

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
 Data File : BF124747.D
 Acq On : 24 Jul 2021 14:56
 Operator : JU/CG
 Sample : M3117-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NJ-CLEAN-4

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: BF124747.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	6	9	13	rBB	9324	9609	6.09%	0.986%
2	5.087	507	510	514	rBB	2924	2750	1.74%	0.282%
3	5.481	573	577	580	rBB	135842	119046	75.44%	12.220%
4	6.492	744	749	752	rBB	133774	124278	78.76%	12.757%
5	6.869	810	813	816	rBB	52233	35946	22.78%	3.690%
6	7.434	904	909	911	rBB	92400	81803	51.84%	8.397%
7	8.051	1011	1014	1017	rBB	25799	18355	11.63%	1.884%
8	8.151	1028	1031	1034	rBB	65696	47566	30.14%	4.883%
9	9.228	1210	1214	1217	rBV	211004	157802	100.00%	16.198%
10	9.904	1326	1329	1332	rBB	61292	47530	30.12%	4.879%
11	10.692	1460	1463	1466	rBB	89058	65980	41.81%	6.773%
12	11.392	1579	1582	1585	rBV	44380	33820	21.43%	3.472%
13	11.910	1668	1670	1672	rBB	11486	7825	4.96%	0.803%
14	12.604	1785	1788	1790	rBB	3628	2625	1.66%	0.269%
15	12.698	1802	1804	1806	rBB	4981	3393	2.15%	0.348%
16	12.833	1824	1827	1829	rBB	4162	2839	1.80%	0.291%
17	12.974	1848	1851	1854	rBV	115002	97433	61.74%	10.001%
18	13.451	1929	1932	1934	rBB	19613	14650	9.28%	1.504%
19	13.880	2000	2005	2013	rBV2	5110	9282	5.88%	0.953%
20	14.027	2025	2030	2033	rBV	35017	30518	19.34%	3.133%
21	14.804	2158	2162	2166	rVB	2409	3199	2.03%	0.328%
22	15.062	2203	2206	2208	rBV2	2701	2514	1.59%	0.258%
23	15.145	2217	2220	2225	rVB2	2833	3287	2.08%	0.337%
24	15.368	2255	2258	2262	rBV3	1532	2413	1.53%	0.248%
25	15.498	2277	2280	2283	rBV	21717	25472	16.14%	2.615%
26	15.533	2283	2286	2289	rVB2	3098	3526	2.23%	0.362%
27	15.739	2317	2321	2325	rBV2	1381	2150	1.36%	0.221%
28	15.968	2355	2360	2366	rVB	4235	6414	4.06%	0.658%
29	16.045	2369	2373	2378	rBV3	1404	2807	1.78%	0.288%
30	16.474	2442	2446	2450	rBV2	3871	6211	3.94%	0.638%
31	17.080	2542	2549	2553	rBV2	1777	3164	2.01%	0.325%

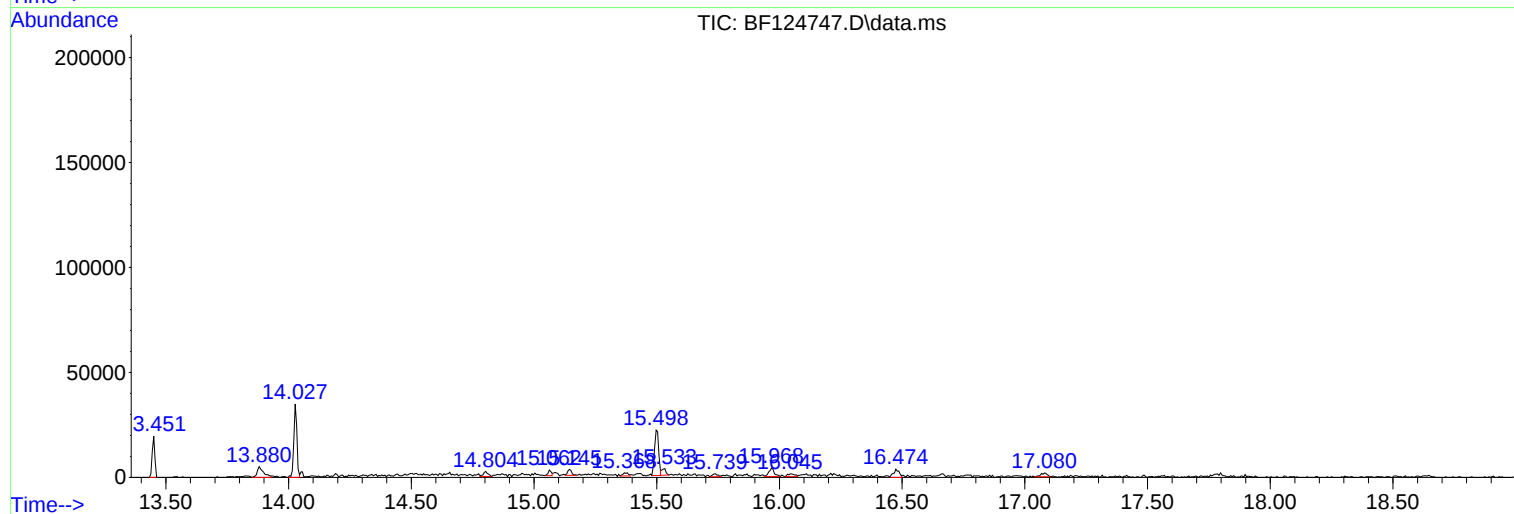
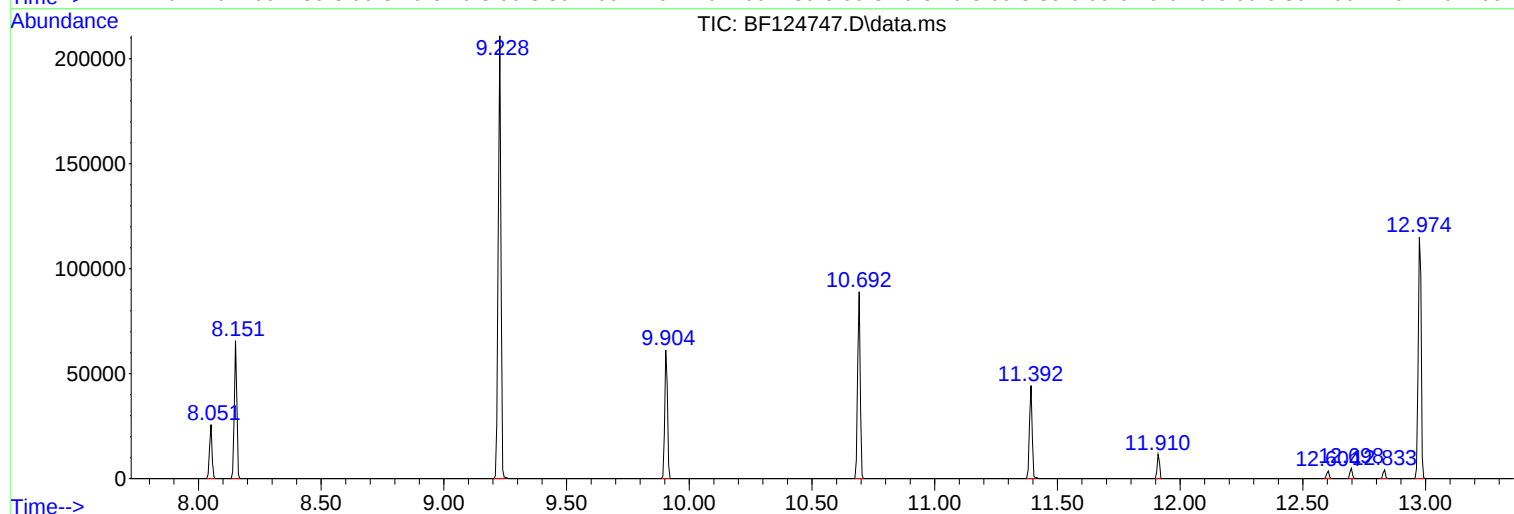
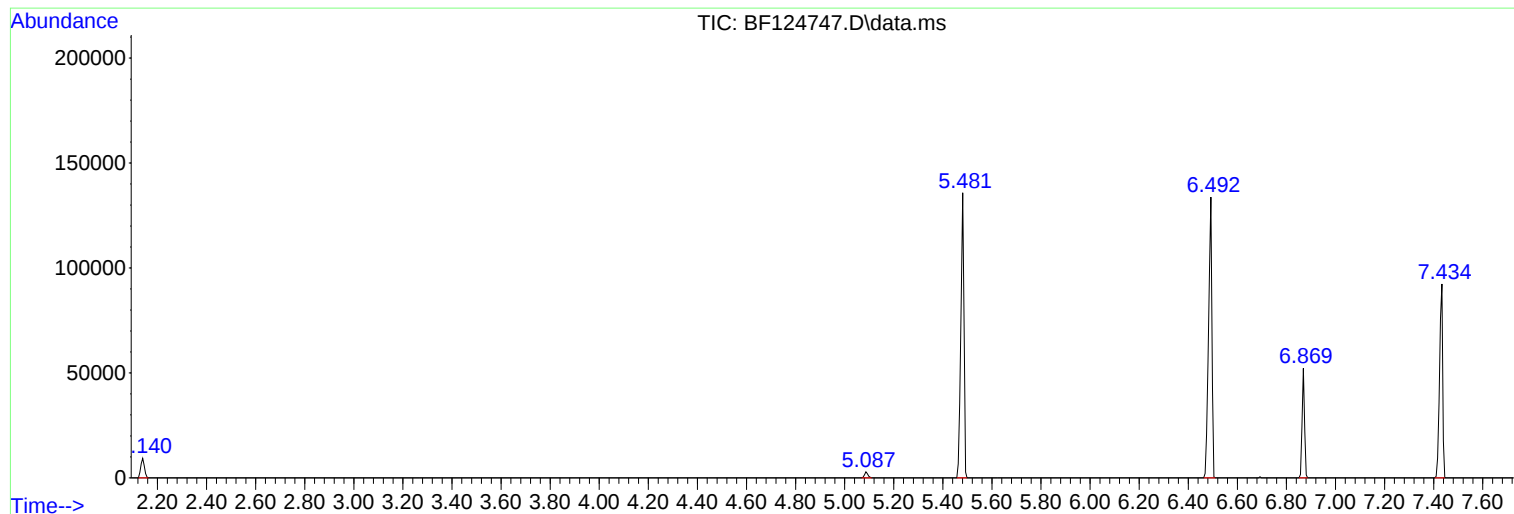
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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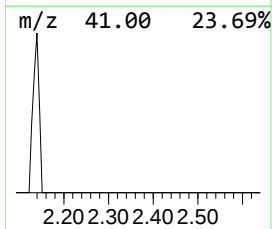
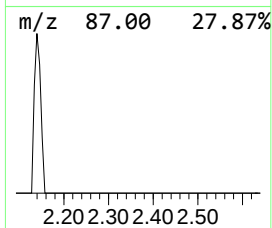
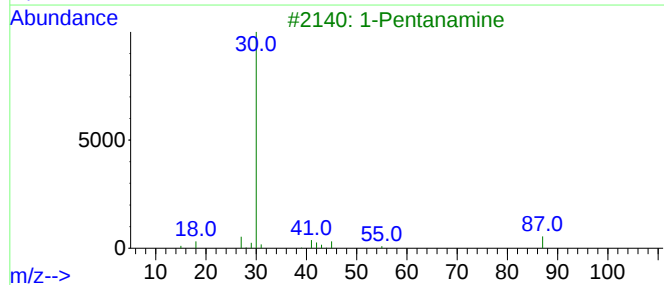
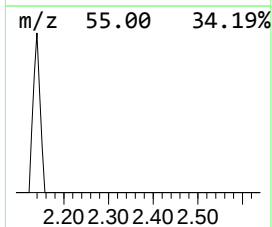
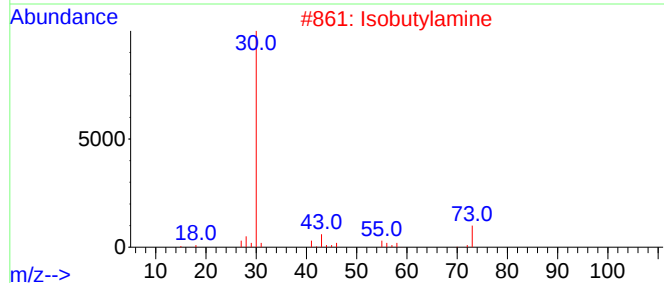
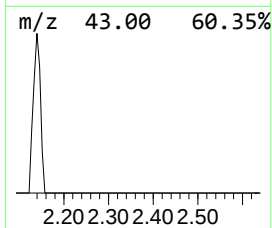
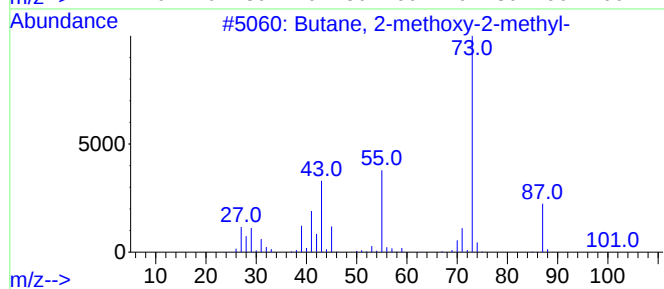
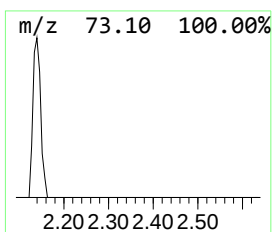
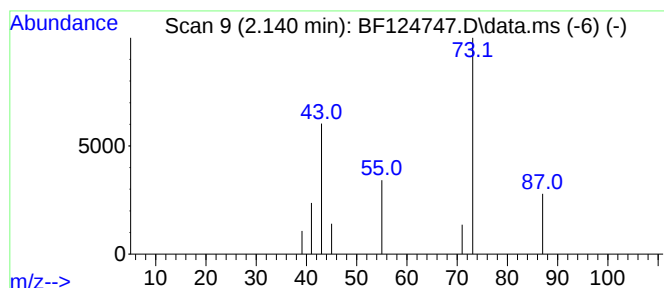
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	5.35 ng	9609	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	64
2			Isobutylamine	73	C4H11N	000078-81-9	7
3			1-Pentanamine	87	C5H13N	000110-58-7	4
4			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4
5			2-Pentanol, acetate	130	C7H14O2	000626-38-0	4



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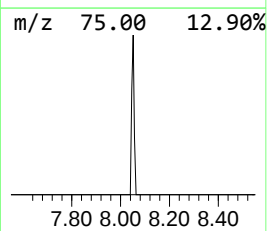
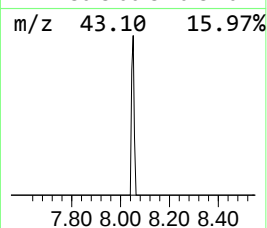
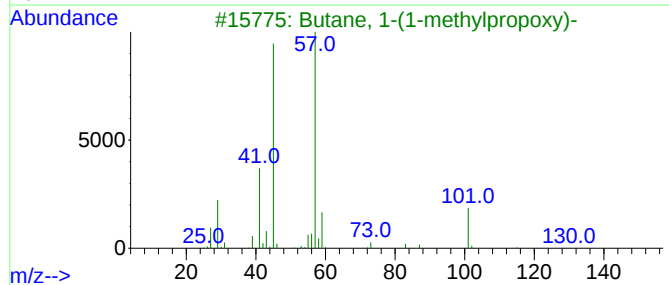
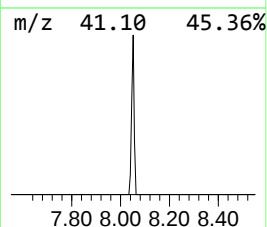
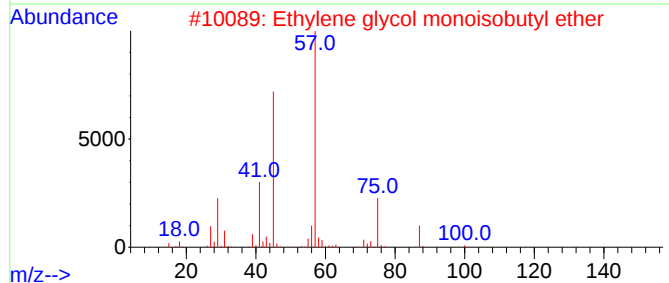
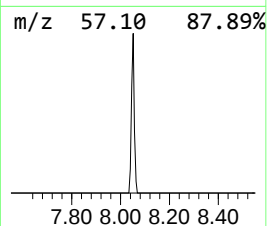
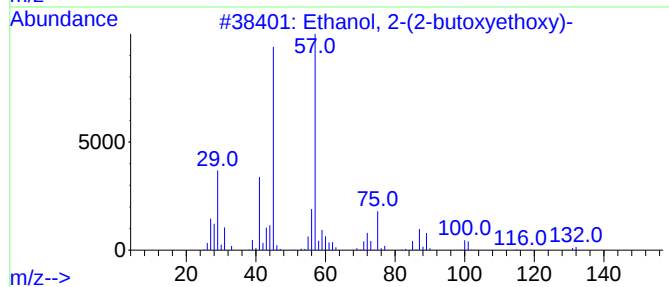
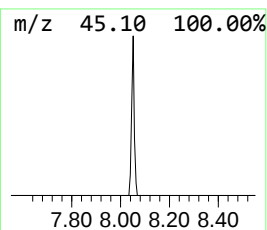
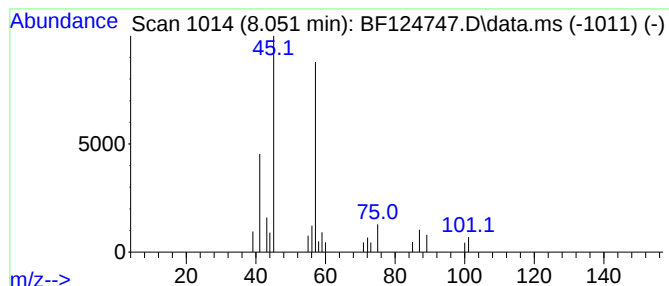
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	7.72 ng	18355	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			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45
3			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	42
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	42
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	40



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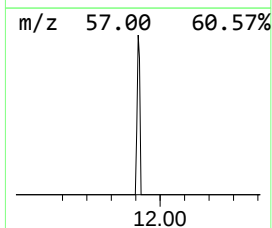
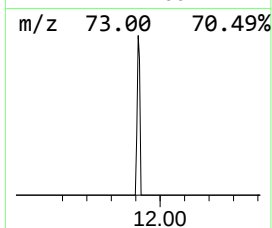
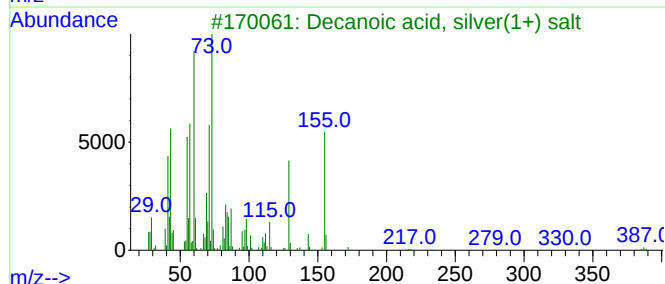
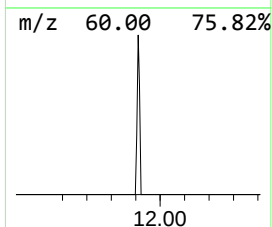
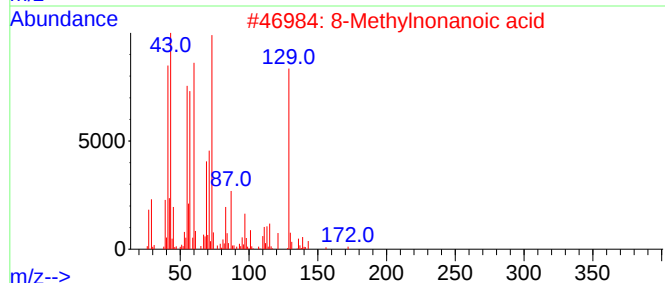
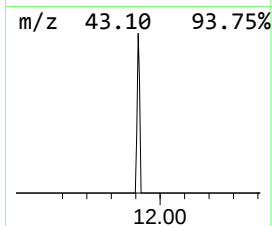
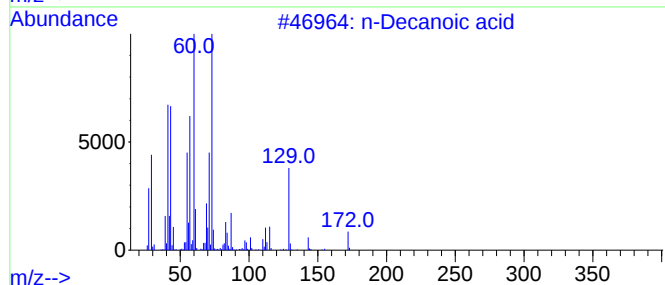
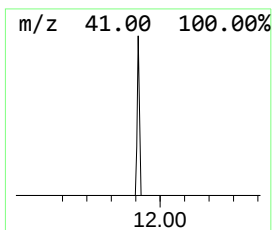
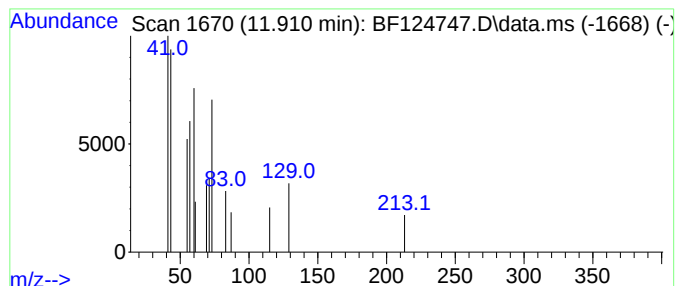
Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-4

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

Peak Number 3 n-Decanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.910	4.63 ng	7825	Phenanthrene-d10		11.392	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Decanoic acid		172	C10H20O2	000334-48-5	53
2	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	53
3	Decanoic acid, silver(1+) salt		278	C10H19AgO2	013126-67-5	38
4	Undecanoic acid		186	C11H22O2	000112-37-8	36
5	2-Deoxy-D-glucose		164	C6H12O5	000154-17-6	36



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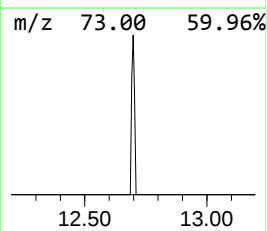
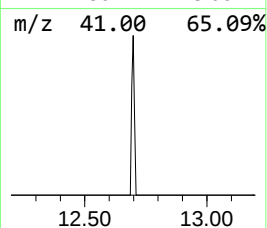
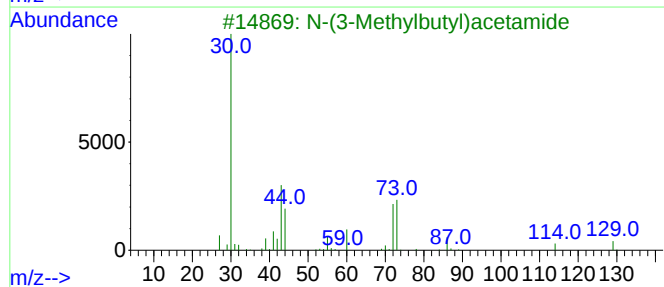
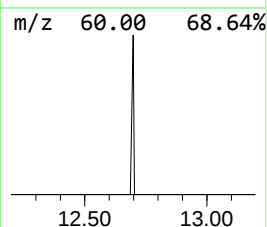
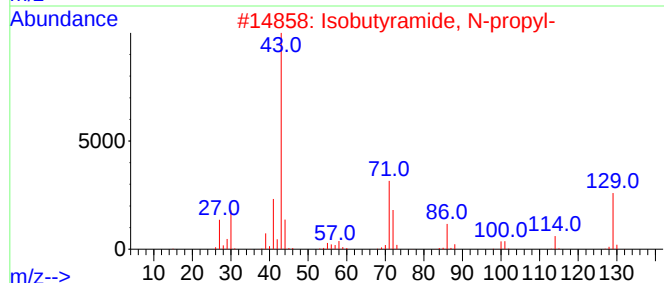
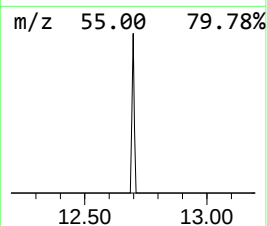
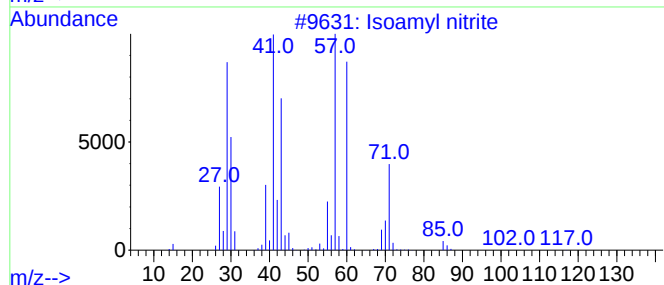
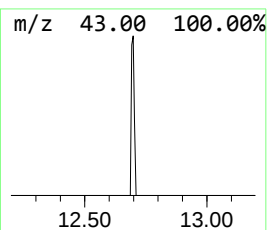
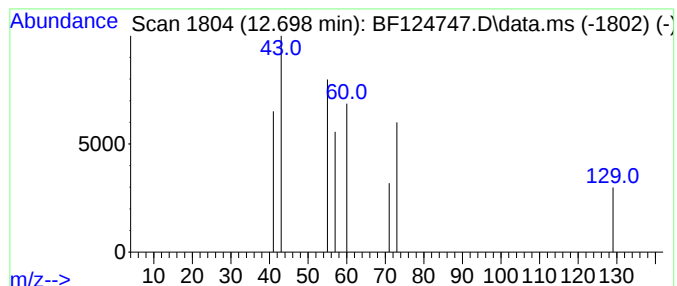
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Peak Number 4 unknown12.698 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	2.01 ng	3393	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isoamyl nitrite	117	C5H11NO2	000110-46-3	9
2			Isobutyramide, N-propyl-	129	C7H15NO	1000407-08-5	7
3			N-(3-Methylbutyl)acetamide	129	C7H15NO	013434-12-3	5
4			Acetic acid	60	C2H4O2	000064-19-7	4
5			Neopentyl isothiocyanate	129	C6H11NS	000597-97-7	4



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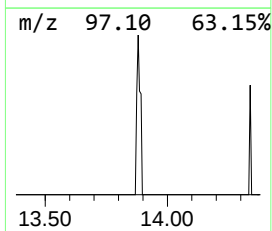
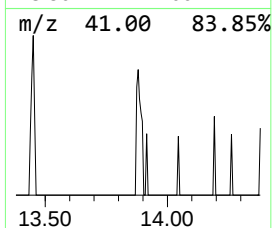
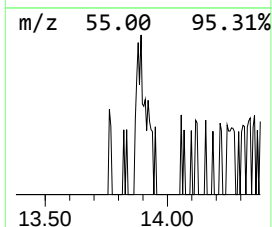
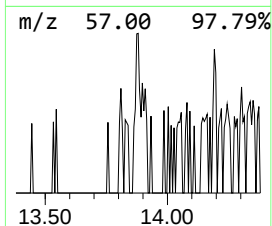
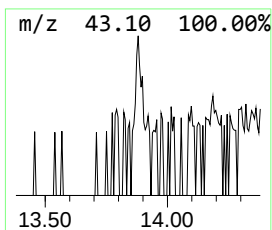
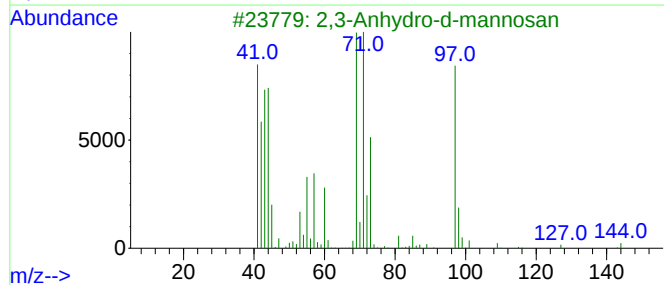
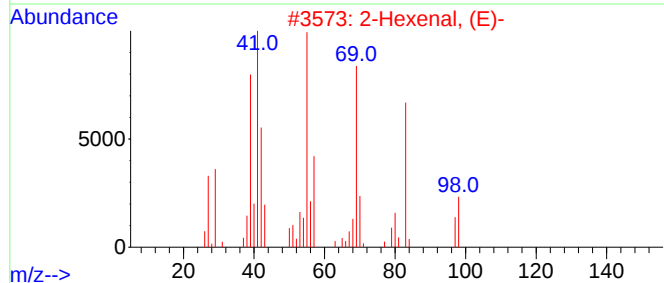
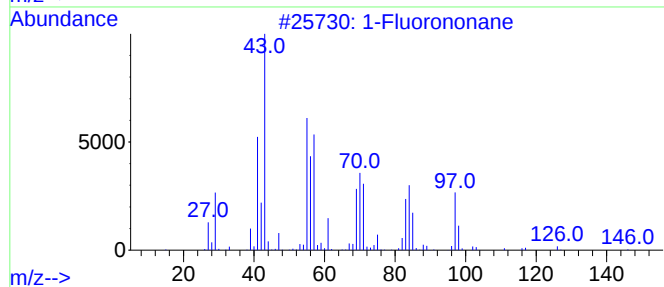
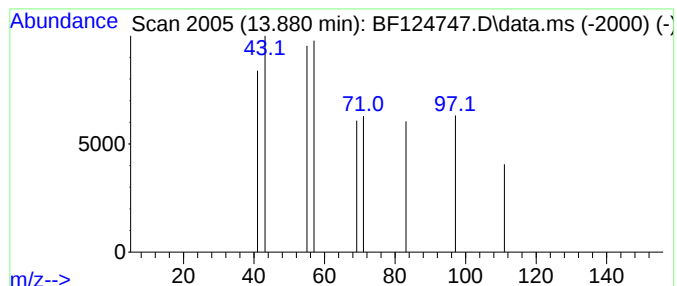
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Peak Number 5 unknown13.880 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	6.08 ng	9282	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Fluorononane	146	C9H19F	000463-18-3	9
2			2-Hexenal, (E)-	98	C6H10O	006728-26-3	9
3			2,3-Anhydro-d-mannosan	144	C6H8O4	1000129-98-0	9
4			Bis(2-ethylhexyl) methylphosphonate	320	C17H37O3P	1000298-35-3	9
5			trans-2-Methylcyclohexanol, 2-me...	184	C11H20O2	1000447-34-0	9



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ClientSampleId :
NJ-CLEAN-4

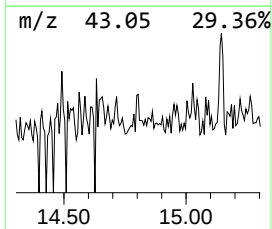
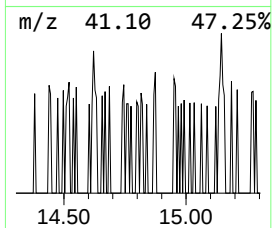
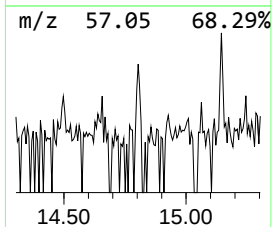
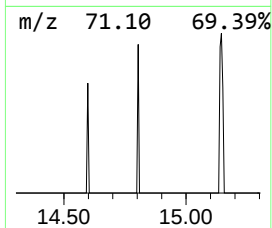
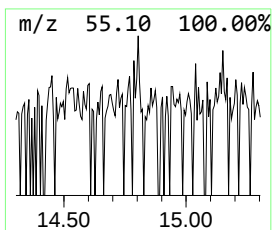
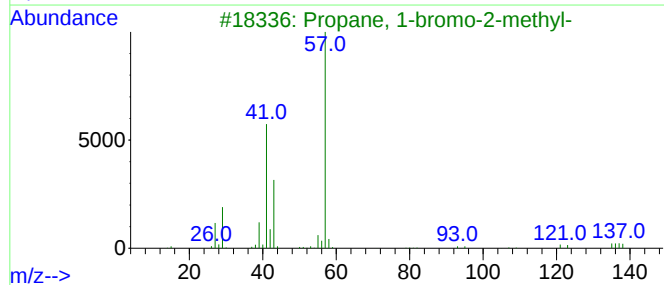
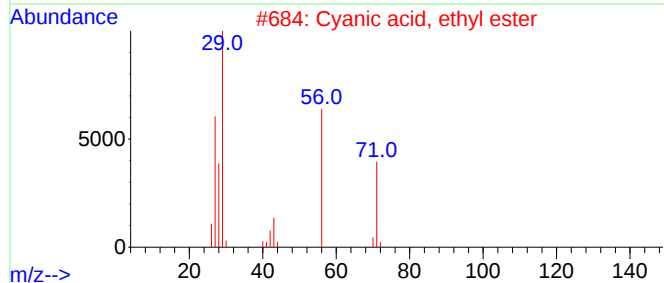
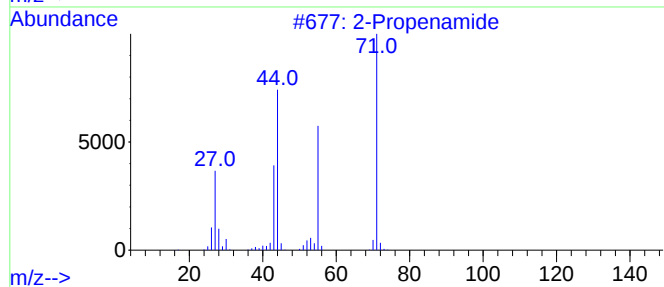
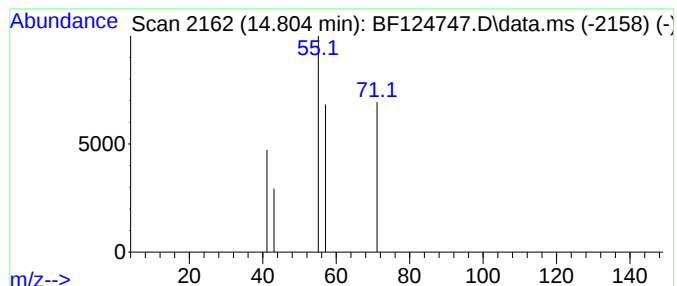
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.804 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	2.51 ng	3199	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenamide			71	C3H5NO	000079-06-1	4
2	Cyanoic acid, ethyl ester			71	C3H5NO	000627-48-5	3
3	Propane, 1-bromo-2-methyl-			136	C4H9Br	000078-77-3	2
4	Ethyl isocyanide			55	C3H5N	000624-79-3	1
5	Methane, isocyanato-			57	C2H3NO	000624-83-9	1



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124747.D
Acq On : 24 Jul 2021 14:56
Operator : JU/CG
Sample : M3117-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-4

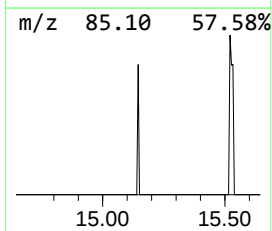
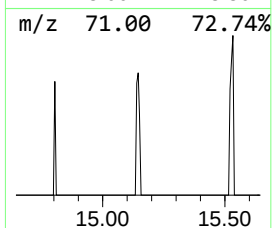
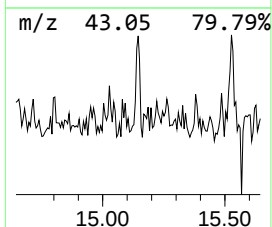
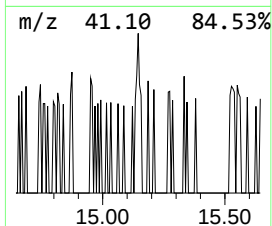
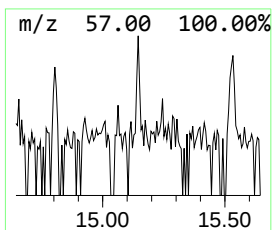
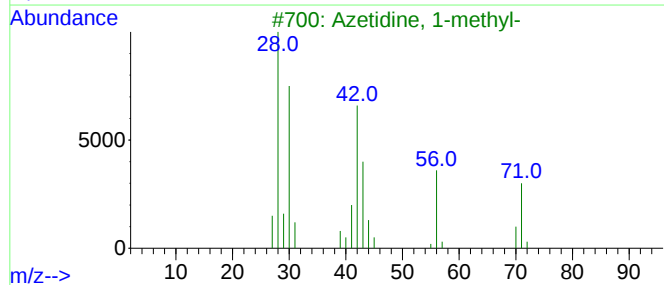
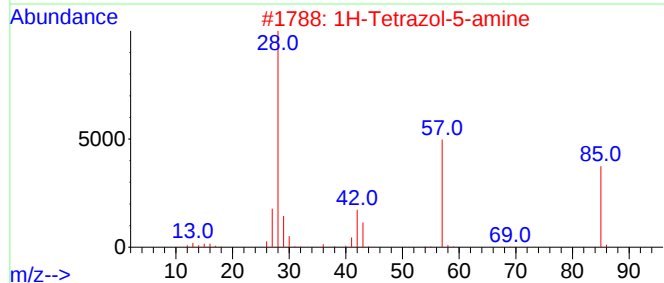
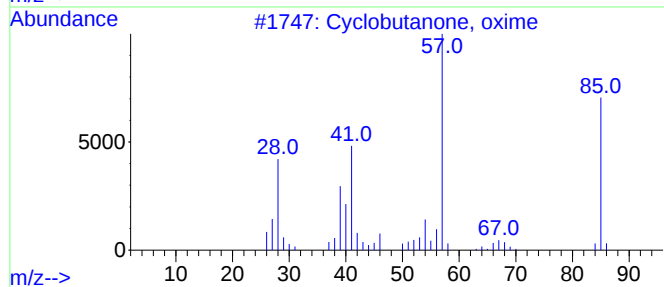
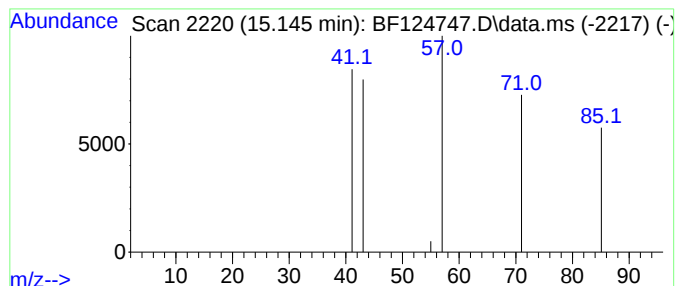
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.145 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	2.58 ng	3287	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutanone, oxime	85	C4H7NO	002972-05-6	7
2			1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
3			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	4
4			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	4
5			5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124747.D
Acq On : 24 Jul 2021 14:56
Operator : JU/CG
Sample : M3117-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-4

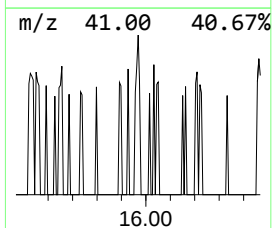
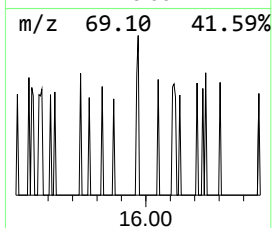
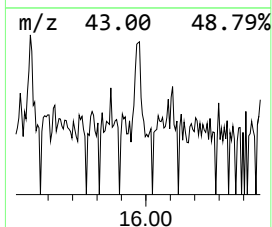
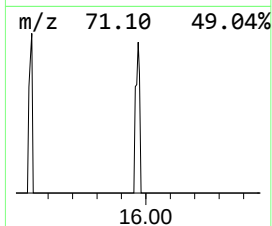
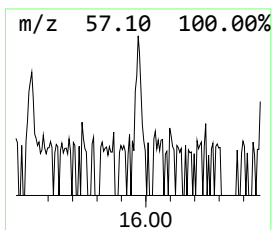
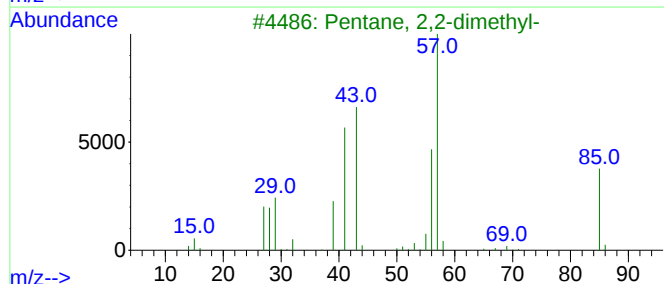
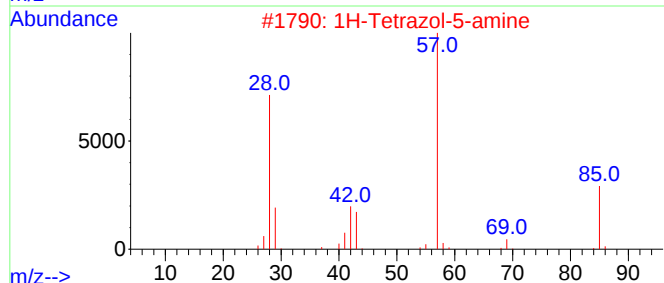
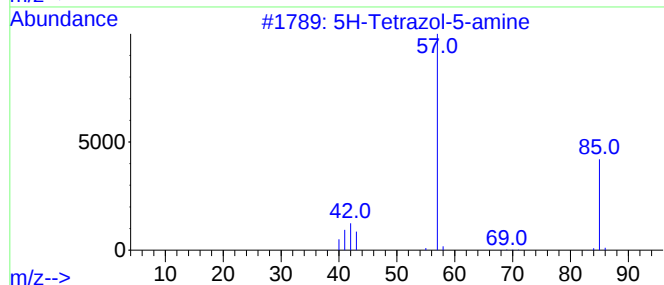
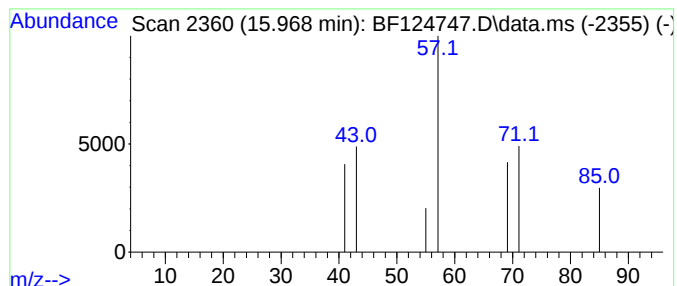
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.968 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.968	5.04 ng	6414	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
2			1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
3			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	4
4			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	4
5			2,2-Dimethylpropionic acid, 4-me...	186	C11H22O2	150588-62-8	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124747.D
Acq On : 24 Jul 2021 14:56
Operator : JU/CG
Sample : M3117-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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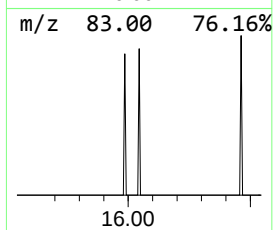
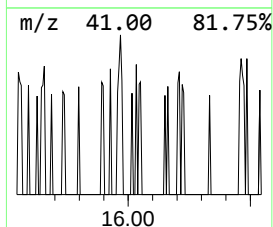
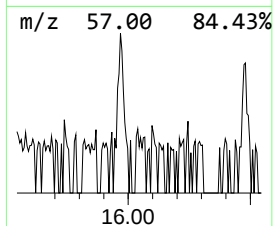
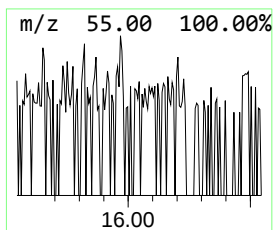
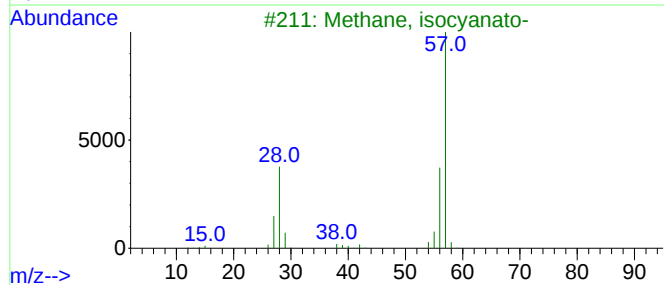
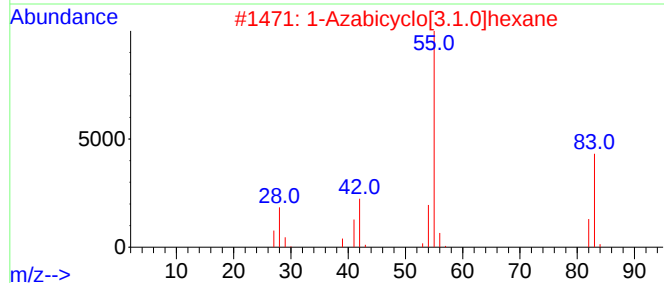
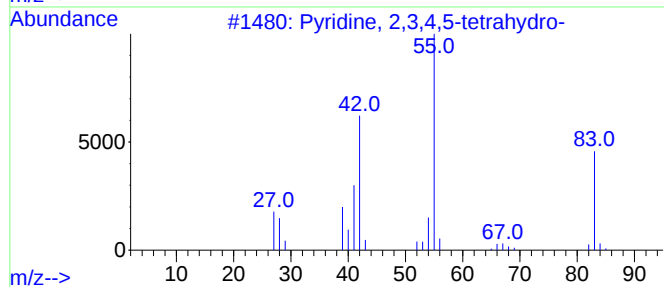
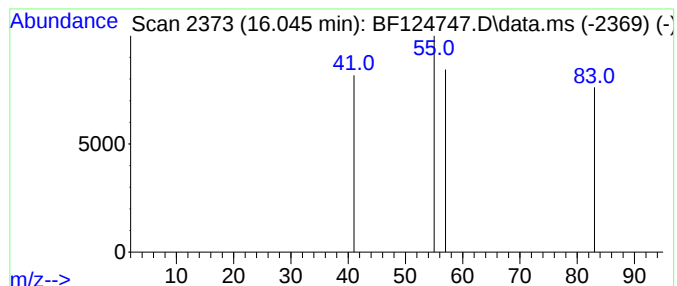
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown16.045 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.045	2.20 ng	2807	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	2
2			1-Azabicyclo[3.1.0]hexane	83	C5H9N	000285-76-7	2
3			Methane, isocyanato-	57	C2H3NO	000624-83-9	1
4			Azetidine	57	C3H7N	000503-29-7	1
5			Cyclobutanecarboxylic acid, pent...	164	C10H12O2	1000299-13-0	1



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124747.D
Acq On : 24 Jul 2021 14:56
Operator : JU/CG
Sample : M3117-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-4

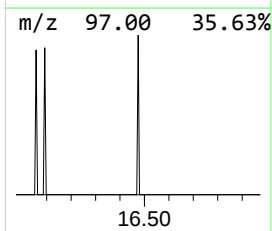
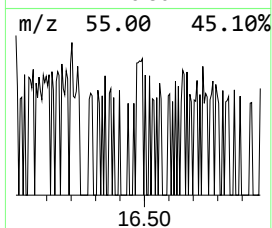
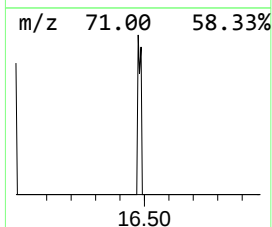
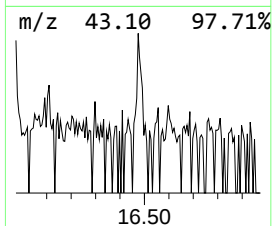
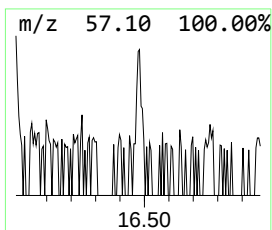
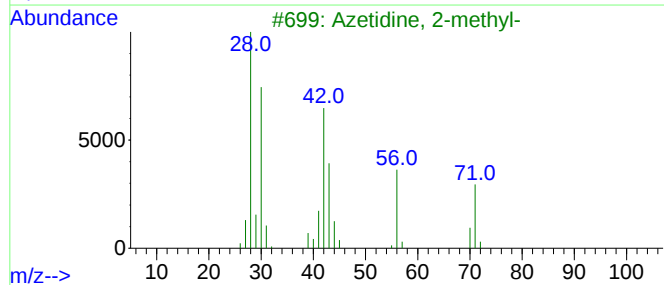
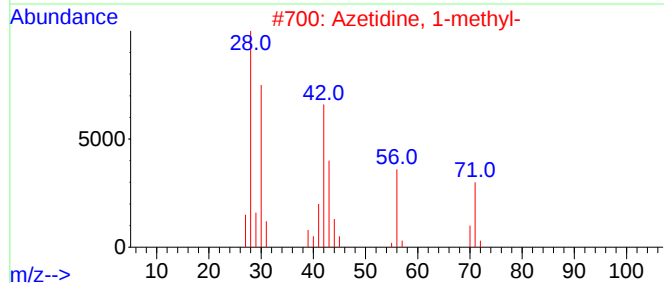
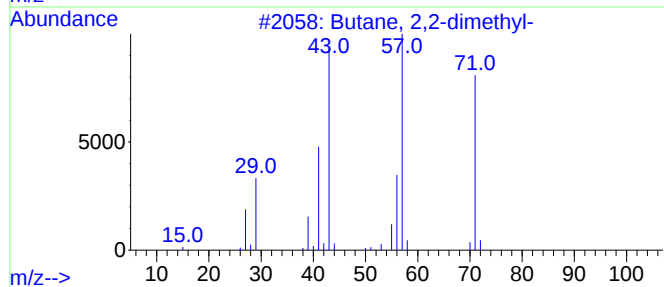
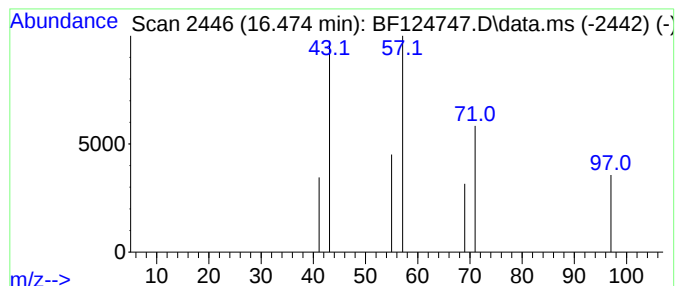
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.474 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.474	4.88 ng	6211	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			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
3			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
4			Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	4
5			2-Propenamide	71	C3H5NO	000079-06-1	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124747.D
Acq On : 24 Jul 2021 14:56
Operator : JU/CG
Sample : M3117-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-4

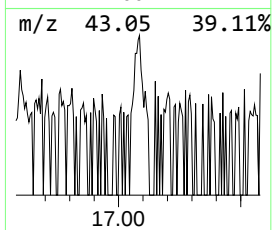
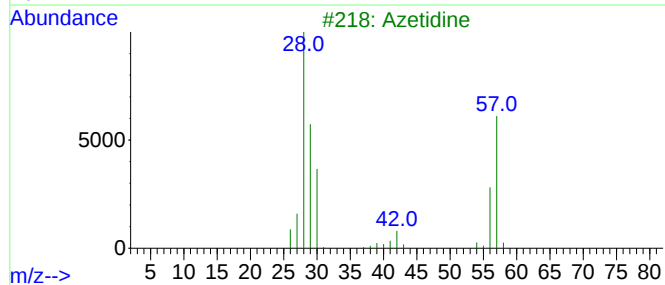
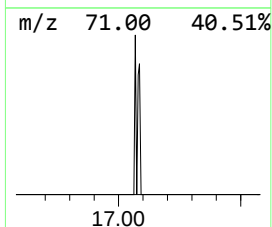
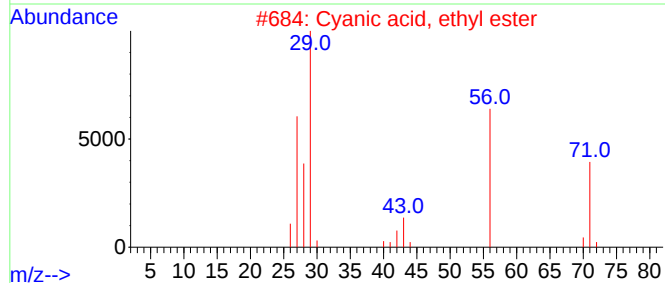
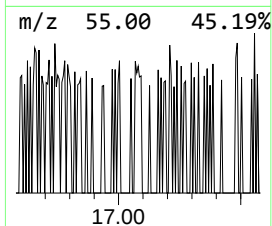
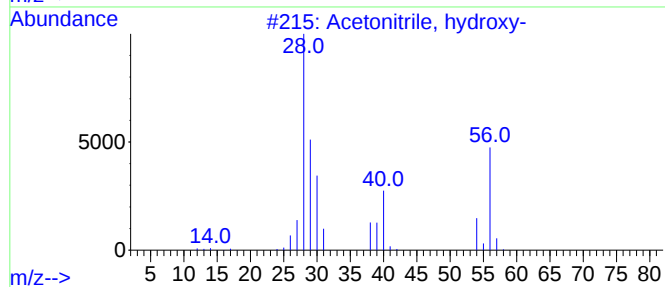
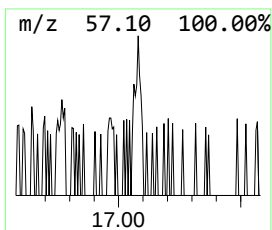
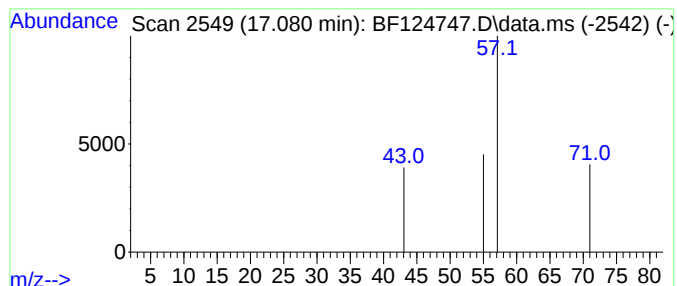
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown17.080 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.080	2.48 ng	3164	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	3
2			Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	2
3			Azetidine	57	C3H7N	000503-29-7	1
4			Methane, isocyanato-	57	C2H3NO	000624-83-9	1
5			Methoxyacetoneitrile	71	C3H5NO	001738-36-9	1



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124747.D
Acq On : 24 Jul 2021 14:56
Operator : JU/CG
Sample : M3117-04
Misc :
ALS Vial : 12 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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Ethanol, 2-(2-b...	8.051	7.7	ng	18355	2	8.151	47566	20.0
n-Decanoic acid	11.910	4.6	ng	7825	4	11.392	33820	20.0
unknown12.698	12.698	2.0	ng	3393	4	11.392	33820	20.0
unknown13.880	13.880	6.1	ng	9282	5	14.027	30518	20.0
unknown14.804	14.804	2.5	ng	3199	6	15.498	25472	20.0
unknown15.145	15.145	2.6	ng	3287	6	15.498	25472	20.0
unknown15.968	15.968	5.0	ng	6414	6	15.498	25472	20.0
unknown16.045	16.045	2.2	ng	2807	6	15.498	25472	20.0
unknown16.474	16.474	4.9	ng	6211	6	15.498	25472	20.0
unknown17.080	17.080	2.5	ng	3164	6	15.498	25472	20.0