LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040816\
Data File : BF086203.D
Acq On : 9 Apr 2016 7:38
Operator : UM/SJ
Sample : H2339-01
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUMPPUMP-5

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-BF040216.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	2.464	31	33	39	rVB	92783	139975	4.07%	0.544%
2	3.584	127	131	140	rBV	94825	183871	5.34%	0.714%
3	4.224	184	187	200	rBV	196785	380216	11.05%	1.477%
4	4.910	244	247	257	rBV	329655	643880	18.71%	2.500%
5	5.333	282	284	302	rBV	1926963	2383498	69.25%	9.256%
6	6.384	373	376	378	rBV	1593506	2235277	64.94%	8.680%
7	6.499	383	386	389	rVB	2596989	2452015	71.24%	9.522%
8	6.727	404	406	412	rBV	830174	727721	21.14%	2.826%
9	6.887	417	420	422	rBV	2106879	2416757	70.21%	9.385%
10	7.173	443	445	450	rBV	22571	50797	1.48%	0.197%
11	7.299	454	456	458	rBV	1839311	1801722	52.34%	6.997%
12	7.790	497	499	503	rBV	32867	57114	1.66%	0.222%
13	7.927	509	511	516	rBV	26416	53656	1.56%	0.208%
14	8.007	516	518	523	rBV	816738	972836	28.26%	3.778%
15	8.956	597	601	604	rBV	338821	546184	15.87%	2.121%
16	9.093	610	613	615	rBV	3196365	3442118	100.00%	13.367%
17	9.208	621	623	629	rVB	49832	51355	1.49%	0.199%
18	9.482	646	647	651	rVB	45277	61162	1.78%	0.238%
19	9.768	669	672	674	rBV	698130	940305	27.32%	3.652%
20	9.985	688	691	693	rBV2	54812	58594	1.70%	0.228%
21	10.202	708	710	711	rVB	29762	39098	1.14%	0.152%
22	10.556	738	741	743	rBV	1489621	1584382	46.03%	6.153%
23	10.671	749	751	755	rVB	47350	56061	1.63%	0.218%
24	11.242	799	801	804	rBV	869319	777228	22.58%	3.018%
25	11.779	846	848	851	rBV	51565	62896	1.83%	0.244%
26	12.568	915	917	922	rBV	25834	46195	1.34%	0.179%
27	12.831	937	940	942	rBV	2102709	2087815	60.65%	8.108%
28	13.391	987	989	990	rBV	46477	39512	1.15%	0.153%
29	13.757	1015	1021	1026	rBV2	17569	42273	1.23%	0.164%
30	13.882	1029	1032	1034	rBV	634701	673215	19.56%	2.614%
31	14.797	1110	1112	1115	rBV	57507	82224	2.39%	0.319%
32	14.888	1118	1120	1122	rVB	43597	41280	1.20%	0.160%
33	15.151	1140	1143	1145	rBV2	29772	36412	1.06%	0.141%
34	15.277	1151	1154	1158	rVB	451233	540003	15.69%	2.097%

LSC Area Percent Report

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Instrument : BNA_F
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Integration Parameters: rteint.p
Integrator: RTE
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.054	1220	1222	1225	rBV3	25926	43479	1.26%	0.169%

Sum of corrected areas: 25751126

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040816\
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Operator : UM/SJ
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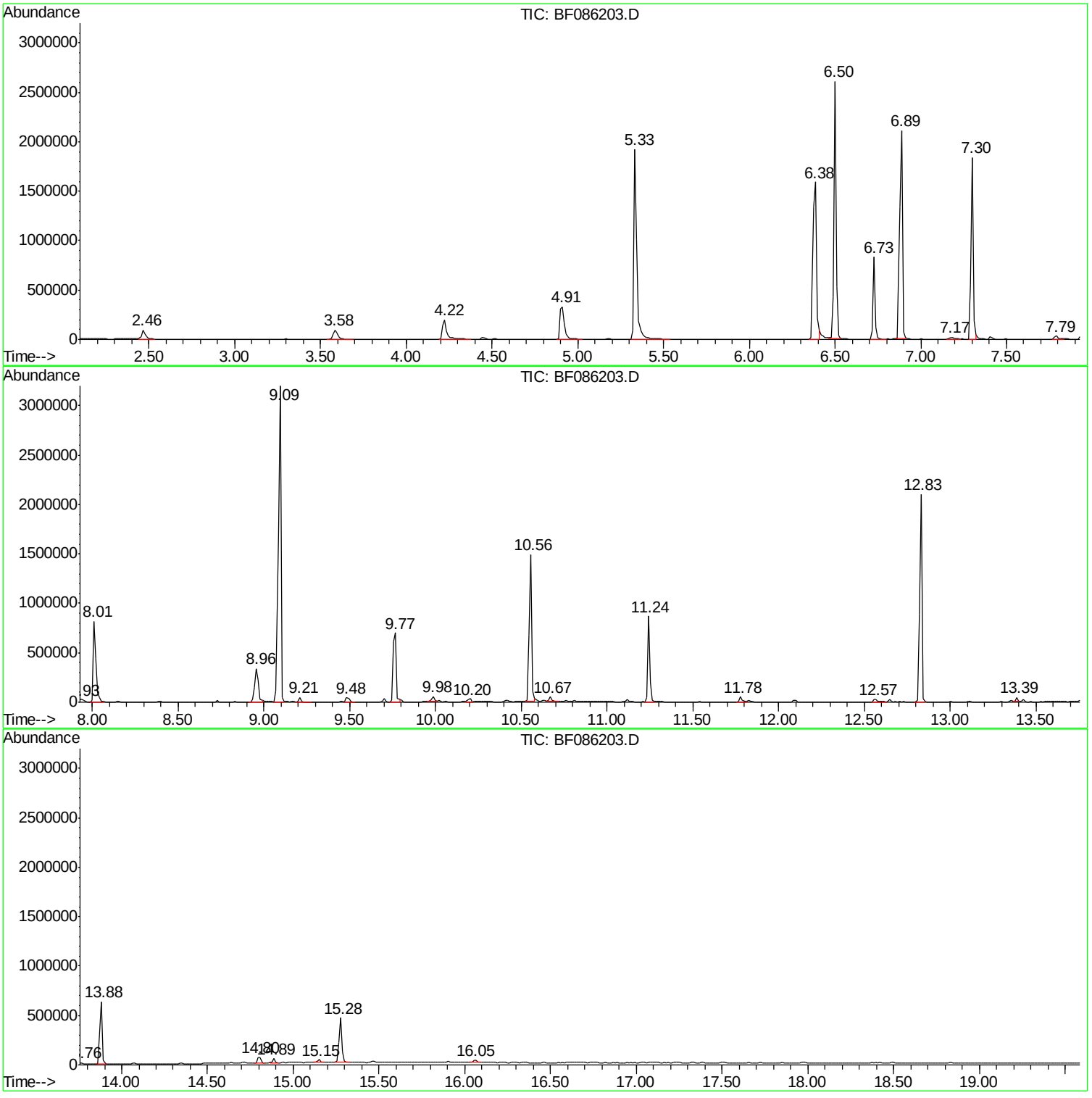
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUMPPUMP-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.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\BF040816\
Data File : BF086203.D
Acq On : 9 Apr 2016 7:38
Operator : UM/SJ
Sample : H2339-01
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUMPPUMP-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

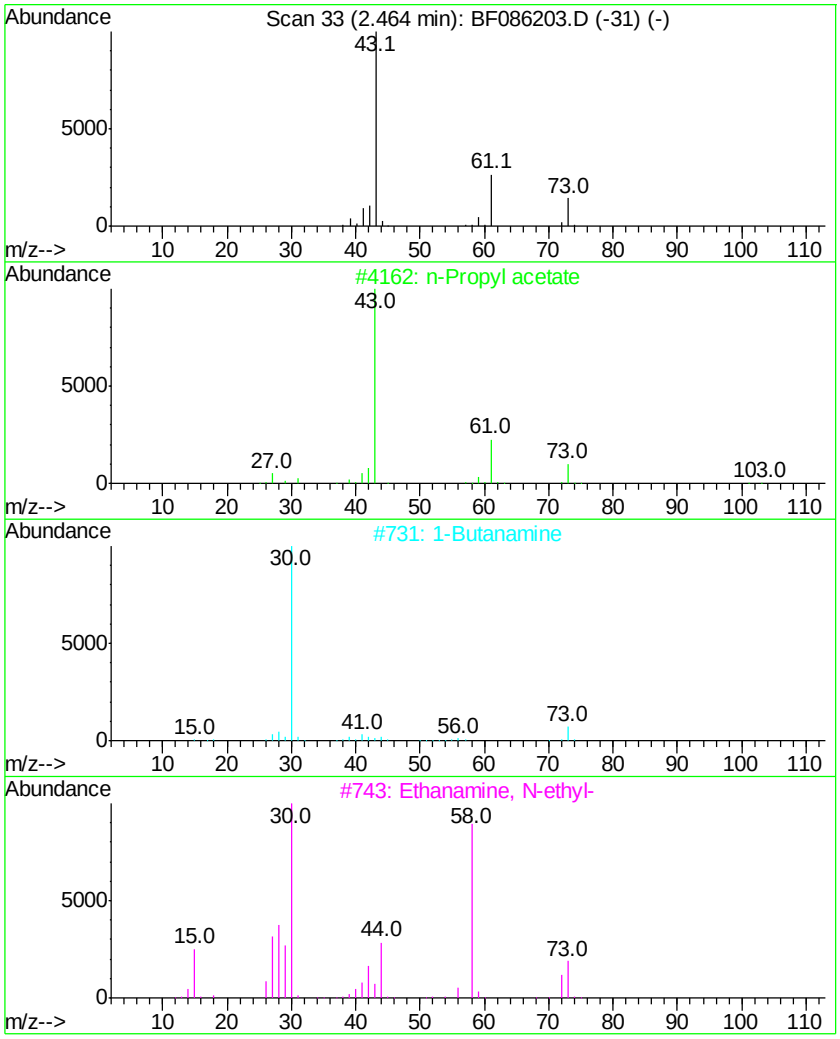
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

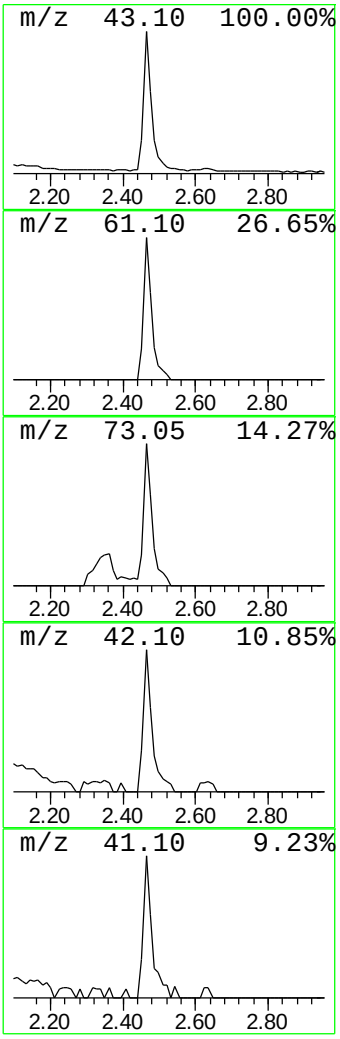
****

Peak Number 1 n-Propyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.46	3.85 ng	139975	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2	1-Butanamine	73	C4H11N	000109-73-9	7
3	Ethanamine, N-ethyl-	73	C4H11N	000109-89-7	7
4	Pentane	72	C5H12	000109-66-0	5
5	Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	5





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040816\
Data File : BF086203.D
Acq On : 9 Apr 2016 7:38
Operator : UM/SJ
Sample : H2339-01
Misc :
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Instrument : BNA_F
ClientSampleId : SUMPPUMP-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

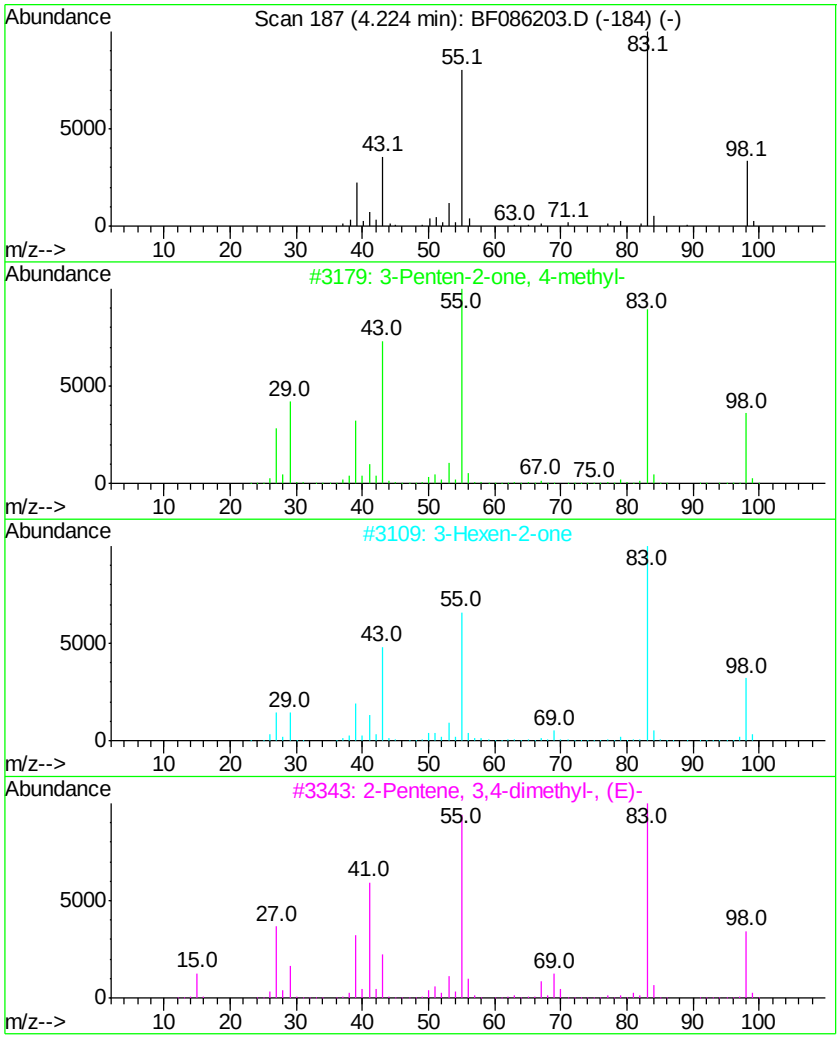
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

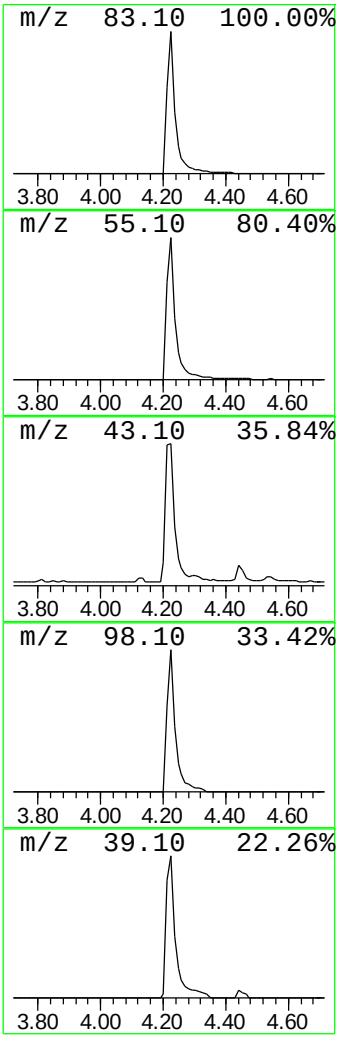
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.22	10.45 ng	380216	1,4-Dichlorobenzene-d4	6.73

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	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040816\
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Acq On : 9 Apr 2016 7:38
Operator : UM/SJ
Sample : H2339-01
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUMPPUMP-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.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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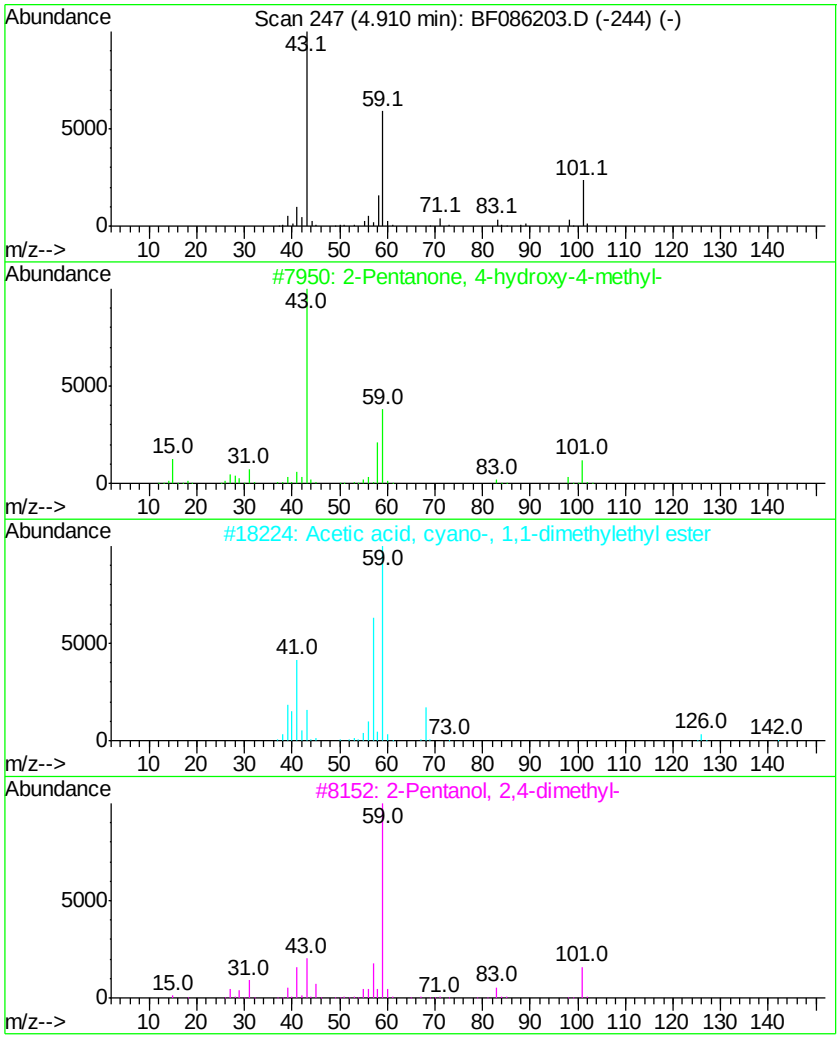
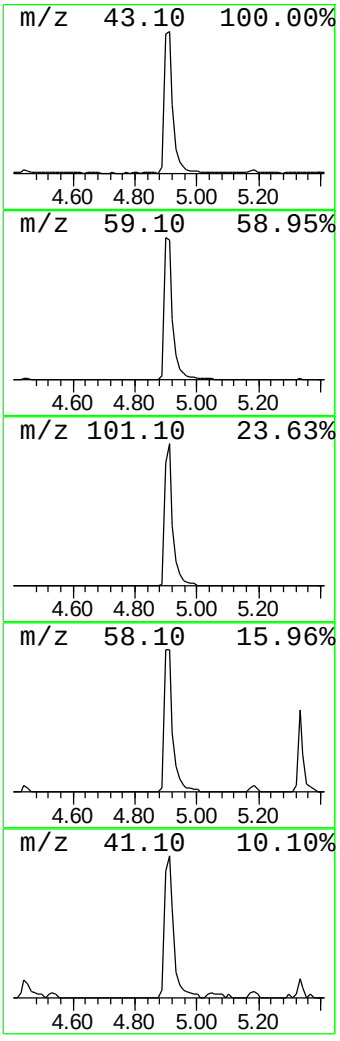
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	17.70 ng	643880	1,4-Dichlorobenzene-d4	6.73

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	25
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	23
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040816\
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Sample : H2339-01
Misc :
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Instrument : BNA_F
ClientSampleId : SUMPPUMP-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
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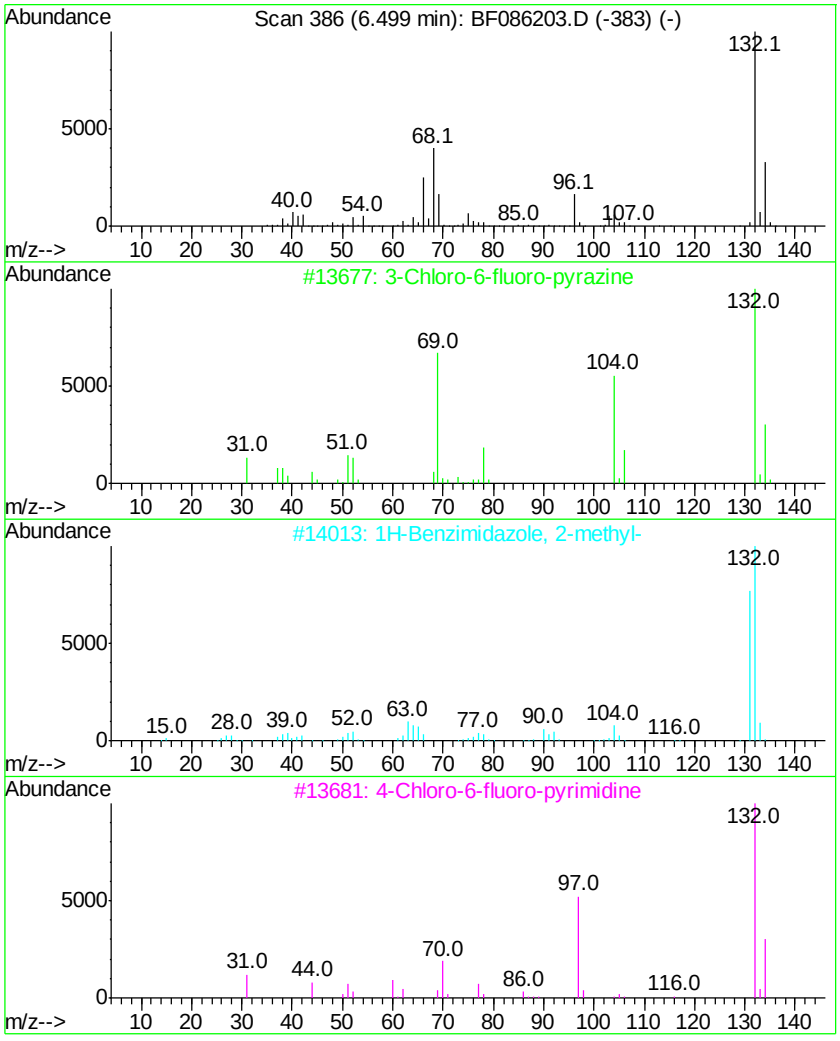
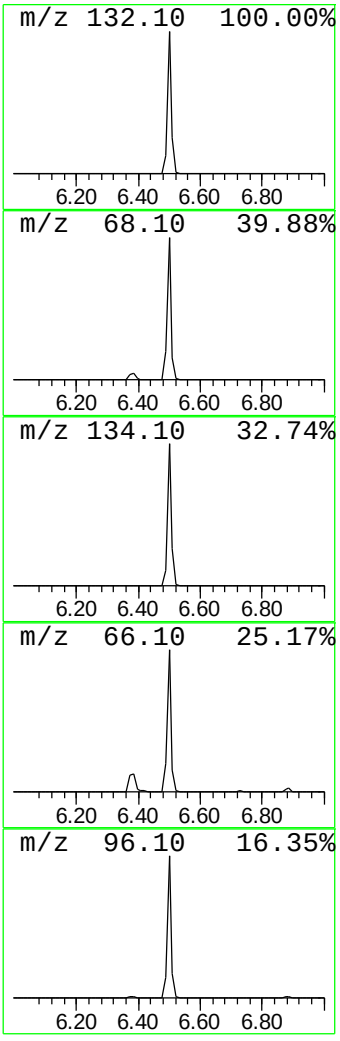
Peak Number 5 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	67.39 ng	2452020	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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ClientSampleId : SUMPPUMP-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

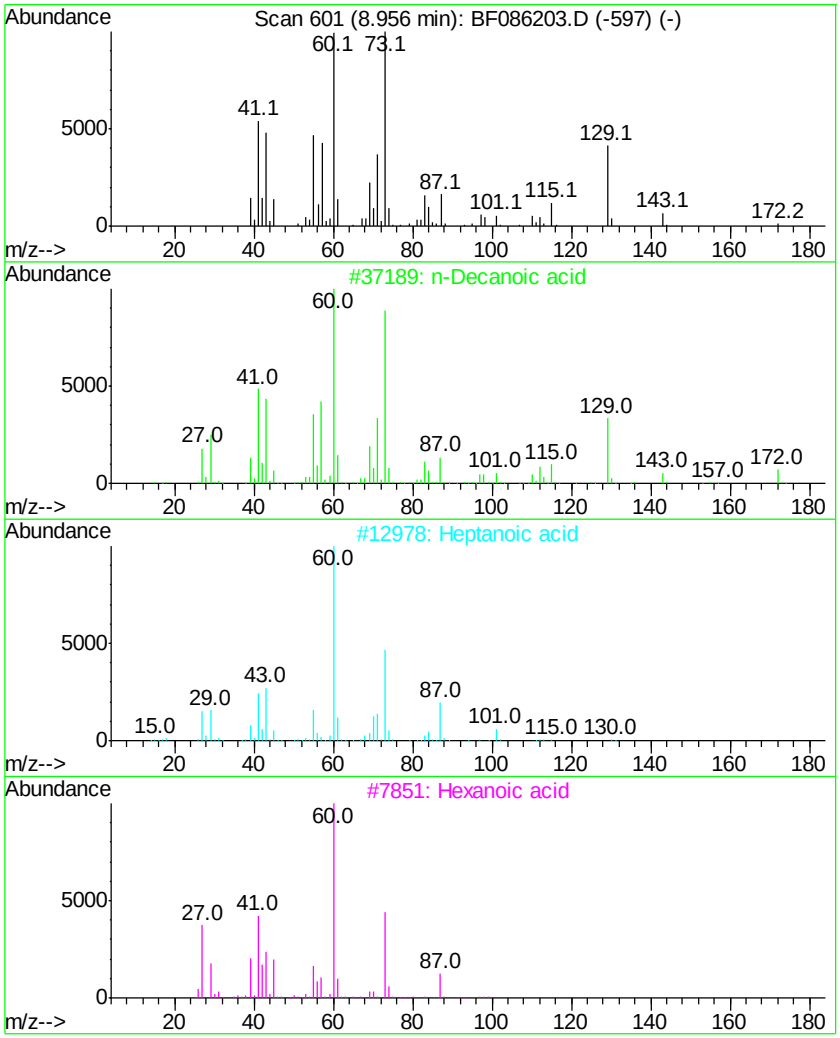
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

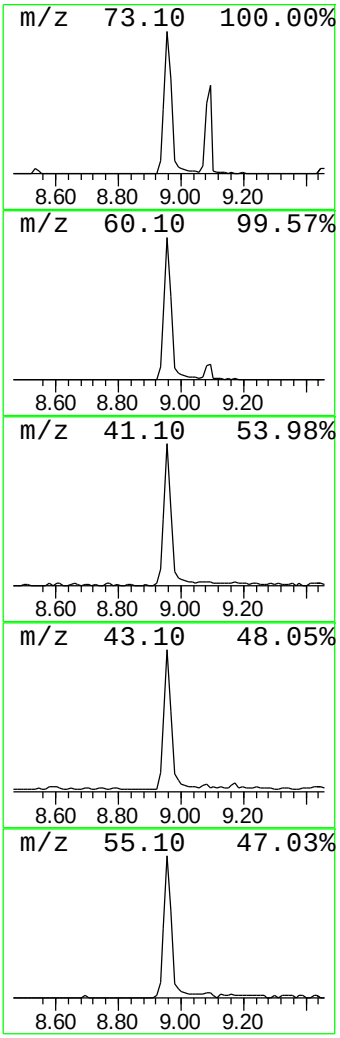
****

Peak Number 7 n-Decanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.96	11.62 ng	546184	Acenaphthene-d10	9.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	90
2	Heptanoic acid	130	C7H14O2	000111-14-8	50
3	Hexanoic acid	116	C6H12O2	000142-62-1	47
4	Pentanoic acid	102	C5H10O2	000109-52-4	43
5	Nonanoic acid	158	C9H18O2	000112-05-0	42





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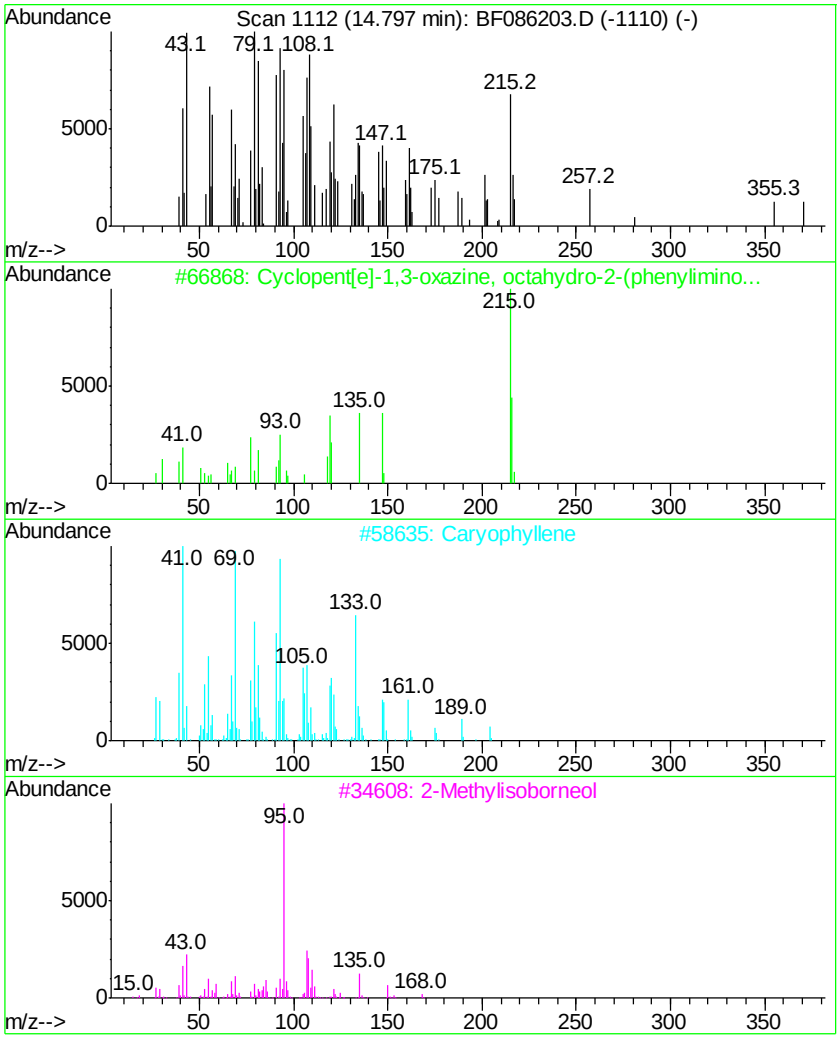
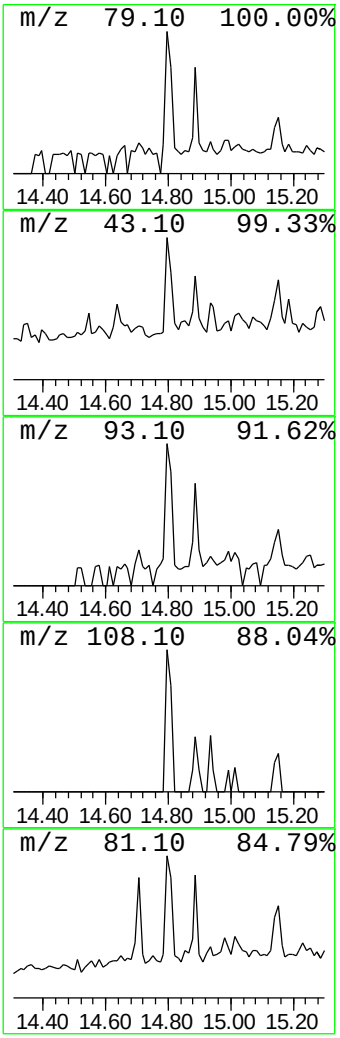
****

Peak Number 8 unknown14.80 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	3.05 ng	82224	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopent[e]-1,3-oxazine, octahy...	216	C13H16N2O	1000138-92-2	38
2	Caryophyllene	204	C15H24	000087-44-5	35
3	2-Methylisoborneol	168	C11H20O	002371-42-8	35
4	Isoaromadendrene epoxide	220	C15H24O	1000159-36-6	30
5	O-Ethyl S-vinyl methylphosphonot...	166	C5H11O2PS	128869-81-8	27





Tentatively Identified Compound (LSC) summary

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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	2.46	3.9	ng	139975	1	6.73	727721	20.0
3-Penten-2-one, 4...	4.22	10.4	ng	380216	1	6.73	727721	20.0
2-Pentanone, 4-hy...	4.91	17.7	ng	643880	1	6.73	727721	20.0
unknown6.50	6.50	67.4	ng	2452020	1	6.73	727721	20.0
n-Decanoic acid	8.96	11.6	ng	546184	3	9.77	940305	20.0
unknown14.80	14.80	3.0	ng	82224	6	15.28	540003	20.0