LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121416\
Data File : BF091613.D
Acq On : 15 Dec 2016 6:41
Operator : UM/SJ
Sample : PB95264BL
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB95264BL

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-BF120916.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	4.967	249	252	255	rBV	1751308	2042121	23.41%	3.824%
2	5.401	287	290	292	rBV	4499486	4662402	53.44%	8.732%
3	6.430	377	380	383	rBV	4885758	4631530	53.09%	8.674%
4	6.556	389	391	394	rBV	3617980	4520212	51.81%	8.465%
5	6.796	409	412	414	rBV	1255466	1371686	15.72%	2.569%
6	6.956	423	426	428	rBV	4544688	6319314	72.43%	11.835%
7	7.356	458	461	464	rBV	4236049	4403509	50.47%	8.247%
8	8.076	522	524	527	rBV	1909981	1838214	21.07%	3.443%
9	9.162	615	619	621	rBV	8782477	8724673	100.00%	16.339%
10	9.836	675	678	680	rBV	1810358	1972486	22.61%	3.694%
11	10.613	744	746	749	rBV2	1554977	1902075	21.80%	3.562%
12	11.310	805	807	810	rBV	1803653	1631257	18.70%	3.055%
13	12.728	929	931	934	rBV	240117	247182	2.83%	0.463%
14	12.899	943	946	949	rBV	5315766	6071855	69.59%	11.371%
15	13.436	990	993	995	rBV	199268	174674	2.00%	0.327%
16	13.939	1035	1037	1040	rBV	1053136	1284290	14.72%	2.405%
17	15.357	1158	1161	1163	rBV	899731	1054226	12.08%	1.974%
18	15.402	1163	1165	1168	rVB	76827	100841	1.16%	0.189%
19	15.814	1198	1201	1204	rVB	75529	128164	1.47%	0.240%
20	16.282	1239	1242	1245	rVB	63039	117502	1.35%	0.220%
21	16.831	1287	1290	1293	rVB	44114	89595	1.03%	0.168%
22	17.483	1343	1347	1352	rBV	44813	108573	1.24%	0.203%

Sum of corrected areas: 53396381

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121416\
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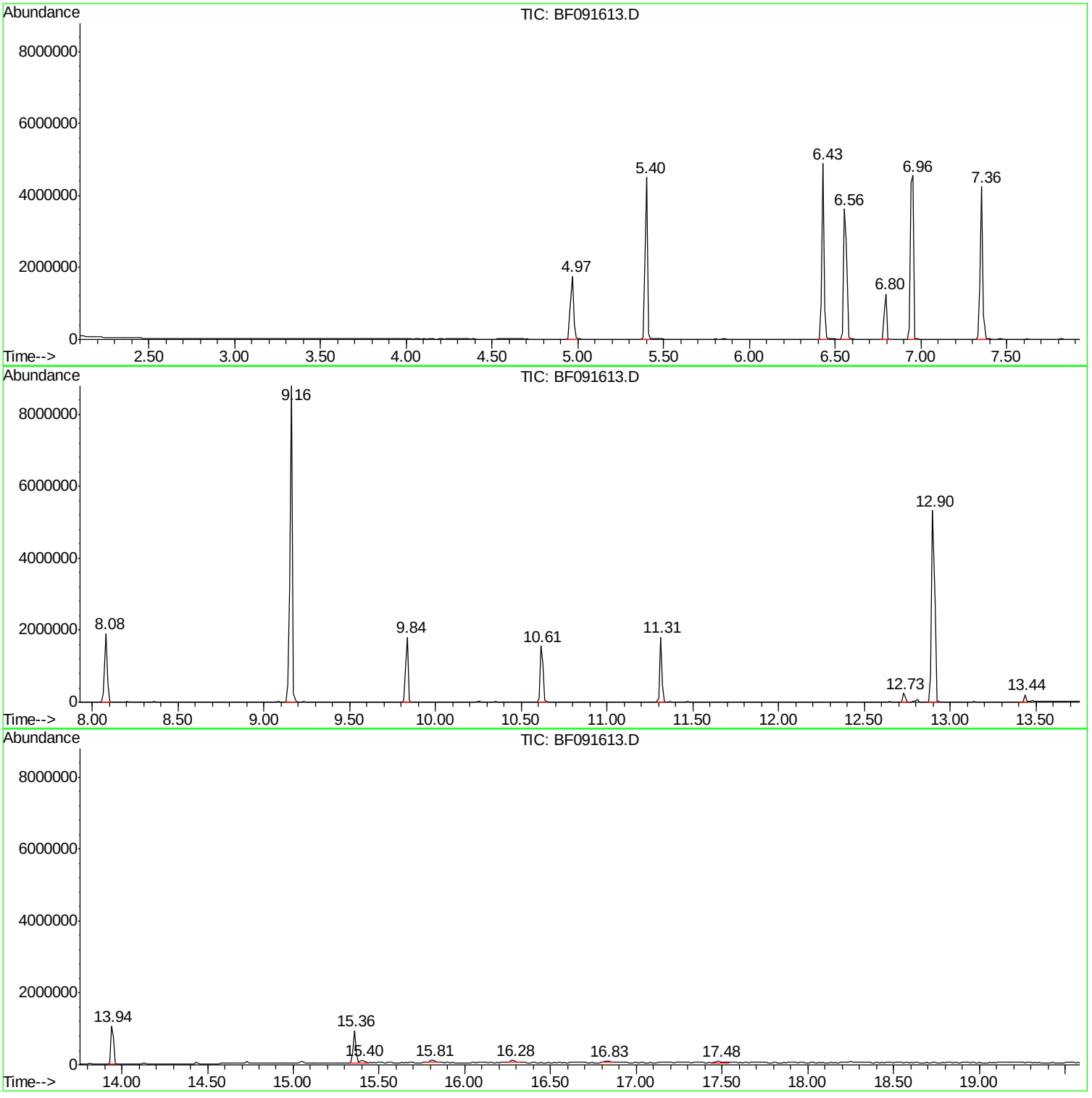
Operator : UM/SJ
Sample : PB95264BL
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB95264BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.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\BF121416\
Data File : BF091613.D
Acq On : 15 Dec 2016 6:41
Operator : UM/SJ
Sample : PB95264BL
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB95264BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

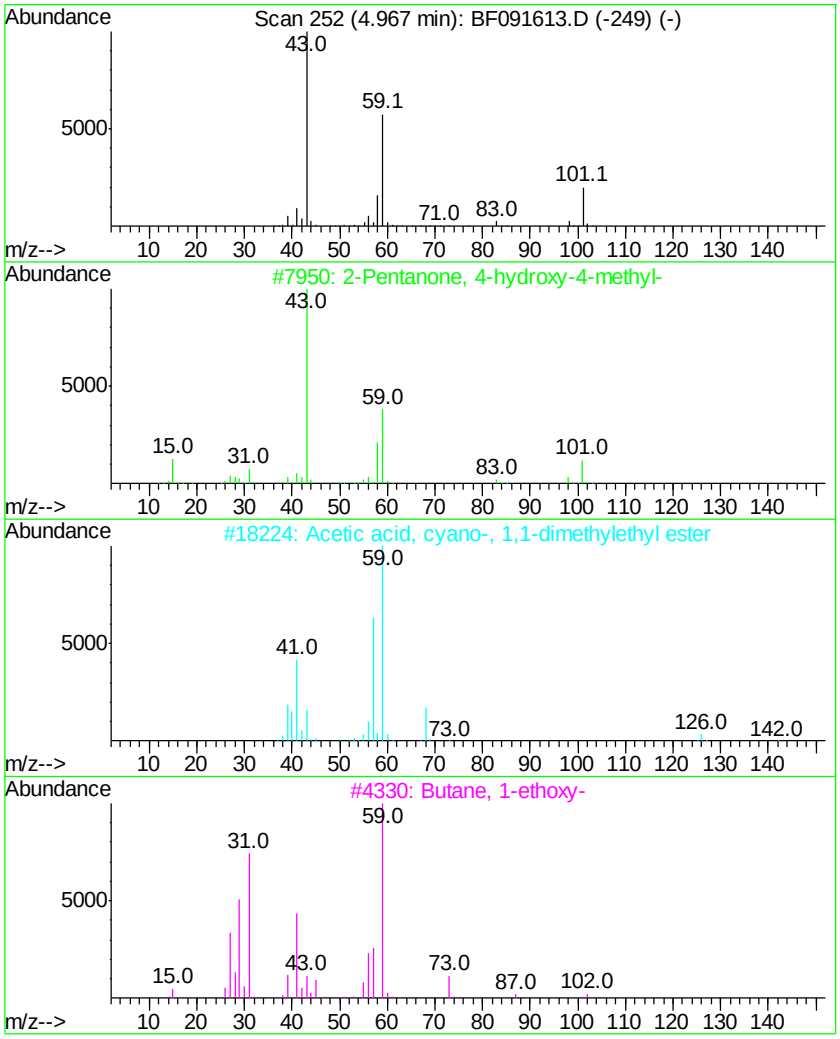
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

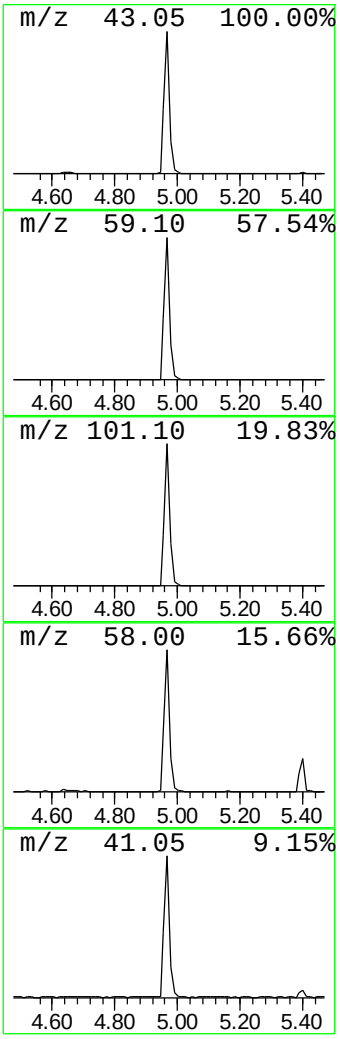
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	29.78 ng	2042120	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121416\
Data File : BF091613.D
Acq On : 15 Dec 2016 6:41
Operator : UM/SJ
Sample : PB95264BL
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB95264BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.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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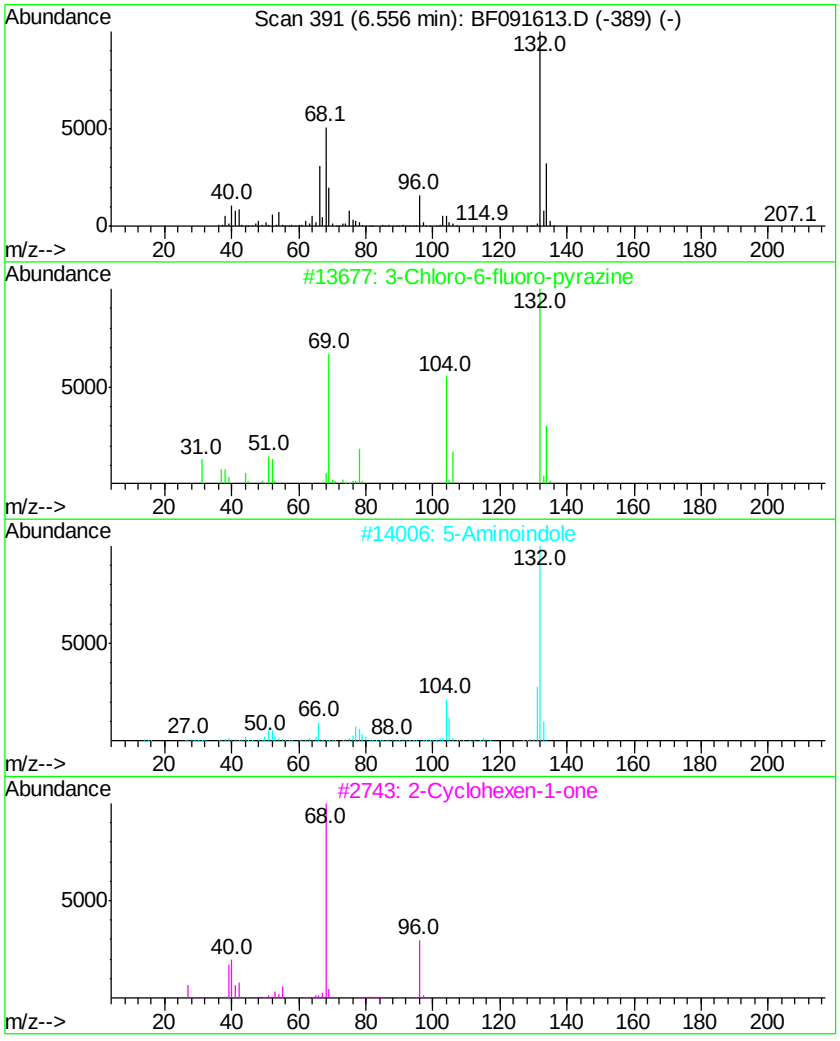
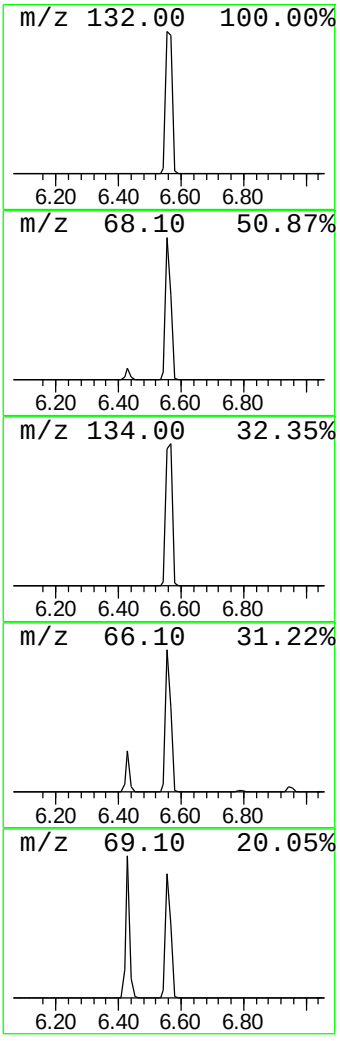
Peak Number 2 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	65.91 ng	4520210	1,4-Dichlorobenzene-d4	6.80

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	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121416\
Data File : BF091613.D
Acq On : 15 Dec 2016 6:41
Operator : UM/SJ
Sample : PB95264BL
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB95264BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.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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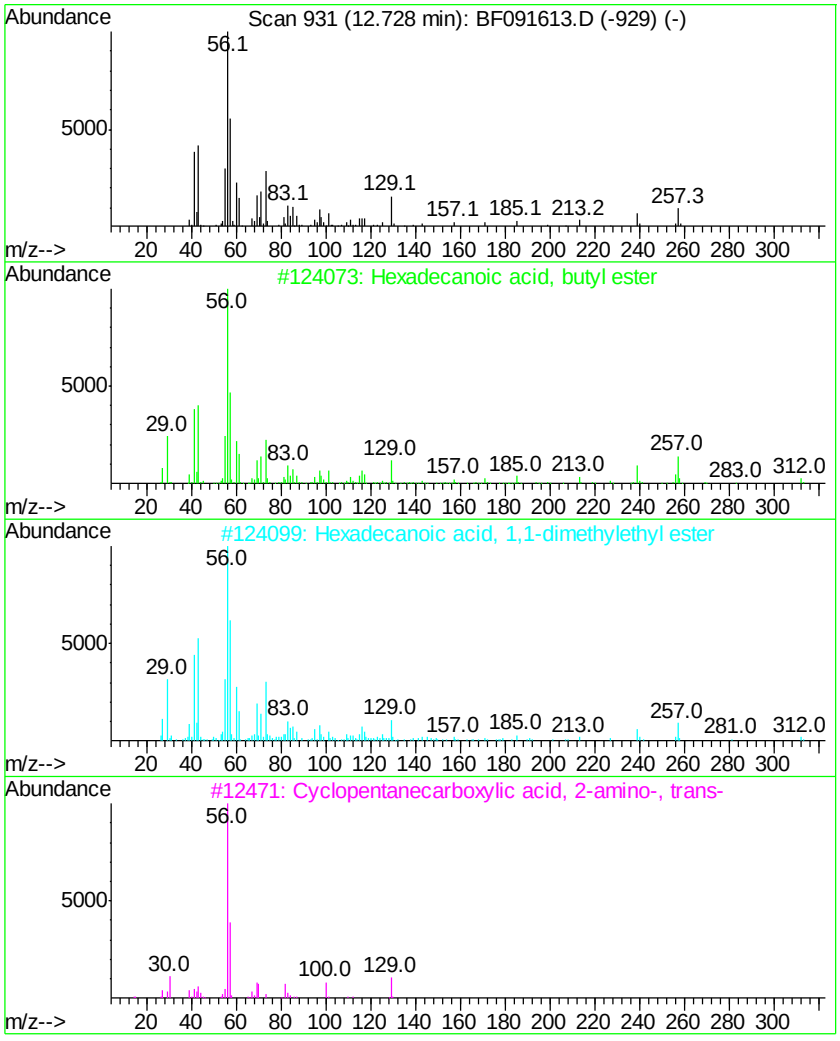
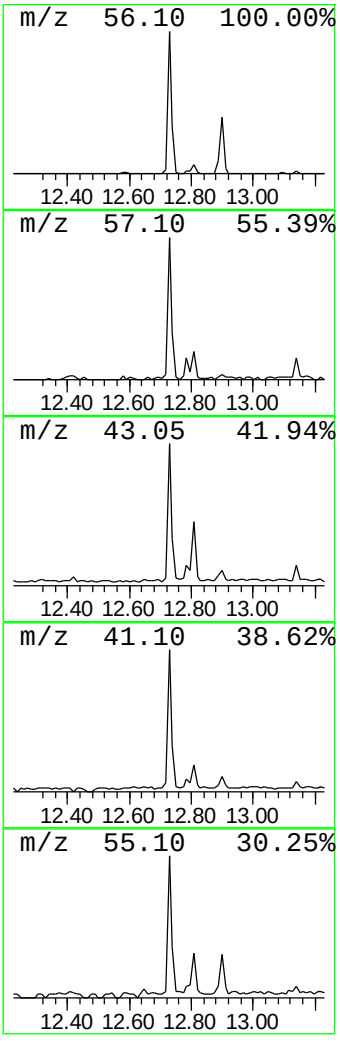
Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	3.85 ng	247182	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	58
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	52
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38
4	Cyclohexanamine	99	C6H13N	000108-91-8	38
5	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	38





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Operator : UM/SJ
Sample : PB95264BL
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB95264BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.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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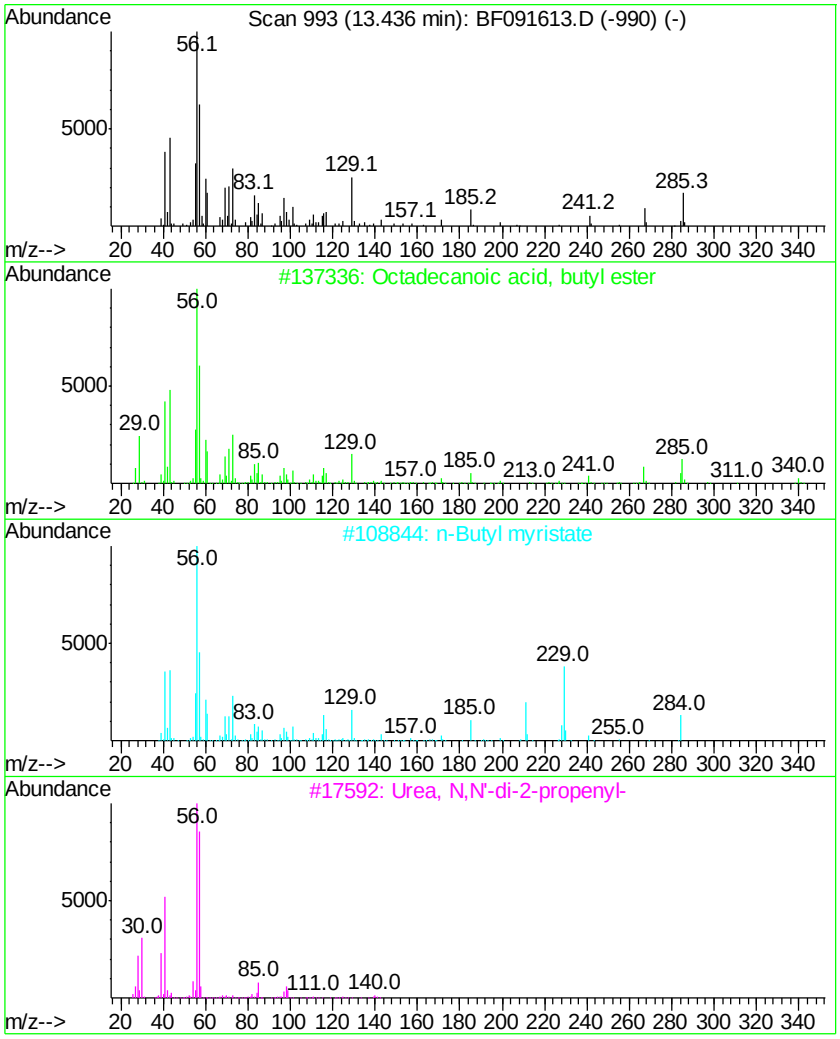
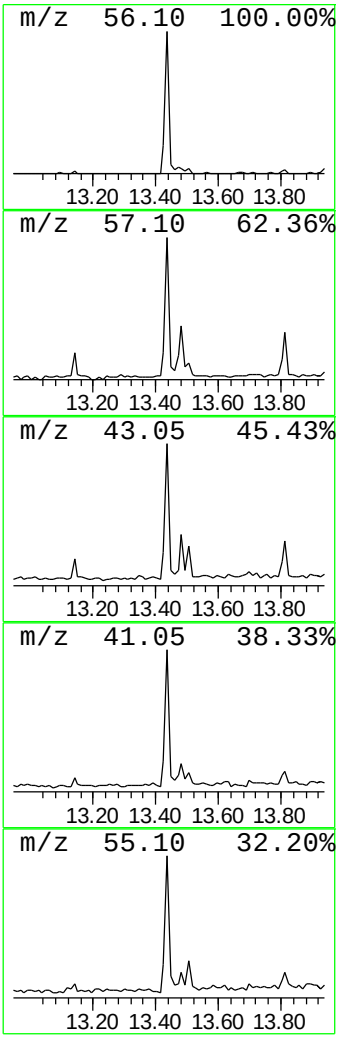
Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	2.72 ng	174674	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	87
2	n-Butyl myristate	284	C18H36O2	000110-36-1	53
3	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35
4	2-Methyl-1-octadecene	266	C19H38	061868-20-0	35
5	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32





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Sample : PB95264BL
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Instrument : BNA_F
ClientSampleId : PB95264BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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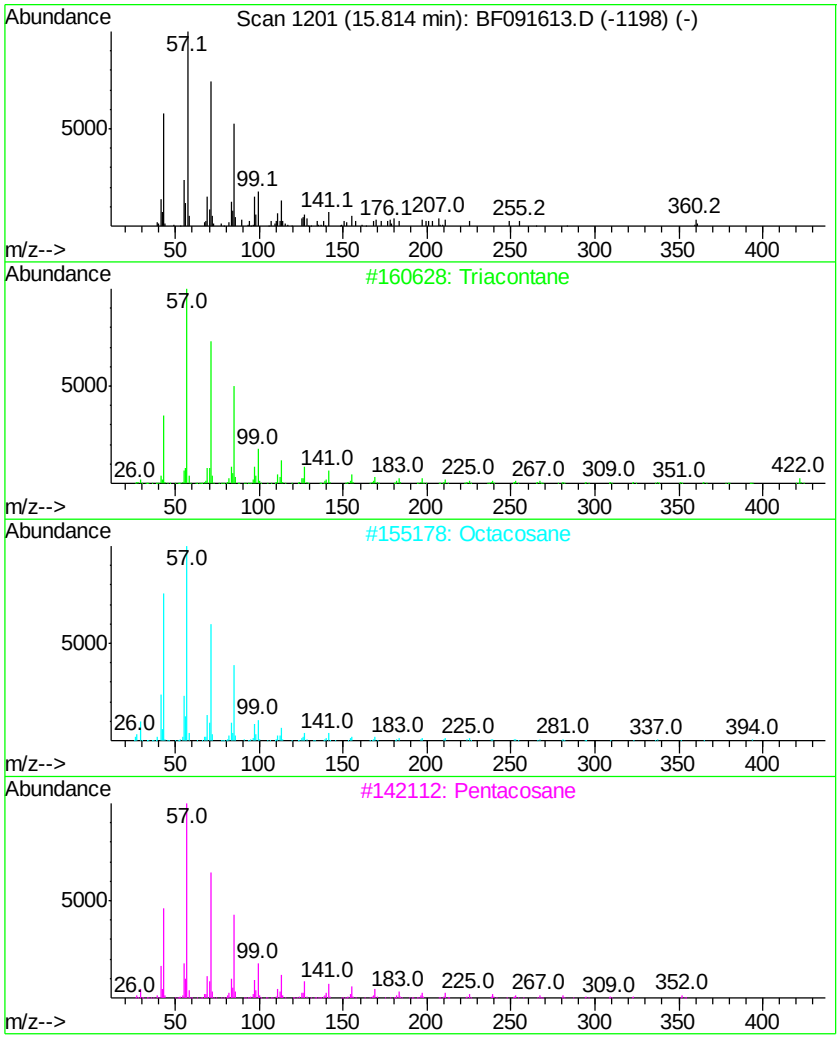
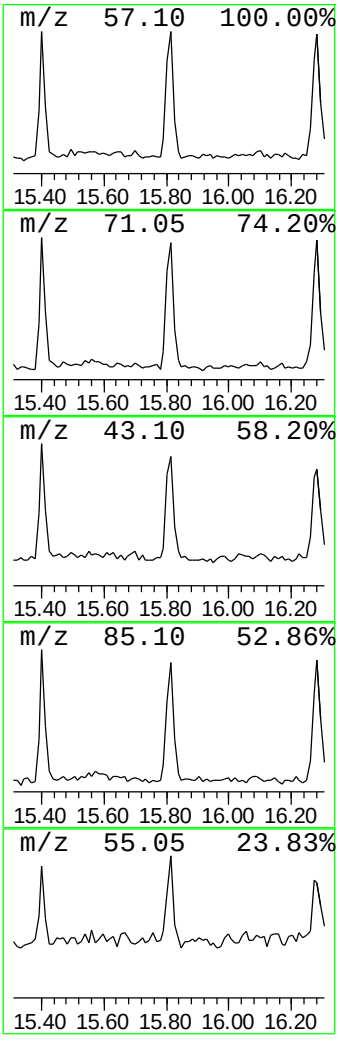
Peak Number 6 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.81	2.43 ng	128164	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Pentacosane	352	C25H52	000629-99-2	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Docosane	310	C22H46	000629-97-0	87





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Sample : PB95264BL
Misc :
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Instrument : BNA_F
ClientSampleId : PB95264BL

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

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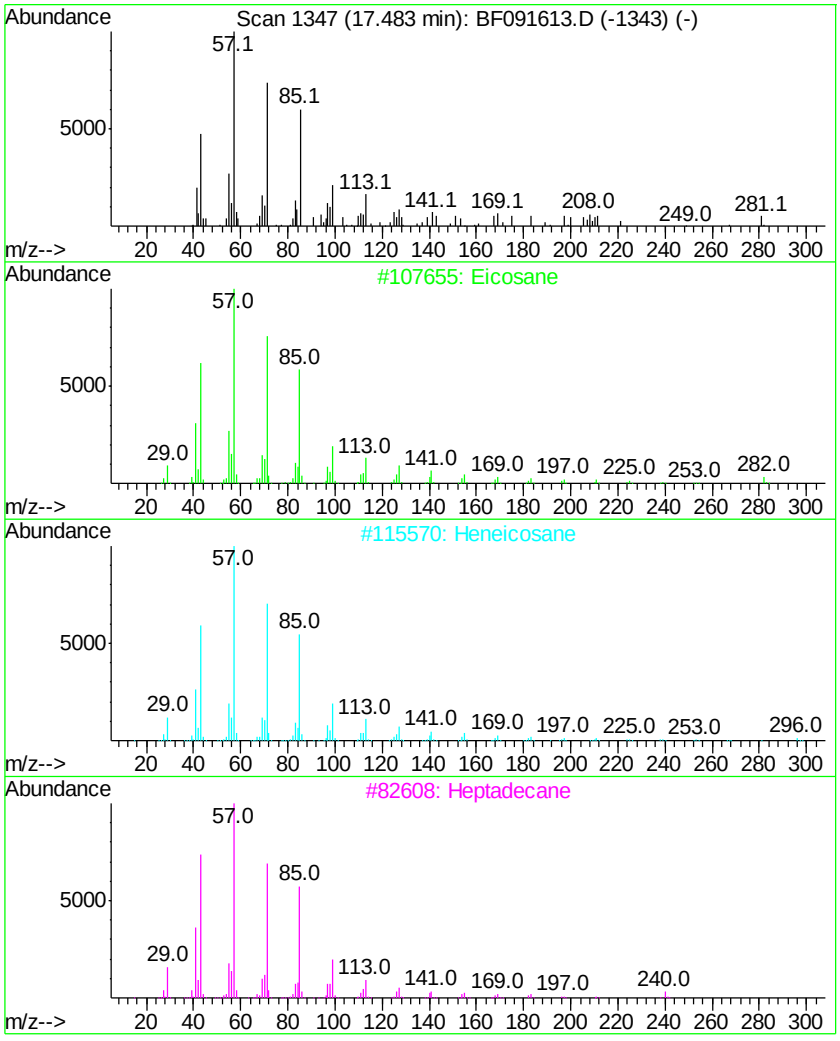
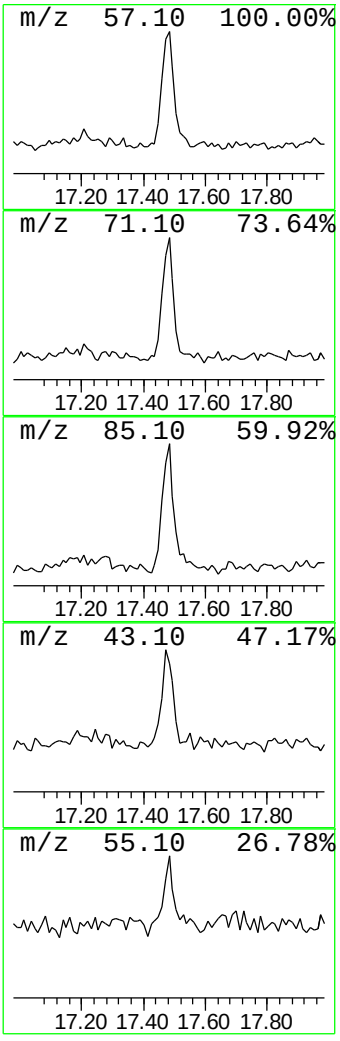
Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.48	2.06 ng	108573	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heneicosane	296	C21H44	000629-94-7	90
3	Heptadecane	240	C17H36	000629-78-7	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Pentacosane	352	C25H52	000629-99-2	87





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
ClientSampleId : PB95264BL

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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...	4.97	29.8	ng	2042120	1	6.80	1371690	20.0
unknown6.56	6.56	65.9	ng	4520210	1	6.80	1371690	20.0
Hexadecanoic acid...	12.73	3.9	ng	247182	5	13.94	1284290	20.0
Octadecanoic acid...	13.44	2.7	ng	174674	5	13.94	1284290	20.0
Triacontane	15.81	2.4	ng	128164	6	15.36	1054230	20.0
Eicosane	17.48	2.1	ng	108573	6	15.36	1054230	20.0