

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
 Data File : BP006548.D
 Acq On : 06 Aug 2021 20:30
 Operator : CG/JU
 Sample : M3278-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 MW-3

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_P\Methods\8270E-BP080321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006548.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.905	305	309	319	rVB	673609	960509	6.13%	1.155%
2	5.358	380	386	394	rBV	2508290	3520786	22.48%	4.232%
3	5.969	485	490	497	rVB	390670	558502	3.57%	0.671%
4	6.934	647	654	665	rBV	1458338	2258356	14.42%	2.715%
5	7.752	787	793	800	rBV	951878	1475074	9.42%	1.773%
6	7.822	800	805	814	rVB	153852	243193	1.55%	0.292%
7	8.910	982	990	1000	rBV	3351475	5412175	34.56%	6.506%
8	10.334	1224	1232	1242	rBV	2522287	4003673	25.56%	4.813%
9	10.534	1259	1266	1273	rVB	1225713	2046469	13.07%	2.460%
10	13.010	1679	1687	1697	rBV	7588069	10740180	68.57%	12.910%
11	14.381	1909	1920	1939	rBV	1788303	2615117	16.70%	3.144%
12	15.875	2163	2174	2184	rBV	6000349	8182295	52.24%	9.836%
13	17.133	2381	2388	2399	rBV	2100446	2958742	18.89%	3.557%
14	17.827	2500	2506	2511	rBV	172536	227948	1.46%	0.274%
15	18.039	2537	2542	2551	rBV	465219	716807	4.58%	0.862%
16	18.751	2659	2663	2679	rBV2	216200	486318	3.11%	0.585%
17	18.963	2695	2699	2706	rVB	179358	215700	1.38%	0.259%
18	19.280	2748	2753	2762	rBV	371549	555871	3.55%	0.668%
19	19.710	2820	2826	2839	rBV	12846389	15662192	100.00%	18.827%
20	20.098	2889	2892	2900	rVB2	162228	200701	1.28%	0.241%
21	20.333	2928	2932	2936	rBV	430922	494134	3.15%	0.594%
22	20.680	2987	2991	2996	rBV	234895	274426	1.75%	0.330%
23	20.957	3035	3038	3046	rBV2	219614	279455	1.78%	0.336%
24	21.233	3080	3085	3091	rVB	2454318	3163888	20.20%	3.803%
25	22.410	3279	3285	3293	rBV	9105753	12569919	80.26%	15.110%
26	23.557	3473	3480	3489	rVB2	1651622	3367739	21.50%	4.048%

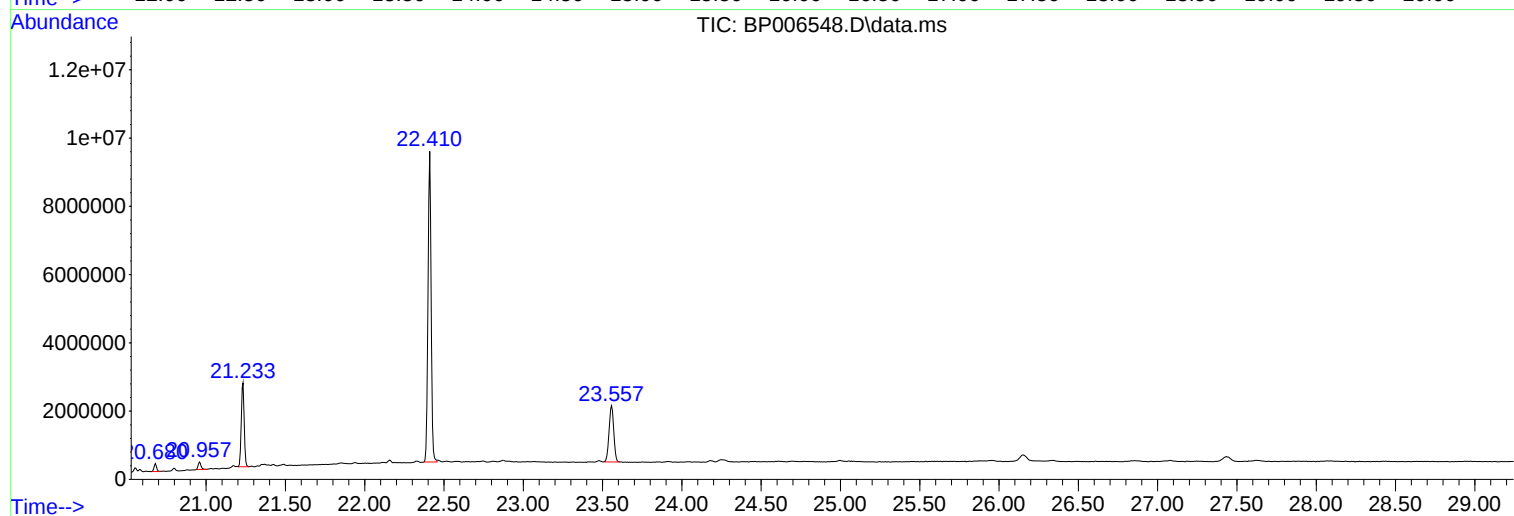
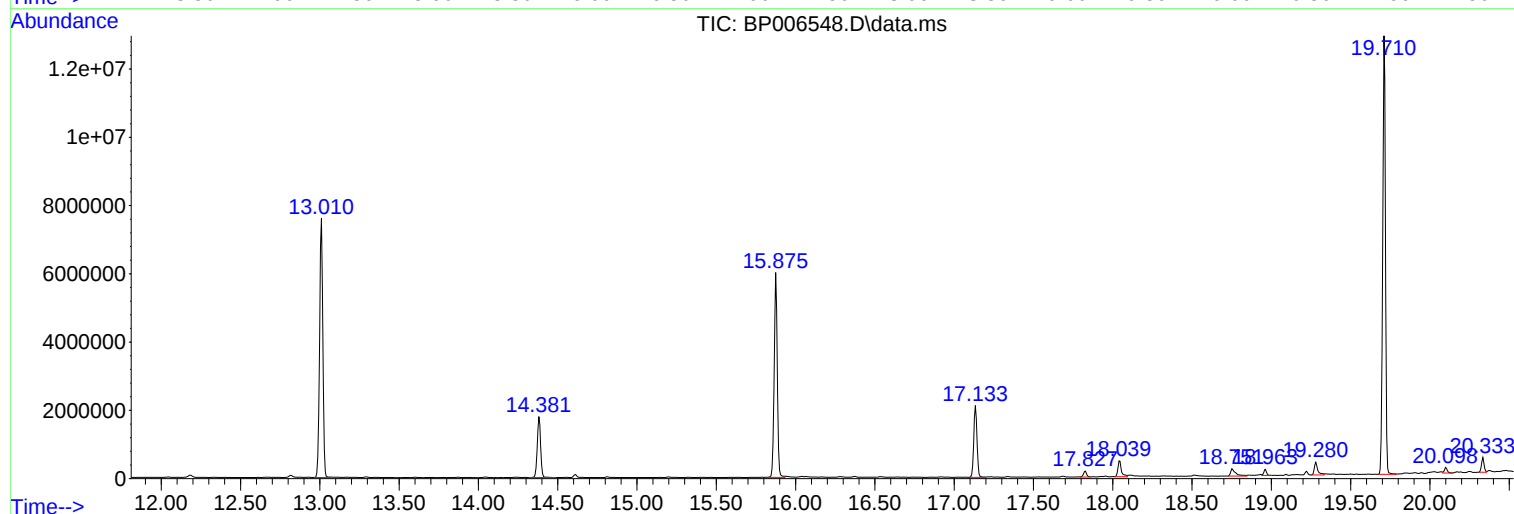
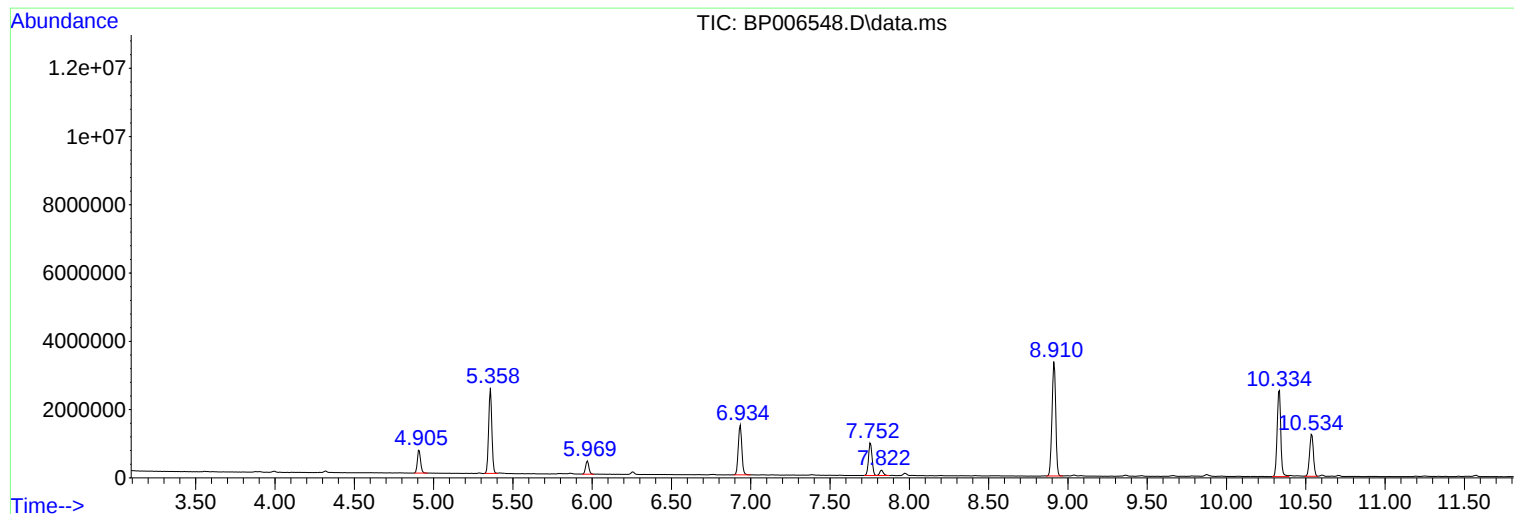
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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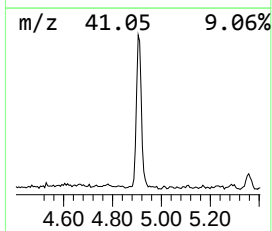
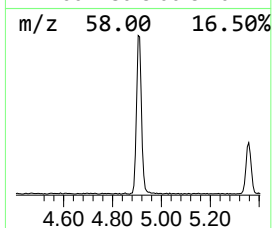
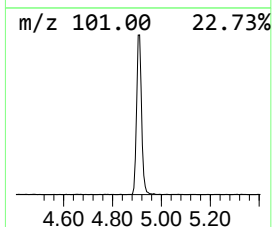
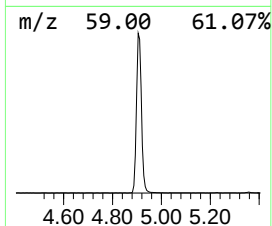
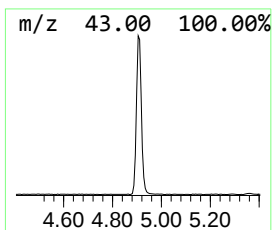
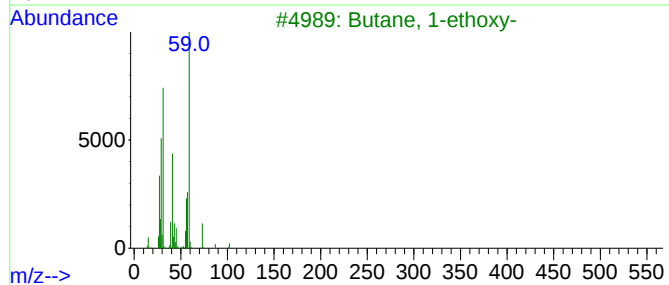
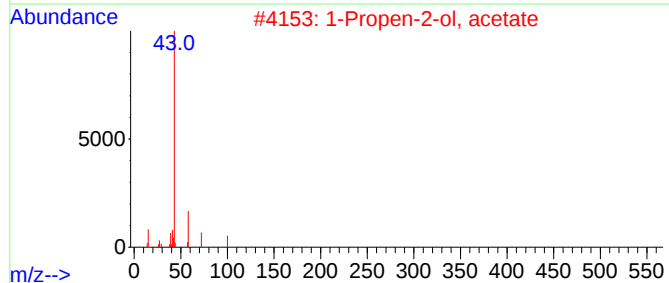
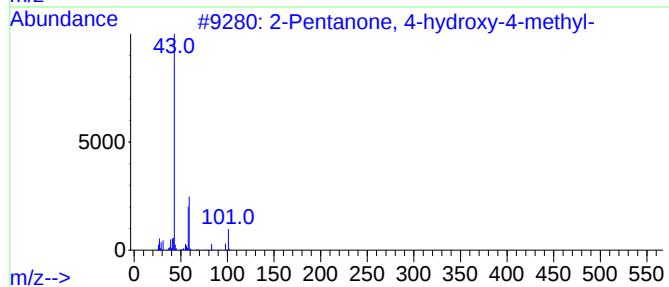
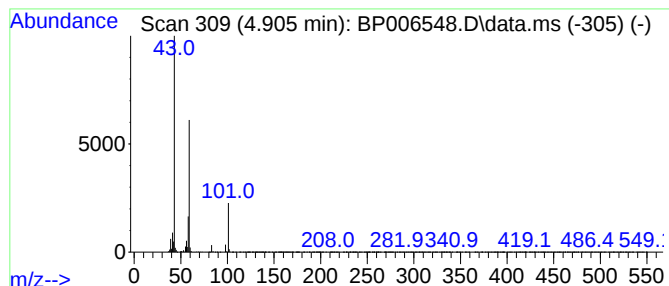
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.905	13.02 ng	960509	1,4-Dichlorobenzene-d4	7.752

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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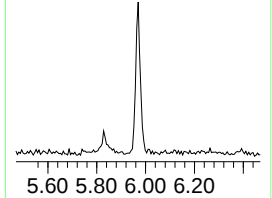
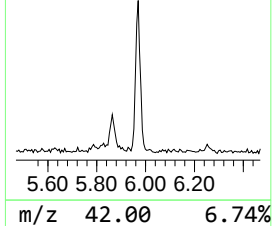
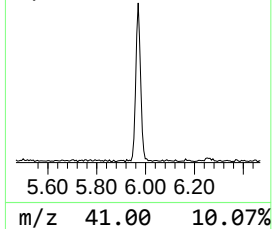
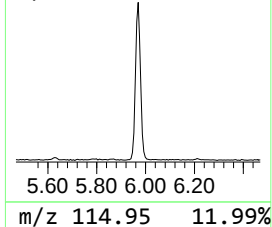
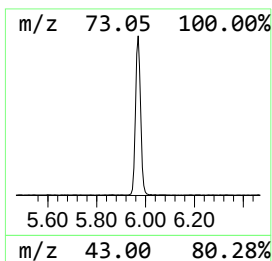
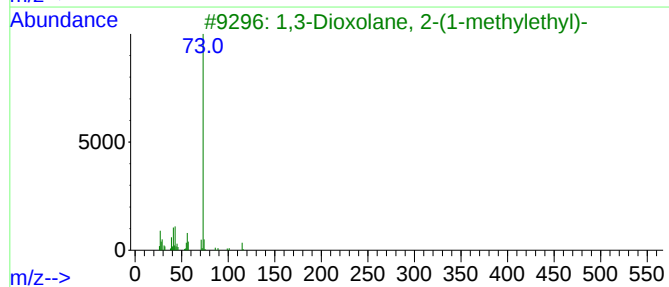
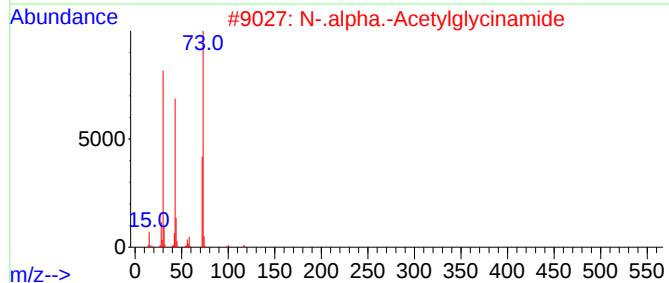
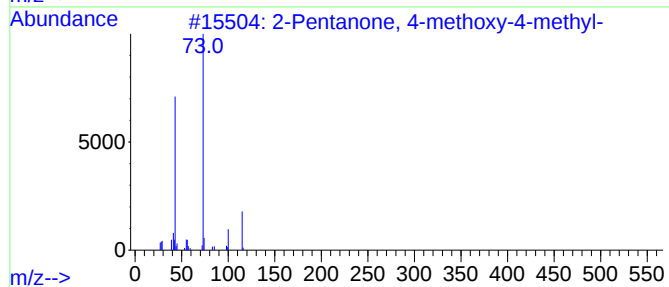
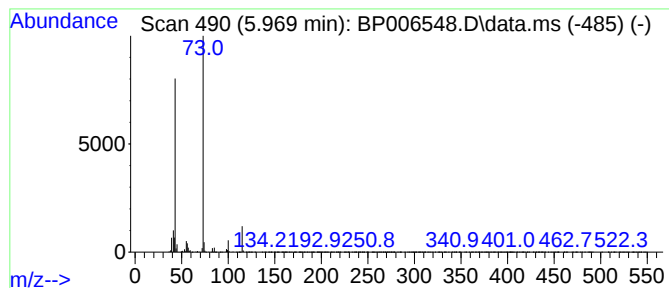
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Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.969	7.57 ng	558502	1,4-Dichlorobenzene-d4	7.752

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	40
3			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
4			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5			Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9



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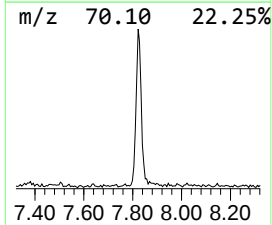
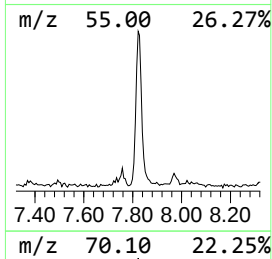
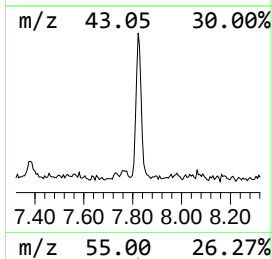
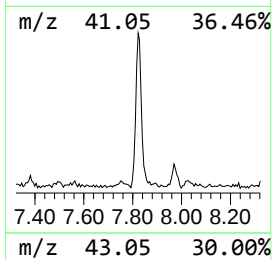
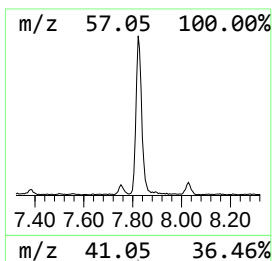
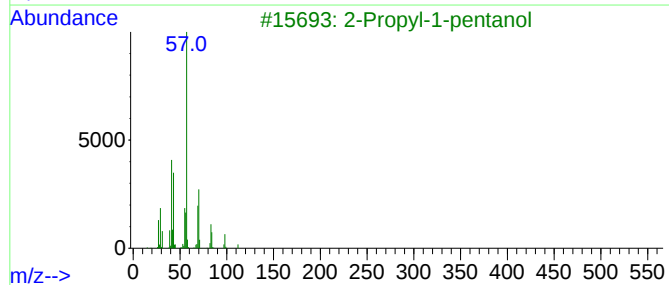
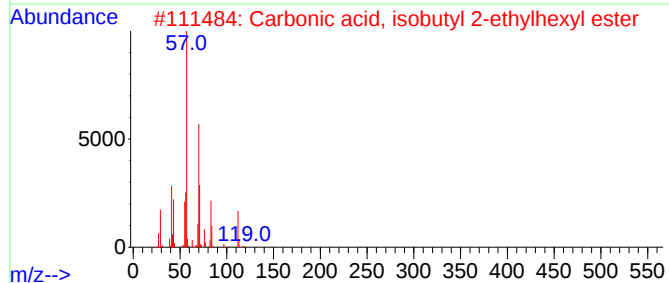
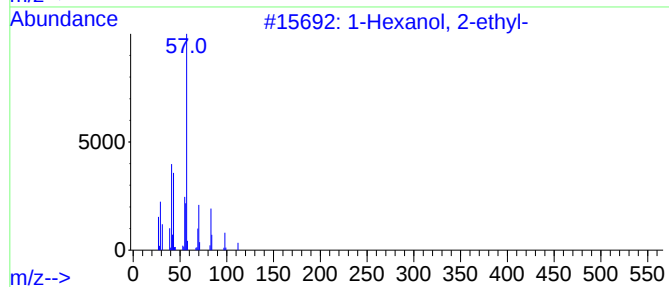
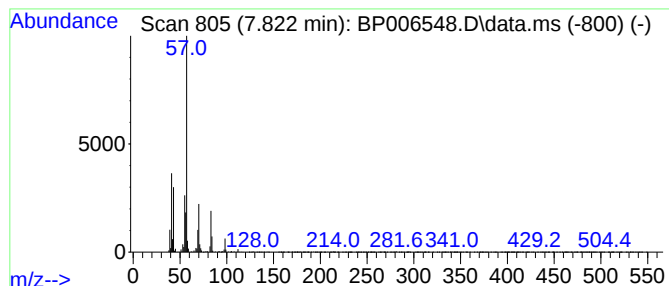
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.822	3.30 ng	243193	1,4-Dichlorobenzene-d4	7.752

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	50
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	43
5			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	43



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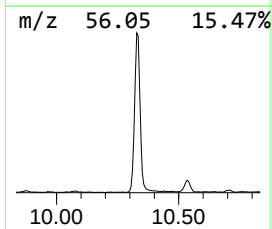
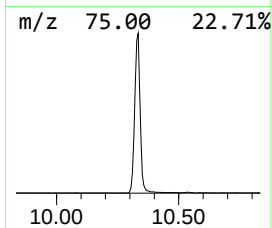
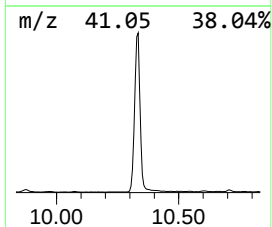
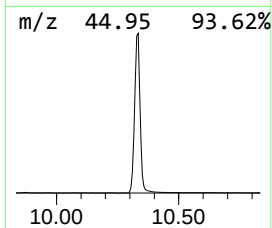
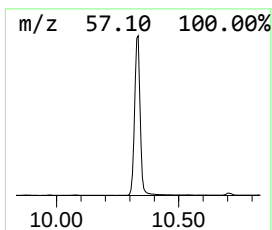
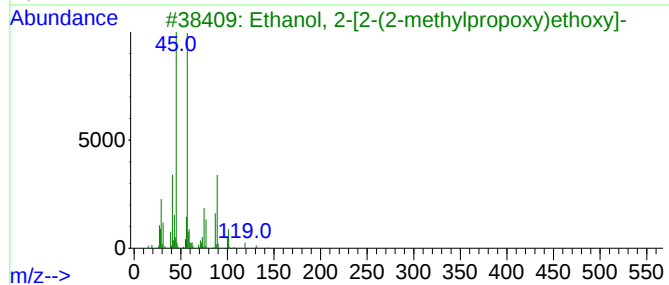
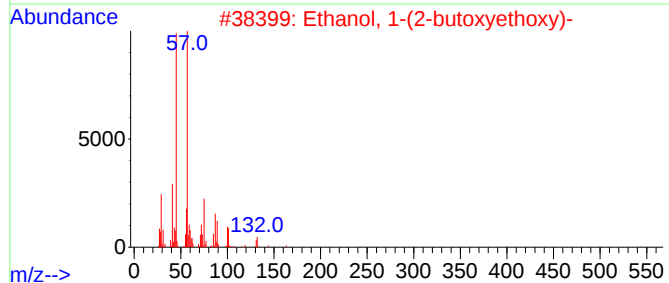
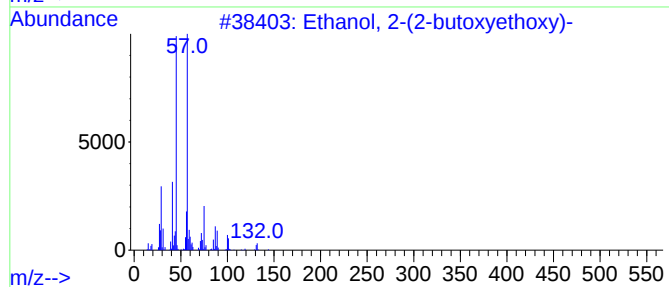
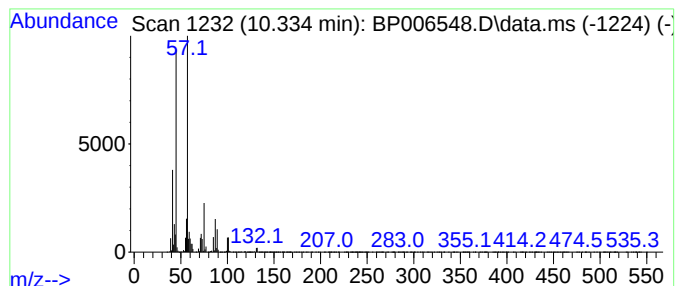
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.334	39.13 ng	4003670	Naphthalene-d8	10.534

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			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50



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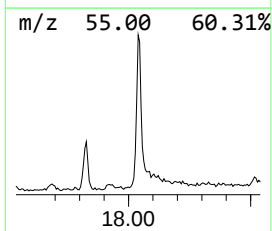
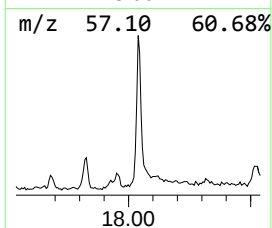
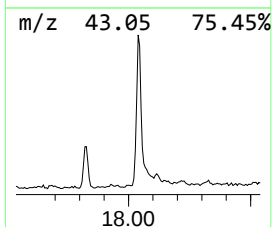
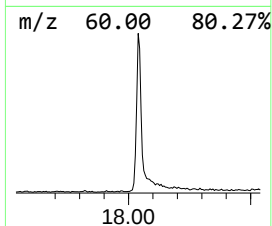
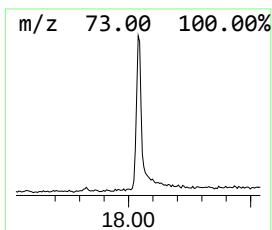
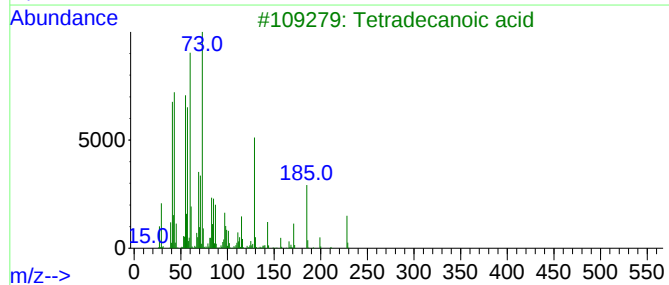
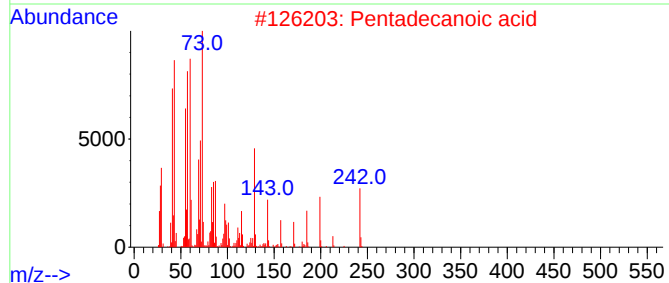
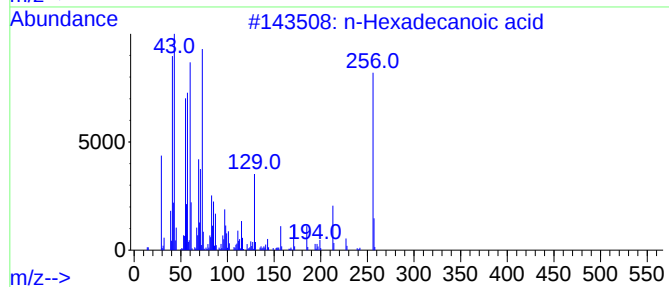
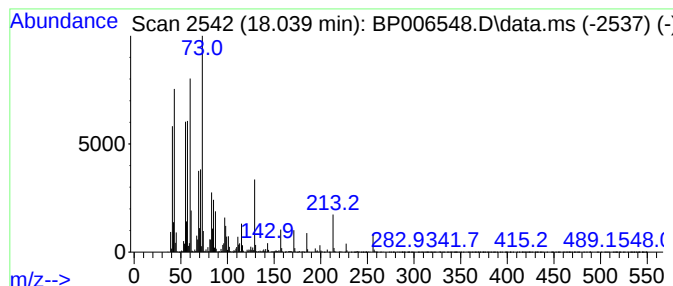
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.039	4.85 ng	716807	Phenanthrene-d10	17.133

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	78
4			Tridecanoic acid	214	C13H26O2	000638-53-9	72
5			Nonanoic acid	158	C9H18O2	000112-05-0	45



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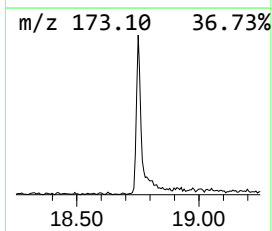
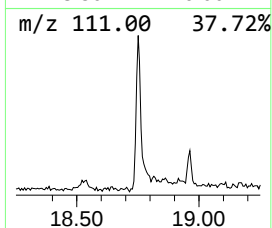
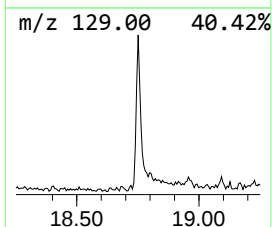
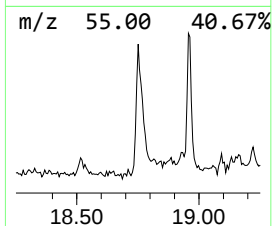
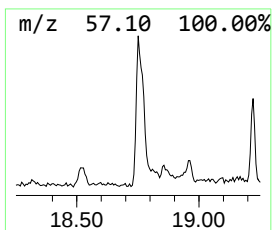
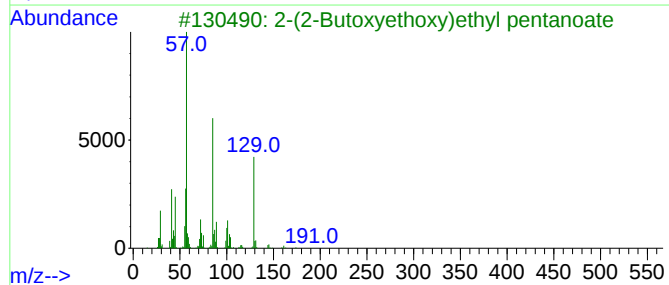
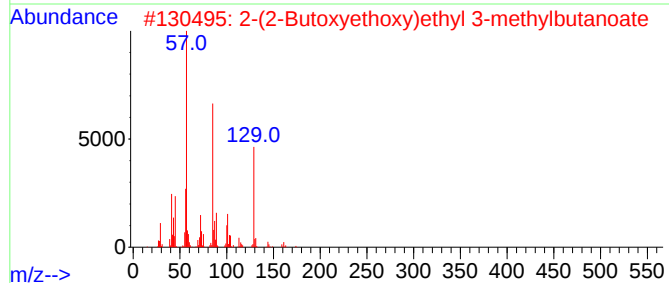
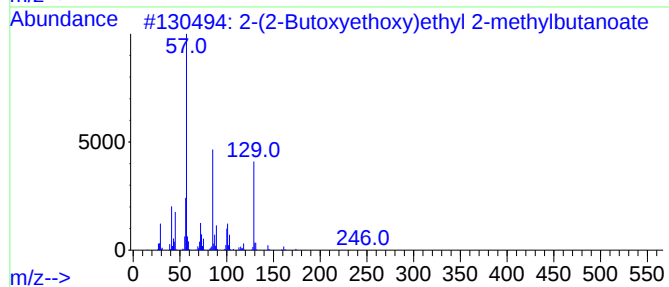
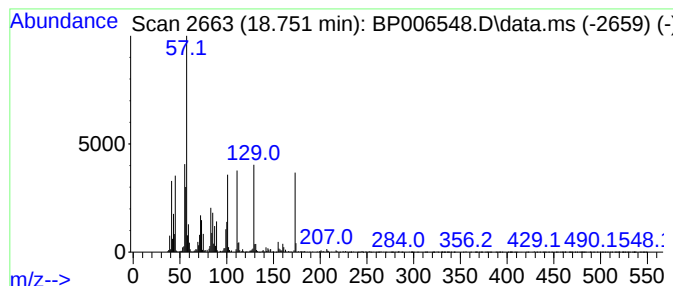
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown18.751 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.751	3.29 ng	486318	Phenanthrene-d10	17.133

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Butoxyethoxy)ethyl 2-methyl...	246	C13H26O4	1000366-96-6	38		
2	2-(2-Butoxyethoxy)ethyl 3-methyl...	246	C13H26O4	1000367-04-5	38		
3	2-(2-Butoxyethoxy)ethyl pentanoate	246	C13H26O4	1000367-00-4	25		
4	DL-Lactamide, N,O-dibutyl-	201	C11H23NO2	1000452-56-2	25		
5	Morpholine, 4-acetyl-	129	C6H11NO2	001696-20-4	14		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006548.D
Acq On : 06 Aug 2021 20:30
Operator : CG/JU
Sample : M3278-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

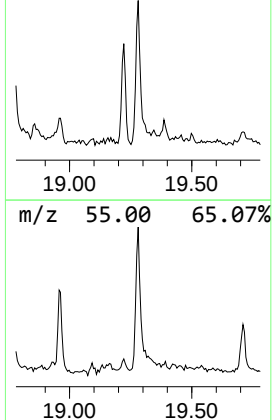
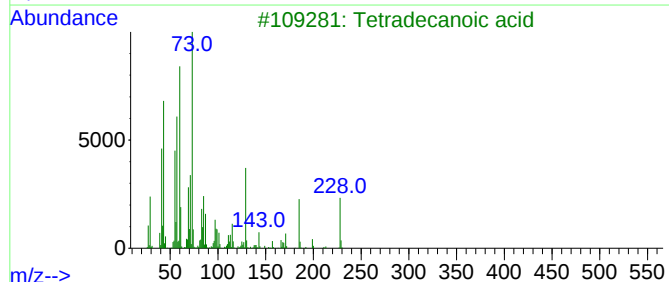
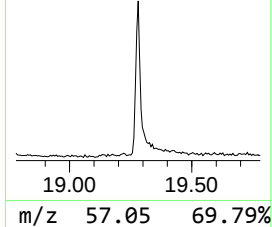
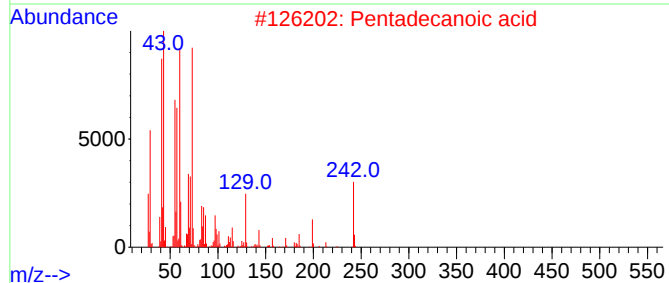
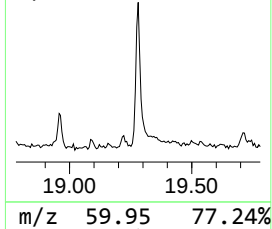
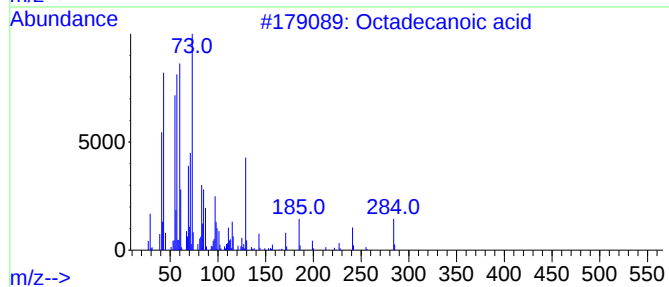
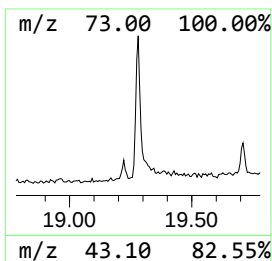
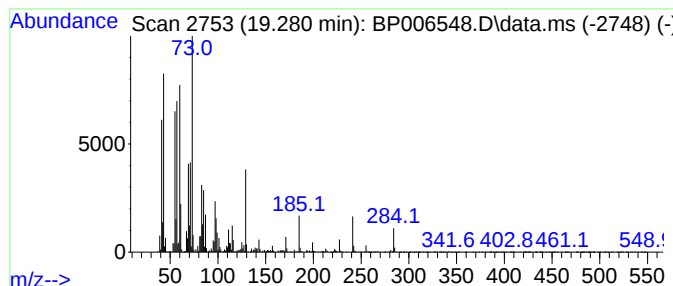
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.280	3.51 ng	555871	Chrysene-d12	21.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006548.D
Acq On : 06 Aug 2021 20:30
Operator : CG/JU
Sample : M3278-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

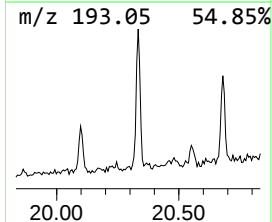
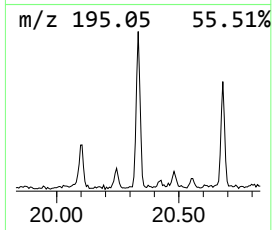
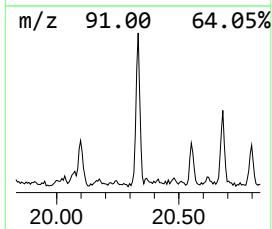
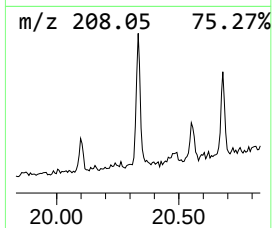
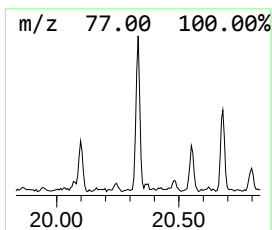
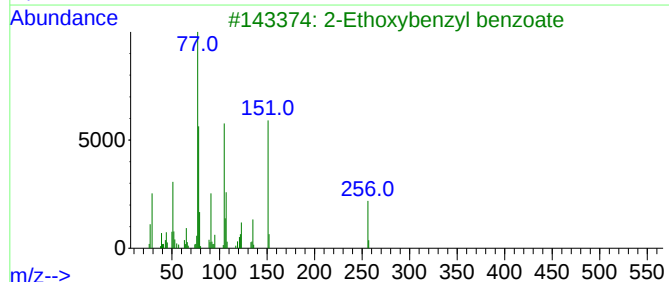
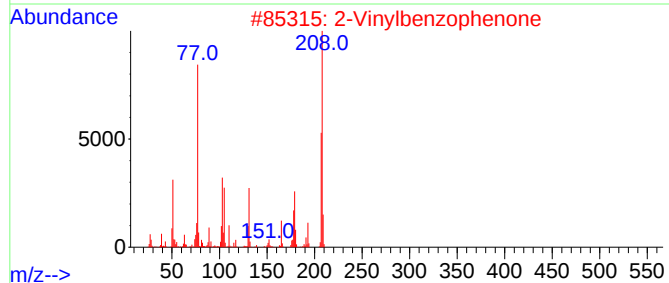
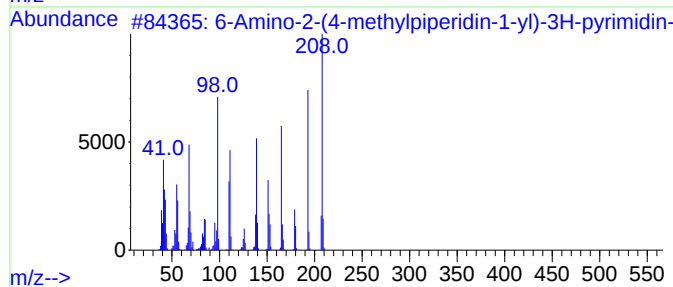
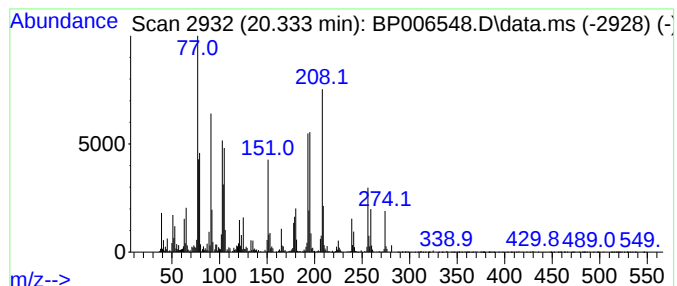
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown20.333 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.333	3.12 ng	494134	Chrysene-d12	21.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Amino-2-(4-methylpiperidin-1-y...	208	C10H16N4O	1000388-65-9	46		
2	2-Vinylbenzophenone	208	C15H12O	052095-42-8	30		
3	2-Ethoxybenzyl benzoate	256	C16H16O3	1000433-46-8	25		
4	2,2',4,4'-Tetramethyldiphenylsul...	274	C16H18O2S	005184-75-8	22		
5	Benzene, 1,1'-(1,2-dimethyl-1,2-...	208	C16H16	000782-06-9	22		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006548.D
Acq On : 06 Aug 2021 20:30
Operator : CG/JU
Sample : M3278-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

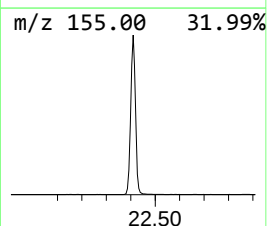
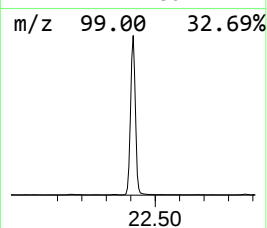
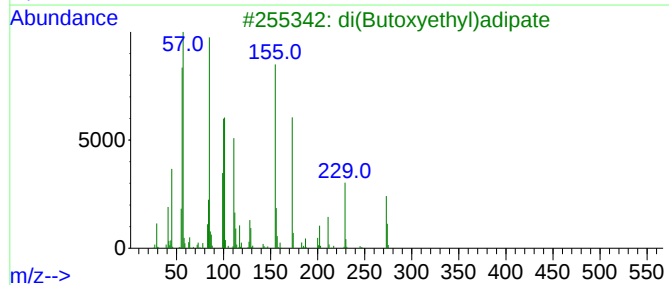
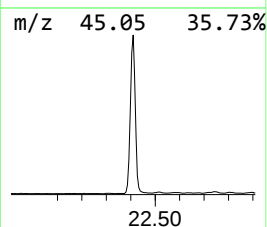
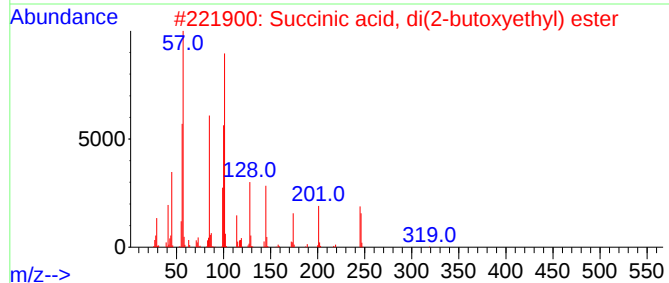
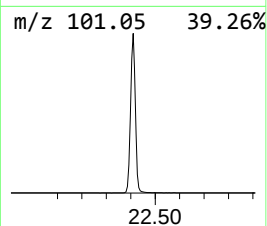
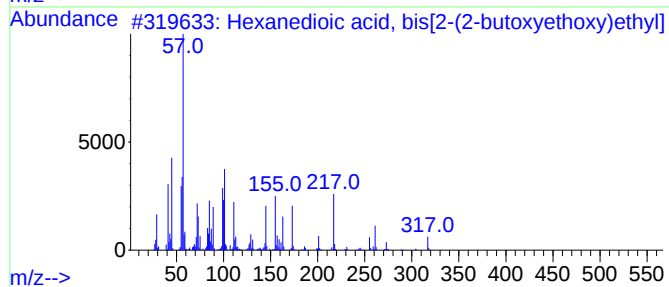
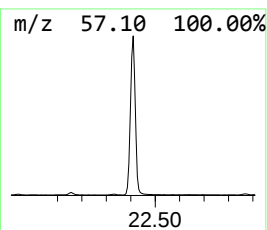
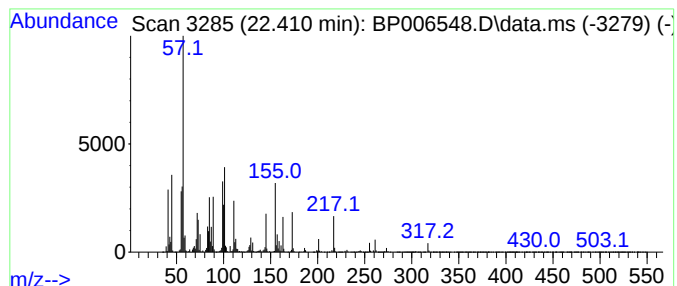
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexanedioic acid, bis[2-(2-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.410	74.65 ng	12569900	Perylene-d12	23.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, bis[2-(2-butox...	434	C22H42O8	000141-17-3	91
2			Succinic acid, di(2-butoxyethyl)...	318	C16H30O6	1010325-84-7	25
3			di(Butoxyethyl)adipate	346	C18H34O6	000141-18-4	23
4			1-Methyl-3-pyrrolidinol	101	C5H11NO	013220-33-2	11
5			Propane, 1,1'-[ethylidenebis(oxy...	174	C10H22O2	005669-09-0	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006548.D
Acq On : 06 Aug 2021 20:30
Operator : CG/JU
Sample : M3278-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.905	13.0	ng	960509	1	7.752	1475070	20.0
2-Pentanone, 4-...	5.969	7.6	ng	558502	1	7.752	1475070	20.0
1-Hexanol, 2-et...	7.822	3.3	ng	243193	1	7.752	1475070	20.0
Ethanol, 2-(2-b...	10.334	39.1	ng	4003670	2	10.534	2046470	20.0
n-Hexadecanoic ...	18.039	4.8	ng	716807	4	17.133	2958740	20.0
unknown18.751	18.751	3.3	ng	486318	4	17.133	2958740	20.0
Octadecanoic acid	19.280	3.5	ng	555871	5	21.233	3163890	20.0
unknown20.333	20.333	3.1	ng	494134	5	21.233	3163890	20.0
Hexanedioic aci...	22.410	74.7	ng	12569900	6	23.557	3367740	20.0