LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
Data File : BF090258.D
Acq On : 27 Sep 2016 18:10
Operator : UM/SJ
Sample : H4933-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B2-14.5-15-BGS

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-BF092016.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	1.644	4	5	55	rVB	3100099	8842945	100.00%	19.222%
2	4.558	257	260	273	rBV	421311	754824	8.54%	1.641%
3	5.039	298	302	304	rBV	2283039	3473536	39.28%	7.551%
4	6.136	394	398	400	rBV	2398367	3748188	42.39%	8.148%
5	6.239	404	407	409	rBV	3235289	3461684	39.15%	7.525%
6	6.467	425	427	430	rBV	904521	830026	9.39%	1.804%
7	6.627	438	441	443	rBV	2790394	2756354	31.17%	5.992%
8	7.039	474	477	480	rBV	1615963	2128273	24.07%	4.626%
9	7.176	486	489	495	rVB	59421	117496	1.33%	0.255%
10	7.759	537	540	542	rBV	1166821	1142085	12.92%	2.483%
11	8.845	631	635	637	rBV	3433750	4316252	48.81%	9.382%
12	9.245	667	670	672	rBV	1502493	1622959	18.35%	3.528%
13	9.496	690	692	695	rVB	1292453	1336614	15.12%	2.905%
14	10.285	758	761	764	rBV	2246016	2629436	29.73%	5.716%
15	10.433	770	774	778	rBV	130342	187723	2.12%	0.408%
16	10.971	818	821	823	rBV	1398004	1418347	16.04%	3.083%
17	11.233	841	844	848	rBV	60221	90970	1.03%	0.198%
18	11.531	868	870	877	rBV3	196586	316238	3.58%	0.687%
19	12.559	957	960	962	rBV	3432178	3914508	44.27%	8.509%
20	13.462	1037	1039	1047	rBV	255497	427573	4.84%	0.929%
21	13.576	1047	1049	1059	rVV	1234688	1340983	15.16%	2.915%
22	14.445	1123	1125	1127	rVB	106025	106134	1.20%	0.231%
23	14.902	1162	1165	1167	rBV	880470	1040503	11.77%	2.262%

Sum of corrected areas: 46003651

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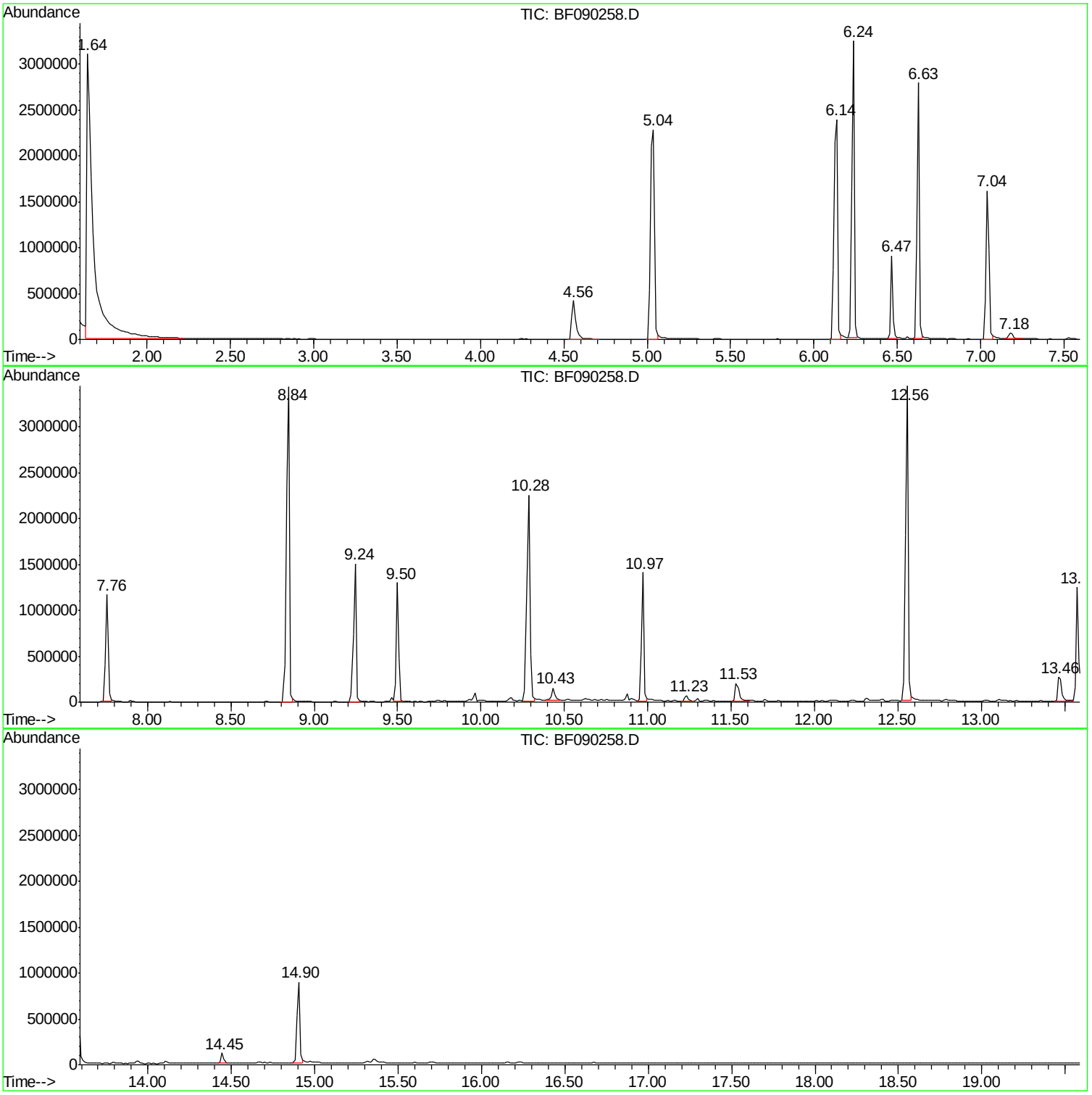
Instrument : BNA_F
ClientSampleId : B2-14.5-15-BGS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
Data File : BF090258.D
Acq On : 27 Sep 2016 18:10
Operator : UM/SJ
Sample : H4933-03
Misc :
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Instrument : BNA_F
ClientSampleId : B2-14.5-15-BGS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

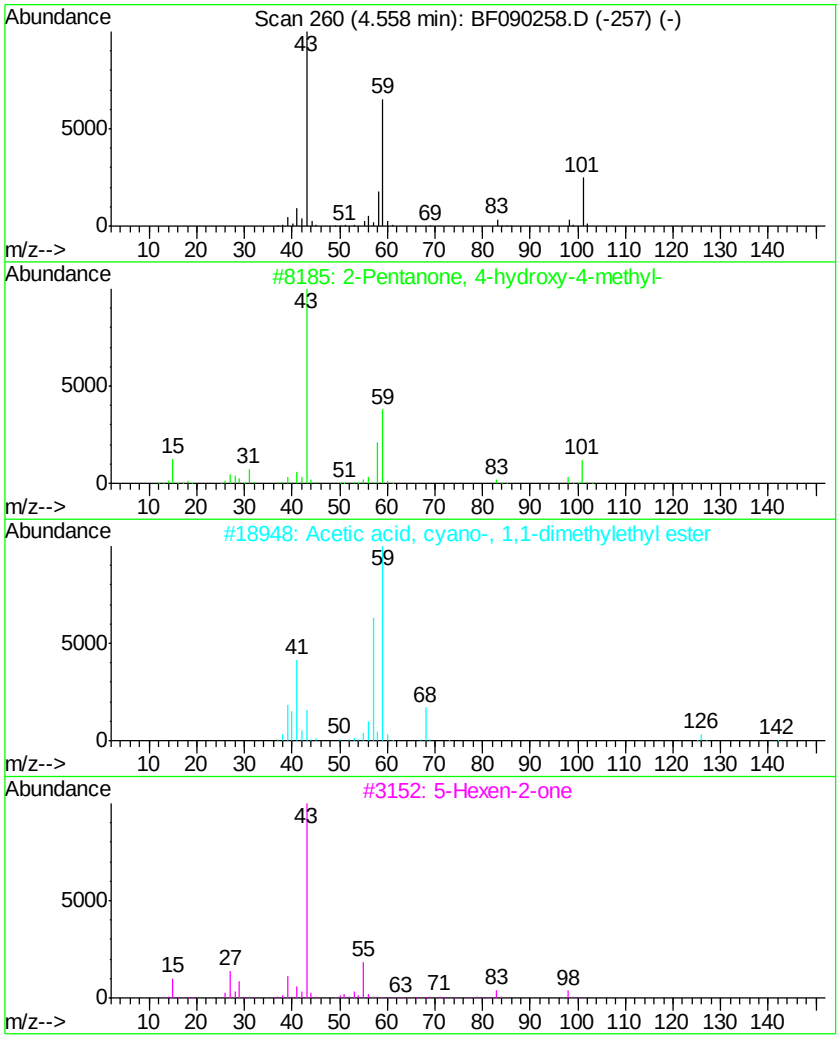
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

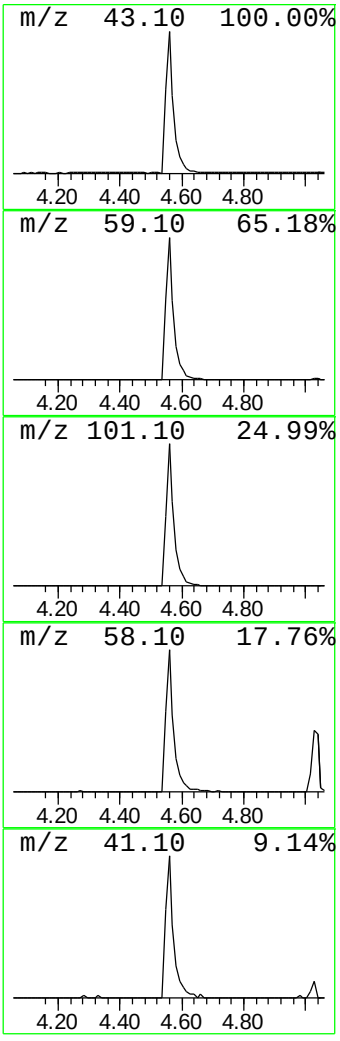
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	18.19 ng	754824	1,4-Dichlorobenzene-d4	6.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Acetone	58	C3H6O	000067-64-1	9





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Operator : UM/SJ
Sample : H4933-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B2-14.5-15-BGS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

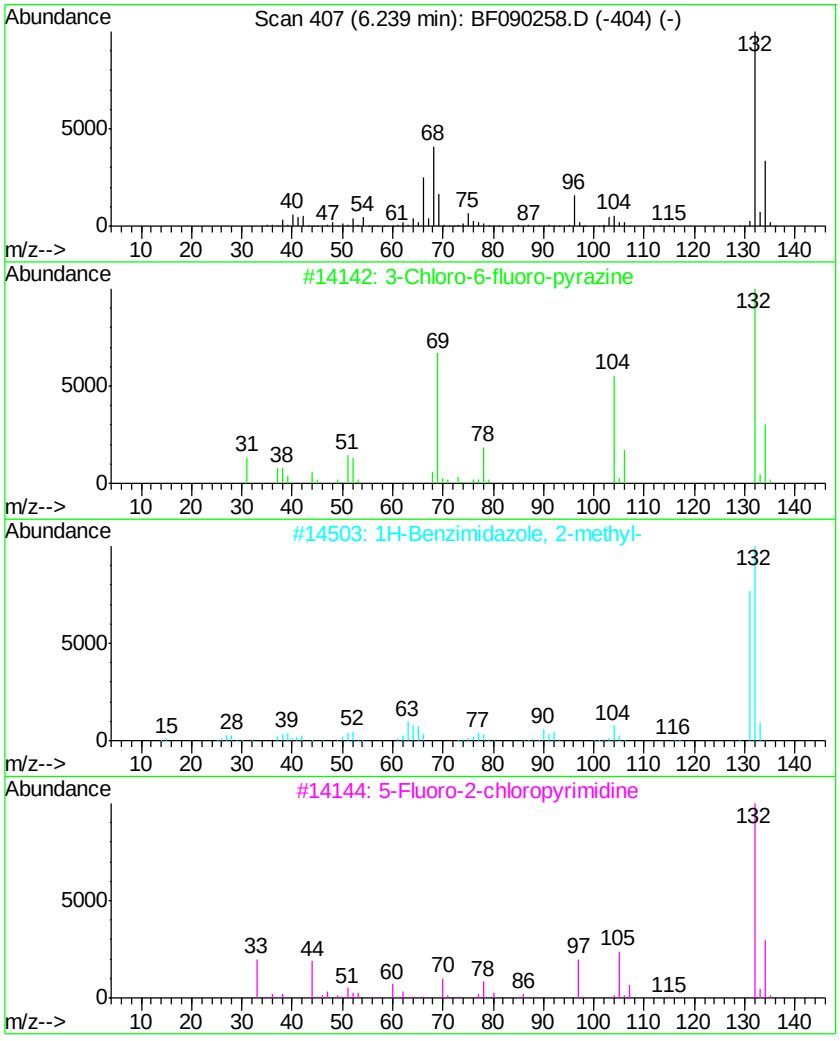
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

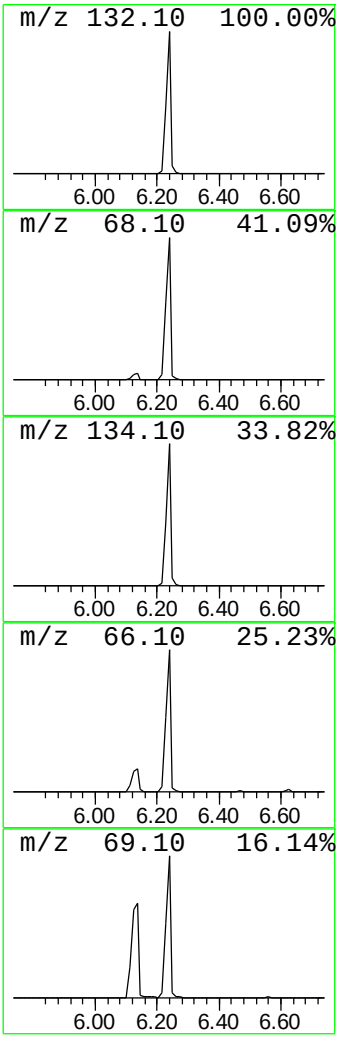
****

Peak Number 3 unknown6.24 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	83.41 ng	3461680	1,4-Dichlorobenzene-d4	6.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





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Data File : BF090258.D
Acq On : 27 Sep 2016 18:10
Operator : UM/SJ
Sample : H4933-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B2-14.5-15-BGS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

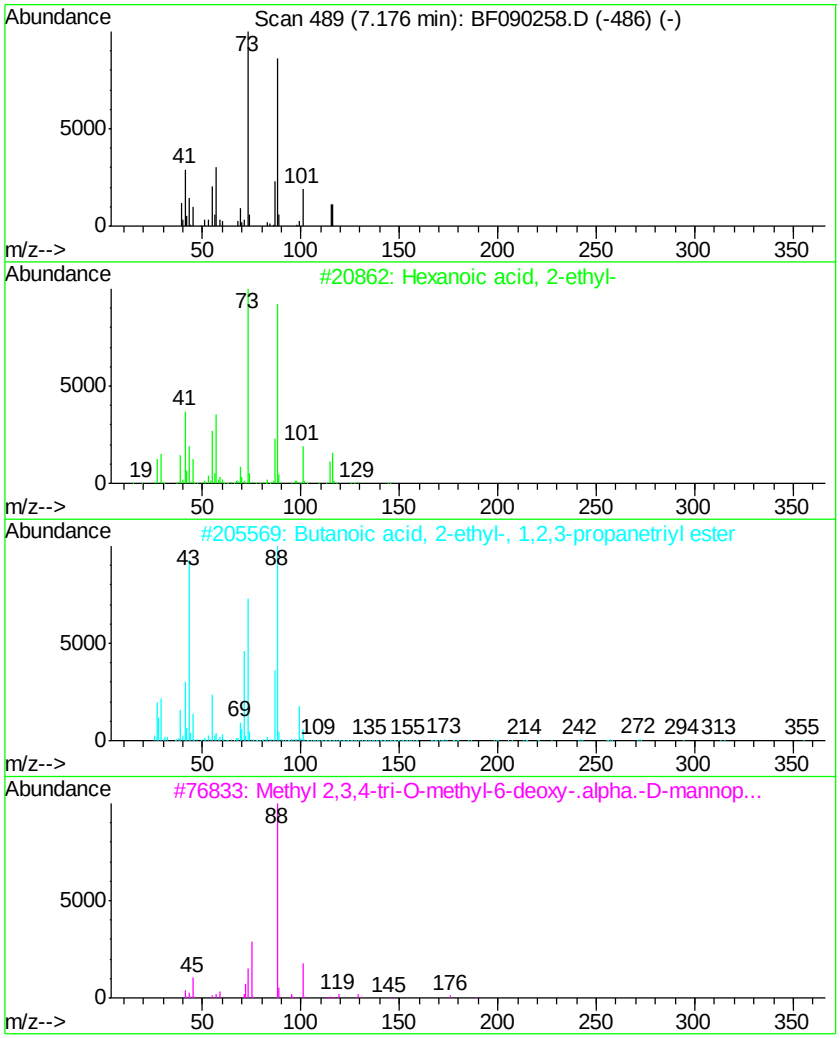
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

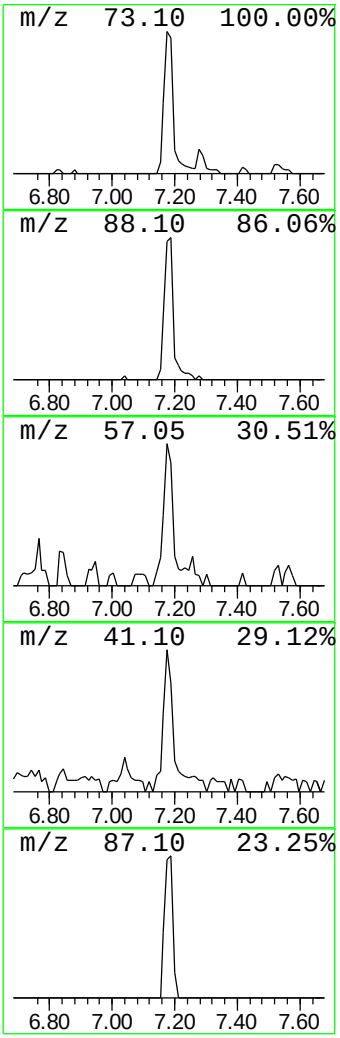
****

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.18	2.06 ng	117496	Naphthalene-d8	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	83
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
3	Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	42
4	1,4-Dioxane	88	C4H8O2	000123-91-1	38
5	Methyl L-(+)-.beta.-hydroxyisobu...	118	C5H10O3	080657-57-4	25





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
Data File : BF090258.D
Acq On : 27 Sep 2016 18:10
Operator : UM/SJ
Sample : H4933-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B2-14.5-15-BGS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

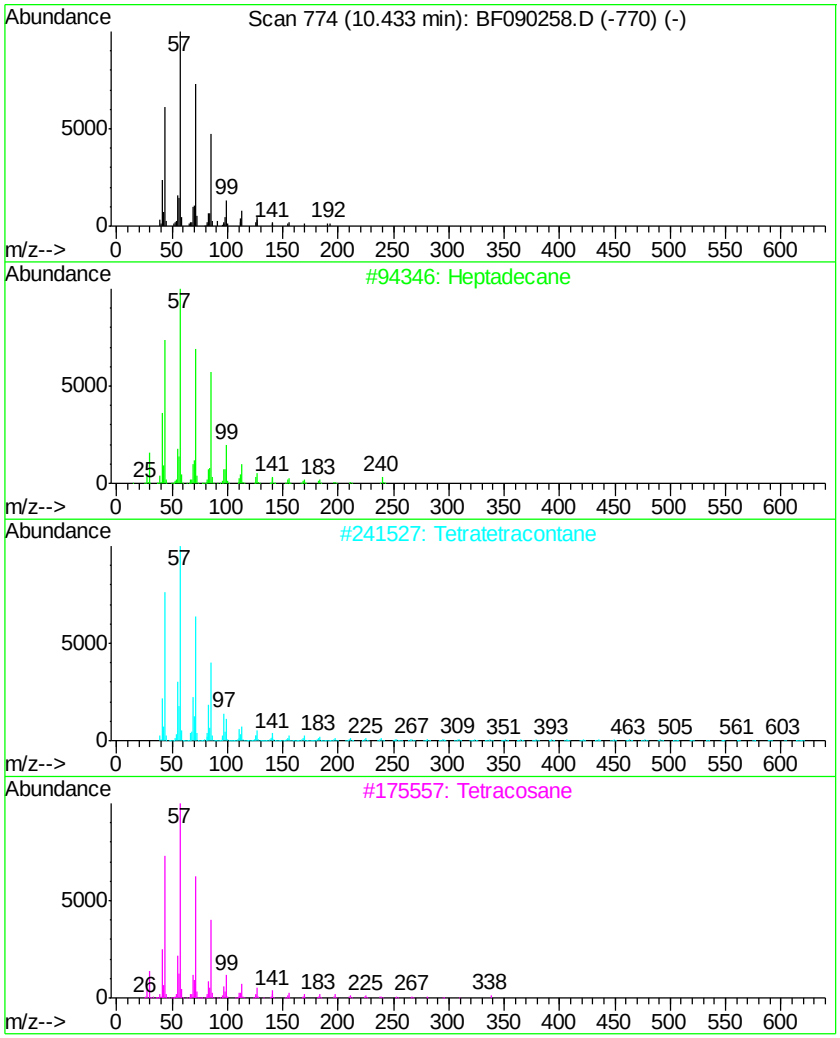
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

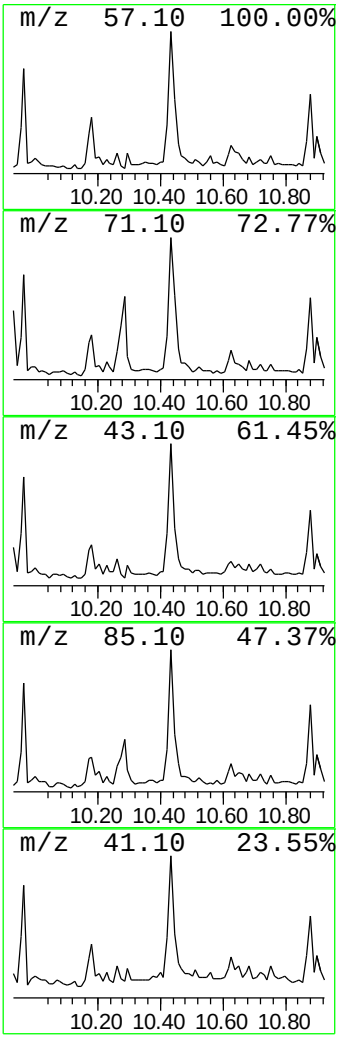
****

Peak Number 6 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.43	2.65 ng	187723	Phenanthrene-d10	10.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Tetracosane	338	C24H50	000646-31-1	90
4	Hexadecane	226	C16H34	000544-76-3	90
5	Tetradecane	198	C14H30	000629-59-4	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
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Operator : UM/SJ
Sample : H4933-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B2-14.5-15-BGS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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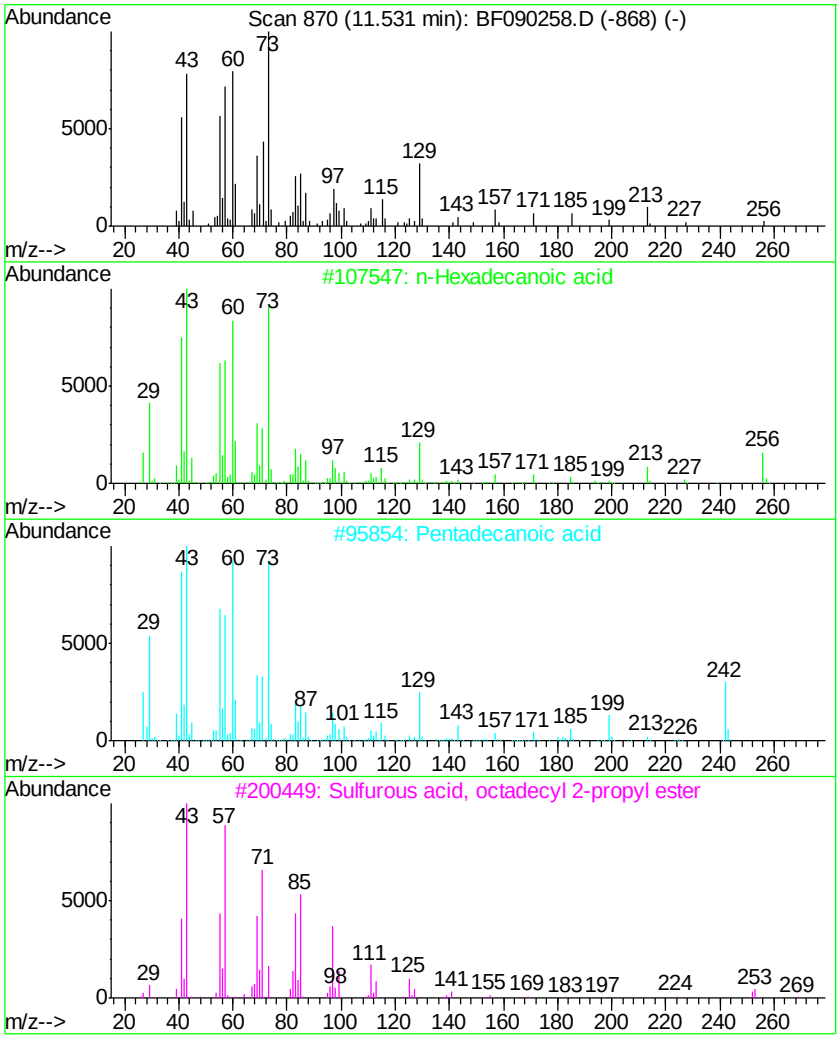
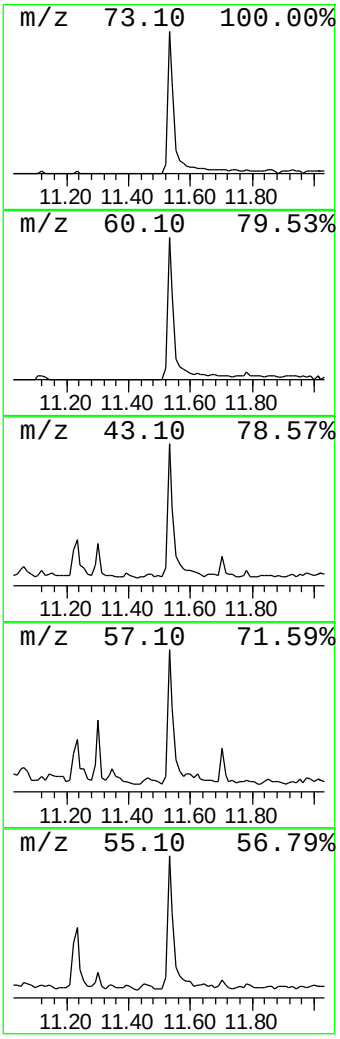
Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.53	4.46 ng	316238	Phenanthrene-d10	10.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	30
4	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	25
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20





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Instrument : BNA_F
ClientSampleId : B2-14.5-15-BGS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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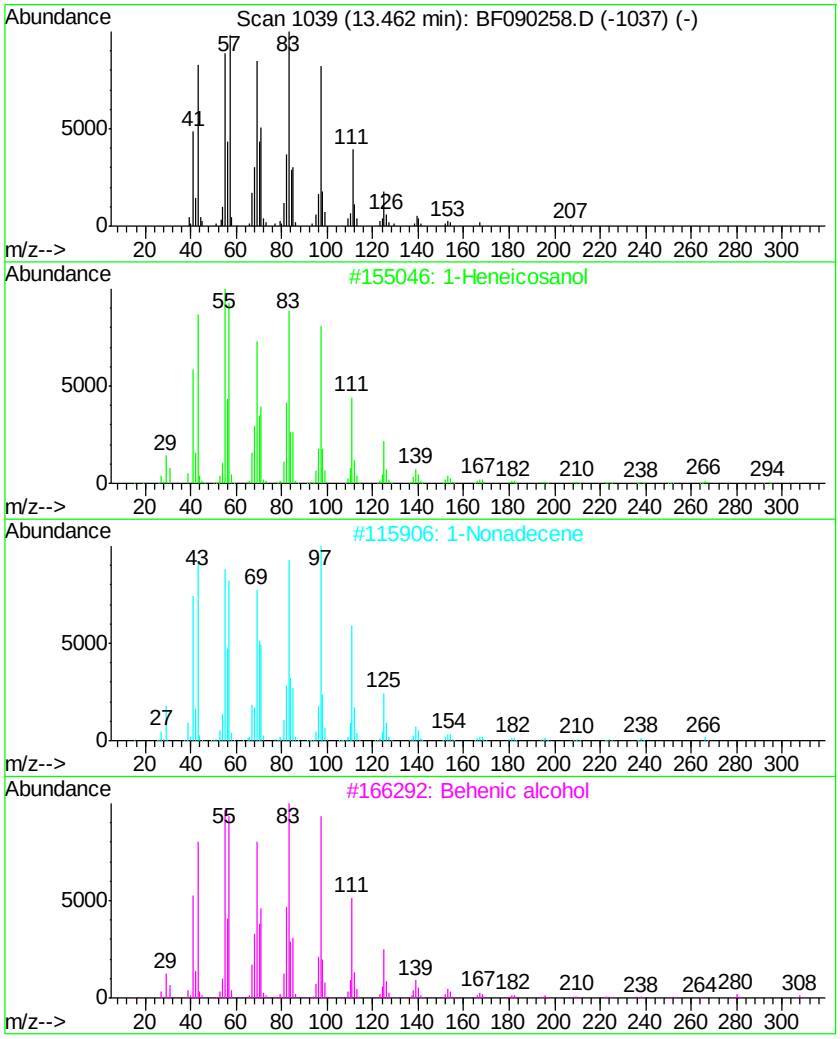
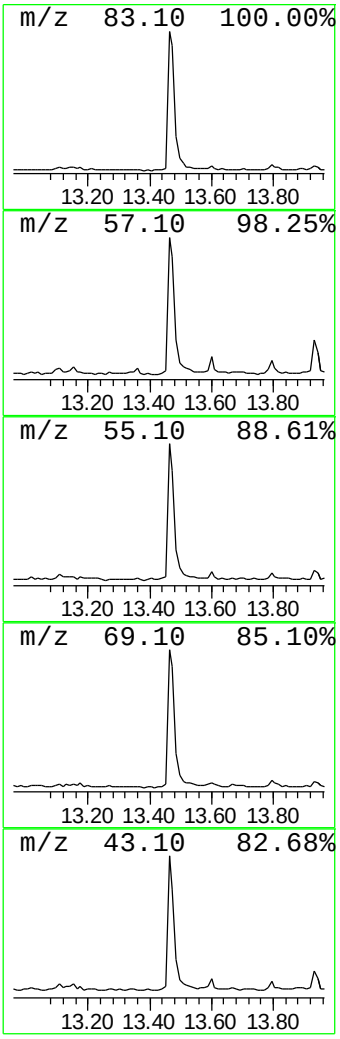
Peak Number 8 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	6.38 ng	427573	Chrysene-d12	13.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	91





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ClientSampleId : B2-14.5-15-BGS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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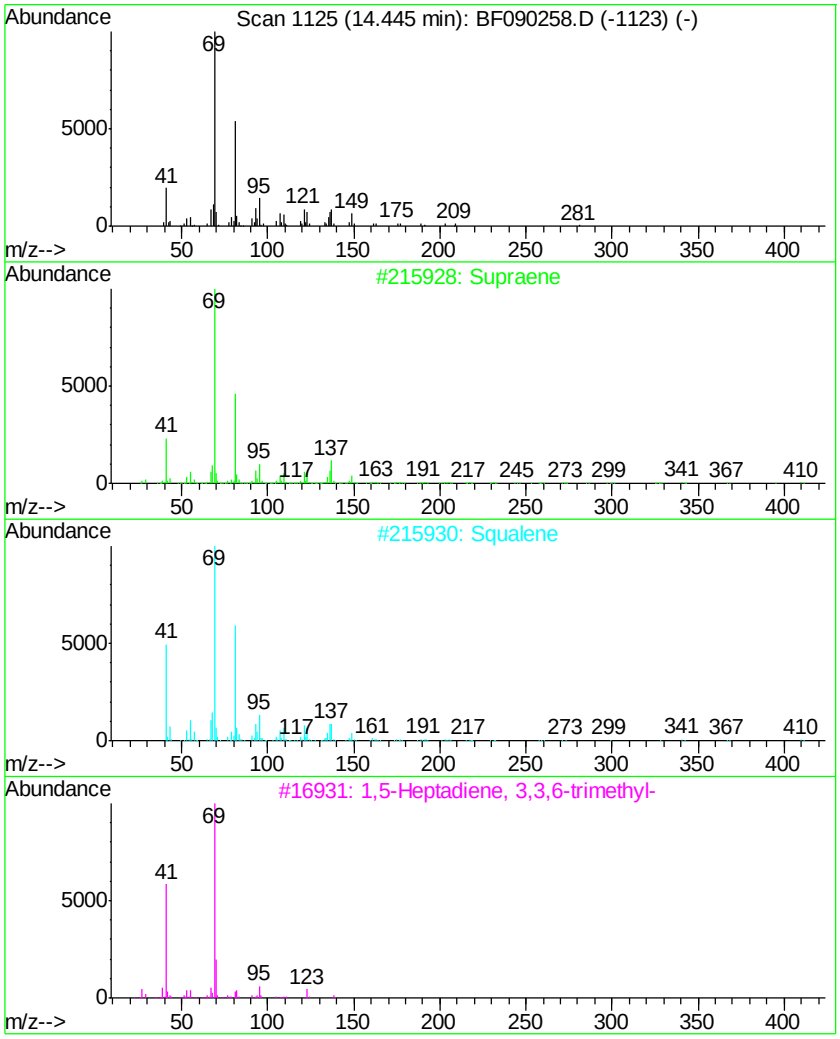
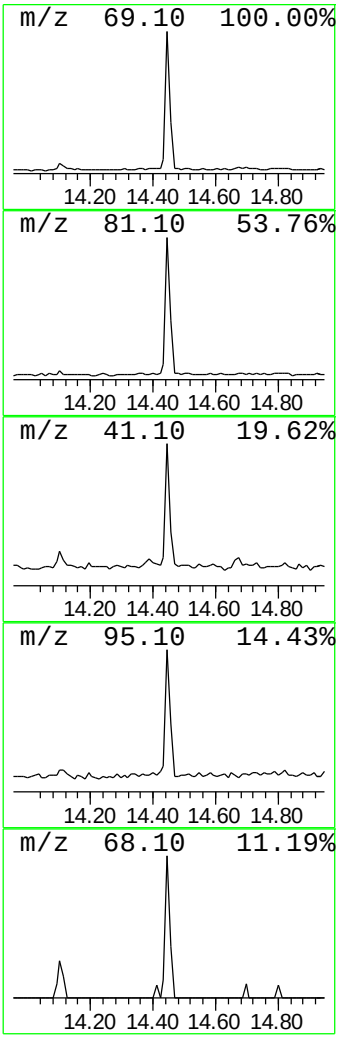
Peak Number 9 Supraene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.04 ng	106134	Perylene-d12	14.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	53
4	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	53
5	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092716\
Data File : BF090258.D
Acq On : 27 Sep 2016 18:10
Operator : UM/SJ
Sample : H4933-03
Misc :
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Instrument : BNA_F
ClientSampleId : B2-14.5-15-BGS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.56	18.2	ng	754824	1	6.47	830026	20.0
unknown6.24	6.24	83.4	ng	3461680	1	6.47	830026	20.0
Hexanoic acid, 2-...	7.18	2.1	ng	117496	2	7.76	1142090	20.0
Heptadecane	10.43	2.6	ng	187723	4	10.97	1418350	20.0
n-Hexadecanoic acid	11.53	4.5	ng	316238	4	10.97	1418350	20.0
1-Heneicosanol	13.46	6.4	ng	427573	5	13.58	1340980	20.0
Supraene	14.45	2.0	ng	106134	6	14.90	1040500	20.0