LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093634.D
Acq On : 14 Mar 2017 3:53
Operator : SJ/MA
Sample : I2199-26
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-103

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-BF030717.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	2.458	48	50	61	rVB	61969	188041	2.82%	0.341%
2	3.132	106	109	125	rBV	359863	845573	12.68%	1.533%
3	4.173	198	200	217	rVB	884821	1872162	28.07%	3.394%
4	4.401	218	220	223	rVV	51025	102758	1.54%	0.186%
5	4.458	223	225	229	rVB	56926	79958	1.20%	0.145%
6	4.881	260	262	282	rBV	640322	1295927	19.43%	2.349%
7	5.316	298	300	327	rBV	4644597	6472683	97.03%	11.735%
8	6.367	391	392	400	rBV	3388834	5962691	89.39%	10.810%
9	6.481	400	402	405	rVB	5100650	5366390	80.45%	9.729%
10	6.710	420	422	431	rVB	1107444	1238018	18.56%	2.244%
11	6.859	433	435	438	rBV	4115429	4463260	66.91%	8.092%
12	7.281	470	472	475	rBV	3114639	4049661	60.71%	7.342%
13	8.002	533	535	549	rBV	1384147	1637688	24.55%	2.969%
14	9.087	627	630	632	rBV	4628972	6670718	100.00%	12.094%
15	9.762	686	689	691	rBV	1389564	1725513	25.87%	3.128%
16	10.550	756	758	761	rBV	2302461	3499121	52.45%	6.344%
17	11.248	817	819	824	rBV	1825074	1817236	27.24%	3.295%
18	12.836	955	958	961	rBV	4573851	5651095	84.71%	10.245%
19	13.899	1049	1051	1060	rBV	1151718	1421829	21.31%	2.578%
20	15.317	1171	1175	1185	rBV2	260858	598044	8.97%	1.084%
21	15.682	1204	1207	1212	rBV	68210	106193	1.59%	0.193%
22	16.128	1243	1246	1251	rBV	55709	94337	1.41%	0.171%

Sum of corrected areas: 55158896

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093634.D
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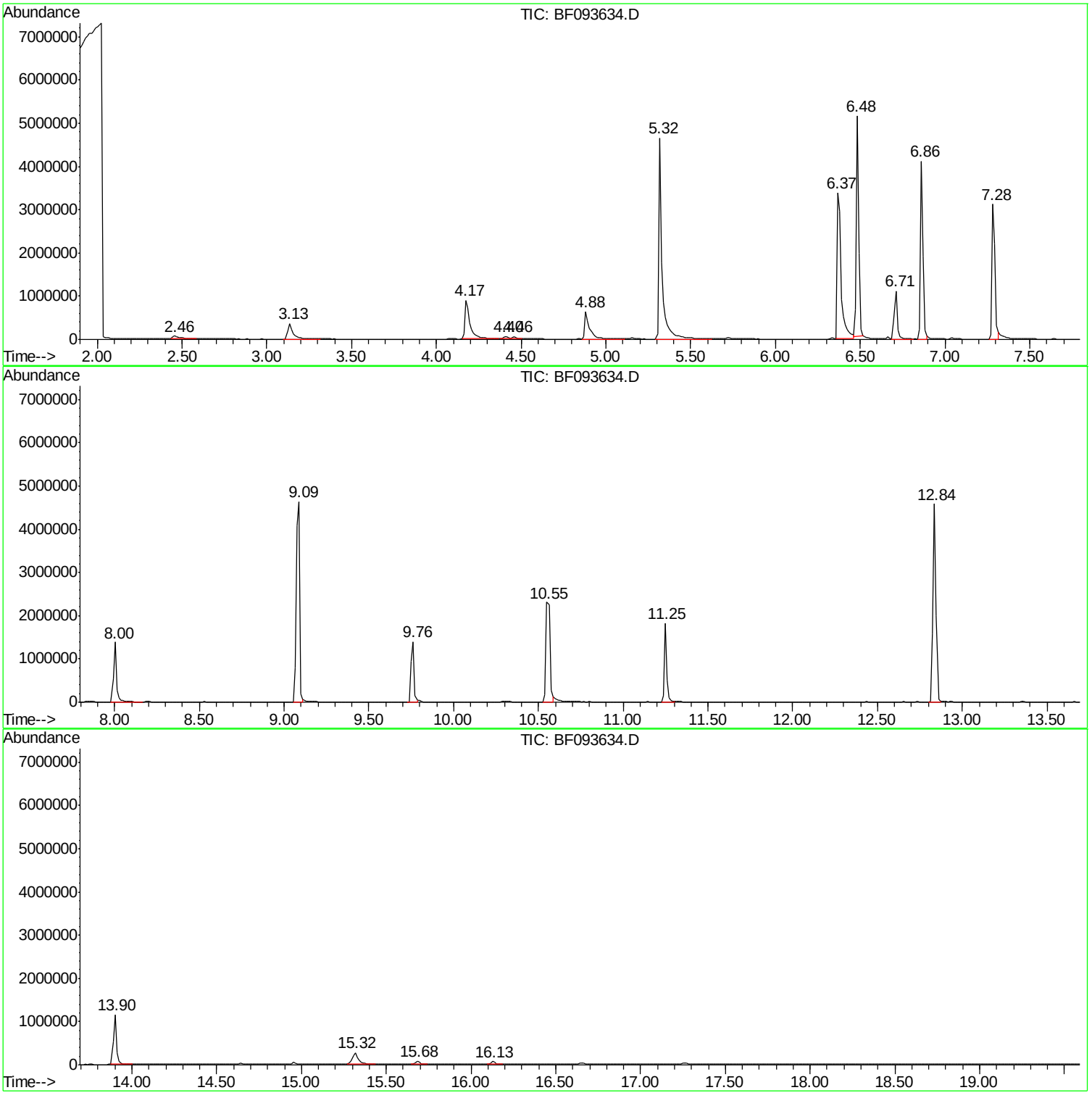
Operator : SJ/MA
Sample : I2199-26
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-103

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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\BF031317\
Data File : BF093634.D
Acq On : 14 Mar 2017 3:53
Operator : SJ/MA
Sample : I2199-26
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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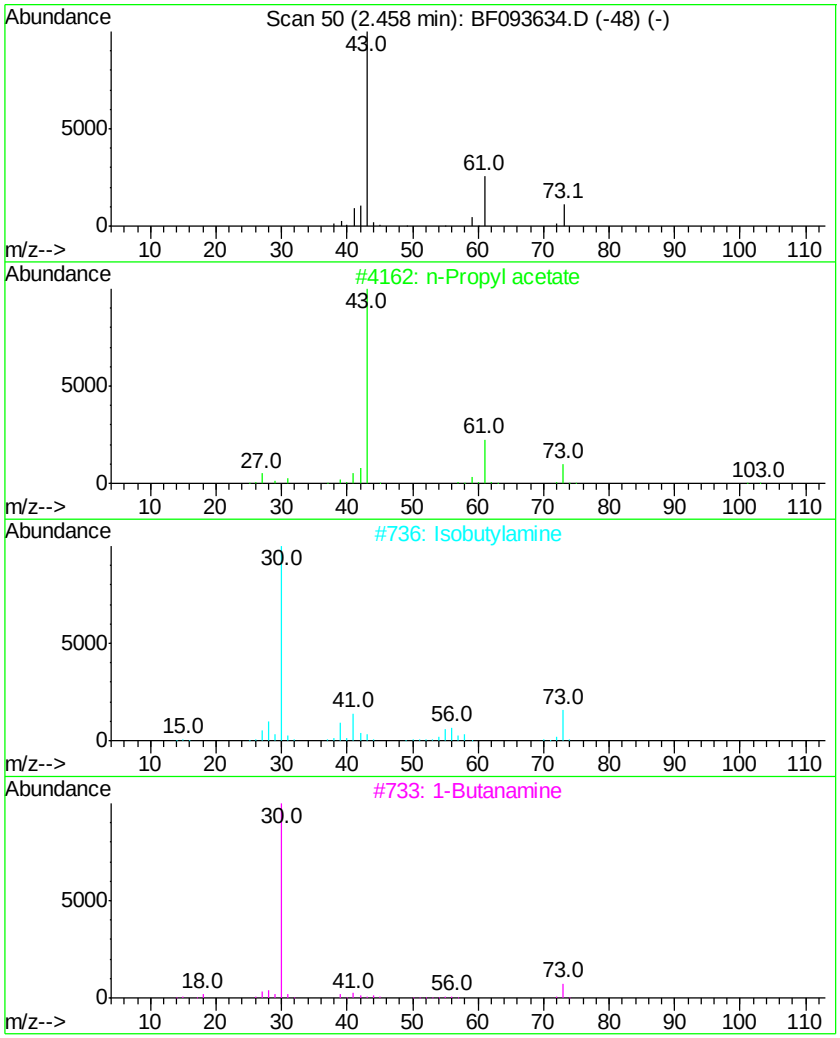
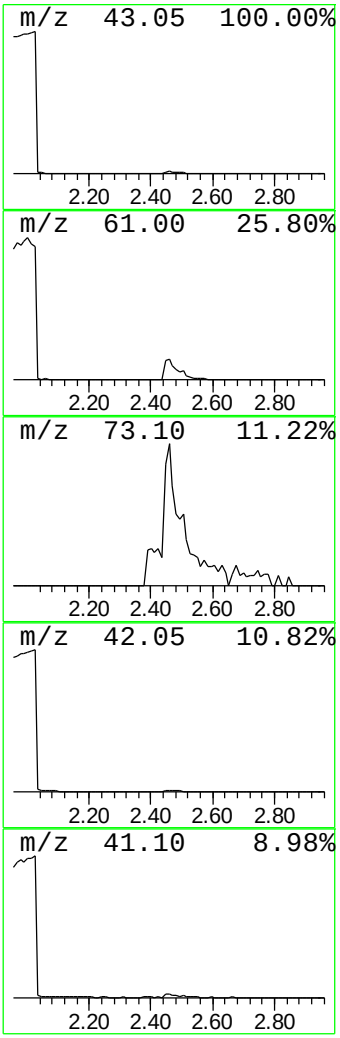
****

Peak Number 1 n-Propyl acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.46	3.04 ng	188041	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2	Isobutylamine	73	C4H11N	000078-81-9	7
3	1-Butanamine	73	C4H11N	000109-73-9	5
4	Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	5
5	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4





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Acq On : 14 Mar 2017 3:53
Operator : SJ/MA
Sample : I2199-26
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-103

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

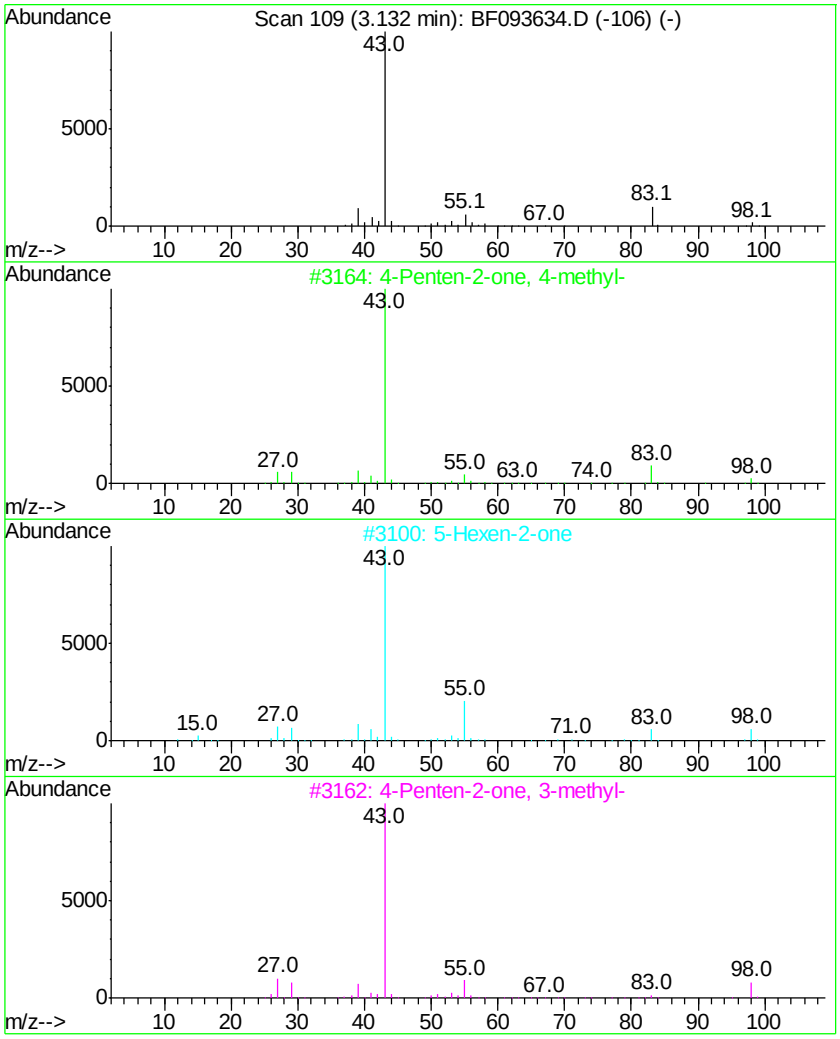
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

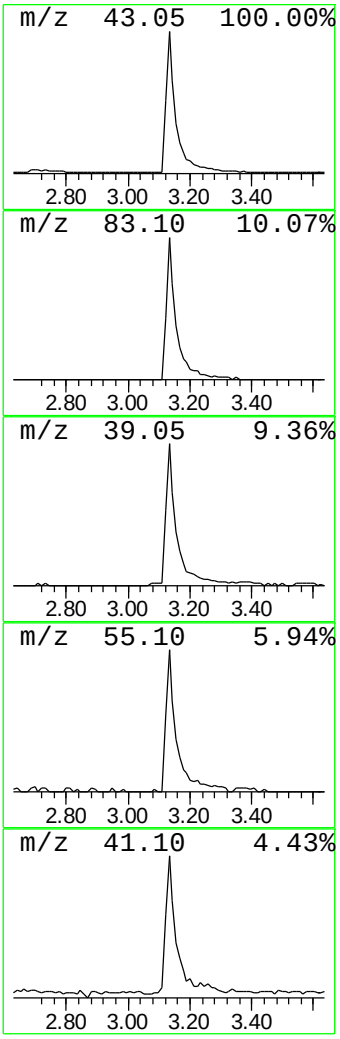
****

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	13.66 ng	845573	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2	5-Hexen-2-one	98	C6H10O	000109-49-9	38
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	9
4	4-Hexen-2-one	98	C6H10O	025659-22-7	9
5	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093634.D
Acq On : 14 Mar 2017 3:53
Operator : SJ/MA
Sample : I2199-26
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-103

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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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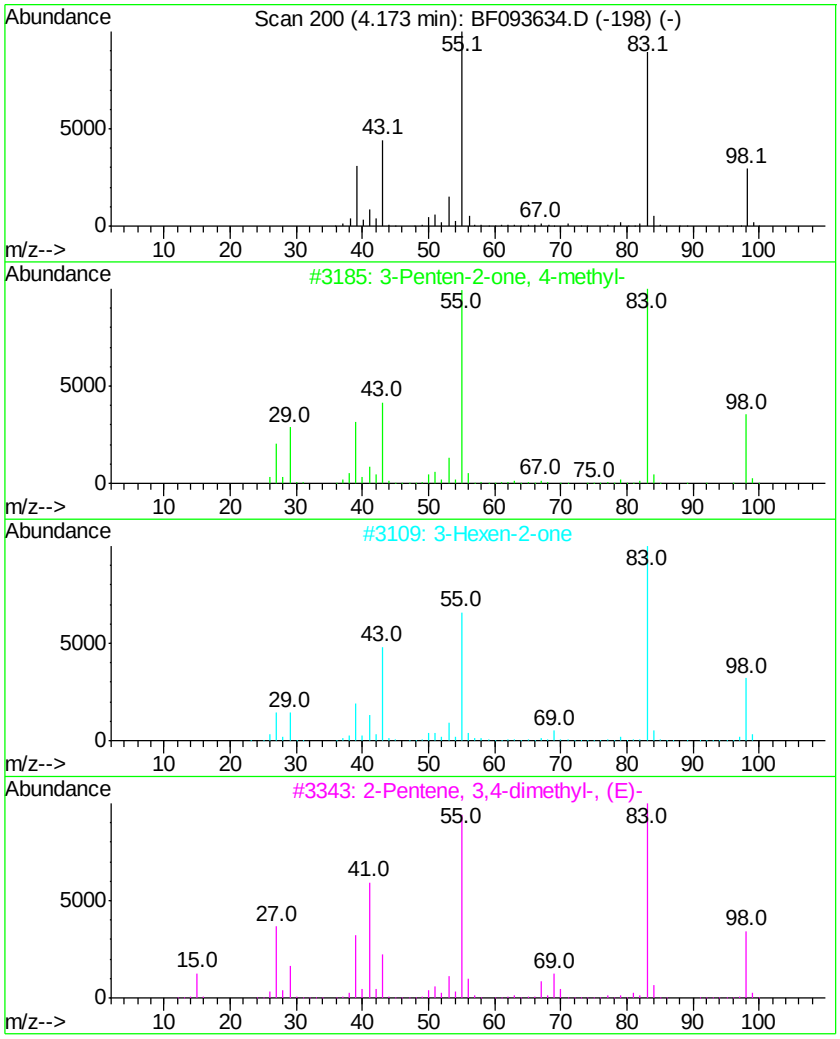
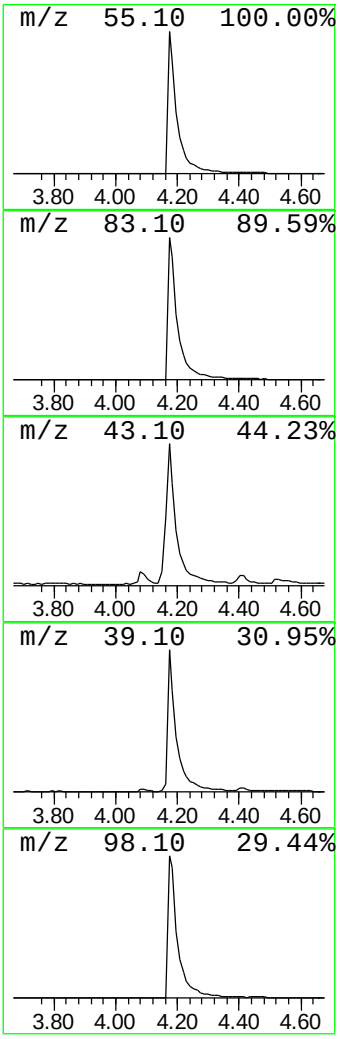
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.17	30.24 ng	1872160	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
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Acq On : 14 Mar 2017 3:53
Operator : SJ/MA
Sample : I2199-26
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-103

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

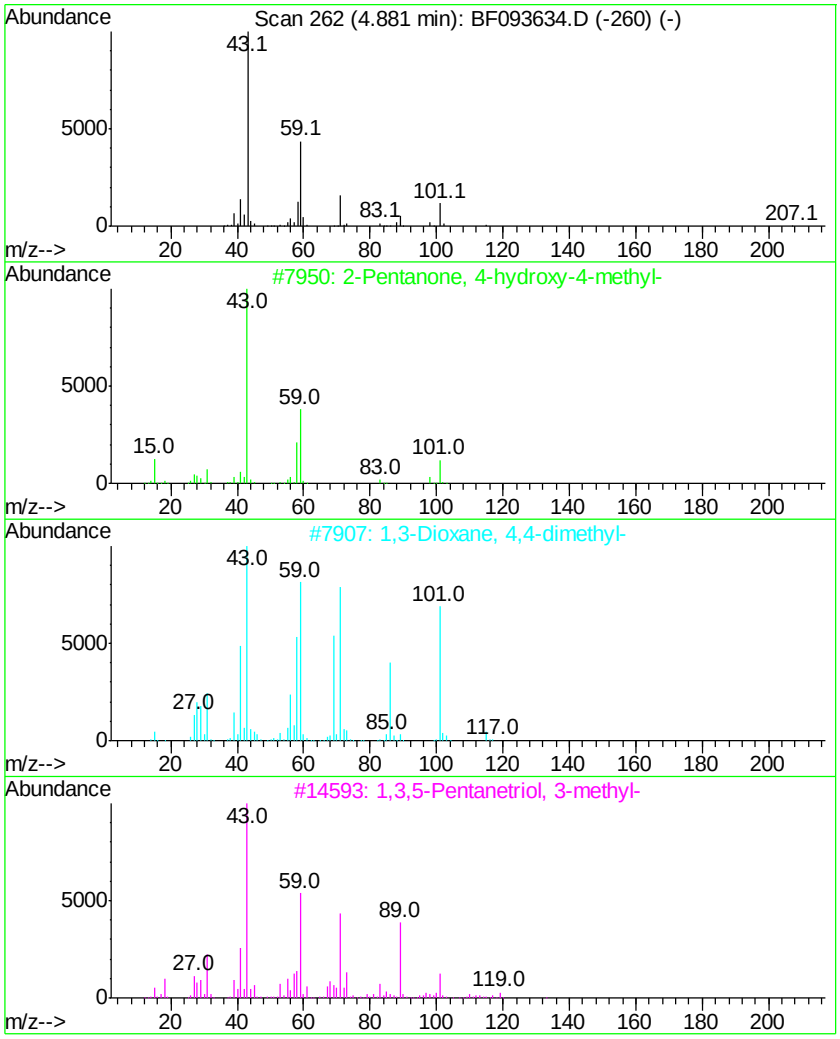
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

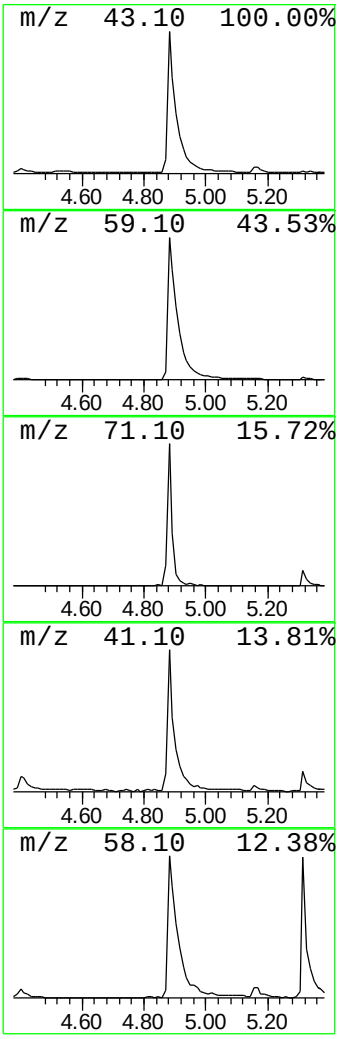
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	20.94 ng	1295930	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	38
3	1,3,5-Pentanetriol, 3-methyl-	134	C6H14O3	007564-64-9	38
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093634.D
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Operator : SJ/MA
Sample : I2199-26
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-103

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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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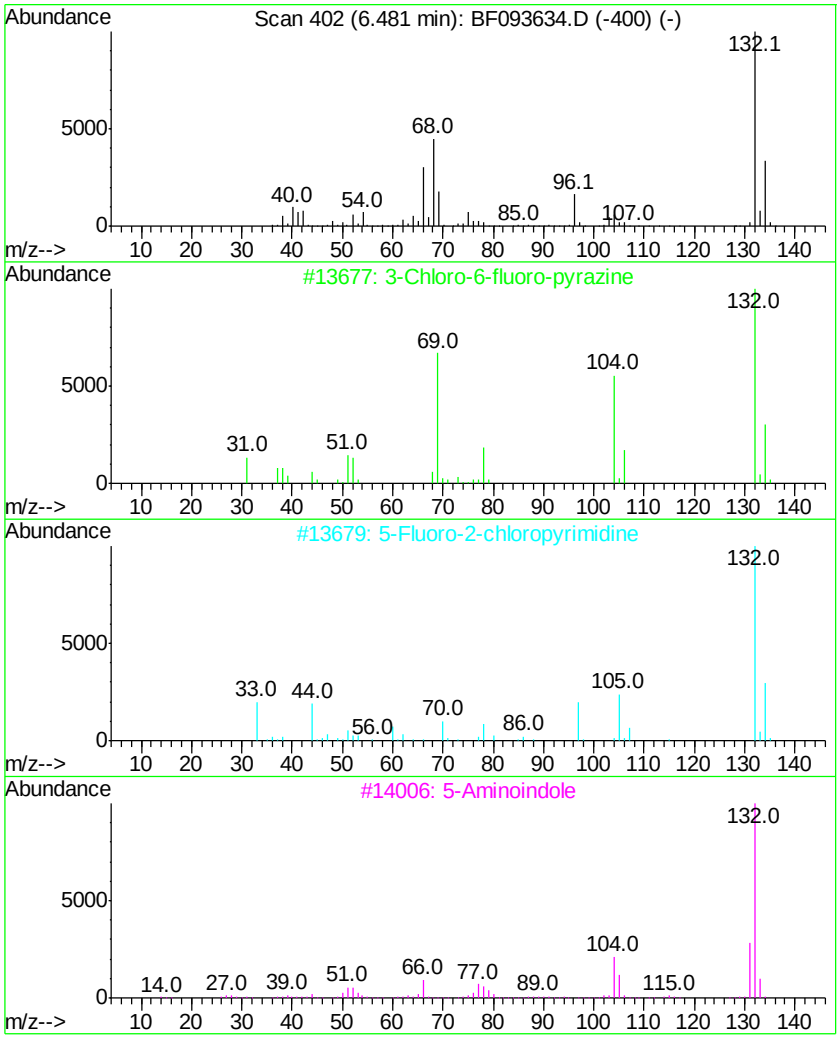
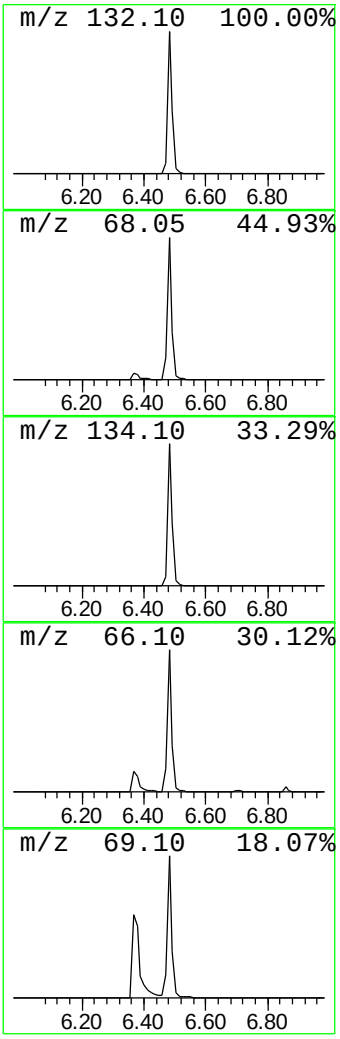
Peak Number 5 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	86.69 ng	5366390	1,4-Dichlorobenzene-d4	6.71

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	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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ClientSampleId : D-103

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

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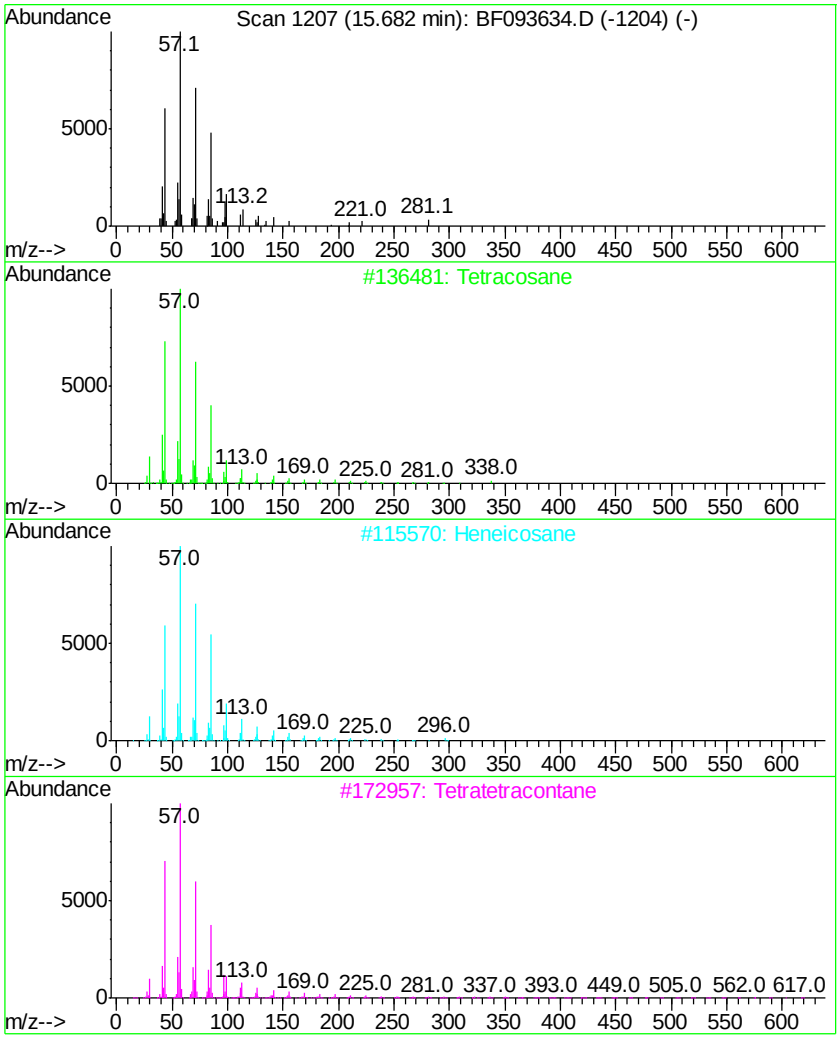
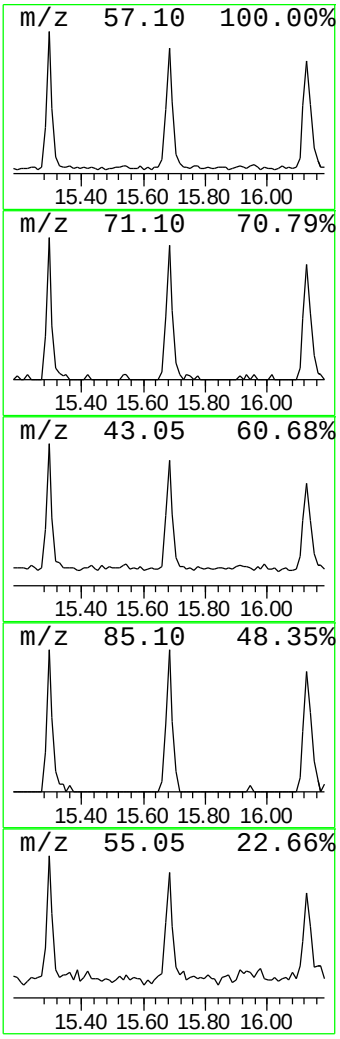
Peak Number 7 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.68	3.55 ng	106193	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Hexatriacontane	507	C36H74	000630-06-8	91
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90





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Data File : BF093634.D
Acq On : 14 Mar 2017 3:53
Operator : SJ/MA
Sample : I2199-26
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-103

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

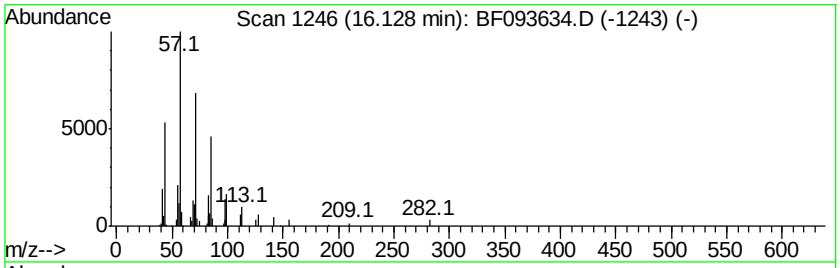
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

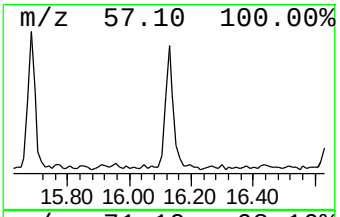
****

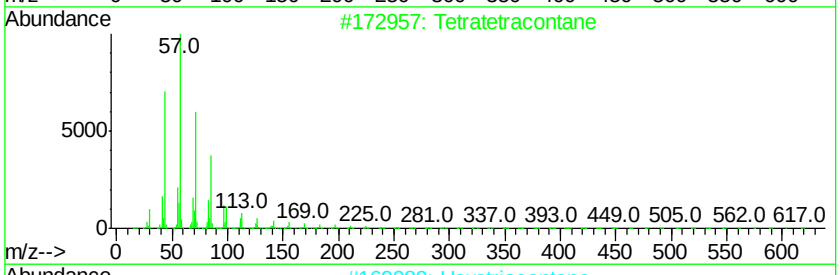
Peak Number 8 Tetratetracontane Concentration Rank 7

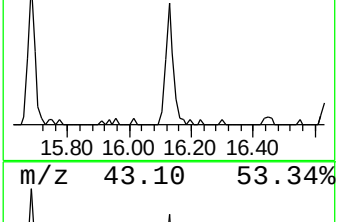
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	3.15 ng	94337	Perylene-d12	15.32

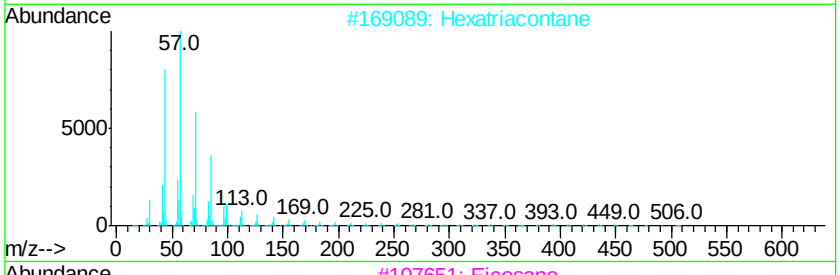
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	91
2	Hexatriacontane	507	C36H74	000630-06-8	91
3	Eicosane	282	C20H42	000112-95-8	90
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90

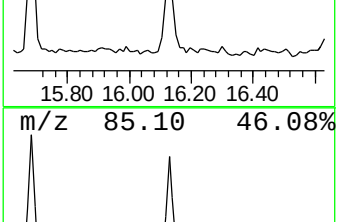


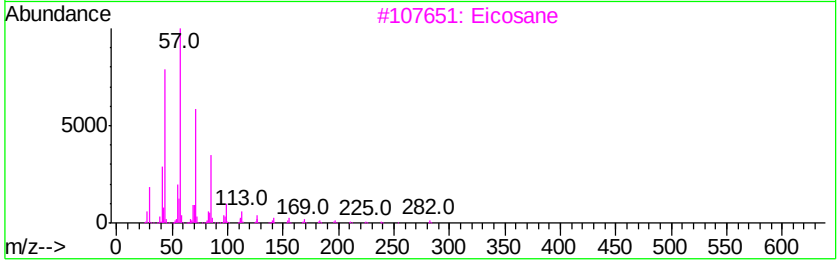


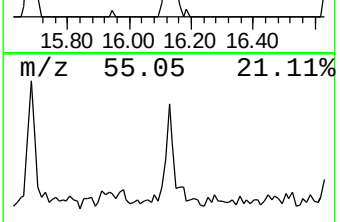












Tentatively Identified Compound (LSC) summary

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Operator : SJ/MA
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Misc :
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Instrument : BNA_F
ClientSampleId : D-103

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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
n-Propyl acetate	2.46	3.0	ng	188041	1	6.71	1238020	20.0
4-Penten-2-one, 4...	3.13	13.7	ng	845573	1	6.71	1238020	20.0
3-Penten-2-one, 4...	4.17	30.2	ng	1872160	1	6.71	1238020	20.0
2-Pentanone, 4-hy...	4.88	20.9	ng	1295930	1	6.71	1238020	20.0
unknown6.48	6.48	86.7	ng	5366390	1	6.71	1238020	20.0
Tetracosane	15.68	3.5	ng	106193	6	15.32	598044	20.0
Tetratetracontane	16.13	3.1	ng	94337	6	15.32	598044	20.0