LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124748.D
Acq On : 24 Jul 2021 15:28
Operator : JU/CG
Sample : M3117-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NJ-CLEAN-7

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: BF124748.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	9208	9946	8.59%	1.299%
2	5.087	507	510	513	rBB	2452	2679	2.31%	0.350%
3	5.481	573	577	580	rBB	110151	97947	84.58%	12.792%
4	6.492	744	749	752	rBB	112826	100554	86.83%	13.132%
5	6.869	810	813	816	rBB	44595	32577	28.13%	4.254%
6	7.434	905	909	911	rBB	76724	65751	56.78%	8.587%
7	8.051	1011	1014	1017	rBB	36507	24036	20.76%	3.139%
8	8.151	1028	1031	1034	rBB	60405	43339	37.43%	5.660%
9	9.228	1210	1214	1217	rBV	160321	115800	100.00%	15.123%
10	9.904	1326	1329	1332	rBB	49231	41200	35.58%	5.381%
11	10.692	1460	1463	1466	rBB	65947	47383	40.92%	6.188%
12	11.392	1579	1582	1585	rBB	41477	30338	26.20%	3.962%
13	11.910	1668	1670	1672	rBB	2800	1769	1.53%	0.231%
14	12.974	1848	1851	1854	rBB	91359	69440	59.97%	9.069%
15	13.874	2001	2004	2007	rBV2	3997	5150	4.45%	0.673%
16	14.027	2027	2030	2033	rBV	35313	28183	24.34%	3.681%
17	14.498	2106	2110	2113	rBV	2127	2142	1.85%	0.280%
18	14.804	2160	2162	2166	rVB2	1938	2050	1.77%	0.268%
19	15.145	2217	2220	2225	rVB3	3397	4973	4.29%	0.649%
20	15.498	2274	2280	2284	rBV	18282	24854	21.46%	3.246%
21	15.527	2284	2285	2289	rVB2	3413	2766	2.39%	0.361%
22	15.968	2355	2360	2364	rVB2	3026	4148	3.58%	0.542%
23	16.051	2369	2374	2376	rBB3	1469	2042	1.76%	0.267%
24	16.480	2443	2447	2452	rVB2	2669	3708	3.20%	0.484%
25	17.080	2544	2549	2555	rBB	2073	2936	2.54%	0.383%

Sum of corrected areas: 765711

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Misc :
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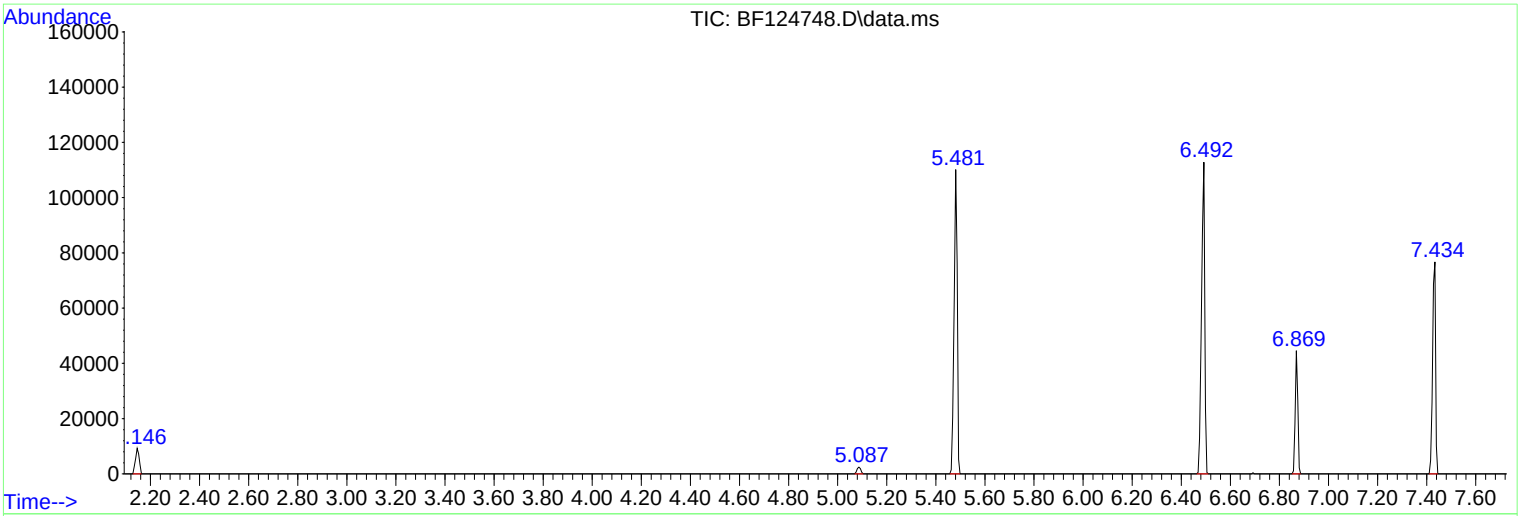
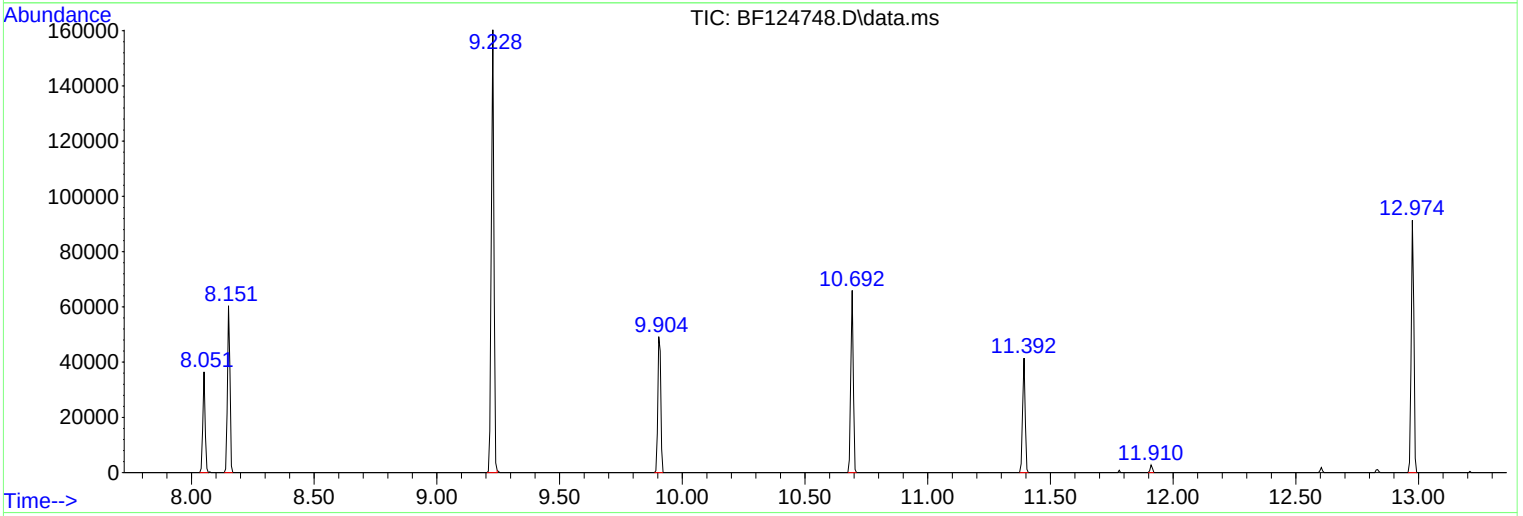
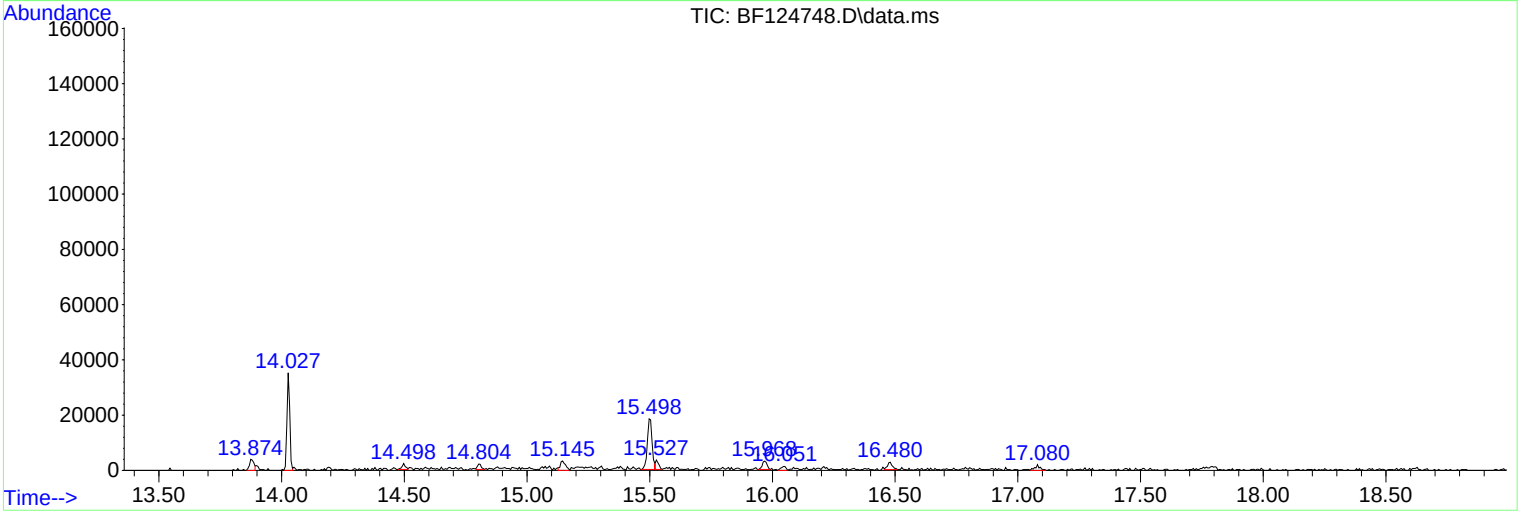
Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-7

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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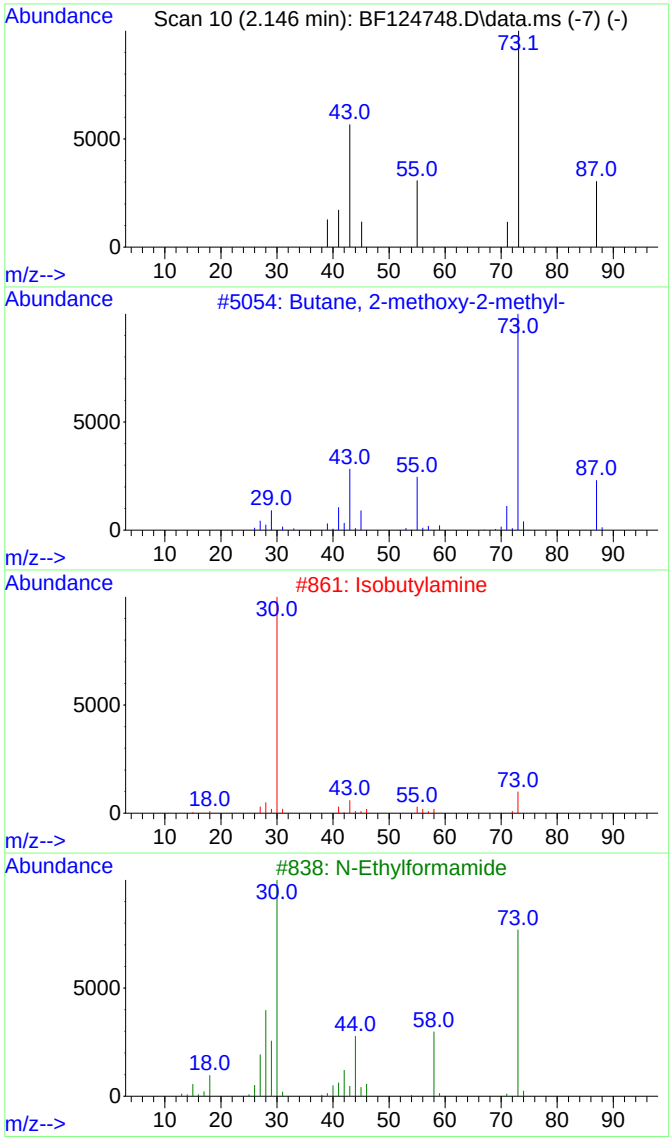
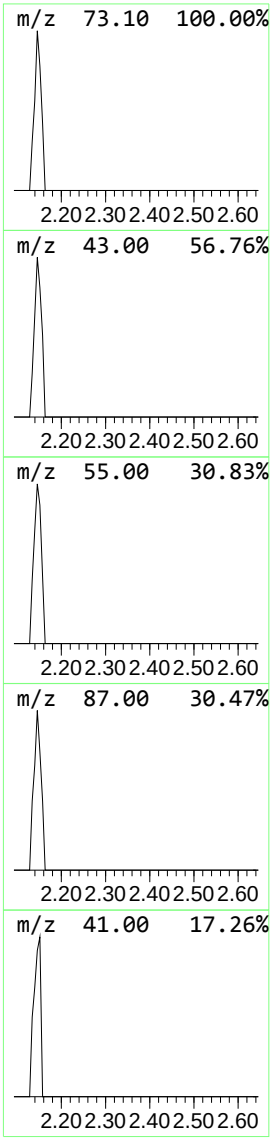
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	6.11 ng	9946	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Isobutylamine	73	C4H11N	000078-81-9	5
3	N-Ethylformamide	73	C3H7NO	000627-45-2	4
4	3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	4
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	4





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Operator : JU/CG
Sample : M3117-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NJ-CLEAN-7

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
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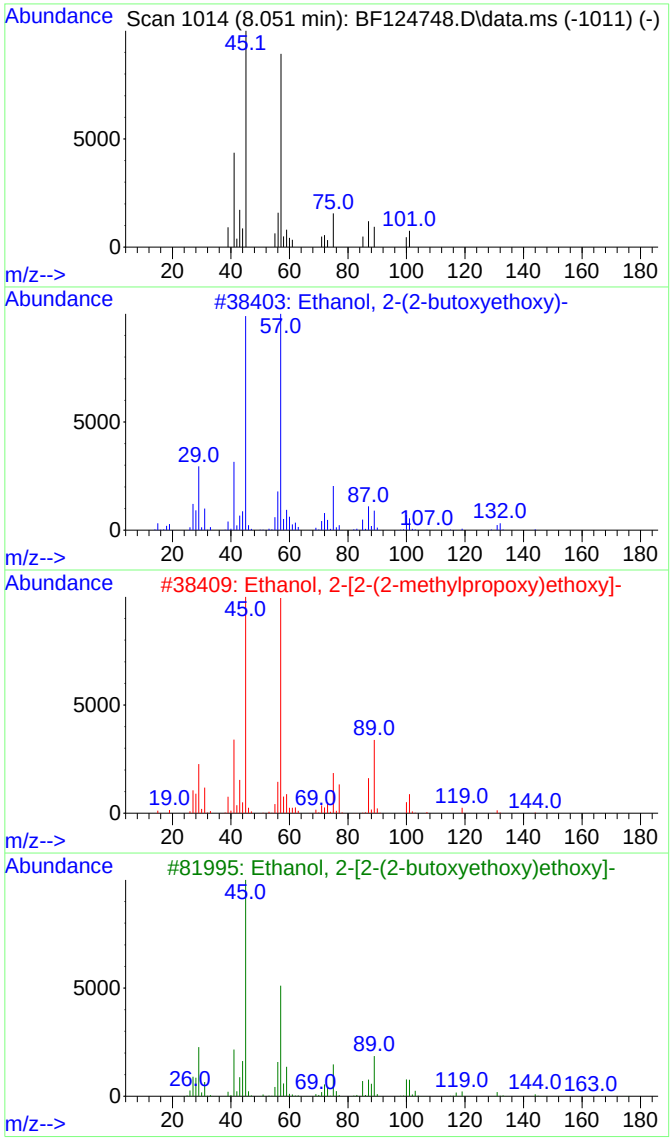
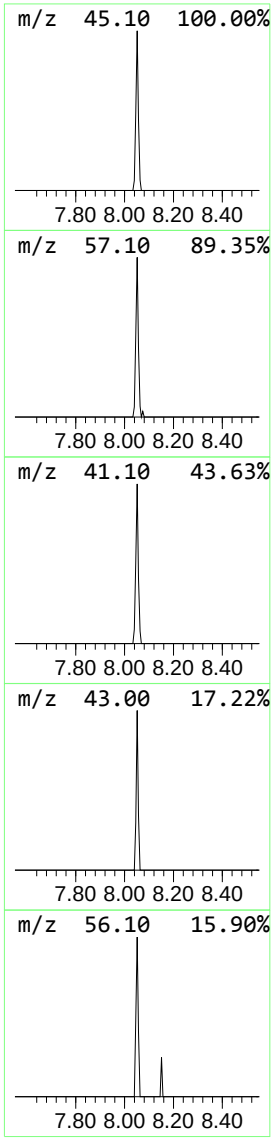
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	11.09 ng	24036	Naphthalene-d8	8.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	59
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	43
4	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	40
5	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	40





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Operator : JU/CG
Sample : M3117-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-7

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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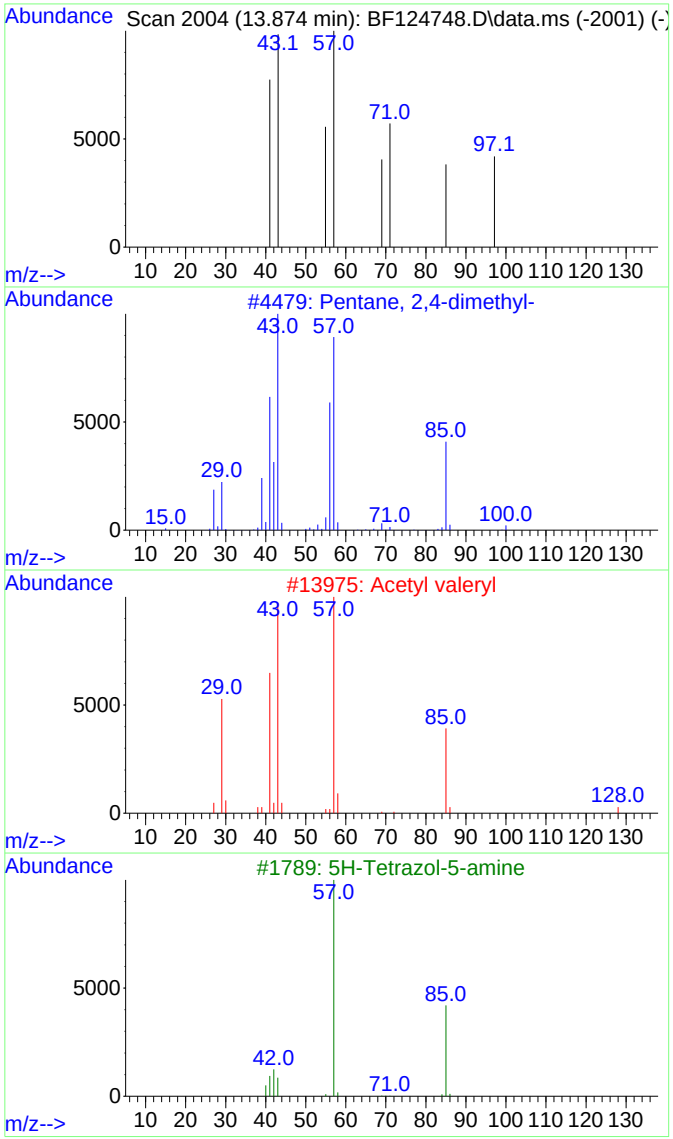
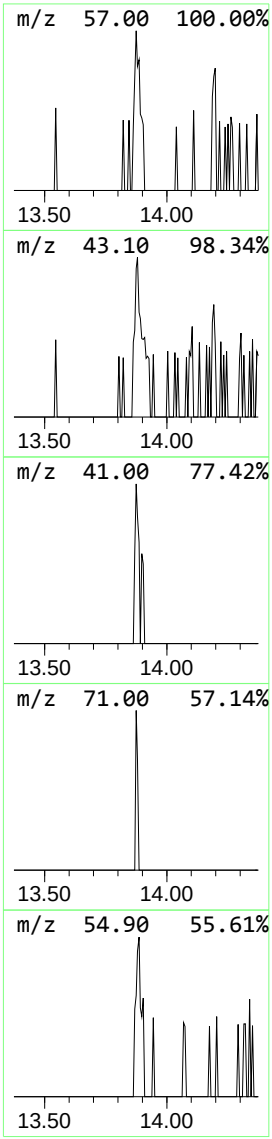
Peak Number 3 unknown13.874 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	3.65 ng	5150	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	9
2	Acetyl valeryl	128	C7H12O2	000096-04-8	9
3	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
4	Oxazole, 4,5-dihydro-2-methyl-	85	C4H7NO	001120-64-5	4
5	trans-Crotonamide	85	C4H7NO	000625-37-6	4





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Acq On : 24 Jul 2021 15:28
Operator : JU/CG
Sample : M3117-07
Misc :
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Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-7

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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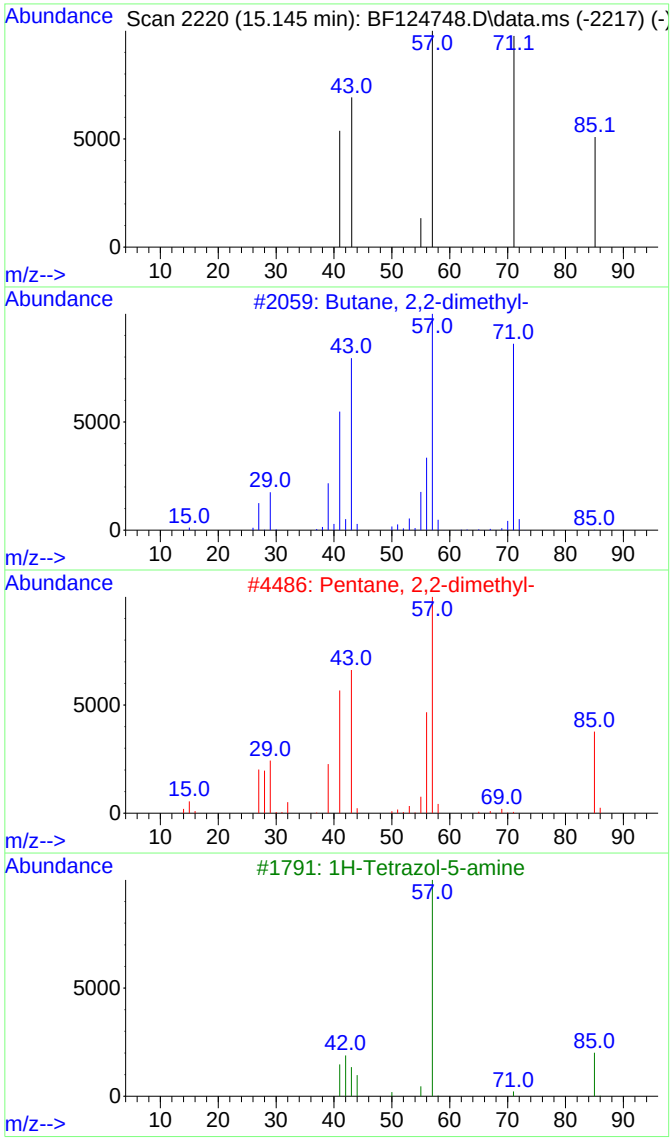
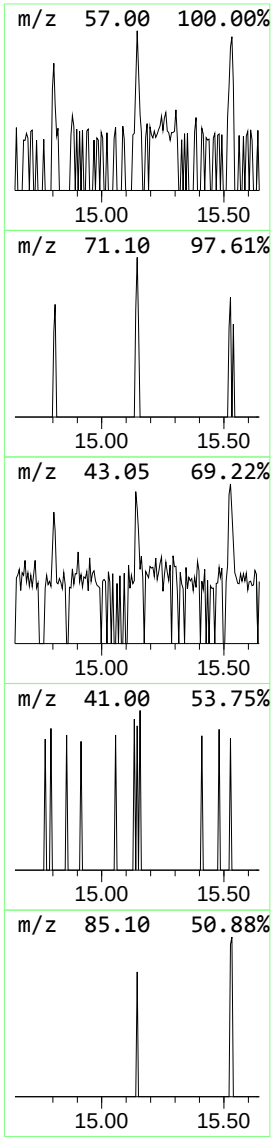
Peak Number 4 unknown15.145 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	4.00 ng	4973	Perylene-d12	15.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	36
2	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	9
3	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
4	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
5	Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4





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Operator : JU/CG
Sample : M3117-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NJ-CLEAN-7

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
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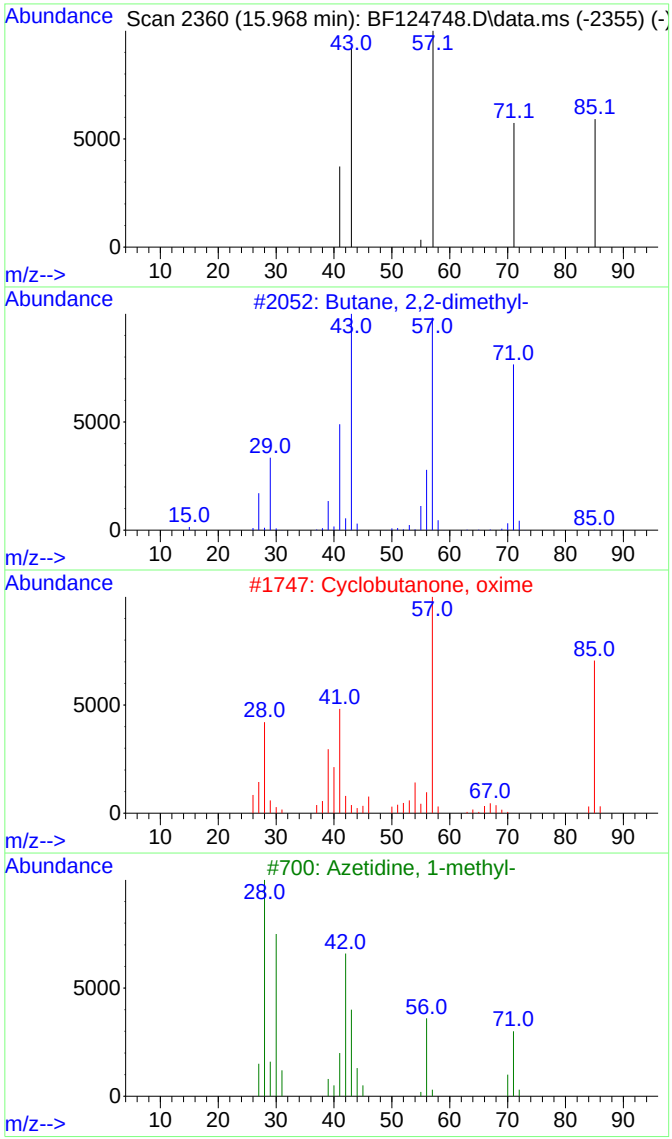
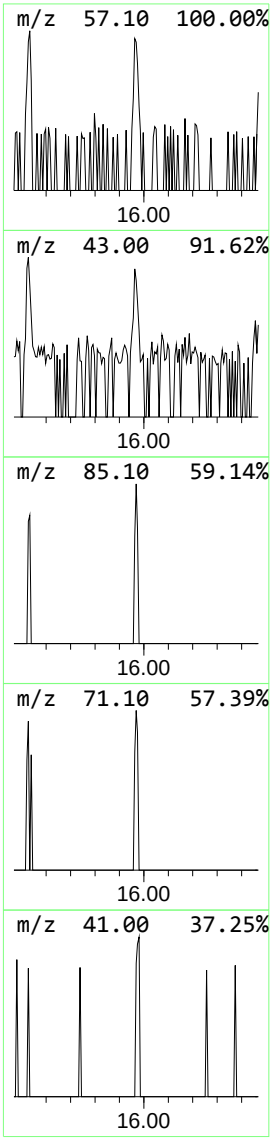
Peak Number 5 unknown15.968 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.968	3.34 ng	4148	Perylene-d12	15.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	9
2	Cyclobutanone, oxime	85	C4H7NO	002972-05-6	7
3	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	7
4	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	7
5	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4





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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
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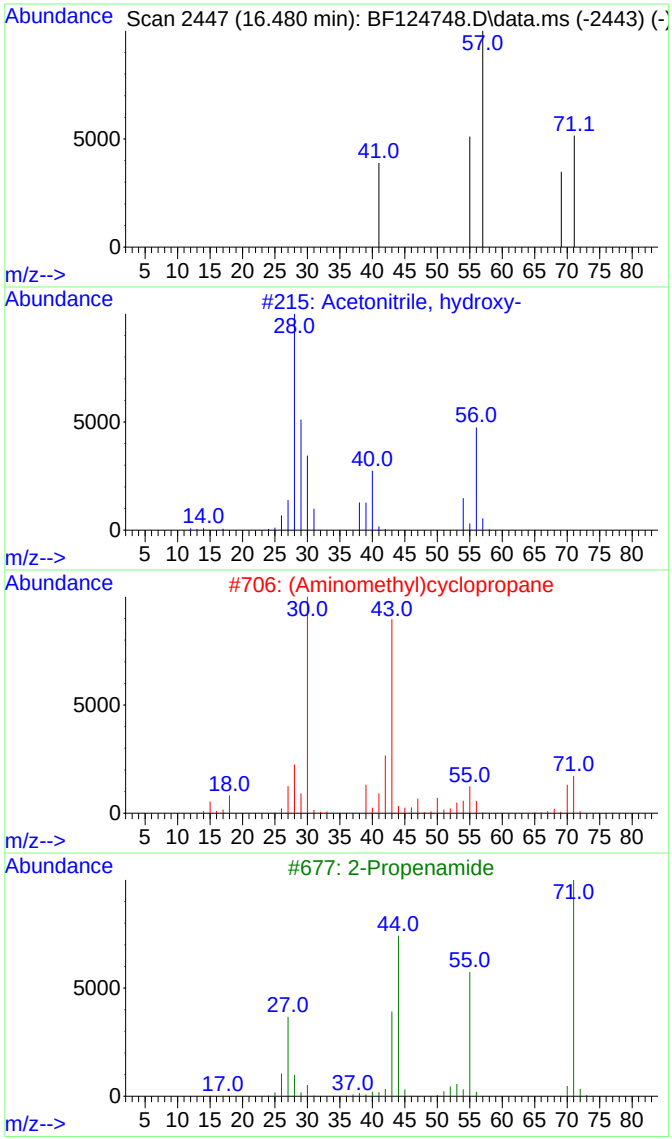
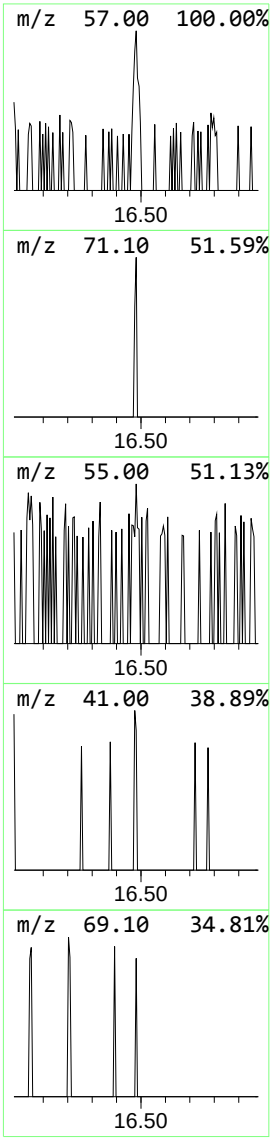
Peak Number 6 unknown16.480 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.480	2.98 ng	3708	Perylene-d12	15.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	4
2	(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	3
3	2-Propenamide	71	C3H5NO	000079-06-1	2
4	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	2
5	Azetidine	57	C3H7N	000503-29-7	1





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Sample : M3117-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NJ-CLEAN-7

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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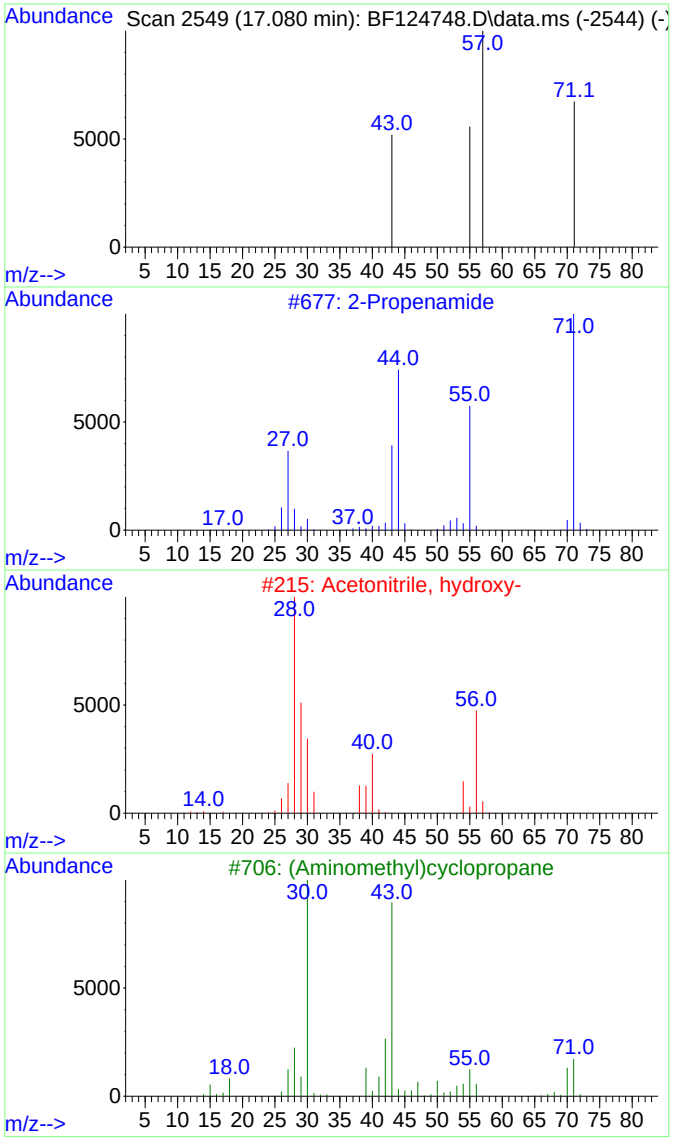
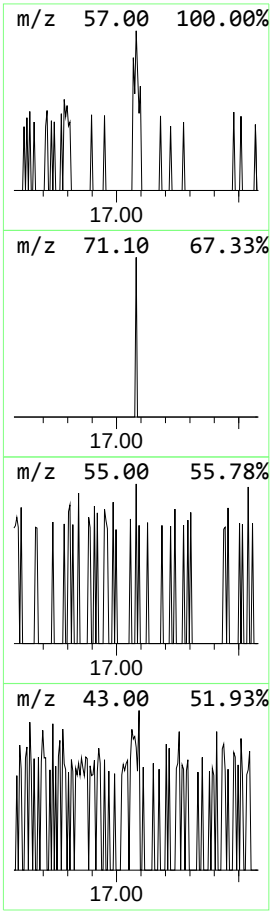
Peak Number 7 unknown17.080 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.080	2.36 ng	2936	Perylene-d12	15.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenamide	71	C3H5NO	000079-06-1	4
2	Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	3
3	(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	3
4	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	2
5	Azetidine	57	C3H7N	000503-29-7	1





Tentatively Identified Compound (LSC) summary

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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...	2.146	6.1	ng	9946	1	6.869	32577	20.0
Ethanol, 2-(2-b...	8.051	11.1	ng	24036	2	8.151	43339	20.0
unknown13.874	13.874	3.6	ng	5150	5	14.027	28183	20.0
unknown15.145	15.145	4.0	ng	4973	6	15.498	24854	20.0
unknown15.968	15.968	3.3	ng	4148	6	15.498	24854	20.0
unknown16.480	16.480	3.0	ng	3708	6	15.498	24854	20.0
unknown17.080	17.080	2.4	ng	2936	6	15.498	24854	20.0