LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
Data File : BF094717.D
Acq On : 30 Apr 2017 16:26
Operator : SJ/MA
Sample : I2860-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TANK-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-BF041717.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	3.372	240	244	257	rBV	505302	543121	15.09%	2.238%
2	3.919	332	337	349	rBV	1248524	1547164	43.00%	6.376%
3	4.319	402	405	420	rBV	808513	866341	24.08%	3.570%
4	4.695	466	469	480	rVB	281577	281877	7.83%	1.162%
5	5.384	583	586	599	rBV	495955	565461	15.72%	2.330%
6	5.513	604	608	616	rVB	1674856	1633435	45.40%	6.732%
7	5.760	647	650	661	rVB	674665	650728	18.09%	2.682%
8	5.942	676	681	684	rBV	2342419	2180370	60.60%	8.986%
9	6.419	756	762	765	rBV	1629532	1820996	50.61%	7.505%
10	7.254	900	904	913	rBV	947839	888511	24.69%	3.662%
11	8.583	1125	1130	1133	rBV	3400870	3598127	100.00%	14.829%
12	9.083	1211	1215	1222	rBV	278489	254472	7.07%	1.049%
13	9.389	1255	1267	1276	rBV2	1054905	1045274	29.05%	4.308%
14	9.725	1321	1324	1329	rBV	69594	76378	2.12%	0.315%
15	9.989	1365	1369	1372	rVB	39358	36198	1.01%	0.149%
16	10.366	1429	1433	1442	rBV	1281527	1396751	38.82%	5.756%
17	10.572	1464	1468	1475	rBV	43646	57834	1.61%	0.238%
18	11.213	1573	1577	1587	rBV	1024860	1023663	28.45%	4.219%
19	11.948	1698	1702	1712	rBV2	120189	150219	4.17%	0.619%
20	12.918	1863	1867	1877	rBV	193499	253873	7.06%	1.046%
21	13.195	1908	1914	1918	rBV2	2931593	3504748	97.40%	14.444%
22	14.354	2107	2111	2120	rBV	56450	91592	2.55%	0.377%
23	14.465	2125	2130	2136	rBV	788087	850098	23.63%	3.504%
24	15.483	2299	2303	2311	rVB	300691	334977	9.31%	1.381%
25	16.089	2402	2406	2414	rBV	509101	612026	17.01%	2.522%

Sum of corrected areas: 24264234

LSC Report - Integrated Chromatogram

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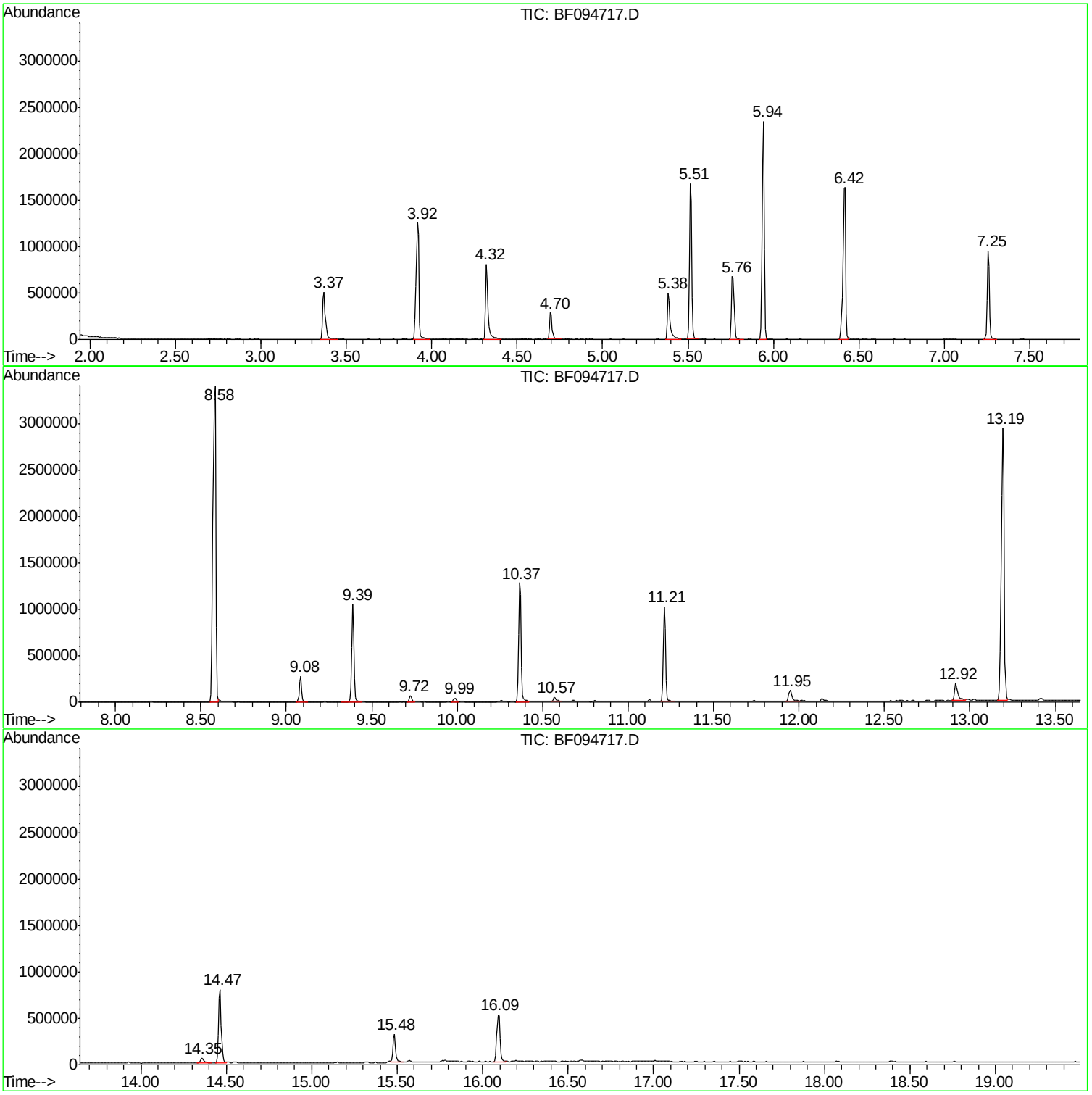
Operator : SJ/MA
Sample : I2860-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TANK-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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\BF043017\
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Acq On : 30 Apr 2017 16:26
Operator : SJ/MA
Sample : I2860-05
Misc :
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Instrument : BNA_F
ClientSampleId : TANK-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

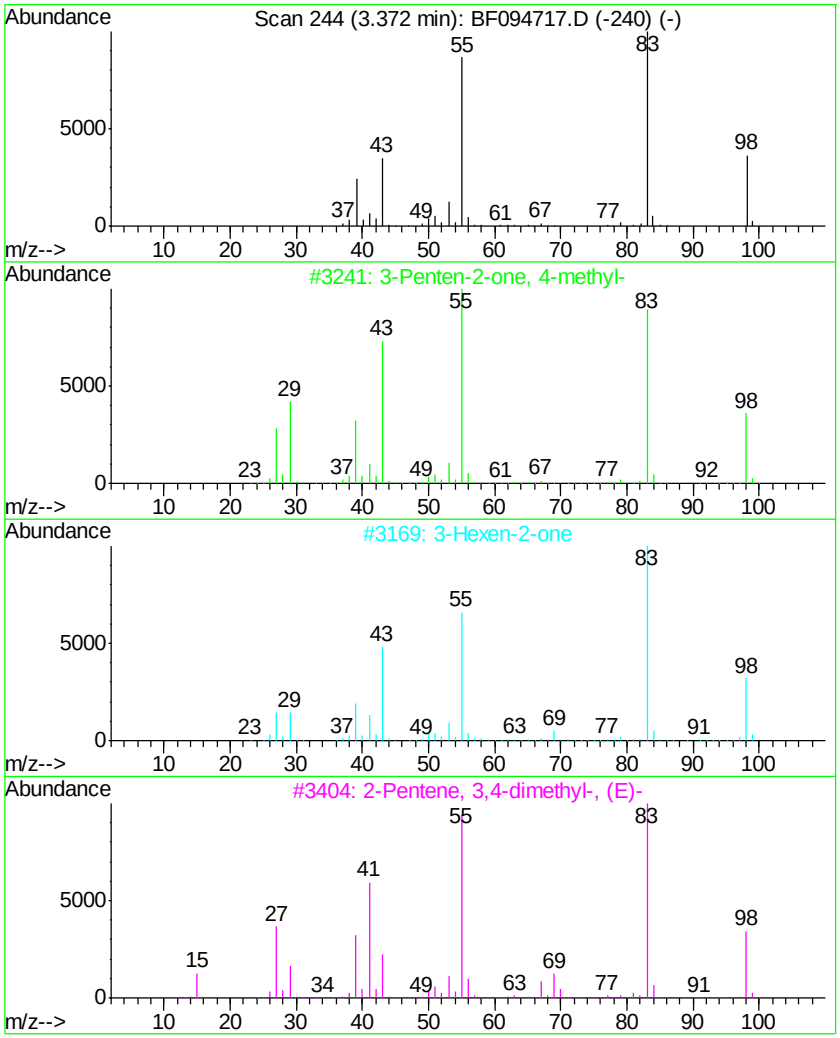
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

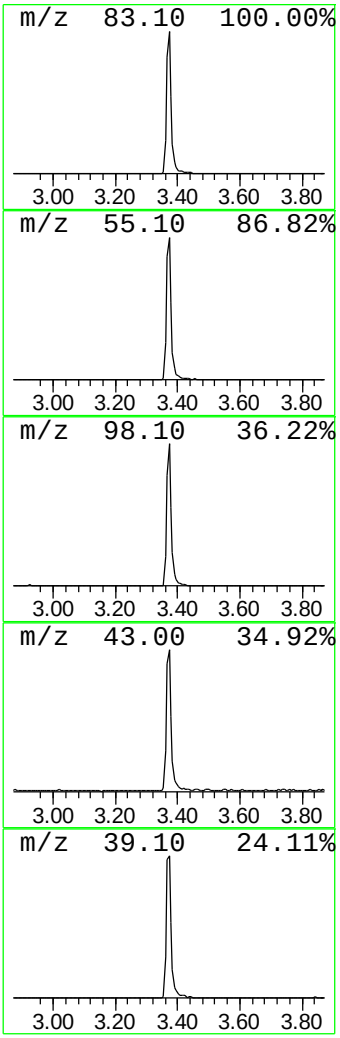
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.37	16.69 ng	543121	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





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Operator : SJ/MA
Sample : I2860-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TANK-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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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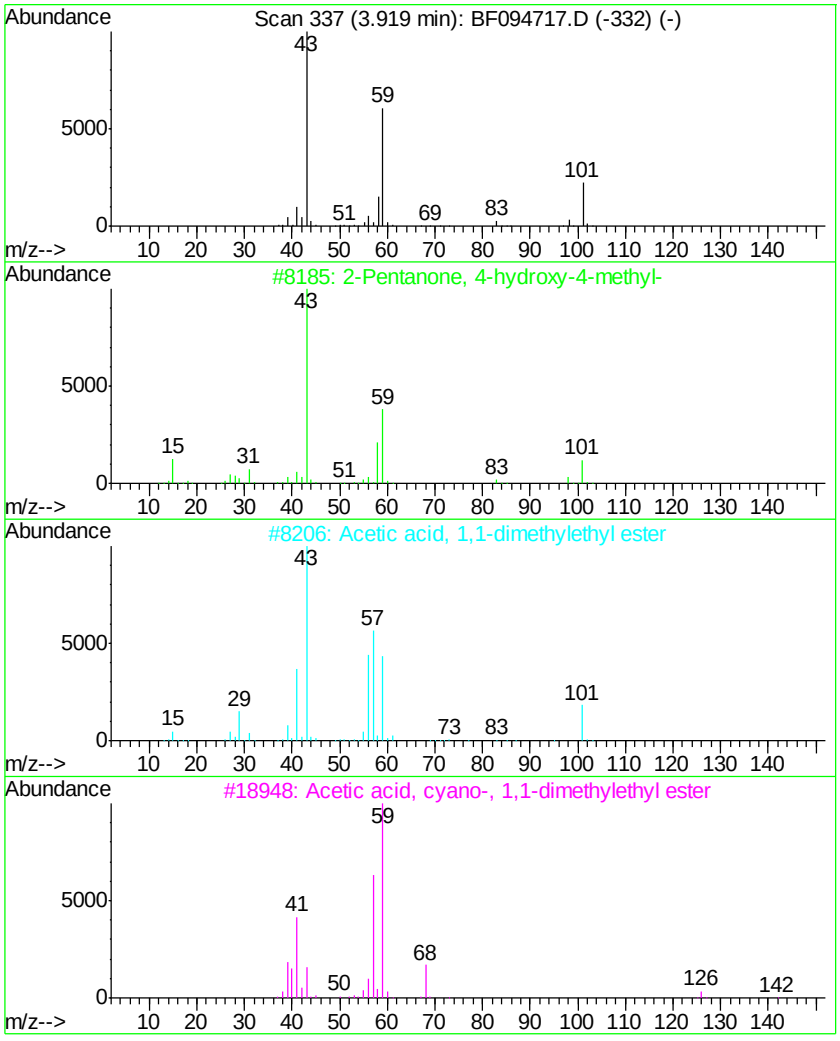
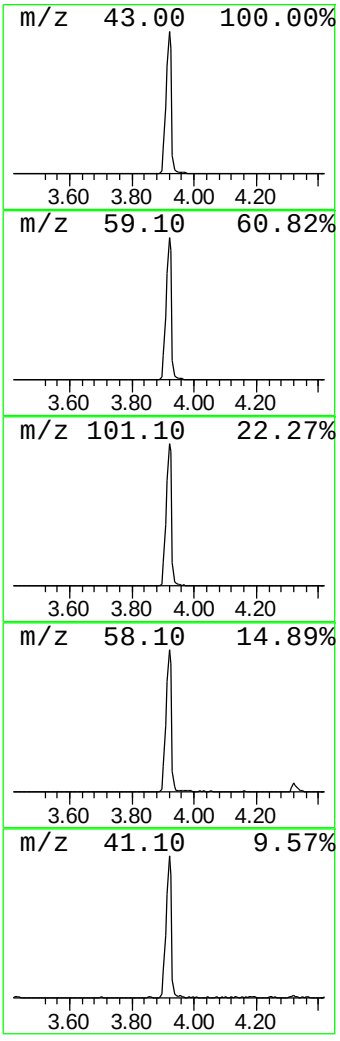
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.92	47.55 ng	1547160	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
Data File : BF094717.D
Acq On : 30 Apr 2017 16:26
Operator : SJ/MA
Sample : I2860-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TANK-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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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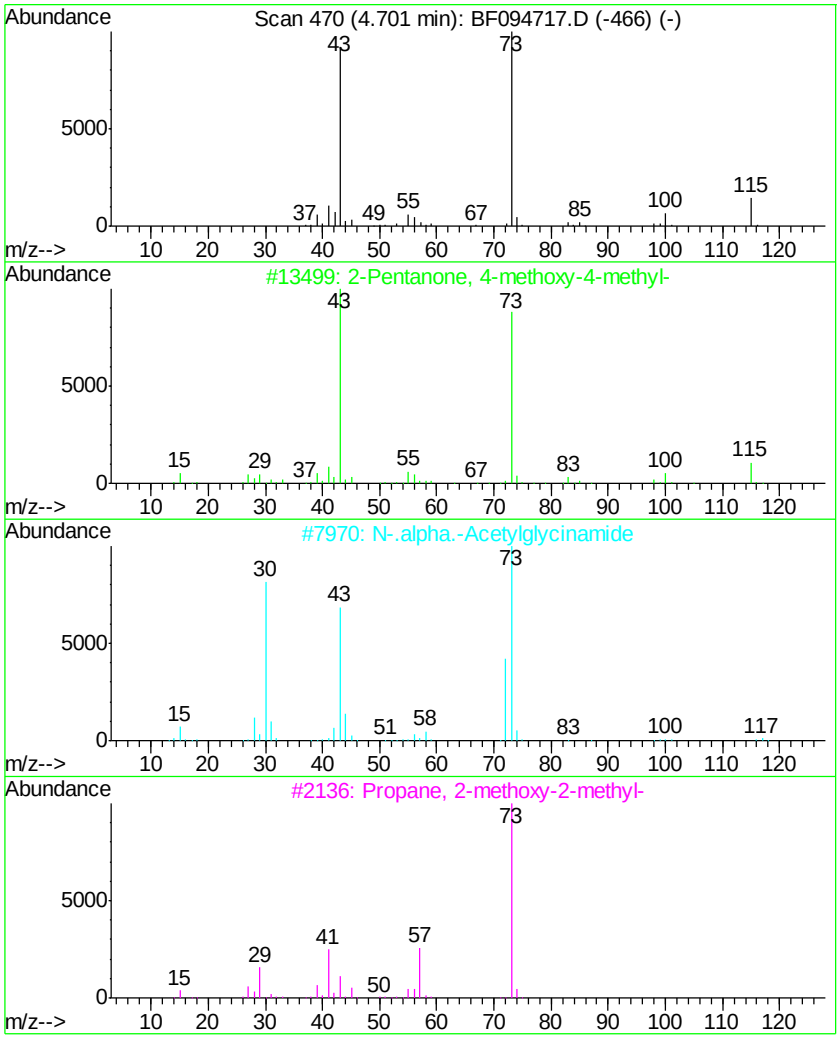
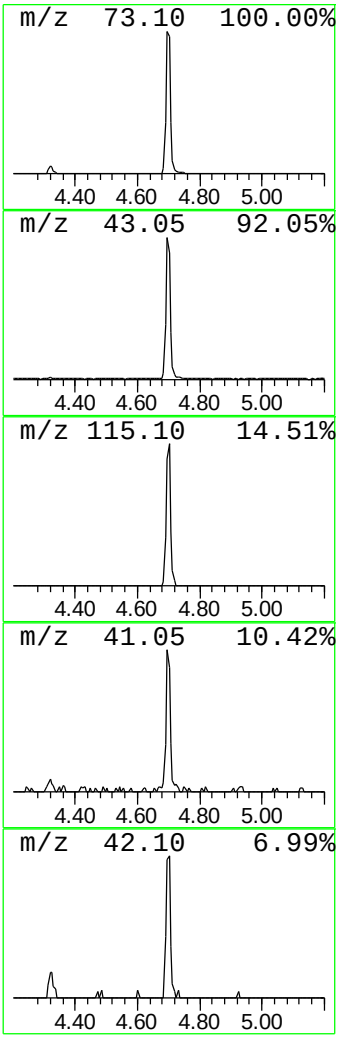
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	8.66 ng	281877	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	47
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	12
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
5	N-Formylmorpholine	115	C5H9NO2	004394-85-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
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Operator : SJ/MA
Sample : I2860-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TANK-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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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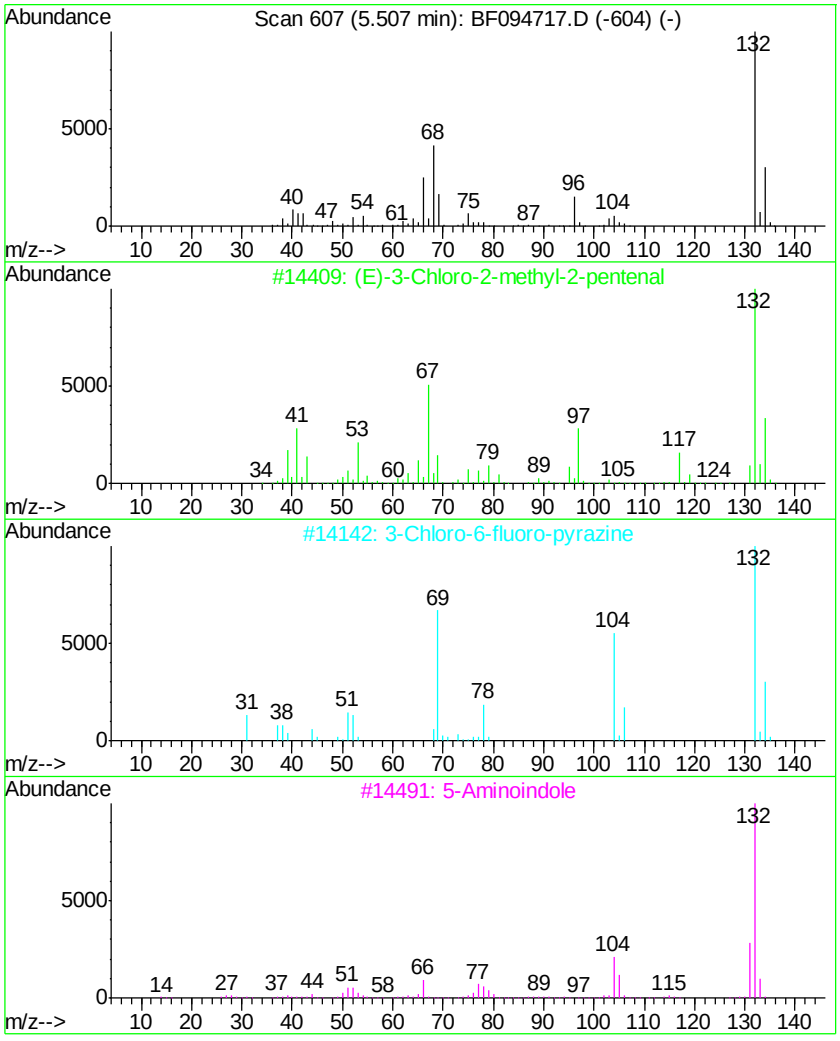
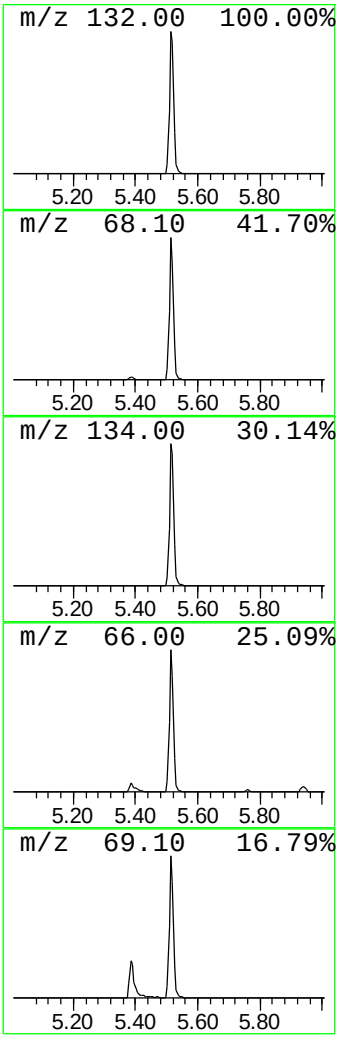
Peak Number 4 unknown5.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.51	50.20 ng	1633440	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
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Acq On : 30 Apr 2017 16:26
Operator : SJ/MA
Sample : I2860-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TANK-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

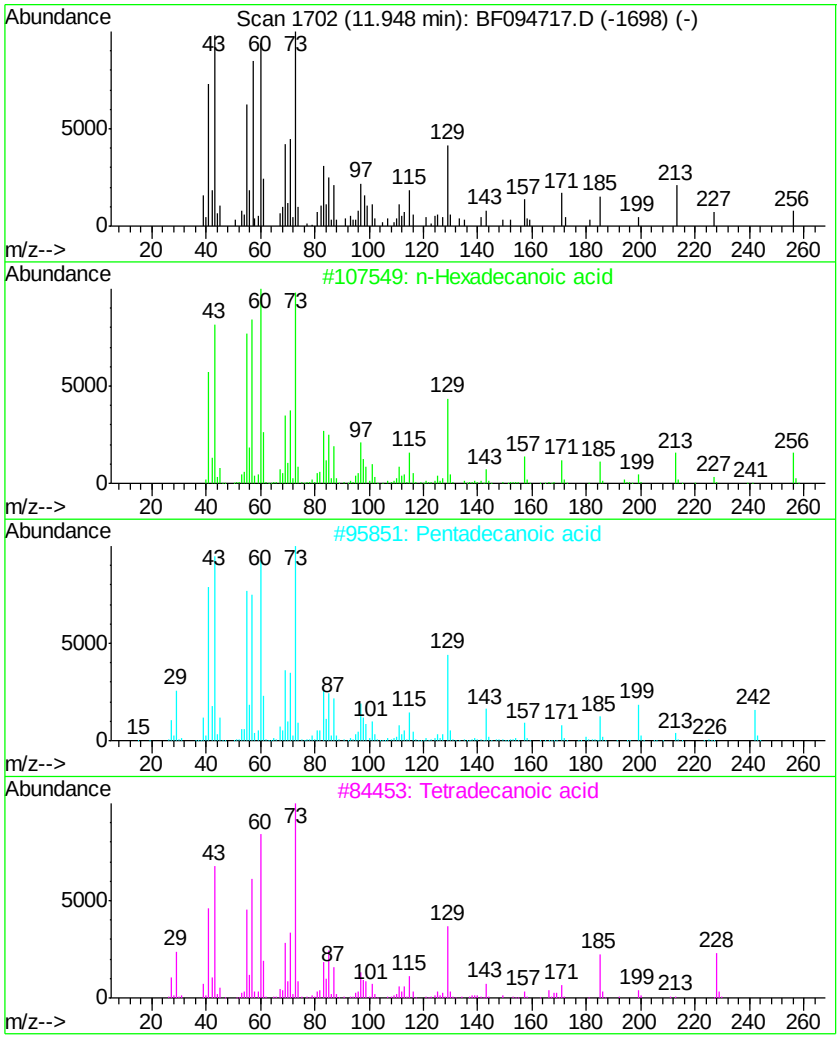
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

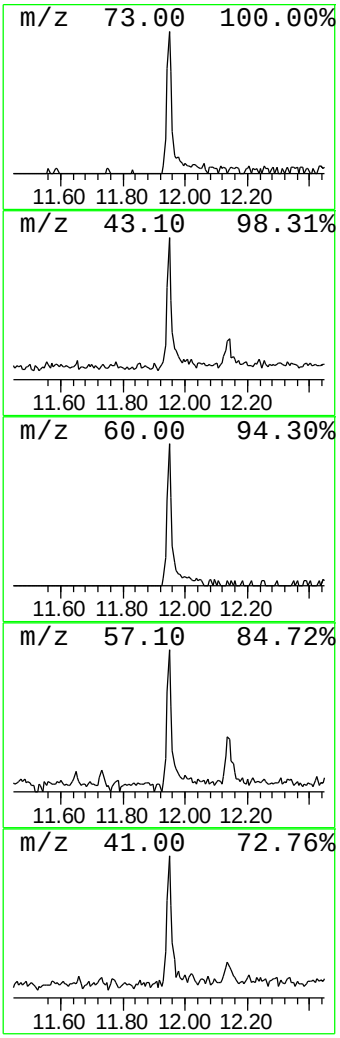
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	2.93 ng	150219	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72





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Operator : SJ/MA
Sample : I2860-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TANK-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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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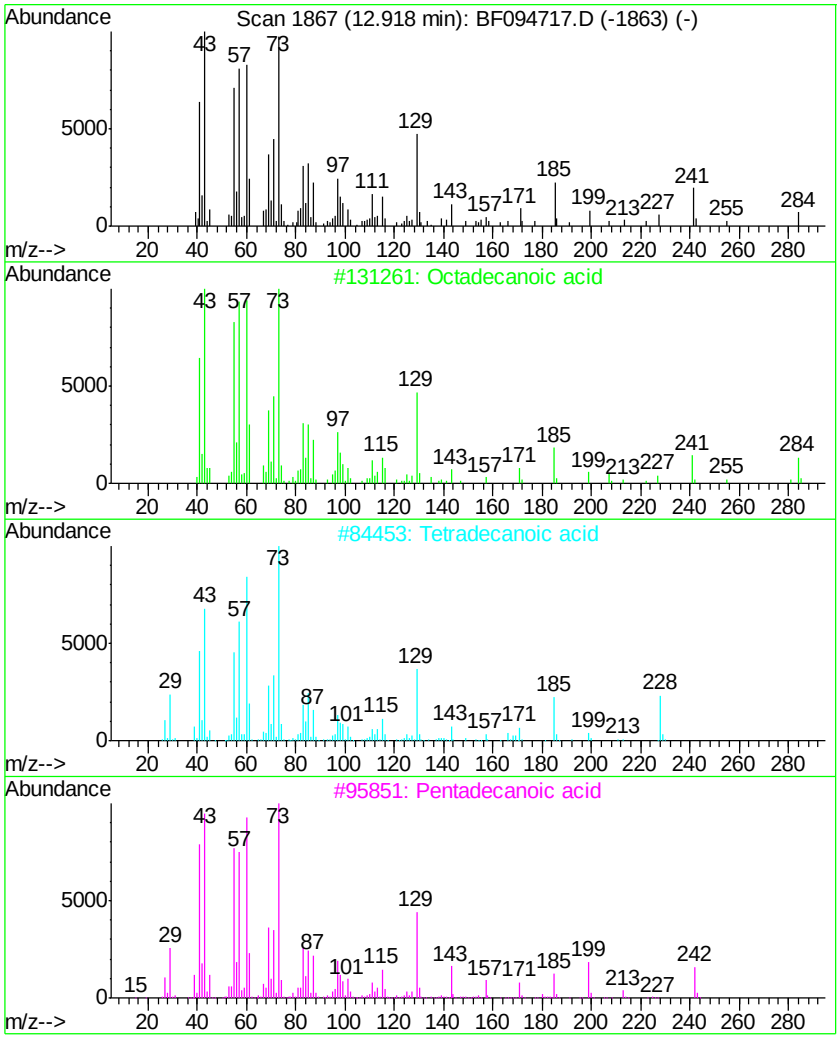
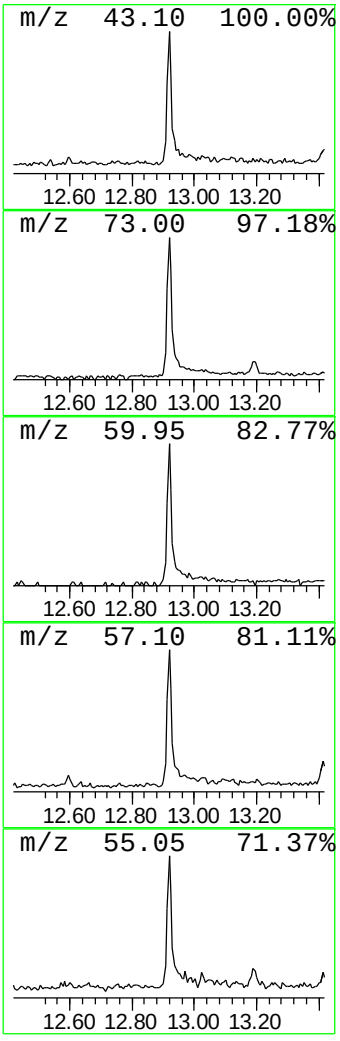
Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.92	5.97 ng	253873	Chrysene-d12	14.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5	Undecanoic acid	186	C11H22O2	000112-37-8	62





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Operator : SJ/MA
Sample : I2860-05
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Instrument : BNA_F
ClientSampleId : TANK-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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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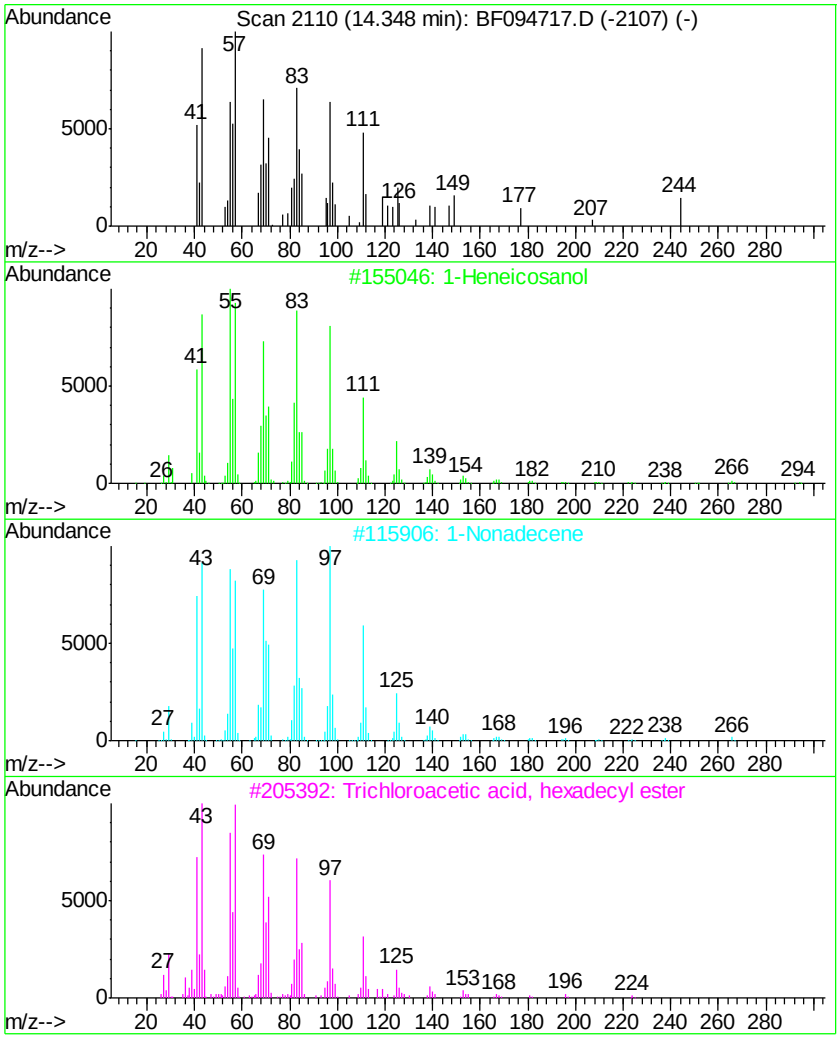
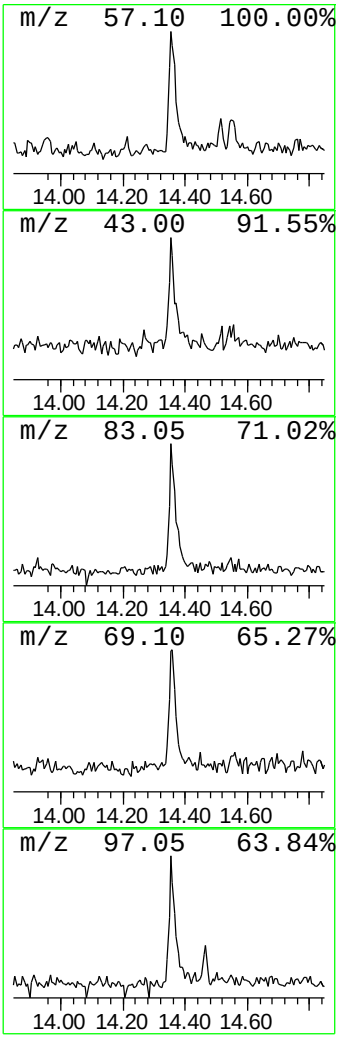
Peak Number 8 1-Heneicosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	2.15 ng	91592	Chrysene-d12	14.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	11-Tricosene	322	C23H46	052078-56-5	91





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Sample : I2860-05
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ClientSampleId : TANK-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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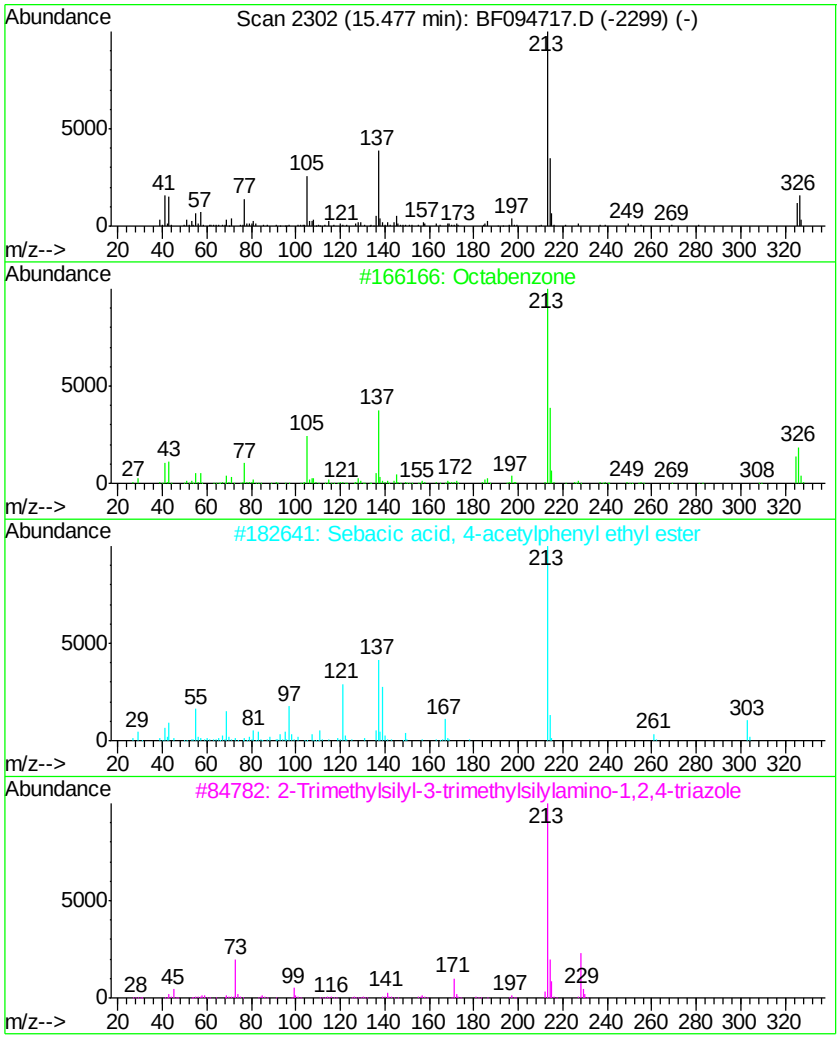
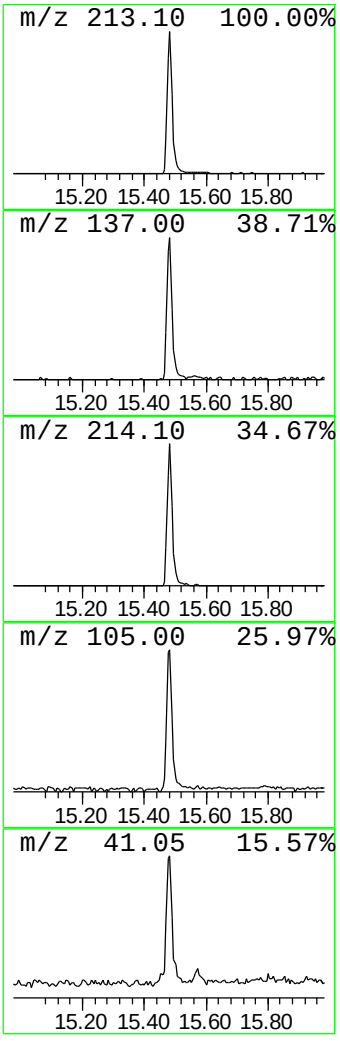
Peak Number 9 Octabenzone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.48	10.95 ng	334977	Perylene-d12	16.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octabenzone	326	C21H26O3	001843-05-6	99
2	Sebacic acid, 4-acetylphenyl eth...	348	C20H28O5	1000354-96-0	25
3	2-Trimethylsilyl-3-trimethylsilv...	228	C8H20N4Si2	1000373-05-5	23
4	1,3,4-Thiadiazole, 2-(5-nitropyr...	325	C10H7N5O4S2	1000260-74-4	23
5	Sebacic acid, 2,2-dichloroethyl ...	326	C14H24Cl2O4	1000355-46-5	12





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
3-Penten-2-one, 4...	3.37	16.7	ng	543121	1	5.77	650728	20.0
2-Pentanone, 4-hy...	3.92	47.5	ng	1547160	1	5.77	650728	20.0
2-Pentanone, 4-me...	4.70	8.7	ng	281877	1	5.77	650728	20.0
unknown5.51	5.51	50.2	ng	1633440	1	5.77	650728	20.0
n-Hexadecanoic acid	11.95	2.9	ng	150219	4	11.21	1023660	20.0
Octadecanoic acid	12.92	6.0	ng	253873	5	14.47	850098	20.0
1-Heneicosanol	14.35	2.1	ng	91592	5	14.47	850098	20.0
Octabenzone	15.48	10.9	ng	334977	6	16.09	612026	20.0