

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061421\
 Data File : BM030441.D
 Acq On : 14 Jun 2021 17:46
 Operator : CG/JU
 Sample : M2687-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 17-B6(108-112)

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_M\Methods\8270-BM060921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM030441.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.581	79	84	89	rBV2	131986	194969	2.86%	0.416%
2	4.040	158	162	168	rVB	53766	79510	1.17%	0.170%
3	4.599	252	257	262	rVB	63184	92507	1.36%	0.198%
4	4.963	313	319	327	rBV	268501	394110	5.78%	0.842%
5	5.352	380	385	391	rVB	45450	70931	1.04%	0.151%
6	5.428	391	398	404	rBV	3108643	4485478	65.81%	9.580%
7	5.487	404	408	417	rVB	126310	268442	3.94%	0.573%
8	5.857	464	471	477	rBV	57248	89524	1.31%	0.191%
9	6.034	493	501	508	rBV	45842	77146	1.13%	0.165%
10	7.010	657	667	683	rBV	3001890	4856948	71.26%	10.373%
11	7.834	800	807	814	rVB	583940	913947	13.41%	1.952%
12	8.987	996	1003	1012	rVB	1679238	2746796	40.30%	5.866%
13	10.398	1234	1243	1261	rBV	1178083	1952972	28.65%	4.171%
14	10.622	1274	1281	1296	rVB	706590	1213882	17.81%	2.592%
15	11.898	1489	1498	1510	rBV2	47282	107949	1.58%	0.231%
16	13.080	1691	1699	1710	rBV	3541841	5223697	76.64%	11.156%
17	13.280	1726	1733	1741	rVB	54245	84167	1.23%	0.180%
18	13.886	1827	1836	1843	rBV	47198	94750	1.39%	0.202%
19	14.457	1926	1933	1946	rVB	1060241	1607937	23.59%	3.434%
20	15.863	2167	2172	2176	rBV	181579	233149	3.42%	0.498%
21	15.939	2179	2185	2204	rVB	3368083	4863047	71.35%	10.386%
22	17.192	2392	2398	2406	rBV	1315424	1898100	27.85%	4.054%
23	17.310	2414	2418	2425	rVB	185842	255640	3.75%	0.546%
24	17.839	2503	2508	2518	rVB3	637959	1059511	15.55%	2.263%
25	18.080	2545	2549	2556	rBV2	165465	262348	3.85%	0.560%
26	18.980	2697	2702	2707	rBV	400406	550556	8.08%	1.176%
27	19.027	2707	2710	2715	rVB	230914	272707	4.00%	0.582%
28	19.356	2763	2766	2775	rVB3	98979	146717	2.15%	0.313%
29	19.804	2836	2842	2849	rBV	5659235	6815631	100.00%	14.556%
30	20.492	2956	2959	2966	rVB3	61092	79944	1.17%	0.171%
31	20.562	2968	2971	2975	rVV	109807	117976	1.73%	0.252%
32	21.062	3053	3056	3066	rBV	257557	355256	5.21%	0.759%
33	21.268	3087	3091	3097	rBV	265759	304698	4.47%	0.651%
34	21.350	3101	3105	3114	rVV	1799266	2346816	34.43%	5.012%
35	22.203	3247	3250	3257	rVB	209650	258535	3.79%	0.552%
36	23.627	3486	3492	3500	rVB2	1269865	2446801	35.90%	5.226%

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17-B6(108-112)

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_M\Methods\8270-BM060921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

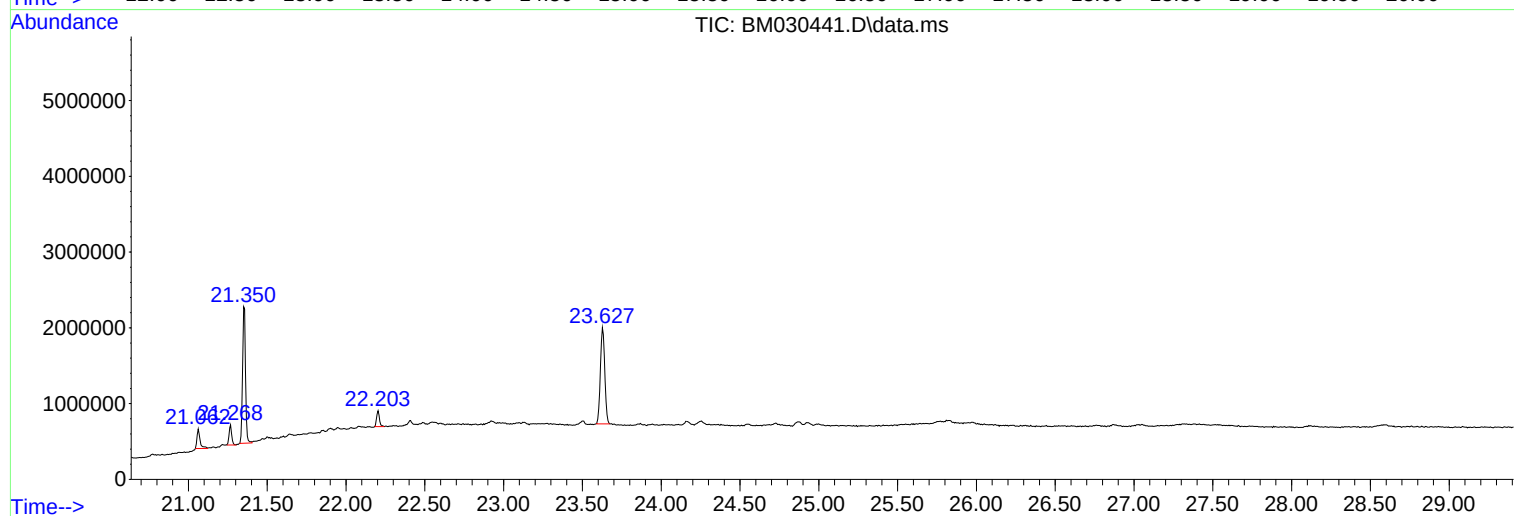
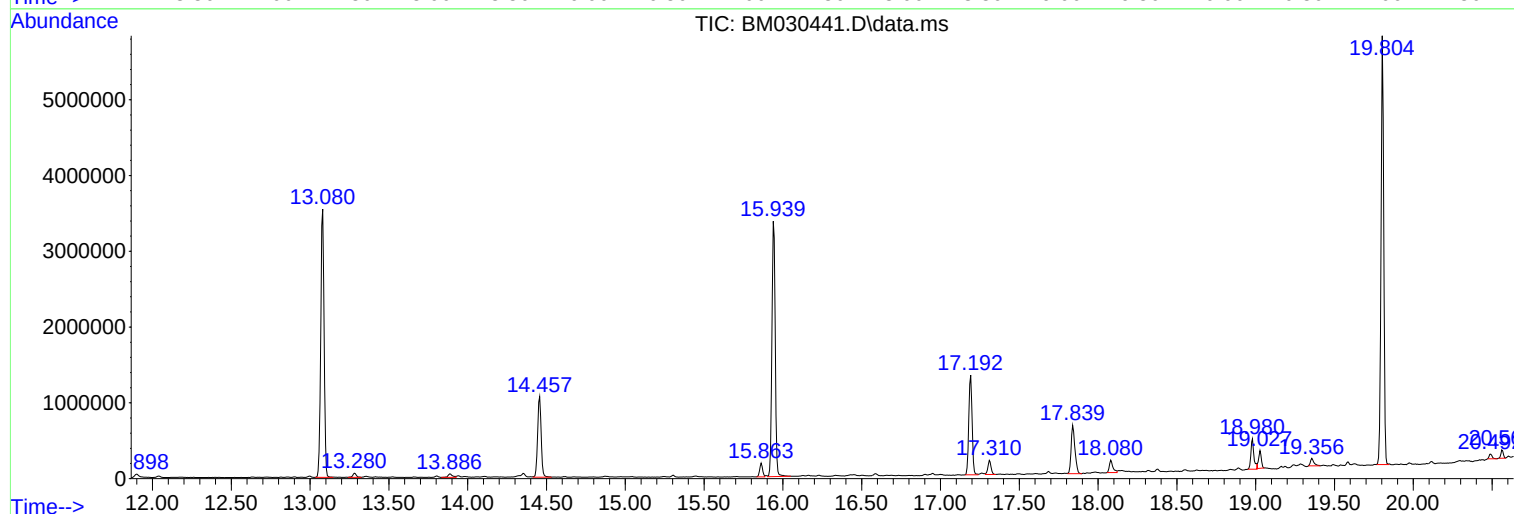
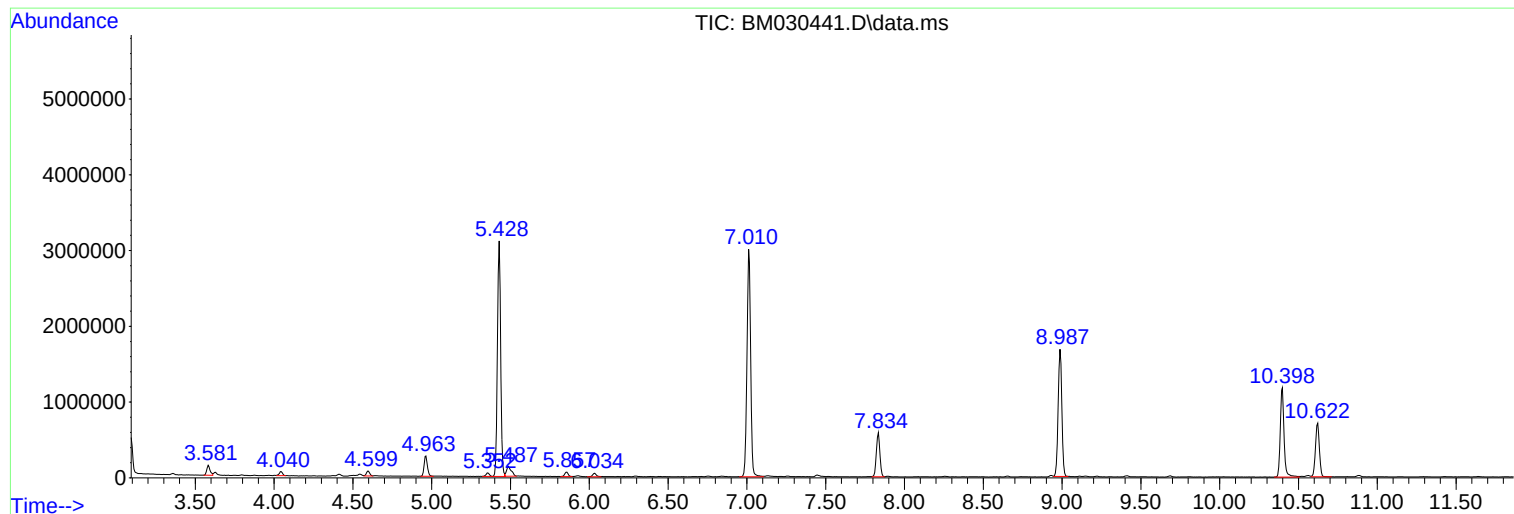
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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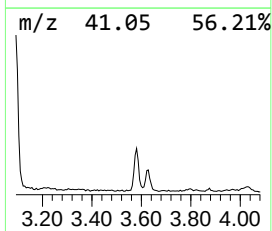
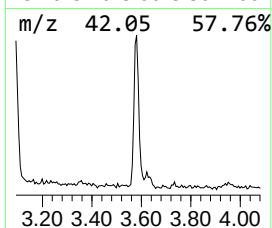
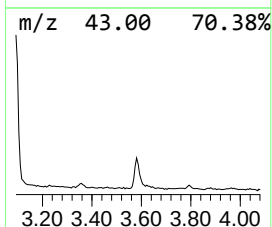
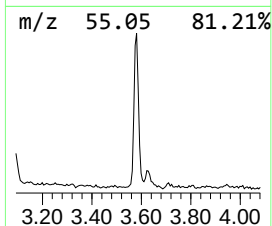
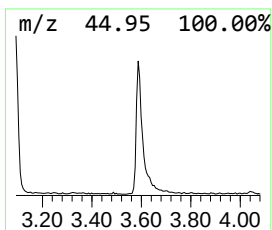
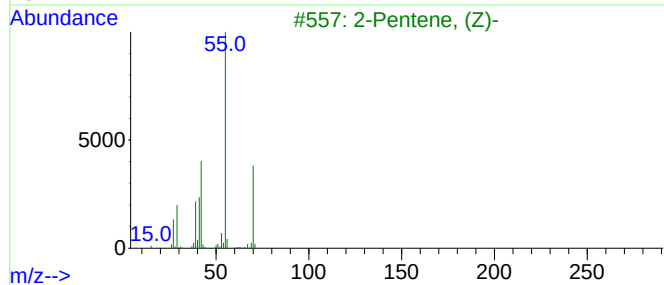
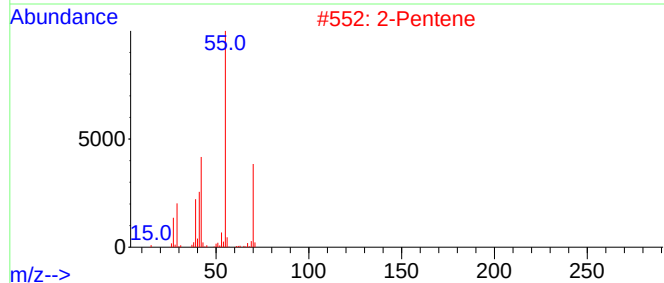
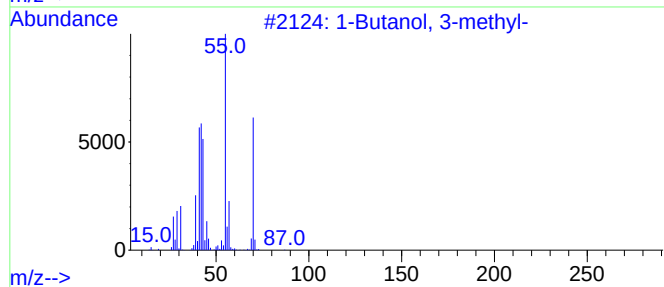
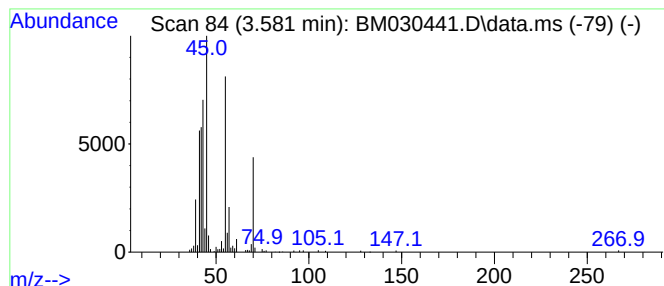
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.581 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.581	4.27 ng	194969	1,4-Dichlorobenzene-d4	7.834

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	47
2		2-Pentene	70	C5H10	000109-68-2	38
3		2-Pentene, (Z)-	70	C5H10	000627-20-3	38
4		1-Pentanol	88	C5H12O	000071-41-0	32
5		Ethoxyacetylene	70	C4H6O	000927-80-0	27



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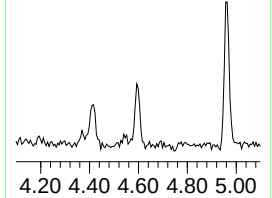
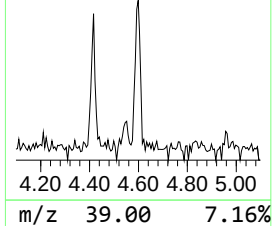
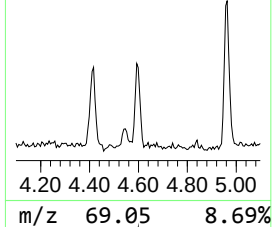
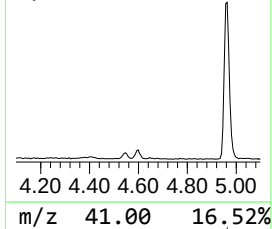
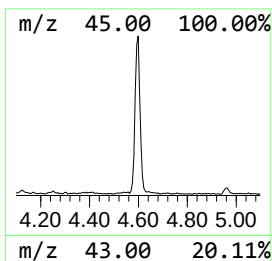
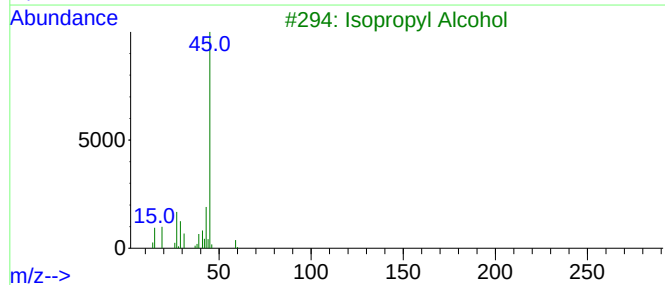
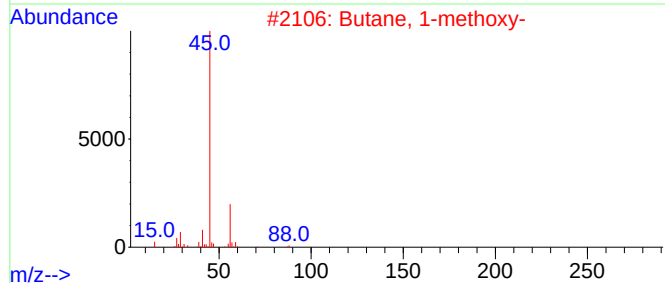
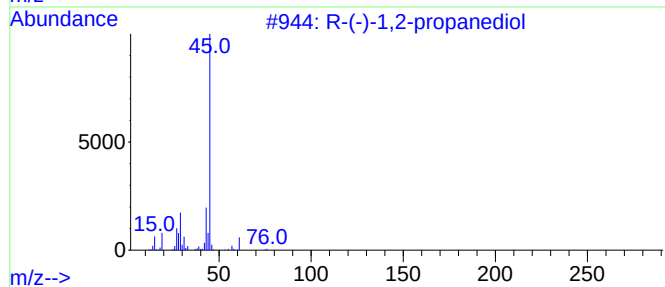
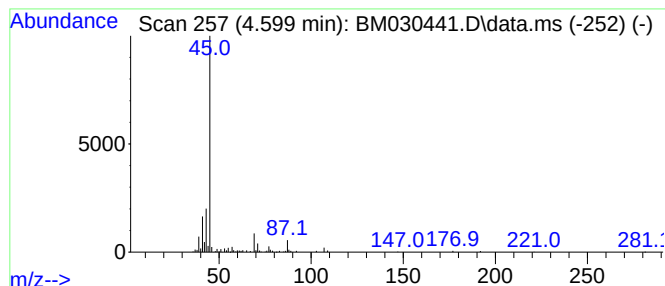
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060921.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown4.599 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.599	2.02 ng	92507	1,4-Dichlorobenzene-d4	7.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	45
2	Butane, 1-methoxy-			88	C5H12O	000628-28-4	45
3	Isopropyl Alcohol			60	C3H8O	000067-63-0	45
4	2-Hexanol			102	C6H14O	000626-93-7	40
5	1-Propanol, 2-(1-methylethoxy)-			118	C6H14O2	003944-37-4	40



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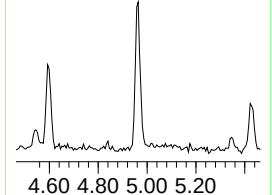
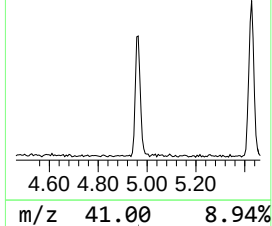
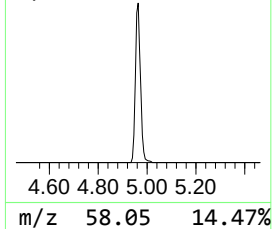
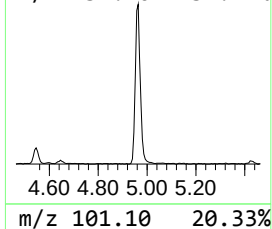
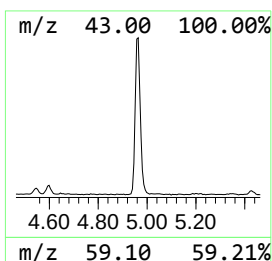
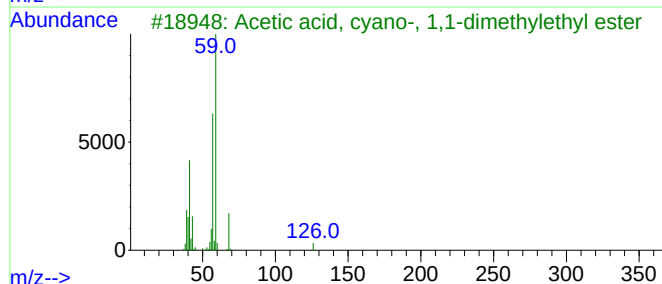
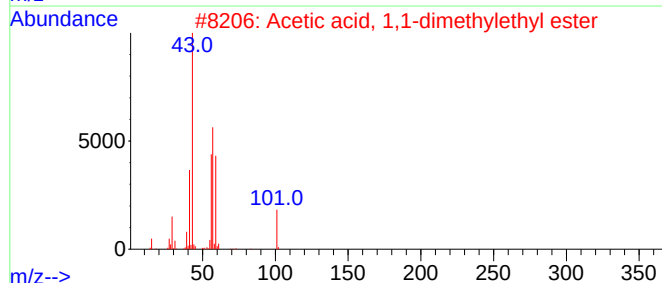
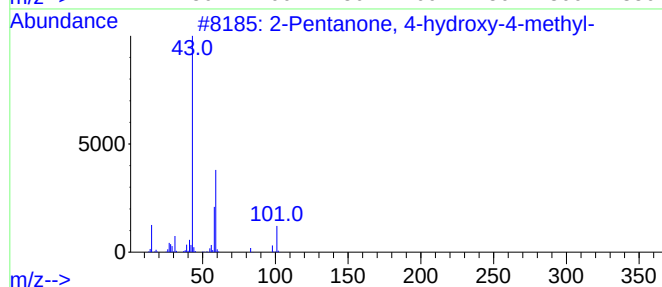
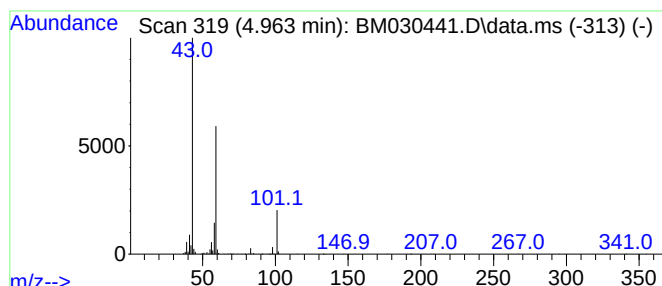
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	8.62 ng	394110	1,4-Dichlorobenzene-d4	7.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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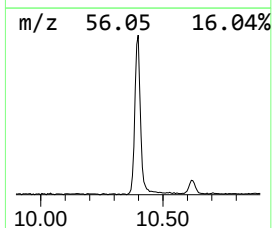
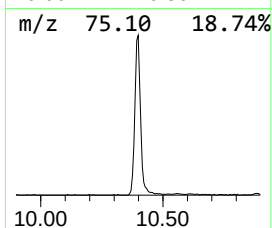
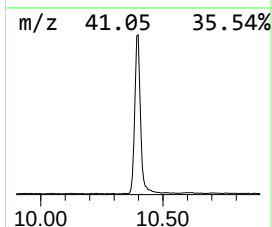
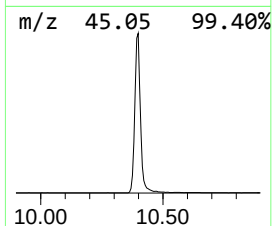
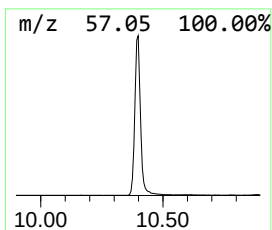
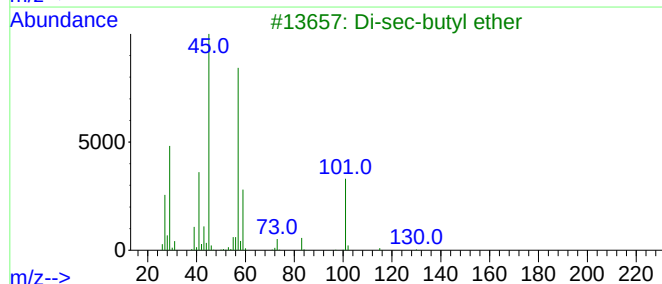
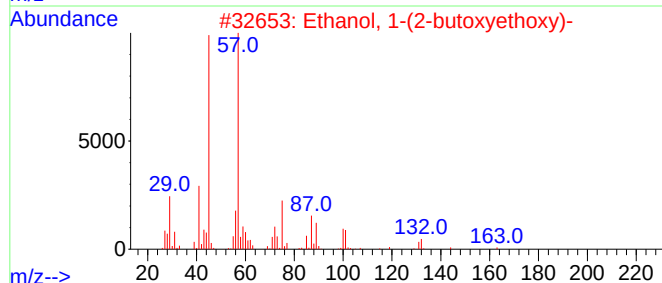
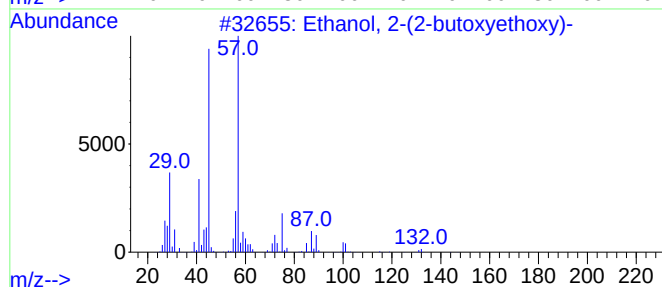
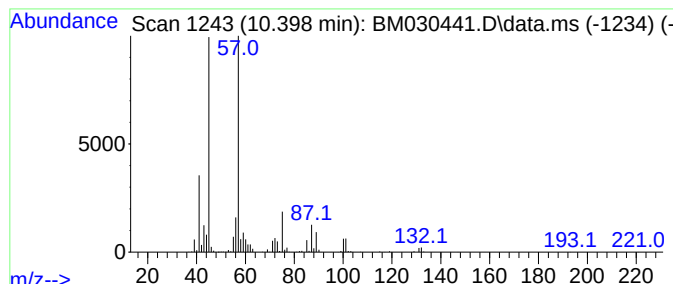
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.398	32.18 ng	1952970	Naphthalene-d8	10.622

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	83
3			Di-sec-butyl ether	130	C8H18O	006863-58-7	50
4			2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	50
5			Propanoic acid, 2-hydroxy-, buty...	146	C7H14O3	000138-22-7	47



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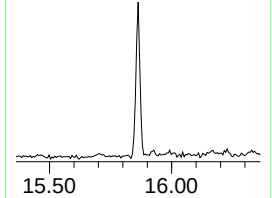
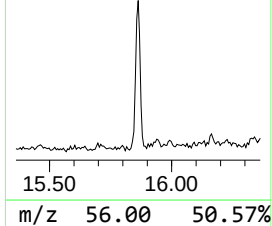
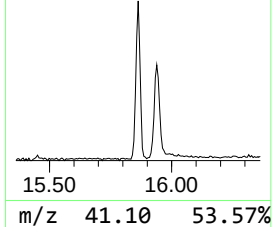
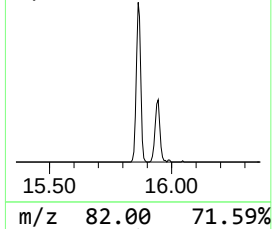
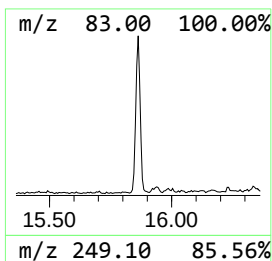
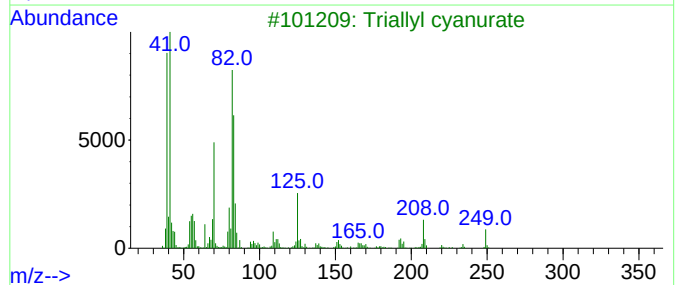
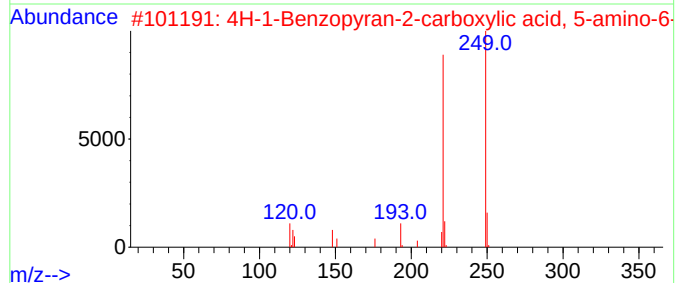
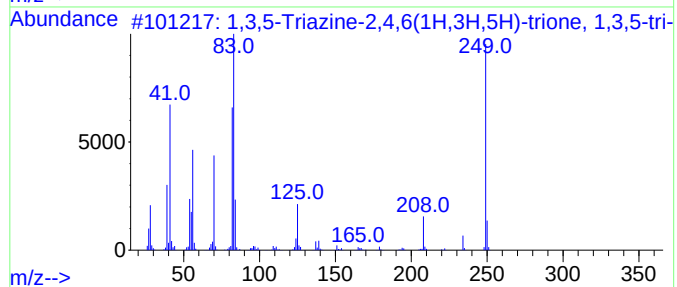
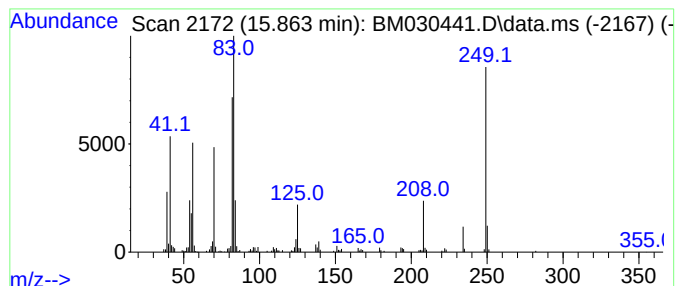
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.863	2.46 ng	233149	Phenanthrene-d10		17.192	
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	99
2	4H-1-Benzopyran-2-carboxylic aci...		249	C12H11NO5	032142-43-1	50
3	Triallyl cyanurate		249	C12H15N3O3	000101-37-1	32
4	n-Nonylcyclohexane		210	C15H30	002883-02-5	22
5	Cyclohexane, 1,1'-(1,4-butanedi...		222	C16H30	006165-44-2	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061421\
Data File : BM030441.D
Acq On : 14 Jun 2021 17:46
Operator : CG/JU
Sample : M2687-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
17-B6(108-112)

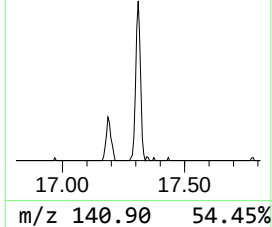
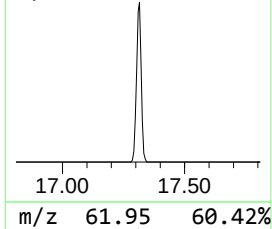
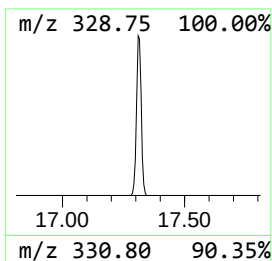
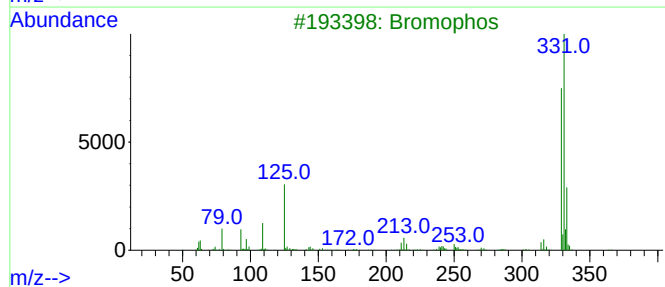
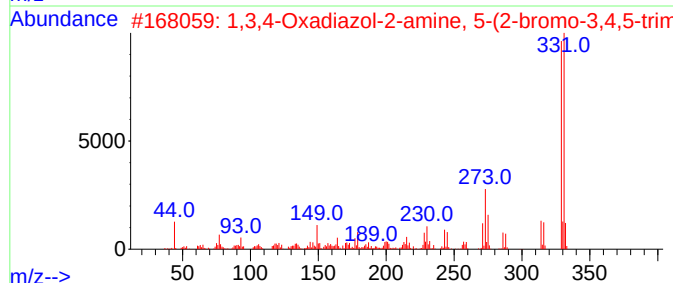
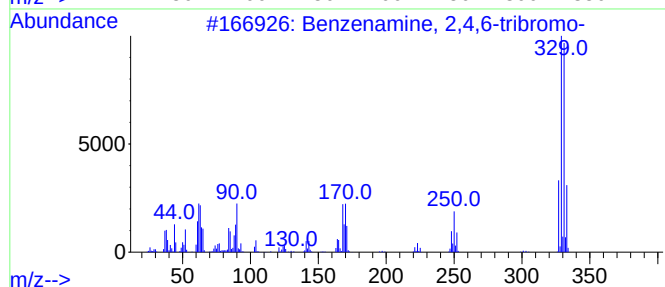
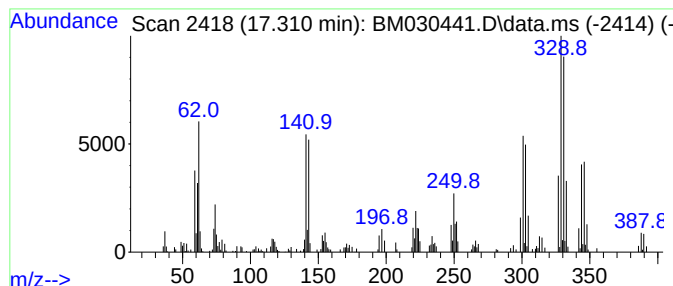
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzenamine, 2,4,6-tribromo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.310	2.69 ng	255640	Phenanthrene-d10	17.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	70
2			1,3,4-Oxadiazol-2-amine, 5-(2-br...	329	C11H12BrN3O4	1000350-74-8	14
3			Bromophos	364	C8H8BrCl2O3PS	002104-96-3	10
4			1-[4-Chloro-6-methyl-2-pyrimidyl...	329	C12H10ClN5	051387-79-2	10
5			4,4'-(p-Phenylenediisopropyliden...	344	C24H28N2	002716-10-1	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061421\
Data File : BM030441.D
Acq On : 14 Jun 2021 17:46
Operator : CG/JU
Sample : M2687-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
17-B6(108-112)

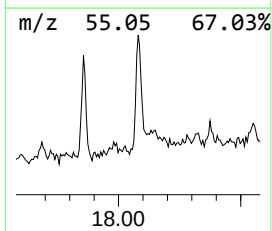
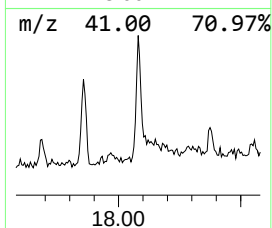
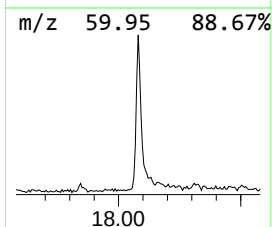
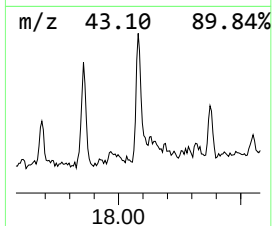
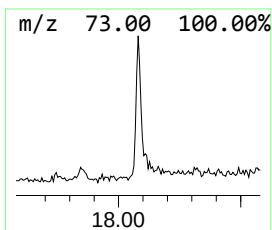
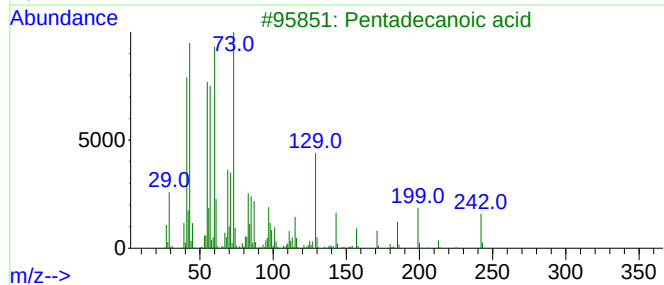
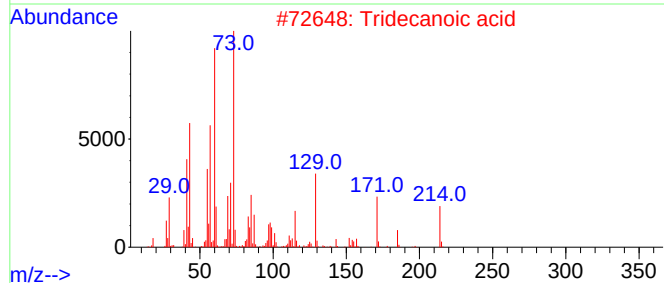
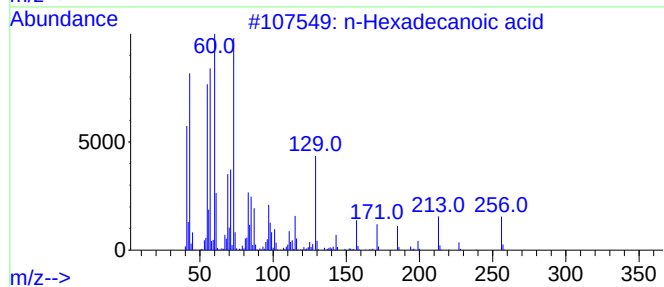
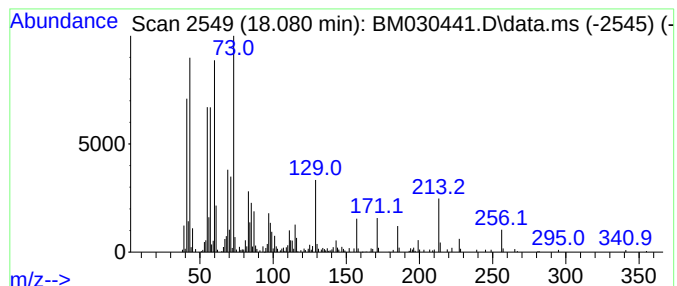
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.080	2.76 ng	262348	Phenanthrene-d10	17.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Octadecanoic acid	284	C18H36O2	000057-11-4	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061421\
Data File : BM030441.D
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Operator : CG/JU
Sample : M2687-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

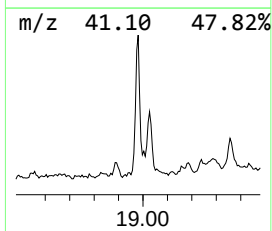
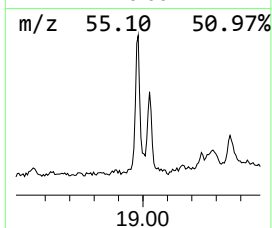
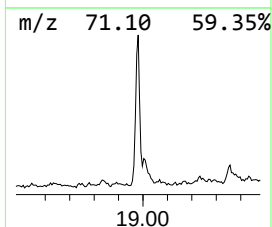
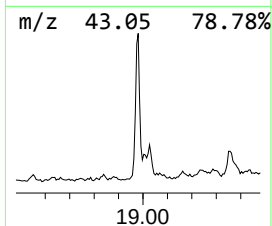
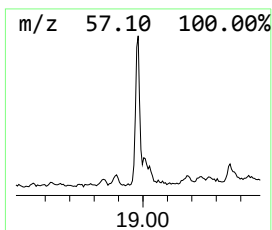
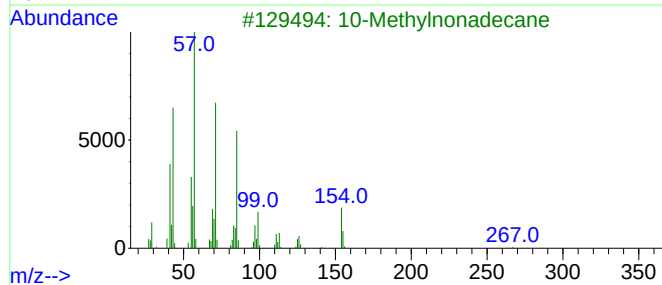
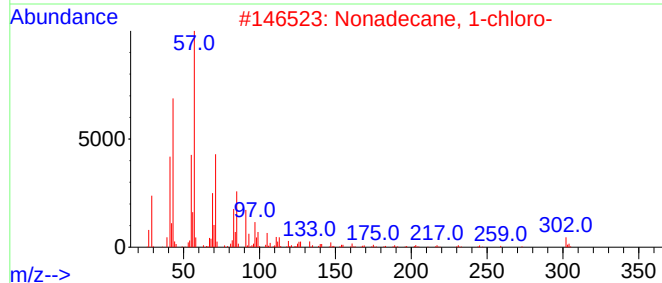
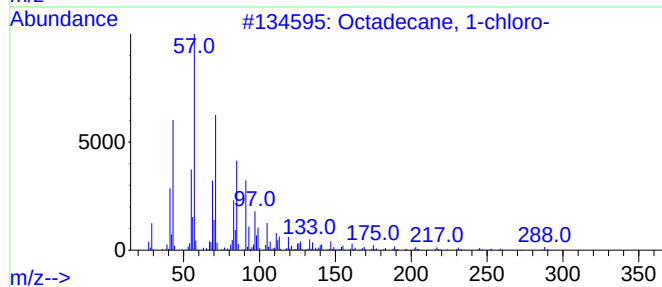
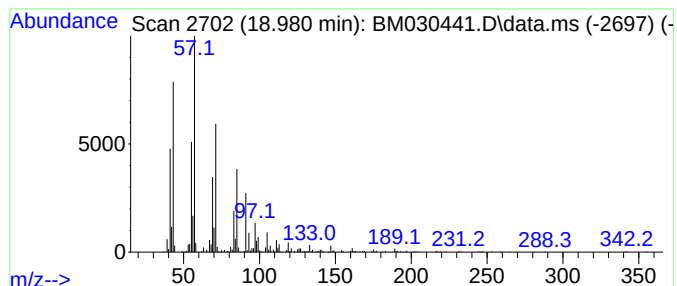
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecane, 1-chloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.980	5.80 ng	550556	Phenanthrene-d10		17.192	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecane, 1-chloro-		288	C18H37Cl	003386-33-2	90
2	Nonadecane, 1-chloro-		302	C19H39Cl	062016-76-6	80
3	10-Methylnonadecane		282	C20H42	056862-62-5	58
4	Hexadecane, 1-chloro-		260	C16H33Cl	004860-03-1	58
5	Nonadecane		268	C19H40	000629-92-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061421\
Data File : BM030441.D
Acq On : 14 Jun 2021 17:46
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Sample : M2687-03
Misc :
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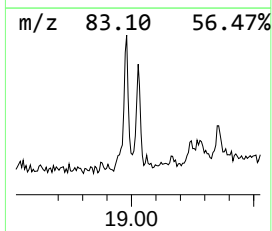
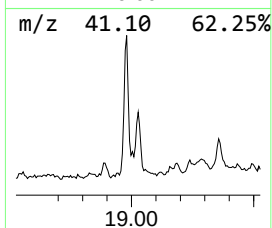
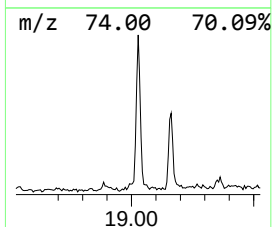
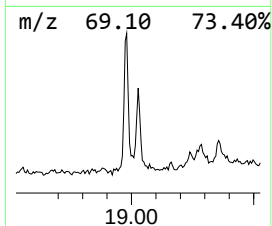
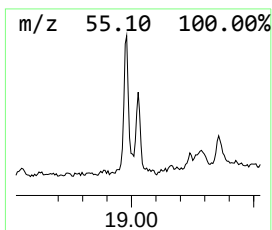
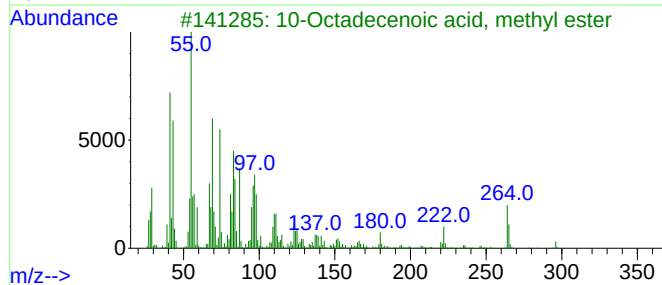
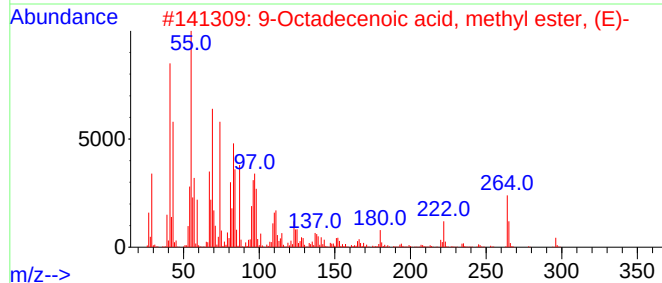
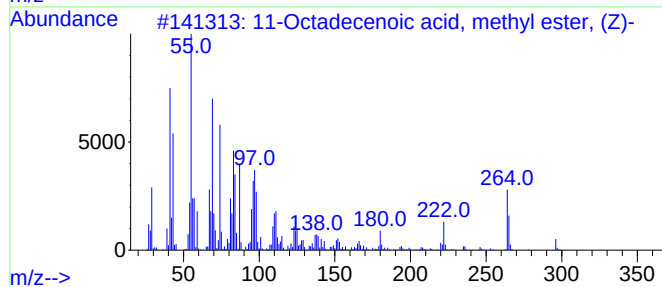
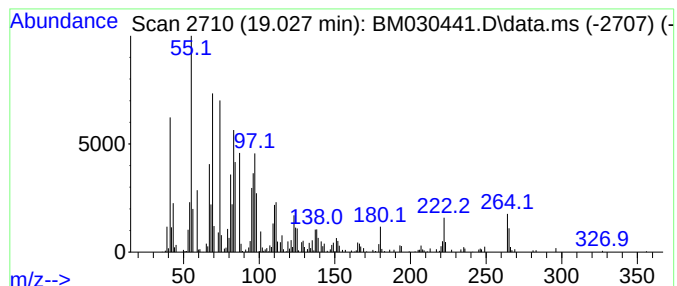
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 11-Octadecenoic acid, methyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.027	2.87 ng	272707	Phenanthrene-d10	17.192	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
2	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
4	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	99
5	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061421\
Data File : BM030441.D
Acq On : 14 Jun 2021 17:46
Operator : CG/JU
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ClientSampleId :
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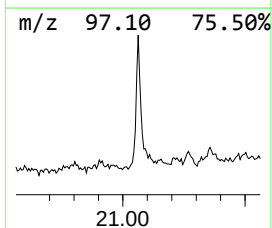
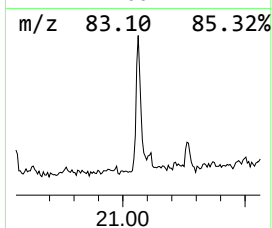
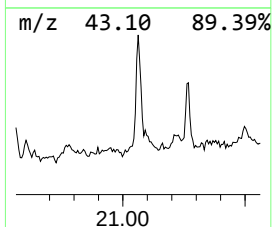
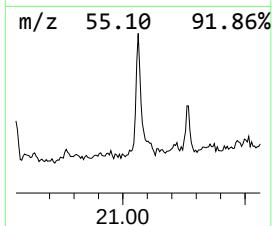
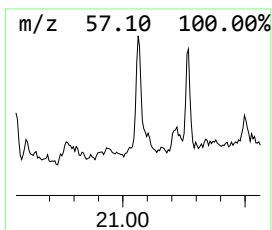
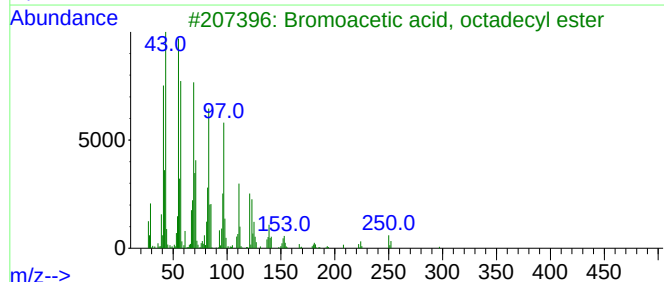
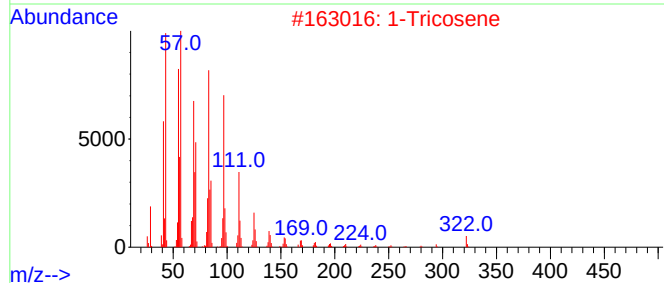
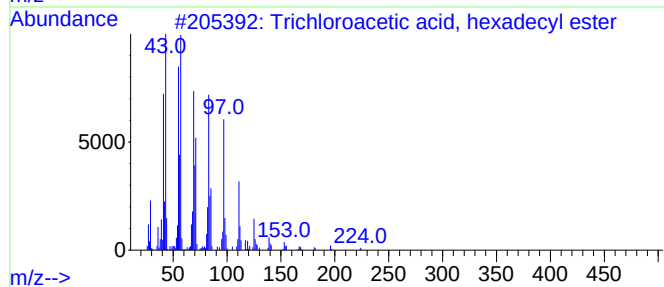
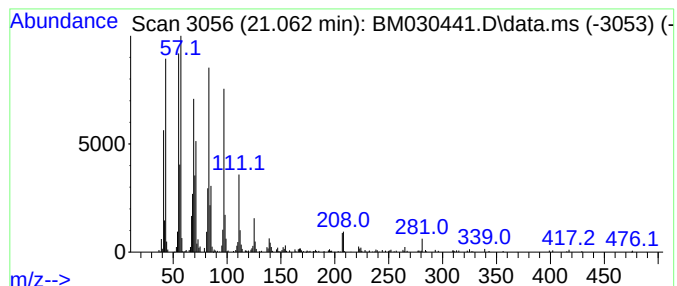
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Trichloroacetic acid, hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.062	3.03 ng	355256	Chrysene-d12	21.351

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		1-Tricosene	322	C23H46	018835-32-0	91
3		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	90
4		1-Docosene	308	C22H44	001599-67-3	90
5		n-Heptadecanol-1	256	C17H36O	001454-85-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061421\
Data File : BM030441.D
Acq On : 14 Jun 2021 17:46
Operator : CG/JU
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Misc :
ALS Vial : 12 Sample Multiplier: 1

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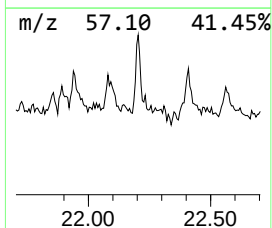
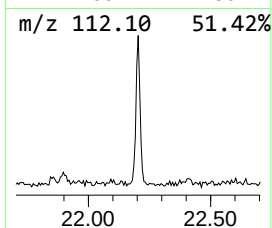
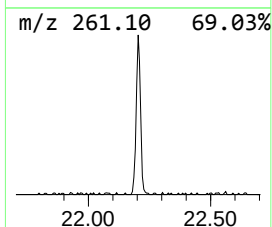
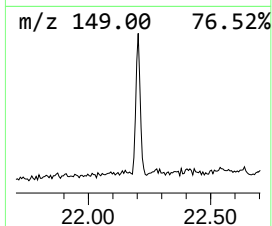
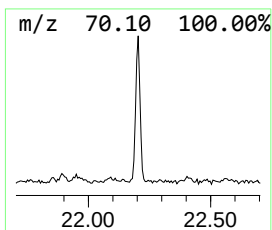
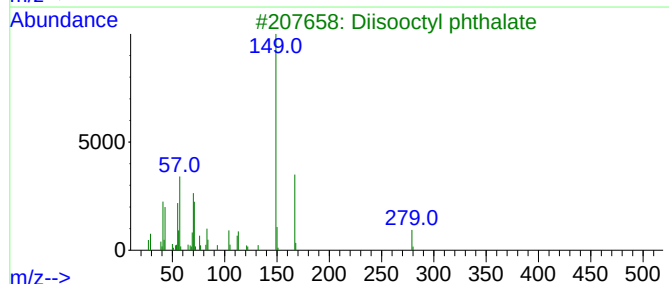
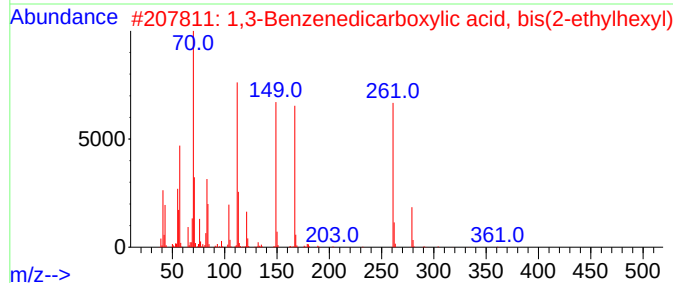
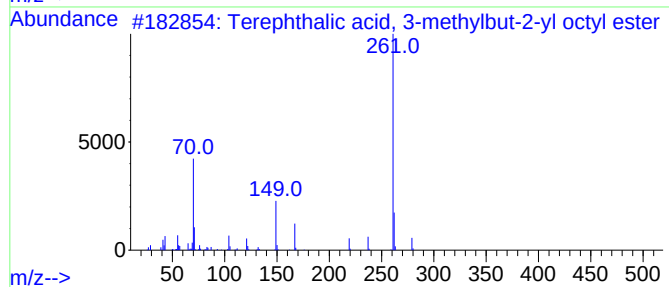
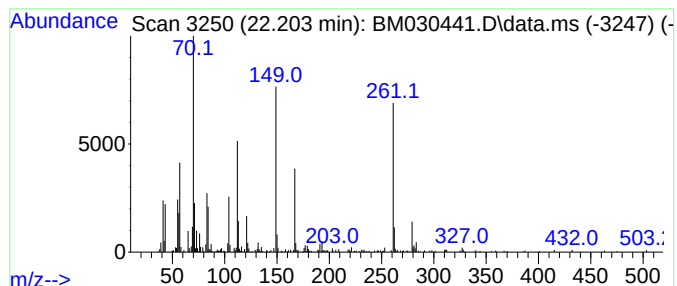
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Terephthalic acid, 3-methyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.203	2.20 ng	258535	Chrysene-d12	21.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	72
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	49
3			Diisooctyl phthalate	390	C24H38O4	000131-20-4	38
4			Terephthalic acid, 3-hexyl octyl...	362	C22H34O4	1000356-23-1	27
5			Phthalic acid, 3,5-difluoropheny...	390	C22H24F2O4	1000315-51-3	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061421\
Data File : BM030441.D
Acq On : 14 Jun 2021 17:46
Operator : CG/JU
Sample : M2687-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
17-B6(108-112)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060921.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
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unknown4.599	4.599	2.0	ng	92507	1	7.834	913947	20.0
2-Pentanone, 4-...	4.963	8.6	ng	394110	1	7.834	913947	20.0
Ethanol, 2-(2-b...	10.398	32.2	ng	1952970	2	10.622	1213880	20.0
1,3,5-Triazine-...	15.863	2.5	ng	233149	4	17.192	1898100	20.0
Benzenamine, 2,...	17.310	2.7	ng	255640	4	17.192	1898100	20.0
n-Hexadecanoic ...	18.080	2.8	ng	262348	4	17.192	1898100	20.0
Octadecane, 1-c...	18.980	5.8	ng	550556	4	17.192	1898100	20.0
11-Octadecenoic...	19.027	2.9	ng	272707	4	17.192	1898100	20.0
Trichloroacetic...	21.062	3.0	ng	355256	5	21.351	2346820	20.0
Terephthalic ac...	22.203	2.2	ng	258535	5	21.351	2346820	20.0