

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061121\
 Data File : BF124262.D
 Acq On : 11 Jun 2021 15:50
 Operator : JU/CG
 Sample : M2625-06
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 18-B12(158-162)

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: BF124262.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	13	18	23	rBV2	19661	24173	1.46%	0.247%
2	5.057	501	505	512	rVB	120248	155087	9.37%	1.584%
3	5.475	571	576	579	rBV	1334448	1214249	73.39%	12.405%
4	5.851	637	640	645	rBB	23778	20740	1.25%	0.212%
5	6.487	743	748	751	rBV	1276090	1224644	74.01%	12.511%
6	6.839	805	808	811	rBV	268838	202536	12.24%	2.069%
7	7.404	899	904	907	rBV	913360	843701	50.99%	8.619%
8	8.022	1006	1009	1016	rBV	36327	41663	2.52%	0.426%
9	8.122	1022	1026	1029	rBV	309024	248604	15.03%	2.540%
10	9.204	1205	1210	1212	rBV	1765719	1611691	97.41%	16.465%
11	9.880	1321	1325	1328	rBV	386807	318301	19.24%	3.252%
12	10.674	1455	1460	1463	rBV	1339485	1205877	72.88%	12.319%
13	11.369	1574	1578	1581	rBV	381398	326317	19.72%	3.334%
14	11.892	1664	1667	1673	rBV	70492	60768	3.67%	0.621%
15	12.680	1797	1801	1806	rBV2	24728	26947	1.63%	0.275%
16	12.957	1843	1848	1851	rBV	1853418	1654590	100.00%	16.903%
17	13.868	1996	2003	2014	rBV5	42694	101797	6.15%	1.040%
18	14.010	2023	2027	2031	rBV	252335	224118	13.55%	2.290%
19	14.762	2152	2155	2162	rVB	45833	48971	2.96%	0.500%
20	15.492	2274	2279	2284	rBV	189436	233835	14.13%	2.389%

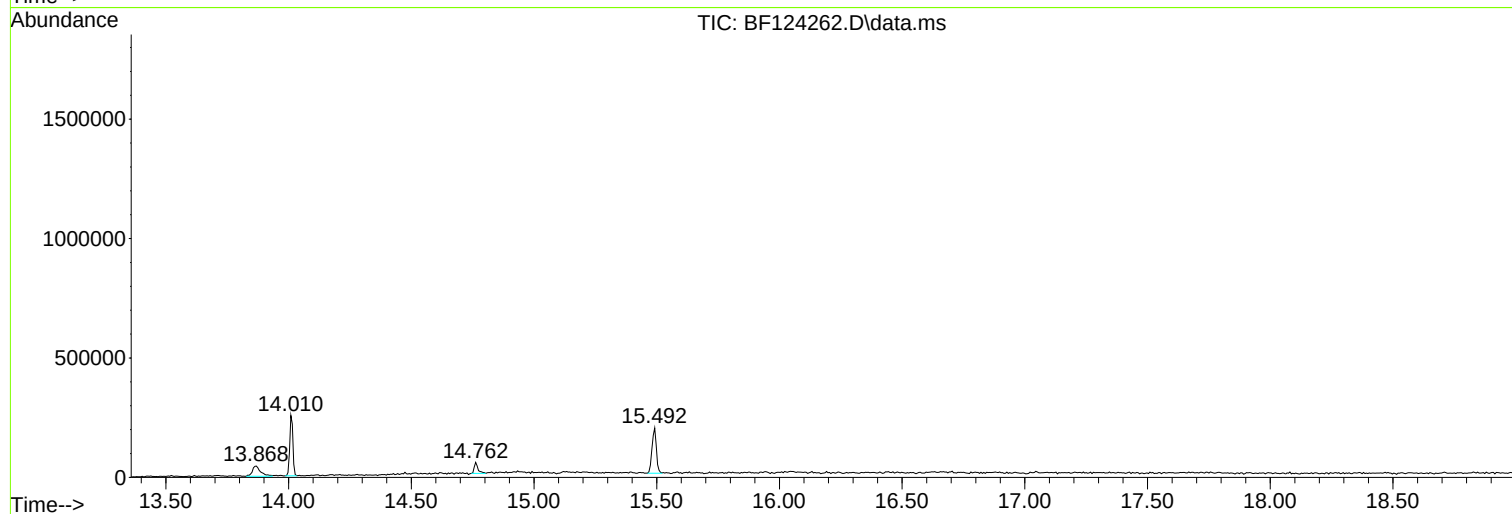
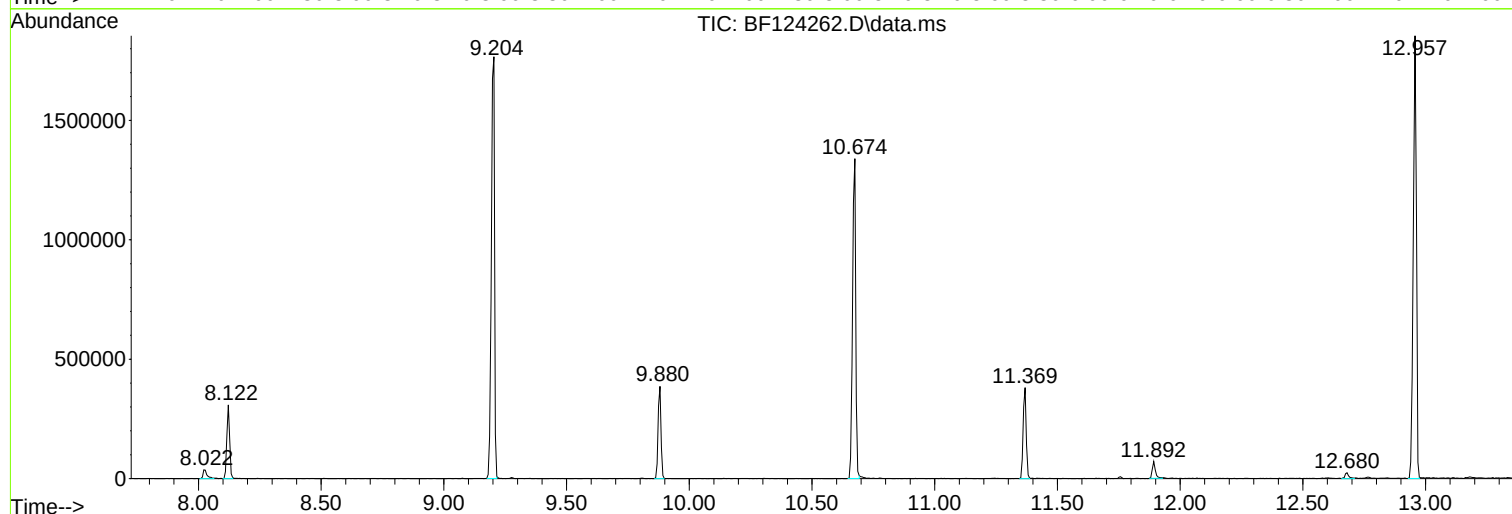
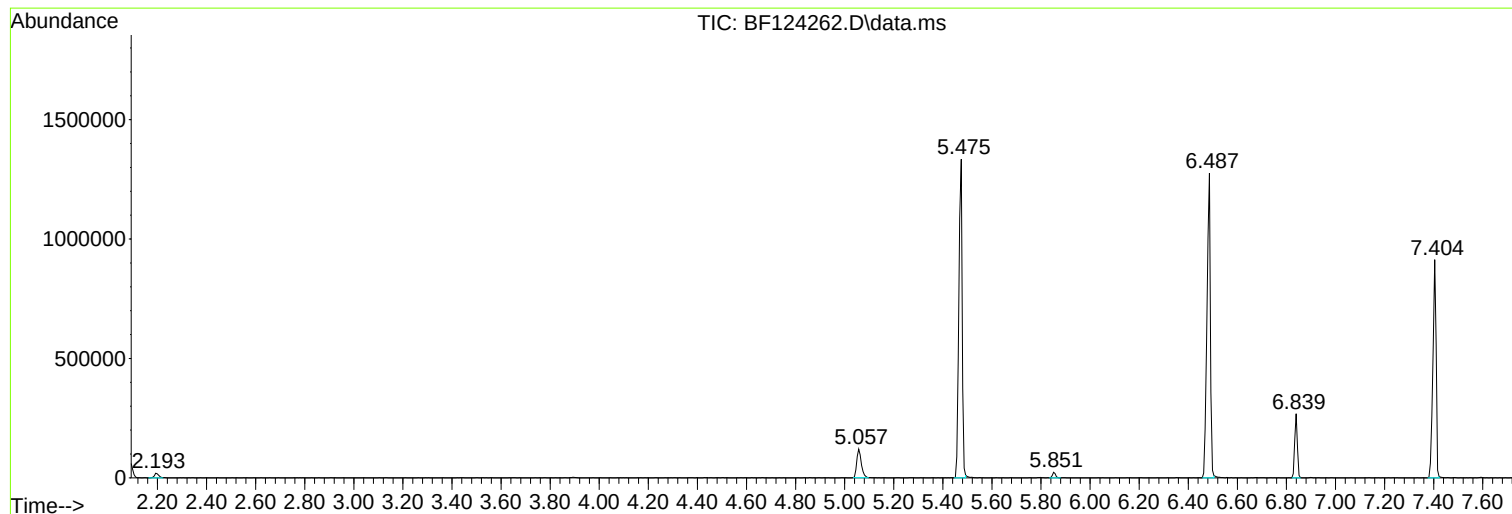
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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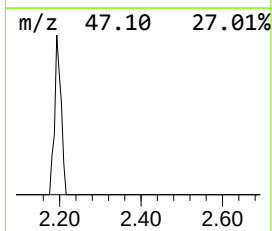
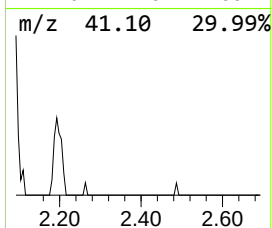
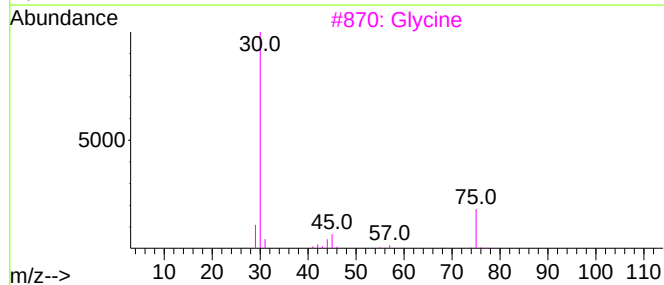
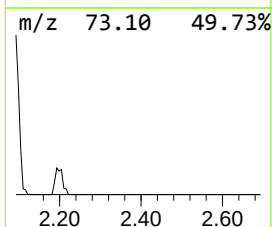
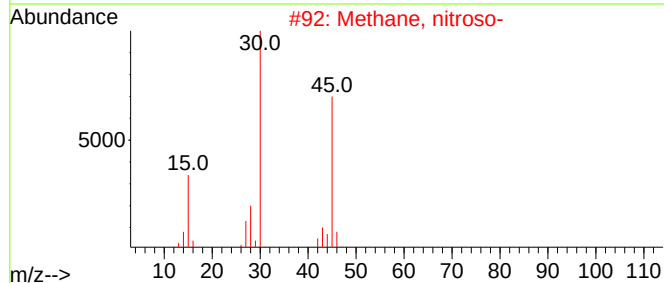
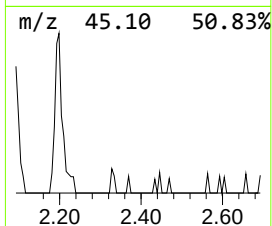
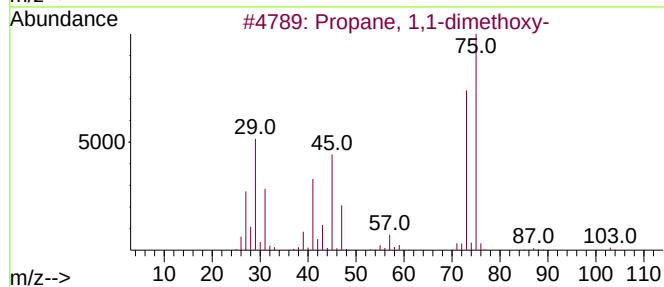
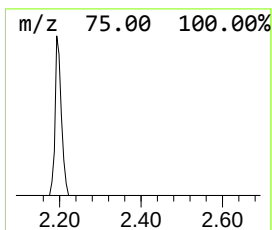
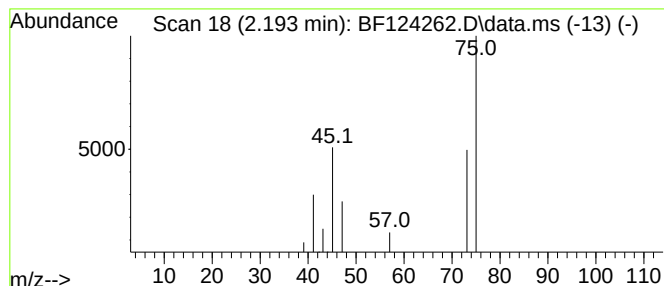
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.193 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	2.39 ng	24173	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	9
2			Methane, nitroso-	45	CH3NO	000865-40-7	4
3			Glycine	75	C2H5NO2	000056-40-6	4
4			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	2
5			Formamide	45	CH3NO	000075-12-7	2



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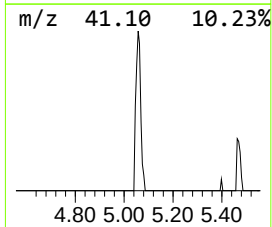
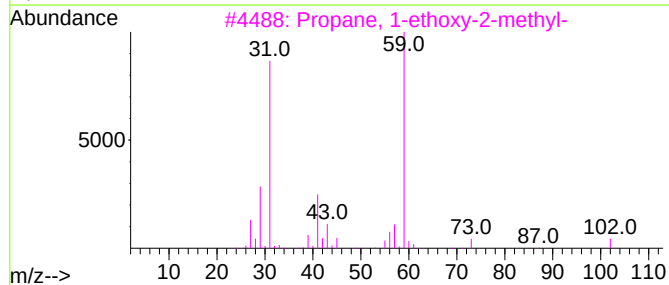
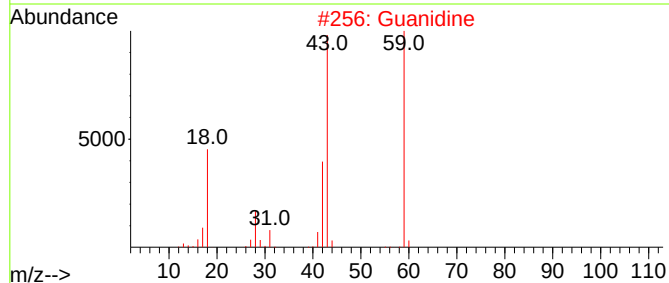
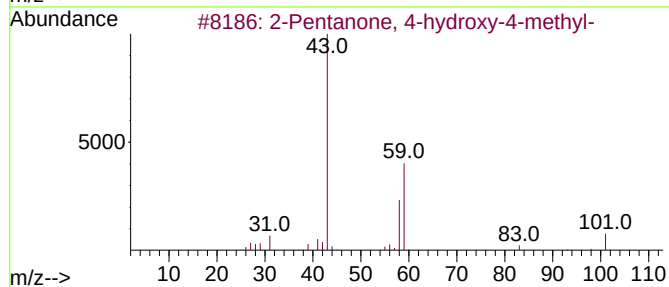
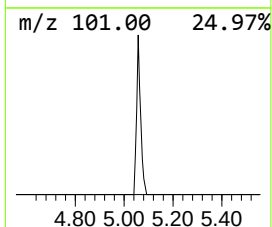
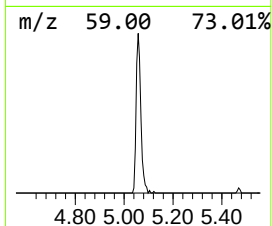
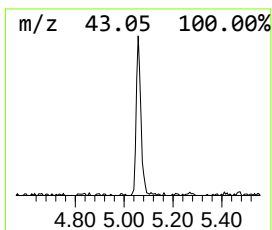
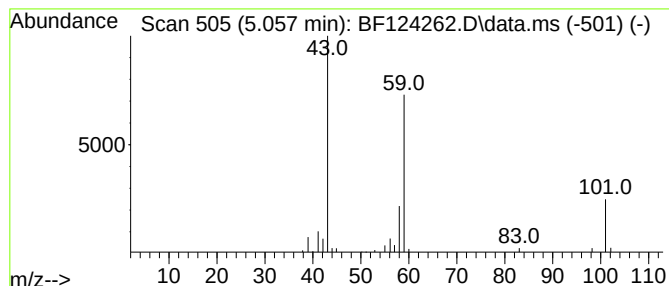
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	15.31 ng	155087	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Guanidine	59	CH5N3	000113-00-8	38		
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25		
4	3-Pentanol	88	C5H12O	000584-02-1	17		
5	2-Nonanone	142	C9H18O	000821-55-6	12		



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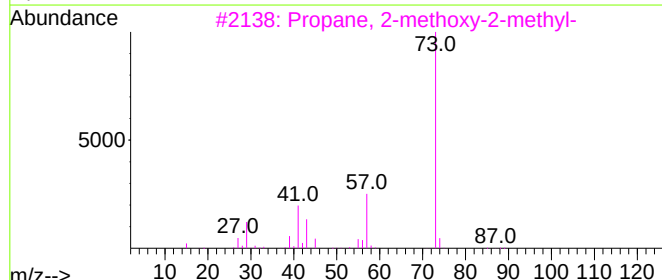
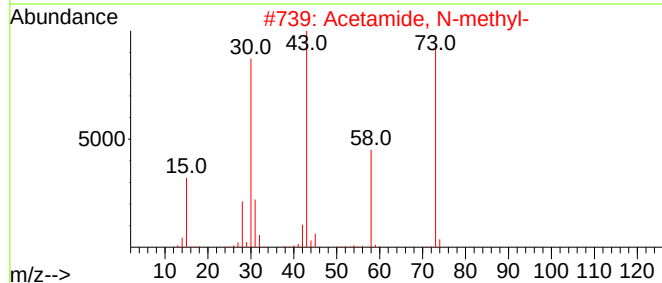
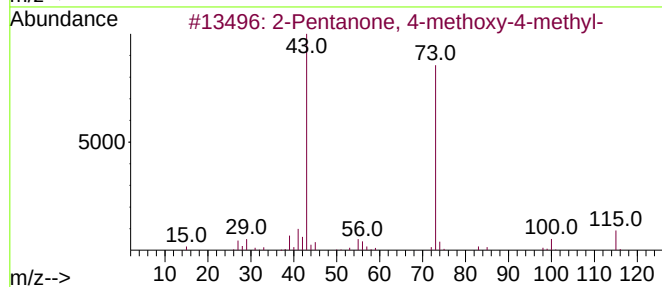
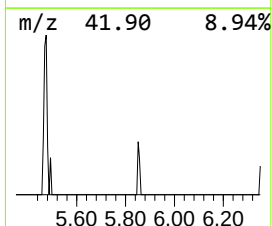
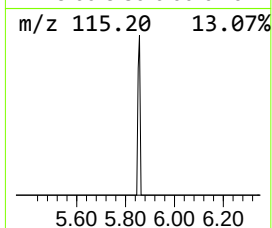
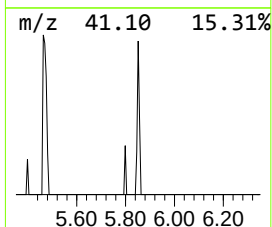
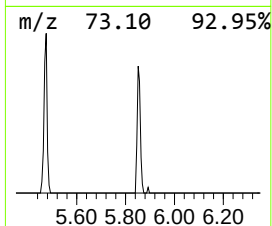
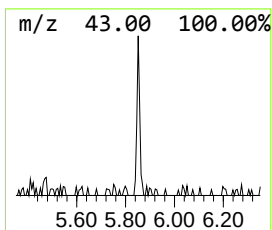
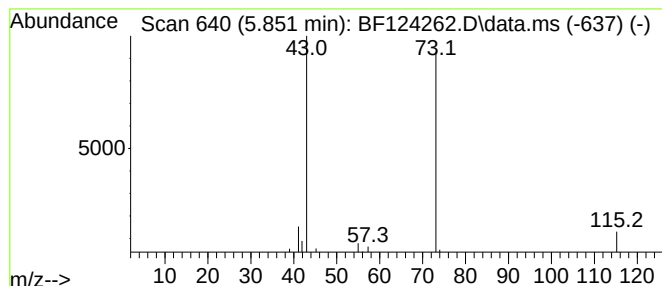
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.851	2.05 ng	20740	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	40
3			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4			Guanidine, methyl-	73	C2H7N3	000471-29-4	7
5			N-Ethylformamide	73	C3H7NO	000627-45-2	7



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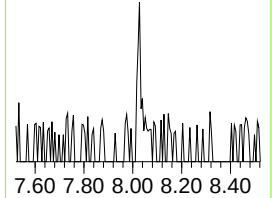
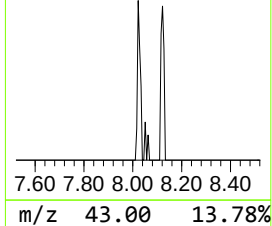
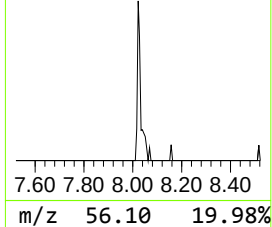
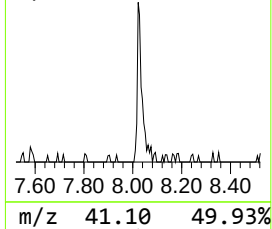
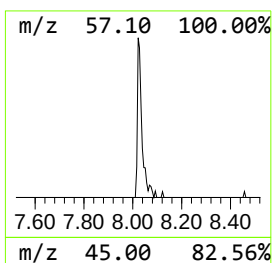
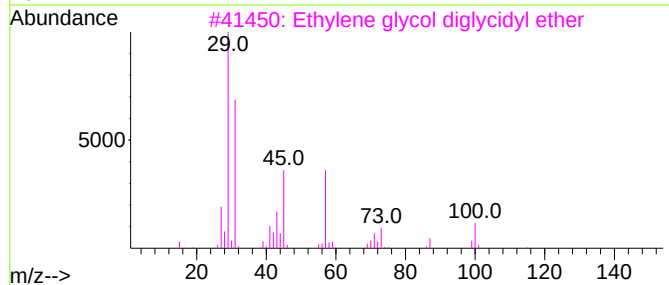
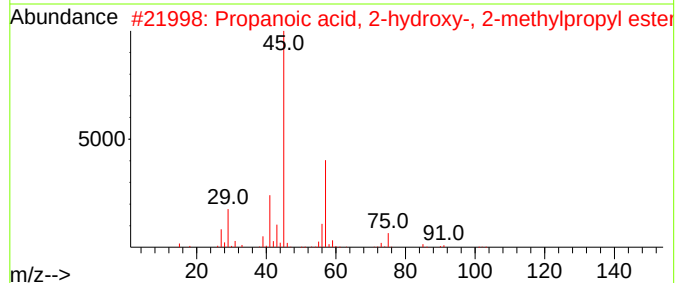
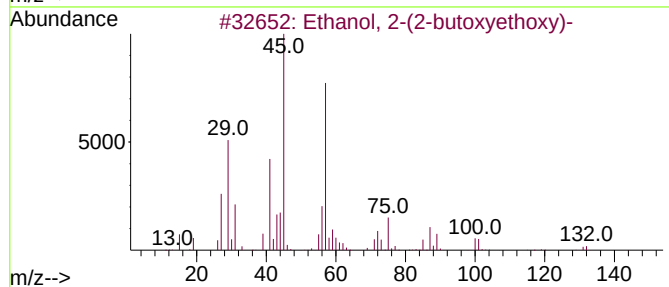
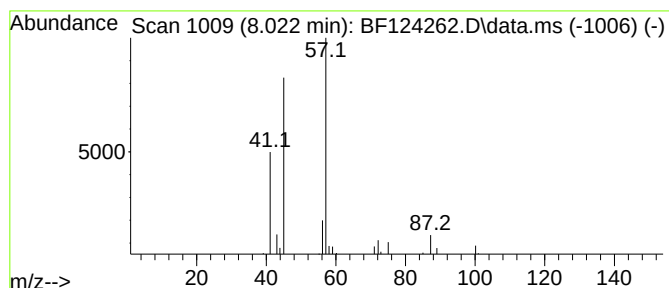
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.022	3.35 ng	41663	Naphthalene-d8	8.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
2			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	53
3			Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	42
4			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	42
5			2-Hexanol	102	C6H14O	000626-93-7	36



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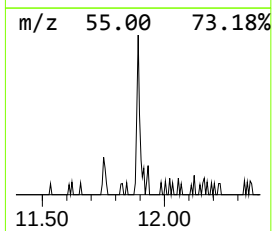
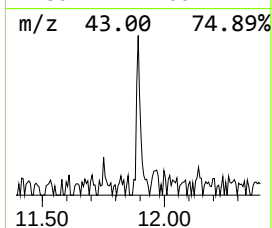
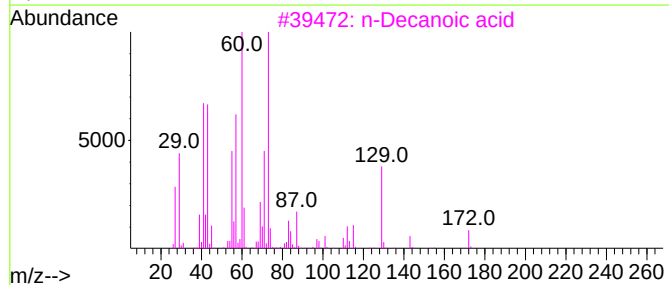
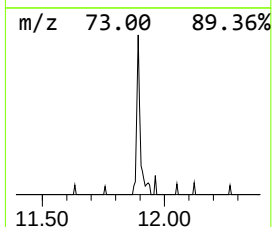
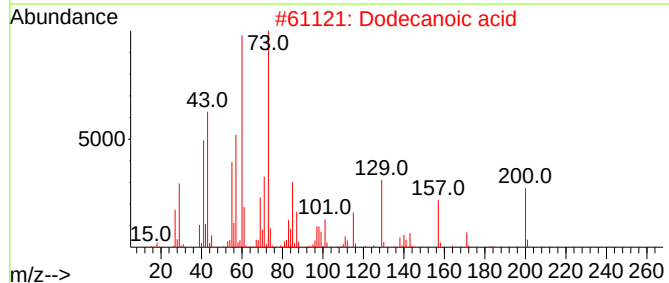
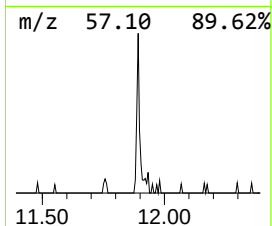
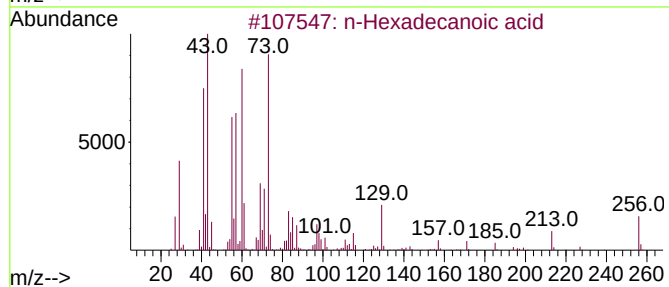
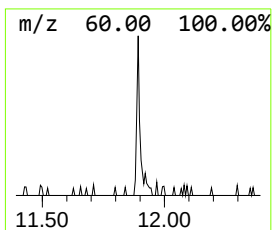
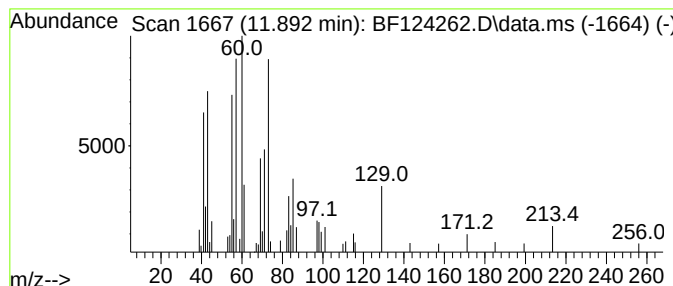
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	3.72 ng	60768	Phenanthrene-d10	11.368

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Dodecanoic acid	200	C12H24O2	000143-07-7	64
3			n-Decanoic acid	172	C10H20O2	000334-48-5	53
4			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	43
5			Undecanoic acid, 10-bromo-	264	C11H21BrO2	018294-93-4	35



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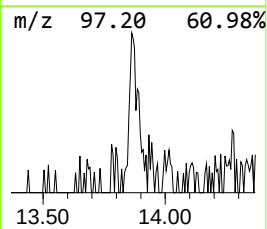
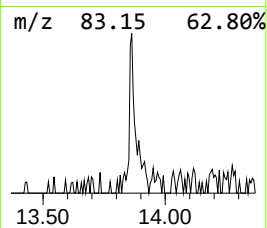
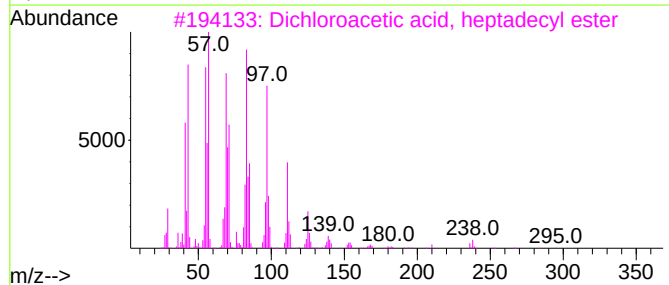
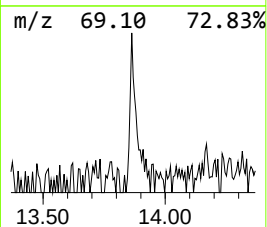
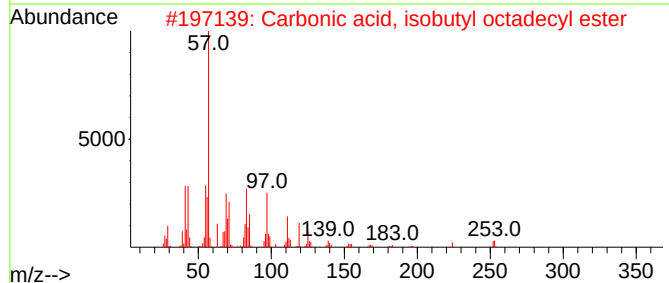
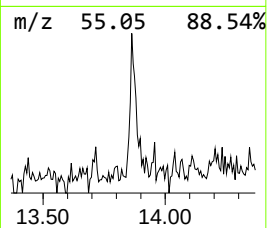
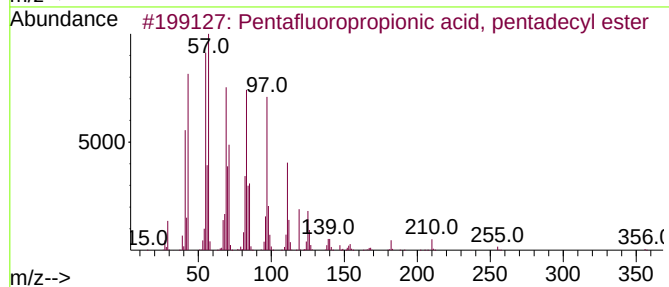
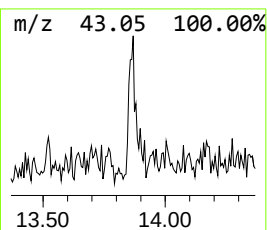
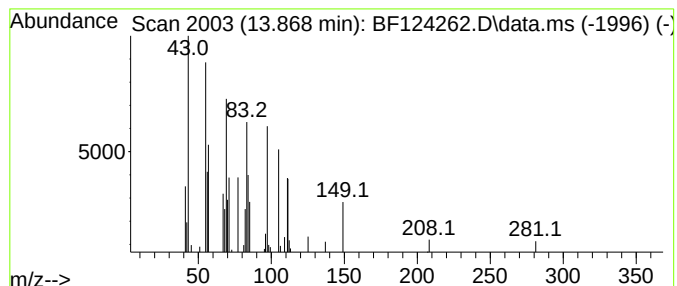
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown13.868 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	9.08 ng	101797	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	43
2			Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	43
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	43
4			1-Dodecanol, 2-octyl-, acetate	340	C22H44O2	074051-84-6	43
5			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061121\
Data File : BF124262.D
Acq On : 11 Jun 2021 15:50
Operator : JU/CG
Sample : M2625-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
18-B12(158-162)

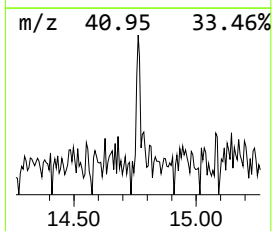
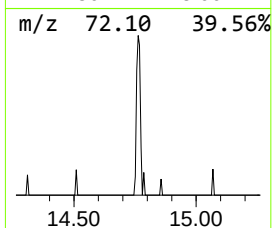
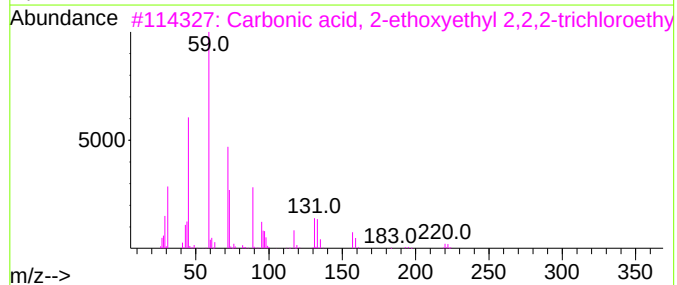
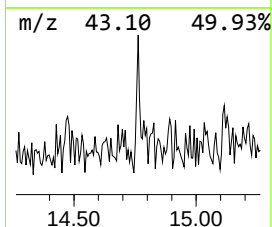
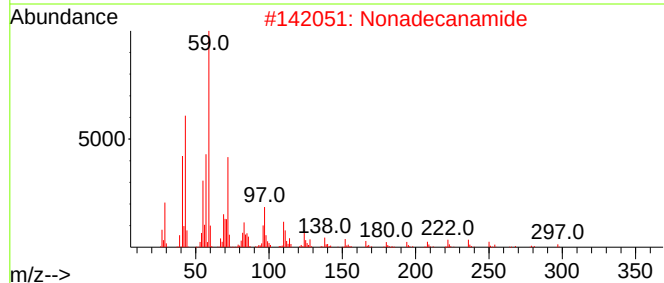
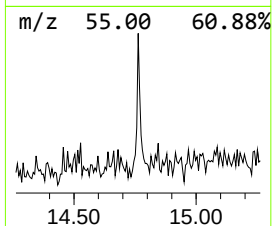
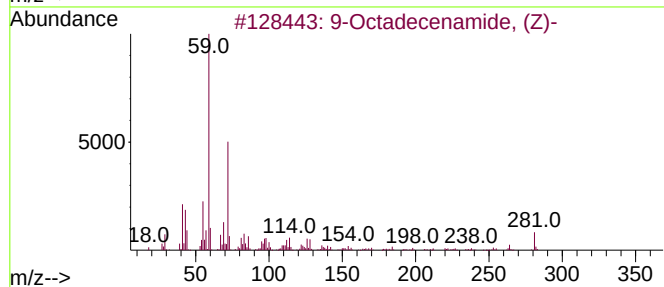
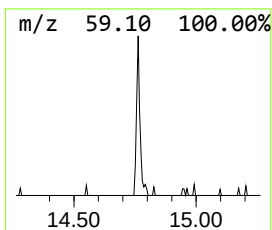
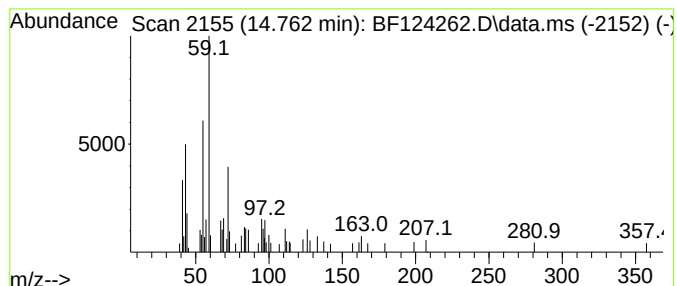
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.762	4.19 ng	48971	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	68
2			Nonadecanamide	297	C19H39NO	058185-32-3	64
3			Carbonic acid, 2-ethoxyethyl 2,2...	264	C7H11Cl3O4	1000331-44-6	53
4			Tetradecanamide	227	C14H29NO	000638-58-4	53
5			Dodecanamide	199	C12H25NO	001120-16-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061121\
Data File : BF124262.D
Acq On : 11 Jun 2021 15:50
Operator : JU/CG
Sample : M2625-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
18-B12(158-162)

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
unknown2.193	2.193	2.4	ng	24173	1	6.839	202536	20.0
2-Pentanone, 4-...	5.057	15.3	ng	155087	1	6.839	202536	20.0
2-Pentanone, 4-...	5.851	2.0	ng	20740	1	6.839	202536	20.0
Ethanol, 2-(2-b...	8.022	3.4	ng	41663	2	8.122	248604	20.0
n-Hexadecanoic ...	11.892	3.7	ng	60768	4	11.368	326317	20.0
unknown13.868	13.868	9.1	ng	101797	5	14.010	224118	20.0
9-Octadecenamid...	14.762	4.2	ng	48971	6	15.492	233835	20.0