LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011016\
Data File : BF084364.D
Acq On : 10 Jan 2016 14:55
Operator : SJ/UM
Sample : H1043-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1COMP

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-BF123115.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	5.047	257	259	269	rVB	1426350	2344046	27.10%	3.117%
2	5.481	294	297	299	rBV	7043889	8630405	99.78%	11.475%
3	6.510	384	387	389	rBV	6764615	7736476	89.45%	10.286%
4	6.636	395	398	400	rBV	7230365	8649249	100.00%	11.500%
5	6.853	415	417	420	rBV	2201722	1830454	21.16%	2.434%
6	7.013	428	431	433	rBV	6611105	5897534	68.19%	7.841%
7	7.425	464	467	469	rBV	4991362	5135283	59.37%	6.828%
8	7.539	475	477	482	rBV	158090	220541	2.55%	0.293%
9	8.145	527	530	532	rBV	2582357	2486363	28.75%	3.306%
10	9.219	621	624	627	rBV	7516772	7539155	87.17%	10.024%
11	9.619	656	659	661	rBV	2347180	2166649	25.05%	2.881%
12	9.893	681	683	686	rBV	2744293	2547848	29.46%	3.388%
13	10.328	717	721	723	rVB3	119699	152991	1.77%	0.203%
14	10.545	737	740	744	rBV	44536	88165	1.02%	0.117%
15	10.682	750	752	755	rBV2	3842660	5315922	61.46%	7.068%
16	10.808	760	763	769	rVB2	142100	257286	2.97%	0.342%
17	11.254	800	802	803	rBV	149201	133575	1.54%	0.178%
18	11.379	811	813	815	rBV	2846354	2411960	27.89%	3.207%
19	12.797	934	937	939	rBV	374500	404982	4.68%	0.538%
20	12.854	939	942	949	rVB2	244004	415065	4.80%	0.552%
21	12.968	949	952	955	rBV	6127793	6283790	72.65%	8.355%
22	13.494	996	998	1000	rBV2	241646	270246	3.12%	0.359%
23	13.871	1029	1031	1039	rBV	335047	558502	6.46%	0.743%
24	14.019	1041	1044	1046	rBV	1287938	1665526	19.26%	2.214%
25	14.191	1056	1059	1061	rBV	79301	87231	1.01%	0.116%
26	14.340	1070	1072	1074	rBV2	75608	94789	1.10%	0.126%
27	14.488	1083	1085	1090	rBV2	73432	110580	1.28%	0.147%
28	15.448	1166	1169	1171	rBV	982609	1371377	15.86%	1.823%
29	16.374	1248	1250	1256	rVB3	39391	99458	1.15%	0.132%
30	16.945	1297	1300	1304	rVB2	39741	92994	1.08%	0.124%
31	17.608	1355	1358	1363	rVB2	42721	121751	1.41%	0.162%
32	18.397	1425	1427	1433	rVB	31995	92155	1.07%	0.123%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011016\
Data File : BF084364.D
Acq On : 10 Jan 2016 14:55
Operator : SJ/UM
Sample : H1043-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1COMP

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-BF123115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

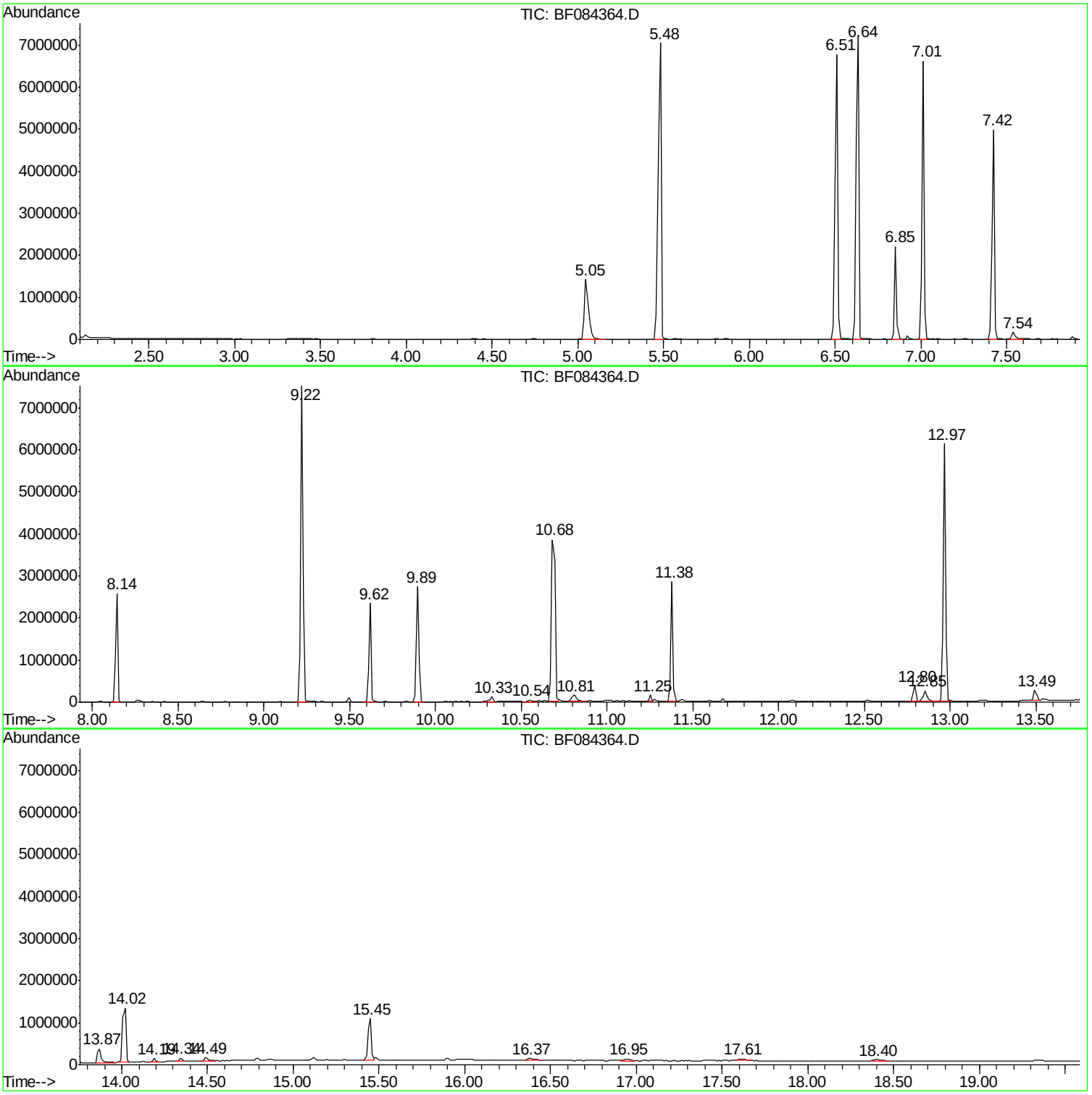
Sum of corrected areas: 75212348

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011016\
Data File : BF084364.D
Acq On : 10 Jan 2016 14:55
Operator : SJ/UM
Sample : H1043-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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\BF011016\
Data File : BF084364.D
Acq On : 10 Jan 2016 14:55
Operator : SJ/UM
Sample : H1043-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

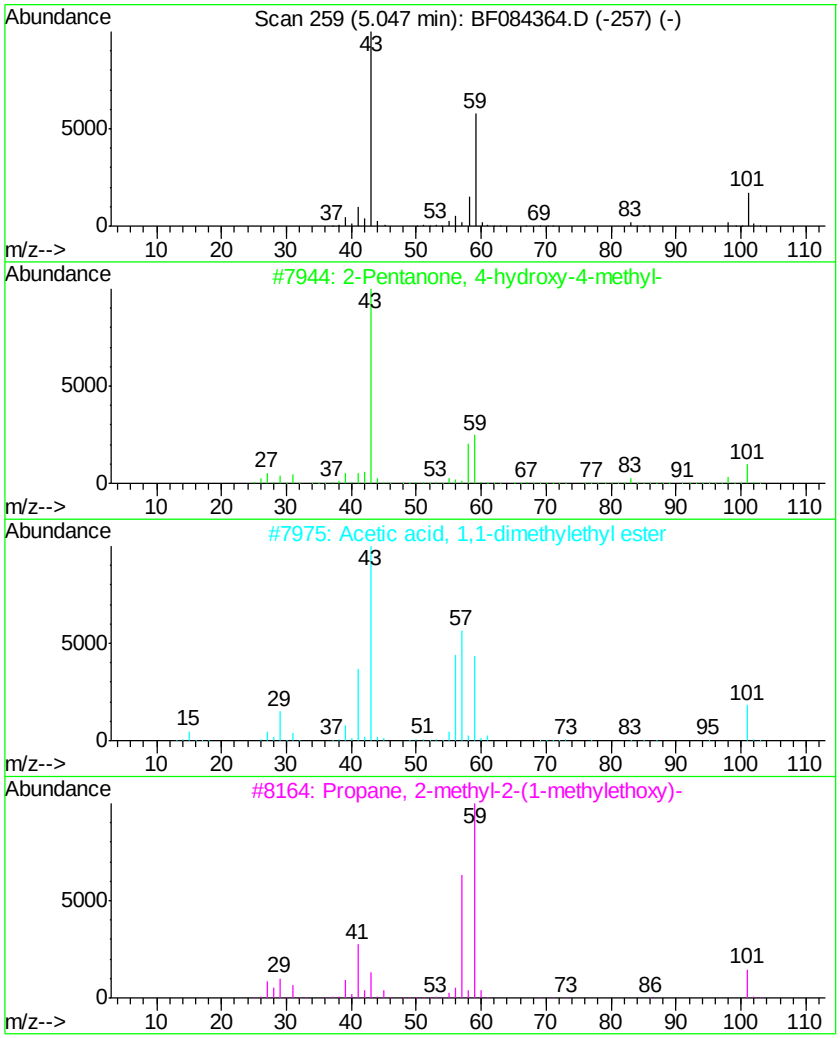
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

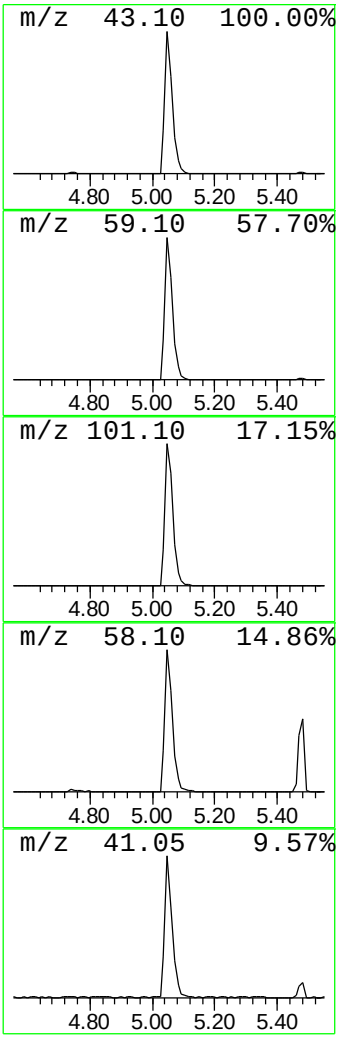
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	25.61 ng	2344050	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	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011016\
Data File : BF084364.D
Acq On : 10 Jan 2016 14:55
Operator : SJ/UM
Sample : H1043-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

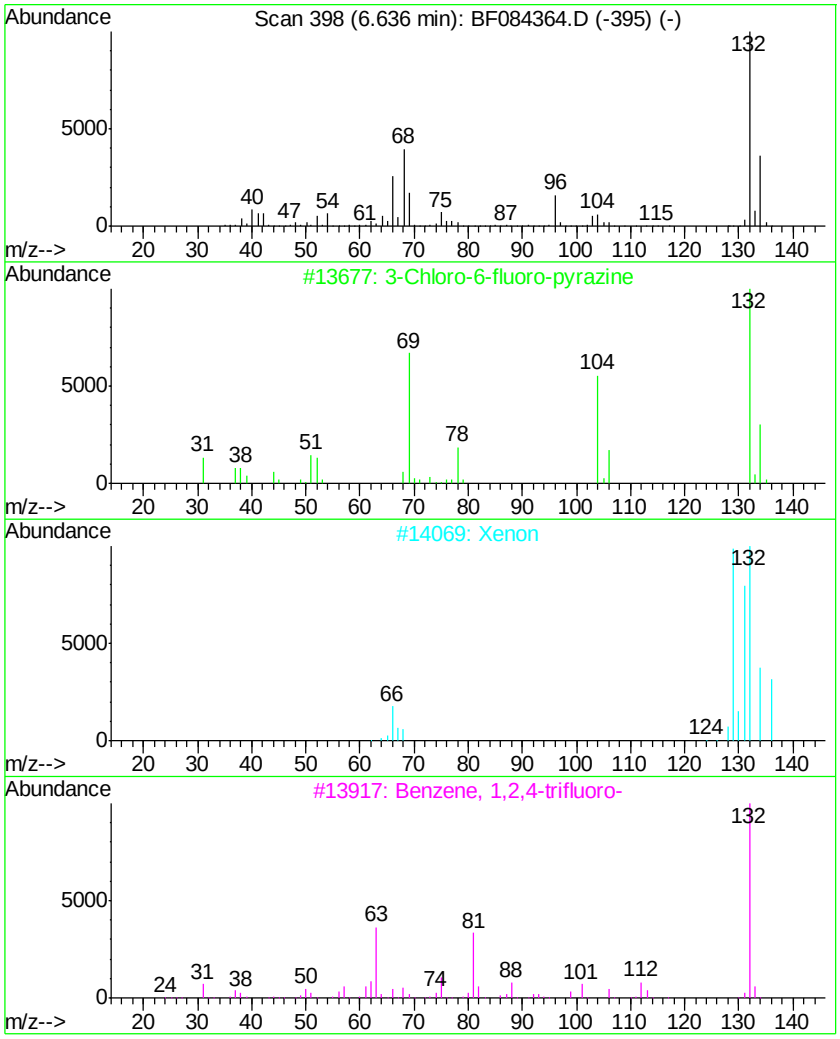
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

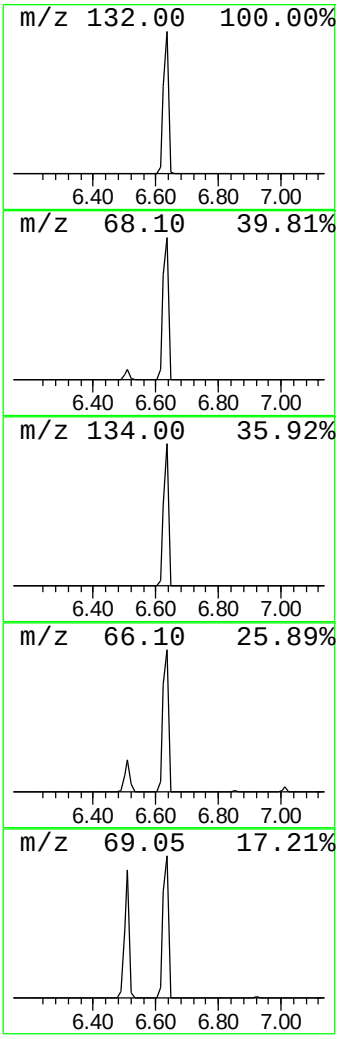
****

Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	94.50 ng	8649250	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Xenon	132	Xe	007440-63-3	9
3	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011016\
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Sample : H1043-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

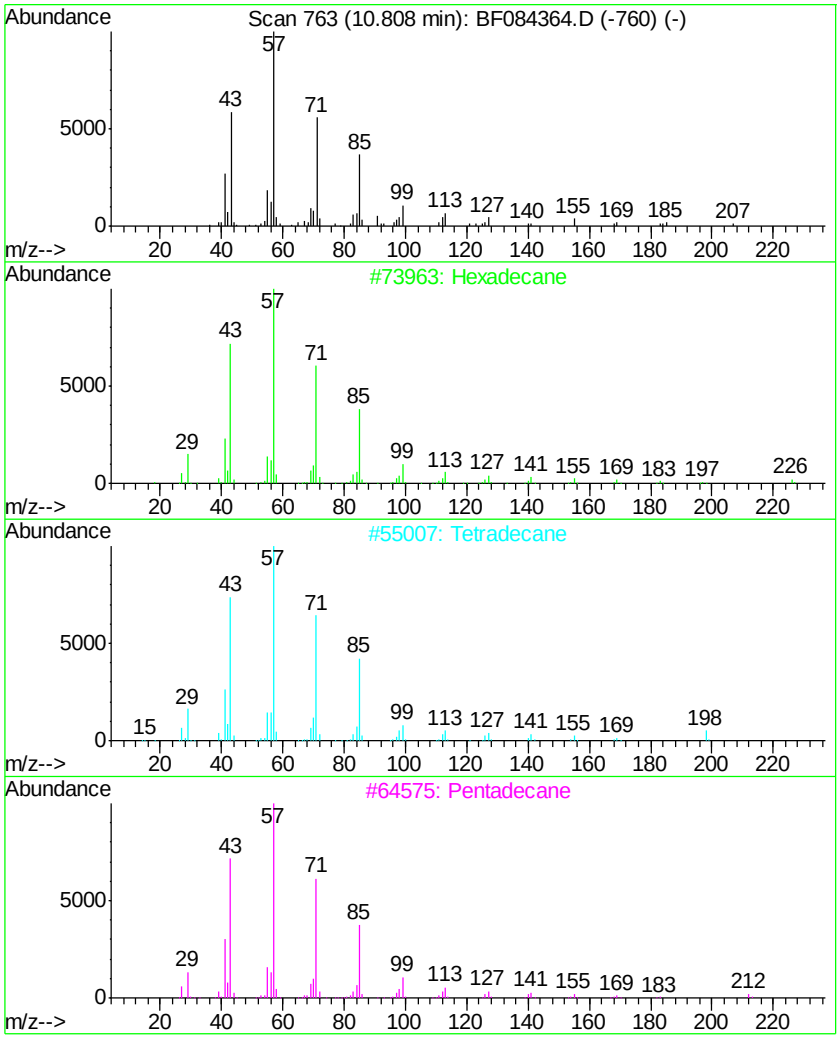
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

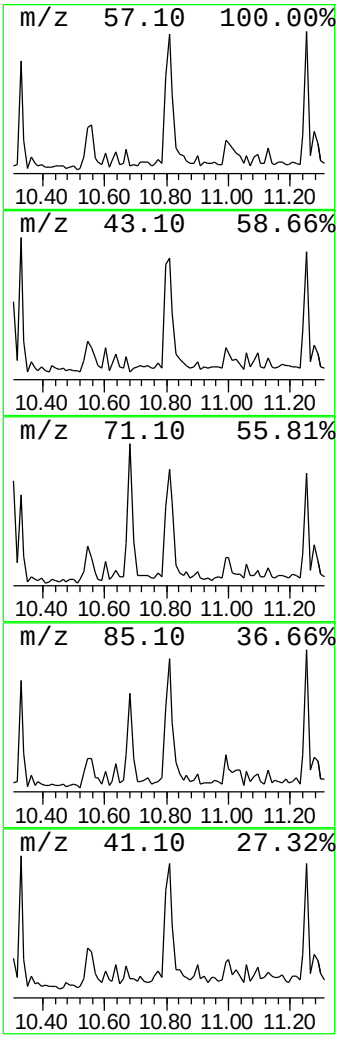
****

Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.81	2.13 ng	257286	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Tetradecane	198	C14H30	000629-59-4	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Eicosane	282	C20H42	000112-95-8	87
5	Heptacosane	380	C27H56	000593-49-7	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011016\
Data File : BF084364.D
Acq On : 10 Jan 2016 14:55
Operator : SJ/UM
Sample : H1043-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

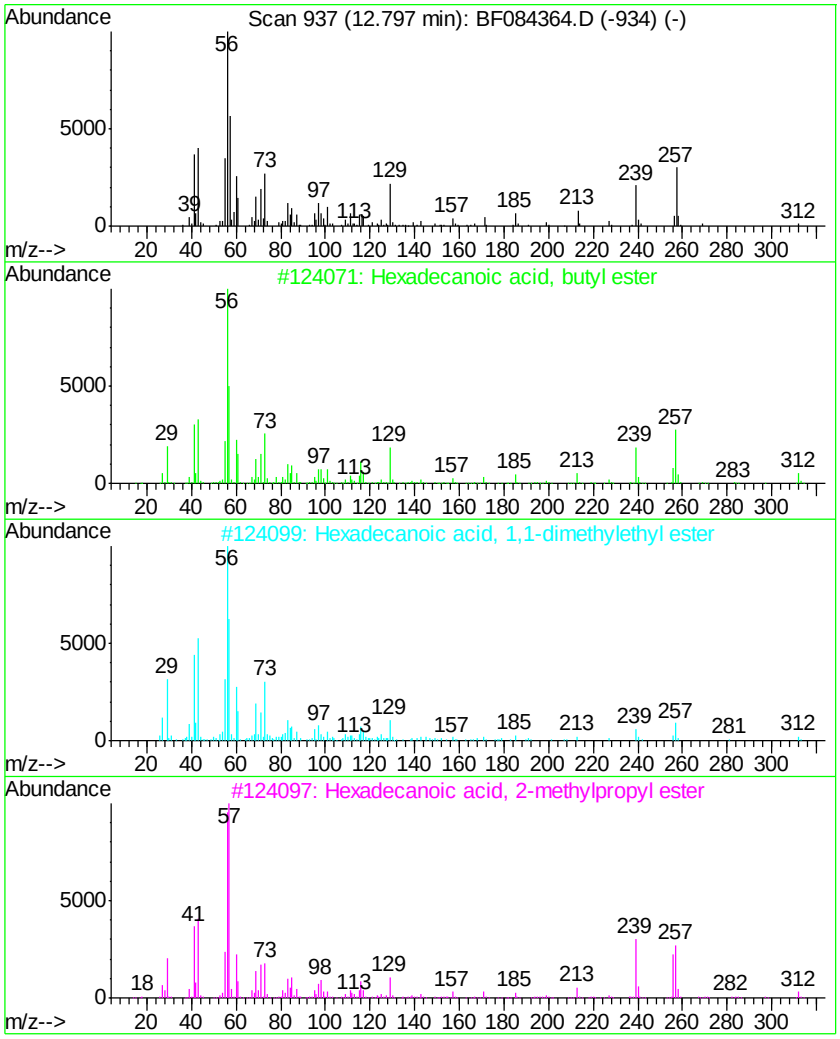
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

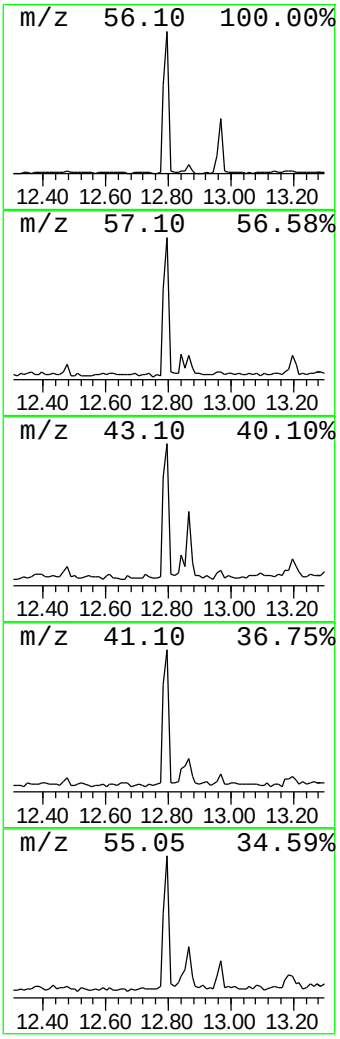
****

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	4.86 ng	404982	Chrysene-d12	14.02

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	64
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	38
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	27
5	2-Methyl-1-octadecene	266	C19H38	061868-20-0	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011016\
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Operator : SJ/UM
Sample : H1043-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

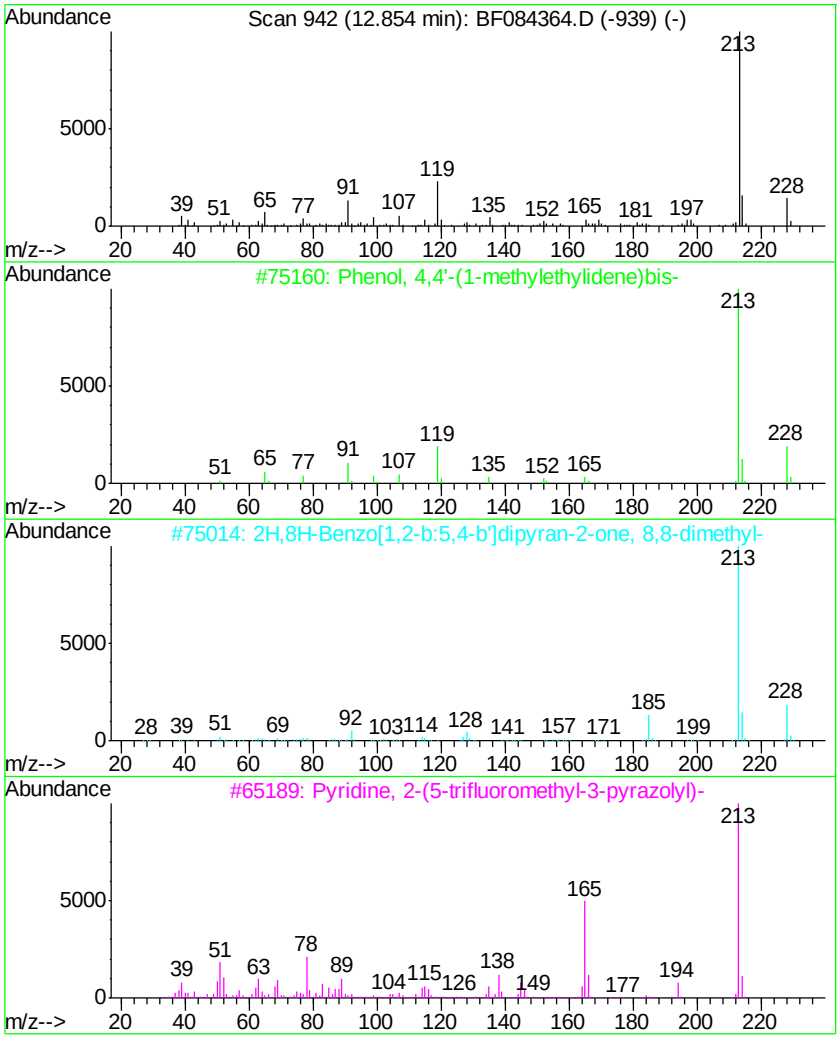
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

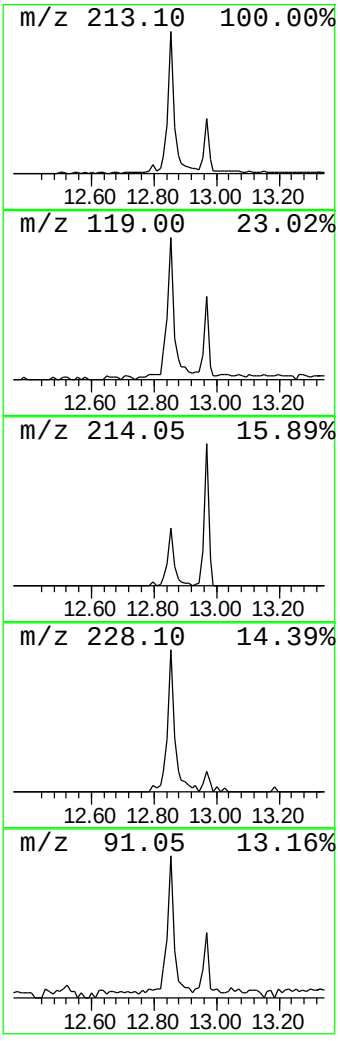
****

Peak Number 6 Phenol, 4,4'-(1-methylethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	4.98 ng	415065	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	91
2	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	58
3	Pyridine, 2-(5-trifluoromethyl-3...	213	C9H6F3N3	003974-71-8	53
4	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	50
5	4H-Pyrazolo[5,1-c]-1,4-benzodiaz...	213	C11H7N3O2	1000277-20-1	50





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Operator : SJ/UM
Sample : H1043-12
Misc :
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Instrument : BNA_F
ClientSampleId : SB-1COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

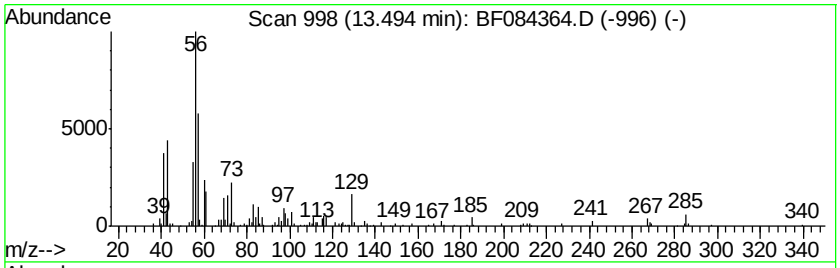
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

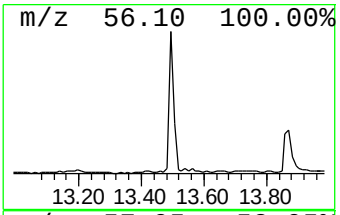
****

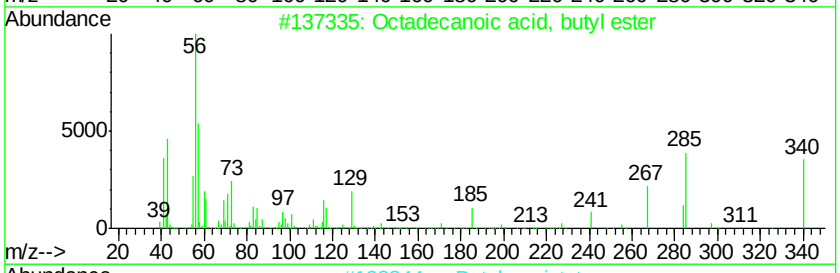
Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 7

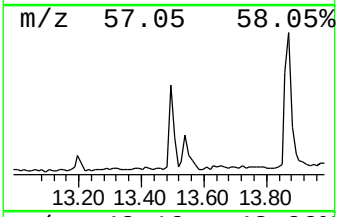
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	3.25 ng	270246	Chrysene-d12	14.02

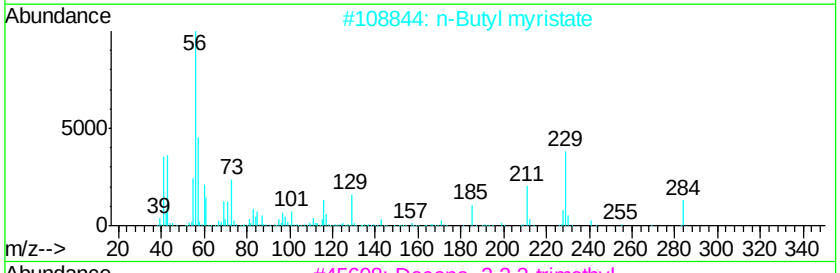
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	94
2	n-Butyl myristate	284	C18H36O2	000110-36-1	83
3	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	37
4	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	37
5	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	37

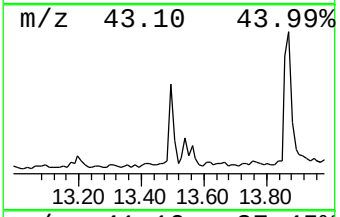


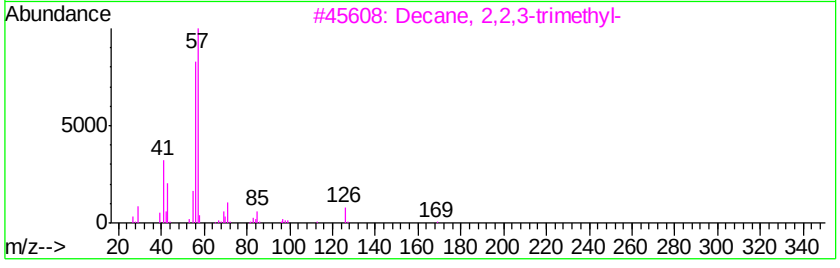


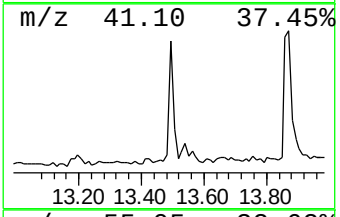


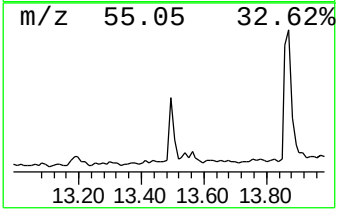












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Instrument : BNA_F
ClientSampleId : SB-1COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

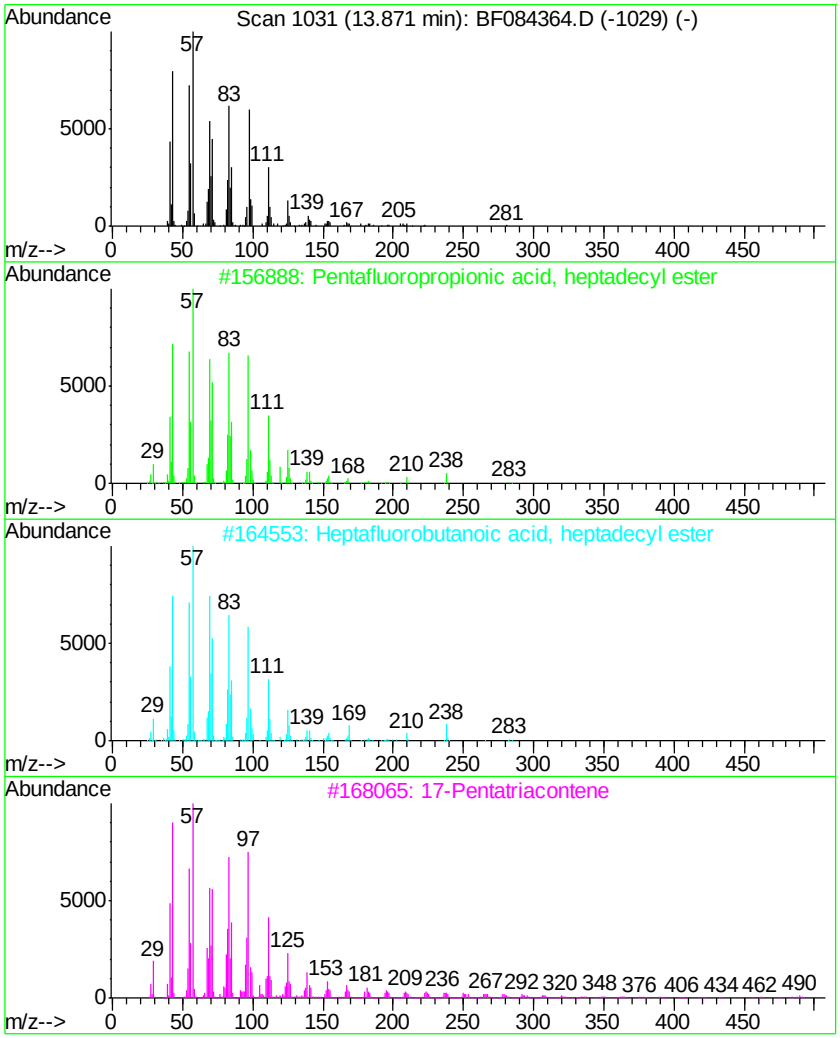
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

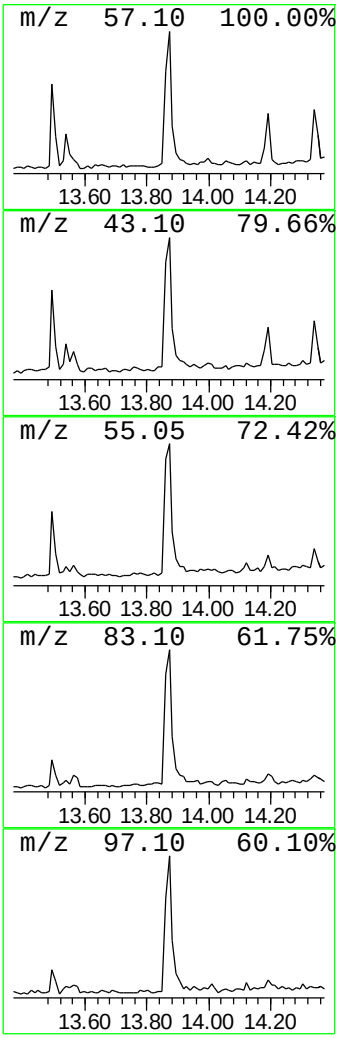
****

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	6.71 ng	558502	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	94
2	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
3	17-Pentatriacontene	491	C35H70	006971-40-0	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011016\
Data File : BF084364.D
Acq On : 10 Jan 2016 14:55
Operator : SJ/UM
Sample : H1043-12
Misc :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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
2-Pentanone, 4-hy...	5.05	25.6	ng	2344050	1	6.85	1830450	20.0
unknown6.64	6.64	94.5	ng	8649250	1	6.85	1830450	20.0
Hexadecane	10.81	2.1	ng	257286	4	11.38	2411960	20.0
Hexadecanoic acid...	12.80	4.9	ng	404982	5	14.02	1665530	20.0
Phenol, 4,4'-(1-m...	12.85	5.0	ng	415065	5	14.02	1665530	20.0
Octadecanoic acid...	13.49	3.3	ng	270246	5	14.02	1665530	20.0
Pentafluoropropio...	13.87	6.7	ng	558502	5	14.02	1665530	20.0