LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100215\
Data File : BF081997.D
Acq On : 3 Oct 2015 00:05
Operator : UM/IZ
Sample : G3887-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OS-SB-25(55-57)

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-BF092815.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	5.074	254	257	268	rVB	937257	1405794	42.47%	5.043%
2	5.486	290	293	295	rBV	2033778	2488340	75.17%	8.927%
3	6.514	380	383	385	rBV	2189315	2315351	69.94%	8.306%
4	6.652	392	395	397	rBV	2599968	2491915	75.28%	8.940%
5	6.892	413	416	418	rBV	389112	575802	17.39%	2.066%
6	7.040	427	429	432	rBV	2218665	1991583	60.16%	7.145%
7	7.452	462	465	471	rBV	1373314	1533833	46.34%	5.503%
8	8.172	526	528	537	rBV	868461	890411	26.90%	3.194%
9	9.120	608	611	613	rBV	54113	50487	1.53%	0.181%
10	9.258	619	623	625	rBV	2532755	3286953	99.29%	11.792%
11	9.646	655	657	660	rBV	442452	435677	13.16%	1.563%
12	9.932	679	682	685	rBV	1125247	1026009	30.99%	3.681%
13	10.721	749	751	754	rBV2	1472485	1973265	59.61%	7.079%
14	10.835	760	761	766	rVB	31328	41551	1.26%	0.149%
15	10.938	768	770	772	rBV	75796	65277	1.97%	0.234%
16	11.418	810	812	815	rBV	680290	987355	29.83%	3.542%
17	11.646	830	832	836	rBV	41639	86179	2.60%	0.309%
18	11.955	857	859	870	rBV	104808	151678	4.58%	0.544%
19	12.481	902	905	907	rBV	22593	50142	1.51%	0.180%
20	12.835	934	936	939	rBV	204262	179979	5.44%	0.646%
21	13.018	949	952	955	rBV	3172948	3310301	100.00%	11.876%
22	13.498	992	994	996	rBV	20088	34433	1.04%	0.124%
23	13.544	996	998	1000	rVB	147763	132878	4.01%	0.477%
24	13.921	1028	1031	1040	rBV	66684	154711	4.67%	0.555%
25	14.069	1041	1044	1052	rVB	1022407	1124427	33.97%	4.034%
26	14.835	1108	1111	1116	rBV2	96295	162294	4.90%	0.582%
27	15.532	1168	1172	1187	rBV	566965	927980	28.03%	3.329%

Sum of corrected areas: 27874605

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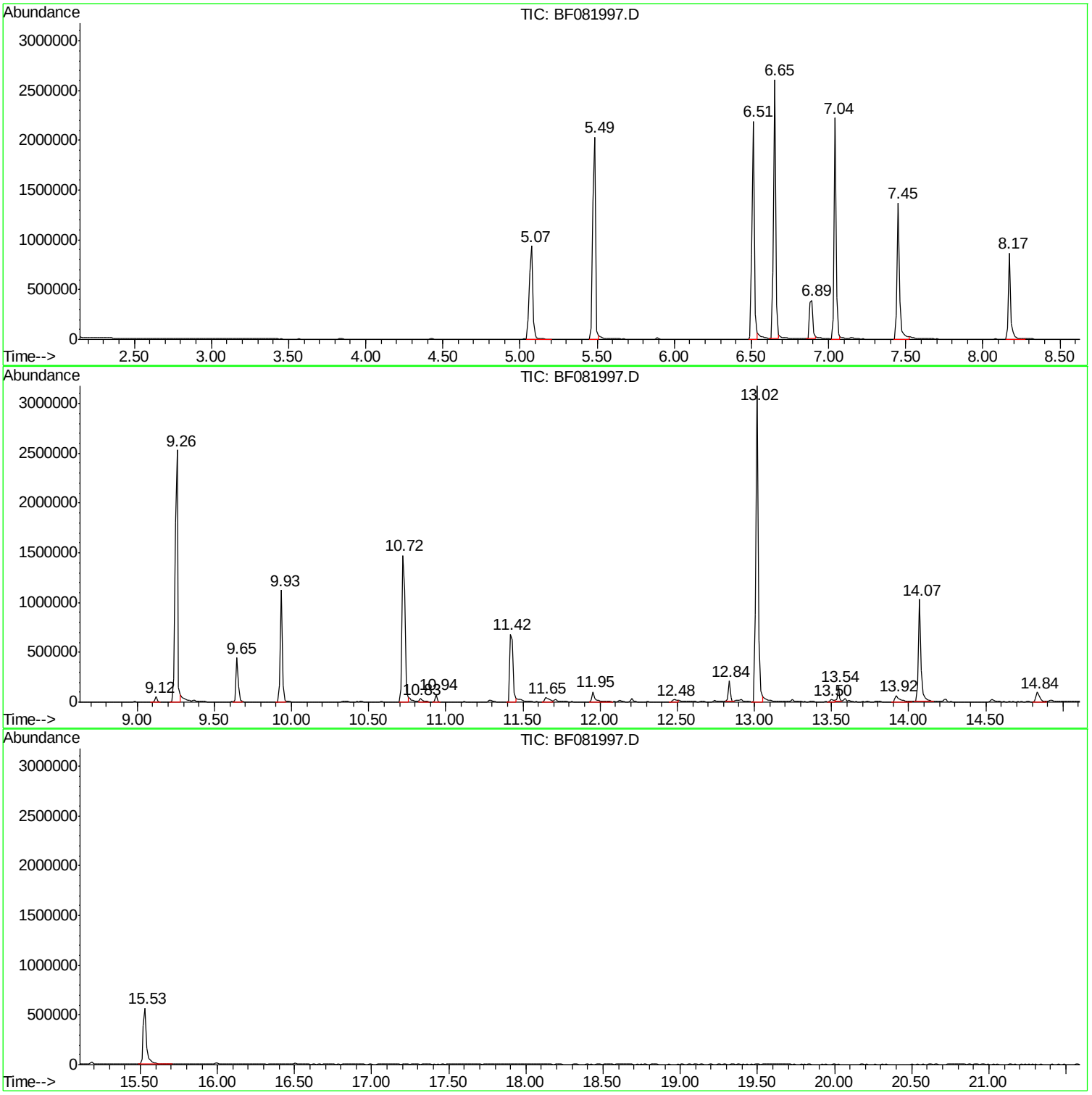
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OS-SB-25(55-57)

Quant Method : H:\HPCHEM1\BNA_F\Method\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100215\
Data File : BF081997.D
Acq On : 3 Oct 2015 00:05
Operator : UM/IZ
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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

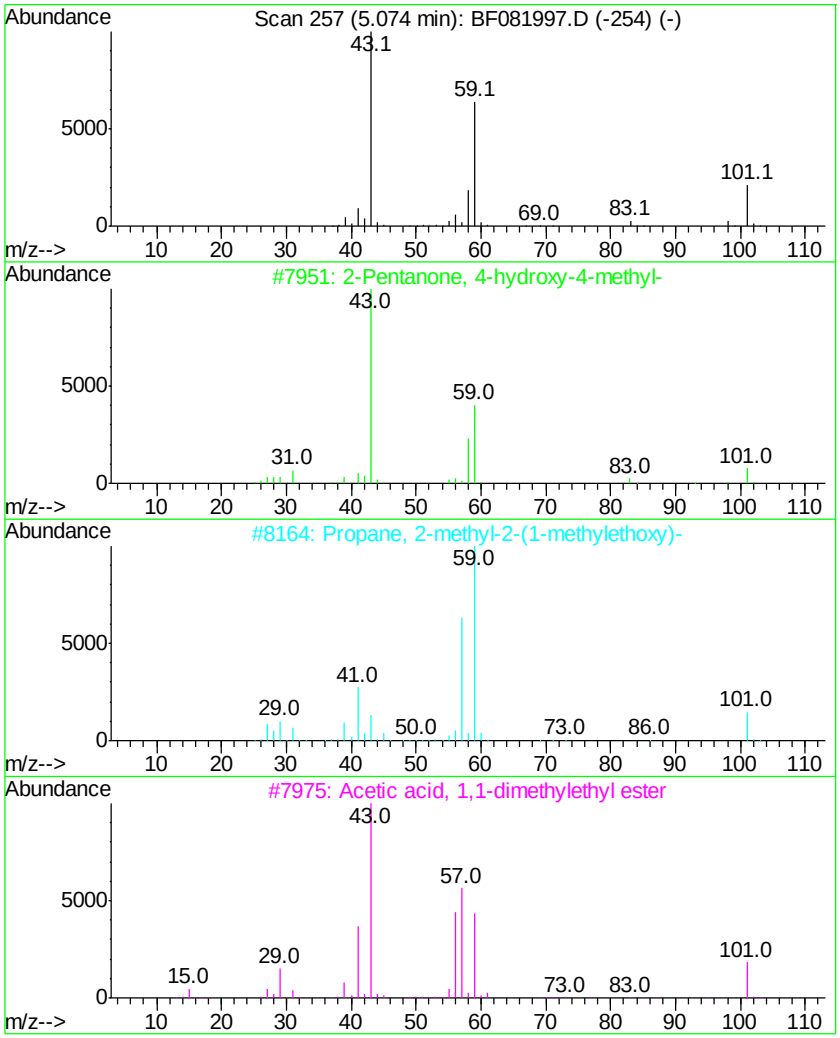
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

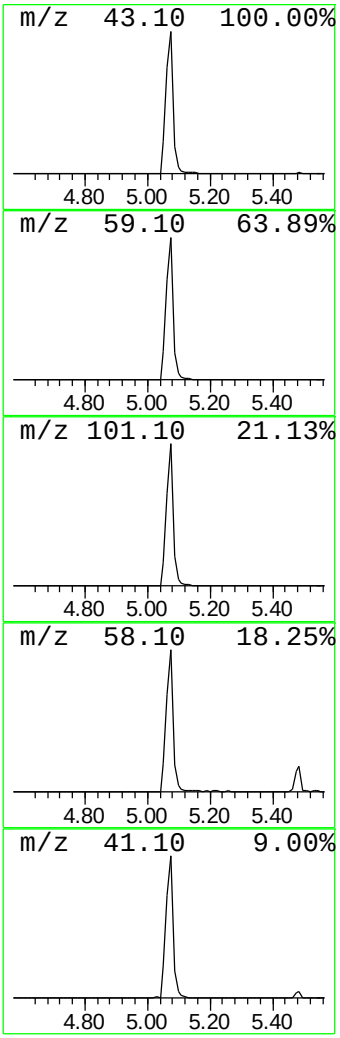
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	48.83 ng	1405790	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100215\
Data File : BF081997.D
Acq On : 3 Oct 2015 00:05
Operator : UM/IZ
Sample : G3887-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OS-SB-25(55-57)

Quant Method : H:\HPCHEM1\BNA_F\Method\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

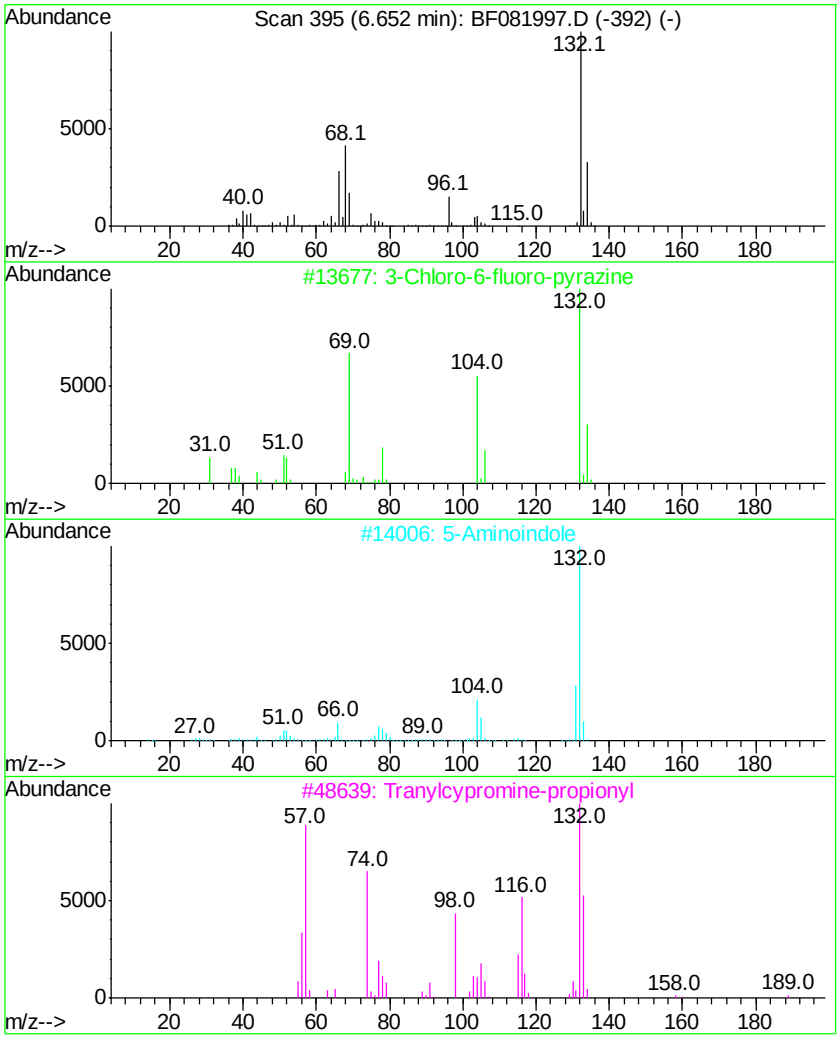
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

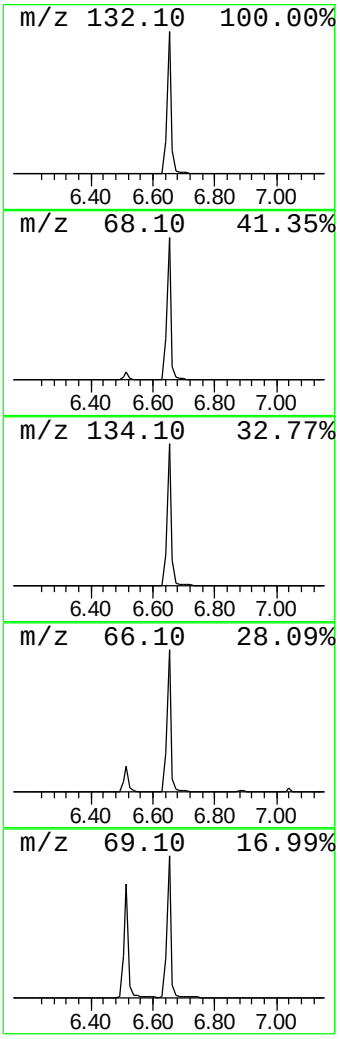
****

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	86.55 ng	2491920	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100215\
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Acq On : 3 Oct 2015 00:05
Operator : UM/IZ
Sample : G3887-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OS-SB-25(55-57)

Quant Method : H:\HPCHEM1\BNA_F\Method\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

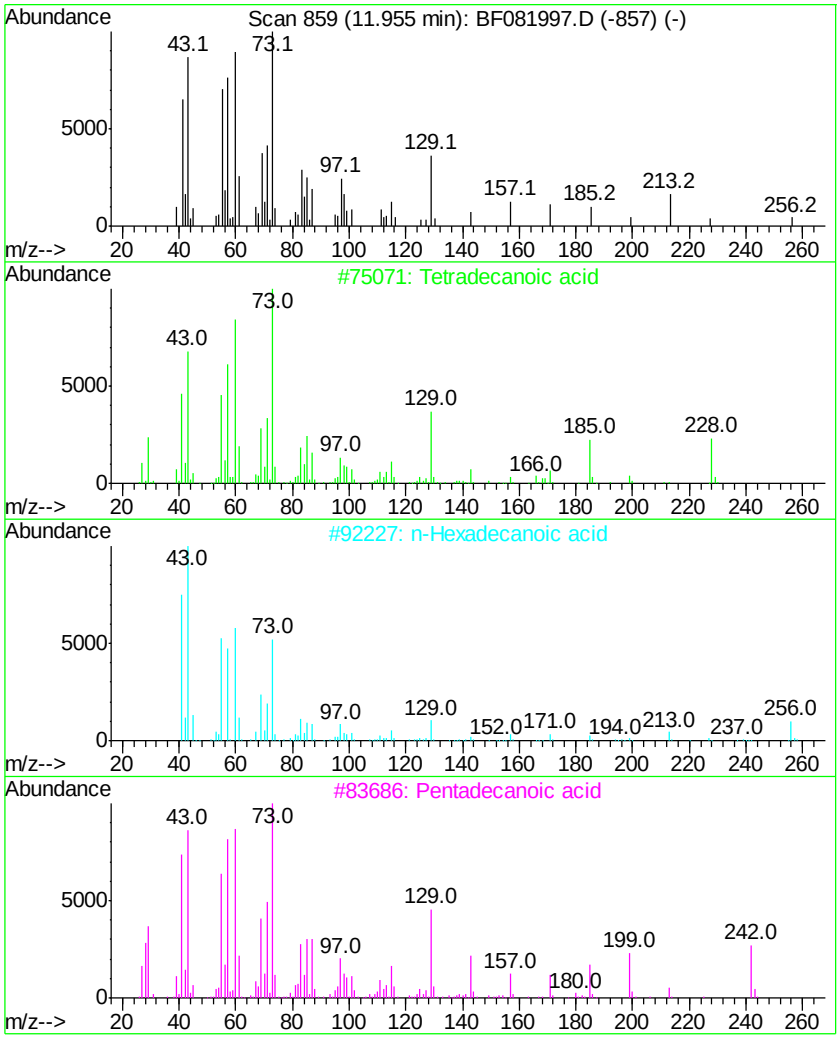
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

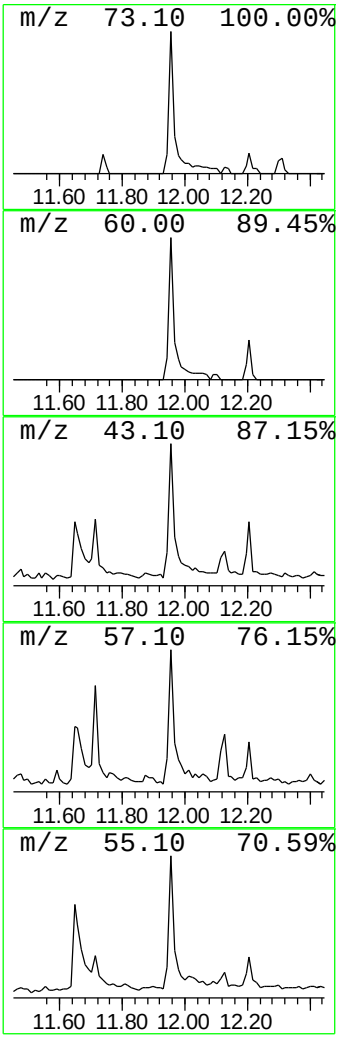
****

Peak Number 4 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	3.07 ng	151678	Phenanthrene-d10	11.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	59
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4	Tridecanoic acid	214	C13H26O2	000638-53-9	53
5	Tridecane	184	C13H28	000629-50-5	11





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100215\
Data File : BF081997.D
Acq On : 3 Oct 2015 00:05
Operator : UM/IZ
Sample : G3887-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OS-SB-25(55-57)

Quant Method : H:\HPCHEM1\BNA_F\Method\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

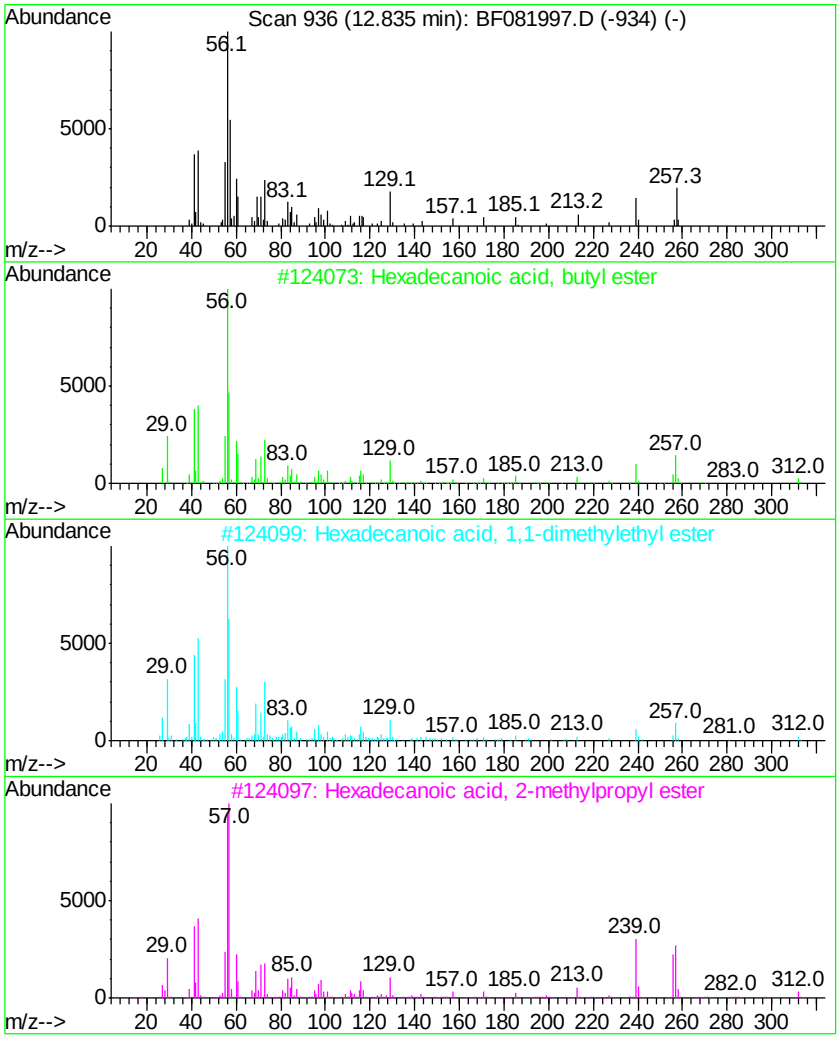
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

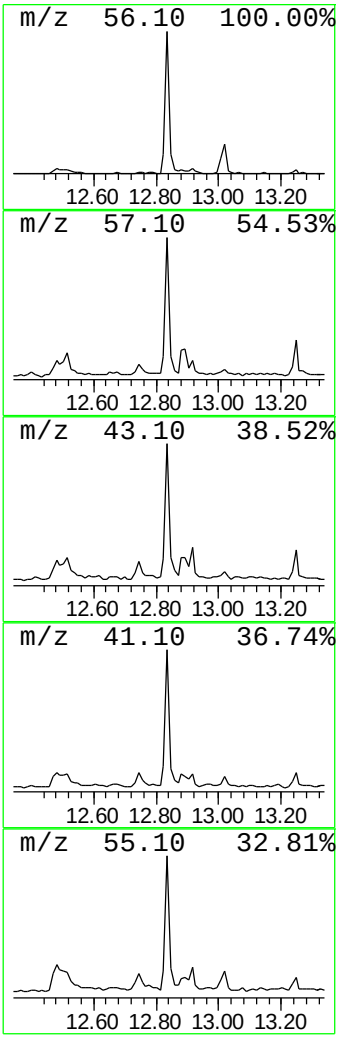
****

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	3.20 ng	179979	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	64
4	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
5	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100215\
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Operator : UM/IZ
Sample : G3887-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OS-SB-25(55-57)

Quant Method : H:\HPCHEM1\BNA_F\Method\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

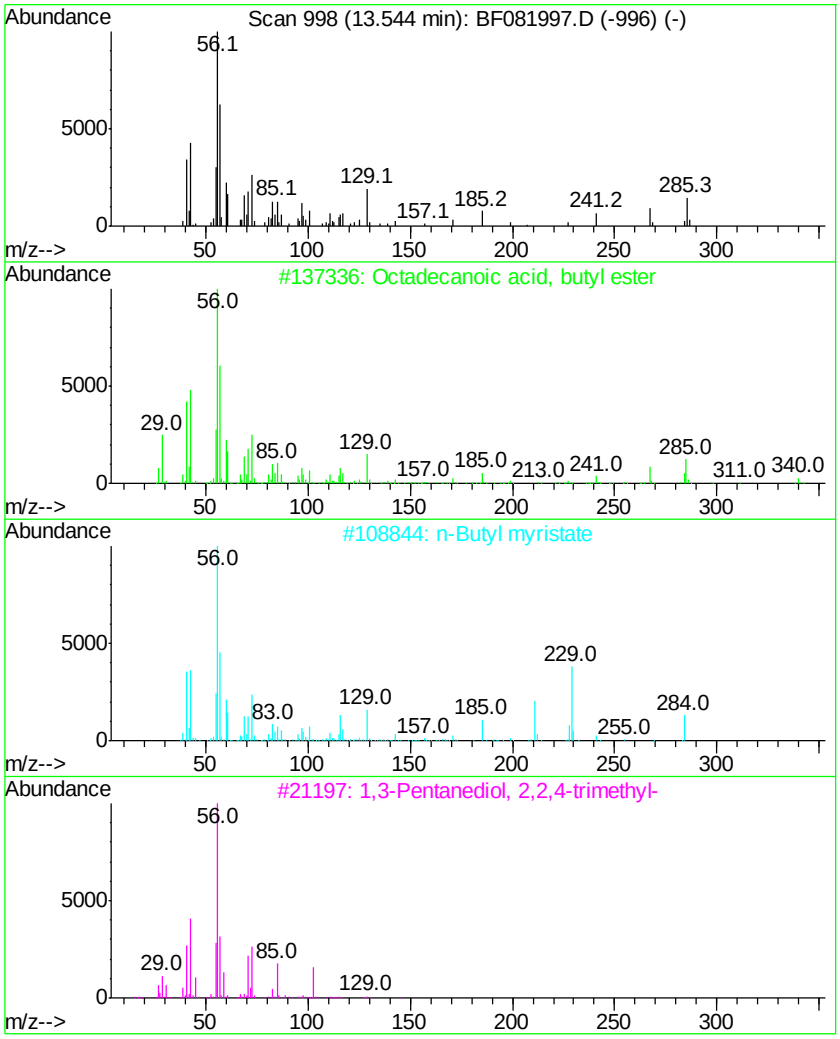
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

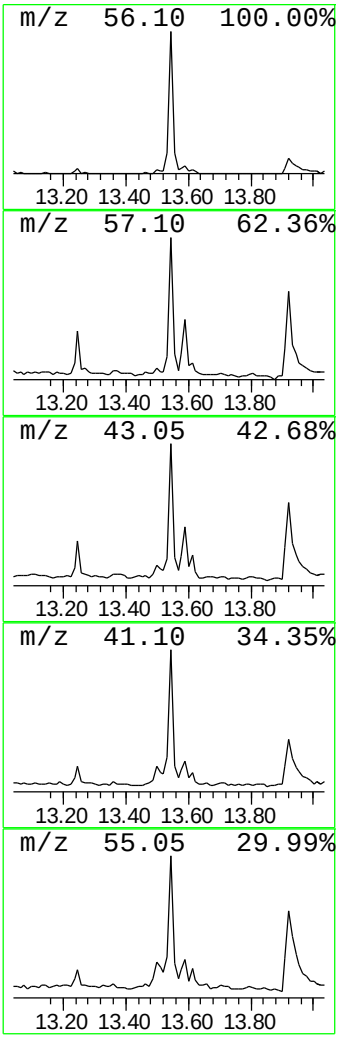
****

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	2.36 ng	132878	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2	n-Butyl myristate	284	C18H36O2	000110-36-1	64
3	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	37
4	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
5	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35





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Operator : UM/IZ
Sample : G3887-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OS-SB-25(55-57)

Quant Method : H:\HPCHEM1\BNA_F\Method\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

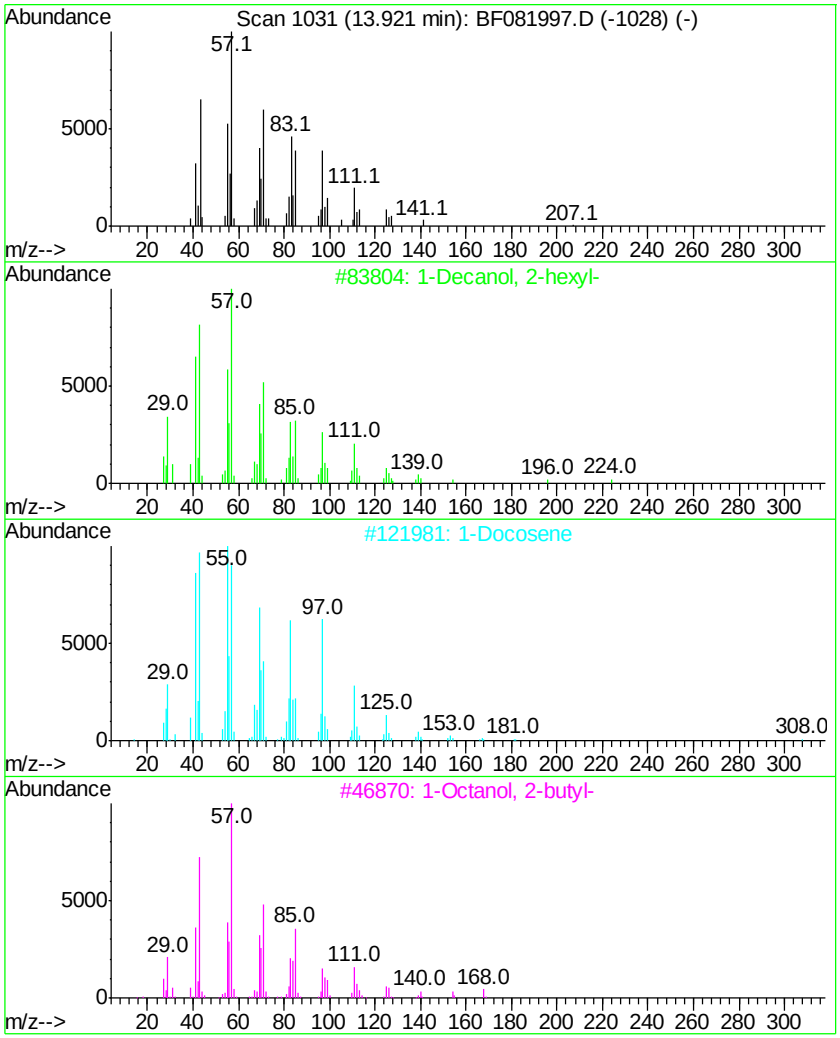
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

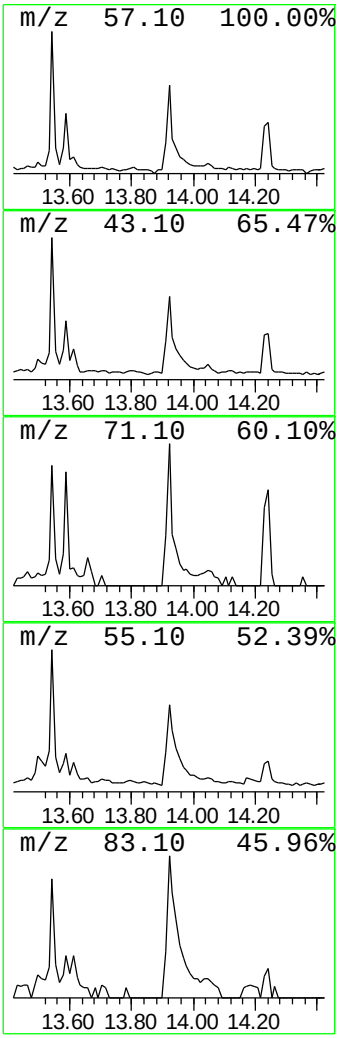
****

Peak Number 7 1-Decanol, 2-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	2.75 ng	154711	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	72
2	1-Docosene	308	C22H44	001599-67-3	70
3	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	64
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	62
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	62





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Operator : UM/IZ
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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OS-SB-25(55-57)

Quant Method : H:\HPCHEM1\BNA_F\Method\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

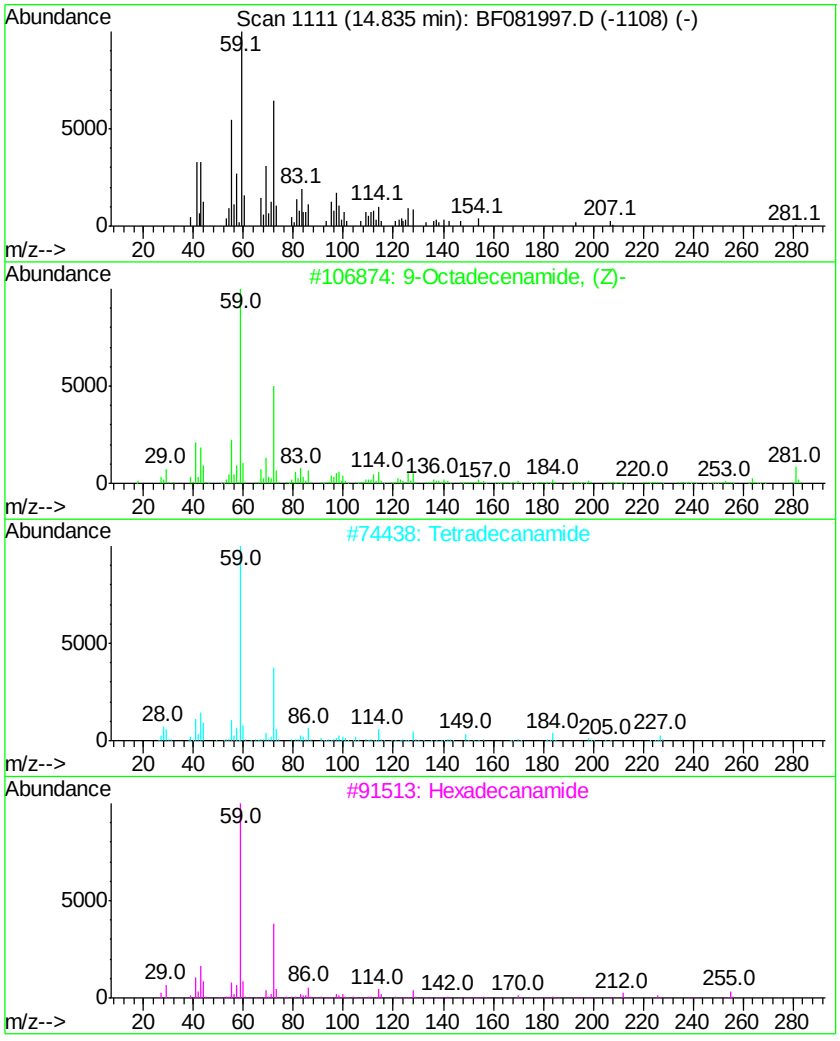
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

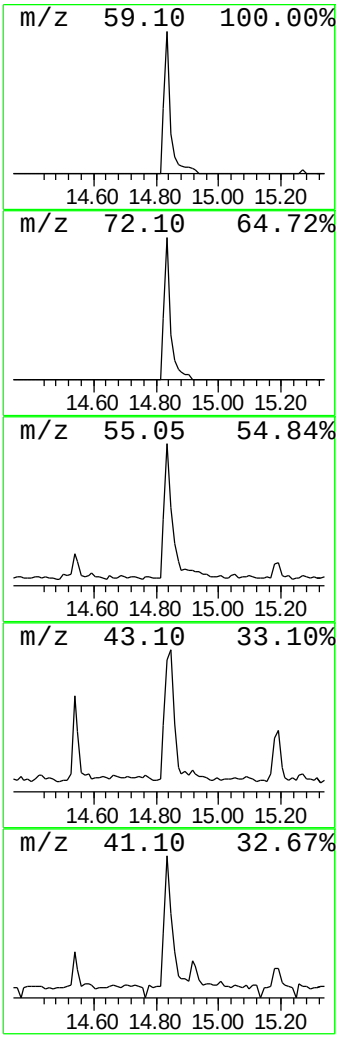
****

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	3.50 ng	162294	Perylene-d12	15.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
2	Tetradecanamide	227	C14H29NO	000638-58-4	59
3	Hexadecanamide	255	C16H33NO	000629-54-9	53
4	Dodecanamide	199	C12H25NO	001120-16-7	53
5	7-Nonenamide	155	C9H17NO	090949-53-4	53





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	5.07	48.8	ng	1405790	1	6.89	575802	20.0
unknown6.65	6.65	86.5	ng	2491920	1	6.89	575802	20.0
Tetradecanoic acid	11.95	3.1	ng	151678	4	11.43	987355	20.0
Hexadecanoic acid...	12.84	3.2	ng	179979	5	14.07	1124430	20.0
Octadecanoic acid...	13.54	2.4	ng	132878	5	14.07	1124430	20.0
1-Decanol, 2-hexyl-	13.92	2.8	ng	154711	5	14.07	1124430	20.0
9-Octadecenamide,...	14.84	3.5	ng	162294	6	15.53	927980	20.0