LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101916\
Data File : BF090651.D
Acq On : 19 Oct 2016 16:52
Operator : UM/SJ
Sample : H5296-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C2-GW

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-BF101316.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	5.080	236	240	242	rBV	2940490	3962604	100.00%	11.594%
2	5.491	273	276	289	rBV	645126	727151	18.35%	2.128%
3	6.509	363	365	375	rBV	661360	989412	24.97%	2.895%
4	6.646	375	377	380	rBV	791211	887724	22.40%	2.597%
5	6.886	396	398	400	rBV	1258194	1196221	30.19%	3.500%
6	7.034	409	411	414	rBV	1684042	2343198	59.13%	6.856%
7	7.446	442	447	453	rBV	1881056	2058893	51.96%	6.024%
8	7.663	462	466	468	rVB3	29306	55568	1.40%	0.163%
9	7.823	478	480	482	rBV	32389	42012	1.06%	0.123%
10	7.903	485	487	489	rBV	35968	45159	1.14%	0.132%
11	8.166	508	510	513	rBV	1269223	1757016	44.34%	5.141%
12	8.372	525	528	530	rBV	83596	83065	2.10%	0.243%
13	8.417	530	532	534	rBV	76215	66883	1.69%	0.196%
14	8.554	542	544	547	rVB	54130	54538	1.38%	0.160%
15	8.646	547	552	553	rBV3	49051	89376	2.26%	0.261%
16	8.737	558	560	561	rVV	65549	69557	1.76%	0.204%
17	8.760	561	562	564	rVV2	32858	46854	1.18%	0.137%
18	8.829	567	568	570	rVB2	43707	45652	1.15%	0.134%
19	9.000	578	583	587	rBV2	70163	161049	4.06%	0.471%
20	9.114	587	593	596	rBV8	43847	132782	3.35%	0.388%
21	9.252	602	605	607	rBV	3976326	3887306	98.10%	11.374%
22	9.400	616	618	619	rVB	48122	43344	1.09%	0.127%
23	9.526	625	629	631	rBV4	22237	48855	1.23%	0.143%
24	9.583	631	634	637	rVV3	47827	135229	3.41%	0.396%
25	9.640	637	639	641	rVV	239736	268651	6.78%	0.786%
26	9.720	643	646	650	rVV3	67363	160209	4.04%	0.469%
27	9.789	650	652	656	rVV5	26123	42956	1.08%	0.126%
28	9.926	661	664	666	rBV	2213837	2098037	52.95%	6.139%
29	10.086	675	678	680	rBV3	33303	54946	1.39%	0.161%
30	10.132	680	682	684	rVV3	48432	76235	1.92%	0.223%
31	10.246	689	692	694	rBV2	54085	73301	1.85%	0.214%
32	10.360	701	702	704	rVB	74957	53490	1.35%	0.157%
33	10.429	706	708	710	rBV2	33040	55455	1.40%	0.162%
34	10.543	713	718	721	rBV	172191	230133	5.81%	0.673%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101916\
Data File : BF090651.D
Acq On : 19 Oct 2016 16:52
Operator : UM/SJ
Sample : H5296-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C2-GW

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-BF101316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.715	730	733	740	rBV	450438	527633	13.32%	1.544%
36	10.840	740	744	747	rBV3	103031	164788	4.16%	0.482%
37	10.898	747	749	757	rVB5	48417	84454	2.13%	0.247%
38	11.058	761	763	766	rBV2	47204	72632	1.83%	0.213%
39	11.160	771	772	775	rVB2	32440	43825	1.11%	0.128%
40	11.286	779	783	784	rBV2	44881	78076	1.97%	0.228%
41	11.366	788	790	792	rBV	33178	55088	1.39%	0.161%
42	11.412	792	794	797	rBV	1875772	1949273	49.19%	5.703%
43	11.629	811	813	818	rVB4	23154	63087	1.59%	0.185%
44	12.189	859	862	867	rVB3	26946	56780	1.43%	0.166%
45	12.452	883	885	888	rBV2	37057	58972	1.49%	0.173%
46	13.001	931	933	936	rBV	3882425	3888456	98.13%	11.377%
47	13.344	961	963	968	rVB	135937	169811	4.29%	0.497%
48	13.561	978	982	988	rVB3	40851	82641	2.09%	0.242%
49	13.892	1009	1011	1019	rBV2	112426	200912	5.07%	0.588%
50	14.052	1023	1025	1028	rVB	1733136	1773779	44.76%	5.190%
51	14.212	1038	1039	1047	rVB2	22148	42531	1.07%	0.124%
52	14.521	1064	1066	1070	rBV3	19559	42637	1.08%	0.125%
53	14.909	1096	1100	1102	rBV	596706	896229	22.62%	2.622%
54	15.504	1149	1152	1165	rBV	1316962	1883814	47.54%	5.512%

Sum of corrected areas: 34178279

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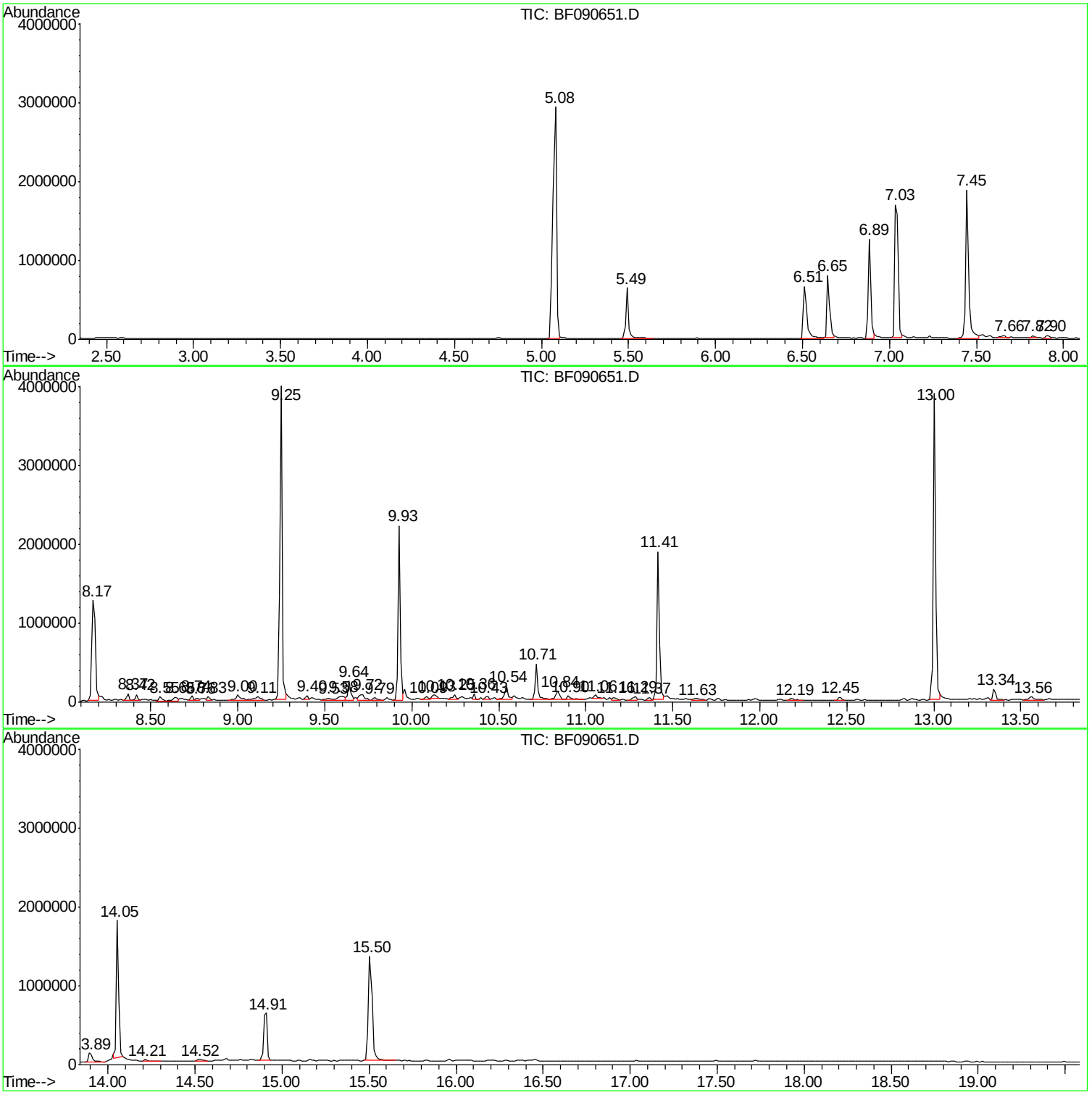
Operator : UM/SJ
Sample : H5296-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OWL-C2-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101916\
Data File : BF090651.D
Acq On : 19 Oct 2016 16:52
Operator : UM/SJ
Sample : H5296-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C2-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

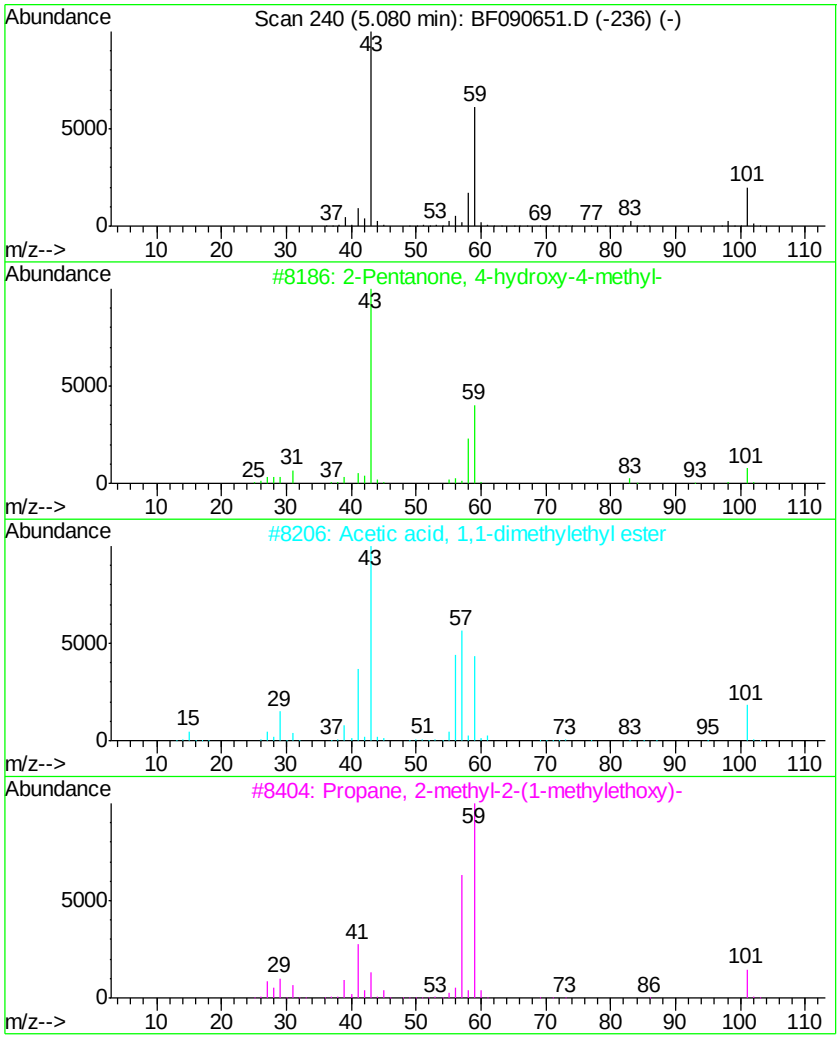
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

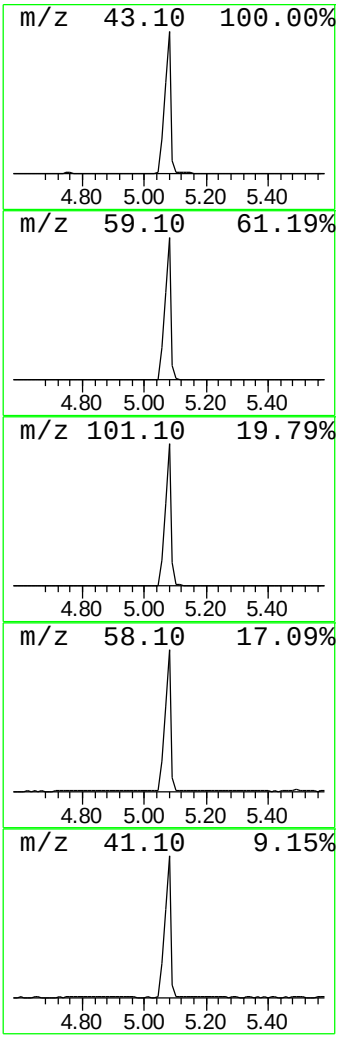
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	66.25 ng	3962600	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101916\
Data File : BF090651.D
Acq On : 19 Oct 2016 16:52
Operator : UM/SJ
Sample : H5296-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C2-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

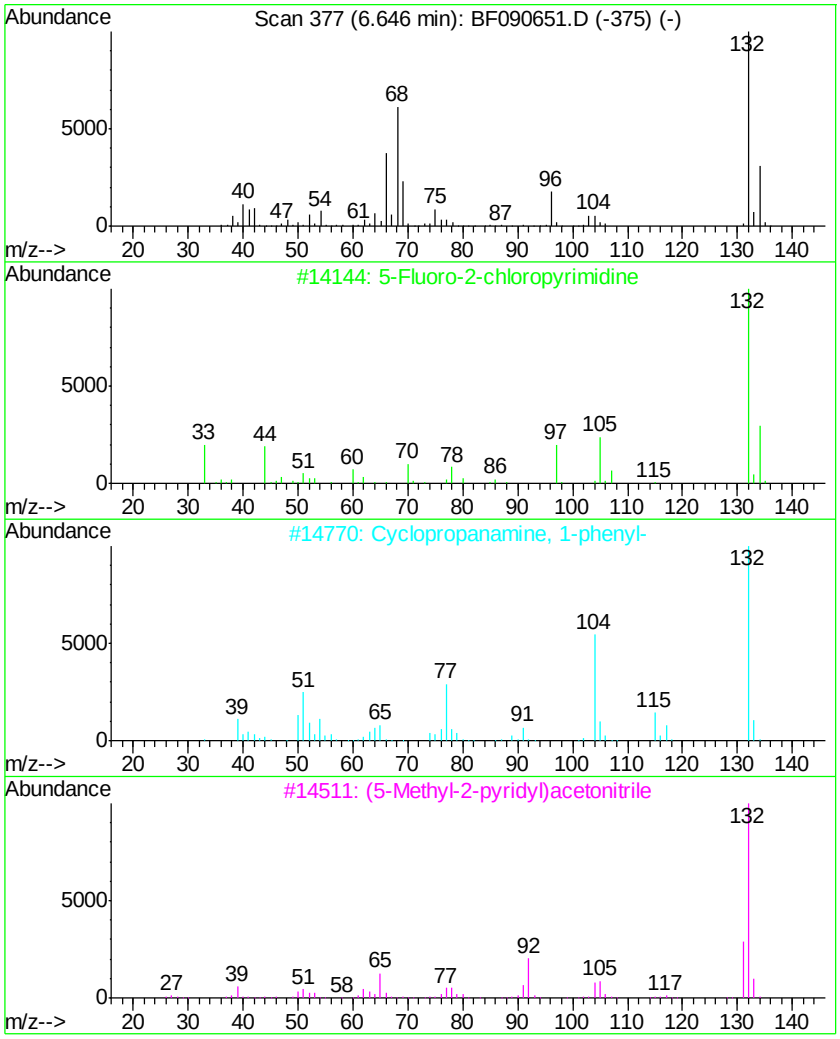
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

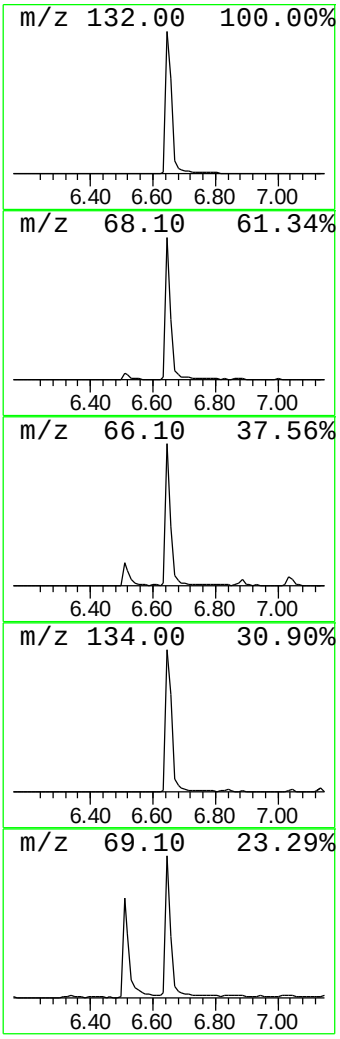
****

Peak Number 2 unknown6.65 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	14.84 ng	887724	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5	5-Aminoindole	132	C8H8N2	005192-03-0	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101916\
Data File : BF090651.D
Acq On : 19 Oct 2016 16:52
Operator : UM/SJ
Sample : H5296-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C2-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.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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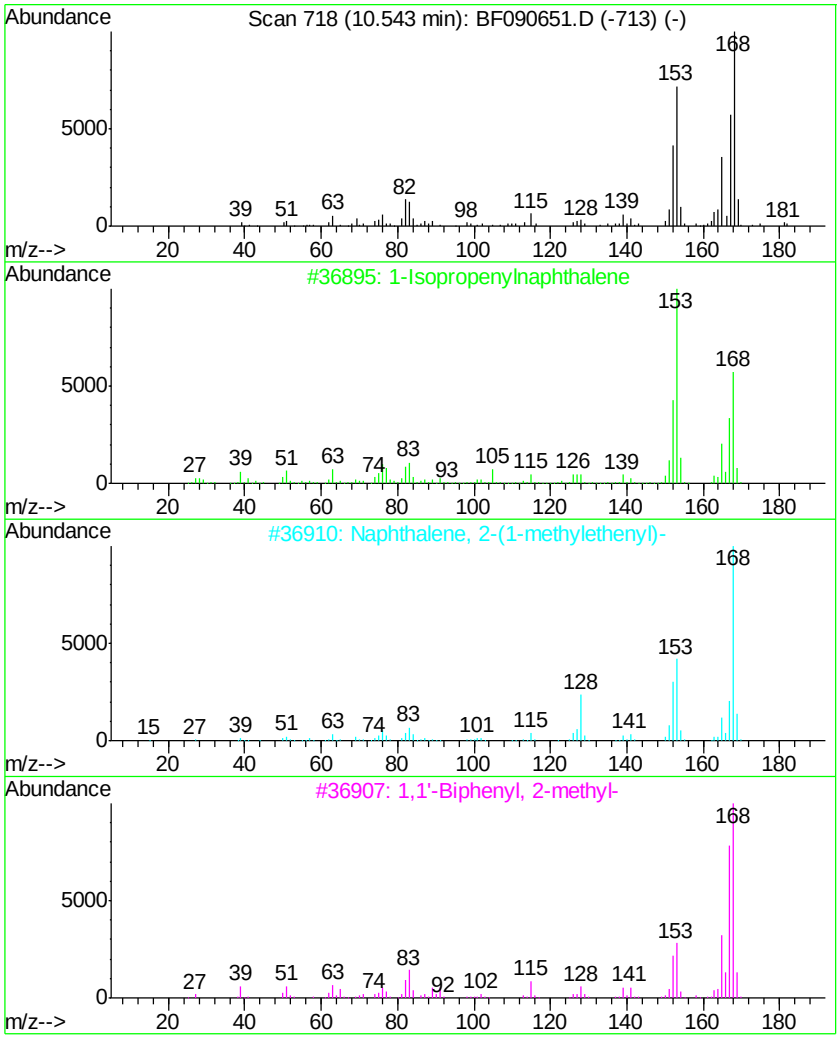
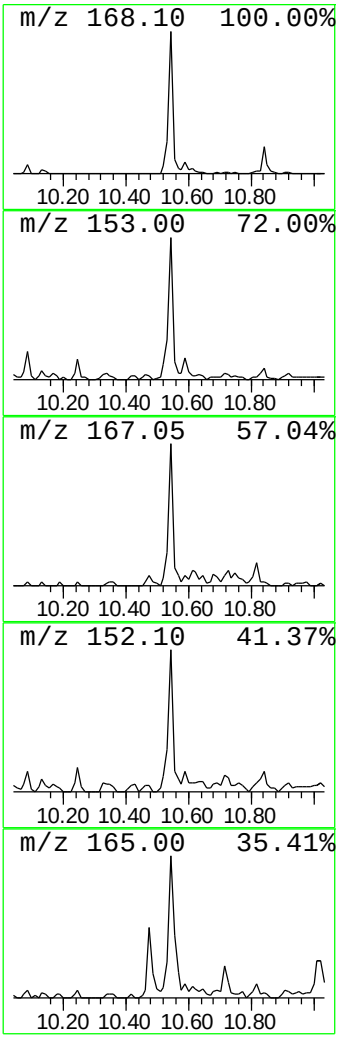
Peak Number 4 1-Isopropenylnaphthalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.54	2.19 ng	230133	Acenaphthene-d10	9.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Isopropenylnaphthalene	168	C13H12	001855-47-6	81
2	Naphthalene, 2-(1-methylethenyl)-	168	C13H12	003710-23-4	80
3	1,1'-Biphenyl, 2-methyl-	168	C13H12	000643-58-3	70
4	Fluorene, 2,4a-dihydro-	168	C13H12	059247-36-8	53
5	Benzene, [1-(2,4-cyclopentadien-...	168	C13H12	002320-32-3	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101916\
Data File : BF090651.D
Acq On : 19 Oct 2016 16:52
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Sample : H5296-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C2-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

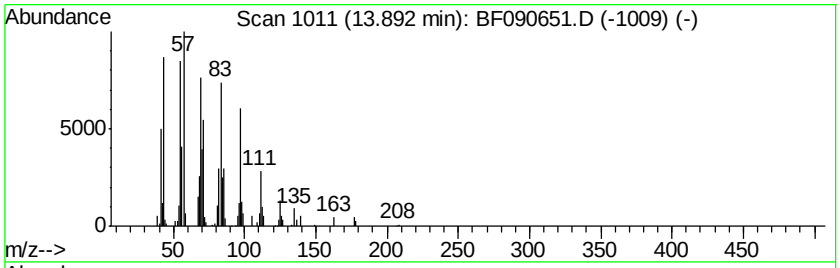
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

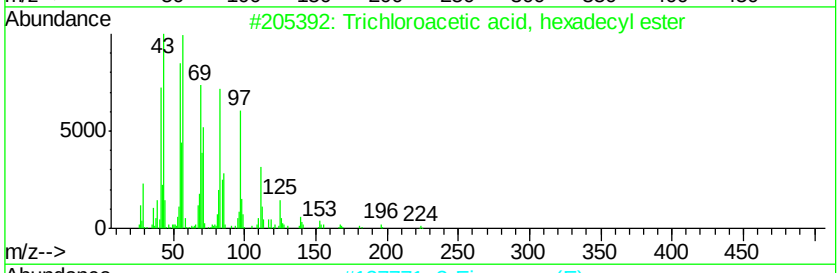
****

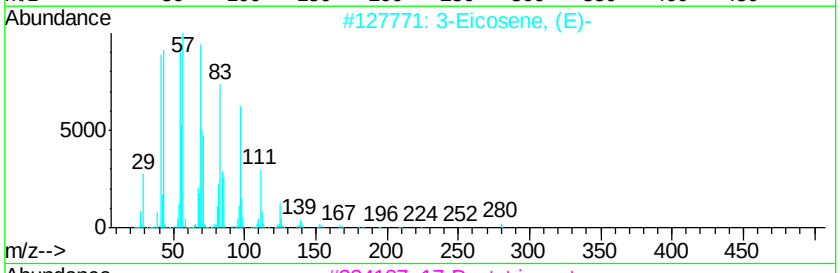
Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 5

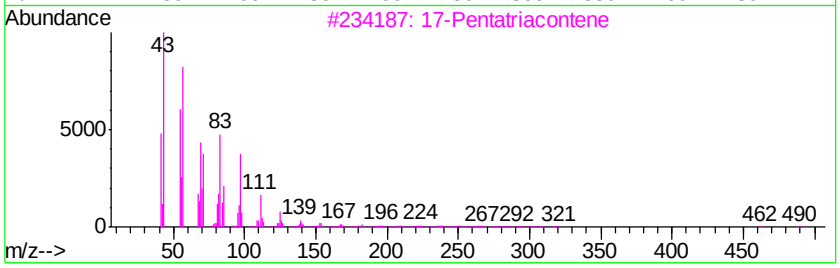
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	2.27 ng	200912	Chrysene-d12	14.05

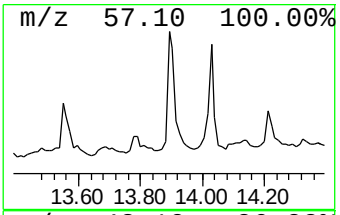
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	17-Pentatriacontene	491	C35H70	006971-40-0	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	Behenic alcohol	326	C22H46O	000661-19-8	90

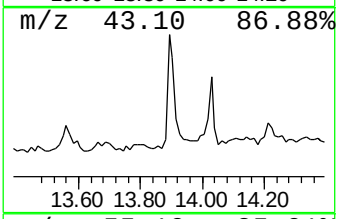


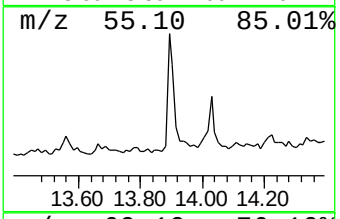


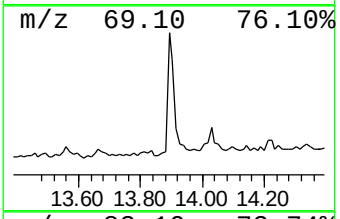


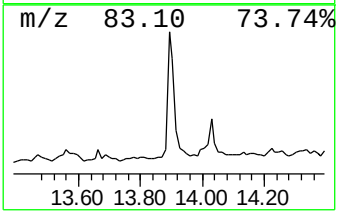












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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

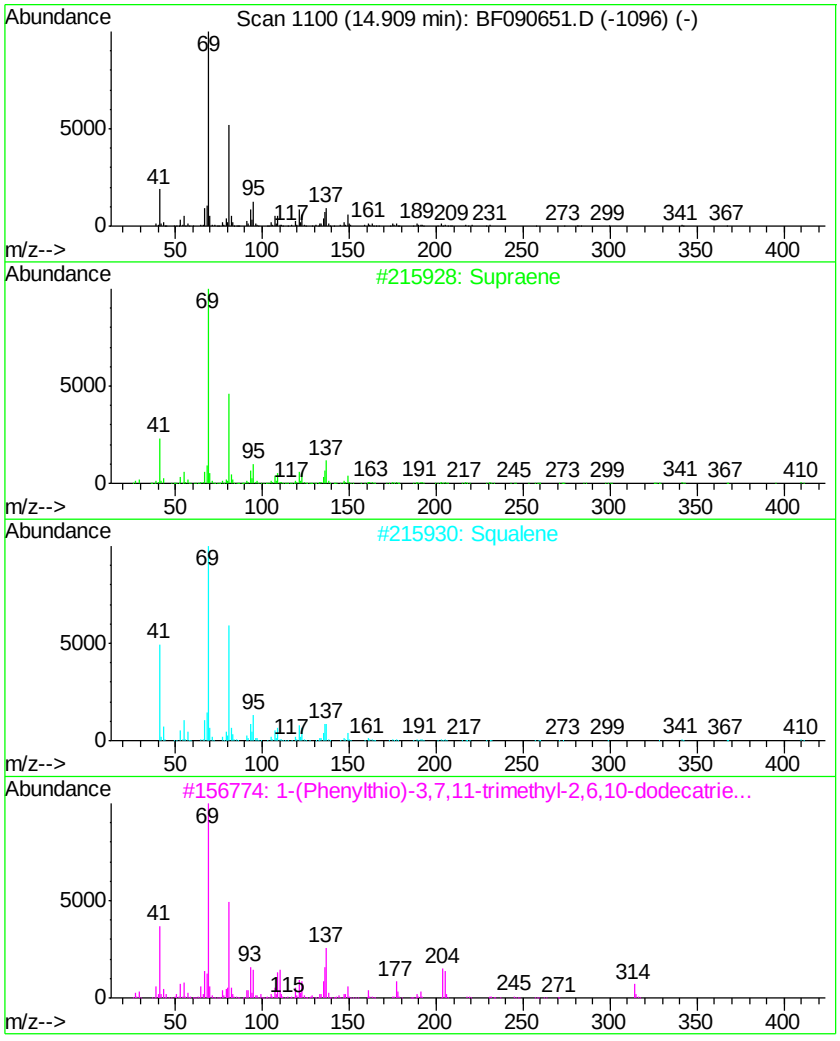
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

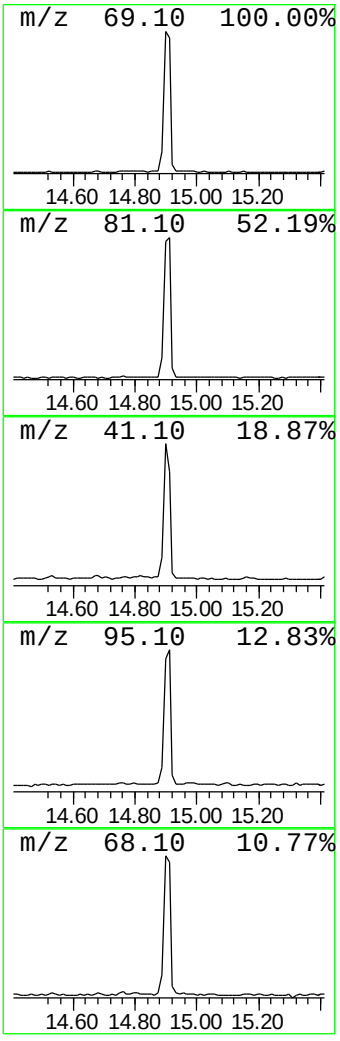
****

Peak Number 6 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	9.52 ng	896229	Perylene-d12	15.50

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-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	78
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101916\
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Acq On : 19 Oct 2016 16:52
Operator : UM/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : OWL-C2-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.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...	5.08	66.3	ng	3962600	1	6.89	1196220	20.0
unknown6.65	6.65	14.8	ng	887724	1	6.89	1196220	20.0
1-Isopropenylnaph...	10.54	2.2	ng	230133	3	9.93	2098040	20.0
Trichloroacetic a...	13.89	2.3	ng	200912	5	14.05	1773780	20.0
Supraene	14.91	9.5	ng	896229	6	15.50	1883810	20.0