

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061821\
 Data File : BF124378.D
 Acq On : 18 Jun 2021 17:25
 Operator : JU/CG
 Sample : M2709-09
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 0248-AMND-COMP-M

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: BF124378.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.340	380	383	392	rVB	71083	89618	3.58%	1.001%
2	5.022	488	499	502	rBV	1226717	2504770	100.00%	27.972%
3	5.416	564	566	579	rBB	82843	92762	3.70%	1.036%
4	6.428	735	738	751	rVB	521918	447625	17.87%	4.999%
5	6.781	795	798	805	rBB	255002	199030	7.95%	2.223%
6	7.351	891	895	898	rBV	824123	716943	28.62%	8.006%
7	7.981	998	1002	1008	rBV	445304	443601	17.71%	4.954%
8	8.069	1013	1017	1020	rVB	308394	251773	10.05%	2.812%
9	9.145	1196	1200	1203	rBV	1742976	1279536	51.08%	14.289%
10	9.822	1312	1315	1319	rVB	385077	303269	12.11%	3.387%
11	10.616	1447	1450	1455	rVB2	39306	35907	1.43%	0.401%
12	11.310	1565	1568	1571	rBV	415507	337895	13.49%	3.773%
13	11.704	1631	1635	1639	rVB	54678	50853	2.03%	0.568%
14	12.410	1751	1755	1758	rVB3	39466	37540	1.50%	0.419%
15	12.527	1772	1775	1778	rVB	35718	32406	1.29%	0.362%
16	12.757	1808	1814	1819	rVB2	32594	43365	1.73%	0.484%
17	12.898	1834	1838	1841	rBV	1551150	1486502	59.35%	16.600%
18	13.957	2012	2018	2021	rBV	364276	321380	12.83%	3.589%
19	15.356	2253	2256	2261	rBV2	20192	26815	1.07%	0.299%
20	15.415	2261	2266	2271	rBV	219905	253057	10.10%	2.826%

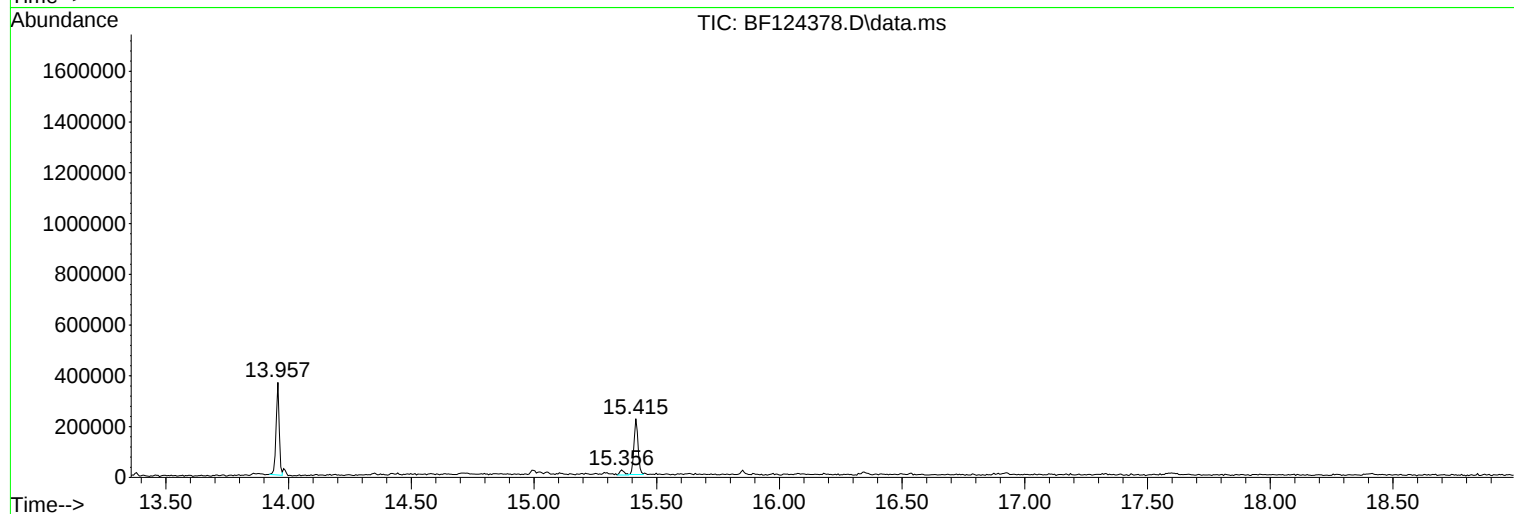
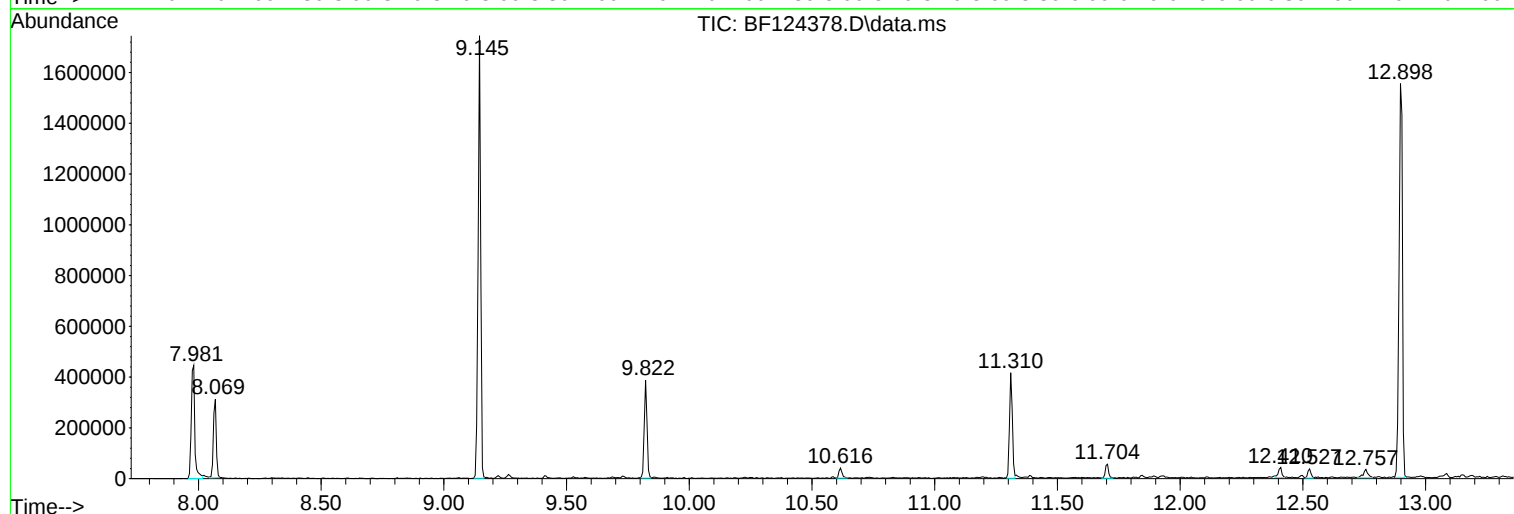
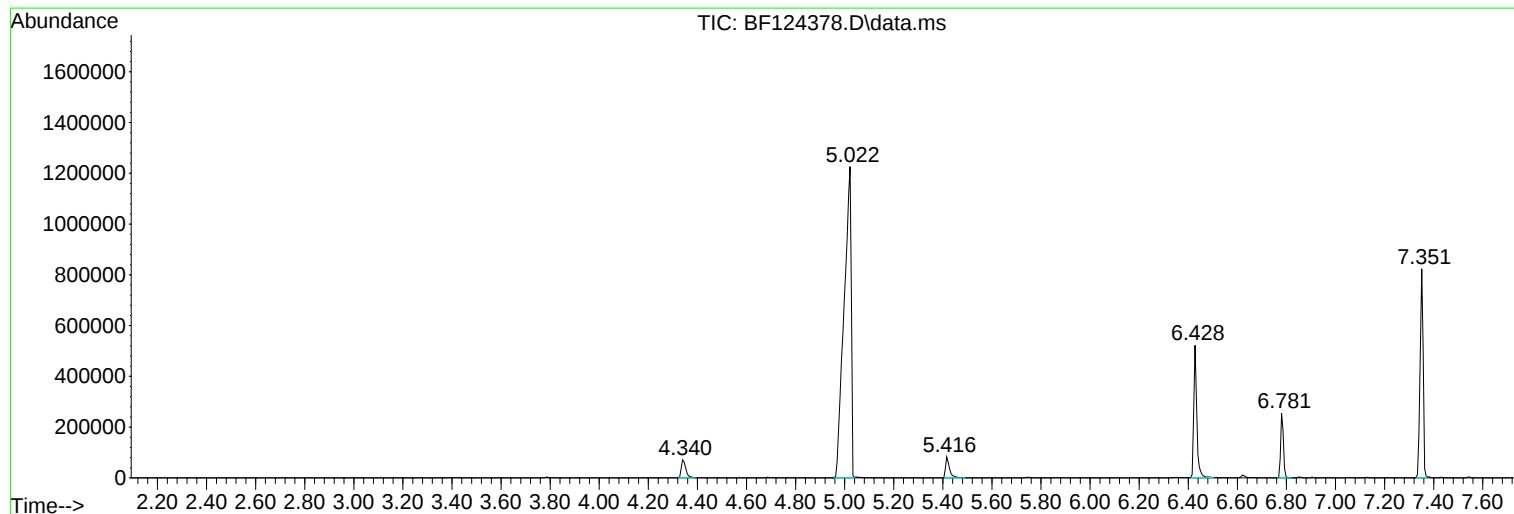
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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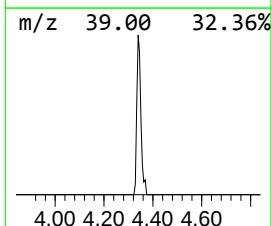
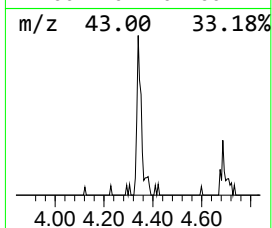
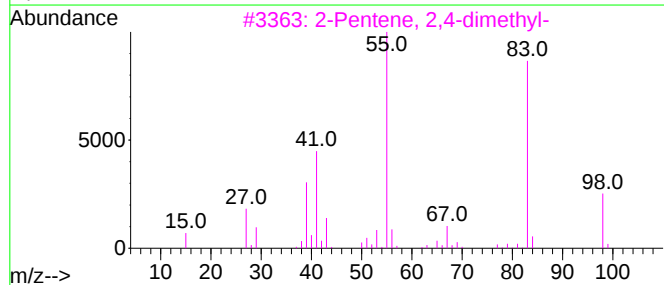
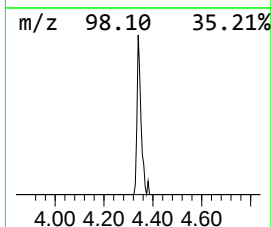
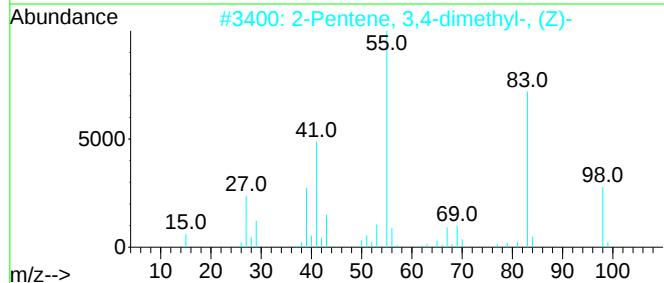
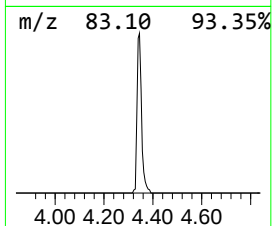
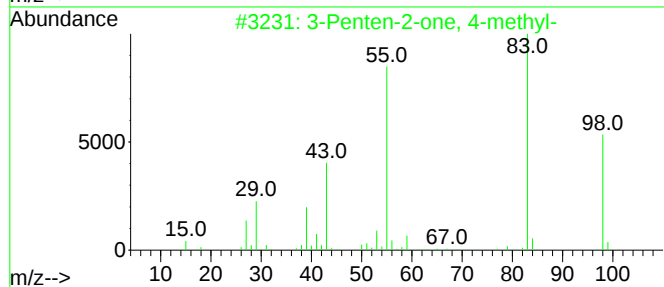
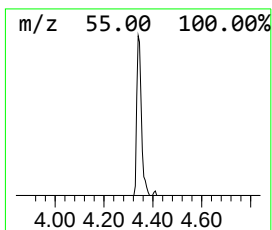
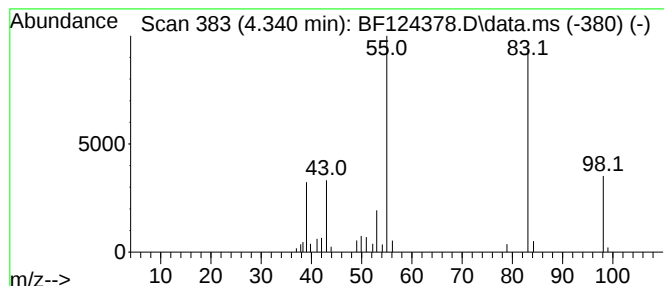
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.340	9.01 ng	89618	1,4-Dichlorobenzene-d4	6.781

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72
4		3-Hexen-2-one	98	C6H10O	000763-93-9	72
5		2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	64



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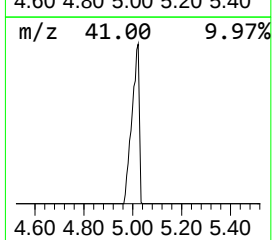
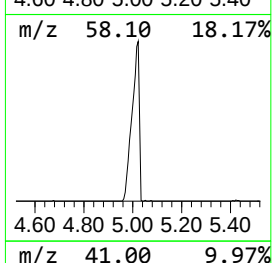
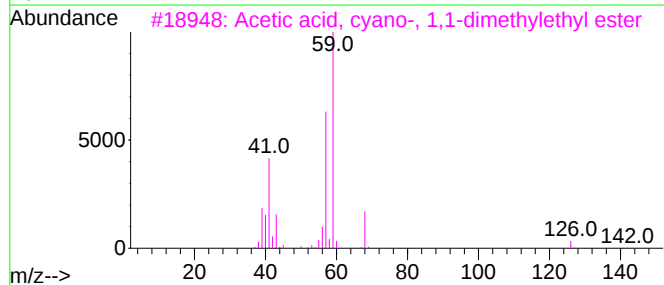
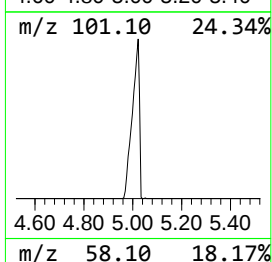
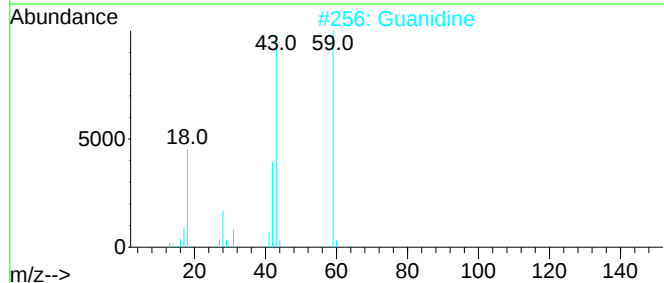
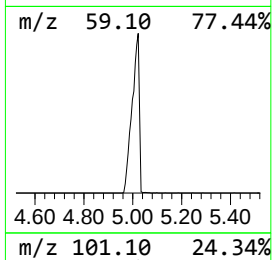
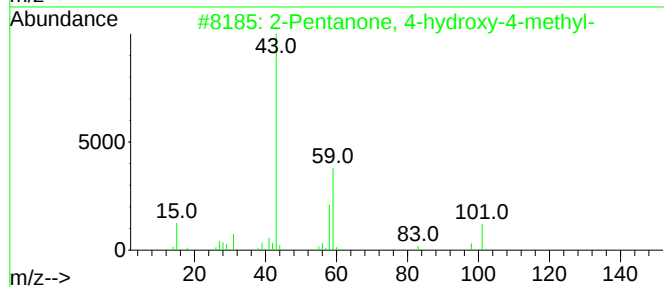
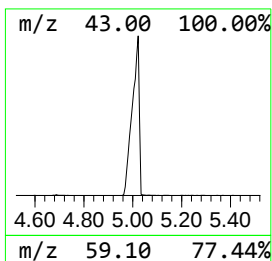
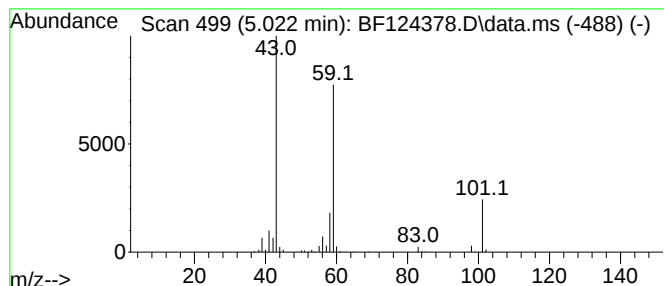
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	251.70 ng	2504770	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Guanidine	59	CH5N3	000113-00-8	50
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	38
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Acetone	58	C3H6O	000067-64-1	9



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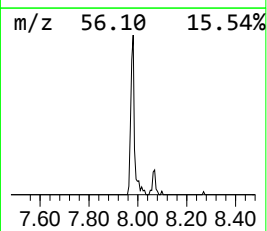
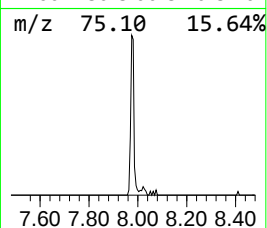
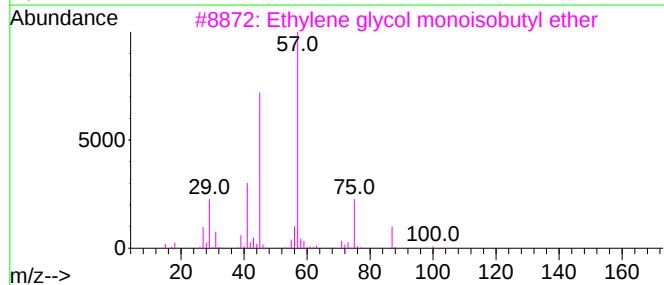
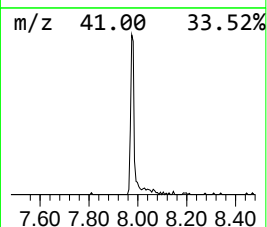
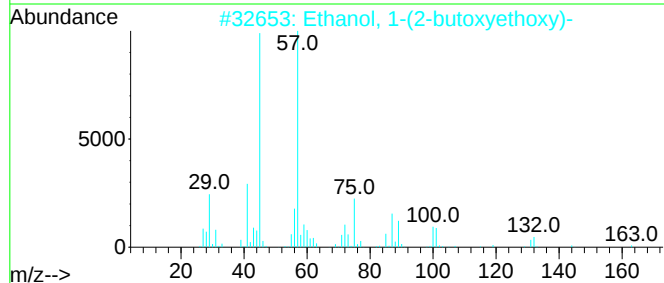
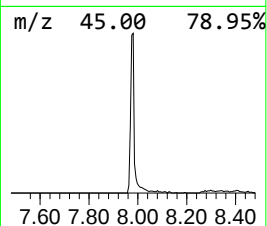
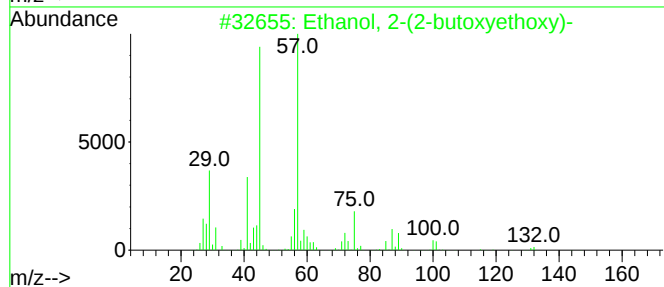
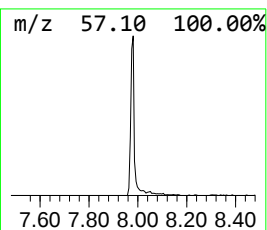
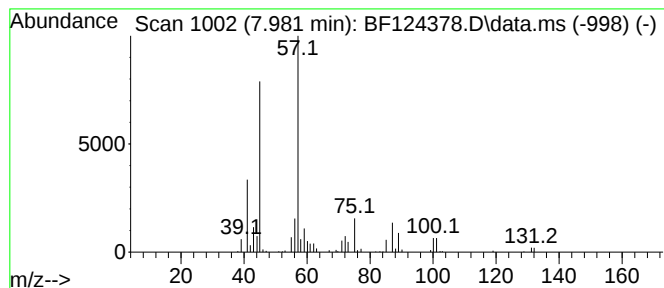
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.981	35.24 ng	443601	Naphthalene-d8	8.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			Diisopropyl ether	102	C6H14O	000108-20-3	50



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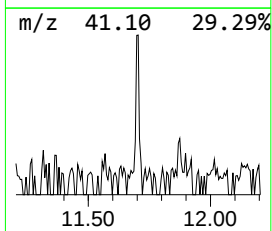
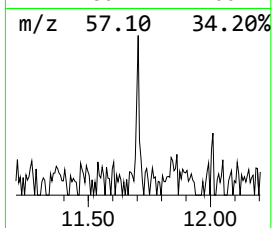
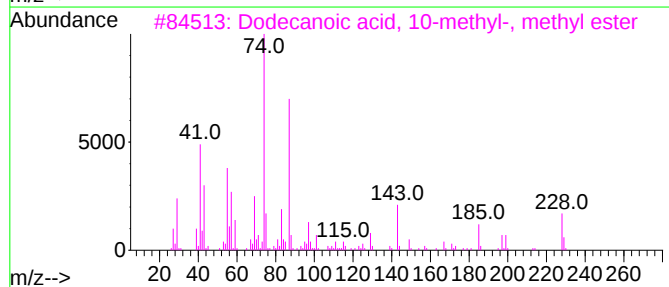
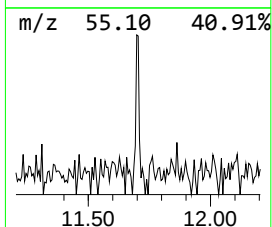
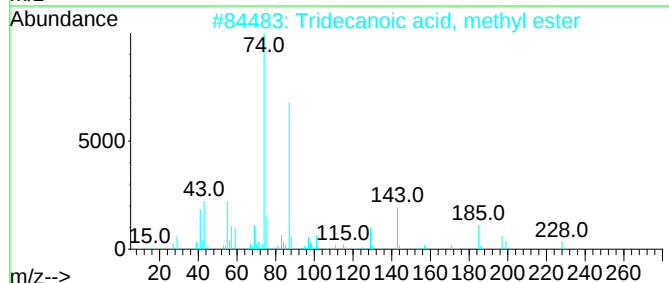
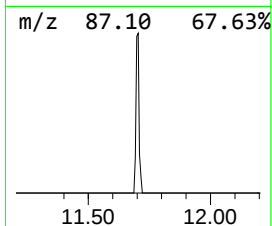
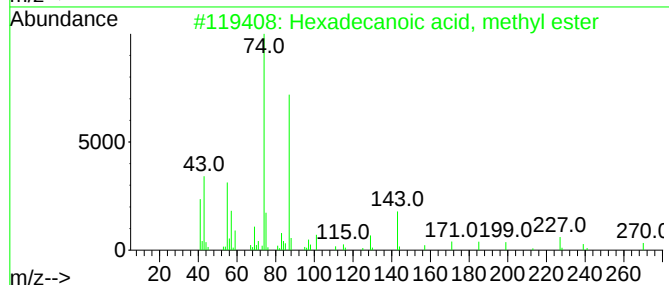
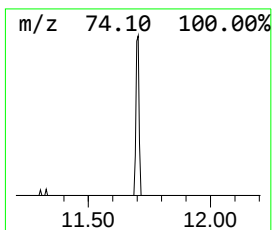
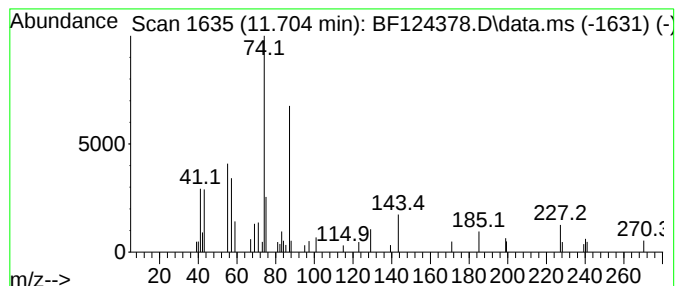
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.704	3.01 ng	50853	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	94
2			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	94
3			Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	81
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	80
5			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	74



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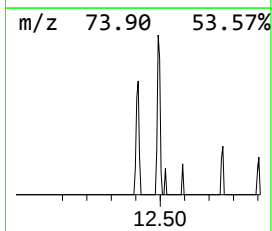
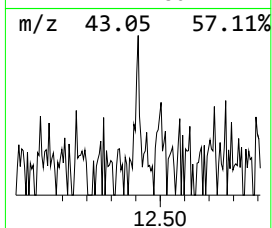
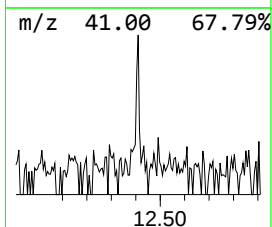
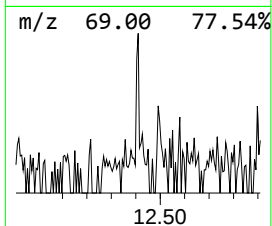
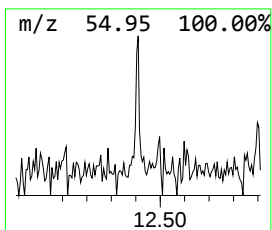
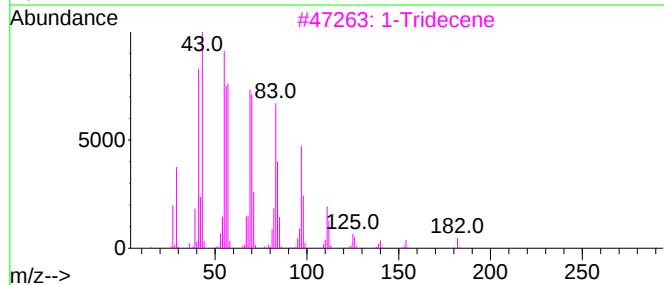
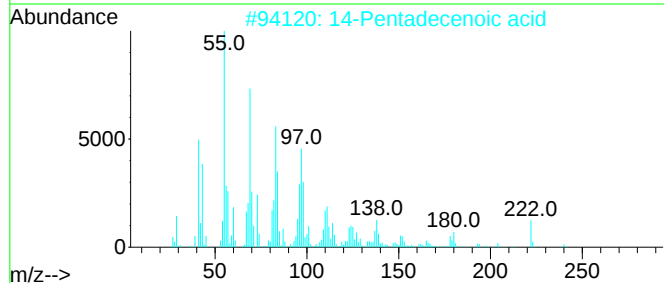
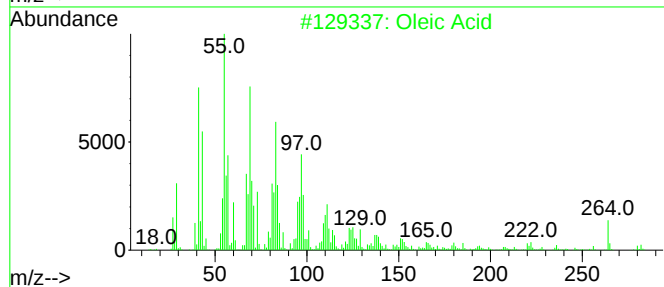
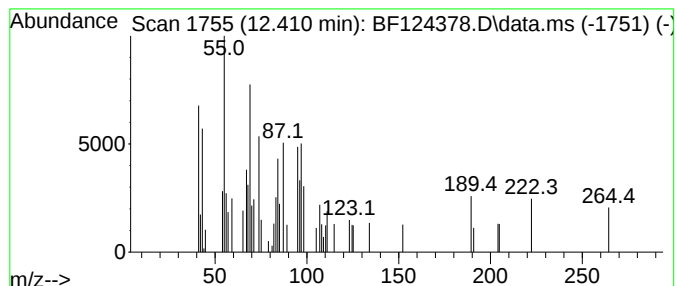
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Oleic Acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	2.22 ng	37540	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oleic Acid	282	C18H34O2	000112-80-1	50
2			14-Pentadecenoic acid	240	C15H28O2	017351-34-7	43
3			1-Tridecene	182	C13H26	002437-56-1	38
4			1-Tetradecanol	214	C14H30O	000112-72-1	38
5			Neoisolongifolane, hydroxy-	222	C15H26O	1000159-37-9	35



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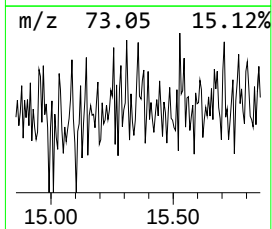
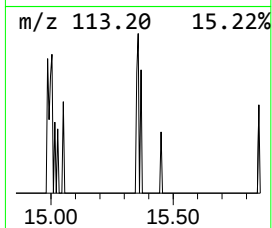
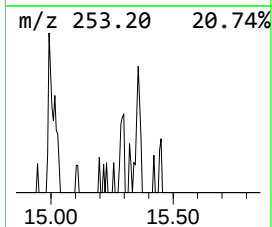
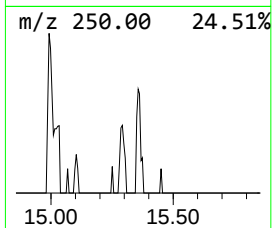
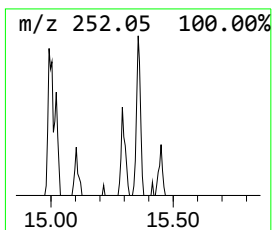
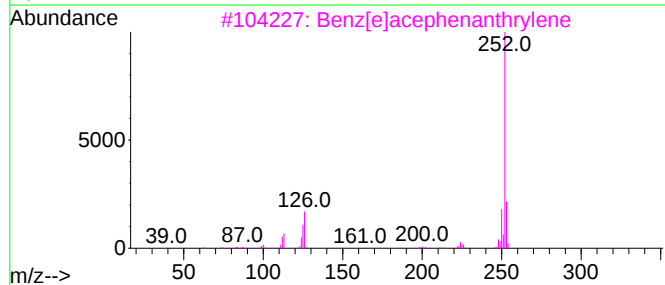
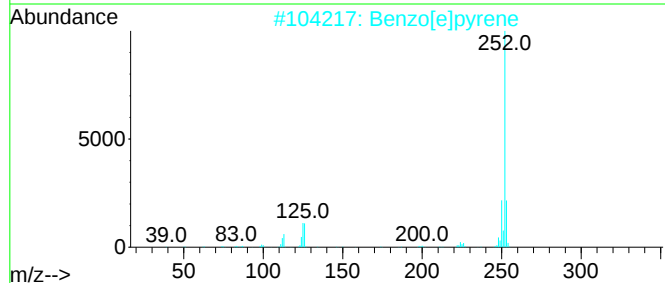
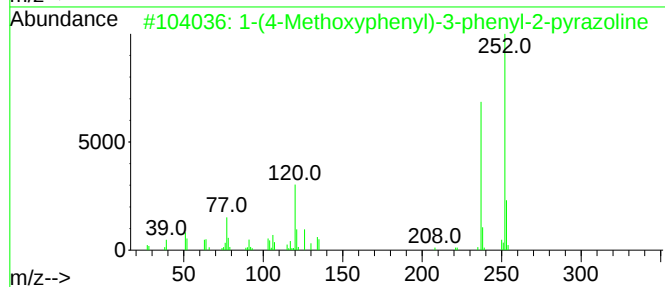
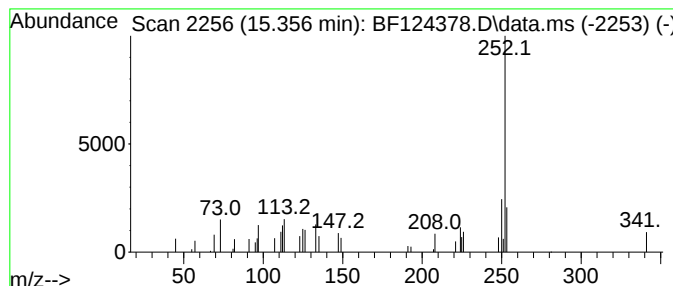
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-(4-Methoxyphenyl)-3-pheny... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.357	2.12 ng	26815	Perylene-d12	15.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(4-Methoxyphenyl)-3-phenyl-2-p...	252	C16H16N2O	002535-59-3	52
2			Benzo[e]pyrene	252	C20H12	000192-97-2	52
3			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	50
4			Benzo[a]pyrene	252	C20H12	000050-32-8	50
5			4H-1-Benzopyran-4-one, 8-methoxy...	252	C16H12O3	026964-26-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061821\
Data File : BF124378.D
Acq On : 18 Jun 2021 17:25
Operator : JU/CG
Sample : M2709-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0248-AMND-COMP-M

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-Penten-2-one,...	4.340	9.0	ng	89618	1	6.781	199030	20.0
2-Pentanone, 4-...	5.022	251.7	ng	2504770	1	6.781	199030	20.0
Ethanol, 2-(2-b...	7.981	35.2	ng	443601	2	8.069	251773	20.0
Hexadecanoic ac...	11.704	3.0	ng	50853	4	11.310	337895	20.0
Oleic Acid	12.410	2.2	ng	37540	4	11.310	337895	20.0
1-(4-Methoxyphe...	15.357	2.1	ng	26815	6	15.415	253057	20.0