LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072516\
Data File : BF089279.D
Acq On : 25 Jul 2016 15:12
Operator : UM/SJ
Sample : H4129-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KSB-14-5.0-7.0

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	1.701	8	10	49	rVB	1254142	2667047	100.00%	16.806%
2	4.696	270	272	280	rBV	53989	96951	3.64%	0.611%
3	5.153	309	312	314	rBV	1206523	1505318	56.44%	9.486%
4	6.227	404	406	413	rBV	1213007	1573888	59.01%	9.918%
5	6.330	413	415	418	rBV	1246833	1481584	55.55%	9.336%
6	6.559	433	435	442	rBV	273634	317765	11.91%	2.002%
7	6.719	446	449	451	rBV	1328617	1252047	46.95%	7.890%
8	7.130	483	485	488	rBV	601645	910908	34.15%	5.740%
9	7.850	545	548	550	rBV	381293	420024	15.75%	2.647%
10	8.925	640	642	645	rBV	1381374	1469184	55.09%	9.258%
11	9.325	675	677	680	rBV	509716	489829	18.37%	3.087%
12	9.588	698	700	703	rBV	408418	416521	15.62%	2.625%
13	10.376	767	769	772	rBV	831739	840045	31.50%	5.293%
14	10.513	779	781	785	rVB	32259	47803	1.79%	0.301%
15	11.062	827	829	835	rBV	373661	364446	13.66%	2.297%
16	12.491	951	954	956	rBV	108546	97866	3.67%	0.617%
17	12.651	965	968	970	rBV	757213	1009389	37.85%	6.361%
18	13.188	1013	1015	1017	rBV	74012	60643	2.27%	0.382%
19	13.554	1044	1047	1051	rBV	71997	94163	3.53%	0.593%
20	13.679	1056	1058	1064	rBV	303615	311943	11.70%	1.966%
21	14.182	1099	1102	1105	rBV	22955	33686	1.26%	0.212%
22	14.594	1136	1138	1141	rVB	34405	34947	1.31%	0.220%
23	14.777	1150	1154	1157	rBV2	31753	73070	2.74%	0.460%
24	15.017	1173	1175	1178	rBV	172719	229533	8.61%	1.446%
25	15.428	1208	1211	1213	rBV	29735	43858	1.64%	0.276%
26	16.685	1318	1321	1327	rVB3	10658	27035	1.01%	0.170%

Sum of corrected areas: 15869493

LSC Report - Integrated Chromatogram

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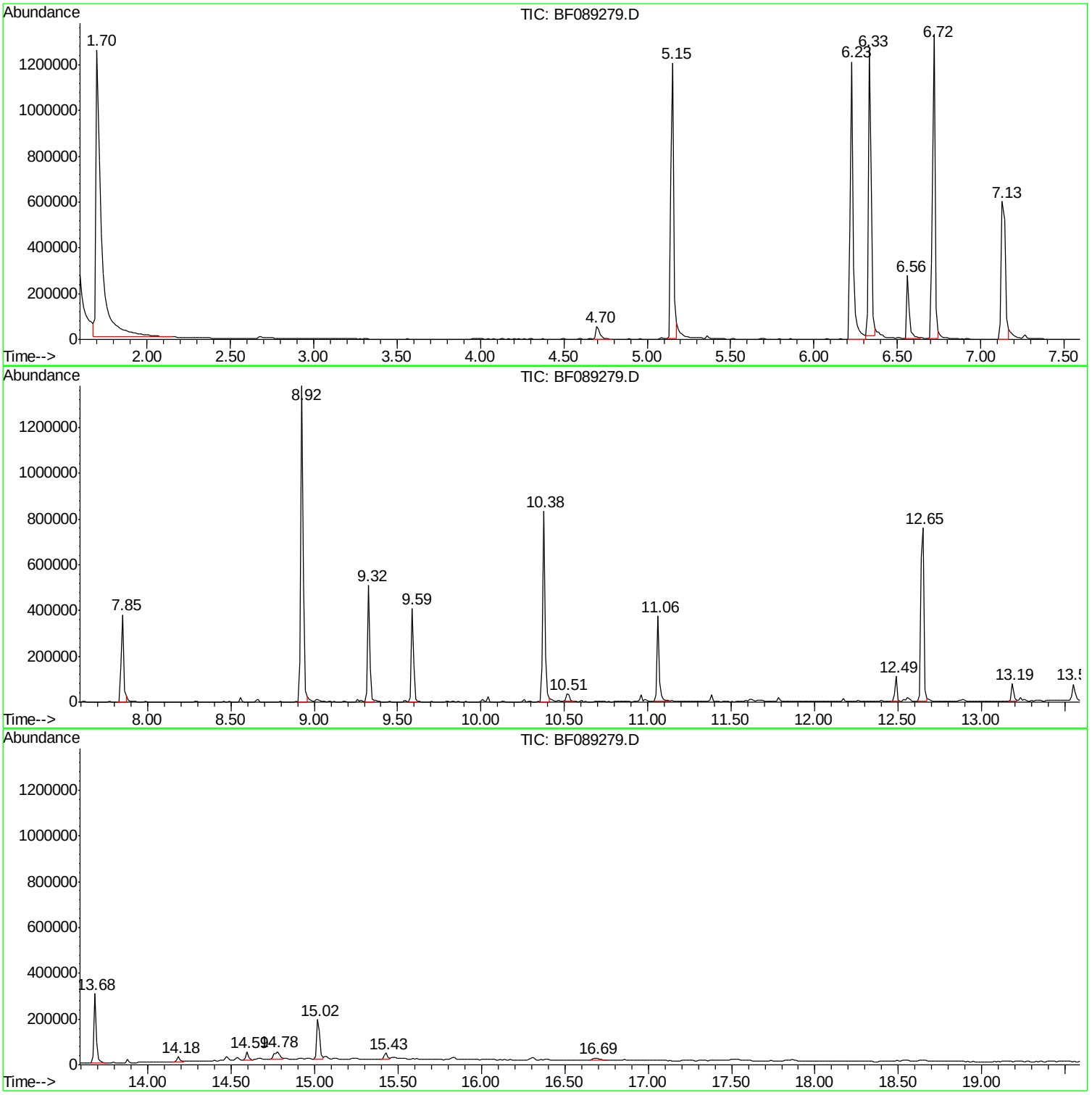
Operator : UM/SJ
Sample : H4129-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KSB-14-5.0-7.0

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\BF072516\
Data File : BF089279.D
Acq On : 25 Jul 2016 15:12
Operator : UM/SJ
Sample : H4129-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KSB-14-5.0-7.0

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

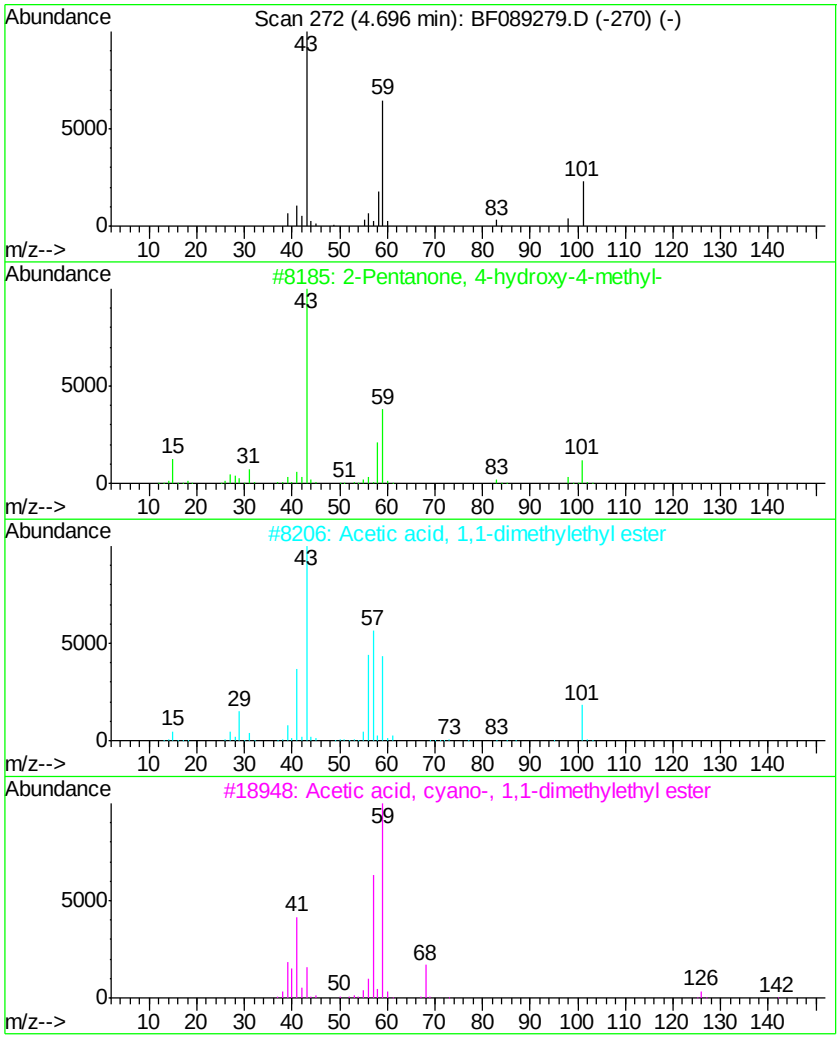
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

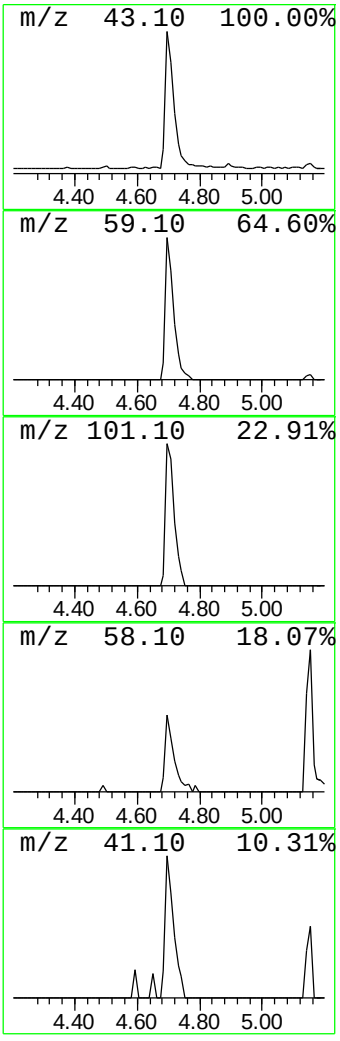
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	6.10 ng	96951	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072516\
Data File : BF089279.D
Acq On : 25 Jul 2016 15:12
Operator : UM/SJ
Sample : H4129-12
Misc :
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Instrument : BNA_F
ClientSampleId : KSB-14-5.0-7.0

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

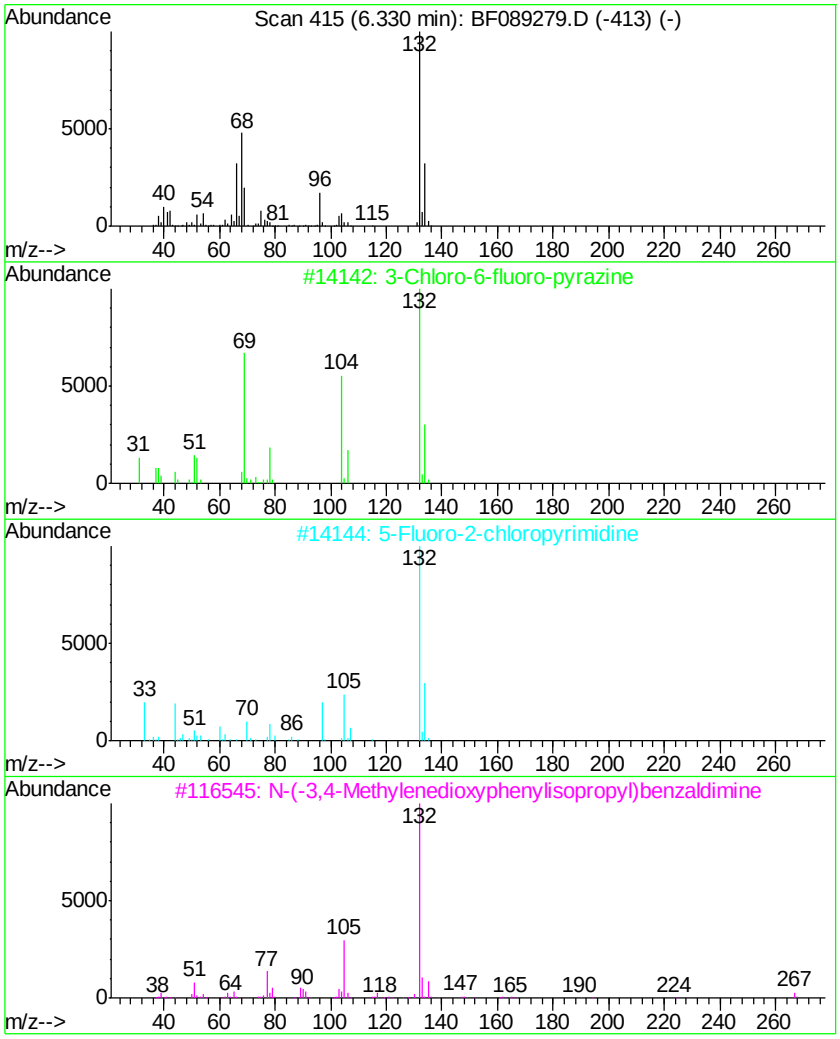
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

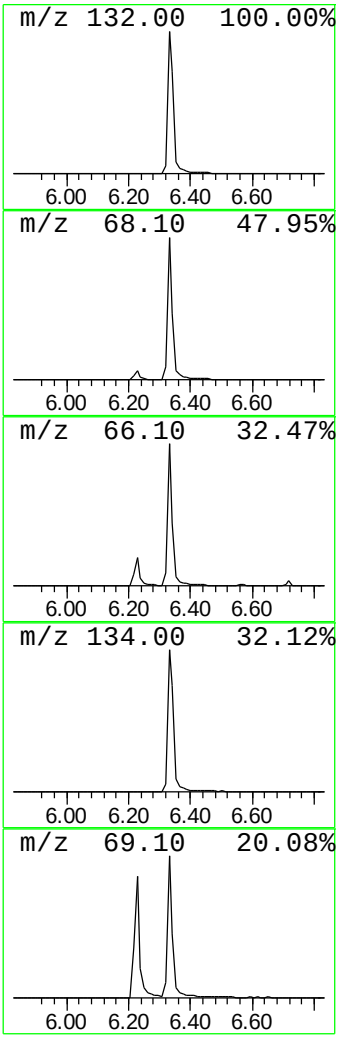
****

Peak Number 3 unknown6.33 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	93.25 ng	1481580	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072516\
Data File : BF089279.D
Acq On : 25 Jul 2016 15:12
Operator : UM/SJ
Sample : H4129-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KSB-14-5.0-7.0

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
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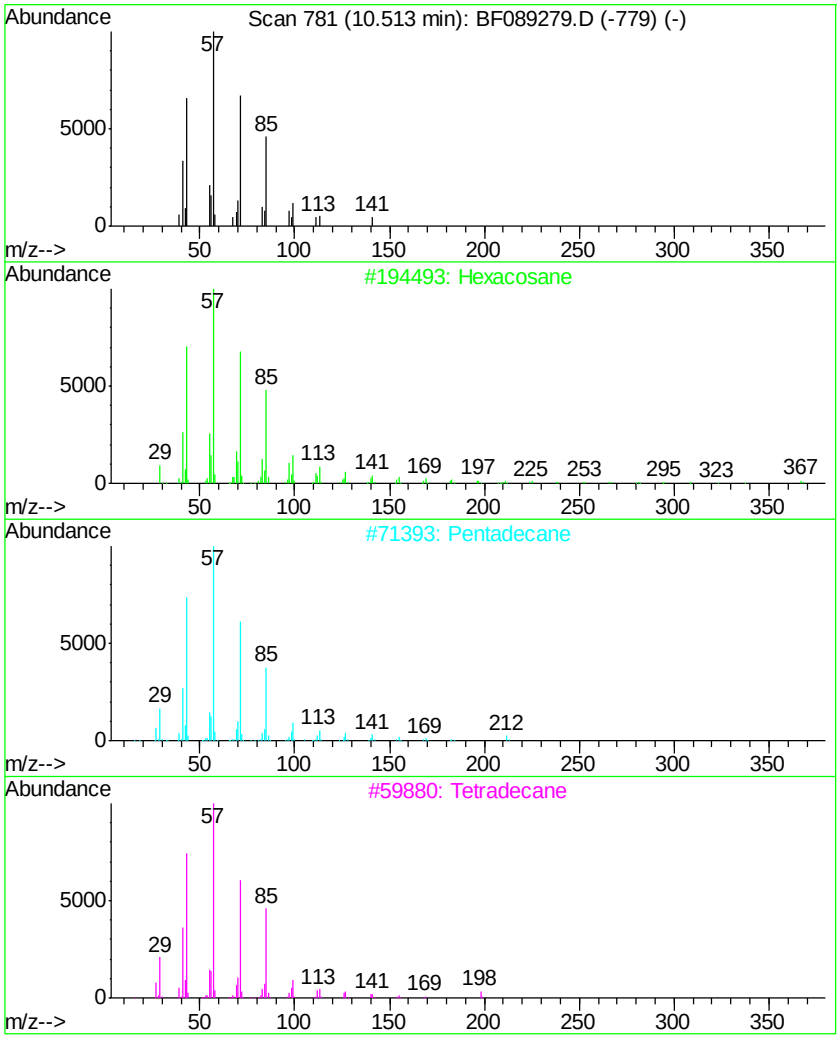
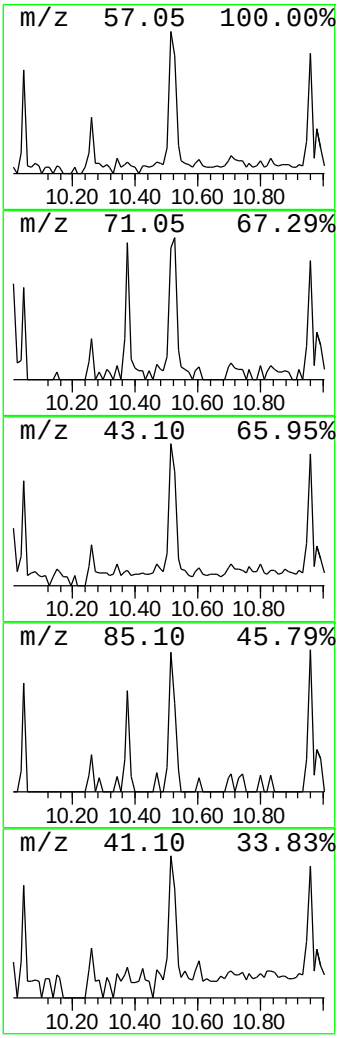
Peak Number 5 Hexacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.51	2.62 ng	47803	Phenanthrene-d10	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Pentadecane	212	C15H32	000629-62-9	86
3	Tetradecane	198	C14H30	000629-59-4	86
4	Nonadecane	268	C19H40	000629-92-5	86
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	83





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Operator : UM/SJ
Sample : H4129-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KSB-14-5.0-7.0

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

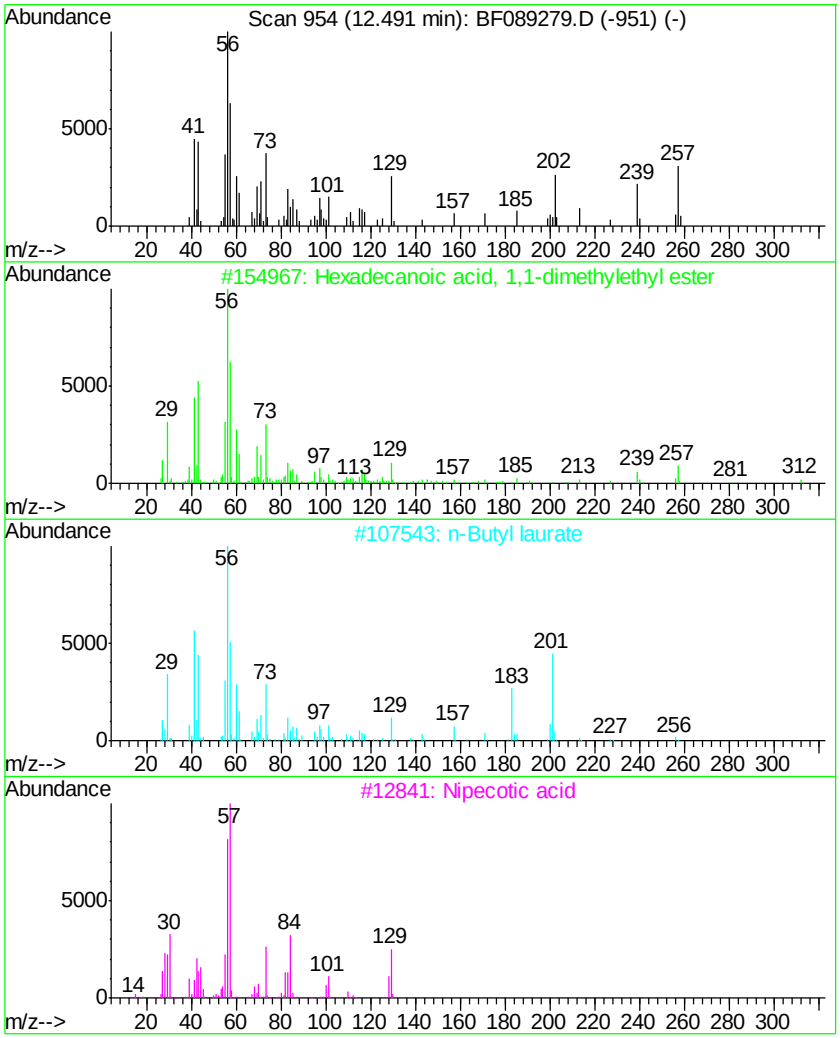
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

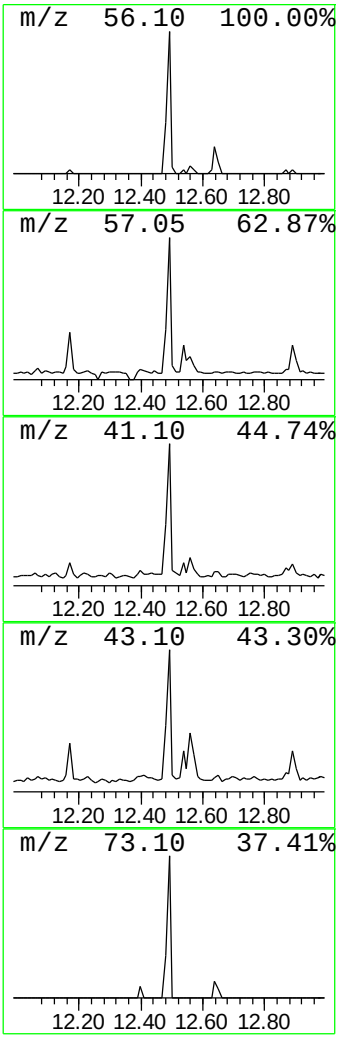
****

Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	6.27 ng	97866	Chrysene-d12	13.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	50
2	n-Butyl laurate	256	C16H32O2	000106-18-3	47
3	Nipecotic acid	129	C6H11NO2	000498-95-3	37
4	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	25
5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072516\
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Sample : H4129-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KSB-14-5.0-7.0

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

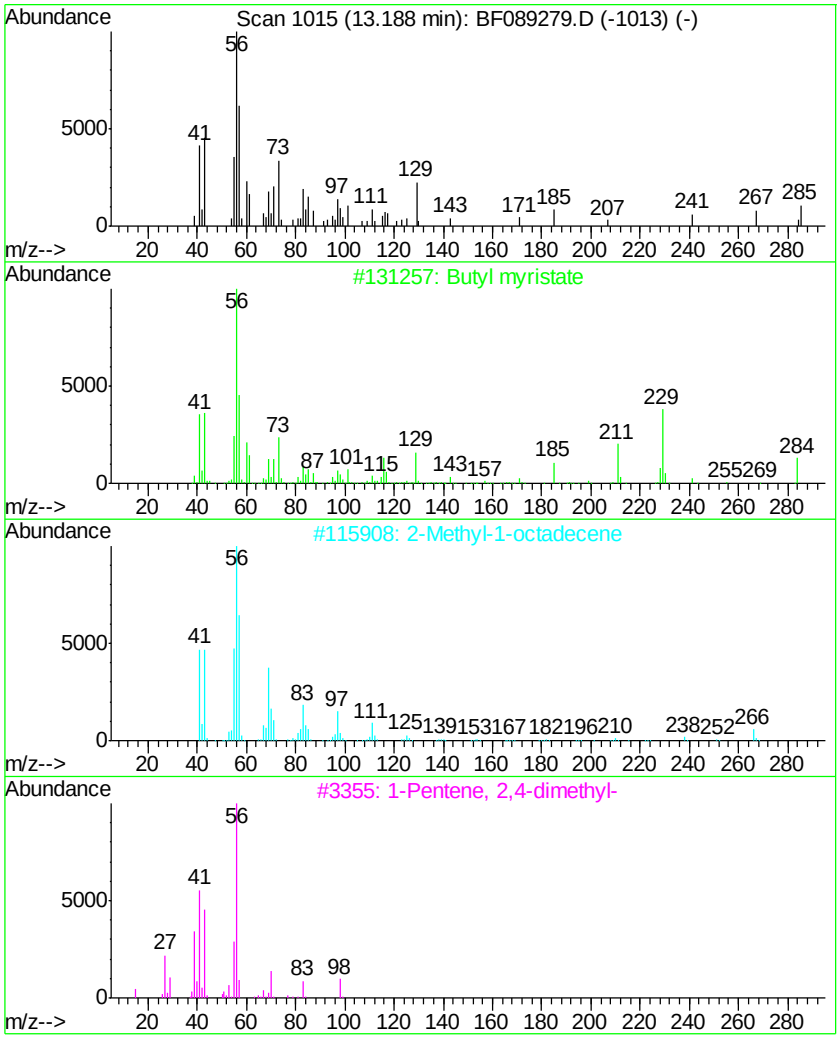
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

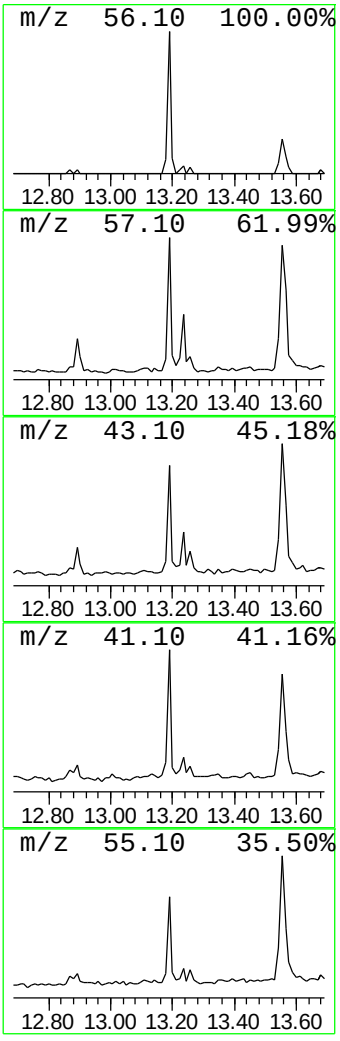
****

Peak Number 7 Butyl myristate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.19	3.89 ng	60643	Chrysene-d12	13.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	80
2	2-Methyl-1-octadecene	266	C19H38	061868-20-0	37
3	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	35
4	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	30
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	27





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Sample : H4129-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KSB-14-5.0-7.0

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

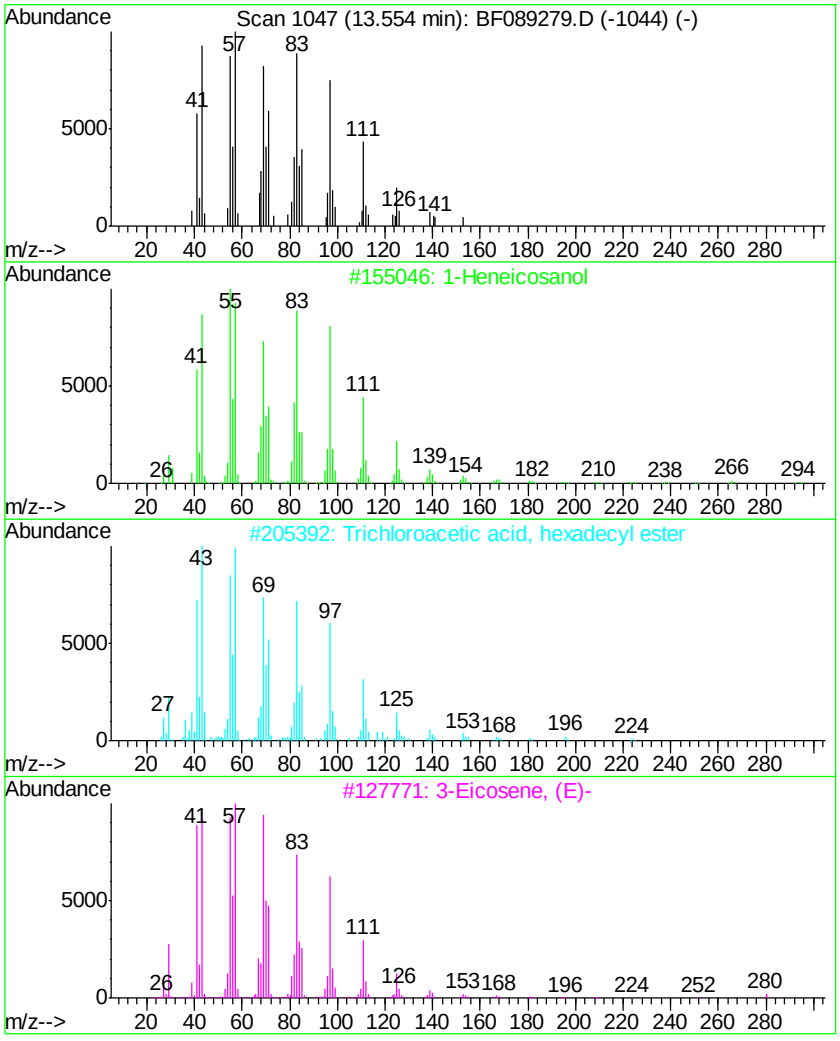
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

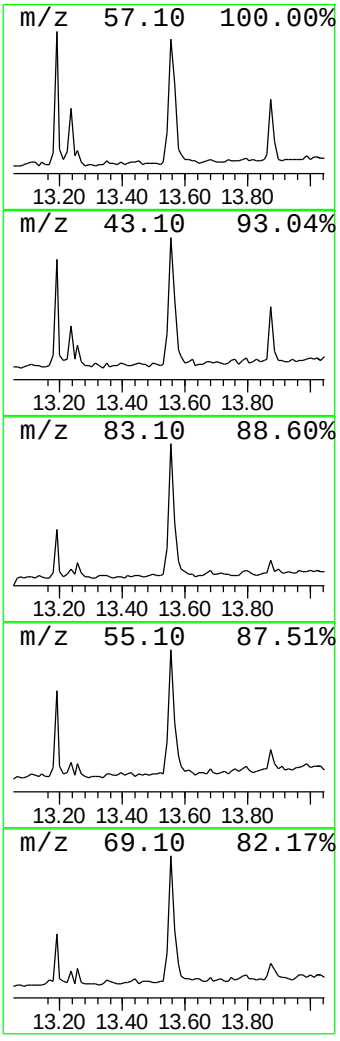
****

Peak Number 8 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	6.04 ng	94163	Chrysene-d12	13.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	90
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90





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Misc :
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Instrument : BNA_F
ClientSampleId : KSB-14-5.0-7.0

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

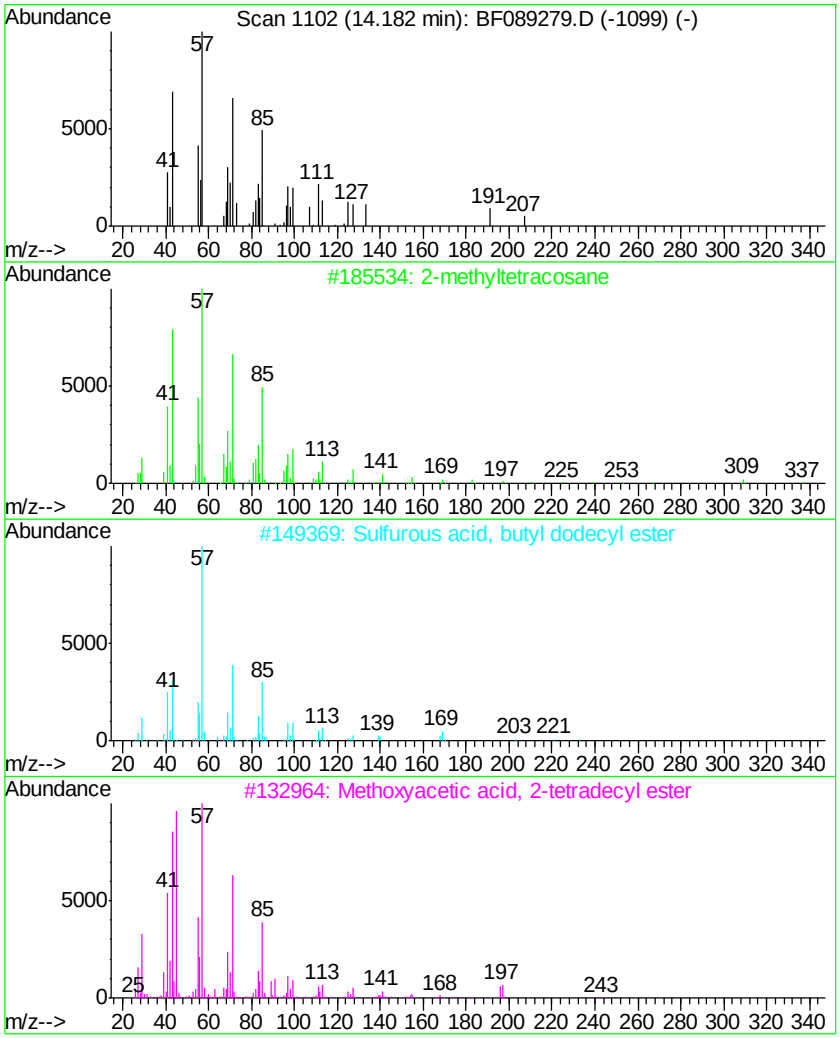
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

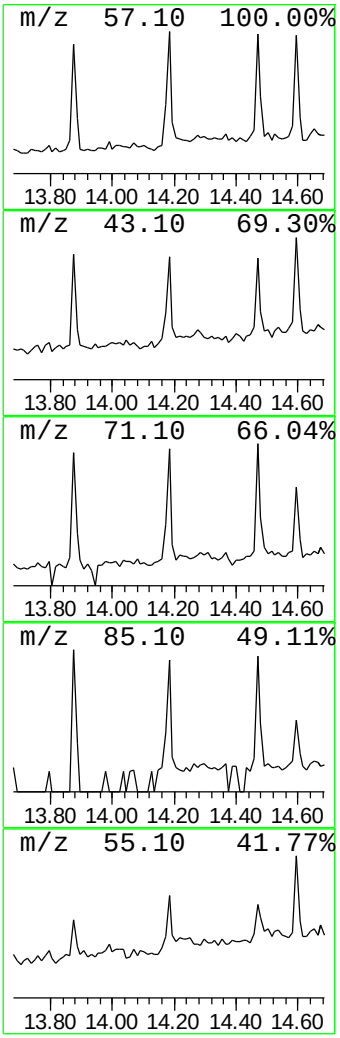
****

Peak Number 9 2-methyltetracosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.18	2.16 ng	33686	Chrysene-d12	13.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyltetracosane	352	C25H52	1000376-72-6	64
2	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	59
3	Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	59
4	Octacosane	394	C28H58	000630-02-4	53
5	2-methyloctacosane	408	C29H60	1000376-72-8	53





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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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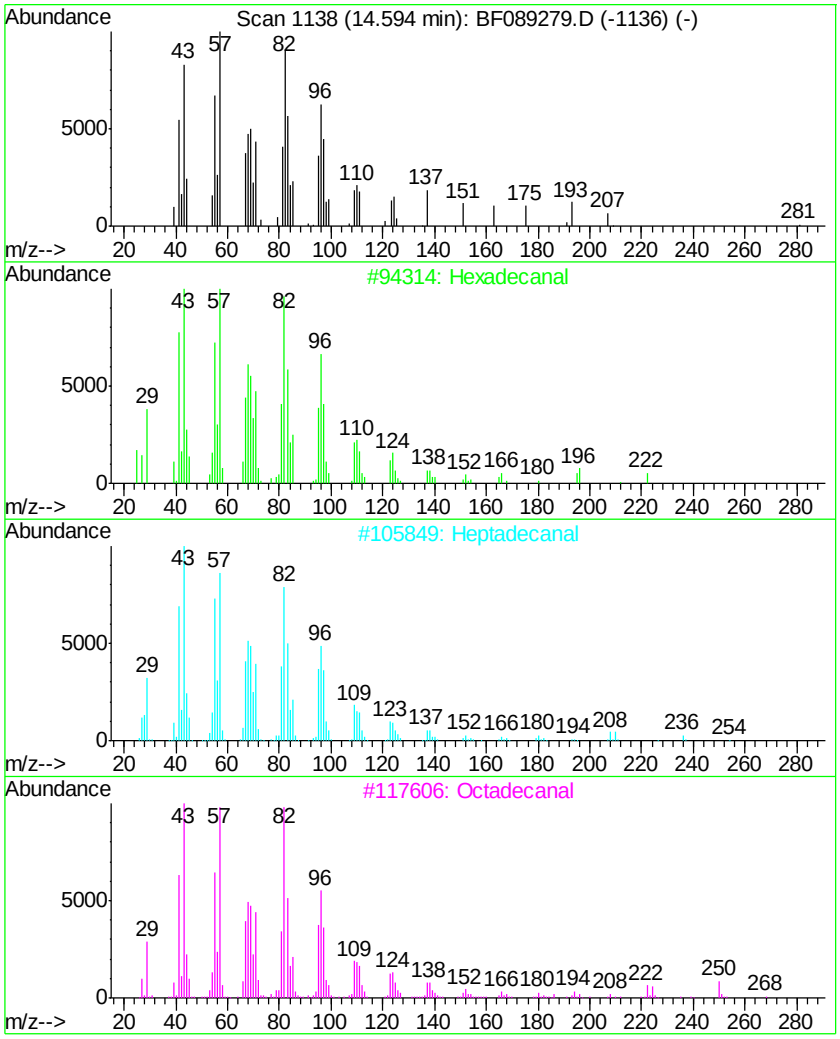
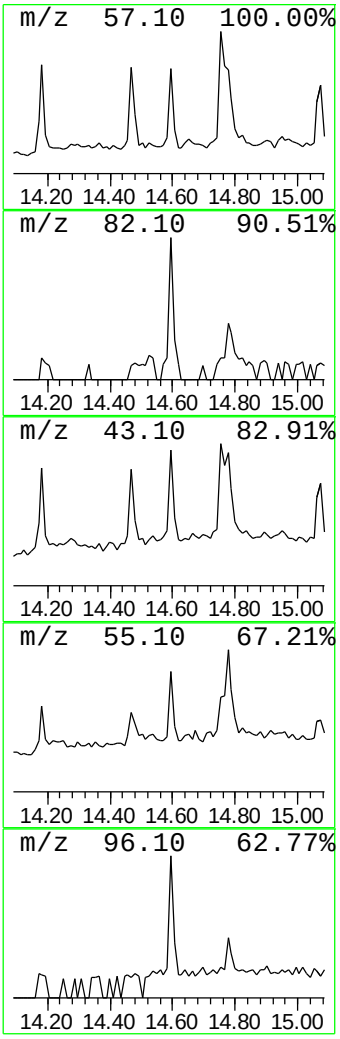
Peak Number 10 Hexadecanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	3.05 ng	34947	Perylene-d12	15.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanal	240	C16H32O	000629-80-1	95
2	Heptadecanal	254	C17H34O	1000376-70-0	91
3	Octadecanal	268	C18H36O	000638-66-4	91
4	16-Octadecenal	266	C18H34O	056554-87-1	91
5	Tetradecanal	212	C14H28O	000124-25-4	91





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Instrument : BNA_F
ClientSampleId : KSB-14-5.0-7.0

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

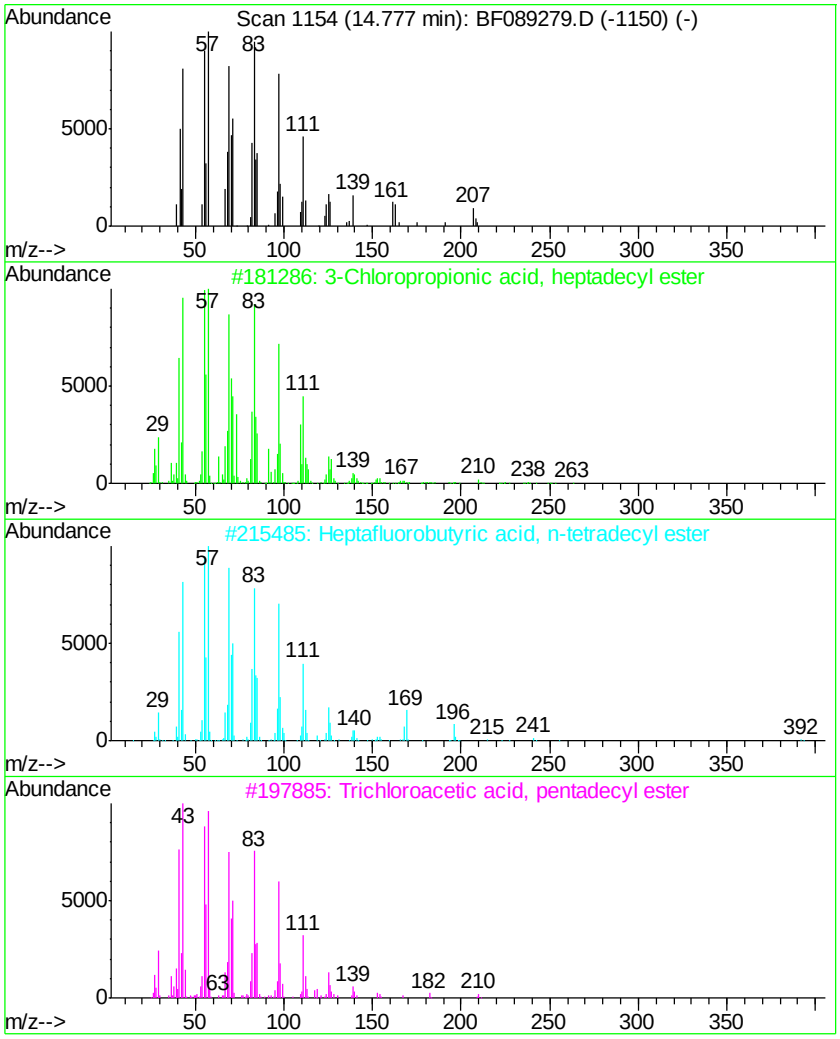
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

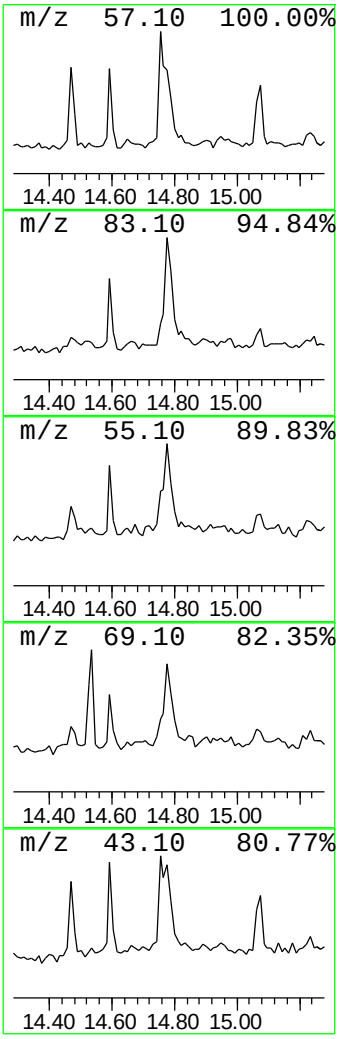
****

Peak Number 11 3-Chloropropionic acid, hep... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.78	6.37 ng	73070	Perylene-d12	15.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072516\
Data File : BF089279.D
Acq On : 25 Jul 2016 15:12
Operator : UM/SJ
Sample : H4129-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KSB-14-5.0-7.0

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
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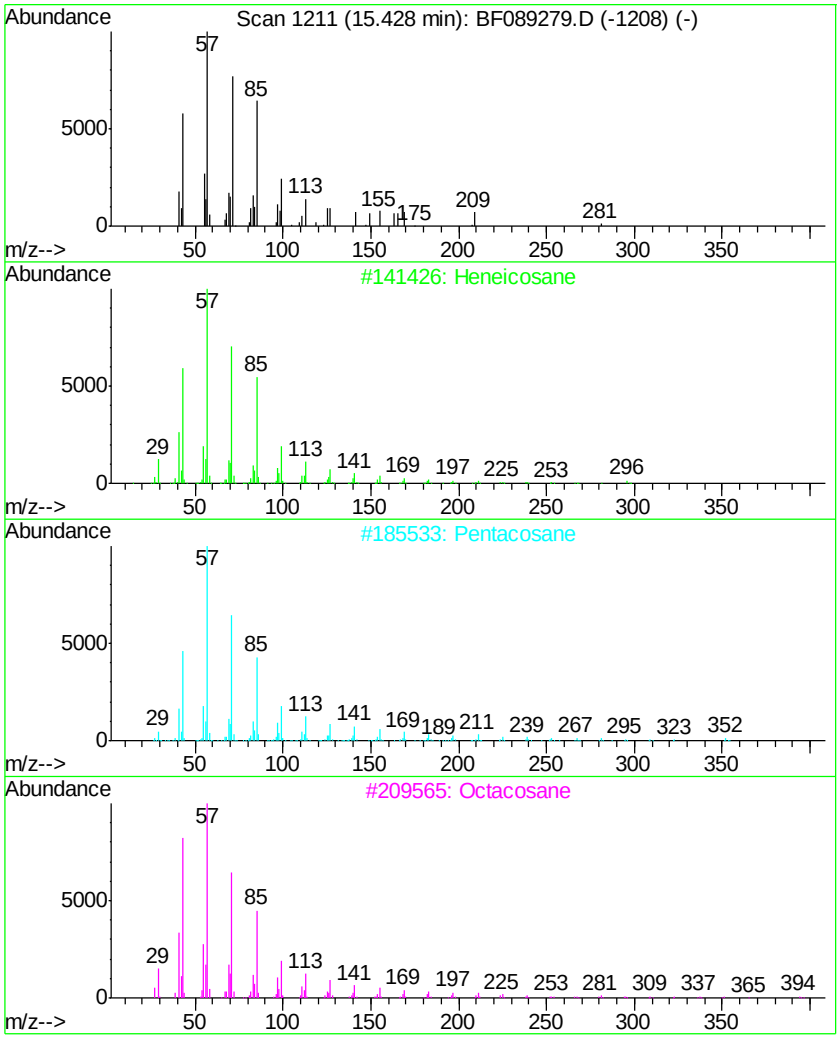
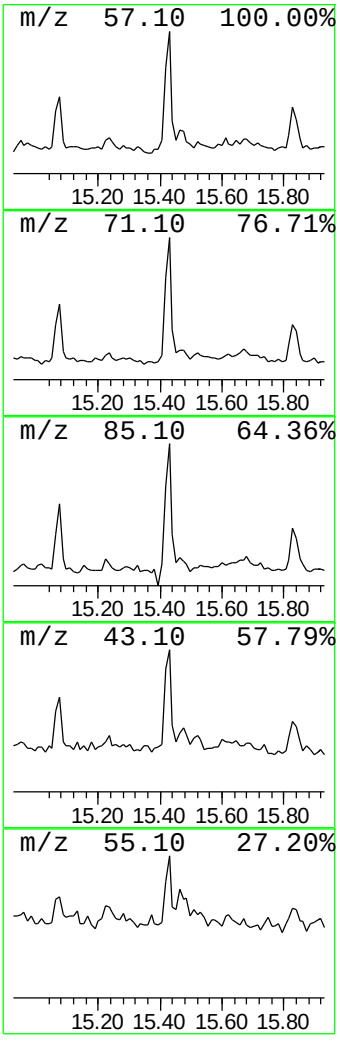
Peak Number 12 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.43	3.82 ng	43858	Perylene-d12	15.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetracosane	338	C24H50	000646-31-1	90
5	Heptadecane	240	C17H36	000629-78-7	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072516\
Data File : BF089279.D
Acq On : 25 Jul 2016 15:12
Operator : UM/SJ
Sample : H4129-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KSB-14-5.0-7.0

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

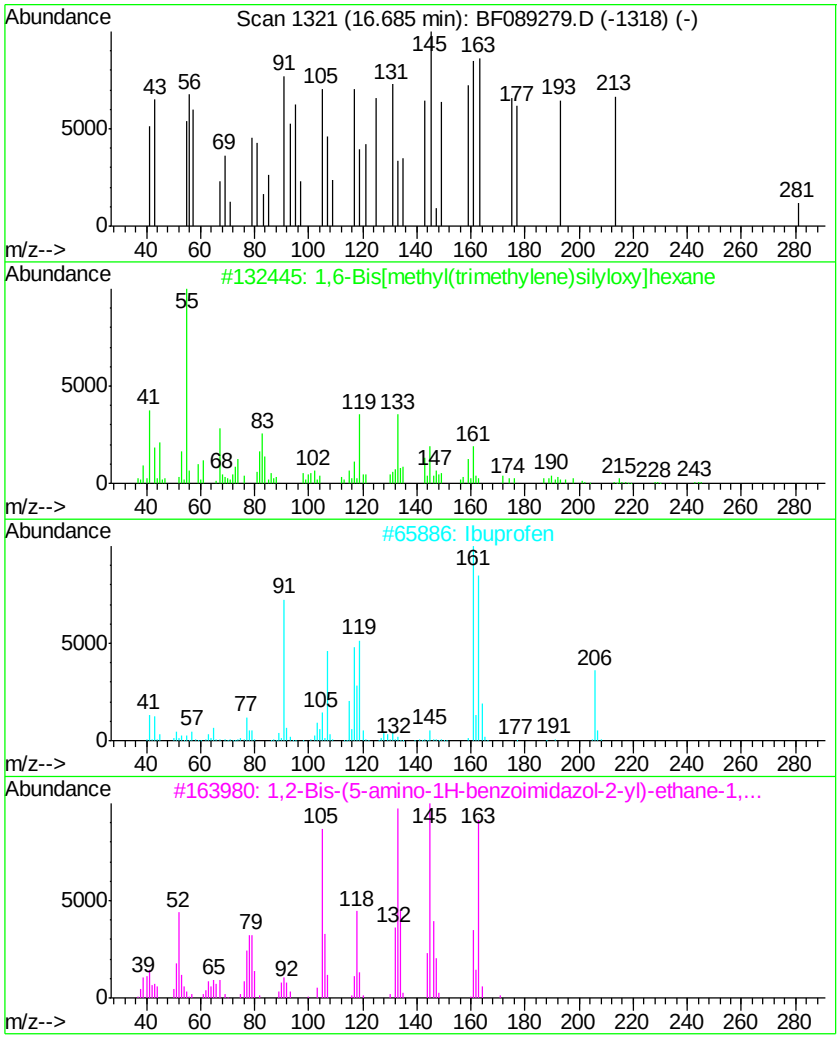
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

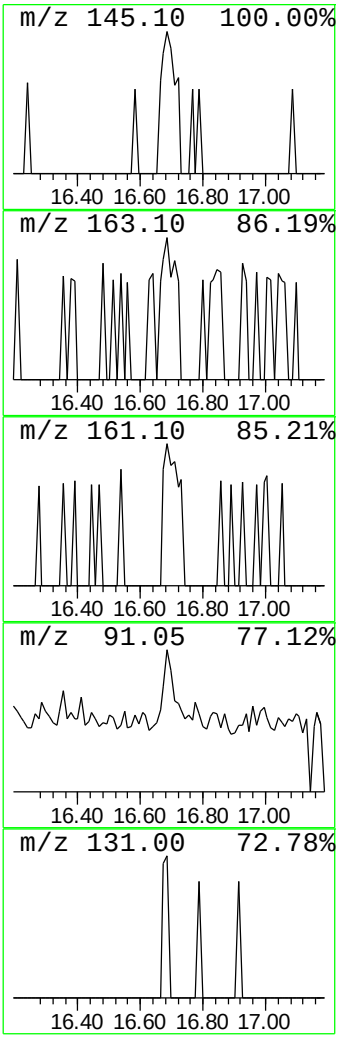
****

Peak Number 13 unknown16.69 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	2.36 ng	27035	Perylene-d12	15.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Bis[methyl(trimethylene)silyl...	286	C14H30O2Si2	1000217-00-5	17
2	Ibuprofen	206	C13H18O2	015687-27-1	10
3	1,2-Bis-(5-amino-1H-benzoimidazo...	324	C16H16N6O2	031545-09-2	10
4	1-(1-Azido-1-methylethyl)-1-brom...	203	C6H10BrN3	1000193-57-5	10
5	2-Propanol, 1,1,1,3-tetrachloro-...	210	C4H6Cl4O	014703-48-1	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072516\
Data File : BF089279.D
Acq On : 25 Jul 2016 15:12
Operator : UM/SJ
Sample : H4129-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : KSB-14-5.0-7.0

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...	4.70	6.1	ng	96951	1	6.56	317765	20.0
unknown6.33	6.33	93.3	ng	1481580	1	6.56	317765	20.0
Hexacosane	10.51	2.6	ng	47803	4	11.06	364446	20.0
Hexadecanoic acid...	12.49	6.3	ng	97866	5	13.68	311943	20.0
Butyl myristate	13.19	3.9	ng	60643	5	13.68	311943	20.0
1-Heneicosanol	13.55	6.0	ng	94163	5	13.68	311943	20.0
2-methyltetracosane	14.18	2.2	ng	33686	5	13.68	311943	20.0
Hexadecanal	14.59	3.0	ng	34947	6	15.02	229533	20.0
3-Chloropropionic...	14.78	6.4	ng	73070	6	15.02	229533	20.0
Heneicosane	15.43	3.8	ng	43858	6	15.02	229533	20.0
unknown16.69	16.69	2.4	ng	27035	6	15.02	229533	20.0