LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060516\
Data File : BF087724.D
Acq On : 5 Jun 2016 23:22
Operator : UM/SJ
Sample : H3379-18
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6

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-BF060416.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	1.770	11	16	18	rBV	4343934	7738274	100.00%	20.409%
2	1.907	26	28	49	rVB	1399367	2962461	38.28%	7.813%
3	2.158	49	50	67	rVB	80213	184849	2.39%	0.488%
4	5.061	301	304	312	rVB	161099	274807	3.55%	0.725%
5	5.461	336	339	341	rBV	2535451	2729175	35.27%	7.198%
6	6.490	425	429	431	rBV	2485625	2840801	36.71%	7.492%
7	6.627	438	441	443	rBV	2774069	2909392	37.60%	7.673%
8	6.856	459	461	464	rBV	807823	684723	8.85%	1.806%
9	7.016	472	475	477	rVB	2553076	2327331	30.08%	6.138%
10	7.427	507	511	513	rBV	1396134	2008617	25.96%	5.297%
11	8.147	571	574	576	rBV	777937	929564	12.01%	2.452%
12	9.222	665	668	671	rBV	2839414	3121350	40.34%	8.232%
13	9.610	700	702	705	rBV	132092	153319	1.98%	0.404%
14	9.896	724	727	730	rBV	1132530	1042489	13.47%	2.749%
15	10.685	793	796	798	rBV	1932389	1975269	25.53%	5.209%
16	11.382	854	857	859	rBV	978345	1053307	13.61%	2.778%
17	12.799	978	981	983	rBV	176025	206593	2.67%	0.545%
18	12.971	993	996	998	rBV	2825474	2988945	38.63%	7.883%
19	13.496	1040	1042	1045	rBV	151403	147915	1.91%	0.390%
20	13.874	1073	1075	1084	rBV	48003	112711	1.46%	0.297%
21	14.011	1084	1087	1089	rBV	952697	859601	11.11%	2.267%
22	15.440	1209	1212	1215	rBV	543172	665310	8.60%	1.755%

Sum of corrected areas: 37916803

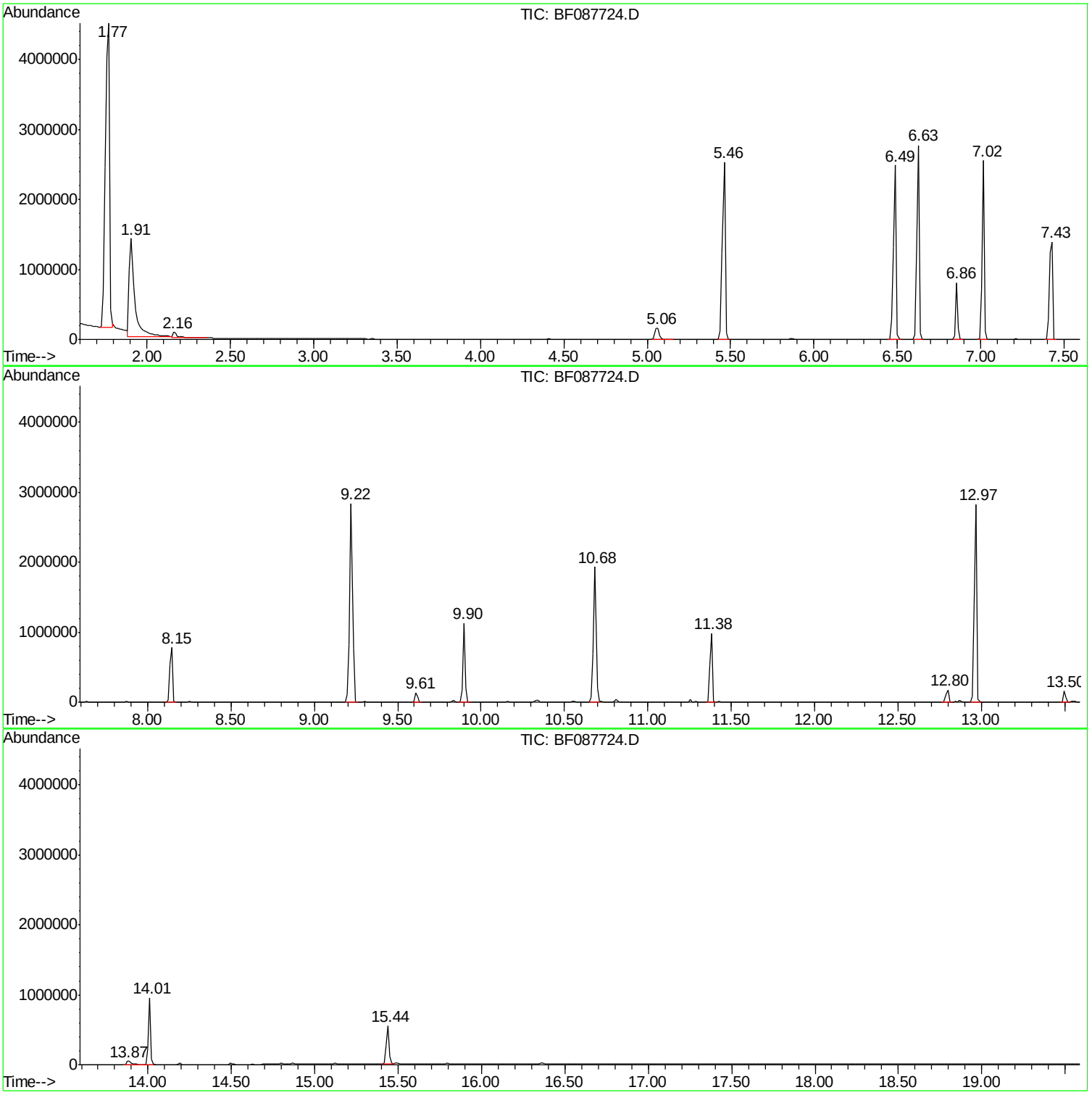
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060516\
Data File : BF087724.D
Acq On : 5 Jun 2016 23:22
Operator : UM/SJ
Sample : H3379-18
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060516\
Data File : BF087724.D
Acq On : 5 Jun 2016 23:22
Operator : UM/SJ
Sample : H3379-18
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

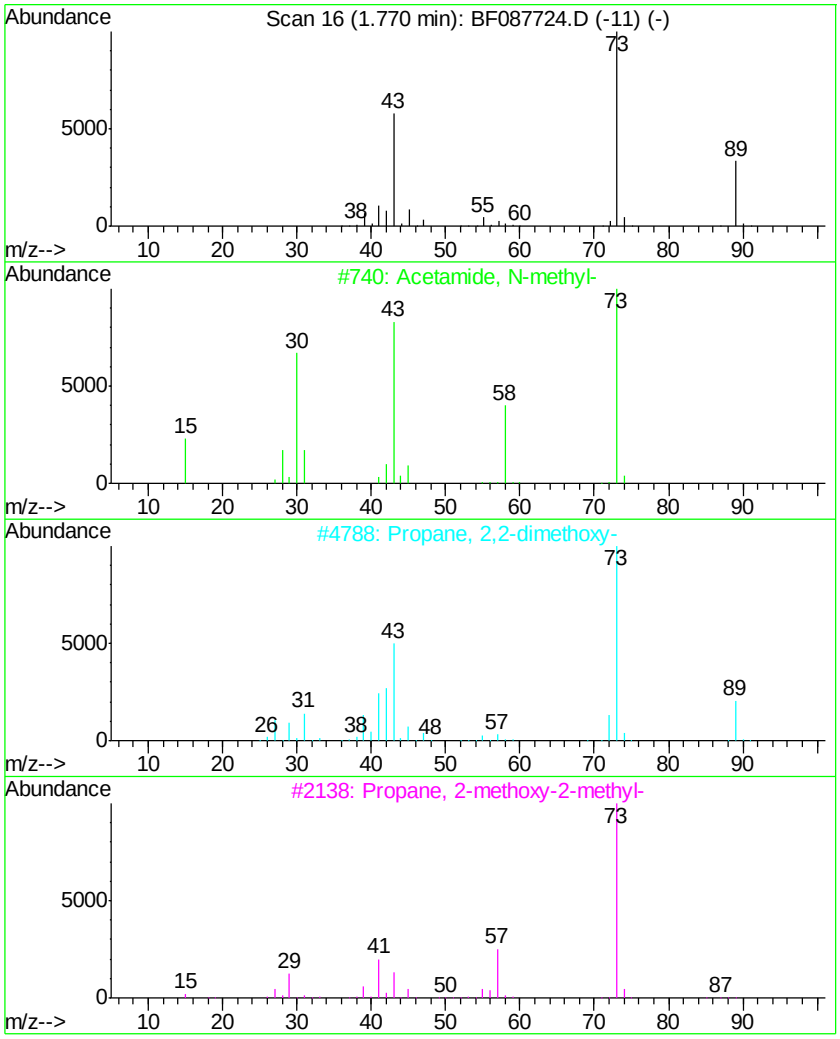
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

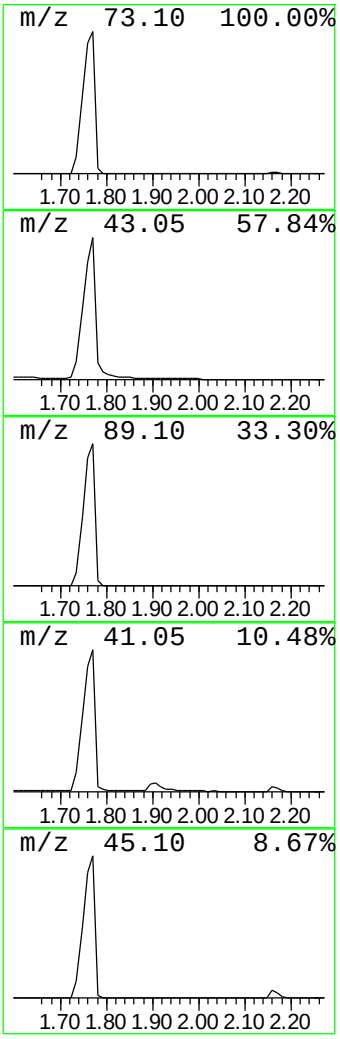
****

Peak Number 1 unknown1.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.77	226.03 ng	7738270	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	43
2	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	17
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9





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Acq On : 5 Jun 2016 23:22
Operator : UM/SJ
Sample : H3379-18
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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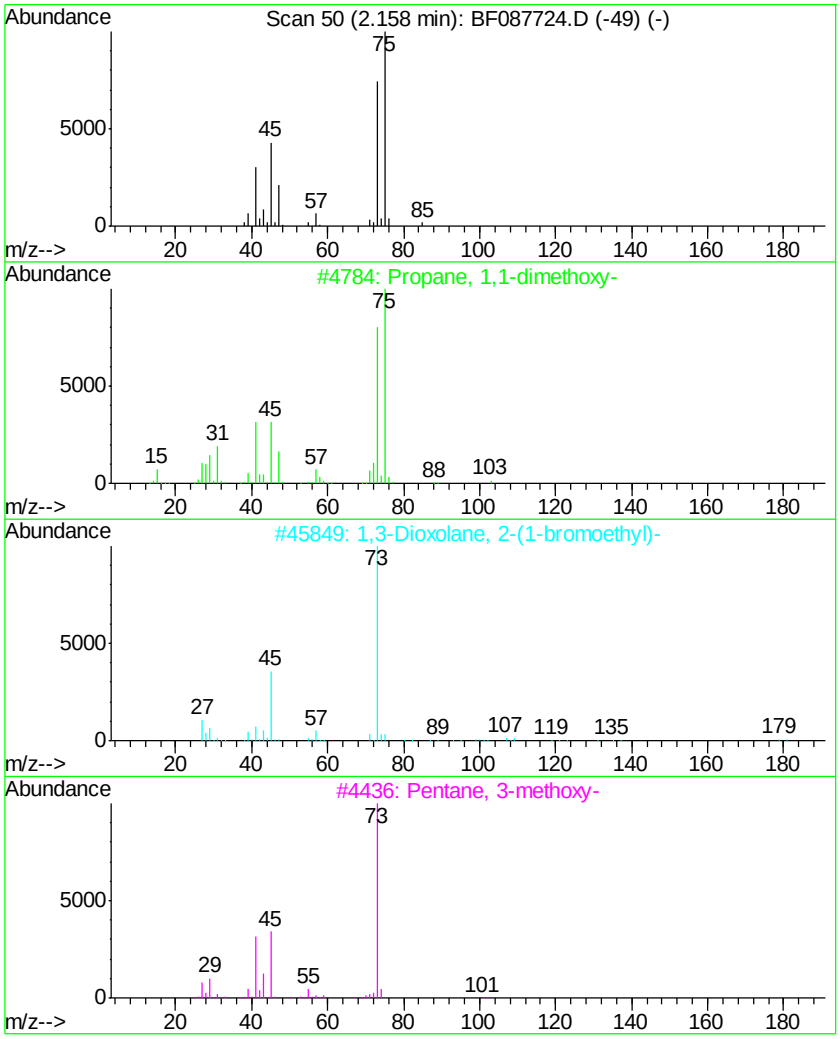
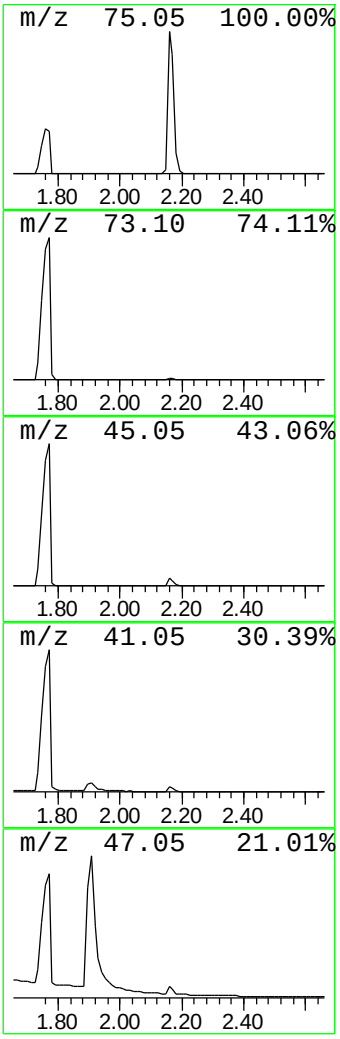
Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	5.40 ng	184849	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	22
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
4	Ethanethioamide	75	C2H5NS	000062-55-5	9
5	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060516\
Data File : BF087724.D
Acq On : 5 Jun 2016 23:22
Operator : UM/SJ
Sample : H3379-18
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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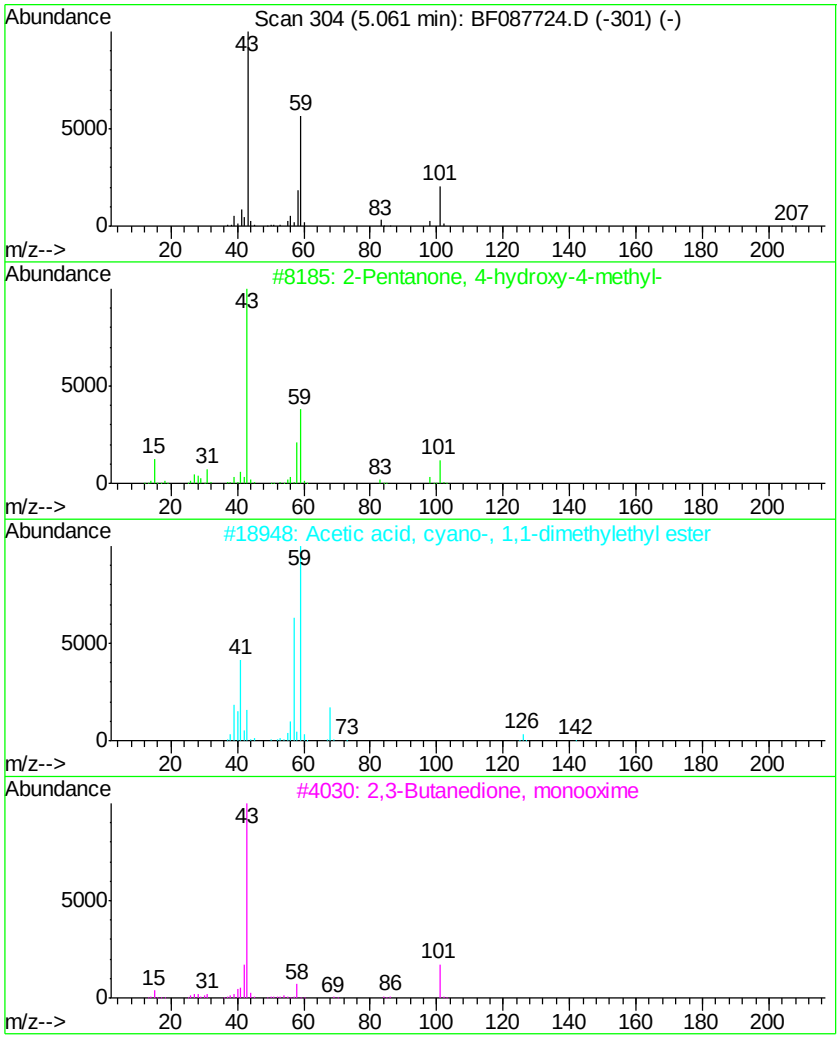
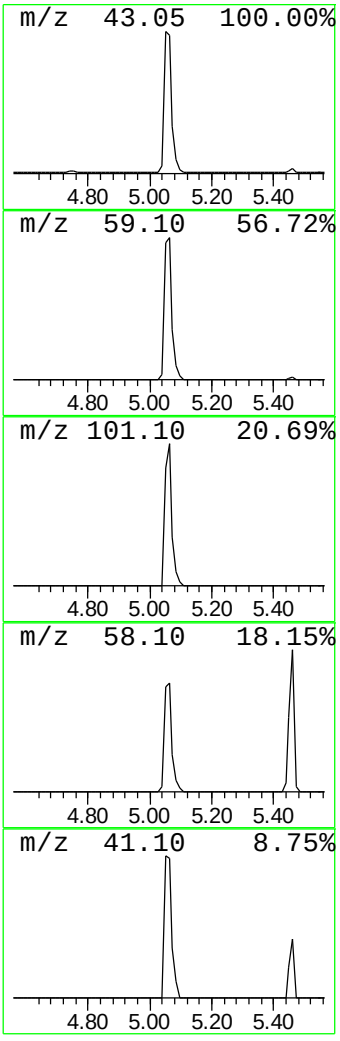
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	8.03 ng	274807	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BF087724.D
Acq On : 5 Jun 2016 23:22
Operator : UM/SJ
Sample : H3379-18
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

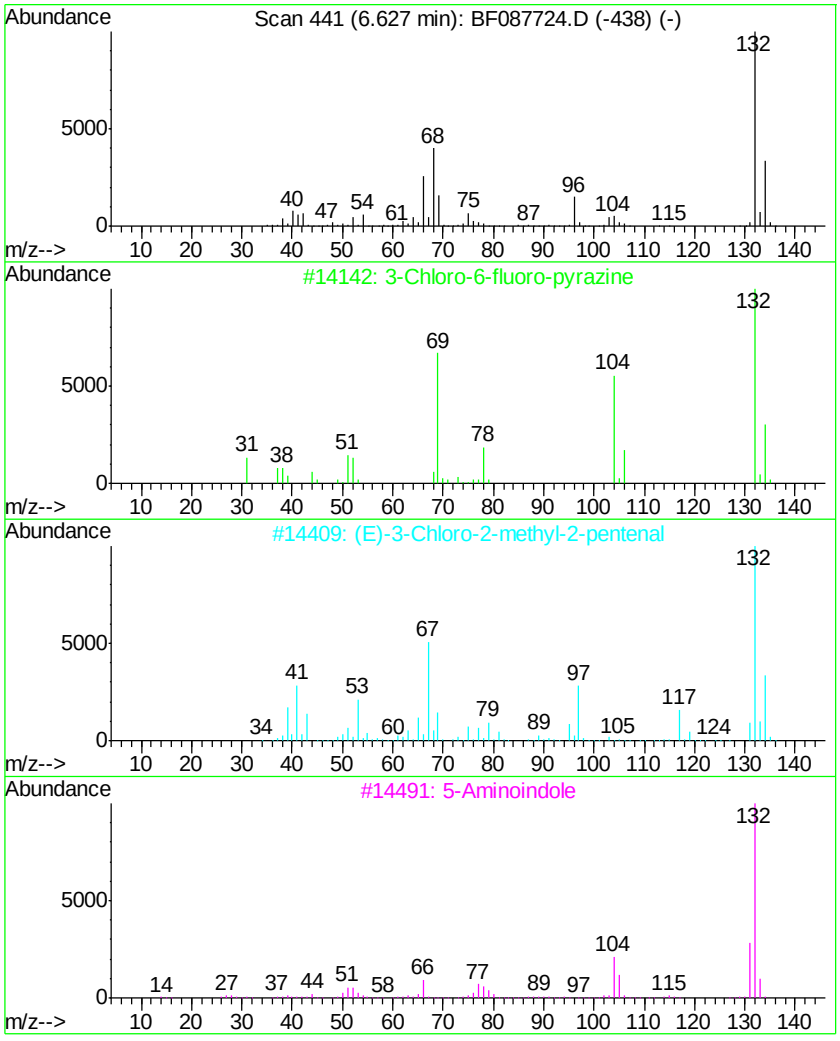
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

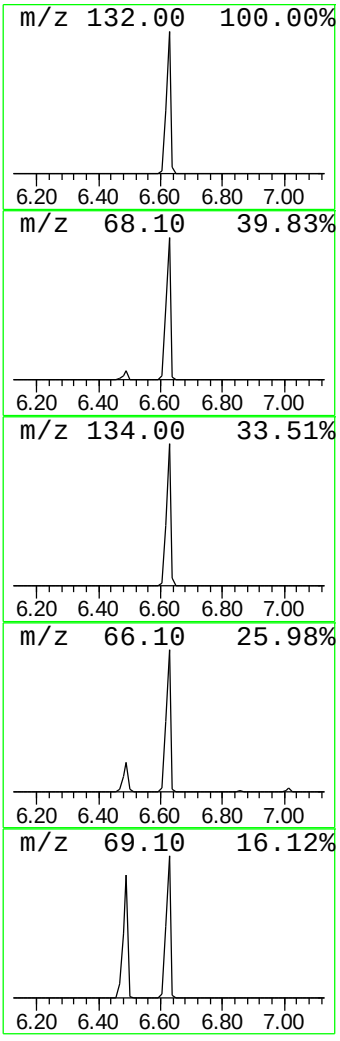
****

Peak Number 5 unknown6.63 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	84.98 ng	2909390	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Sample : H3379-18
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

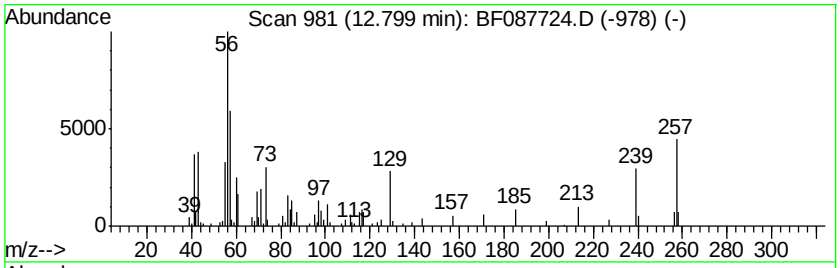
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

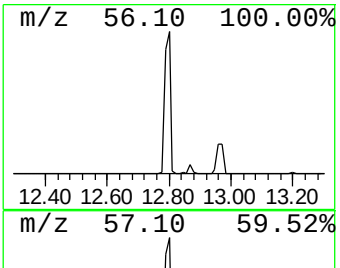
****

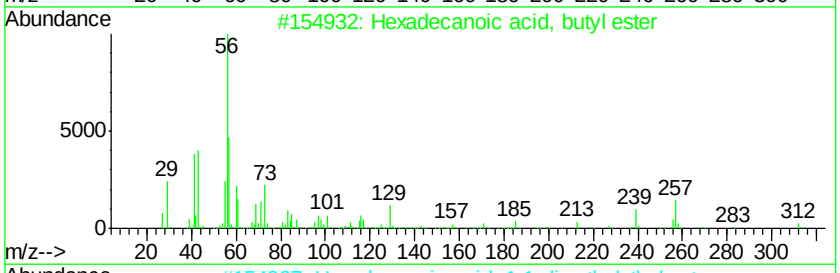
Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 7

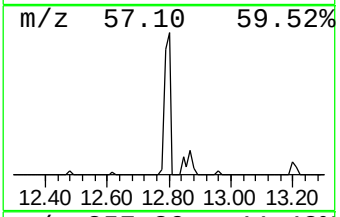
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	4.81 ng	206593	Chrysene-d12	14.01

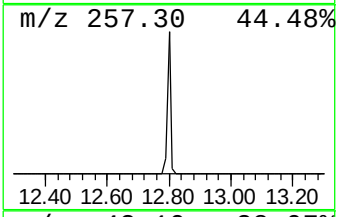
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	62
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	52
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	32
4	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	25
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	22

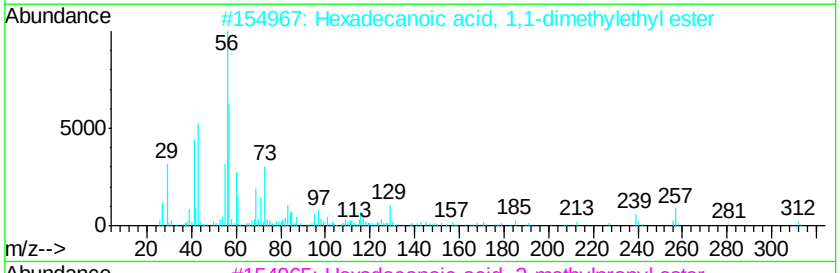


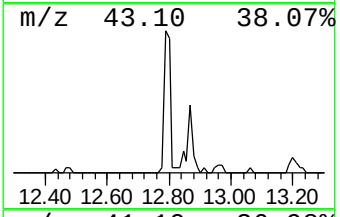


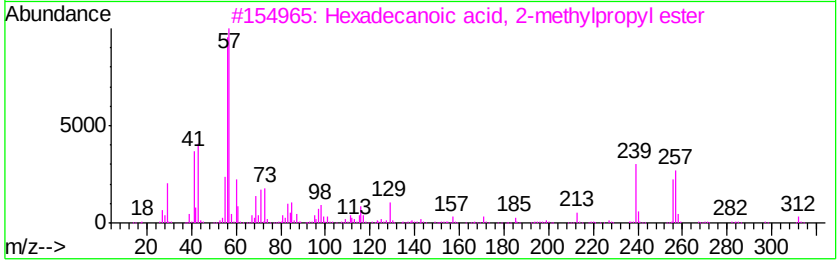


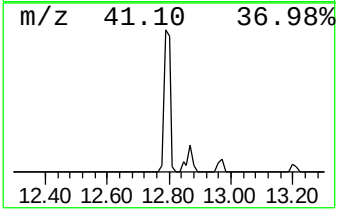












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Acq On : 5 Jun 2016 23:22
Operator : UM/SJ
Sample : H3379-18
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

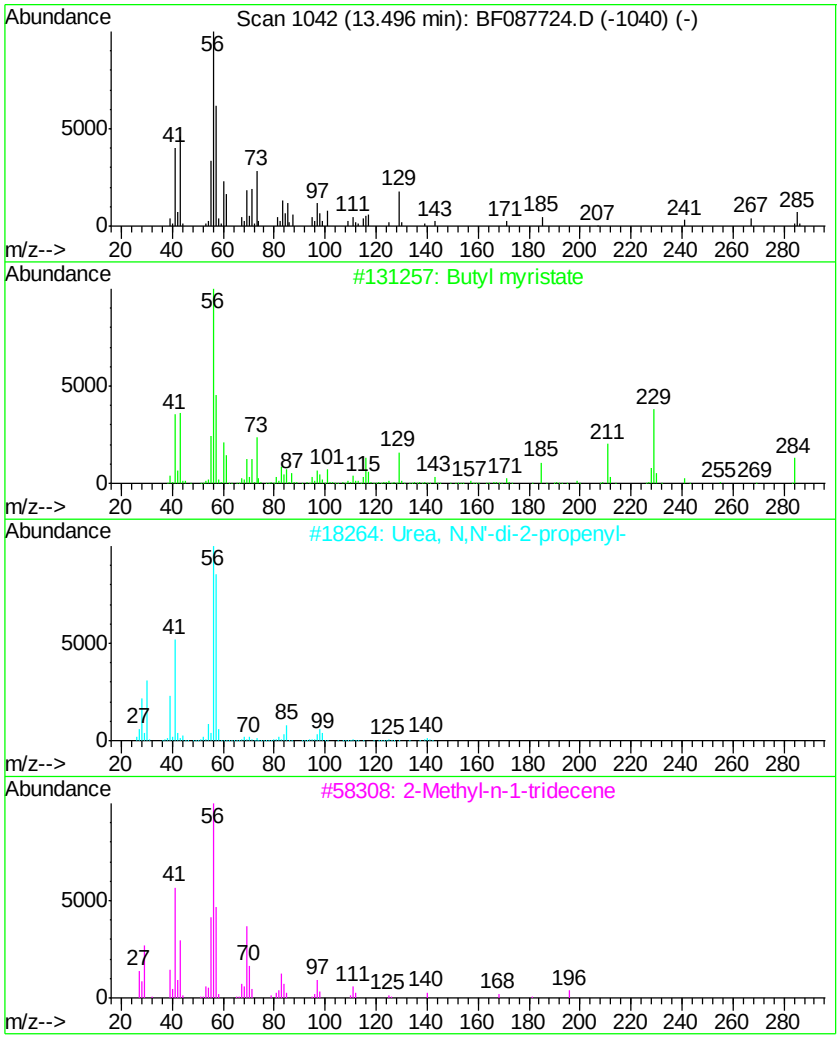
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

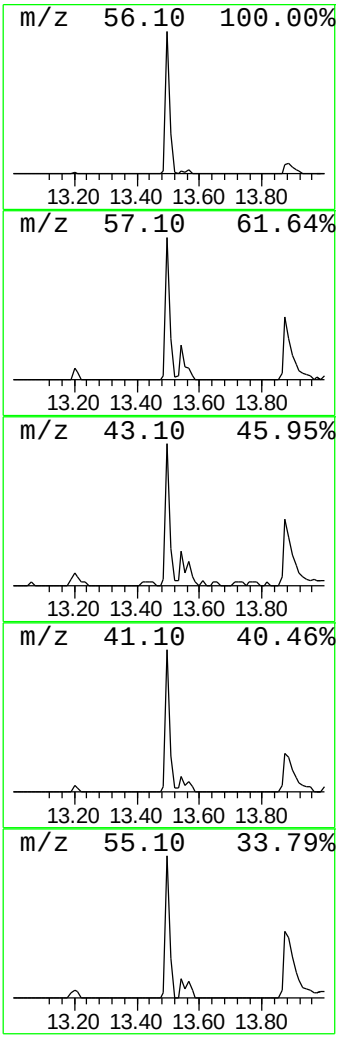
****

Peak Number 8 Butyl myristate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	3.44 ng	147915	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	80
2	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38
3	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
4	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	35
5	Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	32





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TIC Library : C:\Database\NIST11.L
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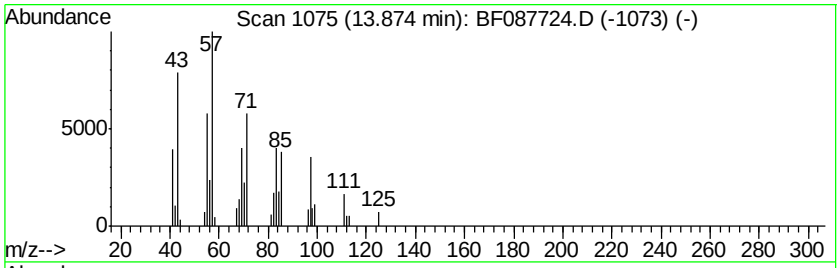
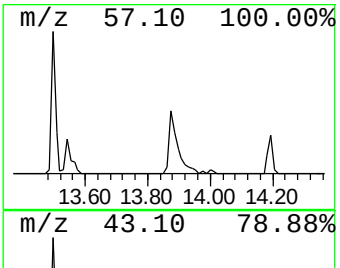
****

Peak Number 9 Oxalic acid, cyclobutyl pen... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	2.62 ng	112711	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	86
2	Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	86
3	Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	86
4	Oxalic acid, cyclobutyl tetradec...	340	C20H36O4	1000309-70-9	78
5	Oxalic acid, cyclobutyl hexadecy...	368	C22H40O4	1000309-70-6	72





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown1.77	1.77	226.0	ng	7738270	1	6.86	684723	20.0
Propane, 1,1-dime...	2.16	5.4	ng	184849	1	6.86	684723	20.0
2-Pentanone, 4-hy...	5.06	8.0	ng	274807	1	6.86	684723	20.0
unknown6.63	6.63	85.0	ng	2909390	1	6.86	684723	20.0
Hexadecanoic acid...	12.80	4.8	ng	206593	5	14.01	859601	20.0
Butyl myristate	13.50	3.4	ng	147915	5	14.01	859601	20.0
Oxalic acid, cycl...	13.87	2.6	ng	112711	5	14.01	859601	20.0