LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124751.D
Acq On : 24 Jul 2021 17:06
Operator : JU/CG
Sample : M3094-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124751.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	7	10	13	rBB	5174	5684	6.17%	0.774%
2	4.598	424	427	430	rBB	15649	14726	15.98%	2.004%
3	5.481	573	577	580	rBB	79057	71423	77.51%	9.720%
4	6.486	744	748	751	rBB	78327	73572	79.85%	10.012%
5	6.869	810	813	816	rBB	55395	43641	47.36%	5.939%
6	7.428	905	908	911	rBB	58597	49189	53.38%	6.694%
7	8.051	1011	1014	1017	rBB	9650	7235	7.85%	0.985%
8	8.151	1028	1031	1034	rBB	76522	59468	64.54%	8.093%
9	9.227	1210	1214	1217	rBV	131404	92143	100.00%	12.540%
10	9.339	1231	1233	1235	rBB	2987	2054	2.23%	0.280%
11	9.910	1327	1330	1333	rBB	84508	60198	65.33%	8.192%
12	10.692	1460	1463	1466	rBB	55884	40246	43.68%	5.477%
13	11.392	1579	1582	1586	rBV	55125	47201	51.23%	6.424%
14	11.916	1668	1671	1673	rBB	6044	4360	4.73%	0.593%
15	12.492	1766	1769	1770	rVB	2294	1668	1.81%	0.227%
16	12.698	1802	1804	1806	rBB	2594	1446	1.57%	0.197%
17	12.980	1848	1852	1855	rBB	71125	54960	59.65%	7.480%
18	13.886	2003	2006	2007	rBV	2101	1491	1.62%	0.203%
19	14.033	2026	2031	2034	rBV	38479	31926	34.65%	4.345%
20	14.509	2107	2112	2114	rBV3	1606	2771	3.01%	0.377%
21	14.551	2117	2119	2124	rVB2	1338	1526	1.66%	0.208%
22	14.598	2124	2127	2130	rVB2	1554	1919	2.08%	0.261%
23	14.627	2130	2132	2134	rBV2	1624	1840	2.00%	0.250%
24	14.709	2145	2146	2149	rBV2	1681	1367	1.48%	0.186%
25	14.745	2151	2152	2156	rBV4	1388	1329	1.44%	0.181%
26	14.886	2171	2176	2179	rBV2	3302	4318	4.69%	0.588%
27	15.104	2212	2213	2216	rVB3	1393	1278	1.39%	0.174%
28	15.151	2216	2221	2222	rBV2	2128	3501	3.80%	0.476%
29	15.209	2226	2231	2232	rBV2	1401	1916	2.08%	0.261%
30	15.392	2261	2262	2265	rVB2	1941	1646	1.79%	0.224%
31	15.415	2265	2266	2269	rBV2	1101	1306	1.42%	0.178%
32	15.509	2277	2282	2285	rBV	20047	24042	26.09%	3.272%
33	15.533	2285	2286	2290	rVB3	1856	2160	2.34%	0.294%
34	15.580	2290	2294	2295	rBV2	1966	1922	2.09%	0.262%
35	15.598	2295	2297	2301	rVB3	1442	1381	1.50%	0.188%
36	15.968	2359	2360	2364	rVB3	1997	1392	1.51%	0.189%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SP-1

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.027	2369	2370	2373	rBV2	1652	1287	1.40%	0.175%
38	16.074	2375	2378	2380	rVB3	1192	1309	1.42%	0.178%
39	16.303	2415	2417	2420	rVB3	1678	1393	1.51%	0.190%
40	16.486	2445	2448	2452	rVB4	1403	2110	2.29%	0.287%
41	16.662	2476	2478	2482	rBV4	1666	2378	2.58%	0.324%
42	16.992	2533	2534	2539	rVB4	1071	1379	1.50%	0.188%
43	17.103	2551	2553	2557	rVB4	1289	1322	1.43%	0.180%
44	17.233	2572	2575	2576	rBV2	1826	1270	1.38%	0.173%
45	17.680	2649	2651	2655	rBV3	1210	1344	1.46%	0.183%
46	18.286	2750	2754	2759	rVB2	966	1449	1.57%	0.197%
47	18.474	2785	2786	2791	rBV	928	1320	1.43%	0.180%

Sum of corrected areas: 734806

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ClientSampleId :
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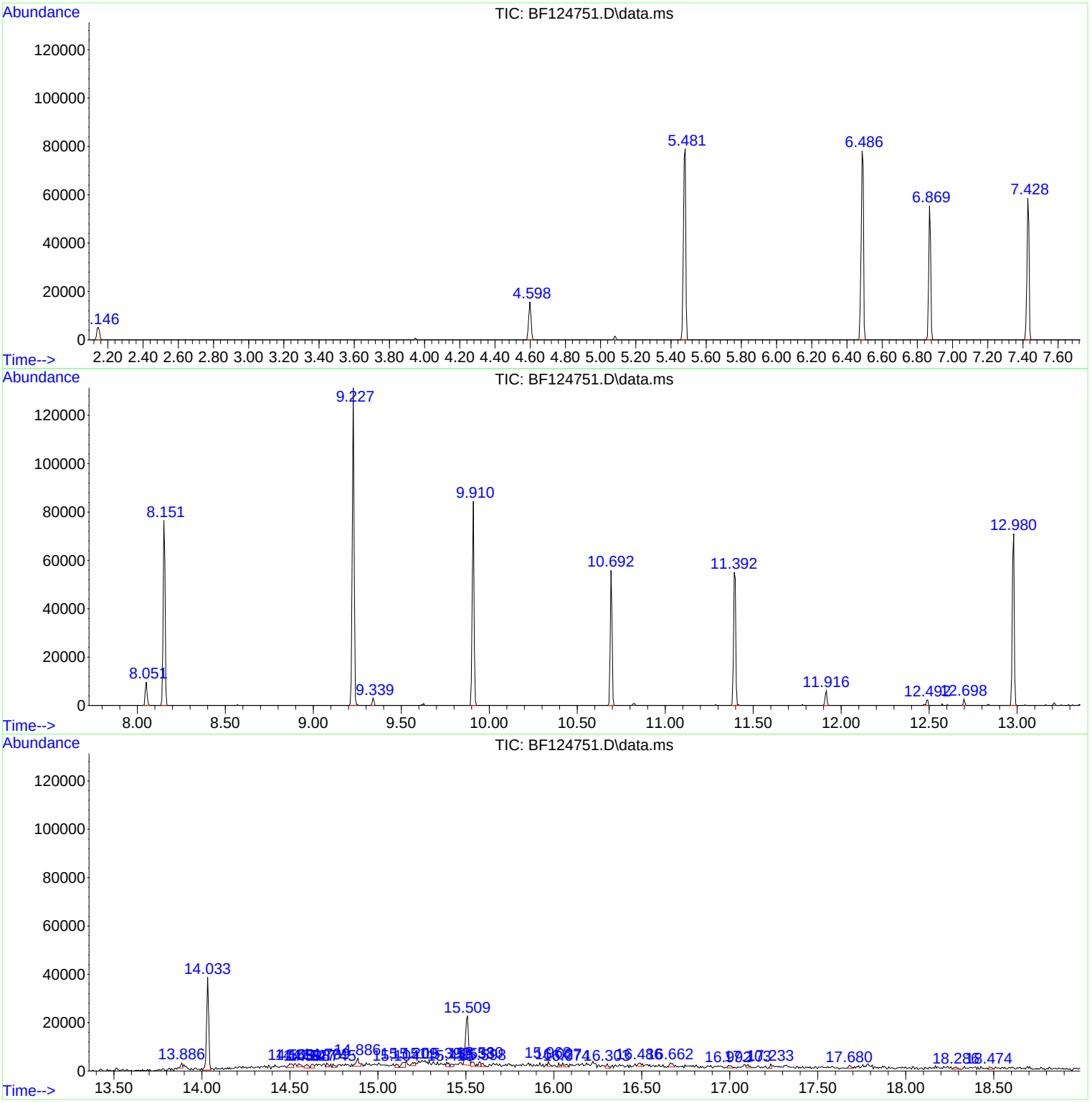
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Data File : BF124751.D
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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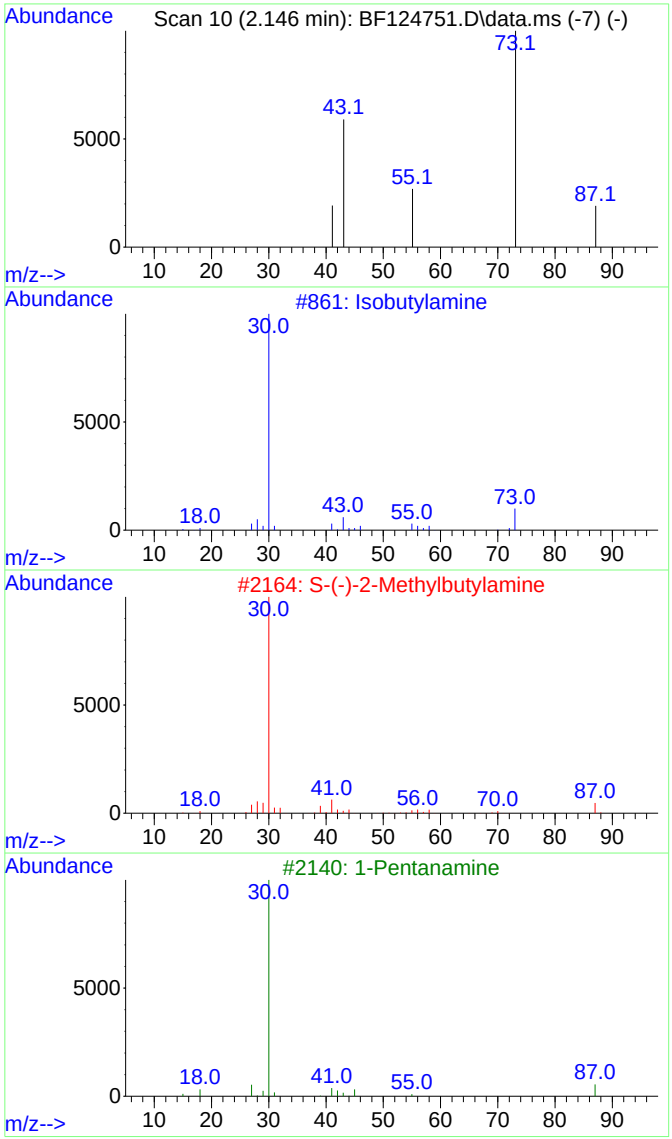
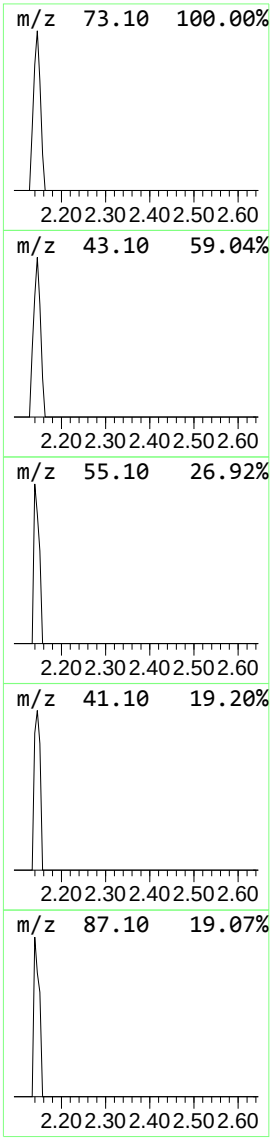
Peak Number 1 unknown2.146 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	2.60 ng	5684	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutylamine	73	C4H11N	000078-81-9	4
2	S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	3
3	1-Pentanamine	87	C5H13N	000110-58-7	3
4	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	3
5	1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	3





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Misc :
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Instrument : BNA_F
ClientSampleId : SP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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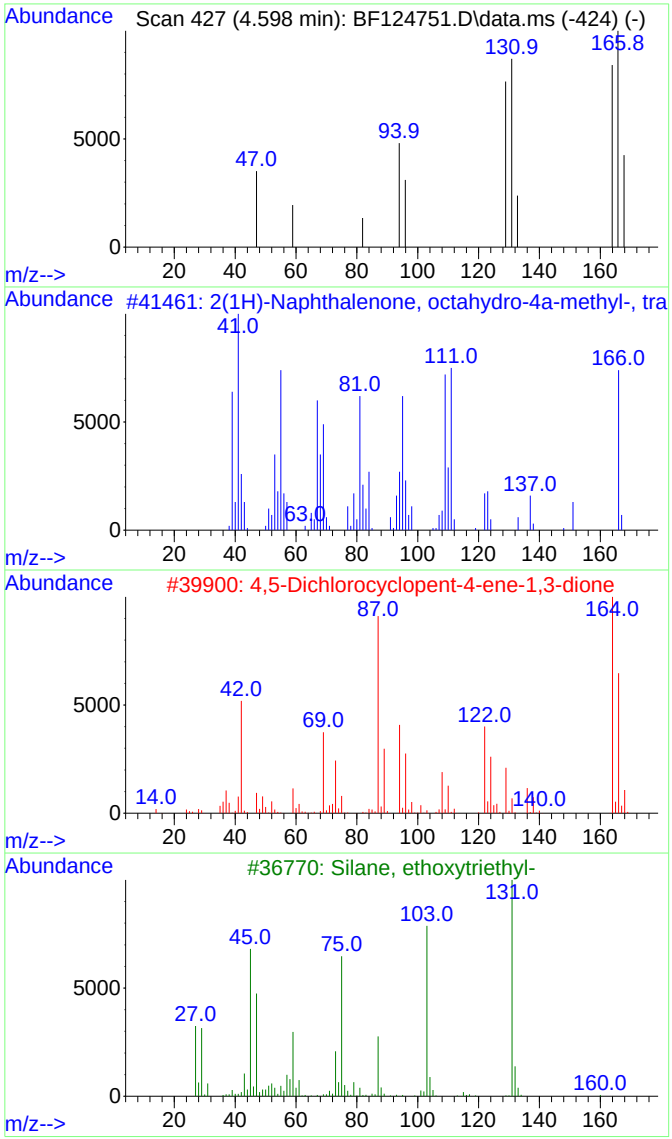
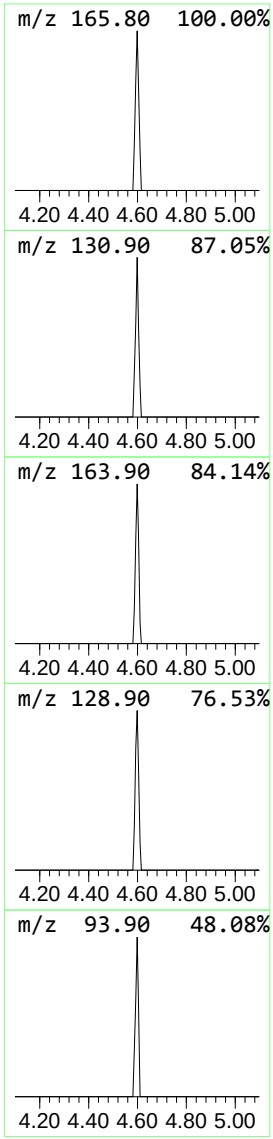
Peak Number 2 unknown4.598 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.598	6.75 ng	14726	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Naphthalenone, octahydro-4...	166	C11H18O	000938-07-8	9
2	4,5-Dichlorocyclopent-4-ene-1,3-...	164	C5H2Cl2O2	003229-28-5	9
3	Silane, ethoxytriethyl-	160	C8H20OSi	000597-67-1	9
4	Benzene, (2-chloro-2-butenyl)-	166	C10H11Cl	054411-12-0	7
5	2-Butene, 3-chloro-1-phenyl-, (Z)-	166	C10H11Cl	016608-68-7	7





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Instrument :
BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
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TIC Library : C:\Database\NIST20.L
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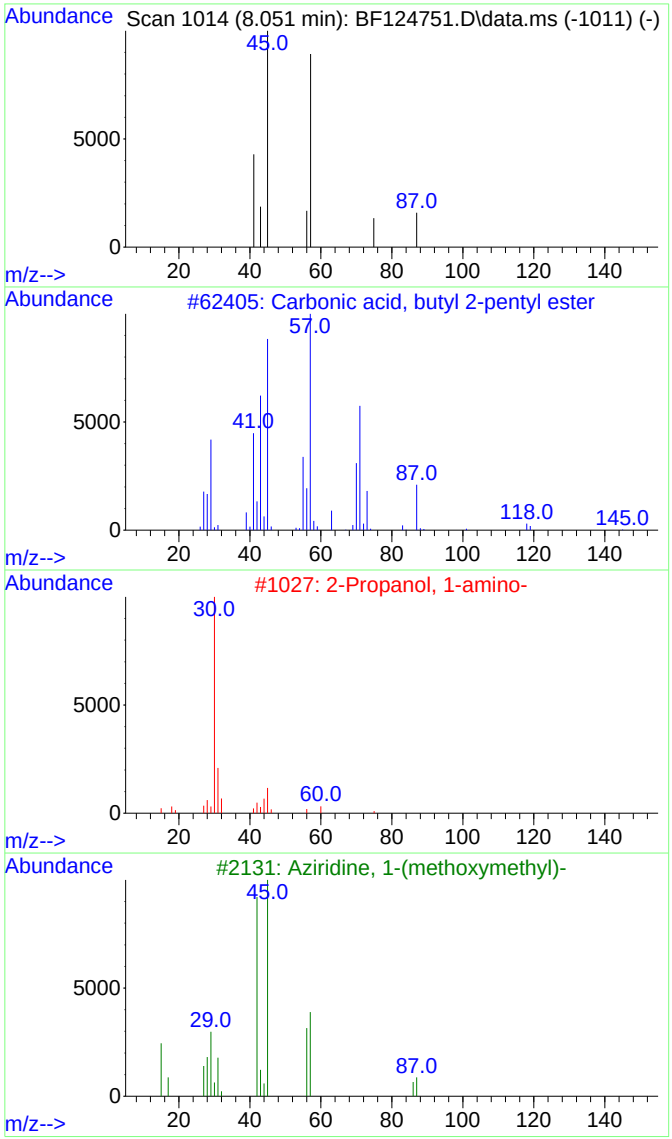
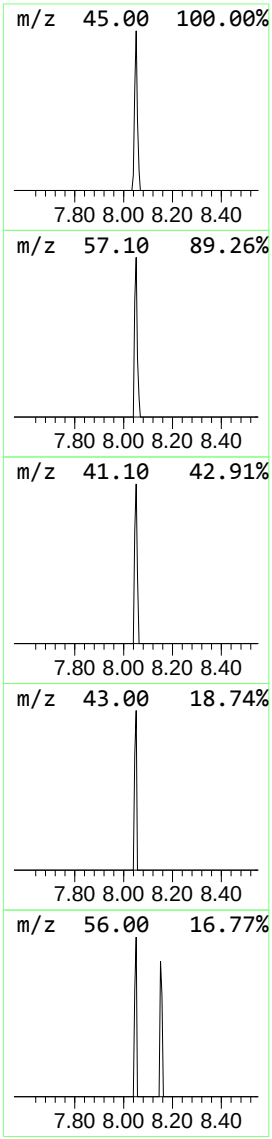
Peak Number 3 unknown8.051 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	2.43 ng	7235	Naphthalene-d8	8.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, butyl 2-pentyl ester	188	C10H20O3	1000357-84-0	9
2	2-Propanol, 1-amino-	75	C3H9NO	000078-96-6	4
3	Aziridine, 1-(methoxymethyl)-	87	C4H9NO	001497-83-2	4
4	Ethanamine, 2-methoxy-	75	C3H9NO	000109-85-3	4
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	4





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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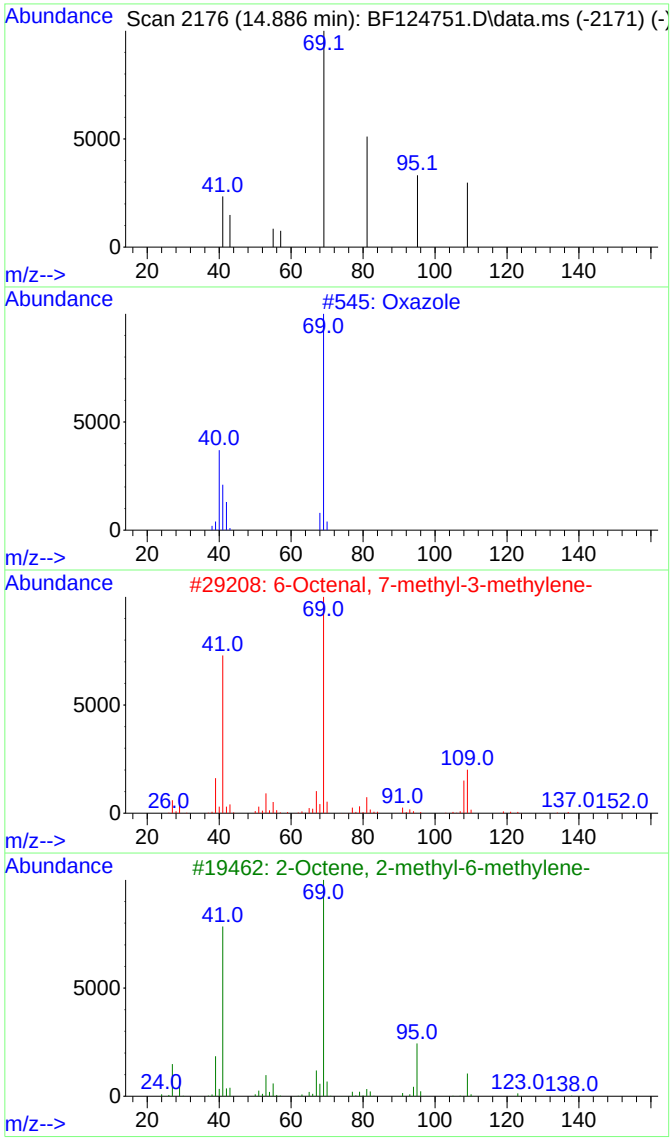
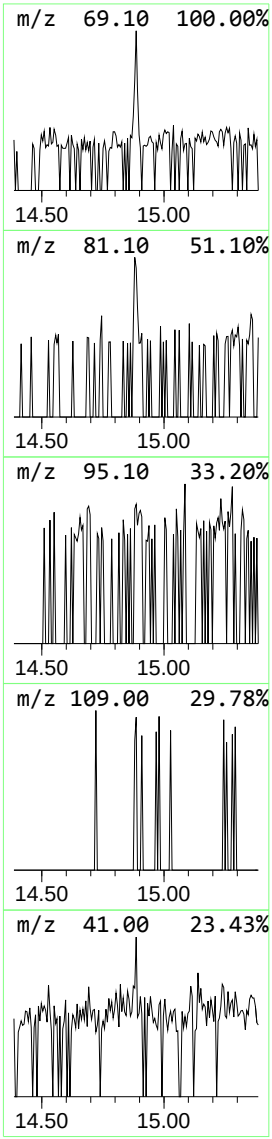
Peak Number 4 unknown14.886 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.886	3.59 ng	4318	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazole	69	C3H3NO	000288-42-6	3
2	6-Octenal, 7-methyl-3-methylene-	152	C10H16O	055050-40-3	2
3	2-Octene, 2-methyl-6-methylene-	138	C10H18	010054-09-8	2
4	1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	2
5	Isoxazole	69	C3H3NO	000288-14-2	2





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Misc :
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Instrument : BNA_F
ClientSampleId : SP-1

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TIC Library : C:\Database\NIST20.L
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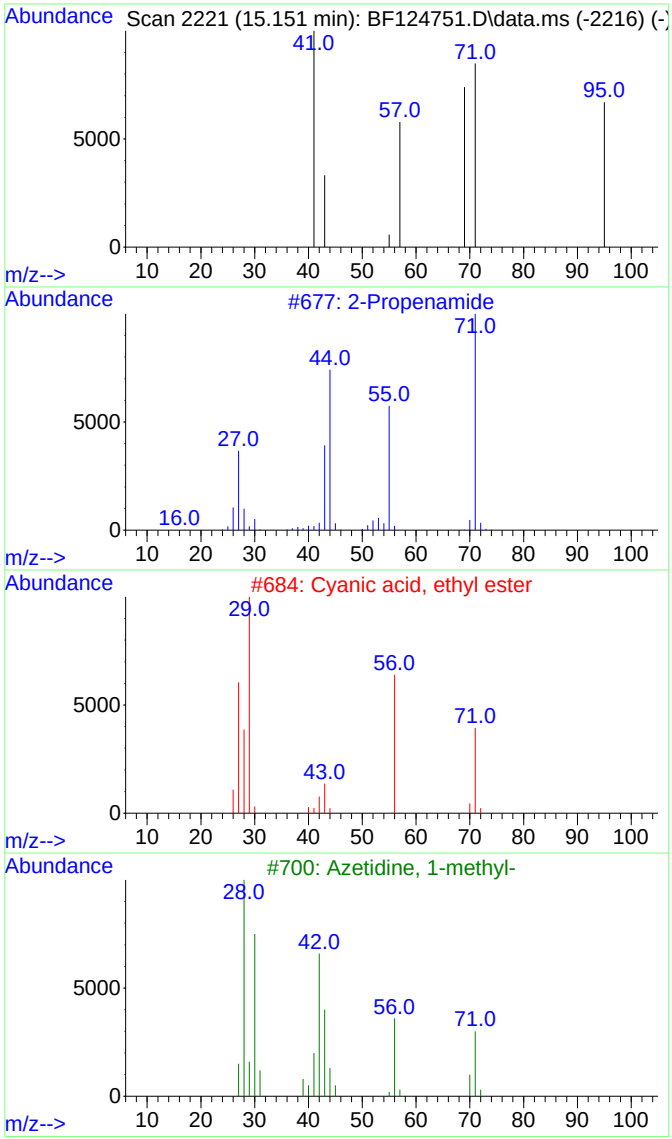
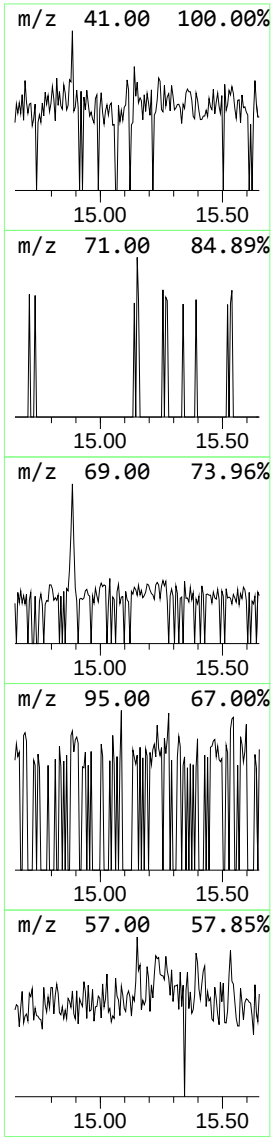
Peak Number 5 unknown15.151 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.151	2.91 ng	3501	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenamide	71	C3H5NO	000079-06-1	4
2	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	3
3	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	3
4	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	3
5	3-Pyridinol	95	C5H5NO	000109-00-2	2





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown2.146	2.146	2.6	ng	5684	1	6.869	43641	20.0
unknown4.598	4.598	6.8	ng	14726	1	6.869	43641	20.0
unknown8.051	8.051	2.4	ng	7235	2	8.151	59468	20.0
unknown14.886	14.886	3.6	ng	4318	6	15.509	24042	20.0
unknown15.151	15.151	2.9	ng	3501	6	15.509	24042	20.0