LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080315\
Data File : BF080830.D
Acq On : 4 Aug 2015 8:12
Operator : TP
Sample : G3172-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BOTTOM-SOUTH-073115

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-BF080315.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	2.167	5	7	10	rBV	70873	88812	1.89%	0.194%
2	4.384	199	201	205	rBV	240663	297506	6.33%	0.650%
3	5.036	254	258	261	rBV	2932002	4578996	97.40%	9.999%
4	5.447	290	294	296	rBV	3217612	4621833	98.31%	10.093%
5	5.847	327	329	331	rBV	192692	213996	4.55%	0.467%
6	6.464	379	383	385	rBV	4417956	4701437	100.00%	10.267%
7	6.602	392	395	397	rBV	4475204	4571638	97.24%	9.983%
8	6.830	413	415	418	rVB	1203017	1029666	21.90%	2.249%
9	6.990	426	429	431	rVB	3620739	3424627	72.84%	7.478%
10	7.390	461	464	467	rBV	2433756	2757791	58.66%	6.022%
11	8.110	524	527	530	rBV	1247148	1241683	26.41%	2.712%
12	9.196	618	622	624	rBV	3581964	4691761	99.79%	10.246%
13	9.585	653	656	658	rBV	747376	631288	13.43%	1.379%
14	9.859	678	680	683	rBV	975966	1331189	28.31%	2.907%
15	10.648	746	749	752	rBV2	2543934	2980523	63.40%	6.509%
16	10.773	758	760	765	rVB	90443	120289	2.56%	0.263%
17	11.219	797	799	801	rBV	83374	93901	2.00%	0.205%
18	11.345	807	810	812	rBV	1589911	1353717	28.79%	2.956%
19	11.653	834	837	838	rBV	52100	66303	1.41%	0.145%
20	11.882	855	857	859	rBV	127000	131726	2.80%	0.288%
21	12.054	871	872	877	rVB2	45148	48359	1.03%	0.106%
22	12.134	877	879	882	rVB	283409	240394	5.11%	0.525%
23	12.762	931	934	936	rBV	81739	93296	1.98%	0.204%
24	12.934	946	949	951	rBV	4140528	3810037	81.04%	8.320%
25	13.414	987	991	994	rBV	1042241	985705	20.97%	2.153%
26	13.974	1037	1040	1042	rBV	997545	881076	18.74%	1.924%
27	14.282	1057	1067	1080	rBV7	21749	193051	4.11%	0.422%
28	15.391	1161	1164	1166	rBV	435052	612514	13.03%	1.338%

Sum of corrected areas: 45793114

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080315\
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Operator : TP
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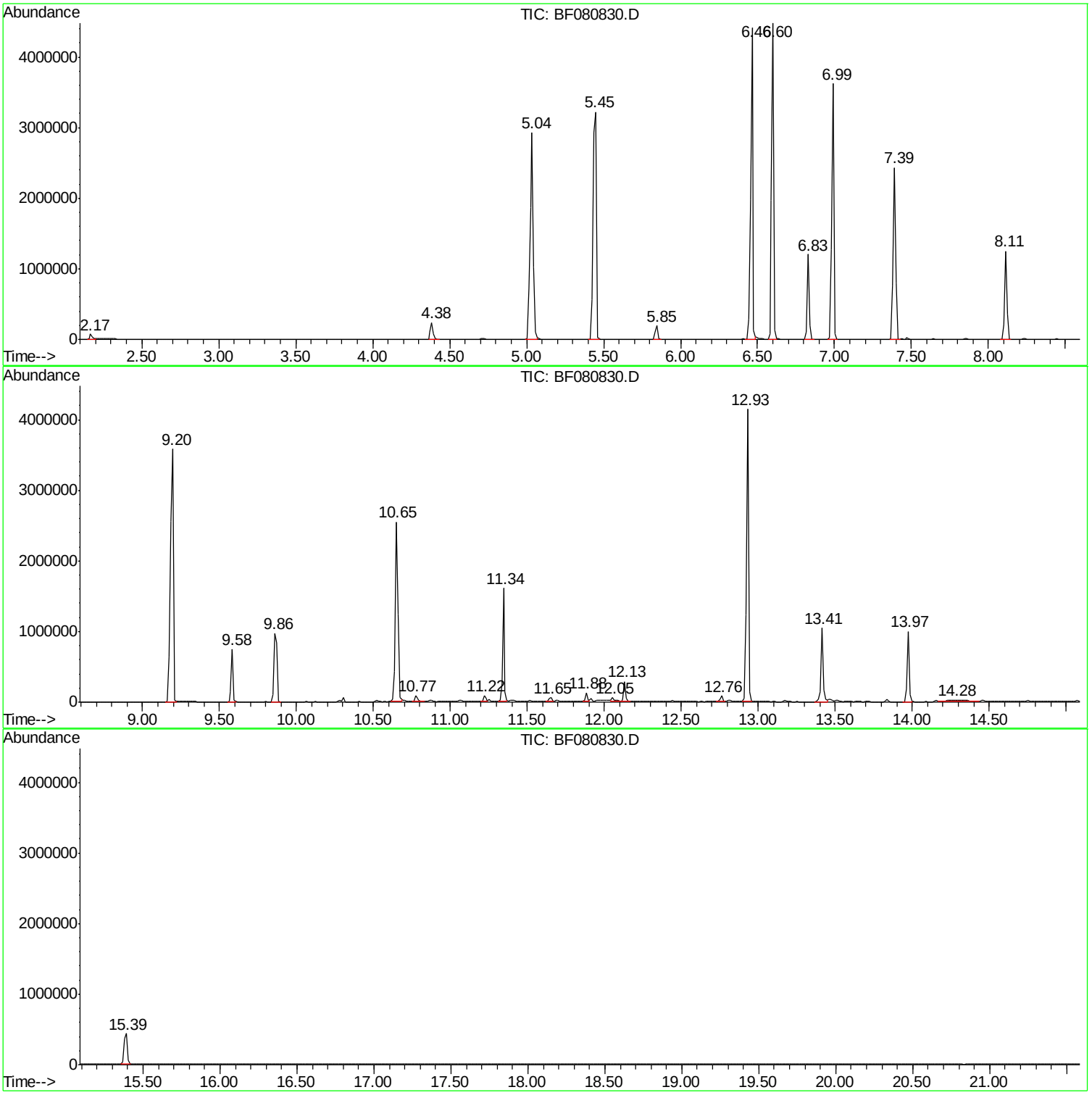
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BOTTOM-SOUTH-073115

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080315.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\BF080315\
Data File : BF080830.D
Acq On : 4 Aug 2015 8:12
Operator : TP
Sample : G3172-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BOTTOM-SOUTH-073115

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

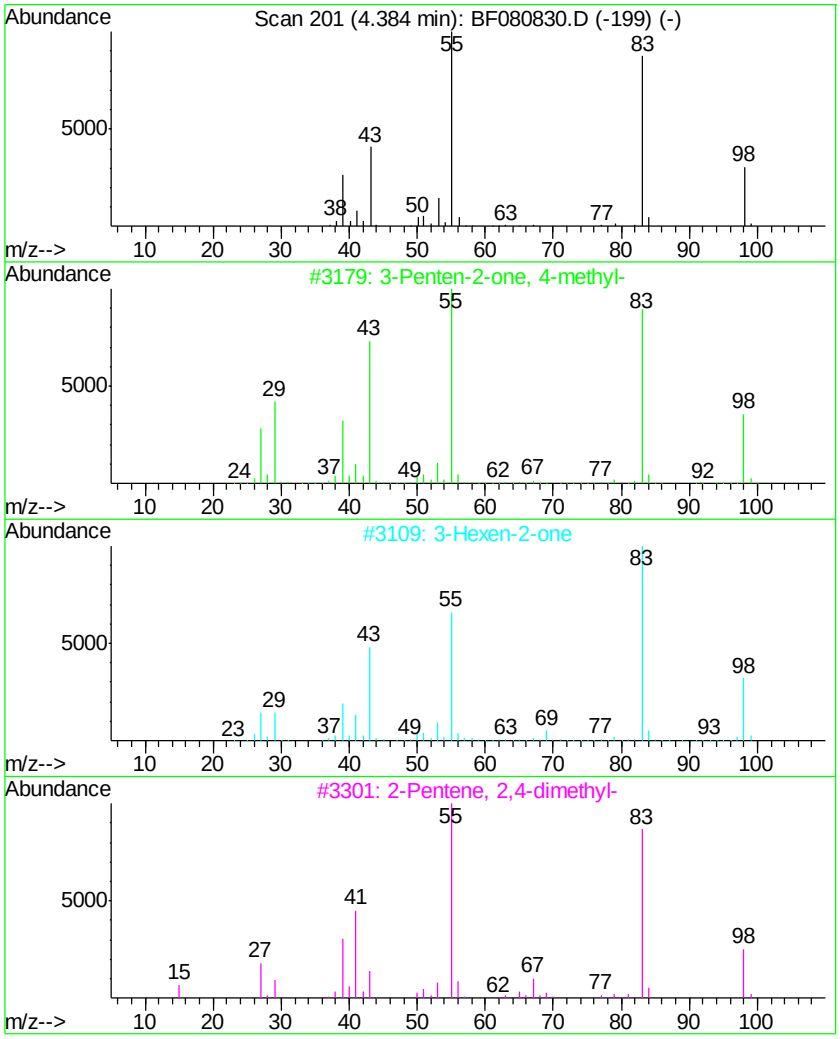
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

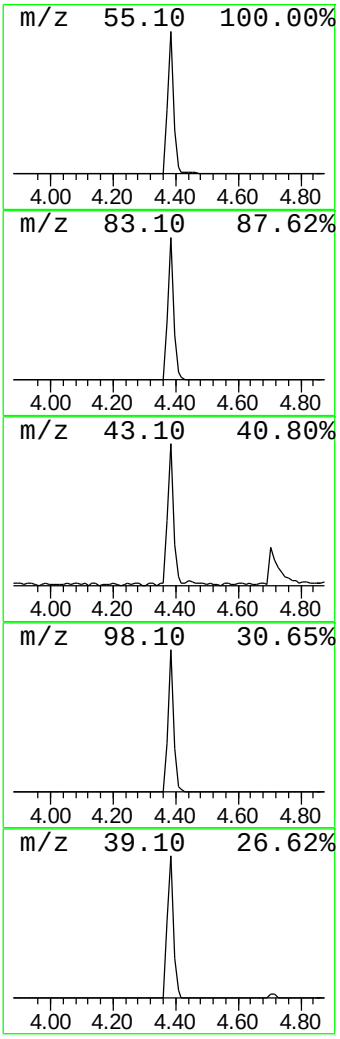
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.38	5.78 ng	297506	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	87
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78





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Data File : BF080830.D
Acq On : 4 Aug 2015 8:12
Operator : TP
Sample : G3172-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BOTTOM-SOUTH-073115

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080315.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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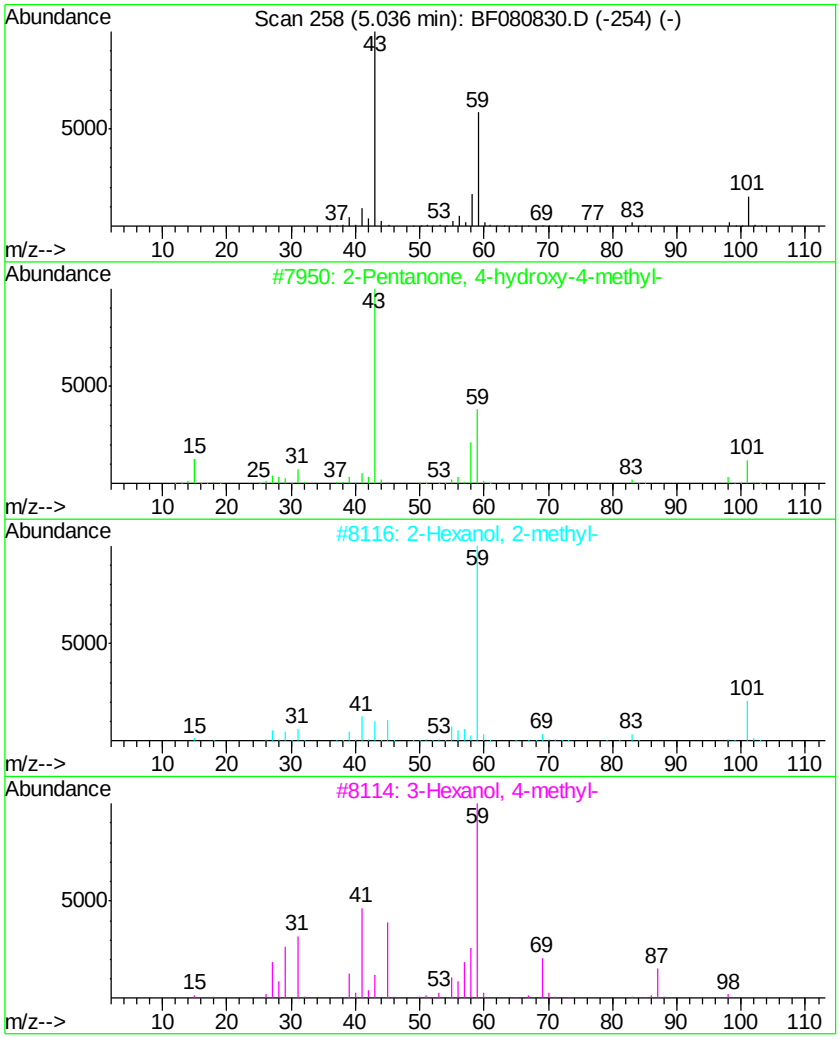
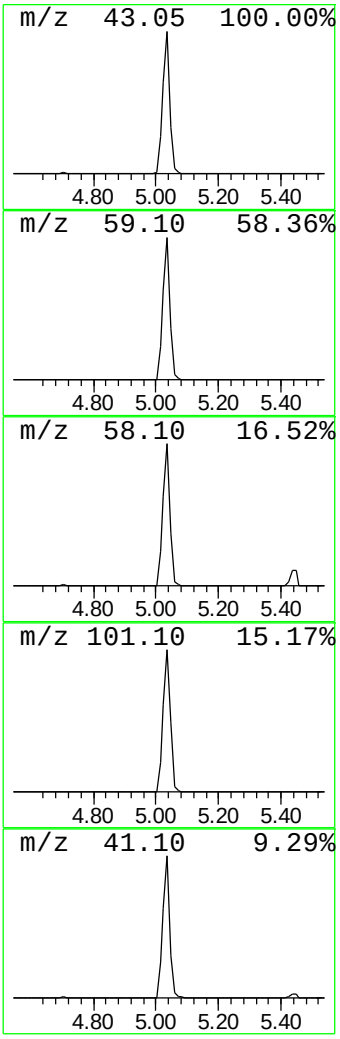
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	88.94 ng	4579000	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
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	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080315\
Data File : BF080830.D
Acq On : 4 Aug 2015 8:12
Operator : TP
Sample : G3172-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BOTTOM-SOUTH-073115

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

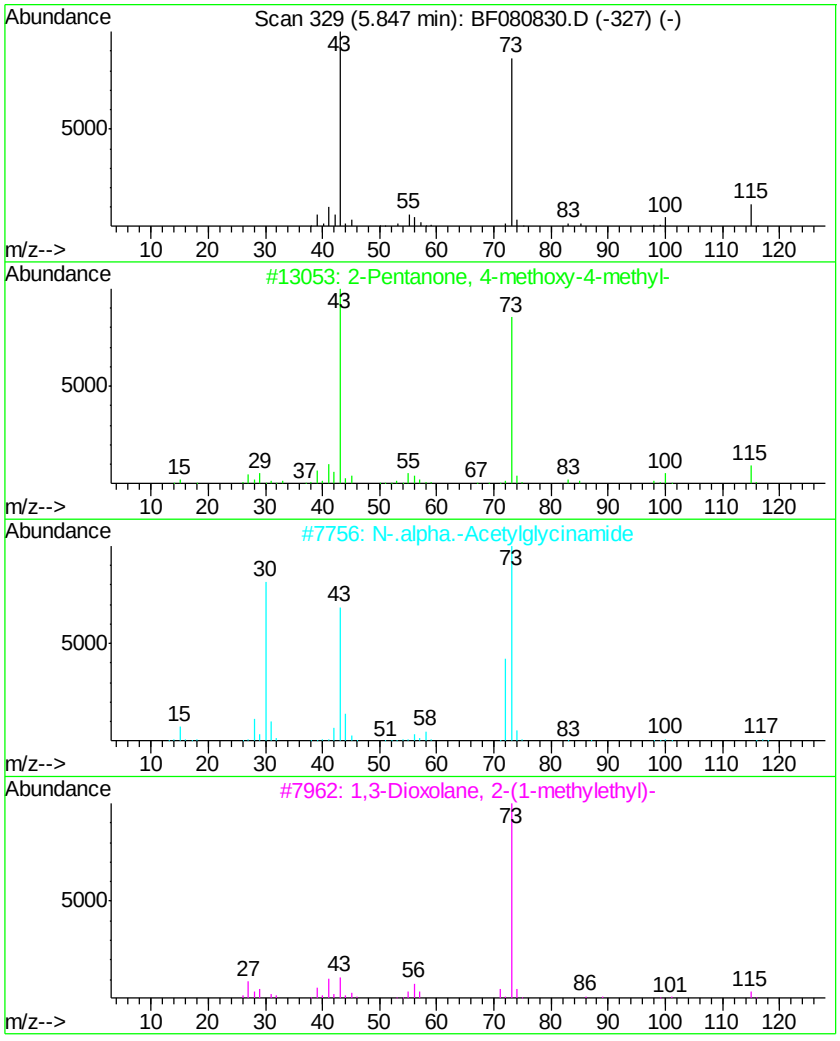
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

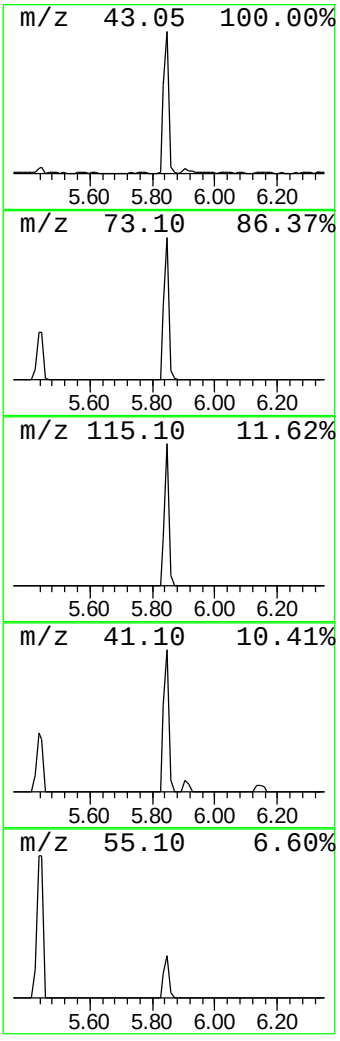
****

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.85	4.16 ng	213996	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	33
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	27
4	3,6-Heptanedione	128	C7H12O2	001703-51-1	17
5	N-Formylmorpholine	115	C5H9NO2	004394-85-8	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080315\
Data File : BF080830.D
Acq On : 4 Aug 2015 8:12
Operator : TP
Sample : G3172-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BOTTOM-SOUTH-073115

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

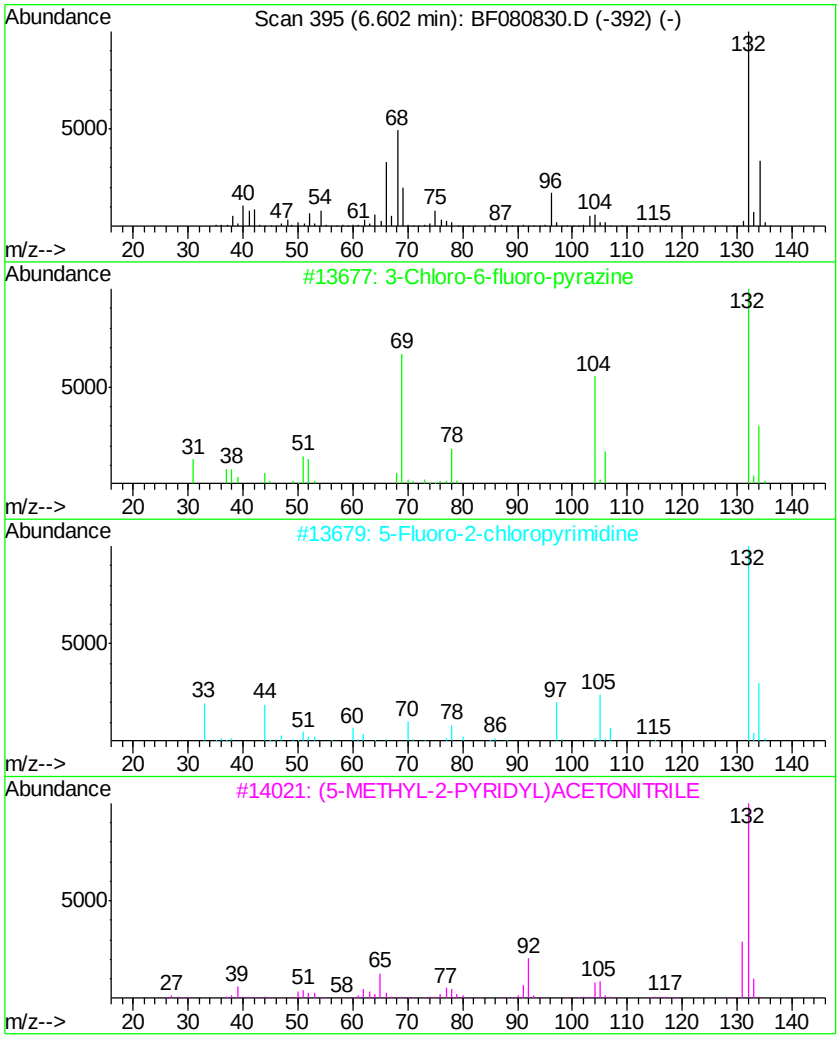
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

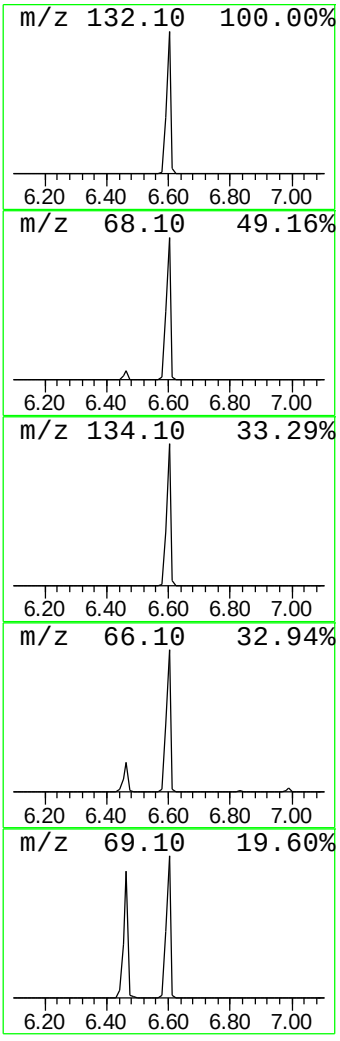
****

Peak Number 4 unknown6.60 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	88.80 ng	4571640	1,4-Dichlorobenzene-d4	6.83

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	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080315\
Data File : BF080830.D
Acq On : 4 Aug 2015 8:12
Operator : TP
Sample : G3172-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BOTTOM-SOUTH-073115

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

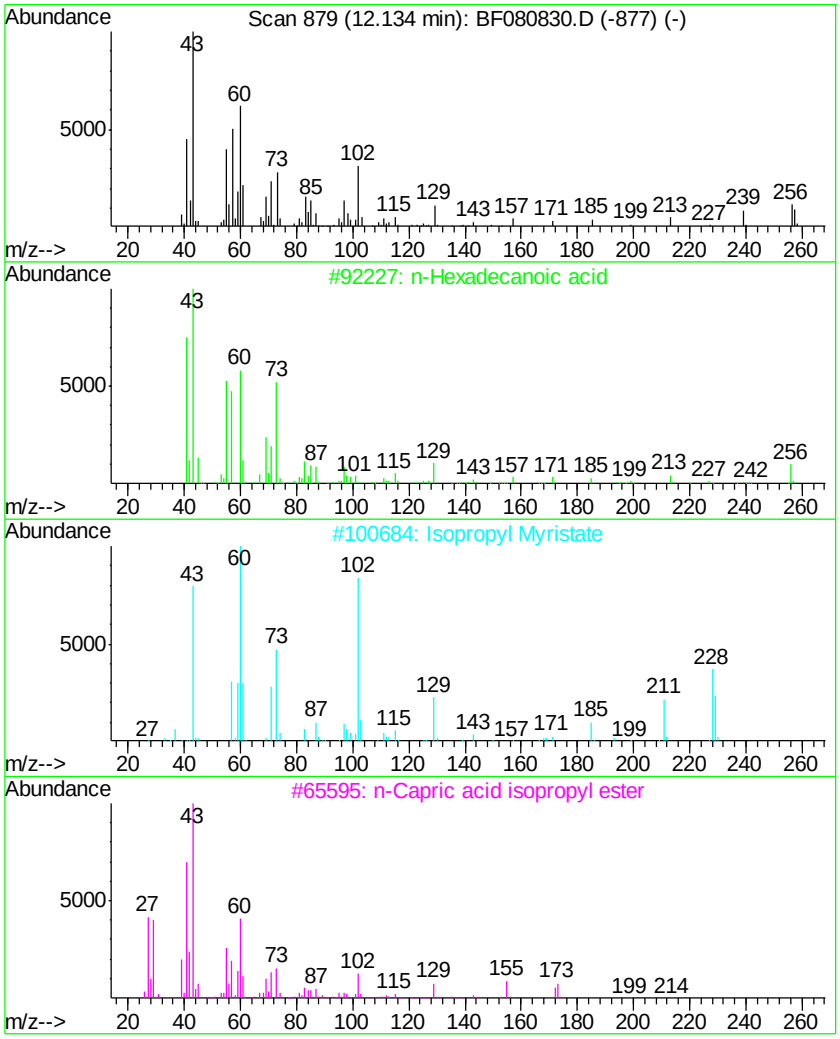
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

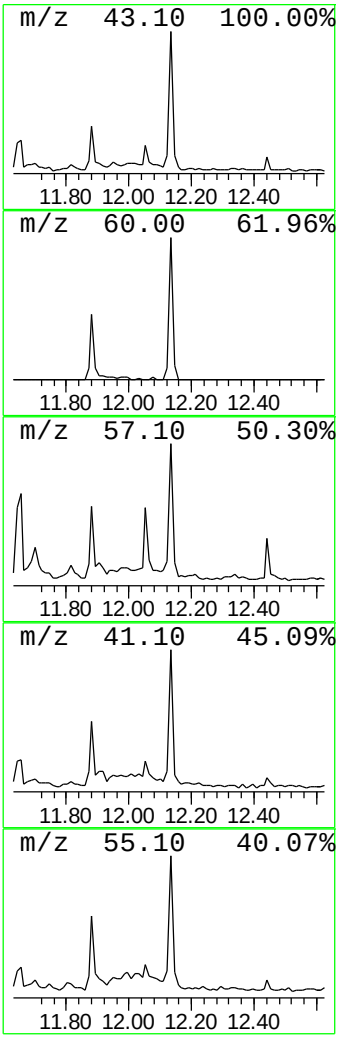
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.13	3.55 ng	240394	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
2	Isopropyl Myristate	270	C17H34O2	000110-27-0	42
3	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	40
4	n-Decanoic acid	172	C10H20O2	000334-48-5	38
5	Hexanoic acid, 1-methylethyl ester	158	C9H18O2	002311-46-8	35





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Data File : BF080830.D
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Sample : G3172-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BOTTOM-SOUTH-073115

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080315.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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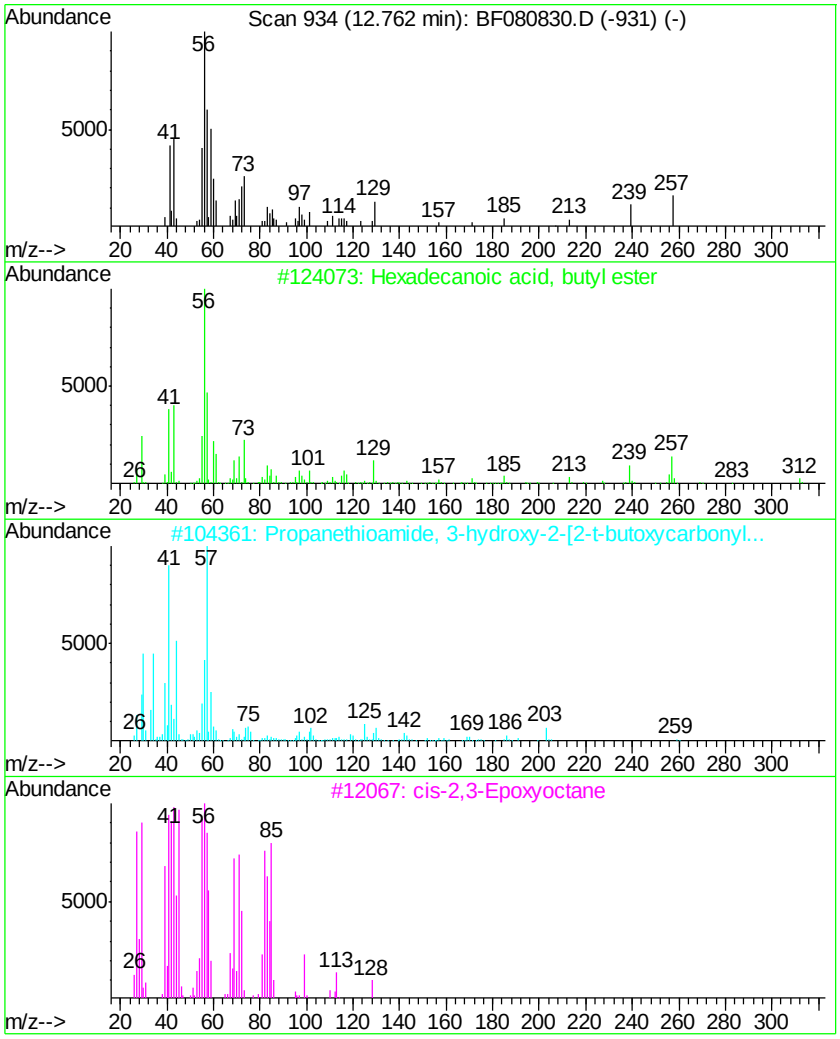
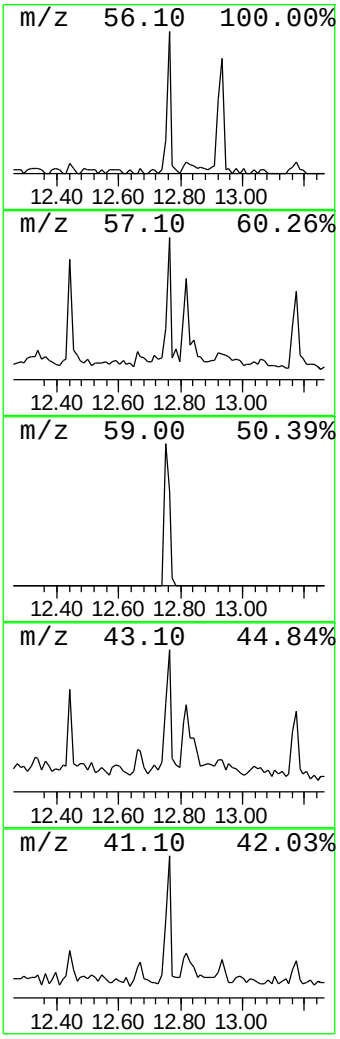
Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	2.12 ng	93296	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	62
2	Propanethioamide, 3-hydroxy-2-[2...	277	C10H19N3O4S	1000190-85-5	40
3	cis-2,3-Epoxyoctane	128	C8H16O	023024-54-6	38
4	Cyclohexanol, 2-amino-, cis-	115	C6H13NO	000931-15-7	38
5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	38





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Data File : BF080830.D
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Operator : TP
Sample : G3172-03
Misc :
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Instrument : BNA_F
ClientSampleId : BOTTOM-SOUTH-073115

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

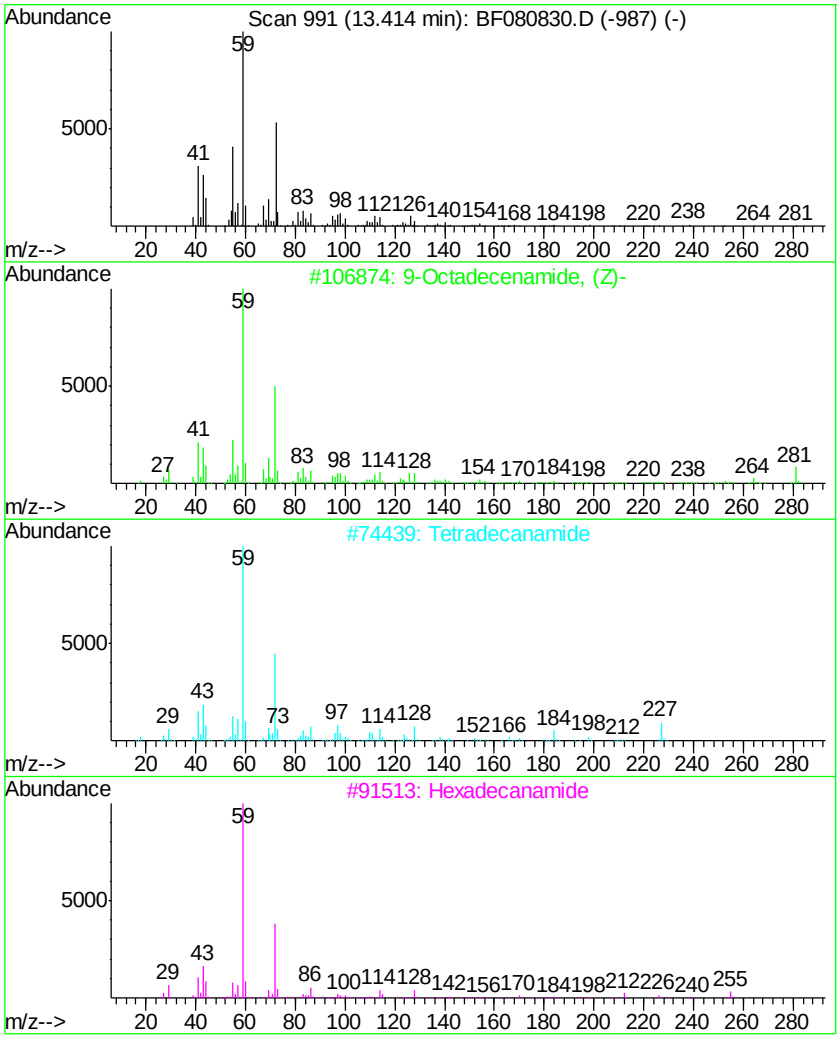
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

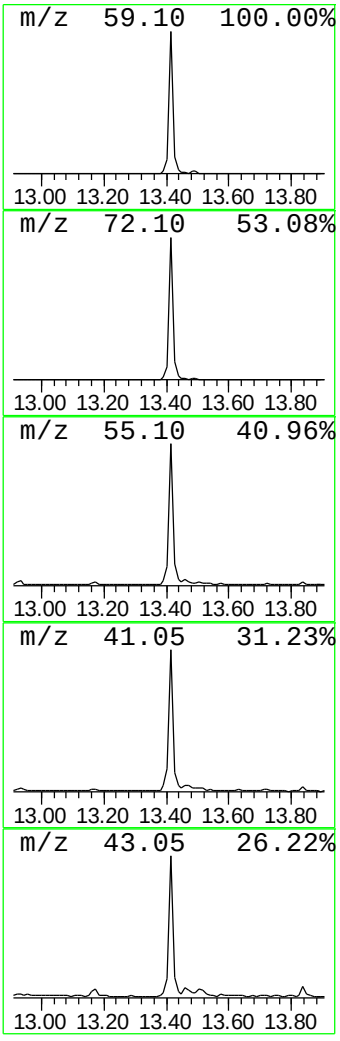
****

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.41	22.38 ng	985705	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
2	Tetradecanamide	227	C14H29NO	000638-58-4	59
3	Hexadecanamide	255	C16H33NO	000629-54-9	56
4	Decanamide-	171	C10H21NO	002319-29-1	56
5	Dodecanamide	199	C12H25NO	001120-16-7	45





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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BOTTOM-SOUTH-073115

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

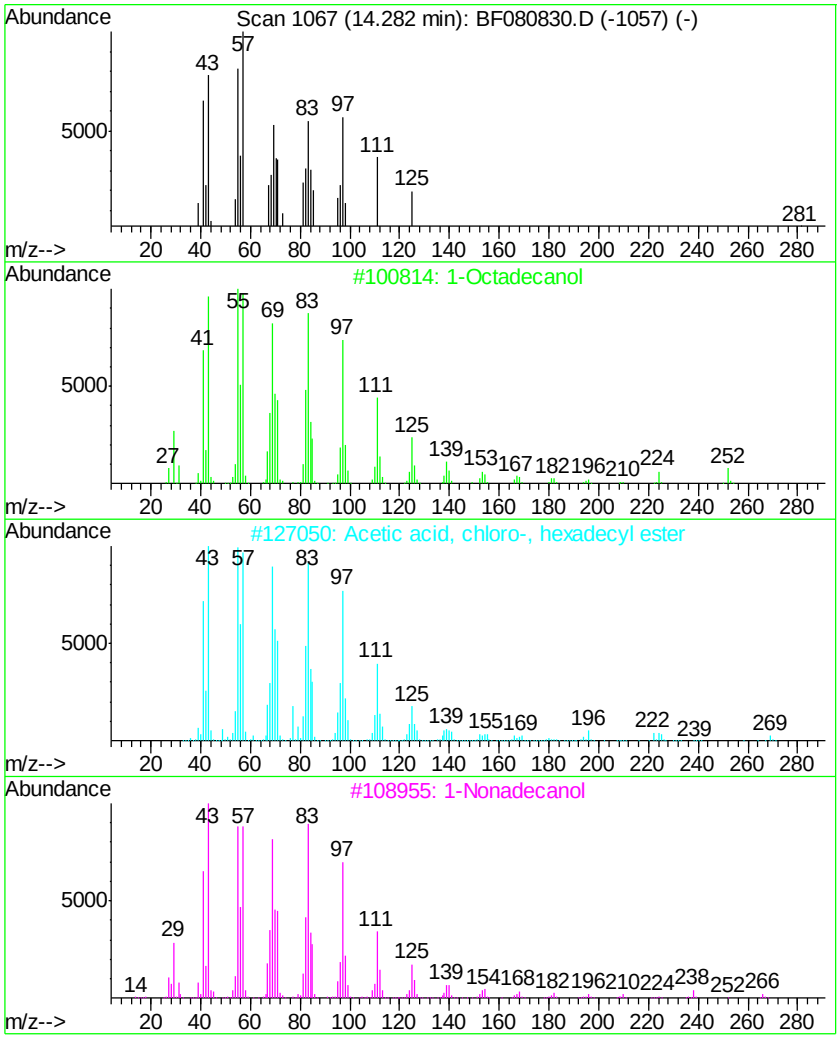
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

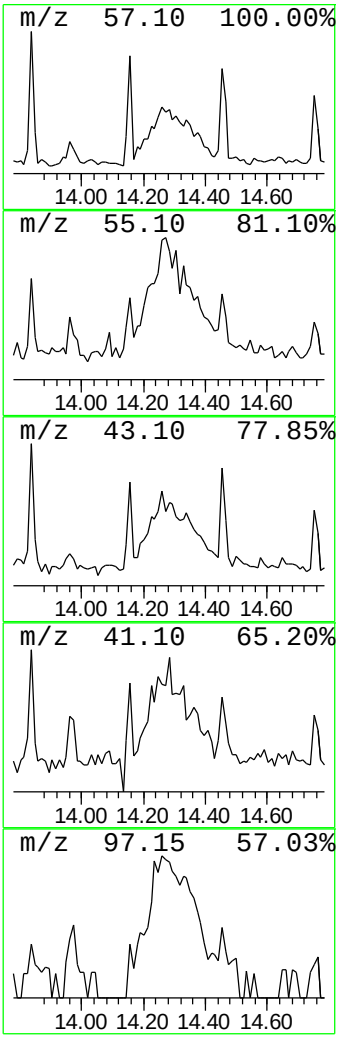
****

Peak Number 9 1-Octadecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.28	4.38 ng	193051	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol	270	C18H38O	000112-92-5	90
2	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	87
3	1-Nonadecanol	284	C19H40O	001454-84-8	83
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	81
5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080315\
Data File : BF080830.D
Acq On : 4 Aug 2015 8:12
Operator : TP
Sample : G3172-03
Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080315.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	5.8	ng	297506	1	6.83	1029670	20.0
2-Pentanone, 4-hy...	5.04	88.9	ng	4579000	1	6.83	1029670	20.0
2-Pentanone, 4-me...	5.85	4.2	ng	213996	1	6.83	1029670	20.0
unknown6.60	6.60	88.8	ng	4571640	1	6.83	1029670	20.0
n-Hexadecanoic acid	12.13	3.5	ng	240394	4	11.34	1353720	20.0
Hexadecanoic acid...	12.76	2.1	ng	93296	5	13.97	881076	20.0
9-Octadecenamide,...	13.41	22.4	ng	985705	5	13.97	881076	20.0
1-Octadecanol	14.28	4.4	ng	193051	5	13.97	881076	20.0