LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072315\
Data File : BF080610.D
Acq On : 24 Jul 2015 00:35
Operator : TP/UM
Sample : G3068-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTHEAST-FLOOR2-72215

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-BF072315.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	3.275	101	104	110	rBV	6089	22117	1.58%	0.191%
2	5.104	262	264	267	rBV	428558	416585	29.84%	3.595%
3	5.527	298	301	303	rBV	1197306	1272115	91.11%	10.977%
4	5.950	335	338	340	rBV	32144	33694	2.41%	0.291%
5	6.167	356	357	368	rVB	73453	88630	6.35%	0.765%
6	6.556	389	391	393	rBV	1707004	1353022	96.91%	11.675%
7	6.704	402	404	407	rBV	1582425	1289799	92.38%	11.129%
8	6.944	423	425	427	rBV	328986	262199	18.78%	2.262%
9	7.104	436	439	441	rVB	1177863	1007051	72.13%	8.690%
10	7.504	472	474	476	rBV	1046535	806748	57.78%	6.961%
11	8.236	535	538	540	rBV	404347	321170	23.00%	2.771%
12	9.185	620	621	623	rVB	33338	27666	1.98%	0.239%
13	9.310	630	632	634	rVB	1688938	1396228	100.00%	12.048%
14	9.710	665	667	669	rBV	70730	88238	6.32%	0.761%
15	9.996	690	692	694	rVB	330738	315491	22.60%	2.722%
16	10.408	726	728	731	rVB	57359	57687	4.13%	0.498%
17	10.773	758	760	763	rBV2	789121	795697	56.99%	6.866%
18	10.899	769	771	774	rBV	23048	31386	2.25%	0.271%
19	11.482	820	822	824	rBV	333958	301742	21.61%	2.604%
20	12.008	865	868	870	rBV	41085	39605	2.84%	0.342%
21	13.094	961	963	966	rBV	1162643	1111989	79.64%	9.595%
22	13.619	1003	1009	1013	rBV	91730	102932	7.37%	0.888%
23	14.088	1048	1050	1056	rVB2	35967	47662	3.41%	0.411%
24	14.248	1062	1064	1067	rBV	215124	236914	16.97%	2.044%
25	15.894	1206	1208	1211	rBV	120124	162801	11.66%	1.405%

Sum of corrected areas: 11589168

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072315\
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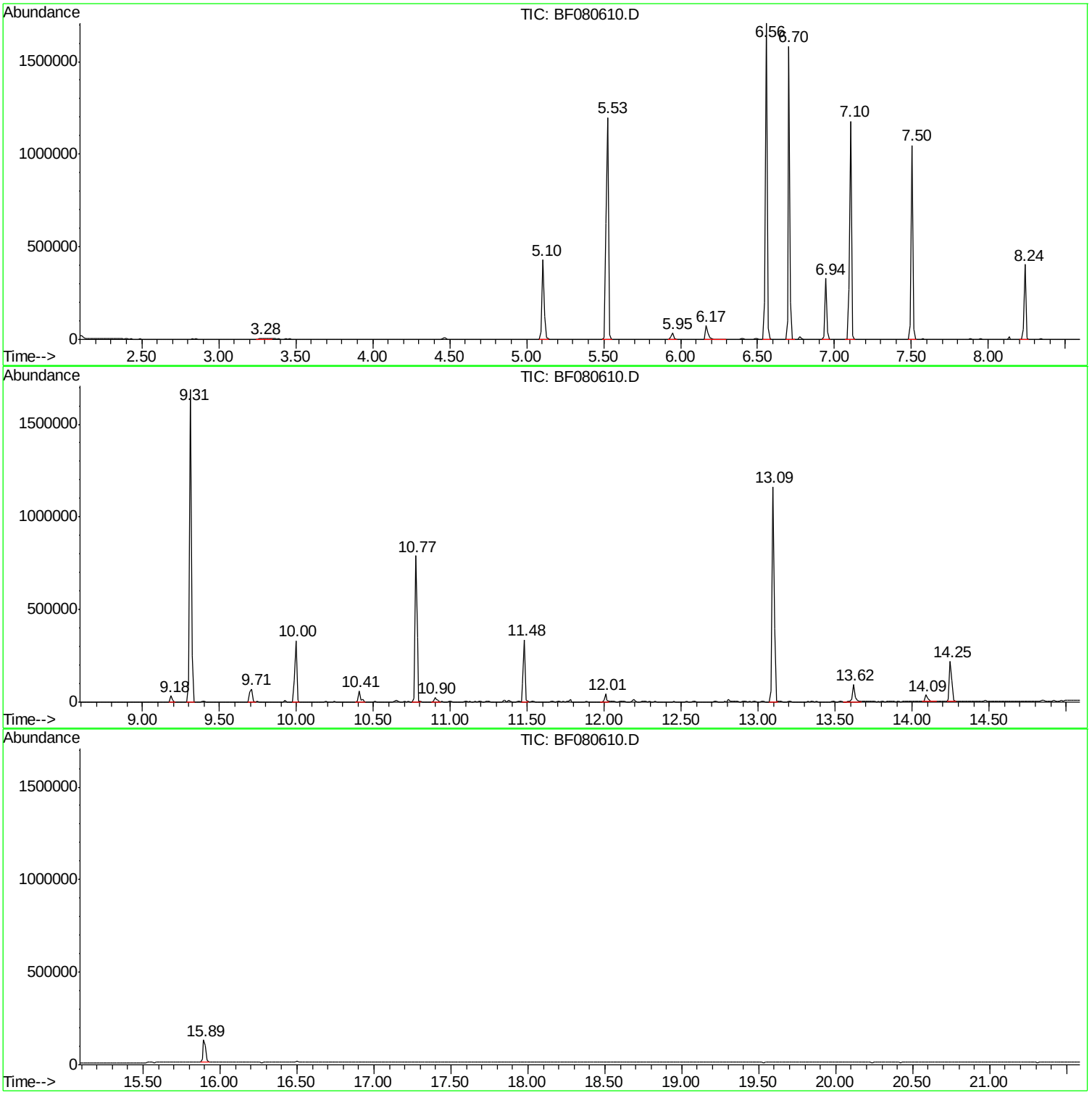
Sample : G3068-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SOUTHEAST-FLOOR2-72215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072315\
Data File : BF080610.D
Acq On : 24 Jul 2015 00:35
Operator : TP/UM
Sample : G3068-03
Misc :
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Instrument : BNA_F
ClientSampleId : SOUTHEAST-FLOOR2-72215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

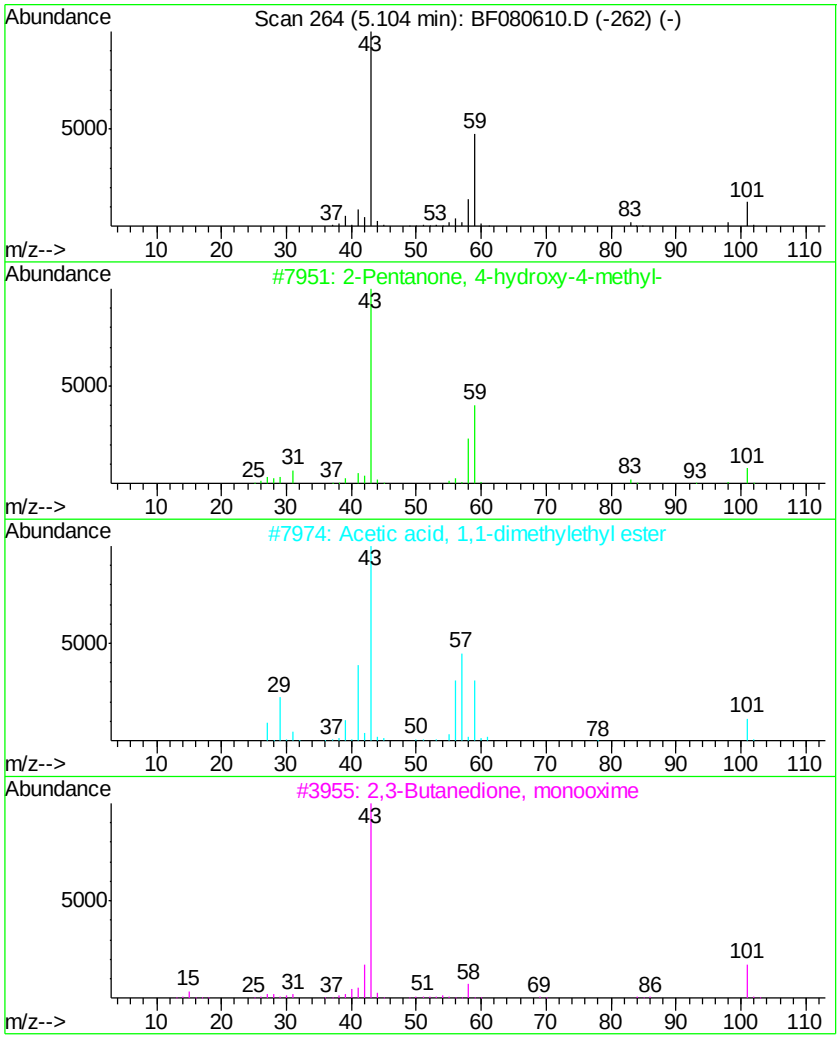
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

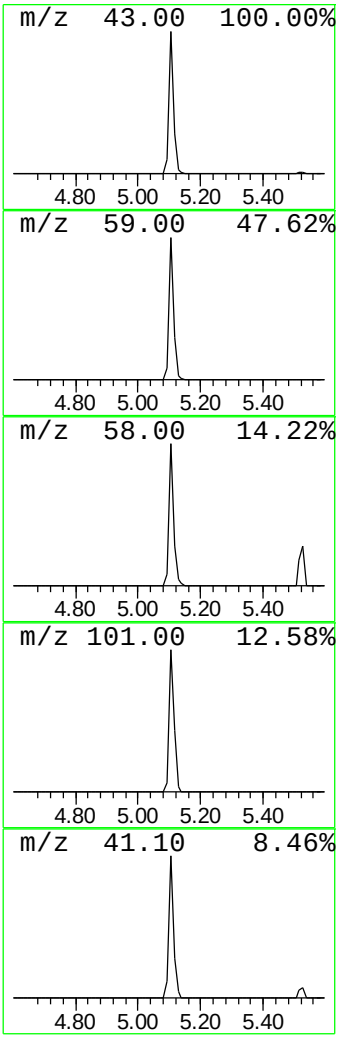
****

Peak Number 1 unknown5.10 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	31.78 ng	416585	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072315\
Data File : BF080610.D
Acq On : 24 Jul 2015 00:35
Operator : TP/UM
Sample : G3068-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SOUTHEAST-FLOOR2-72215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

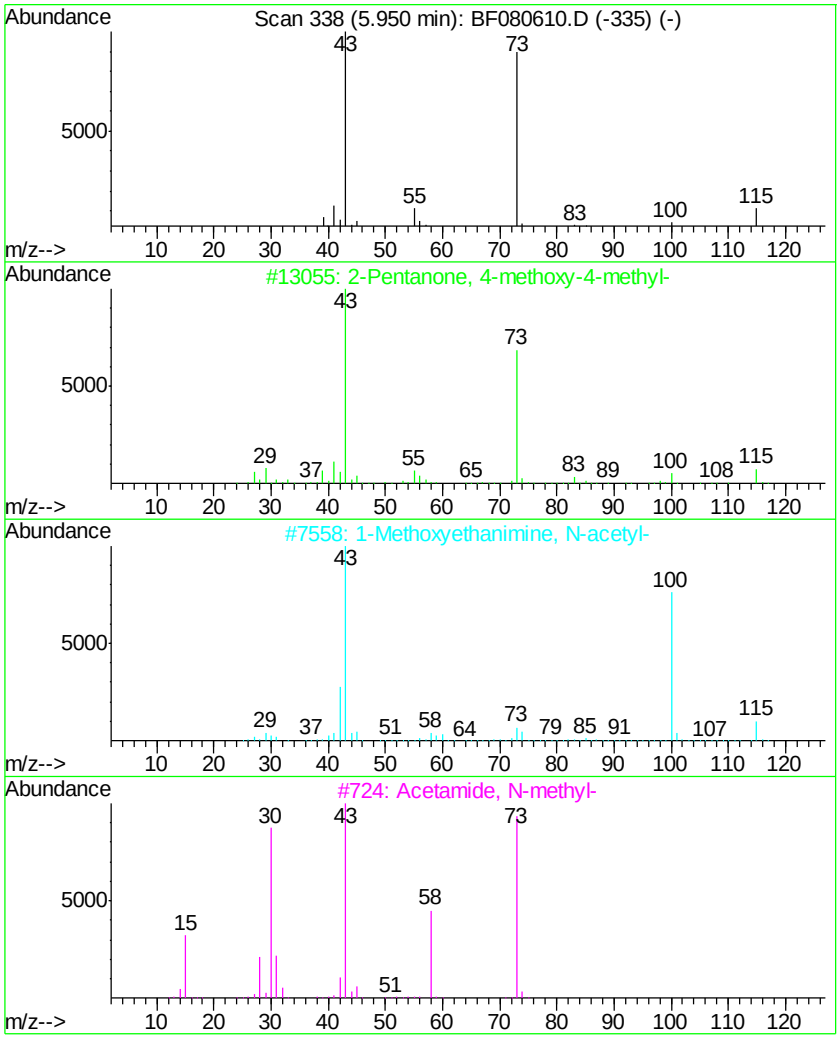
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

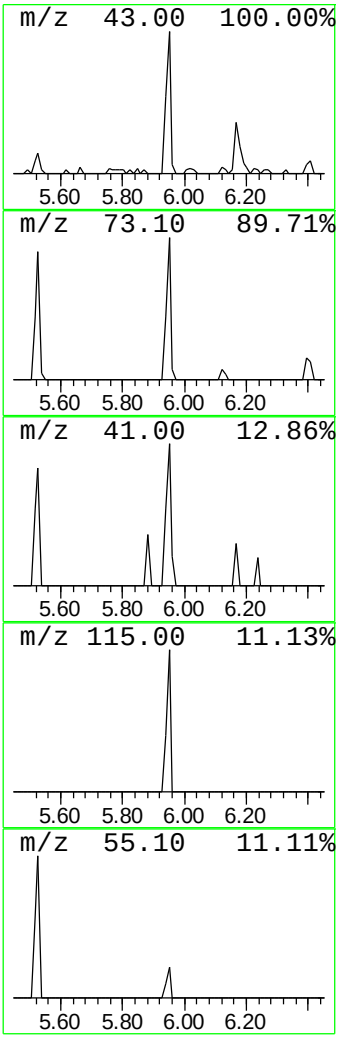
****

Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.95	2.57 ng	33694	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	72
2	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
5	2,6-Dimethyl-3,7,9-trioxabicyclo...	158	C8H14O3	1000143-37-8	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072315\
Data File : BF080610.D
Acq On : 24 Jul 2015 00:35
Operator : TP/UM
Sample : G3068-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SOUTHEAST-FLOOR2-72215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.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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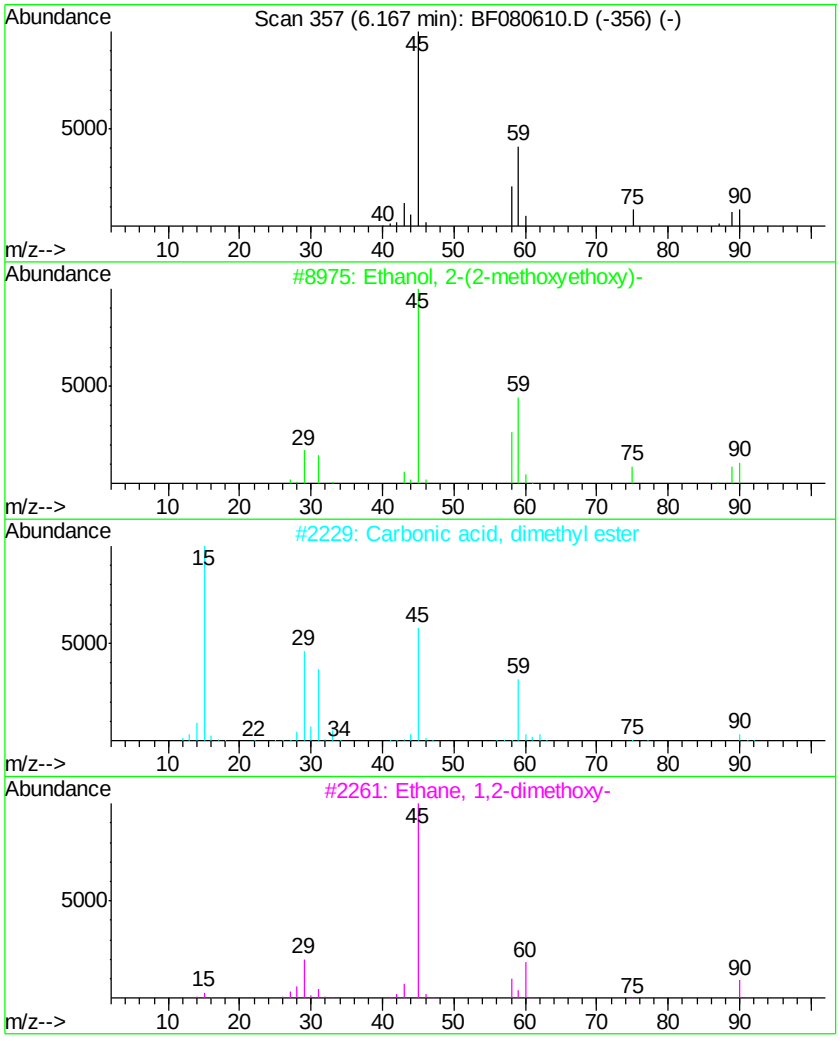
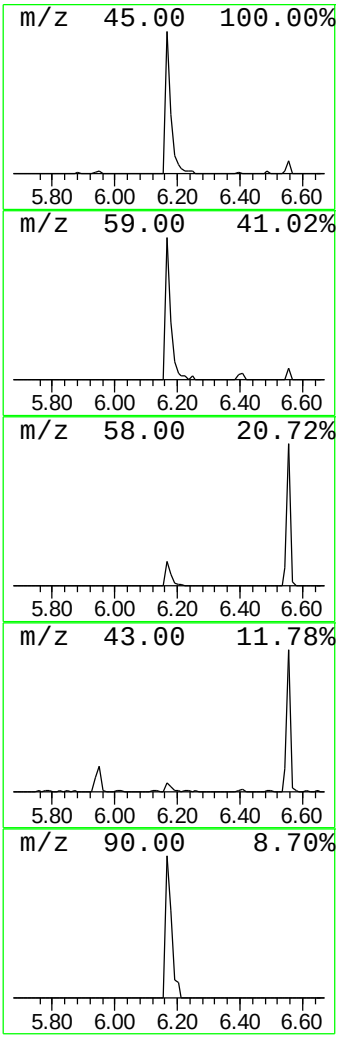
Peak Number 3 Ethanol, 2-(2-methoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.17	6.76 ng	88630	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	83
2	Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	64
3	Ethane, 1,2-dimethoxy-	90	C4H10O2	000110-71-4	28
4	Hydrazine, (2-methoxyethyl)-	90	C3H10N2O	003044-15-3	9
5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072315\
Data File : BF080610.D
Acq On : 24 Jul 2015 00:35
Operator : TP/UM
Sample : G3068-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SOUTHEAST-FLOOR2-72215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

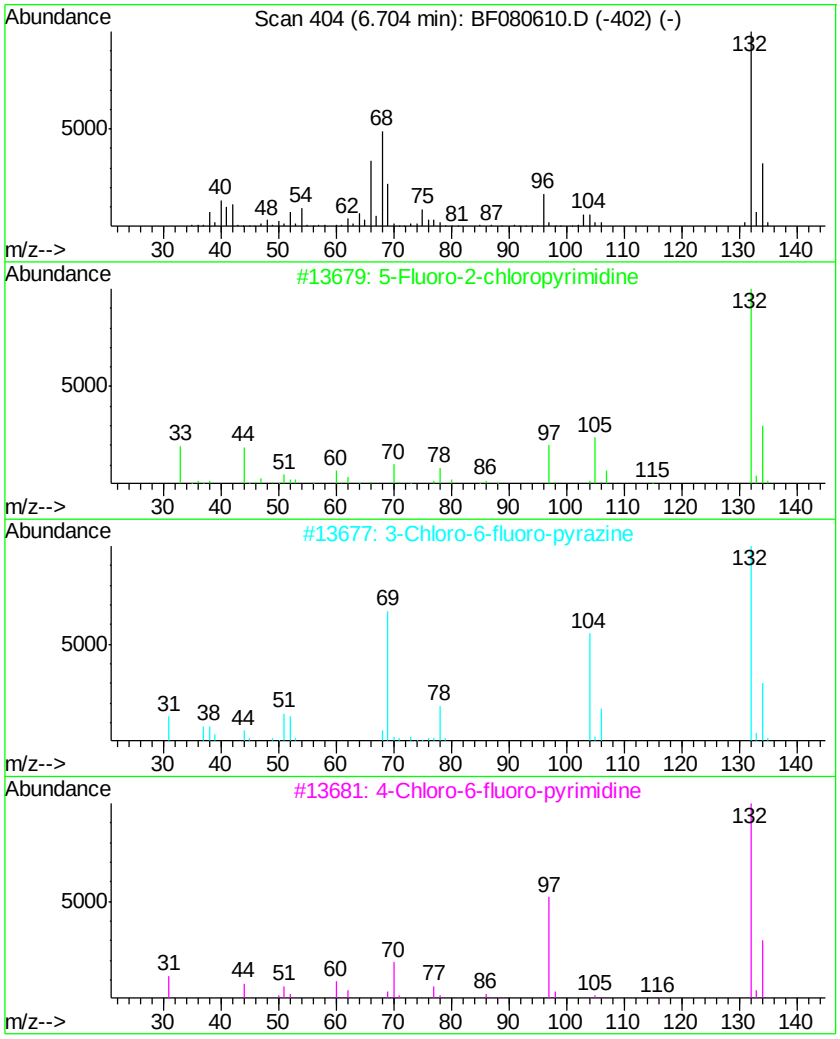
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

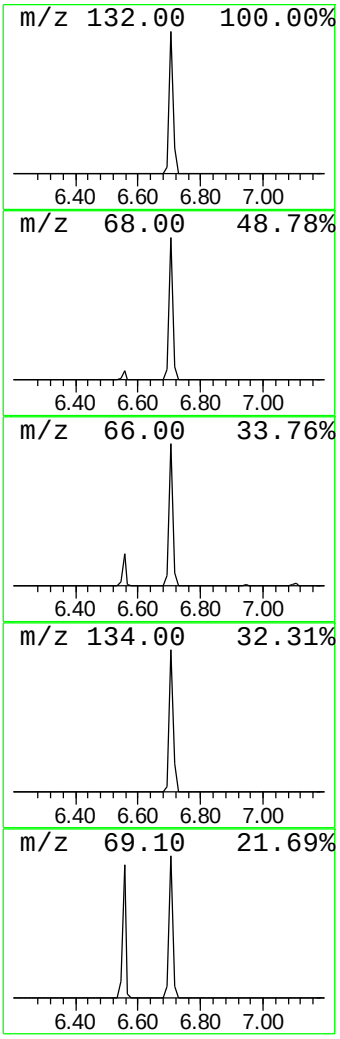
****

Peak Number 4 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	98.38 ng	1289800	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072315\
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Acq On : 24 Jul 2015 00:35
Operator : TP/UM
Sample : G3068-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SOUTHEAST-FLOOR2-72215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

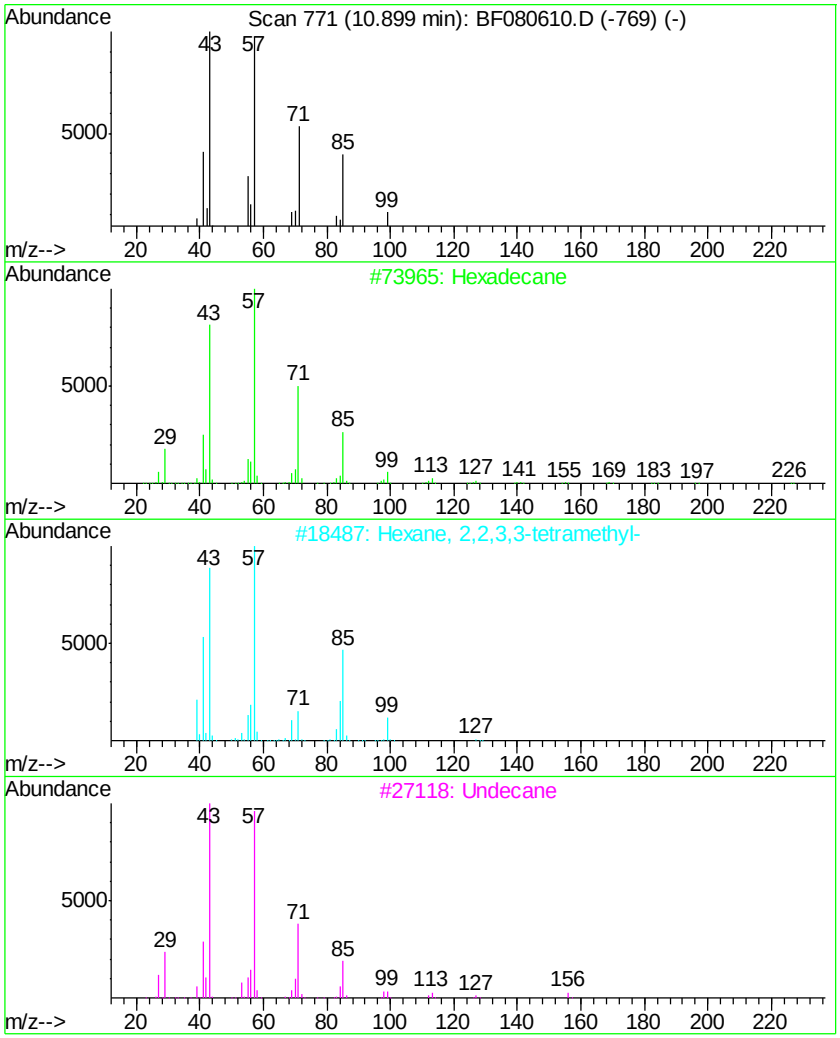
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

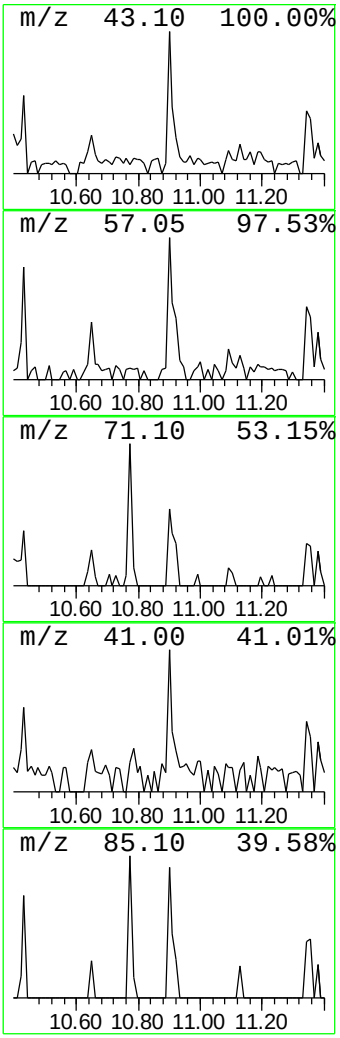
****

Peak Number 6 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	2.08 ng	31386	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	64
2	Hexane, 2,2,3,3-tetramethyl-	142	C10H22	013475-81-5	53
3	Undecane	156	C11H24	001120-21-4	50
4	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	50
5	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	47





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072315\
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Sample : G3068-03
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SOUTHEAST-FLOOR2-72215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.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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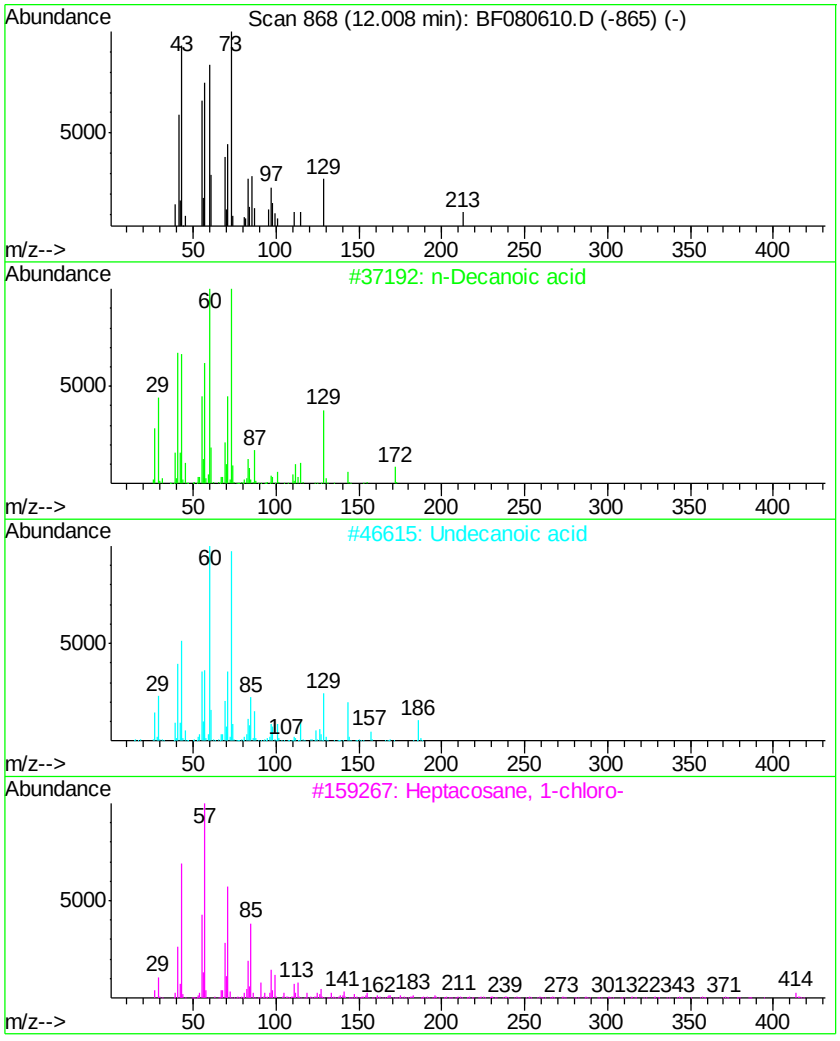
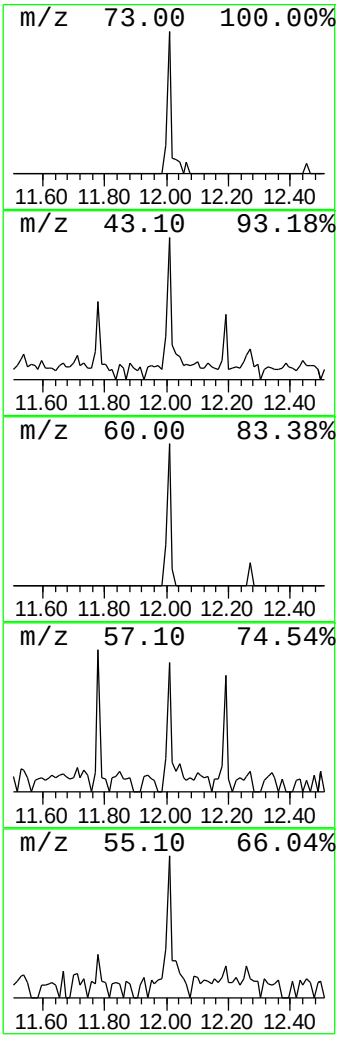
Peak Number 7 n-Decanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	2.63 ng	39605	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	53
2	Undecanoic acid	186	C11H22O2	000112-37-8	50
3	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	22
4	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	14
5	Vinyl lauryl ether	212	C14H28O	000765-14-0	14





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Sample : G3068-03
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Instrument :
BNA_F
ClientSampleId :
SOUTHEAST-FLOOR2-72215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

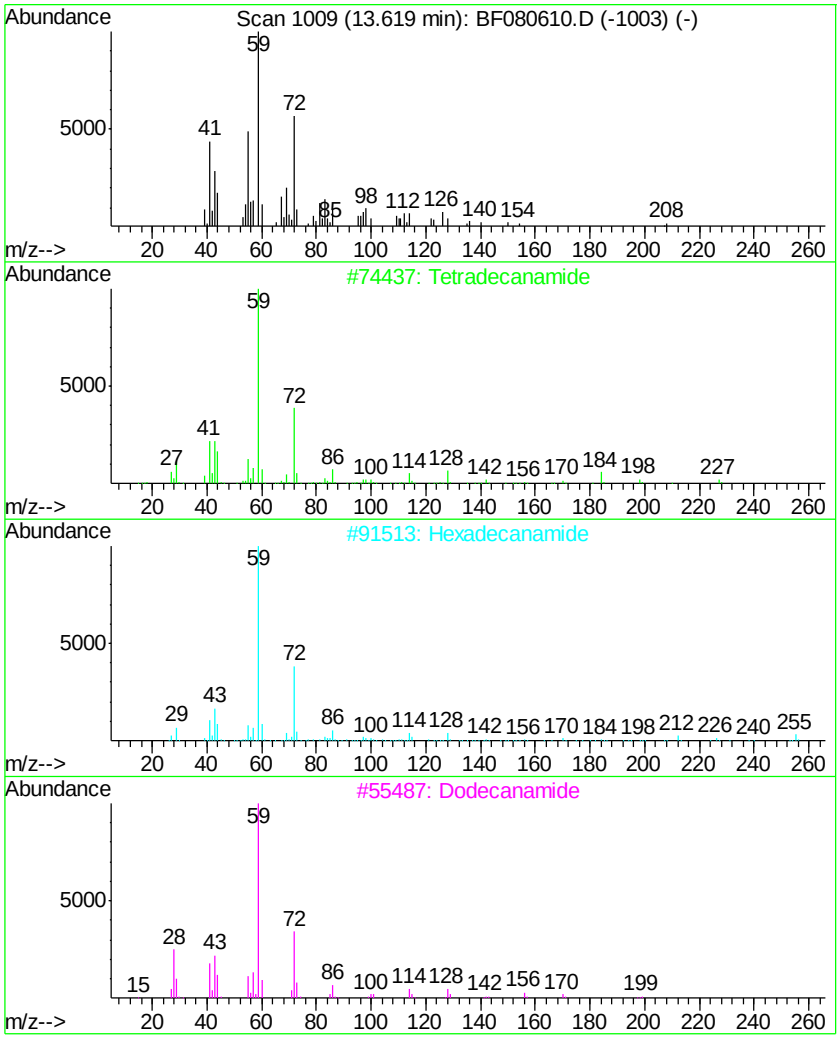
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

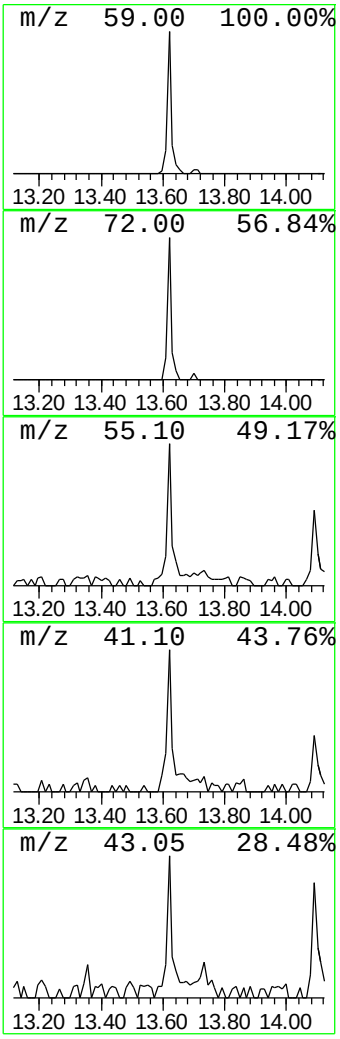
****

Peak Number 8 Tetradecanamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.62	8.69 ng	102932	Chrysene-d12	14.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanamide	227	C14H29NO	000638-58-4	72
2	Hexadecanamide	255	C16H33NO	000629-54-9	72
3	Dodecanamide	199	C12H25NO	001120-16-7	59
4	Octanamide	143	C8H17NO	000629-01-6	53
5	2-Hydroxy-2-methylundec-5-en-3-one	198	C12H22O2	1000191-46-2	38





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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.M
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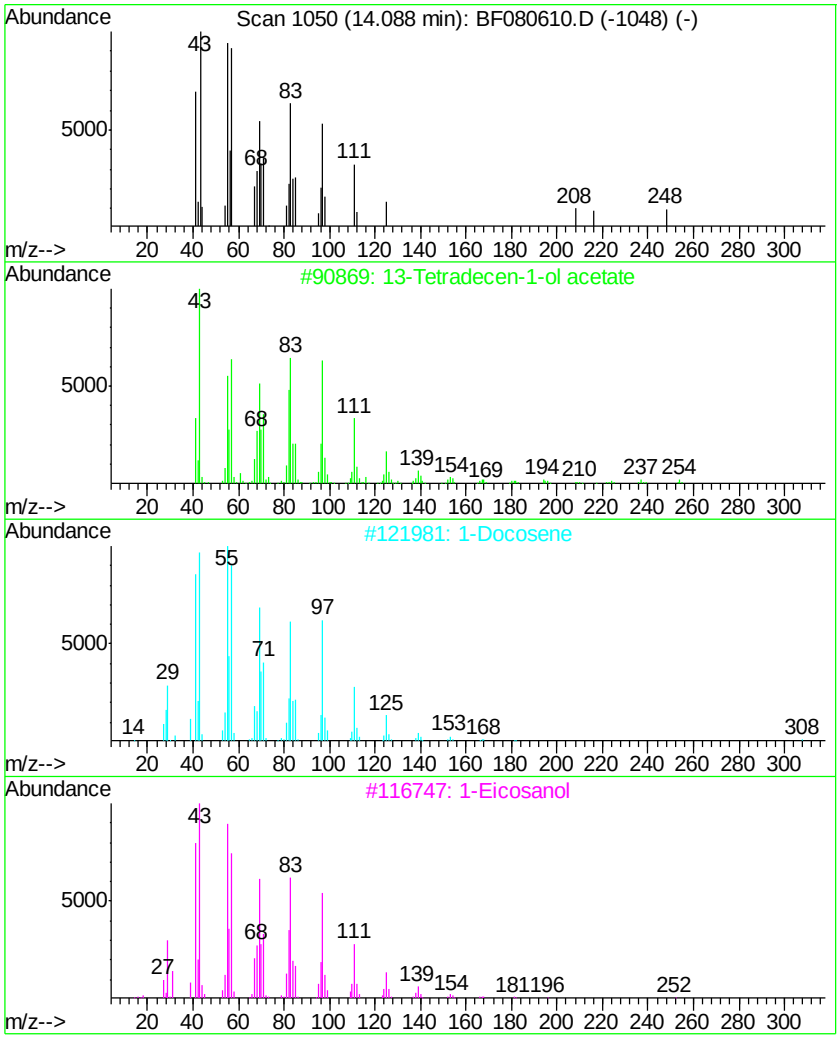
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

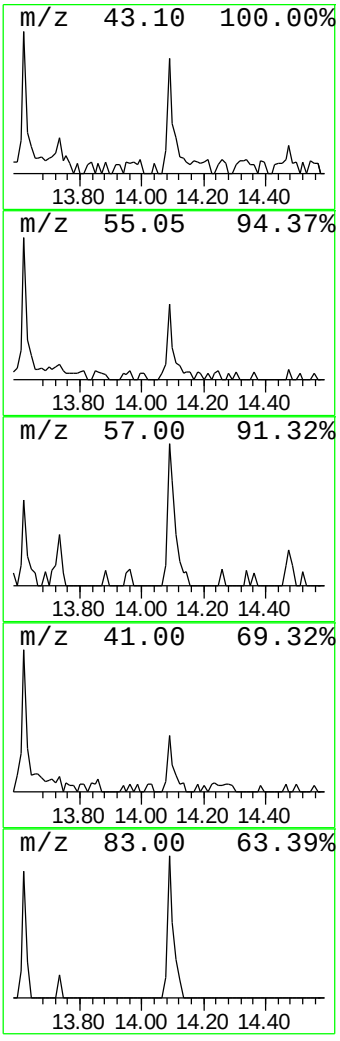
****

Peak Number 9 13-Tetradecen-1-ol acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.09	4.02 ng	47662	Chrysene-d12	14.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	83
2	1-Docosene	308	C22H44	001599-67-3	81
3	1-Eicosanol	298	C20H42O	000629-96-9	81
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	81
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	76





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072315.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
unknown5.10	5.10	31.8	ng	416585	1	6.94	262199	20.0
2-Pentanone, 4-me...	5.95	2.6	ng	33694	1	6.94	262199	20.0
Ethanol, 2-(2-met...	6.17	6.8	ng	88630	1	6.94	262199	20.0
unknown6.70	6.70	98.4	ng	1289800	1	6.94	262199	20.0
Hexadecane	10.90	2.1	ng	31386	4	11.48	301742	20.0
n-Decanoic acid	12.01	2.6	ng	39605	4	11.48	301742	20.0
Tetradecanamide	13.62	8.7	ng	102932	5	14.25	236914	20.0
13-Tetradecen-1-o...	14.09	4.0	ng	47662	5	14.25	236914	20.0