LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\Data\BM033117\
Data File : BM009484.D
Acq On : 31 Mar 2017 21:22
Operator : SJ/MA
Sample : I2475-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : QNWP8-MW25S-GW

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_M\METHODS\8270-BM032217.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	4.969	316	320	333	rVB	88029	123851	1.25%	0.258%
2	5.422	389	397	403	rBV	1469354	2088720	21.04%	4.343%
3	7.004	659	666	676	rBV	844804	1400477	14.11%	2.912%
4	7.375	722	729	740	rBV	2439311	3826406	38.54%	7.956%
5	7.845	803	809	816	rBV	525656	823570	8.30%	1.712%
6	8.169	857	864	871	rVB	2068091	3432873	34.58%	7.138%
7	9.010	999	1007	1015	rBV	1850559	3077224	31.00%	6.398%
8	10.645	1278	1285	1292	rBV	625985	1048039	10.56%	2.179%
9	11.522	1428	1434	1439	rBV3	118441	203979	2.05%	0.424%
10	13.104	1696	1703	1714	rBV	4094119	6118424	61.63%	12.721%
11	13.604	1783	1788	1795	rBV5	182418	307381	3.10%	0.639%
12	13.939	1840	1845	1851	rBV	126515	183952	1.85%	0.382%
13	14.492	1933	1939	1945	rBV3	852501	1399748	14.10%	2.910%
14	15.010	2018	2027	2032	rBV3	83917	156622	1.58%	0.326%
15	15.315	2073	2079	2083	rVB4	119477	212248	2.14%	0.441%
16	15.651	2130	2136	2142	rBV3	156538	245345	2.47%	0.510%
17	15.980	2186	2192	2201	rBV	3497479	4941551	49.78%	10.274%
18	16.180	2222	2226	2236	rVB4	106377	243178	2.45%	0.506%
19	17.239	2400	2406	2412	rBV	1221308	1702674	17.15%	3.540%
20	18.115	2550	2555	2563	rBV	451418	681887	6.87%	1.418%
21	19.392	2768	2772	2784	rBV	359217	540618	5.45%	1.124%
22	19.856	2846	2851	2859	rBV	7974091	9927490	100.00%	20.641%
23	21.109	3060	3064	3070	rBV	407624	510377	5.14%	1.061%
24	21.415	3111	3116	3122	rBV	2071147	2509140	25.27%	5.217%
25	23.738	3504	3511	3519	rVB	1219804	2390033	24.07%	4.969%

Sum of corrected areas: 48095807

LSC Report - Integrated Chromatogram

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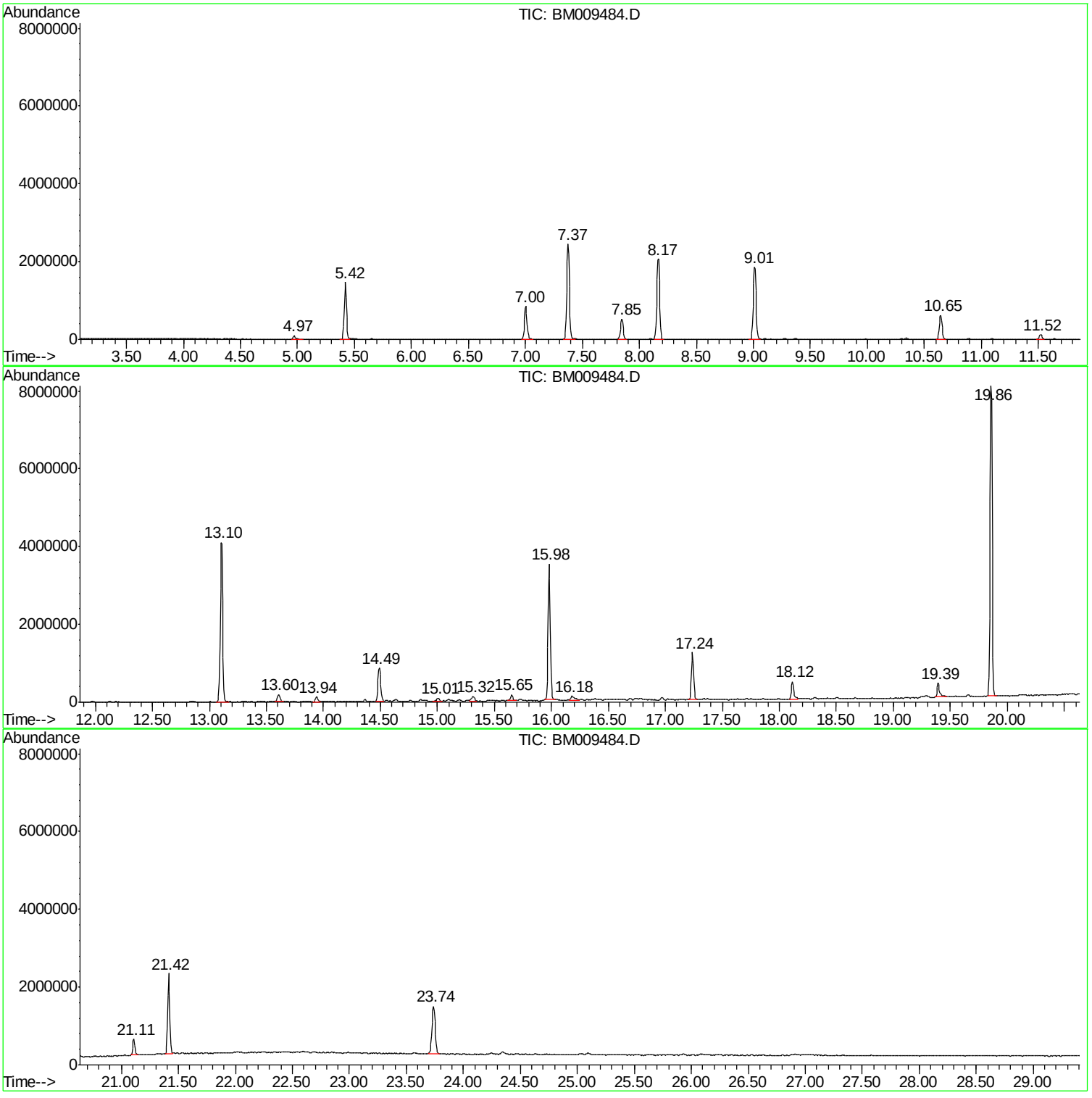
Operator : SJ/MA
Sample : I2475-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : QNWP8-MW25S-GW

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.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 M\Data\BM033117\
Data File : BM009484.D
Acq On : 31 Mar 2017 21:22
Operator : SJ/MA
Sample : I2475-01
Misc :
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Instrument : BNA_M
ClientSampleId : QNWP8-MW25S-GW

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

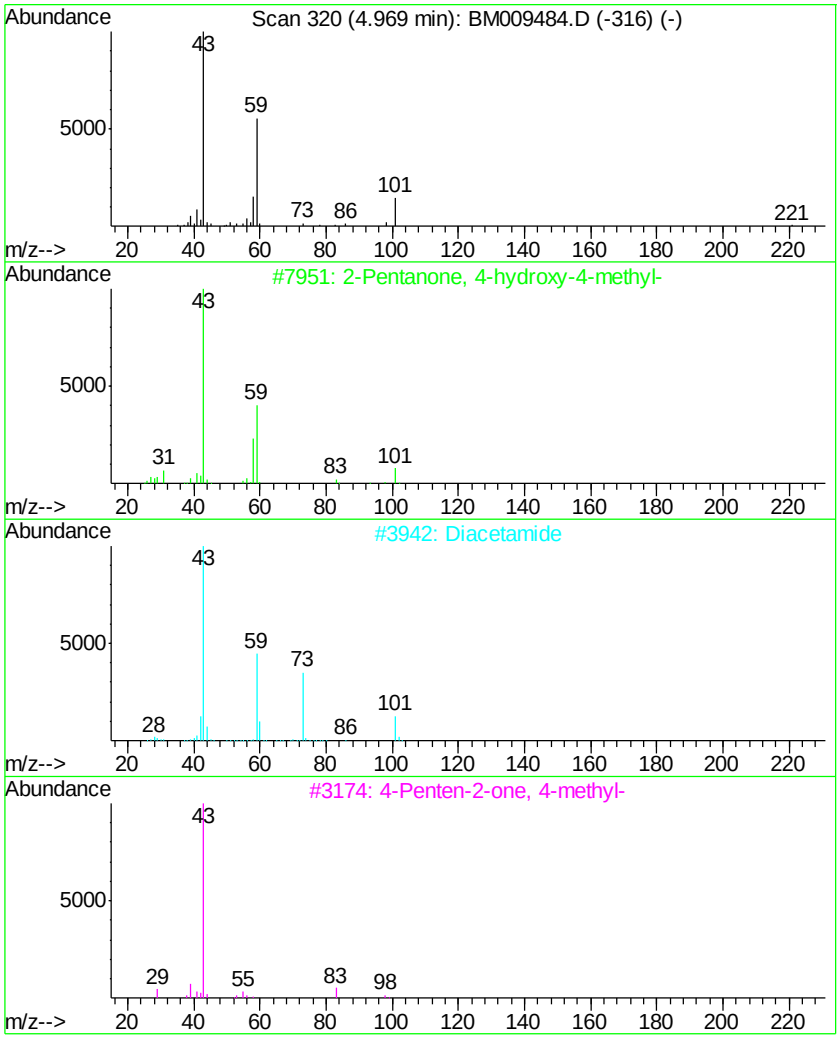
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

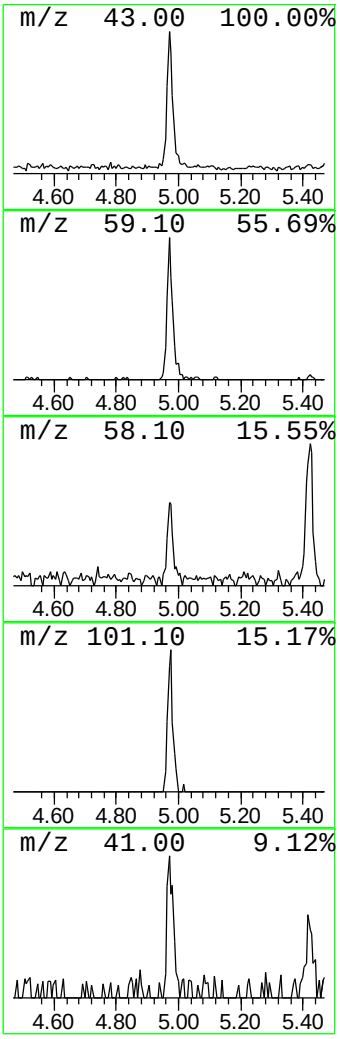
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	3.01 ng	123851	1,4-Dichlorobenzene-d4	7.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Diacetamide	101	C4H7NO2	000625-77-4	9
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4	t-Butyl ethyl ether	102	C6H14O	1000118-18-4	9
5	2-Heptanone, 7,7-dichloro-	182	C7H12Cl2O	066241-43-8	9





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Data File : BM009484.D
Acq On : 31 Mar 2017 21:22
Operator : SJ/MA
Sample : I2475-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : QNWP8-MW25S-GW

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

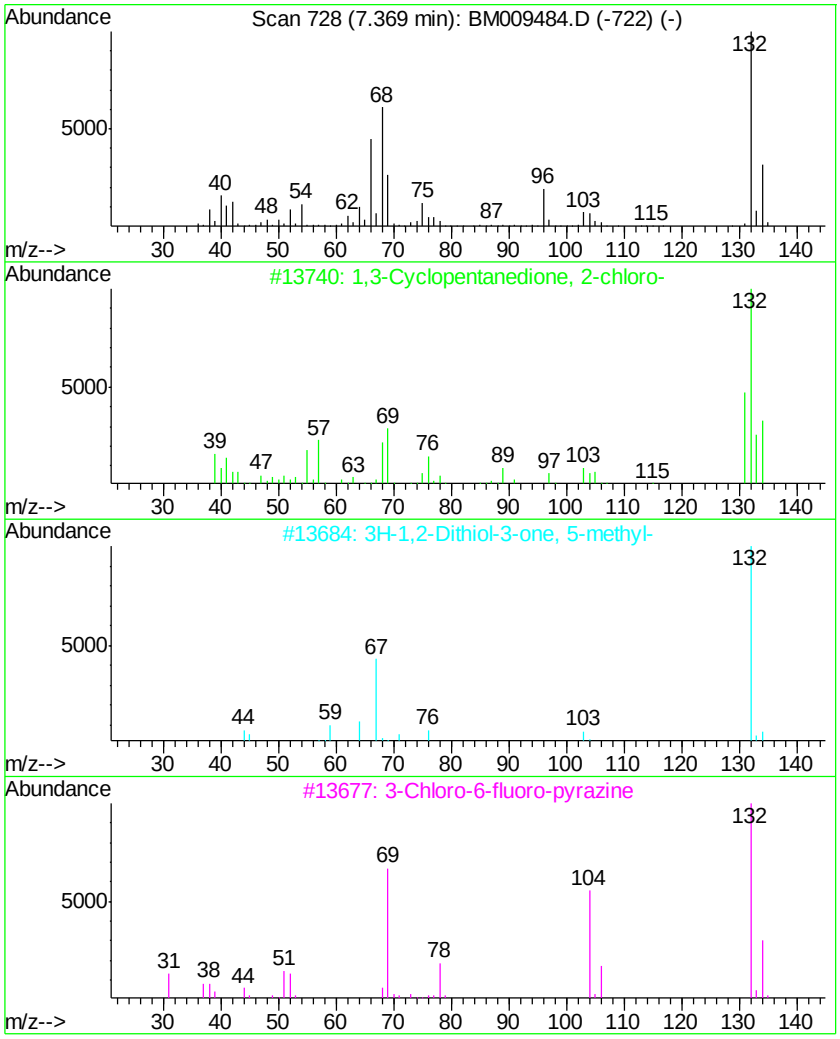
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

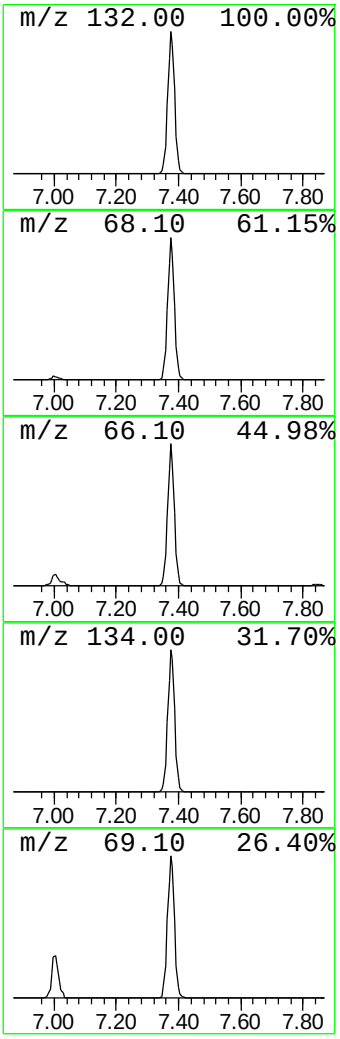
****

Peak Number 2 unknown7.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	92.92 ng	3826410	1,4-Dichlorobenzene-d4	7.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	11
5	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	10





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Operator : SJ/MA
Sample : I2475-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : QNWP8-MW25S-GW

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
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TIC Library : C:\DATABASE\NIST02.L
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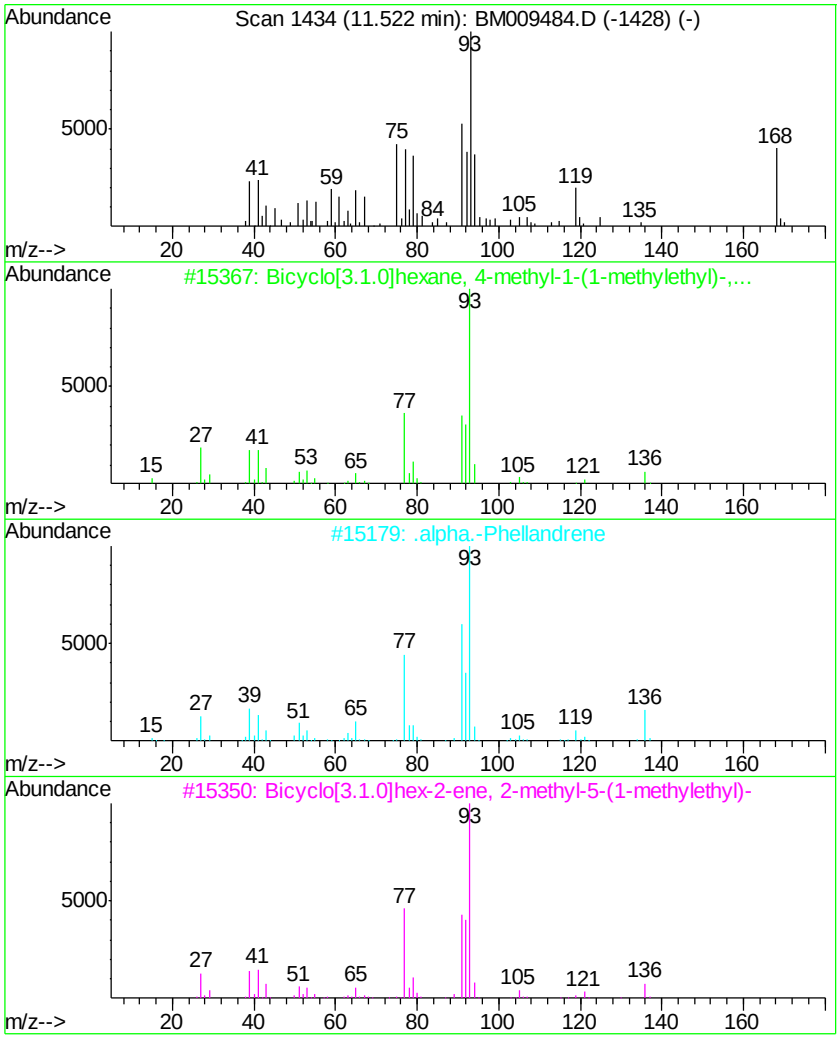
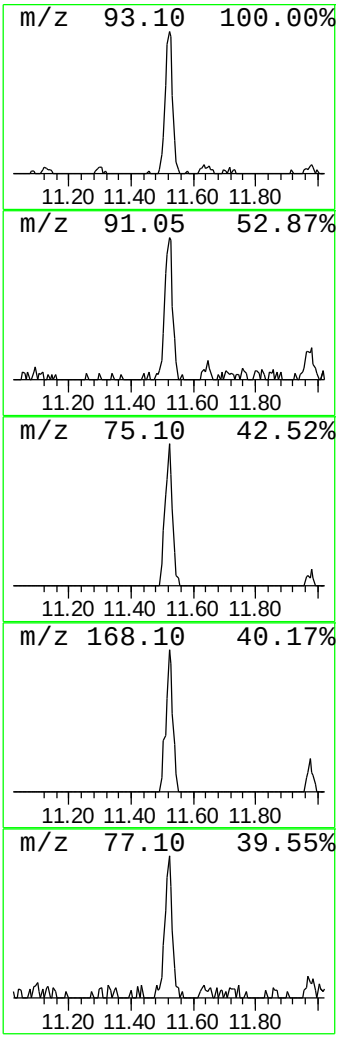
Peak Number 4 unknown11.52 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.52	3.89 ng	203979	Naphthalene-d8	10.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.0]hexane, 4-methyl-1...	136	C10H16	058037-87-9	43
2	.alpha.-Phellandrene	136	C10H16	000099-83-2	38
3	Bicyclo[3.1.0]hex-2-ene, 2-methy...	136	C10H16	002867-05-2	38
4	1,3,6-Octatriene, 3,7-dimethyl-,...	136	C10H16	003779-61-1	38
5	1S-.alpha.-Pinene	136	C10H16	007785-26-4	37





Data Path : Z:\HPCHEM1\BNA M\Data\BM033117\
Data File : BM009484.D
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Sample : I2475-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : QNWP8-MW25S-GW

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

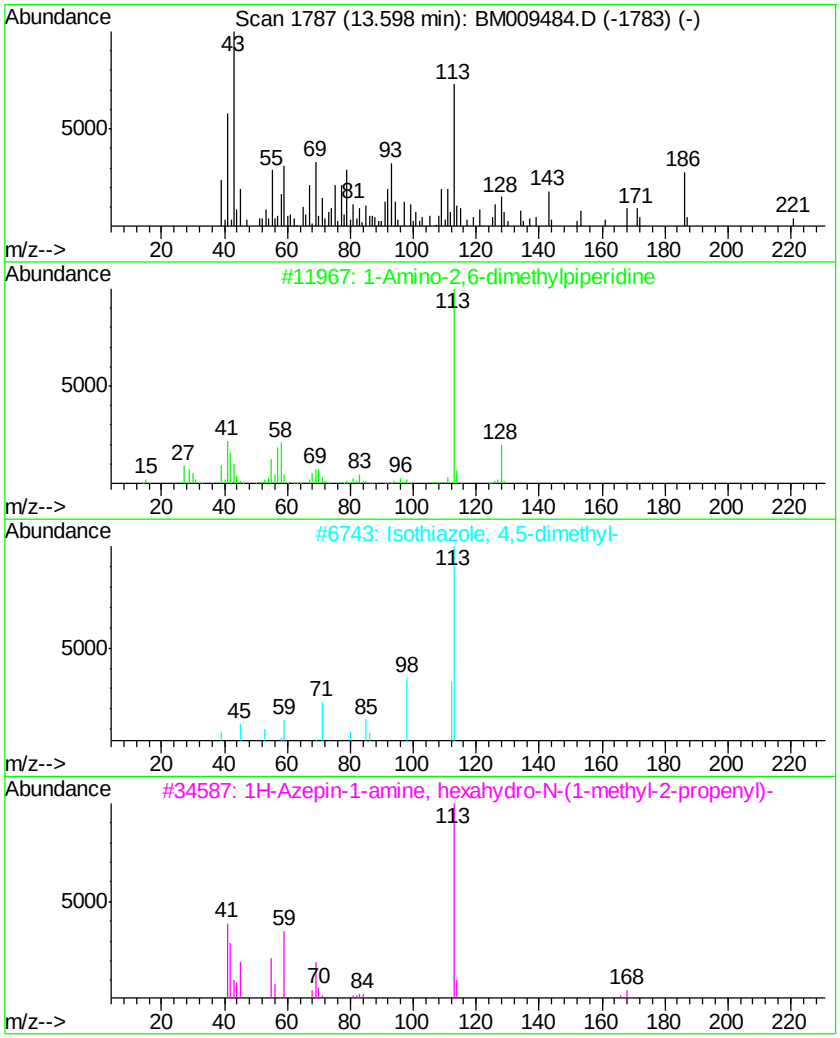
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

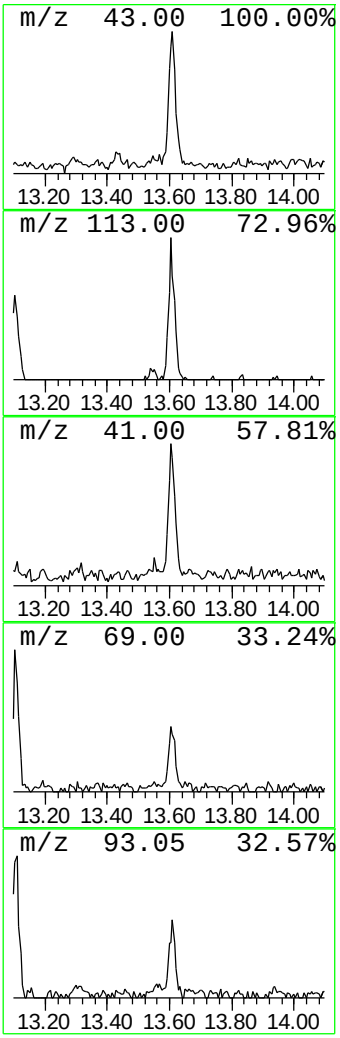
****

Peak Number 5 unknown13.60 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	4.39 ng	307381	Acenaphthene-d10	14.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Amino-2,6-dimethylpiperidine	128	C7H16N2	039135-39-2	38
2	Isothiazole, 4,5-dimethyl-	113	C5H7NS	027330-47-8	35
3	1H-Azepin-1-amine, hexahydro-N-(...	168	C10H20N2	028075-23-2	35
4	Propionaldehyde, diethylhydrazone	128	C7H16N2	028236-90-0	35
5	Acetaldehyde, ethyl(1-methylethy...	128	C7H16N2	075268-00-7	35





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Operator : SJ/MA
Sample : I2475-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : QNWP8-MW25S-GW

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

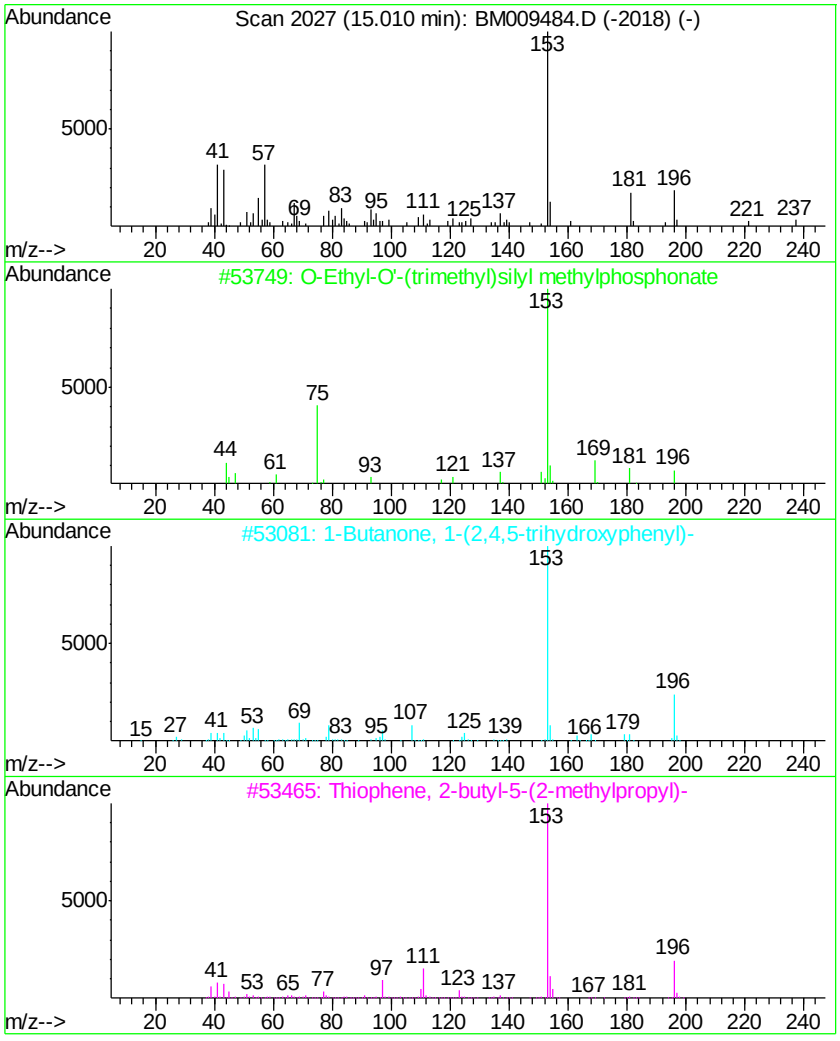
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

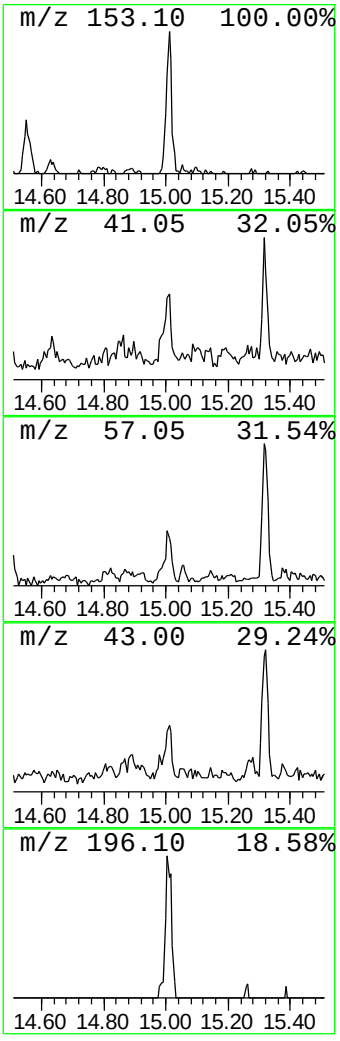
****

Peak Number 6 O-Ethyl-O'-(trimethyl)silyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.01	2.24 ng	156622	Acenaphthene-d10	14.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	O-Ethyl-O'-(trimethyl)silyl meth...	196	C6H17O3PSi	057451-30-6	72
2	1-Butanone, 1-(2,4,5-trihydroxyp...	196	C10H12O4	001421-63-2	53
3	Thiophene, 2-butyl-5-(2-methylpr...	196	C12H20S	054845-35-1	53
4	Methylphosphonic acid, anhydride...	278	C12H27O3PSi	1000273-46-7	53
5	N-Methyl-6-[2-naphthalenyl]-1,2,...	237	C13H11N5	072115-48-1	53





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Instrument : BNA_M
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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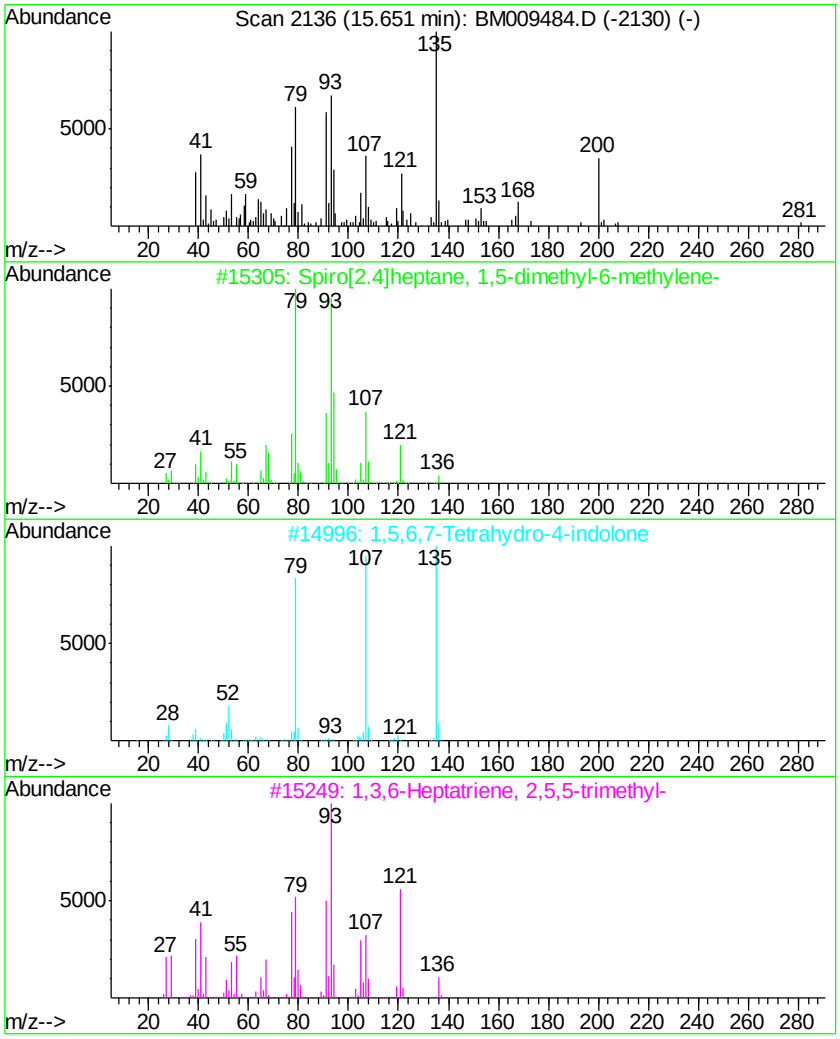
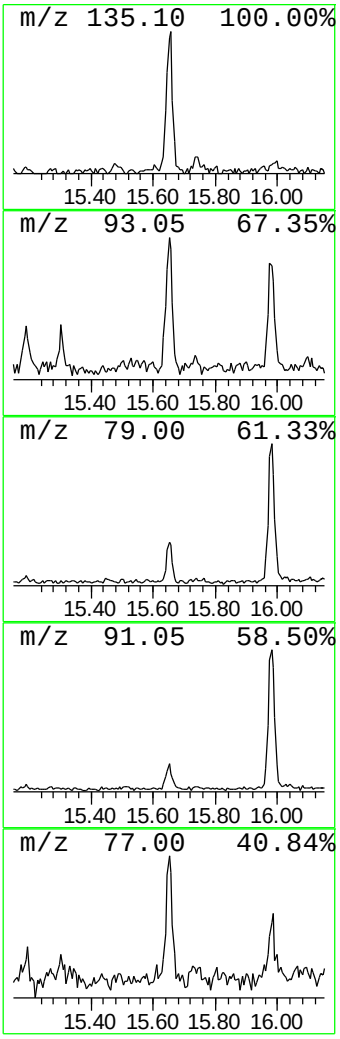
****

Peak Number 7 unknown15.65 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.65	3.51 ng	245345	Acenaphthene-d10	14.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Spiro[2.4]heptane, 1,5-dimethyl-...	136	C10H16	062238-24-8	46
2	1,5,6,7-Tetrahydro-4-indolone	135	C8H9NO	013754-86-4	41
3	1,3,6-Heptatriene, 2,5,5-trimethyl-	136	C10H16	029548-02-5	38
4	Bicyclo[4.1.0]hept-2-ene, 3,7,7-...	136	C10H16	000554-61-0	38
5	Cyclobutane, 2-ethylidene-1-vinyl-	108	C8H12	1000150-32-4	38





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ClientSampleId : QNWP8-MW25S-GW

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

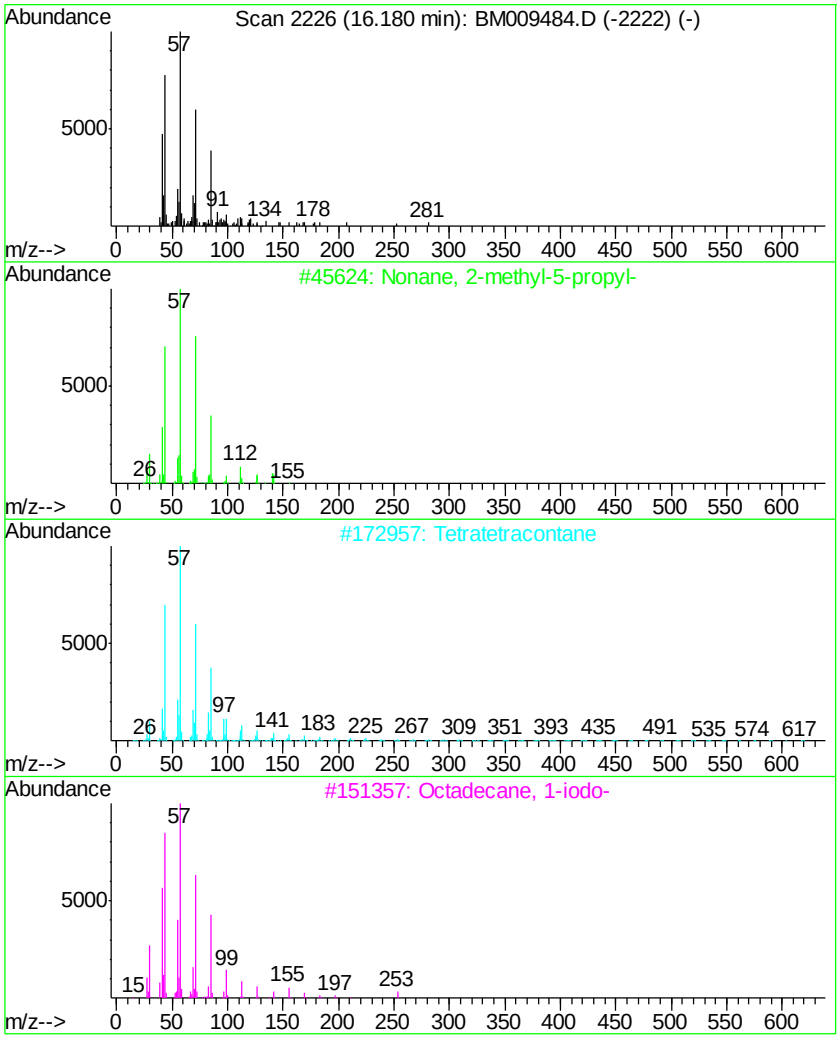
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

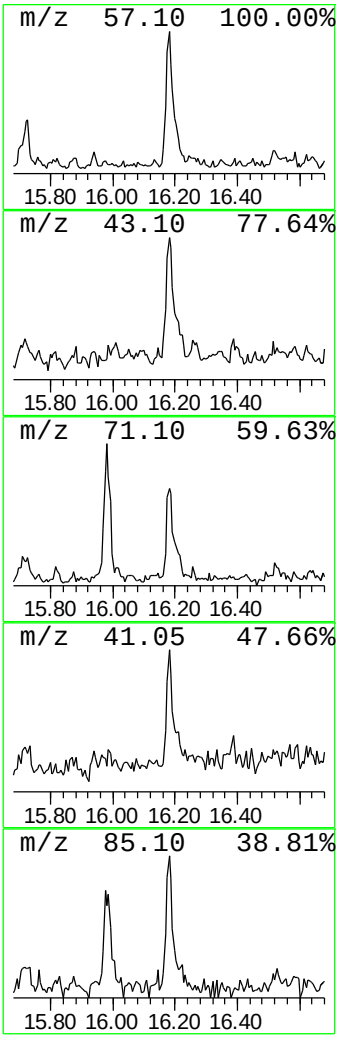
****

Peak Number 8 Nonane, 2-methyl-5-propyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	2.86 ng	243178	Phenanthrene-d10	17.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	64
2	Tetratetracontane	619	C44H90	007098-22-8	64
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	59
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	59
5	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	59





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ClientSampleId : QNWP8-MW25S-GW

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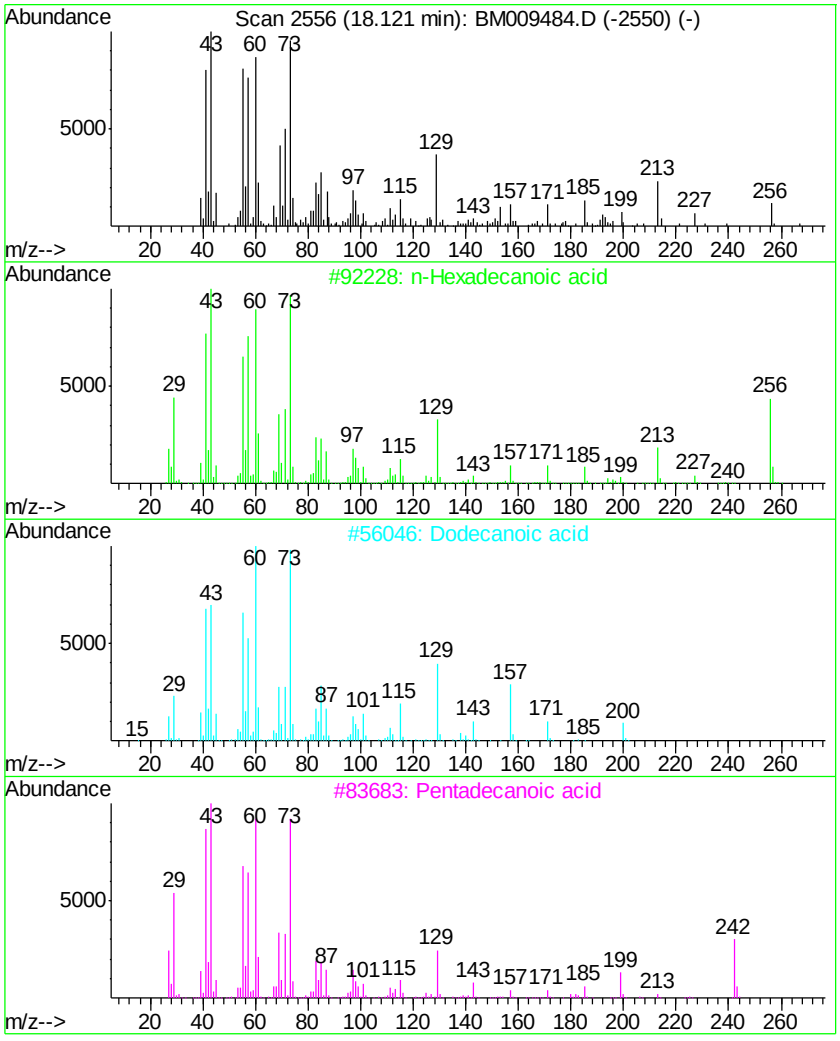
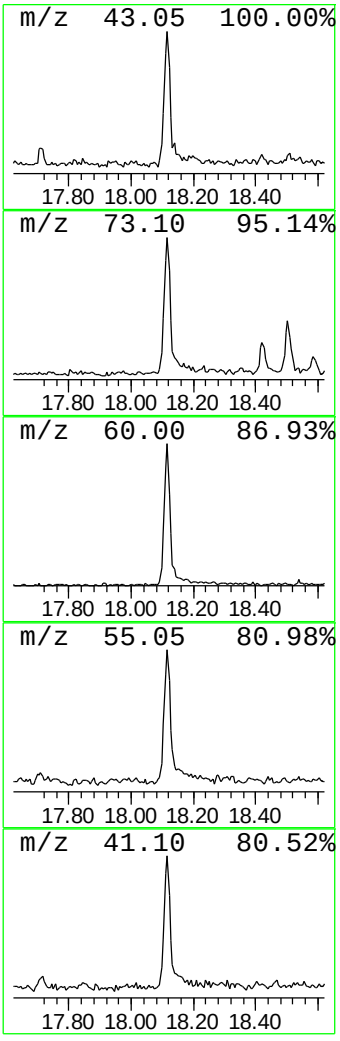
****

Peak Number 9 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.12	8.01 ng	681887	Phenanthrene-d10	17.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Dodecanoic acid	200	C12H24O2	000143-07-7	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Undecanoic acid	186	C11H22O2	000112-37-8	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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Instrument : BNA_M
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
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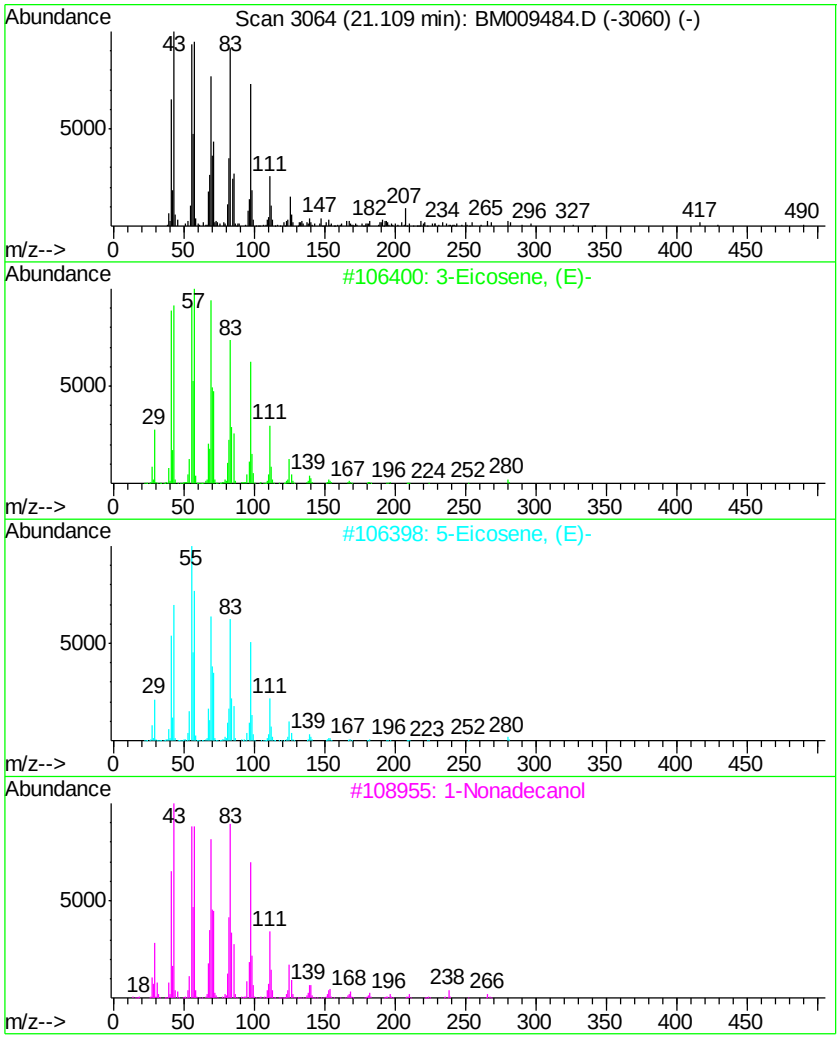
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

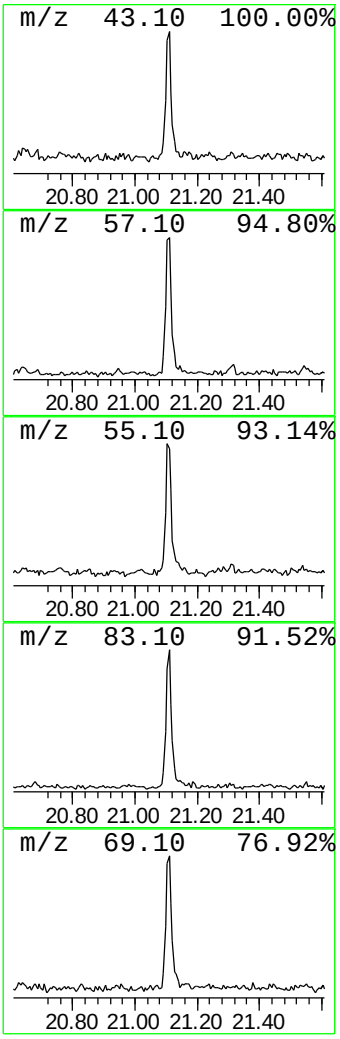
****

Peak Number 11 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.11	4.07 ng	510377	Chrysene-d12	21.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	99
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
3	1-Nonadecanol	284	C19H40O	001454-84-8	94
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
5	17-Pentatriacontene	491	C35H70	006971-40-0	89





Tentatively Identified Compound (LSC) summary

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Acq On : 31 Mar 2017 21:22
Operator : SJ/MA
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : QNWP8-MW25S-GW

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.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
2-Pentanone, 4-hy...	4.97	3.0	ng	123851	1	7.85	823570	20.0
unknown7.37	7.37	92.9	ng	3826410	1	7.85	823570	20.0
unknown11.52	11.52	3.9	ng	203979	2	10.65	1048040	20.0
unknown13.60	13.60	4.4	ng	307381	3	14.49	1399750	20.0
O-Ethyl-O'-(trime...	15.01	2.2	ng	156622	3	14.49	1399750	20.0
unknown15.65	15.65	3.5	ng	245345	3	14.49	1399750	20.0
Nonane, 2-methyl-...	16.18	2.9	ng	243178	4	17.24	1702670	20.0
n-Hexadecanoic acid	18.12	8.0	ng	681887	4	17.24	1702670	20.0
3-Eicosene, (E)-	21.11	4.1	ng	510377	5	21.42	2509140	20.0