

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
 Data File : BF124776.D
 Acq On : 26 Jul 2021 21:31
 Operator : JU/CG
 Sample : M3151-02
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-2

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

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

Signal : TIC: BF124776.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.158	9	12	16	rBB	9332	9949	8.29%	1.098%
2	5.099	509	512	515	rBB	1809	1977	1.65%	0.218%
3	5.493	575	579	582	rBB	132036	112007	93.35%	12.356%
4	6.498	745	750	753	rBV	118793	110502	92.09%	12.190%
5	6.875	811	814	817	rBB	39439	27659	23.05%	3.051%
6	7.434	905	909	912	rBB	77538	71478	59.57%	7.885%
7	8.051	1012	1014	1018	rBB	8119	6789	5.66%	0.749%
8	8.157	1029	1032	1035	rBB	48974	35393	29.50%	3.904%
9	9.234	1211	1215	1218	rBV	151932	119987	100.00%	13.237%
10	9.910	1327	1330	1333	rBB	41947	32948	27.46%	3.635%
11	10.698	1461	1464	1467	rBB	69645	54705	45.59%	6.035%
12	11.398	1580	1583	1586	rBV	37777	27409	22.84%	3.024%
13	11.916	1669	1671	1674	rBB	6501	5264	4.39%	0.581%
14	12.610	1787	1789	1792	rBB	3885	3148	2.62%	0.347%
15	12.704	1803	1805	1808	rBB	7112	4658	3.88%	0.514%
16	12.839	1826	1828	1830	rBB	3649	2314	1.93%	0.255%
17	12.986	1849	1853	1856	rBB	116866	97642	81.38%	10.772%
18	13.210	1889	1891	1893	rBB	2939	1965	1.64%	0.217%
19	13.551	1947	1949	1952	rBB	7378	5371	4.48%	0.593%
20	13.880	2002	2005	2015	rBB3	12759	15469	12.89%	1.706%
21	14.039	2027	2032	2035	rBV	34226	28825	24.02%	3.180%
22	14.198	2055	2059	2064	rBB	16507	13625	11.36%	1.503%
23	14.416	2094	2096	2099	rVB	2073	2160	1.80%	0.238%
24	14.504	2108	2111	2114	rBV	16509	14235	11.86%	1.570%
25	14.616	2124	2130	2132	rBV2	1806	2570	2.14%	0.284%
26	14.721	2145	2148	2152	rVB2	4755	5799	4.83%	0.640%
27	14.810	2155	2163	2167	rVB2	15658	20181	16.82%	2.226%
28	14.886	2174	2176	2180	rBV	1532	1738	1.45%	0.192%
29	14.963	2186	2189	2193	rVB2	1133	1459	1.22%	0.161%
30	15.057	2202	2205	2207	rVB2	1489	1493	1.24%	0.165%
31	15.151	2216	2221	2224	rBV	12444	13975	11.65%	1.542%
32	15.515	2279	2283	2290	rBV2	18278	30733	25.61%	3.390%
33	15.980	2357	2362	2365	rBV2	5085	7210	6.01%	0.795%
34	16.486	2443	2448	2454	rVB3	2503	4677	3.90%	0.516%
35	17.039	2538	2542	2544	rBB2	1390	1807	1.51%	0.199%
36	17.074	2544	2548	2549	rBV	1529	1583	1.32%	0.175%

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37	17.098	2549	2552	2557	rVB2	1648	2706	2.26%	0.299%
38	17.321	2587	2590	2593	rVB2	1209	1633	1.36%	0.180%
39	18.192	2735	2738	2743	rBV2	1005	1854	1.55%	0.205%
40	18.839	2846	2848	2853	rVB	972	1584	1.32%	0.175%

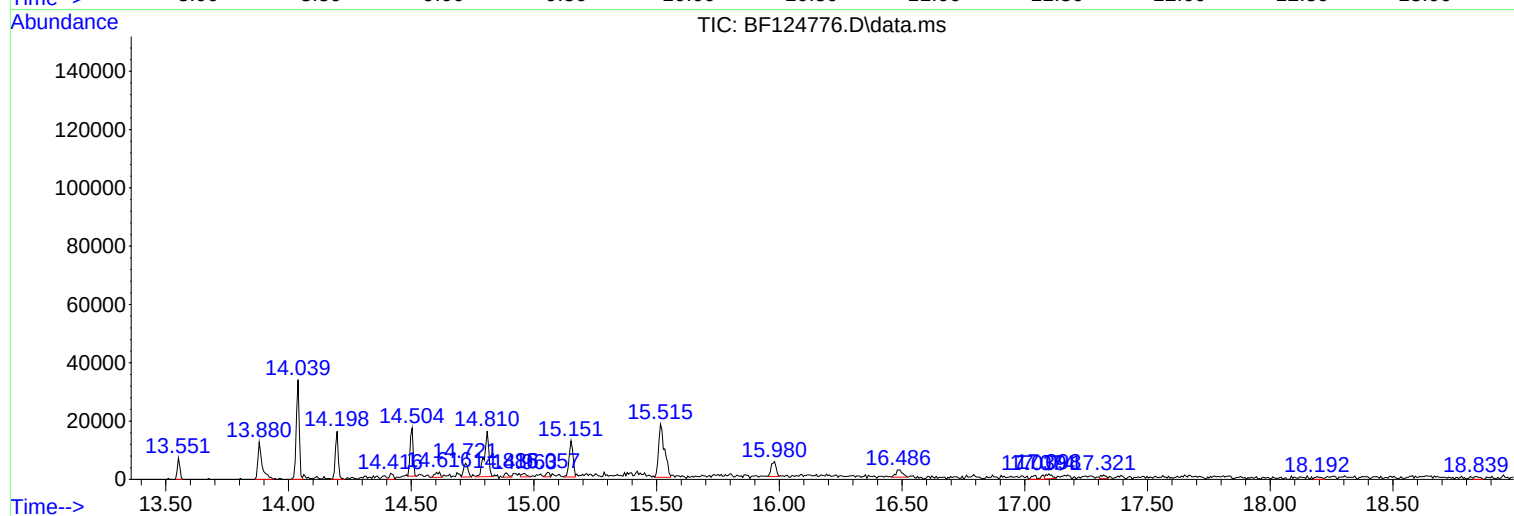
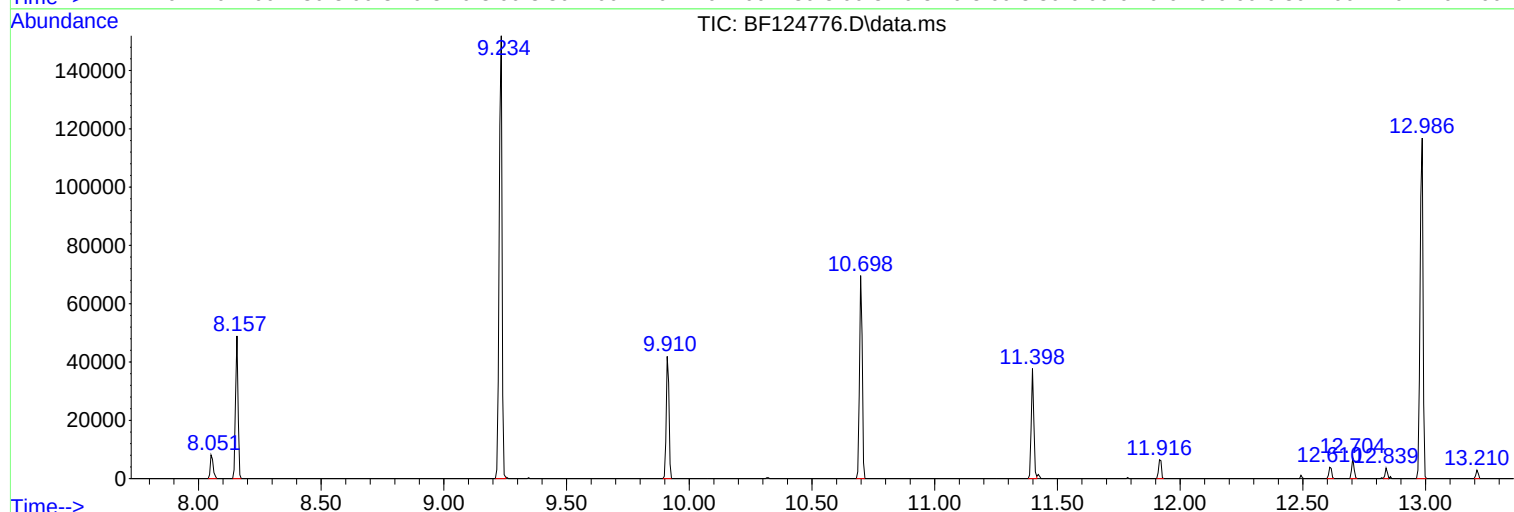
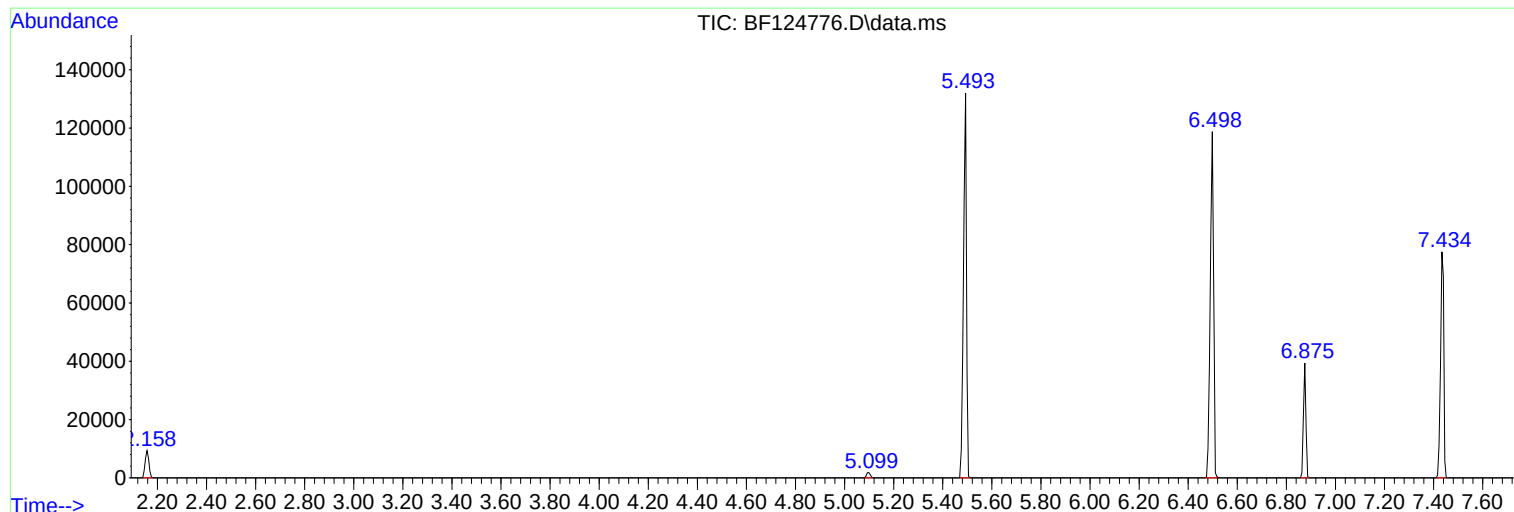
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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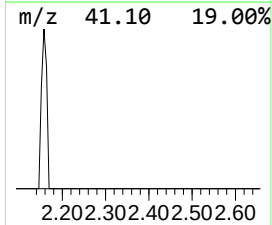
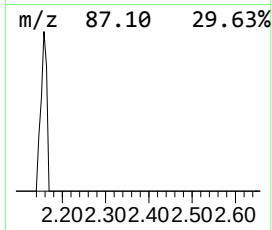
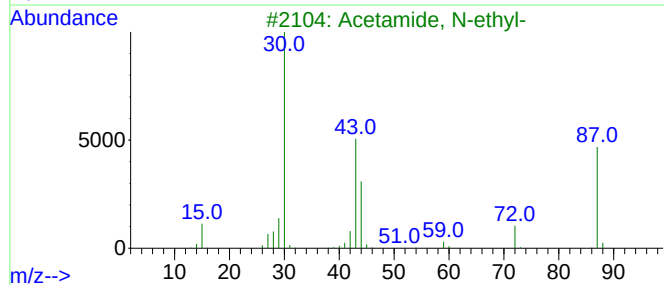
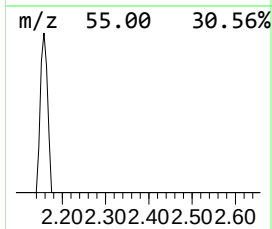
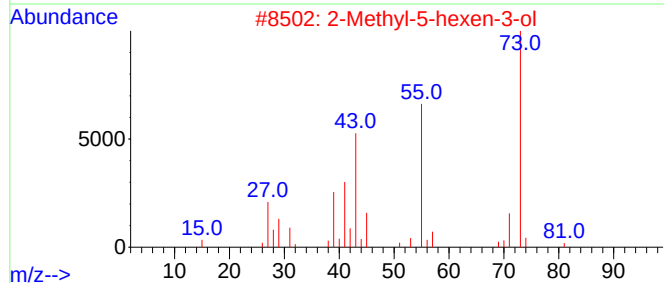
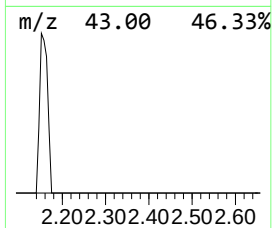
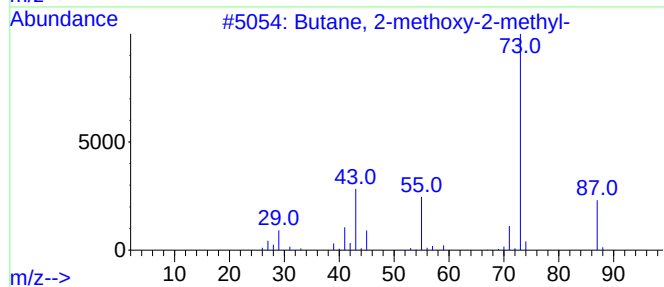
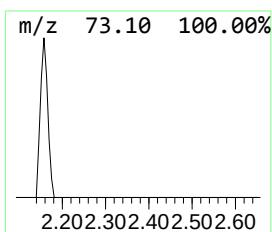
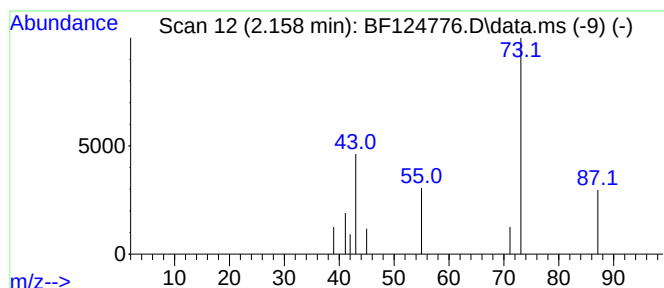
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.158	7.19 ng	9949	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-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	5
4			Isobutylamine	73	C4H11N	000078-81-9	5
5			N-Ethylformamide	73	C3H7NO	000627-45-2	5



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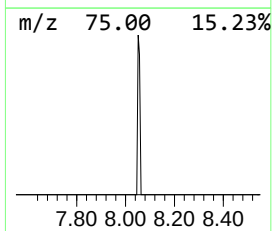
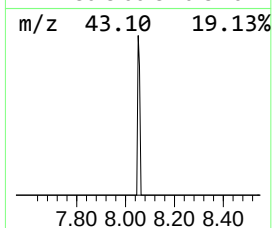
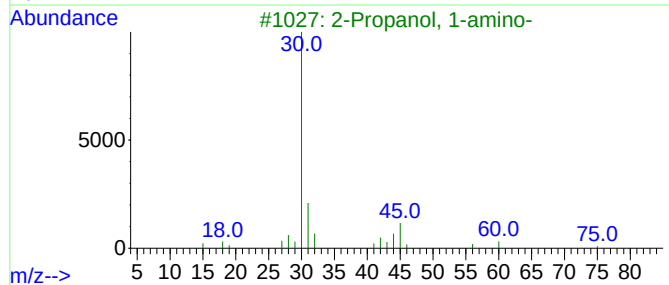
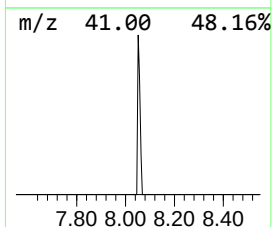
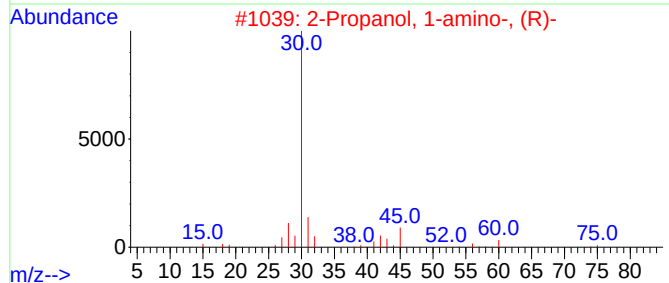
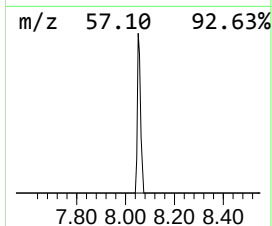
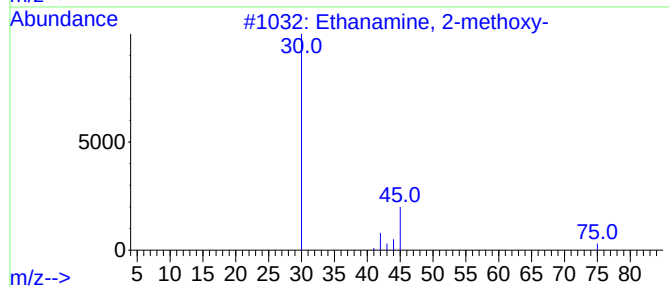
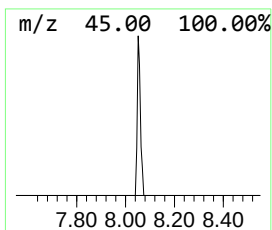
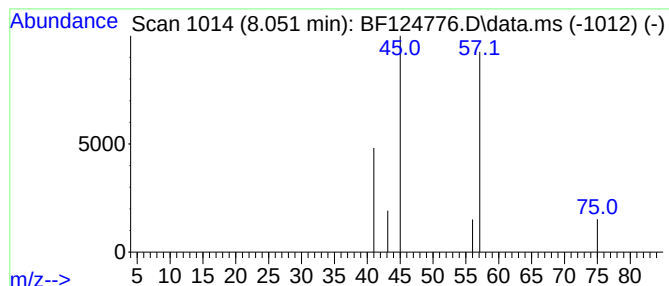
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Peak Number 2 unknown8.051 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	3.84 ng	6789	Naphthalene-d8	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanamine, 2-methoxy-	75	C3H9NO	000109-85-3	4
2			2-Propanol, 1-amino-, (R)-	75	C3H9NO	002799-16-8	3
3			2-Propanol, 1-amino-	75	C3H9NO	000078-96-6	3
4			Formamide	45	CH3NO	000075-12-7	3
5			Methane, nitroso-	45	CH3NO	000865-40-7	3



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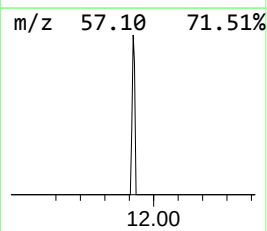
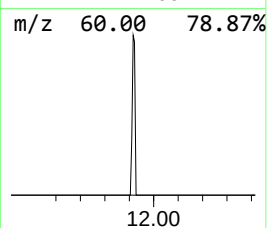
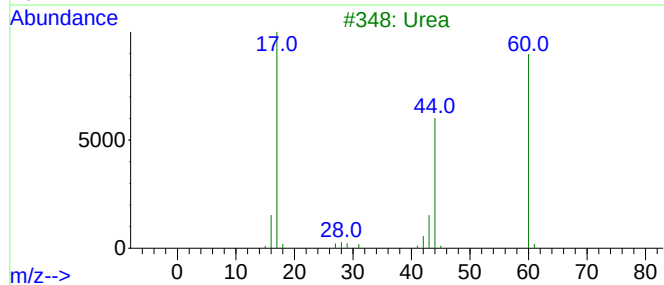
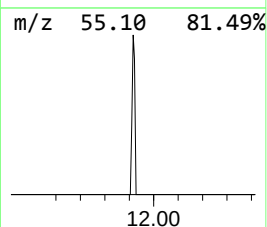
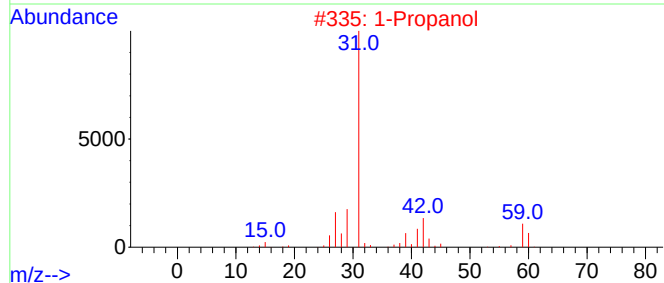
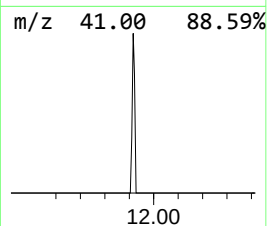
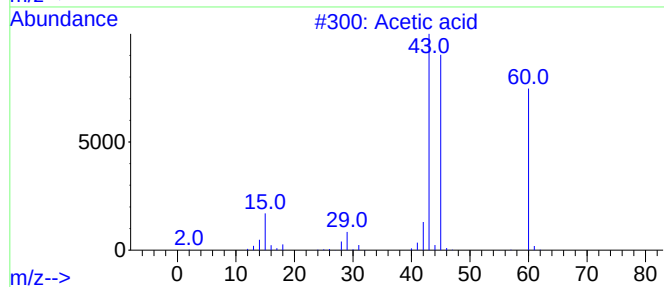
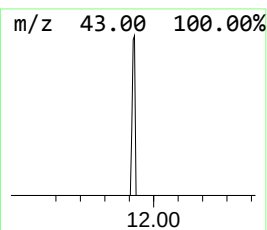
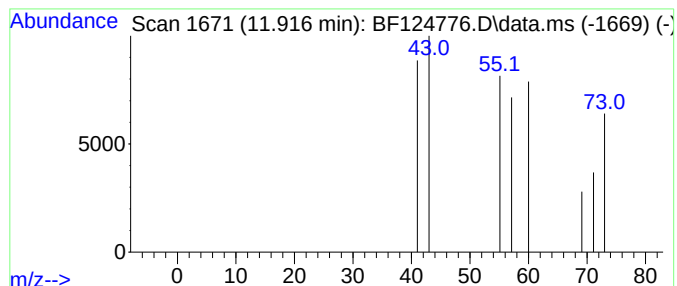
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown11.916 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.84 ng	5264	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid	60	C2H4O2	000064-19-7	4
2			1-Propanol	60	C3H8O	000071-23-8	3
3			Urea	60	CH4N2O	000057-13-6	2
4			Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	2
5			Carbonyl sulfide	60	COS	000463-58-1	2



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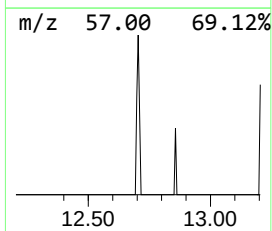
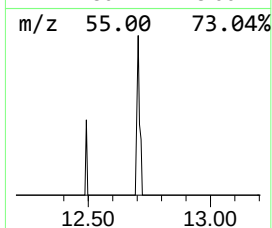
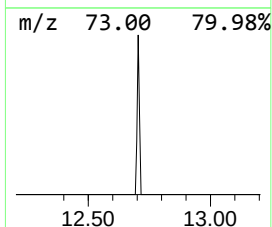
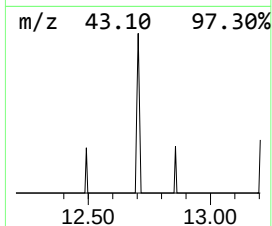
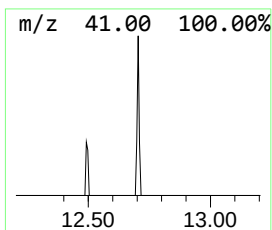
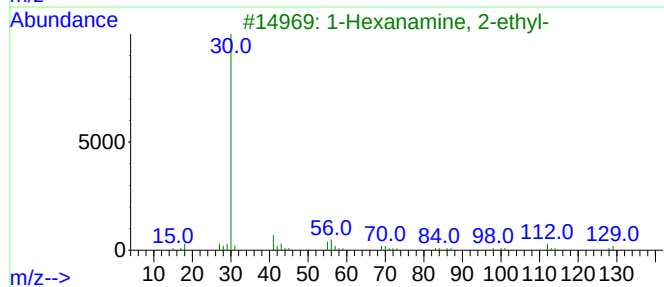
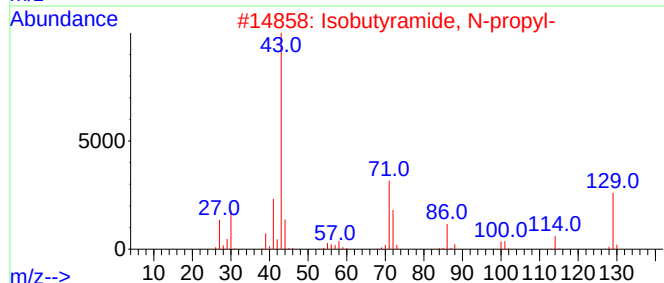
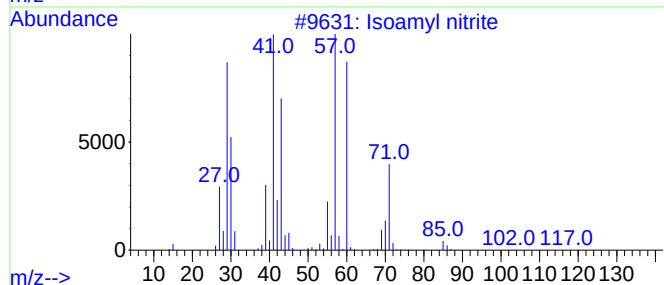
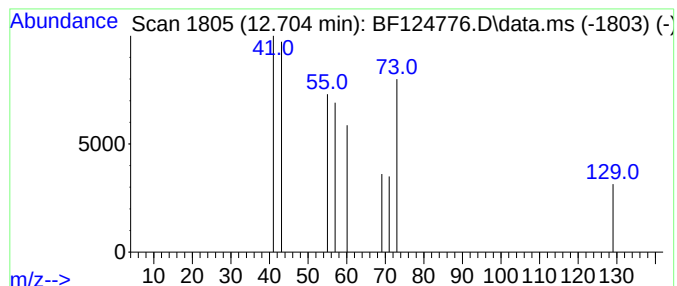
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Peak Number 4 unknown12.704 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	3.40 ng	4658	Phenanthrene-d10	11.398

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			1-Hexanamine, 2-ethyl-	129	C8H19N	000104-75-6	5
4			Neopentyl isothiocyanate	129	C6H11NS	000597-97-7	4
5			Acetic acid	60	C2H4O2	000064-19-7	4



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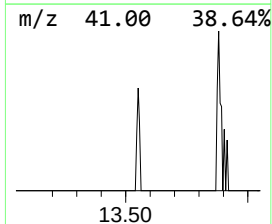
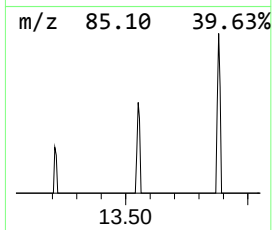
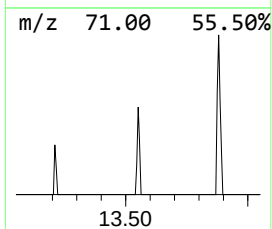
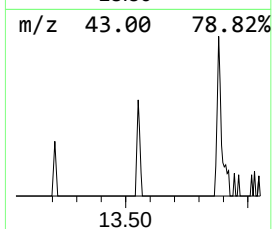
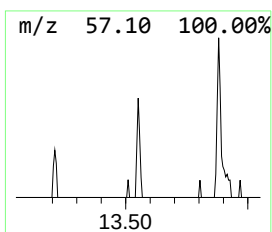
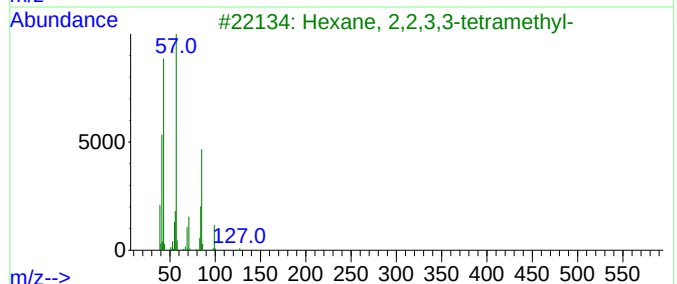
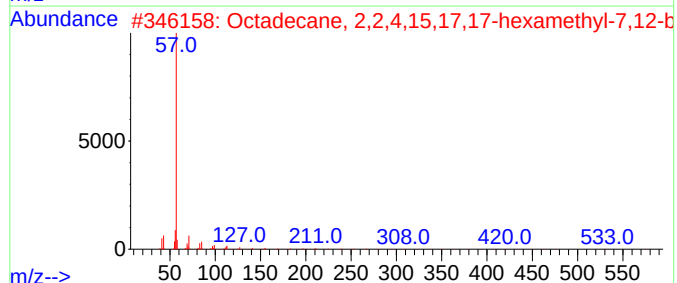
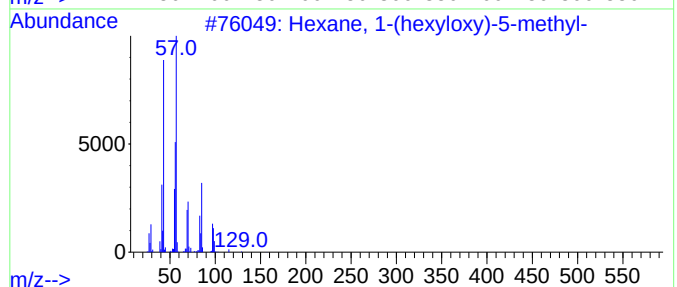
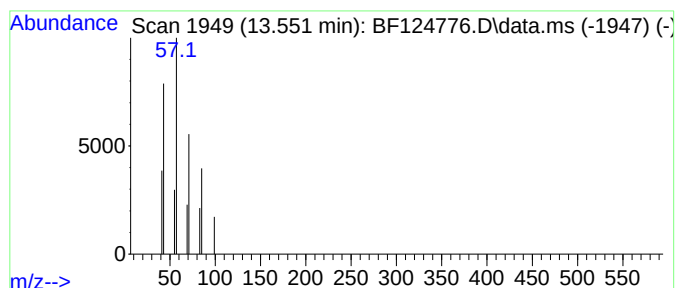
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown13.551 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.551	3.73 ng	5371	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 1-(hexyloxy)-5-methyl-	200	C13H28O	074421-19-5	42		
2	Octadecane, 2,2,4,15,17,17-hexam...	591	C42H86	055470-97-8	39		
3	Hexane, 2,2,3,3-tetramethyl-	142	C10H22	013475-81-5	36		
4	Hexane, 1-(hexyloxy)-3-methyl-	200	C13H28O	074421-18-4	33		
5	1,6:3,4-Dianhydro-2-deoxy-.beta....	128	C6H8O3	050767-53-8	28		



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Sample : M3151-02
Misc :
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ClientSampleId :
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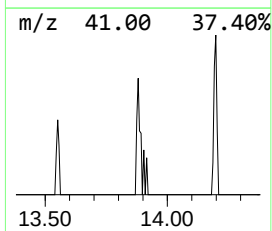
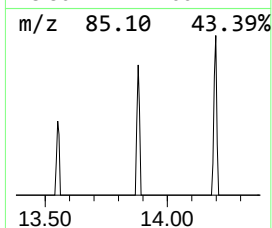
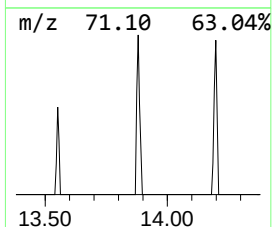
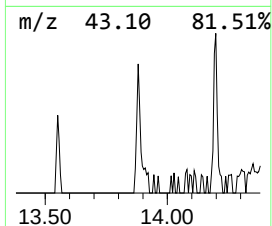
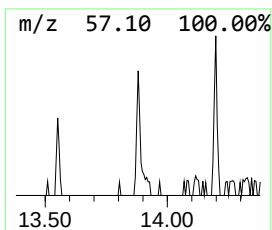
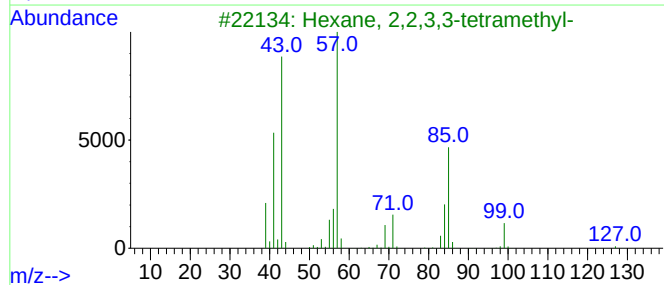
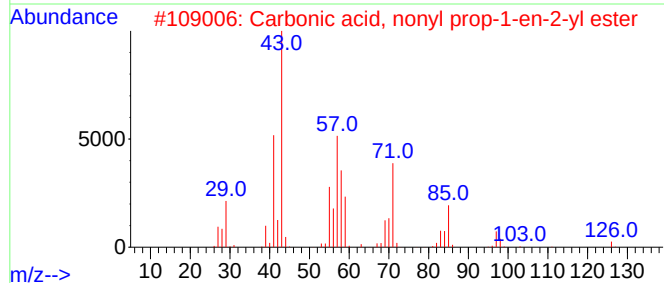
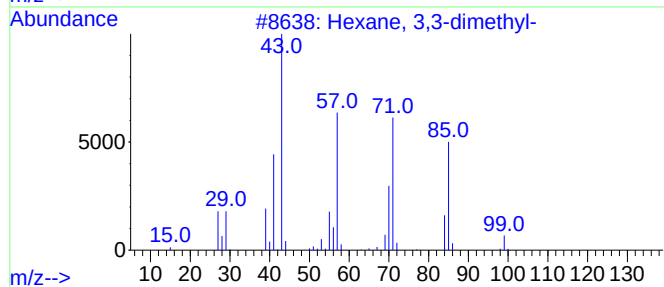
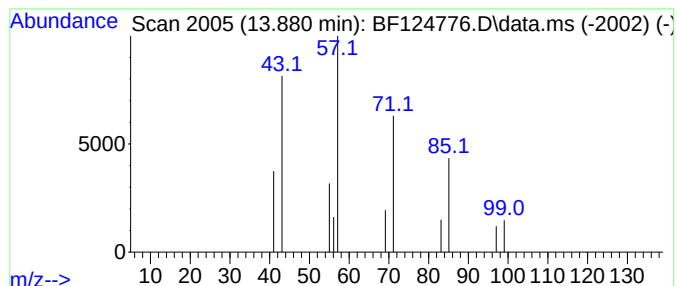
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown13.880 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	10.73 ng	15469	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	45
2			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	42
3			Hexane, 2,2,3,3-tetramethyl-	142	C10H22	013475-81-5	40
4			Sulfurous acid, hexyl heptyl ester	264	C13H28O3S	1000309-12-9	38
5			Ether, heptyl hexyl	200	C13H28O	007289-40-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124776.D
Acq On : 26 Jul 2021 21:31
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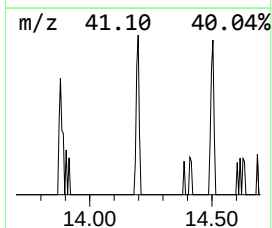
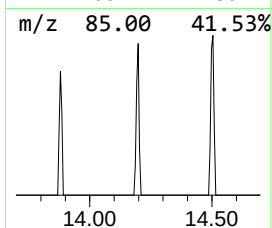
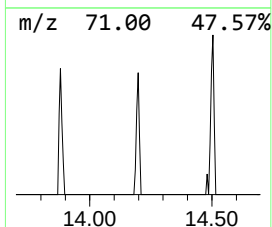
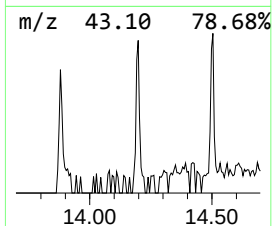
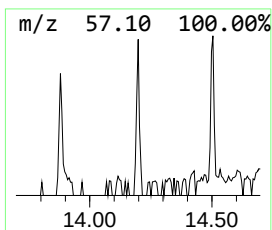
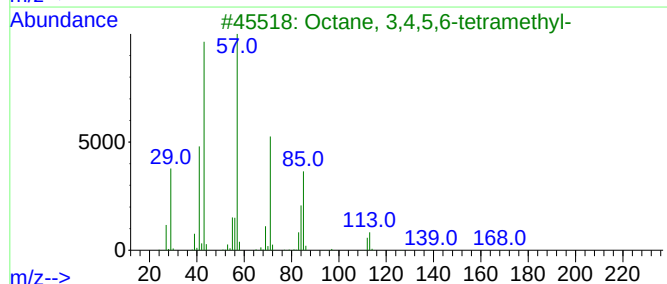
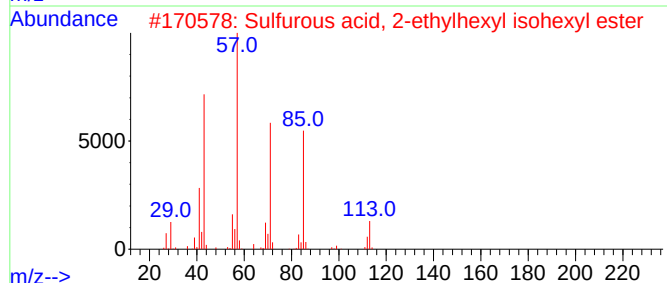
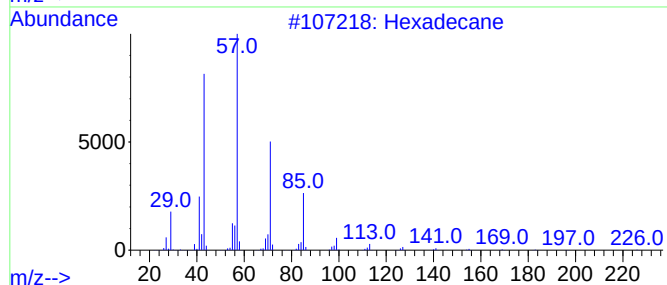
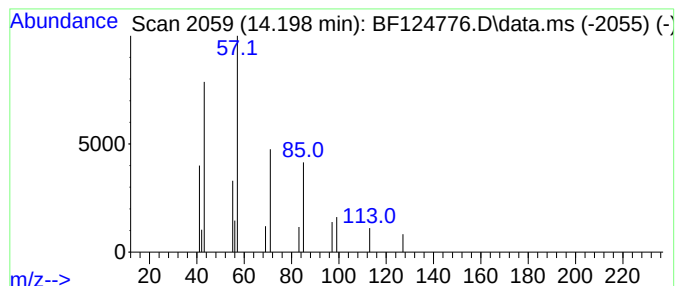
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.198	9.45 ng	13625	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	72
2			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	64
3			Octane, 3,4,5,6-tetramethyl-	170	C12H26	062185-21-1	64
4			Heptadecane	240	C17H36	000629-78-7	64
5			Nonadecane	268	C19H40	000629-92-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124776.D
Acq On : 26 Jul 2021 21:31
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Sample : M3151-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

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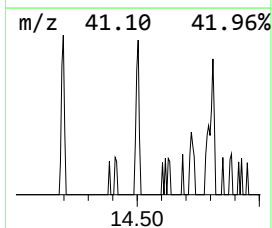
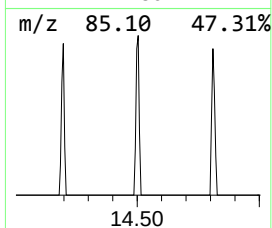
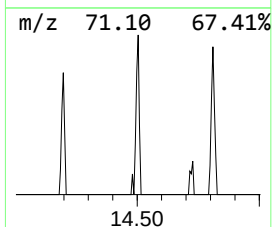
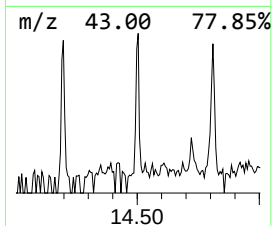
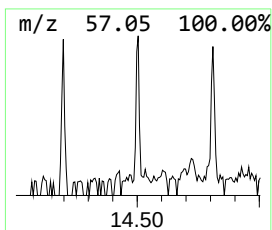
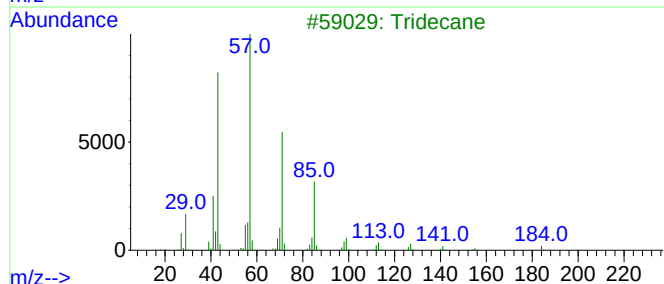
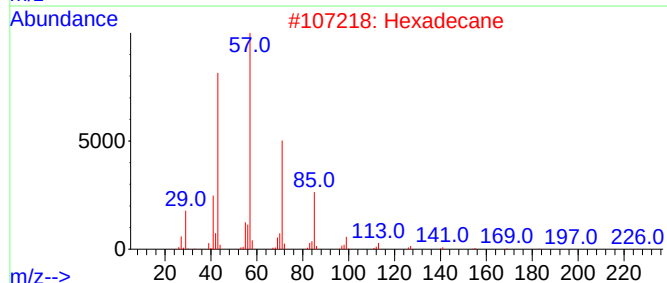
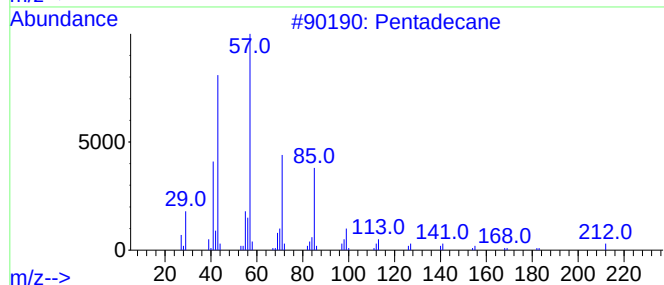
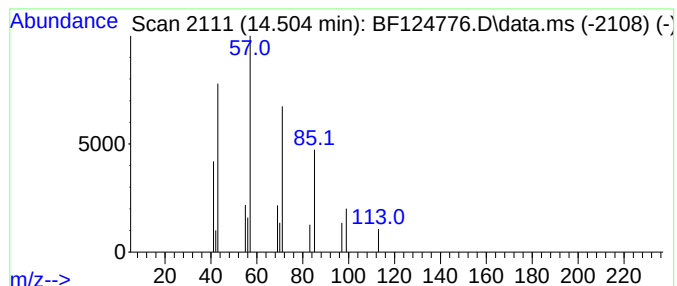
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.504	9.88 ng	14235	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane	212	C15H32	000629-62-9	64
2			Hexadecane	226	C16H34	000544-76-3	64
3			Tridecane	184	C13H28	000629-50-5	59
4			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	53
5			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124776.D
Acq On : 26 Jul 2021 21:31
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Misc :
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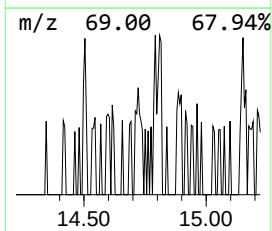
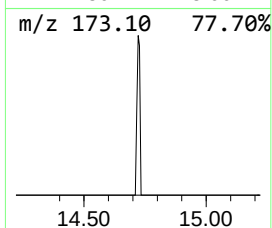
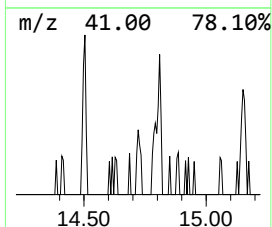
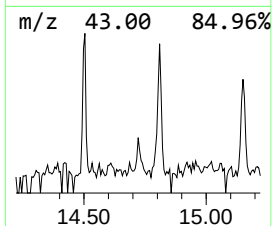
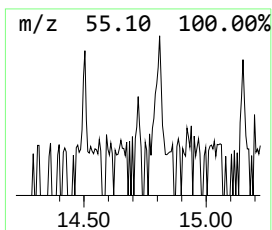
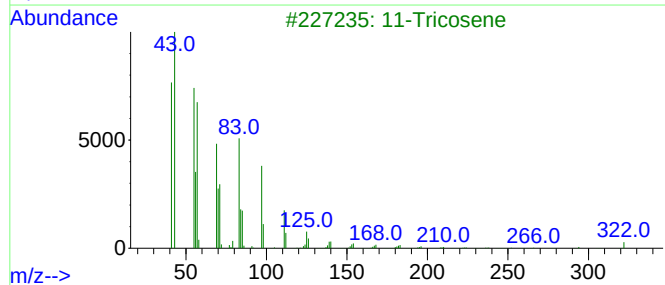
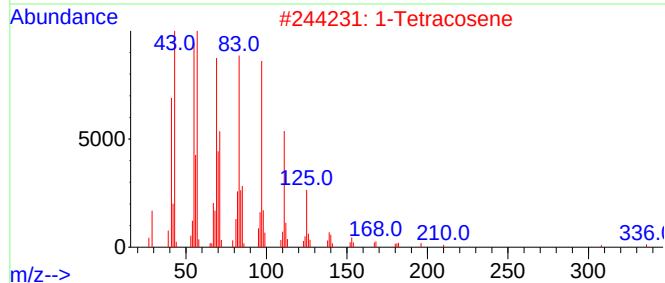
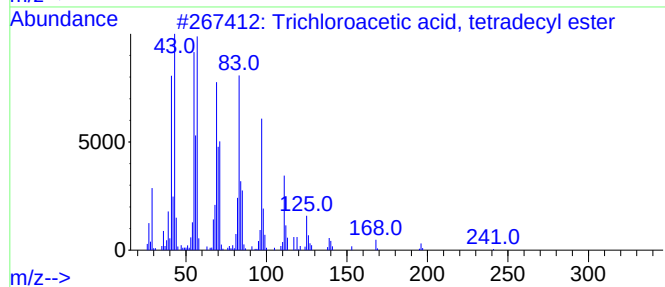
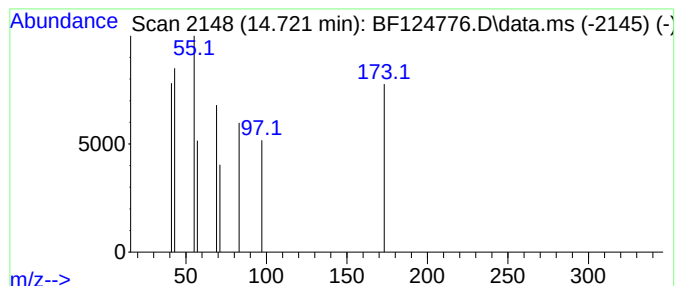
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown14.721 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.721	4.02 ng	5799	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	40
2			1-Tetracosene	336	C24H48	010192-32-2	40
3			11-Tricosene	322	C23H46	052078-56-5	40
4			Cetene	224	C16H32	000629-73-2	40
5			9-Eicosene, (E)-	280	C20H40	074685-29-3	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124776.D
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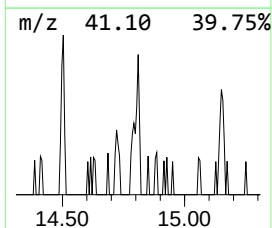
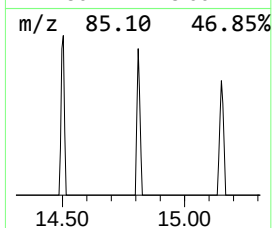
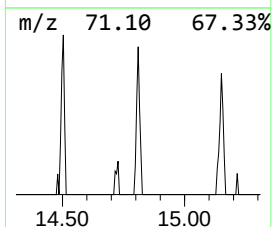
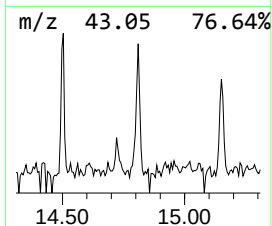
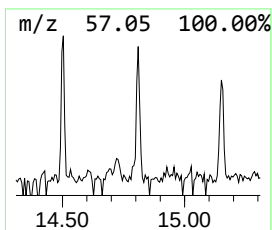
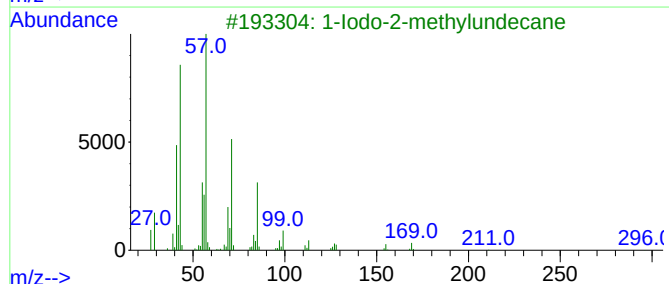
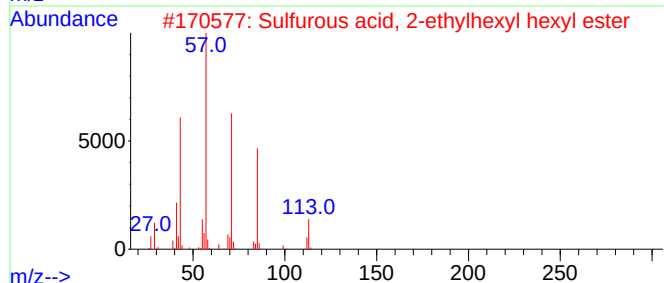
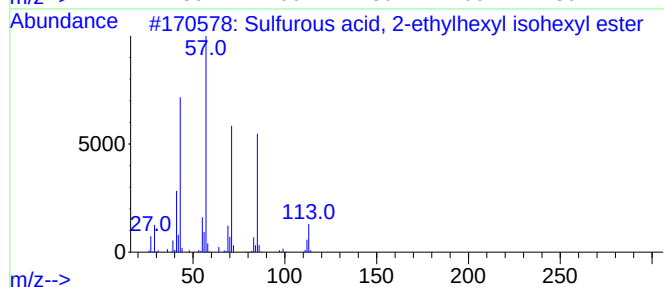
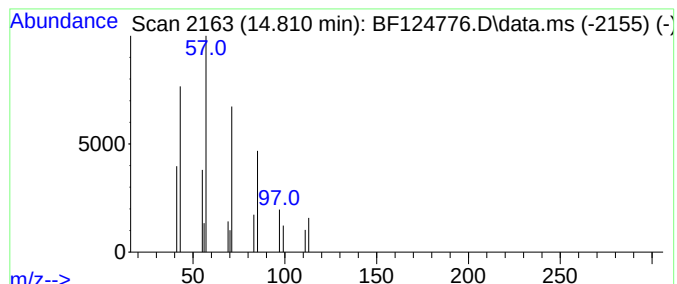
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Sulfurous acid, 2-ethylhexy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.810	13.13 ng	20181	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	59
2			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	59
3			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	59
4			Hexadecane	226	C16H34	000544-76-3	59
5			Tridecane	184	C13H28	000629-50-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
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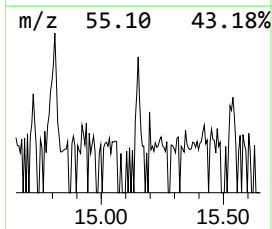
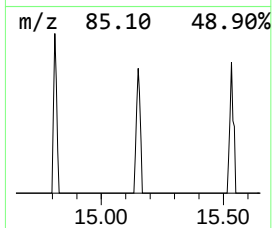
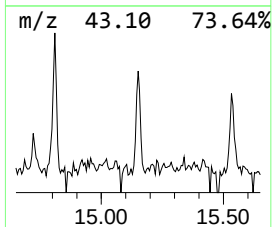
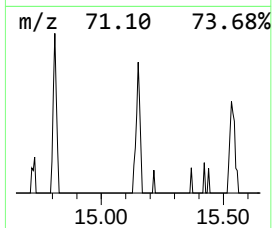
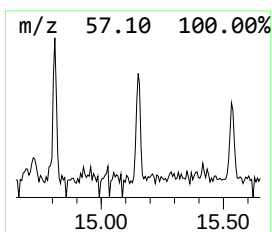
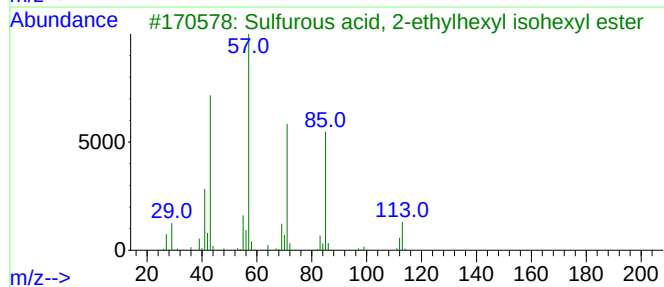
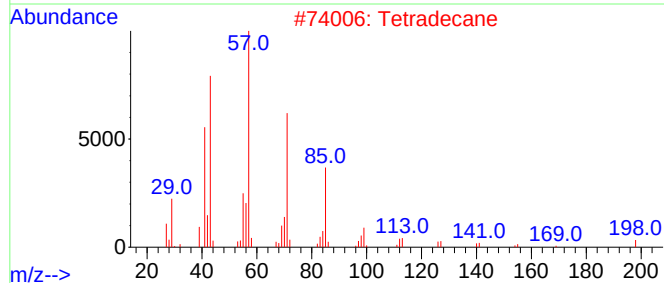
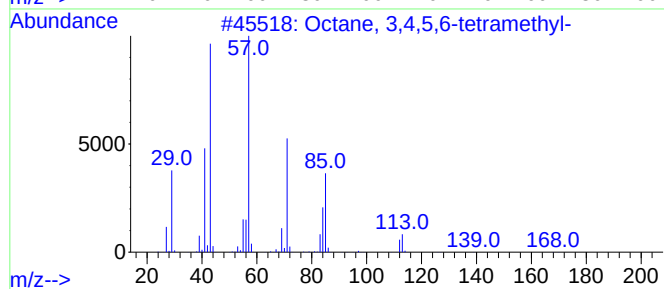
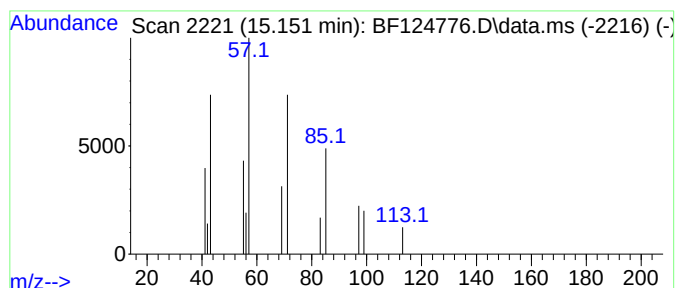
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Octane, 3,4,5,6-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.151	9.09 ng	13975	Perylene-d12	15.515	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,4,5,6-tetramethyl-	170	C12H26	062185-21-1	64
2	Tetradecane	198	C14H30	000629-59-4	64
3	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	64
4	Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	59
5	Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
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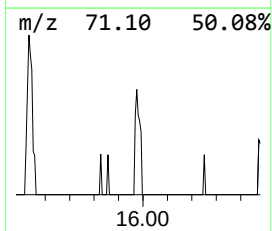
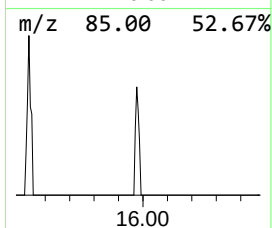
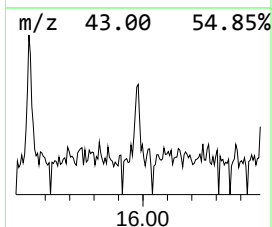
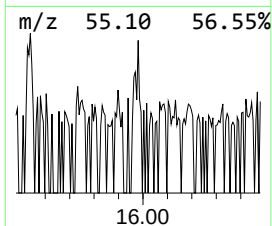
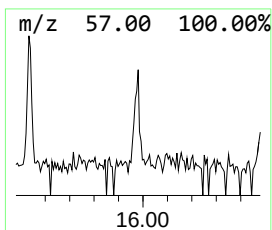
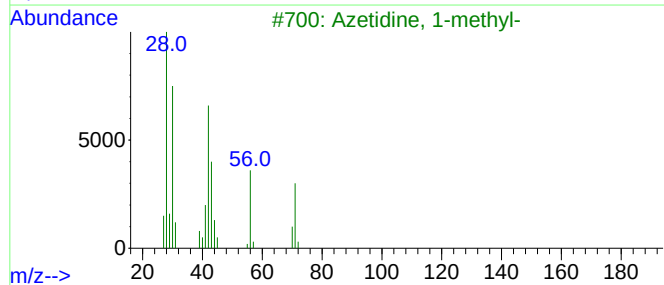
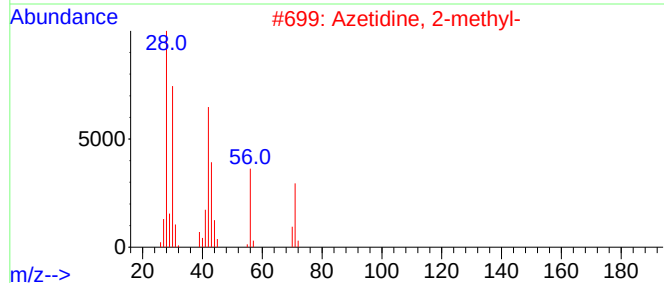
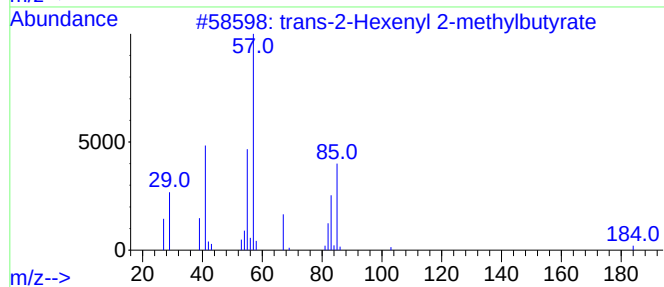
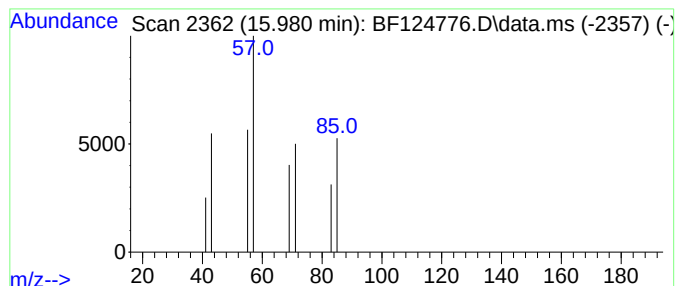
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown15.980 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.980	4.69 ng	7210	Perylene-d12	15.515	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-2-Hexenyl 2-methylbutyrate	184	C11H20O2	1000433-23-8	9
2	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
3	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
4	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
5	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124776.D
Acq On : 26 Jul 2021 21:31
Operator : JU/CG
Sample : M3151-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

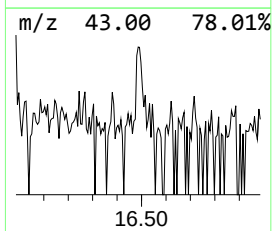
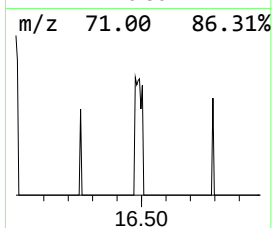
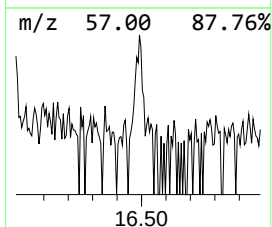
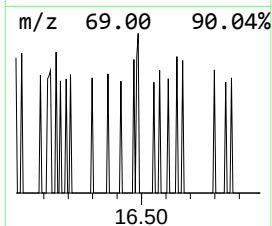
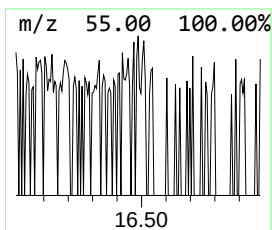
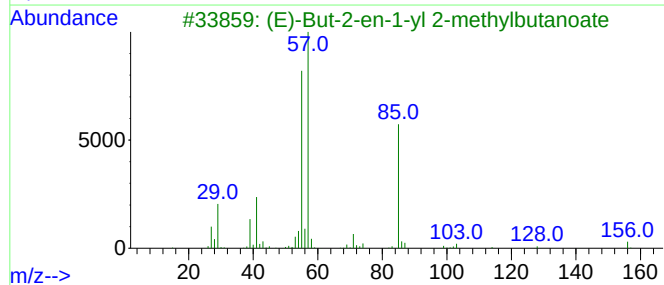
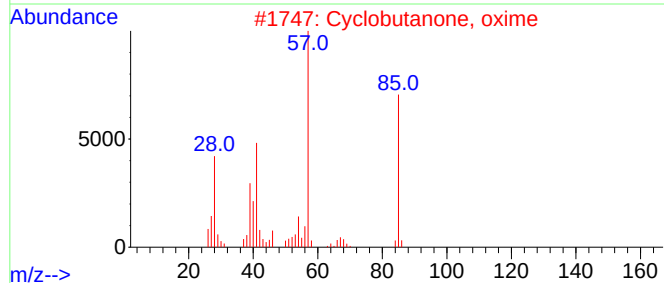
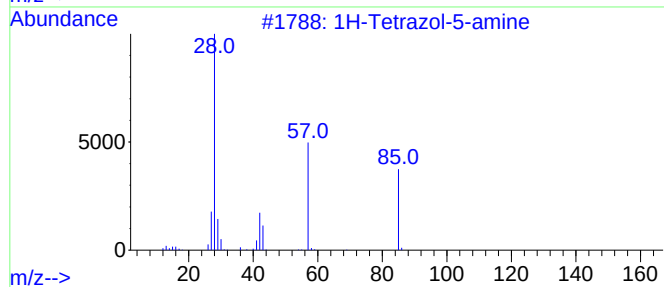
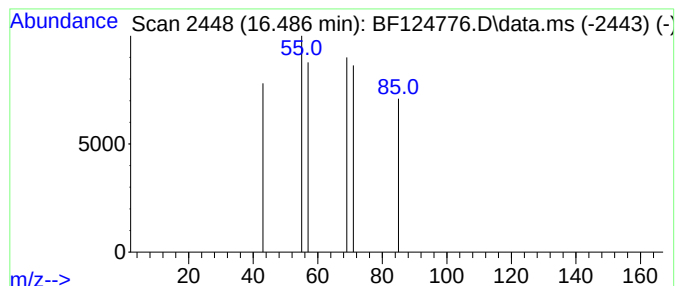
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown16.486 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.486	3.04 ng	4677	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
2			Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4
3			(E)-But-2-en-1-yl 2-methylbutanoate	156	C9H16O2	1000372-81-0	4
4			Oxirane, 2-methyl-3-propyl-, cis-	100	C6H12O	006124-90-9	4
5			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124776.D
Acq On : 26 Jul 2021 21:31
Operator : JU/CG
Sample : M3151-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.158	7.2	ng	9949	1	6.875	27659	20.0
unknown8.051	8.051	3.8	ng	6789	2	8.157	35393	20.0
unknown11.916	11.916	3.8	ng	5264	4	11.398	27409	20.0
unknown12.704	12.704	3.4	ng	4658	4	11.398	27409	20.0
unknown13.551	13.551	3.7	ng	5371	5	14.039	28825	20.0
unknown13.880	13.880	10.7	ng	15469	5	14.039	28825	20.0
Hexadecane	14.198	9.4	ng	13625	5	14.039	28825	20.0
Pentadecane	14.504	9.9	ng	14235	5	14.039	28825	20.0
unknown14.721	14.721	4.0	ng	5799	5	14.039	28825	20.0
Sulfurous acid,...	14.810	13.1	ng	20181	6	15.515	30733	20.0
Octane, 3,4,5,6...	15.151	9.1	ng	13975	6	15.515	30733	20.0
unknown15.980	15.980	4.7	ng	7210	6	15.515	30733	20.0
unknown16.486	16.486	3.0	ng	4677	6	15.515	30733	20.0