LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020616\
Data File : BF084910.D
Acq On : 6 Feb 2016 14:31
Operator : SJ/IZ
Sample : H1325-01
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B016(17-19)

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-BF020116.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	2.350	21	23	28	rVB	196136	230097	4.28%	0.513%
2	4.110	175	177	182	rBV	64921	117707	2.19%	0.263%
3	4.819	237	239	252	rVB	1307403	2271487	42.22%	5.068%
4	5.264	275	278	280	rBV	4536045	4755925	88.39%	10.612%
5	5.664	311	313	316	rBV	69490	64545	1.20%	0.144%
6	6.316	367	370	372	rBV	3868129	3985184	74.06%	8.892%
7	6.430	378	380	383	rBV	4436148	4582786	85.17%	10.225%
8	6.659	398	400	403	rBV	1319868	1078036	20.04%	2.405%
9	6.819	411	414	416	rBV	4533506	4100286	76.20%	9.149%
10	7.230	447	450	453	rBV	2842078	3080287	57.25%	6.873%
11	7.950	510	513	517	rBV	1269805	1581041	29.38%	3.528%
12	9.025	604	607	610	rBV	4850734	5380665	100.00%	12.006%
13	9.116	612	615	618	rVB	87670	83901	1.56%	0.187%
14	9.642	659	661	663	rBV	106967	85171	1.58%	0.190%
15	9.699	663	666	667	rVV	1306478	1439881	26.76%	3.213%
16	9.722	667	668	671	rVB	59150	57828	1.07%	0.129%
17	10.145	701	705	707	rVB2	94509	98275	1.83%	0.219%
18	10.488	732	735	737	rBV	3255776	3523215	65.48%	7.861%
19	10.613	744	746	750	rVB	125645	146705	2.73%	0.327%
20	11.059	783	785	786	rBV	101938	87889	1.63%	0.196%
21	11.173	792	795	797	rBV	1563176	1376986	25.59%	3.072%
22	11.482	820	822	825	rBV	77135	74801	1.39%	0.167%
23	11.894	856	858	862	rBV	99435	108722	2.02%	0.243%
24	12.602	918	920	922	rBV2	173010	231989	4.31%	0.518%
25	12.762	931	934	937	rVB	4448008	4298253	79.88%	9.590%
26	13.299	979	981	983	rBV	179263	154720	2.88%	0.345%
27	13.802	1023	1025	1027	rBV	1079537	962438	17.89%	2.147%
28	15.174	1142	1145	1147	rBV	739938	859172	15.97%	1.917%

Sum of corrected areas: 44817992

LSC Report - Integrated Chromatogram

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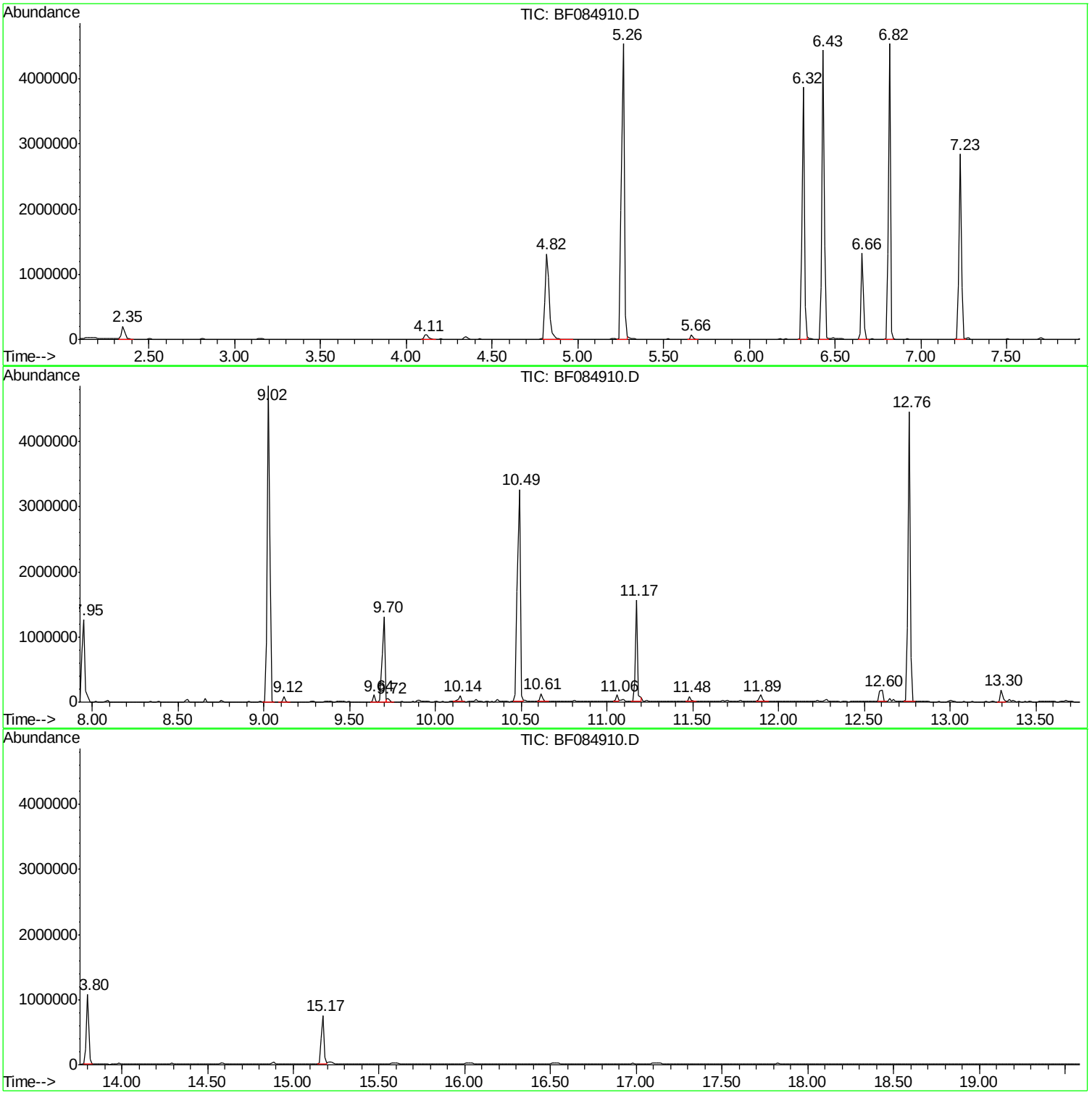
Operator : SJ/IZ
Sample : H1325-01
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S4-B016(17-19)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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\BF020616\
Data File : BF084910.D
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Operator : SJ/IZ
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ClientSampleId : S4-B016(17-19)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

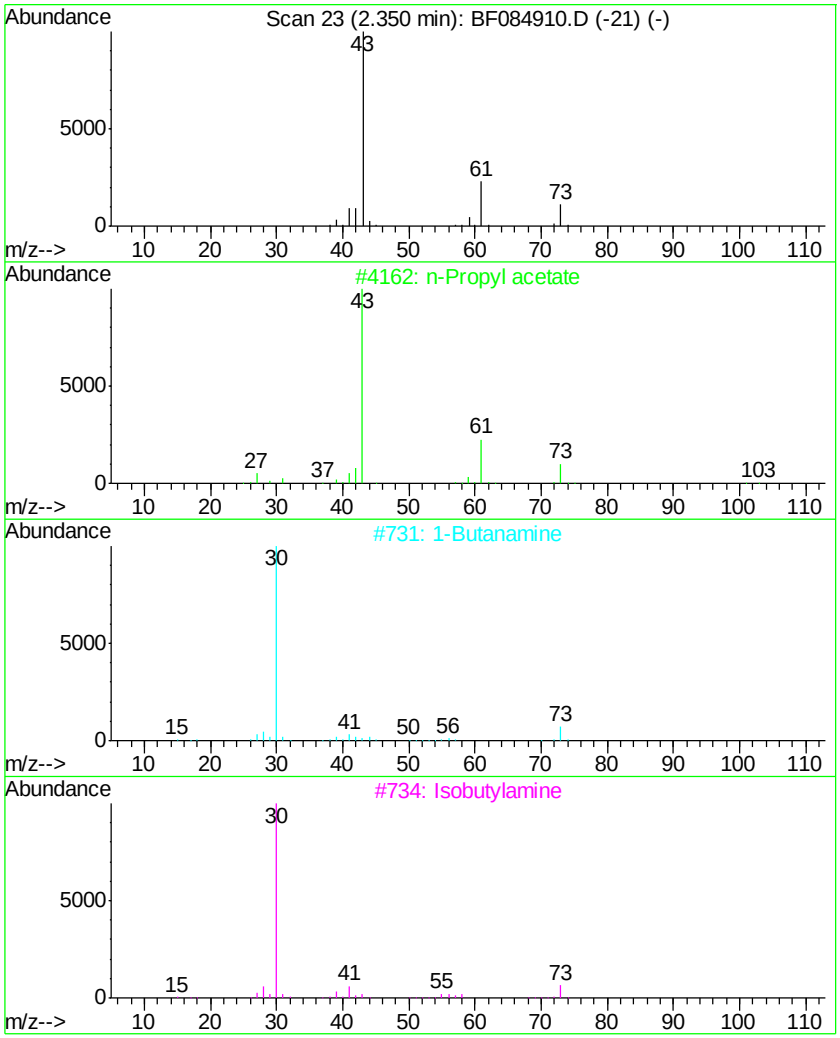
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

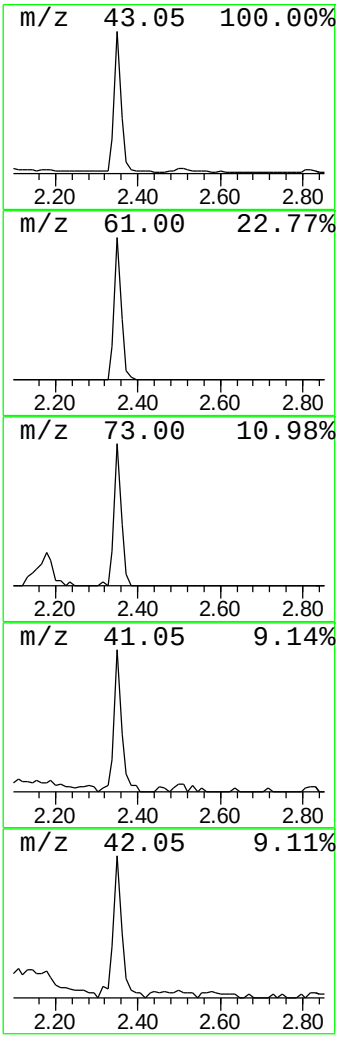
****

Peak Number 1 n-Propyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.35	4.27 ng	230097	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	1-Butanamine	73	C4H11N	000109-73-9	9
3	Isobutylamine	73	C4H11N	000078-81-9	5
4	Ethanamine, N-ethyl-	73	C4H11N	000109-89-7	4
5	Butane, 2-methyl-	72	C5H12	000078-78-4	4





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020616\
Data File : BF084910.D
Acq On : 6 Feb 2016 14:31
Operator : SJ/IZ
Sample : H1325-01
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B016(17-19)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

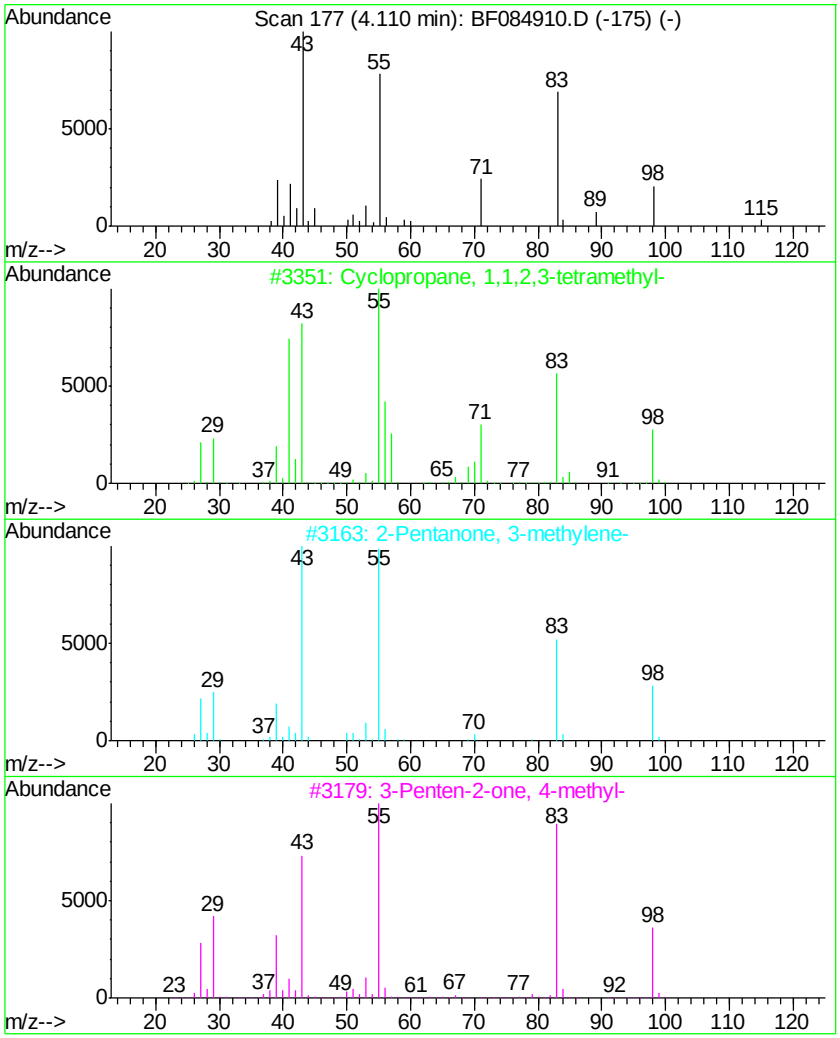
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

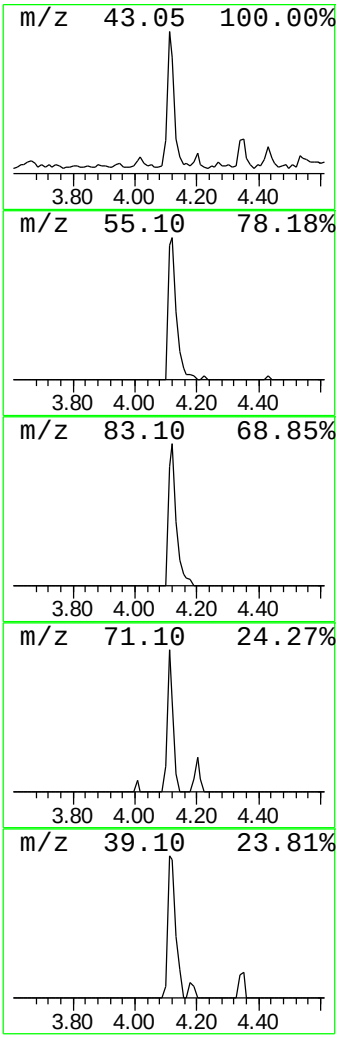
****

Peak Number 2 Cyclopropane, 1,1,2,3-tetra... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.11	2.18 ng	117707	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,1,2,3-tetramethyl-	98	C7H14	074752-93-5	64
2	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	64
3	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	58
4	2,4-Azetidinedione, 3,3-diethyl-...	155	C8H13NO2	069315-91-9	50
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020616\
Data File : BF084910.D
Acq On : 6 Feb 2016 14:31
Operator : SJ/IZ
Sample : H1325-01
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B016(17-19)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

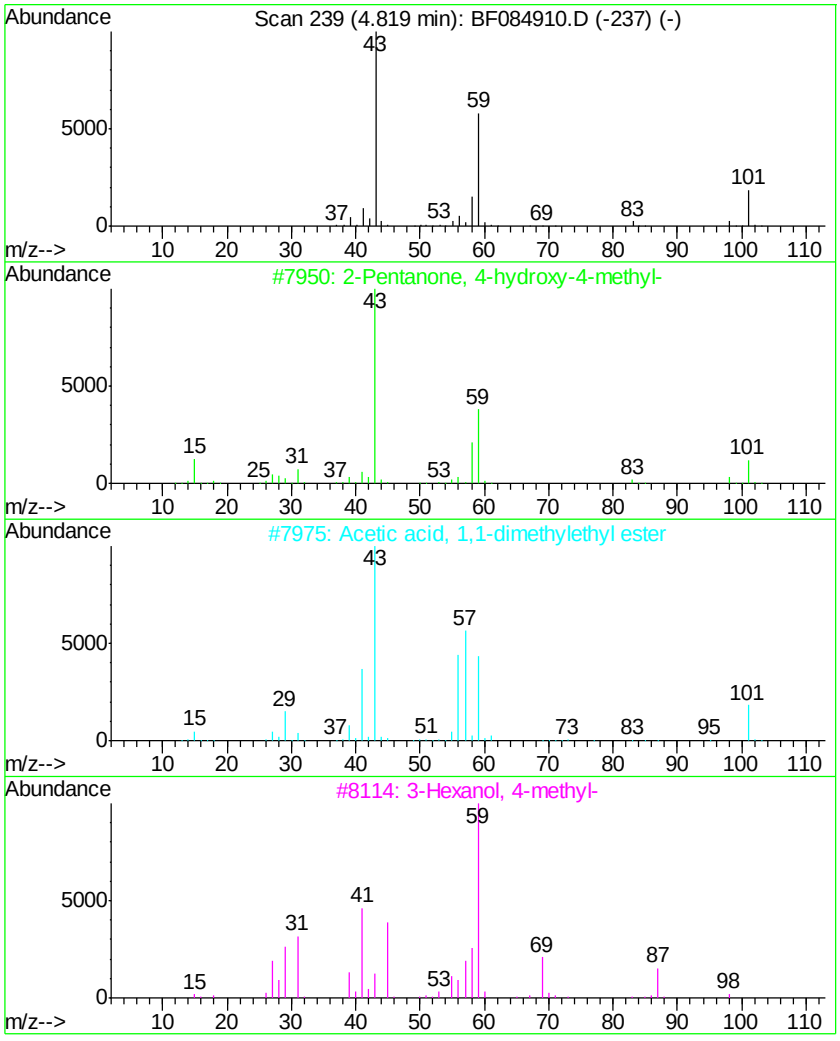
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

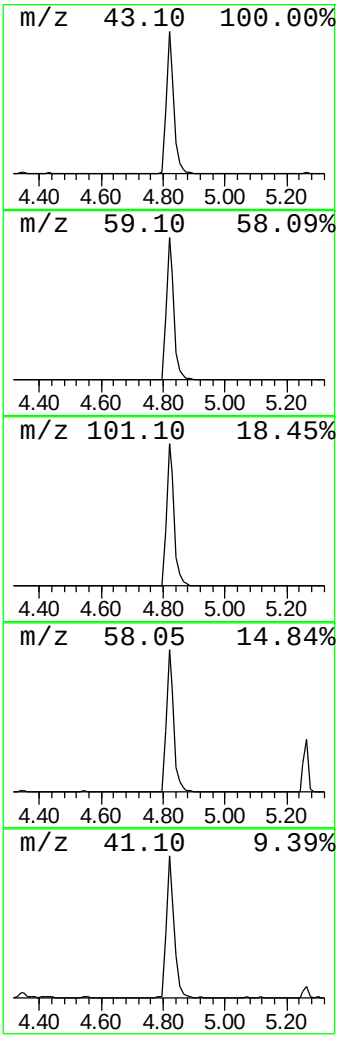
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	42.14 ng	2271490	1,4-Dichlorobenzene-d4	6.66

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	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020616\
Data File : BF084910.D
Acq On : 6 Feb 2016 14:31
Operator : SJ/IZ
Sample : H1325-01
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B016(17-19)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

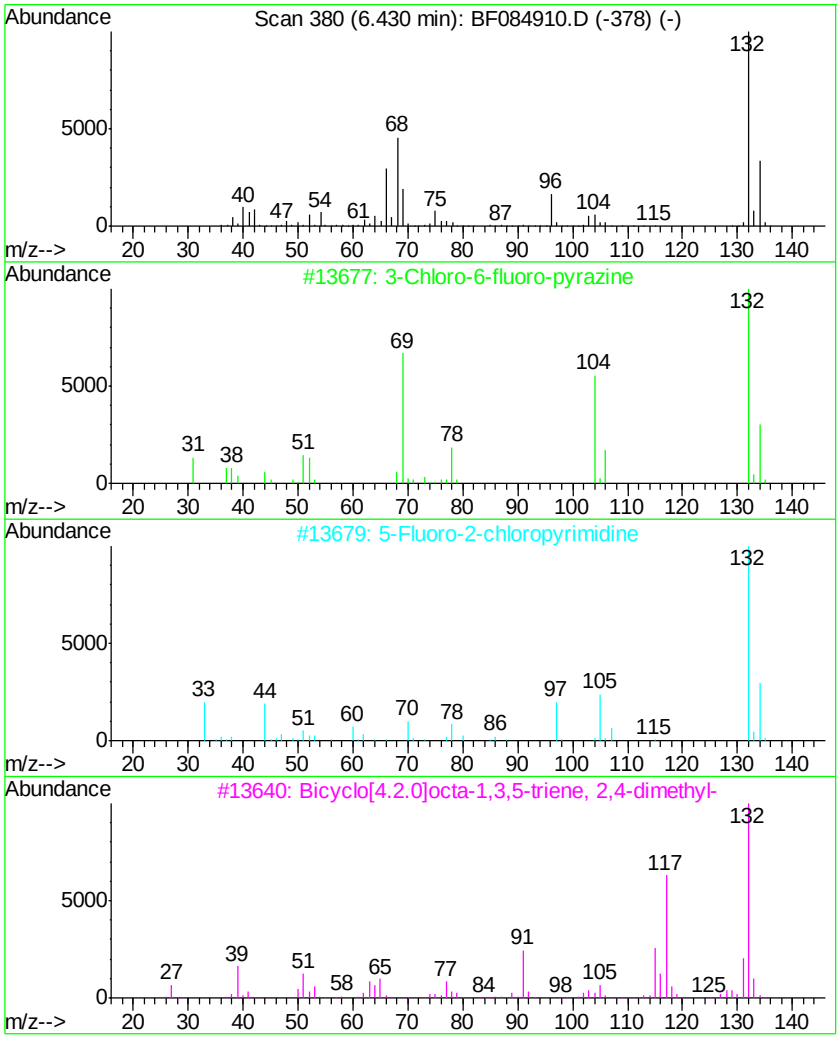
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

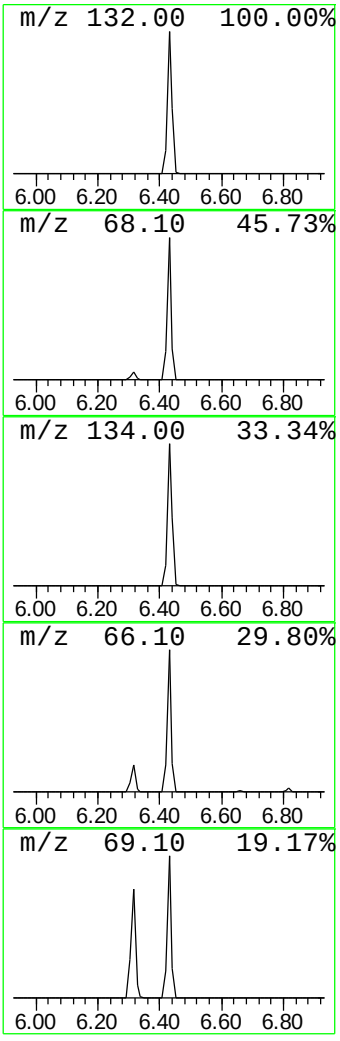
****

Peak Number 4 unknown6.43 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	85.02 ng	4582790	1,4-Dichlorobenzene-d4	6.66

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	16
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020616\
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Operator : SJ/IZ
Sample : H1325-01
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B016(17-19)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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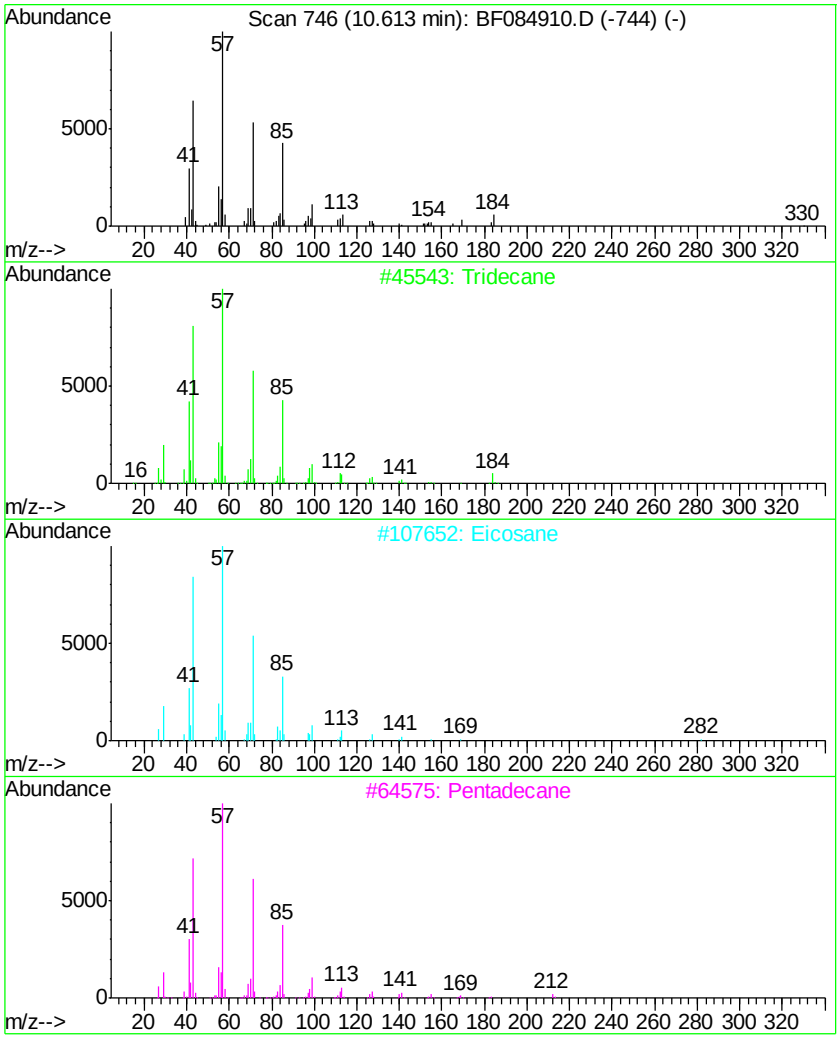
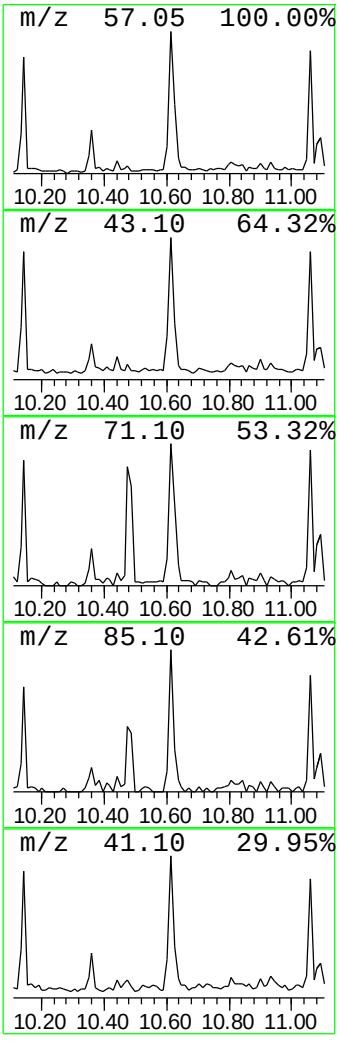
****

Peak Number 6 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.61	2.13 ng	146705	Phenanthrene-d10	11.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	Eicosane	282	C20H42	000112-95-8	91
3	Pentadecane	212	C15H32	000629-62-9	86
4	Tetradecane	198	C14H30	000629-59-4	86
5	Tetracosane	338	C24H50	000646-31-1	86





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Instrument : BNA_F
ClientSampleId : S4-B016(17-19)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

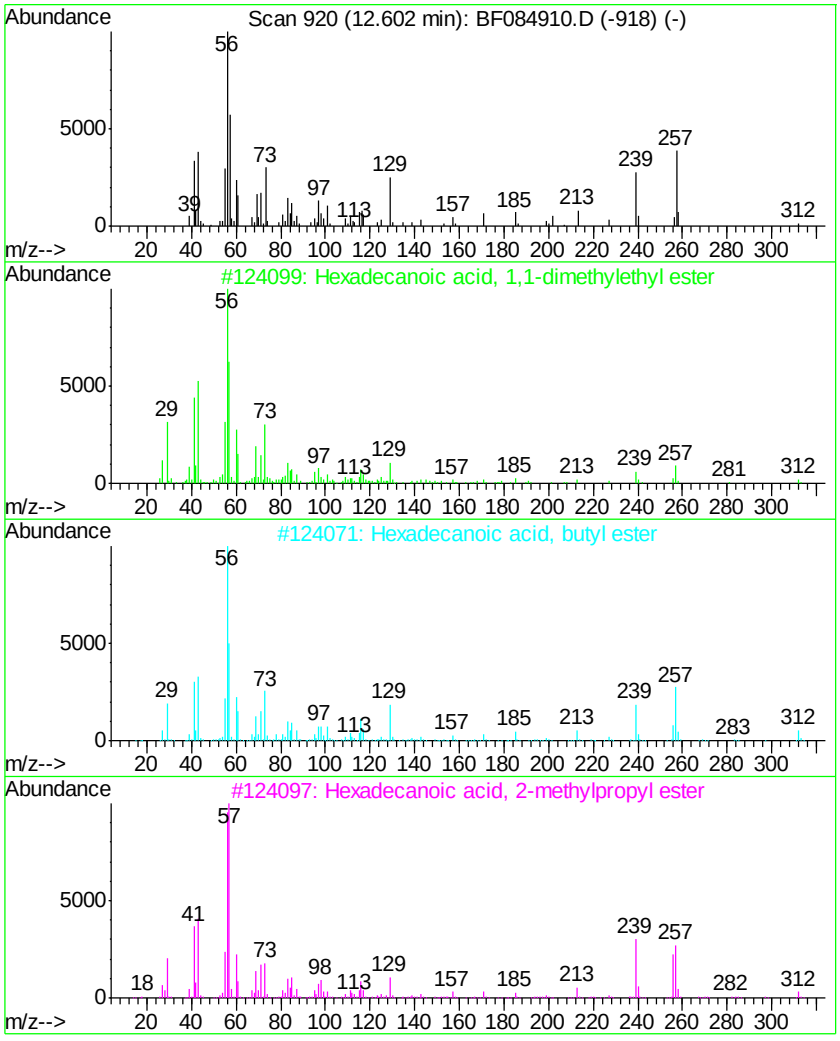
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

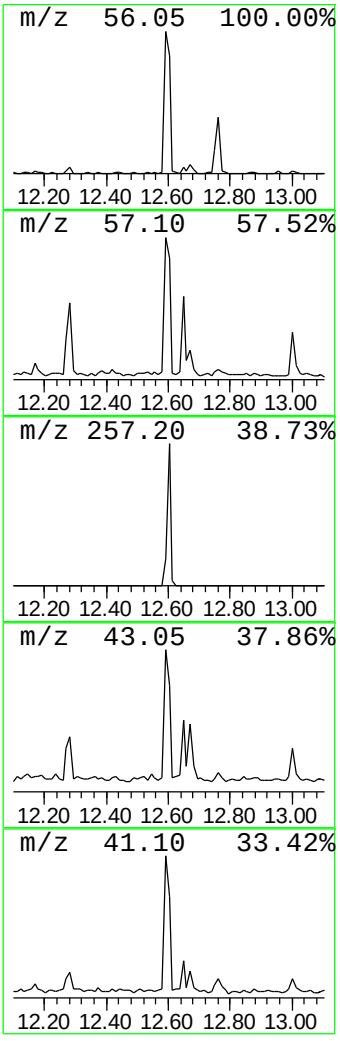
****

Peak Number 7 Hexadecanoic acid, 1,1-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.60	4.82 ng	231989	Chrysene-d12	13.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	64
4	Nipecotic acid	129	C6H11NO2	000498-95-3	43
5	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	27





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

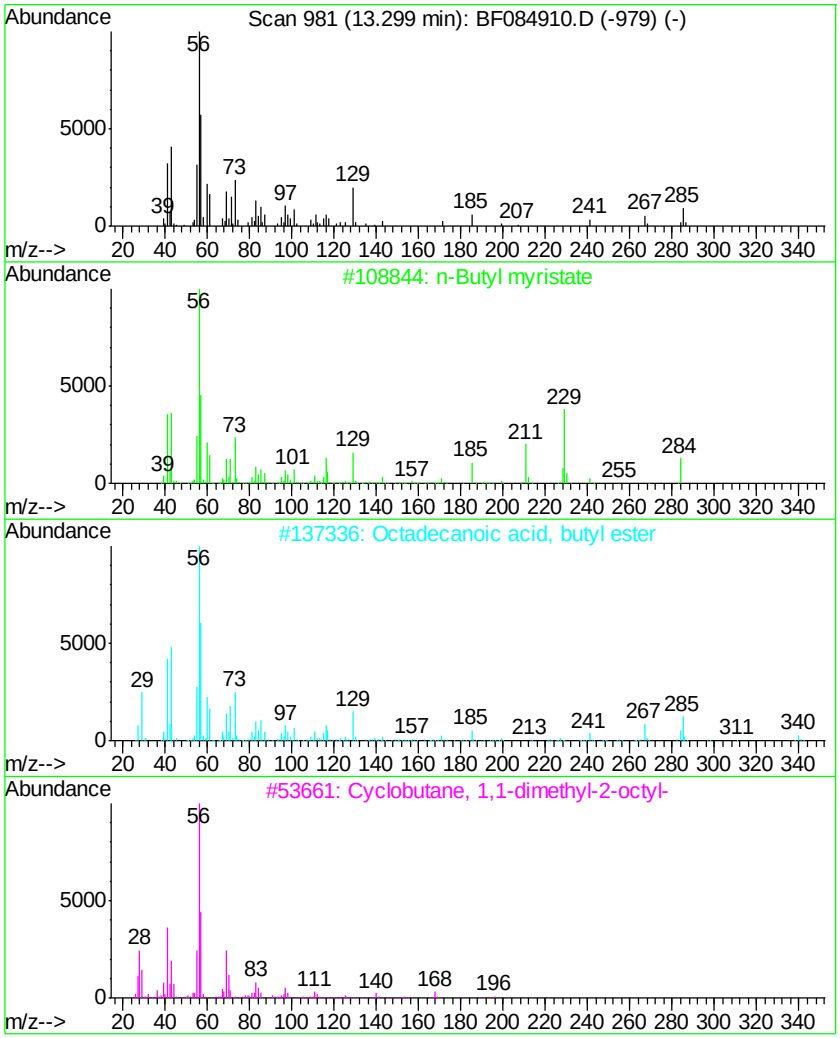
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

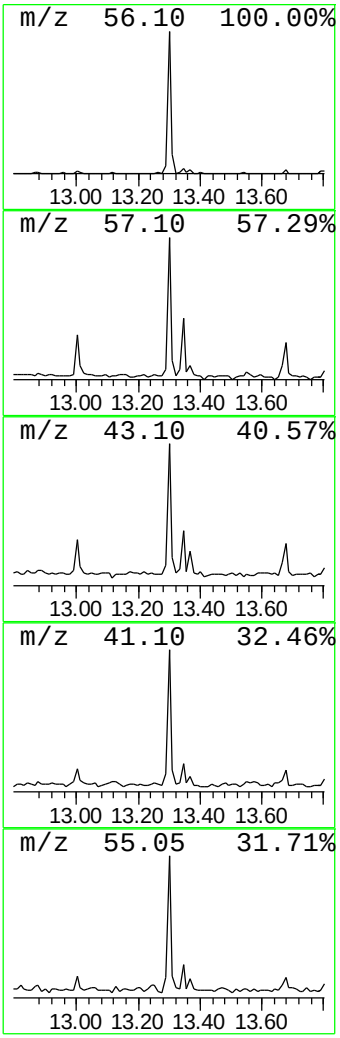
****

Peak Number 8 n-Butyl myristate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.30	3.22 ng	154720	Chrysene-d12	13.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Butyl myristate	284	C18H36O2	000110-36-1	72
2	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	49
3	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
4	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37
5	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	35





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	2.35	4.3	ng	230097	1	6.66	1078040	20.0
Cyclopropane, 1,1...	4.11	2.2	ng	117707	1	6.66	1078040	20.0
2-Pentanone, 4-hy...	4.82	42.1	ng	2271490	1	6.66	1078040	20.0
unknown6.43	6.43	85.0	ng	4582790	1	6.66	1078040	20.0
Tridecane	10.61	2.1	ng	146705	4	11.17	1376990	20.0
Hexadecanoic acid...	12.60	4.8	ng	231989	5	13.80	962438	20.0
n-Butyl myristate	13.30	3.2	ng	154720	5	13.80	962438	20.0