LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092916\
Data File : BF090295.D
Acq On : 29 Sep 2016 17:10
Operator : UM/SJ
Sample : H4982-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-23

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	38	rVB	696770	1862079	69.07%	6.368%
2	4.547	256	259	267	rBV	293641	535937	19.88%	1.833%
3	5.027	298	301	303	rBV	2349845	2687170	99.68%	9.190%
4	6.124	394	397	399	rBV	2384168	2668645	98.99%	9.127%
5	6.227	403	406	409	rVB	2585397	2529634	93.83%	8.651%
6	6.456	424	426	429	rBV	688613	743904	27.59%	2.544%
7	6.616	437	440	443	rBV	2246498	2092386	77.61%	7.156%
8	7.039	474	477	479	rBV	1441553	1772015	65.73%	6.060%
9	7.747	537	539	542	rBV	1037724	970765	36.01%	3.320%
10	8.833	631	634	637	rBV	2835217	2695920	100.00%	9.220%
11	9.233	667	669	672	rBV	771161	693589	25.73%	2.372%
12	9.359	677	680	682	rVB	42564	47141	1.75%	0.161%
13	9.496	690	692	694	rBV	1197338	1021416	37.89%	3.493%
14	9.953	730	732	734	rVB	57633	65524	2.43%	0.224%
15	10.170	748	751	754	rBV2	24968	48430	1.80%	0.166%
16	10.285	758	761	763	rBV	1325836	1510448	56.03%	5.166%
17	10.433	772	774	778	rVB	64640	108440	4.02%	0.371%
18	10.868	810	812	814	rBV2	37697	46092	1.71%	0.158%
19	10.970	818	821	824	rBV	579196	924821	34.30%	3.163%
20	11.039	824	827	830	rVB2	45449	47958	1.78%	0.164%
21	11.222	841	843	846	rVV2	104142	113119	4.20%	0.387%
22	11.291	848	849	852	rVB	20577	29542	1.10%	0.101%
23	11.462	862	864	866	rBV3	31022	42883	1.59%	0.147%
24	11.531	868	870	872	rVV2	97162	112597	4.18%	0.385%
25	11.576	872	874	878	rVB2	45799	88692	3.29%	0.303%
26	11.782	888	892	896	rVB3	30205	59893	2.22%	0.205%
27	12.011	909	912	914	rBV	37097	48306	1.79%	0.165%
28	12.091	918	919	922	rVB2	29617	29923	1.11%	0.102%
29	12.159	923	925	928	rBV	194774	267583	9.93%	0.915%
30	12.216	928	930	932	rBV3	24004	30349	1.13%	0.104%
31	12.308	936	938	942	rBV2	41600	73786	2.74%	0.252%
32	12.388	942	945	950	rVV	309650	390779	14.50%	1.336%
33	12.456	950	951	955	rVB2	21135	30813	1.14%	0.105%
34	12.548	957	959	962	rBV	1581570	1817074	67.40%	6.214%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
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Integrator: RTE
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Sampling : 1 Min Area: 3 % of largest Peak
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.616	962	965	969	rVB3	30048	49055	1.82%	0.168%
36	12.719	970	974	976	rVB	54996	89797	3.33%	0.307%
37	12.788	976	980	981	rBV	46929	63458	2.35%	0.217%
38	12.822	981	983	987	rVB2	43596	57159	2.12%	0.195%
39	12.948	992	994	996	rVB2	20071	29564	1.10%	0.101%
40	13.108	1005	1008	1009	rBV	62136	73661	2.73%	0.252%
41	13.325	1025	1027	1029	rBV	27789	50001	1.85%	0.171%
42	13.474	1038	1040	1043	rBV2	143397	235611	8.74%	0.806%
43	13.576	1046	1049	1056	rVV2	677753	1085226	40.25%	3.711%
44	13.794	1066	1068	1073	rBV3	25220	39784	1.48%	0.136%
45	13.965	1081	1083	1085	rBV	34346	49862	1.85%	0.171%
46	14.102	1093	1095	1098	rBV3	61665	77339	2.87%	0.264%
47	14.514	1129	1131	1133	rVB2	49089	46800	1.74%	0.160%
48	14.571	1133	1136	1140	rBV	145424	306899	11.38%	1.050%
49	14.799	1155	1156	1159	rBV	69948	96108	3.56%	0.329%
50	14.857	1159	1161	1163	rBV	95631	109719	4.07%	0.375%
51	14.902	1163	1165	1170	rBV	418499	572875	21.25%	1.959%

Sum of corrected areas: 29240571

LSC Report - Integrated Chromatogram

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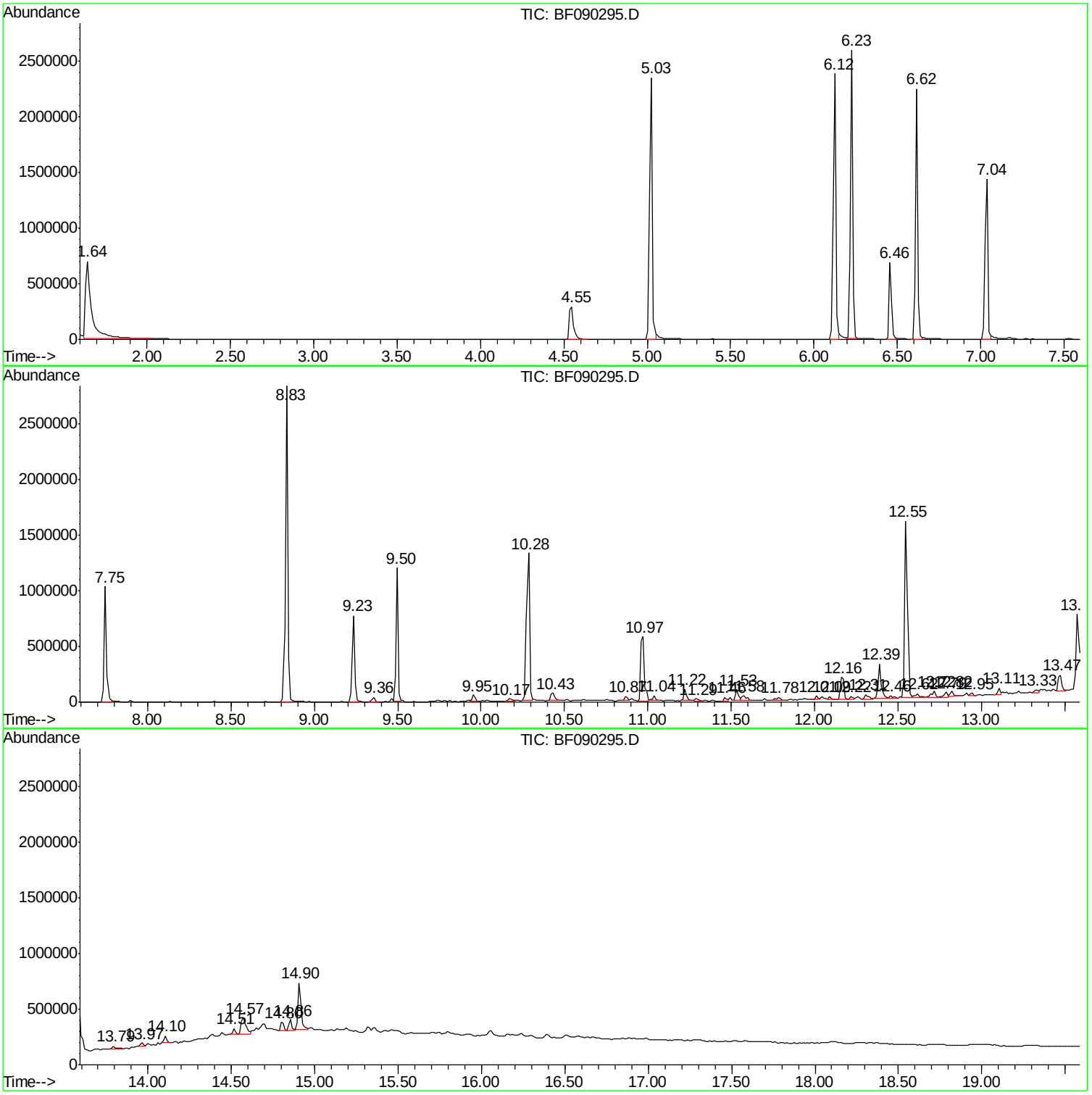
Sample : H4982-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-23

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 : BF090295.D
Acq On : 29 Sep 2016 17:10
Operator : UM/SJ
Sample : H4982-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-23

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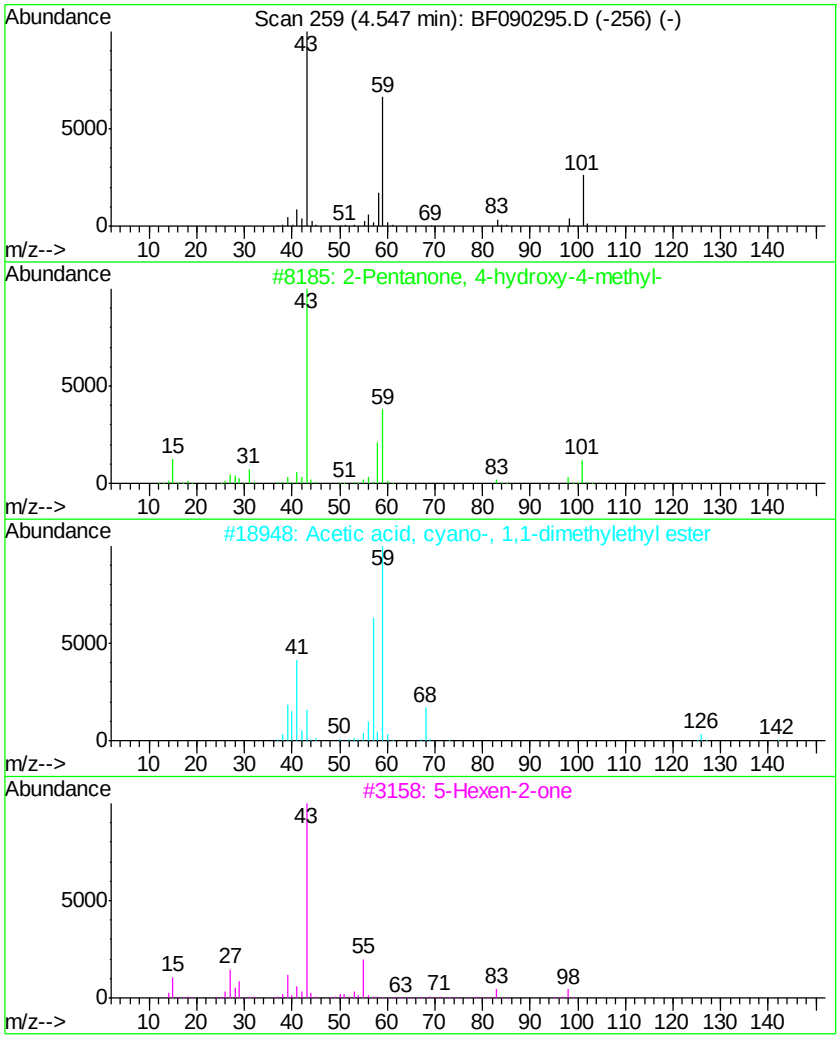
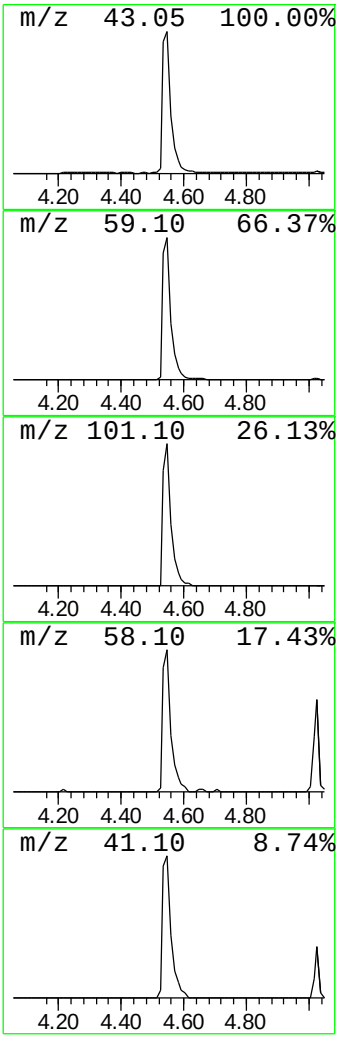
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	14.41 ng	535937	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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Acetone	58	C3H6O	000067-64-1	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092916\
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Acq On : 29 Sep 2016 17:10
Operator : UM/SJ
Sample : H4982-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-23

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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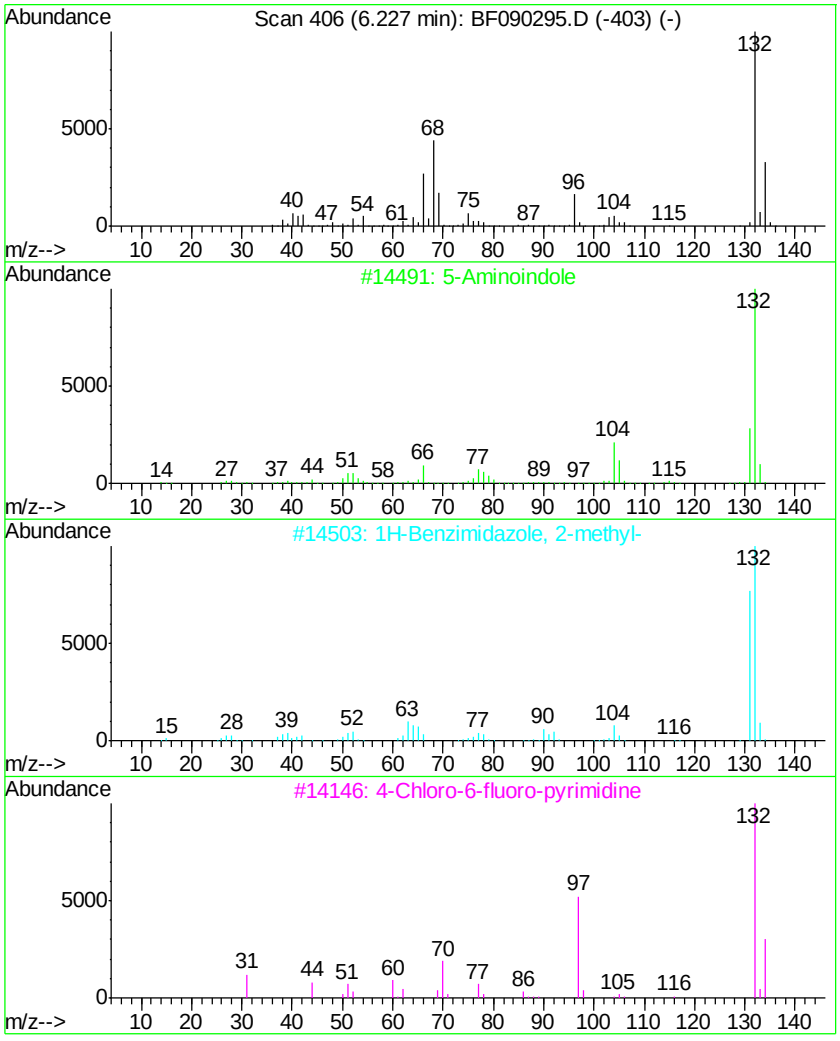
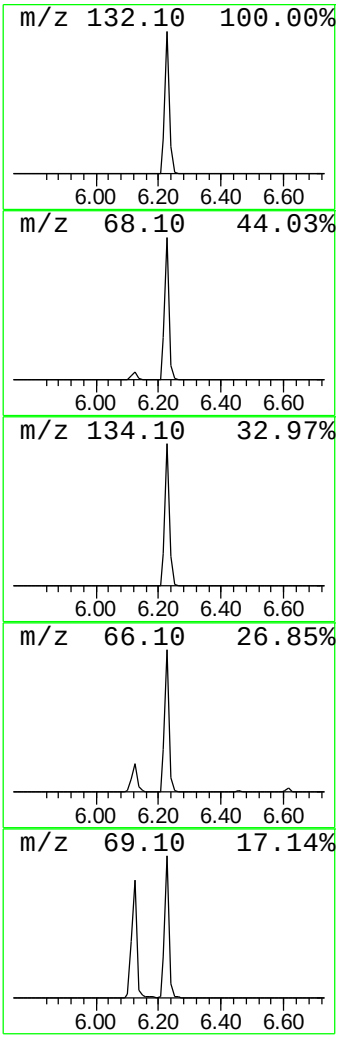
Peak Number 3 unknown6.23 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.23	68.01 ng	2529630	1,4-Dichlorobenzene-d4	6.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Sample : H4982-08
Misc :
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Instrument : BNA_F
ClientSampleId : S-23

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
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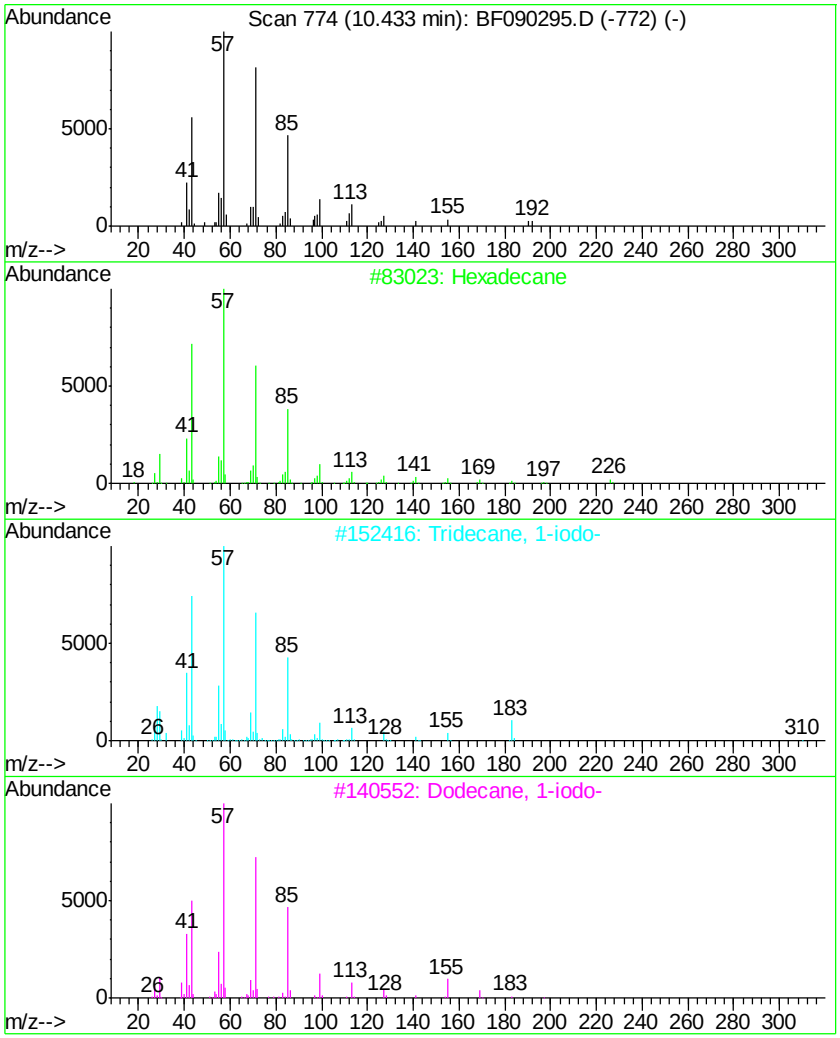
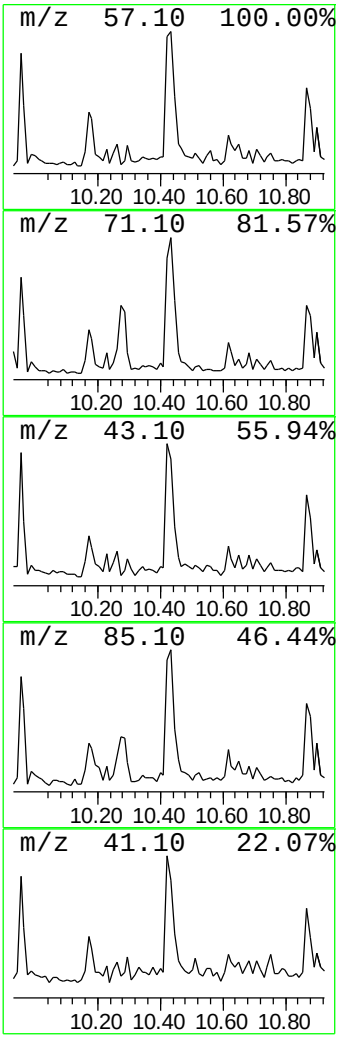
Peak Number 5 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.43	2.35 ng	108440	Phenanthrene-d10	10.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
4	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	86
5	Pentadecane	212	C15H32	000629-62-9	86





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Instrument : BNA_F
ClientSampleId : S-23

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TIC Library : C:\DATABASE\NIST11.L
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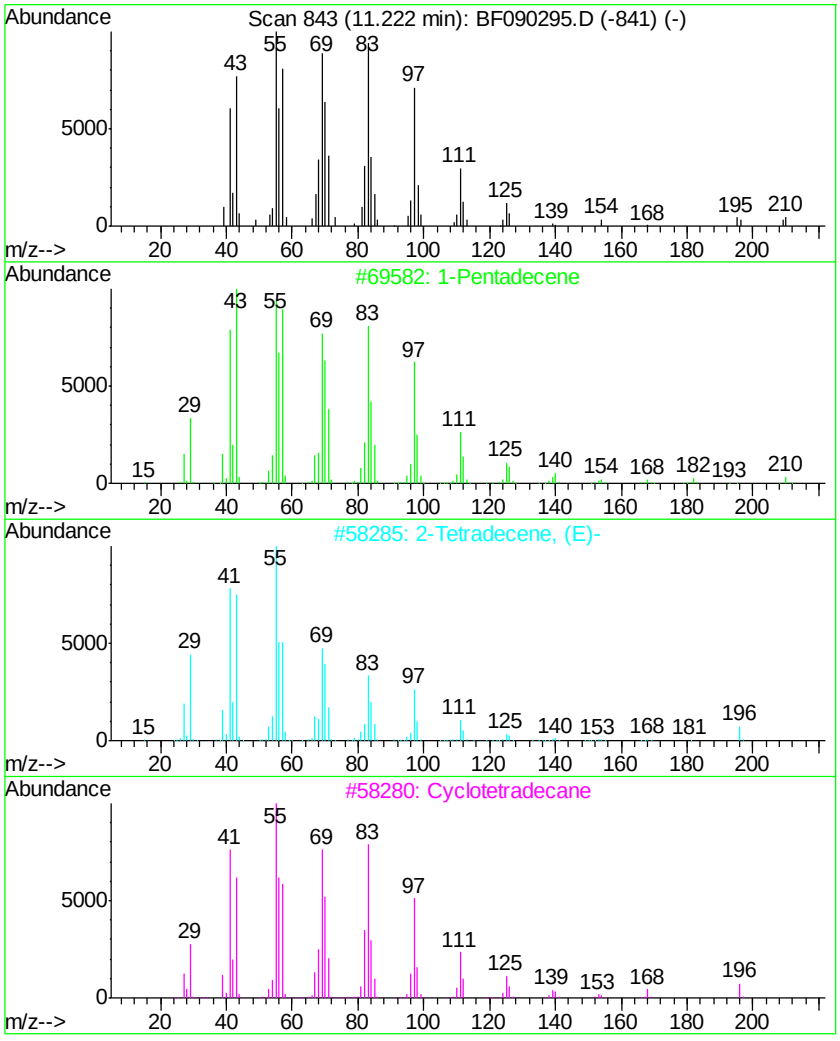
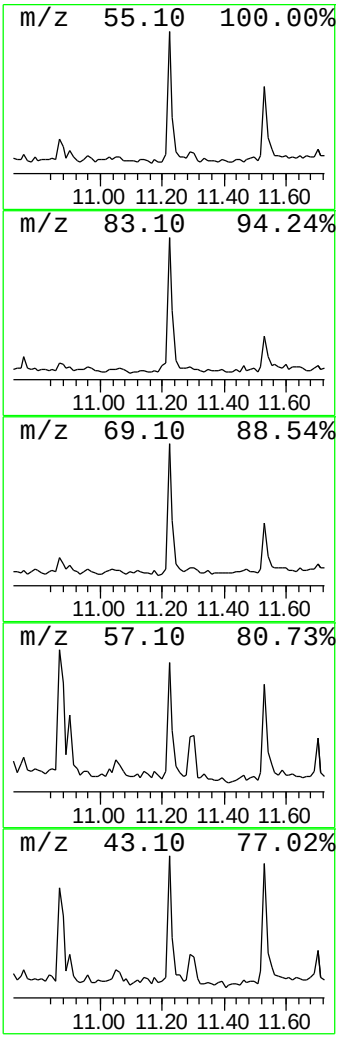
Peak Number 6 1-Pentadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.22	2.45 ng	113119	Phenanthrene-d10	10.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecene	210	C15H30	013360-61-7	99
2	2-Tetradecene, (E)-	196	C14H28	035953-54-9	97
3	Cyclotetradecane	196	C14H28	000295-17-0	94
4	1-Hexadecanol	242	C16H34O	036653-82-4	94
5	1-Tetradecene	196	C14H28	001120-36-1	91





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TIC Library : C:\DATABASE\NIST11.L
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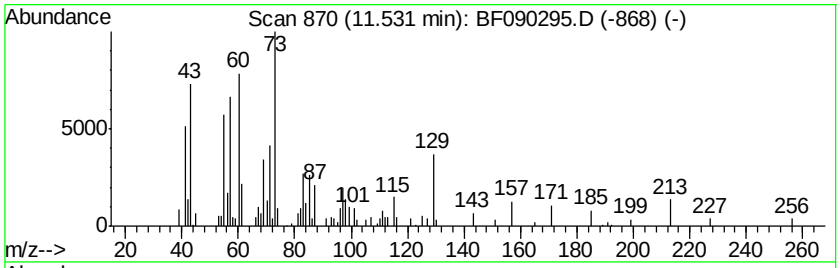
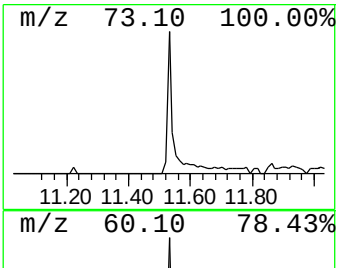
****

Peak Number 7 Pentadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.53	2.44 ng	112597	Phenanthrene-d10	10.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tetratetracontane	619	C44H90	007098-22-8	18
5	Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	18





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ClientSampleId : S-23

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

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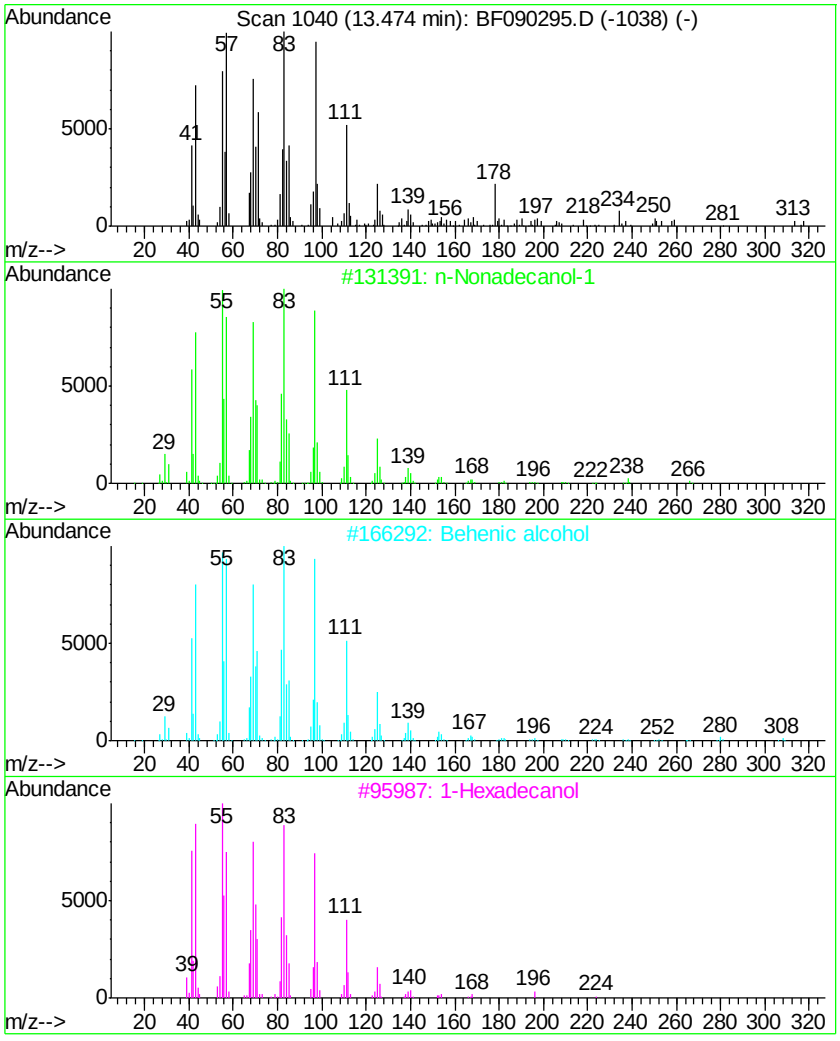
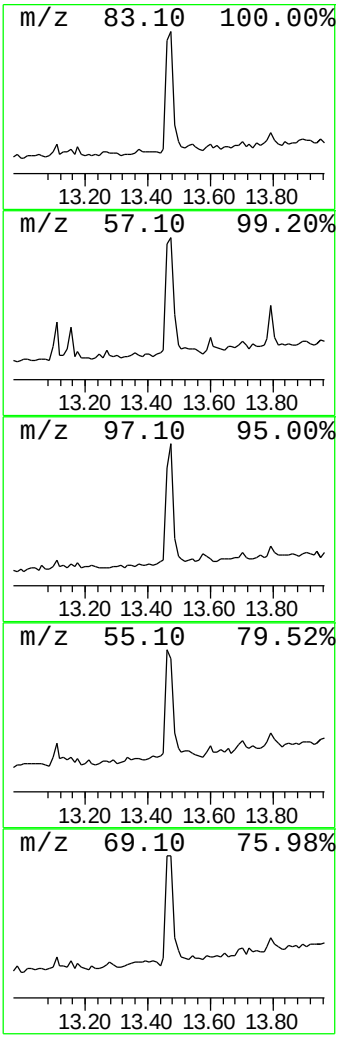
Peak Number 8 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	4.34 ng	235611	Chrysene-d12	13.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	1-Hexadecanol	242	C16H34O	036653-82-4	87
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
5	1-Heneicosanol	312	C21H44O	015594-90-8	87





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	14.4	ng	535937	1	6.46	743904	20.0
unknown6.23	6.23	68.0	ng	2529630	1	6.46	743904	20.0
Hexadecane	10.43	2.4	ng	108440	4	10.97	924821	20.0
1-Pentadecene	11.22	2.5	ng	113119	4	10.97	924821	20.0
Pentadecanoic acid	11.53	2.4	ng	112597	4	10.97	924821	20.0
n-Nonadecanol-1	13.47	4.3	ng	235611	5	13.58	1085230	20.0