

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
 Data File : BF124750.D
 Acq On : 24 Jul 2021 16:34
 Operator : JU/CG
 Sample : M3117-08
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NJ-CLEAN-8

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: BF124750.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	4	8	11	rBB	8481	9145	9.03%	1.295%
2	5.087	507	510	512	rBB	1682	1697	1.68%	0.240%
3	5.481	573	577	580	rBB	109371	89566	88.46%	12.680%
4	6.492	745	749	752	rBB	104355	90297	89.18%	12.783%
5	6.869	810	813	816	rBB	44431	32273	31.87%	4.569%
6	7.434	905	909	911	rBB	72023	59262	58.53%	8.389%
7	8.051	1011	1014	1017	rBB	21067	13990	13.82%	1.981%
8	8.151	1028	1031	1034	rBB	54220	41341	40.83%	5.852%
9	9.228	1210	1214	1217	rBV	139322	101250	100.00%	14.334%
10	9.910	1327	1330	1333	rBB	50109	39412	38.93%	5.579%
11	10.692	1460	1463	1466	rBB2	55868	41717	41.20%	5.906%
12	11.392	1579	1582	1585	rBB	39596	28561	28.21%	4.043%
13	11.910	1668	1670	1672	rBB	5333	3792	3.75%	0.537%
14	12.698	1802	1804	1806	rBB	2965	1953	1.93%	0.276%
15	12.974	1848	1851	1854	rBB	75833	62359	61.59%	8.828%
16	13.880	2002	2005	2011	rBB2	4117	5717	5.65%	0.809%
17	14.033	2027	2031	2034	rBV	30269	25567	25.25%	3.619%
18	14.192	2053	2058	2061	rBV	2402	2766	2.73%	0.392%
19	14.492	2108	2109	2112	rBV	1548	1525	1.51%	0.216%
20	14.686	2141	2142	2150	rVB2	961	1785	1.76%	0.253%
21	14.809	2159	2163	2164	rBV2	2759	2650	2.62%	0.375%
22	15.074	2204	2208	2212	rBV2	1857	3037	3.00%	0.430%
23	15.145	2216	2220	2224	rVV2	2508	3132	3.09%	0.443%
24	15.380	2256	2260	2262	rVB	1537	1622	1.60%	0.230%
25	15.504	2277	2281	2284	rBV	17584	20817	20.56%	2.947%
26	15.527	2284	2285	2289	rVB2	2650	2847	2.81%	0.403%
27	15.645	2303	2305	2308	rBV2	1258	1518	1.50%	0.215%
28	15.968	2355	2360	2365	rVB2	3039	5338	5.27%	0.756%
29	16.033	2368	2371	2374	rBV	1055	1458	1.44%	0.206%
30	16.339	2419	2423	2425	rBV	1148	1723	1.70%	0.244%
31	16.486	2441	2448	2452	rBV	2531	5125	5.06%	0.726%
32	17.103	2551	2553	2556	rVB	1368	1330	1.31%	0.188%
33	18.662	2815	2818	2820	rVB2	1471	1811	1.79%	0.256%

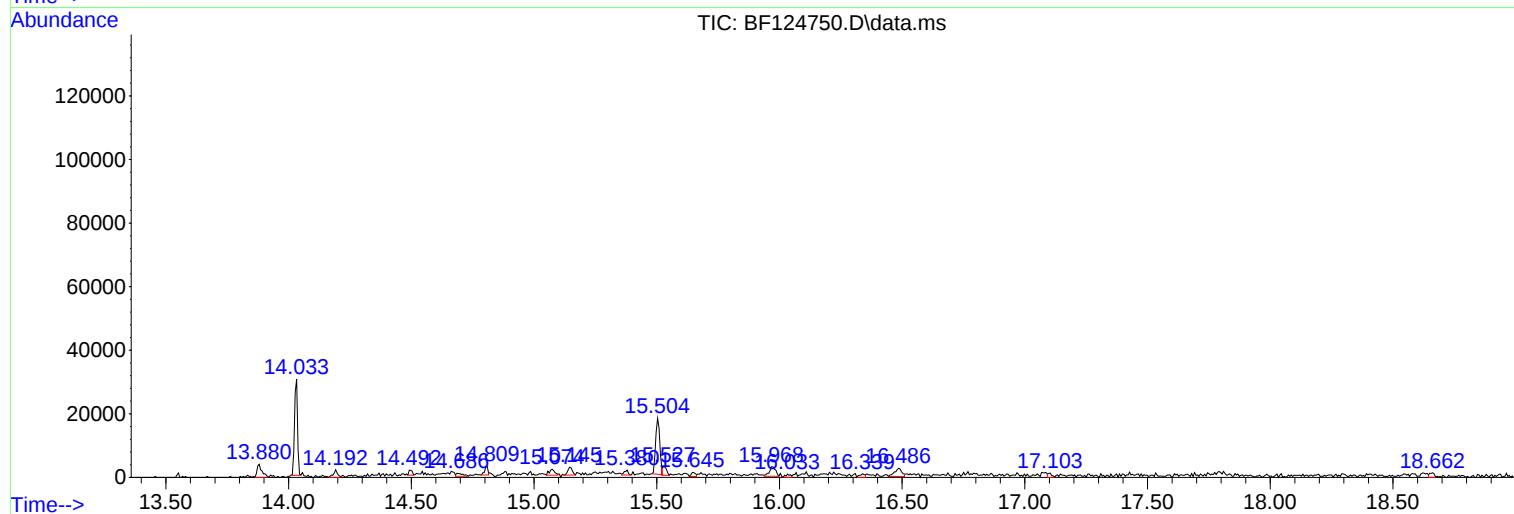
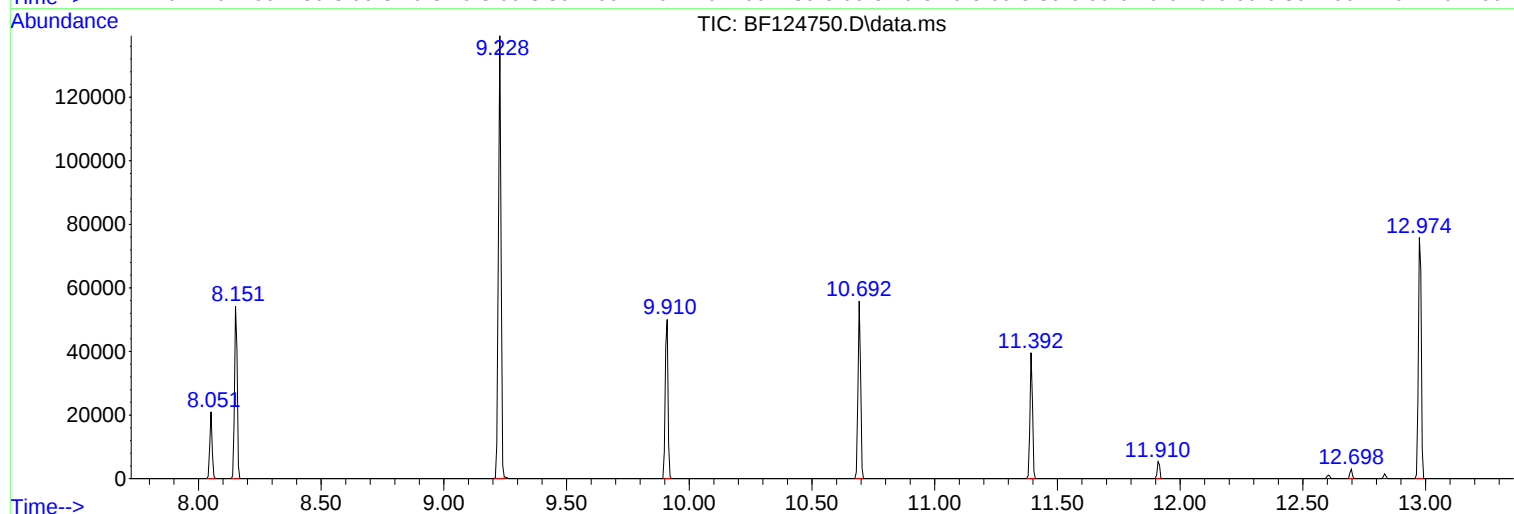
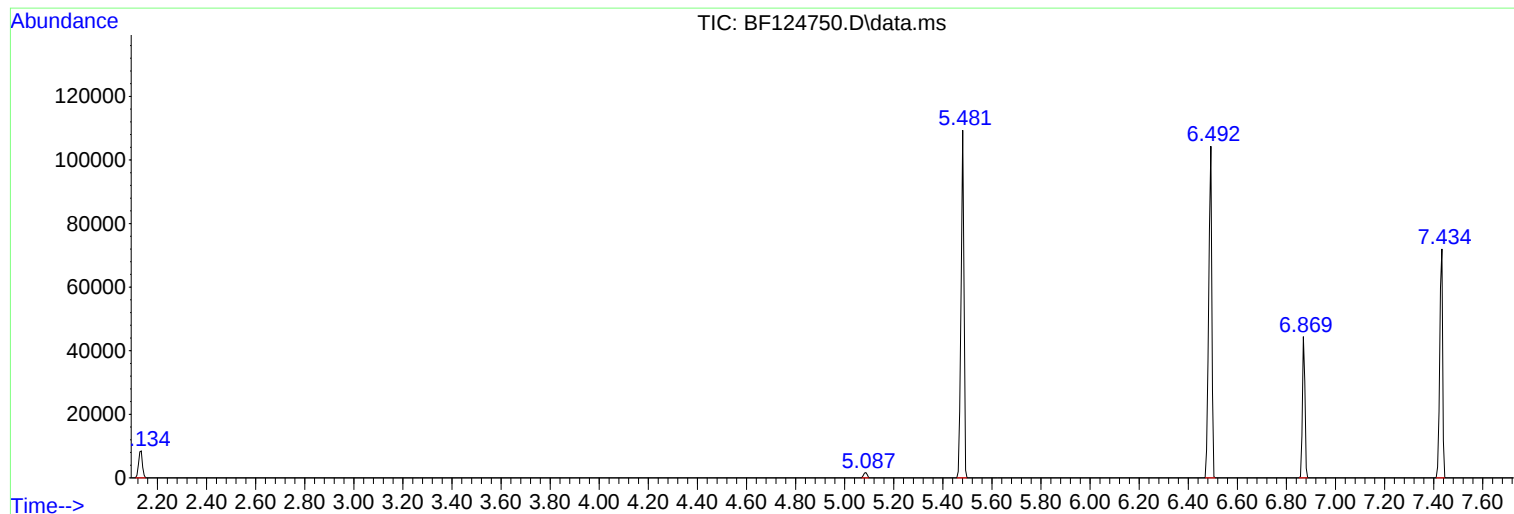
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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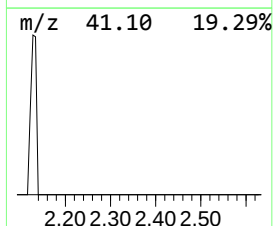
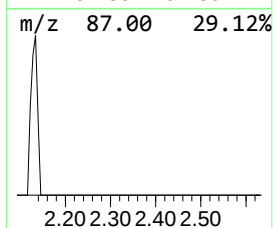
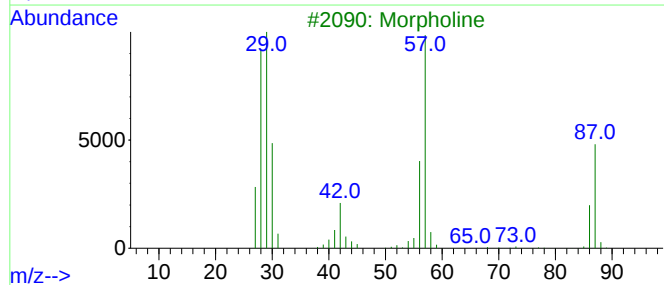
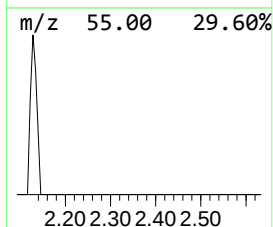
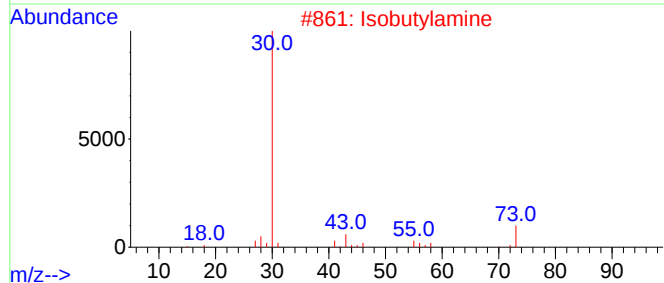
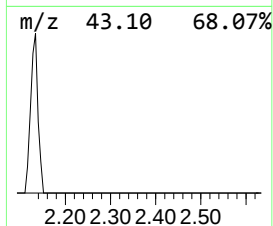
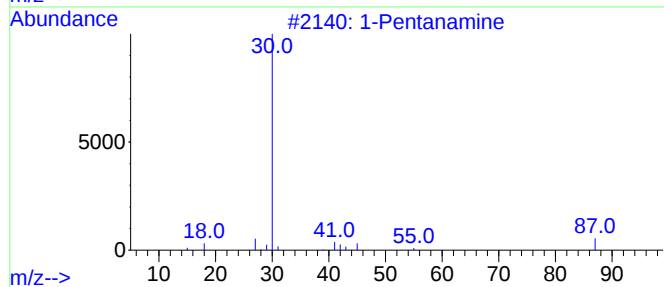
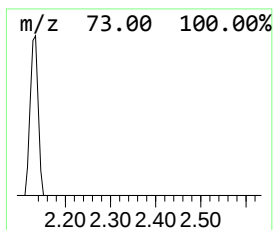
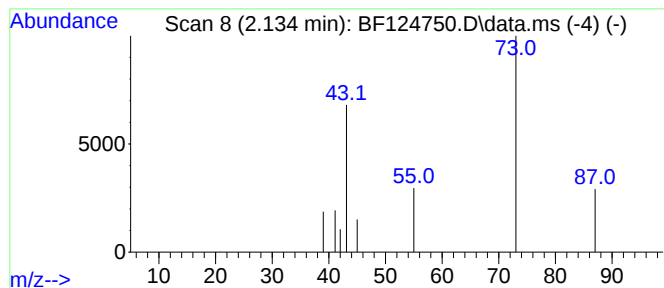
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.134 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	5.67 ng	9145	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentanamine	87	C5H13N	000110-58-7	5
2			Isobutylamine	73	C4H11N	000078-81-9	4
3			Morpholine	87	C4H9NO	000110-91-8	4
4			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4
5			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	4



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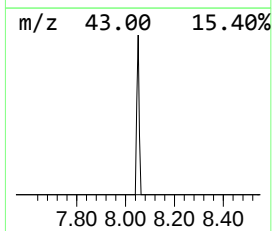
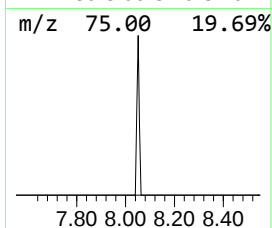
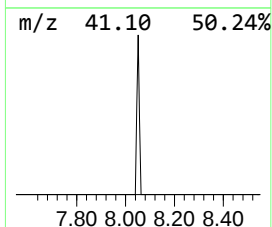
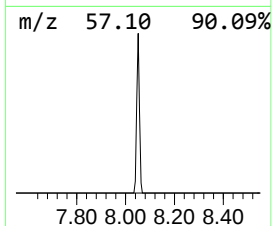
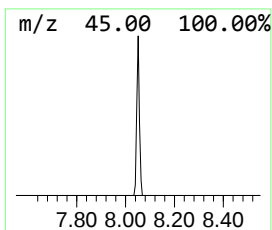
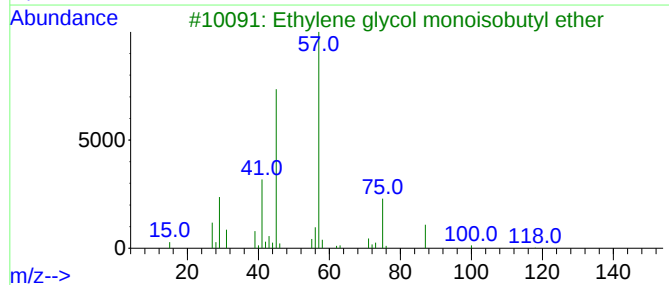
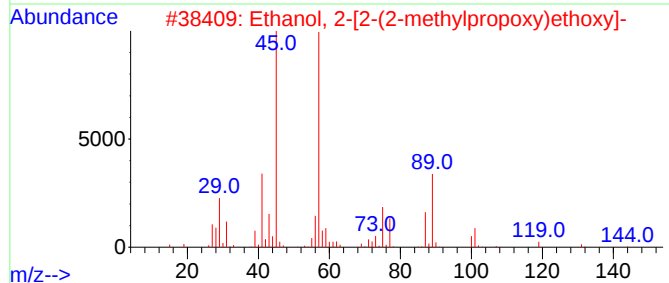
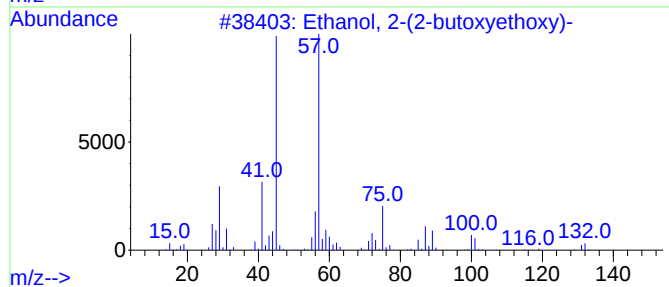
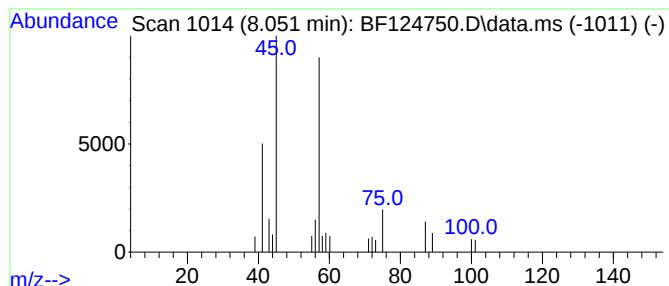
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	6.77 ng	13990	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	45
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	40
4			Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	40
5			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	39



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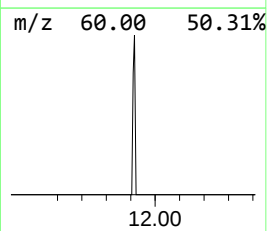
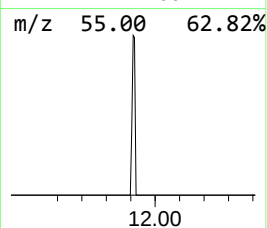
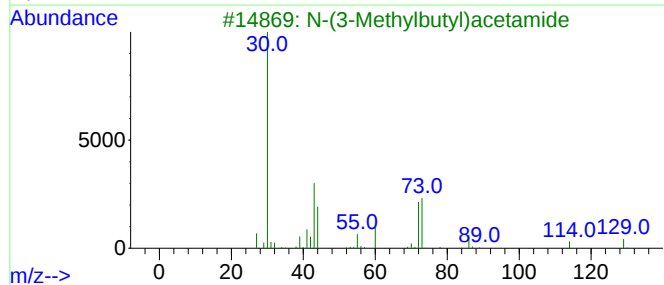
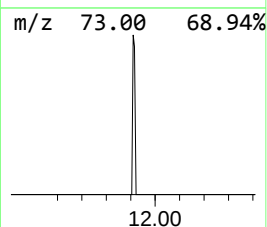
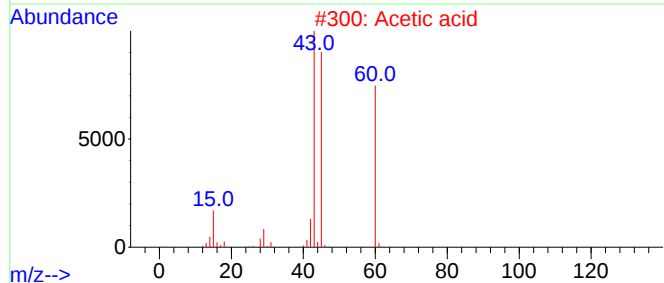
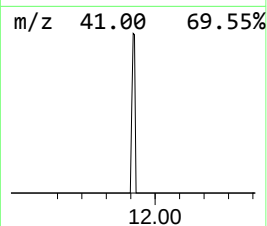
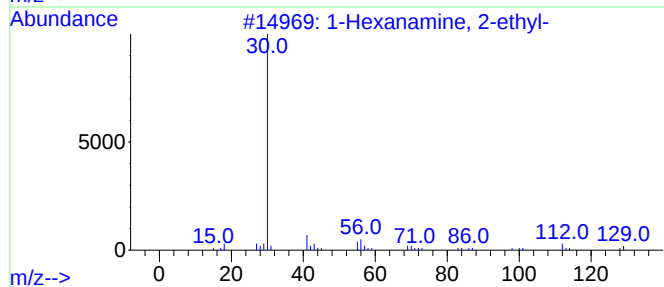
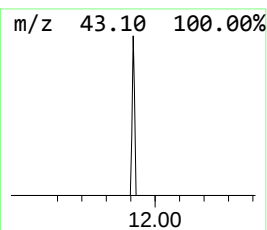
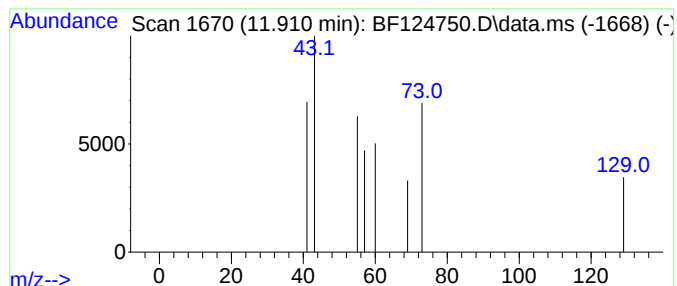
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Peak Number 3 unknown11.910 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	2.66 ng	3792	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanamine, 2-ethyl-	129	C8H19N	000104-75-6	5
2			Acetic acid	60	C2H4O2	000064-19-7	4
3			N-(3-Methylbutyl)acetamide	129	C7H15NO	013434-12-3	4
4			N-Pentylacetamide	129	C7H15NO	002524-60-9	4
5			3-Pentane isothiocyanate	129	C6H11NS	201224-89-7	4



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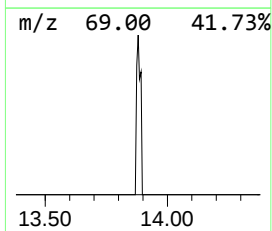
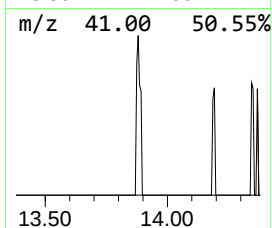
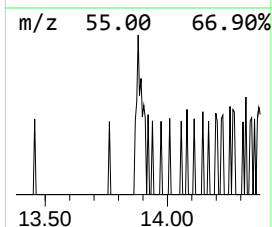
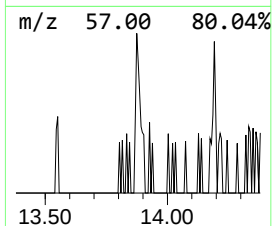
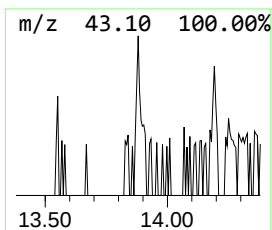
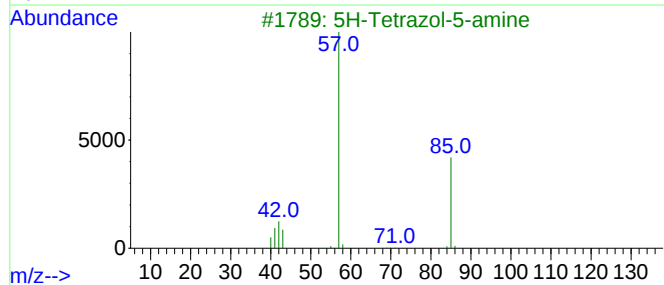
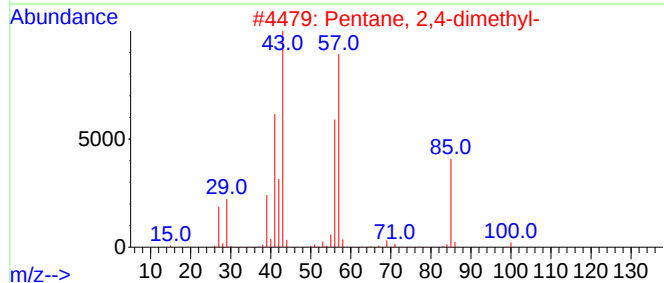
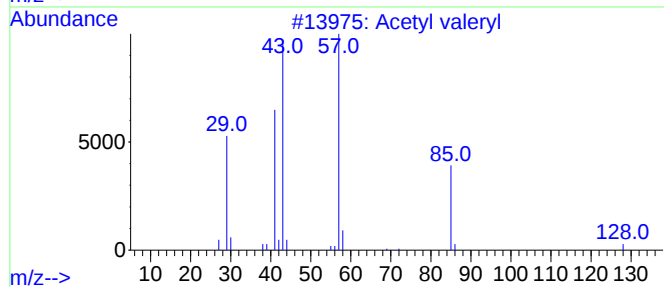
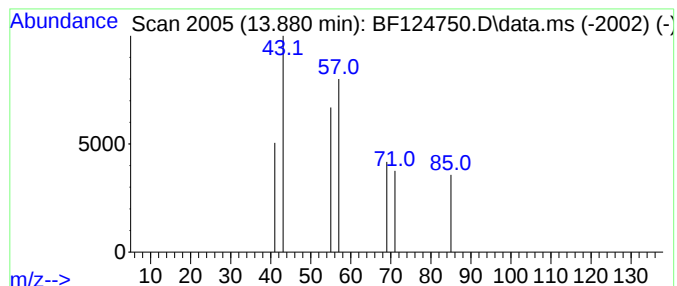
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Peak Number 4 unknown13.880 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	4.47 ng	5717	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetyl valeryl	128	C7H12O2	000096-04-8	9
2			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	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			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	4



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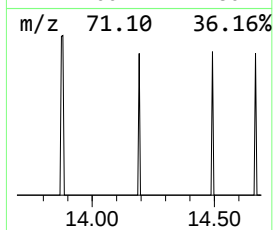
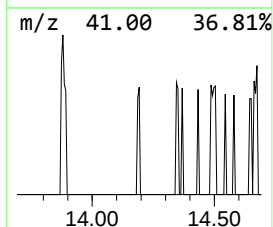
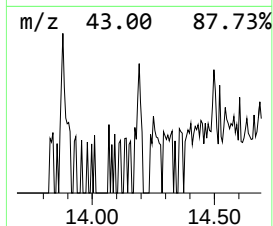
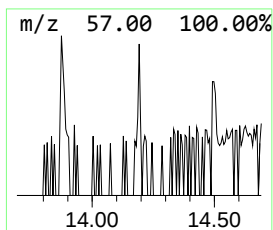
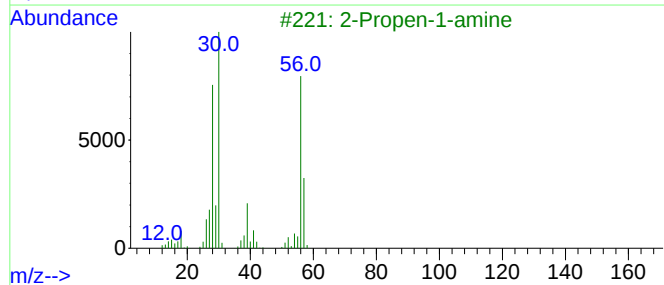
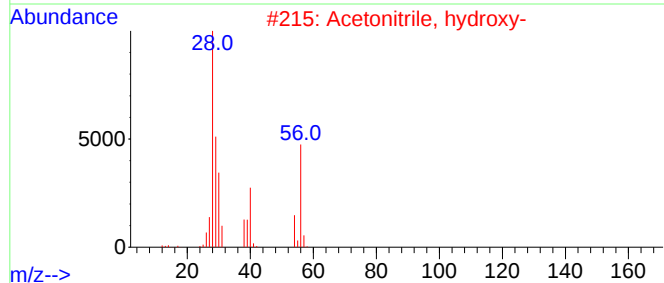
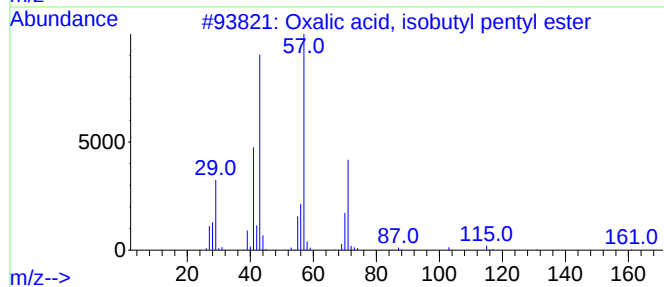
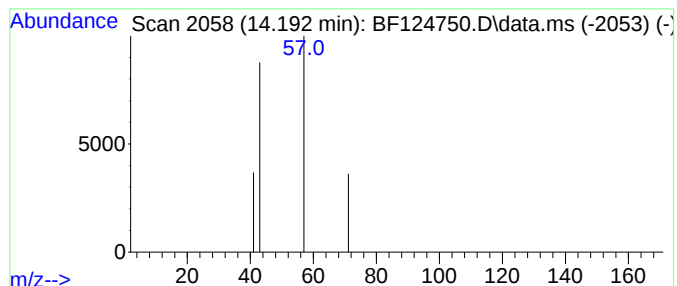
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Peak Number 5 unknown14.192 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.192	2.16 ng	2766	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	4
2			Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	3
3			2-Propen-1-amine	57	C3H7N	000107-11-9	2
4			Propanoic acid, 2-methyl-, 2-pro...	128	C7H12O2	015727-77-2	2
5			1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	2



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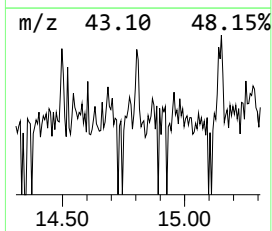
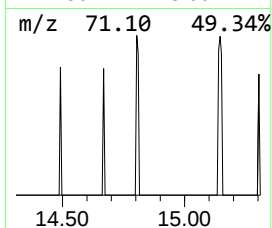
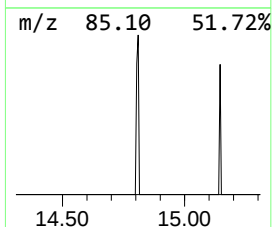
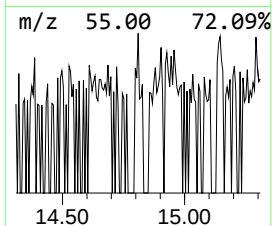
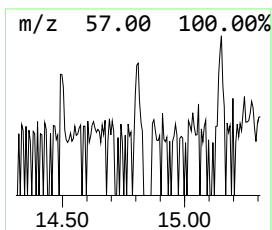
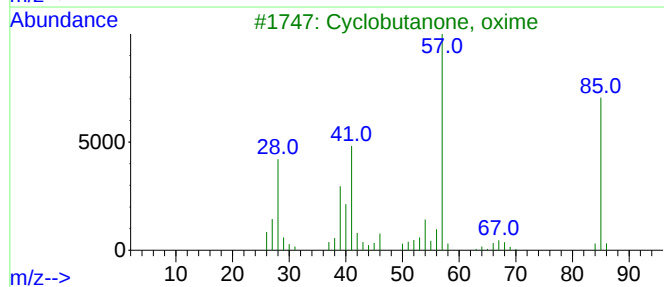
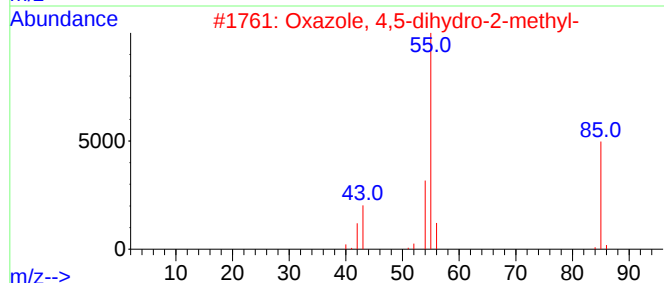
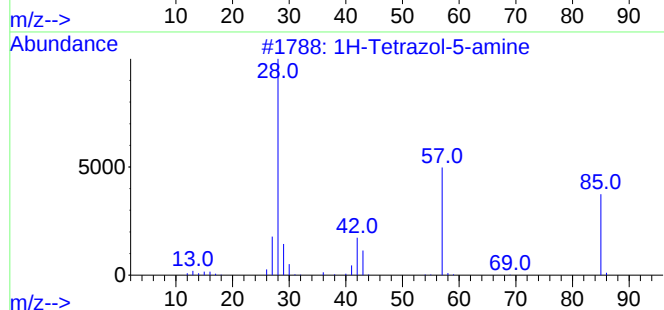
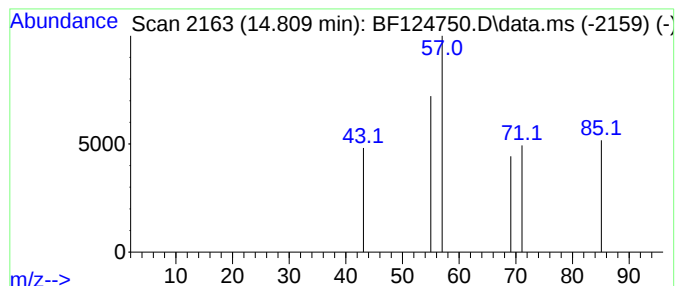
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.810 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.810	2.55 ng	2650	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
2			Oxazole, 4,5-dihydro-2-methyl-	85	C4H7NO	001120-64-5	4
3			Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4
4			5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
5			Oxalic acid, allyl nonyl ester	256	C14H24O4	1000309-23-7	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124750.D
Acq On : 24 Jul 2021 16:34
Operator : JU/CG
Sample : M3117-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-8

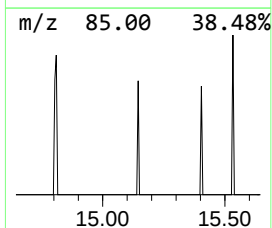
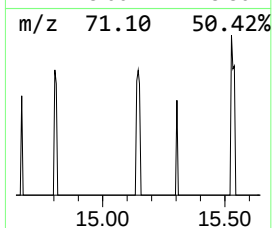
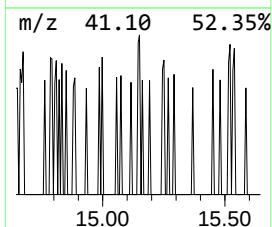
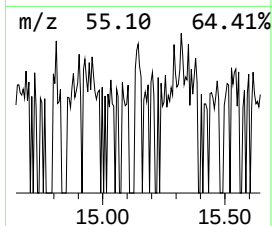
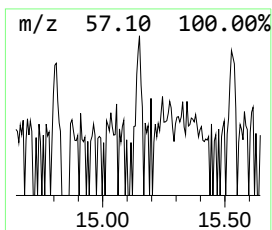
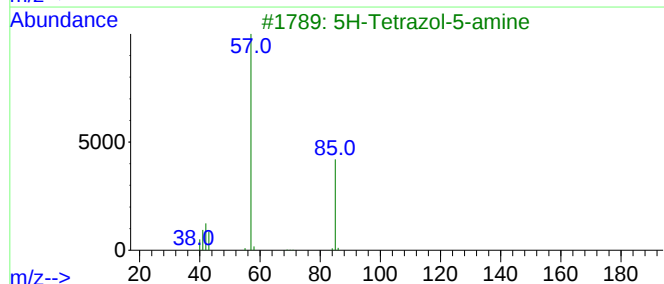
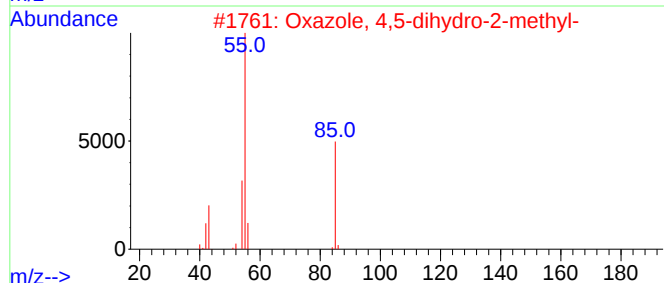
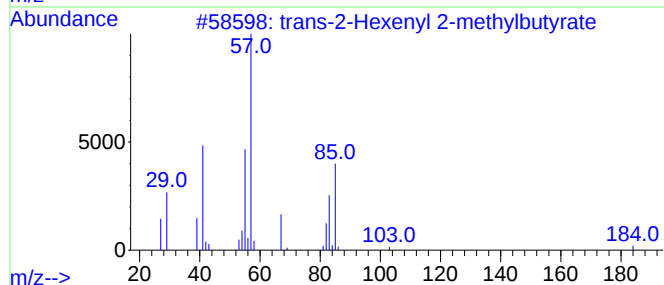
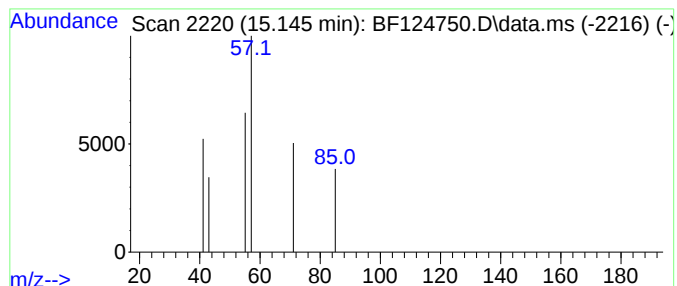
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.145 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	3.01 ng	3132	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-2-Hexenyl 2-methylbutyrate	184	C11H20O2	1000433-23-8	9
2			Oxazole, 4,5-dihydro-2-methyl-	85	C4H7NO	001120-64-5	4
3			5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
4			1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
5			(E)-But-2-en-1-yl 2-methylbutanoate	156	C9H16O2	1000372-81-0	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124750.D
Acq On : 24 Jul 2021 16:34
Operator : JU/CG
Sample : M3117-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-8

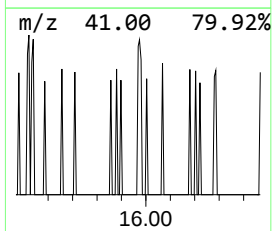
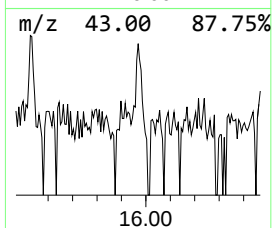
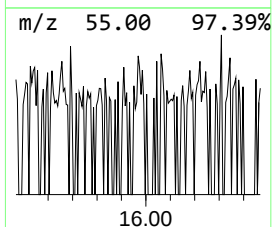
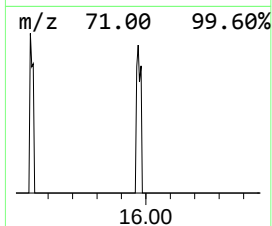
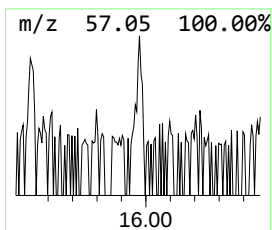
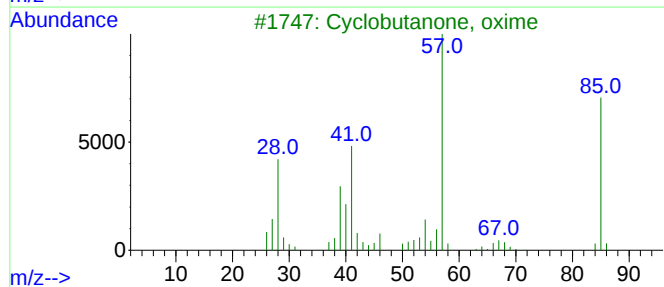
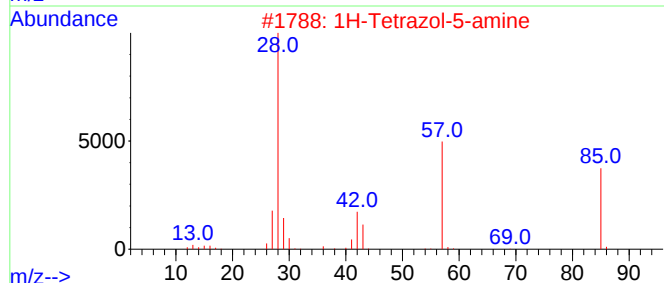
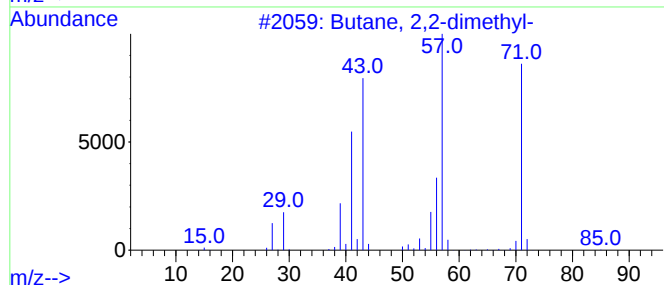
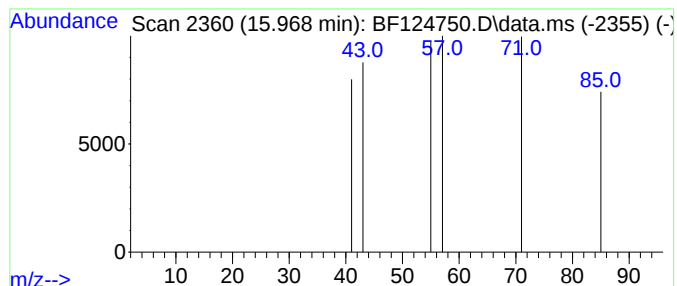
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.968 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.968	5.13 ng	5338	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	9
2			1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
3			Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4
4			(E)-But-2-en-1-yl 2-methylbutanoate	156	C9H16O2	1000372-81-0	4
5			Oxirane, 2-methyl-3-propyl-, cis-	100	C6H12O	006124-90-9	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124750.D
Acq On : 24 Jul 2021 16:34
Operator : JU/CG
Sample : M3117-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-8

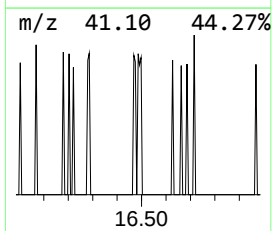
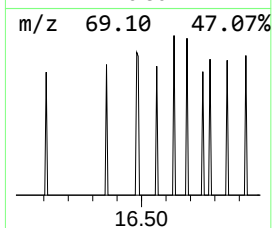
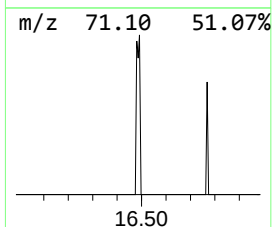
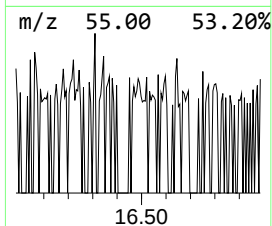
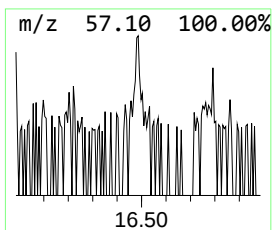
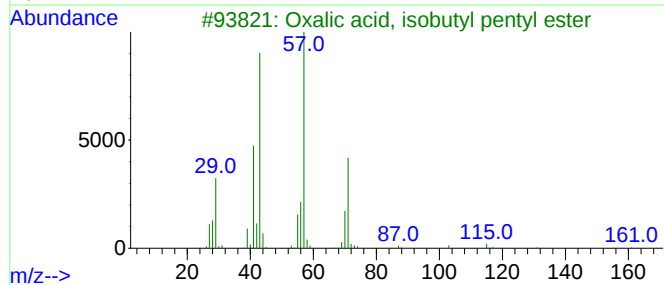
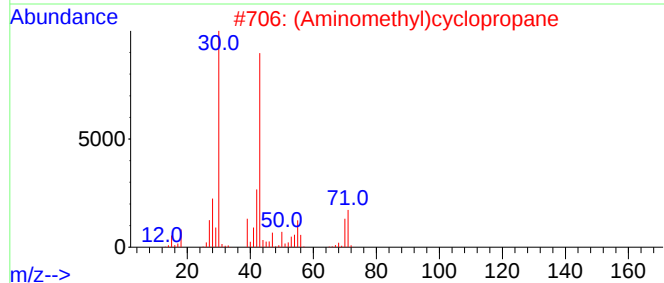
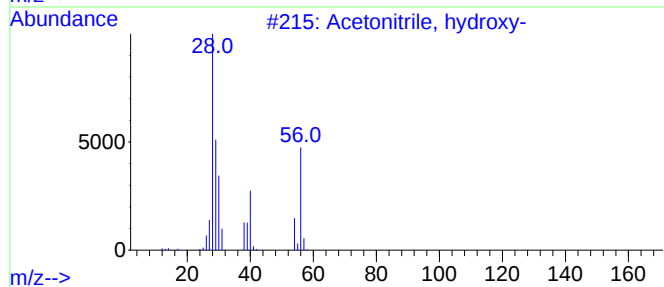
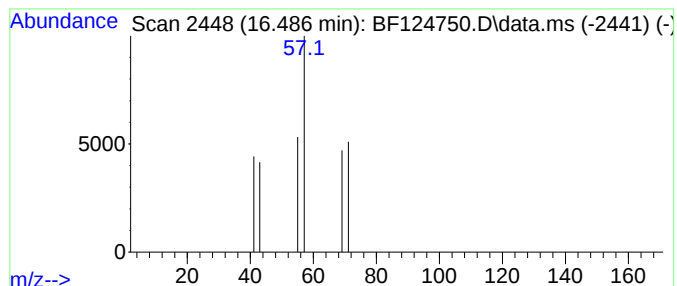
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown16.486 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.486	4.92 ng	5125	Perylene-d12	15.504

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			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	2
4			2-Propenamide	71	C3H5NO	000079-06-1	2
5			Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124750.D
Acq On : 24 Jul 2021 16:34
Operator : JU/CG
Sample : M3117-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-8

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

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					#	RT	Resp	Conc
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Ethanol, 2-(2-b...	8.051	6.8	ng	13990	2	8.151	41341	20.0
unknown11.910	11.910	2.7	ng	3792	4	11.392	28561	20.0
unknown13.880	13.880	4.5	ng	5717	5	14.033	25567	20.0
unknown14.192	14.192	2.2	ng	2766	5	14.033	25567	20.0
unknown14.810	14.810	2.5	ng	2650	6	15.504	20817	20.0
unknown15.145	15.145	3.0	ng	3132	6	15.504	20817	20.0
unknown15.968	15.968	5.1	ng	5338	6	15.504	20817	20.0
unknown16.486	16.486	4.9	ng	5125	6	15.504	20817	20.0