LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM033017\
Data File : BM009456.D
Acq On : 30 Mar 2017 18:21
Operator : SJ/MA
Sample : I2445-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 032717-PRRT-F-U-M

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	4.375	213	219	226	rBV	103018	151597	1.55%	0.376%
2	4.969	315	320	330	rVB	621690	872029	8.92%	2.164%
3	5.422	390	397	408	rBV	887466	1277595	13.07%	3.171%
4	6.040	497	502	506	rBV	110808	149792	1.53%	0.372%
5	7.004	658	666	677	rBV	507723	804045	8.23%	1.996%
6	7.381	722	730	739	rBV	1472605	2377478	24.33%	5.901%
7	7.851	804	810	816	rVB	475759	749416	7.67%	1.860%
8	8.169	857	864	871	rBV	2150765	3401863	34.81%	8.443%
9	9.016	1001	1008	1017	rBV	1888792	3045373	31.17%	7.558%
10	10.645	1278	1285	1294	rVB	559406	958519	9.81%	2.379%
11	13.110	1696	1704	1712	rBV	4381188	6141322	62.85%	15.242%
12	13.945	1840	1846	1851	rBV	101938	146941	1.50%	0.365%
13	14.492	1933	1939	1946	rBV2	776654	1185537	12.13%	2.942%
14	15.986	2186	2193	2202	rBV	2046170	2974134	30.44%	7.382%
15	16.186	2223	2227	2235	rBV2	67979	118973	1.22%	0.295%
16	17.239	2399	2406	2414	rBV2	1036433	1509288	15.45%	3.746%
17	18.109	2551	2554	2560	rBV2	106770	151672	1.55%	0.376%
18	19.392	2768	2772	2777	rBV4	85953	110548	1.13%	0.274%
19	19.862	2846	2852	2860	rBV	8044700	9771349	100.00%	24.252%
20	21.103	3059	3063	3069	rBV	194900	243305	2.49%	0.604%
21	21.415	3111	3116	3122	rBV	1687042	2094901	21.44%	5.199%
22	23.738	3505	3511	3522	rVB	1019702	2055262	21.03%	5.101%

Sum of corrected areas: 40290939

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA M\DATA\BM033017\
Data File : BM009456.D
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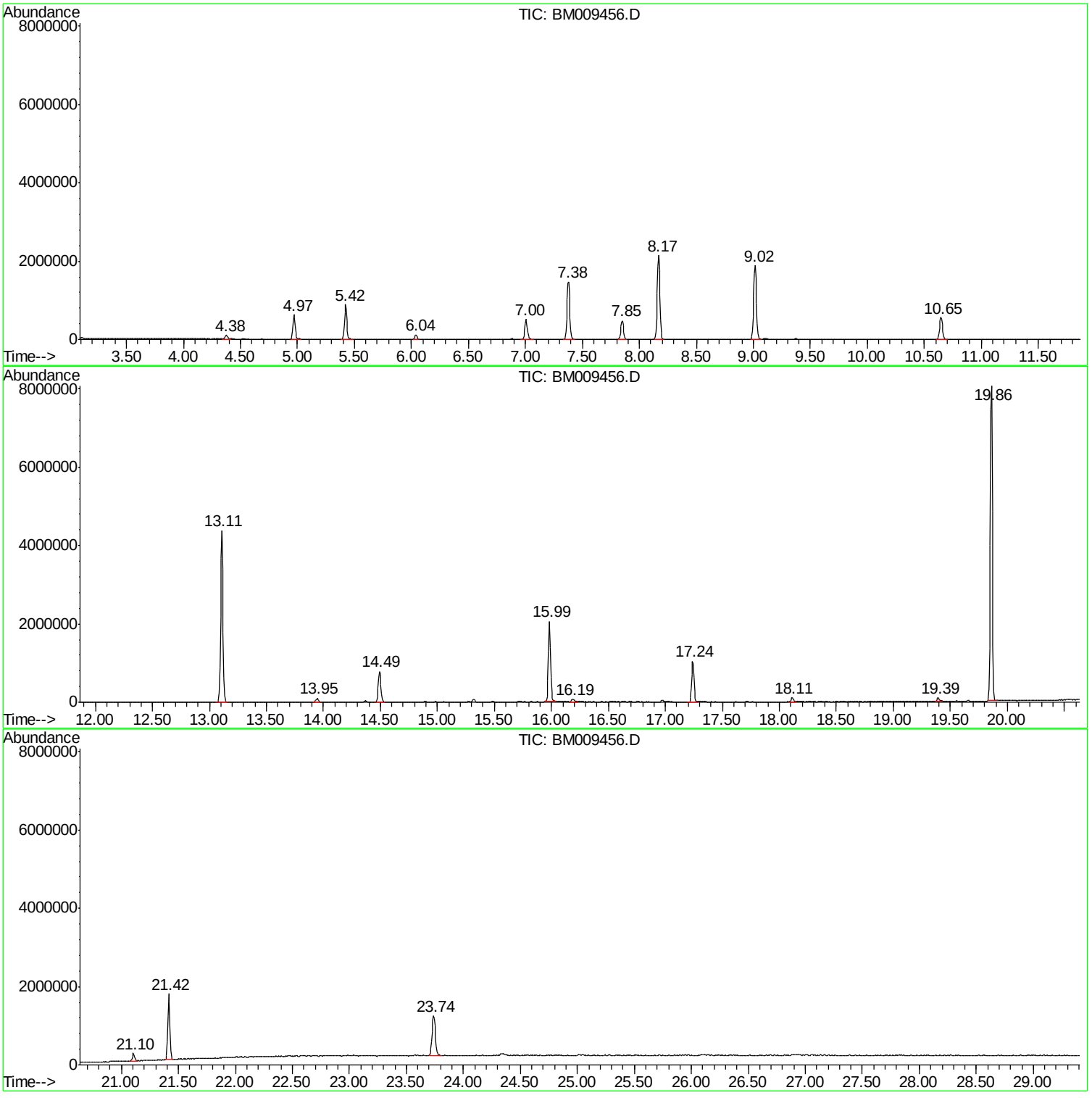
Operator : SJ/MA
Sample : I2445-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
032717-PRRT-F-U-M

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



Data Path : Z:\HPCHEM1\BNA M\DATA\BM033017\
Data File : BM009456.D
Acq On : 30 Mar 2017 18:21
Operator : SJ/MA
Sample : I2445-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 032717-PRRT-F-U-M

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

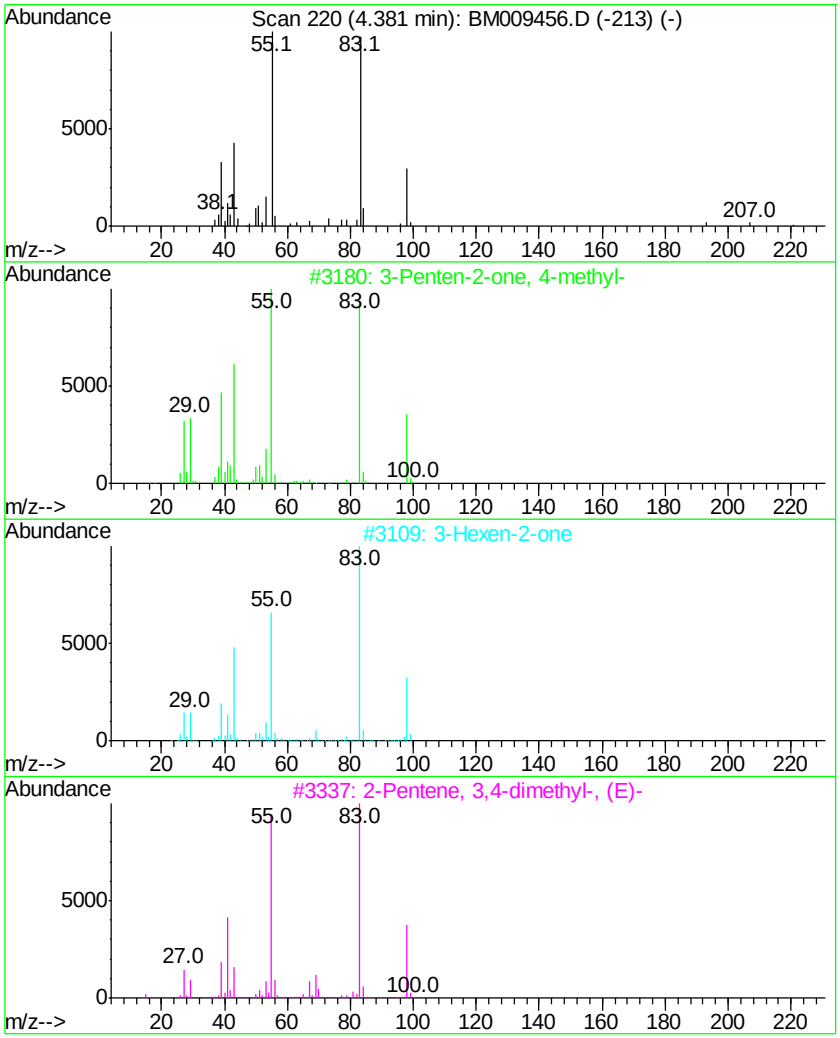
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

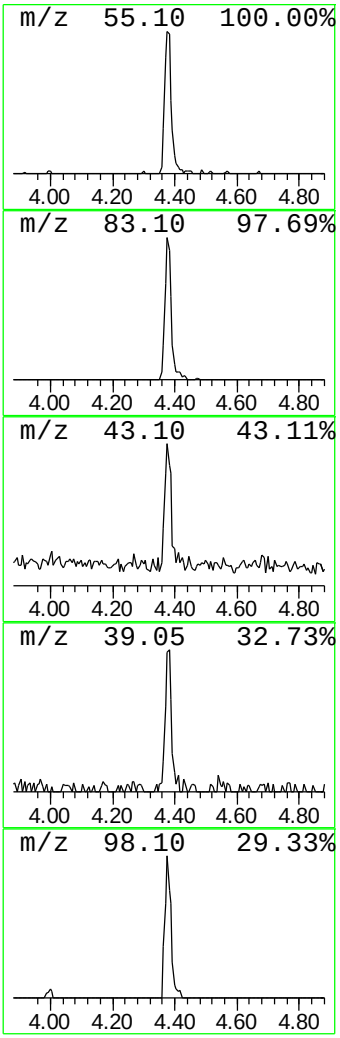
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.38	4.05 ng	151597	1,4-Dichlorobenzene-d4	7.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	86
2	3-Hexen-2-one	98	C6H10O	000763-93-9	83
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	72
5	Cyclohexane, methyl-	98	C7H14	000108-87-2	72





Data Path : Z:\HPCHEM1\BNA M\DATA\BM033017\
Data File : BM009456.D
Acq On : 30 Mar 2017 18:21
Operator : SJ/MA
Sample : I2445-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 032717-PRRT-F-U-M

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

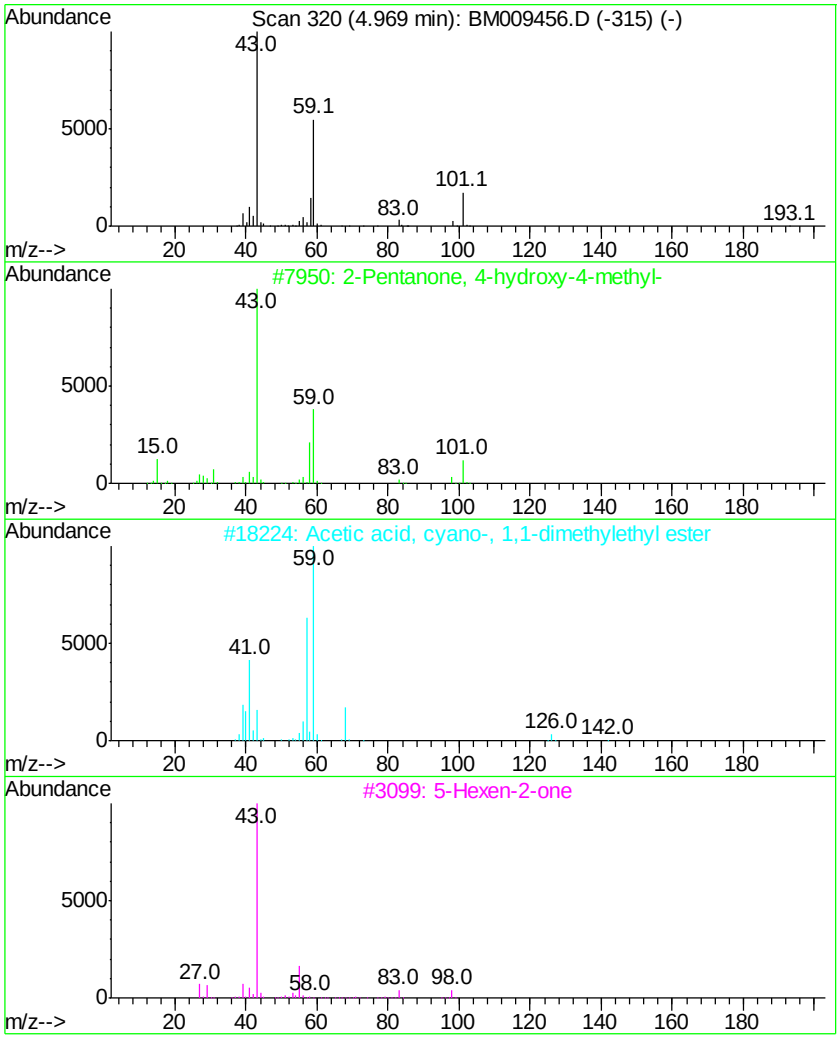
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

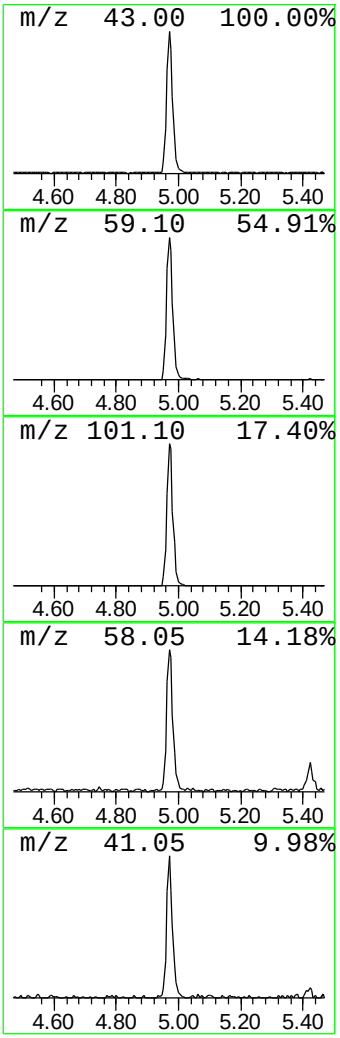
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	23.27 ng	872029	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	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM033017\
Data File : BM009456.D
Acq On : 30 Mar 2017 18:21
Operator : SJ/MA
Sample : I2445-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 032717-PRRT-F-U-M

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

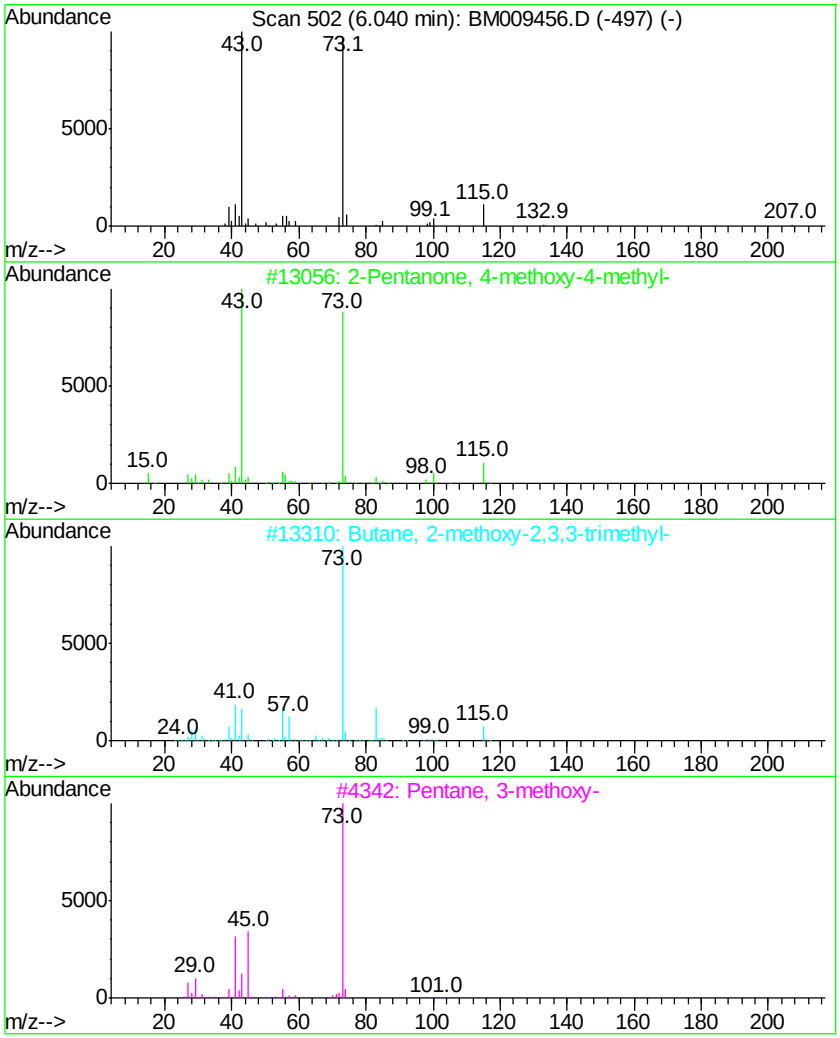
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

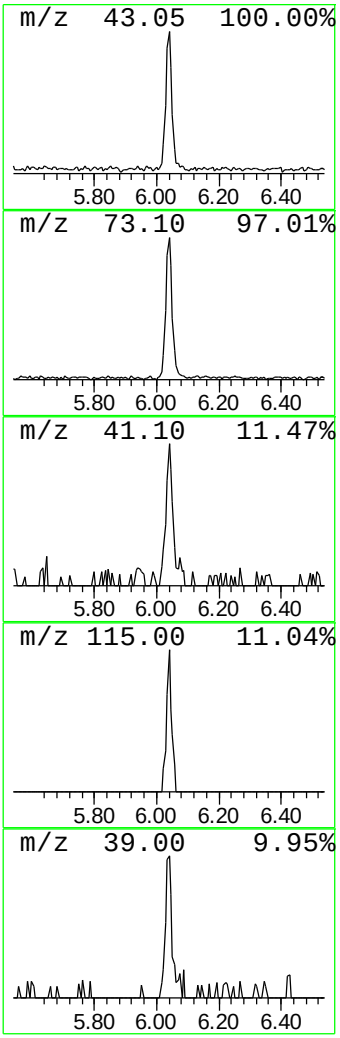
****

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.04	4.00 ng	149792	1,4-Dichlorobenzene-d4	7.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2	Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	23
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	2-Methyl-2,4-dimethoxybutane	132	C7H16O2	039836-89-0	12
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10





Data Path : Z:\HPCHEM1\BNA M\DATA\BM033017\
Data File : BM009456.D
Acq On : 30 Mar 2017 18:21
Operator : SJ/MA
Sample : I2445-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 032717-PRRT-F-U-M

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

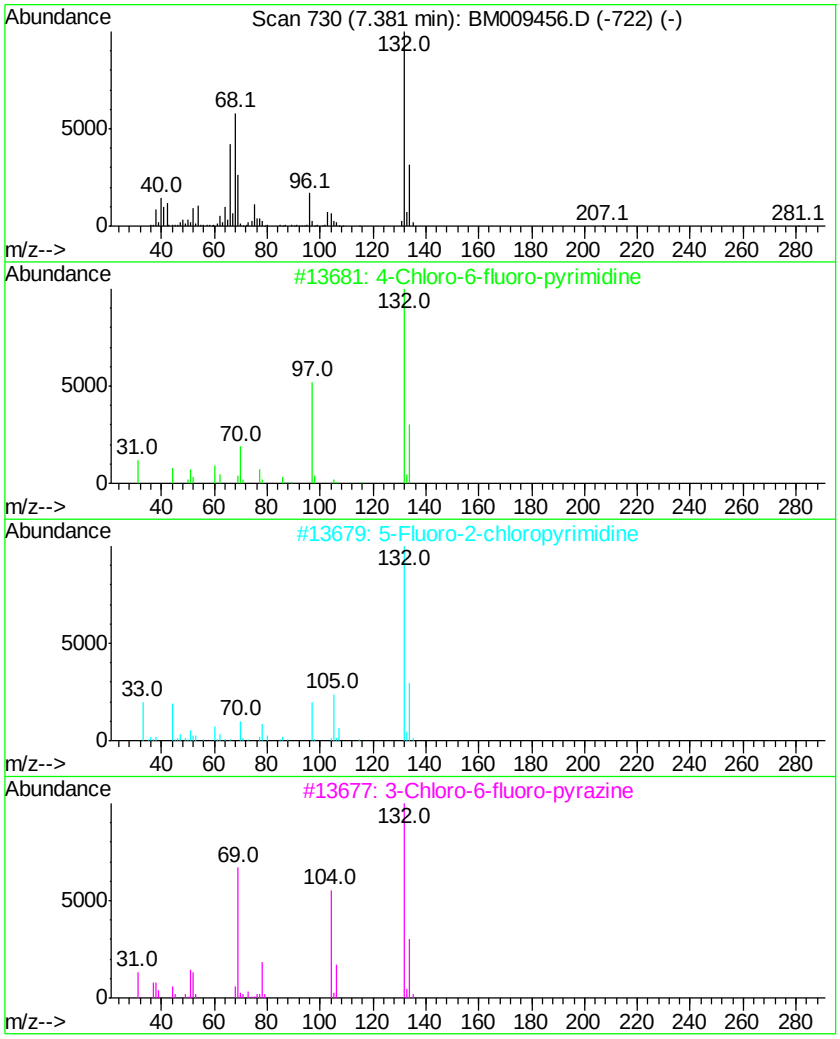
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

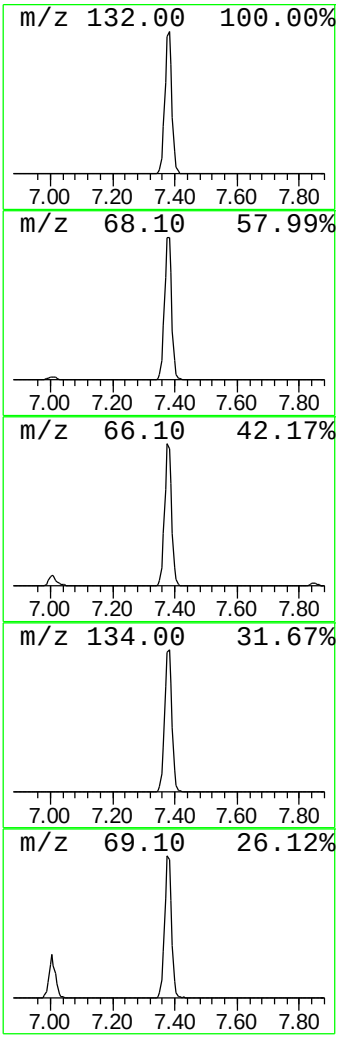
****

Peak Number 4 unknown7.38 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	63.45 ng	2377480	1,4-Dichlorobenzene-d4	7.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12





Data Path : Z:\HPCHEM1\BNA M\DATA\BM033017\
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Acq On : 30 Mar 2017 18:21
Operator : SJ/MA
Sample : I2445-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 032717-PRRT-F-U-M

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

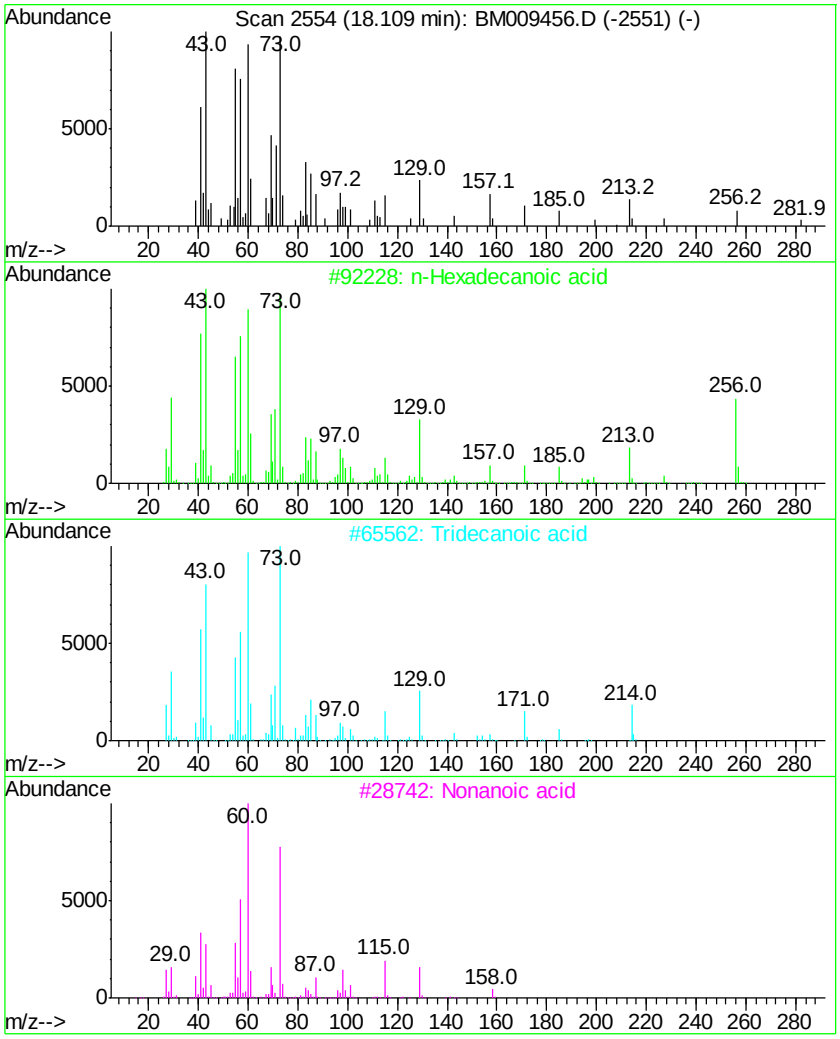
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

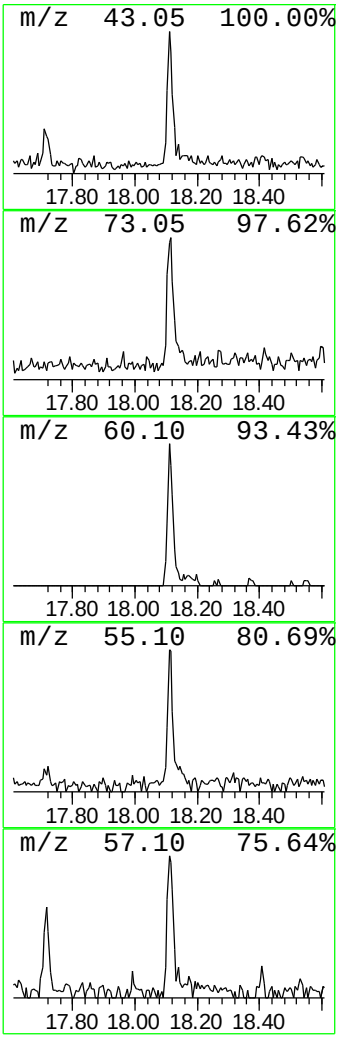
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.11	2.01 ng	151672	Phenanthrene-d10	17.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	81
3	Nonanoic acid	158	C9H18O2	000112-05-0	38
4	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	25
5	Eicosane	282	C20H42	000112-95-8	11





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Data File : BM009456.D
Acq On : 30 Mar 2017 18:21
Operator : SJ/MA
Sample : I2445-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 032717-PRRT-F-U-M

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

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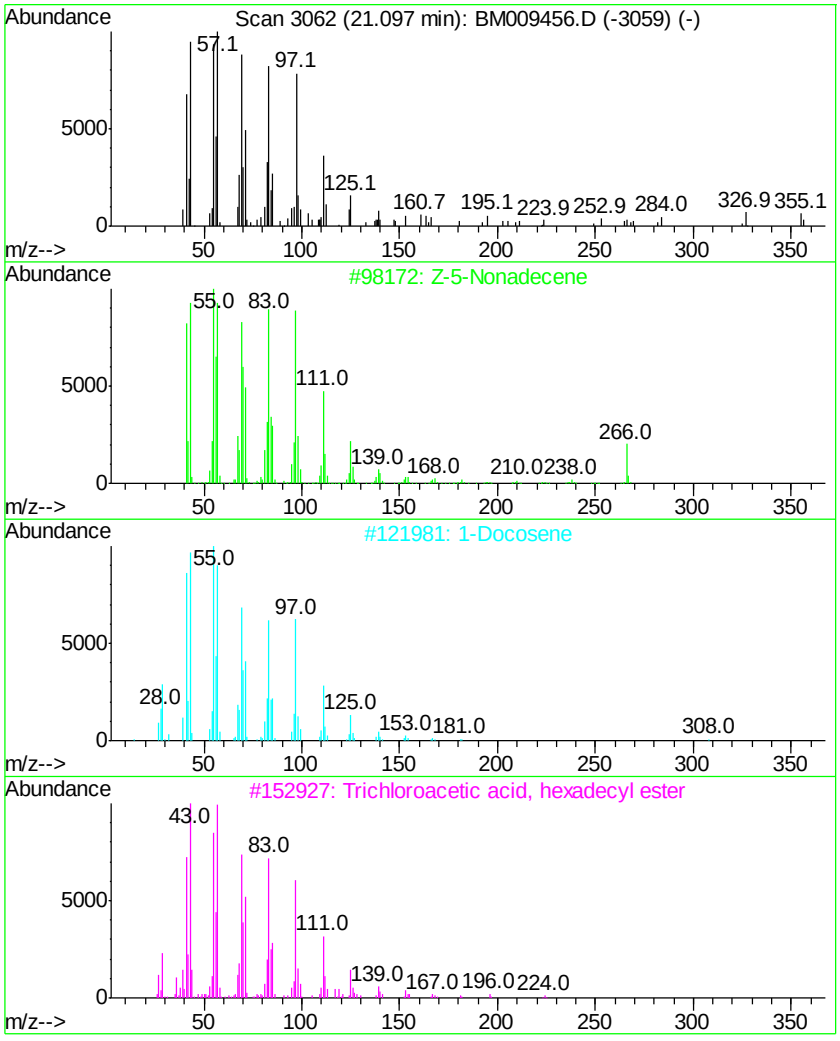
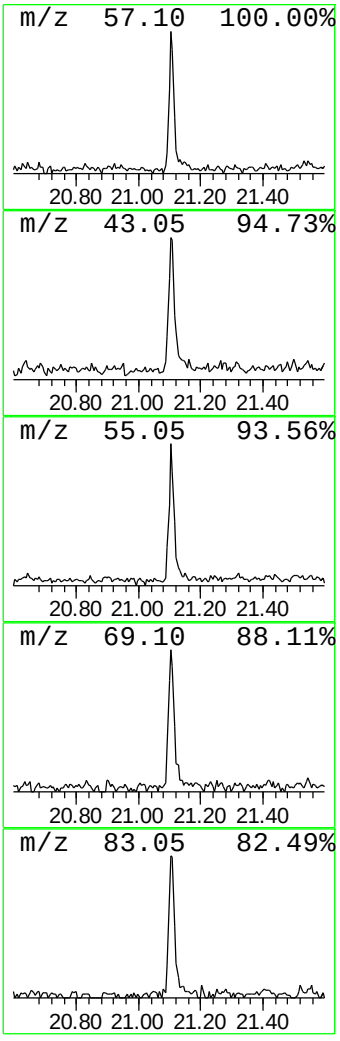
Peak Number 7 Z-5-Nonadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.10	2.32 ng	243305	Chrysene-d12	21.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-5-Nonadecene	266	C19H38	1000131-11-8	97
2	1-Docosene	308	C22H44	001599-67-3	93
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	Cyclotetracosane	336	C24H48	000297-03-0	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM033017\
Data File : BM009456.D
Acq On : 30 Mar 2017 18:21
Operator : SJ/MA
Sample : I2445-02
Misc :
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Instrument : BNA_M
ClientSampleId : 032717-PRRT-F-U-M

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
3-Penten-2-one, 4...	4.38	4.0	ng	151597	1	7.85	749416	20.0
2-Pentanone, 4-hy...	4.97	23.3	ng	872029	1	7.85	749416	20.0
2-Pentanone, 4-me...	6.04	4.0	ng	149792	1	7.85	749416	20.0
unknown7.38	7.38	63.5	ng	2377480	1	7.85	749416	20.0
n-Hexadecanoic acid	18.11	2.0	ng	151672	4	17.24	1509290	20.0
Z-5-Nonadecene	21.10	2.3	ng	243305	5	21.42	2094900	20.0