

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061421\
 Data File : BF124310.D
 Acq On : 14 Jun 2021 17:13
 Operator : JU/CG
 Sample : M2687-09
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DUP-02

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-BF060321.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124310.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	9	17	25	rVB2	61815	93743	12.90%	1.620%
2	2.681	96	101	107	rBB3	9936	16060	2.21%	0.278%
3	3.193	184	188	194	rBV2	14905	24296	3.34%	0.420%
4	3.287	199	204	211	rBB2	4686	9534	1.31%	0.165%
5	3.869	298	303	307	rBB	8706	9532	1.31%	0.165%
6	4.616	427	430	434	rBB	8188	9742	1.34%	0.168%
7	5.034	498	501	511	rBB	57596	66838	9.20%	1.155%
8	5.410	562	565	567	rBV	28450	26609	3.66%	0.460%
9	5.457	570	573	584	rVB	843419	726411	100.00%	12.555%
10	5.669	606	609	613	rBB	12464	11117	1.53%	0.192%
11	5.839	636	638	641	rBV	9378	8584	1.18%	0.148%
12	6.469	742	745	756	rBV	755091	720252	99.15%	12.448%
13	6.828	803	806	809	rBV	235437	174930	24.08%	3.023%
14	7.392	898	902	905	rBV	565152	452270	62.26%	7.817%
15	8.016	1006	1008	1017	rBV3	28090	40899	5.63%	0.707%
16	8.110	1021	1024	1028	rBV	260373	224877	30.96%	3.887%
17	9.186	1204	1207	1210	rBV	821818	656109	90.32%	11.340%
18	9.869	1319	1323	1327	rBV	352926	275711	37.96%	4.765%
19	10.604	1445	1448	1451	rBB	42034	34527	4.75%	0.597%
20	10.663	1454	1458	1461	rBV	710894	590139	81.24%	10.200%
21	11.221	1548	1553	1556	rBV	7115	8193	1.13%	0.142%
22	11.357	1573	1576	1580	rBV	326900	287450	39.57%	4.968%
23	11.427	1585	1588	1593	rVB	41392	35193	4.84%	0.608%
24	11.733	1638	1640	1646	rBV3	23486	21477	2.96%	0.371%
25	11.886	1662	1666	1669	rBV2	31207	30639	4.22%	0.530%
26	12.445	1758	1761	1766	rBV4	10399	13530	1.86%	0.234%
27	12.668	1796	1799	1801	rBV3	8922	8827	1.22%	0.153%
28	12.768	1810	1816	1818	rBV4	9511	13440	1.85%	0.232%
29	12.821	1823	1825	1827	rVB2	13481	10548	1.45%	0.182%
30	12.945	1842	1846	1850	rBV	707784	566982	78.05%	9.799%
31	13.427	1924	1928	1934	rBV8	10001	12389	1.71%	0.214%
32	13.486	1934	1938	1940	rBV3	17157	18123	2.49%	0.313%
33	13.880	2001	2005	2006	rBV3	9517	12866	1.77%	0.222%
34	13.980	2020	2022	2024	rBV	27761	23791	3.28%	0.411%
35	14.010	2024	2027	2030	rVB	246722	229402	31.58%	3.965%
36	14.380	2086	2090	2093	rBV6	4772	8289	1.14%	0.143%

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37	14.633	2130	2133	2136	rBV4	23767	23410	3.22%	0.405%
38	14.851	2168	2170	2175	rBV5	19656	23273	3.20%	0.402%
39	14.892	2175	2177	2181	rVB5	7175	8620	1.19%	0.149%
40	15.292	2240	2245	2246	rBV5	14950	19444	2.68%	0.336%
41	15.309	2246	2248	2253	rVB6	18836	30257	4.17%	0.523%
42	15.486	2274	2278	2284	rVB2	159396	198879	27.38%	3.437%
43	16.439	2437	2440	2442	rBV4	7728	8737	1.20%	0.151%

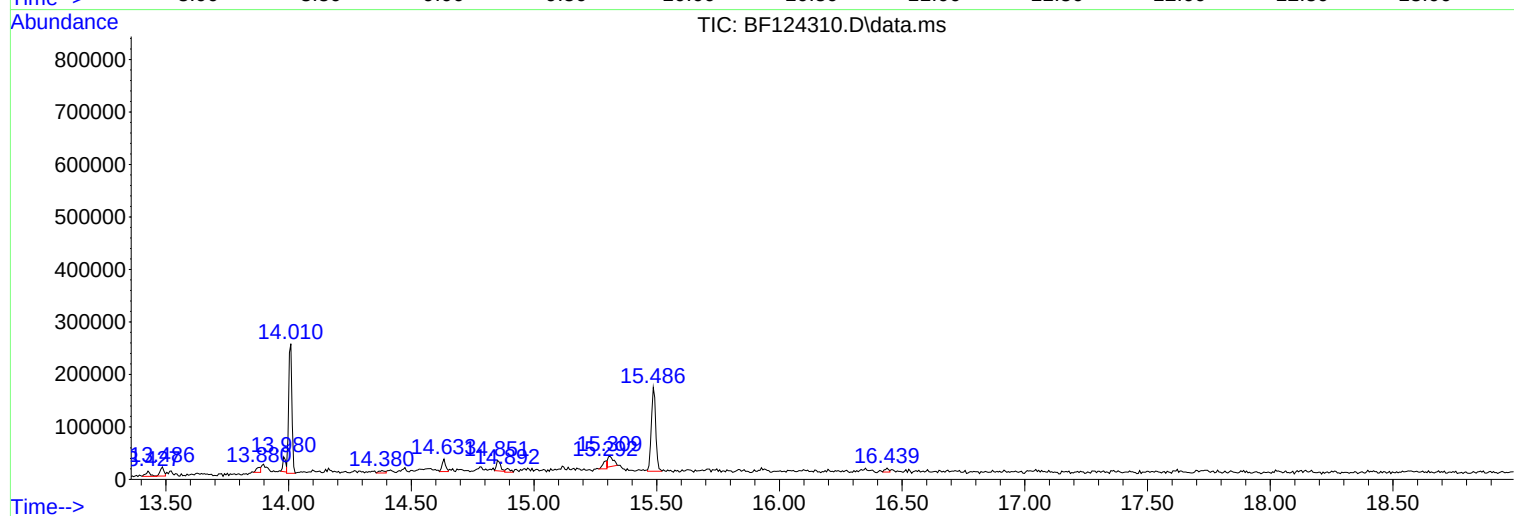
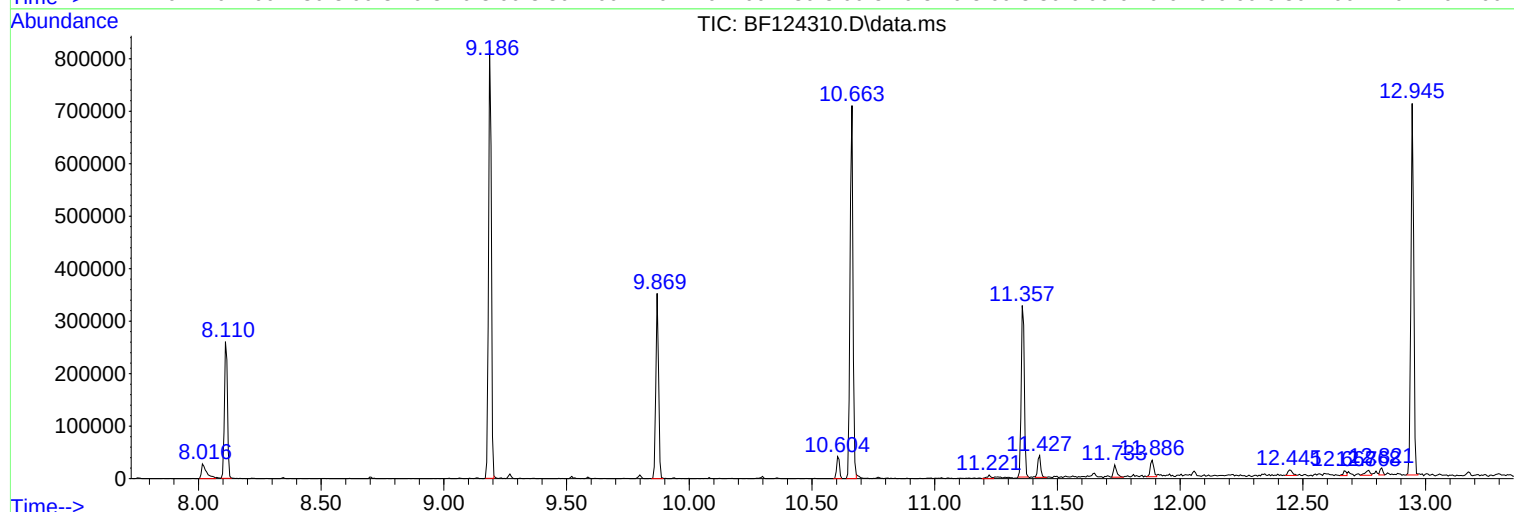
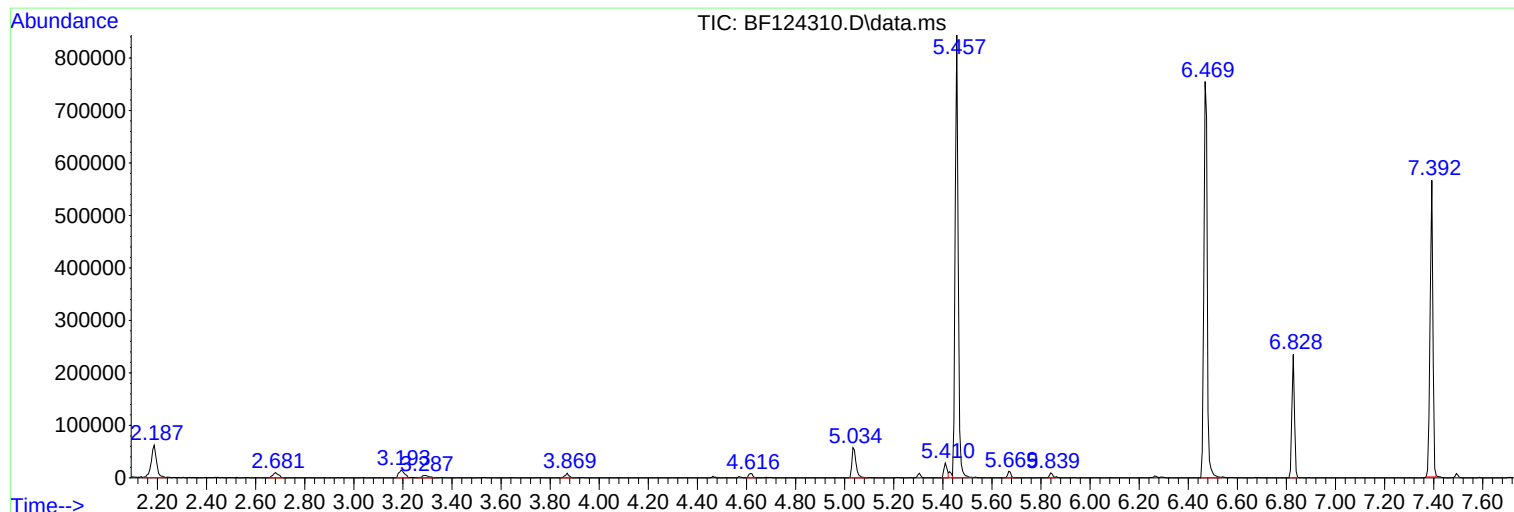
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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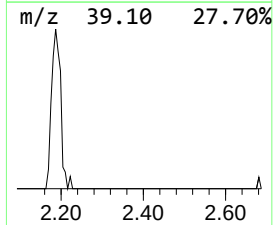
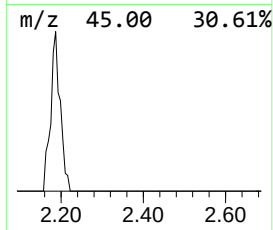
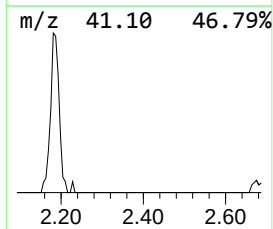
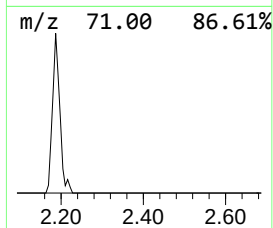
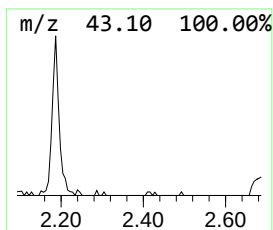
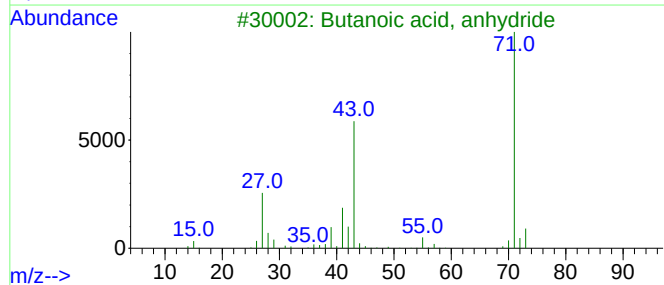
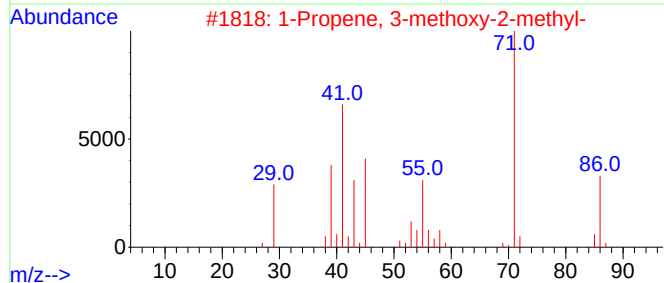
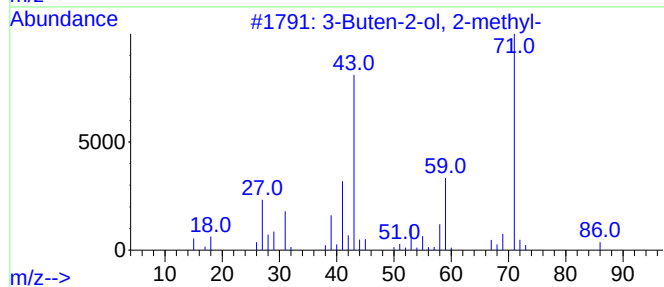
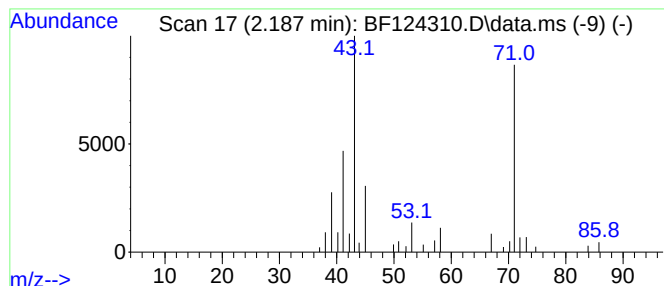
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Buten-2-ol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	10.72 ng	93743	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	72
2			1-Propene, 3-methoxy-2-methyl-	86	C5H10O	022418-49-1	59
3			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	50
4			3-Penten-2-ol	86	C5H10O	001569-50-2	50
5			trans-3-Penten-2-ol	86	C5H10O	003899-34-1	42



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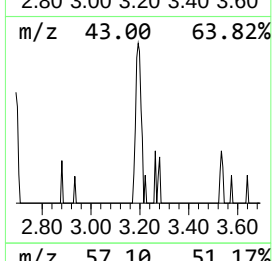
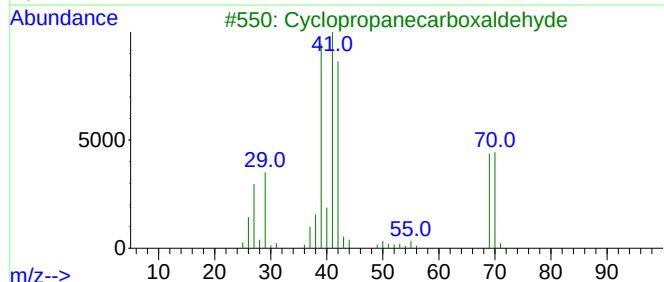
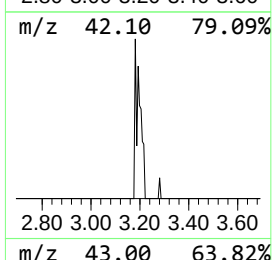
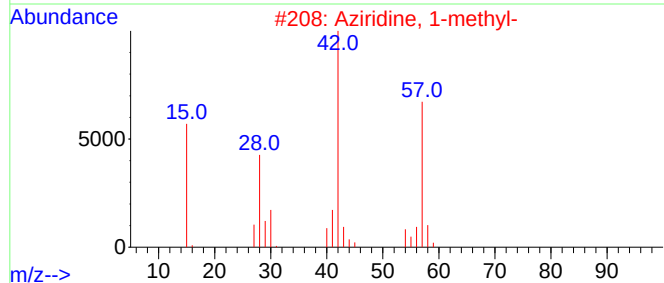
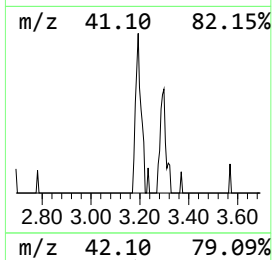
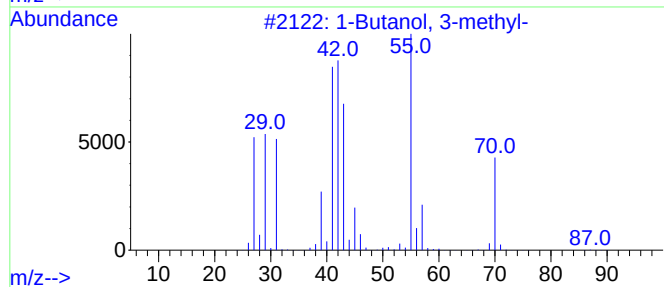
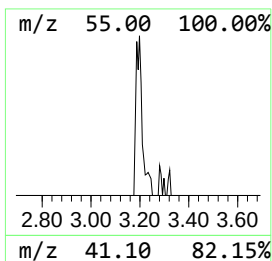
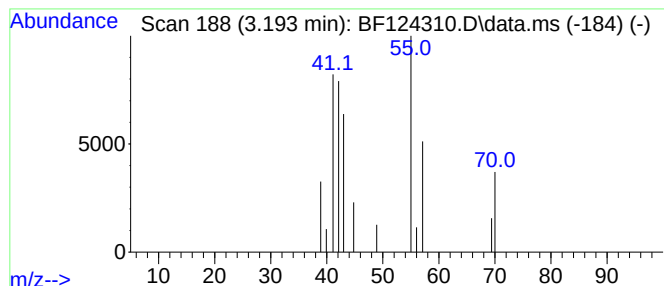
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Butanol, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.193	2.78 ng	24296	1,4-Dichlorobenzene-d4	6.828

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	56
2		Aziridine, 1-methyl-	57	C3H7N	001072-44-2	9
3		Cyclopropanecarboxaldehyde	70	C4H6O	001489-69-6	9
4		Butane, 1-chloro-3-methyl-	106	C5H11Cl	000107-84-6	9
5		Methyl vinyl ketone	70	C4H6O	000078-94-4	7



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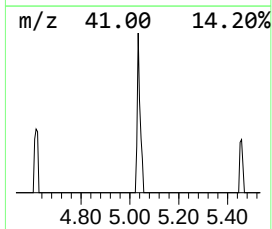
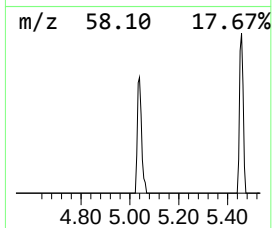
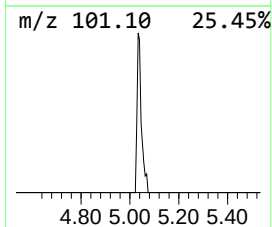
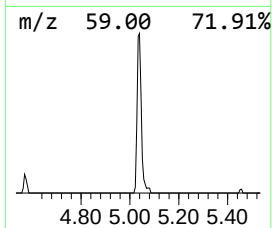
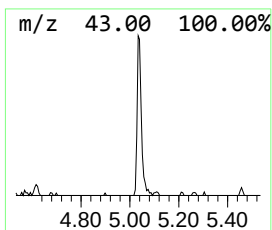
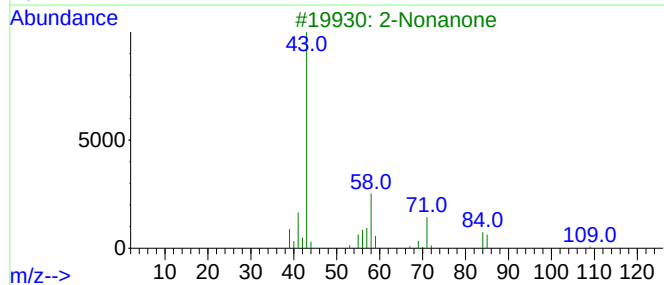
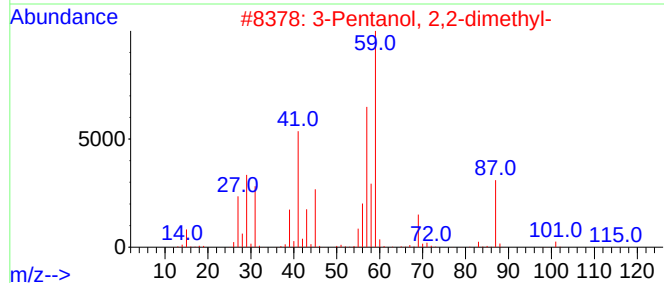
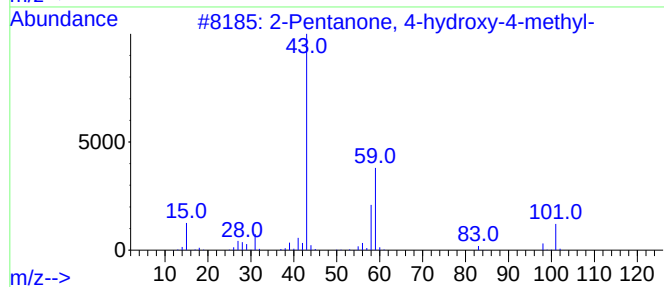
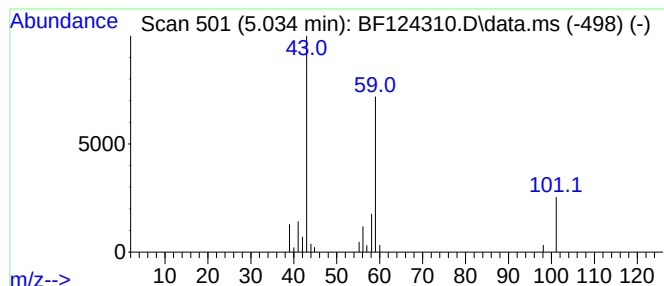
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	7.64 ng	66838	1,4-Dichlorobenzene-d4	6.828

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	36	
2	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	28	
3	2-Nonanone	142	C9H18O	000821-55-6	23	
4	3-Pentanol	88	C5H12O	000584-02-1	17	
5	Guanidine	59	CH5N3	000113-00-8	9	



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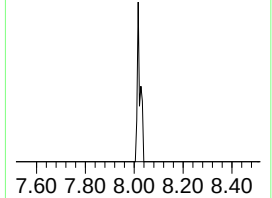
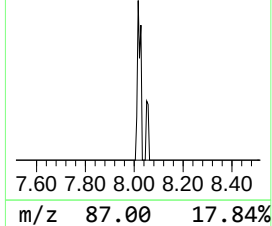
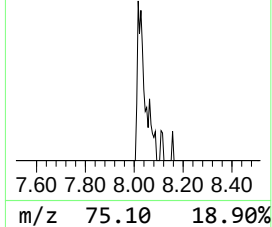
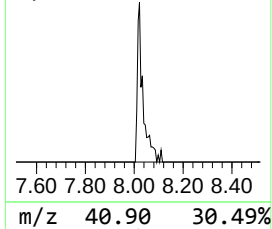
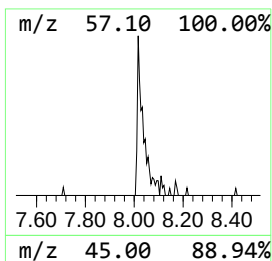
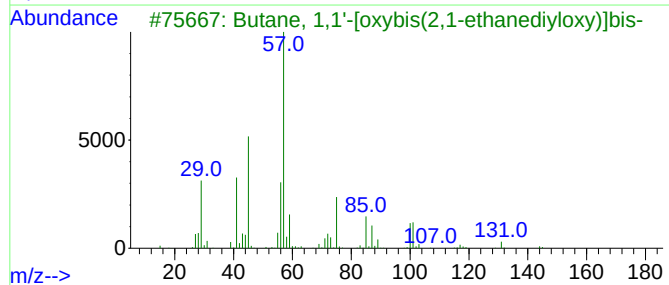
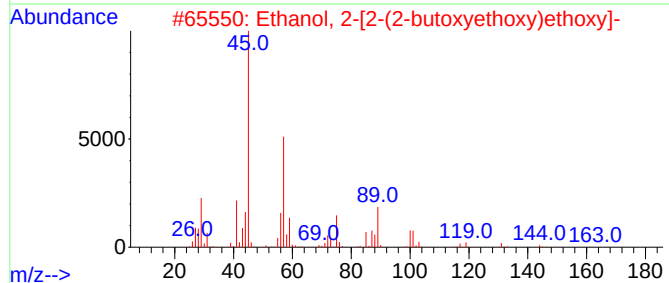
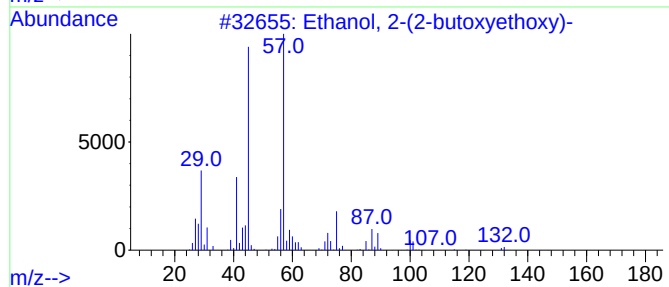
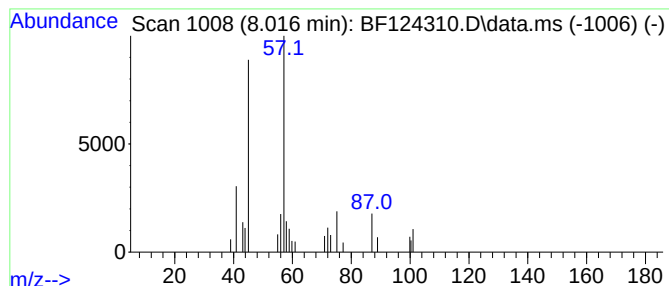
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.016	3.64 ng	40899	Naphthalene-d8	8.110

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-butoxyethoxy)et...	206	C10H22O4	000143-22-6	42
3			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	40
4			Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	39
5			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	38



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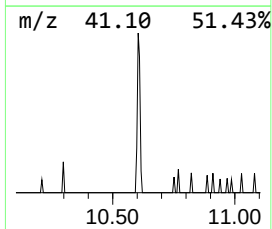
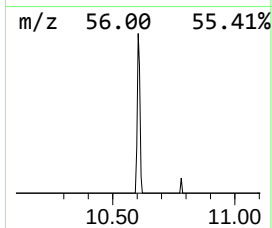
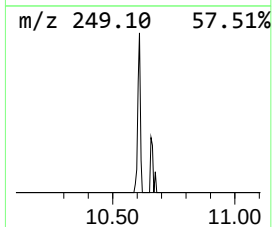
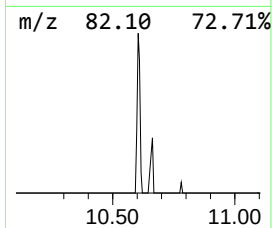
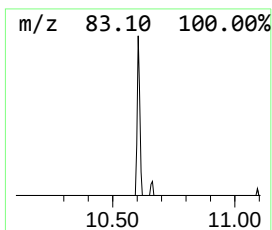
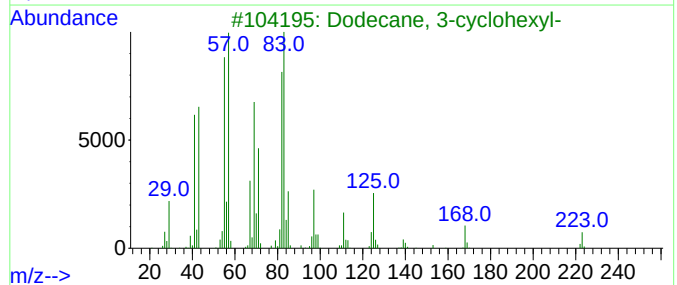
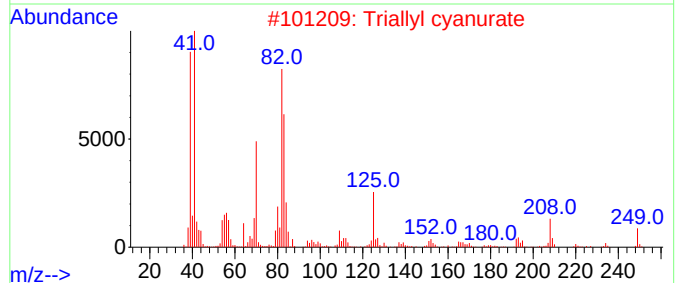
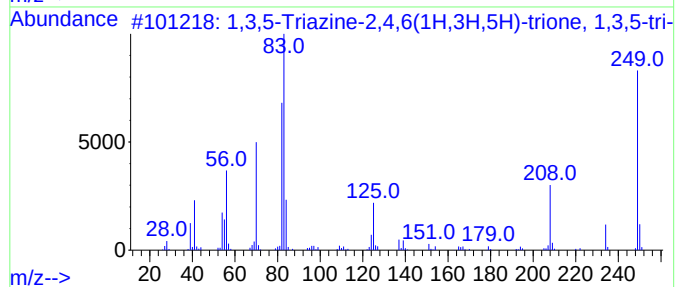
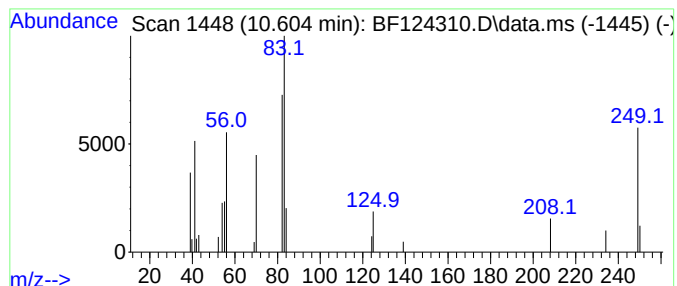
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.604	2.50 ng	34527	Acenaphthene-d10	9.869	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	249	C12H15N3O3	001025-15-6	93
2	Triallyl cyanurate	249	C12H15N3O3	000101-37-1	25
3	Dodecane, 3-cyclohexyl-	252	C18H36	013151-83-2	23
4	Tridecane, 3-cyclohexyl-	266	C19H38	013151-88-7	23
5	Glycine, N-(3-methyl-1-oxo-2-but...	171	C8H13NO3	056009-34-8	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061421\
Data File : BF124310.D
Acq On : 14 Jun 2021 17:13
Operator : JU/CG
Sample : M2687-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
DUP-02

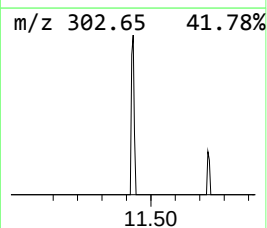
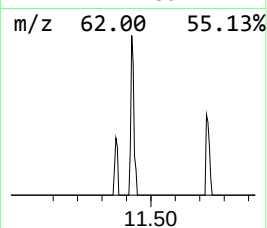
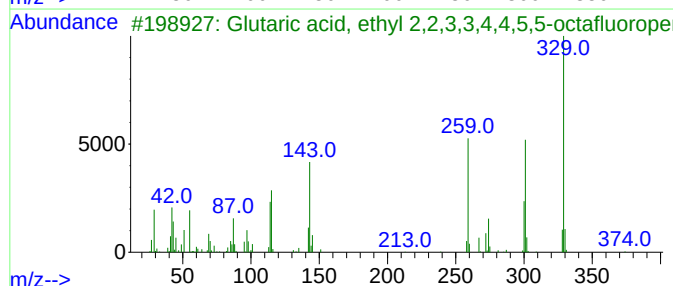
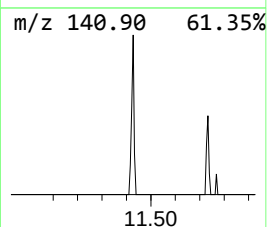
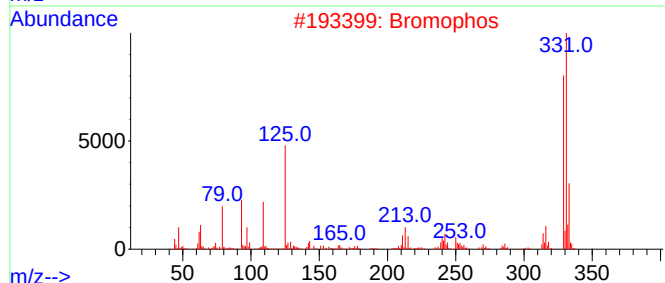
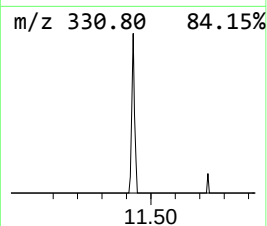
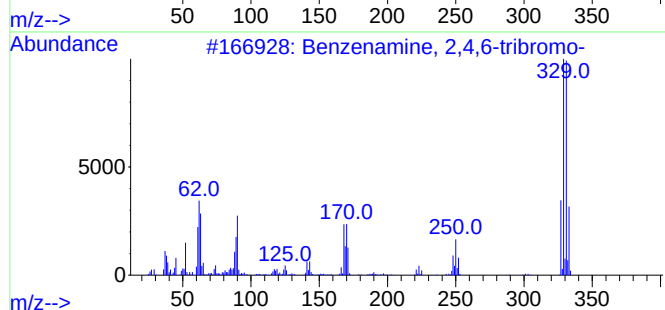
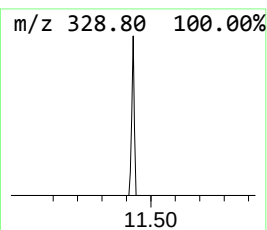
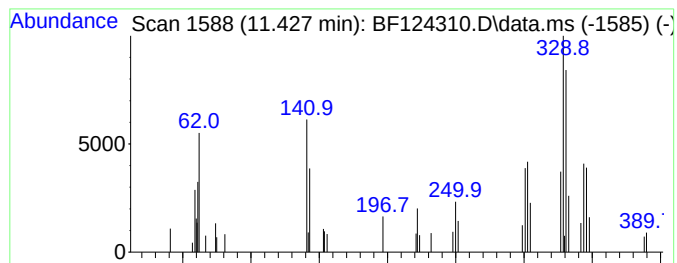
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzenamine, 2,4,6-tribromo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.427	2.45 ng	35193	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	50
2			Bromophos	364	C8H8BrCl2O3PS	002104-96-3	10
3			Glutaric acid, ethyl 2,2,3,3,4,4...	374	C12H14F8O4	1000359-67-5	10
4			2,5-Di(trifluoroacetyloxy)acetop...	344	C12H6F6O5	1000365-30-5	9
5			Glutaric acid, hexyl 2,2,3,3,4,4...	430	C16H22F8O4	1000359-68-1	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061421\
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Acq On : 14 Jun 2021 17:13
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Sample : M2687-09
Misc :
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Instrument :
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ClientSampleId :
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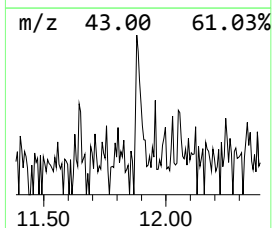
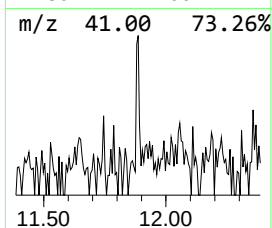
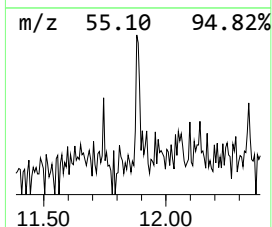
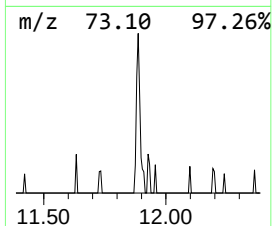
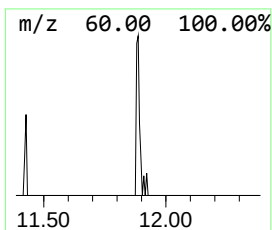
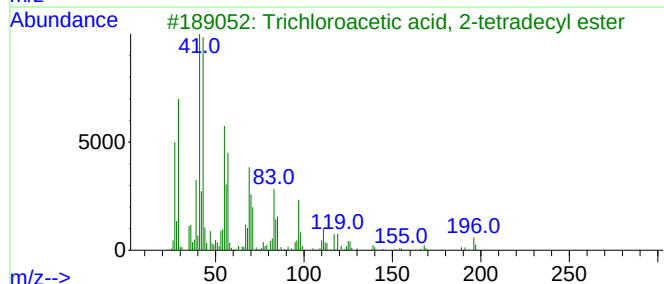
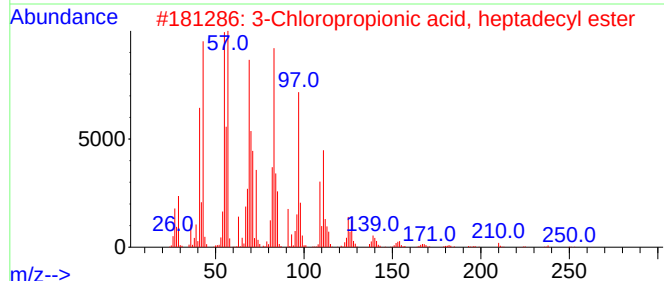
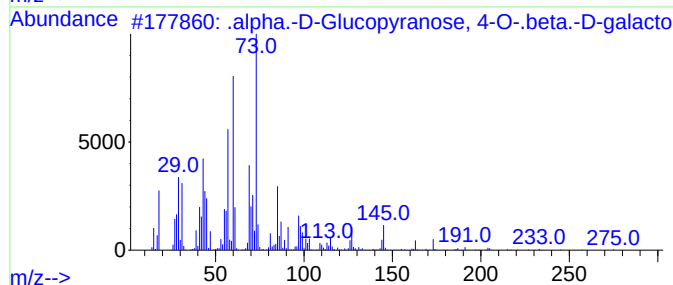
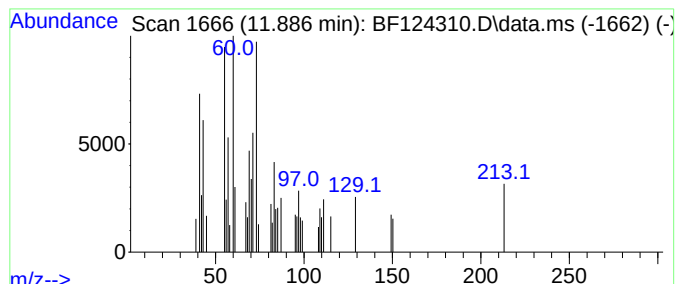
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown11.886 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	2.13 ng	30639	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.		.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	27
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	27		
3	Trichloroacetic acid, 2-tetradec...	358	C16H29Cl3O2	1000282-06-6	25		
4	Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	25		
5	Butyraldehyde, semicarbazone	129	C5H11N3O	013183-21-6	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061421\
Data File : BF124310.D
Acq On : 14 Jun 2021 17:13
Operator : JU/CG
Sample : M2687-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

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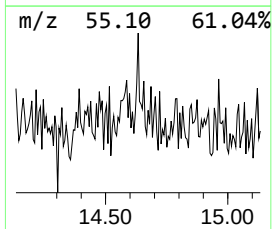
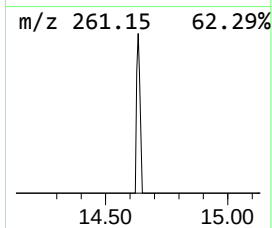
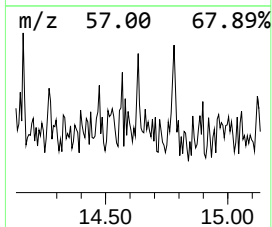
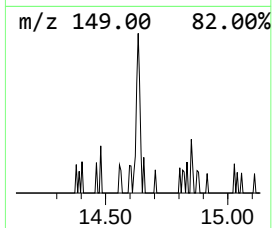
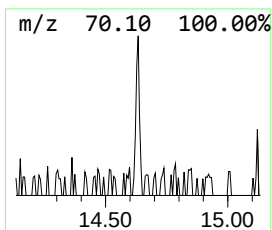
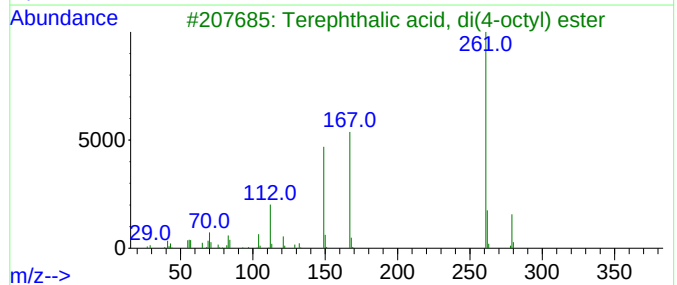
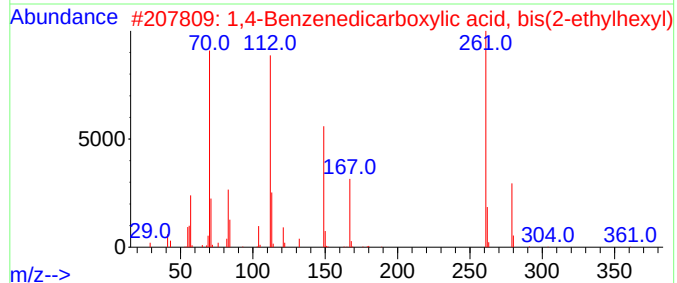
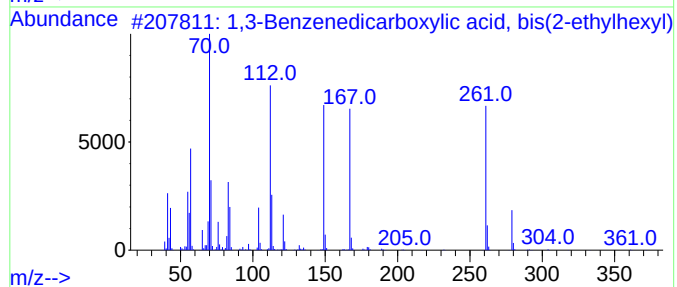
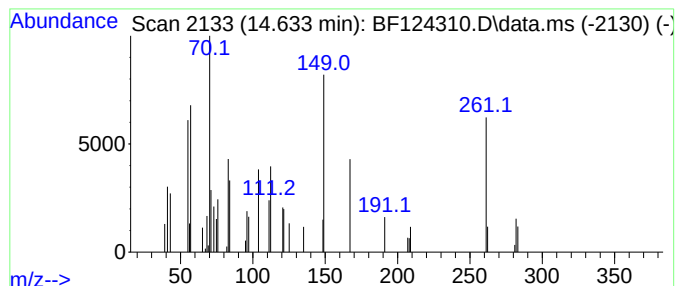
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown14.633 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.633	2.04 ng	23410	Chrysene-d12	14.009

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	38
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	37
3			Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	36
4			Phthalic acid, 2-ethylhexyl hexy...	362	C22H34O4	1000309-02-5	12
5			Terephthalic acid, 3-hexyl octyl...	362	C22H34O4	1000356-23-1	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061421\
Data File : BF124310.D
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Operator : JU/CG
Sample : M2687-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-02

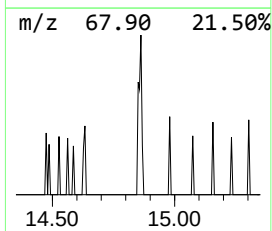
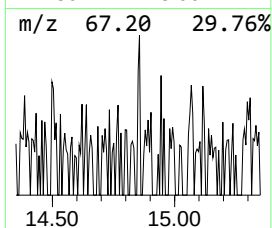
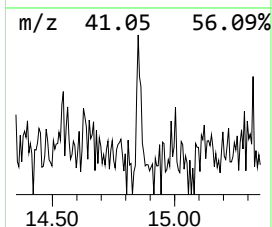
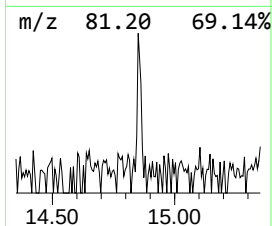
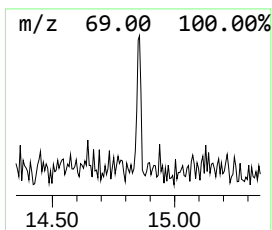
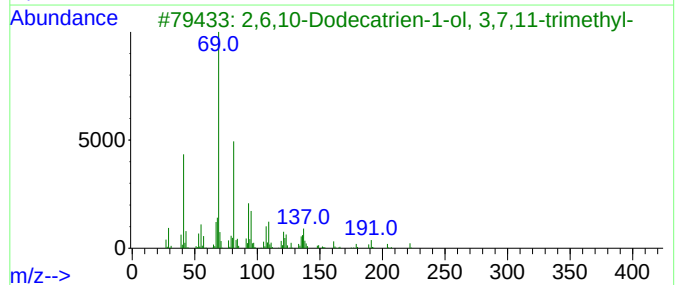
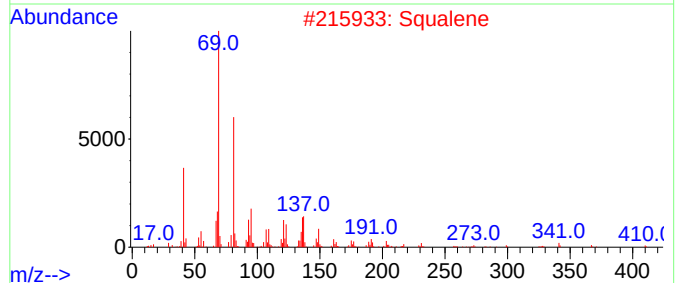
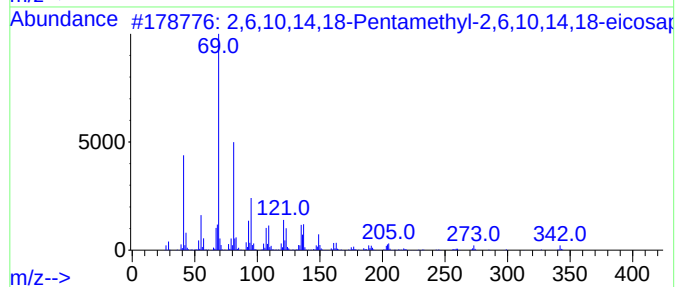
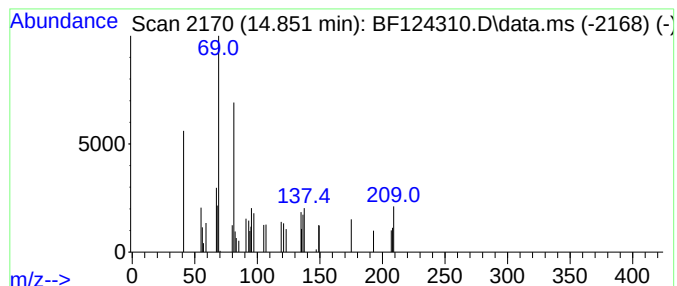
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown14.851 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.851	2.34 ng	23273	Perylene-d12	15.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	43		
2	Squalene	410	C30H50	000111-02-4	43		
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	37		
4	Geranyl phenylacetate	272	C18H24O2	000102-22-7	27		
5	Nerolidol 2	222	C15H26O	1000285-43-6	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061421\
Data File : BF124310.D
Acq On : 14 Jun 2021 17:13
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Sample : M2687-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

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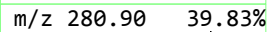
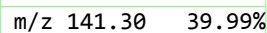
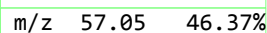
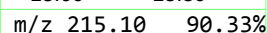
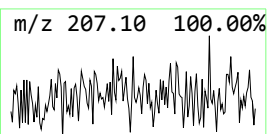
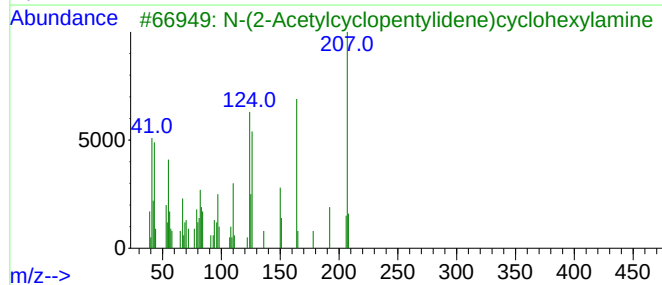
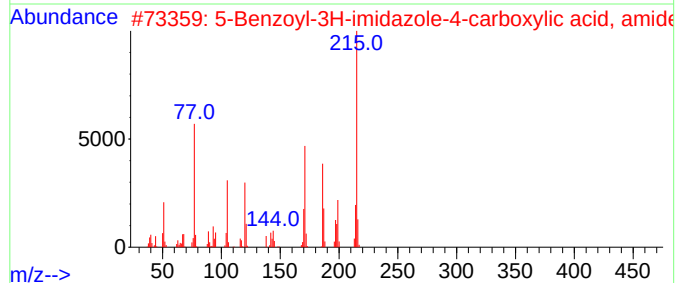
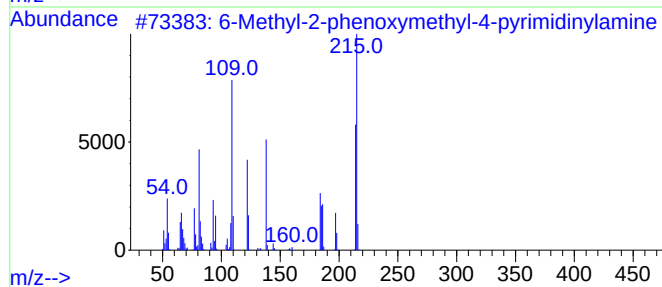
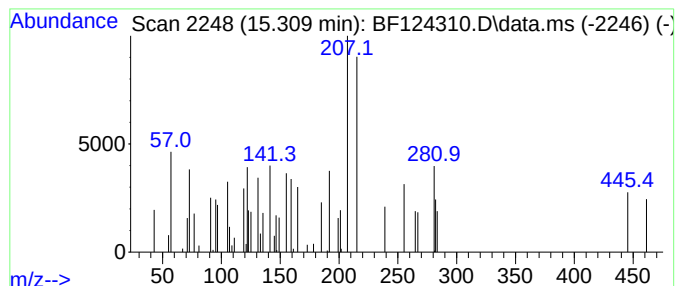
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown15.309 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.309	3.04 ng	30257	Perylene-d12	15.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Methyl-2-phenoxyethyl-4-pyrim...	215	C12H13N3O	067386-50-9	18
2			5-Benzoyl-3H-imidazole-4-carboxy...	215	C11H9N3O2	1000317-72-1	9
3			N-(2-Acetylcyclopentylidene)cycl...	207	C13H21NO	1000100-48-5	9
4			N-Methyl-1-adamantaneacetamide	207	C13H21NO	031897-93-5	9
5			Carbonic acid, monoamide, N-(2-e...	207	C12H17NO2	1000340-19-1	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061421\
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Buten-2-ol, 2...	2.187	10.7	ng	93743	1	6.828	174930	20.0
1-Butanol, 3-me...	3.193	2.8	ng	24296	1	6.828	174930	20.0
2-Pentanone, 4-...	5.034	7.6	ng	66838	1	6.828	174930	20.0
Ethanol, 2-(2-b...	8.016	3.6	ng	40899	2	8.110	224877	20.0
1,3,5-Triazine-...	10.604	2.5	ng	34527	3	9.869	275711	20.0
Benzenamine, 2,...	11.427	2.5	ng	35193	4	11.357	287450	20.0
unknown11.886	11.886	2.1	ng	30639	4	11.357	287450	20.0
unknown14.633	14.633	2.0	ng	23410	5	14.009	229402	20.0
unknown14.851	14.851	2.3	ng	23273	6	15.486	198879	20.0
unknown15.309	15.309	3.0	ng	30257	6	15.486	198879	20.0