LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020616\
Data File : BF084913.D
Acq On : 6 Feb 2016 15:53
Operator : SJ/IZ
Sample : H1330-01
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B010(5-7)

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	2.224	7	12	19	rVB4	18744	75505	1.30%	0.158%
2	2.384	24	26	29	rVB	142466	210450	3.62%	0.442%
3	3.058	82	85	91	rVB	68568	117483	2.02%	0.247%
4	4.121	175	178	184	rBV	1463458	2016272	34.65%	4.231%
5	4.830	237	240	252	rVB	845537	1498139	25.75%	3.144%
6	5.264	275	278	281	rBV	4170270	4607118	79.18%	9.668%
7	6.316	367	370	373	rBV	3750883	4094856	70.38%	8.593%
8	6.430	377	380	383	rBV	4219817	5059581	86.96%	10.618%
9	6.659	398	400	403	rVB	1378501	1118855	19.23%	2.348%
10	6.819	412	414	416	rVB	4871215	4358432	74.91%	9.146%
11	7.230	447	450	453	rBV	2897106	3333938	57.30%	6.996%
12	7.356	458	461	463	rBV	58399	68930	1.18%	0.145%
13	7.950	510	513	515	rBV	1211437	1518660	26.10%	3.187%
14	7.985	515	516	518	rVB	89207	65295	1.12%	0.137%
15	8.613	567	571	573	rVB	83167	95885	1.65%	0.201%
16	9.025	604	607	610	rBV	5129907	5818173	100.00%	12.210%
17	9.699	663	666	668	rBV	1237808	1493661	25.67%	3.135%
18	10.122	701	703	706	rBV	97490	106905	1.84%	0.224%
19	10.488	732	735	737	rBV	3458067	3701880	63.63%	7.769%
20	11.173	792	795	797	rBV	1594802	1378707	23.70%	2.893%
21	11.894	856	858	862	rBV	77935	93073	1.60%	0.195%
22	12.602	917	920	922	rBV	183201	235123	4.04%	0.493%
23	12.762	931	934	937	rBV	4589521	4525036	77.77%	9.496%
24	13.299	979	981	983	rBV	172915	150972	2.59%	0.317%
25	13.802	1023	1025	1027	rBV	1096442	980471	16.85%	2.058%
26	15.174	1142	1145	1147	rBV	717623	861032	14.80%	1.807%
27	15.802	1196	1200	1204	rBV2	44335	67692	1.16%	0.142%

Sum of corrected areas: 47652124

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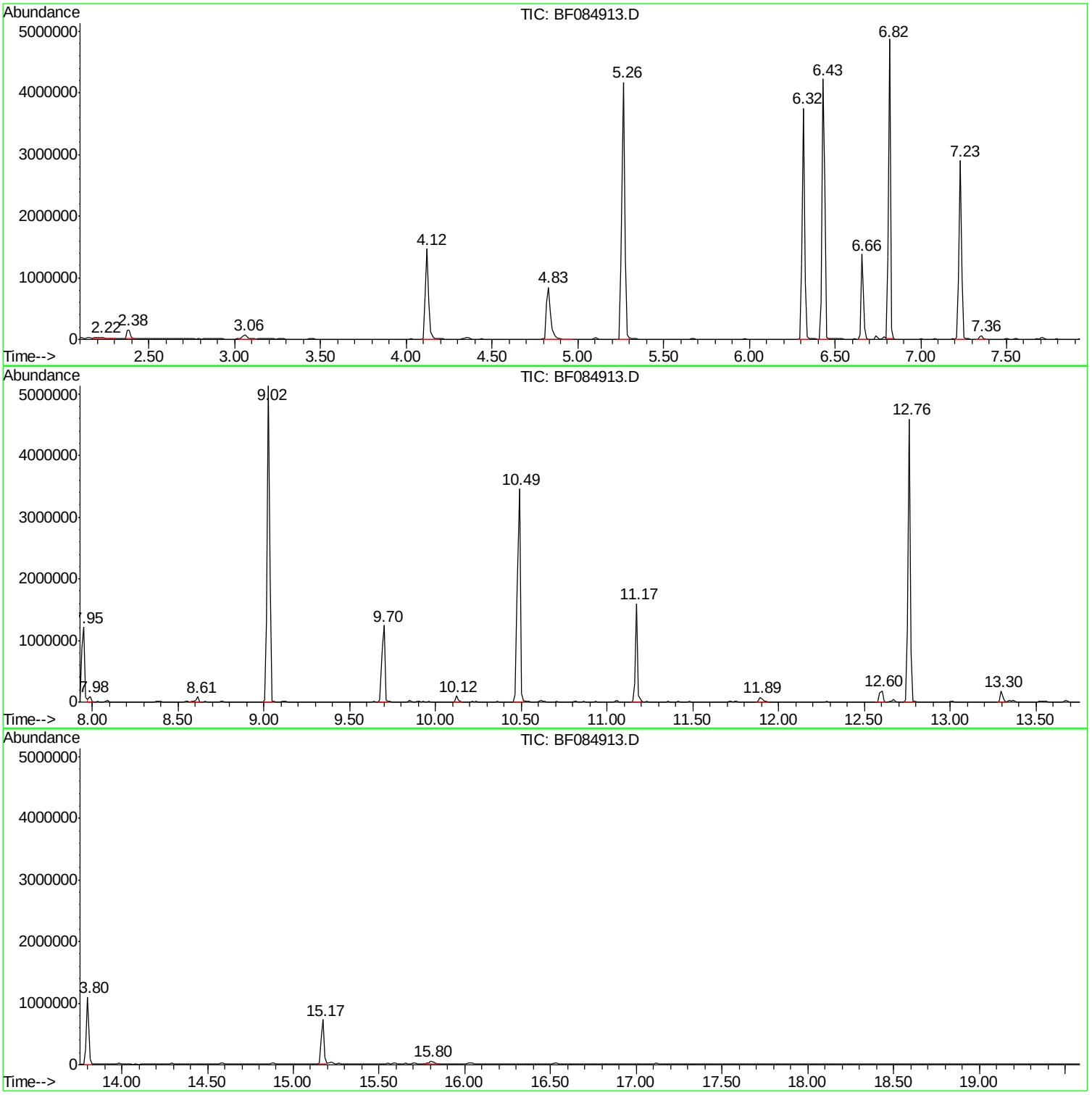
ClientSampleId : S4-B010(5-7)

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



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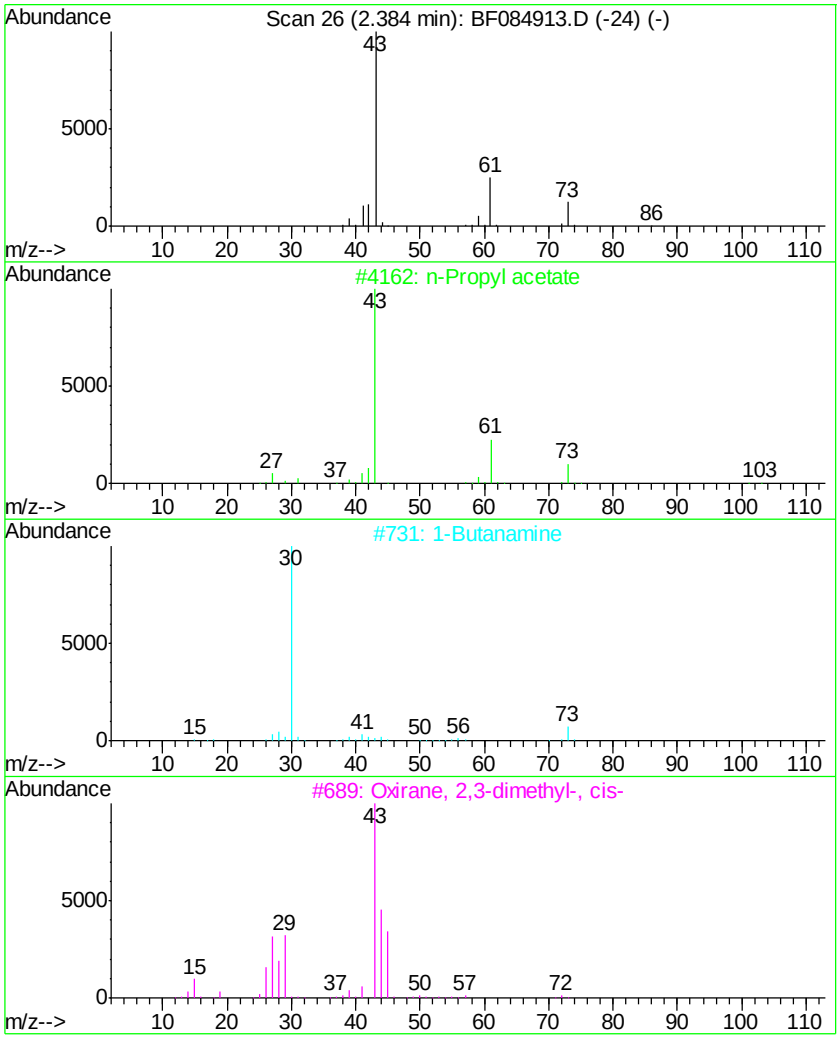
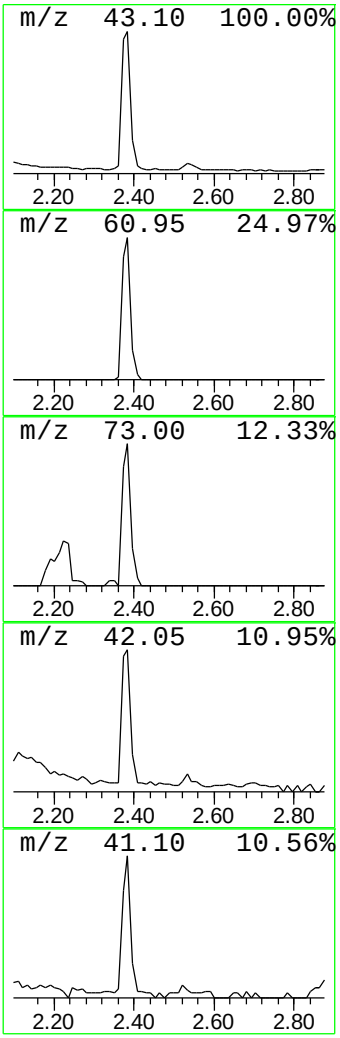
Peak Number 1 n-Propyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.38	3.76 ng	210450	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	7
3	Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	7
4	Isobutylamine	73	C4H11N	000078-81-9	5
5	Butane, 2-methyl-	72	C5H12	000078-78-4	4





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Sample : H1330-01
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Instrument : BNA_F
ClientSampleId : S4-B010(5-7)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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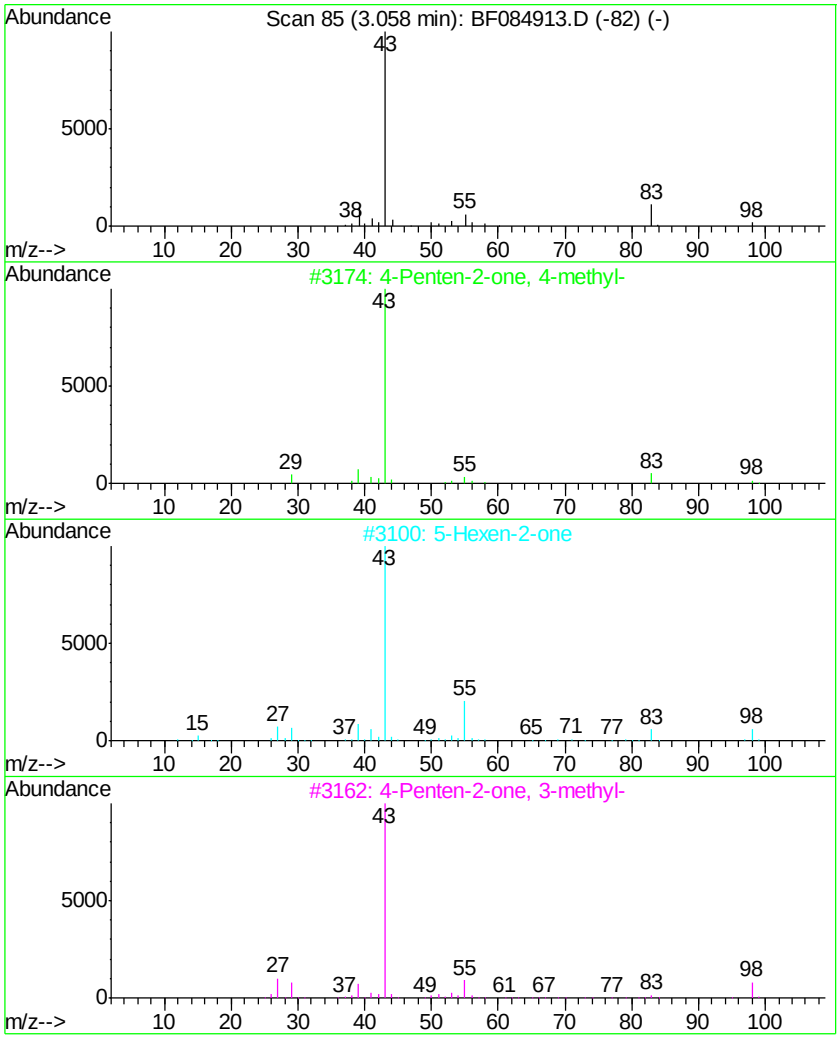
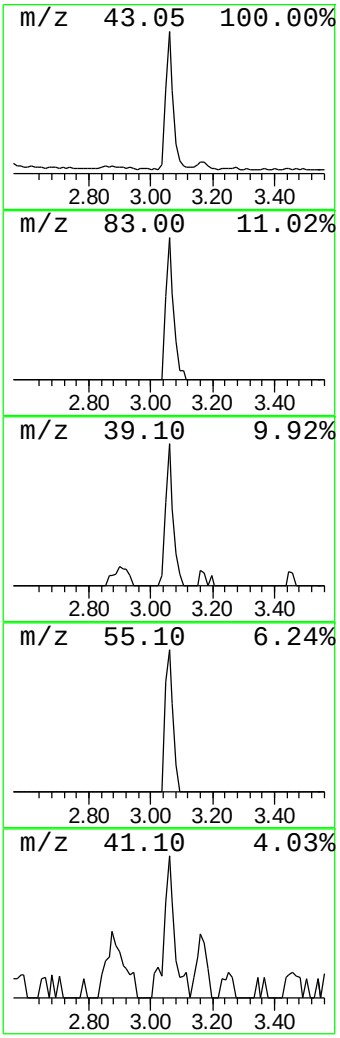
Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.06	2.10 ng	117483	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2	5-Hexen-2-one	98	C6H10O	000109-49-9	38
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	25
4	4-Hexen-2-one	98	C6H10O	025659-22-7	9
5	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	7





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Misc :
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Instrument : BNA_F
ClientSampleId : S4-B010(5-7)

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

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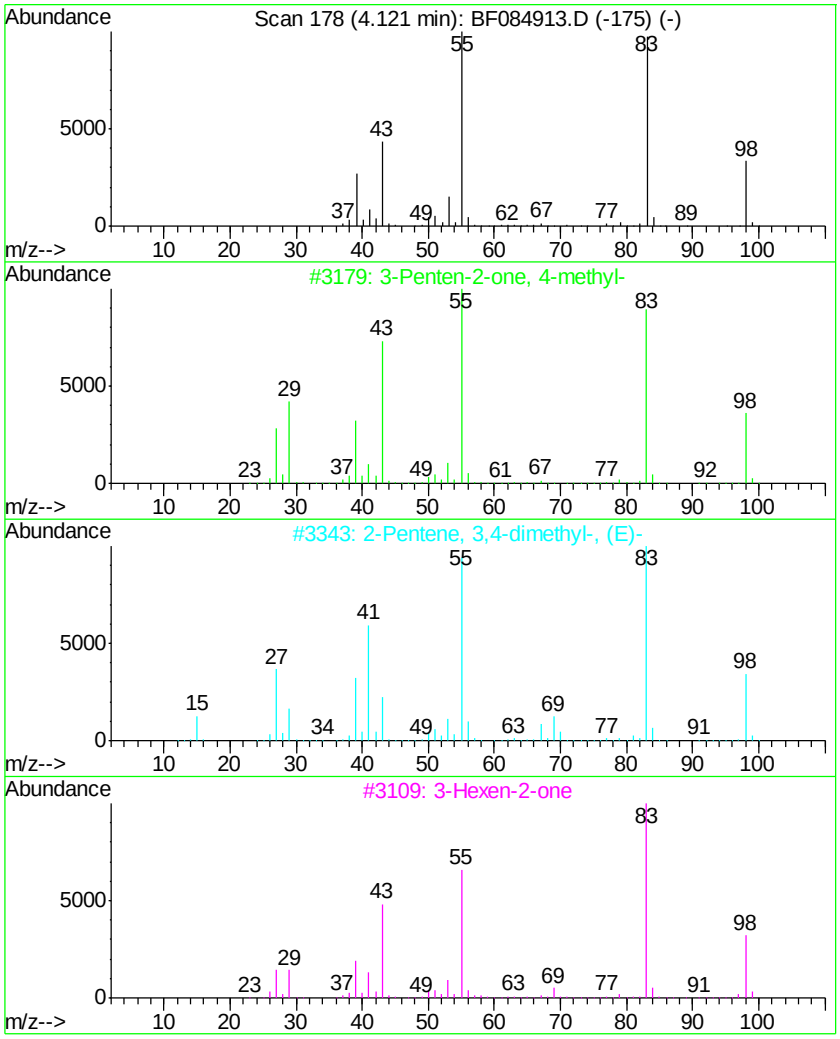
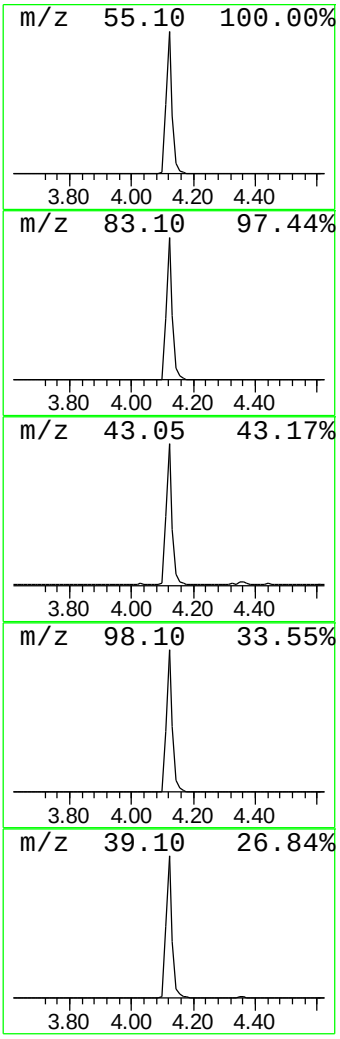
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.12	36.04 ng	2016270	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3	3-Hexen-2-one	98	C6H10O	000763-93-9	87
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86





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Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B010(5-7)

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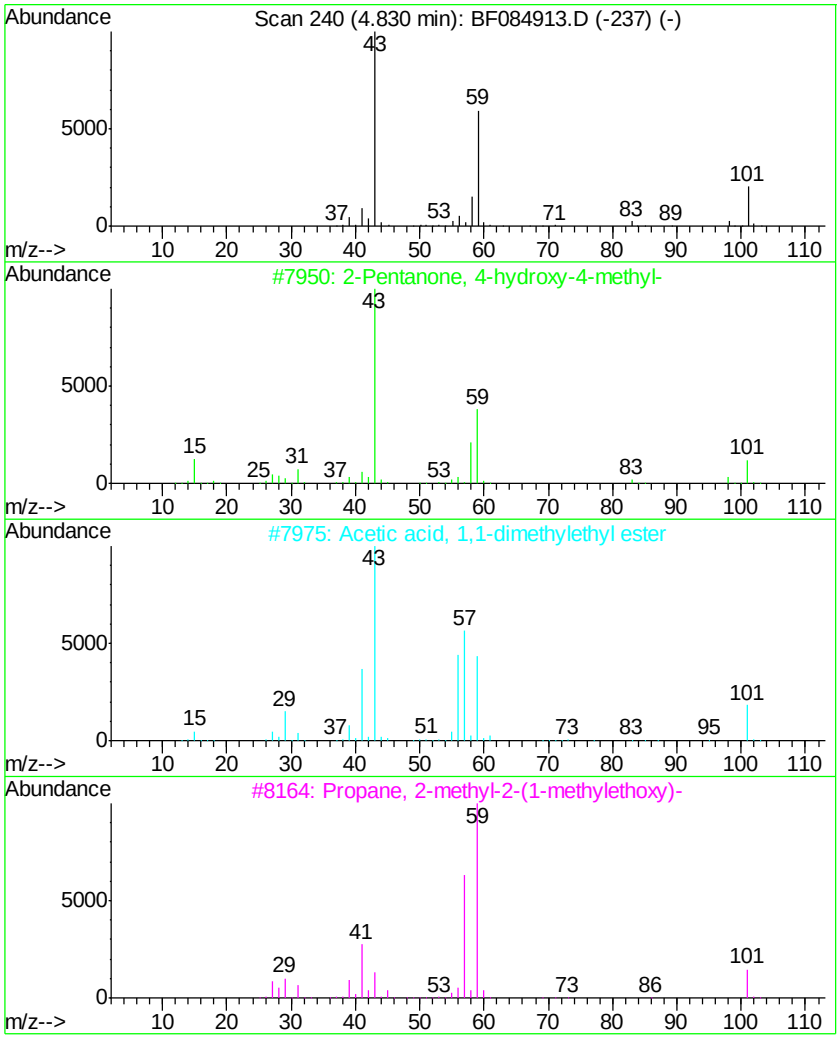
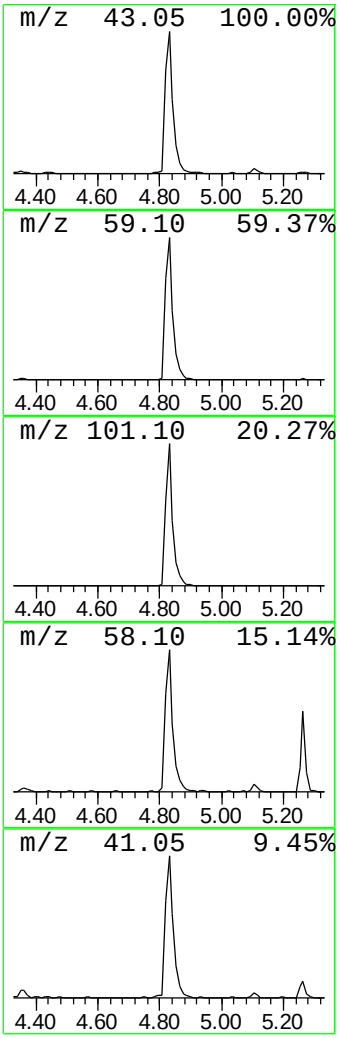
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	26.78 ng	1498140	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	72
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	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Sample : H1330-01
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B010(5-7)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
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TIC Library : C:\DATABASE\NIST02.L
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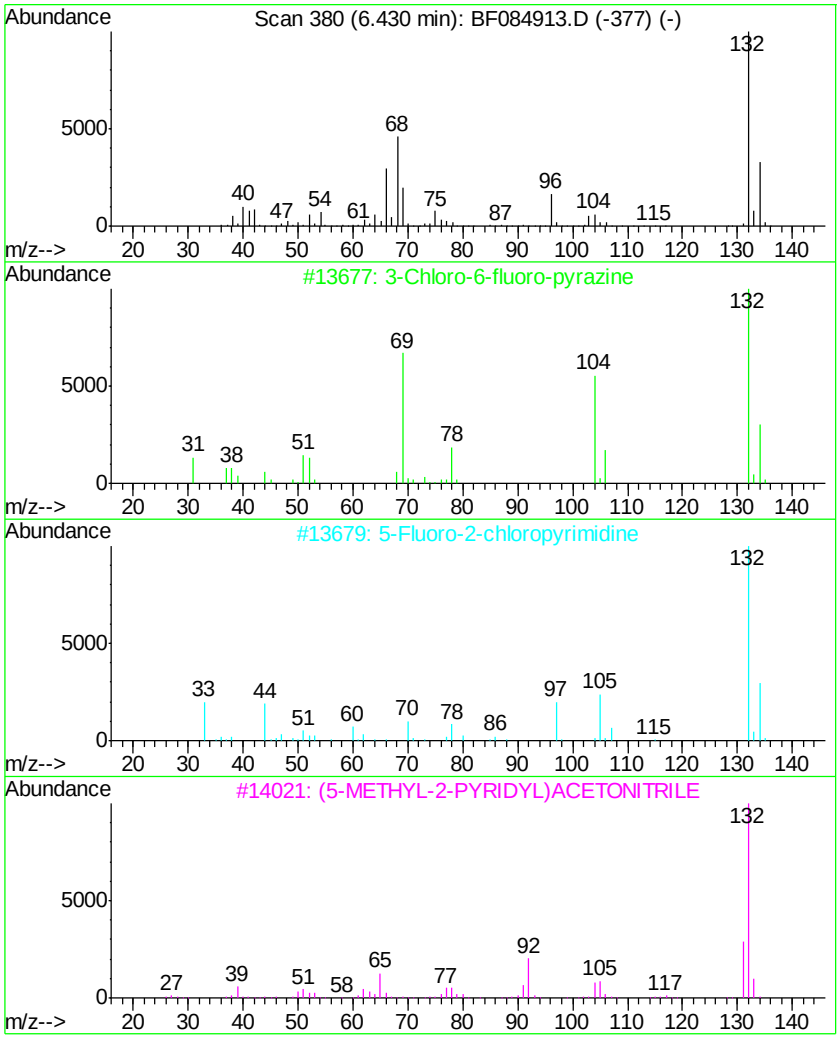
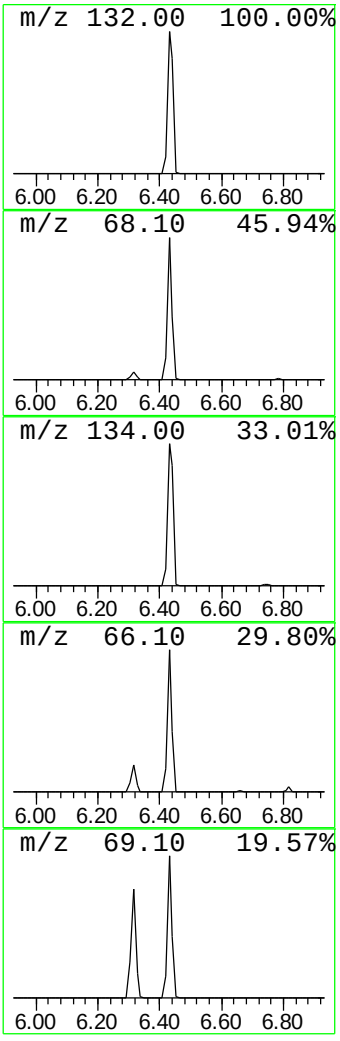
Peak Number 5 unknown6.43 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	90.44 ng	5059580	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	12
3	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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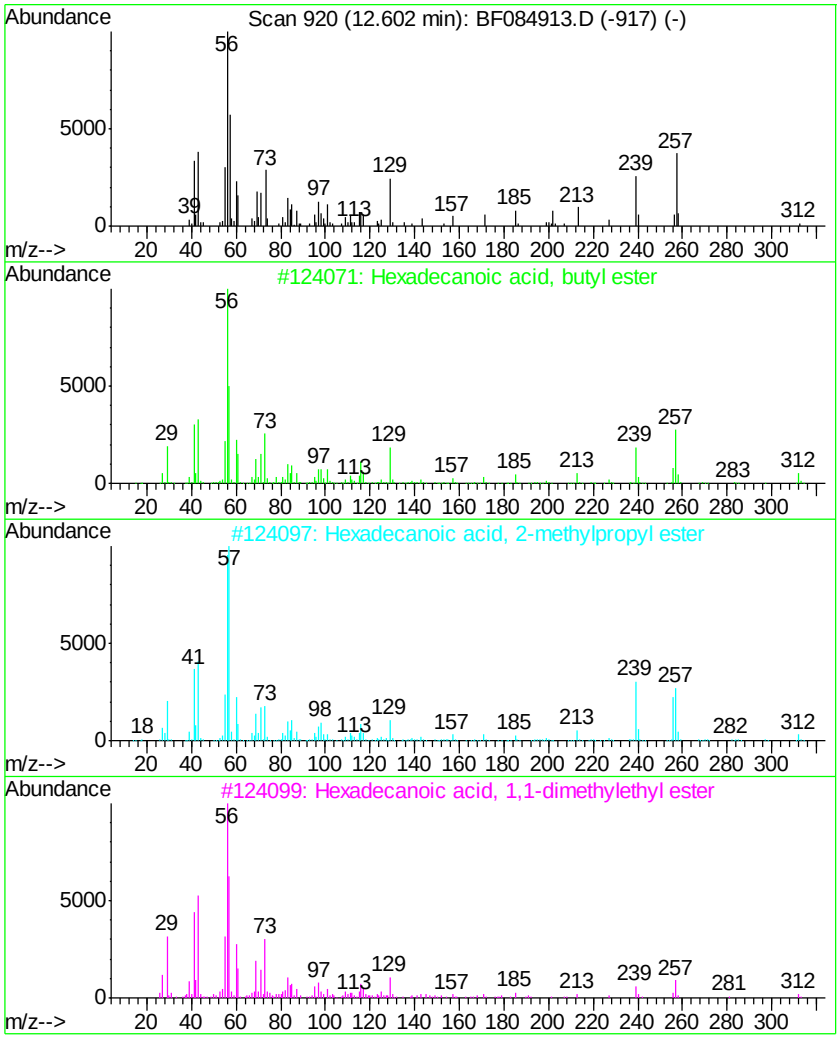
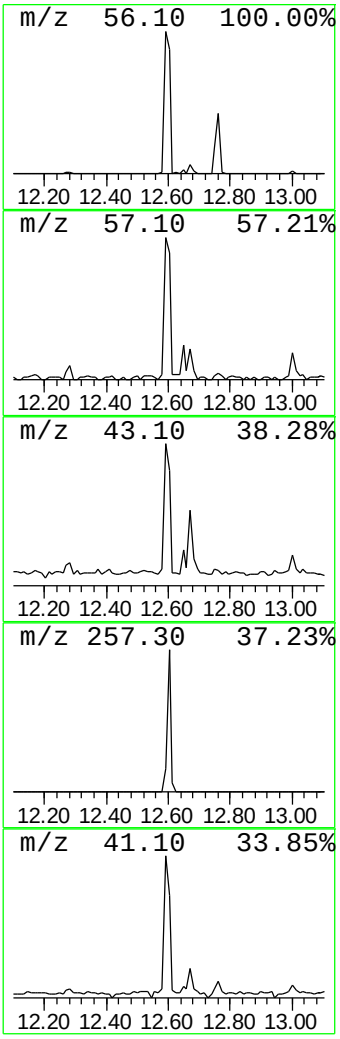
Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.60	4.80 ng	235123	Chrysene-d12	13.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	80
3	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	64
4	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	35
5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	22





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

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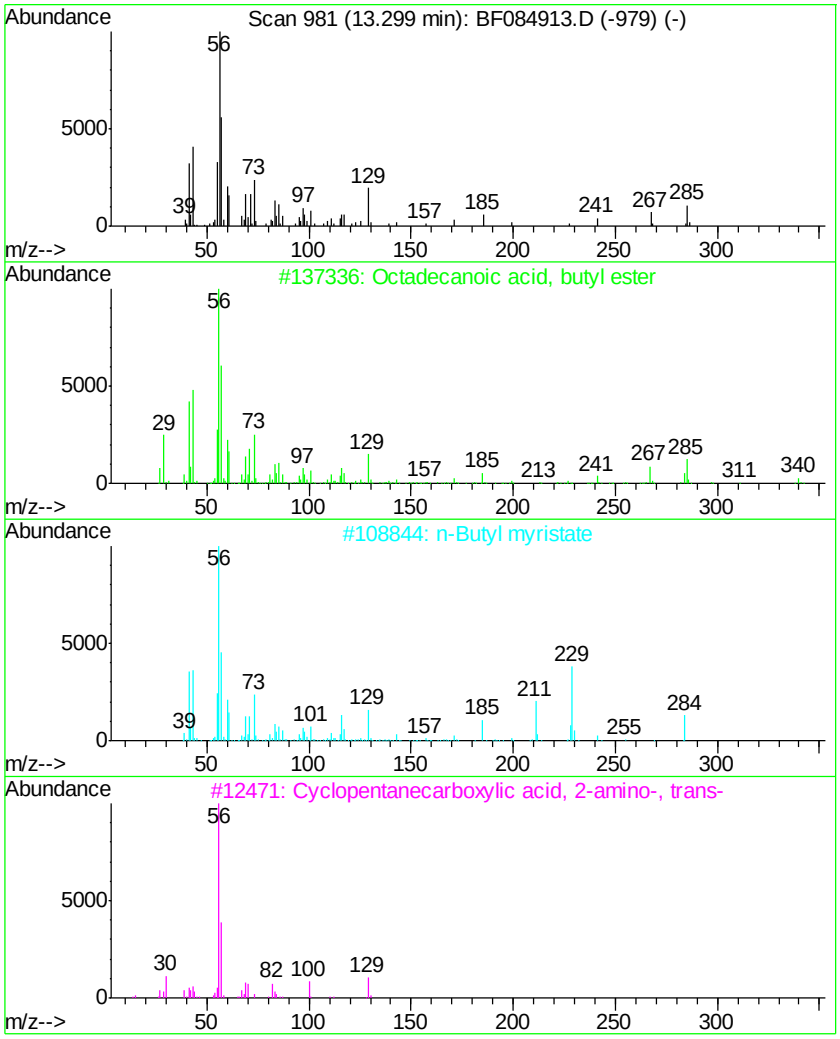
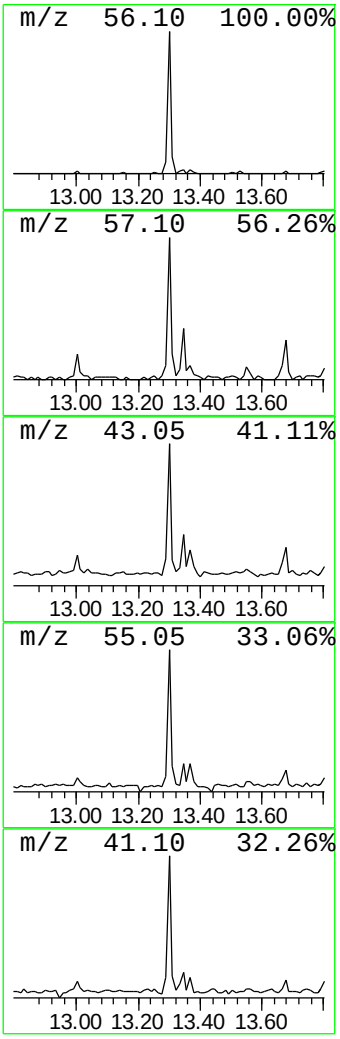
Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.30	3.08 ng	150972	Chrysene-d12	13.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2	n-Butyl myristate	284	C18H36O2	000110-36-1	86
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
5	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37





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	2.38	3.8	ng	210450	1	6.66	1118860	20.0
4-Penten-2-one, 4...	3.06	2.1	ng	117483	1	6.66	1118860	20.0
3-Penten-2-one, 4...	4.12	36.0	ng	2016270	1	6.66	1118860	20.0
2-Pentanone, 4-hy...	4.83	26.8	ng	1498140	1	6.66	1118860	20.0
unknown6.43	6.43	90.4	ng	5059580	1	6.66	1118860	20.0
Hexadecanoic acid...	12.60	4.8	ng	235123	5	13.80	980471	20.0
Octadecanoic acid...	13.30	3.1	ng	150972	5	13.80	980471	20.0