LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092916\
Data File : BF090306.D
Acq On : 30 Sep 2016 00:42
Operator : UM/SJ
Sample : H5015-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-2

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	3	5	24	rVB	118469	304430	9.30%	0.990%
2	4.547	256	259	276	rVB	368788	720510	22.02%	2.344%
3	5.027	298	301	304	rBV	2693111	3167755	96.82%	10.304%
4	6.124	394	397	400	rBV	2506117	3222626	98.49%	10.482%
5	6.227	403	406	409	rVV	2815431	3154872	96.42%	10.262%
6	6.456	424	426	429	rBV	652633	682332	20.85%	2.219%
7	6.616	437	440	443	rBV	2687616	2528963	77.29%	8.226%
8	7.039	474	477	479	rBV	1982635	2293773	70.11%	7.461%
9	7.747	537	539	542	rBV	1019833	908252	27.76%	2.954%
10	8.833	631	634	637	rBV	3214235	3271889	100.00%	10.643%
11	9.233	667	669	672	rBV	1042963	973918	29.77%	3.168%
12	9.496	690	692	694	rBV	1147164	968988	29.62%	3.152%
13	9.702	707	710	712	rBV	27091	34107	1.04%	0.111%
14	9.953	731	732	734	rVB	37622	39727	1.21%	0.129%
15	10.033	738	739	743	rVB3	40969	48520	1.48%	0.158%
16	10.170	749	751	758	rBV2	17358	47906	1.46%	0.156%
17	10.285	758	761	763	rBV	1655185	1782820	54.49%	5.799%
18	10.433	771	774	778	rVB	41277	72979	2.23%	0.237%
19	10.868	810	812	814	rBV	33527	39663	1.21%	0.129%
20	10.959	818	820	825	rBV2	508468	1054011	32.21%	3.428%
21	11.039	825	827	830	rVB	50111	52522	1.61%	0.171%
22	11.222	838	843	846	rBV4	23336	43978	1.34%	0.143%
23	11.531	869	870	872	rVV2	26203	33444	1.02%	0.109%
24	11.576	872	874	879	rVB2	36851	63254	1.93%	0.206%
25	11.782	888	892	895	rVB3	24751	41240	1.26%	0.134%
26	12.159	923	925	928	rBV	308222	357215	10.92%	1.162%
27	12.388	942	945	947	rBV	318766	327188	10.00%	1.064%
28	12.548	957	959	962	rBV	1746467	2160699	66.04%	7.028%
29	12.788	978	980	981	rBV	35247	35583	1.09%	0.116%
30	13.474	1037	1040	1044	rBV2	103426	160967	4.92%	0.524%
31	13.576	1046	1049	1056	rVV2	653563	880313	26.91%	2.863%
32	14.102	1092	1095	1099	rVB2	37557	56165	1.72%	0.183%
33	14.445	1123	1125	1127	rVB	106979	112749	3.45%	0.367%
34	14.559	1133	1135	1140	rBV	101861	190216	5.81%	0.619%

LSC Area Percent Report

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Operator : UM/SJ
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Misc :
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Instrument : BNA_F
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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

35	14.674	1141	1145	1148	rVV2	16156	46472	1.42%	0.151%
36	14.799	1154	1156	1159	rBV	55233	64914	1.98%	0.211%
37	14.857	1159	1161	1163	rBV	58730	80609	2.46%	0.262%
38	14.902	1163	1165	1169	rBV	465524	522834	15.98%	1.701%
39	16.045	1262	1265	1269	rVB2	28114	52038	1.59%	0.169%
40	16.388	1292	1295	1301	rBV	25792	57790	1.77%	0.188%
41	18.057	1437	1441	1448	rBV7	26288	85349	2.61%	0.278%

Sum of corrected areas: 30743580

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092916\
Data File : BF090306.D
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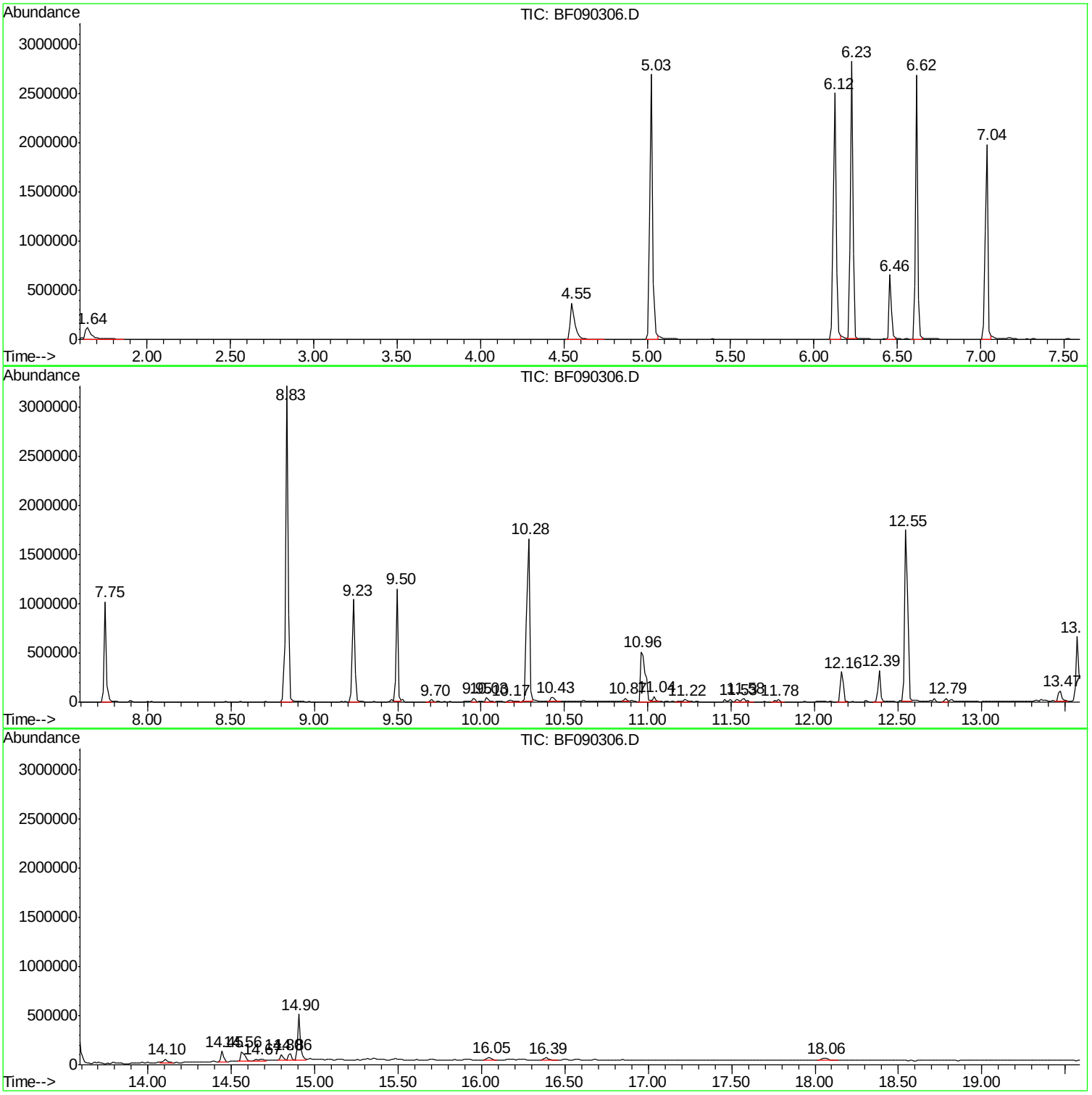
Operator : UM/SJ
Sample : H5015-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-2

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\BF092916\
Data File : BF090306.D
Acq On : 30 Sep 2016 00:42
Operator : UM/SJ
Sample : H5015-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-2

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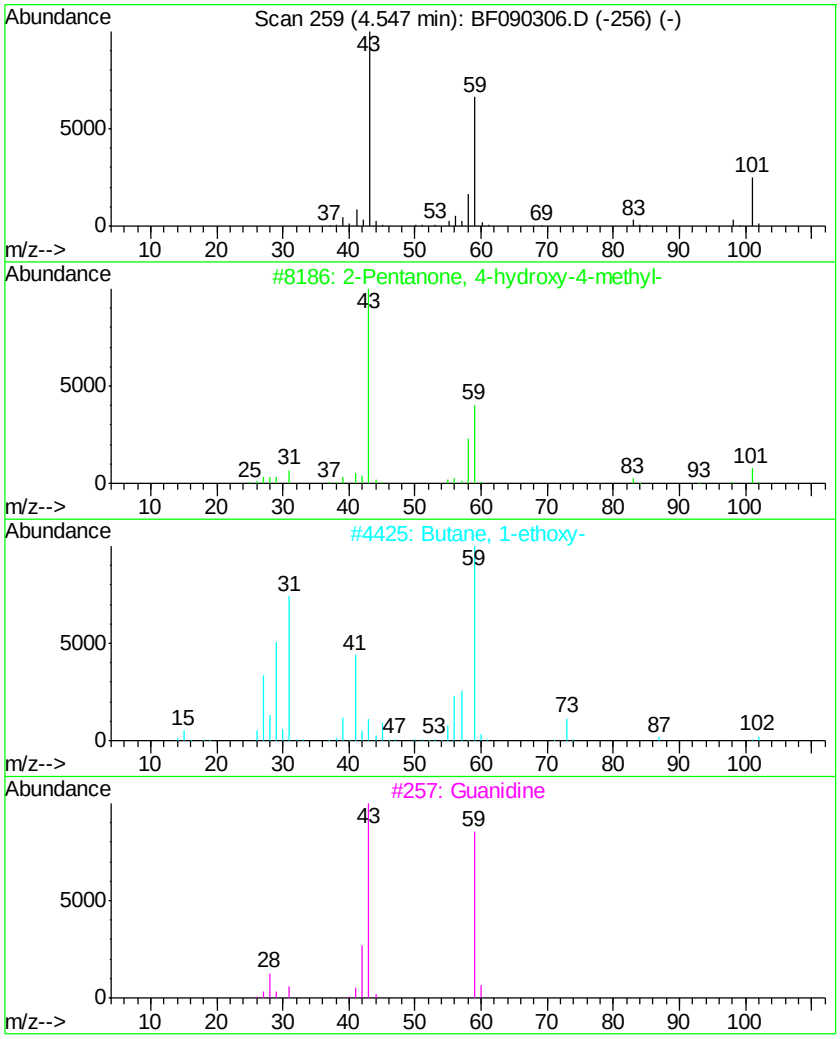
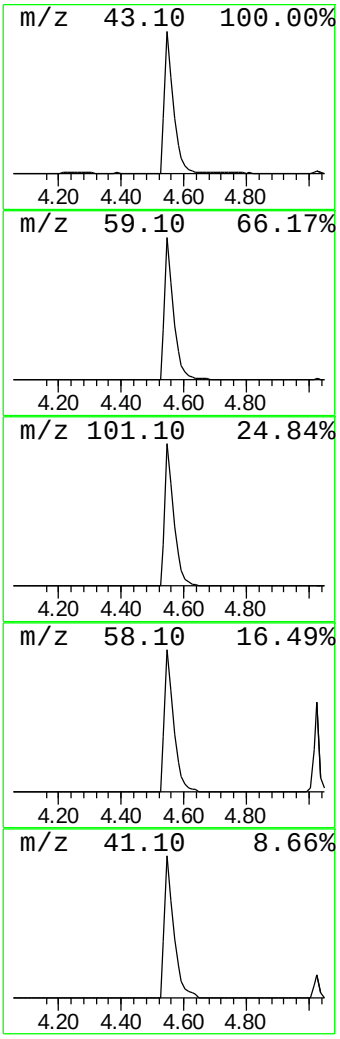
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	21.12 ng	720510	1,4-Dichlorobenzene-d4	6.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
3	Guanidine	59	CH5N3	000113-00-8	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092916\
Data File : BF090306.D
Acq On : 30 Sep 2016 00:42
Operator : UM/SJ
Sample : H5015-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-2

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

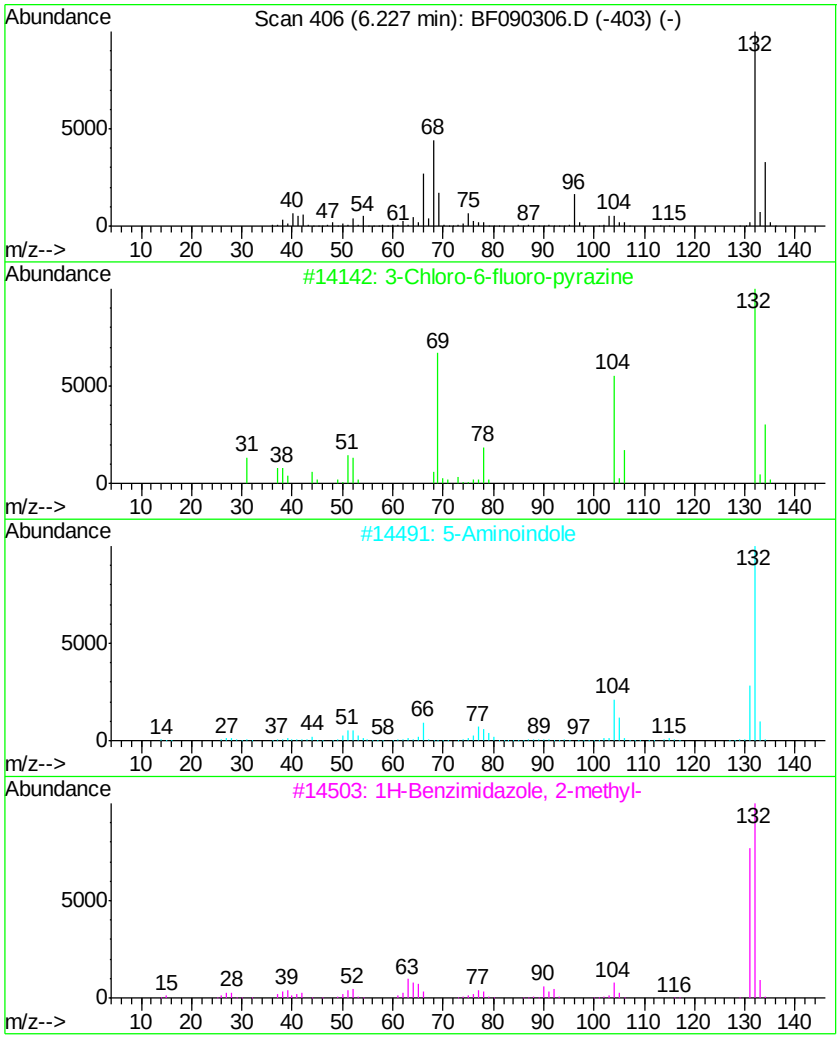
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

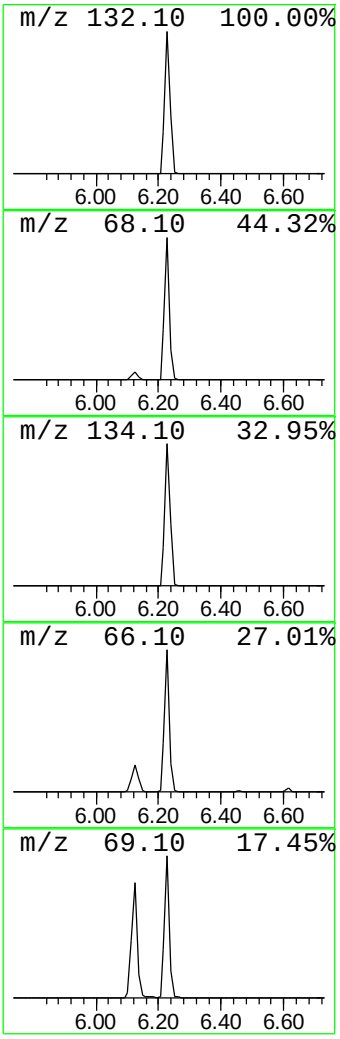
****

Peak Number 3 unknown6.23 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.23	92.47 ng	3154870	1,4-Dichlorobenzene-d4	6.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092916\
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ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-2

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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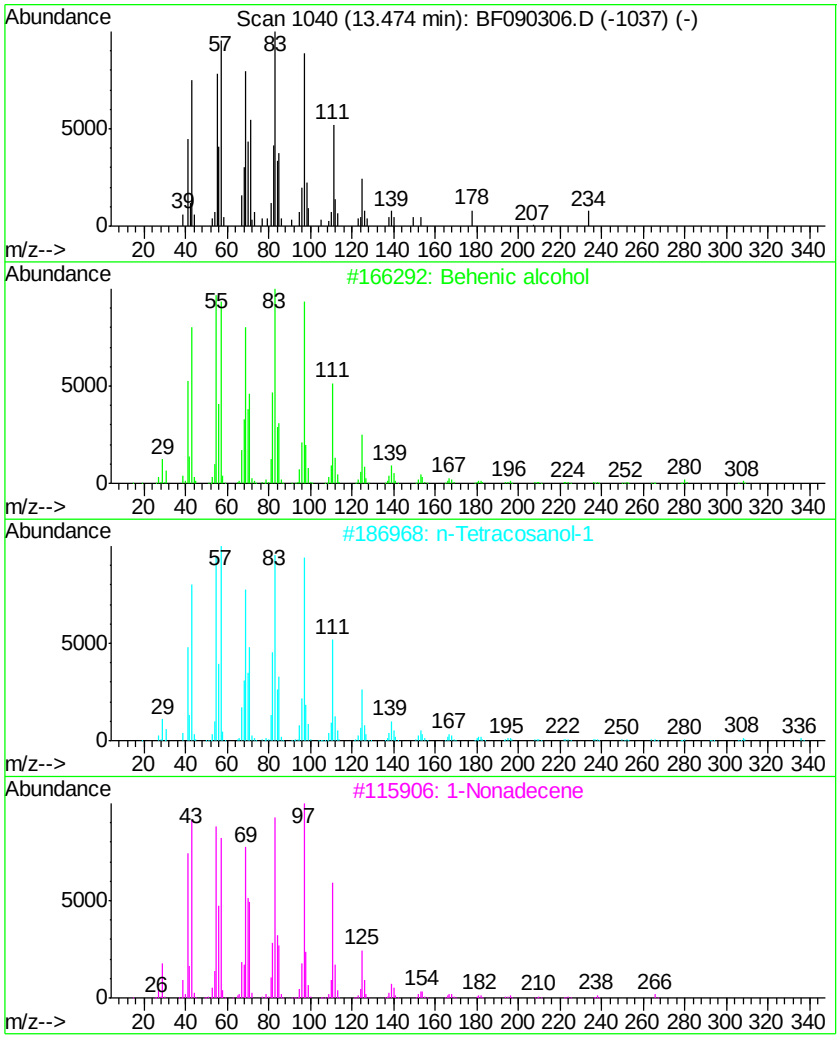
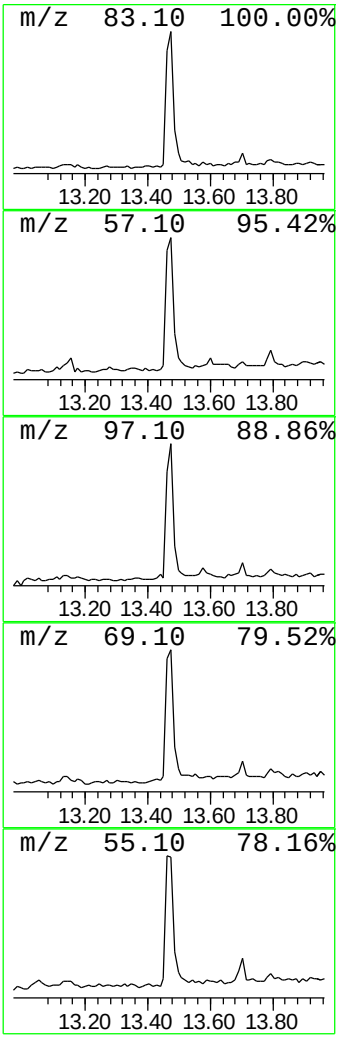
Peak Number 5 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	3.66 ng	160967	Chrysene-d12	13.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	1-Nonadecene	266	C19H38	018435-45-5	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	94
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	94





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Operator : UM/SJ
Sample : H5015-02
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Instrument : BNA_F
ClientSampleId : COMPOSITE-2

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

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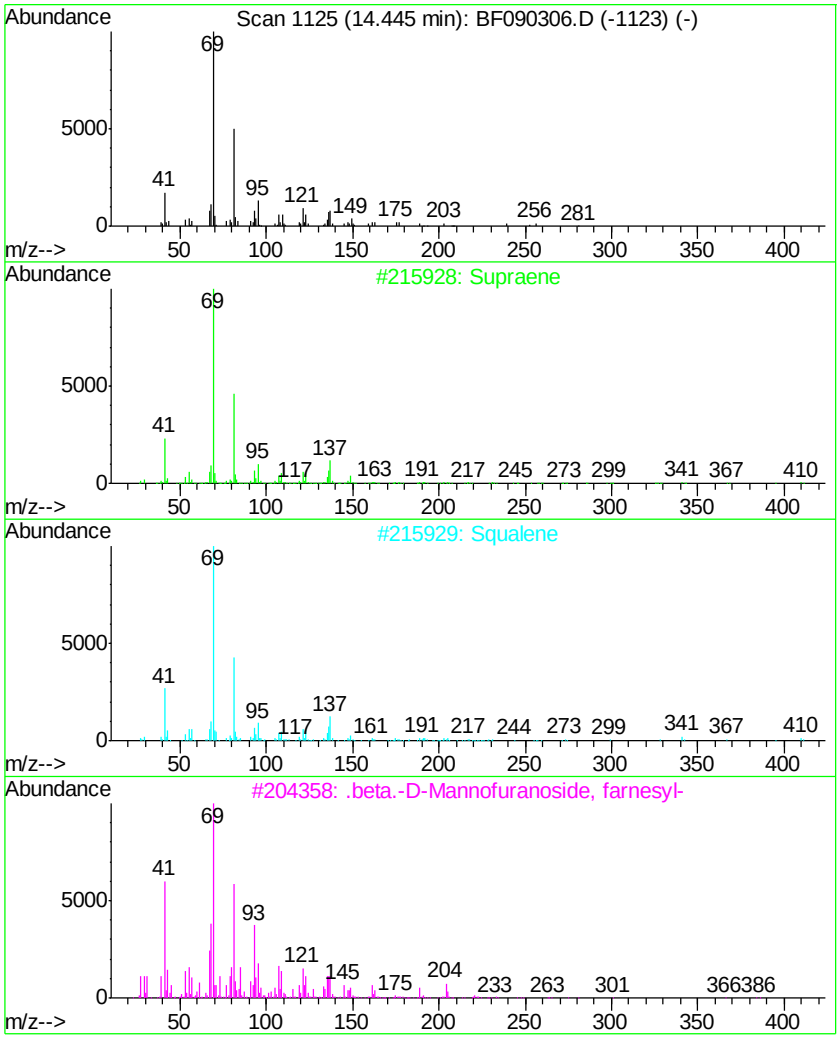
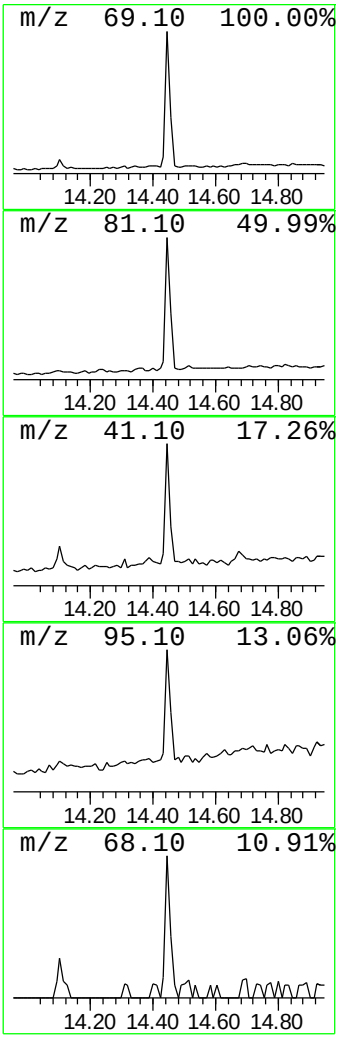
Peak Number 6 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	4.31 ng	112749	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	.beta.-D-Mannofuranoside, farnesyl-	384	C21H36O6	1000155-15-5	78
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	50
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50





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Sample : H5015-02
Misc :
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Instrument : BNA_F
ClientSampleId : COMPOSITE-2

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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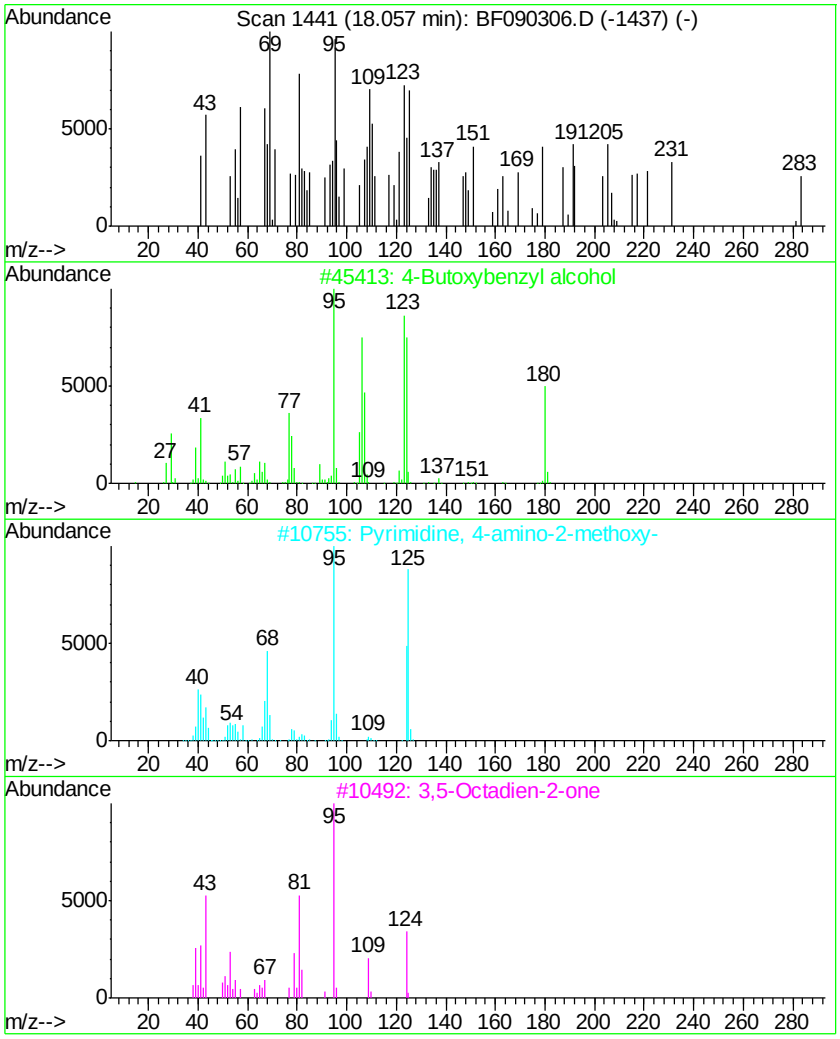
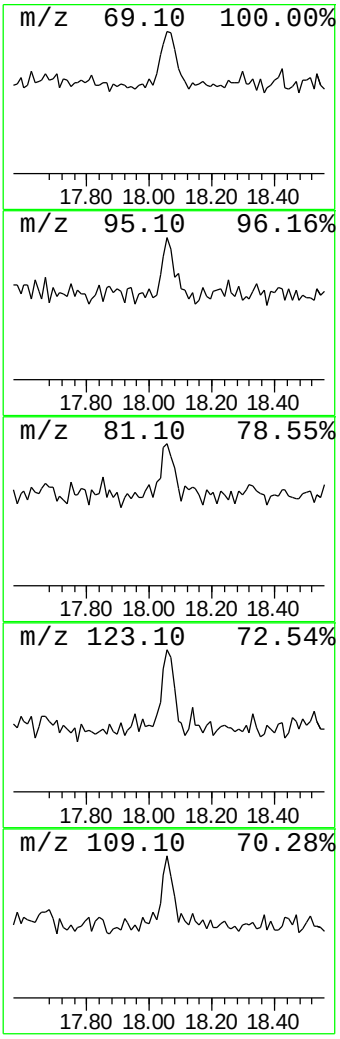
Peak Number 8 unknown18.06 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.06	3.26 ng	85349	Perylene-d12	14.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Butoxybenzyl alcohol	180	C11H16O2	006214-45-5	27
2	Pyrimidine, 4-amino-2-methoxy-	125	C5H7N3O	003289-47-2	25
3	3,5-Octadien-2-one	124	C8H12O	038284-27-4	18
4	3-Cyclohexene-1-carboxaldehyde, ...	124	C8H12O	000931-96-4	15
5	3-Cyclopentylpropionic acid, 3-c...	216	C11H17ClO2	1000292-47-2	14





Tentatively Identified Compound (LSC) summary

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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...	4.55	21.1	ng	720510	1	6.46	682332	20.0
unknown6.23	6.23	92.5	ng	3154870	1	6.46	682332	20.0
Behenic alcohol	13.47	3.7	ng	160967	5	13.58	880313	20.0
Supraene	14.45	4.3	ng	112749	6	14.90	522834	20.0
unknown18.06	18.06	3.3	ng	85349	6	14.90	522834	20.0