LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124773.D
Acq On : 26 Jul 2021 19:47
Operator : JU/CG
Sample : M3143-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STOCK-PILE-2

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: BF124773.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	10	13	17	rBB	7647	8436	8.72%	1.162%
2	5.098	509	512	514	rBB	1613	1732	1.79%	0.239%
3	5.493	575	579	582	rBB	117047	96721	100.00%	13.324%
4	6.498	746	750	753	rBV	110806	93393	96.56%	12.866%
5	6.875	811	814	817	rBB	37133	26021	26.90%	3.585%
6	7.434	905	909	912	rBB	68936	60221	62.26%	8.296%
7	8.057	1012	1015	1018	rBB	5366	4500	4.65%	0.620%
8	8.157	1029	1032	1035	rBB	46678	32771	33.88%	4.515%
9	9.233	1211	1215	1218	rBV	113106	92372	95.50%	12.725%
10	9.910	1327	1330	1333	rBB	39688	31043	32.10%	4.276%
11	10.698	1461	1464	1467	rBB	66108	47228	48.83%	6.506%
12	11.398	1580	1583	1586	rBV	34089	27097	28.02%	3.733%
13	11.422	1586	1587	1591	rVB	4495	2799	2.89%	0.386%
14	11.916	1669	1671	1675	rBB	3248	2181	2.25%	0.300%
15	12.610	1787	1789	1792	rBB	7478	5584	5.77%	0.769%
16	12.839	1826	1828	1831	rVB	7590	6034	6.24%	0.831%
17	12.986	1849	1853	1856	rBB	98777	79191	81.88%	10.909%
18	13.792	1987	1990	1992	rBV	1159	1318	1.36%	0.182%
19	13.892	2003	2007	2016	rVB5	2795	4834	5.00%	0.666%
20	14.039	2029	2032	2035	rBV	30072	25094	25.94%	3.457%
21	14.063	2035	2036	2038	rVB	1906	1267	1.31%	0.175%
22	14.298	2074	2076	2078	rBV	1164	1250	1.29%	0.172%
23	14.539	2112	2117	2120	rBV4	1668	2358	2.44%	0.325%
24	14.957	2186	2188	2196	rVB5	2115	2992	3.09%	0.412%
25	15.080	2205	2209	2213	rBV4	2174	3818	3.95%	0.526%
26	15.151	2218	2221	2225	rVB4	2543	3085	3.19%	0.425%
27	15.204	2227	2230	2232	rBV2	1533	2222	2.30%	0.306%
28	15.251	2237	2238	2243	rVV3	2678	3484	3.60%	0.480%
29	15.304	2246	2247	2251	rVB3	1500	1693	1.75%	0.233%
30	15.445	2267	2271	2274	rBV2	1194	1379	1.43%	0.190%
31	15.515	2279	2283	2288	rBV	19193	21995	22.74%	3.030%
32	15.968	2357	2360	2362	rBV2	1149	1365	1.41%	0.188%
33	16.133	2386	2388	2391	rVB3	1618	1202	1.24%	0.166%
34	16.233	2404	2405	2408	rVB2	2072	1414	1.46%	0.195%
35	16.268	2408	2411	2413	rBV2	1773	1441	1.49%	0.199%
36	16.298	2413	2416	2417	rBV2	1068	1121	1.16%	0.154%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124773.D
Acq On : 26 Jul 2021 19:47
Operator : JU/CG
Sample : M3143-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STOCK-PILE-2

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	16.374	2427	2429	2432	rVB2	1267	1233	1.27%	0.170%
38	16.492	2447	2449	2455	rVB3	1609	2306	2.38%	0.318%
39	16.598	2464	2467	2470	rBV2	1392	1484	1.53%	0.204%
40	16.698	2481	2484	2487	rVB	1018	1254	1.30%	0.173%
41	16.768	2493	2496	2499	rBV3	1464	1576	1.63%	0.217%
42	17.086	2547	2550	2554	rBV3	1132	1549	1.60%	0.213%
43	17.615	2635	2640	2641	rBV4	922	1259	1.30%	0.173%
44	17.756	2662	2664	2669	rVB3	1288	1470	1.52%	0.203%
45	17.951	2695	2697	2700	rVB2	1682	1354	1.40%	0.187%
46	17.974	2700	2701	2704	rBV2	1621	1145	1.18%	0.158%
47	18.103	2720	2723	2725	rVB	1418	1438	1.49%	0.198%
48	18.127	2725	2727	2729	rBV	1125	1188	1.23%	0.164%
49	18.168	2732	2734	2739	rVB2	981	1592	1.65%	0.219%
50	18.327	2758	2761	2762	rBV2	1161	1168	1.21%	0.161%
51	18.521	2791	2794	2798	rBV3	1070	1525	1.58%	0.210%
52	18.774	2835	2837	2841	rBV4	1372	1460	1.51%	0.201%
53	18.886	2851	2856	2860	rBV3	1128	2244	2.32%	0.309%

Sum of corrected areas: 725901

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Misc :
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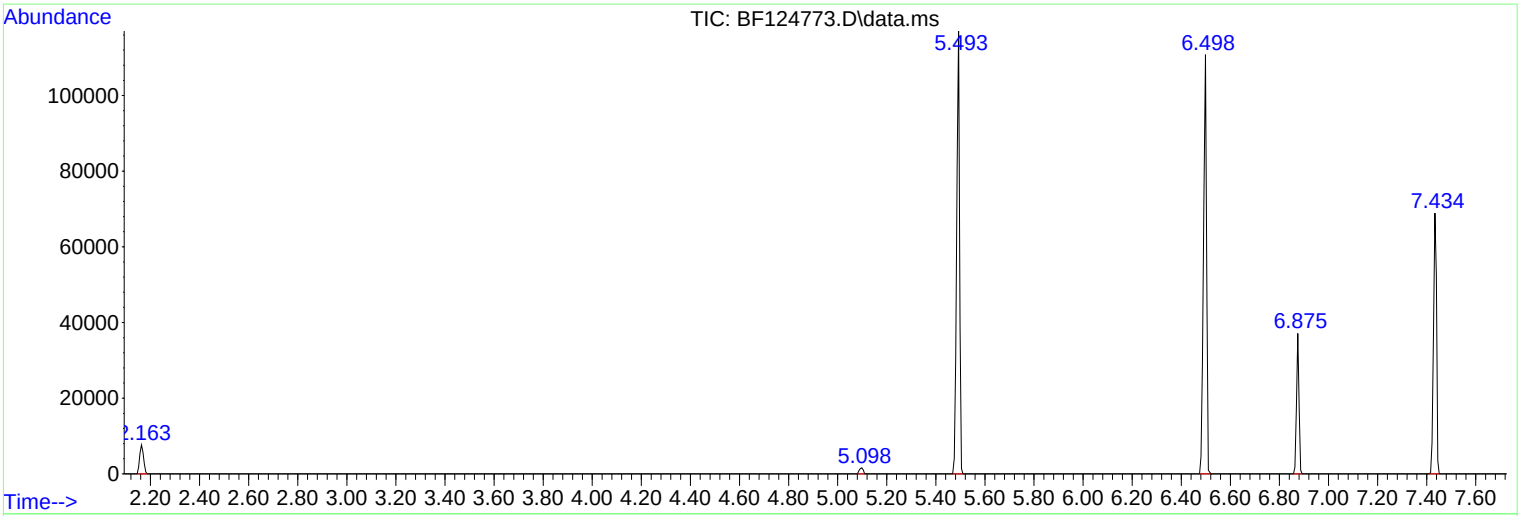
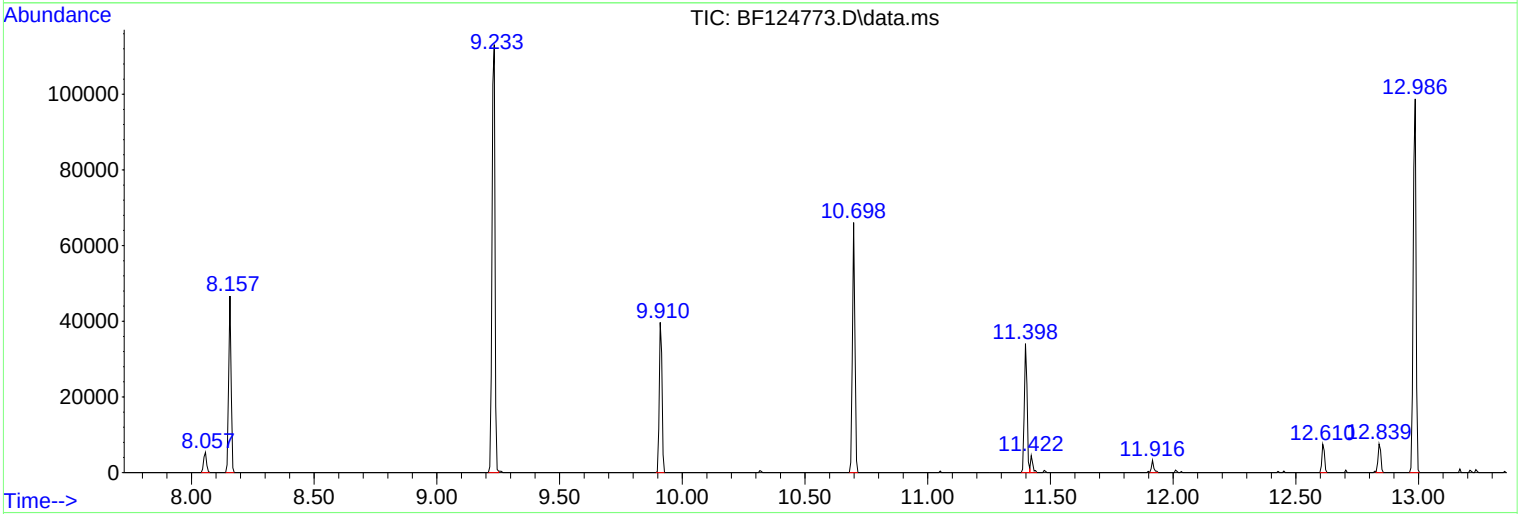
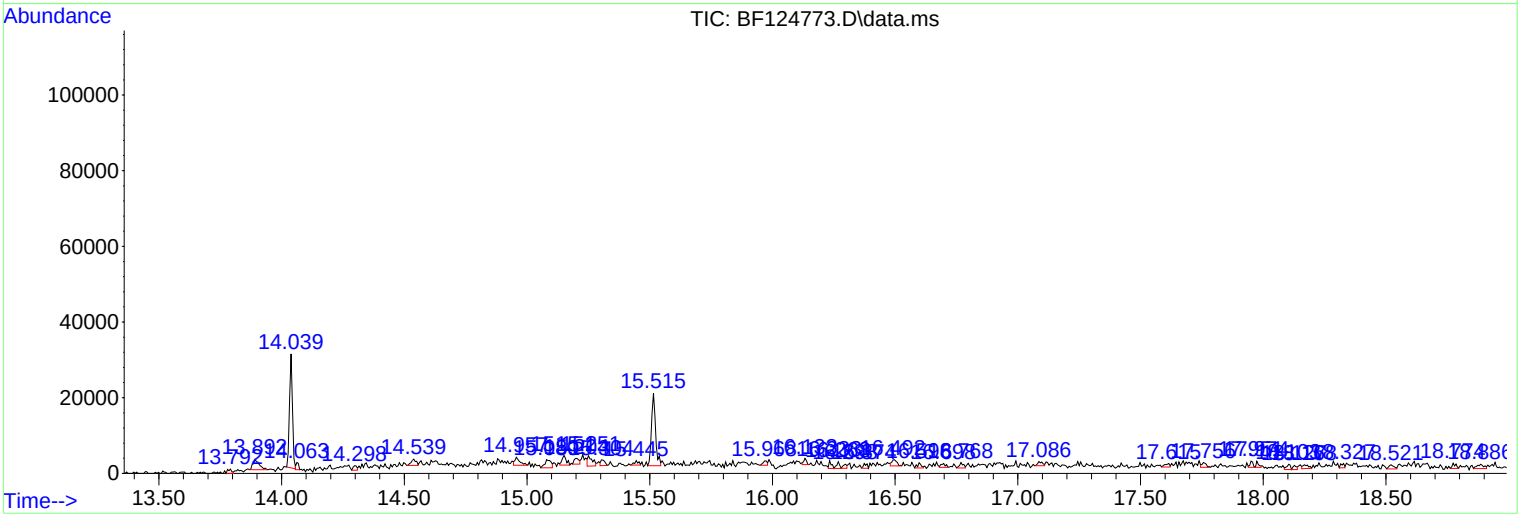
Instrument :
BNA_F
ClientSampleId :
STOCK-PILE-2

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124773.D
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Operator : JU/CG
Sample : M3143-03
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Instrument :
BNA_F
ClientSampleId :
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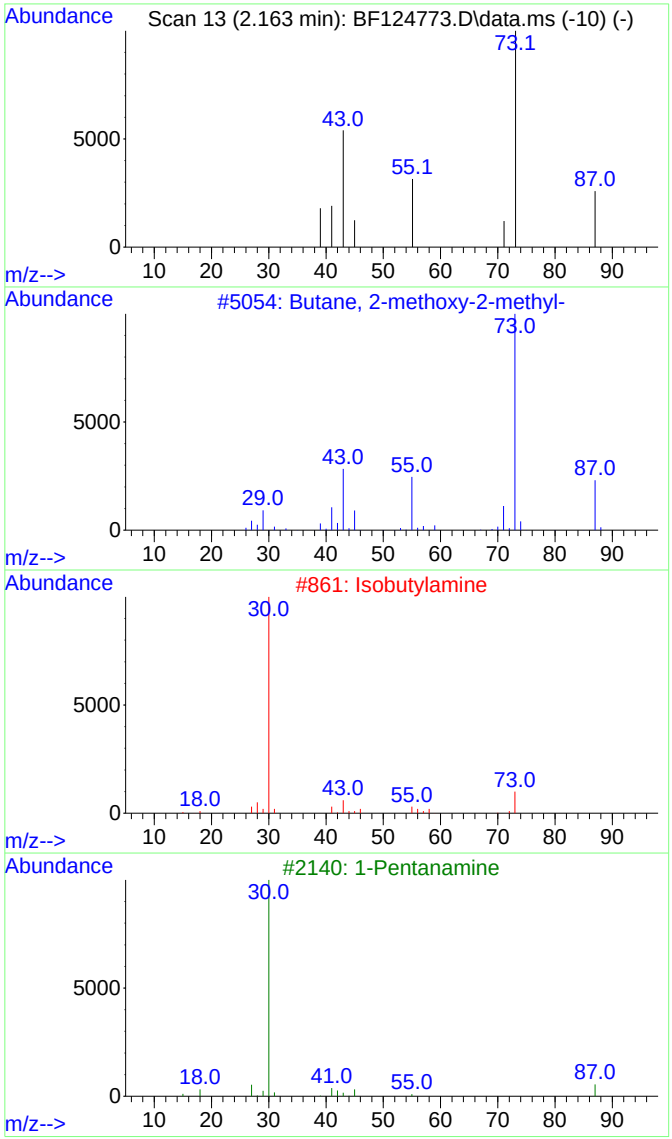
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

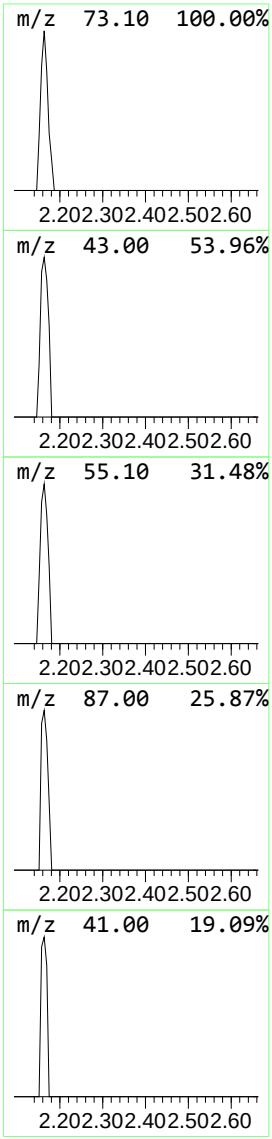
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	6.48 ng	8436	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2	Isobutylamine	73	C4H11N	000078-81-9	5
3	1-Pentanamine	87	C5H13N	000110-58-7	4
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	4
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124773.D
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Operator : JU/CG
Sample : M3143-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STOCK-PILE-2

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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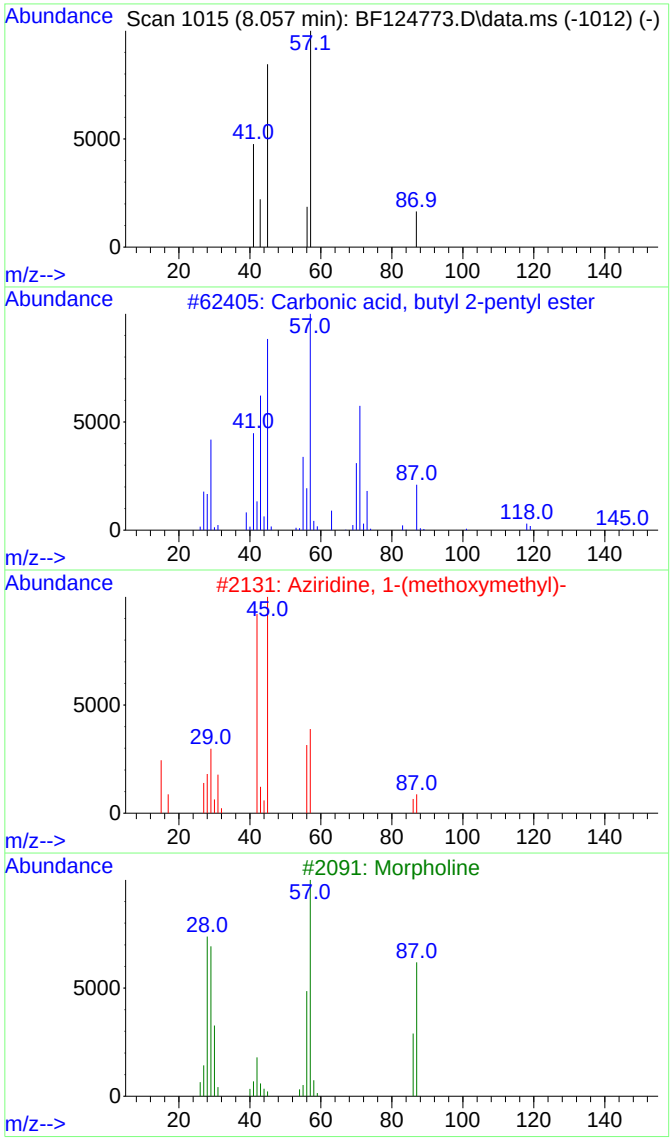
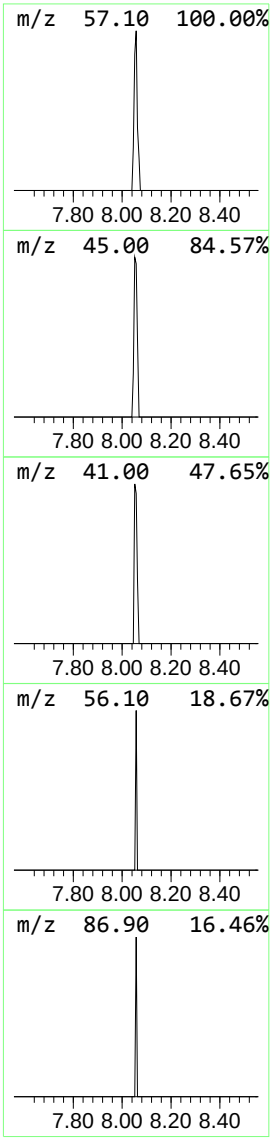
Peak Number 2 unknown8.057 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.057	2.75 ng	4500	Naphthalene-d8	8.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, butyl 2-pentyl ester	188	C10H20O3	1000357-84-0	9
2	Aziridine, 1-(methoxymethyl)-	87	C4H9NO	001497-83-2	4
3	Morpholine	87	C4H9NO	000110-91-8	4
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	4
5	Neopentylamine	87	C5H13N	005813-64-9	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124773.D
Acq On : 26 Jul 2021 19:47
Operator : JU/CG
Sample : M3143-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STOCK-PILE-2

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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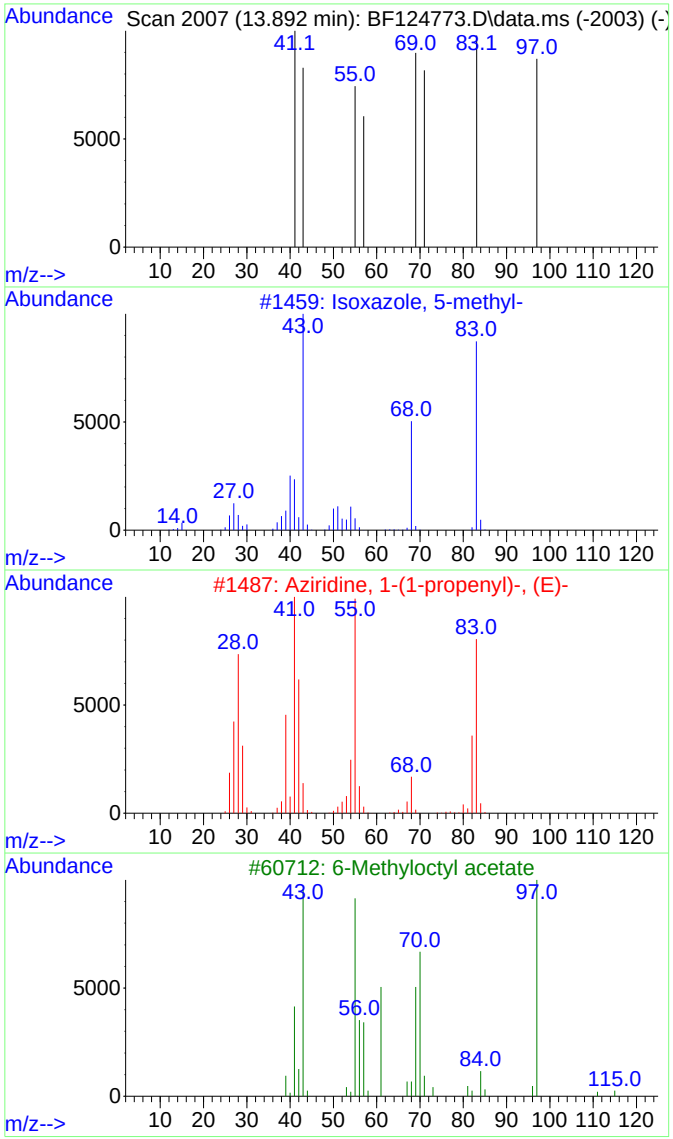
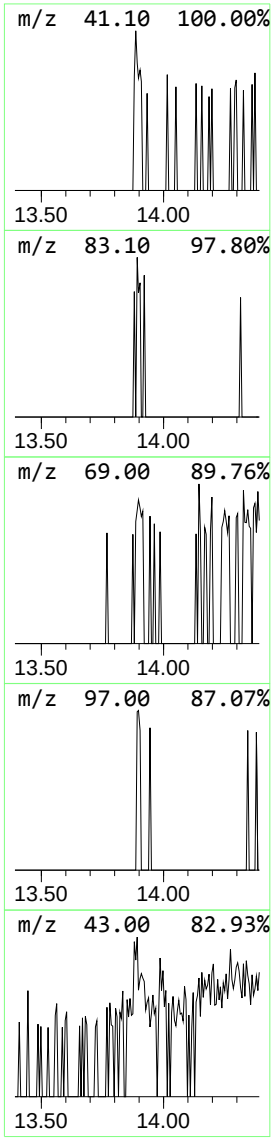
Peak Number 3 unknown13.892 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	3.85 ng	4834	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	4
2	Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	4
3	6-Methyloctyl acetate	186	C11H22O2	1000439-66-5	4
4	2,3'-Bifuran, octahydro-	142	C8H14O2	073373-15-6	4
5	Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124773.D
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Sample : M3143-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STOCK-PILE-2

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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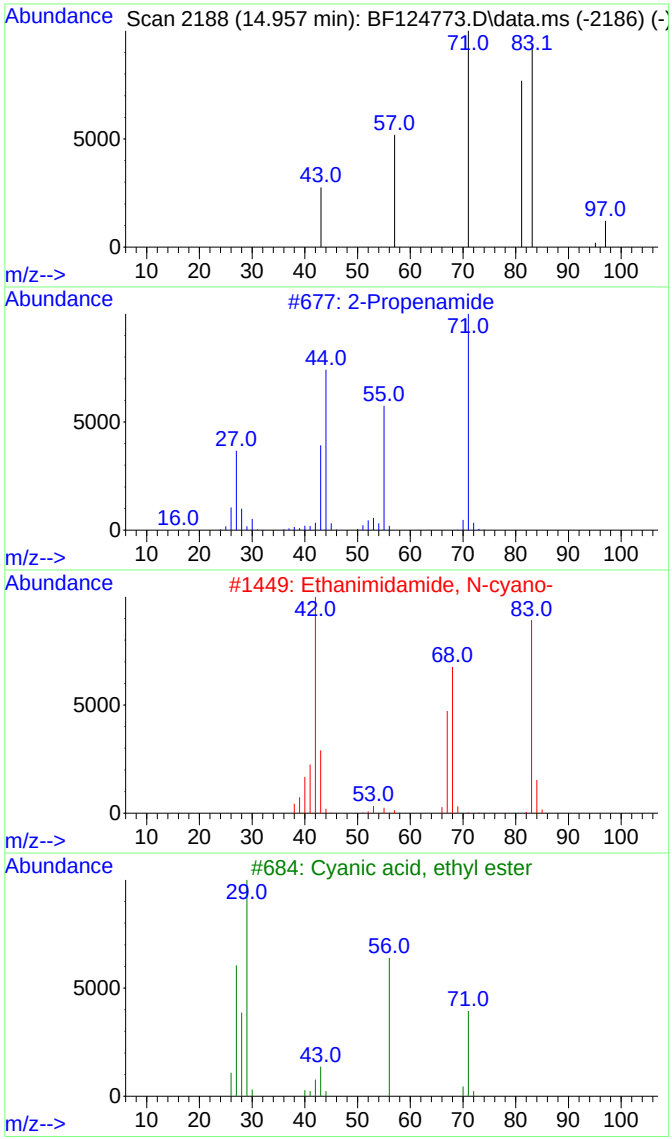
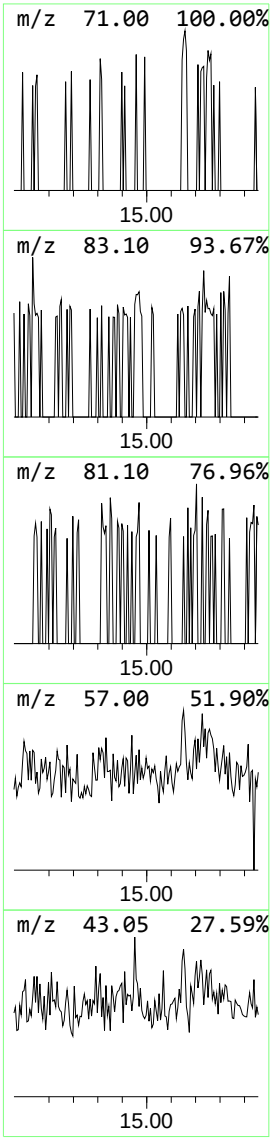
Peak Number 4 unknown14.957 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.957	2.72 ng	2992	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenamide	71	C3H5NO	000079-06-1	4
2	Ethanimidamide, N-cyano-	83	C3H5N3	056563-07-6	3
3	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	3
4	2,4-Dimethylcyclopentanol	114	C7H14O	089794-28-5	2
5	1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	2





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Operator : JU/CG
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ClientSampleId :
STOCK-PILE-2

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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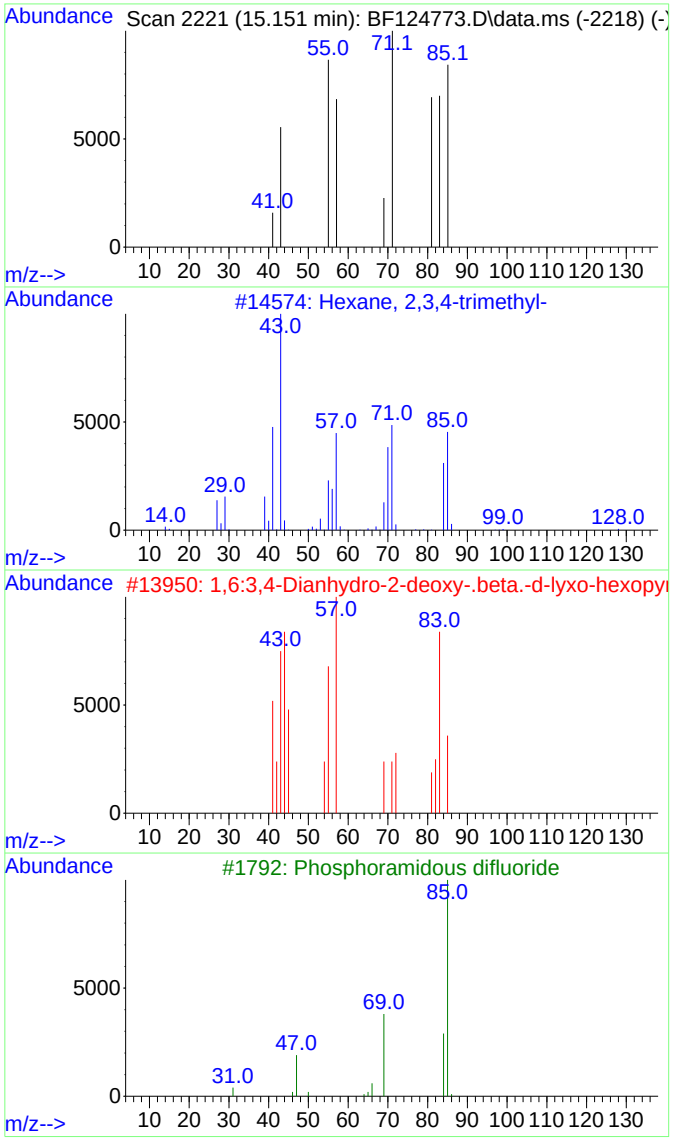
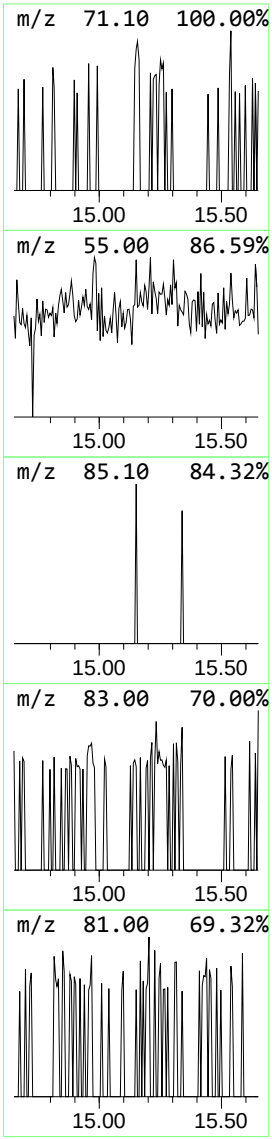
Peak Number 5 unknown15.151 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.151	2.81 ng	3085	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	9
2	1,6:3,4-Dianhydro-2-deoxy-.beta....	128	C6H8O3	050767-53-8	9
3	Phosphoramidous difluoride	85	F2H2NP	025757-74-8	4
4	Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	4
5	2-Propenamide	71	C3H5NO	000079-06-1	4





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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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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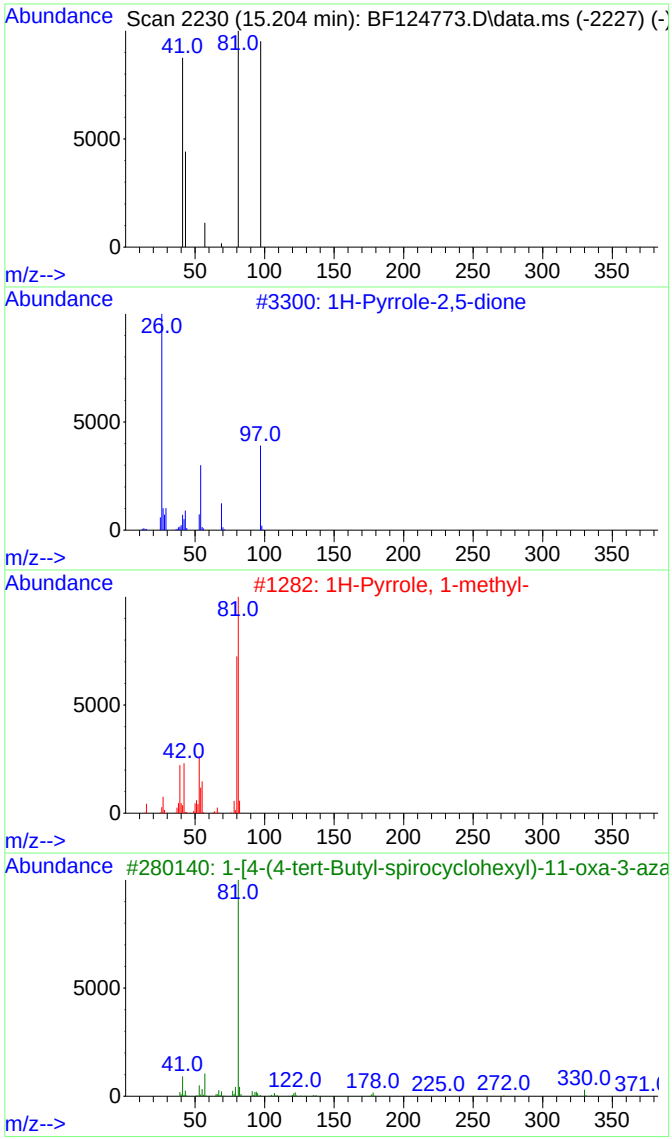
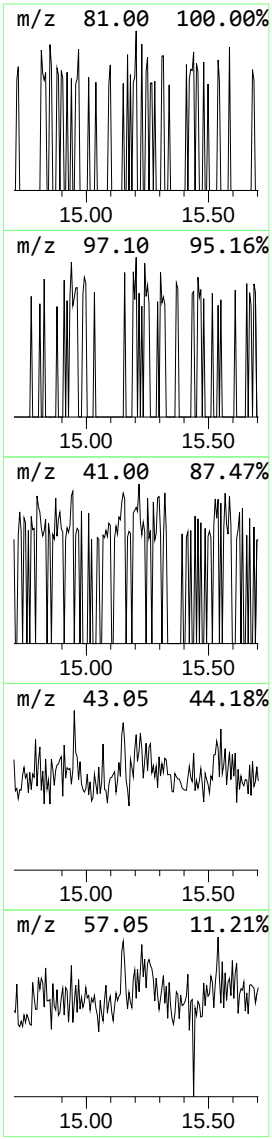
Peak Number 6 unknown15.204 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.204	2.02 ng	2222	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrrole-2,5-dione	97	C4H3NO2	000541-59-3	2
2	1H-Pyrrole, 1-methyl-	81	C5H7N	000096-54-8	2
3	1-[4-(4-tert-Butyl-spirocyclohex...	371	C20H28F3NO2	1000301-43-3	2
4	1-Allylazetidine	97	C6H11N	1000195-02-5	2
5	Formic acid, trans-4-methylcyclo...	142	C8H14O2	1000368-24-5	2





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Data File : BF124773.D
Acq On : 26 Jul 2021 19:47
Operator : JU/CG
Sample : M3143-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STOCK-PILE-2

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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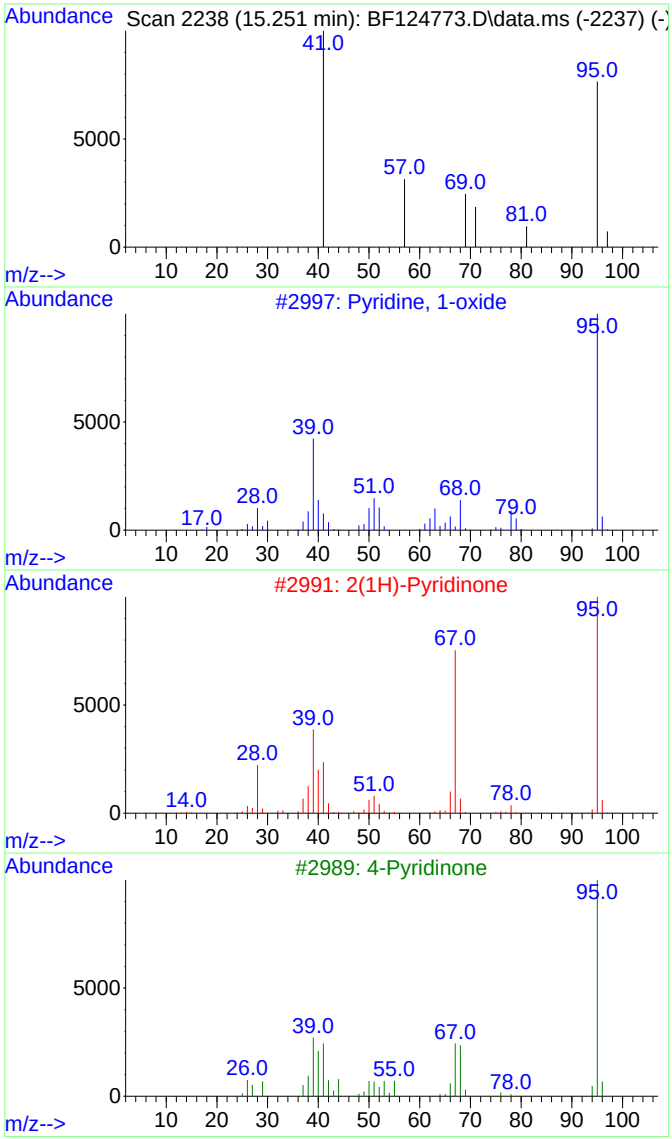
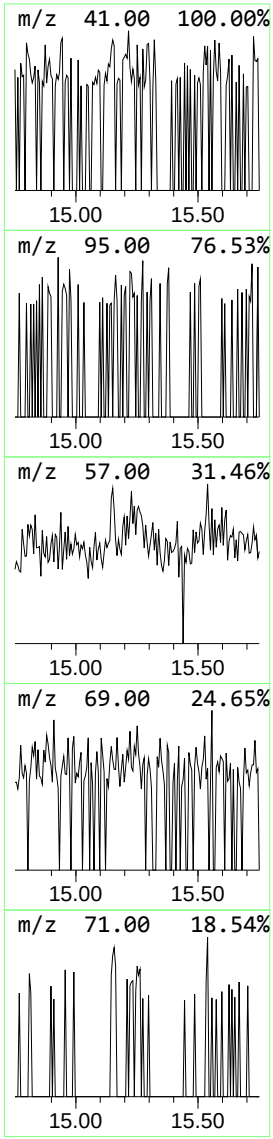
Peak Number 7 unknown15.251 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.251	3.17 ng	3484	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 1-oxide	95	C5H5NO	000694-59-7	2
2	2(1H)-Pyridinone	95	C5H5NO	000142-08-5	2
3	4-Pyridinone	95	C5H5NO	1000433-50-4	2
4	1H-1,2,4-Triazole, 1-vinyl-	95	C4H5N3	002764-83-2	2
5	4-Aminopyrimidine	95	C4H5N3	000591-54-8	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124773.D
Acq On : 26 Jul 2021 19:47
Operator : JU/CG
Sample : M3143-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STOCK-PILE-2

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

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TIC Integration Parameters: LSCINT.P

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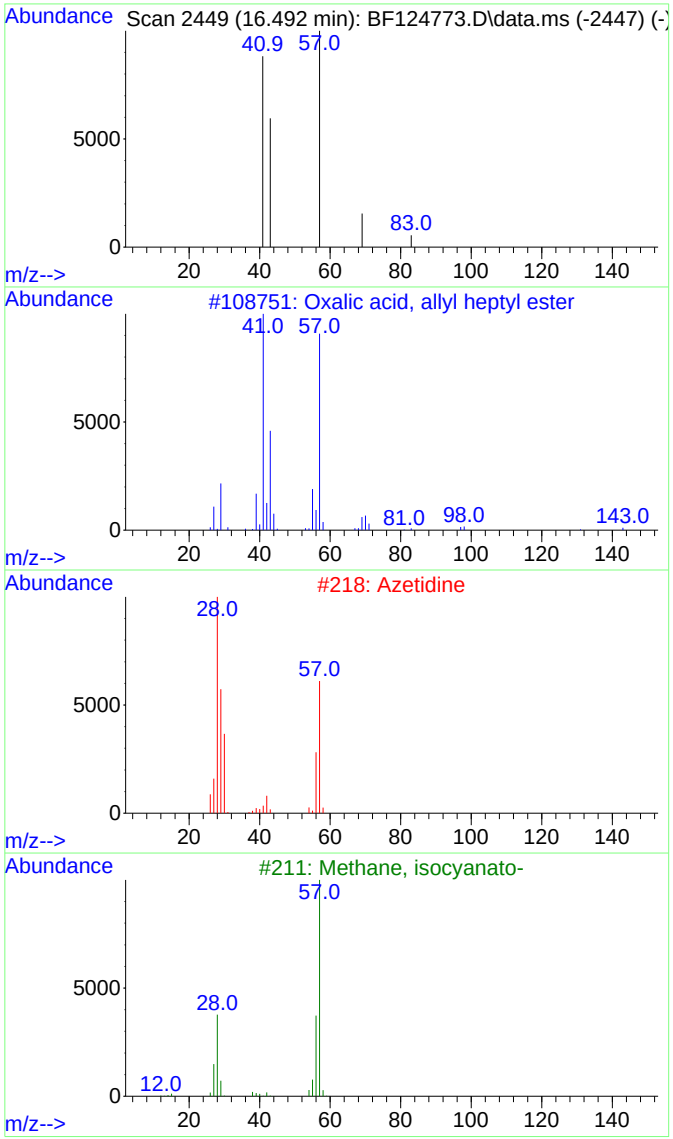
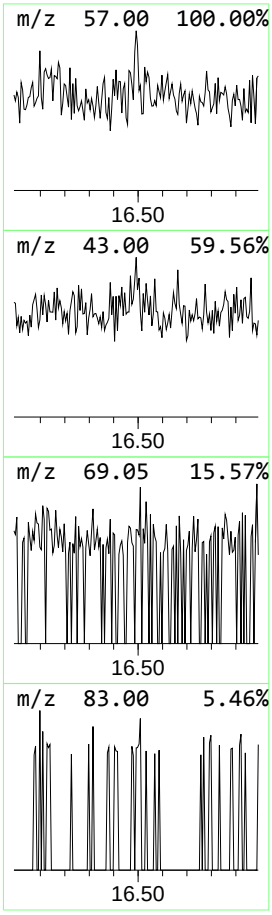
Peak Number 8 unknown16.492 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.492	2.10 ng	2306	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, allyl heptyl ester	228	C12H20O4	1000309-23-5	2
2	Azetidine	57	C3H7N	000503-29-7	1
3	Methane, isocyanato-	57	C2H3NO	000624-83-9	1
4	Acetonitrile	41	C2H3N	000075-05-8	1
5	Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	1





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124773.D
Acq On : 26 Jul 2021 19:47
Operator : JU/CG
Sample : M3143-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STOCK-PILE-2

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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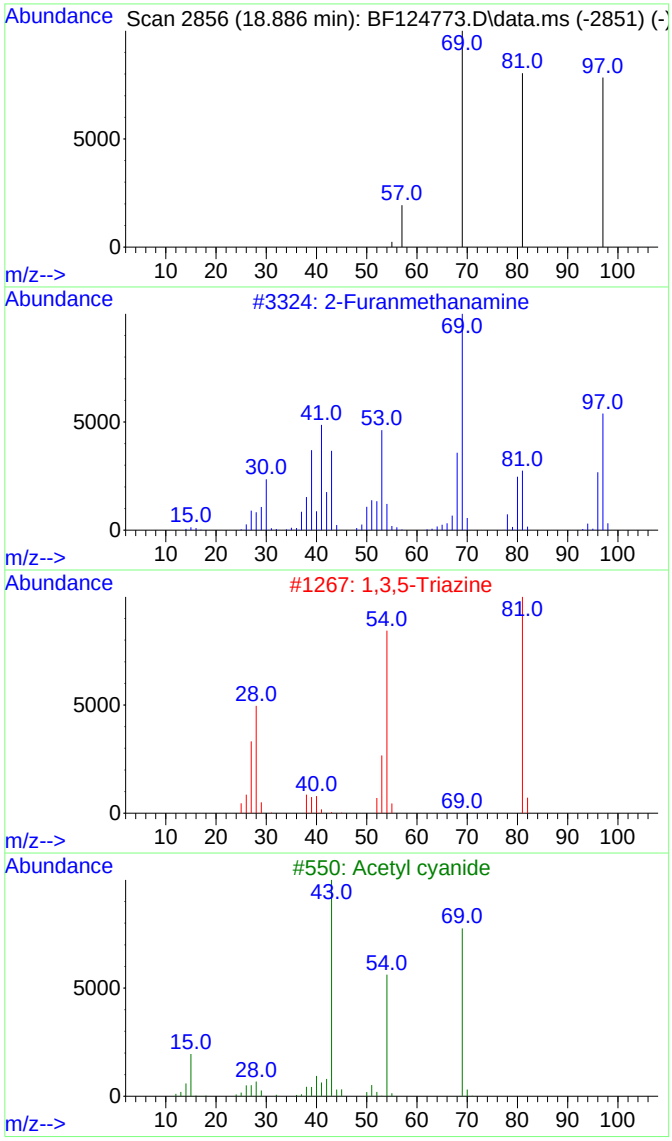
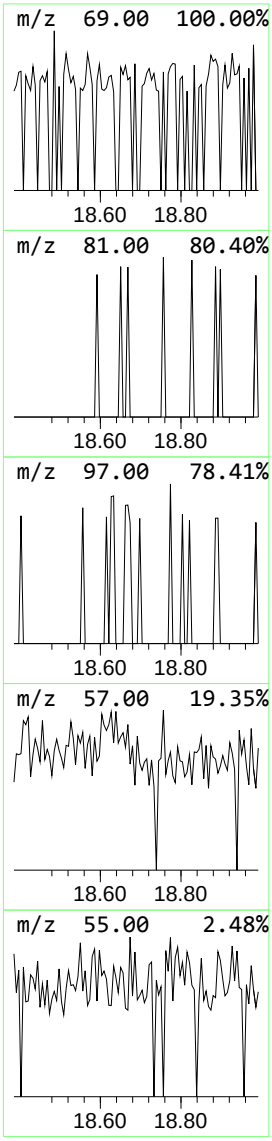
Peak Number 9 unknown18.886 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.886	2.04 ng	2244	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Furanmethanamine	97	C5H7NO	000617-89-0	5
2	1,3,5-Triazine	81	C3H3N3	000290-87-9	3
3	Acetyl cyanide	69	C3H3NO	000631-57-2	3
4	1H-Pyrrole-2,5-dione	97	C4H3NO2	000541-59-3	3
5	Aziridine, 2-methylene-1-(1-meth...	97	C6H11N	055268-35-4	3





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124773.D
Acq On : 26 Jul 2021 19:47
Operator : JU/CG
Sample : M3143-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STOCK-PILE-2

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.163	6.5	ng	8436	1	6.875	26021	20.0
unknown8.057	8.057	2.8	ng	4500	2	8.157	32771	20.0
unknown13.892	13.892	3.9	ng	4834	5	14.039	25094	20.0
unknown14.957	14.957	2.7	ng	2992	6	15.515	21995	20.0
unknown15.151	15.151	2.8	ng	3085	6	15.515	21995	20.0
unknown15.204	15.204	2.0	ng	2222	6	15.515	21995	20.0
unknown15.251	15.251	3.2	ng	3484	6	15.515	21995	20.0
unknown16.492	16.492	2.1	ng	2306	6	15.515	21995	20.0
unknown18.886	18.886	2.0	ng	2244	6	15.515	21995	20.0