LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010617\
Data File : BF092120.D
Acq On : 6 Jan 2017 16:43
Operator : UM/SJ
Sample : I1025-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP7-8-COMP10

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-BF122116.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	2.321	36	38	49	rVB	218859	321519	5.51%	0.614%
2	4.093	190	193	199	rBV	107325	171432	2.94%	0.327%
3	4.801	252	255	272	rVB	1484875	2421420	41.47%	4.621%
4	5.259	292	295	297	rBV	3803258	5379040	92.12%	10.266%
5	6.310	384	387	389	rBV	4909423	5839441	100.00%	11.144%
6	6.413	394	396	399	rVV	5066242	5416380	92.76%	10.337%
7	6.642	414	416	418	rBV	1435779	1221516	20.92%	2.331%
8	6.802	427	430	432	rBV	3762521	4276708	73.24%	8.162%
9	7.213	463	466	468	rBV	3261509	3292597	56.39%	6.284%
10	7.922	526	528	531	rBV	1249776	1428292	24.46%	2.726%
11	9.008	620	623	625	rBV	5949170	5672977	97.15%	10.827%
12	9.671	679	681	683	rBV	1695043	1588803	27.21%	3.032%
13	9.911	699	702	712	rVB	482752	508377	8.71%	0.970%
14	10.459	747	750	753	rBV2	2687062	3605174	61.74%	6.880%
15	10.848	782	784	794	rVB	86073	125108	2.14%	0.239%
16	11.145	808	810	813	rBV	1156420	1609313	27.56%	3.071%
17	11.705	856	859	861	rBV	398708	421617	7.22%	0.805%
18	12.231	902	905	912	rBV	142722	353291	6.05%	0.674%
19	12.482	925	927	934	rBV	344301	406968	6.97%	0.777%
20	12.745	947	950	952	rBV	4500339	5604447	95.98%	10.696%
21	13.774	1038	1040	1043	rVB	1488910	1564650	26.79%	2.986%
22	15.145	1157	1160	1163	rBV	1055516	1169483	20.03%	2.232%

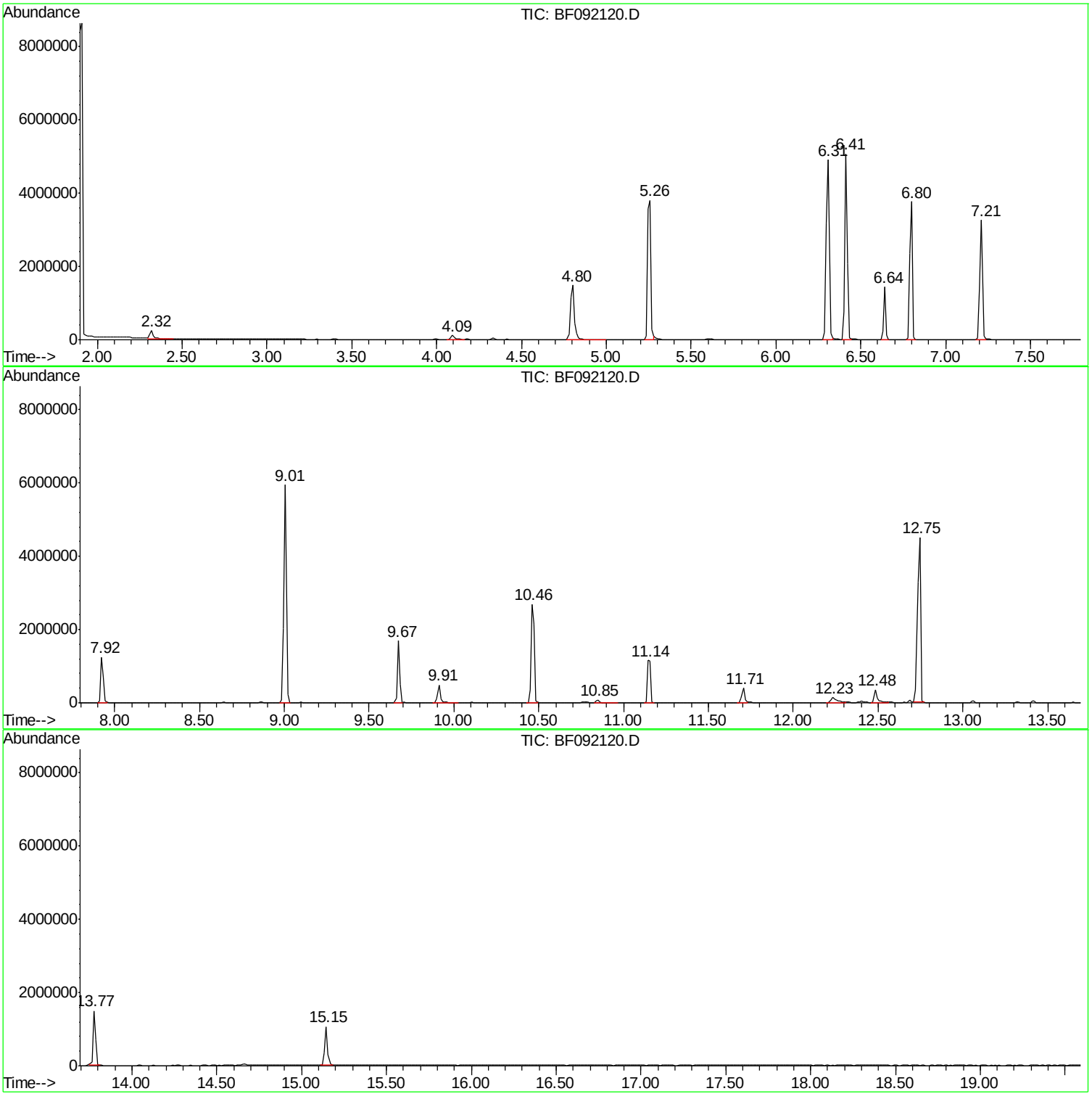
Sum of corrected areas: 52398553

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010617\
Data File : BF092120.D
Acq On : 6 Jan 2017 16:43
Operator : UM/SJ
Sample : I1025-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP7-8-COMP10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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\BF010617\
Data File : BF092120.D
Acq On : 6 Jan 2017 16:43
Operator : UM/SJ
Sample : I1025-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP7-8-COMP10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

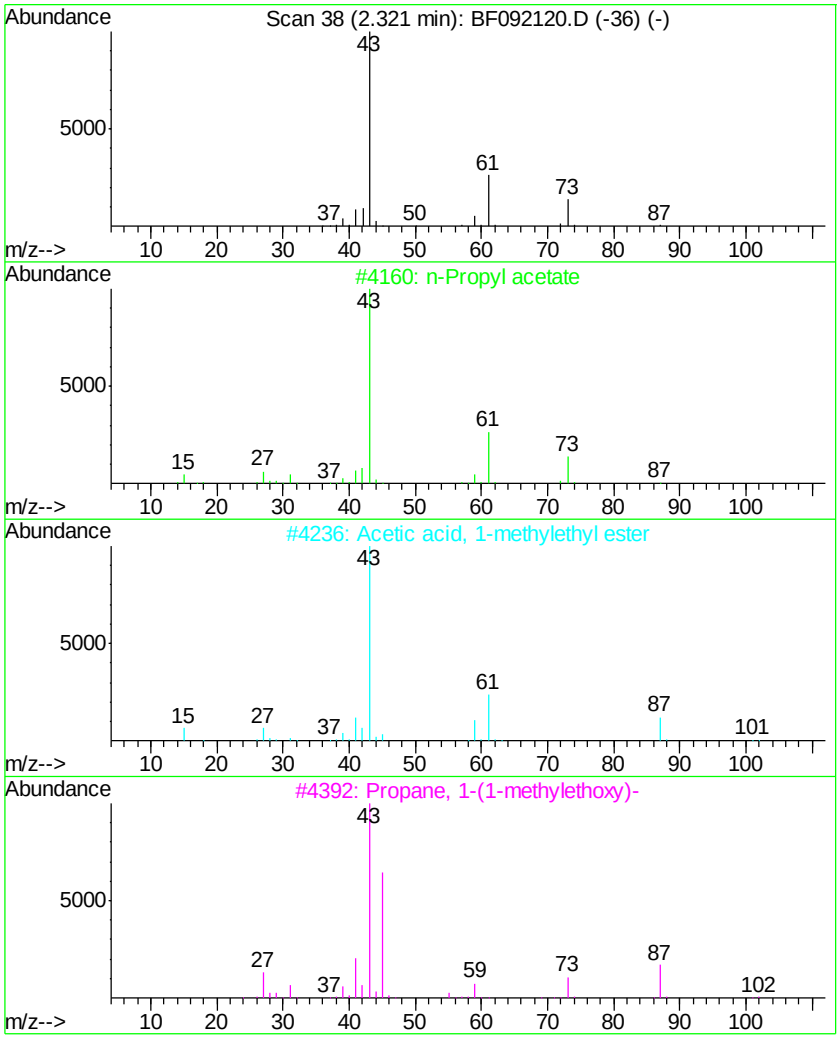
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

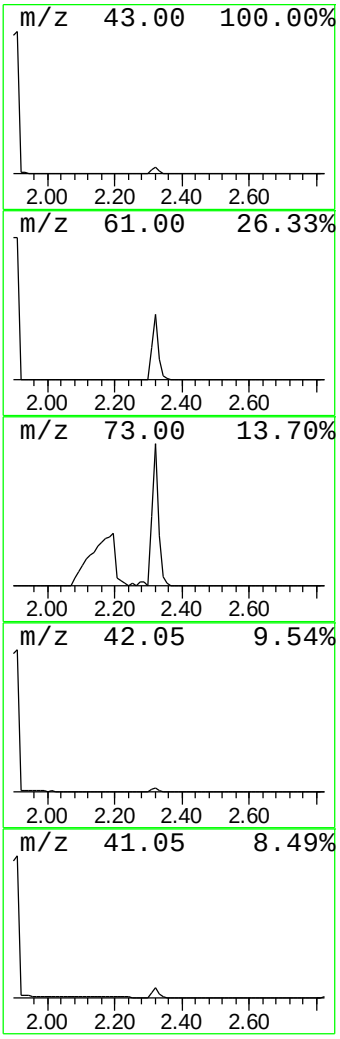
****

Peak Number 1 n-Propyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	5.26 ng	321519	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	Acetic acid, 1-methylethyl ester	102	C5H10O2	000108-21-4	38
3	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	9
4	1-Butanamine	73	C4H11N	000109-73-9	7
5	Pentane	72	C5H12	000109-66-0	5





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010617\
Data File : BF092120.D
Acq On : 6 Jan 2017 16:43
Operator : UM/SJ
Sample : I1025-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP7-8-COMP10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

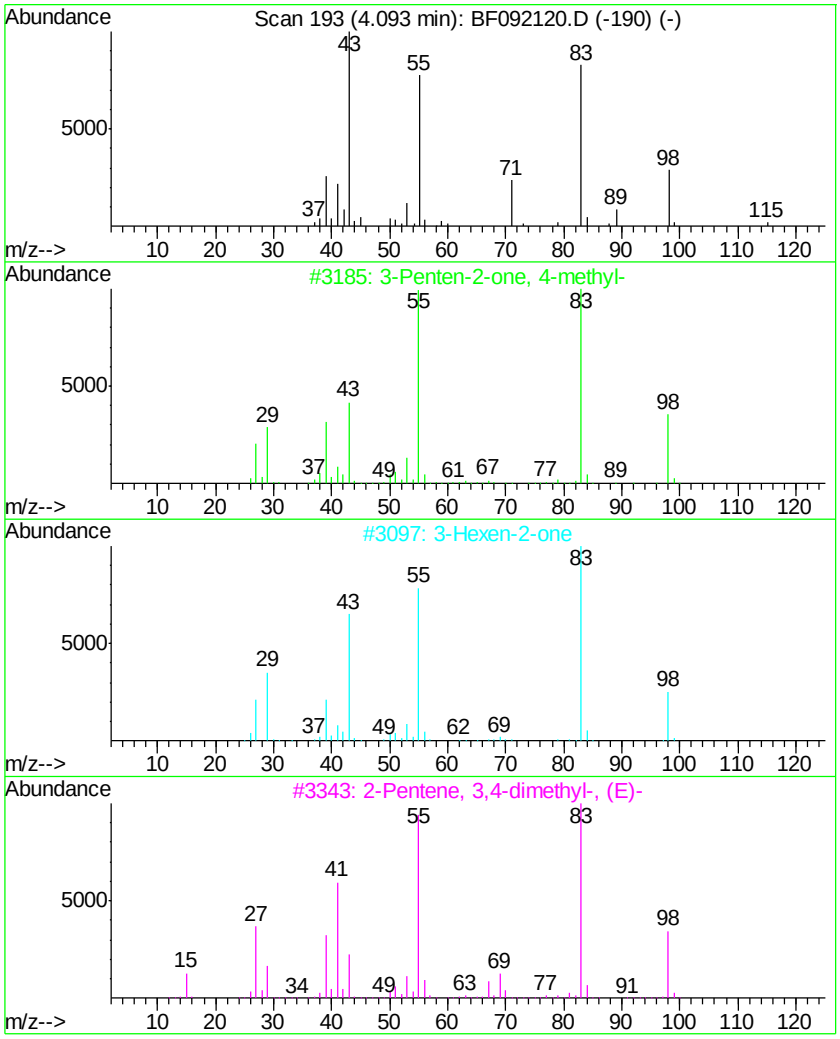
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

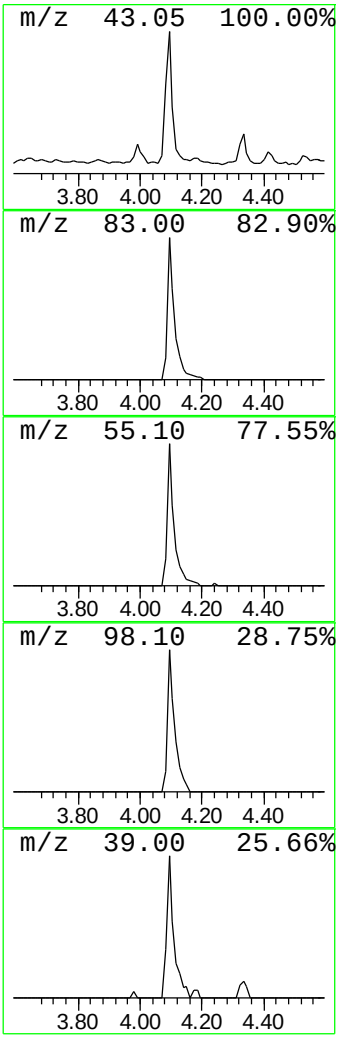
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.09	2.81 ng	171432	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	76
2	3-Hexen-2-one	98	C6H10O	000763-93-9	72
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	64
4	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	64
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010617\
Data File : BF092120.D
Acq On : 6 Jan 2017 16:43
Operator : UM/SJ
Sample : I1025-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP7-8-COMP10

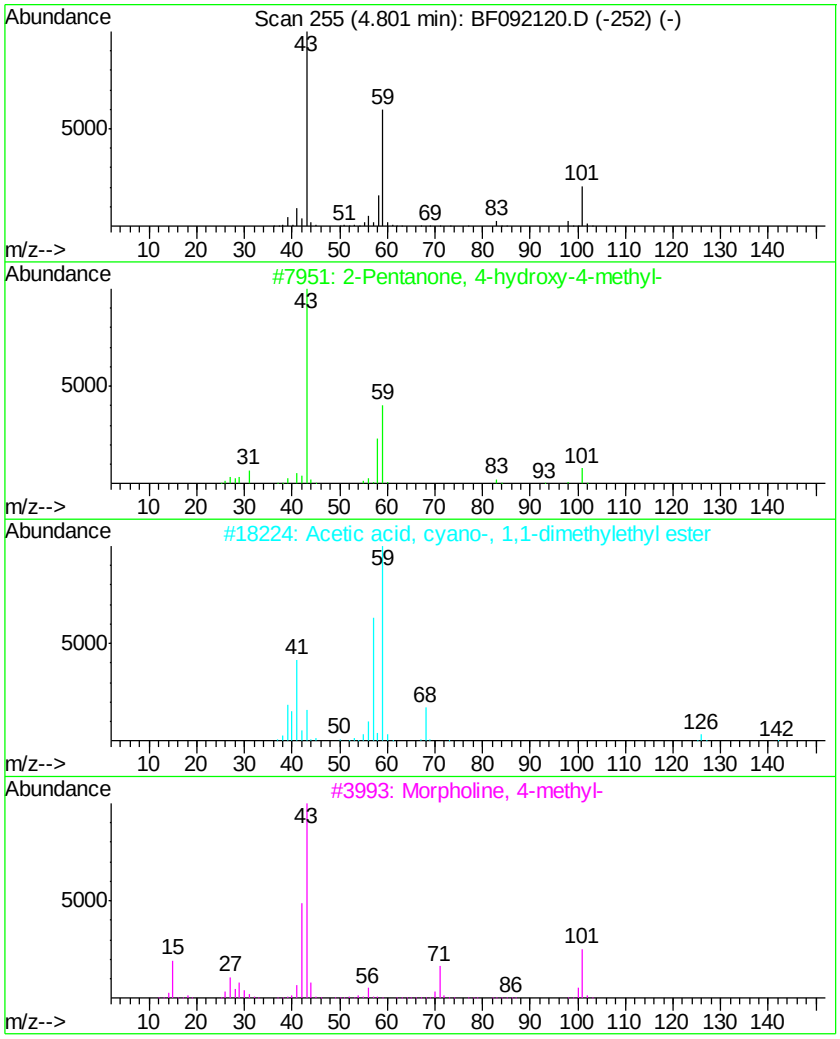
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

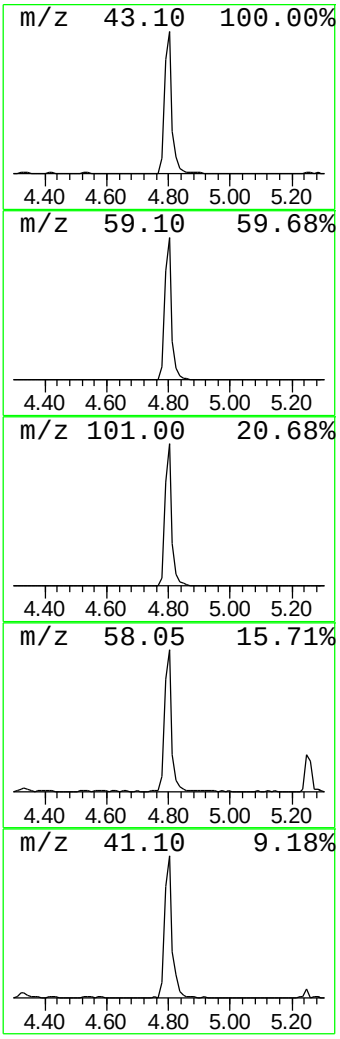
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	39.65 ng	2421420	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010617\
Data File : BF092120.D
Acq On : 6 Jan 2017 16:43
Operator : UM/SJ
Sample : I1025-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP7-8-COMP10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

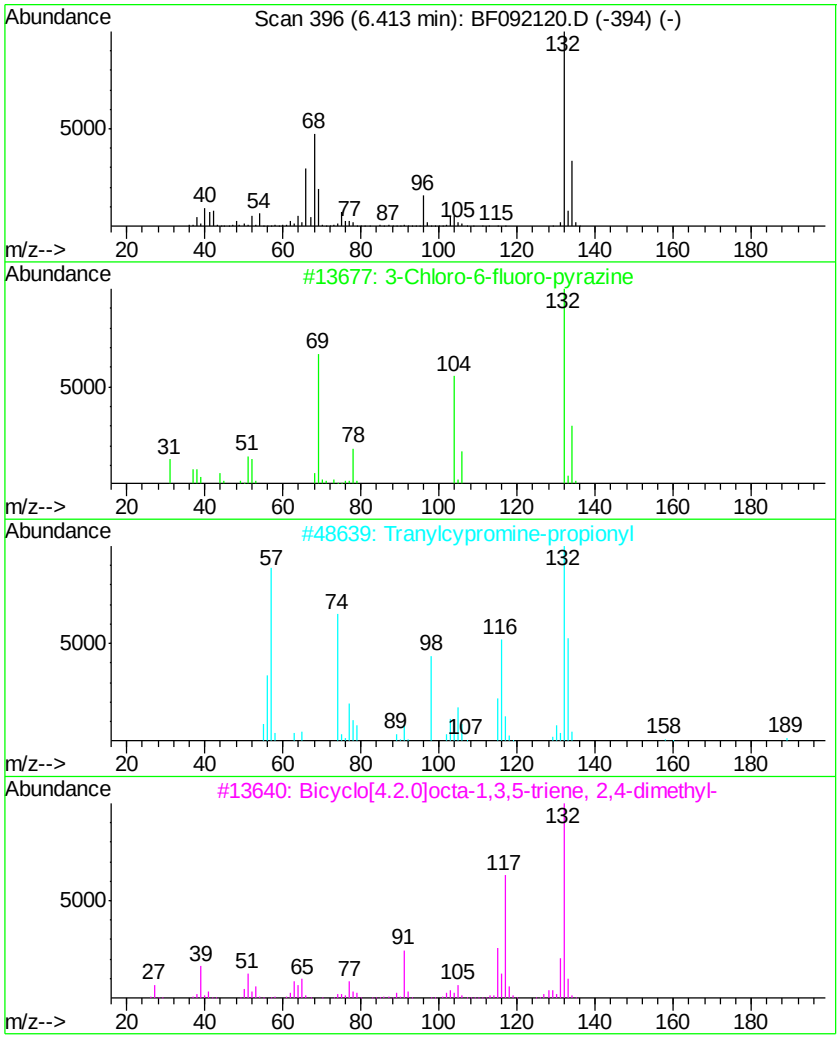
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

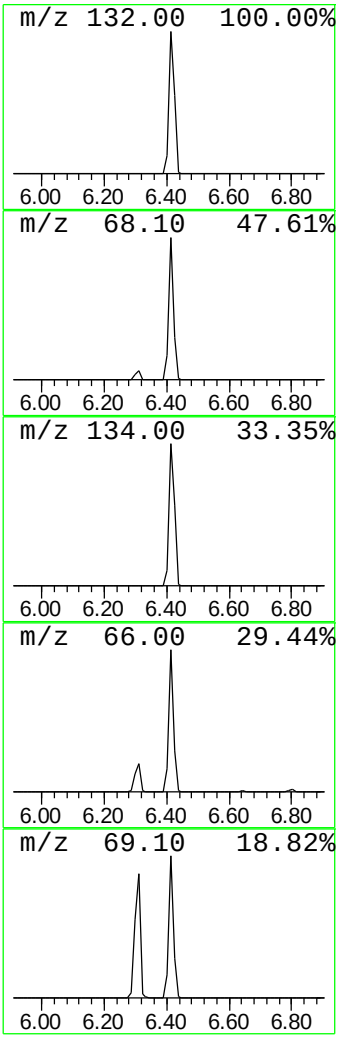
****

Peak Number 4 unknown6.41 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	88.68 ng	5416380	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010617\
Data File : BF092120.D
Acq On : 6 Jan 2017 16:43
Operator : UM/SJ
Sample : I1025-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP7-8-COMP10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

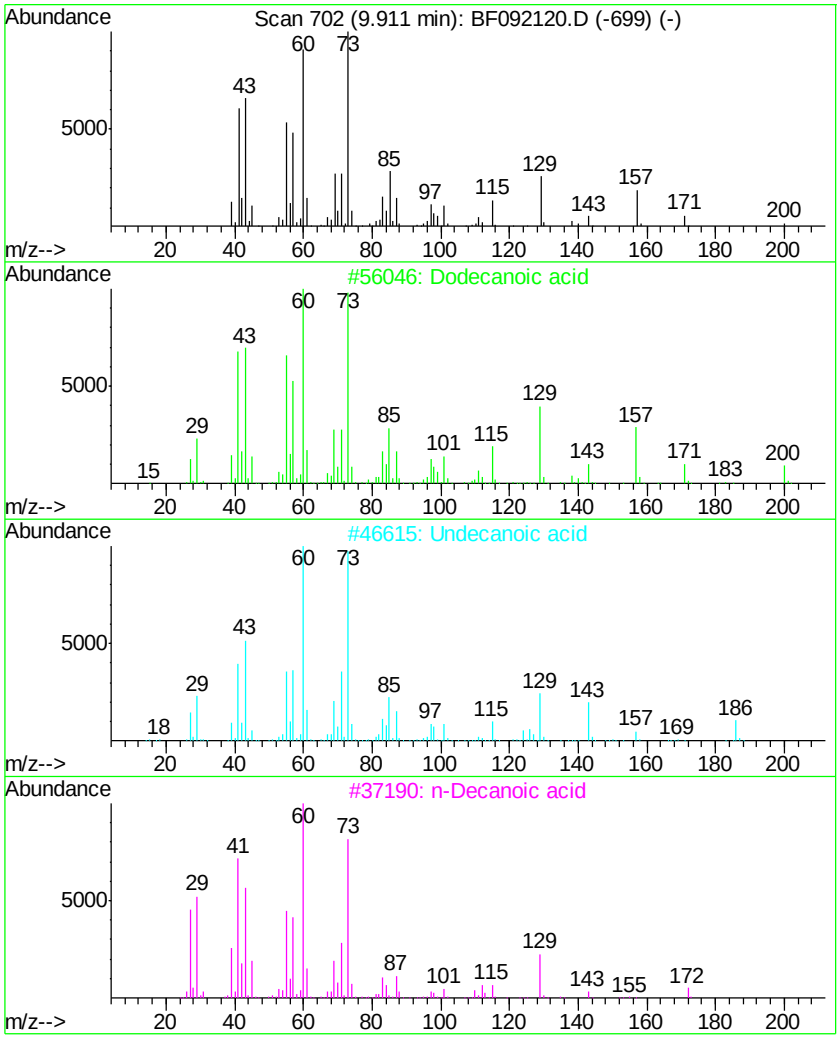
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

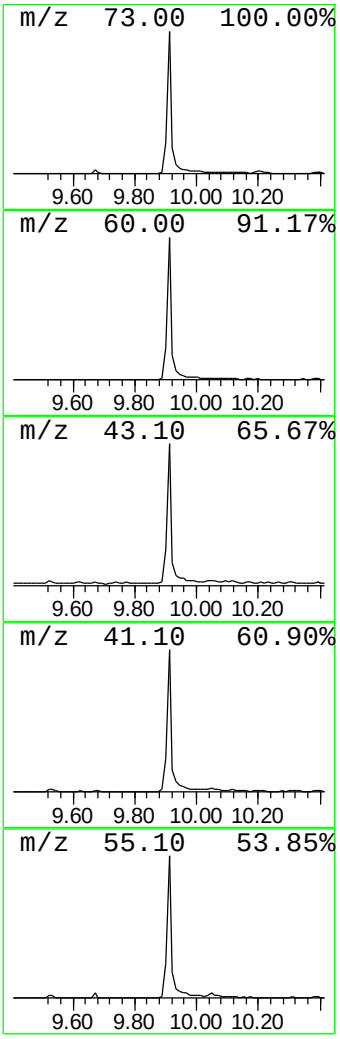
****

Peak Number 6 Dodecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.91	6.40 ng	508377	Acenaphthene-d10	9.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	98
2	Undecanoic acid	186	C11H22O2	000112-37-8	86
3	n-Decanoic acid	172	C10H20O2	000334-48-5	81
4	Nonanoic acid	158	C9H18O2	000112-05-0	62
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010617\
Data File : BF092120.D
Acq On : 6 Jan 2017 16:43
Operator : UM/SJ
Sample : I1025-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP7-8-COMP10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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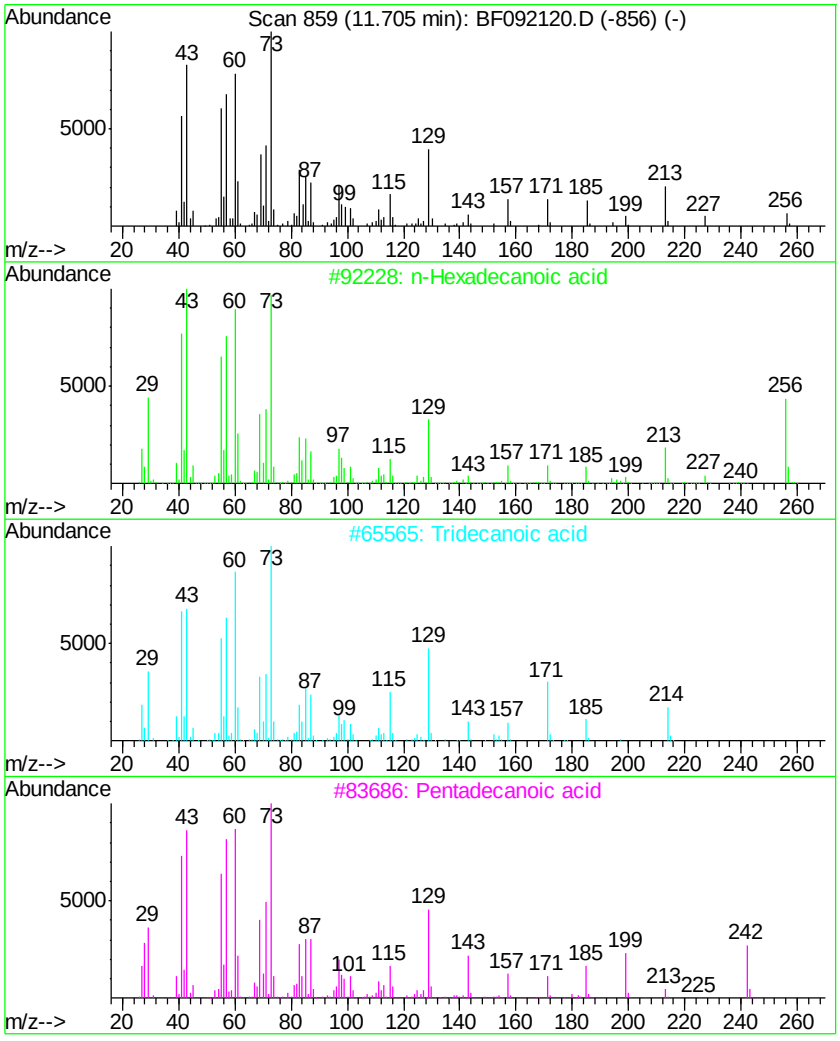
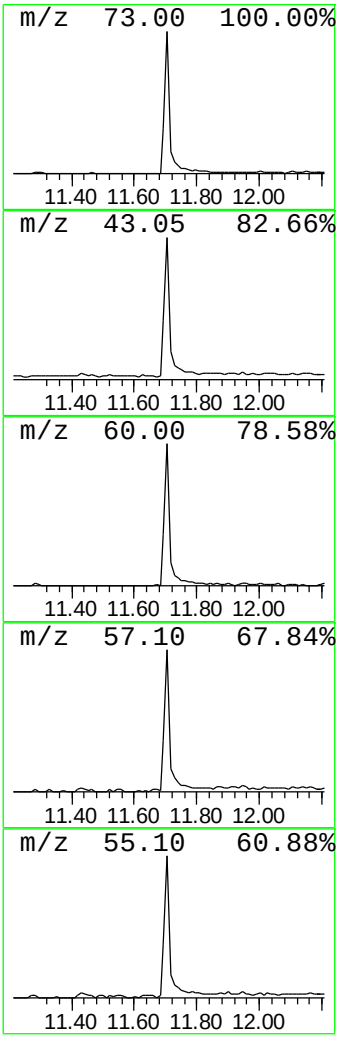
Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	5.24 ng	421617	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





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Data File : BF092120.D
Acq On : 6 Jan 2017 16:43
Operator : UM/SJ
Sample : I1025-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP7-8-COMP10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

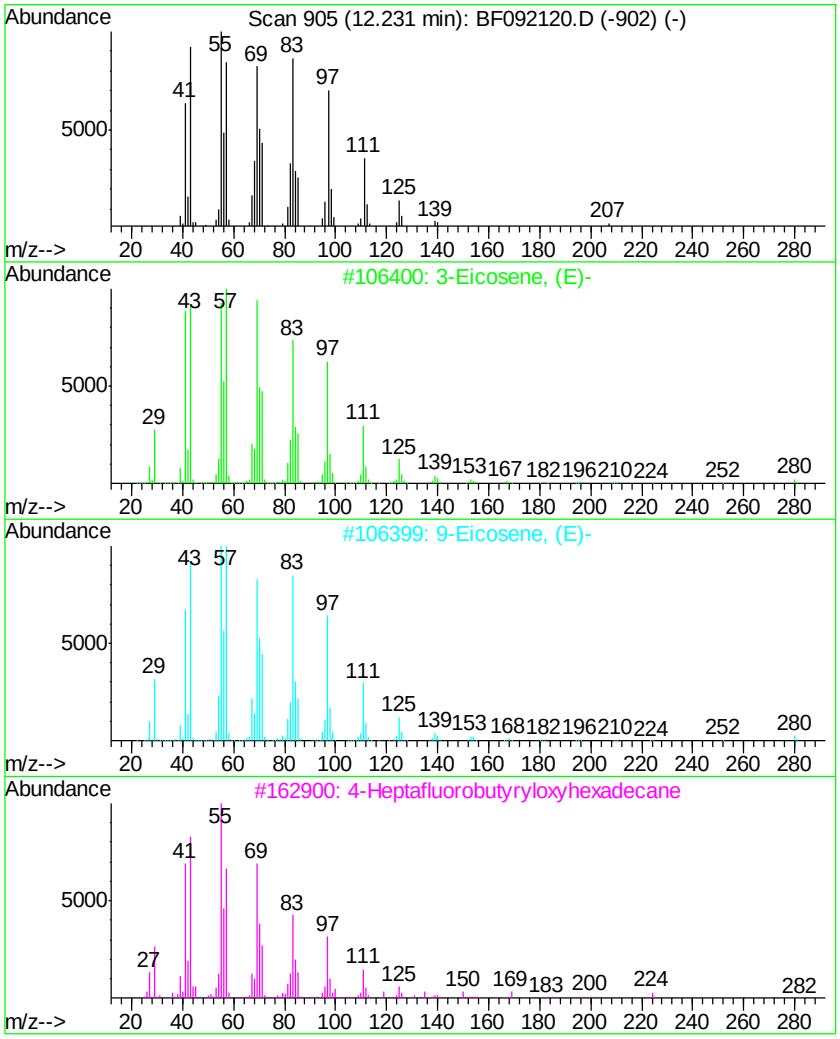
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

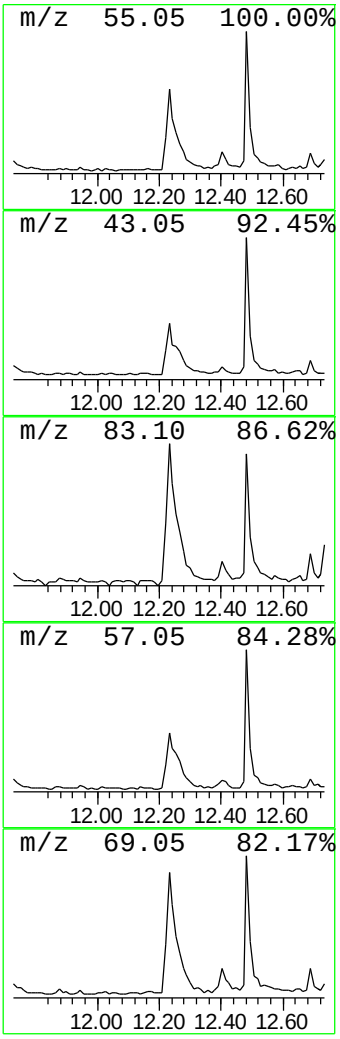
****

Peak Number 8 3-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.23	4.39 ng	353291	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	94
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
3	4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1000282-97-2	91
4	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
5	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010617\
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Acq On : 6 Jan 2017 16:43
Operator : UM/SJ
Sample : I1025-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP7-8-COMP10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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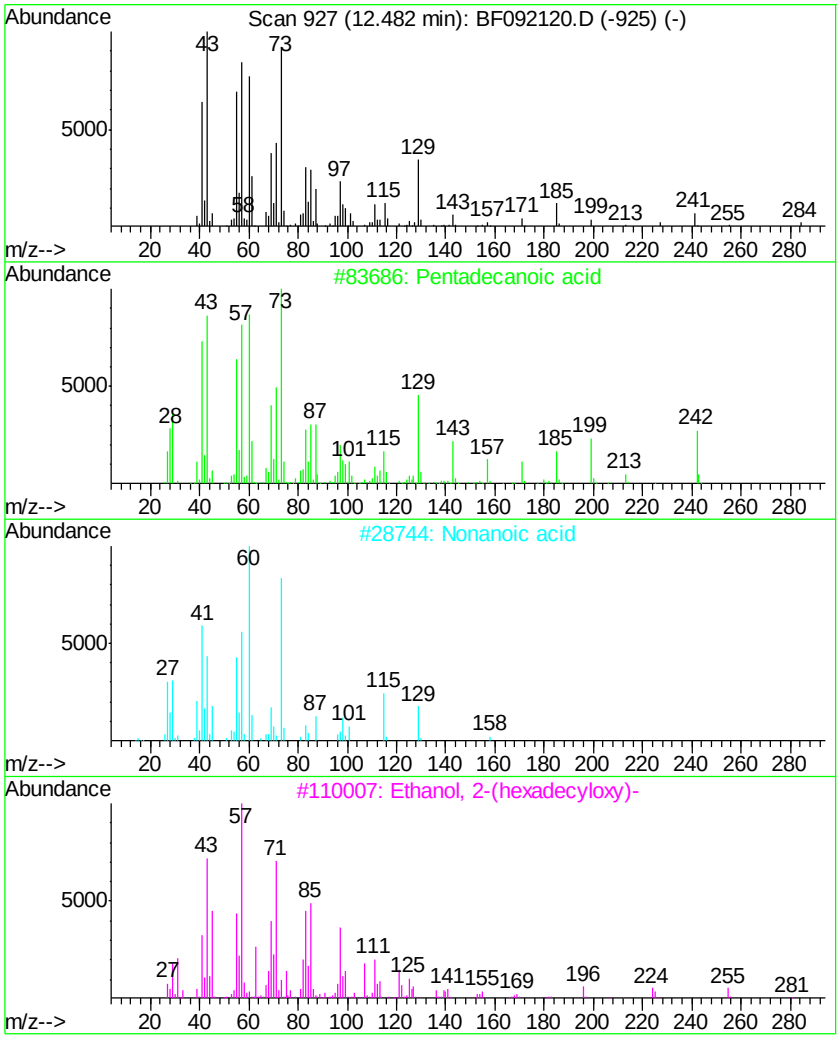
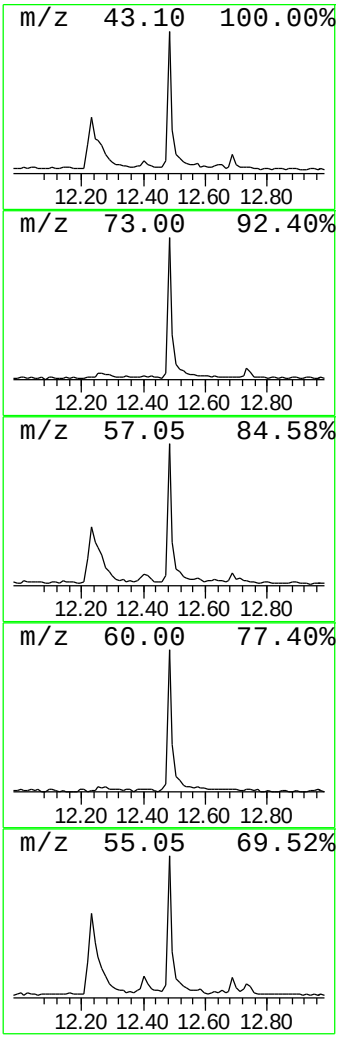
Peak Number 9 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	5.20 ng	406968	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	78
2	Nonanoic acid	158	C9H18O2	000112-05-0	27
3	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	22
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	11
5	Tridecane	184	C13H28	000629-50-5	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010617\
Data File : BF092120.D
Acq On : 6 Jan 2017 16:43
Operator : UM/SJ
Sample : I1025-04
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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	2.32	5.3	ng	321519	1	6.64	1221520	20.0
3-Penten-2-one, 4...	4.09	2.8	ng	171432	1	6.64	1221520	20.0
2-Pentanone, 4-hy...	4.80	39.6	ng	2421420	1	6.64	1221520	20.0
unknown6.41	6.41	88.7	ng	5416380	1	6.64	1221520	20.0
Dodecanoic acid	9.91	6.4	ng	508377	3	9.67	1588800	20.0
n-Hexadecanoic acid	11.71	5.2	ng	421617	4	11.16	1609310	20.0
3-Eicosene, (E)-	12.23	4.4	ng	353291	4	11.16	1609310	20.0
Pentadecanoic acid	12.48	5.2	ng	406968	5	13.77	1564650	20.0