LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085602.D
Acq On : 20 Mar 2016 7:07
Operator : UM/SJ
Sample : H1804-11
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-8C

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-BF031816.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	2.435	7	13	18	rVB	15106	51018	1.33%	0.152%
2	2.698	34	36	43	rVB	119585	159655	4.15%	0.477%
3	5.053	239	242	248	rBV	265080	427824	11.12%	1.278%
4	5.464	275	278	280	rBV	2787392	2937827	76.33%	8.777%
5	6.493	365	368	370	rBV	2333047	3042001	79.03%	9.089%
6	6.619	377	379	382	rBV	2613633	3200216	83.15%	9.561%
7	6.847	397	399	402	rBV	655423	878074	22.81%	2.623%
8	7.007	411	413	416	rVB	2571272	2514034	65.32%	7.511%
9	7.419	446	449	451	rBV	2216381	2215818	57.57%	6.620%
10	8.162	509	514	516	rBV2	1465591	2671668	69.41%	7.982%
11	8.207	516	518	520	rVB	40208	38543	1.00%	0.115%
12	8.847	572	574	578	rBV	139911	118222	3.07%	0.353%
13	8.950	580	583	585	rBV	65198	64441	1.67%	0.193%
14	9.213	603	606	609	rBV	3711281	3828019	99.46%	11.437%
15	9.887	663	665	667	rBV	1341028	1298369	33.73%	3.879%
16	9.922	667	668	670	rVB	158094	116286	3.02%	0.347%
17	10.093	681	683	685	rBV	73412	60164	1.56%	0.180%
18	10.436	711	713	715	rVB	72726	58815	1.53%	0.176%
19	10.676	731	734	737	rBV2	1978987	2456636	63.83%	7.340%
20	11.373	792	795	797	rBV	1497370	1356817	35.25%	4.054%
21	12.779	916	918	921	rBV	352399	296648	7.71%	0.886%
22	12.859	921	925	927	rVB2	41865	48904	1.27%	0.146%
23	12.962	931	934	936	rBV	3849914	3848943	100.00%	11.499%
24	13.488	977	980	982	rBV	161951	164187	4.27%	0.491%
25	14.002	1023	1025	1028	rBV	875134	875740	22.75%	2.616%
26	15.431	1147	1150	1153	rBV	581995	741937	19.28%	2.217%

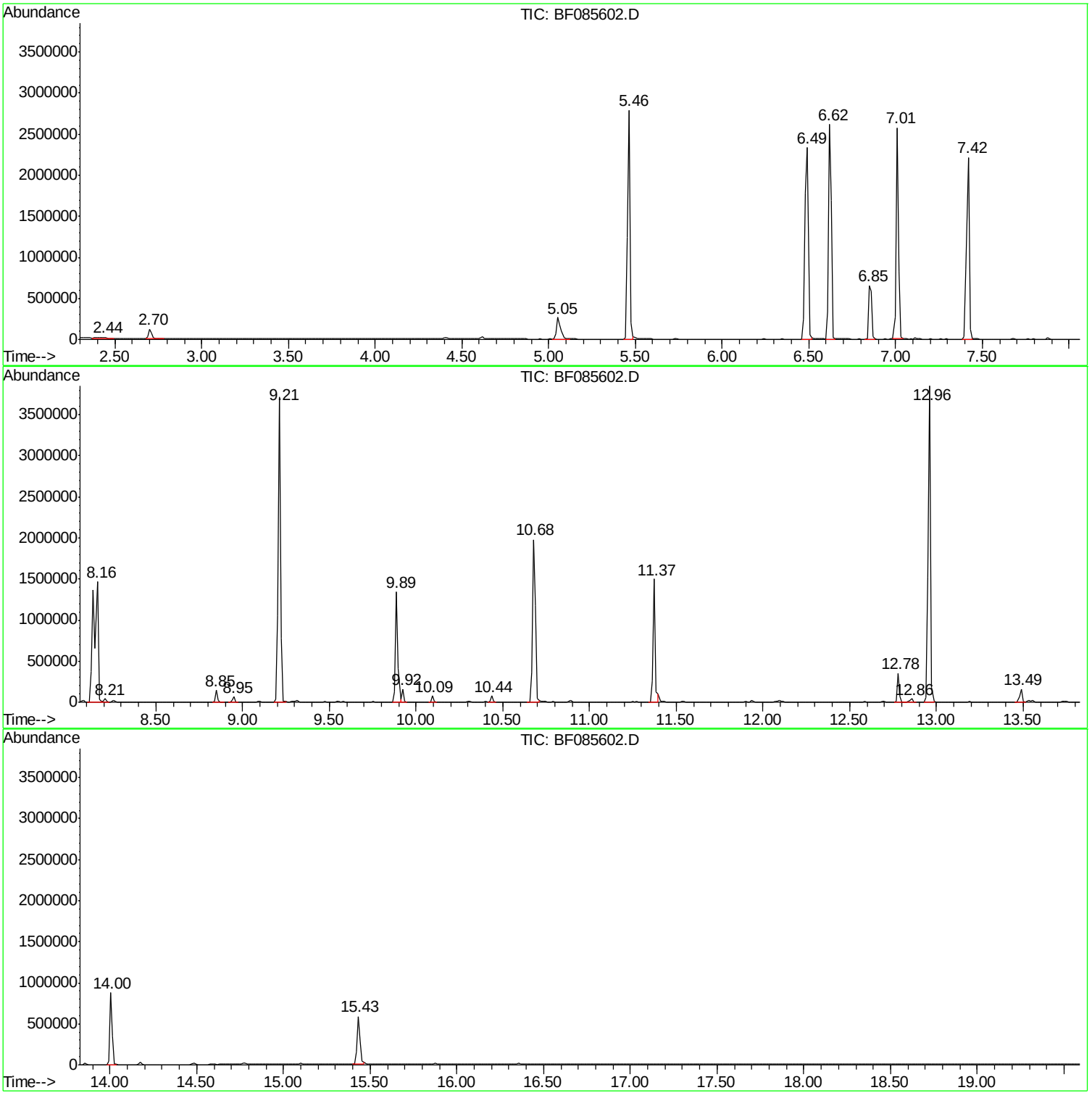
Sum of corrected areas: 33470806

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085602.D
Acq On : 20 Mar 2016 7:07
Operator : UM/SJ
Sample : H1804-11
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRACK-D-GRID-8C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.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\BF031816\
Data File : BF085602.D
Acq On : 20 Mar 2016 7:07
Operator : UM/SJ
Sample : H1804-11
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-8C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

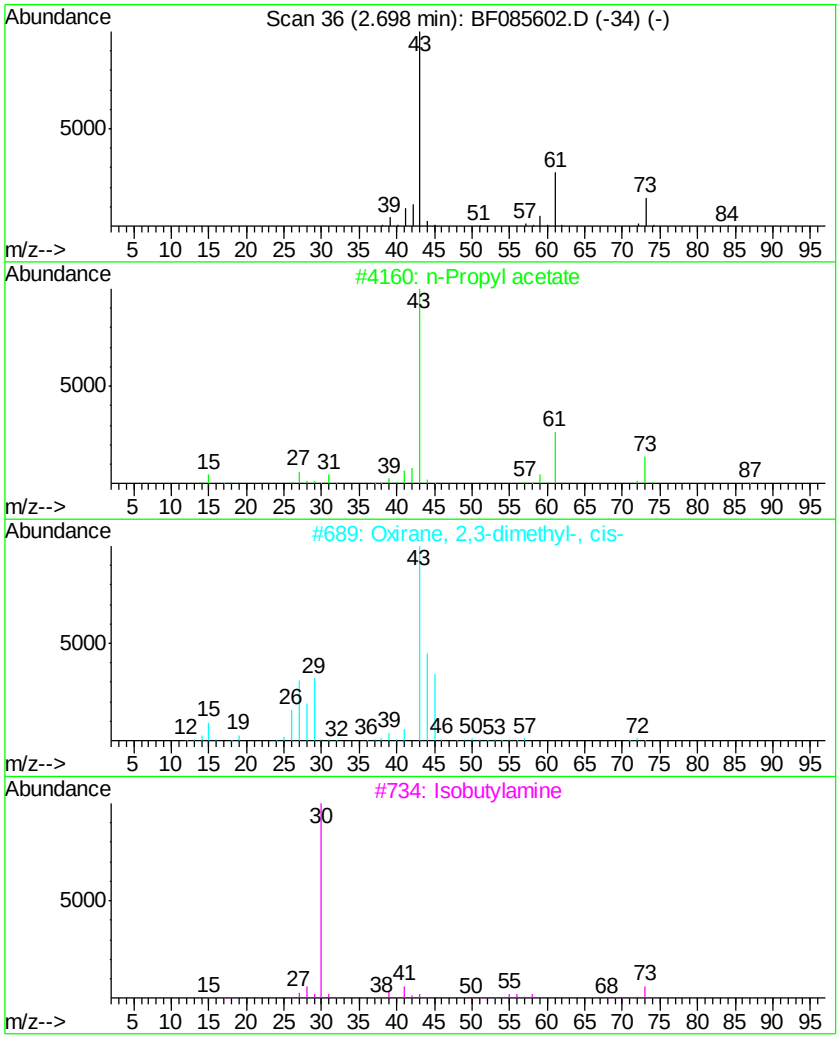
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

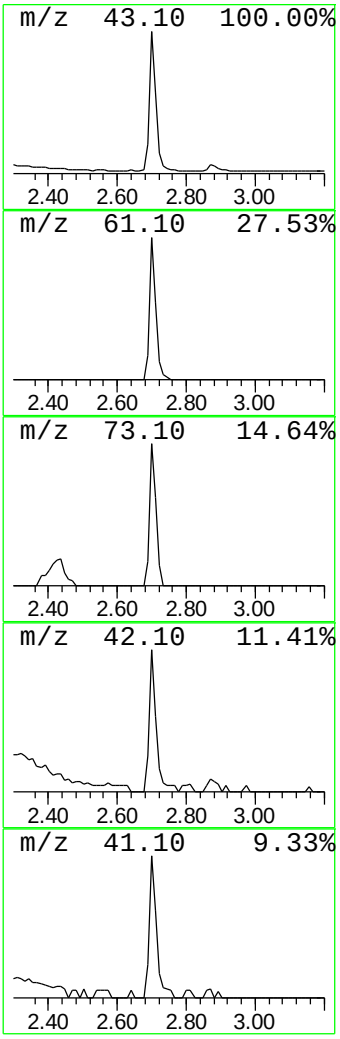
****

Peak Number 1 n-Propyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.70	3.64 ng	159655	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	7
3	Isobutylamine	73	C4H11N	000078-81-9	7
4	1-Butanamine	73	C4H11N	000109-73-9	7
5	Pentane	72	C5H12	000109-66-0	5





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085602.D
Acq On : 20 Mar 2016 7:07
Operator : UM/SJ
Sample : H1804-11
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-8C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

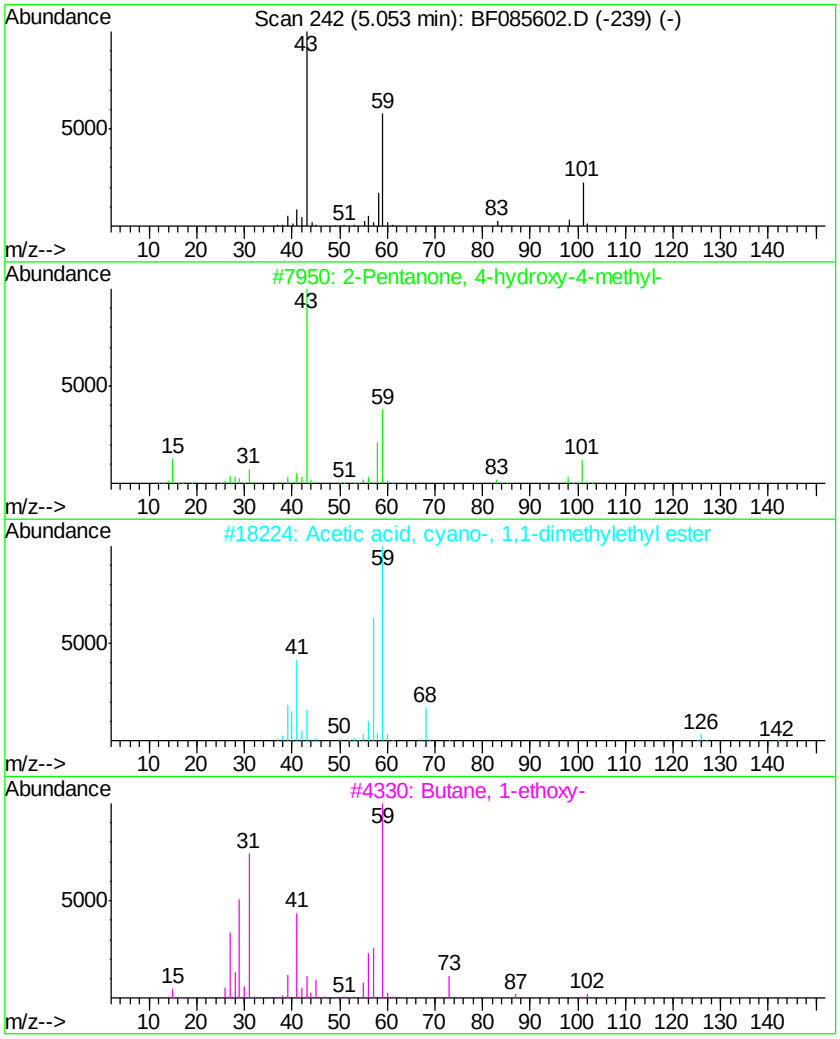
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

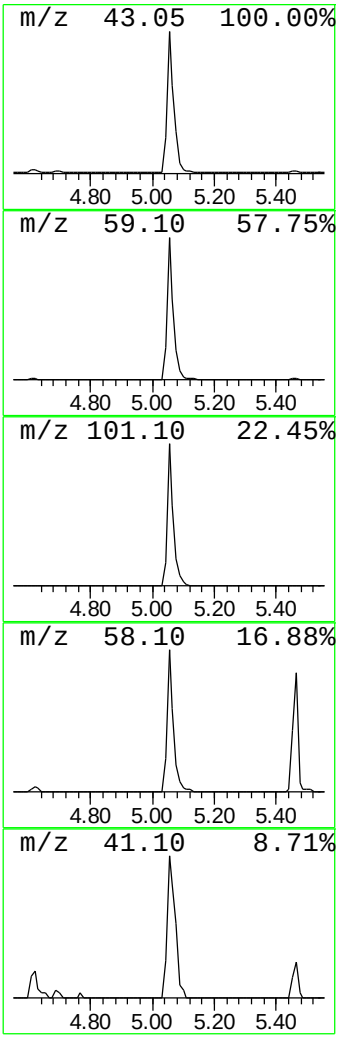
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	9.74 ng	427824	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	23
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085602.D
Acq On : 20 Mar 2016 7:07
Operator : UM/SJ
Sample : H1804-11
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-8C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

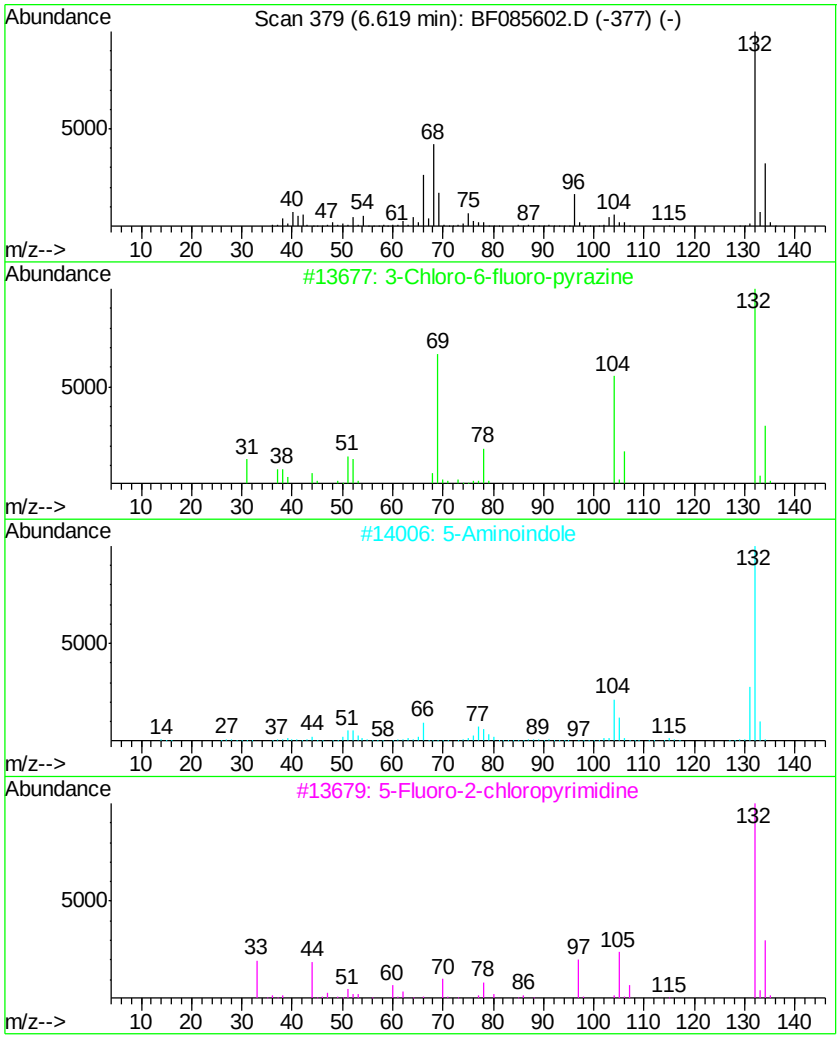
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

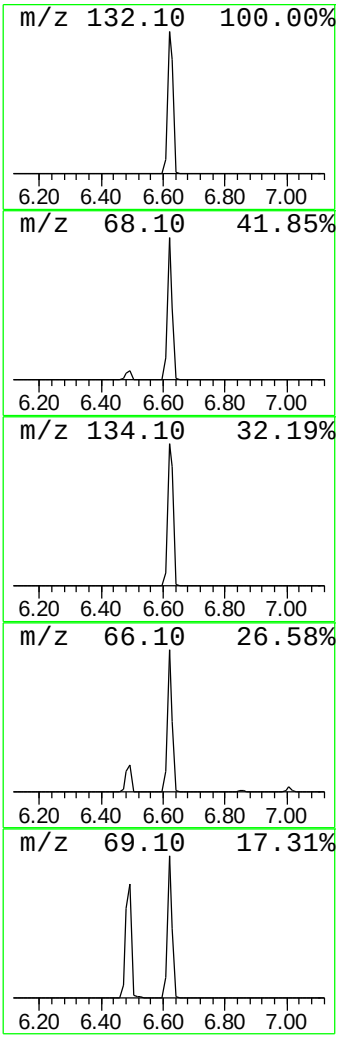
****

Peak Number 3 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	72.89 ng	3200220	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	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085602.D
Acq On : 20 Mar 2016 7:07
Operator : UM/SJ
Sample : H1804-11
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-8C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

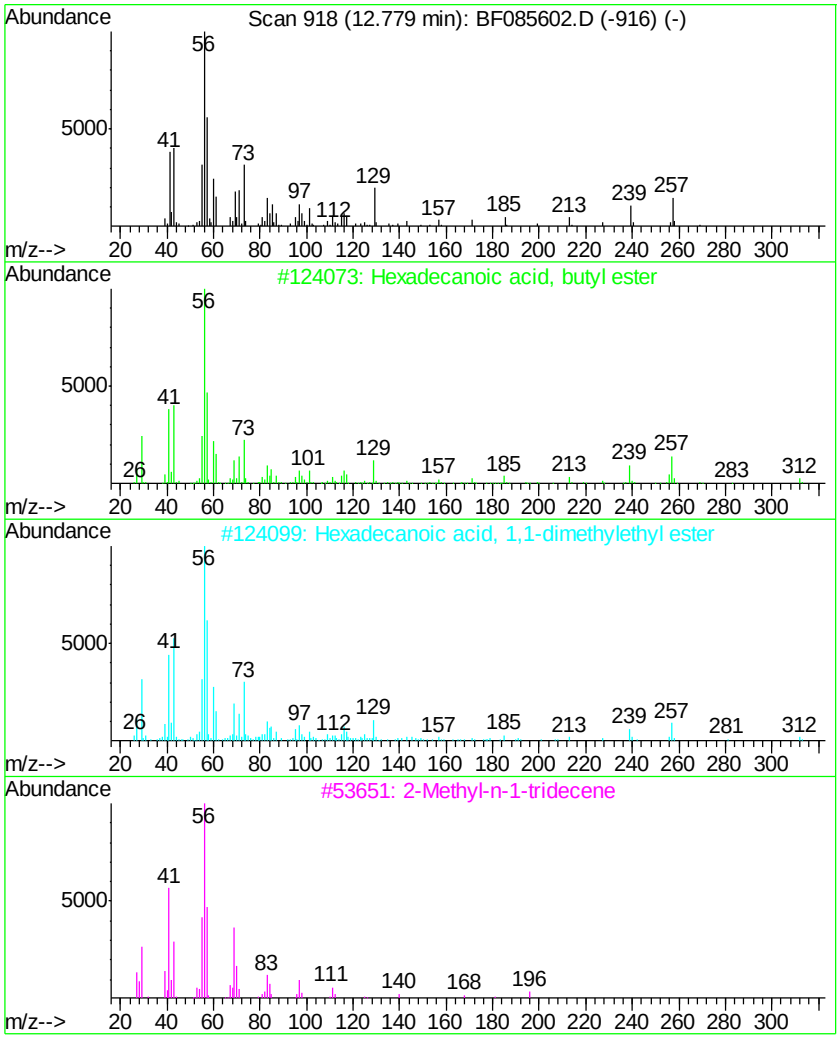
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

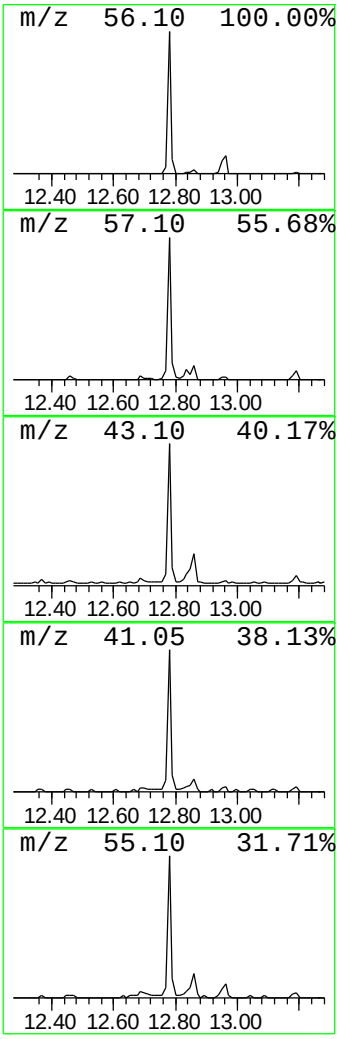
****

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	6.77 ng	296648	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	90
3	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
4	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	27





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085602.D
Acq On : 20 Mar 2016 7:07
Operator : UM/SJ
Sample : H1804-11
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-8C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

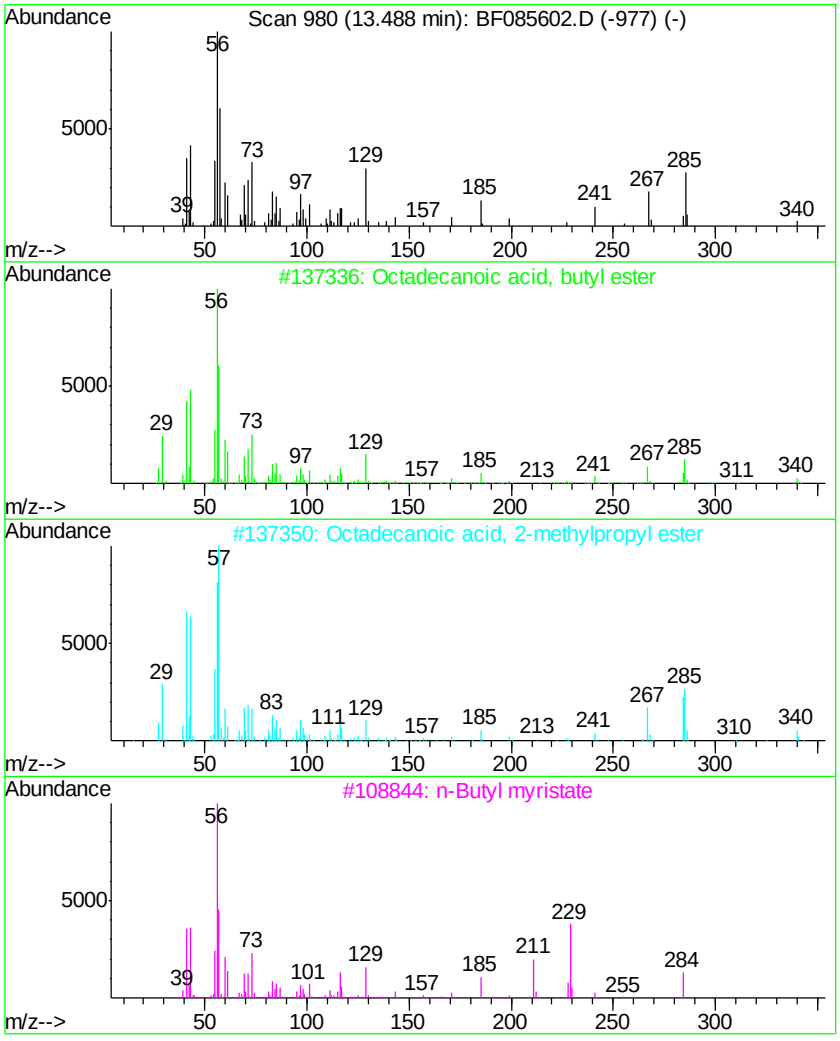
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

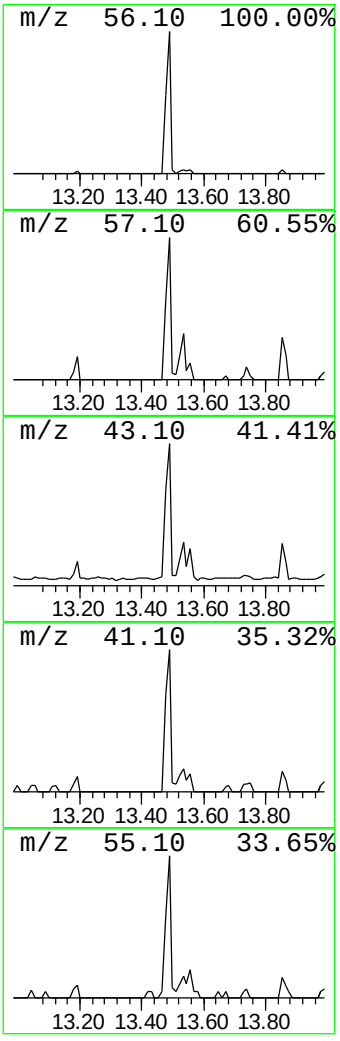
****

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	3.75 ng	164187	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	96
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	64
3	n-Butyl myristate	284	C18H36O2	000110-36-1	53
4	Nipecotic acid	129	C6H11NO2	000498-95-3	47
5	Cyclohexanamine	99	C6H13N	000108-91-8	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085602.D
Acq On : 20 Mar 2016 7:07
Operator : UM/SJ
Sample : H1804-11
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-8C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.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	2.70	3.6	ng	159655	1	6.86	878074	20.0
2-Pentanone, 4-hy...	5.05	9.7	ng	427824	1	6.86	878074	20.0
unknown6.62	6.62	72.9	ng	3200220	1	6.86	878074	20.0
Hexadecanoic acid...	12.78	6.8	ng	296648	5	14.00	875740	20.0
Octadecanoic acid...	13.49	3.8	ng	164187	5	14.00	875740	20.0