LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124650.D
Acq On : 21 Jul 2021 3:40
Operator : JU/CG
Sample : M3047-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-020-ABCD

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-BF070721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124650.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	13	16	19	rBB	2176	2097	2.43%	0.289%
2	5.510	578	582	585	rBB	74514	60016	69.52%	8.259%
3	6.516	749	753	756	rBB	71732	61401	71.12%	8.450%
4	6.904	816	819	822	rBB	49561	35450	41.06%	4.878%
5	7.463	910	914	917	rBB	52160	38306	44.37%	5.271%
6	8.081	1017	1019	1022	rBB	6846	5434	6.29%	0.748%
7	8.186	1034	1037	1040	rBB	61745	44837	51.94%	6.170%
8	9.263	1217	1220	1223	rBB	95833	66763	77.33%	9.187%
9	9.945	1333	1336	1339	rBB	55568	40334	46.72%	5.550%
10	10.727	1466	1469	1472	rBB	37453	24382	28.24%	3.355%
11	11.433	1585	1589	1591	rBV	36046	31730	36.75%	4.366%
12	11.633	1619	1623	1626	rBB	5934	5869	6.80%	0.808%
13	11.945	1673	1676	1680	rBB2	2550	1825	2.11%	0.251%
14	12.645	1792	1795	1797	rBB	6801	5583	6.47%	0.768%
15	12.733	1808	1810	1812	rBB	1468	1002	1.16%	0.138%
16	12.892	1826	1837	1846	rBV2	53514	86332	100.00%	11.880%
17	13.016	1855	1858	1861	rBV	66090	47491	55.01%	6.535%
18	13.092	1868	1871	1874	rBV	1132	937	1.09%	0.129%
19	13.180	1883	1886	1887	rBV2	1134	1160	1.34%	0.160%
20	13.210	1887	1891	1896	rVB2	5085	8365	9.69%	1.151%
21	13.263	1898	1900	1903	rVB2	1973	1822	2.11%	0.251%
22	13.304	1903	1907	1910	rBB	2366	1802	2.09%	0.248%
23	13.398	1921	1923	1925	rBB	2058	1497	1.73%	0.206%
24	13.815	1992	1994	1997	rBV	1123	1296	1.50%	0.178%
25	13.845	1997	1999	2002	rVV2	1584	1281	1.48%	0.176%
26	13.910	2007	2010	2014	rVV2	1827	2469	2.86%	0.340%
27	14.015	2024	2028	2030	rBV2	806	1211	1.40%	0.167%
28	14.068	2032	2037	2040	rVV2	31821	36715	42.53%	5.052%
29	14.092	2040	2041	2044	rVB	6749	5390	6.24%	0.742%
30	14.174	2053	2055	2057	rVB	1842	1154	1.34%	0.159%
31	14.227	2063	2064	2067	rBV2	1430	1724	2.00%	0.237%
32	14.457	2098	2103	2106	rVB2	2227	3011	3.49%	0.414%
33	14.486	2106	2108	2111	rBV2	1301	1376	1.59%	0.189%
34	14.539	2113	2117	2121	rBV2	1212	2070	2.40%	0.285%
35	14.604	2126	2128	2133	rVB2	806	1143	1.32%	0.157%
36	14.768	2154	2156	2160	rVB3	942	1285	1.49%	0.177%

LSC Area Percent Report

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Acq On : 21 Jul 2021 3:40
Operator : JU/CG
Sample : M3047-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-020-ABCD

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-BF070721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.810	2160	2163	2164	rBV2	1525	1138	1.32%	0.157%
38	14.833	2164	2167	2169	rBV2	791	976	1.13%	0.134%
39	14.998	2194	2195	2198	rVB2	1230	934	1.08%	0.129%
40	15.121	2213	2216	2219	rBV	5561	6843	7.93%	0.942%
41	15.145	2219	2220	2225	rVB2	3534	3274	3.79%	0.451%
42	15.198	2225	2229	2231	rBV2	1815	2363	2.74%	0.325%
43	15.221	2231	2233	2237	rVB2	1322	1482	1.72%	0.204%
44	15.280	2241	2243	2247	rVB2	1019	986	1.14%	0.136%
45	15.433	2262	2269	2272	rBV	4506	6635	7.69%	0.913%
46	15.492	2275	2279	2282	rVV	6864	7419	8.59%	1.021%
47	15.562	2286	2291	2294	rVV	14567	17791	20.61%	2.448%
48	15.586	2294	2295	2300	rVB3	2208	2430	2.81%	0.334%
49	15.645	2300	2305	2306	rBV2	873	1003	1.16%	0.138%
50	15.715	2314	2317	2320	rBV	1163	1211	1.40%	0.167%
51	15.768	2323	2326	2328	rBV	1375	1450	1.68%	0.200%
52	15.851	2337	2340	2341	rBV2	1374	1132	1.31%	0.156%
53	15.986	2360	2363	2366	rBV2	1214	1827	2.12%	0.251%
54	16.033	2369	2371	2373	rVB	1267	1160	1.34%	0.160%
55	16.109	2380	2384	2385	rVB4	832	959	1.11%	0.132%
56	16.233	2403	2405	2408	rVB2	1022	959	1.11%	0.132%
57	16.292	2413	2415	2417	rBV2	1673	1707	1.98%	0.235%
58	16.445	2439	2441	2444	rBV2	904	961	1.11%	0.132%
59	16.486	2446	2448	2451	rBV2	945	1230	1.42%	0.169%
60	16.568	2458	2462	2464	rVB3	1177	1271	1.47%	0.175%
61	16.651	2472	2476	2481	rVB2	1132	1980	2.29%	0.272%
62	16.692	2481	2483	2484	rBV2	1350	1085	1.26%	0.149%
63	16.739	2487	2491	2496	rVB2	1051	1796	2.08%	0.247%
64	16.809	2501	2503	2508	rVB2	619	955	1.11%	0.131%
65	17.051	2541	2544	2548	rVB	1677	1918	2.22%	0.264%
66	17.104	2550	2553	2555	rBV2	1407	2240	2.59%	0.308%
67	17.180	2562	2566	2568	rVB2	892	1211	1.40%	0.167%
68	17.221	2571	2573	2576	rBV2	883	992	1.15%	0.137%
69	17.321	2586	2590	2592	rBV	1250	1670	1.93%	0.230%
70	17.509	2619	2622	2625	rVB2	1701	2177	2.52%	0.300%
71	17.709	2653	2656	2659	rBV2	1268	1593	1.85%	0.219%
72	17.898	2683	2688	2690	rBV2	981	1311	1.52%	0.180%
73	18.115	2722	2725	2728	rVB	1442	1920	2.22%	0.264%
74	18.298	2754	2756	2758	rVB	1182	1011	1.17%	0.139%
75	18.327	2758	2761	2762	rBV	785	1055	1.22%	0.145%
76	18.692	2819	2823	2824	rVB	827	988	1.14%	0.136%

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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
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77	18.756	2832	2834	2837	rBV	857	1071	1.24%	0.147%

Sum of corrected areas: 726674

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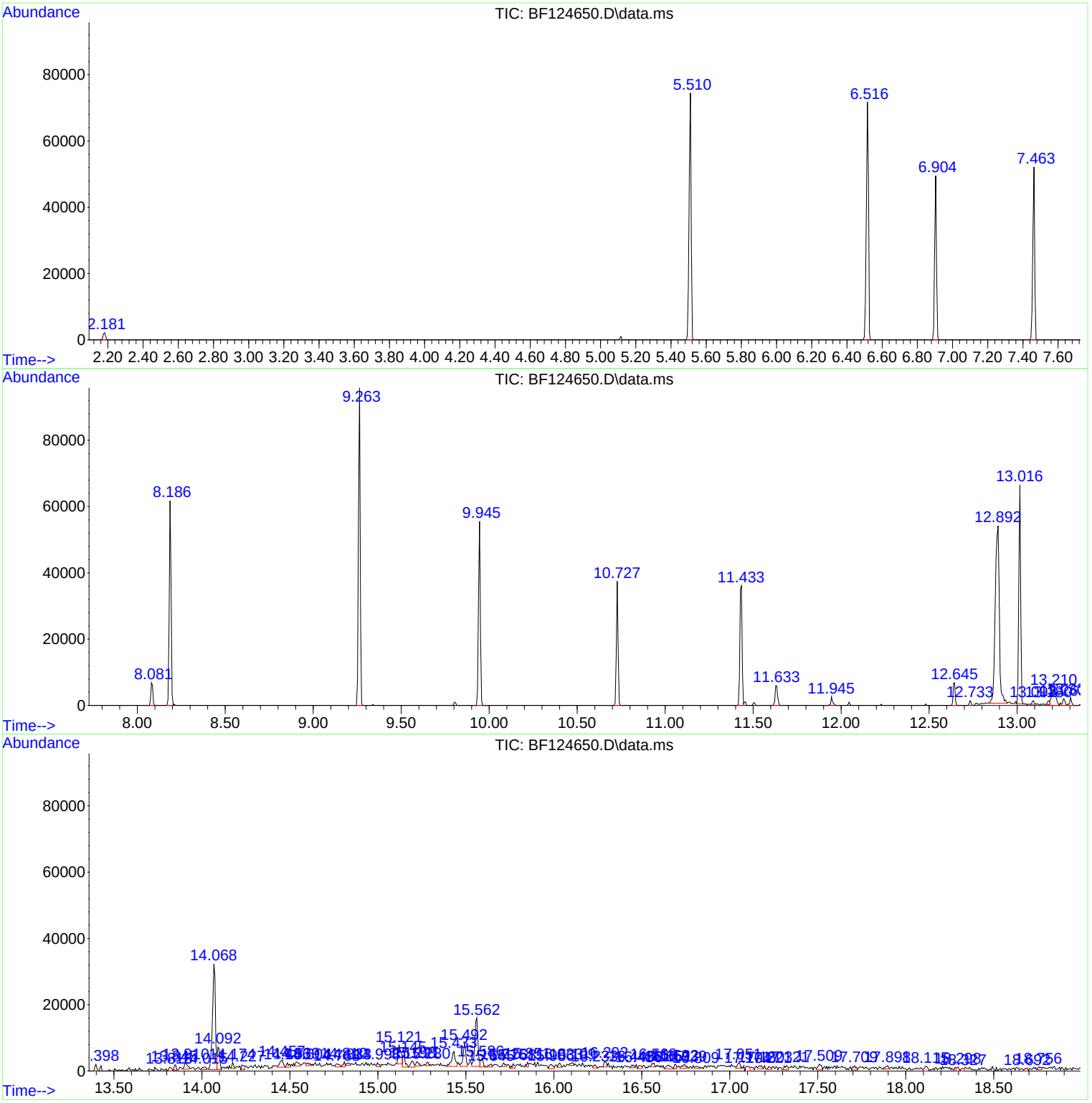
Instrument :
BNA_F
ClientSampleId :
FK-EF-01-020-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124650.D
Acq On : 21 Jul 2021 3:40
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

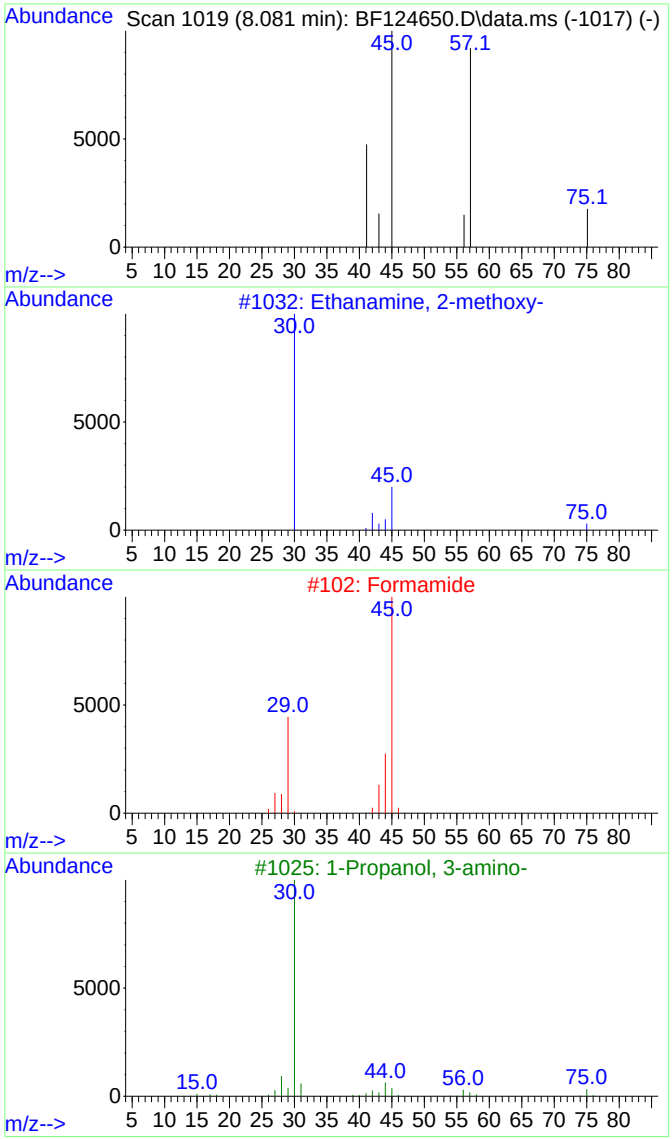
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

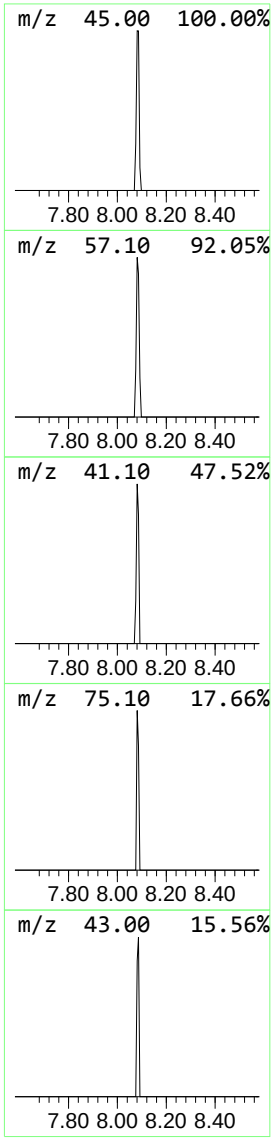
****

Peak Number 1 unknown8.081 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.081	2.42 ng	5434	Naphthalene-d8	8.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanamine, 2-methoxy-	75	C3H9NO	000109-85-3	4
2	Formamide	45	CH3NO	000075-12-7	3
3	1-Propanol, 3-amino-	75	C3H9NO	000156-87-6	3
4	Ethylamine	45	C2H7N	000075-04-7	3
5	Methane, nitroso-	45	CH3NO	000865-40-7	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124650.D
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Sample : M3047-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-020-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

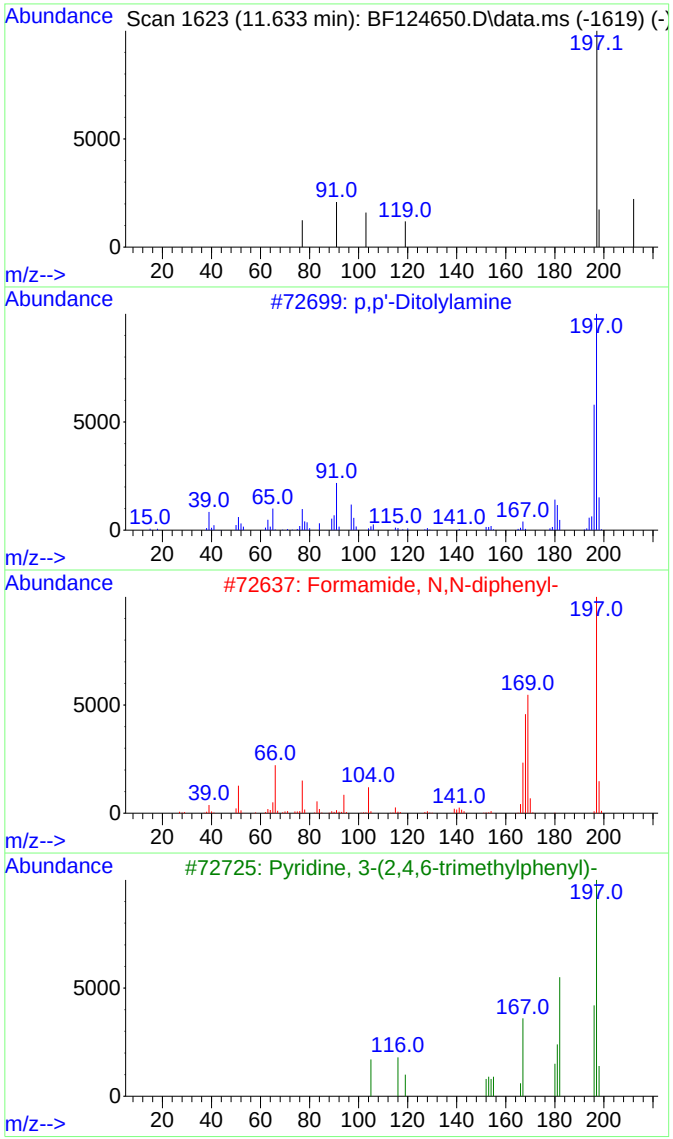
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

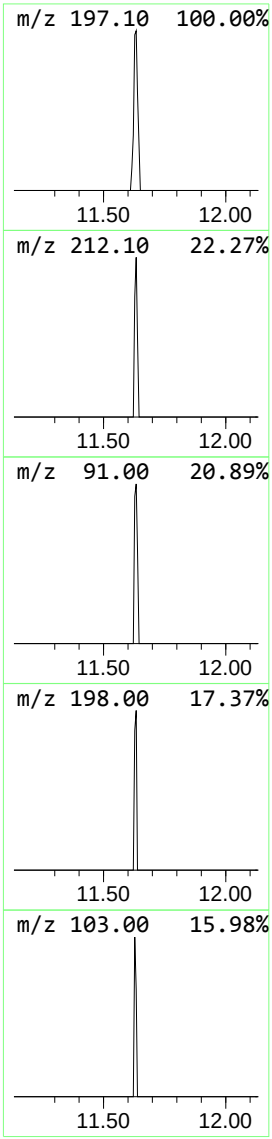
****

Peak Number 2 unknown11.633 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.633	3.70 ng	5869	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p,p'-Ditolylamine	197	C14H15N	000620-93-9	9
2	Formamide, N,N-diphenyl-	197	C13H11NO	000607-00-1	9
3	Pyridine, 3-(2,4,6-trimethylphen...	197	C14H15N	075601-34-2	9
4	Benzo[d,E]isocoumarin, 3,3-dimet...	212	C14H12O2	005723-17-1	9
5	Phenyl-p-tolyl-amine, N-methyl-	197	C14H15N	1000447-00-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124650.D
Acq On : 21 Jul 2021 3:40
Operator : JU/CG
Sample : M3047-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-020-ABCD

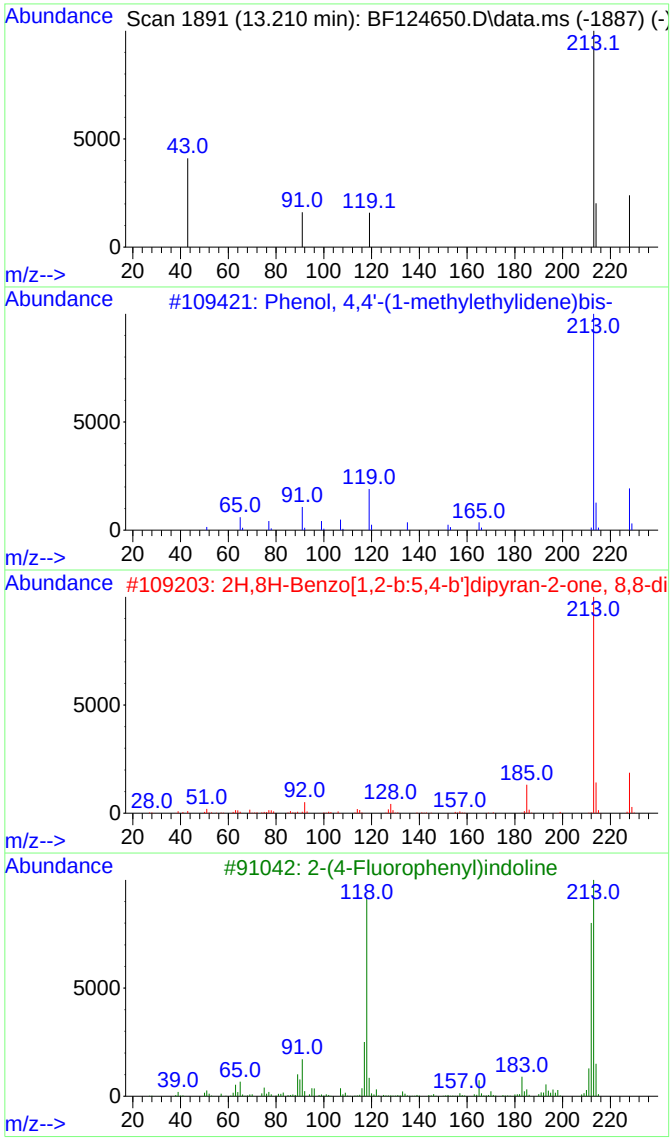
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

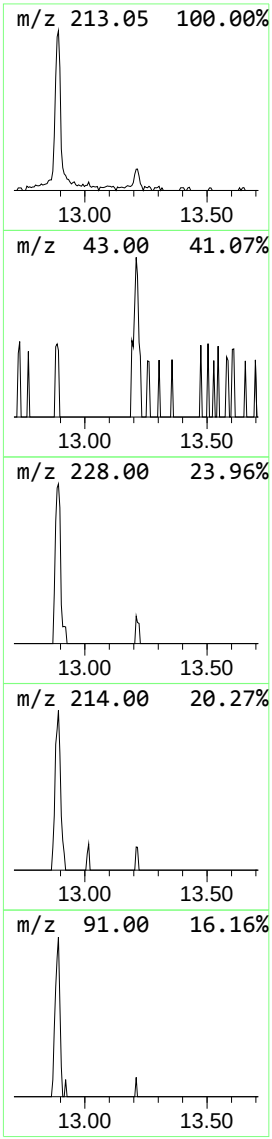
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Phenol, 4,4'-(1-methylethyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.210	4.56 ng	8365	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	64
2	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	9
3	2-(4-Fluorophenyl)indoline	213	C14H12FN	595548-71-3	9
4	Simetryn	213	C8H15N5S	001014-70-6	5
5	2-(p-Nitrobenzyl)pyridine	214	C12H10N2O2	000620-87-1	5





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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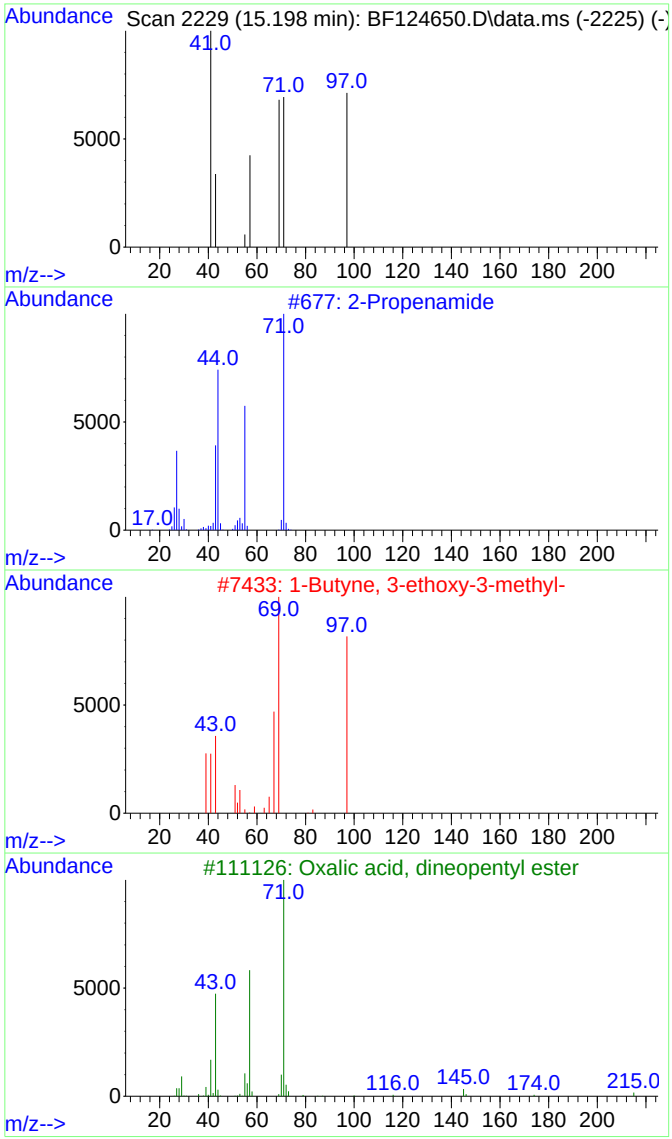
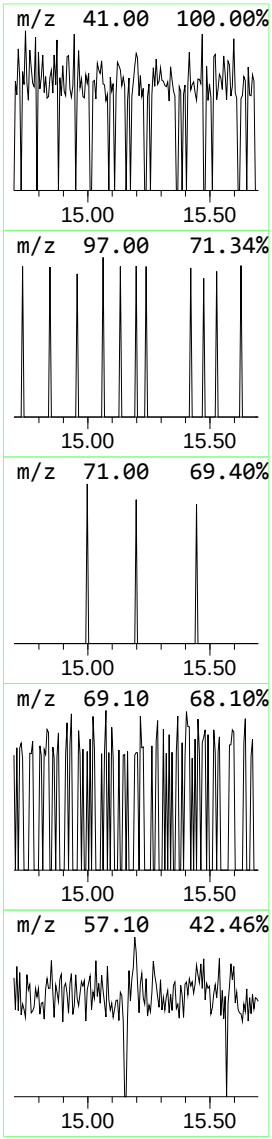
Peak Number 4 unknown15.198 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	2.66 ng	2363	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenamide	71	C3H5NO	000079-06-1	4
2	1-Butyne, 3-ethoxy-3-methyl-	112	C7H12O	007740-69-4	4
3	Oxalic acid, dineopentyl ester	230	C12H22O4	1010309-72-7	4
4	1H-Pyrrole-2,5-dione	97	C4H3NO2	000541-59-3	3
5	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	3





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

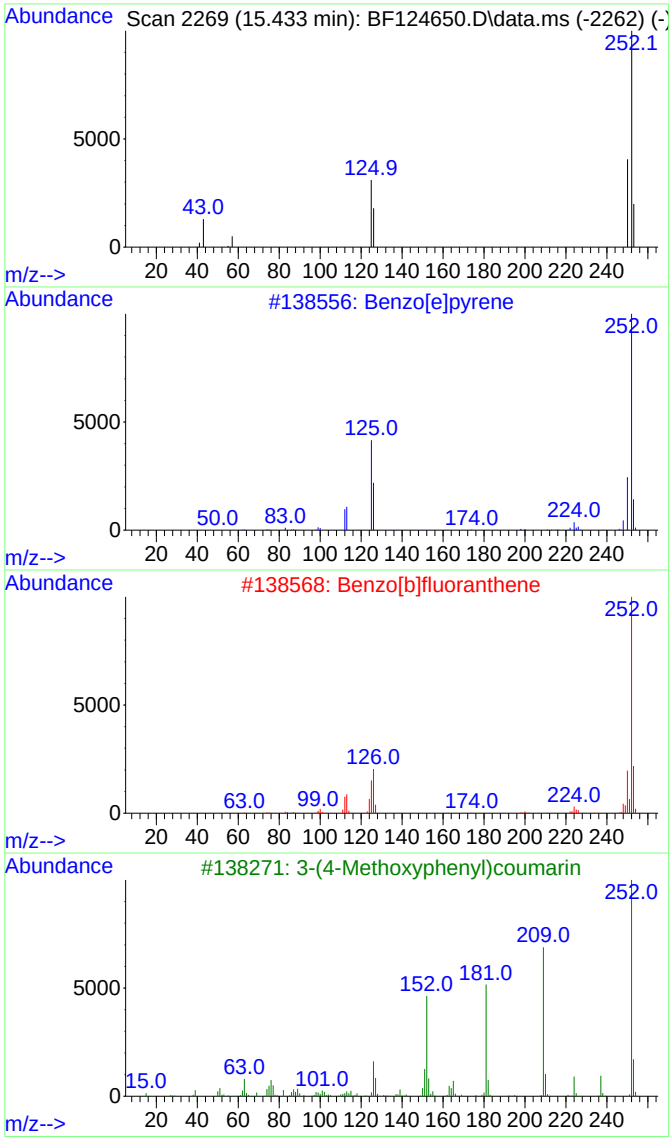
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

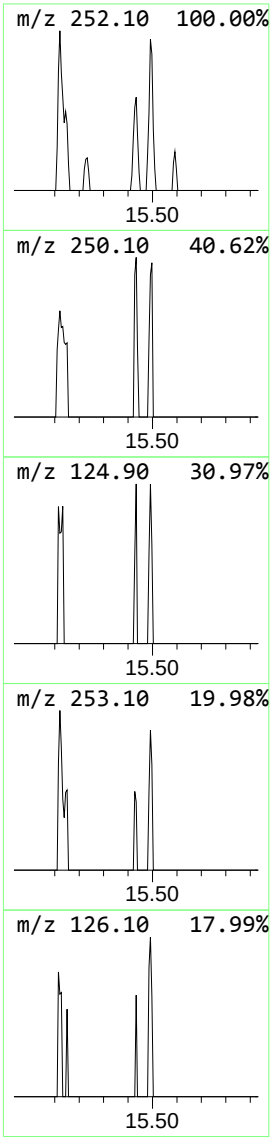
****

Peak Number 5 unknown15.433 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.433	7.46 ng	6635	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	45
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	9
3	3-(4-Methoxyphenyl)coumarin	252	C16H12O3	023000-33-1	9
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	9
5	3-[5-(3-Aminophenyl)-1,3,4-oxadi...	252	C14H12N4O	002588-85-4	9





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Data File : BF124650.D
Acq On : 21 Jul 2021 3:40
Operator : JU/CG
Sample : M3047-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-020-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.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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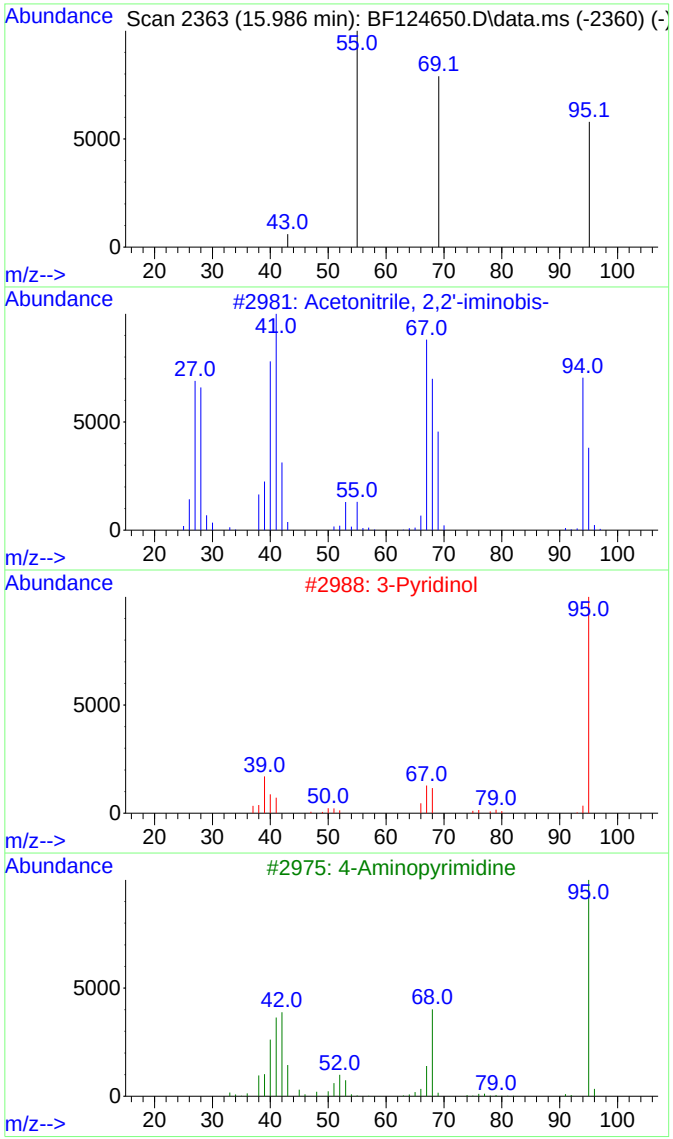
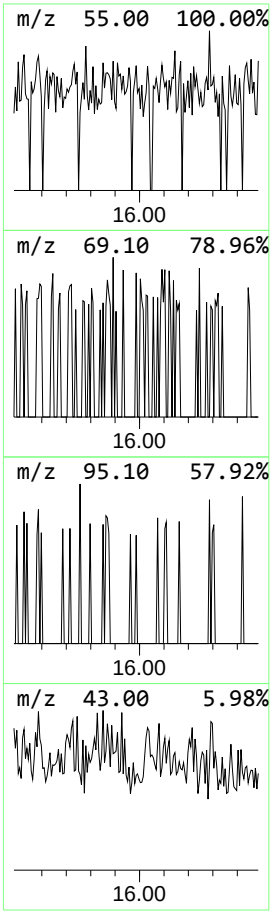
Peak Number 6 unknown15.986 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.986	2.05 ng	1827	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetonitrile, 2,2'-iminobis-	95	C4H5N3	000628-87-5	4
2	3-Pyridinol	95	C5H5NO	000109-00-2	2
3	4-Aminopyrimidine	95	C4H5N3	000591-54-8	2
4	Oxazole	69	C3H3NO	000288-42-6	2
5	1H-1,2,4-Triazole	69	C2H3N3	000288-88-0	2





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Data File : BF124650.D
Acq On : 21 Jul 2021 3:40
Operator : JU/CG
Sample : M3047-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-020-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.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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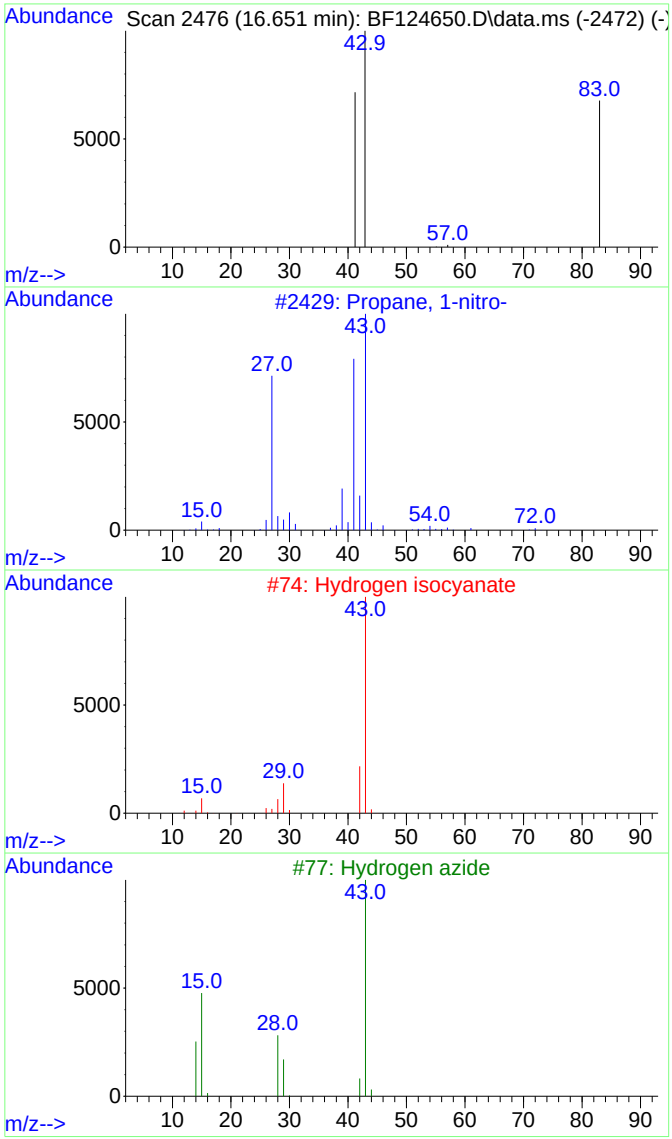
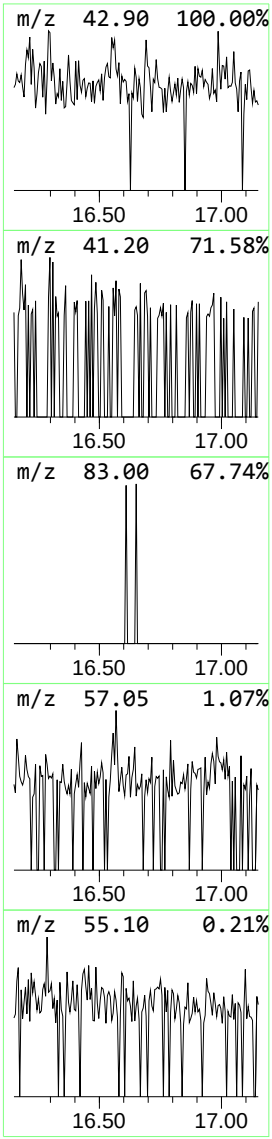
Peak Number 7 unknown16.651 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.651	2.23 ng	1980	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	1
2	Hydrogen isocyanate	43	CHNO	000075-13-8	1
3	Hydrogen azide	43	HN3	007782-79-8	1
4	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	1
5	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	1





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Data File : BF124650.D
Acq On : 21 Jul 2021 3:40
Operator : JU/CG
Sample : M3047-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-020-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.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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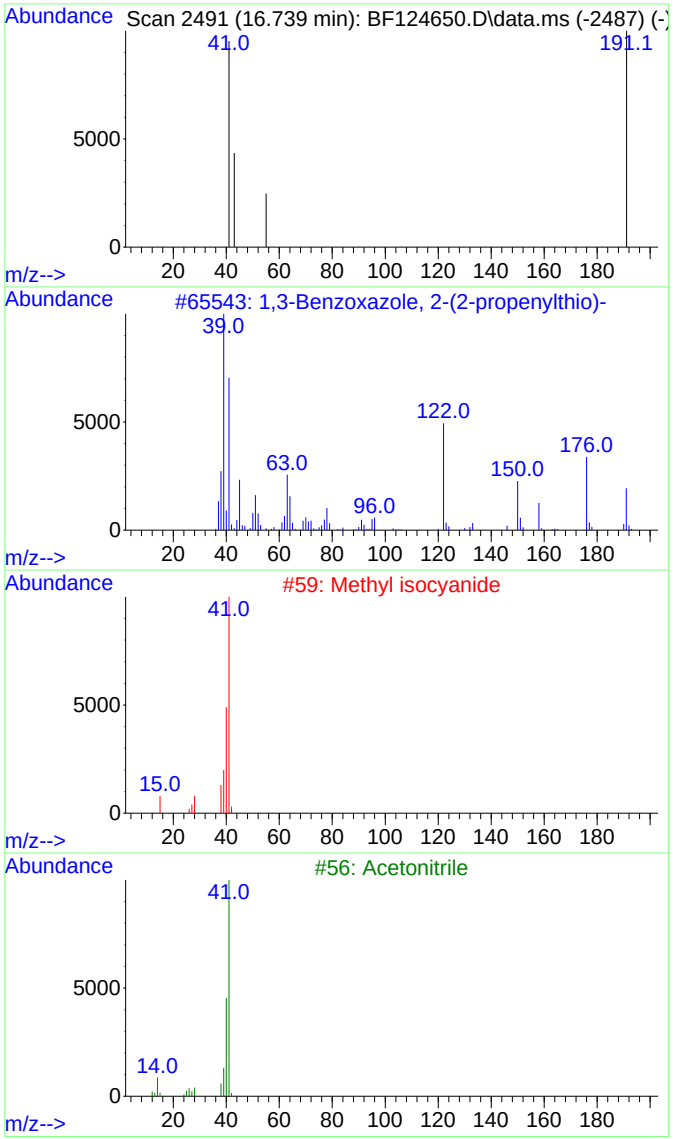
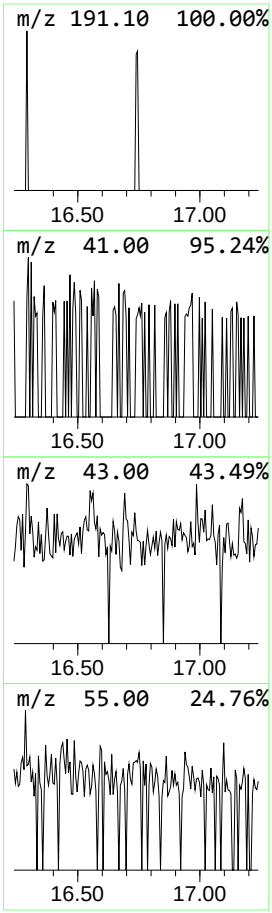
Peak Number 8 unknown16.739 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.739	2.02 ng	1796	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzoxazole, 2-(2-propenylth...	191	C10H9NOS	1010362-66-2	2
2	Methyl isocyanide	41	C2H3N	000593-75-9	1
3	Acetonitrile	41	C2H3N	000075-05-8	1
4	Benzisoxazole-2-acetic acid, hyd...	191	C9H9N3O2	055244-10-5	1
5	Butyramide, 4-chloro-N-3-methylb...	191	C9H18ClNO	1000419-94-5	1





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Data File : BF124650.D
Acq On : 21 Jul 2021 3:40
Operator : JU/CG
Sample : M3047-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-020-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.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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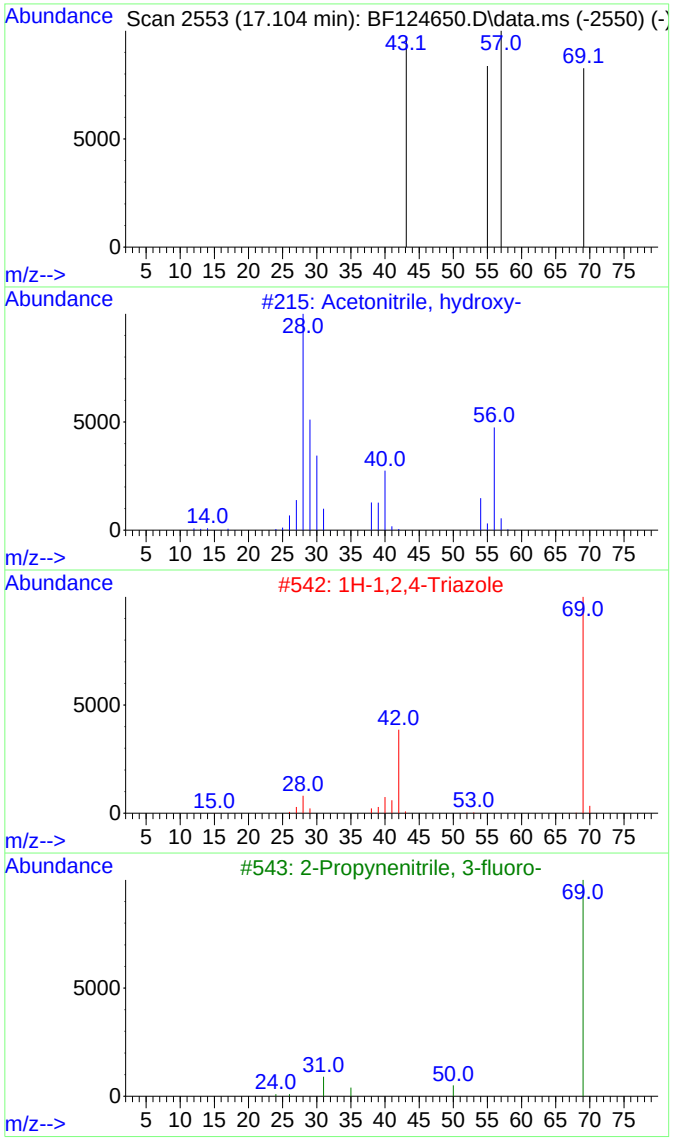
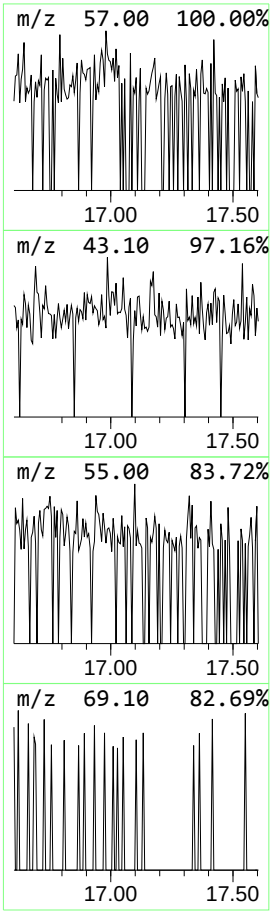
Peak Number 9 unknown17.104 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.104	2.52 ng	2240	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	3
2	1H-1,2,4-Triazole	69	C2H3N3	000288-88-0	2
3	2-Propynenitrile, 3-fluoro-	69	C3FN	032038-83-8	2
4	Methane, isocyanato-	57	C2H3NO	000624-83-9	1
5	Azetidine	57	C3H7N	000503-29-7	1





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Data File : BF124650.D
Acq On : 21 Jul 2021 3:40
Operator : JU/CG
Sample : M3047-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-020-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.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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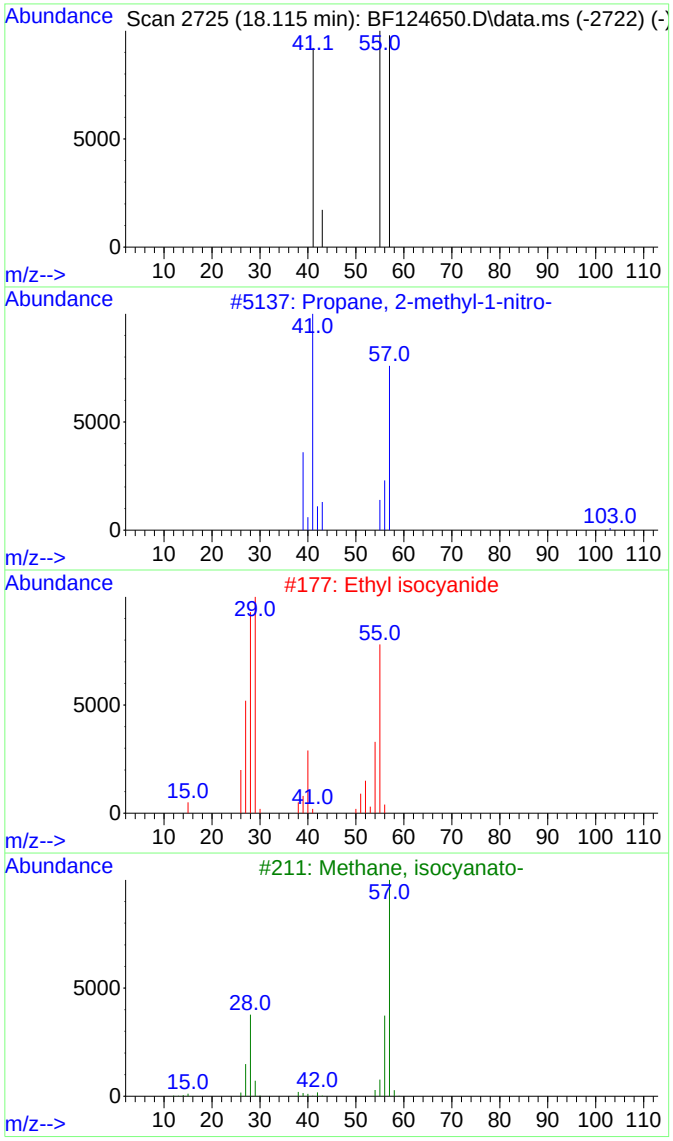
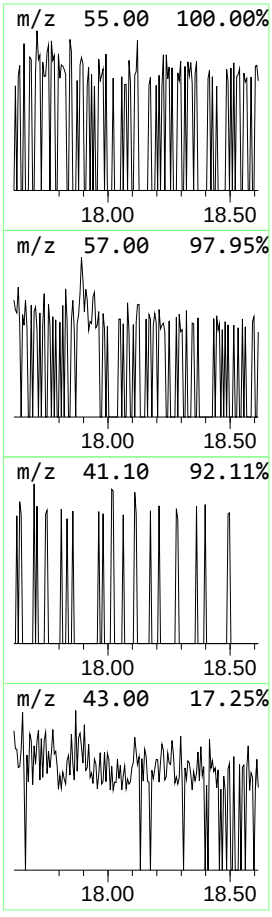
Peak Number 10 unknown18.115 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.115	2.16 ng	1920	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-1-nitro-	103	C4H9NO2	000625-74-1	2
2	Ethyl isocyanide	55	C3H5N	000624-79-3	1
3	Methane, isocyanato-	57	C2H3NO	000624-83-9	1
4	Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	1
5	Azetidine	57	C3H7N	000503-29-7	1





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124650.D
Acq On : 21 Jul 2021 3:40
Operator : JU/CG
Sample : M3047-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-020-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
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
unknown8.081	8.081	2.4	ng	5434	2	8.186	44837	20.0
unknown11.633	11.633	3.7	ng	5869	4	11.433	31730	20.0
Phenol, 4,4'-(1...	13.210	4.6	ng	8365	5	14.068	36715	20.0
unknown15.198	15.198	2.7	ng	2363	6	15.562	17791	20.0
unknown15.433	15.433	7.5	ng	6635	6	15.562	17791	20.0
unknown15.986	15.986	2.0	ng	1827	6	15.562	17791	20.0
unknown16.651	16.651	2.2	ng	1980	6	15.562	17791	20.0
unknown16.739	16.739	2.0	ng	1796	6	15.562	17791	20.0
unknown17.104	17.104	2.5	ng	2240	6	15.562	17791	20.0
unknown18.115	18.115	2.2	ng	1920	6	15.562	17791	20.0