LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089259.D
Acq On : 24 Jul 2016 4:34
Operator : UM/SJ
Sample : H4151-04
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-COMP

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-BF072016.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	1.712	9	11	49	rVB	615333	1281936	74.05%	9.202%
2	4.718	271	274	284	rBV	40330	80703	4.66%	0.579%
3	5.164	311	313	332	rBV	1183320	1480155	85.50%	10.625%
4	6.239	404	407	414	rBV	1193481	1514394	87.48%	10.870%
5	6.353	414	417	419	rBV	1142923	1489433	86.04%	10.691%
6	6.582	434	437	448	rBV	197612	244306	14.11%	1.754%
7	6.730	448	450	453	rBV	1006369	1096017	63.31%	7.867%
8	7.153	484	487	505	rBV	817296	1032570	59.65%	7.412%
9	7.862	547	549	560	rBV	362947	368226	21.27%	2.643%
10	8.947	641	644	646	rBV	1586269	1731155	100.00%	12.426%
11	9.336	676	678	681	rBV	177151	205623	11.88%	1.476%
12	9.610	700	702	704	rBV	387167	375041	21.66%	2.692%
13	10.399	768	771	773	rBV	643877	819809	47.36%	5.885%
14	10.525	781	782	787	rVB	17935	26583	1.54%	0.191%
15	10.971	819	821	823	rBV	18071	18224	1.05%	0.131%
16	11.085	829	831	833	rBV	245537	296629	17.13%	2.129%
17	12.502	953	955	958	rBV	116793	131211	7.58%	0.942%
18	12.662	967	969	972	rBV	927187	965533	55.77%	6.931%
19	13.211	1014	1017	1019	rBV	71579	71957	4.16%	0.517%
20	13.256	1019	1021	1024	rVB2	10444	18590	1.07%	0.133%
21	13.577	1046	1049	1057	rBV	39213	70661	4.08%	0.507%
22	13.702	1057	1060	1065	rBV	221566	257292	14.86%	1.847%
23	13.897	1075	1077	1083	rVB	15352	17690	1.02%	0.127%
24	14.194	1099	1103	1110	rBV2	8912	27160	1.57%	0.195%
25	14.697	1145	1147	1150	rVB	9580	18349	1.06%	0.132%
26	15.040	1175	1177	1180	rBV	155918	228993	13.23%	1.644%
27	15.097	1180	1182	1186	rVB	15937	21326	1.23%	0.153%
28	15.451	1211	1213	1216	rBV	14242	19837	1.15%	0.142%
29	15.862	1246	1249	1254	rVB2	10176	22012	1.27%	0.158%

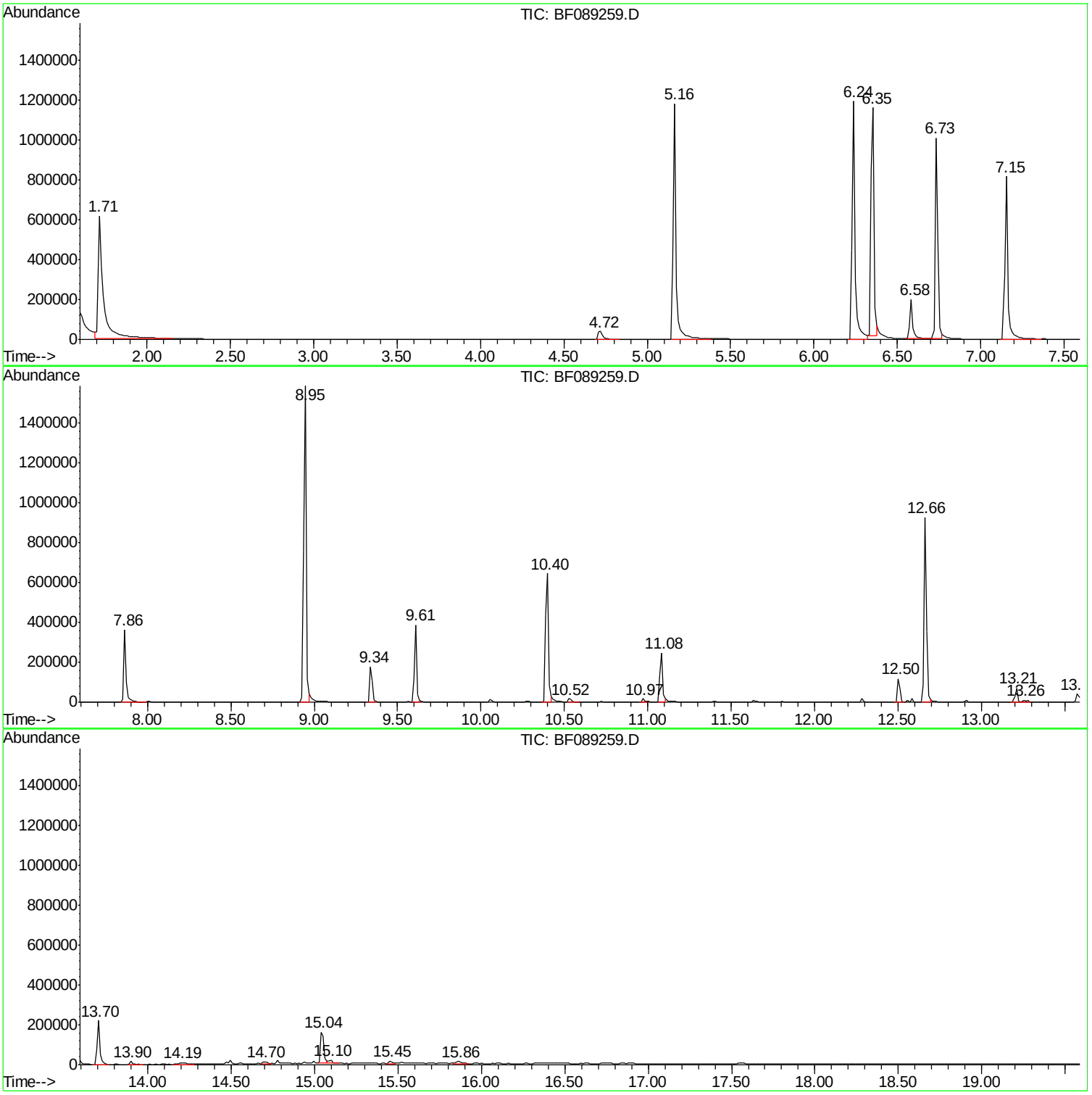
Sum of corrected areas: 13931415

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089259.D
Acq On : 24 Jul 2016 4:34
Operator : UM/SJ
Sample : H4151-04
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089259.D
Acq On : 24 Jul 2016 4:34
Operator : UM/SJ
Sample : H4151-04
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

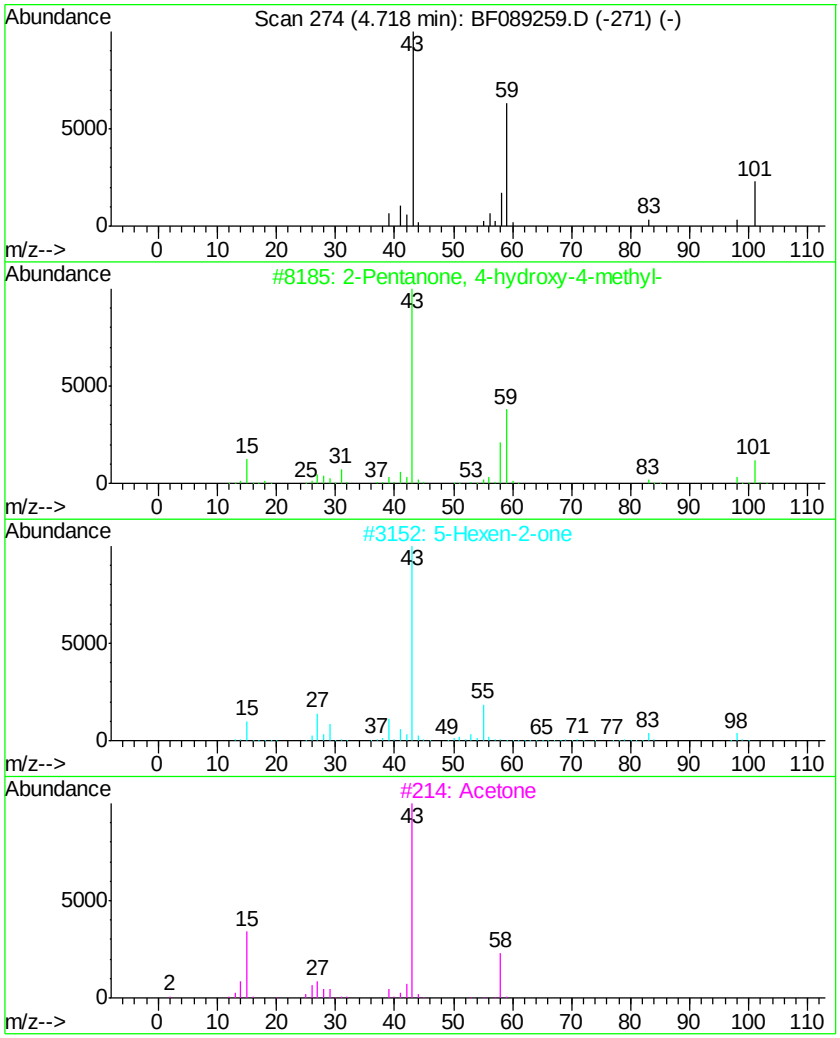
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

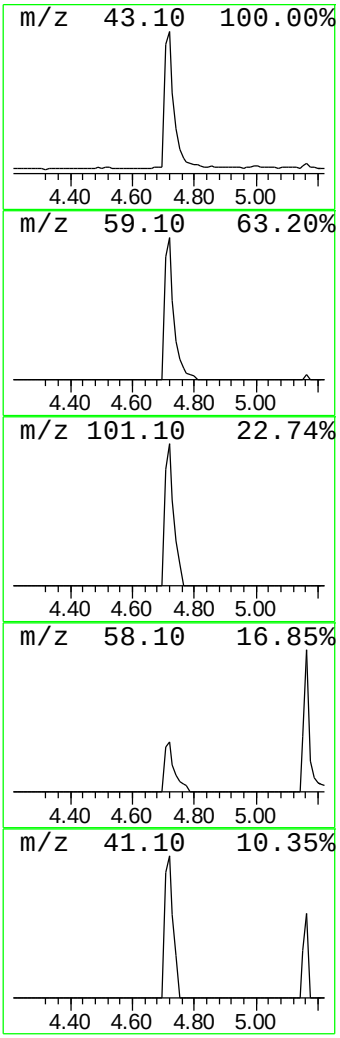
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	6.61 ng	80703	1,4-Dichlorobenzene-d4	6.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	Acetone	58	C3H6O	000067-64-1	9
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089259.D
Acq On : 24 Jul 2016 4:34
Operator : UM/SJ
Sample : H4151-04
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

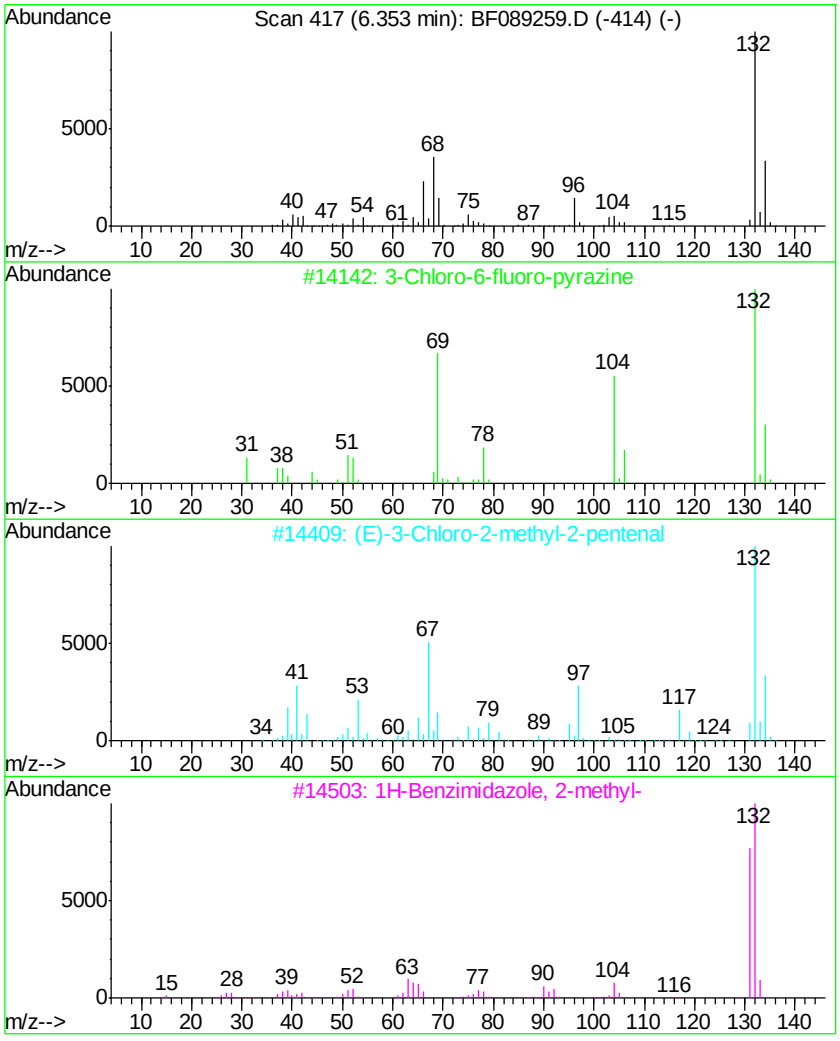
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

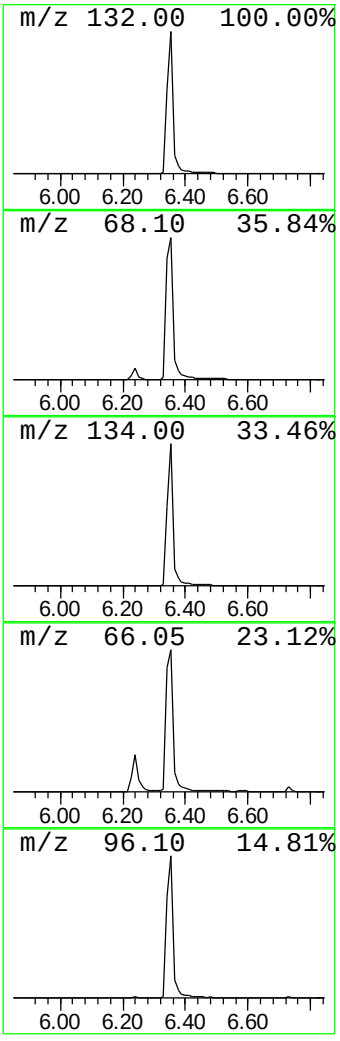
****

Peak Number 3 unknown6.35 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	121.93 ng	1489430	1,4-Dichlorobenzene-d4	6.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089259.D
Acq On : 24 Jul 2016 4:34
Operator : UM/SJ
Sample : H4151-04
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

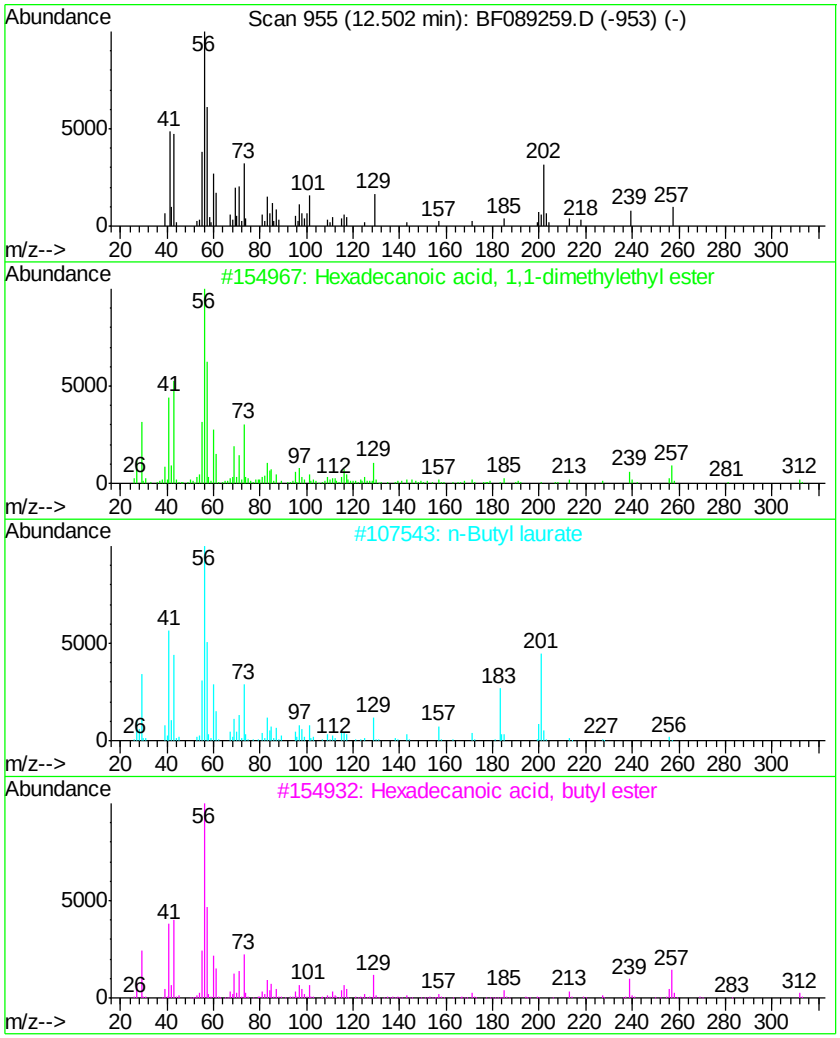
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

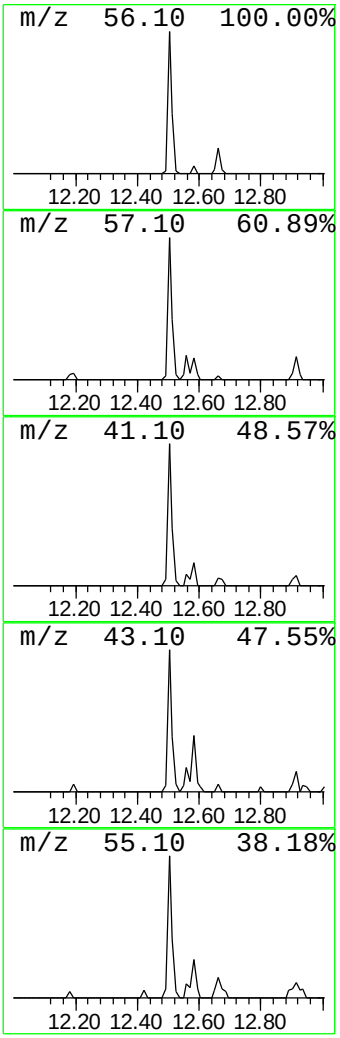
****

Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	10.20 ng	131211	Chrysene-d12	13.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
2	n-Butyl laurate	256	C16H32O2	000106-18-3	58
3	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	58
4	Dodecanoic acid, 1-methylpropyl ...	256	C16H32O2	006937-42-4	47
5	2-Methyl-1-tetradecene	210	C15H30	052254-38-3	35





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089259.D
Acq On : 24 Jul 2016 4:34
Operator : UM/SJ
Sample : H4151-04
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

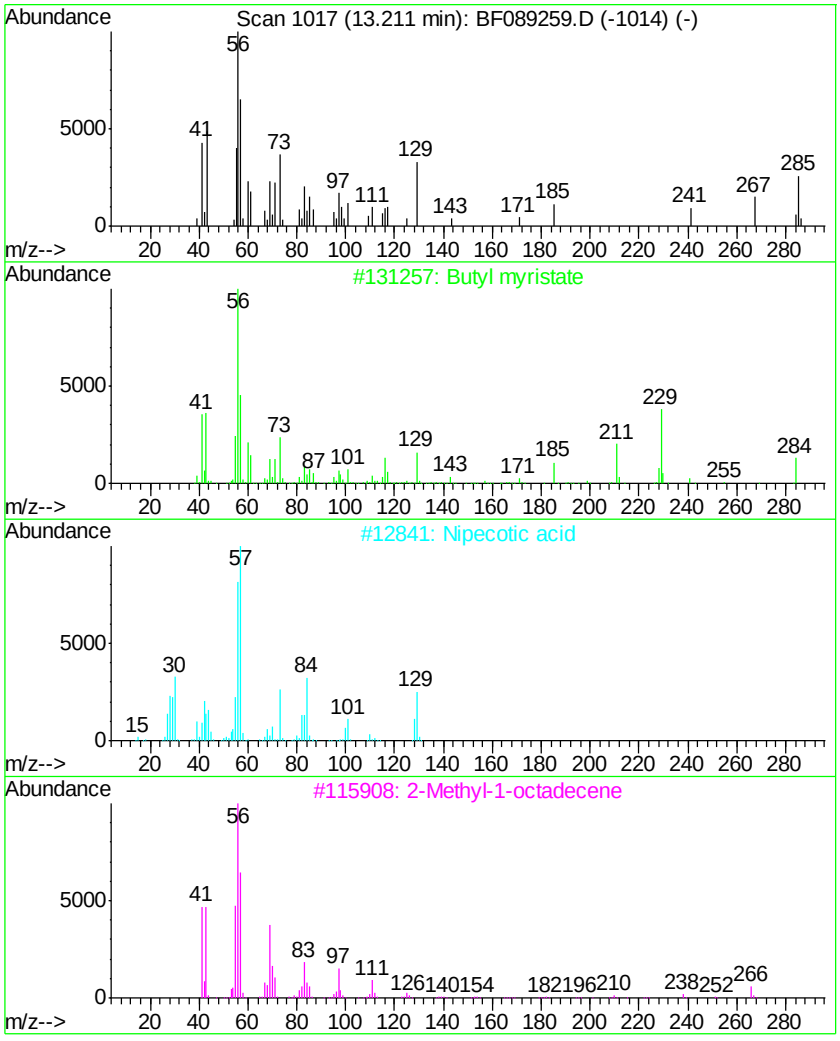
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

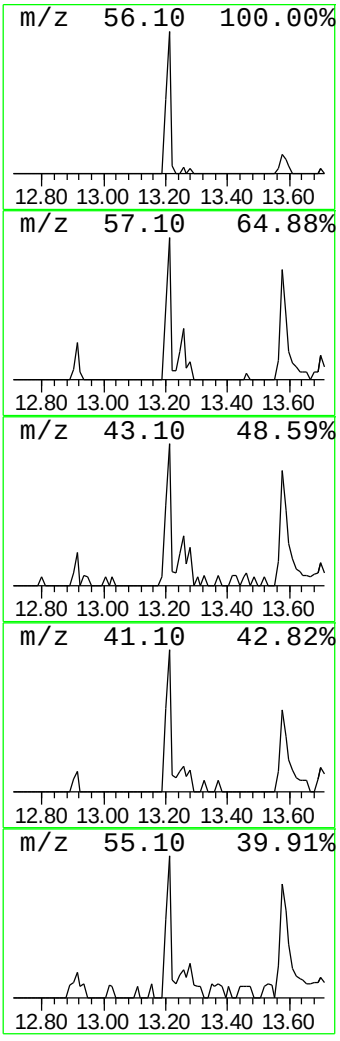
****

Peak Number 6 Butyl myristate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.21	5.59 ng	71957	Chrysene-d12	13.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	53
2	Nipecotic acid	129	C6H11NO2	000498-95-3	38
3	2-Methyl-1-octadecene	266	C19H38	061868-20-0	27
4	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089259.D
Acq On : 24 Jul 2016 4:34
Operator : UM/SJ
Sample : H4151-04
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

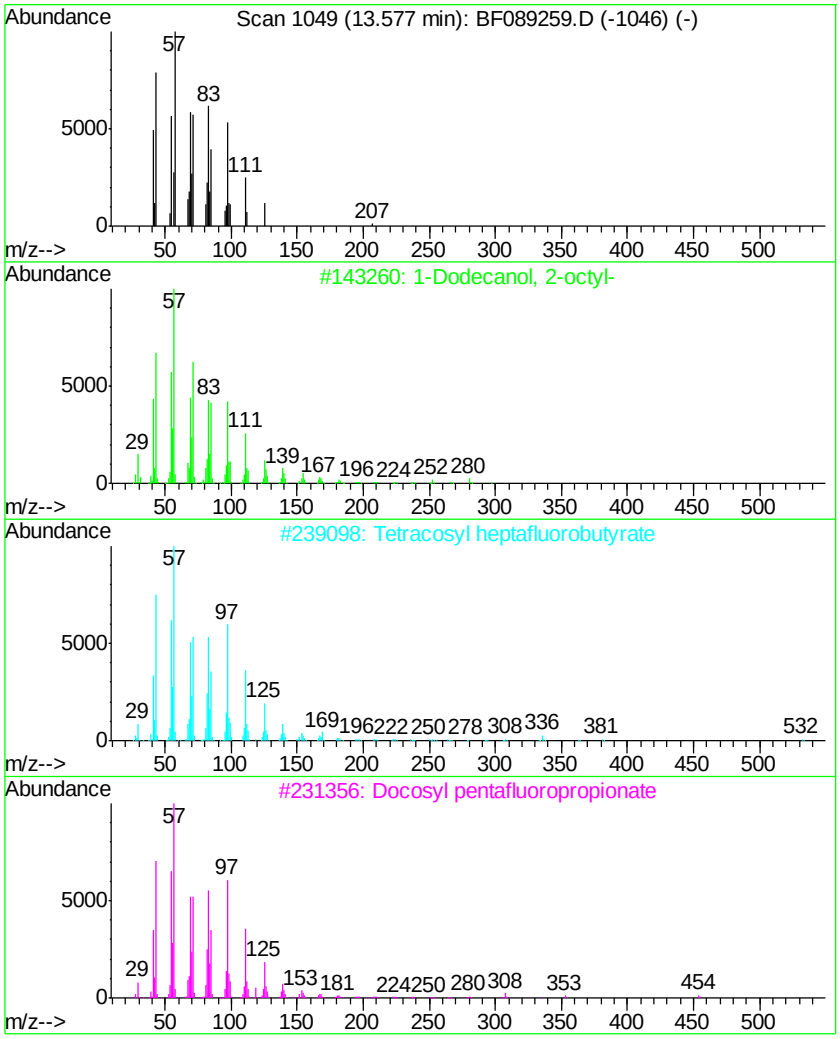
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

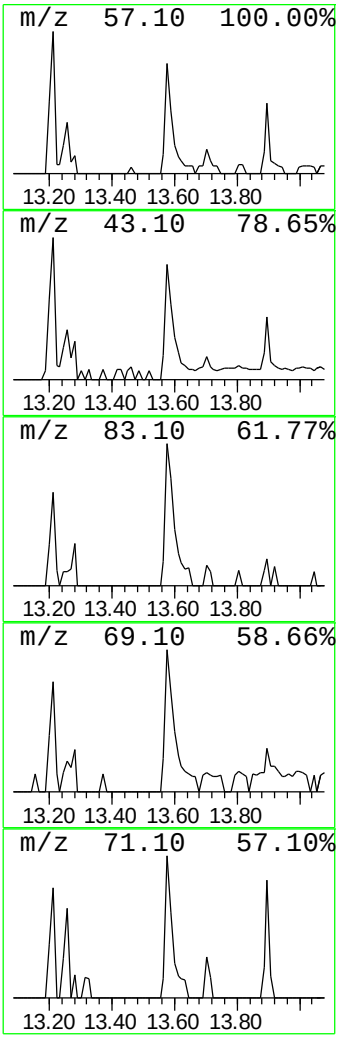
****

Peak Number 7 1-Dodecanol, 2-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.58	5.49 ng	70661	Chrysene-d12	13.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
2	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
4	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089259.D
Acq On : 24 Jul 2016 4:34
Operator : UM/SJ
Sample : H4151-04
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

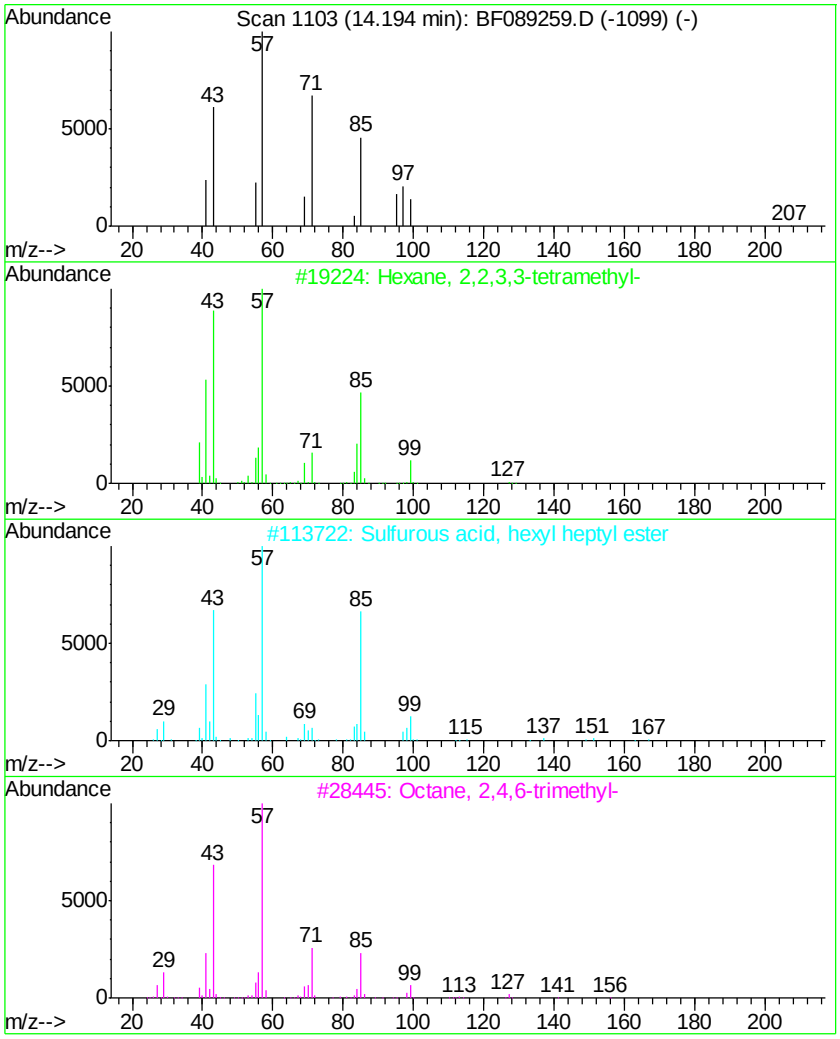
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

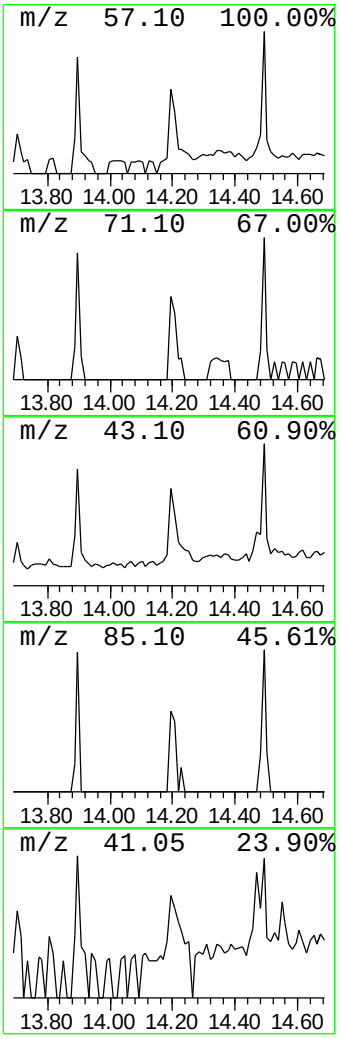
****

Peak Number 8 unknown14.19 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	2.11 ng	27160	Chrysene-d12	13.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2,3,3-tetramethyl-	142	C10H22	013475-81-5	38
2	Sulfurous acid, hexyl heptyl ester	264	C13H28O3S	1000309-12-9	37
3	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	33
4	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	9
5	Sulfurous acid, hexyl 2-pentyl e...	236	C11H24O3S	1000309-15-6	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089259.D
Acq On : 24 Jul 2016 4:34
Operator : UM/SJ
Sample : H4151-04
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
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
2-Pentanone, 4-hy...	4.72	6.6	ng	80703	1	6.58	244306	20.0
unknown6.35	6.35	121.9	ng	1489430	1	6.58	244306	20.0
Hexadecanoic acid...	12.50	10.2	ng	131211	5	13.70	257292	20.0
Butyl myristate	13.21	5.6	ng	71957	5	13.70	257292	20.0
1-Dodecanol, 2-oc...	13.58	5.5	ng	70661	5	13.70	257292	20.0
unknown14.19	14.19	2.1	ng	27160	5	13.70	257292	20.0