

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092722\
 Data File : BP011821.D
 Acq On : 27 Sep 2022 18:20
 Operator : CG/JU
 Sample : N4833-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 004-2

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-BP092122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP011821.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.046	6	10	38	rVB	8427369	13728537	59.09%	12.021%
2	5.011	337	344	353	rBV	163419	257256	1.11%	0.225%
3	5.469	415	422	440	rBV	2191674	3477292	14.97%	3.045%
4	7.069	686	694	713	rBV	1543321	2606663	11.22%	2.282%
5	7.910	829	837	846	rBV	1228737	2024156	8.71%	1.772%
6	9.075	1027	1035	1050	rBV	3917149	6595890	28.39%	5.776%
7	10.499	1270	1277	1297	rBV	932968	1759218	7.57%	1.540%
8	10.722	1307	1315	1327	rVB	1679332	2943638	12.67%	2.578%
9	12.987	1693	1700	1716	rBV2	164504	350703	1.51%	0.307%
10	13.181	1725	1733	1746	rBV	9815708	15030302	64.69%	13.161%
11	14.551	1959	1966	1979	rBV	2635033	3963864	17.06%	3.471%
12	16.045	2213	2220	2237	rBV	4760216	6812431	29.32%	5.965%
13	17.310	2428	2435	2446	rBV	3409090	4877094	20.99%	4.271%
14	17.975	2544	2548	2556	rVB	288347	347059	1.49%	0.304%
15	18.192	2580	2585	2591	rBV	178416	330368	1.42%	0.289%
16	18.263	2592	2597	2611	rVB	8514045	10599910	45.62%	9.282%
17	19.104	2736	2740	2745	rBV	222543	243634	1.05%	0.213%
18	19.422	2790	2794	2807	rBV	319449	653633	2.81%	0.572%
19	19.869	2864	2870	2879	rBV	17630637	23235080	100.00%	20.346%
20	21.098	3075	3079	3087	rBV2	325049	637578	2.74%	0.558%
21	21.392	3124	3129	3140	rBV	4240036	5500874	23.67%	4.817%
22	21.516	3145	3150	3163	rBV	1548461	2601191	11.20%	2.278%
23	23.833	3538	3544	3554	rVB2	2787080	5625997	24.21%	4.926%

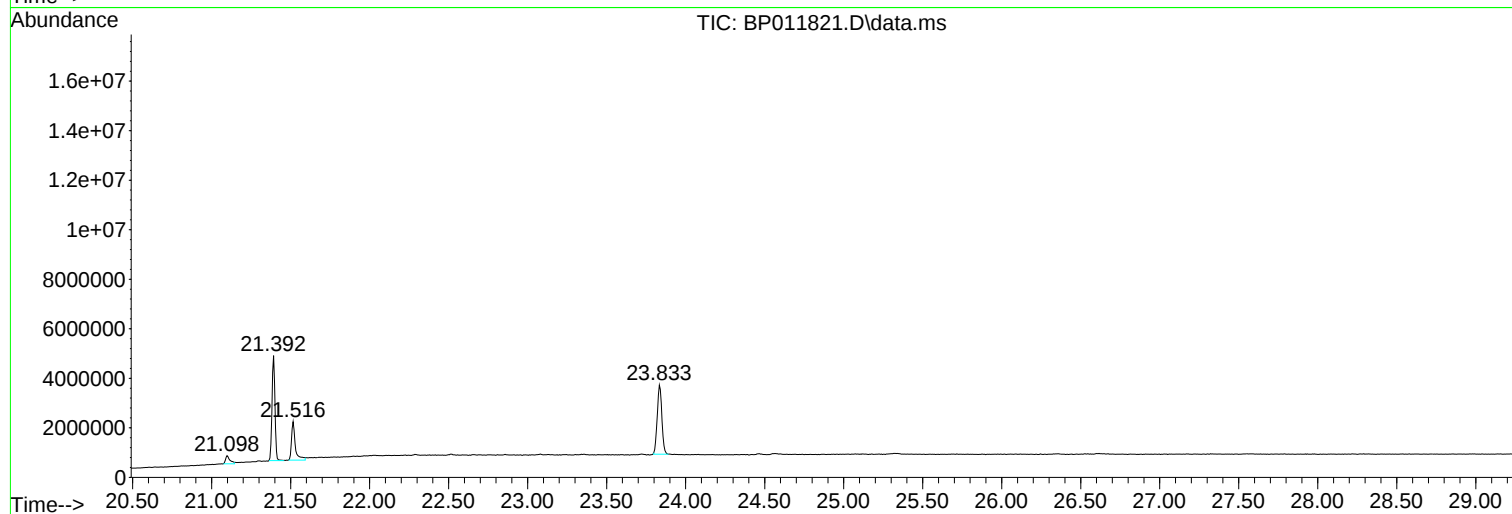
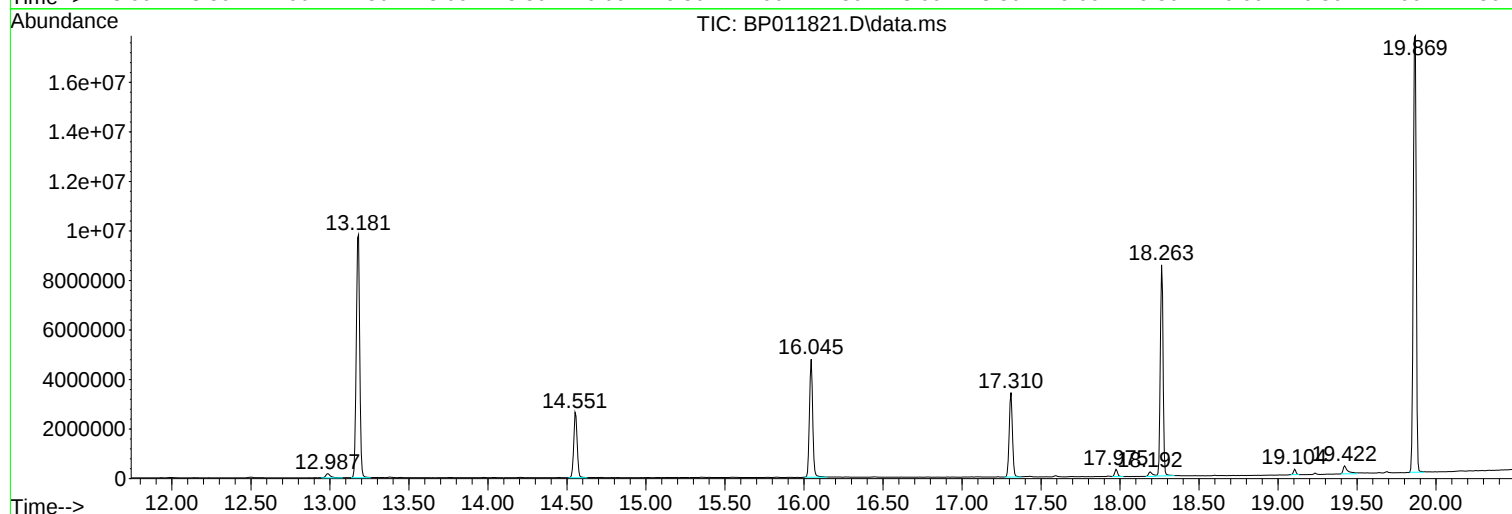
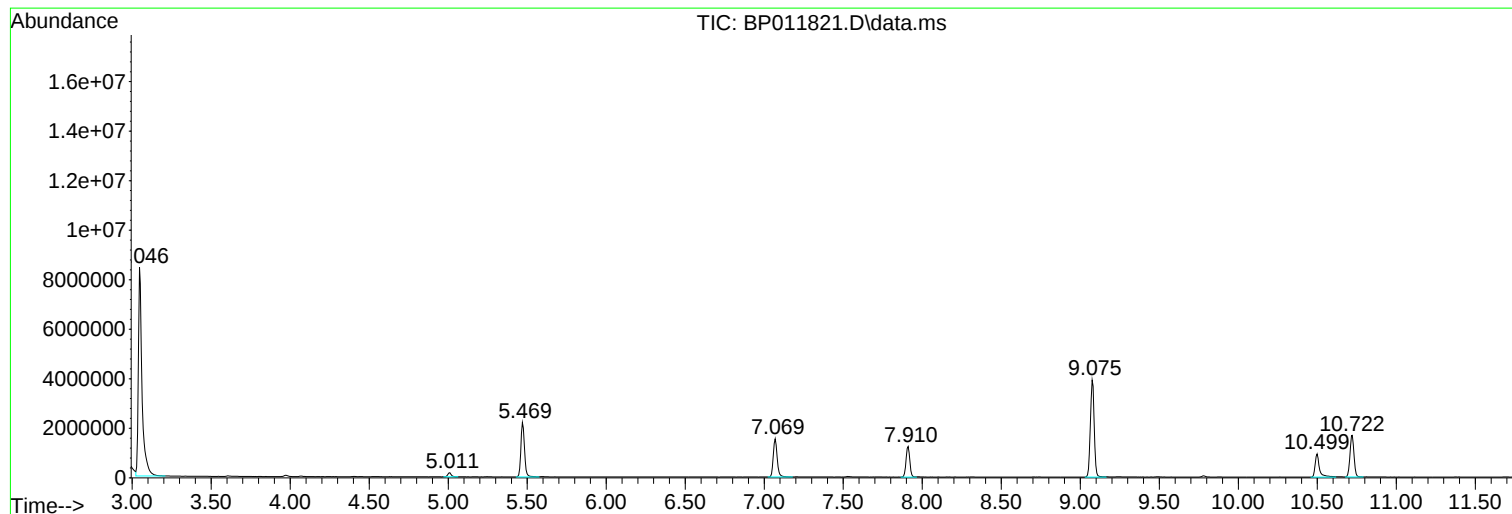
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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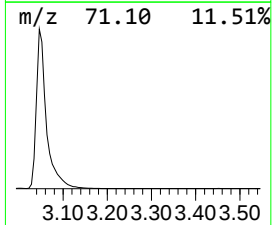
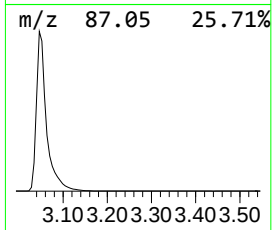
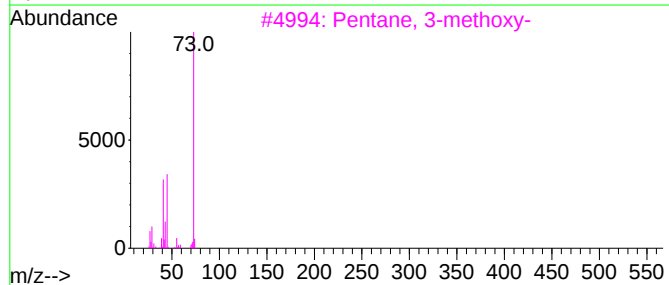
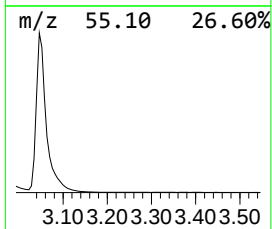
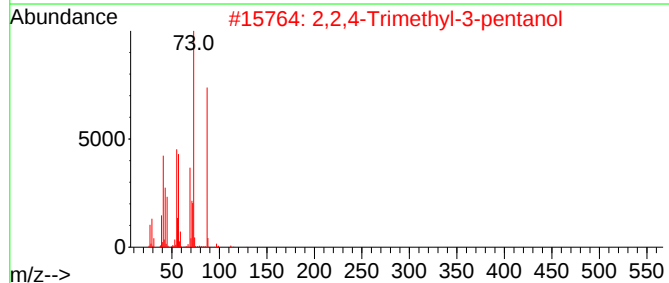
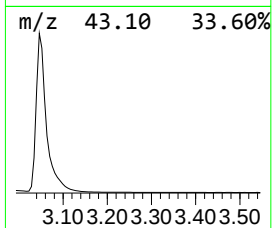
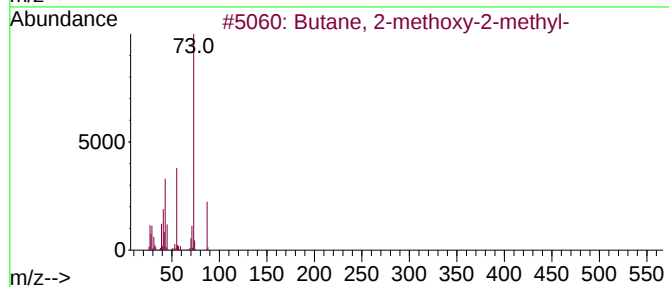
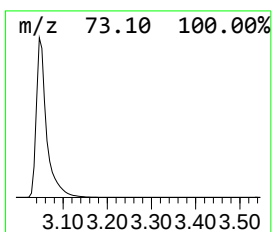
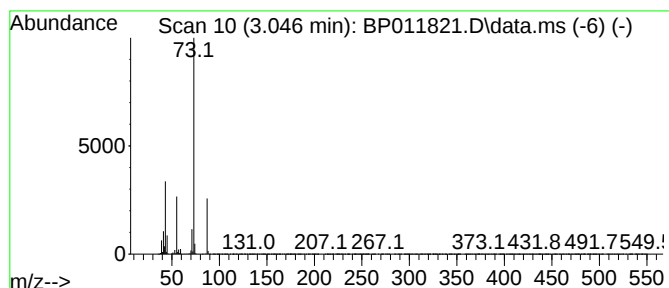
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.046	135.65 ng	13728500	1,4-Dichlorobenzene-d4	7.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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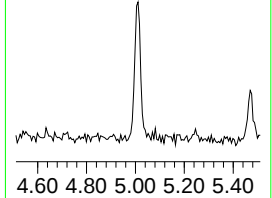
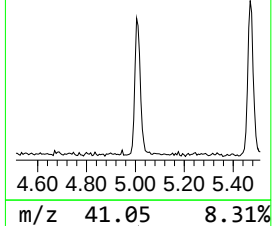
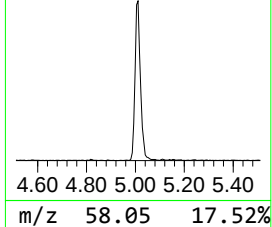
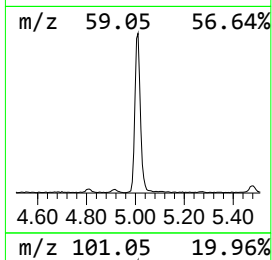
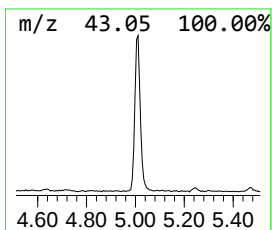
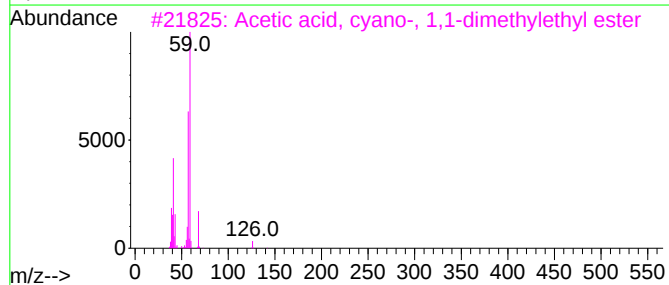
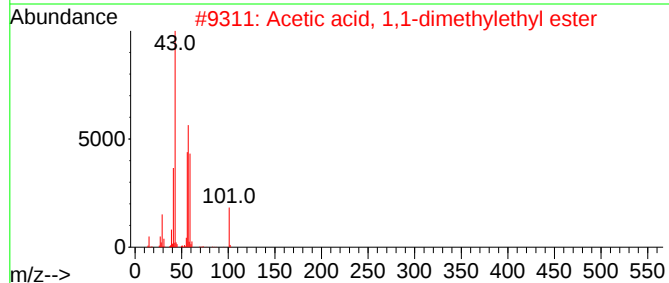
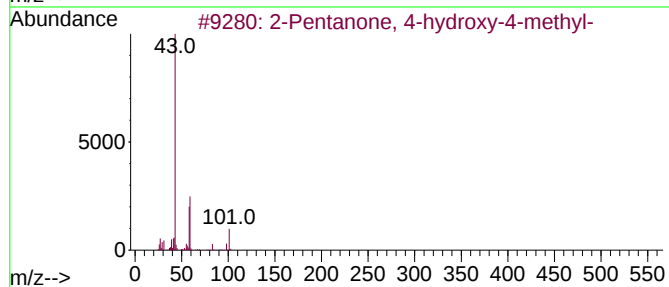
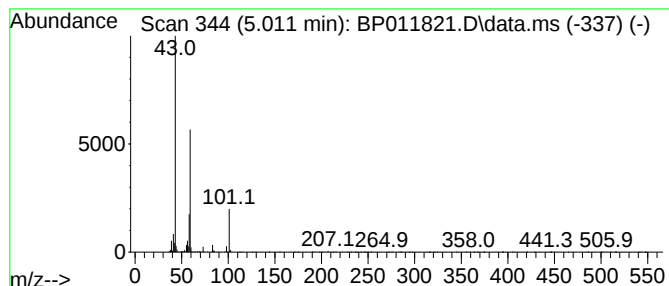
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.011	2.54 ng	257256	1,4-Dichlorobenzene-d4	7.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
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			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25



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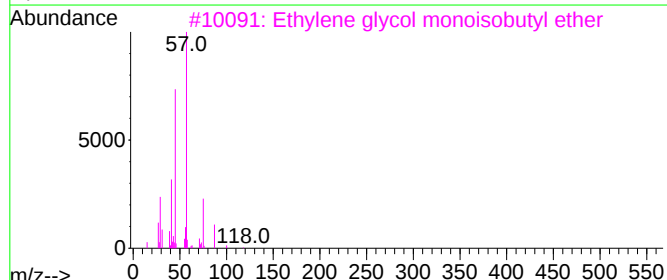
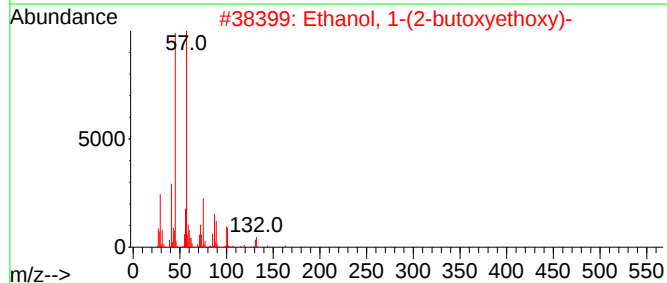
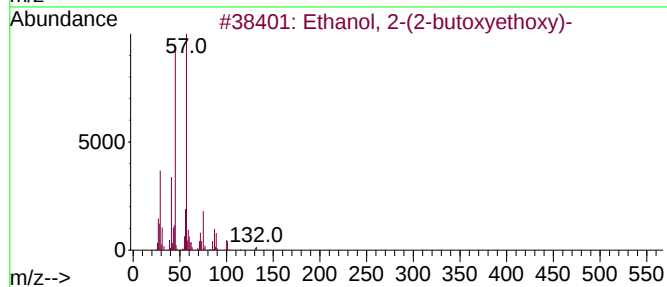
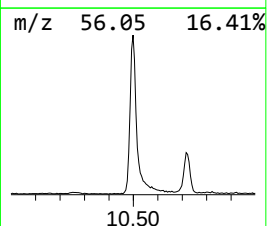
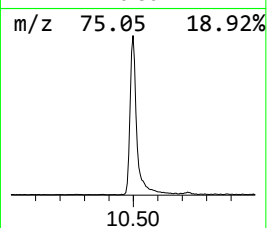
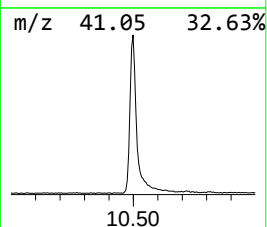
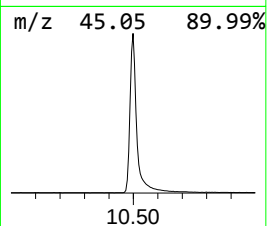
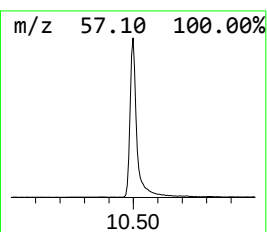
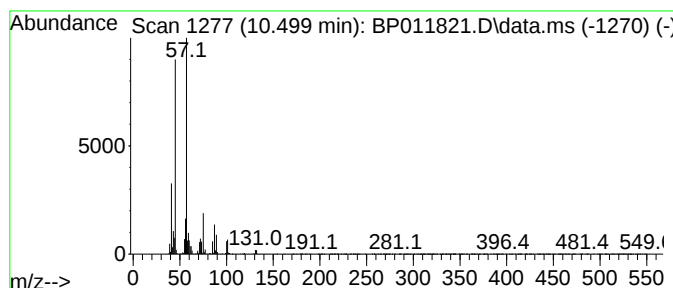
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.499	11.95 ng	1759220	Naphthalene-d8	10.722	
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	78
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	58
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56



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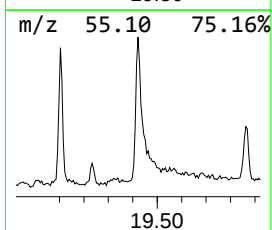
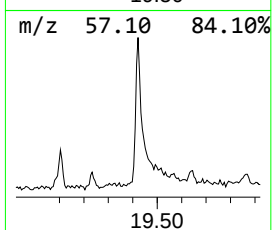
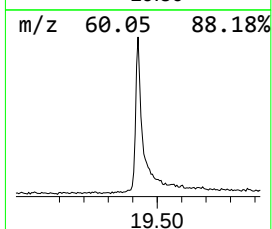
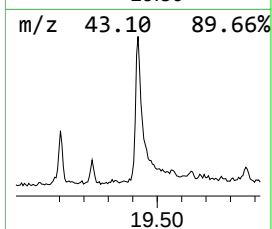
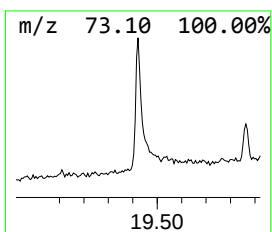
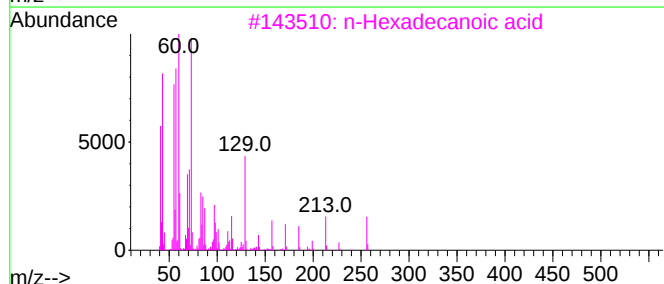
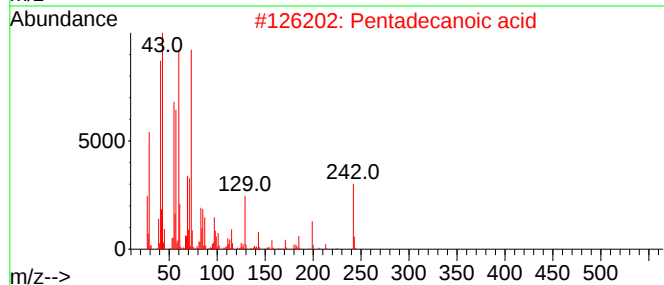
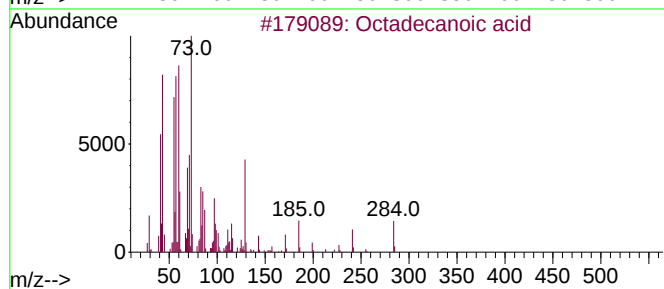
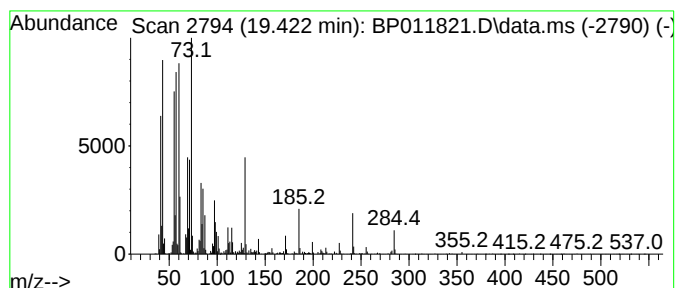
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.422	2.38 ng	653633	Chrysene-d12	21.392

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	94
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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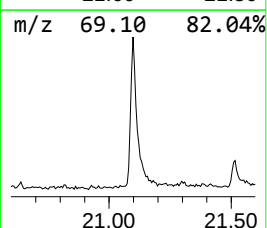
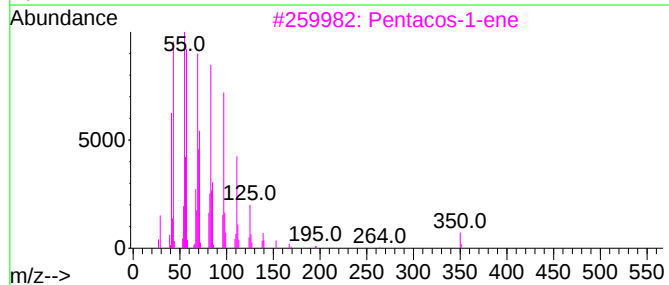
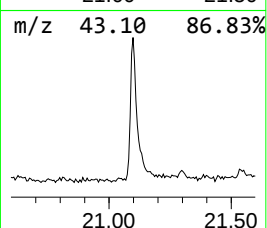
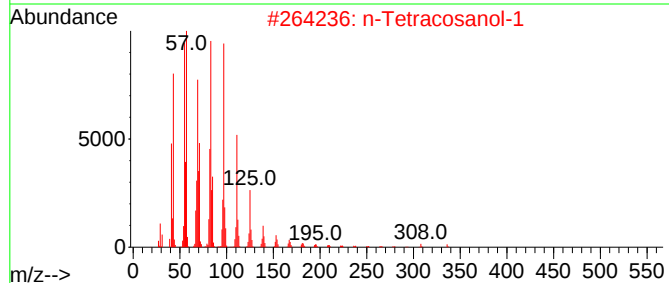
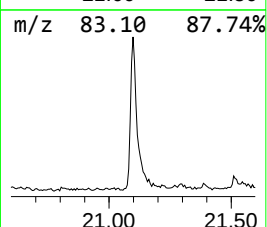
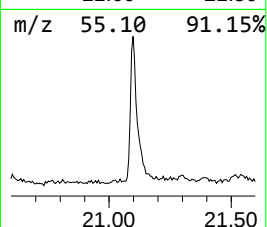
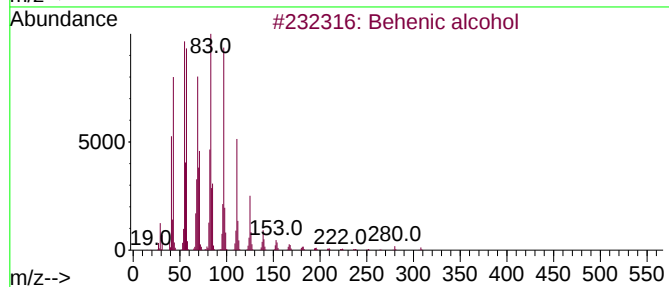
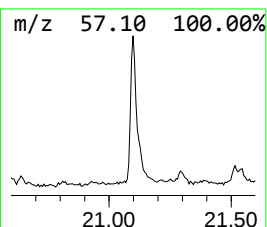
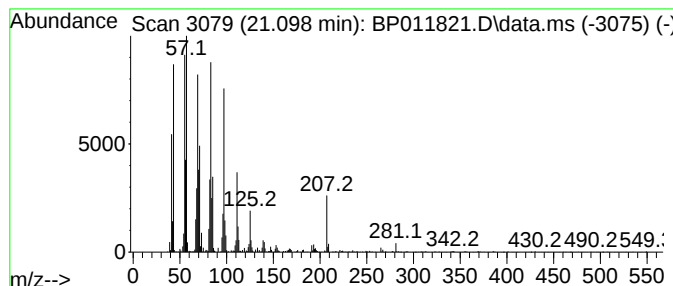
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.098	2.32 ng	637578	Chrysene-d12	21.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	94
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			Pentacos-1-ene	350	C25H50	016980-85-1	94
4			Heptacos-1-ene	378	C27H54	015306-27-1	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91



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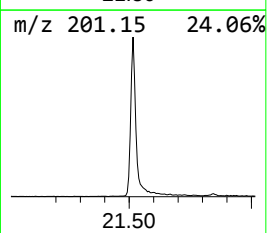
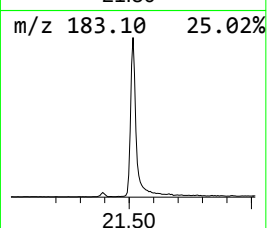
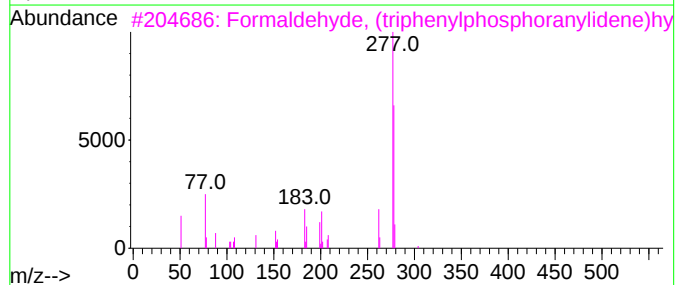
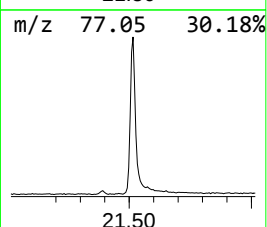
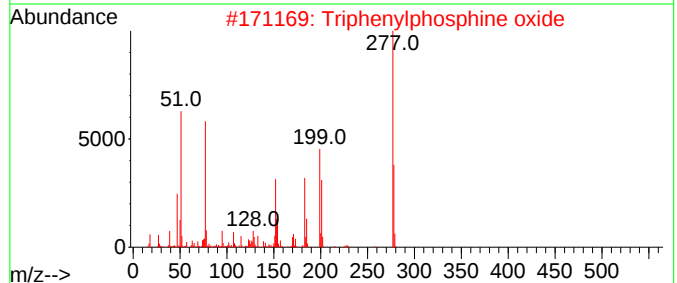
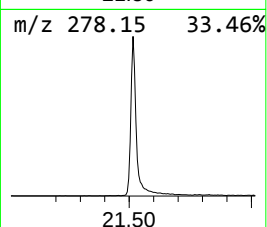
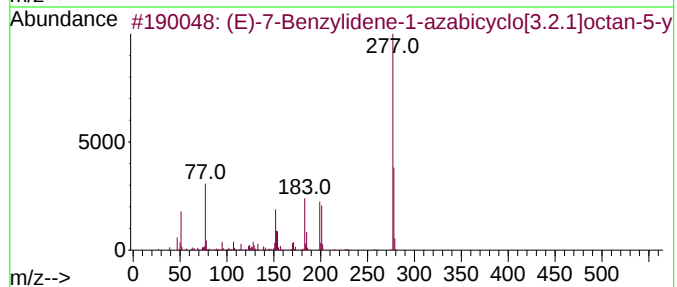
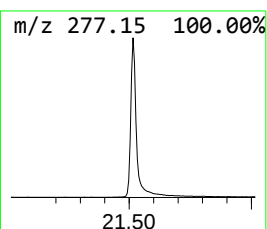
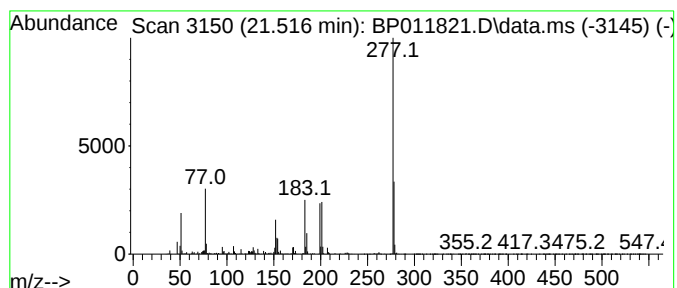
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 (E)-7-Benzylidene-1-azabicyclo... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.516	9.46 ng	2601190	Chrysene-d12	21.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	94		
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	83		
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50		
4	4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	43		
5	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092722\
Data File : BP011821.D
Acq On : 27 Sep 2022 18:20
Operator : CG/JU
Sample : N4833-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
004-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.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
Butane, 2-metho...	3.046	135.7	ng	13728500	1	7.910	2024160	20.0
2-Pentanone, 4-...	5.011	2.5	ng	257256	1	7.910	2024160	20.0
Ethanol, 2-(2-b...	10.499	11.9	ng	1759220	2	10.722	2943640	20.0
Octadecanoic acid	19.422	2.4	ng	653633	5	21.392	5500870	20.0
Behenic alcohol	21.098	2.3	ng	637578	5	21.392	5500870	20.0
(E)-7-Benzylide...	21.516	9.5	ng	2601190	5	21.392	5500870	20.0