LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091917\
Data File : BF098645.D
Acq On : 19 Sep 2017 17:05
Operator : SJ/JU
Sample : I5113-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-3-0-11.75-SPLP

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-BF091117.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	4.822	462	465	481	rBV	232475	452904	3.99%	0.573%
2	5.245	532	537	552	rBV	3765333	4410691	38.83%	5.583%
3	6.281	709	713	719	rBV	2515732	2796912	24.62%	3.540%
4	6.404	729	734	737	rBV	5782037	7218001	63.54%	9.136%
5	6.622	768	771	779	rBV	1069754	989476	8.71%	1.252%
6	6.787	793	799	802	rBV	5547413	6237593	54.91%	7.895%
7	7.210	863	871	874	rBV	3949137	5564801	48.99%	7.044%
8	7.763	947	965	972	rVB	666948	2426899	21.37%	3.072%
9	7.910	985	990	992	rBV	1464614	1587573	13.98%	2.010%
10	7.934	992	994	997	rVB	1005990	815558	7.18%	1.032%
11	8.622	1105	1111	1115	rVB	579877	506937	4.46%	0.642%
12	8.722	1122	1128	1132	rBV	396778	407540	3.59%	0.516%
13	8.892	1141	1157	1159	rBV	997648	2222241	19.56%	2.813%
14	8.998	1167	1175	1177	rVB	6924392	9739463	85.74%	12.328%
15	9.086	1183	1190	1193	rBV	151827	167629	1.48%	0.212%
16	9.245	1212	1217	1222	rBV2	85448	124422	1.10%	0.157%
17	9.322	1225	1230	1232	rBV	135378	161862	1.42%	0.205%
18	9.657	1280	1287	1290	rBV	1510691	1642238	14.46%	2.079%
19	9.692	1290	1293	1296	rVV	1052226	872974	7.69%	1.105%
20	9.733	1297	1300	1303	rVB	133943	125578	1.11%	0.159%
21	9.863	1316	1322	1324	rBV	464949	442863	3.90%	0.561%
22	9.886	1324	1326	1334	rVB4	141131	163763	1.44%	0.207%
23	10.204	1375	1380	1384	rBV	763196	696704	6.13%	0.882%
24	10.463	1415	1424	1427	rBV	4350257	6574993	57.88%	8.322%
25	10.575	1439	1443	1449	rVB	118742	158046	1.39%	0.200%
26	10.745	1468	1472	1476	rBV3	85823	117487	1.03%	0.149%
27	10.957	1503	1508	1517	rVB2	132470	159025	1.40%	0.201%
28	11.039	1517	1522	1526	rVB	187084	221375	1.95%	0.280%
29	11.145	1534	1540	1542	rBV	1920151	1967994	17.33%	2.491%
30	11.169	1542	1544	1546	rVB	1250449	950361	8.37%	1.203%
31	11.204	1546	1550	1551	rBV2	178551	191674	1.69%	0.243%
32	11.380	1574	1580	1583	rBV	1819566	1735204	15.28%	2.196%
33	11.445	1587	1591	1594	rVV3	107236	123386	1.09%	0.156%
34	11.480	1594	1597	1601	rVV	214602	185458	1.63%	0.235%

LSC Area Percent Report

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Sample : I5113-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-3-0-11.75-SPLP

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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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.527	1601	1605	1608	rVB	155819	145300	1.28%	0.184%
36	11.675	1627	1630	1633	rBV2	193481	186705	1.64%	0.236%
37	11.751	1641	1643	1652	rVB3	142550	187252	1.65%	0.237%
38	11.827	1652	1656	1658	rBV	121679	125252	1.10%	0.159%
39	12.351	1740	1745	1752	rBV	267840	266633	2.35%	0.337%
40	12.580	1781	1784	1787	rVB	144018	126853	1.12%	0.161%
41	12.621	1787	1791	1797	rVB2	159034	203470	1.79%	0.258%
42	12.745	1801	1812	1815	rBV	6809375	11359145	100.00%	14.378%
43	12.904	1834	1839	1844	rBV	150163	170685	1.50%	0.216%
44	13.569	1950	1952	1959	rVB	141567	155593	1.37%	0.197%
45	13.780	1980	1988	1992	rBV	2157922	2125246	18.71%	2.690%
46	15.174	2216	2225	2236	rBV	1428545	1790931	15.77%	2.267%

Sum of corrected areas: 79002690

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Instrument :
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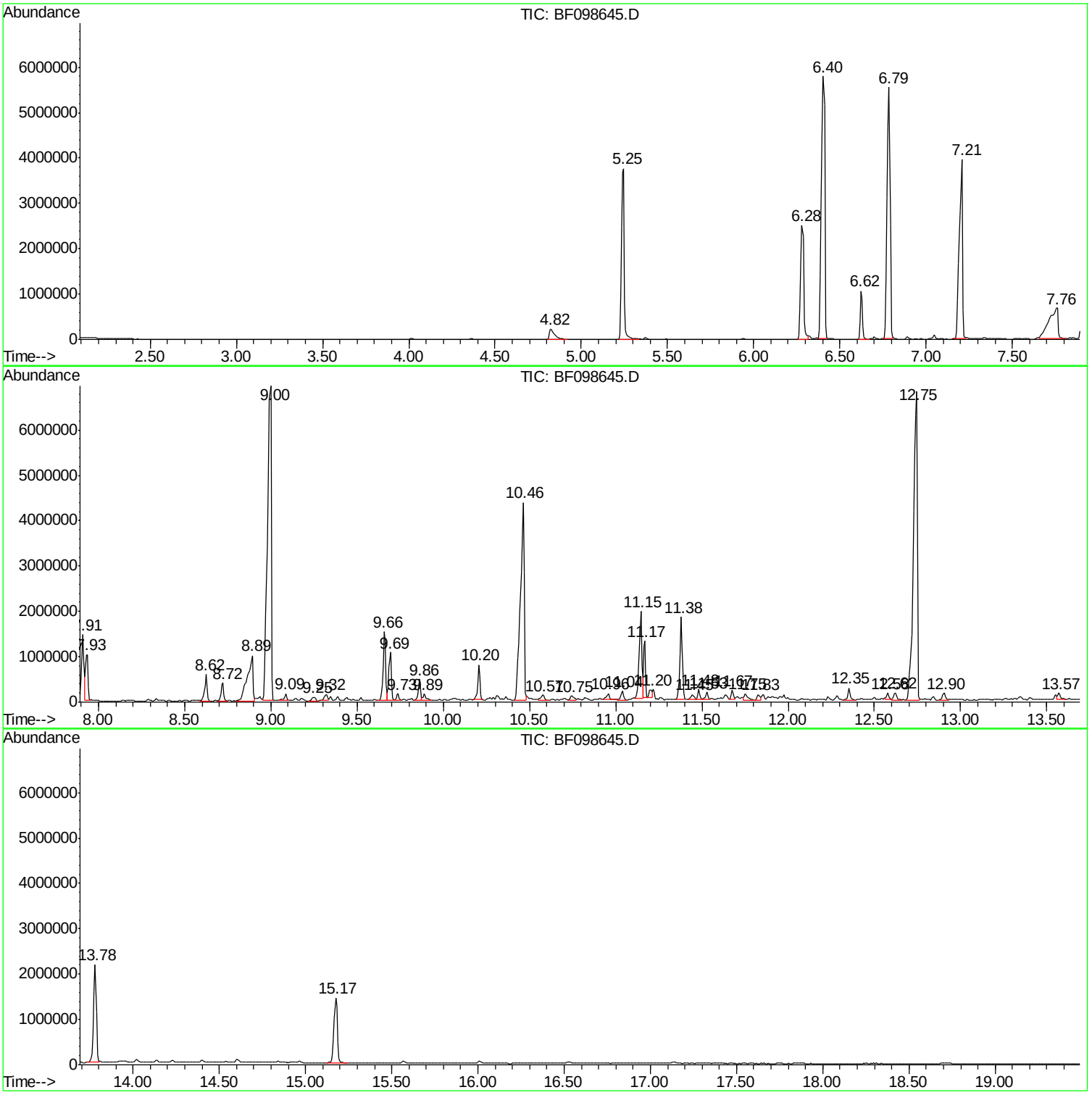
ClientSampleId :
RL-3-0-11.75-SPLP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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-BF091117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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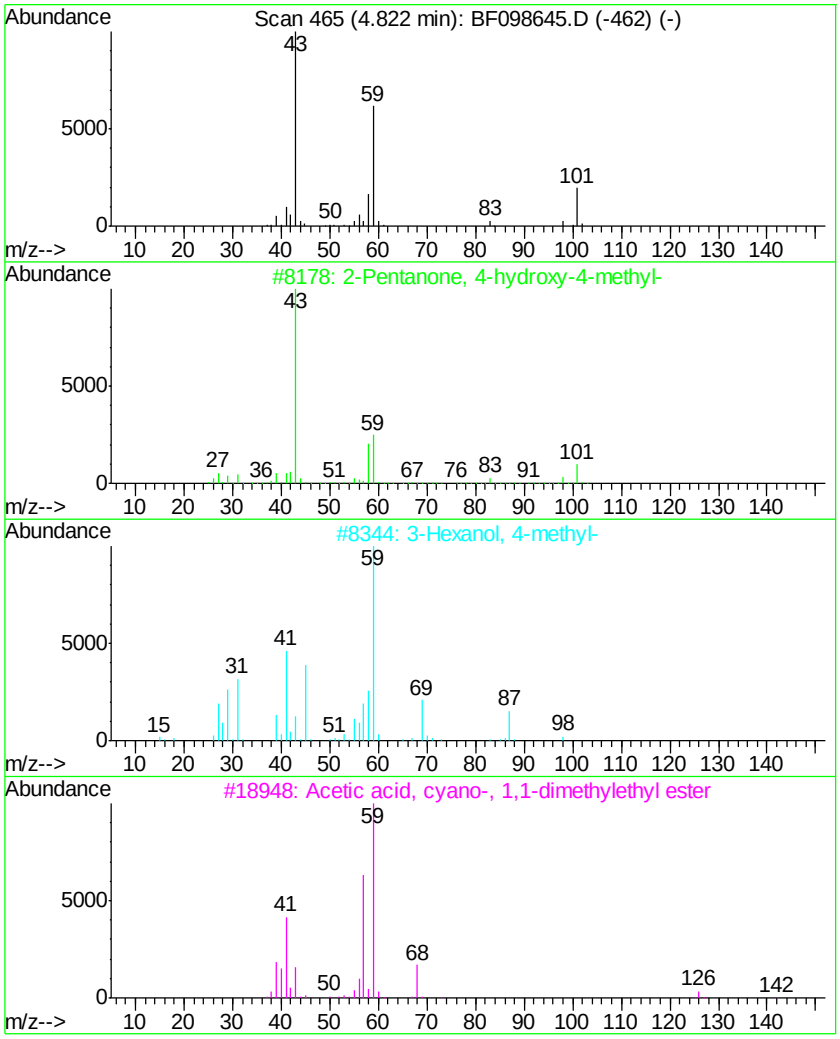
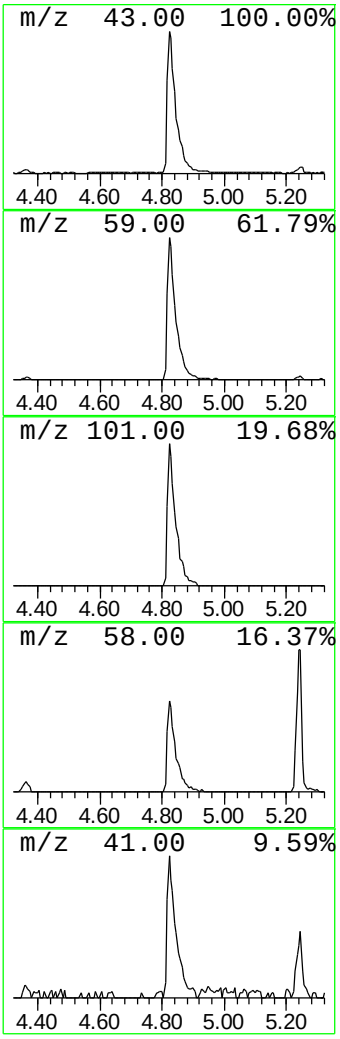
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	9.15 ng	452904	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Acetone	58	C3H6O	000067-64-1	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Instrument : BNA_F
ClientSampleId : RL-3-0-11.75-SPLP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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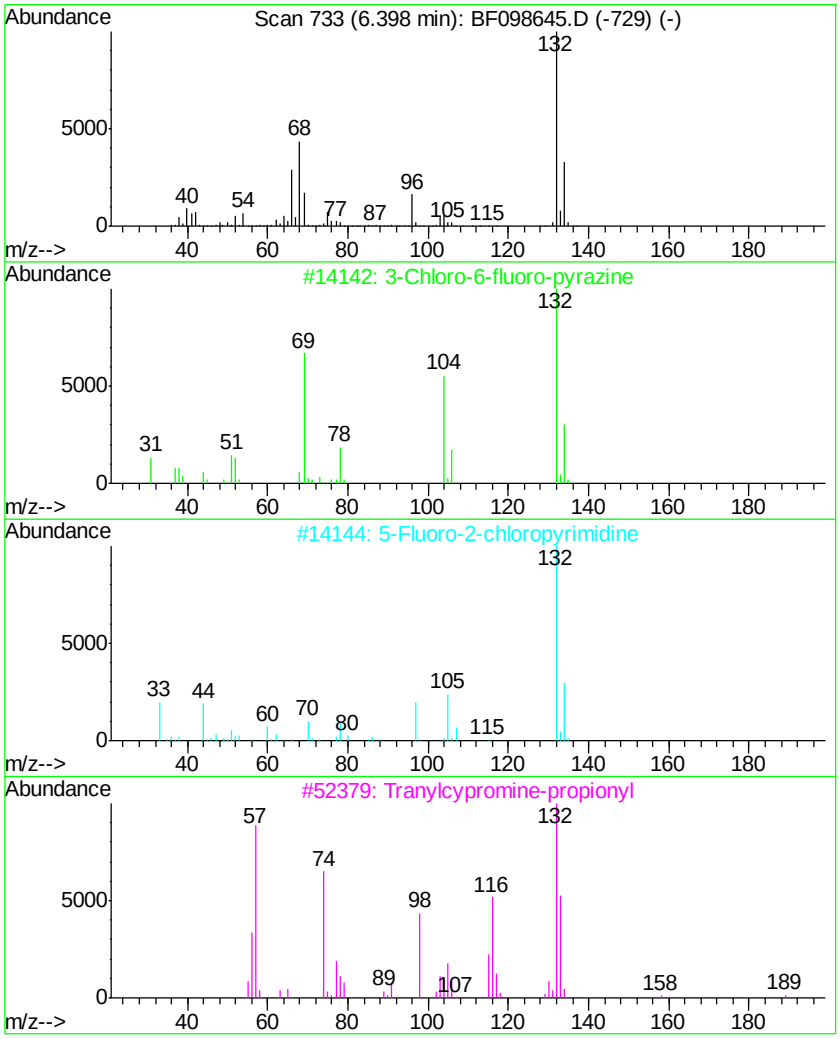
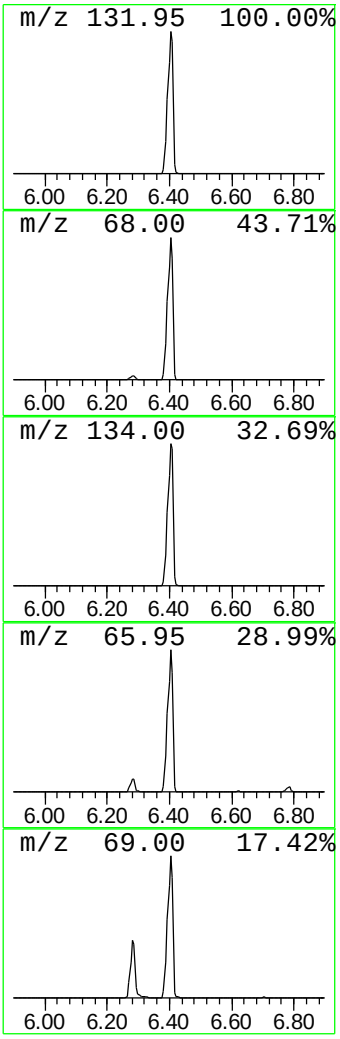
****

Peak Number 2 unknown6.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	145.90 ng	7218000	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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Sample : I5113-06
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ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-3-0-11.75-SPLP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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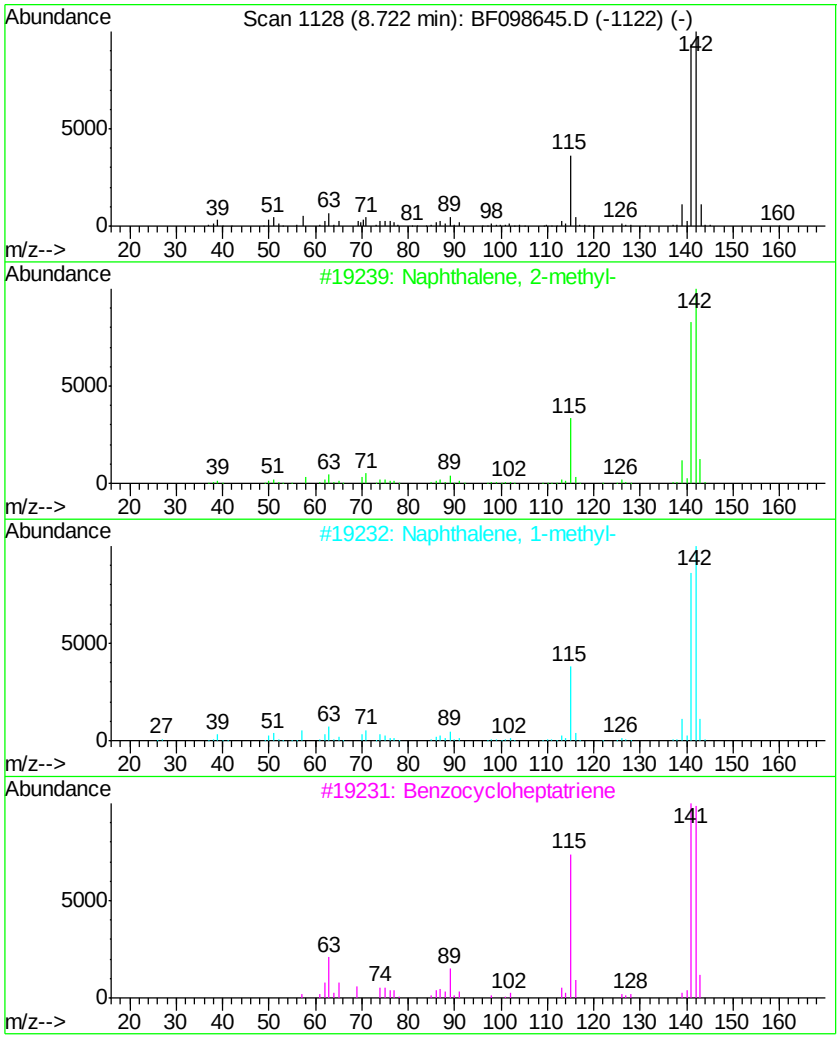
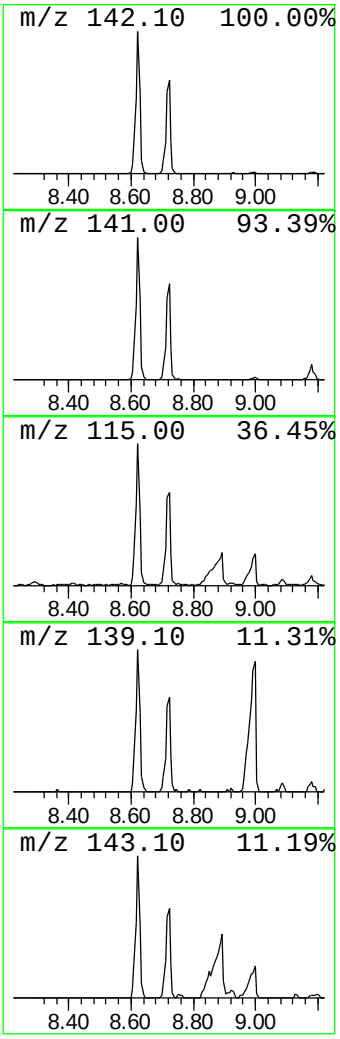
Peak Number 4 Naphthalene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	5.13 ng	407540	Naphthalene-d8	7.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	90





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ClientSampleId : RL-3-0-11.75-SPLP

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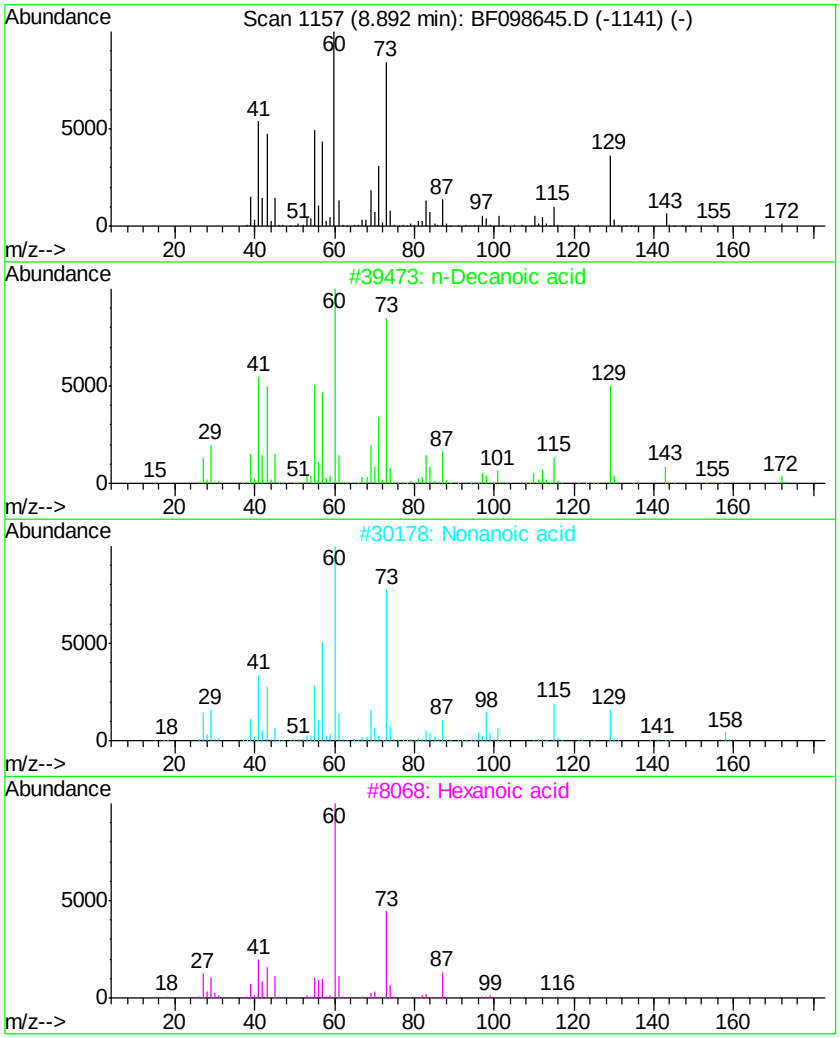
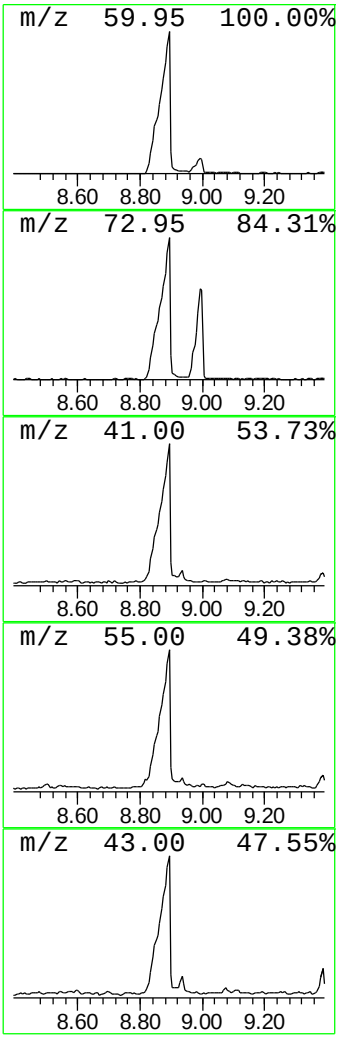
Peak Number 5 n-Decanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.89	27.06 ng	2222240	Acenaphthene-d10	9.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	97
2	Nonanoic acid	158	C9H18O2	000112-05-0	53
3	Hexanoic acid	116	C6H12O2	000142-62-1	52
4	Heptanoic acid	130	C7H14O2	000111-14-8	50
5	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	47





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ClientSampleId : RL-3-0-11.75-SPLP

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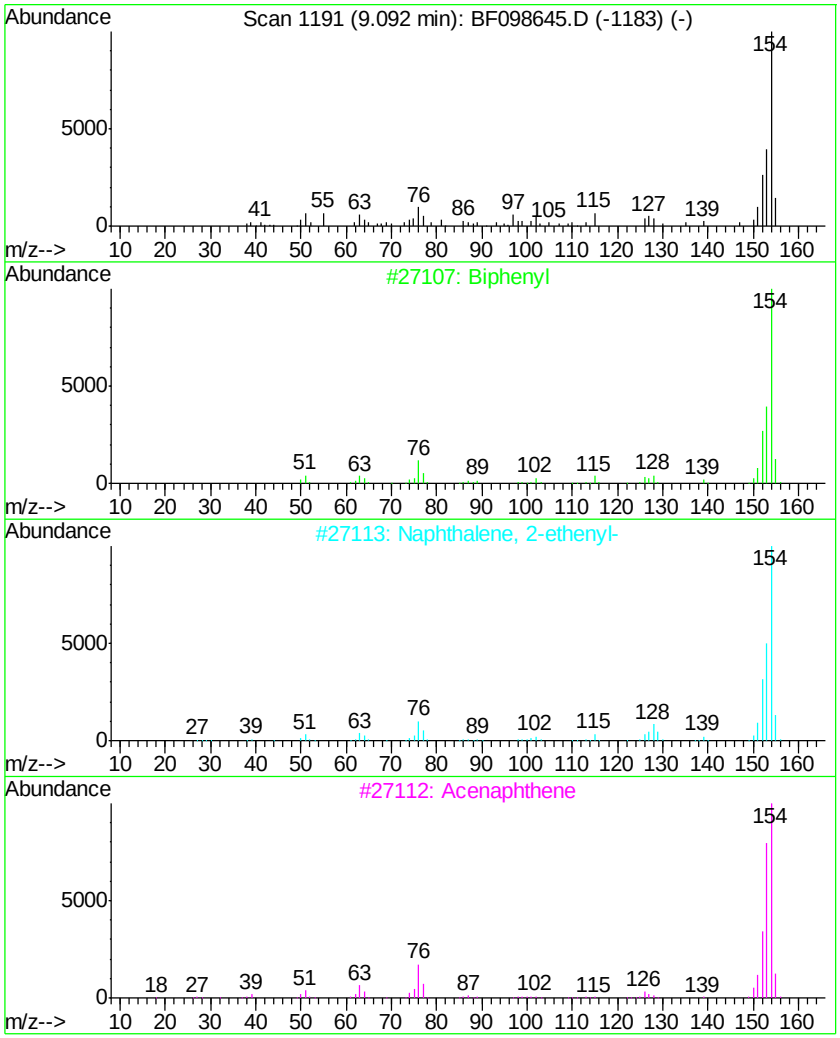
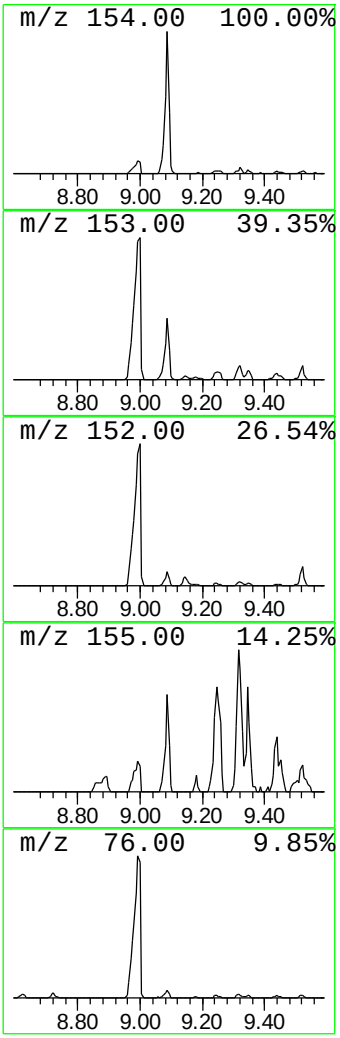
Peak Number 6 Biphenyl Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.09	2.04 ng	167629	Acenaphthene-d10	9.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Biphenyl	154	C12H10	000092-52-4	95
2	Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	90
3	Acenaphthene	154	C12H10	000083-32-9	52
4	Propanedinitrile, 2,4,6-cyclohep...	154	C10H6N2	002860-54-0	50
5	1-Isoquinolinecarbonitrile	154	C10H6N2	001198-30-7	50





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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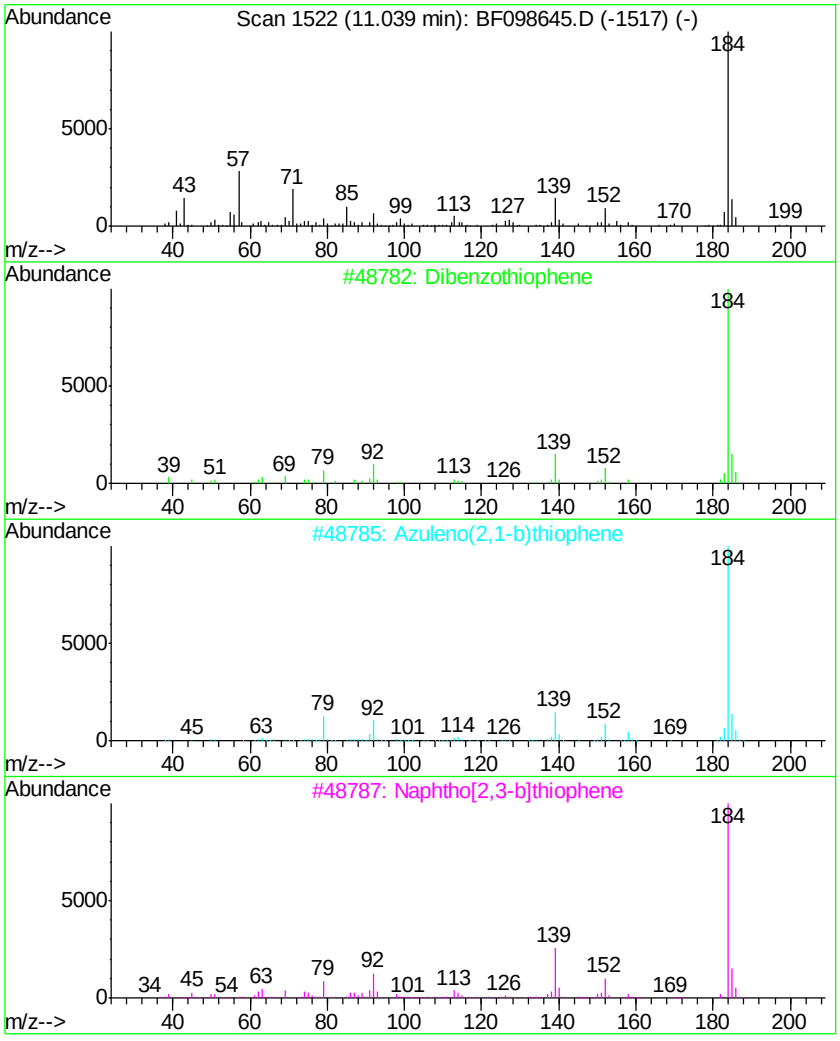
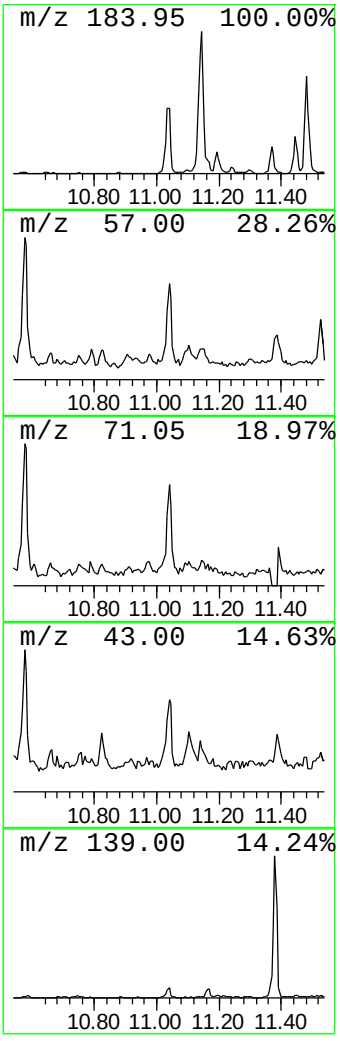
Peak Number 7 Dibenzothiophene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.04	2.25 ng	221375	Phenanthrene-d10	11.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzothiophene	184	C12H8S	000132-65-0	94
2	Azuleno(2,1-b)thiophene	184	C12H8S	000248-13-5	87
3	Naphtho[2,3-b]thiophene	184	C12H8S	000268-77-9	87
4	Naphtho[1,2-b]thiophene	184	C12H8S	000234-41-3	87
5	Naphtho[2,1-b]thiophene	184	C12H8S	000233-02-3	74





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.82	9.2	ng	452904	1	6.62	989476	20.0
unknown6.40	6.40	145.9	ng	7218000	1	6.62	989476	20.0
Naphthalene, 2-me...	8.72	5.1	ng	407540	2	7.91	1587570	20.0
n-Decanoic acid	8.89	27.1	ng	2222240	3	9.66	1642240	20.0
Biphenyl	9.09	2.0	ng	167629	3	9.66	1642240	20.0
Dibenzothiophene	11.04	2.3	ng	221375	4	11.15	1967990	20.0