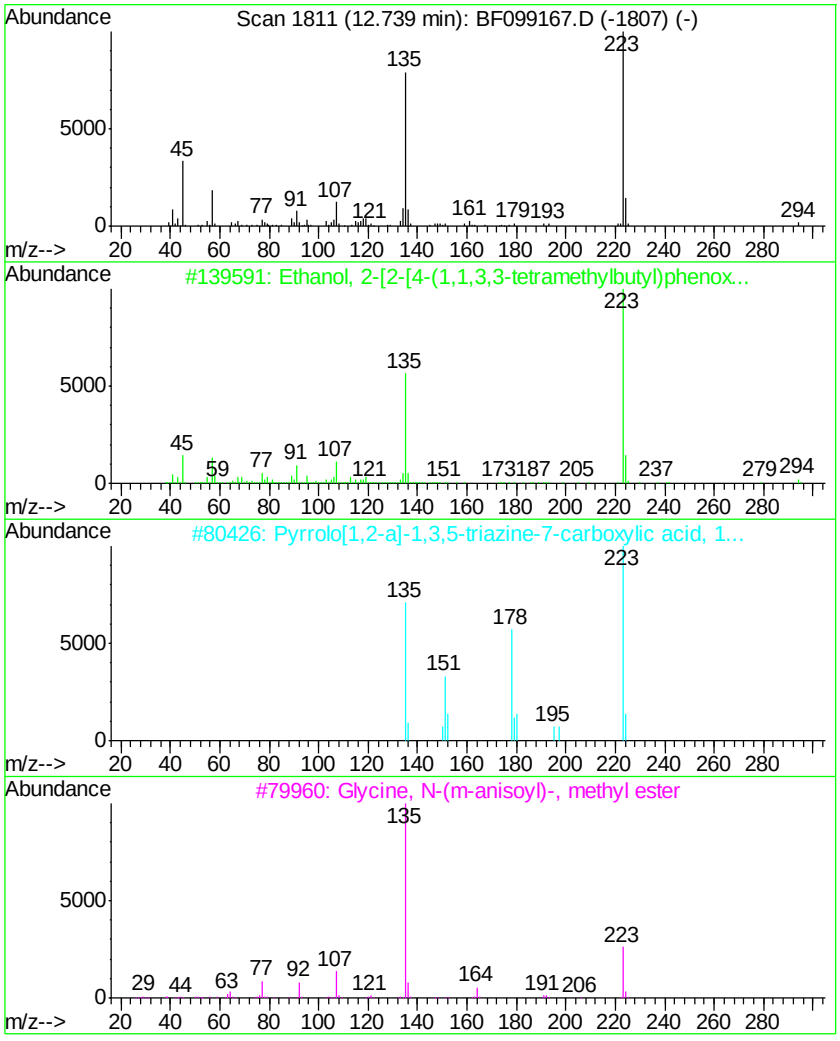
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

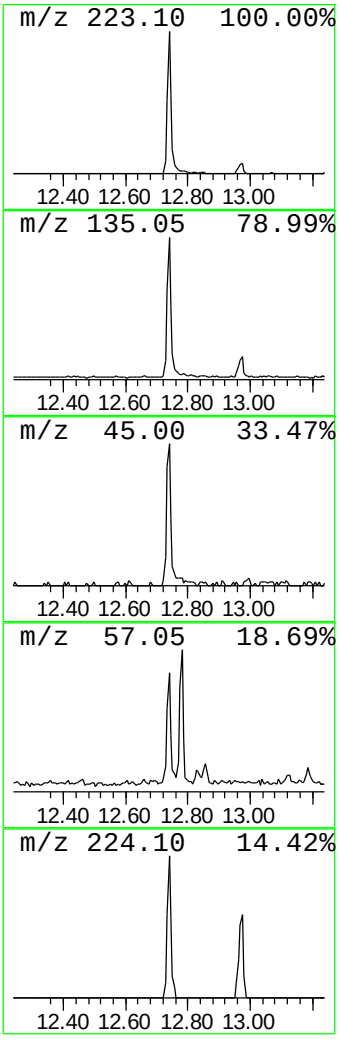
****

Peak Number 6 Ethanol, 2-[2-[4-(1,1,3,3-t... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	3.61 ng	148347	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	93
2	Pyrrolo[1,2-a]-1,3,5-triazine-7-...	223	C9H9N3O4	054449-89-7	90
3	Glycine, N-(m-anisoyl)-, methyl ...	223	C11H13NO4	1000299-70-7	64
4	2-Methoxycarbonyl-2-methylbrendane	194	C12H18O2	148191-16-6	35
5	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	35





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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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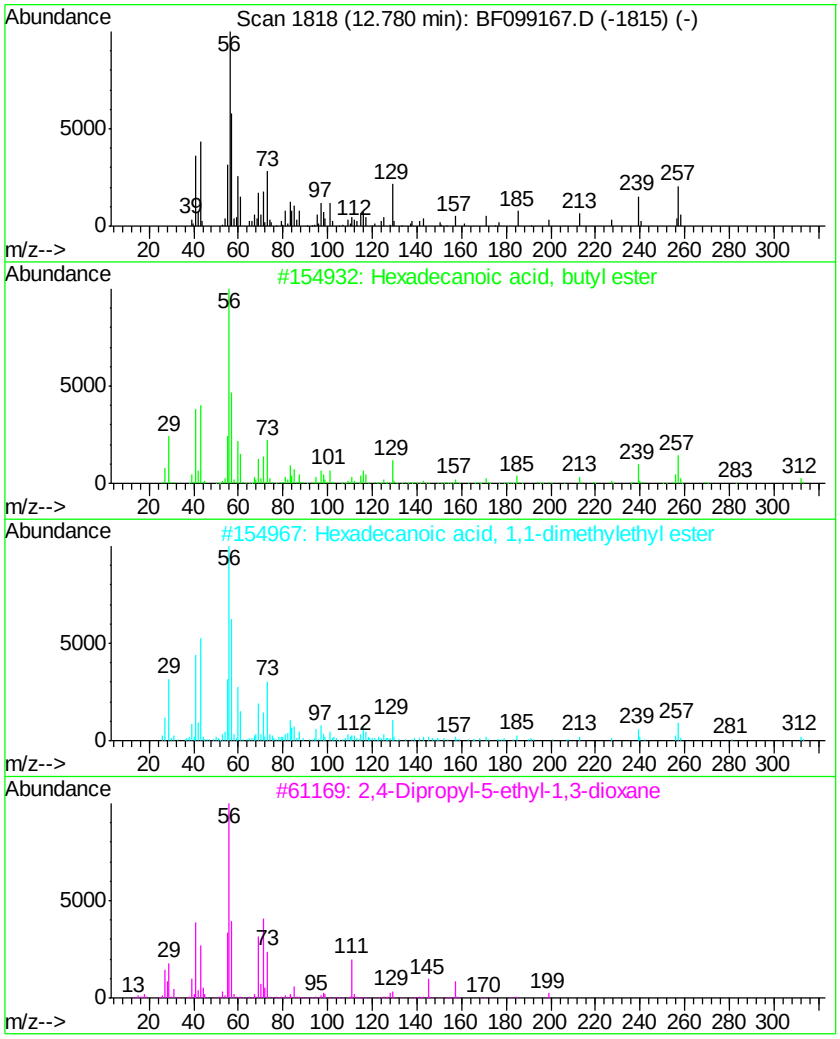
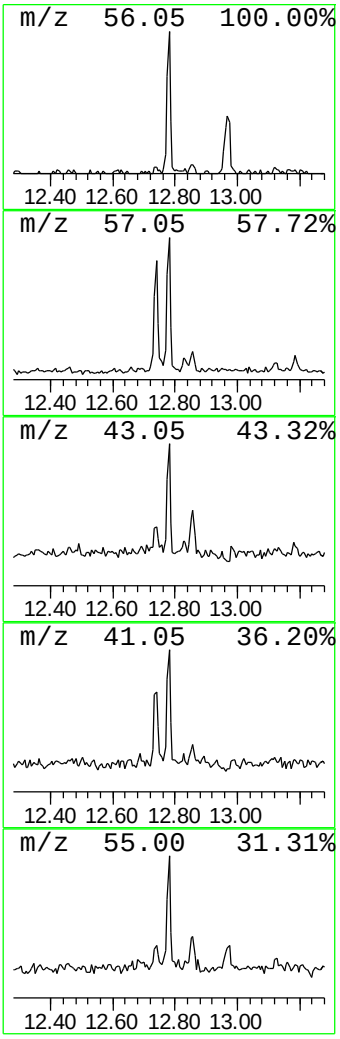
Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	2.06 ng	84791	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	37
4	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	27
5	1-Piperidinyloxy, 4-(hydroxyimin...	185	C9H17N2O2	003229-75-2	27





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TIC Library : C:\DATABASE\NIST11.L
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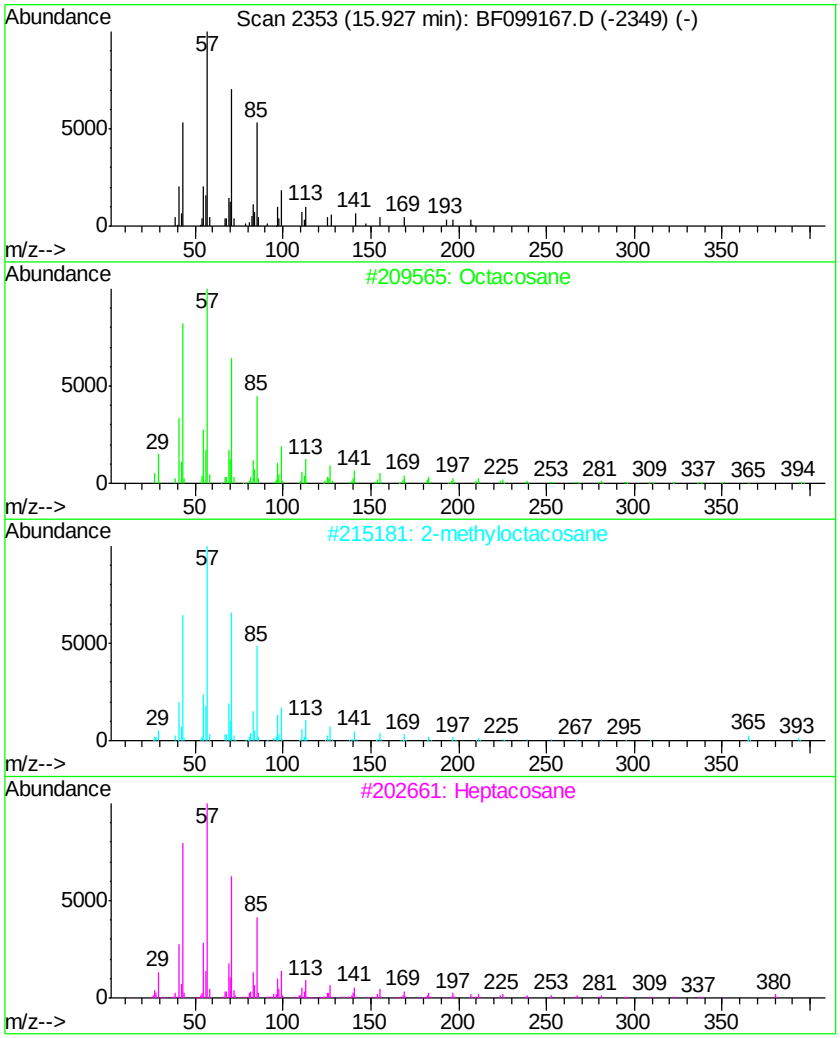
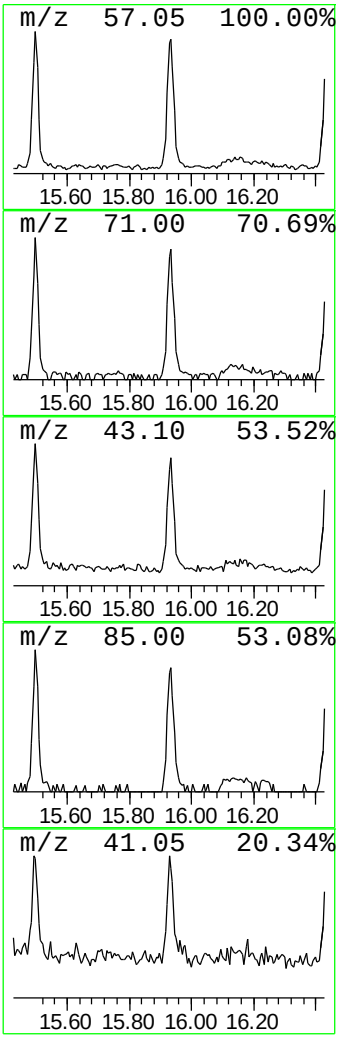
Peak Number 8 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	2.47 ng	86526	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Hexacosane	366	C26H54	000630-01-3	90





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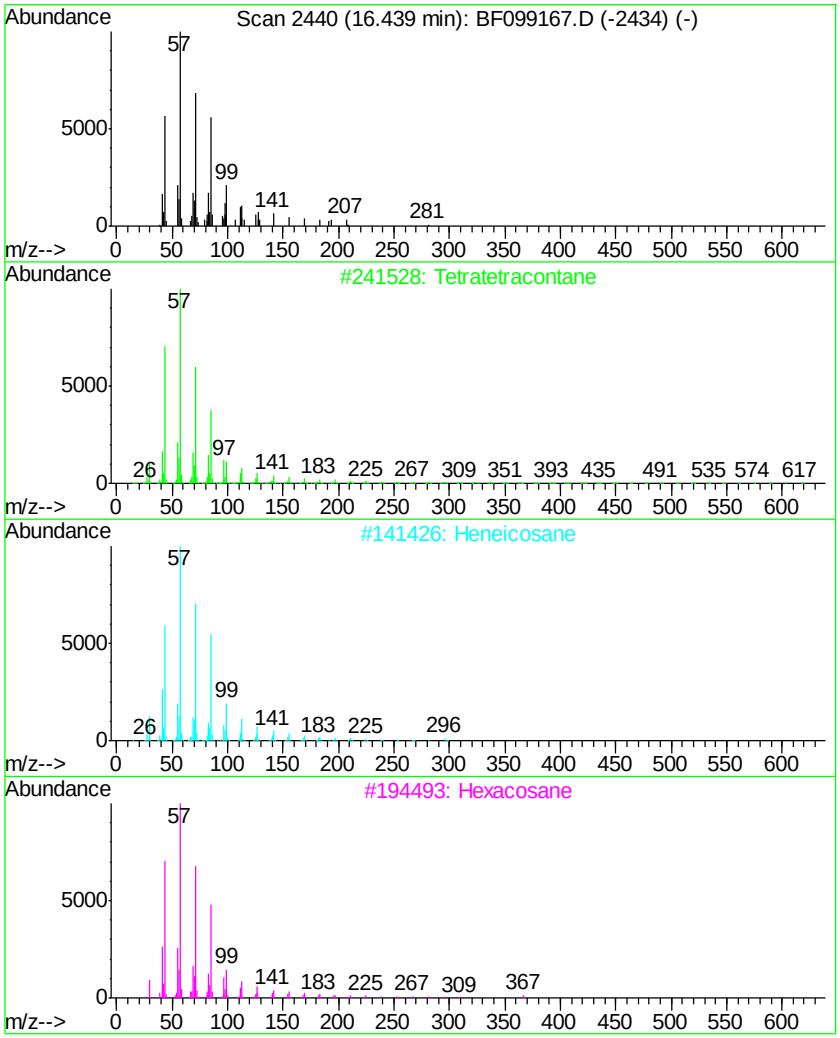
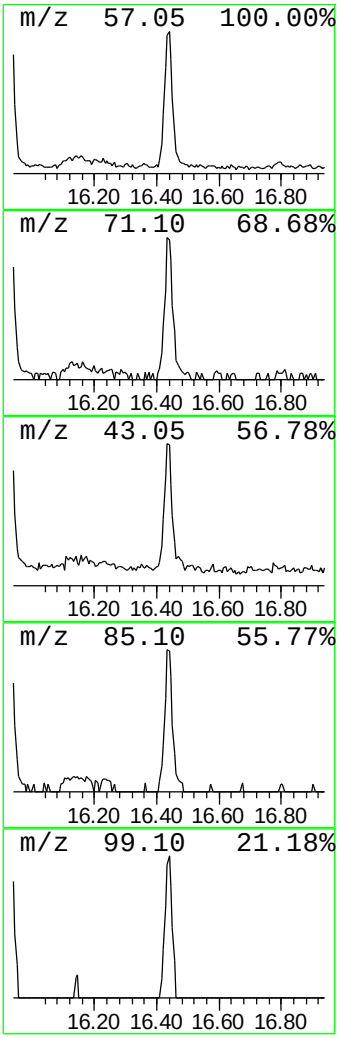
Peak Number 9 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.44	3.22 ng	112666	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Heptadecane	240	C17H36	000629-78-7	87
5	2-methyloctacosane	408	C29H60	1000376-72-8	87





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Instrument : BNA_F
ClientSampleId : MW-9

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

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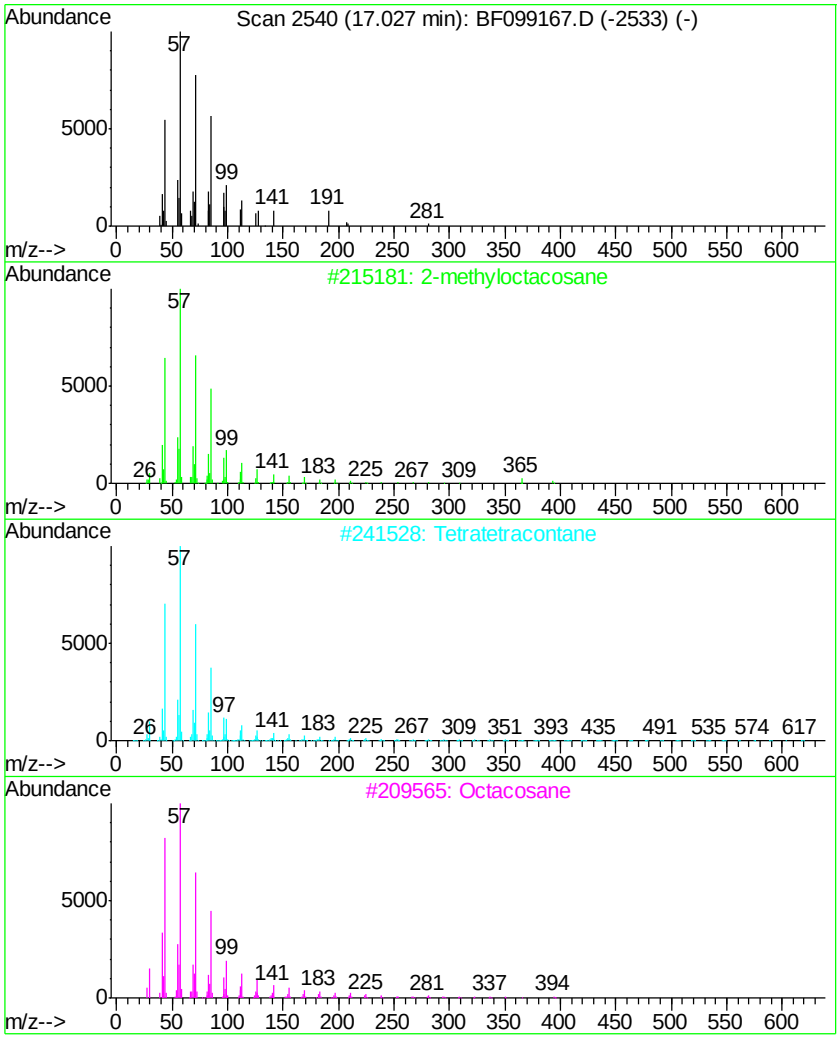
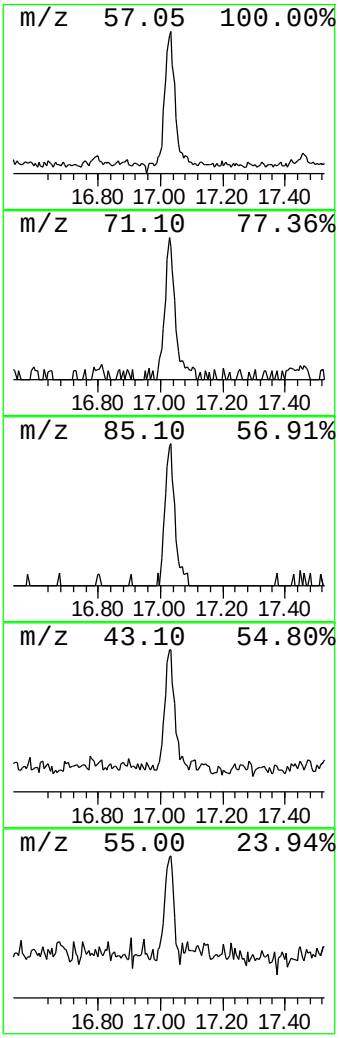
Peak Number 10 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.03	2.67 ng	93483	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	87
2	Tetratetracontane	619	C44H90	007098-22-8	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	86
5	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	86





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...	2.17	20.6	ng	803387	1	6.86	778967	20.0
2-Pentanone, 4-hy...	5.09	5.6	ng	219289	1	6.86	778967	20.0
unknown6.63	6.63	71.9	ng	2801040	1	6.86	778967	20.0
Ethanol, 2-[4-(1,...	11.59	3.1	ng	180731	4	11.39	1178330	20.0
Ethanol, 2-[2-[4-...	12.74	3.6	ng	148347	5	14.02	821282	20.0
Hexadecanoic acid...	12.78	2.1	ng	84791	5	14.02	821282	20.0
Octacosane	15.93	2.5	ng	86526	6	15.49	700262	20.0
Tetratetracontane	16.44	3.2	ng	112666	6	15.49	700262	20.0
2-methyloctacosane	17.03	2.7	ng	93483	6	15.49	700262	20.0