LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051016\
Data File : BF086854.D
Acq On : 10 May 2016 11:43
Operator : UM/SJ
Sample : H2880-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-42-050416

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-BF050916.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	2.361	22	24	35	rVB	43402	109715	2.61%	0.320%
2	4.167	176	182	184	rBV2	23773	80535	1.92%	0.235%
3	4.384	198	201	206	rVB	29291	46414	1.10%	0.135%
4	4.841	239	241	250	rBV	255043	496927	11.82%	1.448%
5	5.287	278	280	296	rBV	2539793	2920754	69.48%	8.512%
6	5.699	314	316	325	rVB	20999	44674	1.06%	0.130%
7	6.339	370	372	380	rBV	2447729	2853595	67.89%	8.317%
8	6.453	380	382	385	rVV	2845582	2983893	70.98%	8.696%
9	6.682	400	402	410	rVB	1147440	1053150	25.05%	3.069%
10	6.842	413	416	418	rBV	2086350	2399627	57.09%	6.994%
11	7.253	450	452	454	rBV	2167831	2043671	48.62%	5.956%
12	7.973	512	515	517	rBV	1105847	1390244	33.07%	4.052%
13	9.048	606	609	611	rBV	3799517	3579539	85.15%	10.432%
14	9.722	665	668	670	rBV	1378365	1493952	35.54%	4.354%
15	10.511	734	737	739	rBV	2074984	2470255	58.77%	7.199%
16	11.196	795	797	799	rBV	1800304	1547228	36.81%	4.509%
17	12.614	918	921	923	rBV	551323	504014	11.99%	1.469%
18	12.682	926	927	930	rVB	121151	149229	3.55%	0.435%
19	12.785	933	936	938	rBV	3731464	4203560	100.00%	12.251%
20	13.311	980	982	984	rBV	372094	345113	8.21%	1.006%
21	13.357	984	986	987	rVV	109173	93871	2.23%	0.274%
22	13.379	987	988	990	rVB	61909	63338	1.51%	0.185%
23	13.551	1001	1003	1010	rBV2	23120	65537	1.56%	0.191%
24	13.688	1013	1015	1017	rBV	108467	107354	2.55%	0.313%
25	13.825	1024	1027	1029	rBV	1445492	1402211	33.36%	4.087%
26	13.997	1040	1042	1045	rBV	132696	134571	3.20%	0.392%
27	14.305	1067	1069	1071	rBV	132337	112521	2.68%	0.328%
28	14.602	1092	1095	1097	rBV	76562	109174	2.60%	0.318%
29	14.900	1118	1121	1123	rVB	65180	75467	1.80%	0.220%
30	15.197	1144	1147	1156	rVB	1035544	1340321	31.89%	3.906%
31	15.608	1180	1183	1186	rBV	34820	45831	1.09%	0.134%
32	16.043	1218	1221	1228	rVB	25052	45723	1.09%	0.133%

LSC Area Percent Report

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Operator : UM/SJ
Sample : H2880-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-42-050416

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-BF050916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 34312008

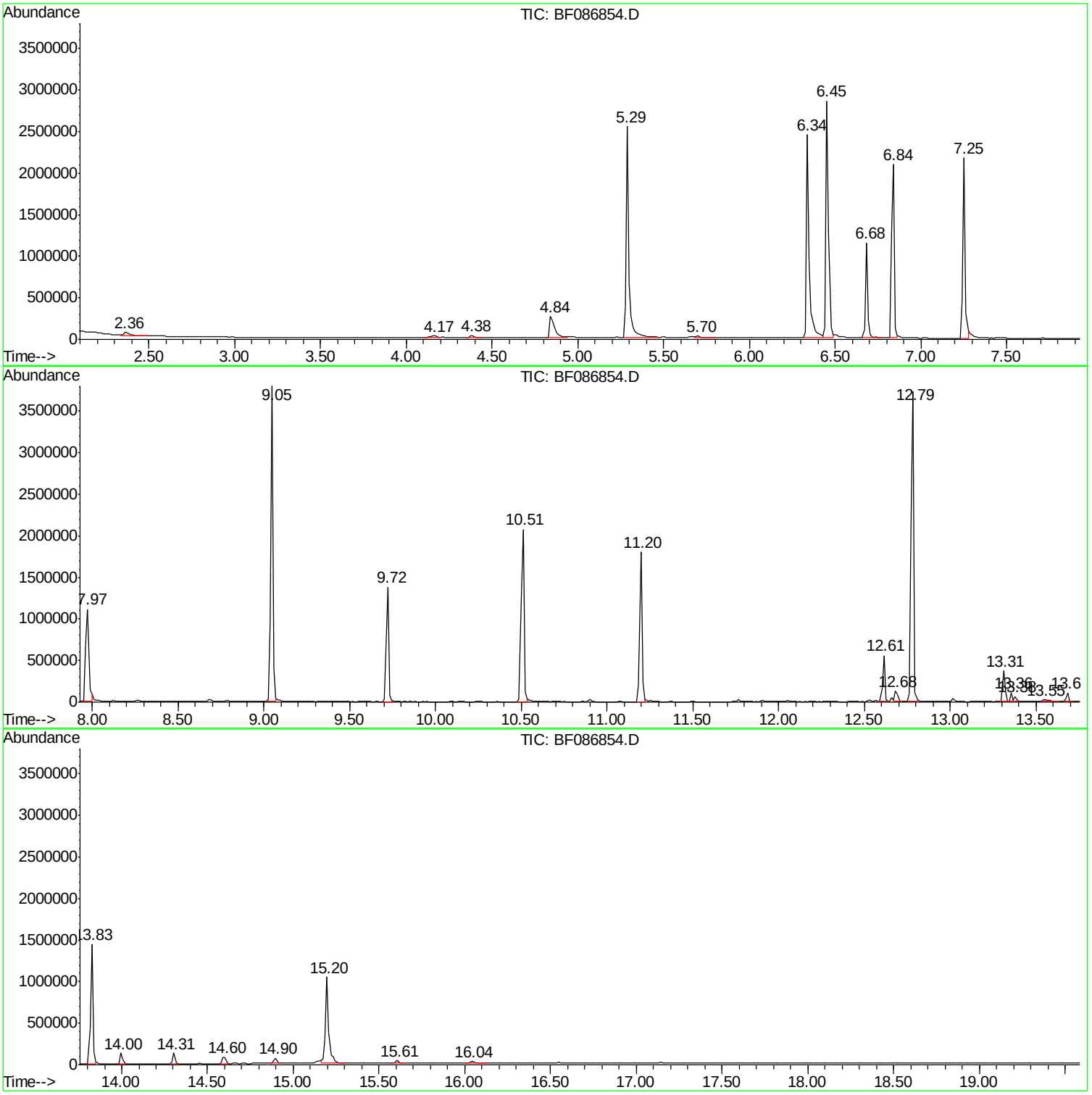
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051016\
Data File : BF086854.D
Acq On : 10 May 2016 11:43
Operator : UM/SJ
Sample : H2880-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-42-050416

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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\BF051016\
Data File : BF086854.D
Acq On : 10 May 2016 11:43
Operator : UM/SJ
Sample : H2880-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-42-050416

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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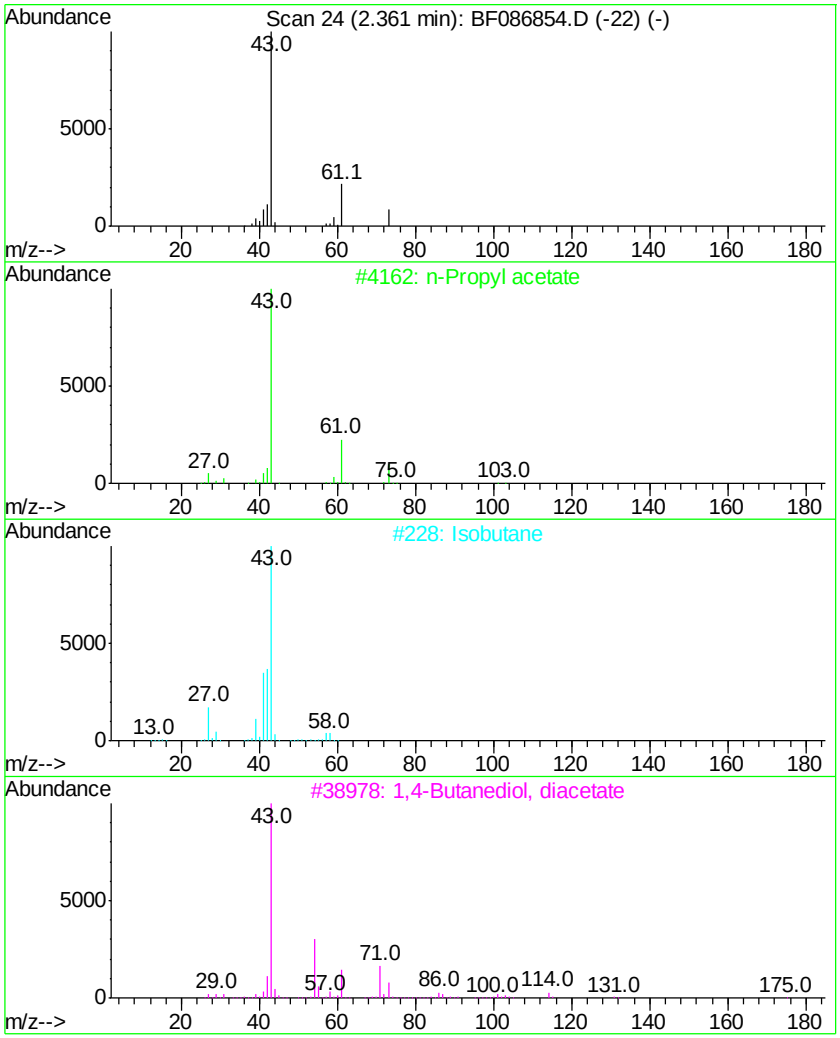
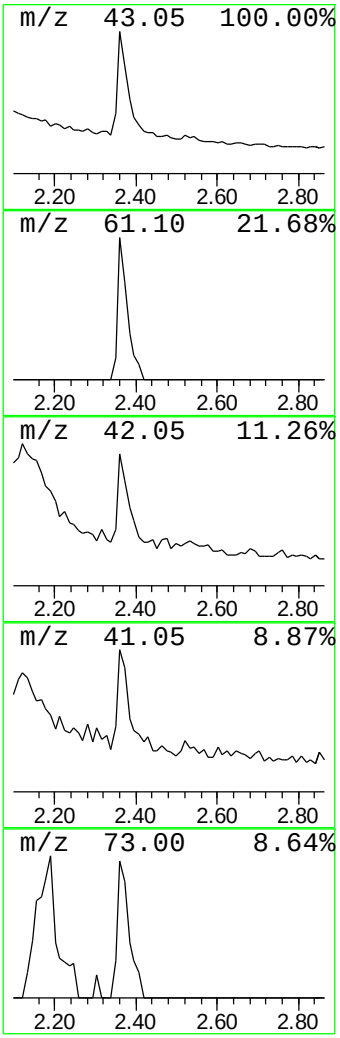
Peak Number 1 n-Propyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.36	2.08 ng	109715	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2	Isobutane	58	C4H10	000075-28-5	5
3	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4
4	Isobutylamine	73	C4H11N	000078-81-9	3
5	Methane, nitro-	61	CH3NO2	000075-52-5	3





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051016\
Data File : BF086854.D
Acq On : 10 May 2016 11:43
Operator : UM/SJ
Sample : H2880-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-42-050416

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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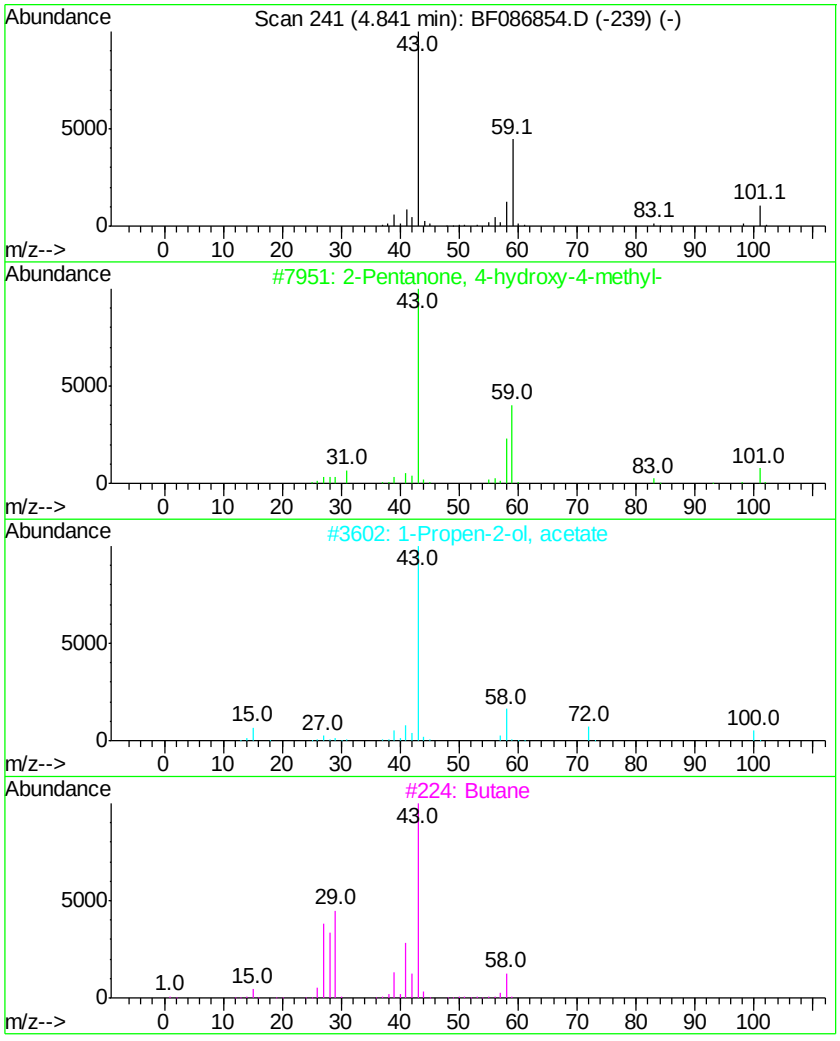
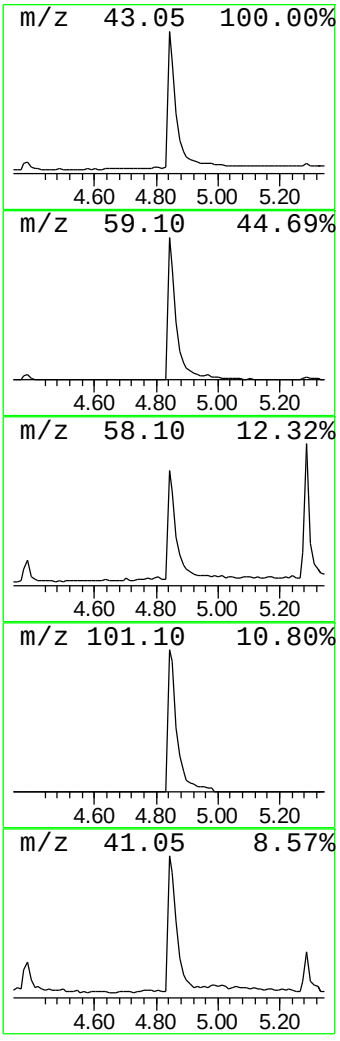
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	9.44 ng	496927	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	Butane	58	C4H10	000106-97-8	9
4	Diacetamide	101	C4H7NO2	000625-77-4	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051016\
Data File : BF086854.D
Acq On : 10 May 2016 11:43
Operator : UM/SJ
Sample : H2880-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-42-050416

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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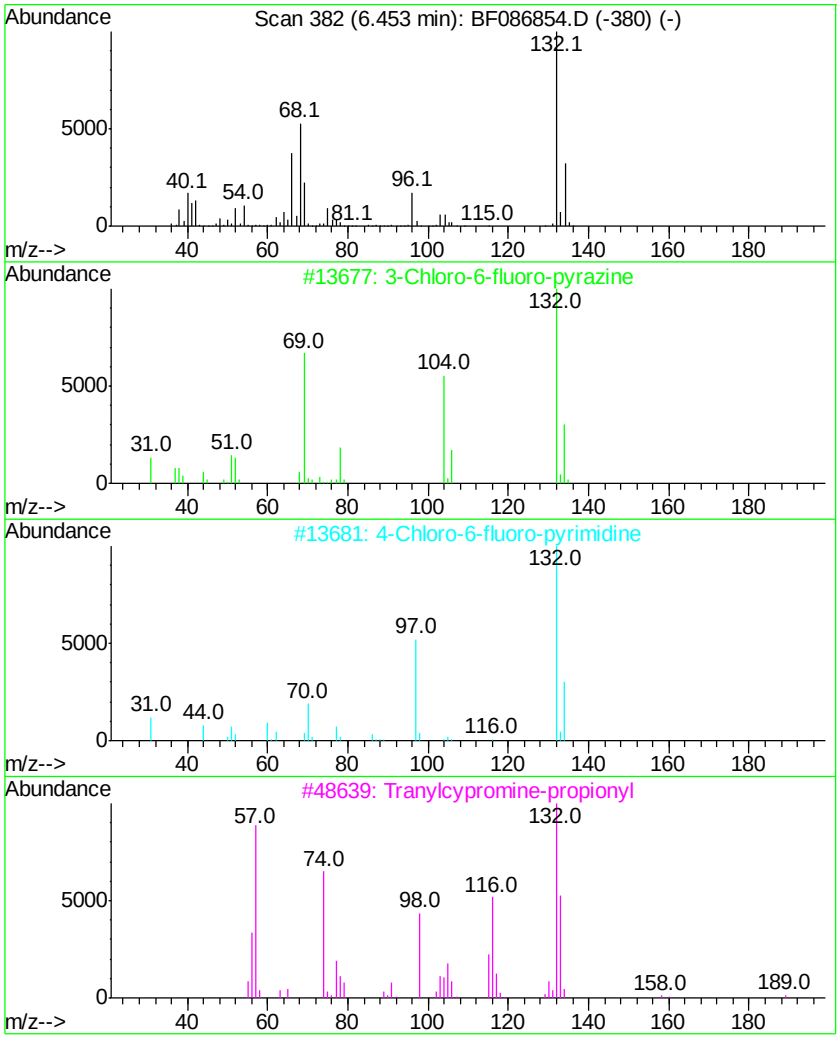
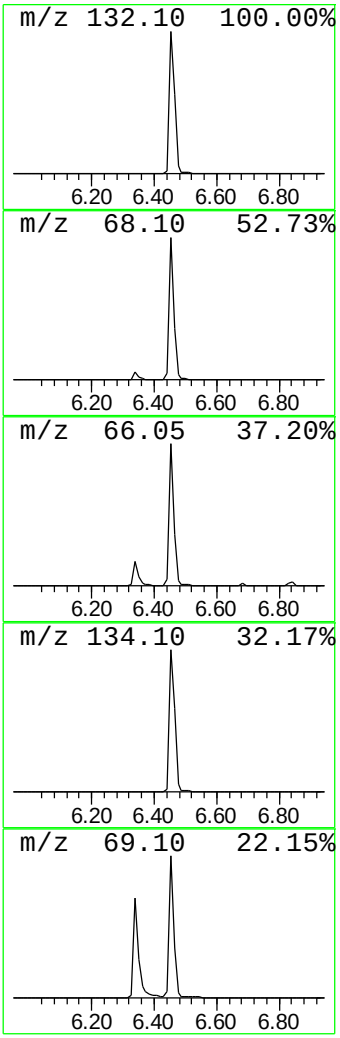
Peak Number 3 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	56.67 ng	2983890	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22





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Misc :
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Instrument : BNA_F
ClientSampleId : HSR-WC-42-050416

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
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TIC Library : C:\DATABASE\NIST02.L
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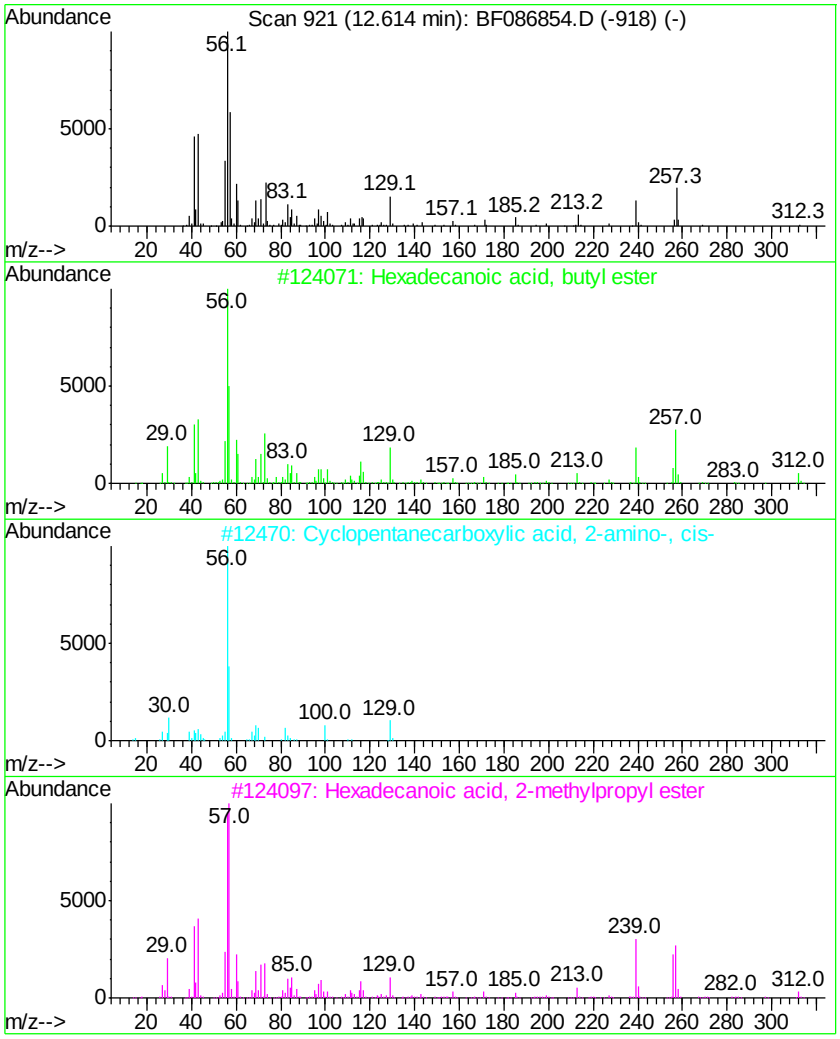
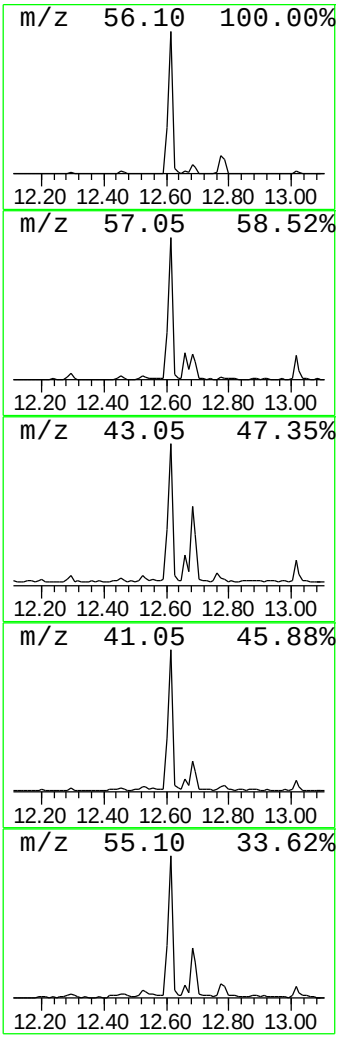
Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.61	7.19 ng	504014	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	38
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	35
4	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	35
5	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	27





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Operator : UM/SJ
Sample : H2880-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-42-050416

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

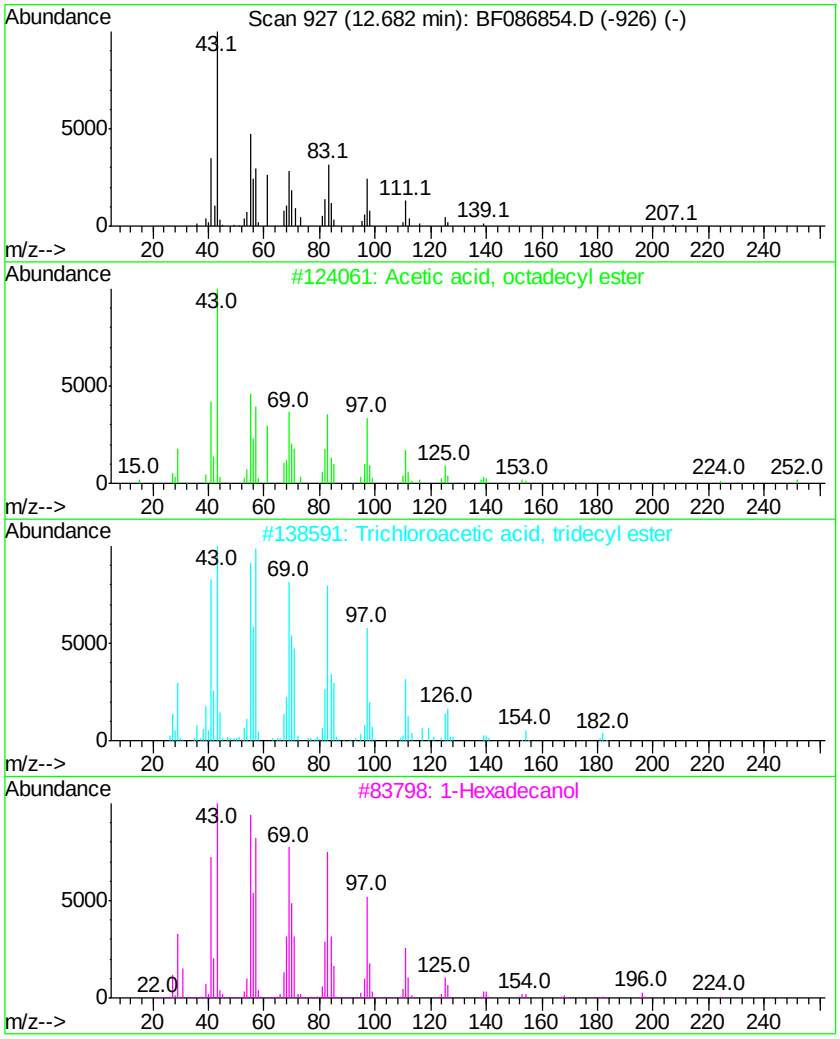
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

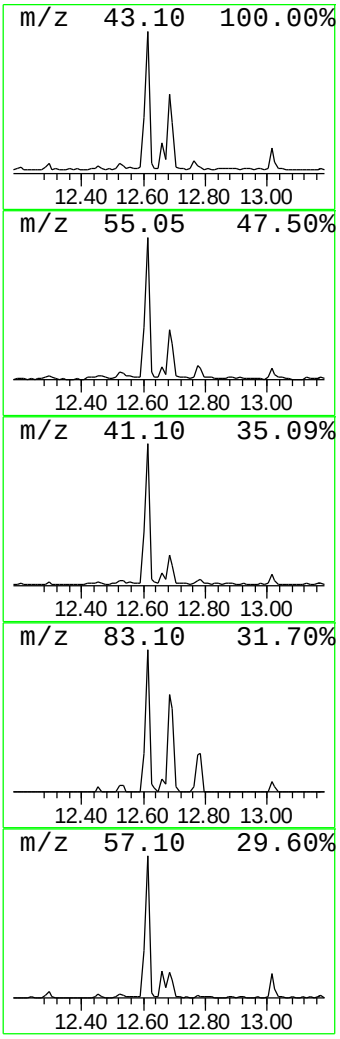
****

Peak Number 6 Acetic acid, octadecyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	2.13 ng	149229	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	90
2	Trichloroacetic acid, tridecyl e...	344	C15H27Cl3O2	074339-51-8	74
3	1-Hexadecanol	242	C16H34O	036653-82-4	74
4	1-Tetracosanol	354	C24H50O	000506-51-4	68
5	1-Hexacosanol	382	C26H54O	000506-52-5	68





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Misc :
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ClientSampleId : HSR-WC-42-050416

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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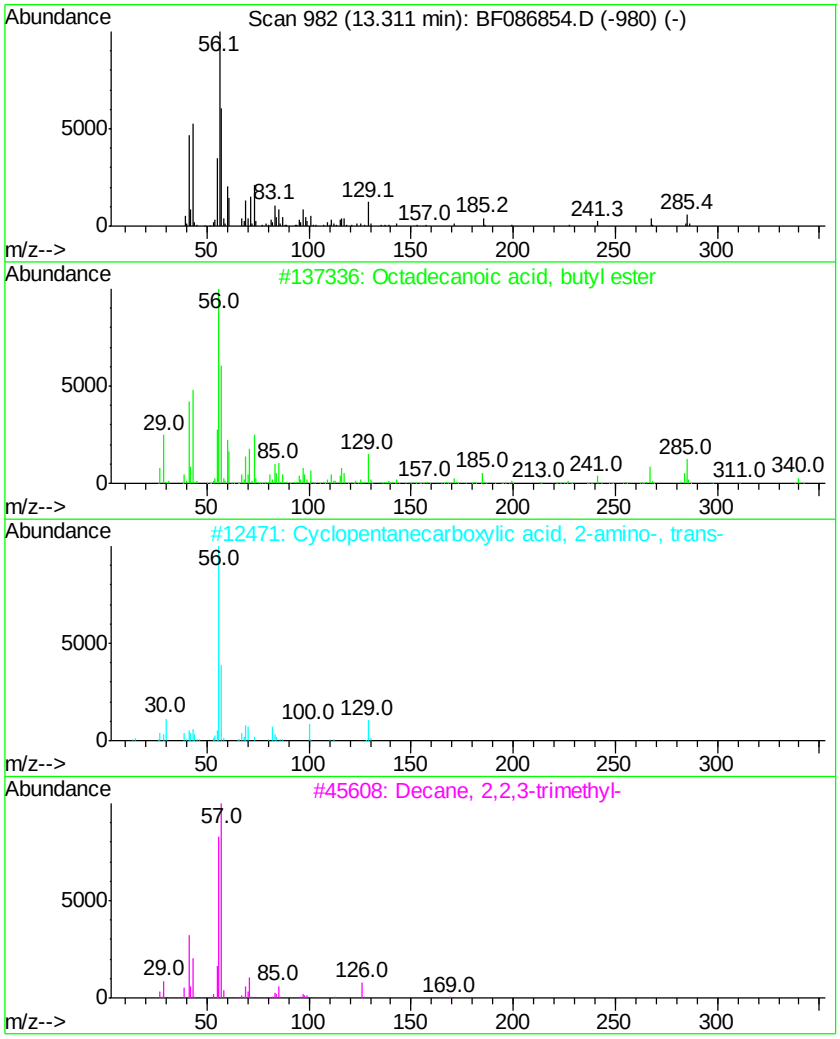
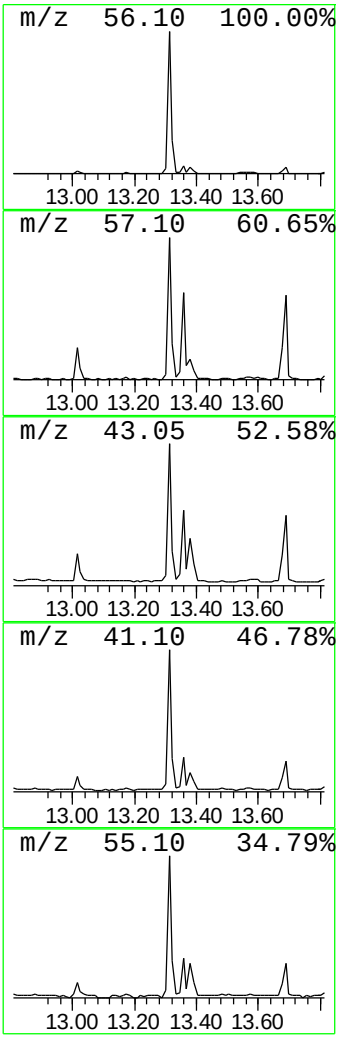
Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.31	4.92 ng	345113	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	46
3	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	38
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	38
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38





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	2.36	2.1	ng	109715	1	6.68	1053150	20.0
2-Pentanone, 4-hy...	4.84	9.4	ng	496927	1	6.68	1053150	20.0
unknown6.45	6.45	56.7	ng	2983890	1	6.68	1053150	20.0
Hexadecanoic acid...	12.61	7.2	ng	504014	5	13.83	1402210	20.0
Acetic acid, octa...	12.68	2.1	ng	149229	5	13.83	1402210	20.0
Octadecanoic acid...	13.31	4.9	ng	345113	5	13.83	1402210	20.0