

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
 Data File : BF124769.D
 Acq On : 26 Jul 2021 17:29
 Operator : JU/CG
 Sample : M3117-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NJ-CLEAN-1

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: BF124769.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	8	11	15	rBB	10724	12341	8.93%	1.336%
2	5.093	507	511	514	rBB	5418	5614	4.06%	0.608%
3	5.487	574	578	581	rBB	130043	115539	83.63%	12.504%
4	6.498	745	750	752	rBV	116525	115737	83.77%	12.525%
5	6.869	811	813	816	rBB	36288	30296	21.93%	3.279%
6	7.434	905	909	912	rBB	88306	75075	54.34%	8.125%
7	8.051	1012	1014	1019	rBB	32000	27190	19.68%	2.943%
8	8.157	1028	1032	1035	rBB	48827	41354	29.93%	4.475%
9	9.228	1210	1214	1217	rBV	168344	138162	100.00%	14.952%
10	9.910	1327	1330	1333	rBB	57320	41836	30.28%	4.528%
11	10.698	1460	1464	1467	rBB	81255	62344	45.12%	6.747%
12	11.398	1579	1583	1586	rBV	42705	33587	24.31%	3.635%
13	11.786	1647	1649	1650	rBB	2664	1656	1.20%	0.179%
14	11.916	1668	1671	1675	rBB	6869	5306	3.84%	0.574%
15	12.610	1786	1789	1791	rBB	3011	2499	1.81%	0.270%
16	12.833	1825	1827	1830	rBB	3381	2725	1.97%	0.295%
17	12.980	1849	1852	1855	rBV	126210	102329	74.06%	11.074%
18	13.557	1945	1950	1952	rBV2	1325	1653	1.20%	0.179%
19	13.798	1986	1991	1992	rBV2	1634	1982	1.43%	0.214%
20	13.886	2001	2006	2016	rVB5	6288	15546	11.25%	1.682%
21	14.033	2028	2031	2034	rBV	32711	28891	20.91%	3.127%
22	14.198	2055	2059	2062	rBV2	1558	2140	1.55%	0.232%
23	14.498	2108	2110	2112	rBV2	2464	1837	1.33%	0.199%
24	15.074	2204	2208	2210	rBV4	2599	3050	2.21%	0.330%
25	15.145	2217	2220	2224	rBV5	3021	4327	3.13%	0.468%
26	15.304	2245	2247	2251	rVB3	2132	2167	1.57%	0.235%
27	15.510	2277	2282	2288	rBV	18106	23713	17.16%	2.566%
28	15.745	2319	2322	2326	rVB3	1731	1988	1.44%	0.215%
29	15.863	2340	2342	2346	rVB3	1805	1808	1.31%	0.196%
30	15.974	2357	2361	2366	rBV4	1996	3416	2.47%	0.370%
31	16.215	2398	2402	2403	rBV2	1908	1713	1.24%	0.185%
32	16.368	2424	2428	2429	rVB3	1538	1813	1.31%	0.196%
33	16.492	2446	2449	2454	rVB3	1573	2100	1.52%	0.227%
34	16.663	2475	2478	2482	rVB3	2506	3517	2.55%	0.381%
35	17.245	2574	2577	2580	rBV2	1865	2630	1.90%	0.285%
36	17.315	2587	2589	2592	rBV2	1581	2311	1.67%	0.250%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.662	2643	2648	2651	rBV2	853	1600	1.16%	0.173%
38	18.545	2795	2798	2802	rBV3	1445	2220	1.61%	0.240%

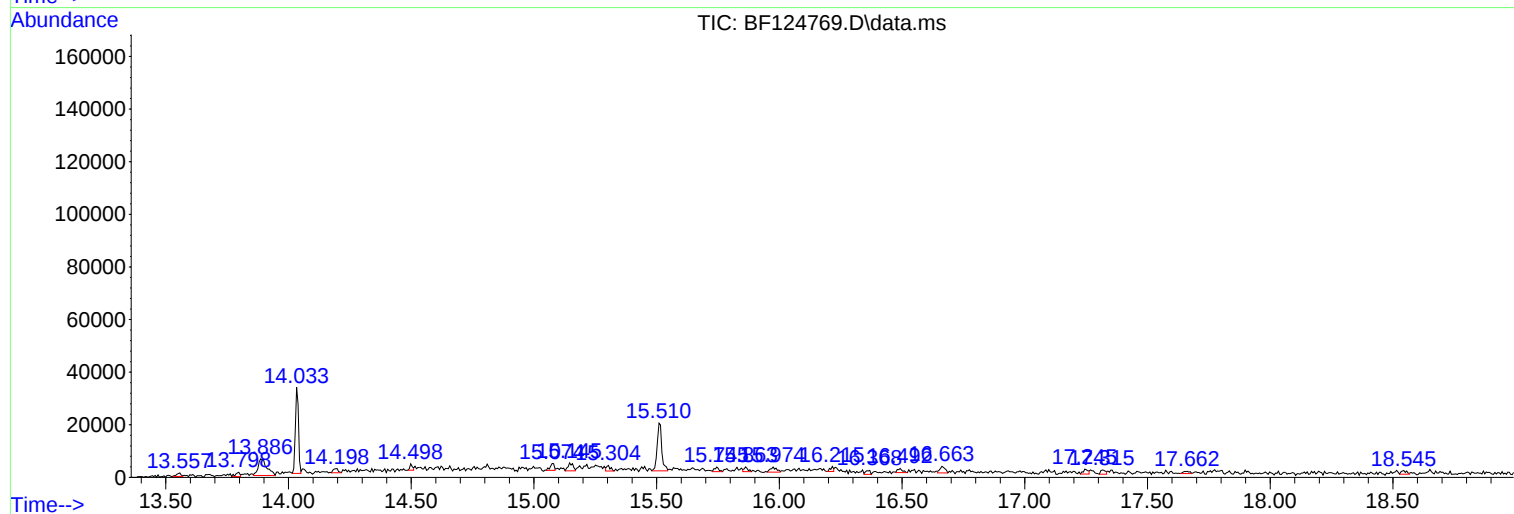
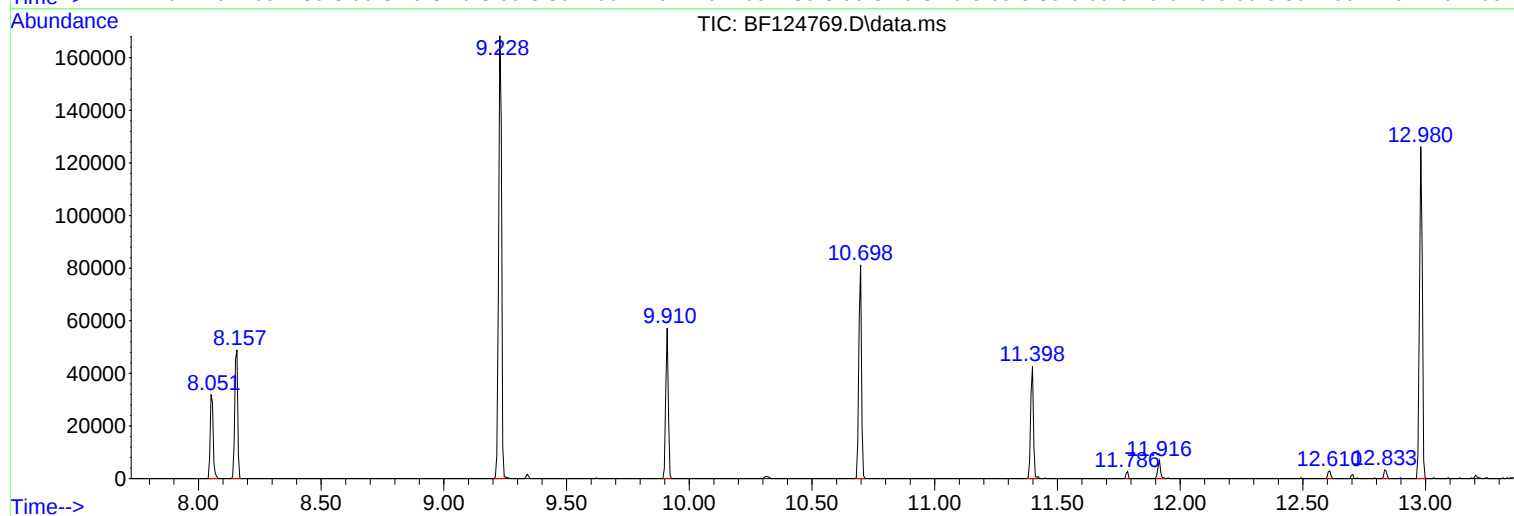
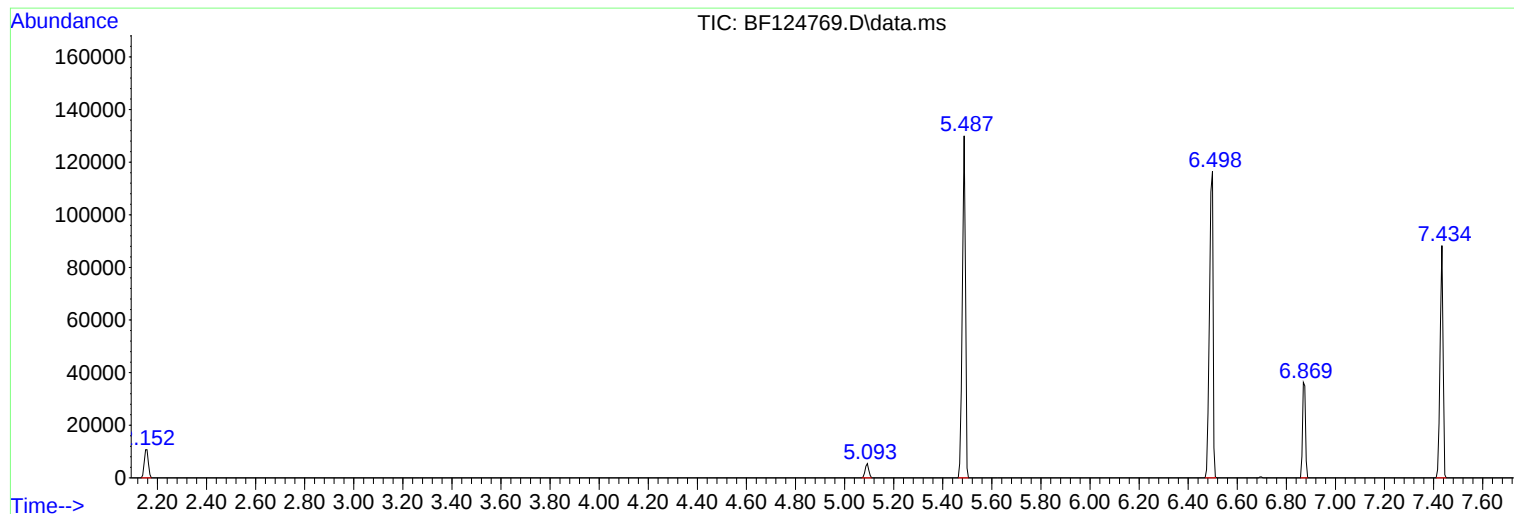
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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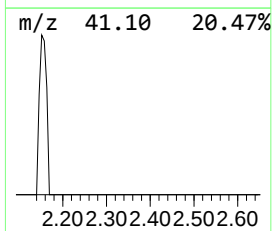
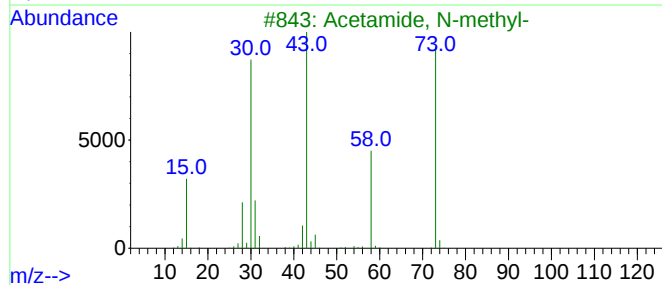
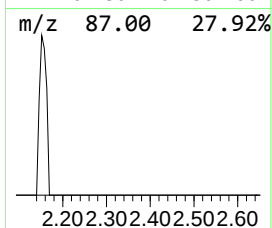
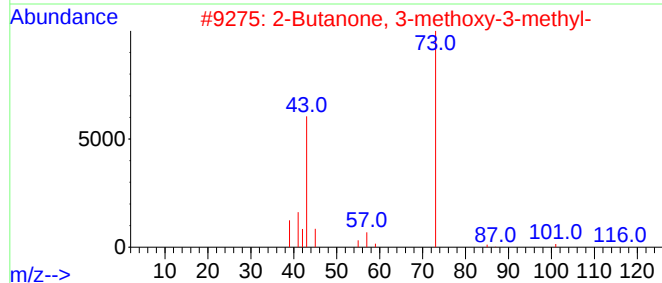
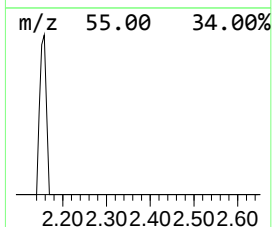
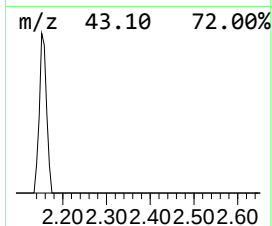
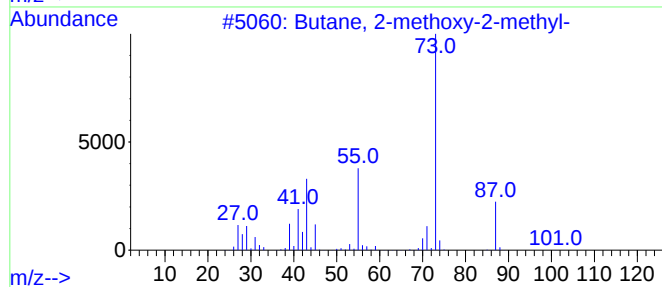
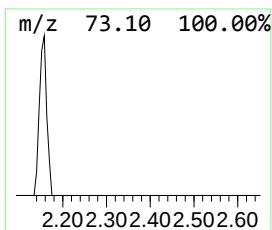
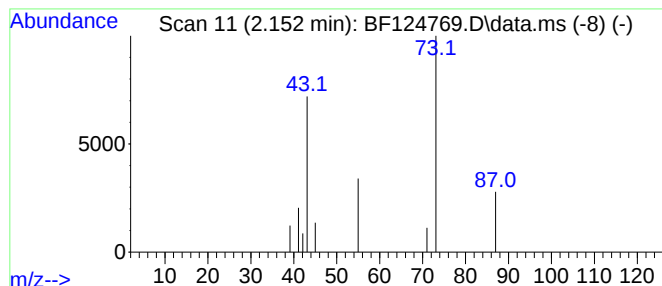
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.152	8.15 ng	12341	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	56
2			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9
3			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	5
4			Isobutylamine	73	C4H11N	000078-81-9	5
5			1-Pentanamine	87	C5H13N	000110-58-7	4



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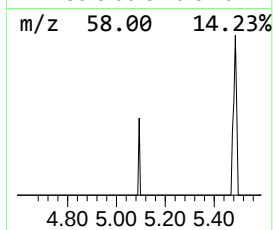
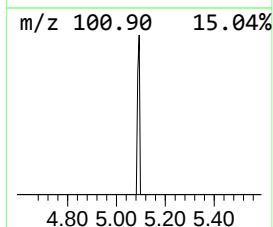
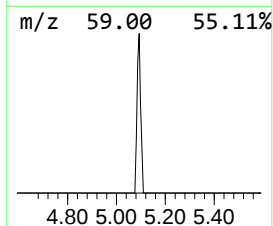
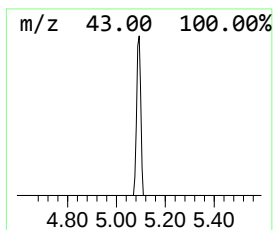
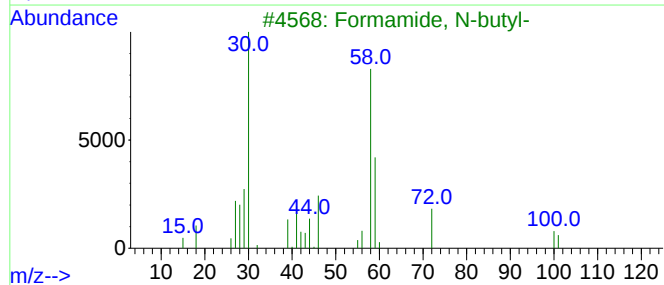
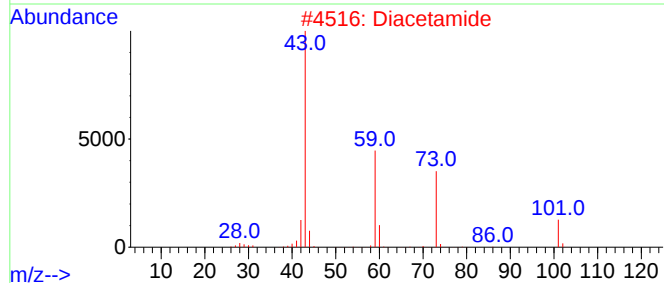
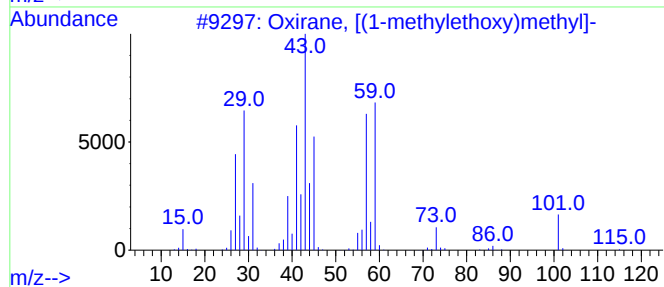
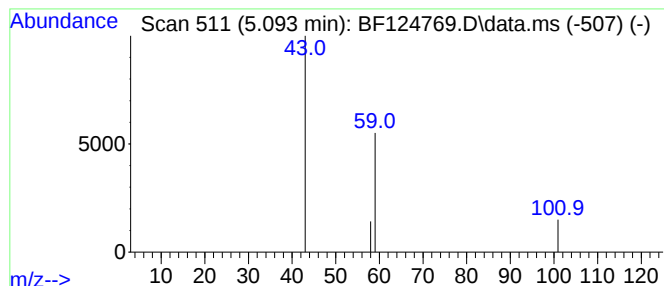
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.093 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	3.71 ng	5614	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	9
2			Diacetamide	101	C4H7NO2	000625-77-4	7
3			Formamide, N-butyl-	101	C5H11NO	000871-71-6	4
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	3
5			Propylamine	59	C3H9N	000107-10-8	3



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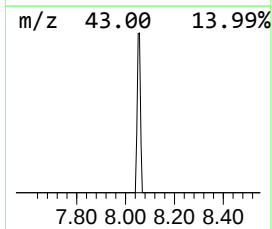
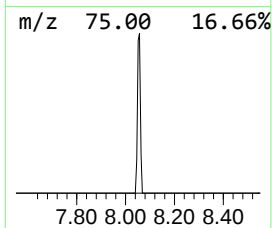
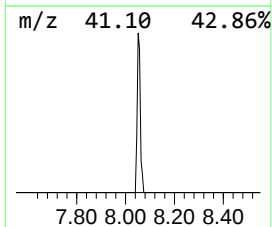
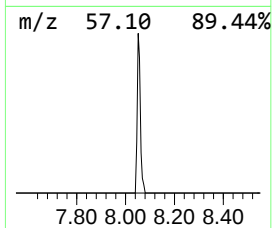
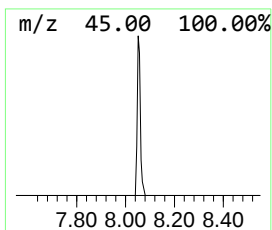
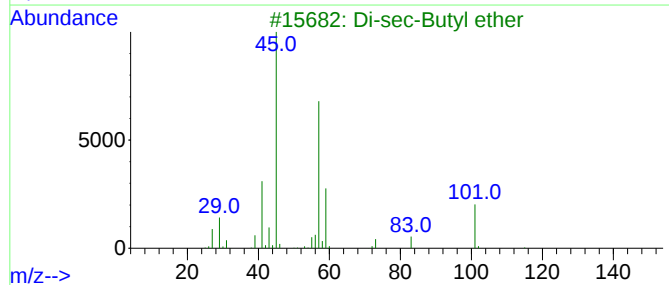
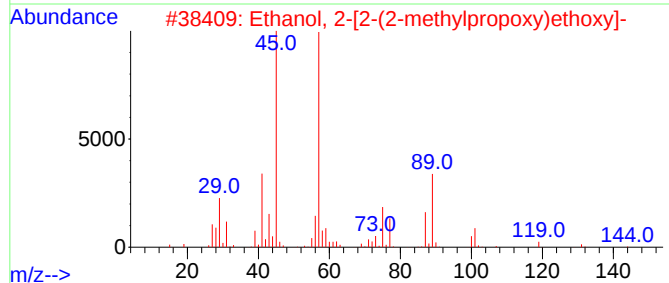
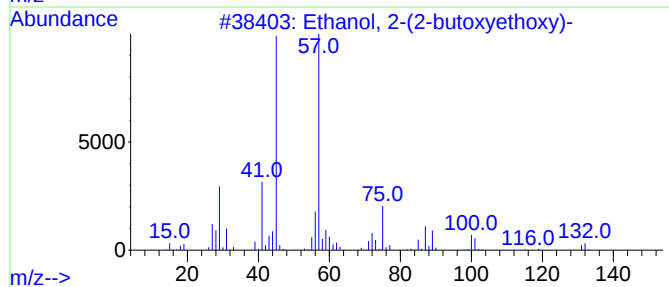
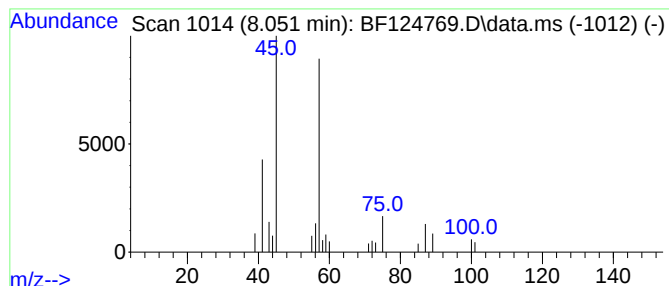
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	13.15 ng	27190	Naphthalene-d8	8.157

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	56
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	42
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	40
5			Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	40



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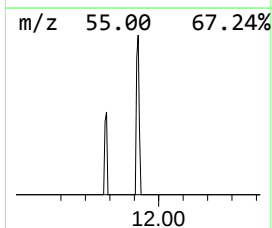
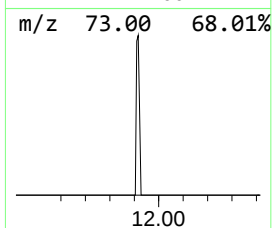
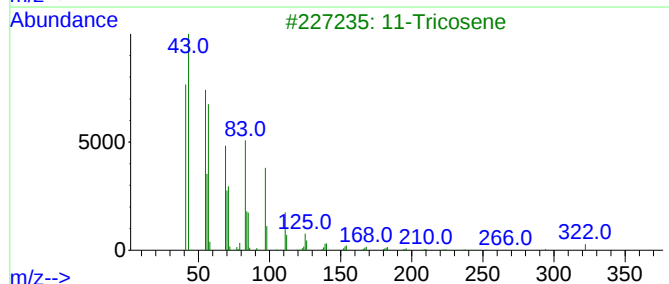
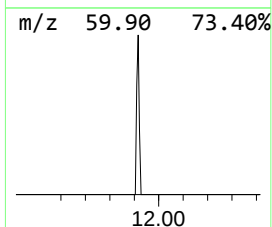
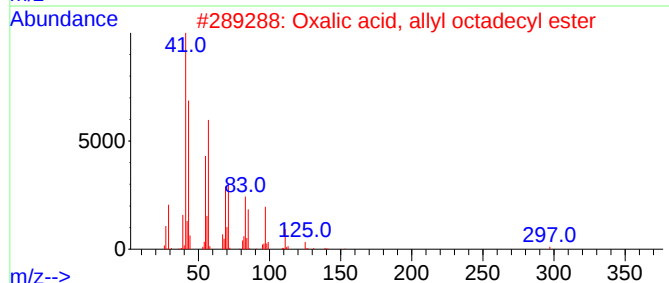
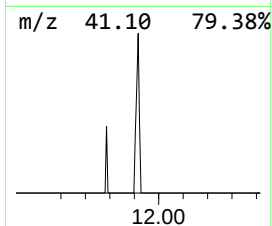
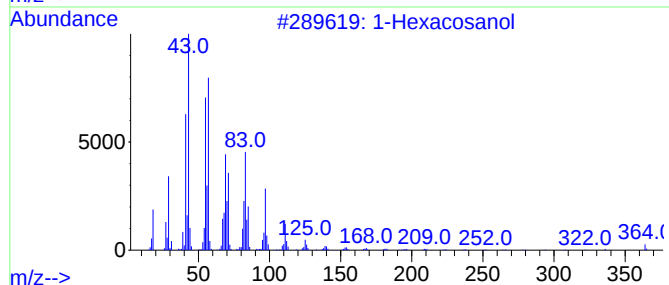
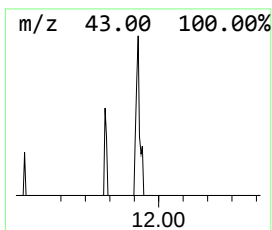
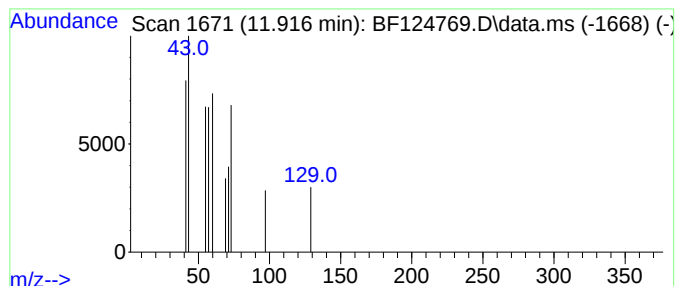
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown11.916 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.16 ng	5306	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol		382	C26H54O		000506-52-5	22
2	Oxalic acid, allyl octadecyl ester		382	C23H42O4		1000309-24-5	10
3	11-Tricosene		322	C23H46		052078-56-5	10
4	N-(3-Methylbutyl)acetamide		129	C7H15NO		013434-12-3	9
5	2-Butenoic acid, 2-methoxy-3-met...		144	C7H12O3		056009-32-6	9



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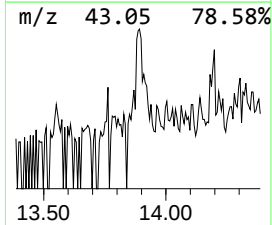
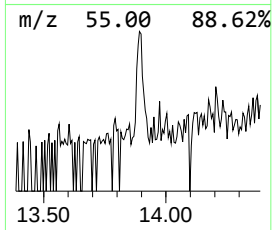
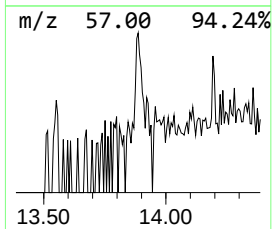
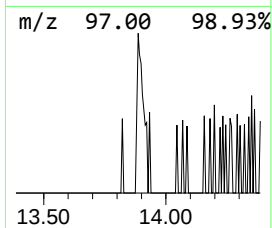
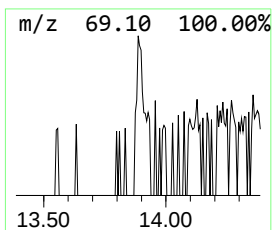
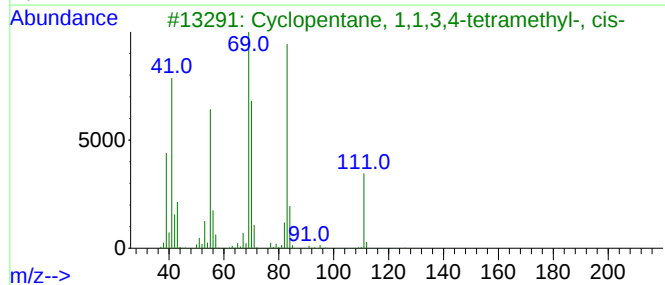
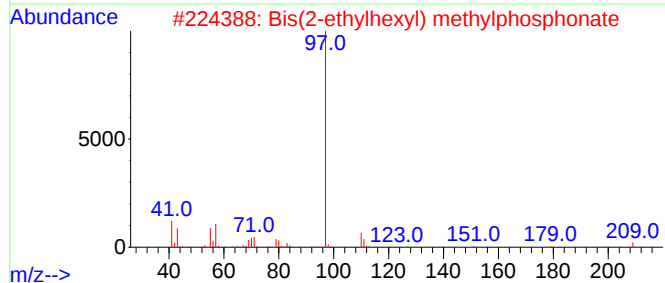
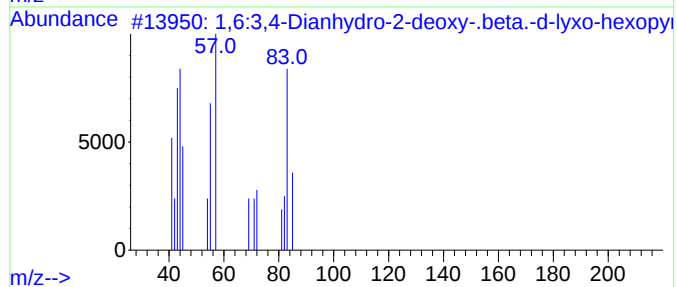
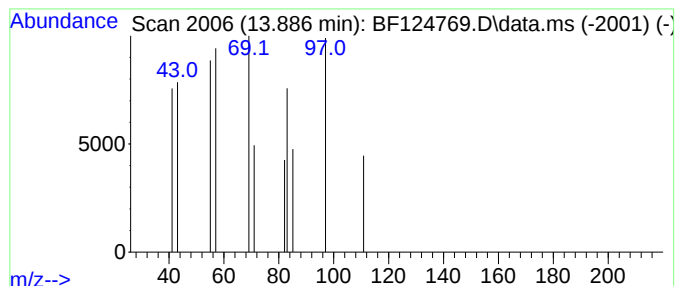
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown13.886 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	10.76 ng	15546	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6:3,4-Dianhydro-2-deoxy-.beta....	128	C6H8O3	050767-53-8	16		
2	Bis(2-ethylhexyl) methylphosphonate	320	C17H37O3P	1000298-35-3	9		
3	Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	053907-60-1	9		
4	Oxirane, 2-butyl-3-methyl-, cis-	114	C7H14O	056052-93-8	9		
5	Octadecane, 1-(ethenylloxy)-	296	C20H40O	000930-02-9	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124769.D
Acq On : 26 Jul 2021 17:29
Operator : JU/CG
Sample : M3117-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-1

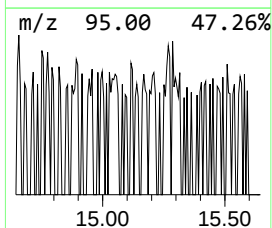
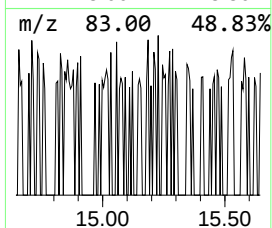
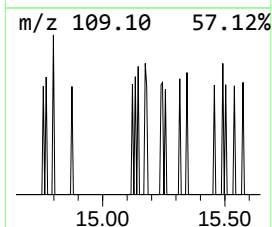
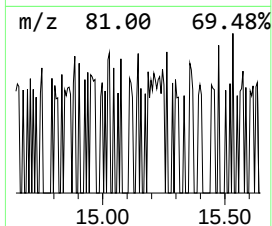
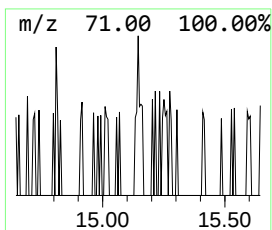
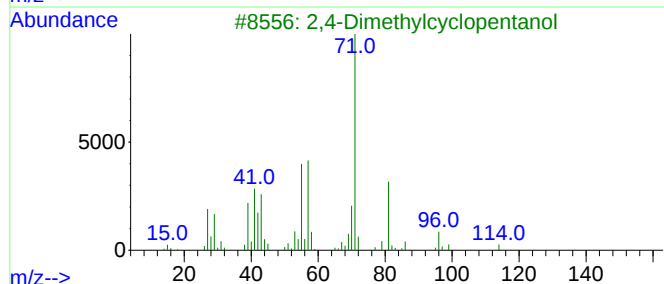
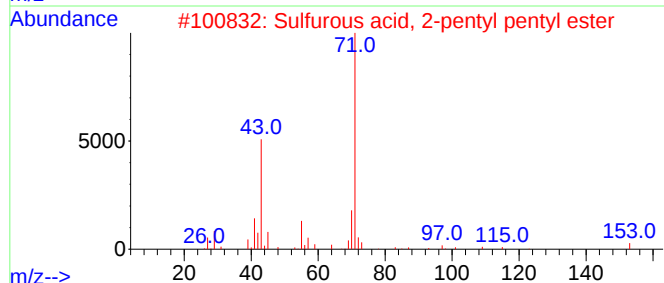
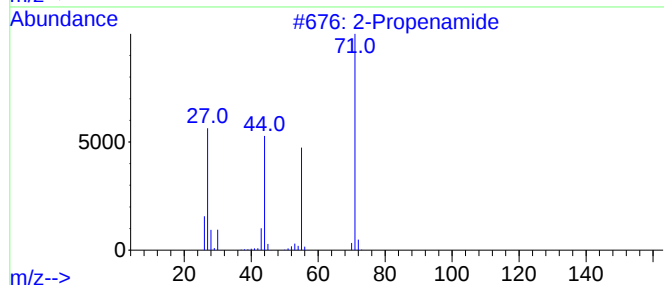
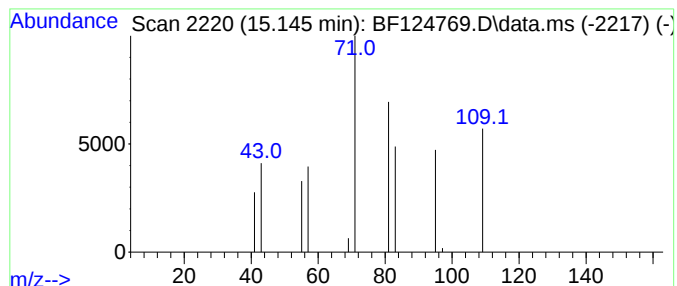
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown15.145 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	3.65 ng	4327	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propenamide	71	C3H5NO	000079-06-1	4
2			Sulfurous acid, 2-pentyl pentyl ...	222	C10H22O3S	1000309-15-4	4
3			2,4-Dimethylcyclopentanol	114	C7H14O	089794-28-5	4
4			Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	3
5			3,4-Pyridinediamine	109	C5H7N3	000054-96-6	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124769.D
Acq On : 26 Jul 2021 17:29
Operator : JU/CG
Sample : M3117-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

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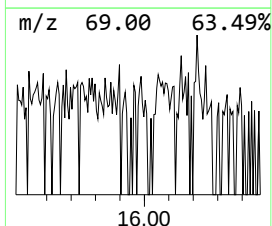
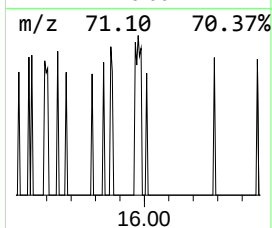
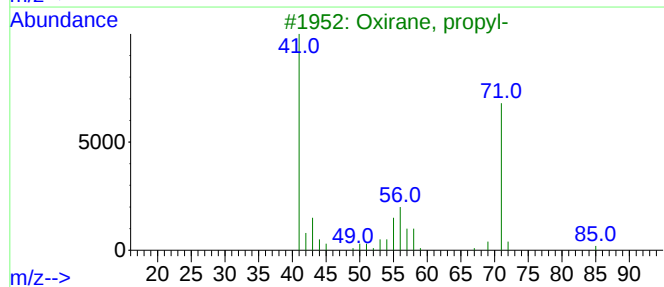
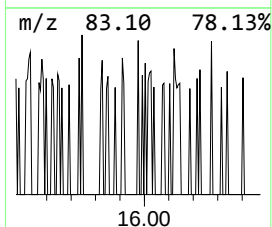
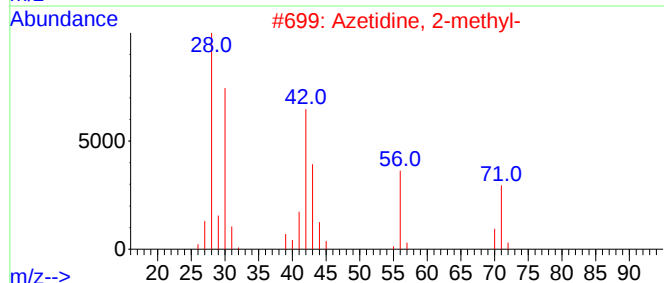
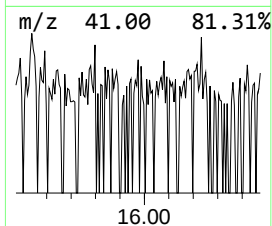
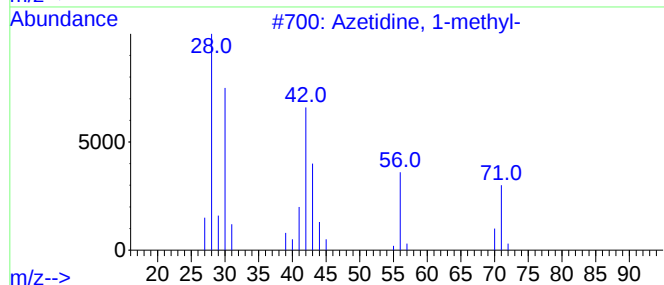
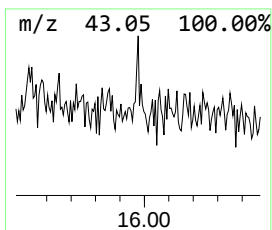
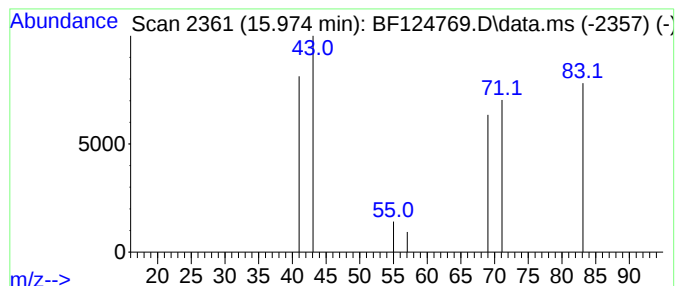
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.974 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.974	2.88 ng	3416	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
2			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
3			Oxirane, propyl-	86	C5H10O	001003-14-1	4
4			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	4
5			Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124769.D
Acq On : 26 Jul 2021 17:29
Operator : JU/CG
Sample : M3117-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-1

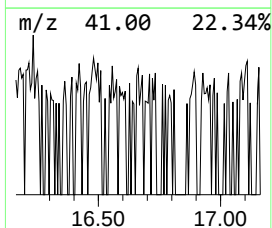
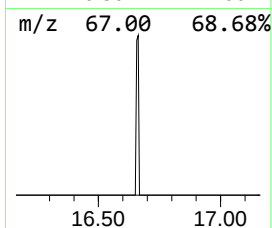
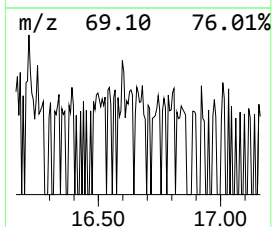
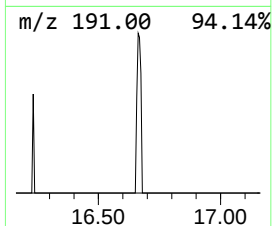
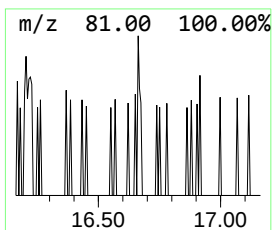
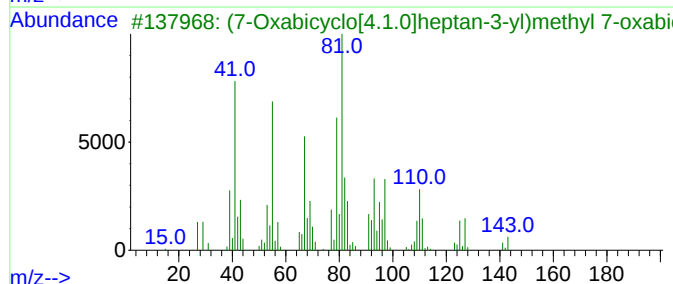
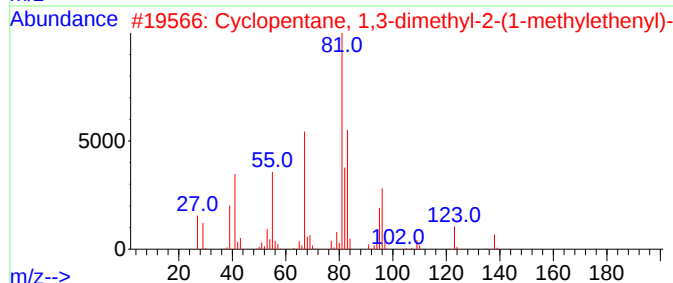
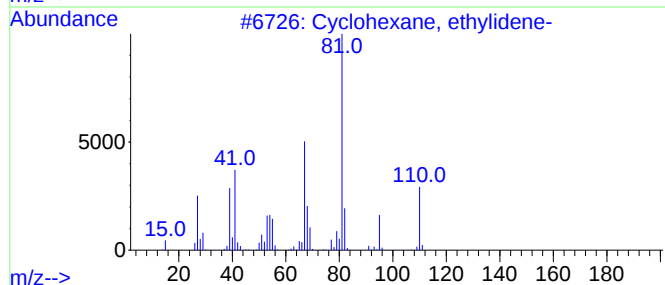
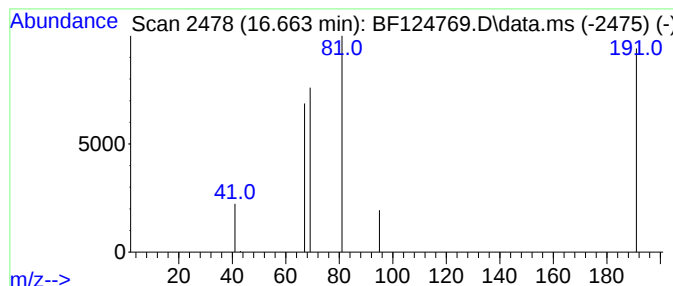
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.663 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.663	2.97 ng	3517	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, ethylidene-	110	C8H14	001003-64-1	4
2			Cyclopentane, 1,3-dimethyl-2-(1-...	138	C10H18	061142-31-2	4
3			(7-Oxabicyclo[4.1.0]heptan-3-yl)...	252	C14H20O4	1000473-40-7	4
4			Spiro[2.5]octane	110	C8H14	000185-65-9	4
5			Cyclohexane, ethenyl-	110	C8H14	000695-12-5	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124769.D
Acq On : 26 Jul 2021 17:29
Operator : JU/CG
Sample : M3117-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

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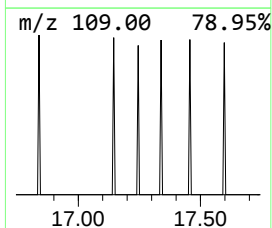
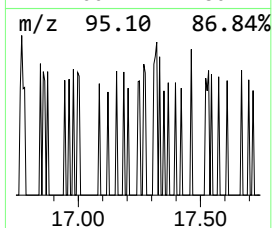
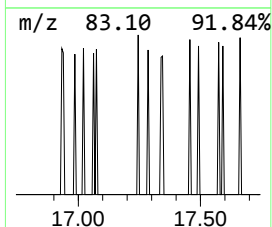
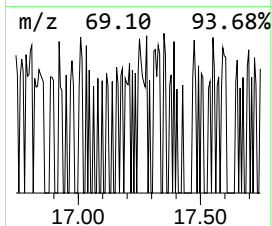
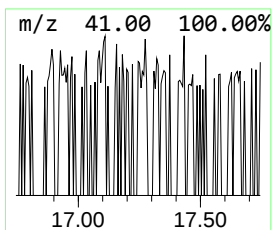
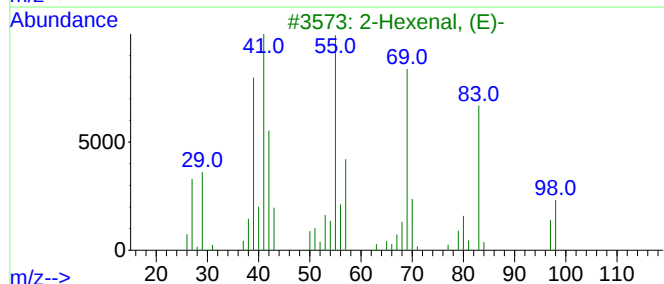
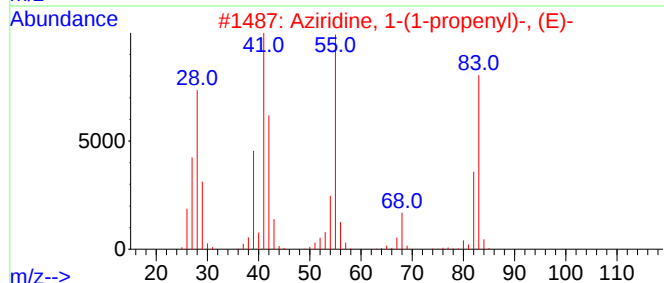
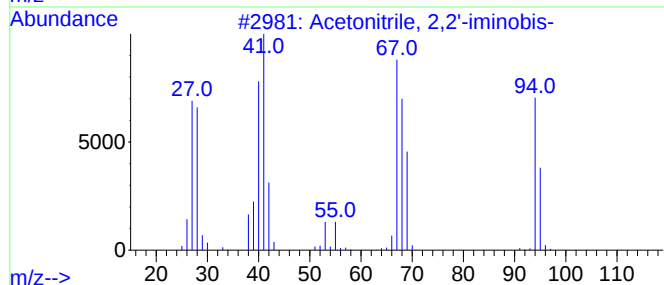
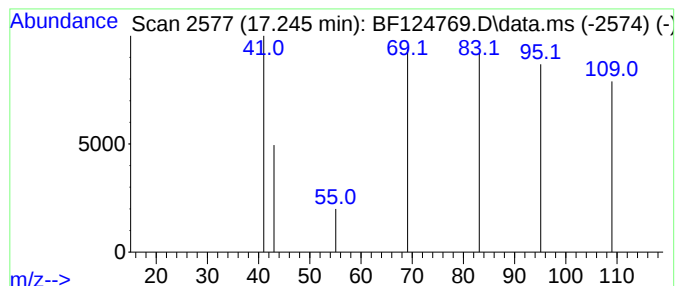
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.245 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.245	2.22 ng	2630	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetonitrile, 2,2'-iminobis-	95	C4H5N3	000628-87-5	4
2			Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	4
3			2-Hexenal, (E)-	98	C6H10O	006728-26-3	4
4			Phosphinous acid, diisopropyl ester	166	C6H15O3P	000691-96-3	4
5			4H-1,2,4-Triazole, 4-methyl-	83	C3H5N3	010570-40-8	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124769.D
Acq On : 26 Jul 2021 17:29
Operator : JU/CG
Sample : M3117-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-1

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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unknown5.093	5.093	3.7	ng	5614	1	6.875	30296	20.0
Ethanol, 2-(2-b...	8.051	13.2	ng	27190	2	8.157	41354	20.0
unknown11.916	11.916	3.2	ng	5306	4	11.398	33587	20.0
unknown13.886	13.886	10.8	ng	15546	5	14.033	28891	20.0
unknown15.145	15.145	3.6	ng	4327	6	15.510	23713	20.0
unknown15.974	15.974	2.9	ng	3416	6	15.510	23713	20.0
unknown16.663	16.663	3.0	ng	3517	6	15.510	23713	20.0
unknown17.245	17.245	2.2	ng	2630	6	15.510	23713	20.0