LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122116\
Data File : BF091855.D
Acq On : 22 Dec 2016 1:13
Operator : UM/SJ
Sample : H6156-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-101

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-BF122116.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	3.630	132	135	139	rBV	66054	123459	1.15%	0.156%
2	4.910	245	247	252	rBV	1032235	1327730	12.36%	1.675%
3	5.344	283	285	288	rBV	3811858	4459255	41.50%	5.626%
4	6.384	374	376	379	rBV	2774480	2860765	26.62%	3.609%
5	6.510	385	387	390	rBV	5381913	8022907	74.66%	10.121%
6	6.739	405	407	410	rBV	1509268	1877905	17.47%	2.369%
7	6.807	410	413	417	rVB2	96673	163711	1.52%	0.207%
8	6.899	418	421	424	rVV	5484358	7221774	67.20%	9.111%
9	7.310	454	457	460	rBV	4318639	6763024	62.93%	8.532%
10	7.402	462	465	466	rVB	147764	180077	1.68%	0.227%
11	7.447	466	469	473	rVB	141027	210742	1.96%	0.266%
12	7.710	486	492	495	rVB2	61988	125090	1.16%	0.158%
13	7.779	495	498	500	rBV2	156740	293322	2.73%	0.370%
14	7.813	500	501	504	rVB	229456	393082	3.66%	0.496%
15	8.030	517	520	524	rBV	2796204	2952735	27.48%	3.725%
16	8.533	556	564	567	rBV3	94415	259740	2.42%	0.328%
17	8.842	588	591	593	rBV2	165006	193034	1.80%	0.244%
18	9.116	611	615	617	rVV	7821431	10746476	100.00%	13.557%
19	9.208	617	623	628	rVV8	49950	157459	1.47%	0.199%
20	9.310	628	632	634	rVB3	115388	167874	1.56%	0.212%
21	9.368	634	637	641	rBV5	45900	119536	1.11%	0.151%
22	9.448	641	644	646	rVV3	61800	113944	1.06%	0.144%
23	9.505	647	649	651	rVV	314084	302056	2.81%	0.381%
24	9.562	651	654	658	rVV	104872	223578	2.08%	0.282%
25	9.642	658	661	663	rVB	193095	215124	2.00%	0.271%
26	9.779	670	673	675	rBV	2582964	3106948	28.91%	3.920%
27	9.813	675	676	678	rVB	1995404	1507902	14.03%	1.902%
28	10.225	707	712	715	rBV6	102388	224695	2.09%	0.283%
29	10.293	715	718	720	rBV2	129930	241849	2.25%	0.305%
30	10.373	724	725	726	rBV	96613	119930	1.12%	0.151%
31	10.419	726	729	730	rVV2	162904	261808	2.44%	0.330%
32	10.465	730	733	734	rVB2	110749	193900	1.80%	0.245%
33	10.579	738	743	745	rBV	3904123	6181201	57.52%	7.798%
34	10.693	752	753	757	rVB	324628	317610	2.96%	0.401%

LSC Area Percent Report

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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
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.139	788	792	797	rBV4	129902	313497	2.92%	0.395%
36	11.265	800	803	805	rVV	2856486	2856707	26.58%	3.604%
37	11.299	805	806	810	rVV4	52983	108169	1.01%	0.136%
38	11.562	827	829	833	rVB4	50831	109369	1.02%	0.138%
39	11.654	833	837	838	rBV2	68710	121863	1.13%	0.154%
40	11.699	838	841	844	rVB3	57647	109183	1.02%	0.138%
41	11.756	844	846	848	rBV2	87297	157012	1.46%	0.198%
42	11.802	848	850	852	rVB3	104256	143875	1.34%	0.182%
43	11.836	852	853	855	rBV	73038	107577	1.00%	0.136%
44	11.871	855	856	859	rVB	237625	251588	2.34%	0.317%
45	11.939	859	862	865	rBV	86944	182976	1.70%	0.231%
46	12.019	865	869	872	rBV5	38664	112301	1.05%	0.142%
47	12.694	925	928	930	rBV	221347	252161	2.35%	0.318%
48	12.854	939	942	944	rBV	7173426	7984660	74.30%	10.073%
49	13.002	953	955	958	rVB	197195	186390	1.73%	0.235%
50	13.768	1019	1022	1026	rBV	138395	235691	2.19%	0.297%
51	13.894	1030	1033	1036	rBV	2593820	2446640	22.77%	3.087%
52	15.288	1152	1155	1158	rBV	1575589	1956379	18.20%	2.468%

Sum of corrected areas: 79266280

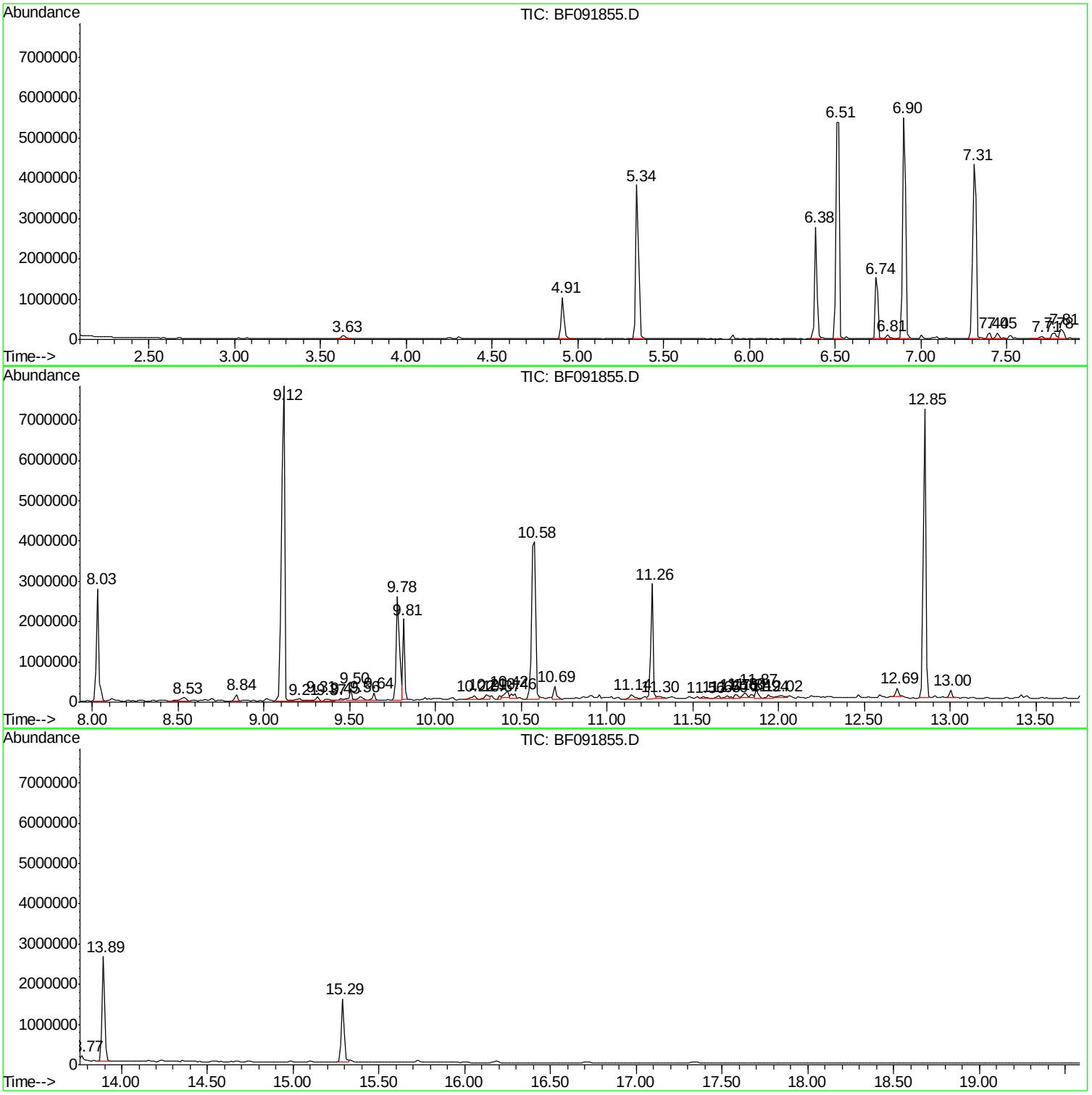
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122116\
Data File : BF091855.D
Acq On : 22 Dec 2016 1:13
Operator : UM/SJ
Sample : H6156-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-101

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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\BF122116\
Data File : BF091855.D
Acq On : 22 Dec 2016 1:13
Operator : UM/SJ
Sample : H6156-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-101

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

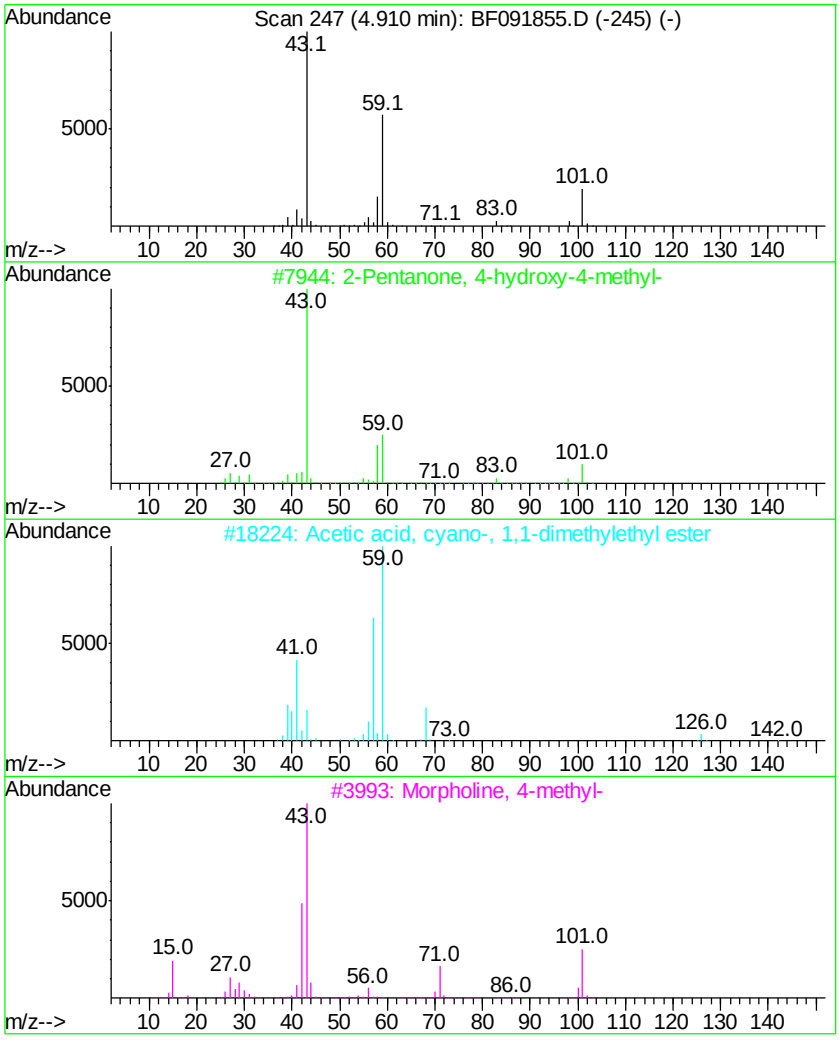
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

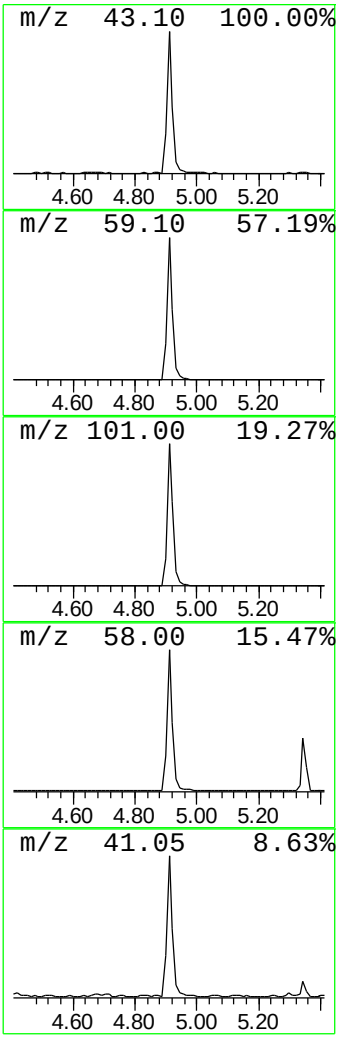
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	14.14 ng	1327730	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122116\
Data File : BF091855.D
Acq On : 22 Dec 2016 1:13
Operator : UM/SJ
Sample : H6156-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-101

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

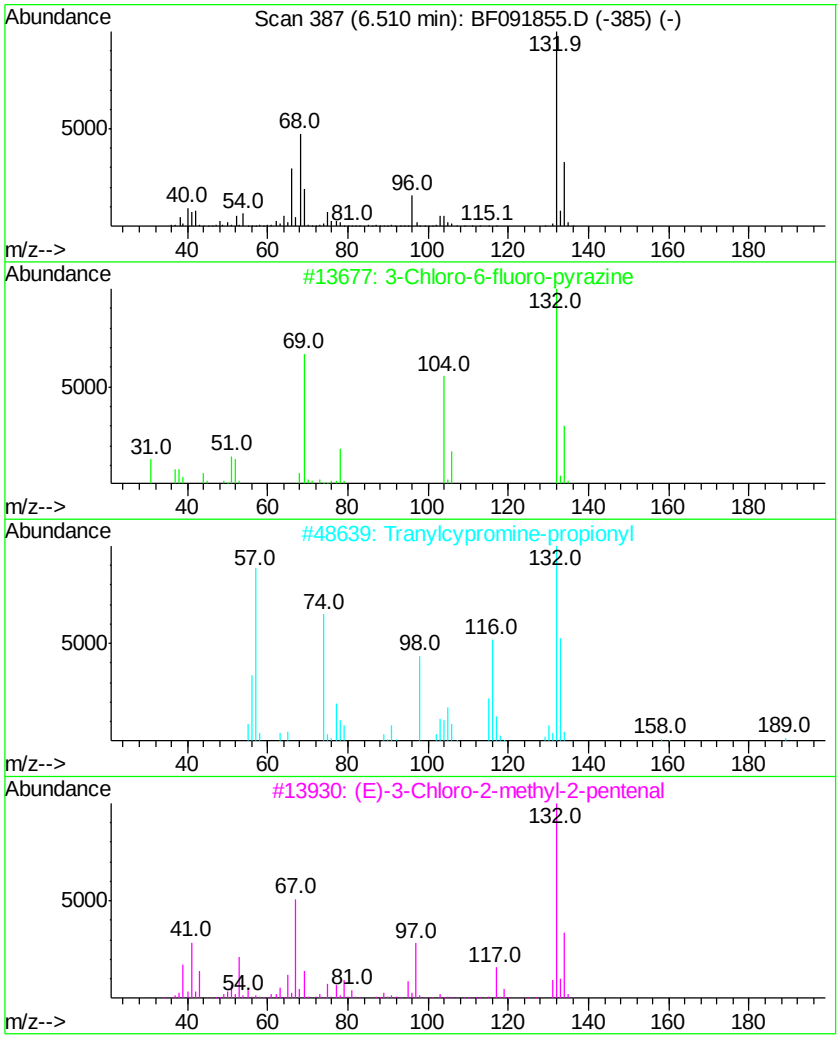
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

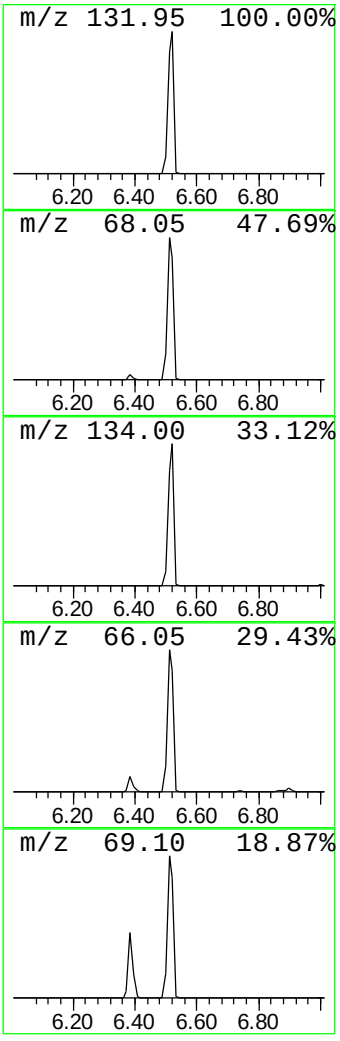
****

Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	85.45 ng	8022910	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122116\
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Sample : H6156-01
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ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-101

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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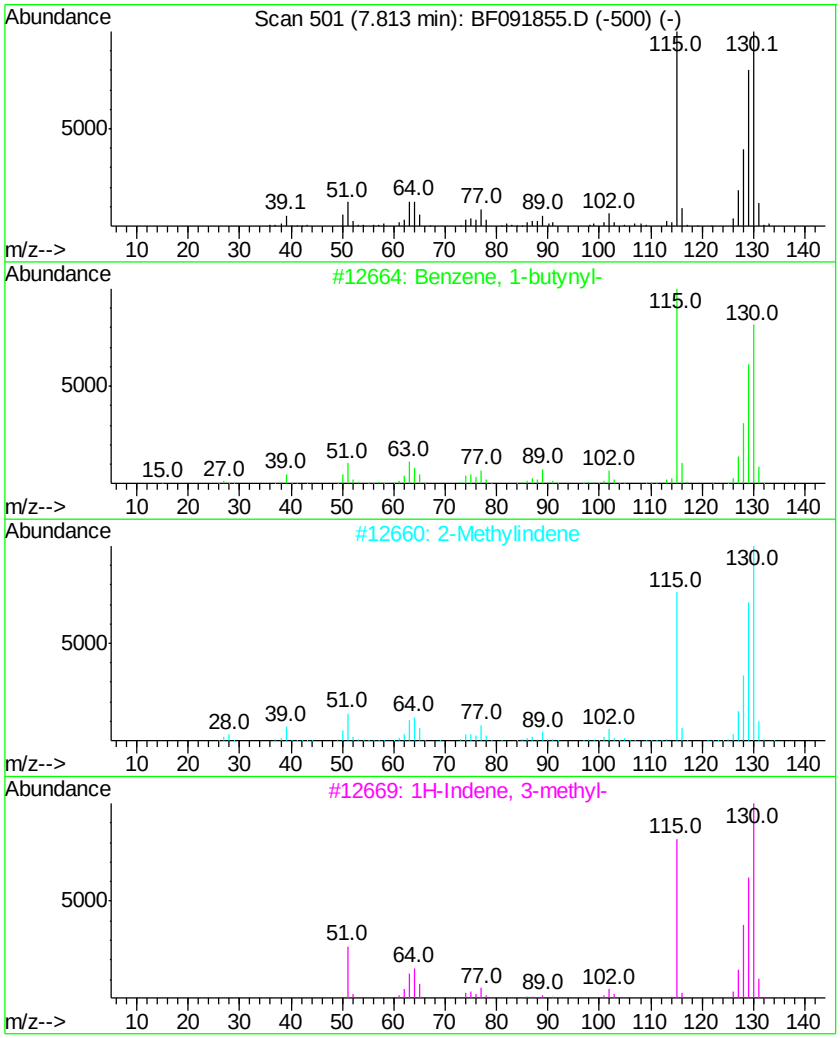
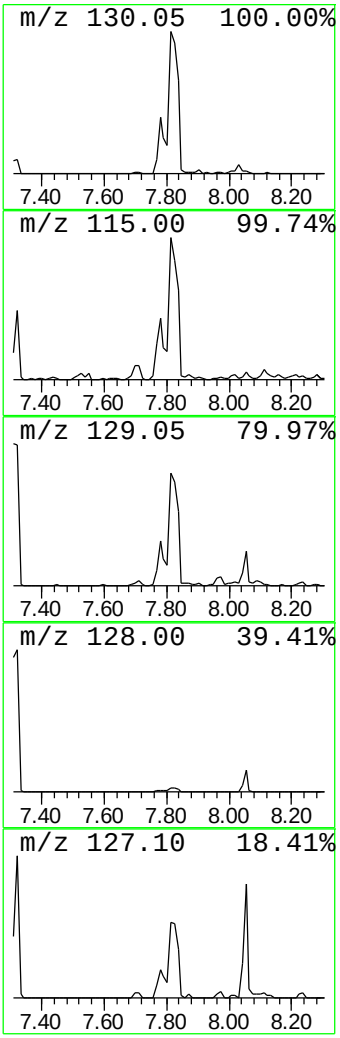
Peak Number 4 Benzene, 1-butynyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.81	2.66 ng	393082	Naphthalene-d8	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-butynyl-	130	C10H10	000622-76-4	96
2	2-Methylindene	130	C10H10	002177-47-1	96
3	1H-Indene, 3-methyl-	130	C10H10	000767-60-2	91
4	Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	91
5	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122116\
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Acq On : 22 Dec 2016 1:13
Operator : UM/SJ
Sample : H6156-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-101

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
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TIC Library : C:\DATABASE\NIST02.L
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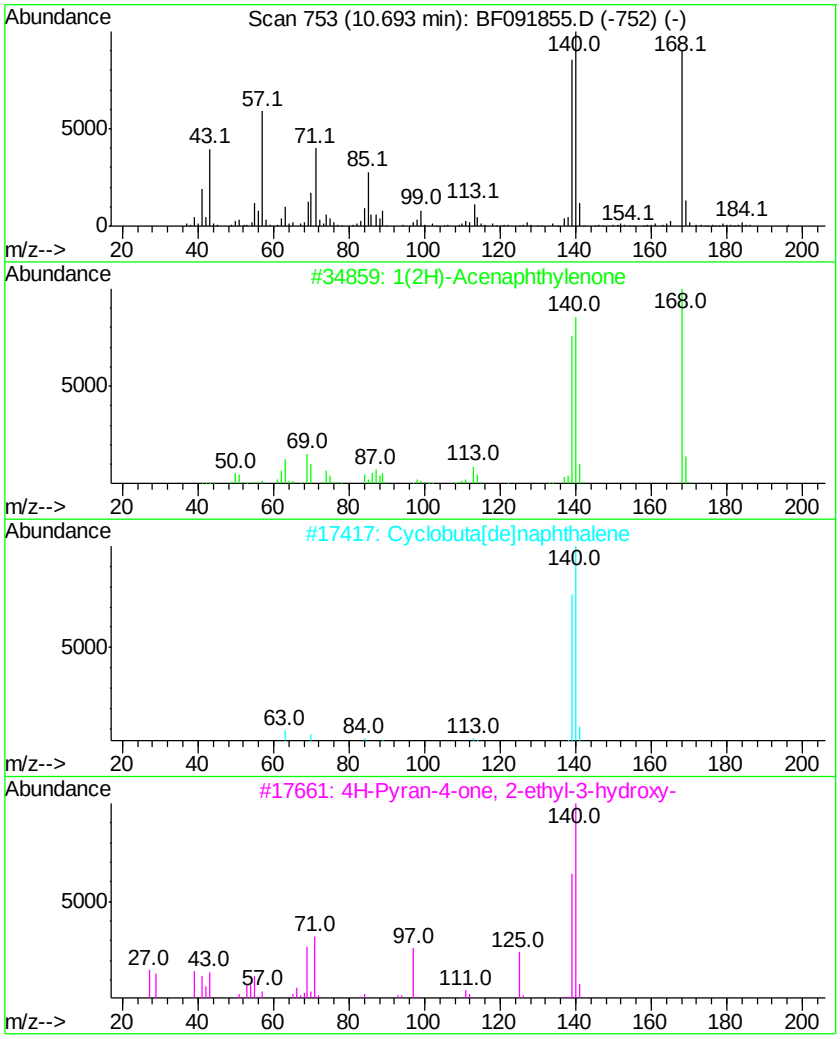
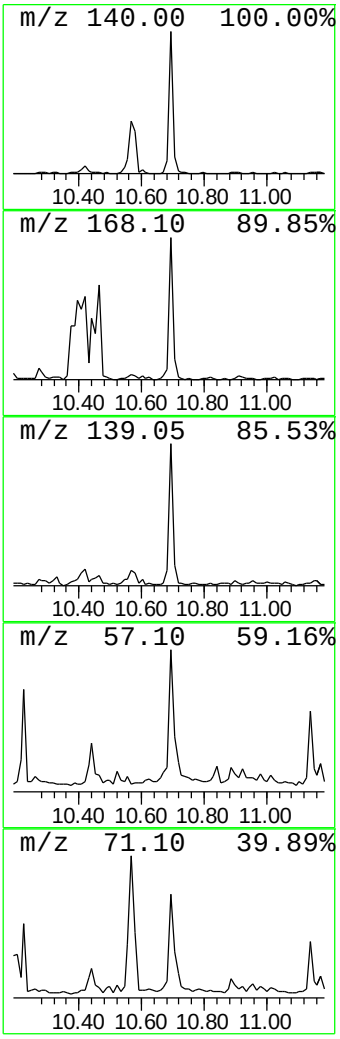
****

Peak Number 5 1(2H)-Acenaphthylenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.69	2.22 ng	317610	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(2H)-Acenaphthylenone	168	C12H8O	002235-15-6	96
2	Cyclobuta[de]naphthalene	140	C11H8	024973-91-9	49
3	4H-Pyran-4-one, 2-ethyl-3-hydroxy-	140	C7H8O3	004940-11-8	47
4	7(4H)-Benzothiazolone, 2-amino-5...	168	C7H8N2OS	017583-10-7	46
5	1H-Inden-1-one, 4,7-difluoro-2,3...	168	C9H6F2O	130408-16-1	43





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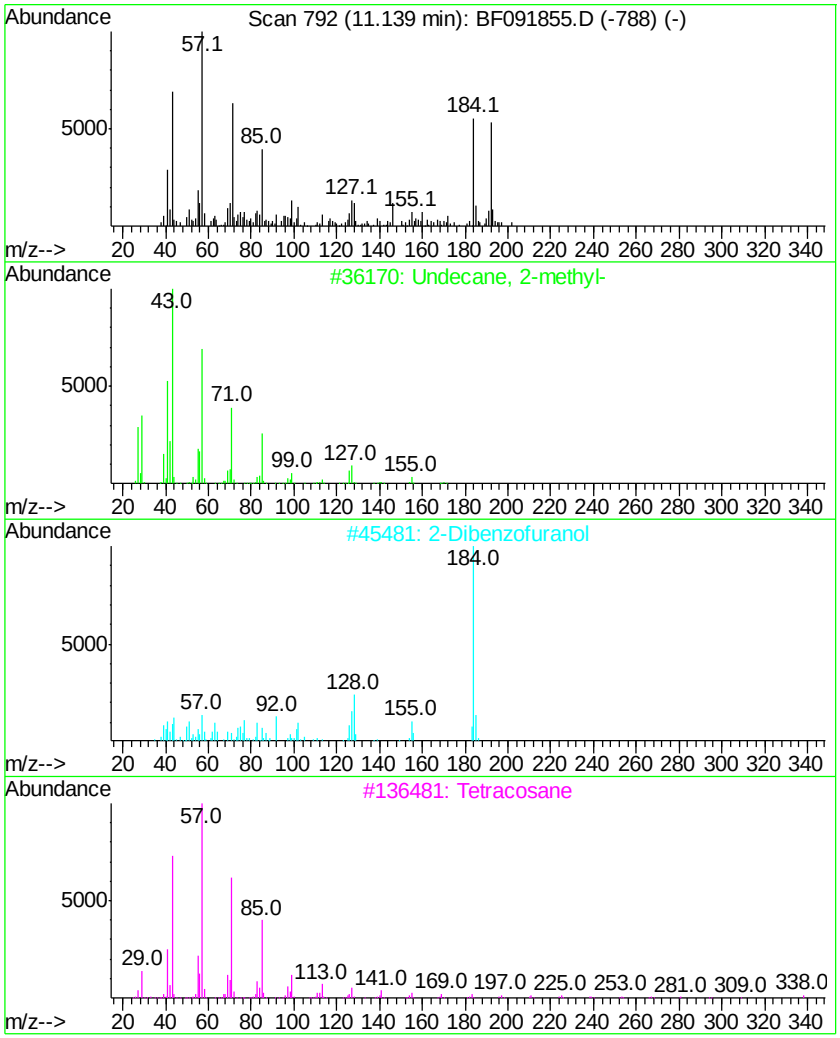
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

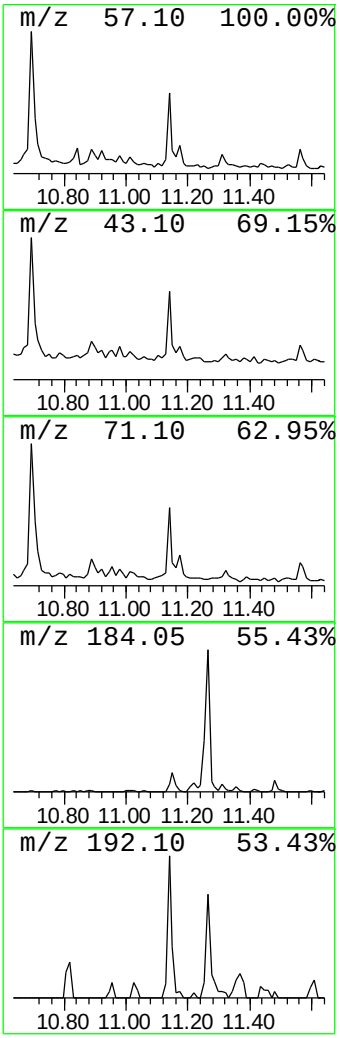
****

Peak Number 6 unknown11.14 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.14	2.19 ng	313497	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2-methyl-	170	C12H26	007045-71-8	42
2	2-Dibenzofuranol	184	C12H8O2	000086-77-1	38
3	Tetracosane	338	C24H50	000646-31-1	38
4	Eicosane	282	C20H42	000112-95-8	30
5	Octacosane	394	C28H58	000630-02-4	30





Tentatively Identified Compound (LSC) summary

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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...	4.91	14.1	ng	1327730	1	6.74	1877910	20.0
unknown6.51	6.51	85.5	ng	8022910	1	6.74	1877910	20.0
Benzene, 1-butynyl-	7.81	2.7	ng	393082	2	8.03	2952740	20.0
1(2H)-Acenaphthyl...	10.69	2.2	ng	317610	4	11.26	2856710	20.0
unknown11.14	11.14	2.2	ng	313497	4	11.26	2856710	20.0