LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086728.D
Acq On : 6 May 2016 17:11
Operator : UM/SJ
Sample : PB90268BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB90268BL

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-BF050416.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	4.933	247	249	256	rBV	222577	399577	8.93%	1.015%
2	5.333	281	284	286	rBV	3726350	4340649	97.00%	11.028%
3	5.744	318	320	329	rVB2	26927	51233	1.14%	0.130%
4	6.373	372	375	377	rBV	3925985	3989973	89.17%	10.137%
5	6.487	382	385	387	rBV	4104516	4463654	99.75%	11.340%
6	6.705	402	404	414	rVB	1047921	1034381	23.12%	2.628%
7	6.865	415	418	420	rBV	3365157	3388019	75.71%	8.608%
8	7.276	451	454	457	rBV	2181575	2526701	56.47%	6.419%
9	7.996	514	517	519	rBV	1140589	1268281	28.34%	3.222%
10	9.070	608	611	614	rBV	4190231	4474808	100.00%	11.369%
11	9.745	667	670	672	rBV	1426877	1457584	32.57%	3.703%
12	10.533	736	739	742	rBV	3152303	3190333	71.30%	8.105%
13	11.219	797	799	802	rBV	1459282	1425352	31.85%	3.621%
14	12.637	921	923	926	rBV	167017	150026	3.35%	0.381%
15	12.808	935	938	941	rBV	4120455	4314113	96.41%	10.960%
16	13.345	982	985	987	rBV	92823	105588	2.36%	0.268%
17	13.711	1015	1017	1019	rBV	56299	54300	1.21%	0.138%
18	13.848	1027	1029	1032	rBV	1204123	1249774	27.93%	3.175%
19	14.031	1042	1045	1047	rBV	93545	108531	2.43%	0.276%
20	14.328	1069	1071	1074	rBV	125072	134994	3.02%	0.343%
21	14.625	1095	1097	1100	rBV	133824	138482	3.09%	0.352%
22	14.922	1121	1123	1126	rBV	69947	111661	2.50%	0.284%
23	15.231	1147	1150	1152	rBV	802395	982763	21.96%	2.497%

Sum of corrected areas: 39360777

LSC Report - Integrated Chromatogram

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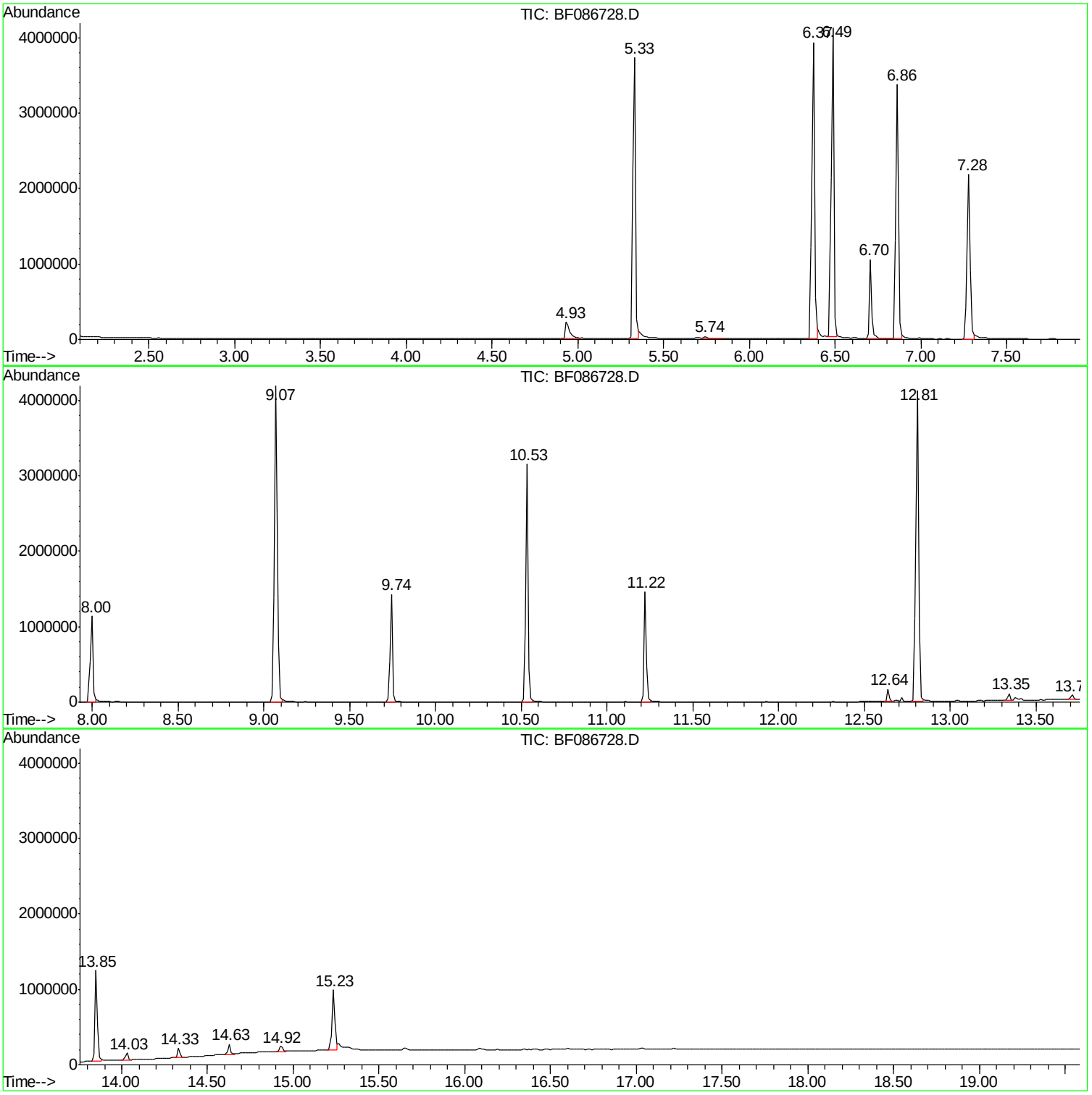
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB90268BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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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Acq On : 6 May 2016 17:11
Operator : UM/SJ
Sample : PB90268BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

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ClientSampleId : PB90268BL

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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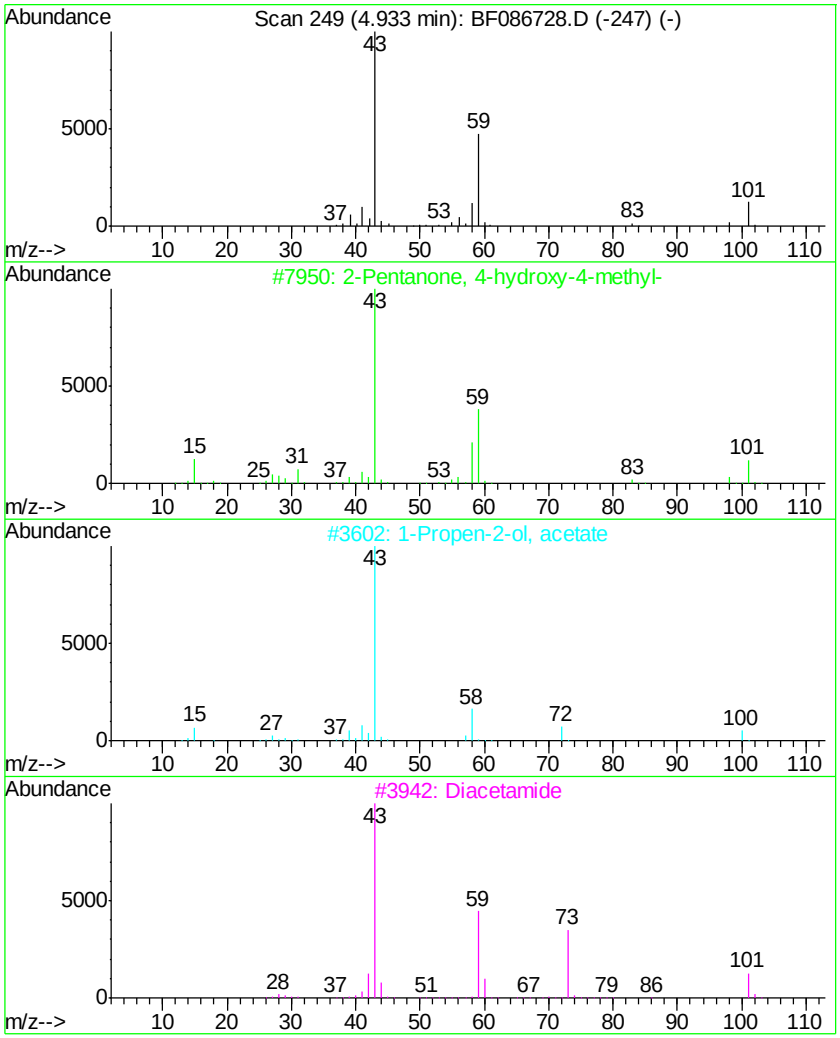
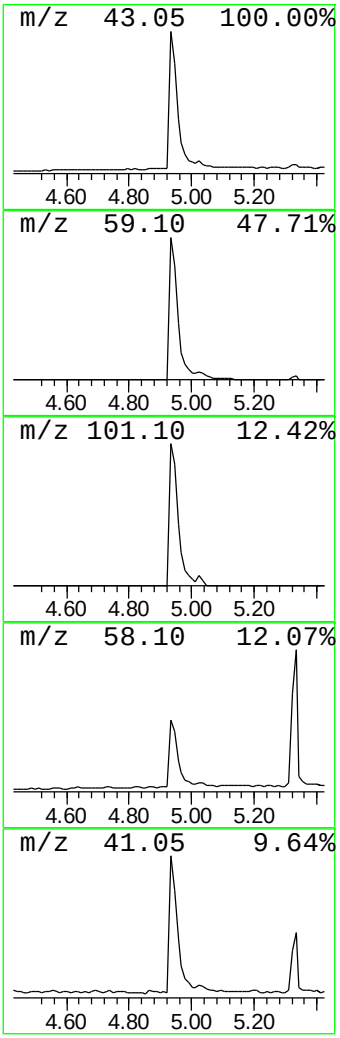
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	15.45 ng	399577	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





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Acq On : 6 May 2016 17:11
Operator : UM/SJ
Sample : PB90268BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB90268BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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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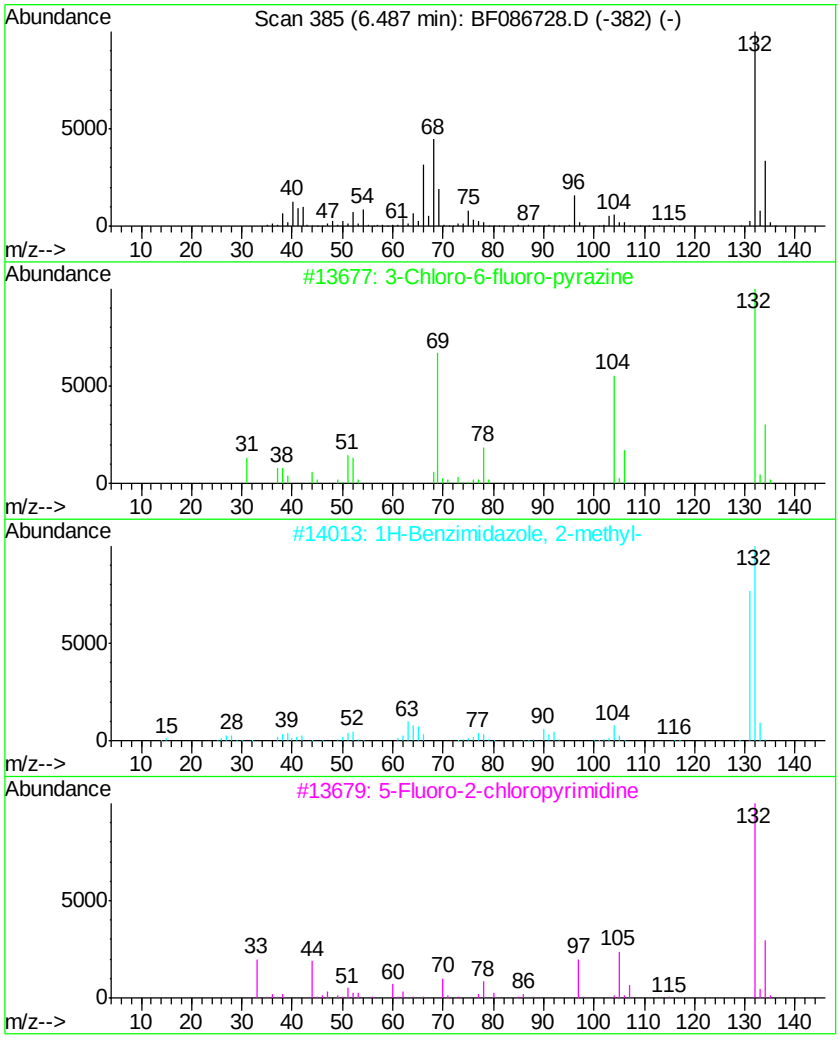
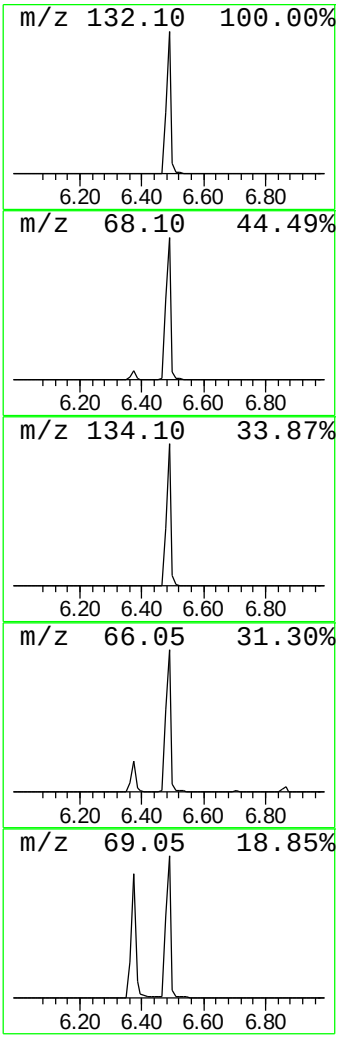
Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	172.61 ng	4463650	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10





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Data File : BF086728.D
Acq On : 6 May 2016 17:11
Operator : UM/SJ
Sample : PB90268BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB90268BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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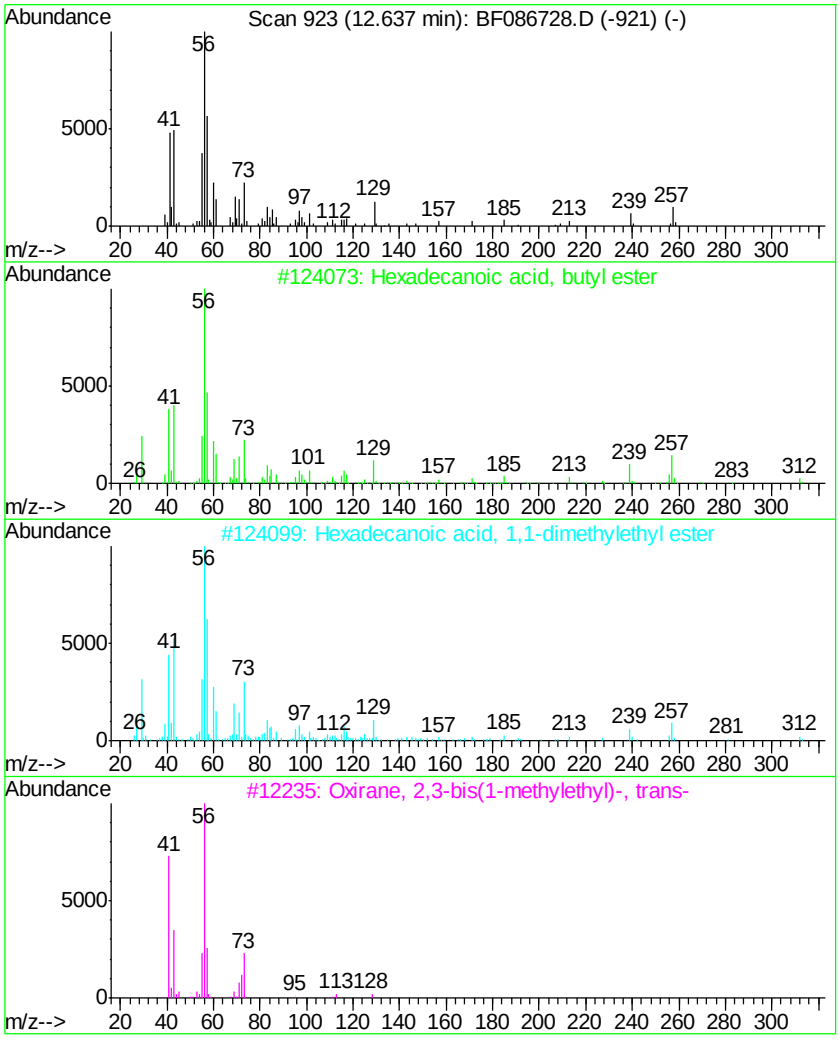
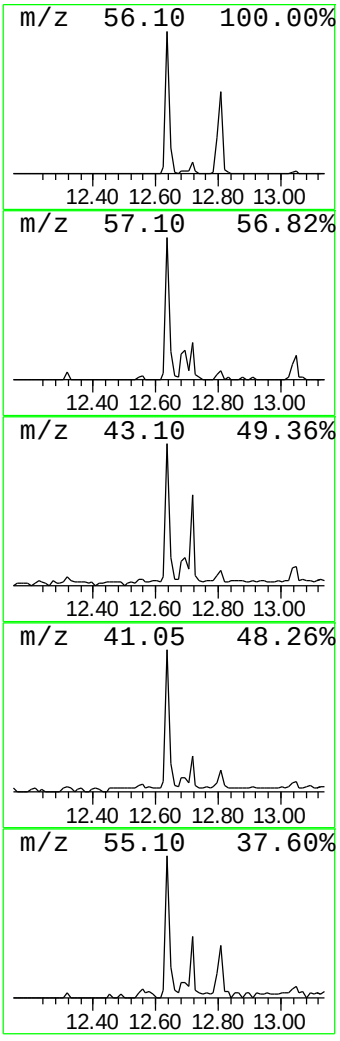
Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	4.80 ng	150026	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	53
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	50
3	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	47
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	46
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38





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Data File : BF086728.D
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Operator : UM/SJ
Sample : PB90268BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB90268BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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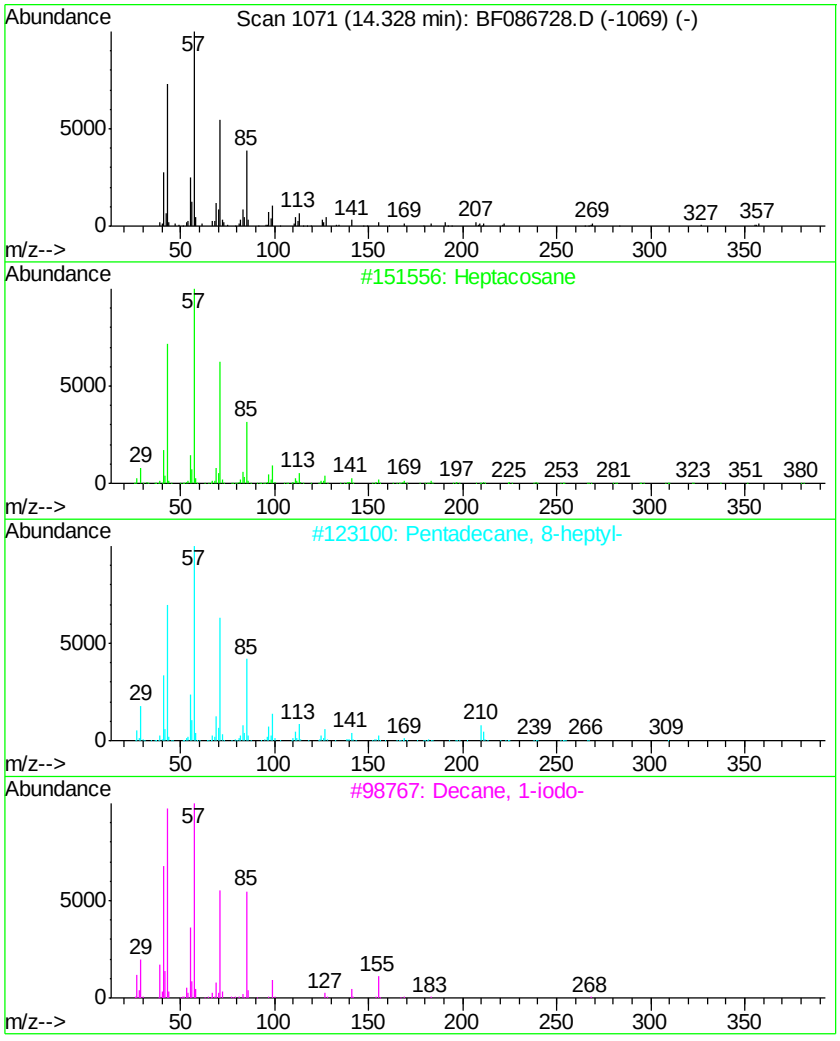
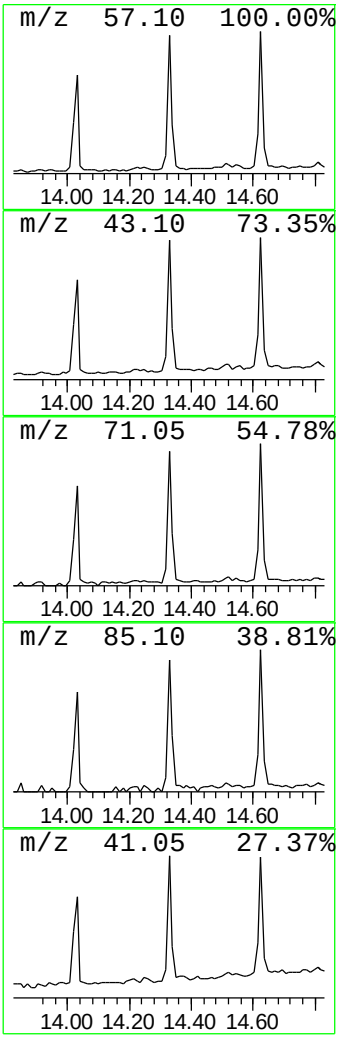
Peak Number 5 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.33	4.32 ng	134994	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
3	Decane, 1-iodo-	268	C10H21I	002050-77-3	90
4	Eicosane	282	C20H42	000112-95-8	90
5	Pentadecane	212	C15H32	000629-62-9	87





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086728.D
Acq On : 6 May 2016 17:11
Operator : UM/SJ
Sample : PB90268BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB90268BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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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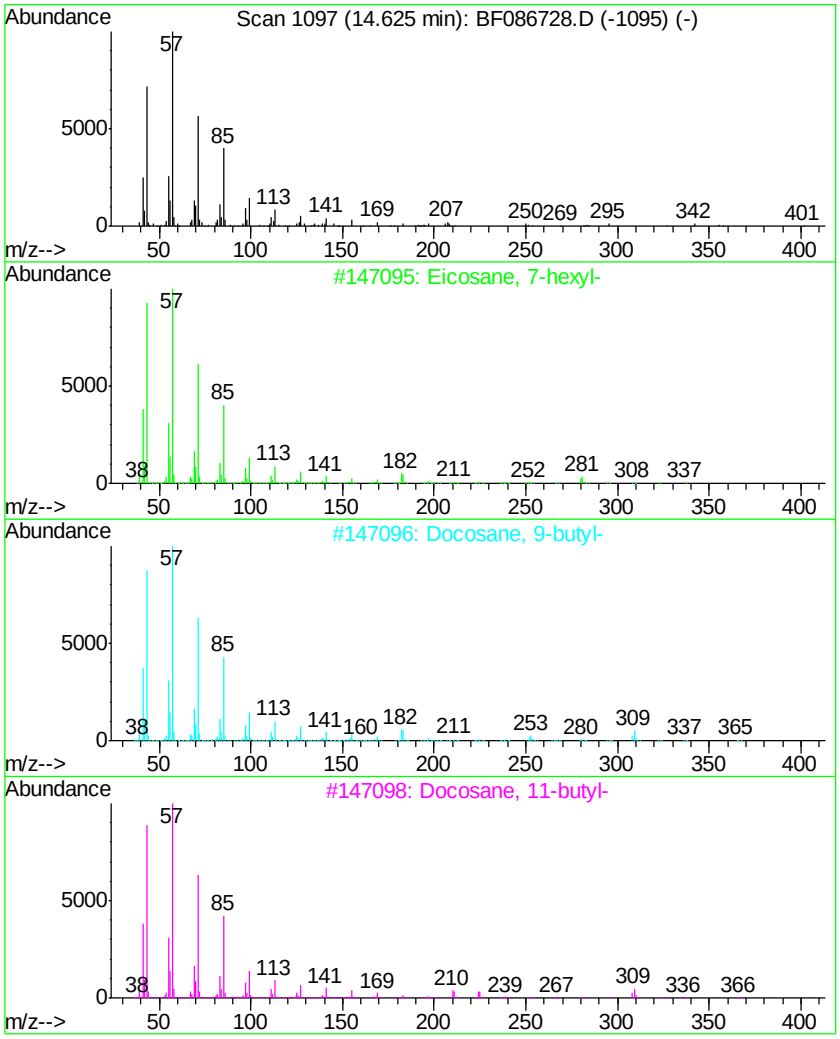
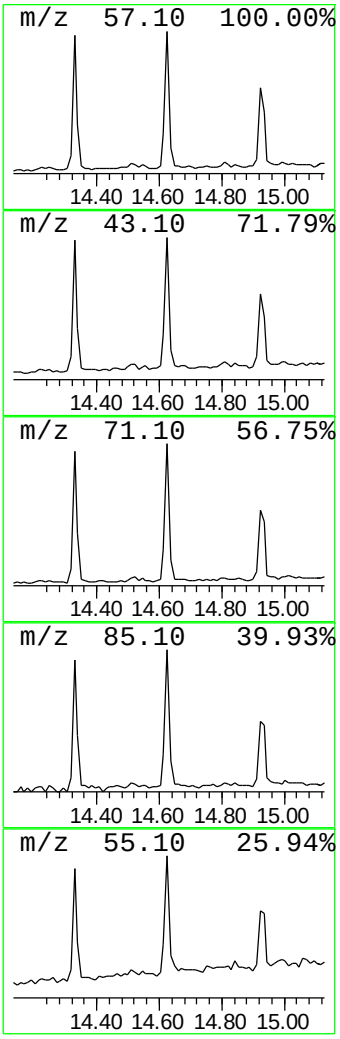
Peak Number 6 Eicosane, 7-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	5.64 ng	138482	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
2	Docosane, 9-butyl-	366	C26H54	055282-14-9	90
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Heptacosane	380	C27H56	000593-49-7	90





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

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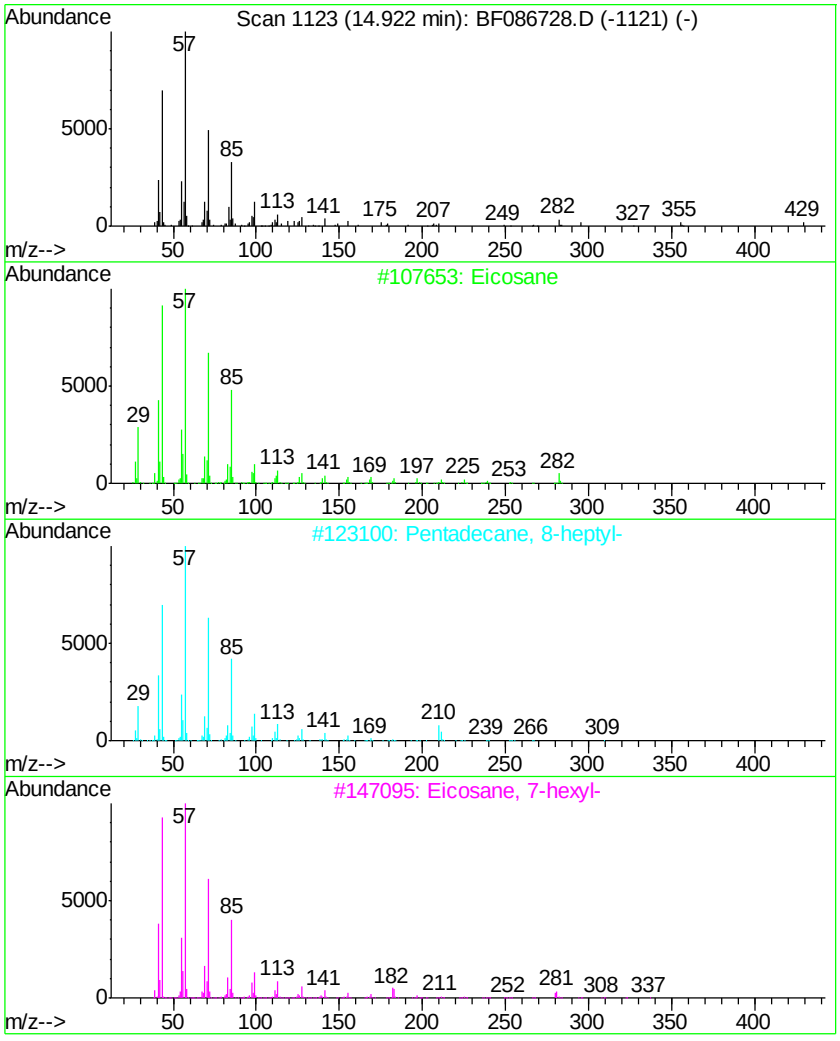
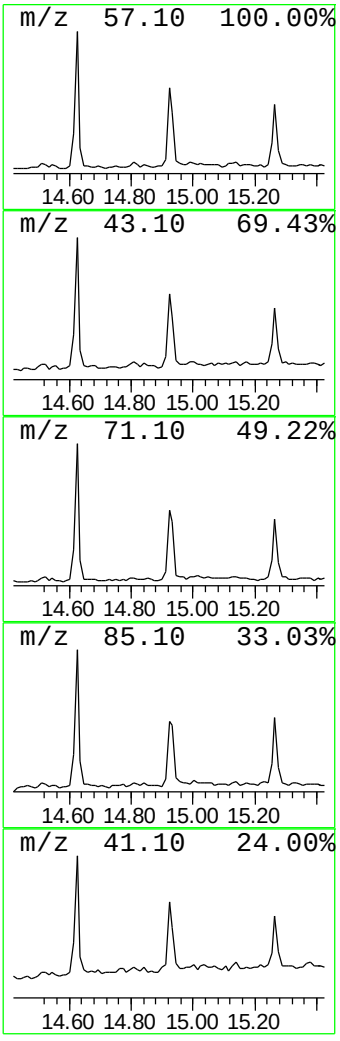
Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	4.54 ng	111661	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	83
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	83
4	Octacosane	394	C28H58	000630-02-4	83
5	Heneicosane	296	C21H44	000629-94-7	81





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
2-Pentanone, 4-hy...	4.93	15.4	ng	399577	1	6.70	1034380	40.0
unknown6.49	6.49	172.6	ng	4463650	1	6.70	1034380	40.0
Hexadecanoic acid...	12.64	4.8	ng	150026	5	13.85	1249770	40.0
Heptacosane	14.33	4.3	ng	134994	5	13.85	1249770	40.0
Eicosane, 7-hexyl-	14.63	5.6	ng	138482	6	15.23	982763	40.0
Eicosane	14.92	4.5	ng	111661	6	15.23	982763	40.0