LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080753.D
Acq On : 1 Aug 2015 1:02
Operator : TP/UM
Sample : G3127-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId :

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-BF073015.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	2.178	4	8	11	rBV	55173	87279	1.94%	0.203%
2	3.218	97	99	113	rBV2	65086	214590	4.76%	0.499%
3	4.407	201	203	207	rBV	188764	236001	5.24%	0.549%
4	5.058	256	260	269	rBV	2576226	3805793	84.44%	8.854%
5	5.459	292	295	298	rBV	3516332	3952807	87.70%	9.196%
6	5.859	328	330	333	rVB	114686	149926	3.33%	0.349%
7	6.476	381	384	387	rVV	2938547	4507072	100.00%	10.486%
8	6.624	394	397	399	rBV	3286695	4304365	95.50%	10.014%
9	6.853	415	417	419	rBV	1083215	939306	20.84%	2.185%
10	7.013	428	431	433	rBV	2269624	2981887	66.16%	6.937%
11	7.413	463	466	468	rBV	2776117	2785740	61.81%	6.481%
12	7.493	468	473	479	rVB	55589	78499	1.74%	0.183%
13	8.133	526	529	531	rVB	1284366	1152280	25.57%	2.681%
14	9.207	620	623	626	rBV	3628555	3816449	84.68%	8.879%
15	9.607	655	658	660	rBV	530164	610800	13.55%	1.421%
16	9.882	680	682	685	rVB	1229010	1210748	26.86%	2.817%
17	10.670	748	751	753	rBV	2761684	2712083	60.17%	6.310%
18	10.796	760	762	767	rBV	54674	67224	1.49%	0.156%
19	11.242	799	801	802	rBV	76015	60391	1.34%	0.140%
20	11.368	809	812	814	rVB	1109977	1204124	26.72%	2.801%
21	11.665	832	838	841	rBV	253950	826740	18.34%	1.923%
22	11.893	857	858	869	rVB	145348	240839	5.34%	0.560%
23	12.076	872	874	876	rVB	49030	47370	1.05%	0.110%
24	12.156	878	881	883	rBV	2563520	2332463	51.75%	5.426%
25	12.614	915	921	923	rBV5	24086	71568	1.59%	0.166%
26	12.682	925	927	933	rVB3	43770	87889	1.95%	0.204%
27	12.854	938	942	944	rVB2	43378	71120	1.58%	0.165%
28	12.945	948	950	953	rBV	2586731	2834595	62.89%	6.595%
29	13.985	1039	1041	1044	rBV	617684	772545	17.14%	1.797%
30	14.099	1044	1051	1055	rVV4	24765	142341	3.16%	0.331%
31	14.168	1055	1057	1064	rVB	47937	67794	1.50%	0.158%
32	15.402	1162	1165	1168	rBV	443941	611191	13.56%	1.422%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080753.D
Acq On : 1 Aug 2015 1:02
Operator : TP/UM
Sample : G3127-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :

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-BF073015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

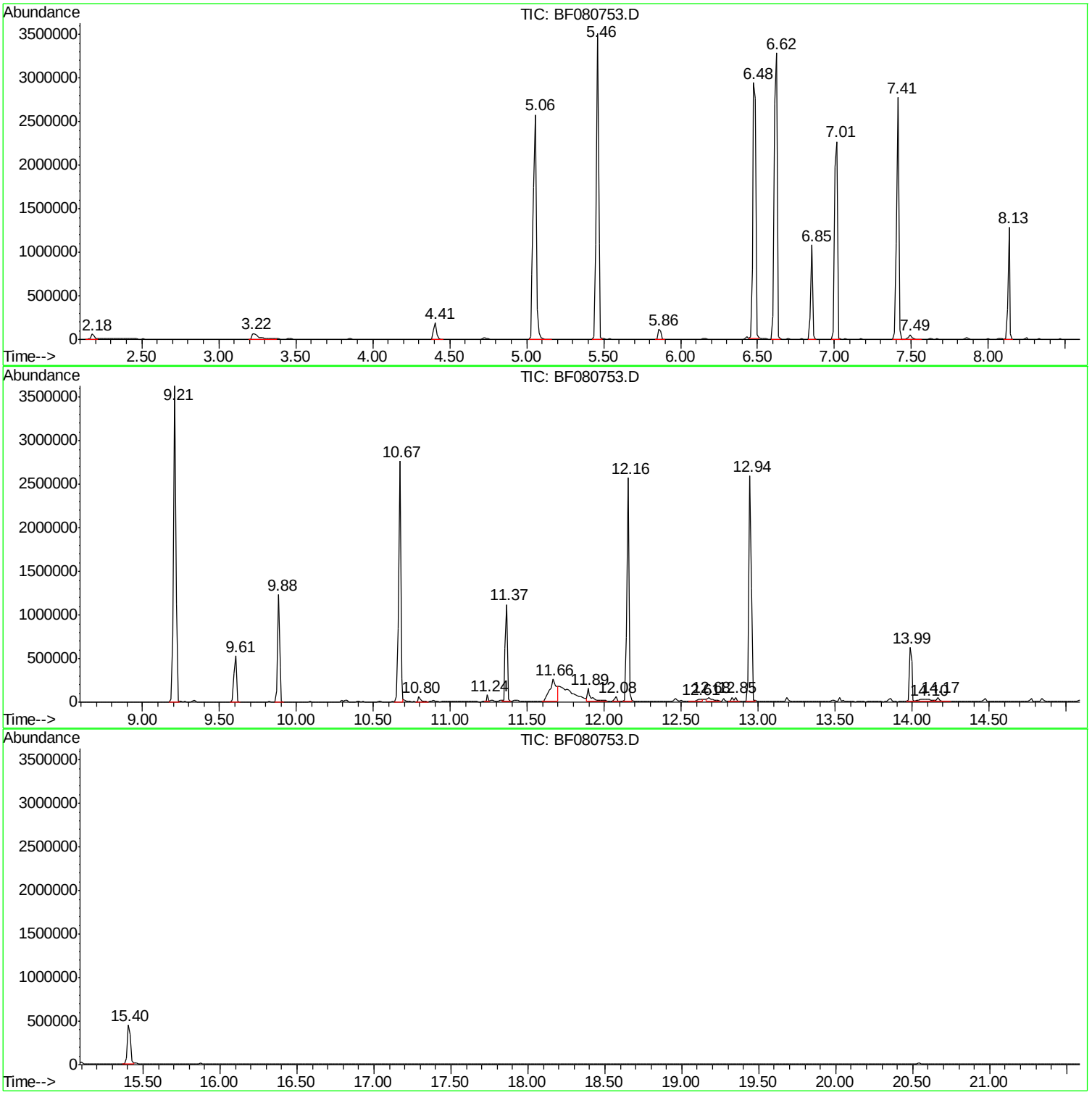
Sum of corrected areas: 42983819

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080753.D
Acq On : 1 Aug 2015 1:02
Operator : TP/UM
Sample : G3127-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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ClientSampleId :

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

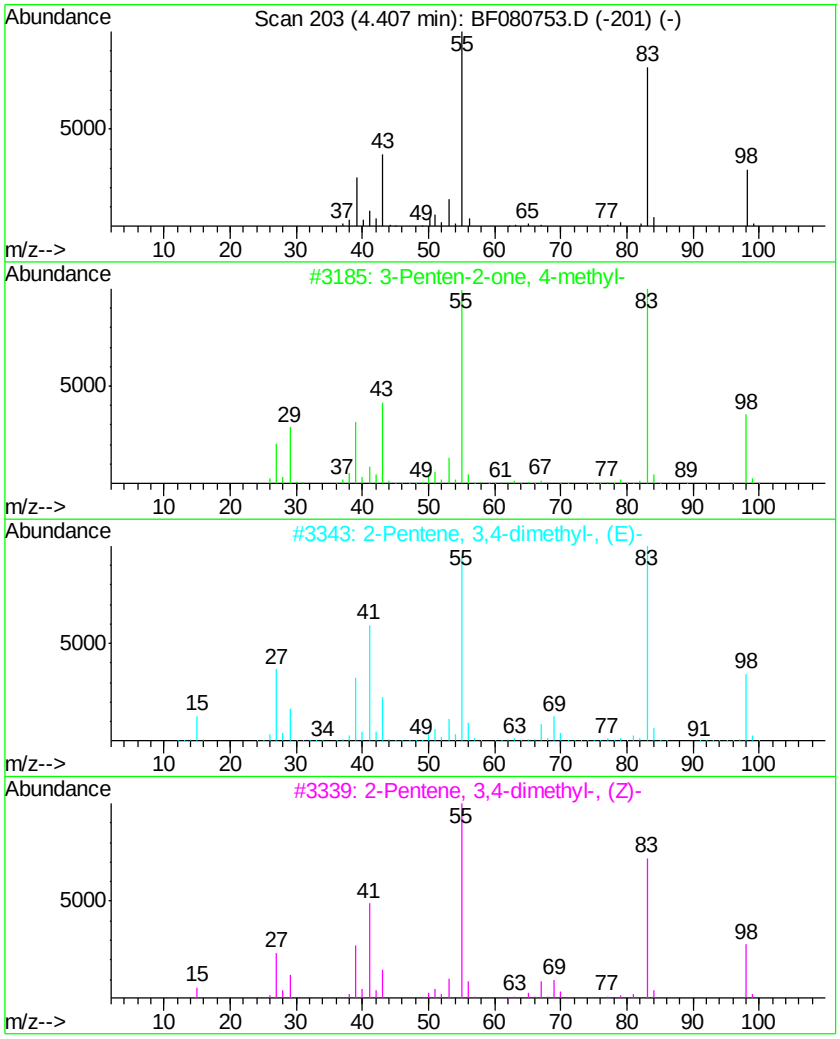
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

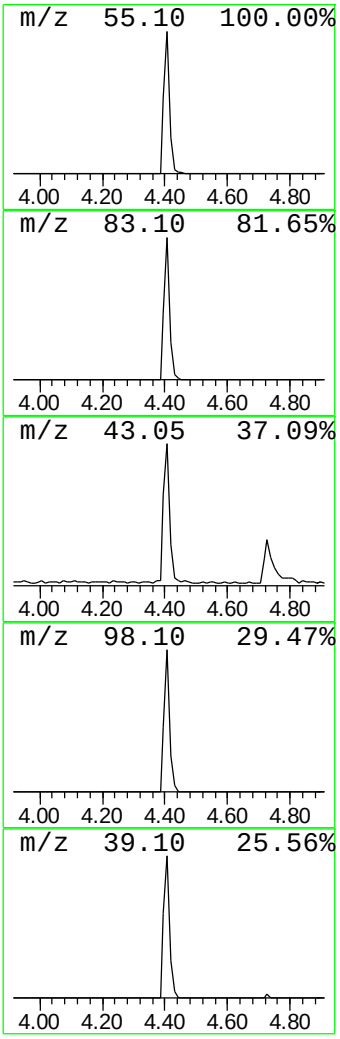
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	5.03 ng	236001	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080753.D
Acq On : 1 Aug 2015 1:02
Operator : TP/UM
Sample : G3127-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

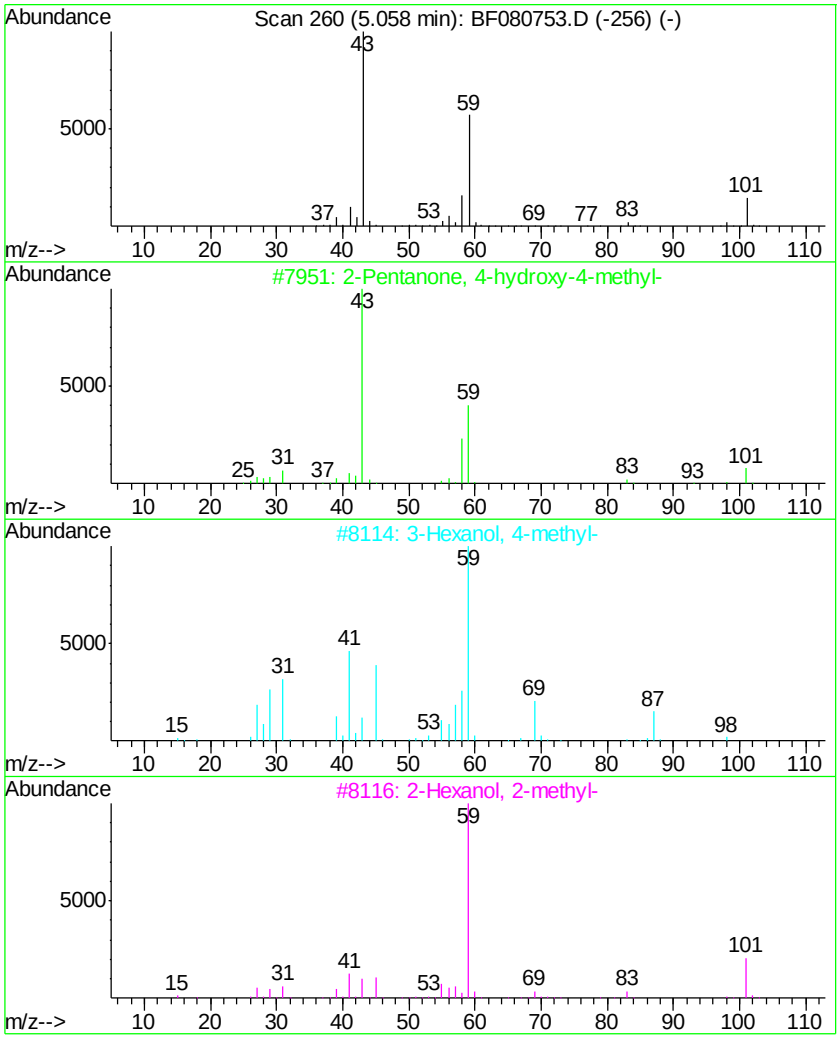
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

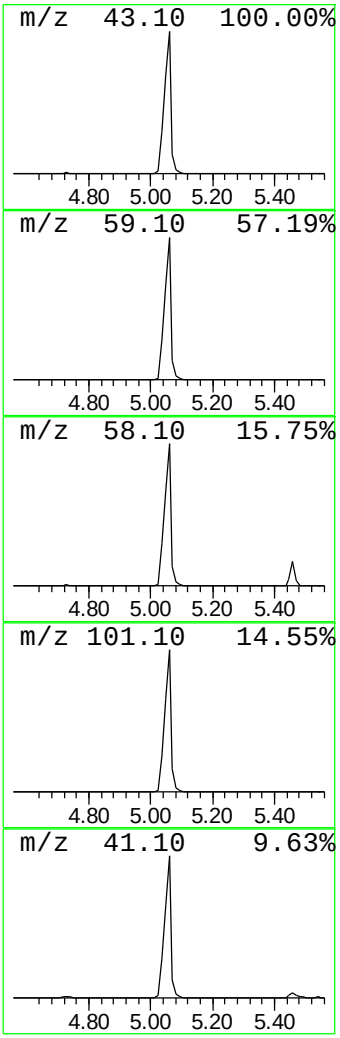
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	81.03 ng	3805790	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	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17





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Acq On : 1 Aug 2015 1:02
Operator : TP/UM
Sample : G3127-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId :

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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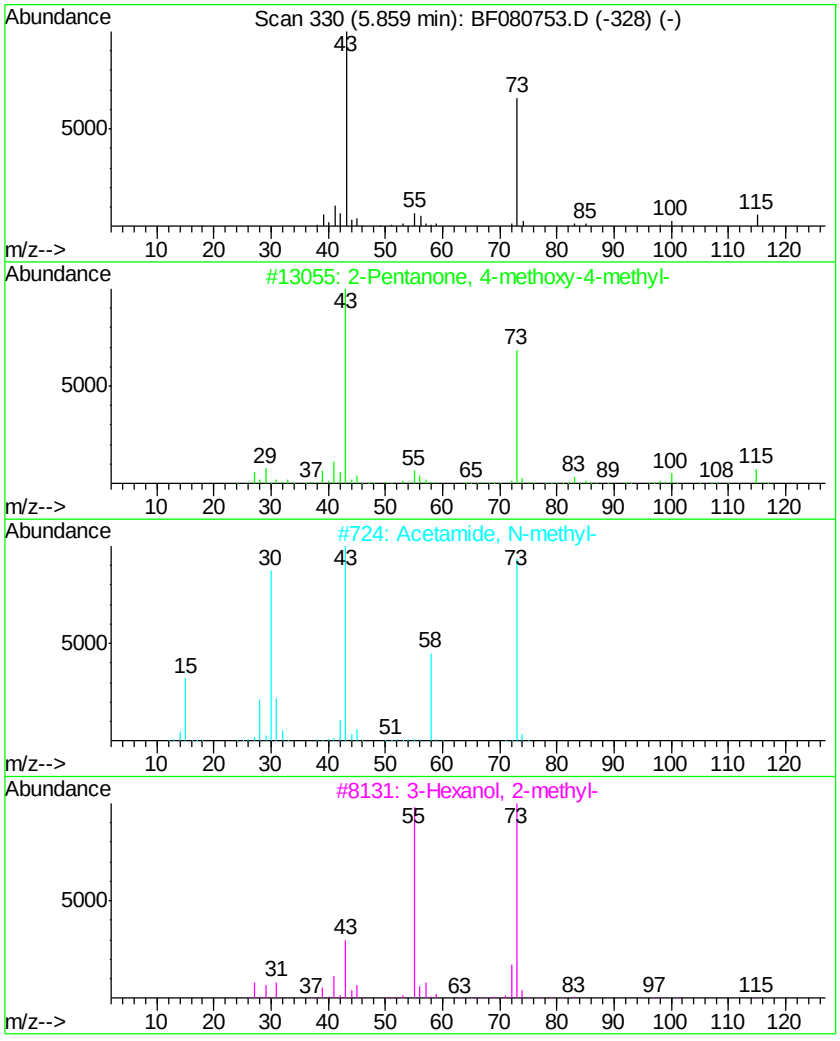
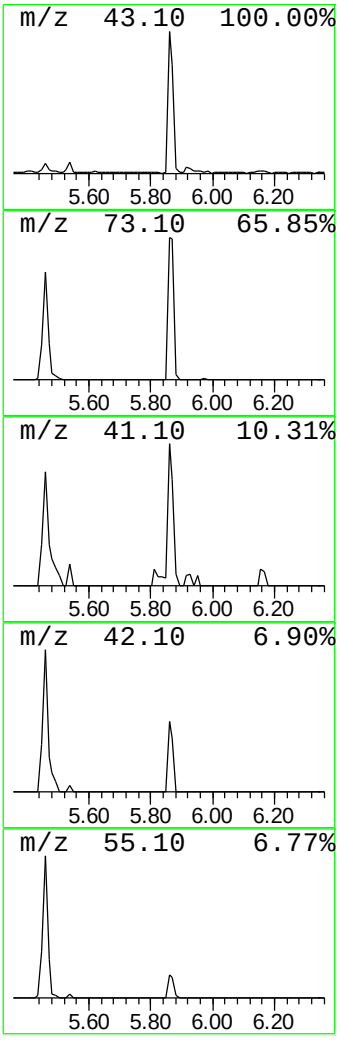
Peak Number 4 unknown5.86 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.86	3.19 ng	149926	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	12
4	N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
5	Hexane, 2-methyl-	100	C7H16	000591-76-4	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080753.D
Acq On : 1 Aug 2015 1:02
Operator : TP/UM
Sample : G3127-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId :

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

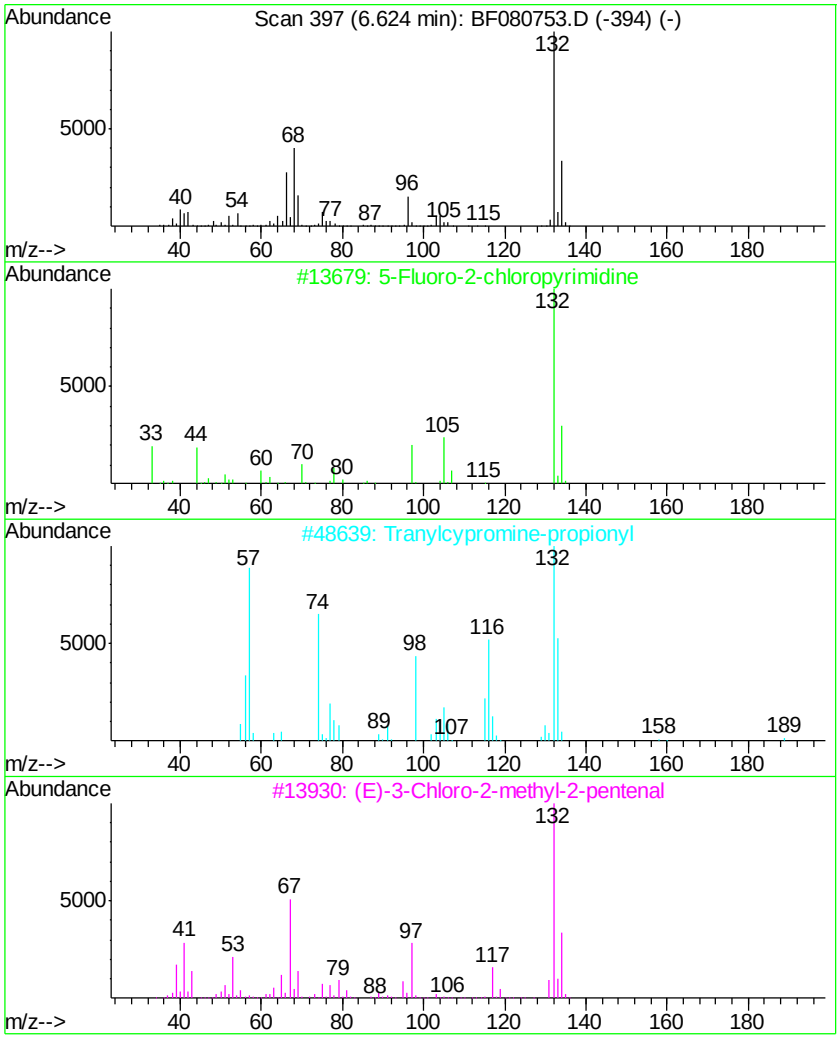
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

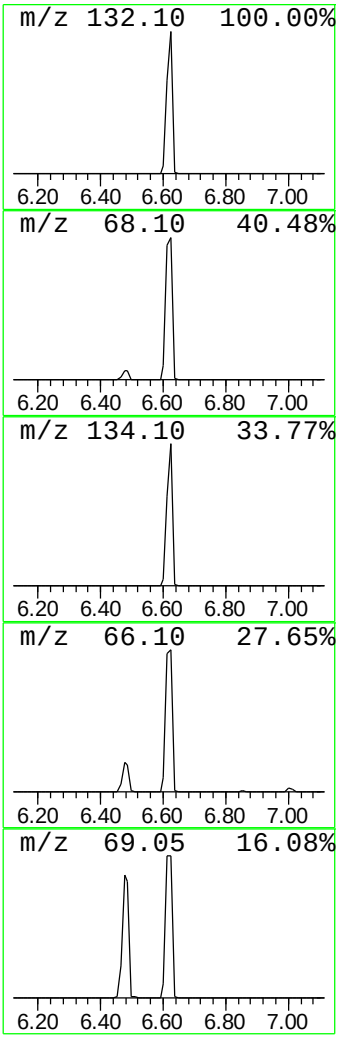
****

Peak Number 5 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	91.65 ng	4304370	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





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Data File : BF080753.D
Acq On : 1 Aug 2015 1:02
Operator : TP/UM
Sample : G3127-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId :

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

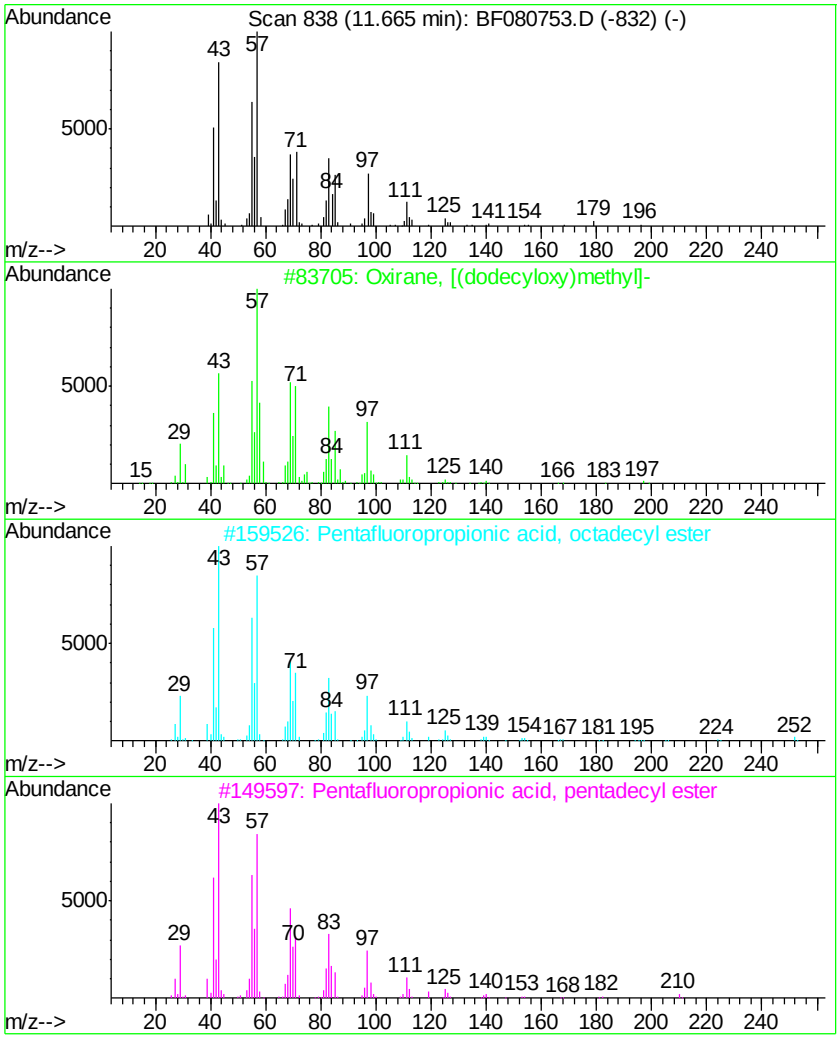
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

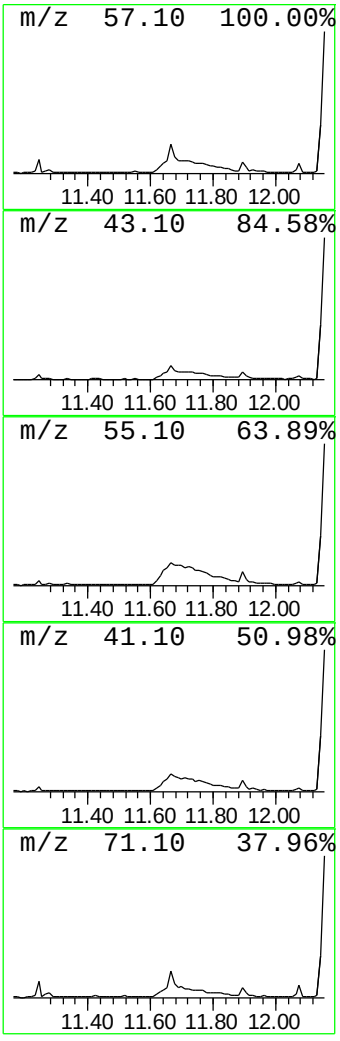
****

Peak Number 7 Oxirane, [(dodecyloxy)methyl]- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	13.73 ng	826740	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	90
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	86
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	83
4	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	83
5	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	83





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Data File : BF080753.D
Acq On : 1 Aug 2015 1:02
Operator : TP/UM
Sample : G3127-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId :

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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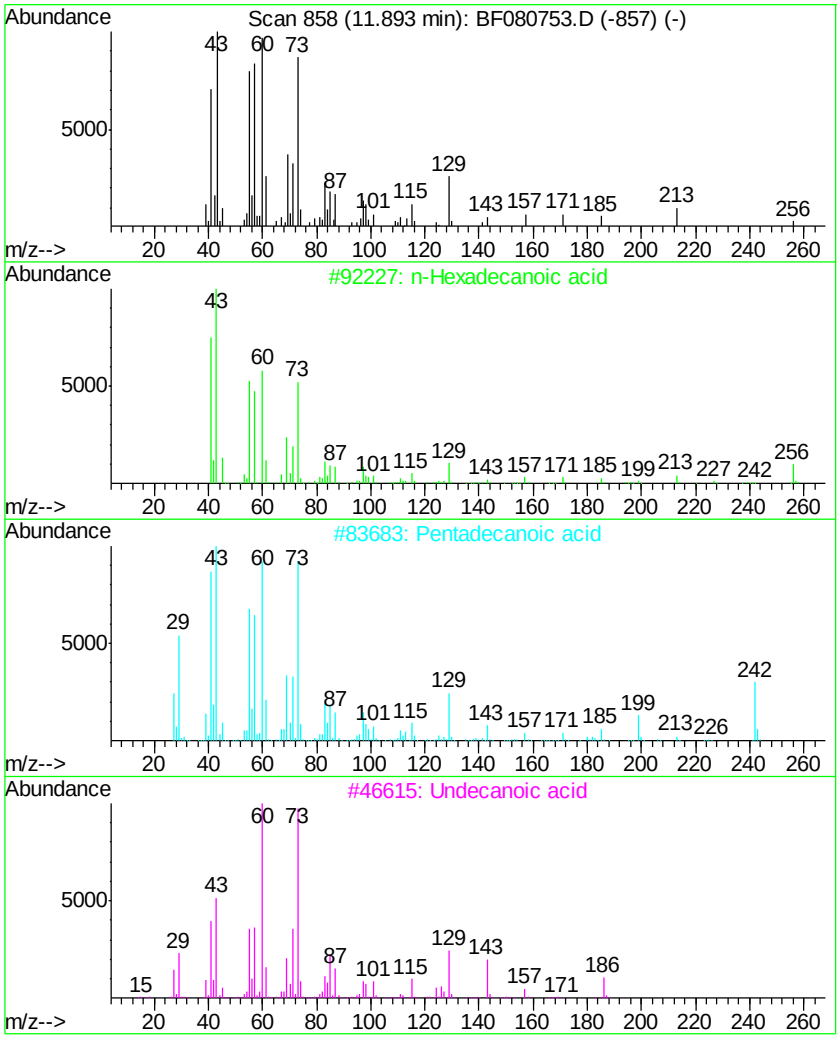
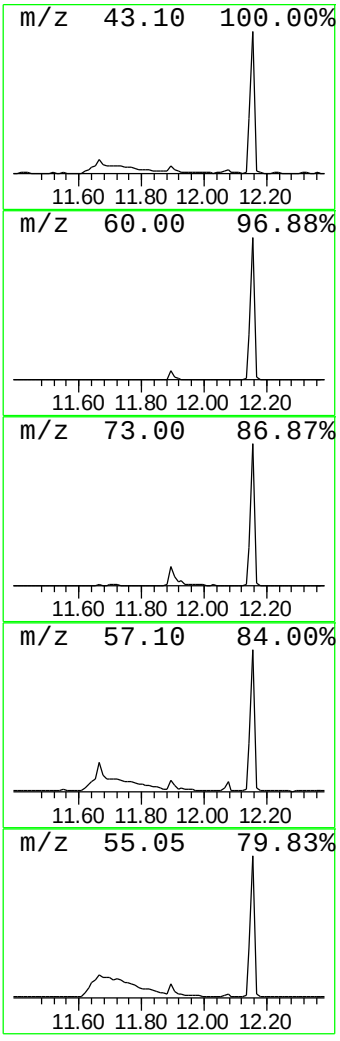
Peak Number 8 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	4.00 ng	240839	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Undecanoic acid	186	C11H22O2	000112-37-8	86
4	Tridecanoic acid	214	C13H26O2	000638-53-9	86
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	83





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Data File : BF080753.D
Acq On : 1 Aug 2015 1:02
Operator : TP/UM
Sample : G3127-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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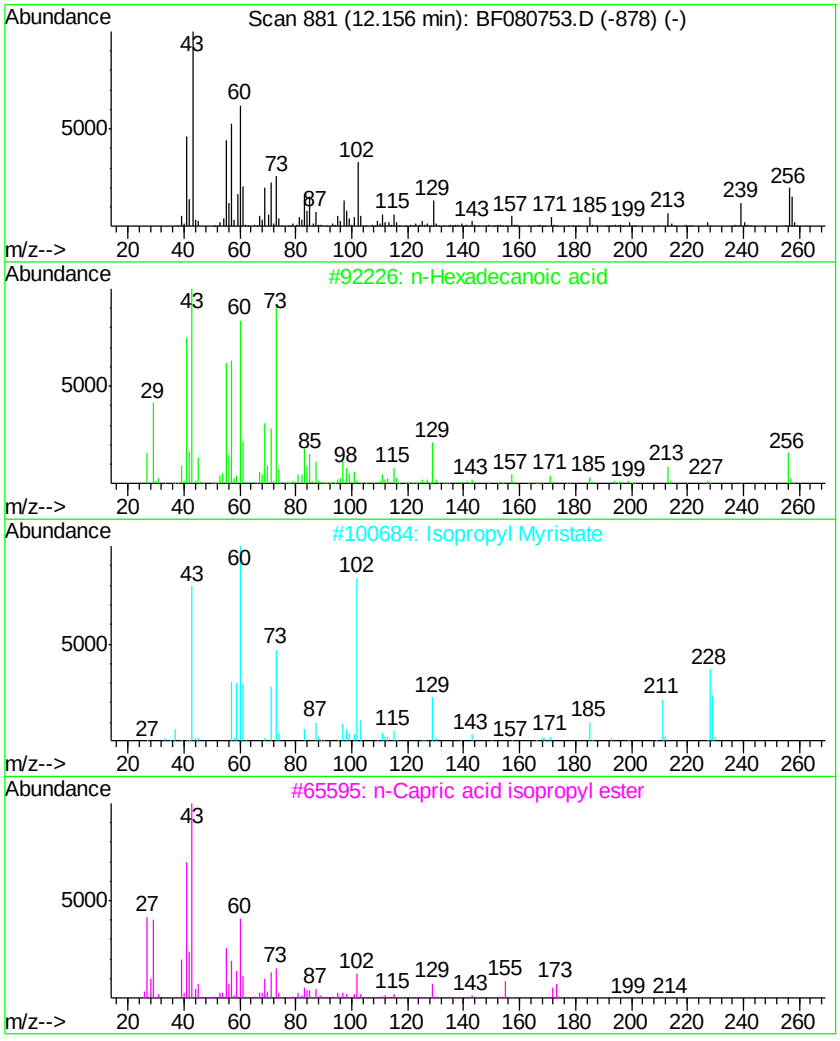
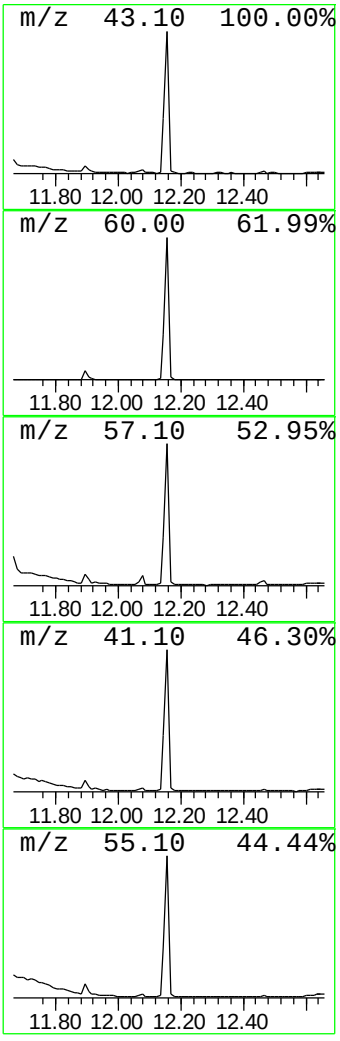
Peak Number 9 unknown12.16 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	38.74 ng	2332460	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	55
2	Isopropyl Myristate	270	C17H34O2	000110-27-0	40
3	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	37
4	Methyl .beta.-d-galactopyranoside	194	C7H14O6	1000126-04-6	32
5	Undecanoic acid	186	C11H22O2	000112-37-8	27





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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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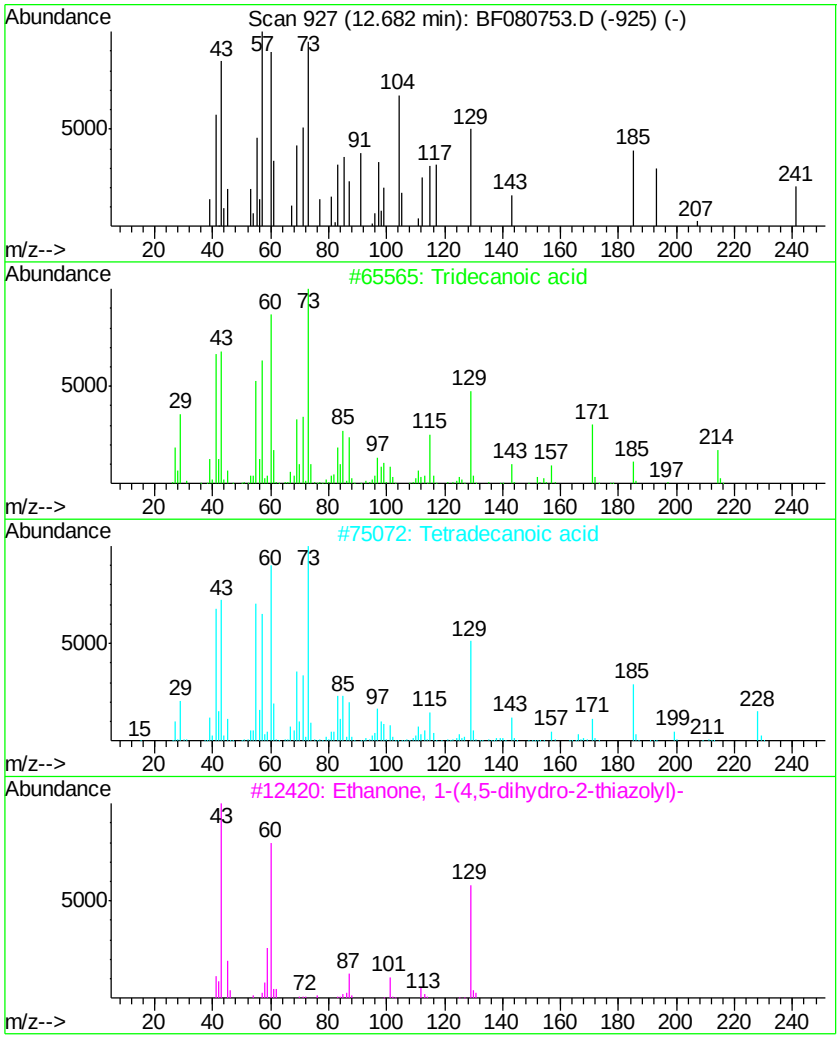
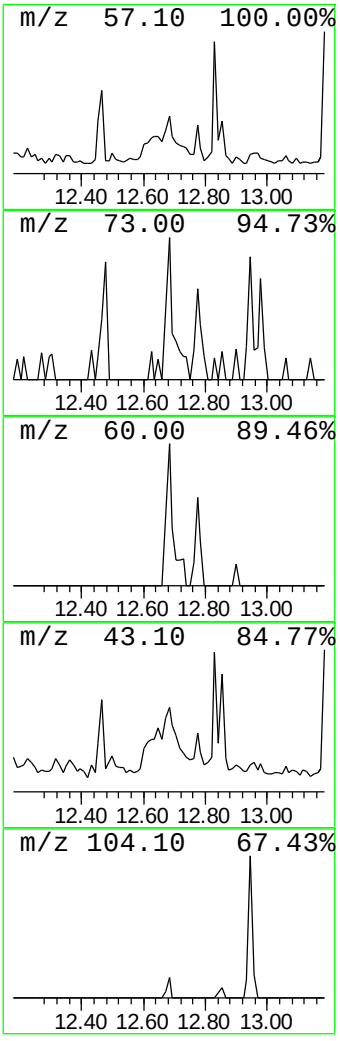
Peak Number 10 unknown12.68 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	2.28 ng	87889	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	35
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	35
3	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	30
4	n-Decanoic acid	172	C10H20O2	000334-48-5	27
5	Methyl 6-O-[1-methylpropyl]-.bet...	250	C11H22O6	1000126-15-7	16





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Data File : BF080753.D
Acq On : 1 Aug 2015 1:02
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Sample : G3127-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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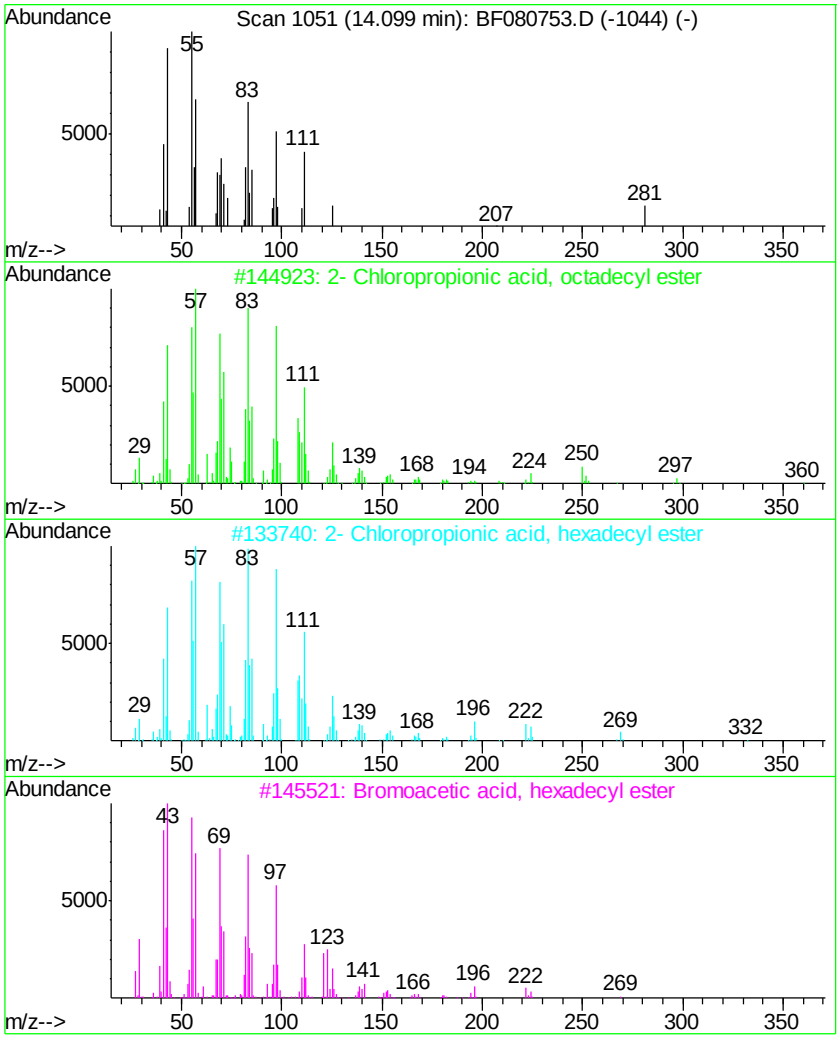
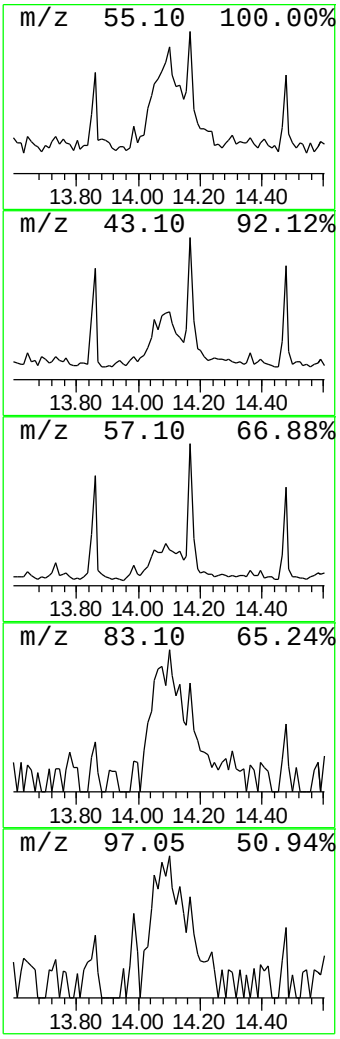
Peak Number 11 2- Chloropropionic acid, oc... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.10	3.68 ng	142341	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90
2	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	78
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	74
4	1-Heptadecanol	256	C17H36O	001454-85-9	64
5	1-Octadecanol	270	C18H38O	000112-92-5	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080753.D
Acq On : 1 Aug 2015 1:02
Operator : TP/UM
Sample : G3127-03
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId :

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.41	5.0	ng	236001	1	6.85	939306	20.0
2-Pentanone, 4-hy...	5.06	81.0	ng	3805790	1	6.85	939306	20.0
unknown5.86	5.86	3.2	ng	149926	1	6.85	939306	20.0
unknown6.62	6.62	91.7	ng	4304370	1	6.85	939306	20.0
Oxirane, [(dodecy...	11.66	13.7	ng	826740	4	11.37	1204120	20.0
n-Hexadecanoic acid	11.89	4.0	ng	240839	4	11.37	1204120	20.0
unknown12.16	12.16	38.7	ng	2332460	4	11.37	1204120	20.0
unknown12.68	12.68	2.3	ng	87889	5	13.99	772545	20.0
2- Chloropropioni...	14.10	3.7	ng	142341	5	13.99	772545	20.0