LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061716\
Data File : BF088097.D
Acq On : 17 Jun 2016 17:10
Operator : UM/SJ
Sample : H3558-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TWP-01

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-BF060716.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	1.667	6	7	16	rVB	153516	297096	8.23%	1.688%
2	1.793	16	18	63	rVB	1520336	3611485	100.00%	20.515%
3	4.136	221	223	233	rVB	216224	318647	8.82%	1.810%
4	4.833	281	284	287	rBV	485519	540068	14.95%	3.068%
5	5.279	321	323	333	rVB	405458	381861	10.57%	2.169%
6	5.690	357	359	361	rBV	67807	62254	1.72%	0.354%
7	6.330	414	415	421	rBV2	255824	278916	7.72%	1.584%
8	6.456	424	426	429	rVV	748378	687964	19.05%	3.908%
9	6.536	431	433	437	rVV	56699	52580	1.46%	0.299%
10	6.696	445	447	449	rBV	624424	594322	16.46%	3.376%
11	6.845	458	460	463	rVB	860105	902808	25.00%	5.128%
12	7.256	494	496	499	rBV	613652	750026	20.77%	4.261%
13	7.976	557	559	562	rBV	738052	813095	22.51%	4.619%
14	9.062	651	654	656	rBV	1634037	1622859	44.94%	9.219%
15	9.462	686	689	690	rBV	142025	165371	4.58%	0.939%
16	9.679	704	708	710	rBV2	42299	55526	1.54%	0.315%
17	9.736	710	713	715	rVV	760153	991619	27.46%	5.633%
18	10.171	747	751	753	rBV2	117967	186233	5.16%	1.058%
19	10.388	767	770	774	rBV	34830	64899	1.80%	0.369%
20	10.513	779	781	784	rBV	633933	590297	16.34%	3.353%
21	10.639	789	792	797	rBV2	117934	211376	5.85%	1.201%
22	11.085	830	831	833	rBV	42628	59800	1.66%	0.340%
23	11.211	840	842	844	rVV	1141978	983466	27.23%	5.587%
24	11.759	887	890	902	rBV2	178981	232067	6.43%	1.318%
25	12.537	956	958	964	rBV	88711	103453	2.86%	0.588%
26	12.788	978	980	983	rBV	1043526	1339633	37.09%	7.610%
27	13.714	1056	1061	1068	rBV2	14561	39980	1.11%	0.227%
28	13.839	1069	1072	1075	rVB	911161	859594	23.80%	4.883%
29	15.222	1190	1193	1206	rVB	569546	806682	22.34%	4.582%

Sum of corrected areas: 17603977

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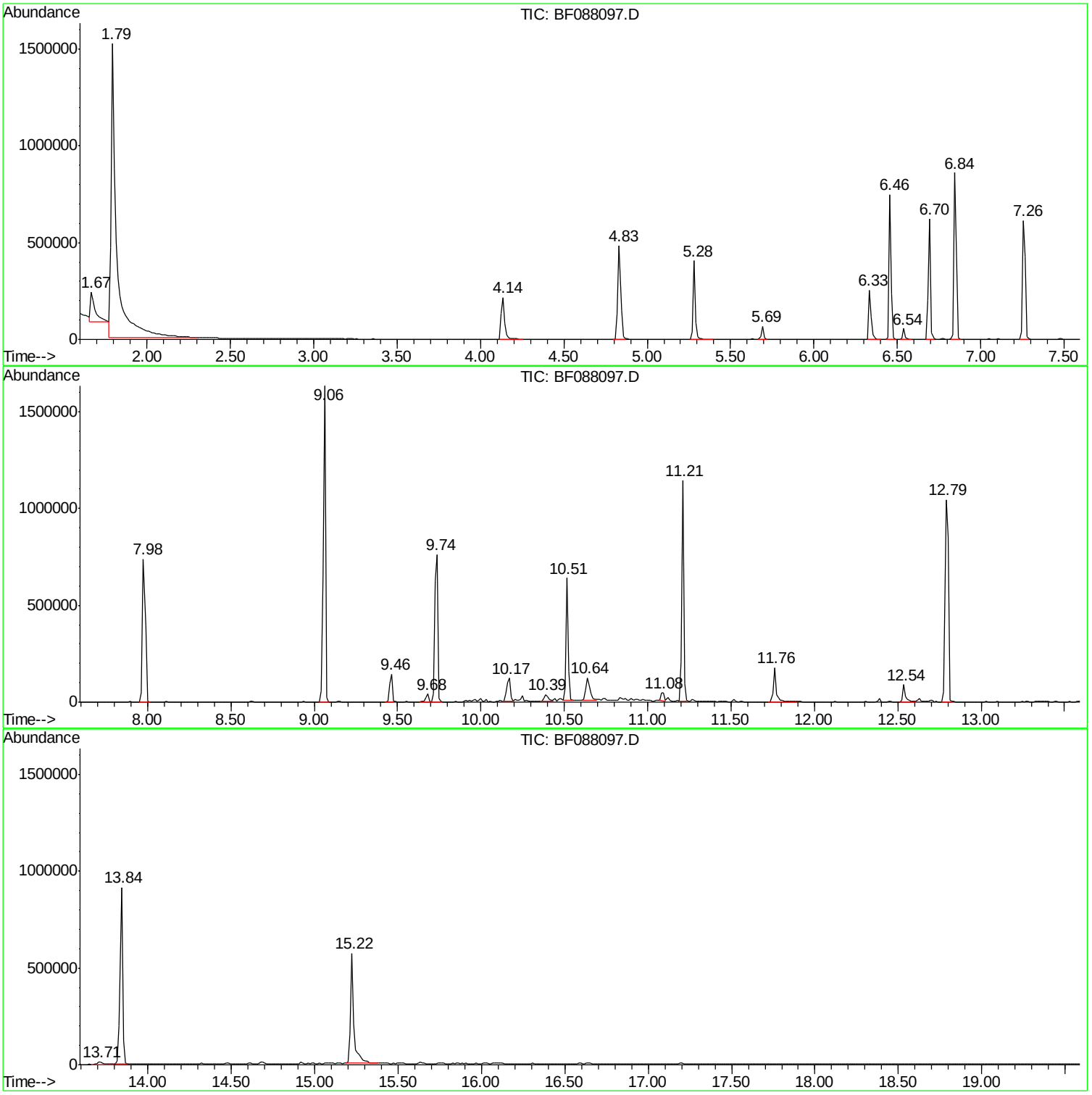
Instrument :
BNA_F
ClientSampleId :
TWP-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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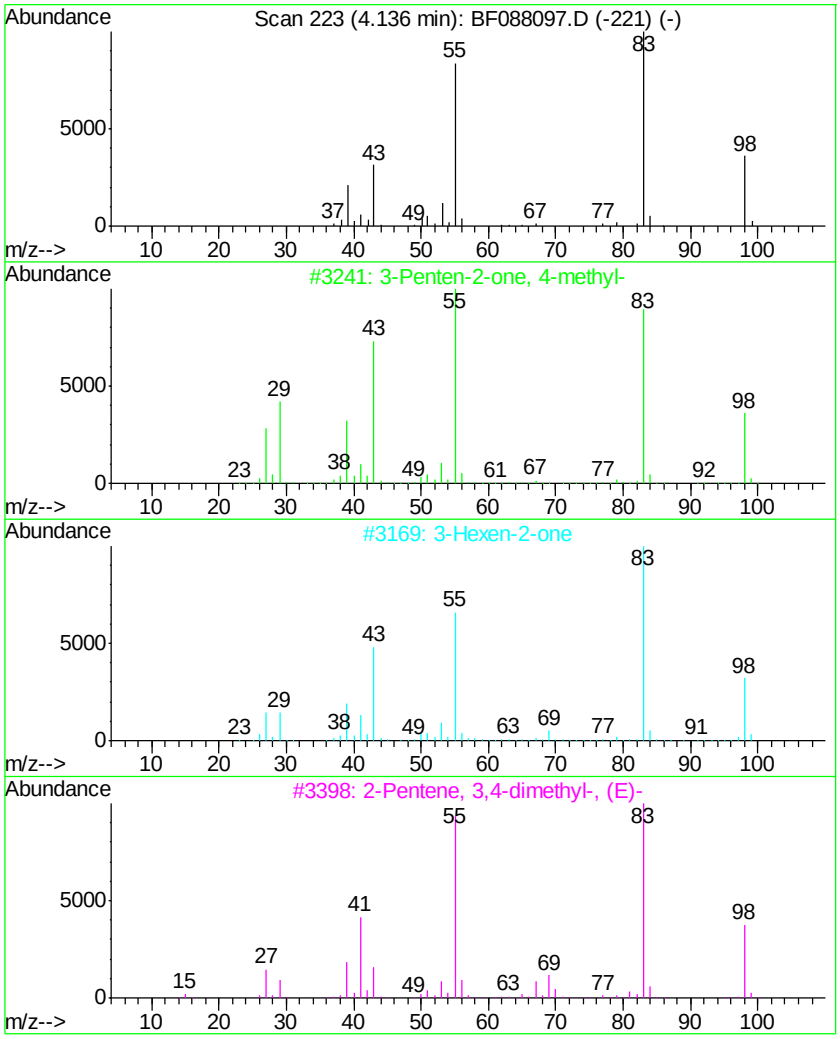
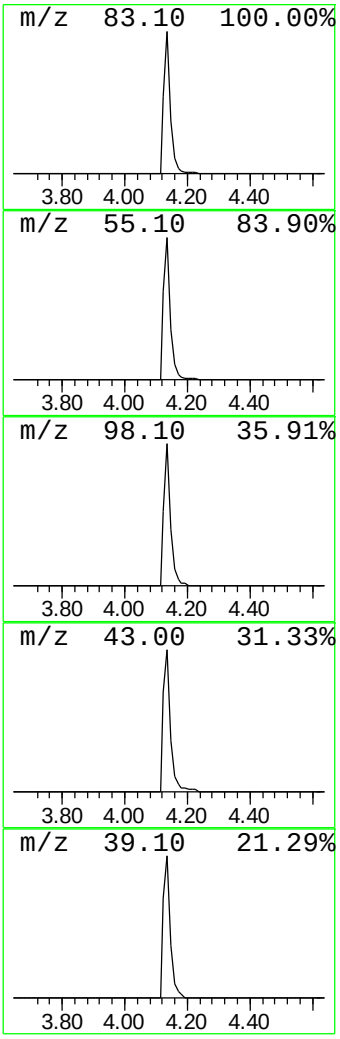
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.14	10.72 ng	318647	1,4-Dichlorobenzene-d4	6.70

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	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78





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Operator : UM/SJ
Sample : H3558-01
Misc :
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Instrument : BNA_F
ClientSampleId : TWP-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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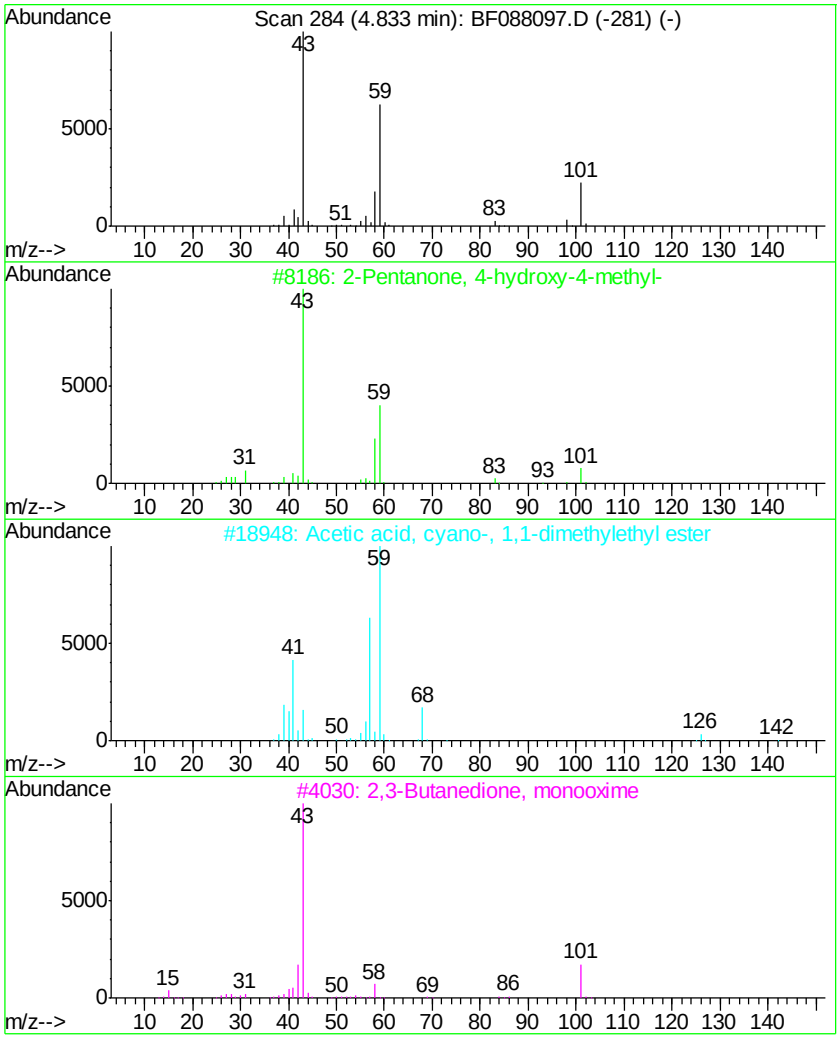
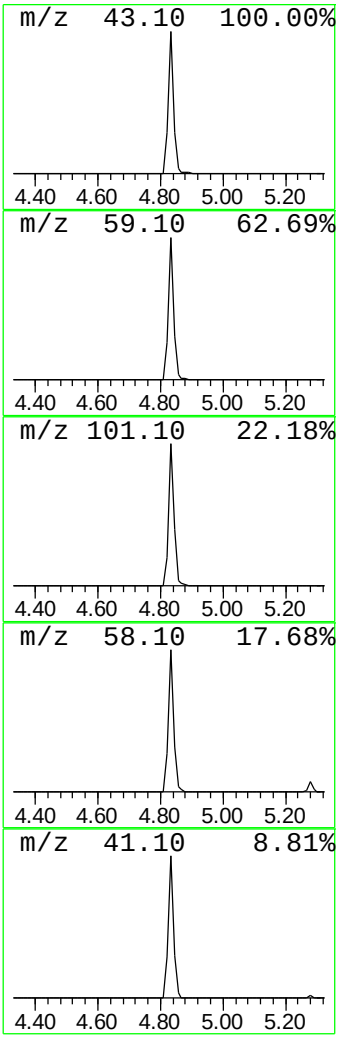
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	18.17 ng	540068	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061716\
Data File : BF088097.D
Acq On : 17 Jun 2016 17:10
Operator : UM/SJ
Sample : H3558-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TWP-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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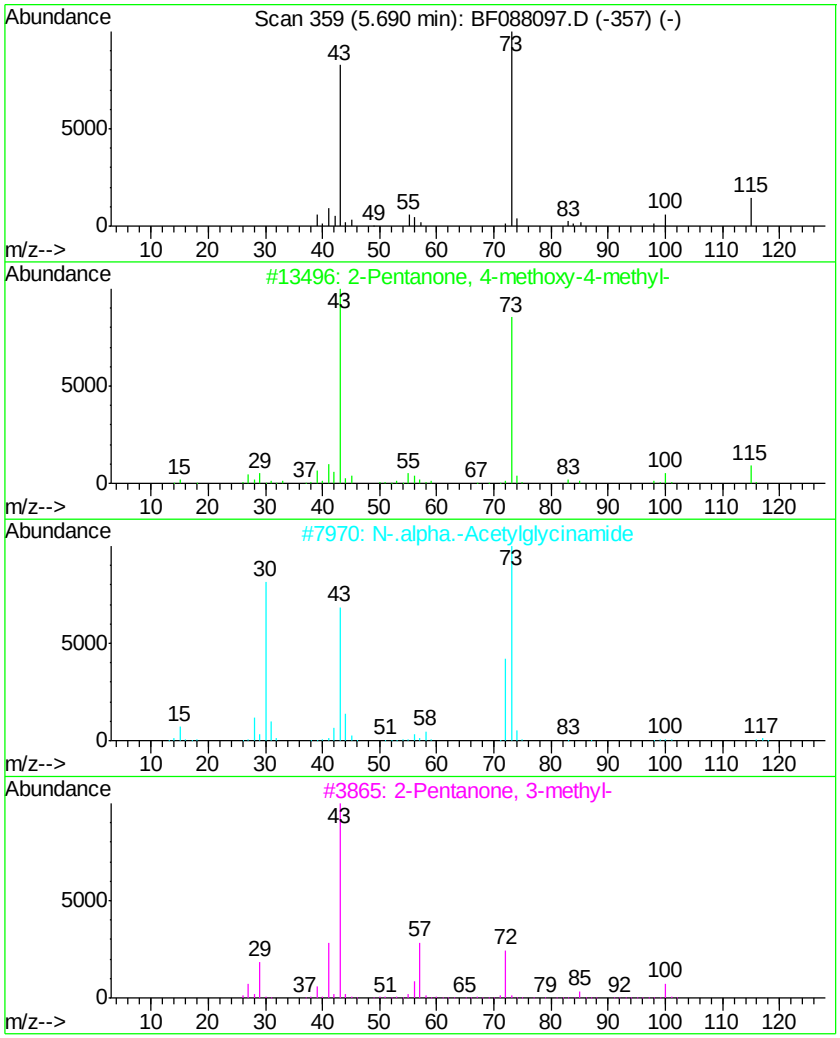
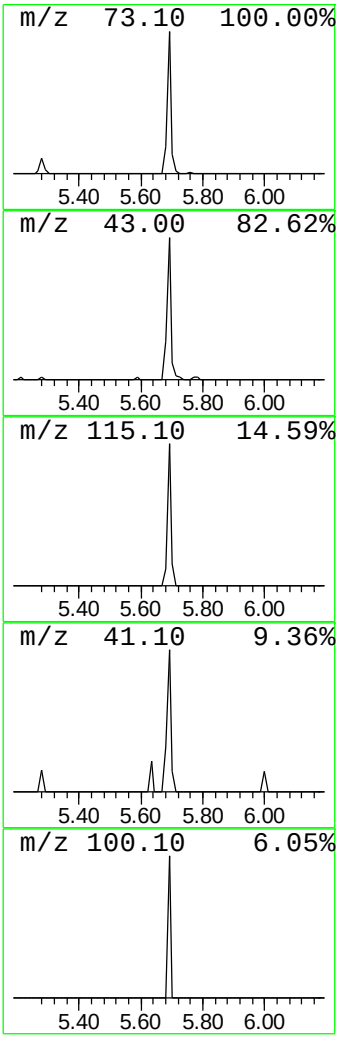
Peak Number 5 2-Pentanone, 4-methoxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.69	2.09 ng	62254	1,4-Dichlorobenzene-d4	6.70

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	33
3	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	16
4	Heptane	100	C7H16	000142-82-5	12
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9





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Misc :
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Instrument : BNA_F
ClientSampleId : TWP-01

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TIC Library : C:\Database\NIST11.L
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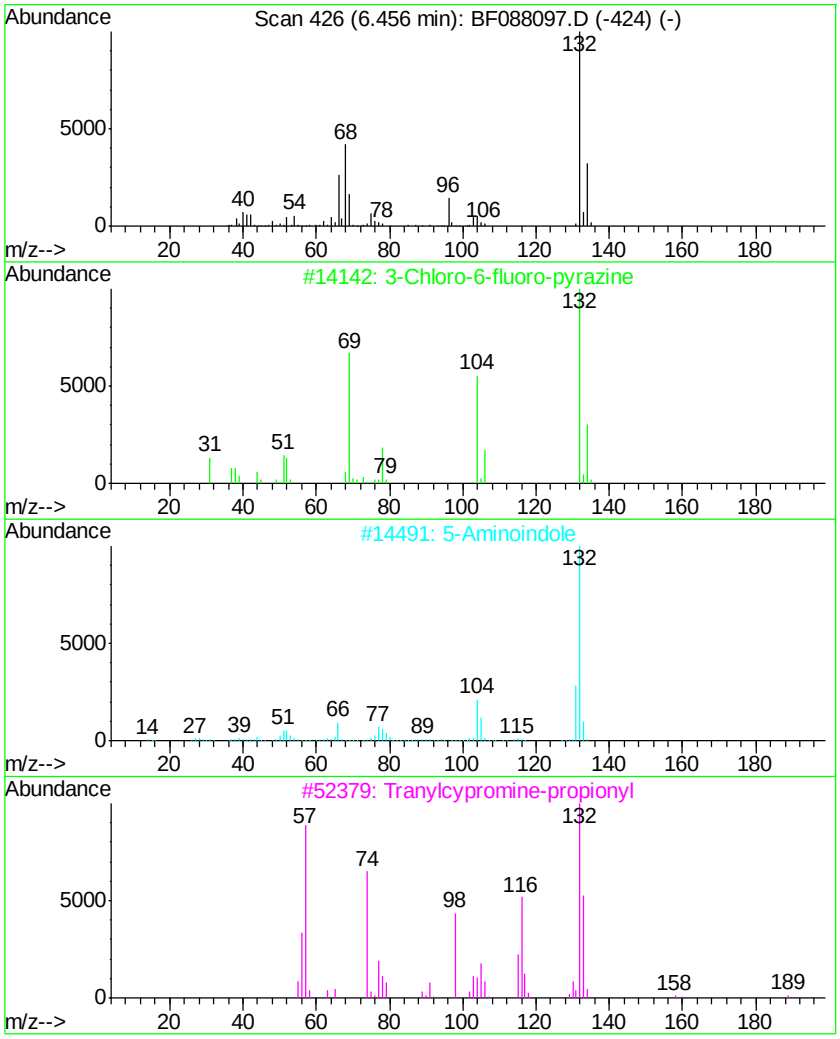
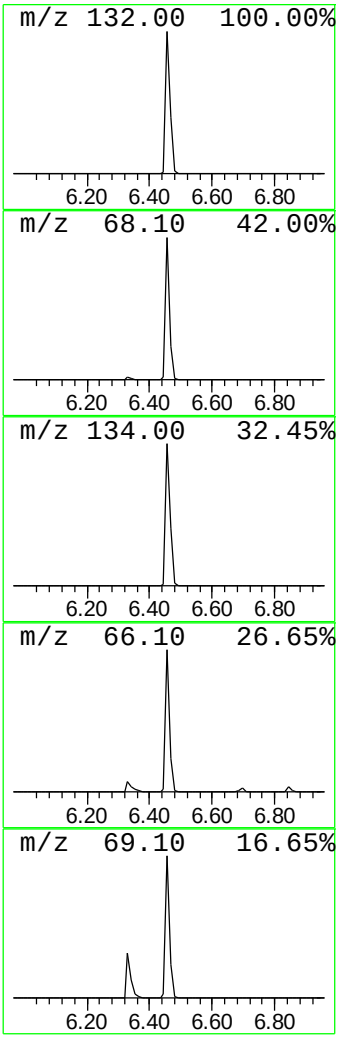
Peak Number 6 unknown6.46 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	23.15 ng	687964	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Sample : H3558-01
Misc :
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Instrument : BNA_F
ClientSampleId : TWP-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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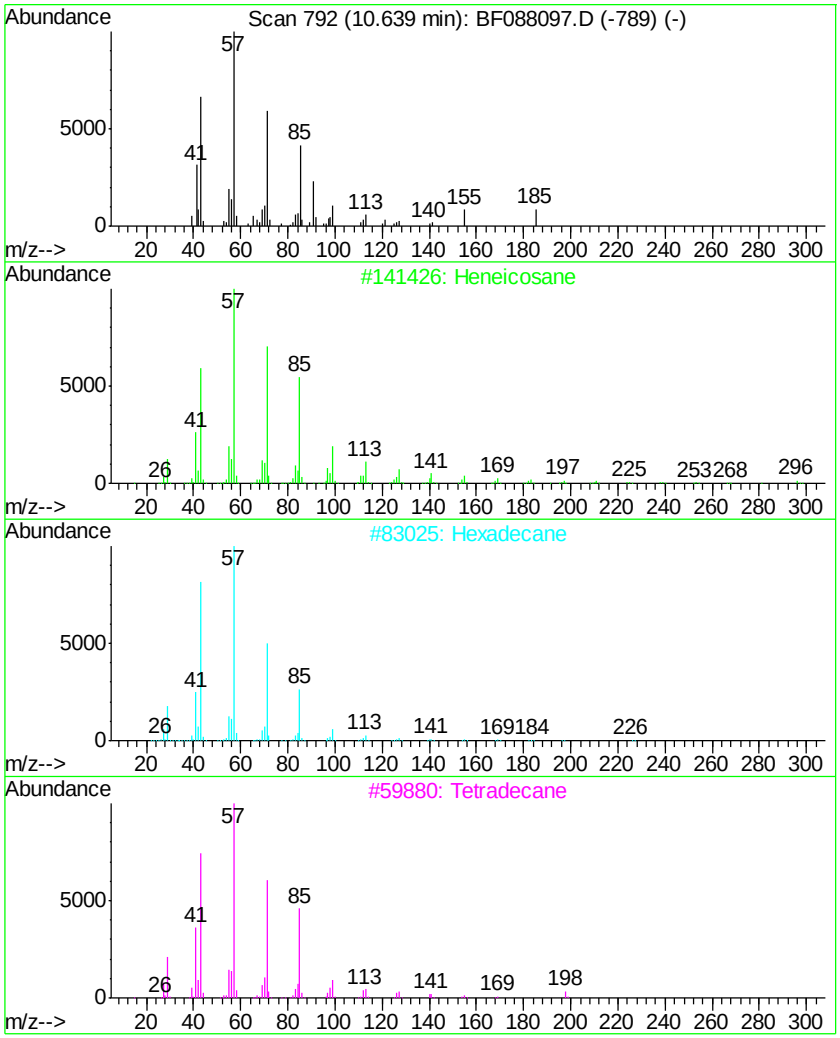
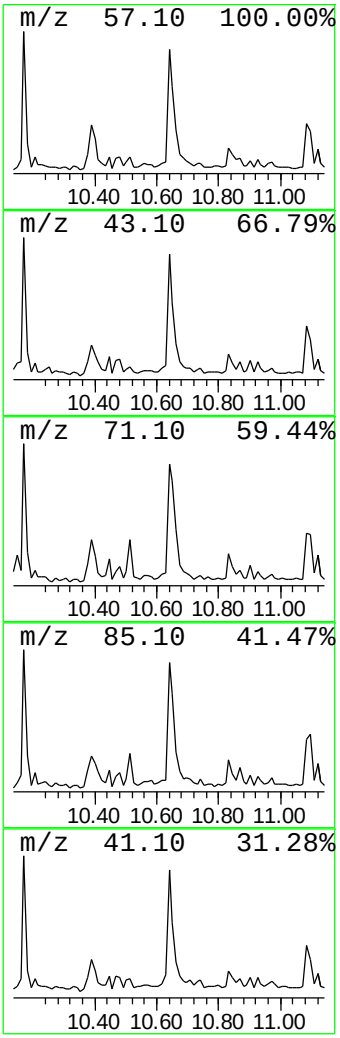
Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	4.30 ng	211376	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	86
2	Hexadecane	226	C16H34	000544-76-3	86
3	Tetradecane	198	C14H30	000629-59-4	83
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	72
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061716\
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Operator : UM/SJ
Sample : H3558-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TWP-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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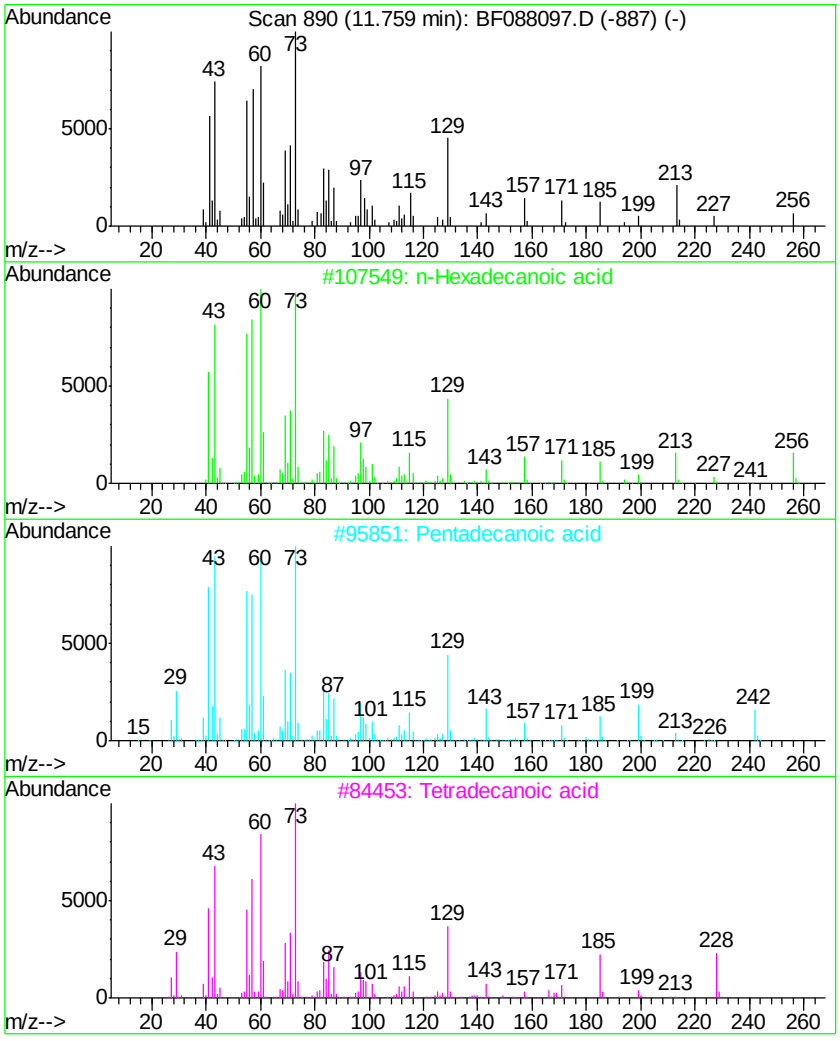
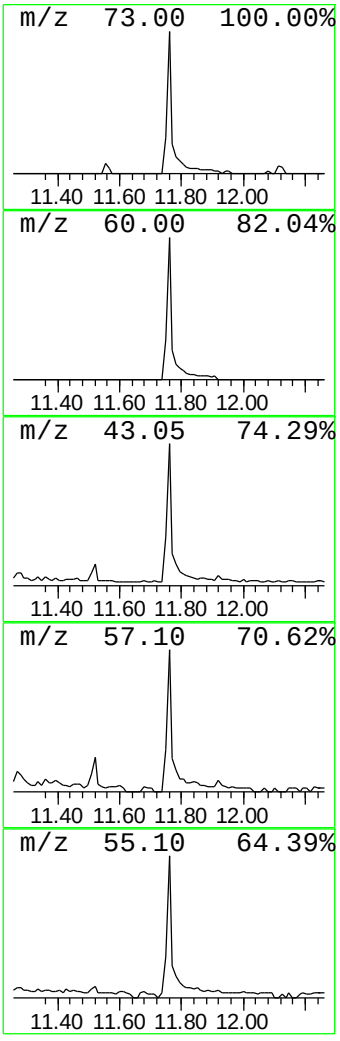
Peak Number 9 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	4.72 ng	232067	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
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	74





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Instrument : BNA_F
ClientSampleId : TWP-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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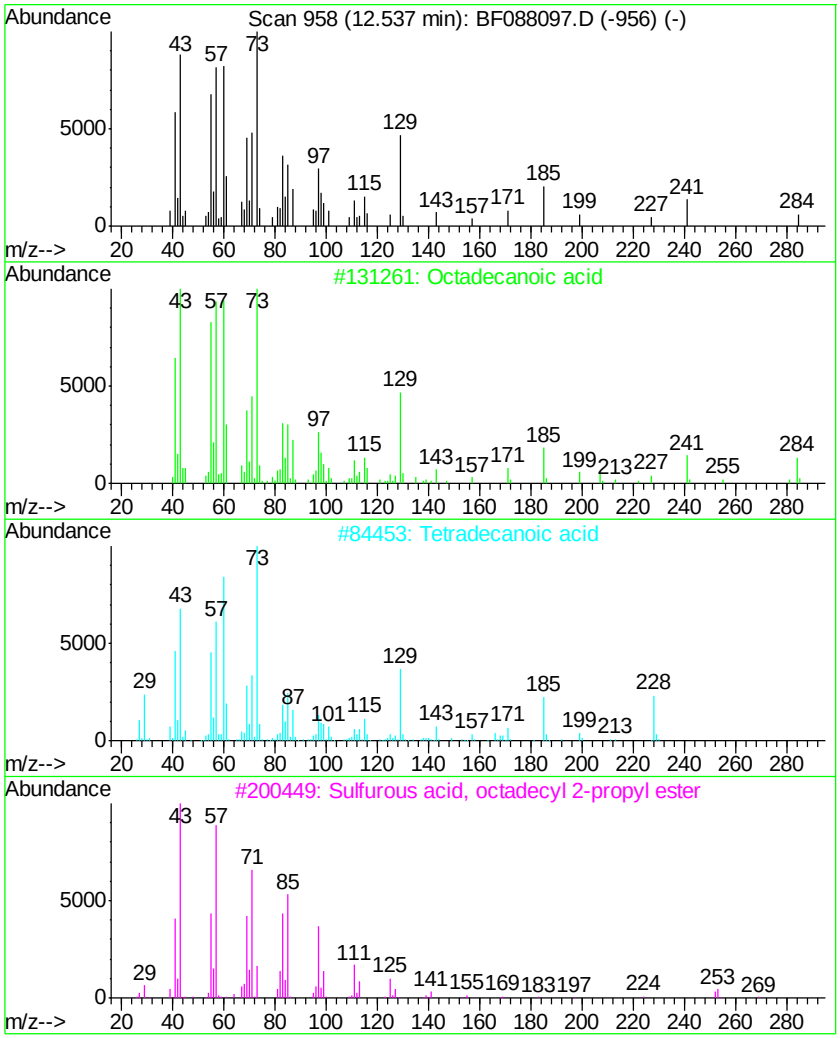
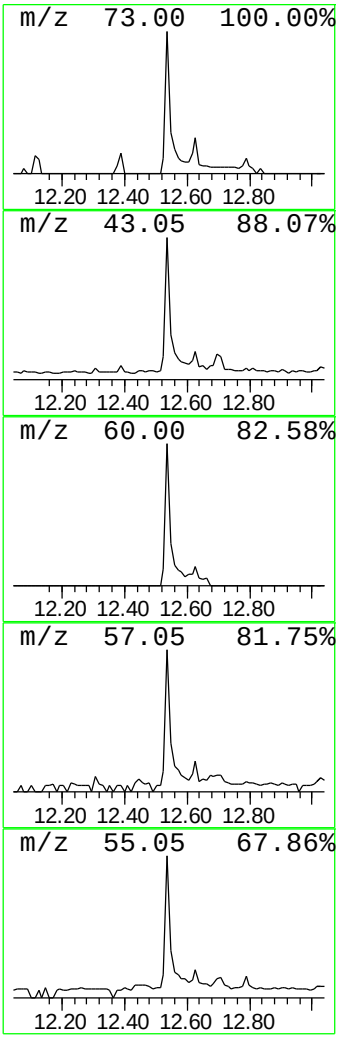
Peak Number 10 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	2.41 ng	103453	Chrysene-d12	13.84

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	80
3	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18
4	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	18
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	14





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...	4.14	10.7	ng	318647	1	6.70	594322	20.0
2-Pentanone, 4-hy...	4.83	18.2	ng	540068	1	6.70	594322	20.0
2-Pentanone, 4-me...	5.69	2.1	ng	62254	1	6.70	594322	20.0
unknown6.46	6.46	23.1	ng	687964	1	6.70	594322	20.0
Heneicosane	10.64	4.3	ng	211376	4	11.21	983466	20.0
n-Hexadecanoic acid	11.76	4.7	ng	232067	4	11.21	983466	20.0
Octadecanoic acid	12.54	2.4	ng	103453	5	13.84	859594	20.0