LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\Data\BF042017\
Data File : BF094554.D
Acq On : 20 Apr 2017 19:38
Operator : SJ/MA
Sample : I2744-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(0-2)20170418

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-BF041717.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	3.472	255	261	265	rBV	51171	54867	1.97%	0.188%
2	3.907	331	335	347	rBV	331021	351742	12.64%	1.207%
3	4.313	400	404	418	rBV	2099822	2064717	74.20%	7.082%
4	5.389	582	587	604	rBV	1983251	2187378	78.61%	7.503%
5	5.513	604	608	611	rBV	2473113	2221138	79.82%	7.619%
6	5.760	647	650	654	rBV	758240	650362	23.37%	2.231%
7	5.936	676	680	684	rBV	1824518	1753261	63.01%	6.014%
8	6.407	755	760	764	rBV	1401247	1375168	49.42%	4.717%
9	7.254	900	904	908	rBV	1021161	897786	32.26%	3.080%
10	8.577	1125	1129	1133	rBV	2864648	2705831	97.24%	9.282%
11	9.077	1210	1214	1218	rBV	628528	558930	20.09%	1.917%
12	9.389	1260	1267	1271	rBV2	1029388	983269	35.34%	3.373%
13	9.989	1365	1369	1373	rVB	49167	41638	1.50%	0.143%
14	10.366	1428	1433	1436	rBV	1388801	1499239	53.88%	5.143%
15	10.571	1464	1468	1476	rBV	63579	86888	3.12%	0.298%
16	11.124	1558	1562	1565	rBV	42905	39549	1.42%	0.136%
17	11.207	1572	1576	1579	rBV	1023422	1024207	36.81%	3.513%
18	11.236	1579	1581	1585	rVV	384497	323973	11.64%	1.111%
19	11.301	1589	1592	1595	rVB	73505	70880	2.55%	0.243%
20	11.507	1625	1627	1631	rBV	29111	29950	1.08%	0.103%
21	11.830	1677	1682	1685	rBV	61439	61715	2.22%	0.212%
22	11.866	1685	1688	1693	rVB	82524	82357	2.96%	0.283%
23	11.960	1699	1704	1707	rVV2	109207	170596	6.13%	0.585%
24	11.989	1707	1709	1716	rVB	46805	54934	1.97%	0.188%
25	12.201	1742	1745	1747	rBV	43992	40781	1.47%	0.140%
26	12.254	1752	1754	1758	rVB2	42855	35285	1.27%	0.121%
27	12.513	1794	1798	1801	rBV	52845	64083	2.30%	0.220%
28	12.607	1812	1814	1824	rVB6	34588	61259	2.20%	0.210%
29	12.695	1825	1829	1833	rBV	670318	685566	24.64%	2.352%
30	12.877	1855	1860	1863	rBV	35087	37912	1.36%	0.130%
31	12.971	1869	1876	1880	rBV	720430	778490	27.98%	2.670%
32	13.130	1900	1903	1906	rBV	29222	30006	1.08%	0.103%
33	13.189	1906	1913	1917	rBV	2494410	2782573	100.00%	9.545%
34	13.260	1919	1925	1929	rBV2	45068	73139	2.63%	0.251%

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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

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.365	1936	1943	1944	rBV3	42973	65845	2.37%	0.226%
36	13.389	1944	1947	1951	rVB	87328	94233	3.39%	0.323%
37	13.471	1957	1961	1965	rBV	46871	47893	1.72%	0.164%
38	13.512	1965	1968	1971	rBV2	82968	93656	3.37%	0.321%
39	13.624	1983	1987	1990	rVB	48897	48157	1.73%	0.165%
40	13.660	1990	1993	1997	rBV2	40332	45440	1.63%	0.156%
41	14.012	2050	2053	2060	rVB	47940	56499	2.03%	0.194%
42	14.142	2069	2075	2078	rBV2	60070	67804	2.44%	0.233%
43	14.177	2078	2081	2083	rVV	48880	53418	1.92%	0.183%
44	14.201	2083	2085	2088	rVV	41786	43483	1.56%	0.149%
45	14.230	2088	2090	2094	rVB2	26372	28882	1.04%	0.099%
46	14.271	2094	2097	2102	rVB	52172	56208	2.02%	0.193%
47	14.354	2103	2111	2119	rBV4	68406	135711	4.88%	0.466%
48	14.454	2119	2128	2131	rBV2	932276	1344456	48.32%	4.612%
49	14.483	2131	2133	2137	rVV	294401	306954	11.03%	1.053%
50	14.512	2137	2138	2142	rVB3	34910	33150	1.19%	0.114%
51	14.577	2145	2149	2153	rVB	52159	60179	2.16%	0.206%
52	14.630	2153	2158	2161	rBV6	17307	29195	1.05%	0.100%
53	14.754	2175	2179	2182	rBV4	28225	48058	1.73%	0.165%
54	14.936	2205	2210	2214	rBV	57790	67866	2.44%	0.233%
55	14.977	2214	2217	2222	rVB	31373	39883	1.43%	0.137%
56	15.048	2226	2229	2232	rVV2	29787	30744	1.10%	0.105%
57	15.089	2232	2236	2238	rVV3	23355	31888	1.15%	0.109%
58	15.142	2241	2245	2250	rVV7	22171	38991	1.40%	0.134%
59	15.189	2250	2253	2260	rVB2	21763	28534	1.03%	0.098%
60	15.312	2271	2274	2278	rBV6	19984	27957	1.00%	0.096%
61	15.501	2303	2306	2308	rBV3	25427	31155	1.12%	0.107%
62	15.571	2314	2318	2324	rBV	185161	205391	7.38%	0.705%
63	15.677	2332	2336	2339	rBV	248065	341064	12.26%	1.170%
64	15.783	2351	2354	2359	rVB	50793	62455	2.24%	0.214%
65	15.965	2381	2385	2389	rBV	165207	157724	5.67%	0.541%
66	16.018	2391	2394	2398	rVB	223379	232699	8.36%	0.798%
67	16.083	2400	2405	2408	rBV	616263	744033	26.74%	2.552%
68	16.106	2408	2409	2412	rVB	61712	33975	1.22%	0.117%
69	16.577	2485	2489	2494	rVB4	39107	53962	1.94%	0.185%
70	17.348	2614	2620	2629	rVB2	105291	195122	7.01%	0.669%
71	17.506	2641	2647	2651	rBV2	41477	79582	2.86%	0.273%

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Integration Parameters: rteint.p
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	17.547	2651	2654	2658	rVB2	20700	32464	1.17%	0.111%
73	17.718	2677	2683	2688	rBV	83442	146065	5.25%	0.501%
74	17.918	2713	2717	2722	rVB2	19779	32599	1.17%	0.112%

Sum of corrected areas: 29152843

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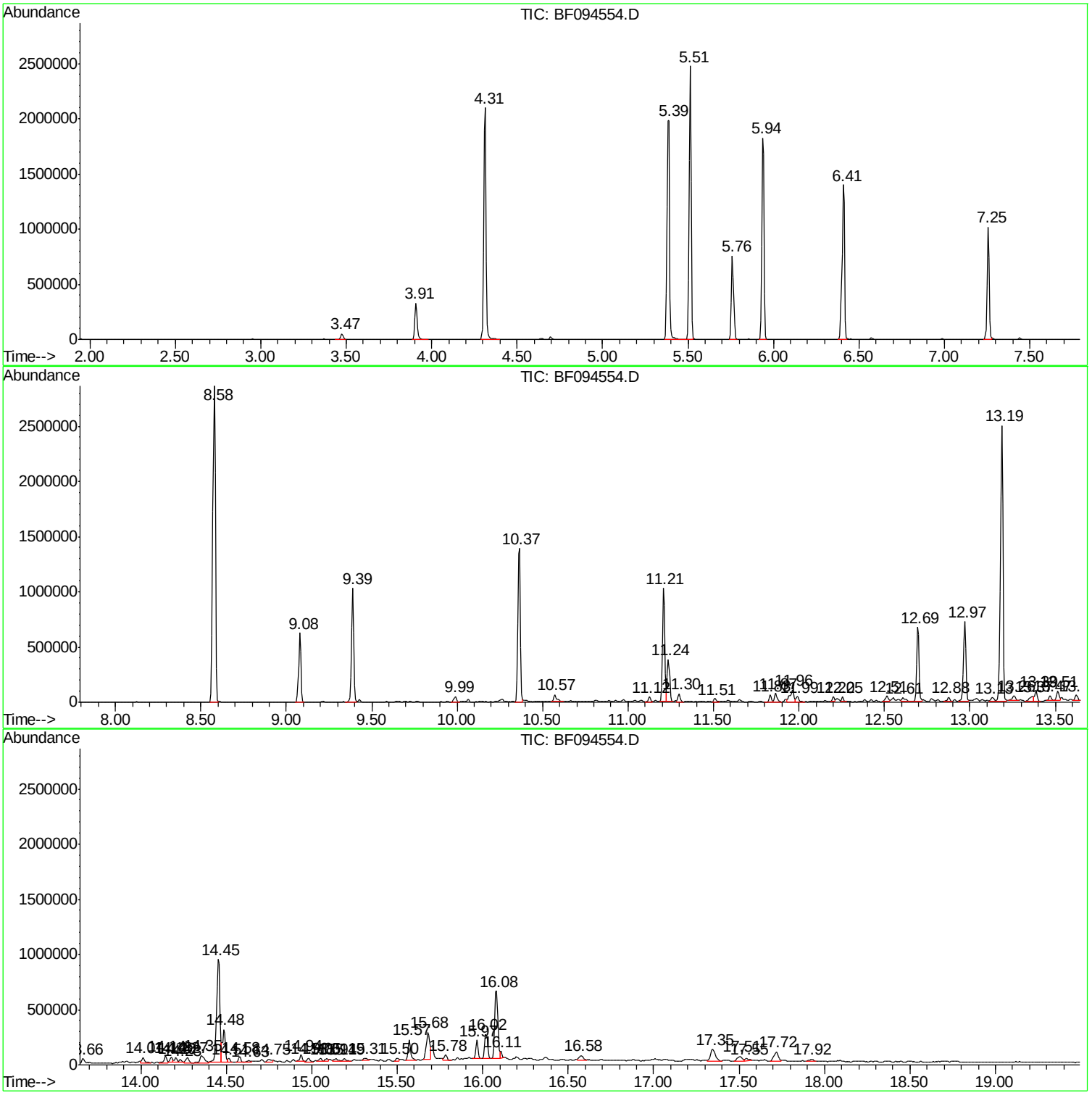
SB-3(0-2)20170418

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
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TIC Library : C:\DATABASE\NIST11.L
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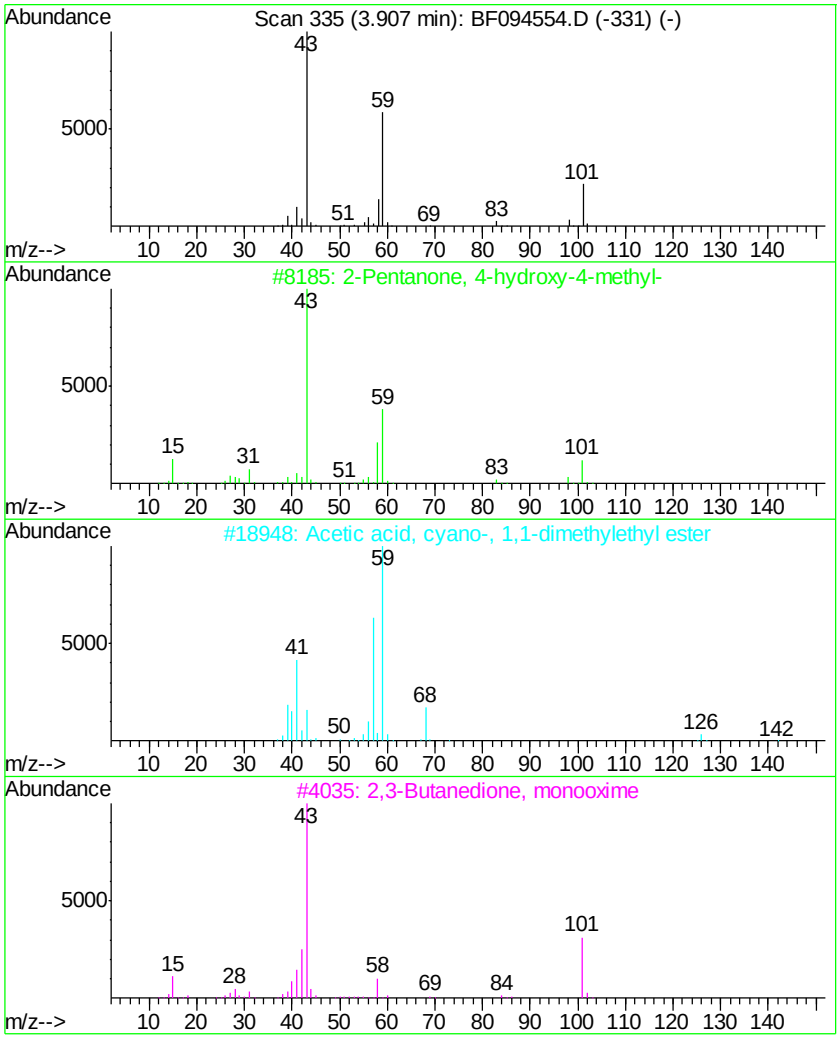
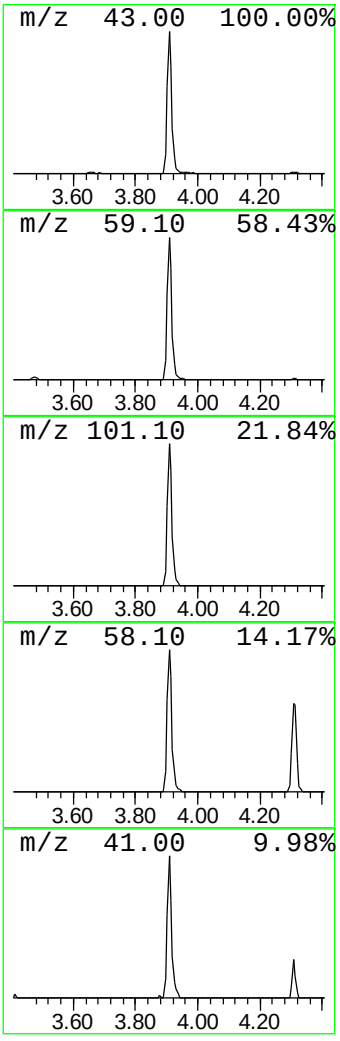
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.91	10.82 ng	351742	1,4-Dichlorobenzene-d4	5.76

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	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
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TIC Library : C:\DATABASE\NIST11.L
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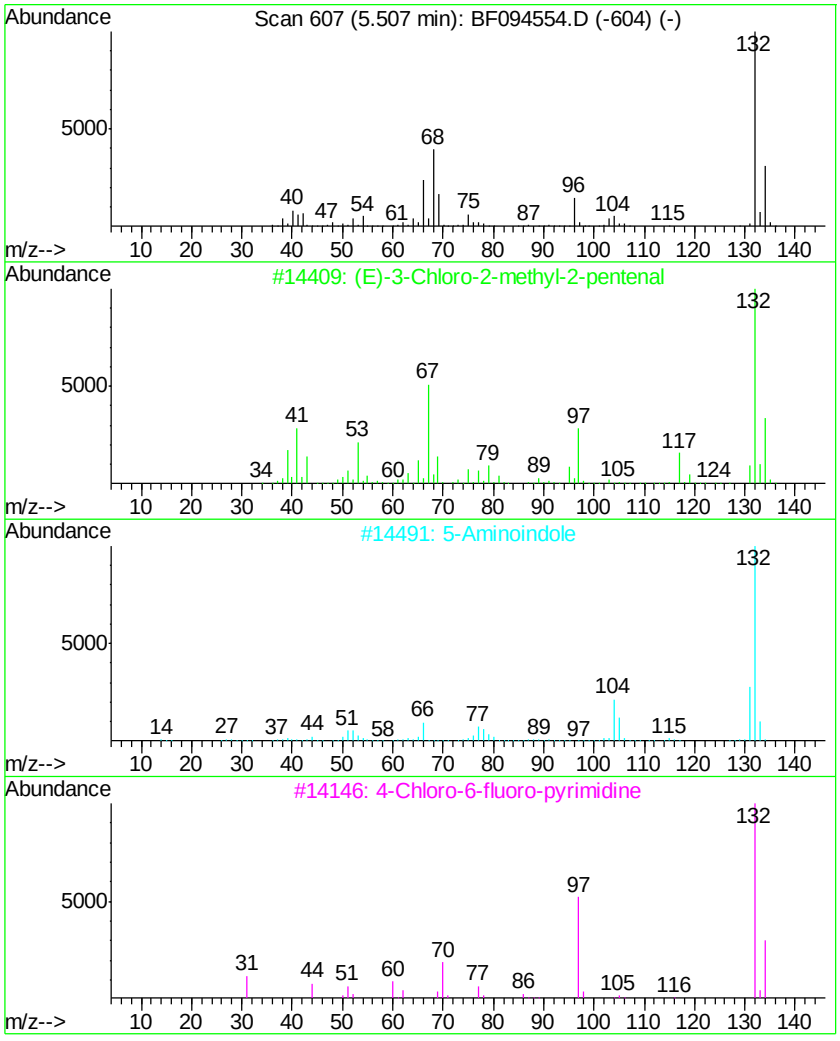
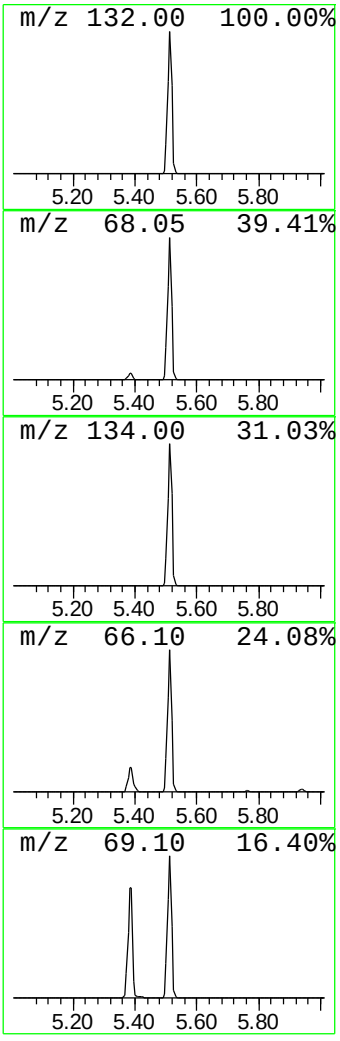
****

Peak Number 2 unknown5.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.51	68.30 ng	2221140	1,4-Dichlorobenzene-d4	5.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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ClientSampleId : SB-3(0-2)20170418

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
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TIC Library : C:\DATABASE\NIST11.L
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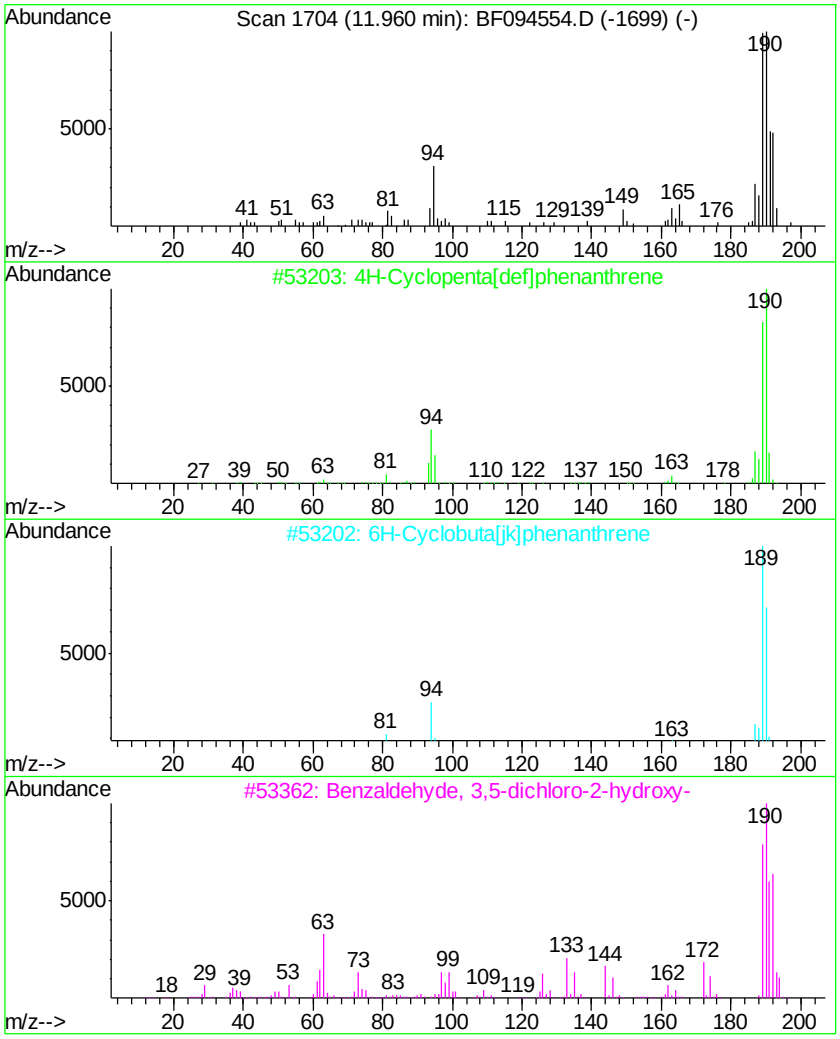
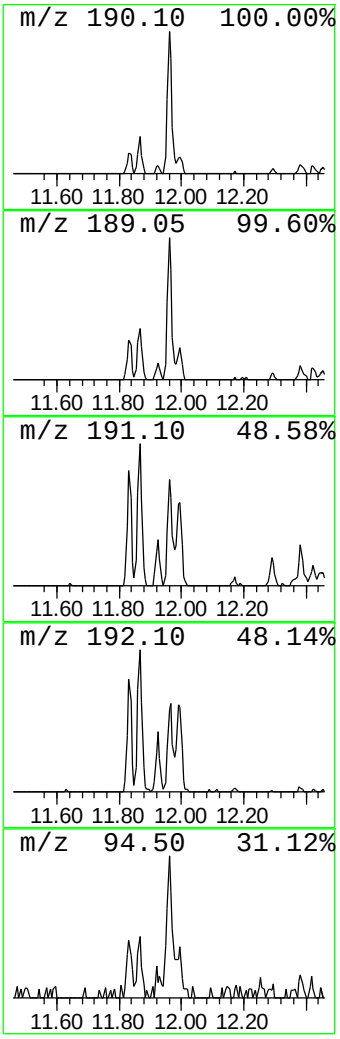
****

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	3.33 ng	170596	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	58
3	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	50
4	Carbonic acid, butyl 2-formyl-4,...	290	C12H12Cl2O4	1000331-42-2	32
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	28





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TIC Library : C:\DATABASE\NIST11.L
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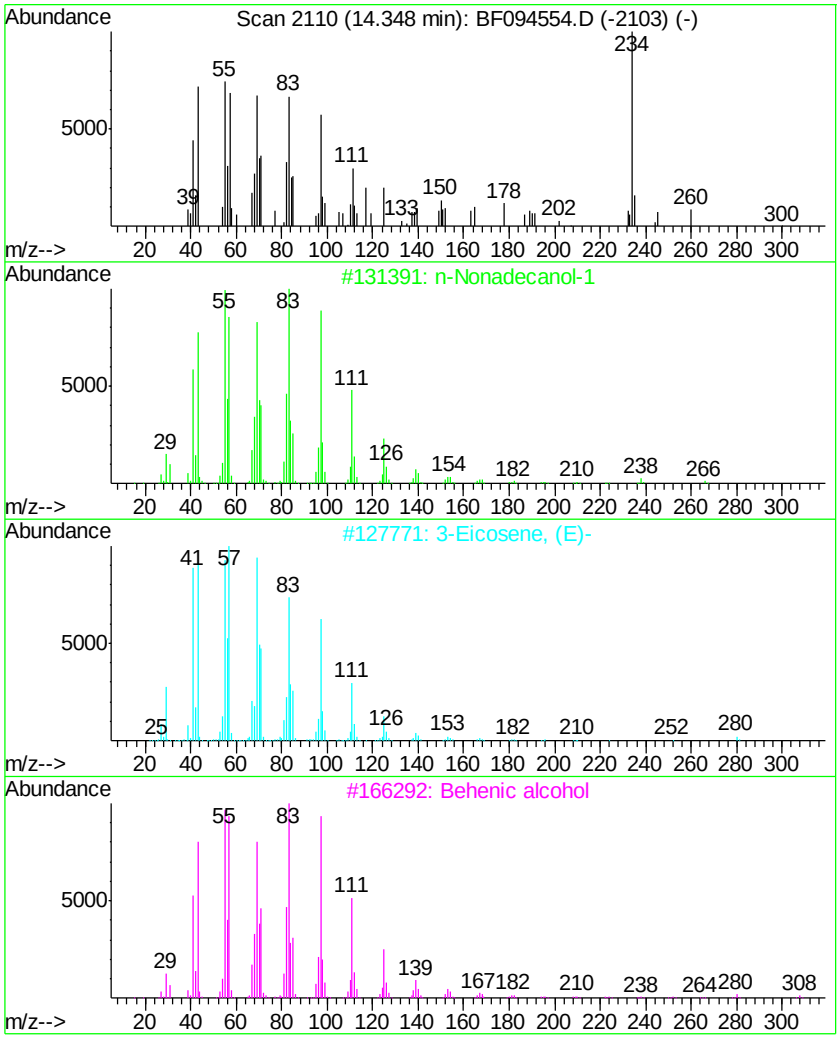
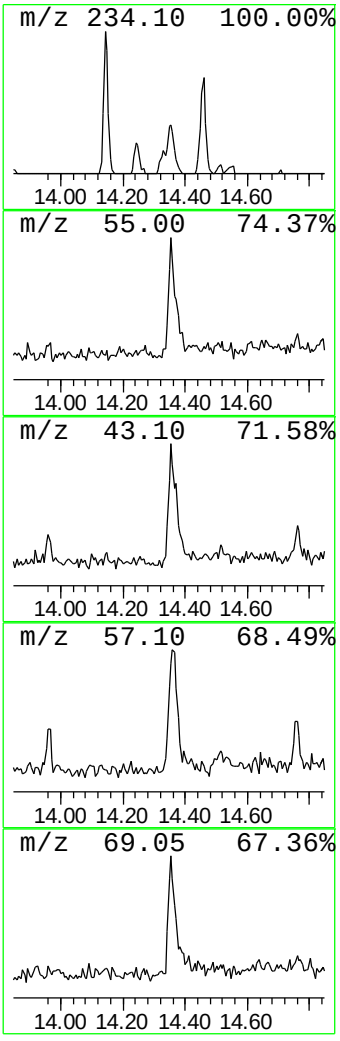
Peak Number 5 n-Nonadecanol-1 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	2.02 ng	135711	Chrysene-d12	14.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	64
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	64
3	Behenic alcohol	326	C22H46O	000661-19-8	64
4	1-Hexadecanol	242	C16H34O	036653-82-4	64
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	64





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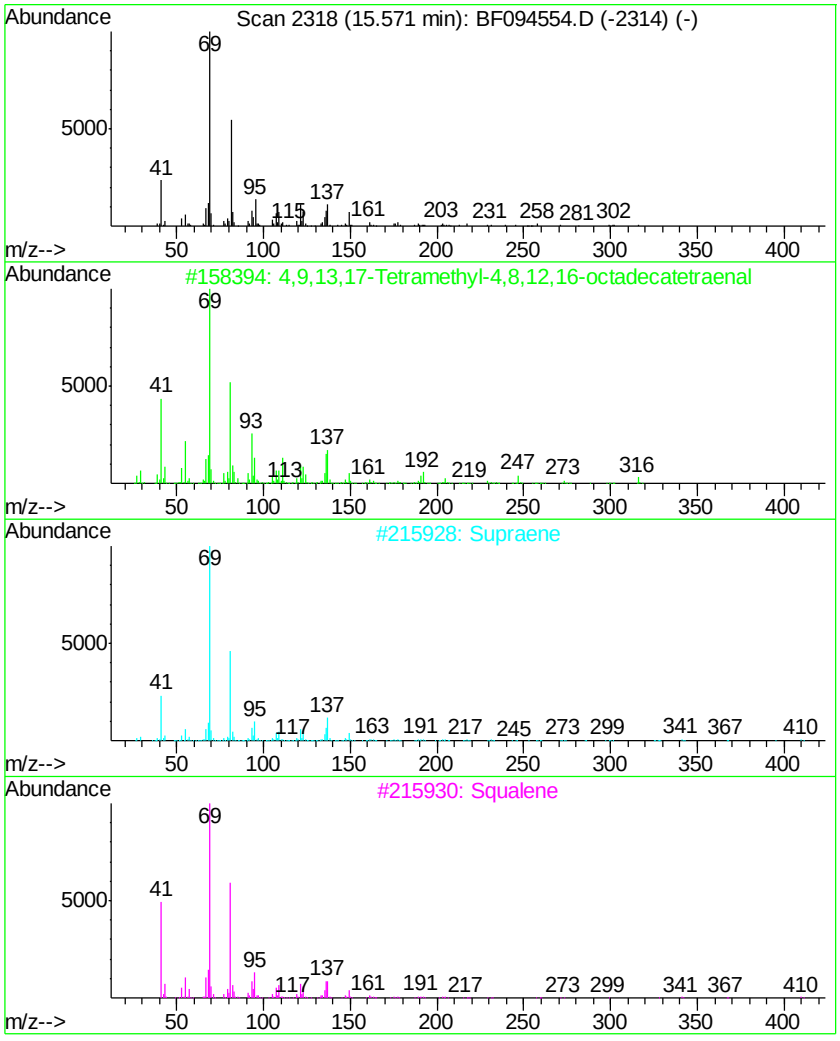
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

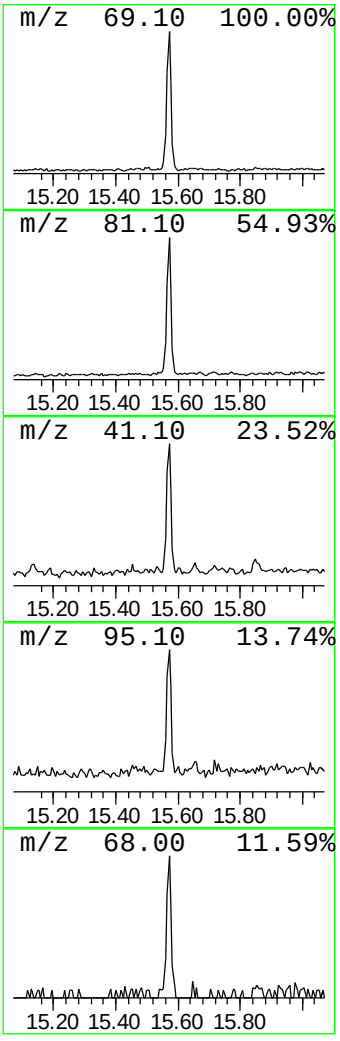
****

Peak Number 6 4,9,13,17-Tetramethyl-4,8,1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.57	5.52 ng	205391	Perylene-d12	16.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	91
2	Supraene	410	C30H50	007683-64-9	91
3	Squalene	410	C30H50	000111-02-4	91
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
5	6,10,14-Hexadecatrien-1-ol, 3,7,...	292	C20H36O	036237-66-8	78





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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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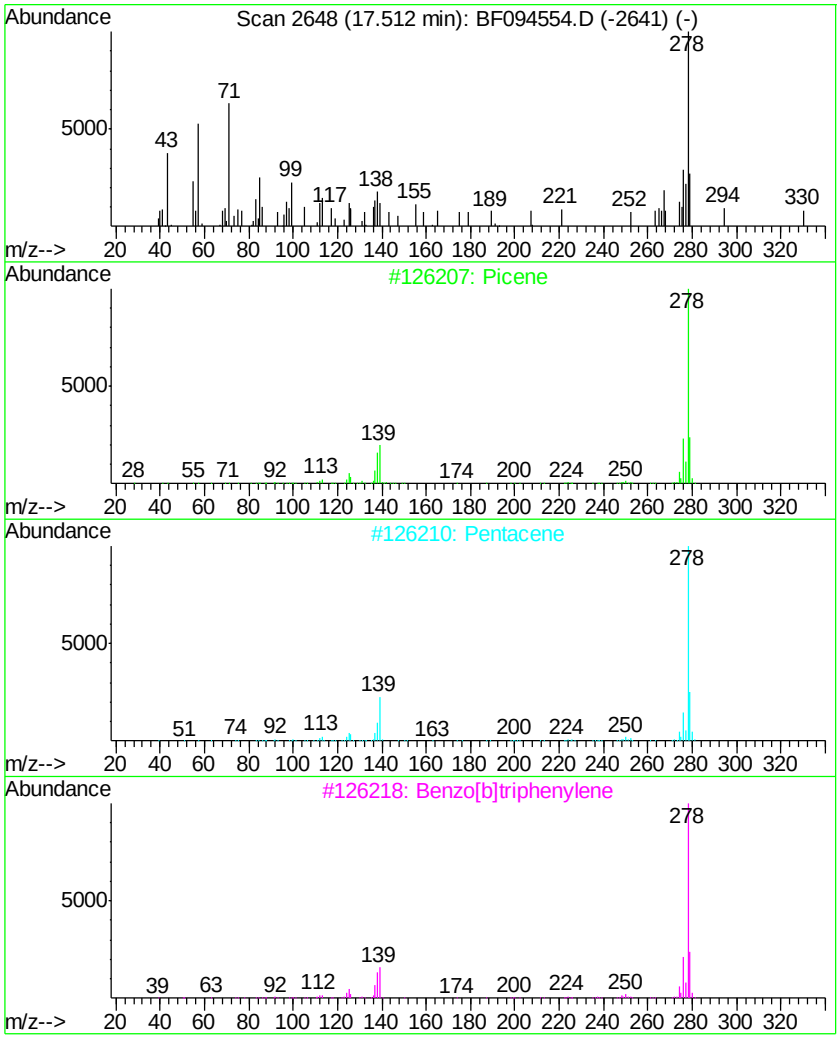
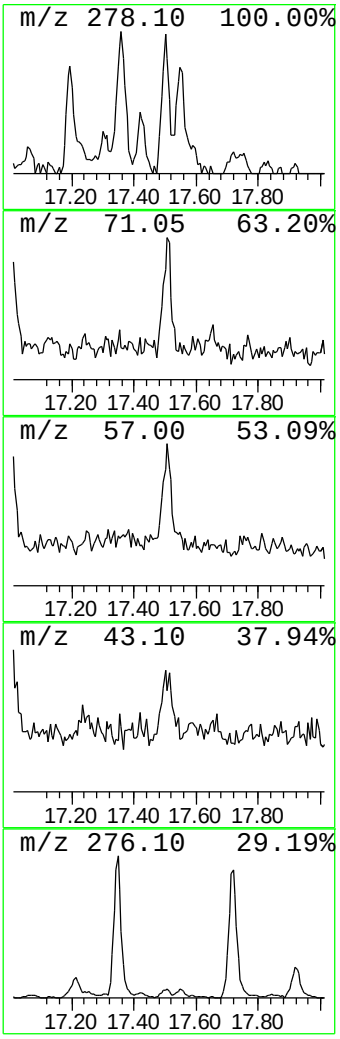
Peak Number 8 Picene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.51	2.14 ng	79582	Perylene-d12	16.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Picene	278	C22H14	000213-46-7	76
2	Pentacene	278	C22H14	000135-48-8	70
3	Benzo[b]triphenylene	278	C22H14	000215-58-7	68
4	Dibenz[a,j]anthracene	278	C22H14	000224-41-9	64
5	Dibenz[a,h]anthracene	278	C22H14	000053-70-3	53





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...	3.91	10.8	ng	351742	1	5.76	650362	20.0
unknown5.51	5.51	68.3	ng	2221140	1	5.76	650362	20.0
4H-Cyclopenta[def...	11.96	3.3	ng	170596	4	11.21	1024210	20.0
n-Nonadecanol-1	14.35	2.0	ng	135711	5	14.46	1344460	20.0
4,9,13,17-Tetrame...	15.57	5.5	ng	205391	6	16.08	744033	20.0
Picene	17.51	2.1	ng	79582	6	16.08	744033	20.0