

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
 Data File : BF124647.D
 Acq On : 21 Jul 2021 2:00
 Operator : JU/CG
 Sample : M3046-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-EF-01-019-ABCD

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-BF070721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124647.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	17	20	24	rBB	6331	7059	5.08%	0.773%
2	5.516	579	583	586	rBB	128264	114111	82.08%	12.502%
3	6.522	749	754	757	rBB	121043	117955	84.85%	12.923%
4	6.904	816	819	821	rBB	45269	35325	25.41%	3.870%
5	7.463	910	914	917	rBB	86902	76838	55.27%	8.418%
6	8.081	1017	1019	1022	rBB	14302	10015	7.20%	1.097%
7	8.186	1033	1037	1040	rBB	63423	47000	33.81%	5.149%
8	9.263	1216	1220	1223	rBV	193018	139019	100.00%	15.230%
9	9.945	1333	1336	1339	rBB	58642	45939	33.05%	5.033%
10	10.727	1466	1469	1472	rBB	76821	56966	40.98%	6.241%
11	11.427	1585	1588	1591	rBV	43427	35285	25.38%	3.866%
12	11.451	1591	1592	1594	rVB	3956	2106	1.51%	0.231%
13	11.945	1674	1676	1680	rBB	6478	5049	3.63%	0.553%
14	12.639	1792	1794	1798	rBB	8072	6324	4.55%	0.693%
15	12.733	1805	1810	1814	rBB	3434	3090	2.22%	0.339%
16	12.869	1831	1833	1837	rVB	8350	7066	5.08%	0.774%
17	13.016	1854	1858	1861	rVB	121452	91541	65.85%	10.029%
18	13.904	2005	2009	2014	rBV3	3693	5849	4.21%	0.641%
19	14.068	2032	2037	2040	rBV	33392	31419	22.60%	3.442%
20	14.092	2040	2041	2043	rVB	4224	1970	1.42%	0.216%
21	14.268	2070	2071	2076	rVB3	1817	2264	1.63%	0.248%
22	14.368	2083	2088	2090	rBV4	1322	2218	1.60%	0.243%
23	14.545	2114	2118	2119	rBV3	3017	3446	2.48%	0.378%
24	14.886	2174	2176	2178	rVB3	2623	1964	1.41%	0.215%
25	15.115	2213	2215	2219	rBV2	5277	6197	4.46%	0.679%
26	15.198	2224	2229	2233	rVV5	2031	3665	2.64%	0.402%
27	15.427	2266	2268	2271	rVB	2383	2314	1.66%	0.254%
28	15.492	2276	2279	2282	rVV3	3435	4756	3.42%	0.521%
29	15.557	2286	2290	2294	rVV	17998	22736	16.35%	2.491%
30	15.592	2294	2296	2300	rVB4	2402	2659	1.91%	0.291%
31	15.668	2305	2309	2311	rVV3	1638	2440	1.76%	0.267%
32	15.715	2314	2317	2321	rVB3	1891	3022	2.17%	0.331%
33	16.086	2375	2380	2381	rBV	1593	1892	1.36%	0.207%
34	16.233	2403	2405	2409	rVB3	1275	1872	1.35%	0.205%
35	16.292	2409	2415	2417	rBV4	3281	5453	3.92%	0.597%
36	16.745	2487	2492	2496	rVB4	2020	3774	2.71%	0.413%

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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.404	2600	2604	2607	rBV3	1510	2170	1.56%	0.238%
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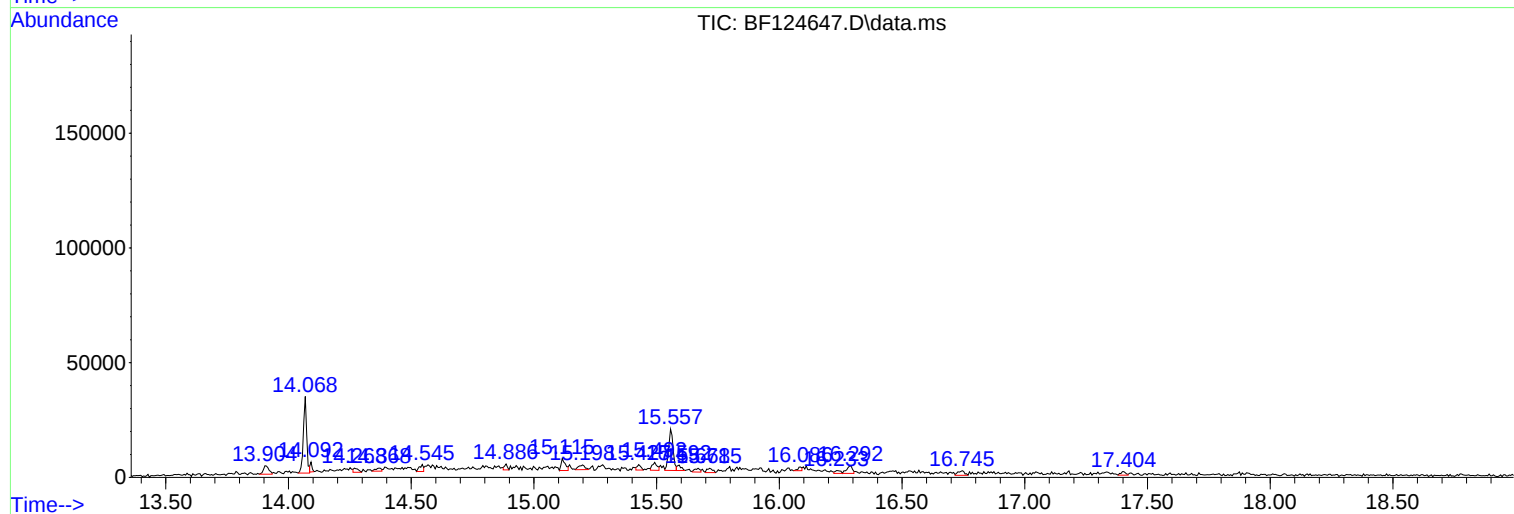
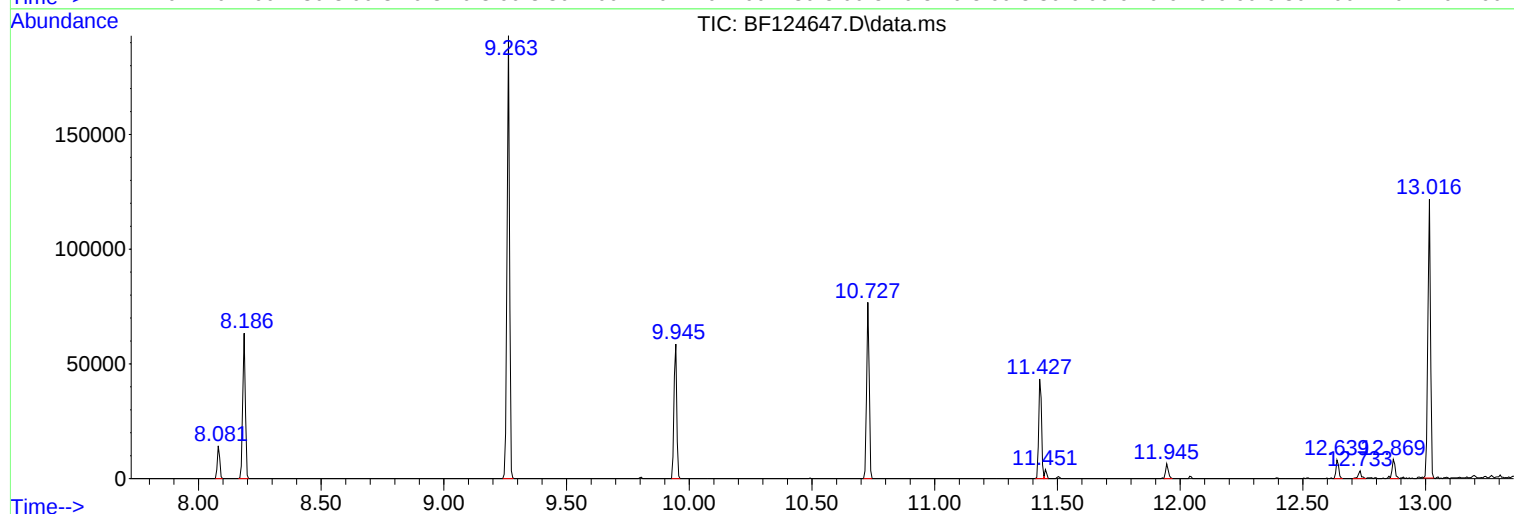
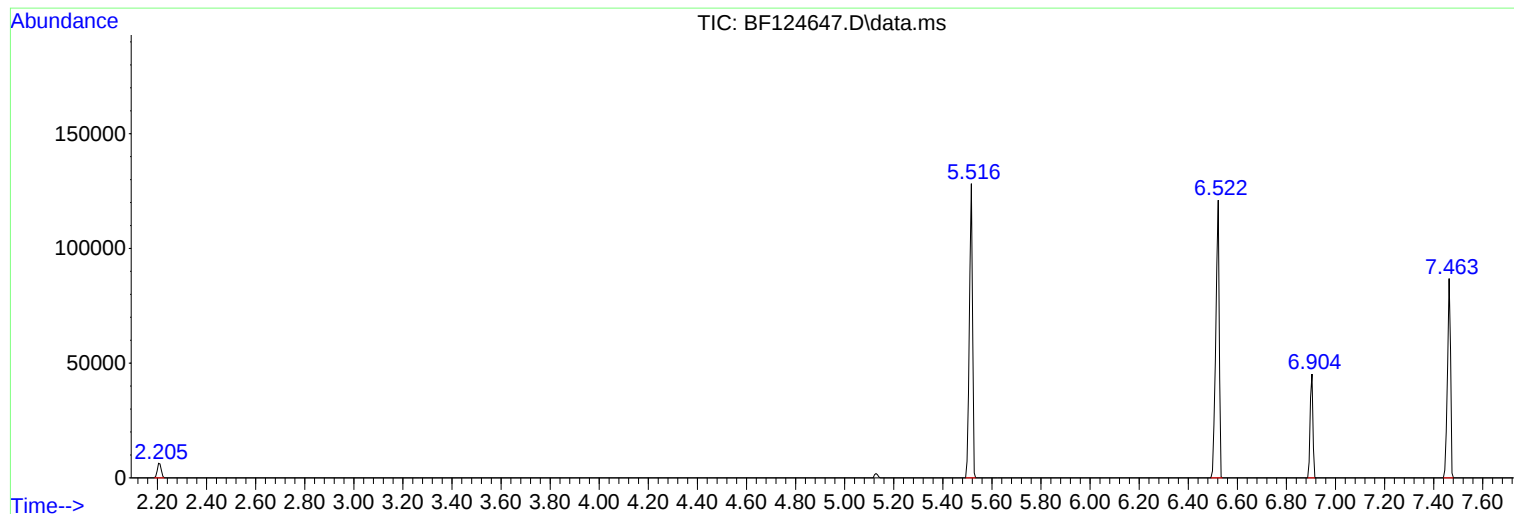
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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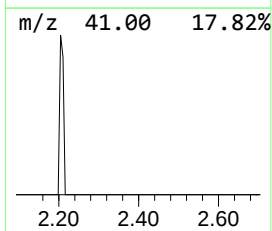
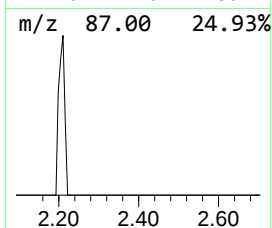
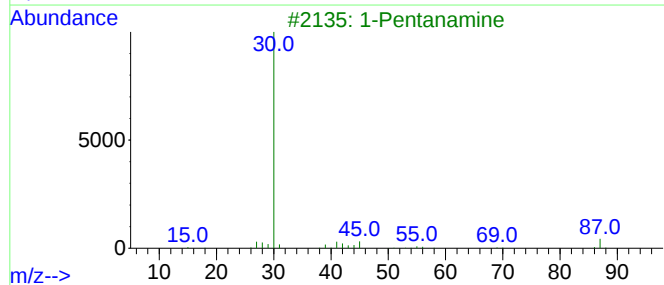
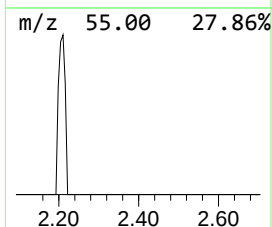
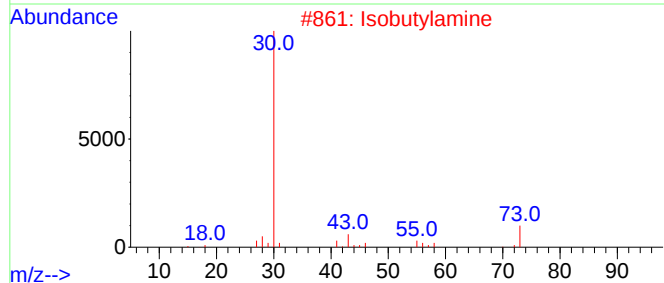
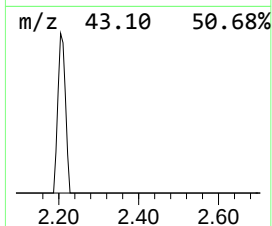
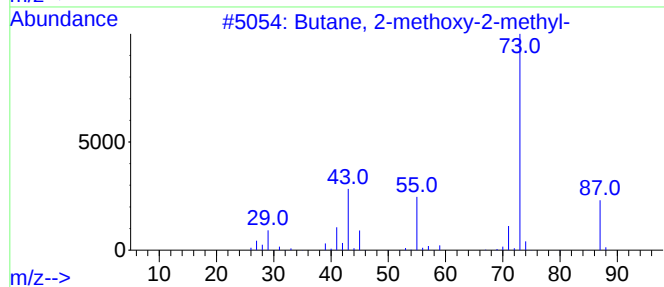
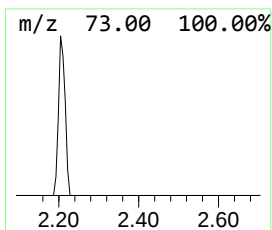
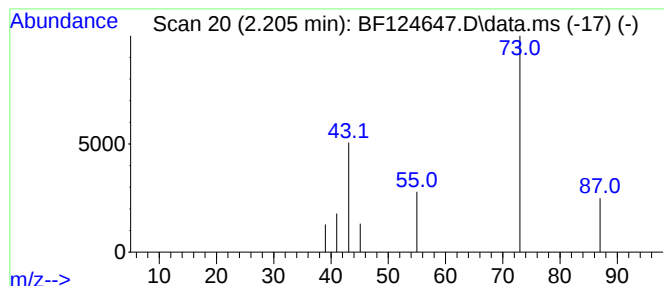
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.205 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.205	4.00 ng	7059	1,4-Dichlorobenzene-d4	6.904

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	9
2		Isobutylamine	73	C4H11N	000078-81-9	5
3		1-Pentanamine	87	C5H13N	000110-58-7	4
4		2-Pentanol, acetate	130	C7H14O2	000626-38-0	4
5		1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4



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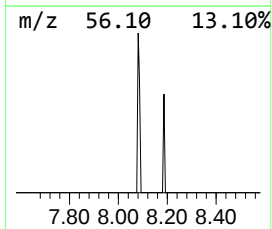
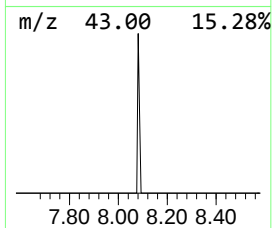
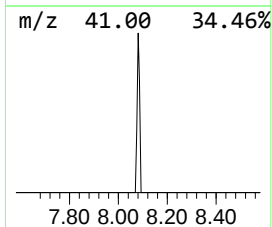
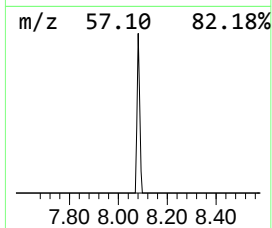
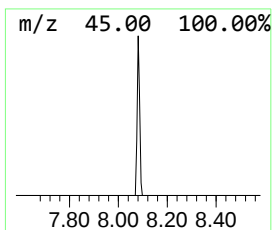
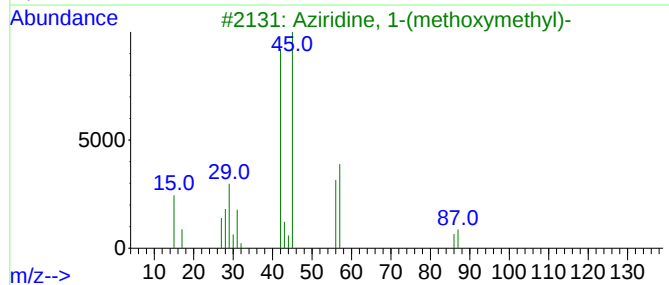
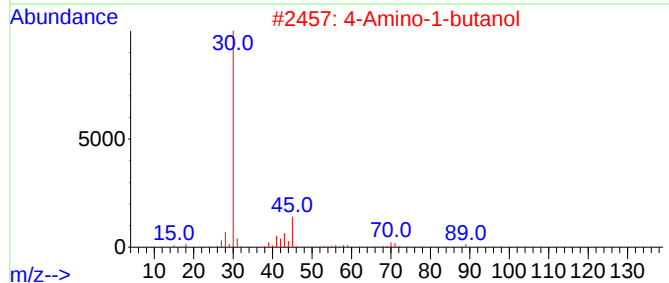
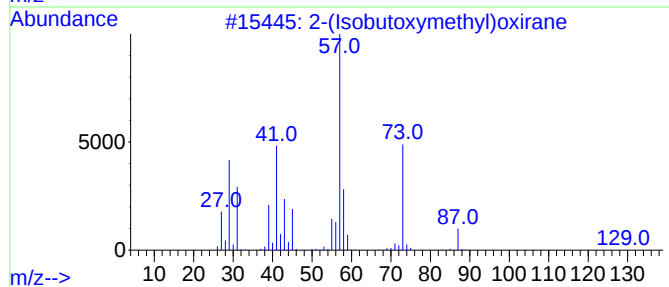
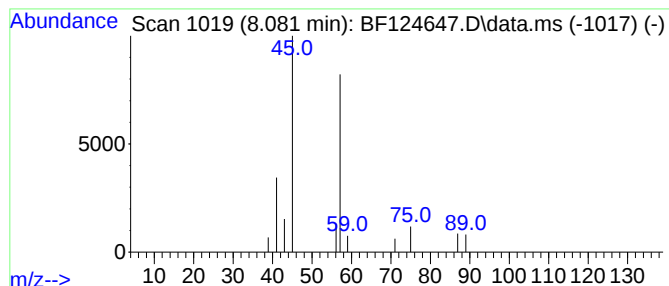
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown8.081 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.081	4.26 ng	10015	Naphthalene-d8	8.186

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
2		4-Amino-1-butanol	89	C4H11NO	013325-10-5	5
3		Aziridine, 1-(methoxymethyl)-	87	C4H9NO	001497-83-2	5
4		2-Propanol, 1-amino-	75	C3H9NO	000078-96-6	4
5		Ethanamine, 2-methoxy-	75	C3H9NO	000109-85-3	4



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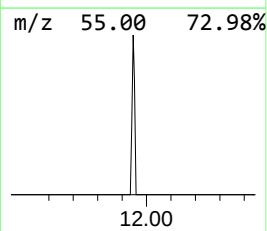
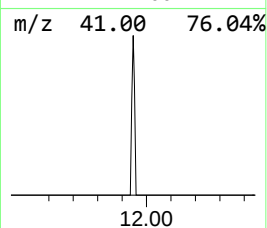
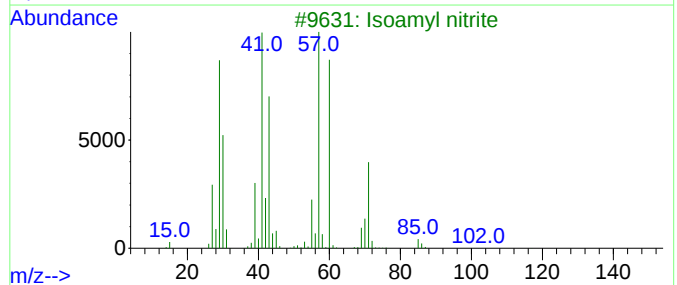
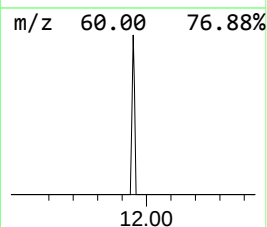
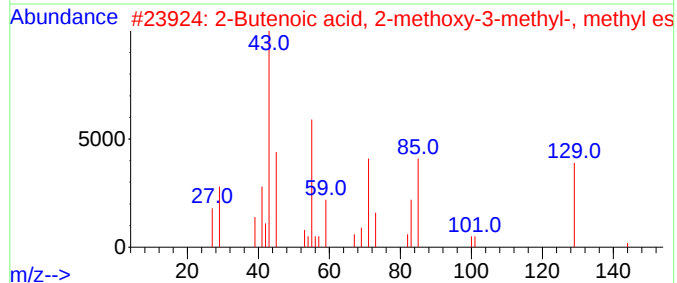
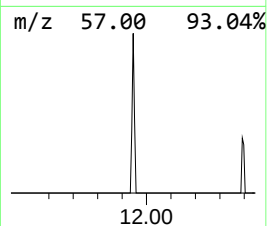
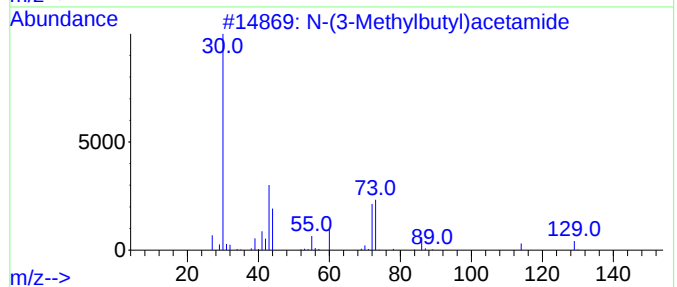
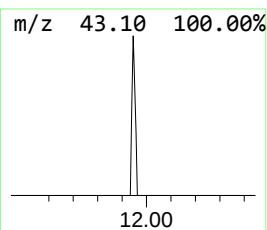
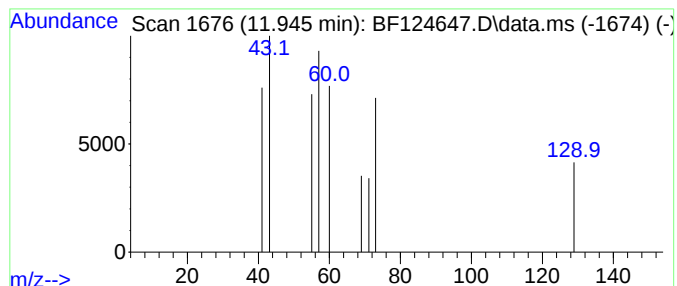
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown11.945 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	2.86 ng	5049	Phenanthrene-d10	11.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-(3-Methylbutyl)acetamide	129	C7H15NO	013434-12-3	9
2			2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	9
3			Isoamyl nitrite	117	C5H11NO2	000110-46-3	9
4			Neopentyl isothiocyanate	129	C6H11NS	000597-97-7	4
5			Acetic acid	60	C2H4O2	000064-19-7	4



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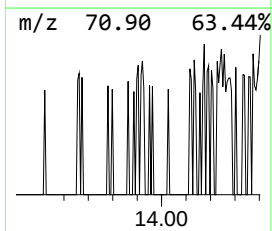
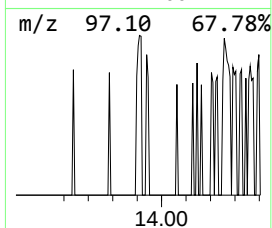
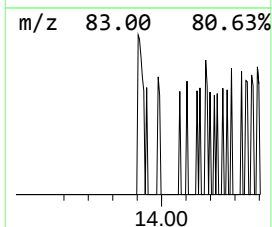
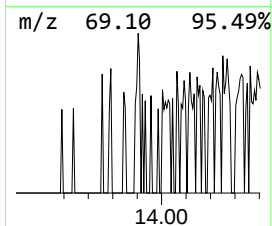
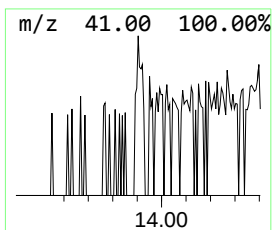
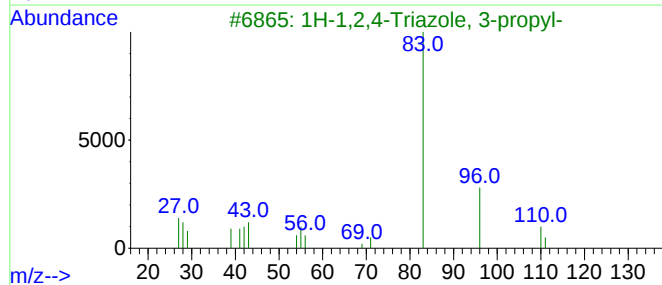
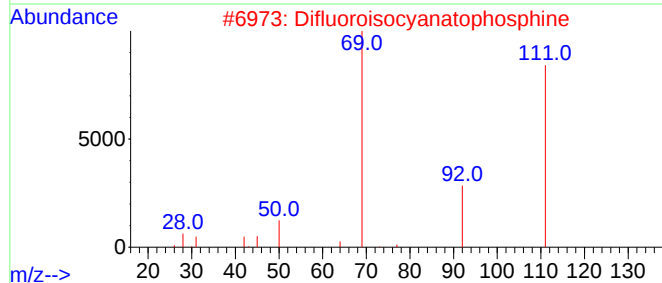
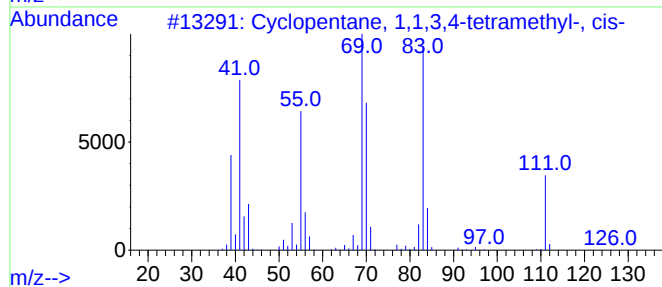
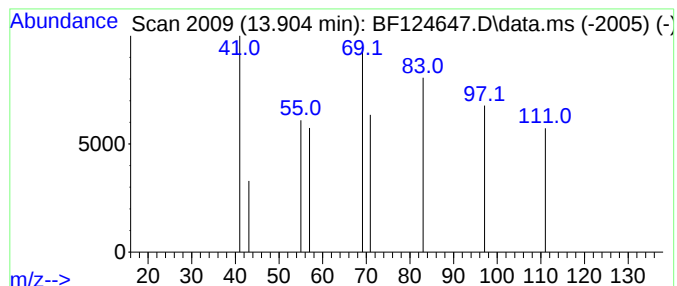
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown13.904 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	3.72 ng	5849	Chrysene-d12	14.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	053907-60-1	9
2			Difluoroisocyanatophosphine	111	CF2NOP	1000306-12-1	5
3			1H-1,2,4-Triazole, 3-propyl-	111	C5H9N3	019932-60-6	4
4			Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	4
5			1-Butyne, 3-ethoxy-3-methyl-	112	C7H12O	007740-69-4	4



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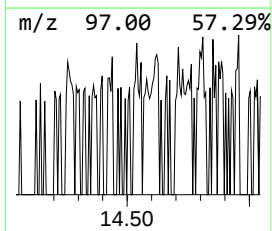
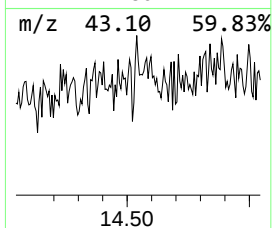
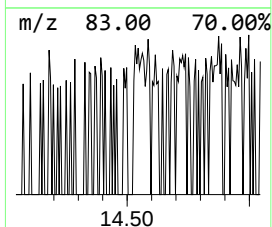
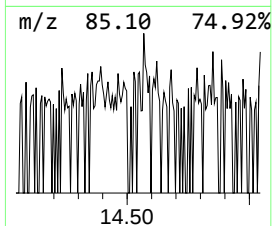
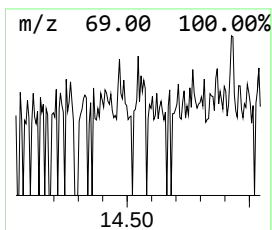
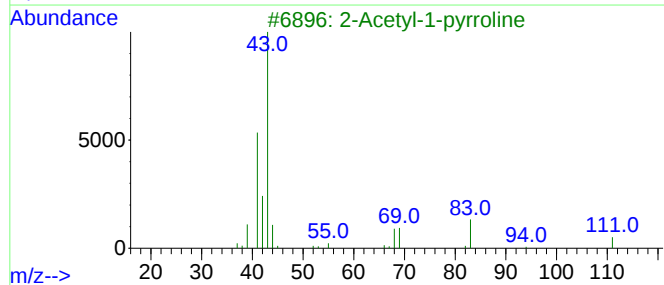
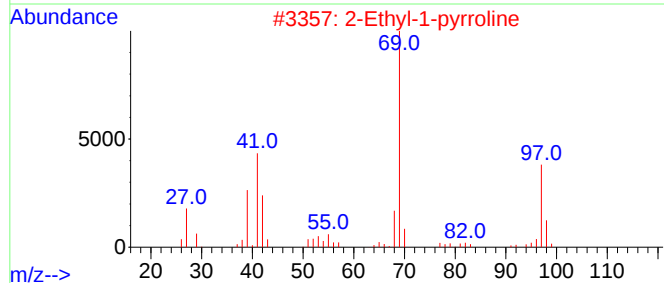
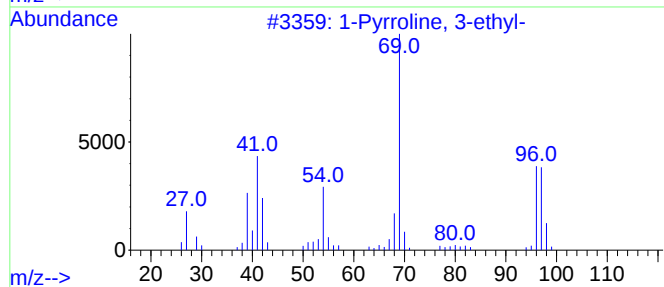
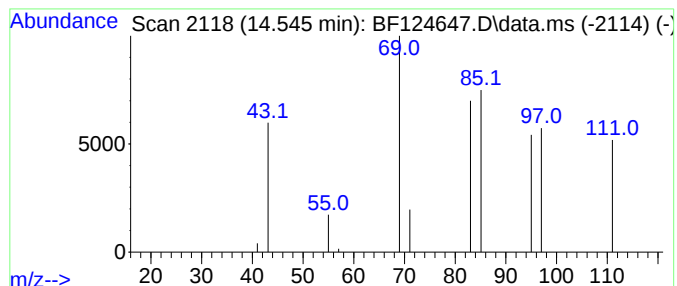
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown14.545 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.545	2.19 ng	3446	Chrysene-d12	14.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pyrroline, 3-ethyl-	97	C6H11N	1000073-06-0	5
2			2-Ethyl-1-pyrroline	97	C6H11N	1000422-81-4	5
3			2-Acetyl-1-pyrroline	111	C6H9NO	085213-22-5	4
4			1-[1,2,4]Triazol-1-ylethanone	111	C4H5N3O	015625-88-4	4
5			Tetrahydropyran 12-tetradecyn-1-...	294	C19H34O2	096249-40-0	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124647.D
Acq On : 21 Jul 2021 2:00
Operator : JU/CG
Sample : M3046-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FK-EF-01-019-ABCD

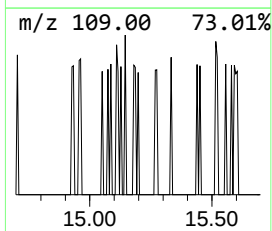
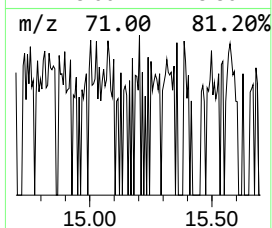
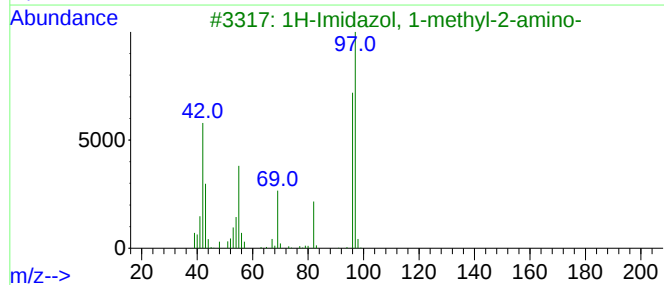
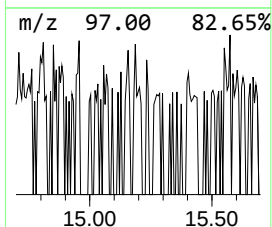
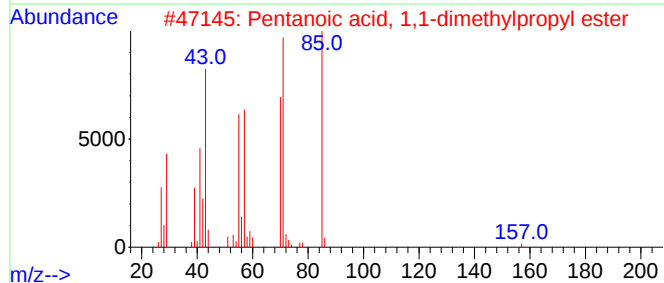
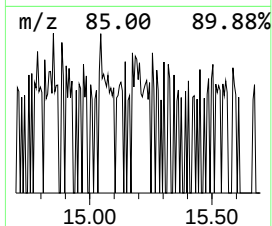
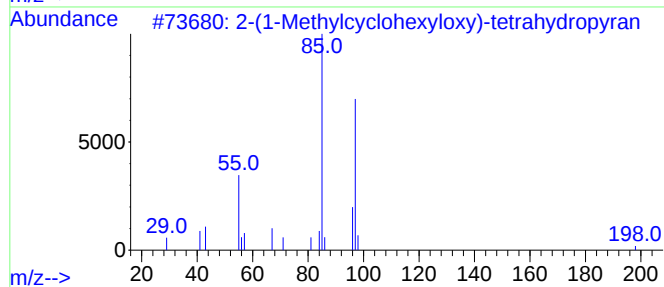
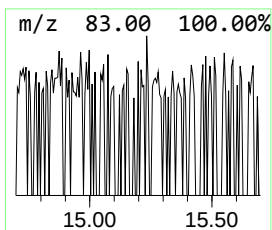
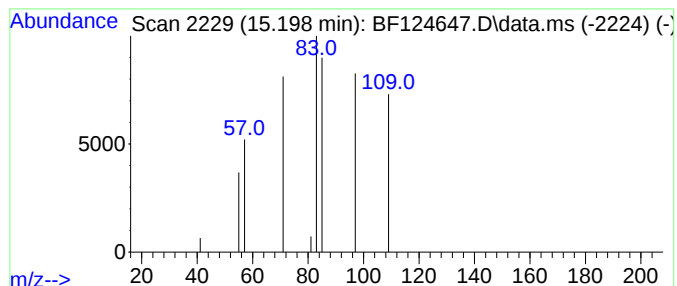
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown15.198 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	3.22 ng	3665	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(1-Methylcyclohexyloxy)-tetrah...	198	C12H22O2	072347-38-7	9		
2	Pentanoic acid, 1,1-dimethylprop...	172	C10H20O2	117421-32-6	9		
3	1H-Imidazol, 1-methyl-2-amino-	97	C4H7N3	006646-51-1	4		
4	2-Propenamide	71	C3H5NO	000079-06-1	4		
5	2,5-Dimethyl-1-pyrroline	97	C6H11N	000822-64-0	4		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124647.D
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Operator : JU/CG
Sample : M3046-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FK-EF-01-019-ABCD

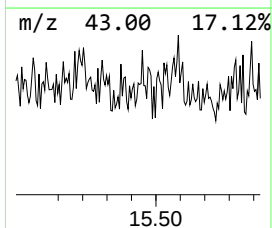
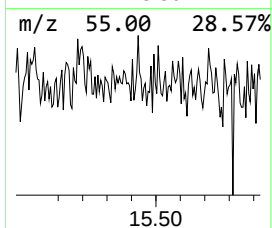
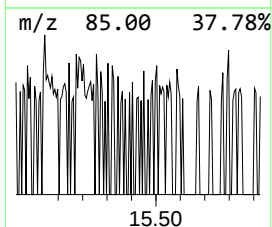
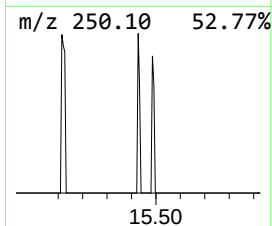
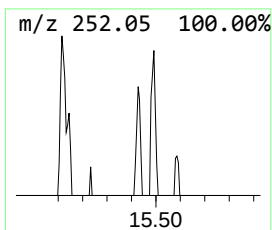
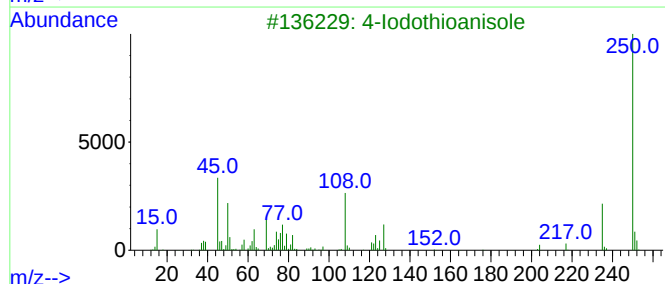
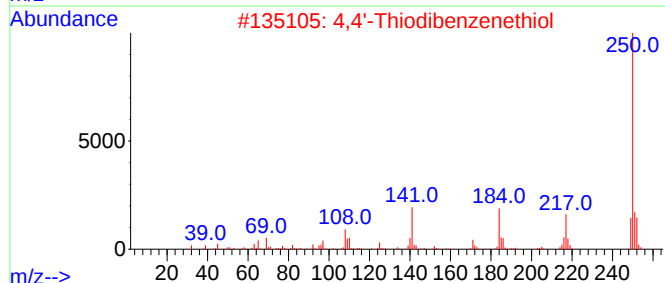
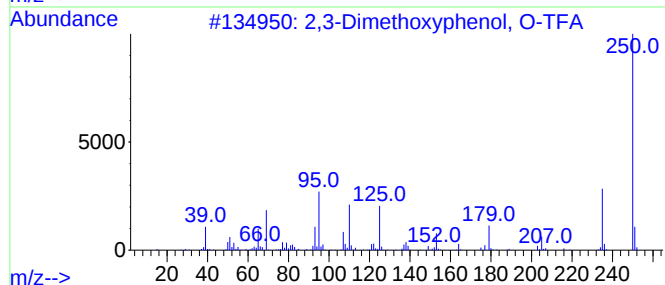
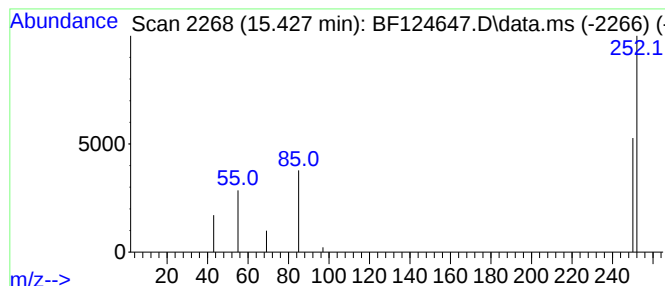
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.427 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.427	2.04 ng	2314	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Dimethoxyphenol, O-TFA	250	C10H9F3O4	1000461-51-9	4		
2	4,4'-Thiodibenzenethiol	250	C12H10S3	019362-77-7	4		
3	4-Iodothioanisole	250	C7H7IS	035371-03-0	4		
4	Methacrylamide	85	C4H7NO	000079-39-0	3		
5	Propargyl alcohol, heptafluorobu...	252	C7H3F7O2	1000352-28-1	3		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124647.D
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Operator : JU/CG
Sample : M3046-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FK-EF-01-019-ABCD

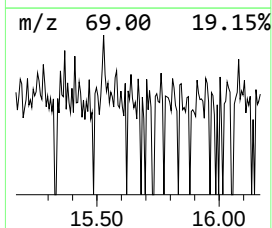
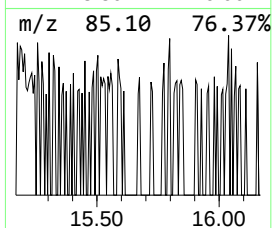
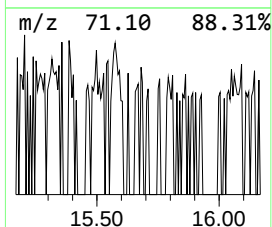
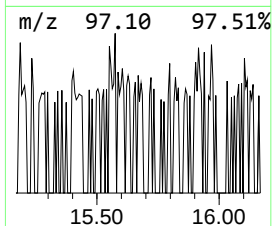
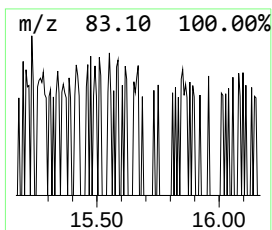
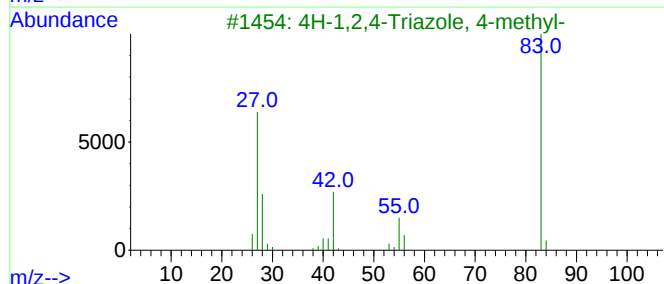
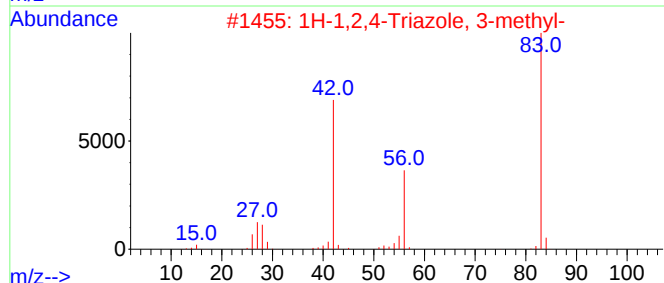
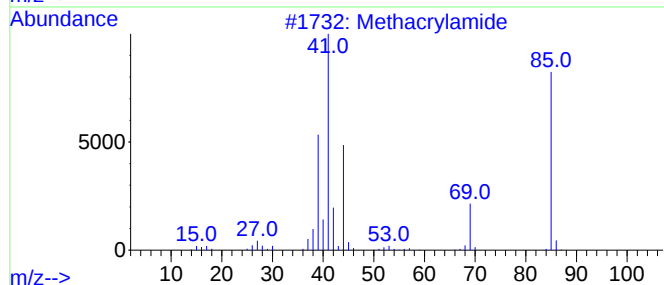
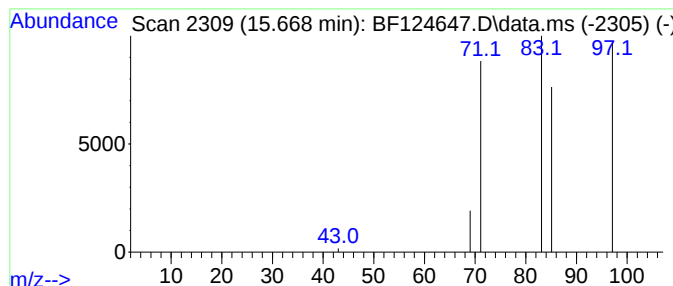
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.668 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.668	2.15 ng	2440	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methacrylamide	85	C4H7NO	000079-39-0	4
2			1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	3
3			4H-1,2,4-Triazole, 4-methyl-	83	C3H5N3	010570-40-8	3
4			3H-1,2,4-Triazol-3-one, 1,2-dihy...	85	C2H3N3O	000930-33-6	2
5			Thiazole	85	C3H3NS	000288-47-1	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124647.D
Acq On : 21 Jul 2021 2:00
Operator : JU/CG
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Misc :
ALS Vial : 12 Sample Multiplier: 1

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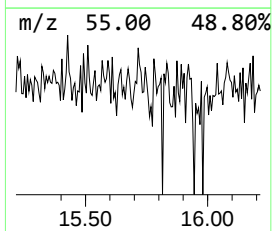
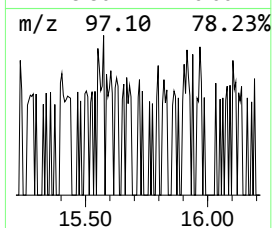
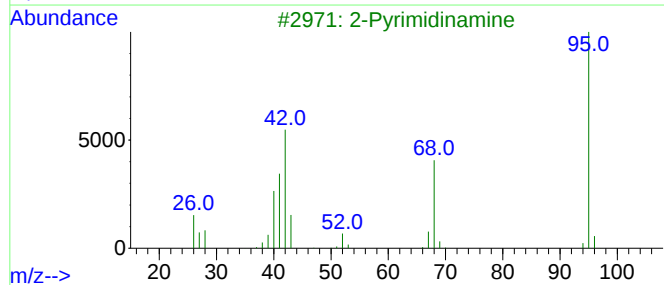
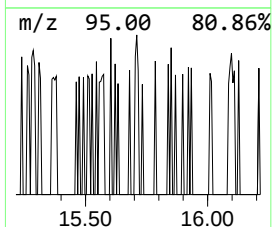
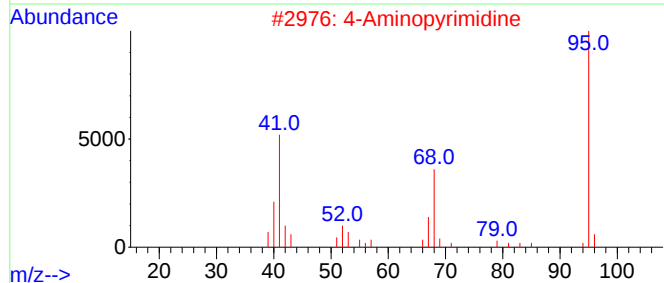
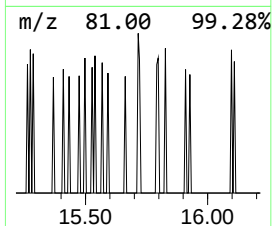
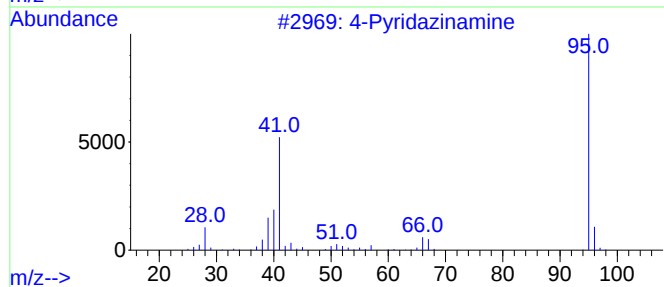
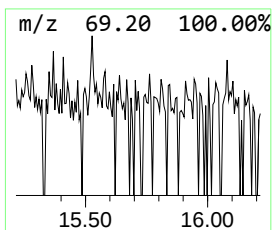
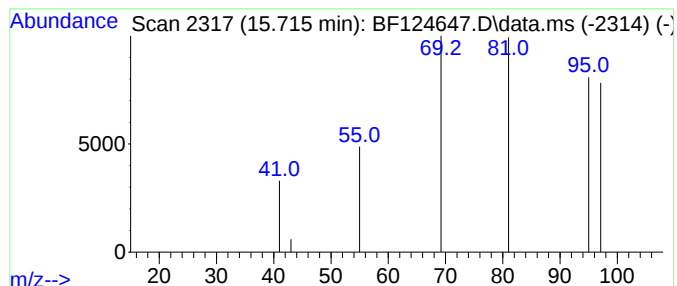
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.715 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.715	2.66 ng	3022	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Pyridazinamine	95	C4H5N3	020744-39-2	4
2			4-Aminopyrimidine	95	C4H5N3	000591-54-8	4
3			2-Pyrimidinamine	95	C4H5N3	000109-12-6	4
4			1-Butyne, 3-ethoxy-3-methyl-	112	C7H12O	007740-69-4	4
5			Isoxazole	69	C3H3NO	000288-14-2	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124647.D
Acq On : 21 Jul 2021 2:00
Operator : JU/CG
Sample : M3046-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-019-ABCD

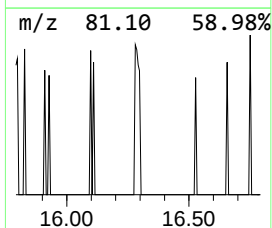
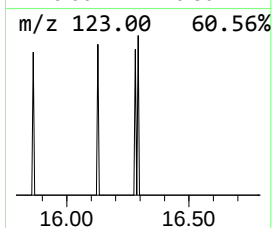
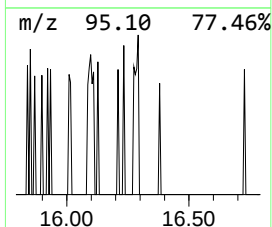
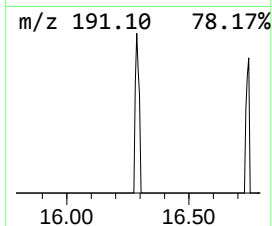
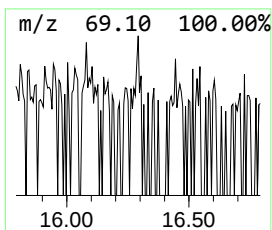
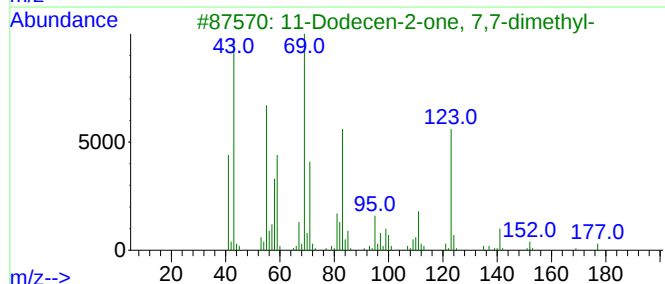
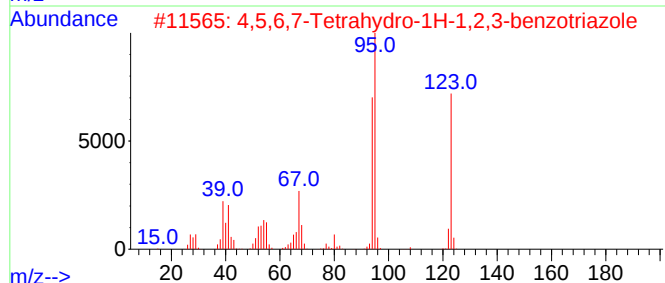
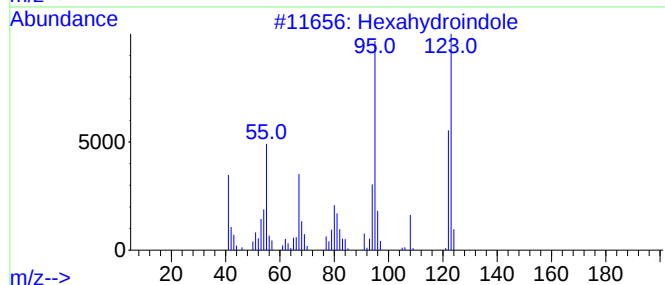
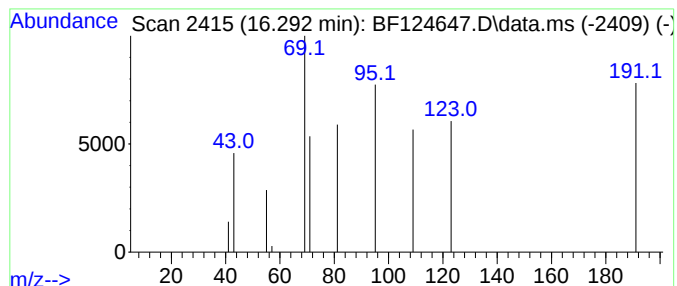
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.292 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.292	4.80 ng	5453	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexahydroindole	123	C8H13N	018159-32-5	5
2			4,5,6,7-Tetrahydro-1H-1,2,3-benz...	123	C6H9N3	006789-99-7	5
3			11-Dodecen-2-one, 7,7-dimethyl-	210	C14H26O	035194-22-0	4
4			Bicyclo[3.3.1]nonan-9-one, 1,2,4...	225	C12H19NO3	129967-65-3	4
5			5-Hexen-1-ol, 2-(2-methyl-1-prop...	154	C10H18O	018675-19-9	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124647.D
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Operator : JU/CG
Sample : M3046-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

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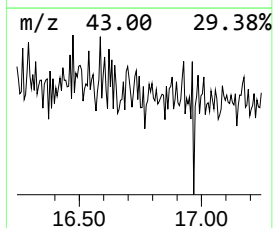
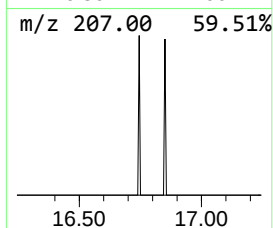
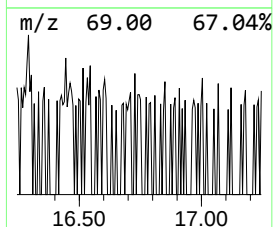
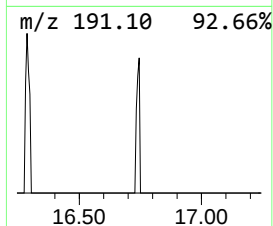
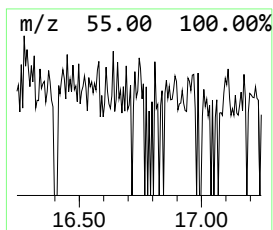
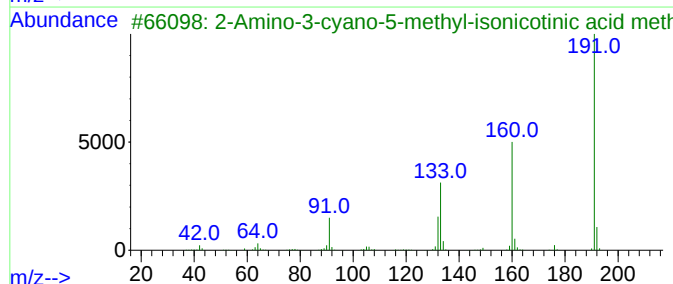
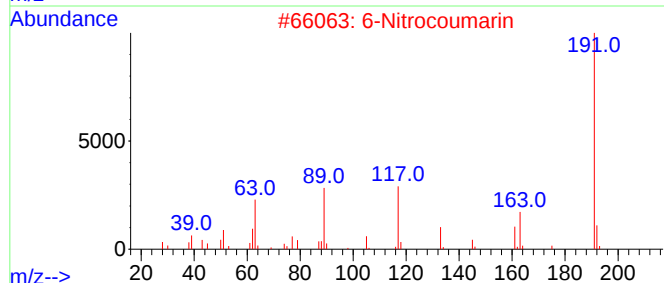
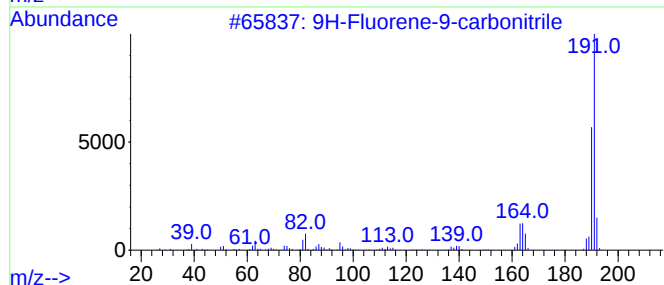
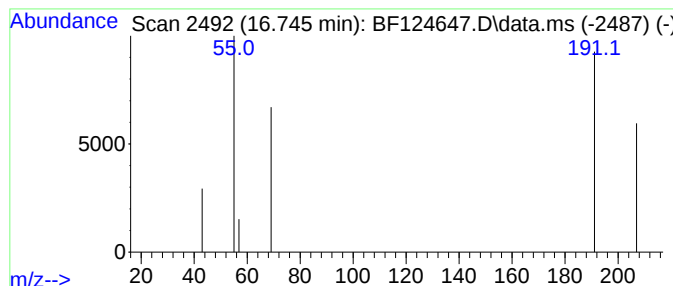
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.745 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.745	3.32 ng	3774	Perylene-d12	15.557

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9H-Fluorene-9-carbonitrile	191	C14H9N	001529-40-4	2
2		6-Nitrocoumarin	191	C9H5NO4	002725-81-7	2
3		2-Amino-3-cyano-5-methyl-isonico...	191	C9H9N3O2	1000296-52-1	2
4		Pyrido[3,4-d]pyrimidine-2,4(1H,3...	191	C9H9N3O2	022389-87-3	2
5		2,4,7-Pteridinetriamine, 6-methyl-	191	C7H9N7	017539-50-3	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FK-EF-01-019-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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unknown8.081	8.081	4.3	ng	10015	2	8.186	47000	20.0
unknown11.945	11.945	2.9	ng	5049	4	11.428	35285	20.0
unknown13.904	13.904	3.7	ng	5849	5	14.069	31419	20.0
unknown14.545	14.545	2.2	ng	3446	5	14.069	31419	20.0
unknown15.198	15.198	3.2	ng	3665	6	15.557	22736	20.0
unknown15.427	15.427	2.0	ng	2314	6	15.557	22736	20.0
unknown15.668	15.668	2.1	ng	2440	6	15.557	22736	20.0
unknown15.715	15.715	2.7	ng	3022	6	15.557	22736	20.0
unknown16.292	16.292	4.8	ng	5453	6	15.557	22736	20.0
unknown16.745	16.745	3.3	ng	3774	6	15.557	22736	20.0