

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
 Data File : BF124877.D
 Acq On : 30 Jul 2021 15:39
 Operator : JU/CG
 Sample : M3210-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-5(1.0-5.0)

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: BF124877.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	10	rVB	11309	12482	5.25%	0.740%
2	4.463	399	404	407	rBB	57848	64786	27.27%	3.843%
3	5.104	505	513	516	rBB	138167	200183	84.27%	11.875%
4	5.487	574	578	581	rBB	69744	57501	24.21%	3.411%
5	6.498	745	750	755	rBB	139416	153824	64.75%	9.125%
6	6.869	810	813	816	rBB	47878	35596	14.98%	2.112%
7	6.928	820	823	826	rBV	42663	31589	13.30%	1.874%
8	7.434	905	909	912	rBV	116880	116521	49.05%	6.912%
9	8.051	1011	1014	1022	rBB	26682	20508	8.63%	1.217%
10	8.151	1028	1031	1034	rBV	64611	50455	21.24%	2.993%
11	9.233	1210	1215	1217	rBV	262740	237556	100.00%	14.092%
12	9.910	1327	1330	1334	rBV	79659	63010	26.52%	3.738%
13	11.398	1579	1583	1585	rBV	82936	65359	27.51%	3.877%
14	11.422	1585	1587	1590	rVB	19318	13779	5.80%	0.817%
15	12.486	1765	1768	1770	rBB	5608	3955	1.66%	0.235%
16	12.610	1786	1789	1792	rBB	18110	13584	5.72%	0.806%
17	12.798	1818	1821	1823	rBV	18817	13950	5.87%	0.828%
18	12.839	1823	1828	1831	rVB	13004	12411	5.22%	0.736%
19	12.986	1848	1853	1856	rBV	271807	229024	96.41%	13.586%
20	13.463	1928	1934	1938	rBV	70956	109898	46.26%	6.519%
21	13.492	1938	1939	1941	rVV	30562	23052	9.70%	1.367%
22	13.516	1941	1943	1945	rVB	26679	18782	7.91%	1.114%
23	13.874	2000	2004	2014	rBB	14852	18805	7.92%	1.116%
24	14.039	2028	2032	2034	rBV2	39251	36837	15.51%	2.185%
25	14.063	2034	2036	2038	rVB	3833	2652	1.12%	0.157%
26	14.139	2047	2049	2055	rBV2	6888	8721	3.67%	0.517%
27	14.192	2055	2058	2063	rVB	3562	4072	1.71%	0.242%
28	14.492	2107	2109	2112	rBV	4238	4364	1.84%	0.259%
29	14.521	2112	2114	2119	rVB	1957	2811	1.18%	0.167%
30	14.804	2159	2162	2166	rBB	3367	3173	1.34%	0.188%
31	14.951	2183	2187	2190	rBB	3676	3598	1.51%	0.213%
32	15.080	2206	2209	2212	rBV2	3012	3726	1.57%	0.221%
33	15.145	2217	2220	2223	rBB	4317	4845	2.04%	0.287%
34	15.192	2223	2228	2232	rBV2	3248	5712	2.40%	0.339%
35	15.515	2279	2283	2289	rBB	26263	31456	13.24%	1.866%
36	15.733	2316	2320	2323	rBB	4592	4012	1.69%	0.238%

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Instrument :
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ClientSampleId :
SB-5(1.0-5.0)

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

37	15.968	2356	2360	2363	rBB	2327	3158	1.33%	0.187%
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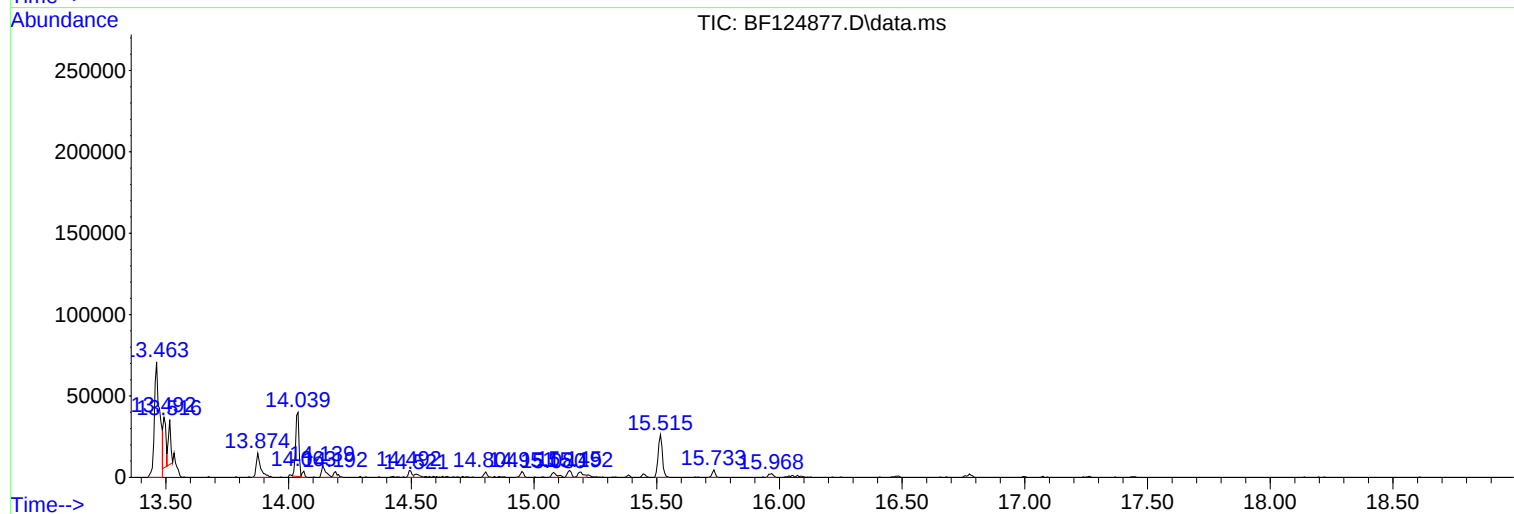
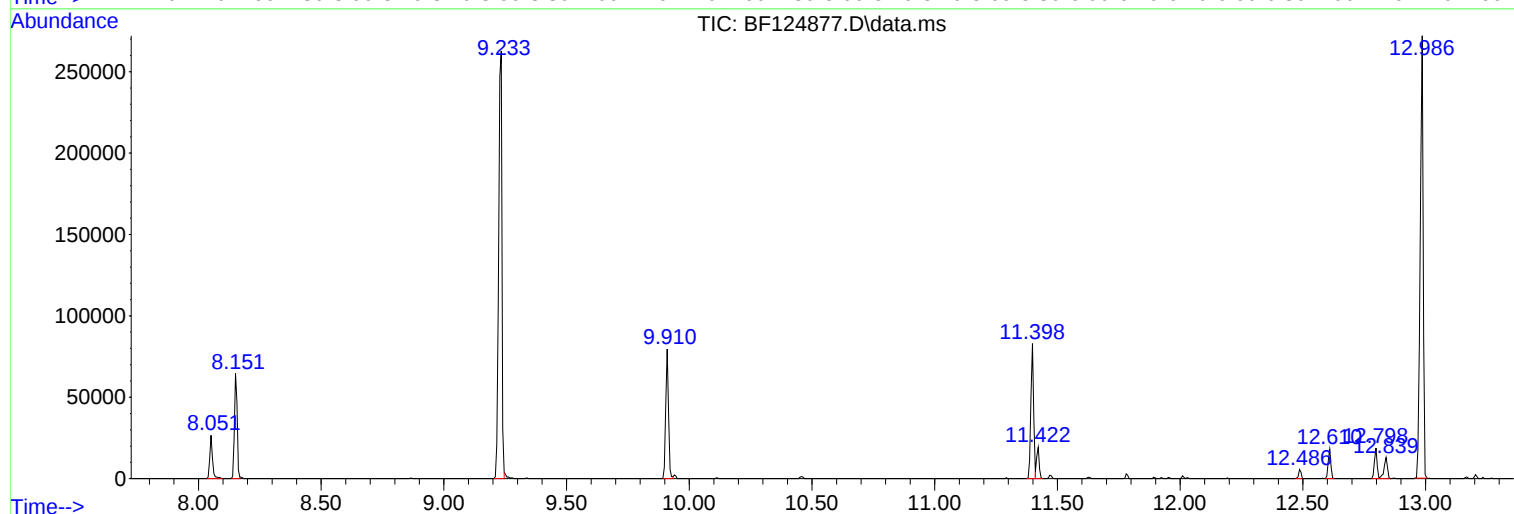
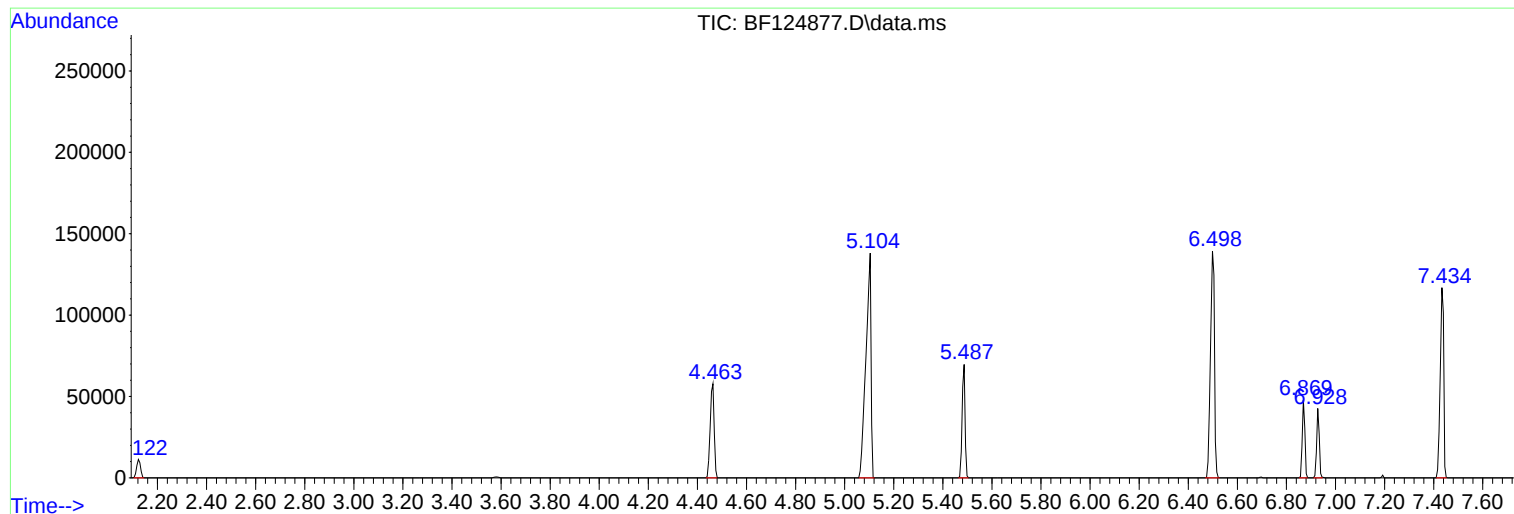
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Instrument :
BNA_F
ClientSampled :
SB-5(1.0-5.0)

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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Sample : M3210-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5(1.0-5.0)

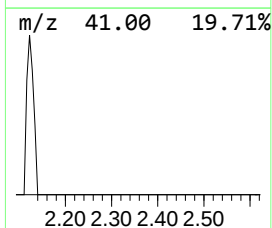
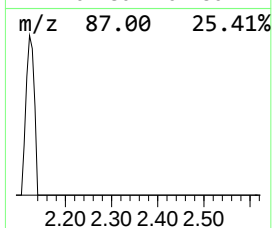
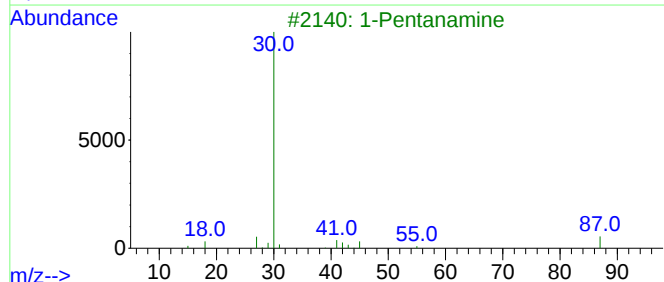
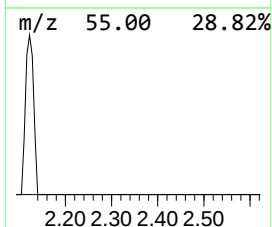
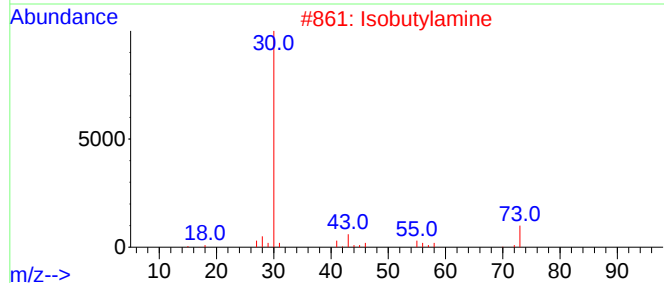
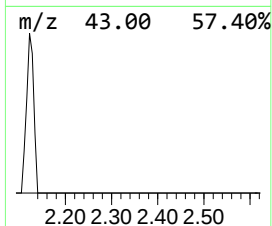
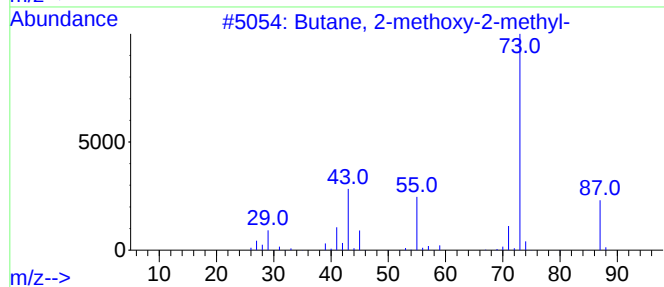
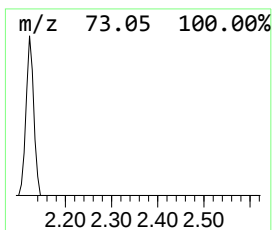
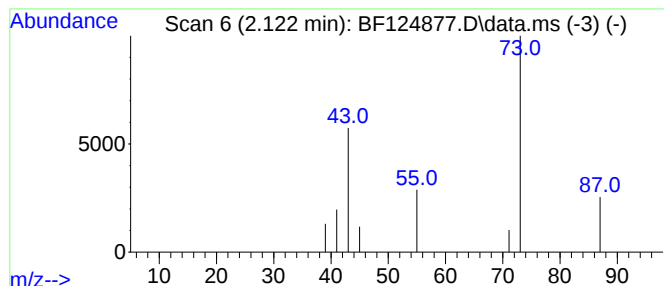
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	7.01 ng	12482	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	74
2			Isobutylamine	73	C4H11N	000078-81-9	5
3			1-Pentanamine	87	C5H13N	000110-58-7	4
4			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	4
5			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4



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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5(1.0-5.0)

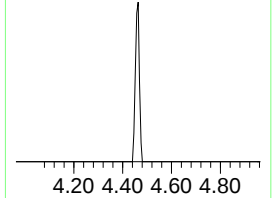
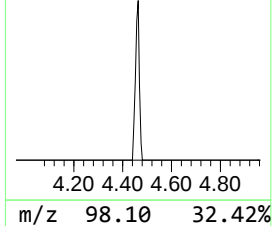
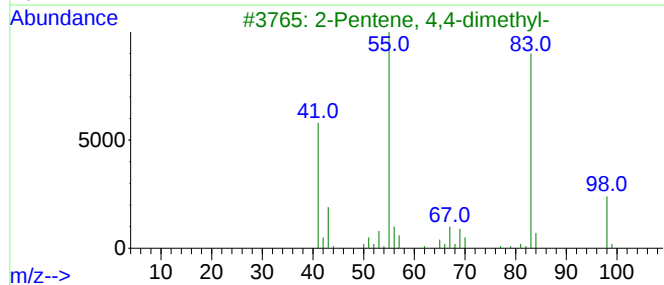
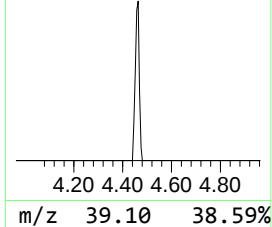
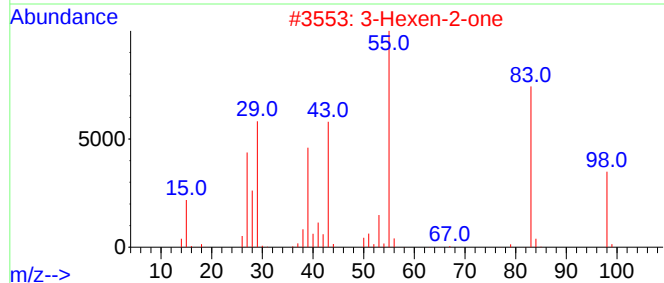
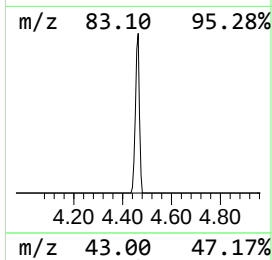
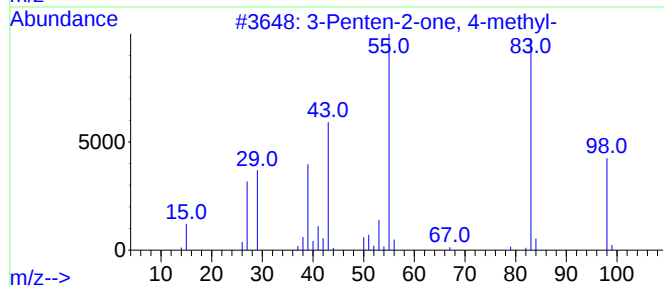
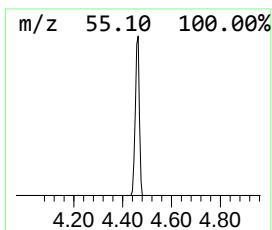
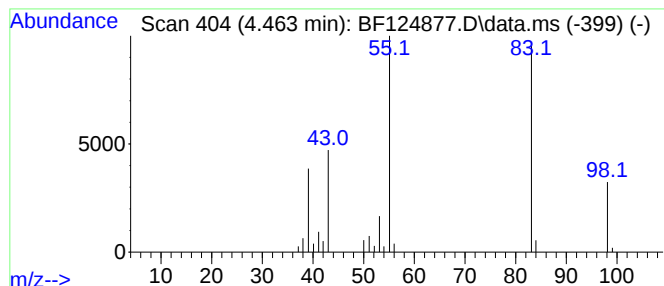
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.463	36.40 ng	64786	1,4-Dichlorobenzene-d4	6.869

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	81
3		2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	78
4		2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	78
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	64



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Instrument :
BNA_F
ClientSampleId :
SB-5(1.0-5.0)

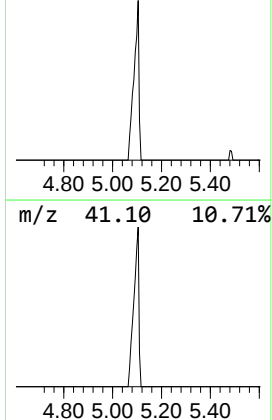
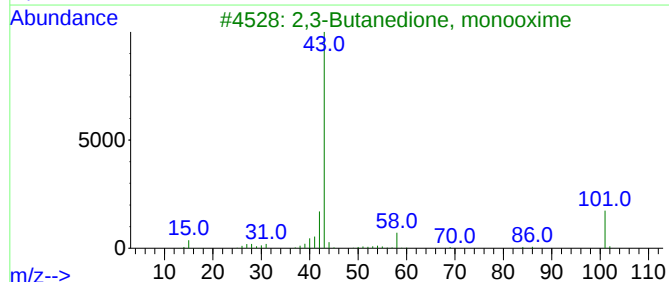
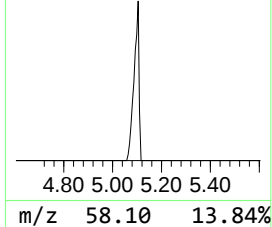
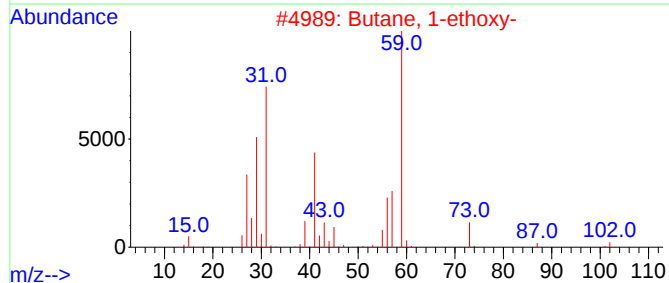
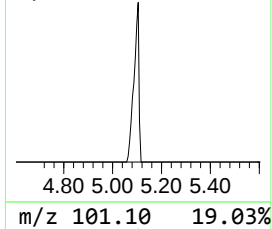
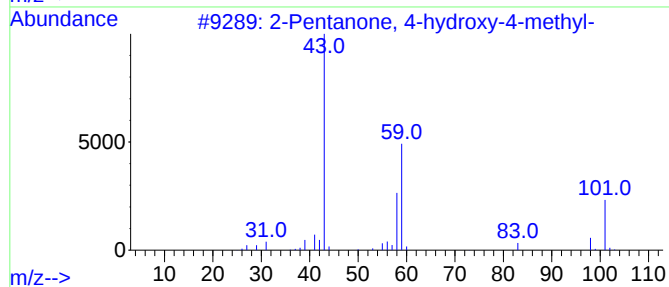
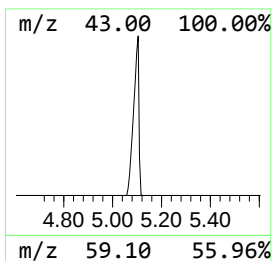
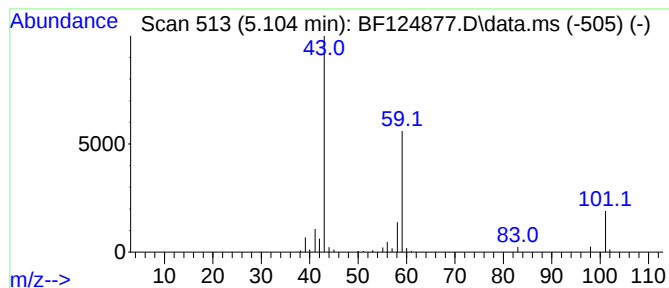
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	112.47 ng	200183	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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ClientSampleId :
SB-5(1.0-5.0)

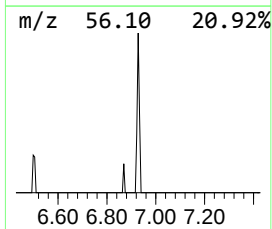
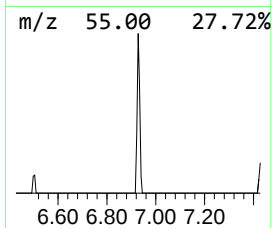
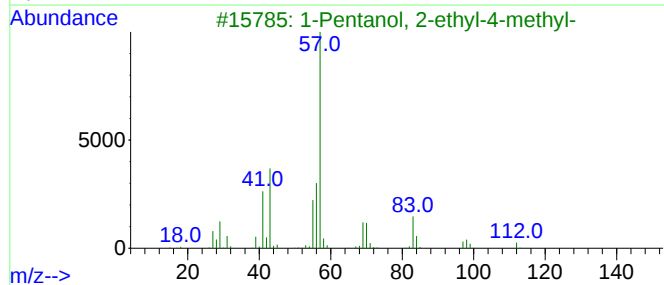
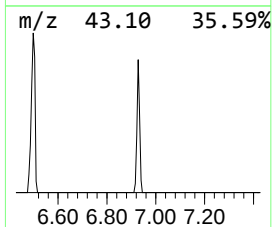
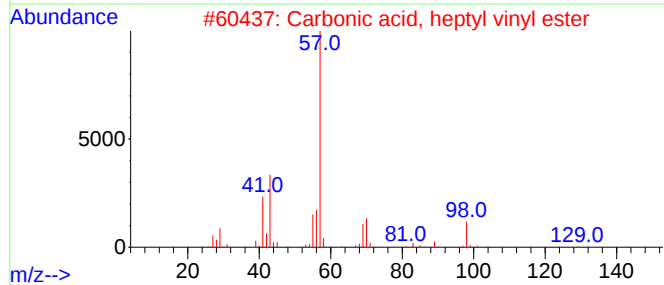
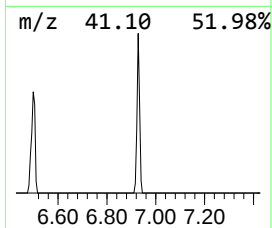
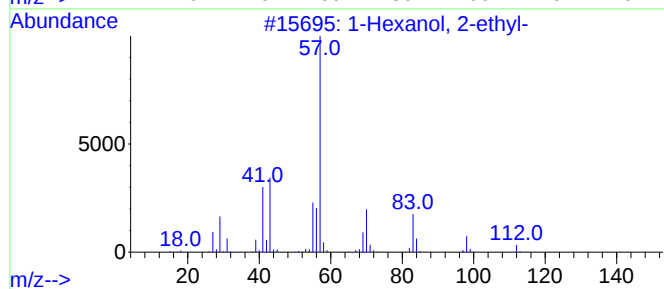
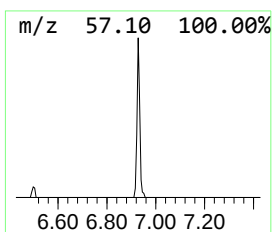
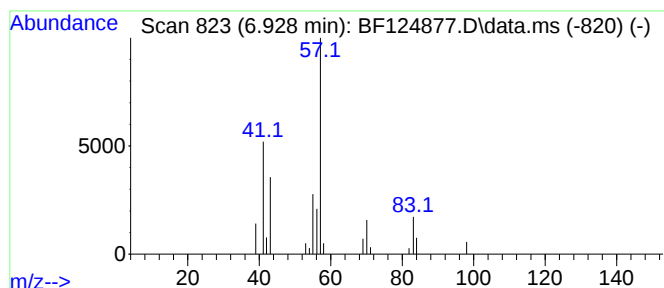
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.928	17.75 ng	31589	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	42
3			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	40
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	38
5			4-Pentenal, 2-ethyl-	112	C7H12O	005204-80-8	37



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BNA_F
ClientSampleId :
SB-5(1.0-5.0)

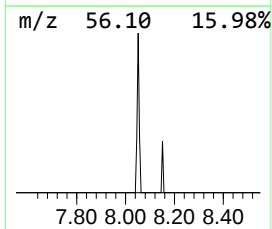
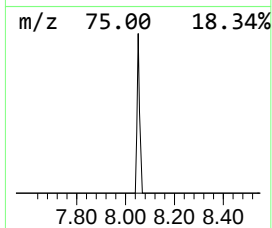
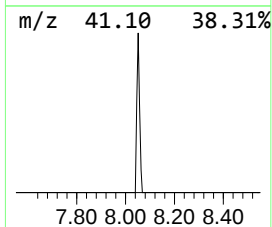
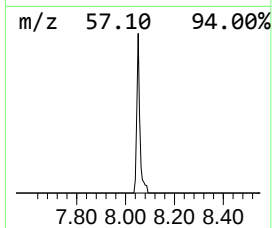
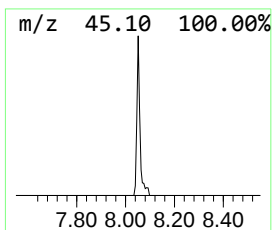
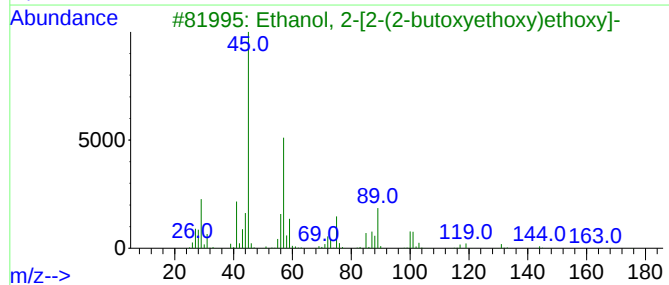
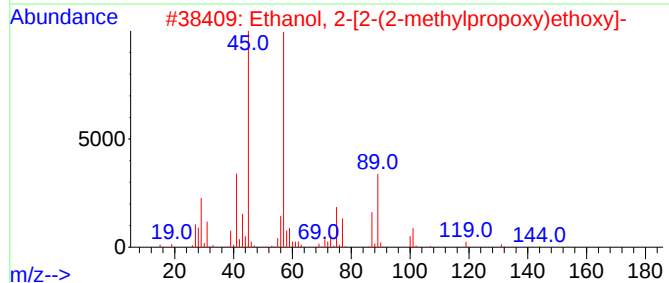
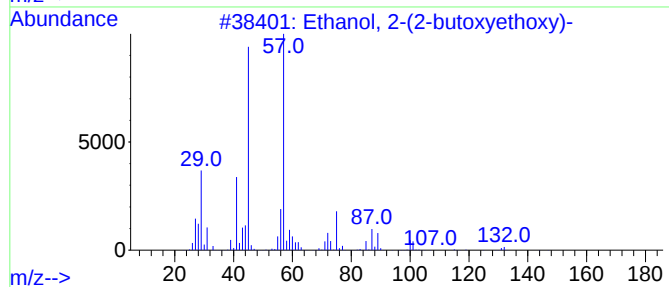
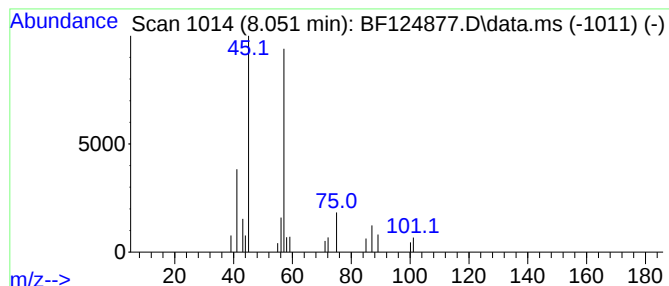
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	8.13 ng	20508	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
3			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
4			Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	39
5			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124877.D
Acq On : 30 Jul 2021 15:39
Operator : JU/CG
Sample : M3210-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

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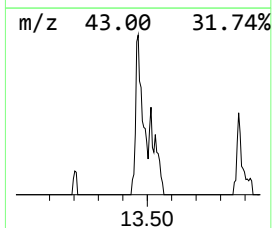
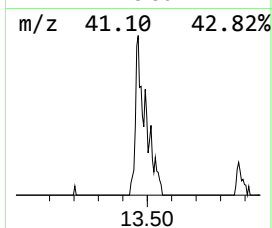
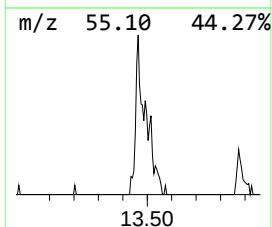
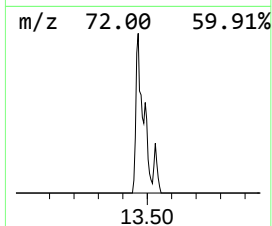
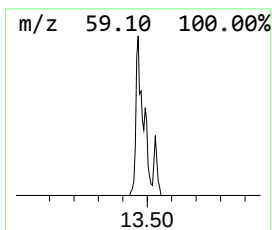
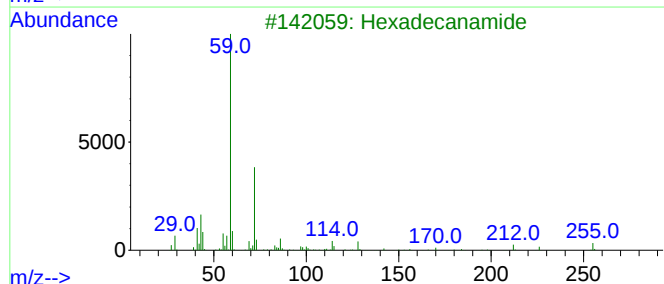
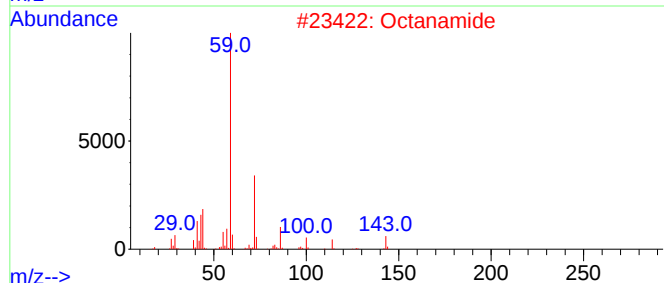
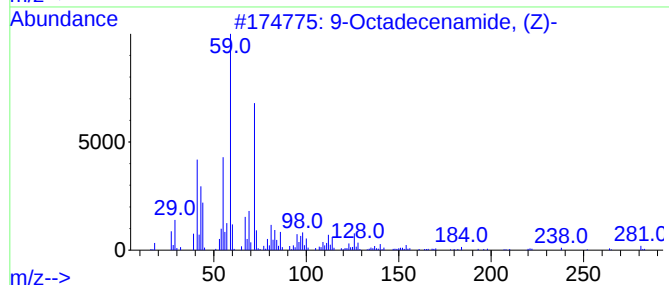
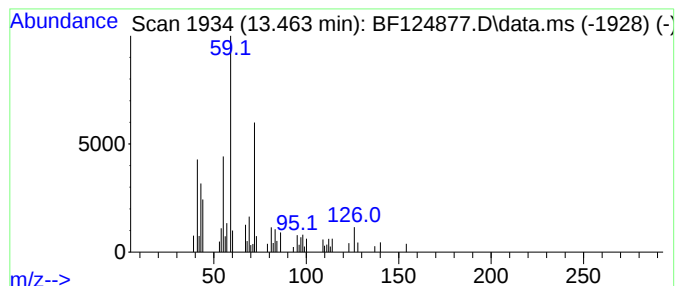
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.463	59.67 ng	109898	Chrysene-d12	14.039

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		Octanamide	143	C8H17NO	000629-01-6	59
3		Hexadecanamide	255	C16H33NO	000629-54-9	59
4		Dodecanamide	199	C12H25NO	001120-16-7	53
5		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124877.D
Acq On : 30 Jul 2021 15:39
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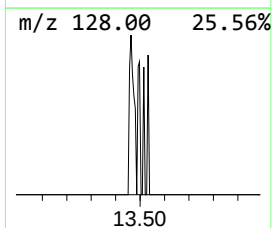
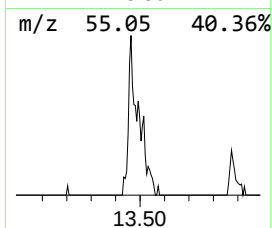
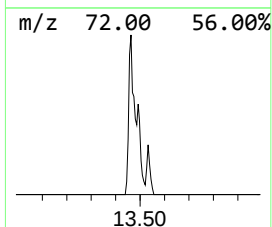
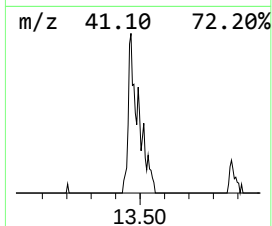
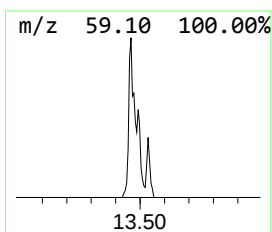
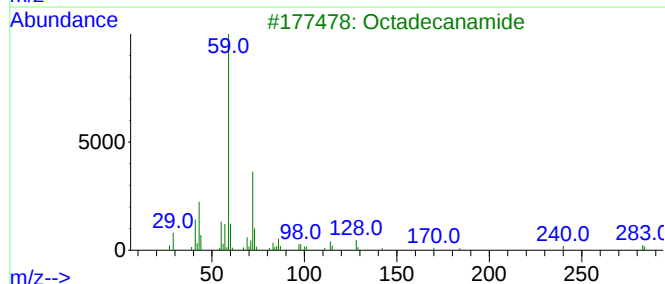
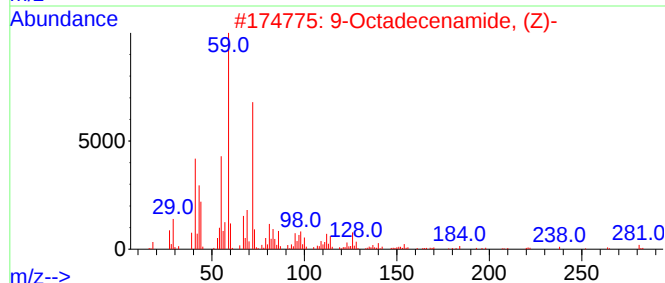
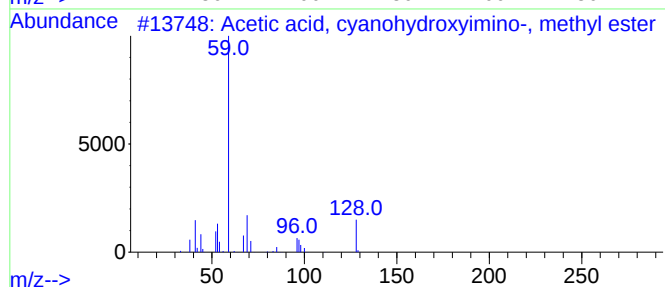
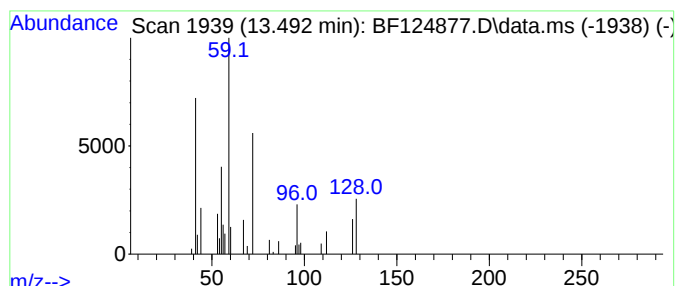
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown13.492 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.492	12.52 ng	23052	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, cyanohydroxyimino-,...	128	C4H4N2O3	061295-92-9	38
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	37
3			Octadecanamide	283	C18H37NO	000124-26-5	23
4			Silane, octyl-	144	C8H20Si	000871-92-1	12
5			Butanoic acid, 3-methyl-2-methyl...	128	C7H12O2	003070-67-5	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
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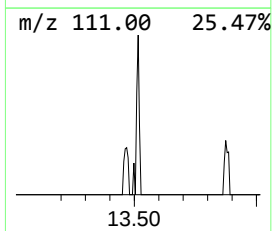
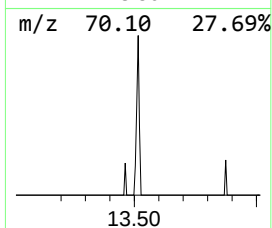
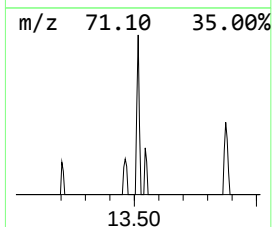
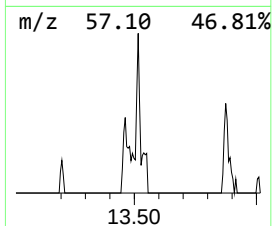
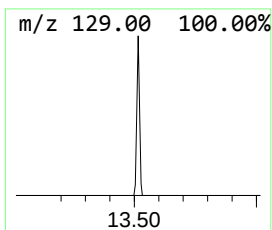
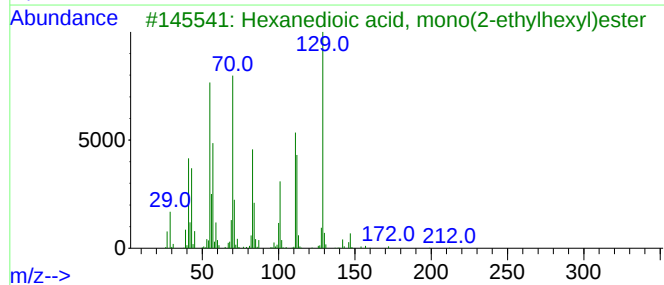
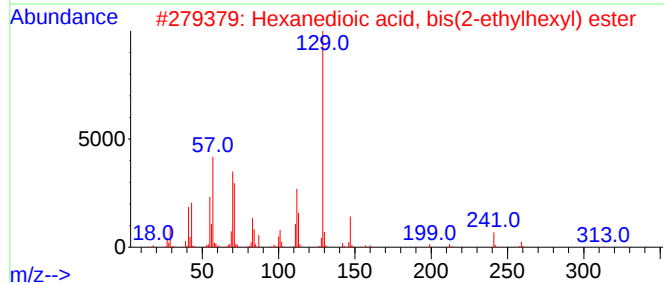
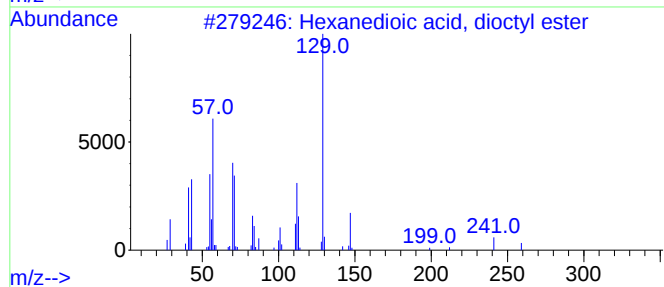
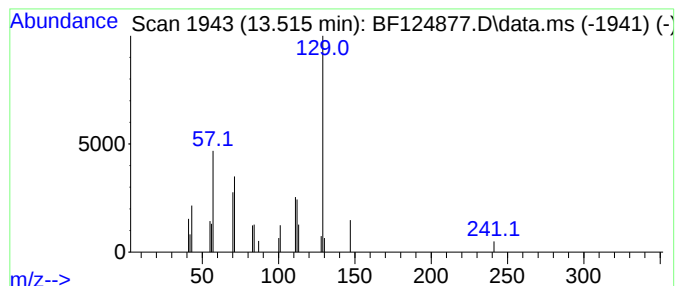
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexanedioic acid, dioctyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.515	10.20 ng	18782	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	90
2			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	86
3			Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	72
4			Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1010324-48-0	59
5			Adipic acid, di(oct-4-yl ester)	370	C22H42O4	1000160-80-1	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
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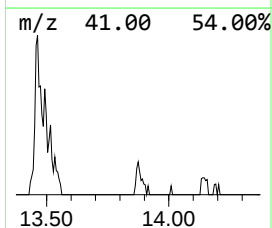
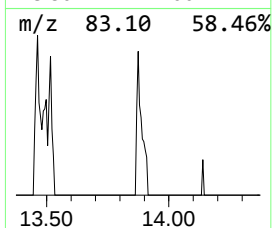
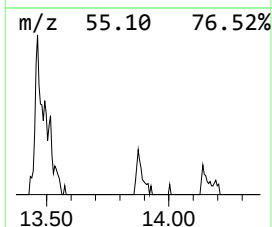
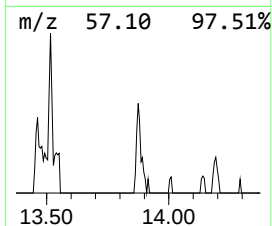
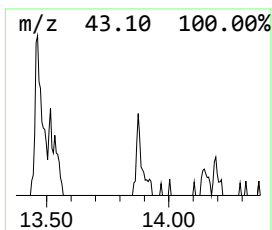
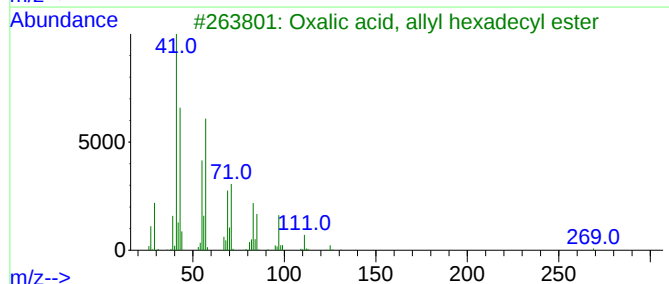
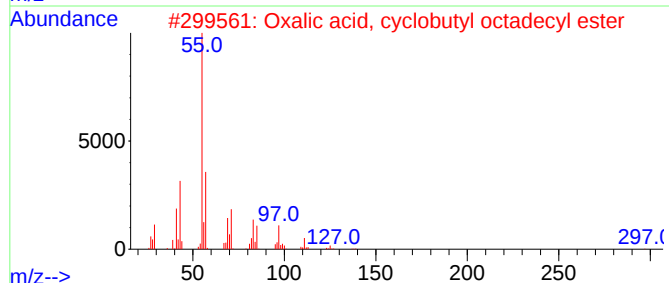
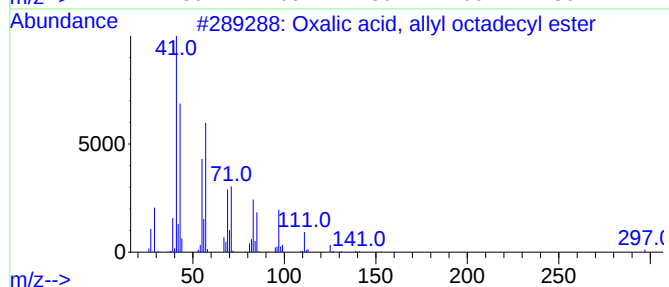
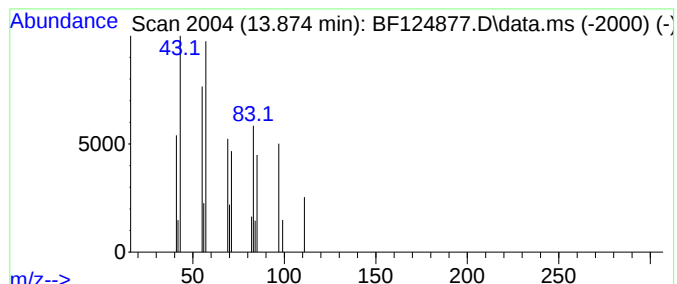
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Oxalic acid, allyl octadecy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	10.21 ng	18805	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	83
2			Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	72
3			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	72
4			Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	72
5			Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
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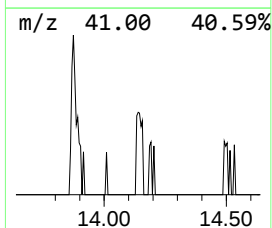
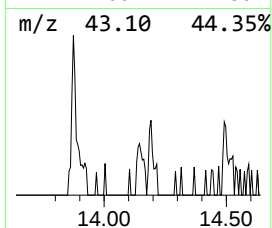
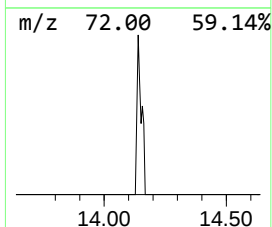
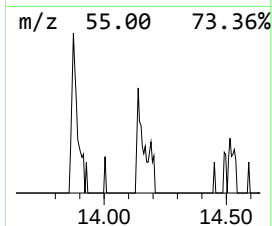
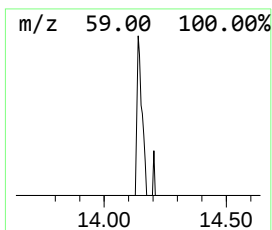
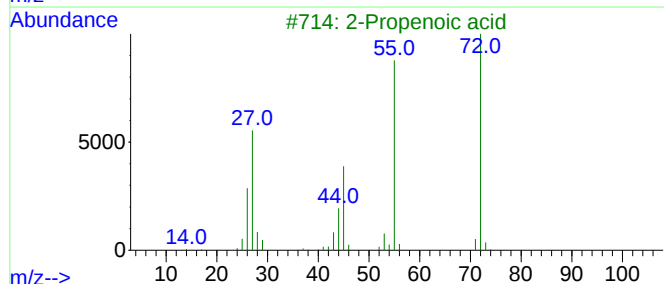
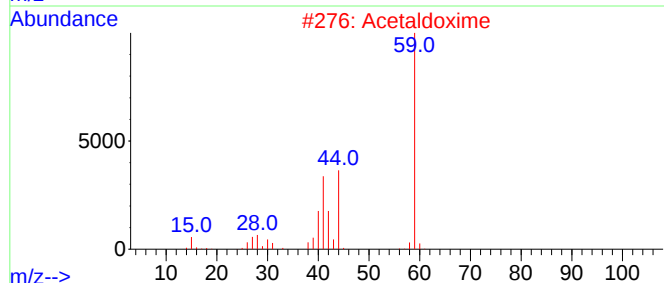
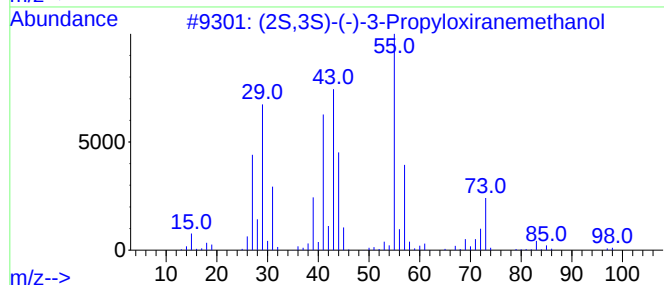
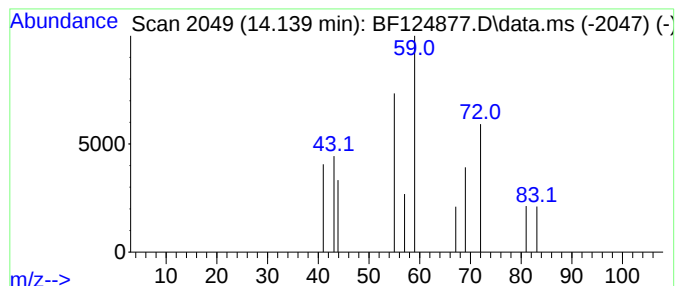
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown14.139 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.139	4.73 ng	8721	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(2S,3S)-(-)-3-Propyloxiranemethanol	116	C6H12O2	089321-71-1	9
2			Acetaldoxime	59	C2H5NO	000107-29-9	7
3			2-Propenoic acid	72	C3H4O2	000079-10-7	4
4			1-Propene, 1-methoxy-	72	C4H8O	007319-16-6	4
5			Acetamide	59	C2H5NO	000060-35-5	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
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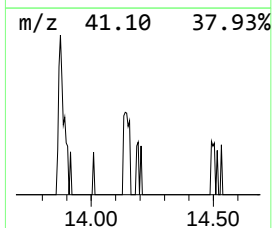
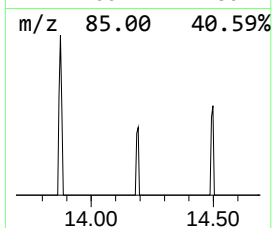
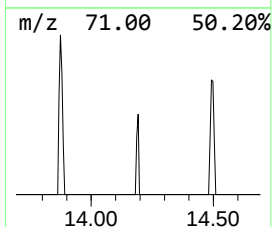
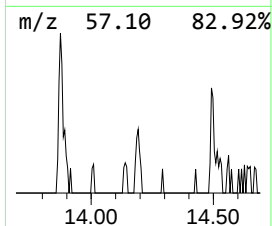
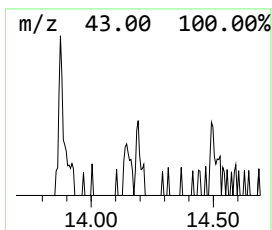
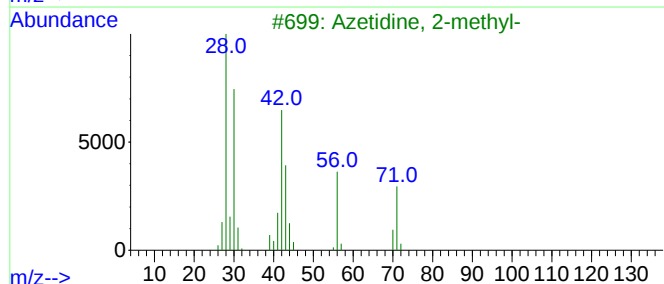
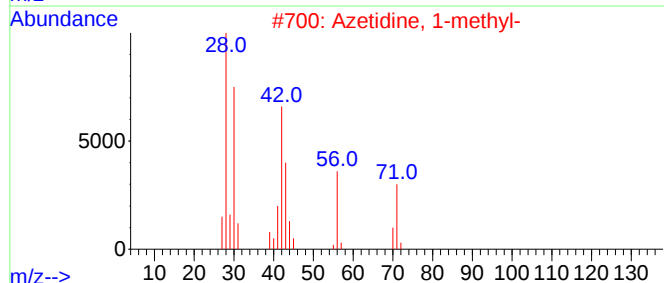
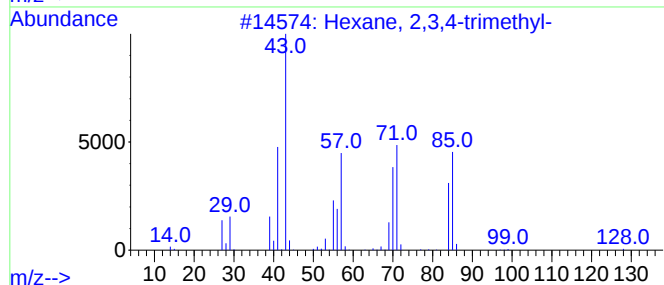
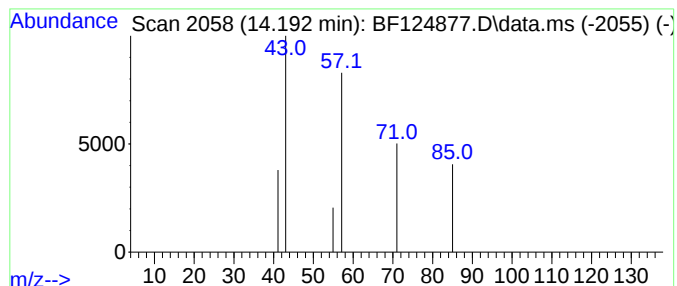
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown14.192 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.192	2.21 ng	4072	Chrysene-d12		14.039

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	9	
2	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5	
3	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5	
4	Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4	
5	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4	



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ALS Vial : 11 Sample Multiplier: 1

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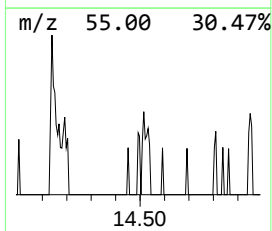
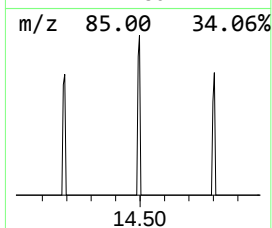
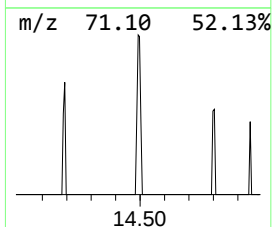
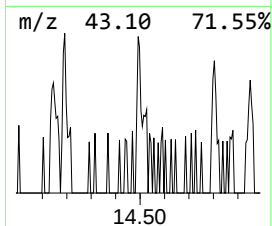
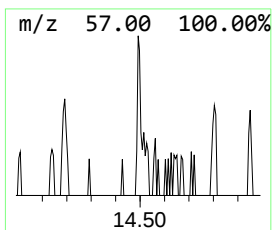
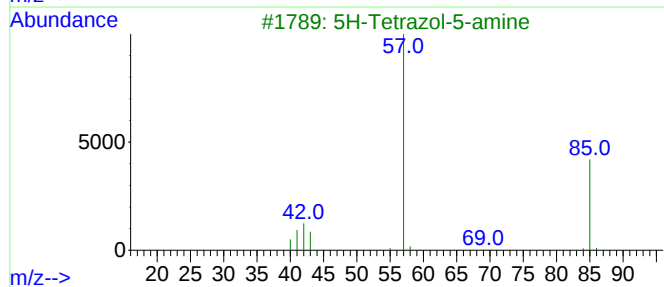
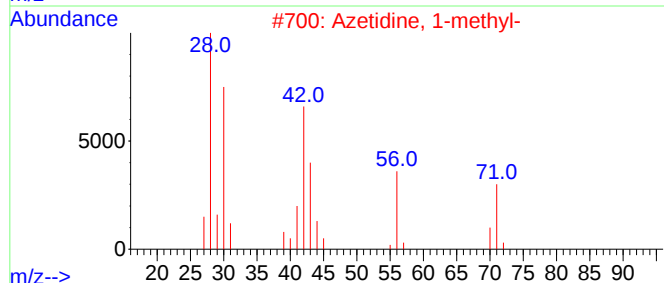
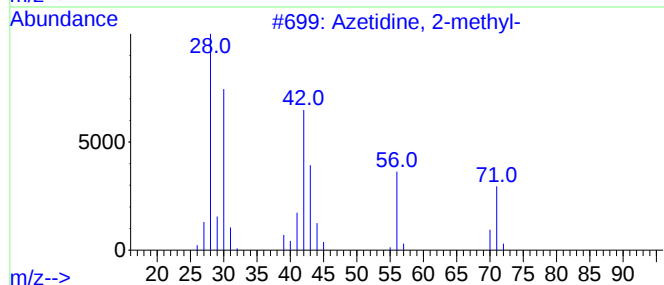
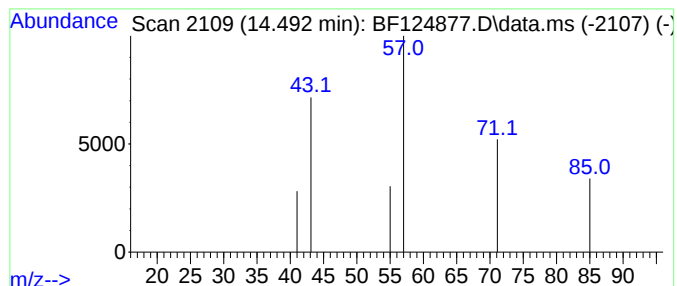
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown14.492 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.492	2.37 ng	4364	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
2			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
3			5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
4			1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
5			2-Propenamide	71	C3H5NO	000079-06-1	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124877.D
Acq On : 30 Jul 2021 15:39
Operator : JU/CG
Sample : M3210-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5(1.0-5.0)

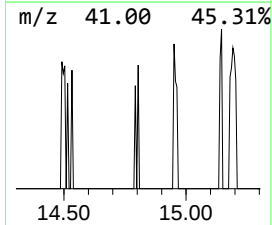
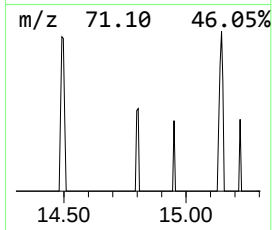
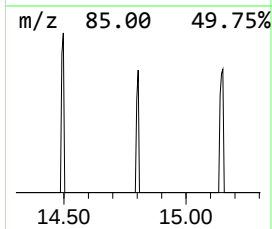
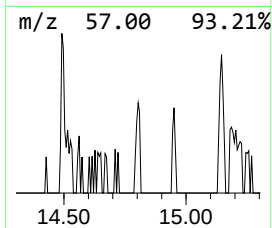
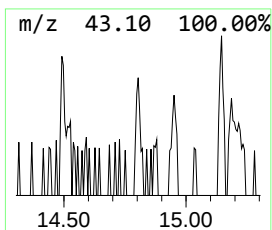
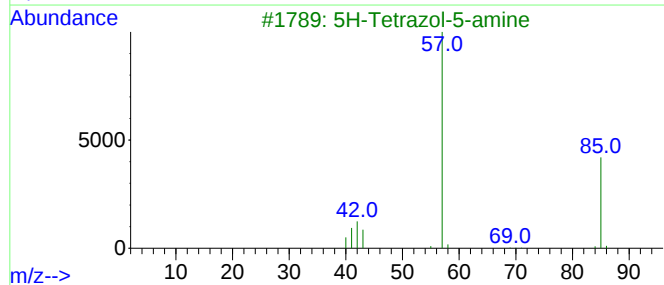
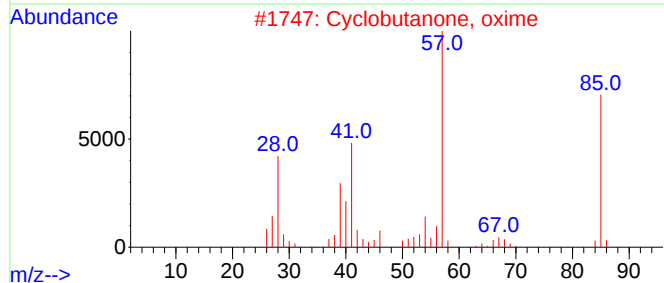
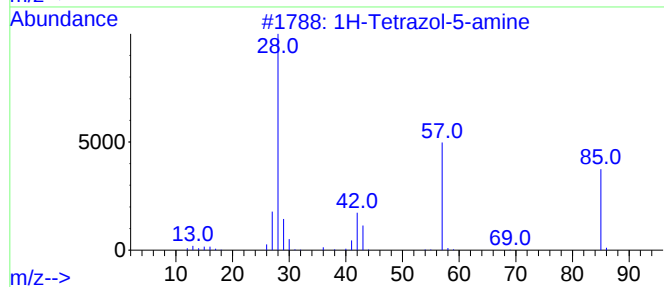
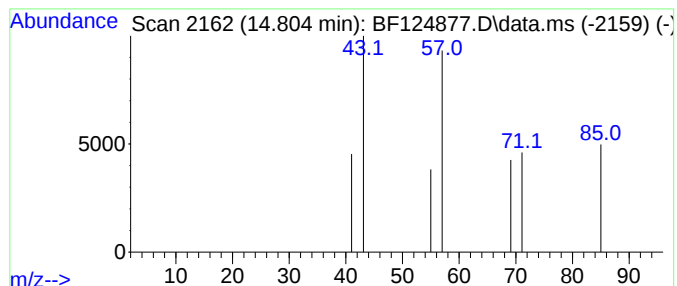
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown14.804 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	2.02 ng	3173	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		5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
4		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	4
5		Oxirane, 2-methyl-3-propyl-, cis-	100	C6H12O	006124-90-9	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124877.D
Acq On : 30 Jul 2021 15:39
Operator : JU/CG
Sample : M3210-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5(1.0-5.0)

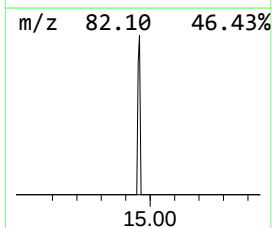
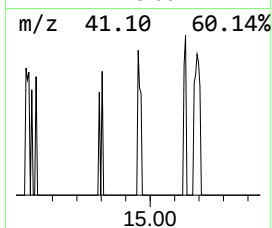
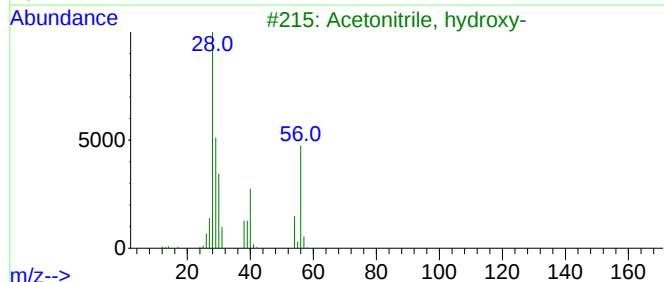
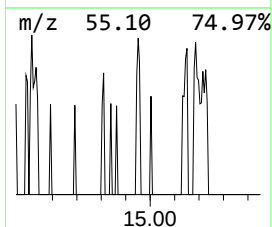
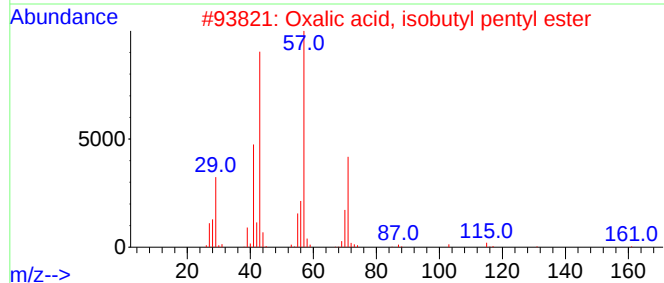
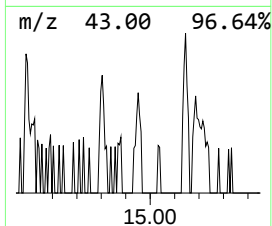
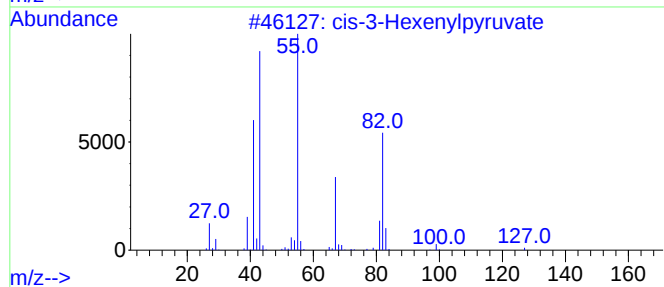
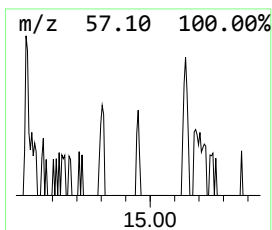
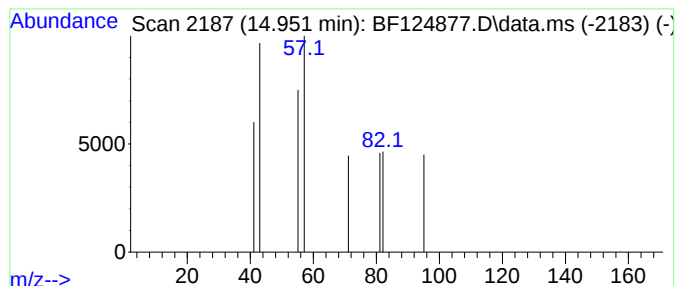
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown14.951 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.951	2.29 ng	3598	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-3-Hexenylpyruvate	170	C9H14O3	068133-76-6	4
2			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	4
3			Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	3
4			Hexanal, 5,5-dimethyl-	128	C8H16O	055320-58-6	2
5			Heptanedinitrile	122	C7H10N2	000646-20-8	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124877.D
Acq On : 30 Jul 2021 15:39
Operator : JU/CG
Sample : M3210-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

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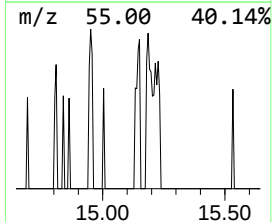
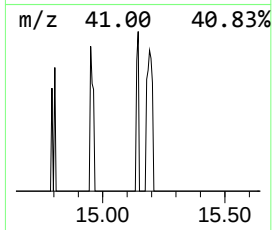
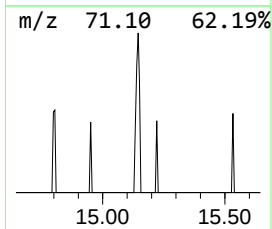
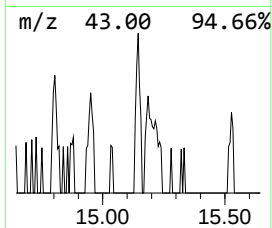
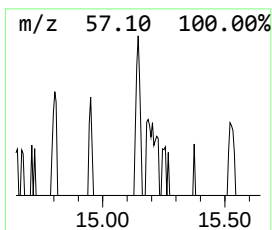
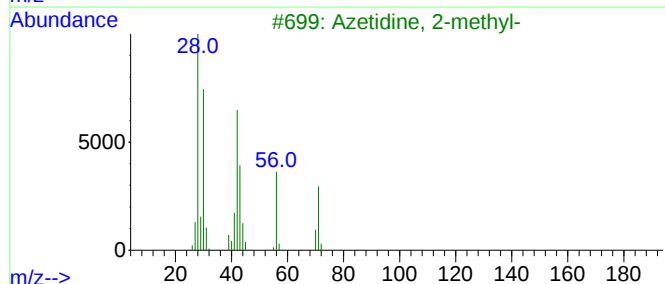
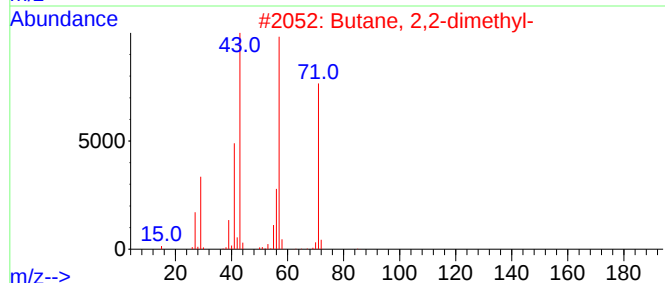
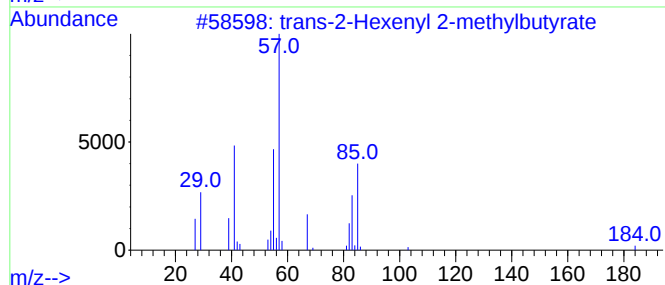
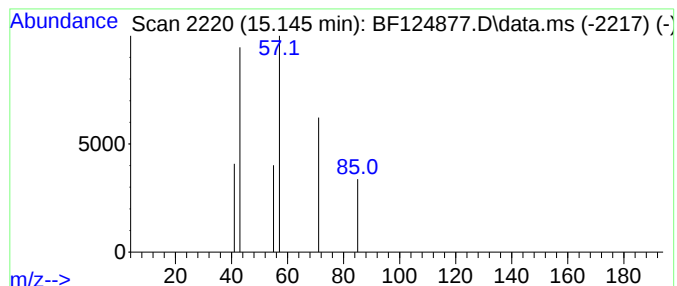
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown15.145 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	3.08 ng	4845	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			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	9
3			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
4			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
5			5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124877.D
Acq On : 30 Jul 2021 15:39
Operator : JU/CG
Sample : M3210-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

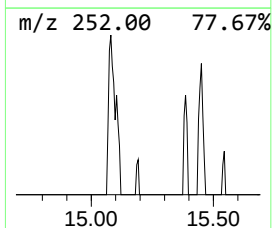
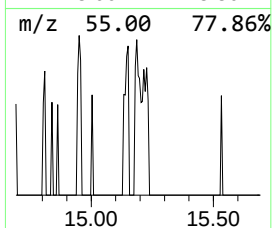
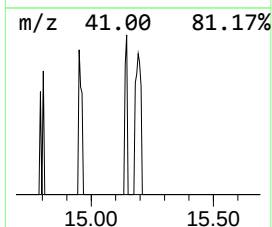
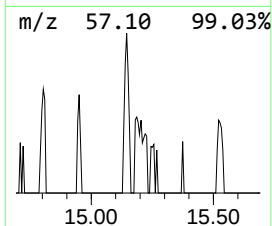
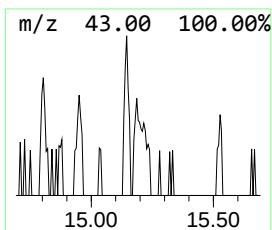
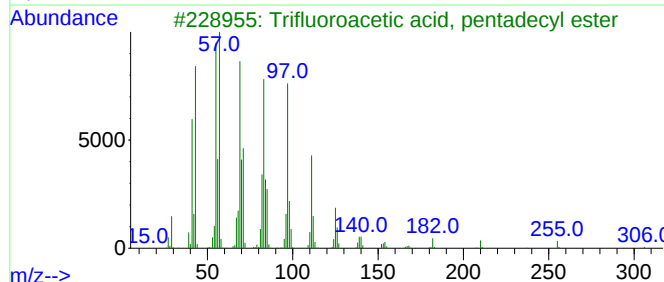
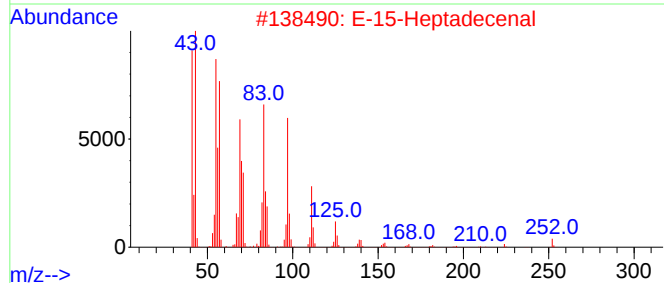
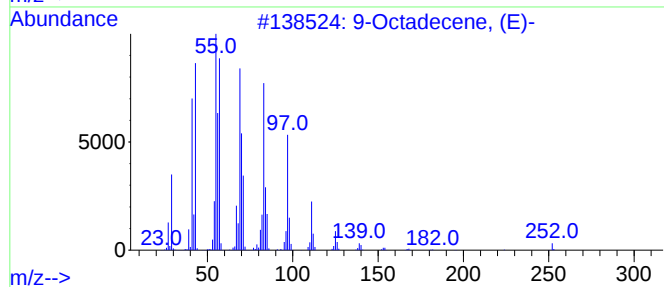
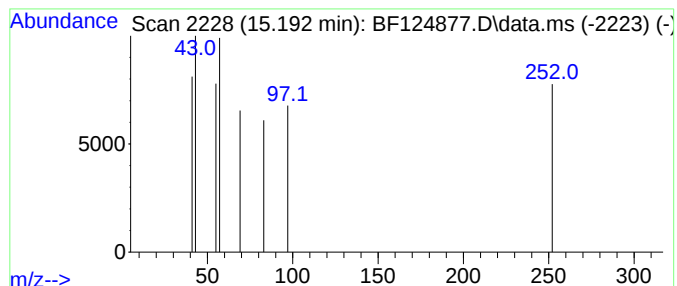
Instrument :
BNA_F
ClientSampleId :
SB-5(1.0-5.0)

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 16 9-Octadecene, (E)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.192	3.63 ng	5712	Perylene-d12		15.515	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9-Octadecene, (E)-		252	C18H36	007206-25-9	83
2	E-15-Heptadecenal		252	C17H32O	1000130-97-9	83
3	Trifluoroacetic acid, pentadecyl...		324	C17H31F3O2	959010-23-2	47
4	Dichloroacetic acid, heptadecyl ...		366	C19H36Cl2O2	1000282-98-2	47
5	Pentafluoropropionic acid, tetra...		360	C17H29F5O2	006222-06-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124877.D
Acq On : 30 Jul 2021 15:39
Operator : JU/CG
Sample : M3210-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-5(1.0-5.0)

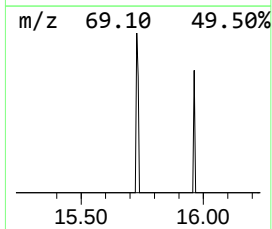
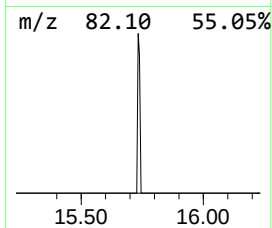
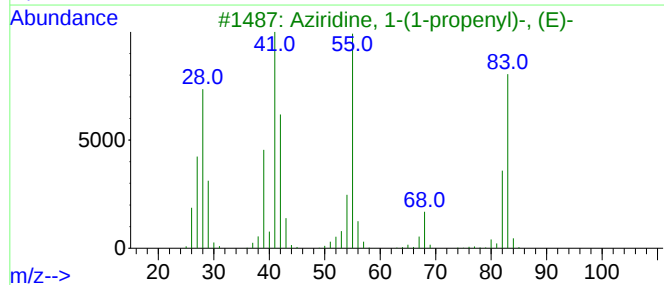
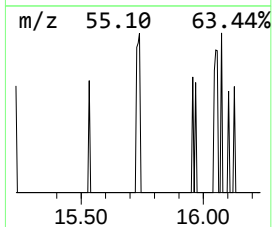
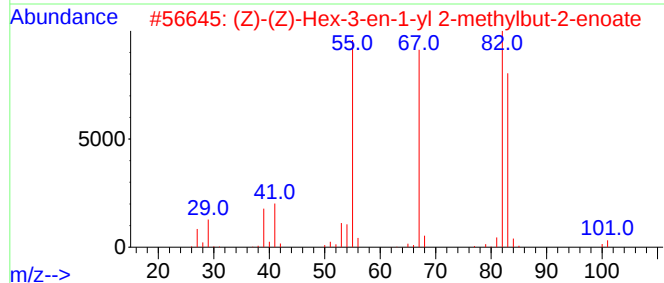
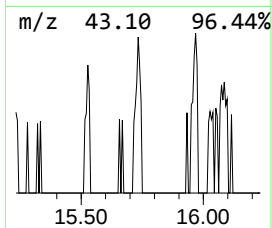
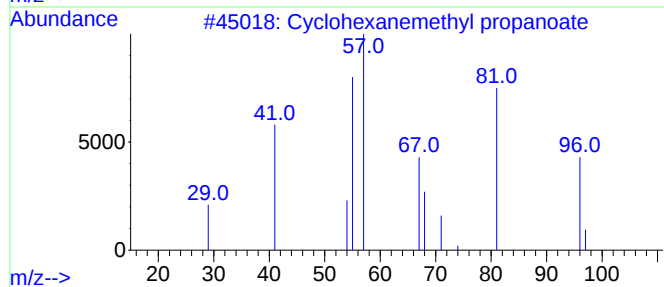
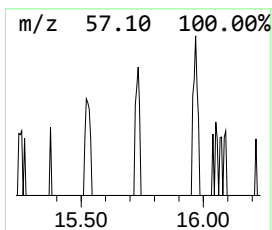
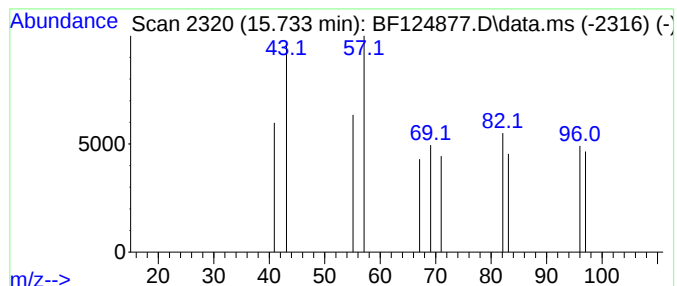
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown15.733 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.733	2.55 ng	4012	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanemethyl propanoate	170	C10H18O2	002890-67-7	25
2			(Z)-(Z)-Hex-3-en-1-yl 2-methylbu...	182	C11H18O2	084060-80-0	9
3			Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	7
4			Pentanenitrile, 4,4-dimethyl-5-oxo-	125	C7H11NO	006140-61-0	7
5			Fomepizole	82	C4H6N2	007554-65-6	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124877.D
Acq On : 30 Jul 2021 15:39
Operator : JU/CG
Sample : M3210-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-5(1.0-5.0)

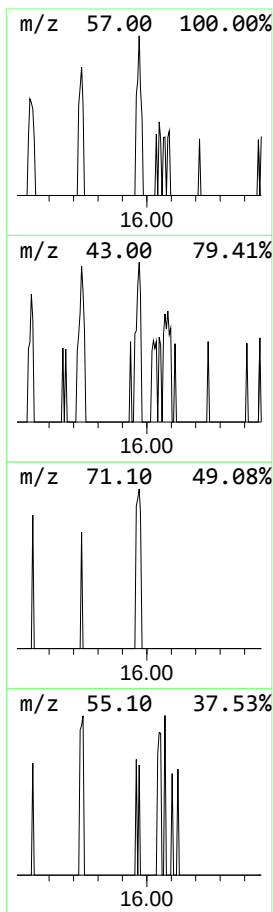
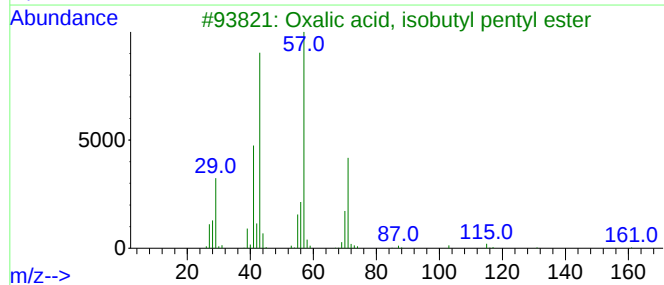
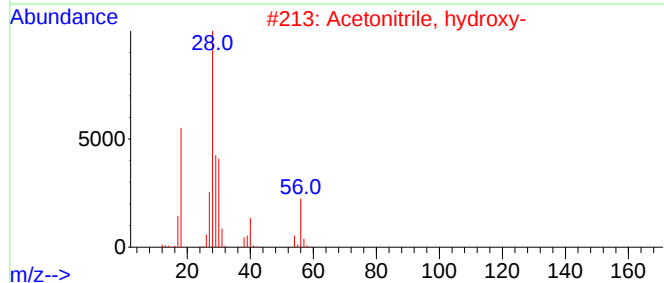
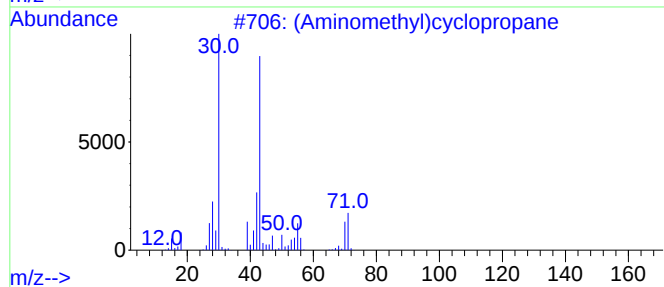
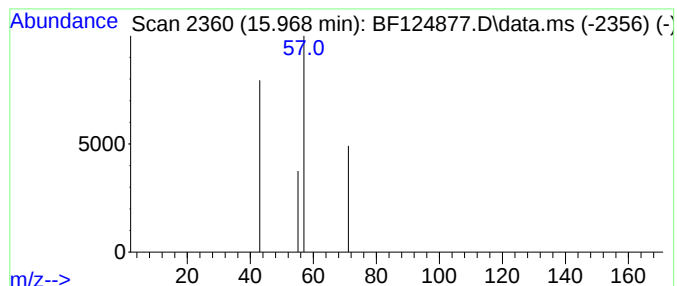
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown15.968 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.968	2.01 ng	3158	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	3
2			Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	3
3			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	2
4			Propanoic acid, 2-methyl-, 2-eth...	286	C16H30O4	074367-30-9	2
5			Hydroxylamine, O-(2-methylpropyl)-	89	C4H11NO	005618-62-2	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
 Data File : BF124877.D
 Acq On : 30 Jul 2021 15:39
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 Sample : M3210-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 SB-5(1.0-5.0)

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...	2.122	7.0	ng	12482	1	6.869	35596	20.0
3-Penten-2-one,...	4.463	36.4	ng	64786	1	6.869	35596	20.0
2-Pentanone, 4-...	5.104	112.5	ng	200183	1	6.869	35596	20.0
1-Hexanol, 2-et...	6.928	17.8	ng	31589	1	6.869	35596	20.0
Ethanol, 2-(2-b...	8.051	8.1	ng	20508	2	8.151	50455	20.0
9-Octadecenamid...	13.463	59.7	ng	109898	5	14.039	36837	20.0
unknown13.492	13.492	12.5	ng	23052	5	14.039	36837	20.0
Hexanedioic aci...	13.515	10.2	ng	18782	5	14.039	36837	20.0
Oxalic acid, al...	13.874	10.2	ng	18805	5	14.039	36837	20.0
unknown14.139	14.139	4.7	ng	8721	5	14.039	36837	20.0
unknown14.192	14.192	2.2	ng	4072	5	14.039	36837	20.0
unknown14.492	14.492	2.4	ng	4364	5	14.039	36837	20.0
unknown14.804	14.804	2.0	ng	3173	6	15.515	31456	20.0
unknown14.951	14.951	2.3	ng	3598	6	15.515	31456	20.0
unknown15.145	15.145	3.1	ng	4845	6	15.515	31456	20.0
9-Octadecene, (E)-	15.192	3.6	ng	5712	6	15.515	31456	20.0
unknown15.733	15.733	2.5	ng	4012	6	15.515	31456	20.0
unknown15.968	15.968	2.0	ng	3158	6	15.515	31456	20.0