

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
 Data File : BP006534.D
 Acq On : 06 Aug 2021 12:04
 Operator : CG/JU
 Sample : M3271-10
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TP-4

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: BP006534.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	304	309	316	rBV	1119491	1505668	16.90%	2.447%
2	5.358	380	386	397	rVB	3489132	4877366	54.74%	7.926%
3	5.970	485	490	496	rVB	220818	312783	3.51%	0.508%
4	6.934	647	654	669	rBV	3418197	5153398	57.84%	8.375%
5	7.752	787	793	800	rVB	851667	1354340	15.20%	2.201%
6	8.911	983	990	997	rBV	2057679	3306421	37.11%	5.373%
7	10.328	1225	1231	1239	rBV	223956	355718	3.99%	0.578%
8	10.540	1258	1267	1272	rBV	1189554	1977411	22.19%	3.213%
9	13.010	1680	1687	1701	rBV	4325092	6248262	70.13%	10.154%
10	14.381	1914	1920	1927	rBV	1670919	2485919	27.90%	4.040%
11	14.446	1927	1931	1939	rVB	76100	116865	1.31%	0.190%
12	15.434	2093	2099	2103	rBV	74923	103208	1.16%	0.168%
13	15.875	2161	2174	2183	rBV	3809308	5317784	59.68%	8.642%
14	17.140	2382	2389	2392	rBV	1974326	2882820	32.36%	4.685%
15	17.175	2392	2395	2402	rVV	787174	1115666	12.52%	1.813%
16	17.269	2402	2411	2417	rVB	140984	240849	2.70%	0.391%
17	18.010	2532	2537	2539	rBV2	96519	136692	1.53%	0.222%
18	18.045	2539	2543	2551	rVV2	857371	1194874	13.41%	1.942%
19	18.192	2563	2568	2572	rBV2	132902	238671	2.68%	0.388%
20	18.228	2572	2574	2581	rVB	81358	106109	1.19%	0.172%
21	18.534	2623	2626	2637	rVB	74290	108976	1.22%	0.177%
22	18.898	2684	2688	2692	rBV2	60064	92424	1.04%	0.150%
23	19.028	2706	2710	2718	rVB4	47651	90827	1.02%	0.148%
24	19.151	2726	2731	2737	rBV	984039	1293772	14.52%	2.102%
25	19.281	2749	2753	2759	rBV	323709	446870	5.02%	0.726%
26	19.504	2782	2791	2796	rBV	888782	1347470	15.12%	2.190%
27	19.710	2818	2826	2836	rBV	7382927	8909776	100.00%	14.479%
28	19.992	2870	2874	2877	rVB	123504	152708	1.71%	0.248%
29	20.145	2896	2900	2904	rVB2	63094	101209	1.14%	0.164%
30	20.957	3035	3038	3044	rBV2	597525	771288	8.66%	1.253%
31	21.163	3070	3073	3077	rVB	157477	157665	1.77%	0.256%
32	21.233	3078	3085	3089	rVV2	2650090	3800582	42.66%	6.176%
33	21.269	3089	3091	3097	rVB	398508	446027	5.01%	0.725%
34	21.863	3187	3192	3196	rBV5	181409	378953	4.25%	0.616%
35	22.857	3356	3361	3367	rBV2	276675	743158	8.34%	1.208%
36	23.457	3459	3463	3472	rVB2	242954	512344	5.75%	0.833%

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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

37 23.563 3474 3481 3487 rBV2 1596523 3151660 35.37% 5.122%

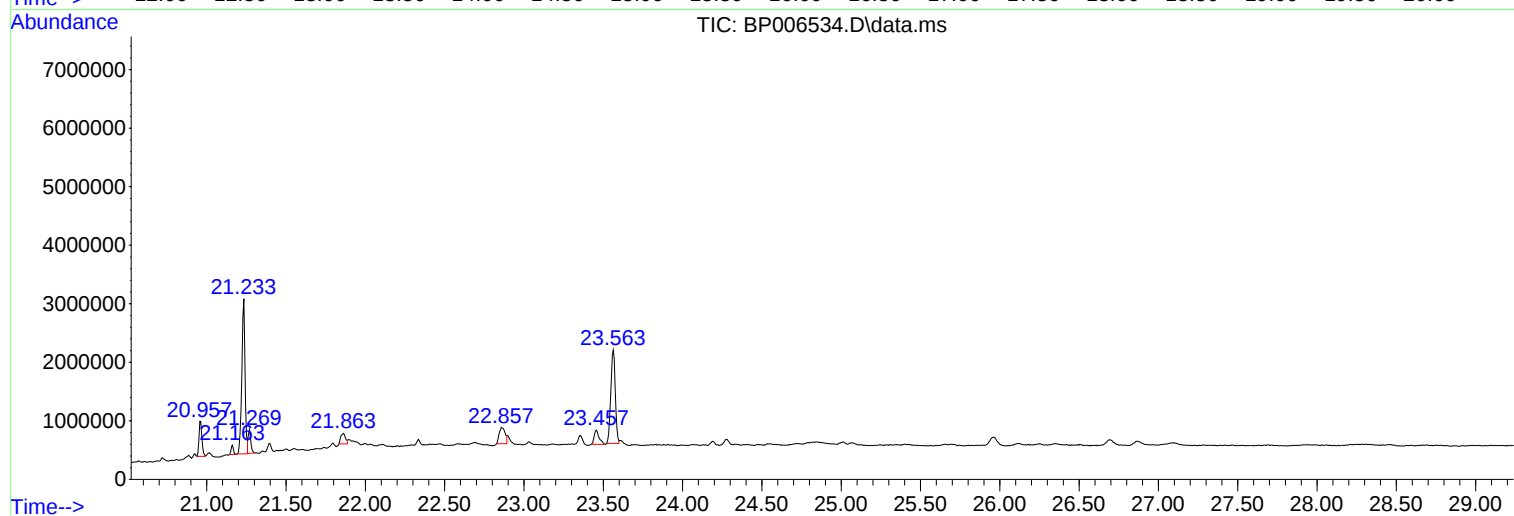
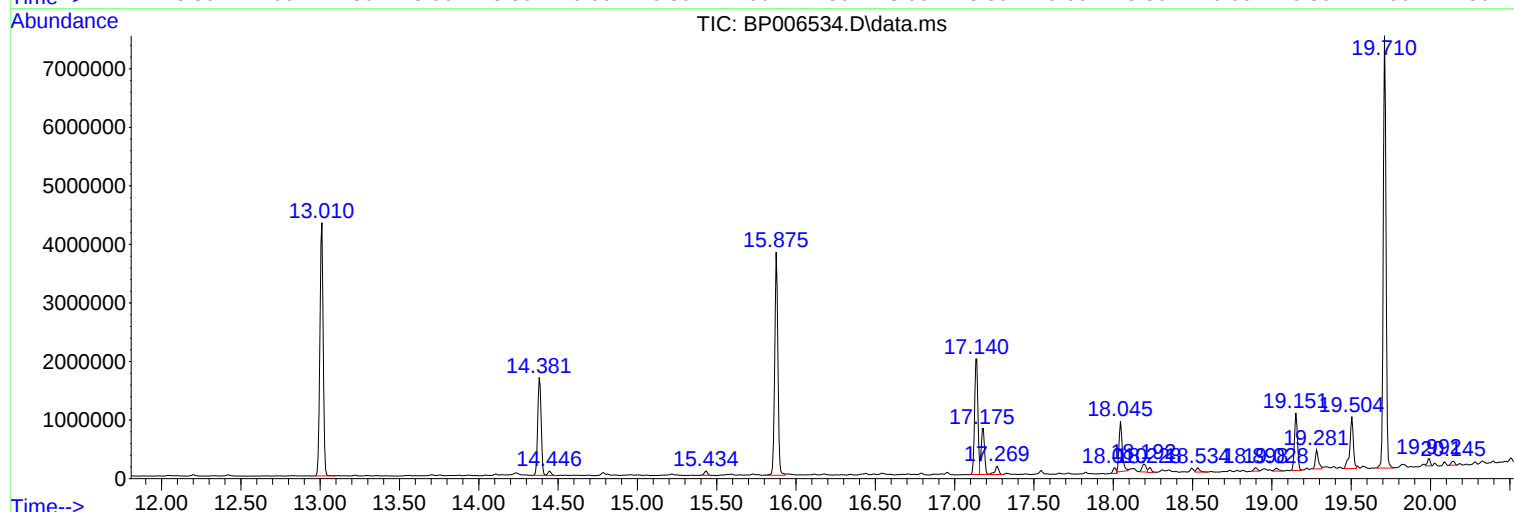
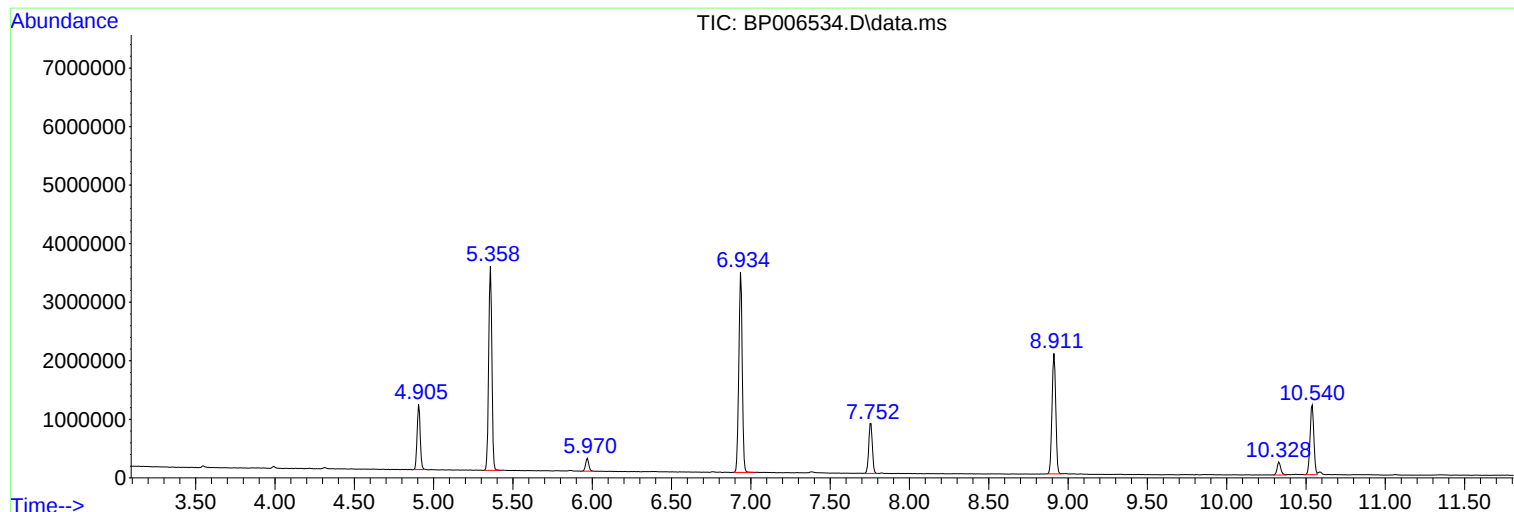
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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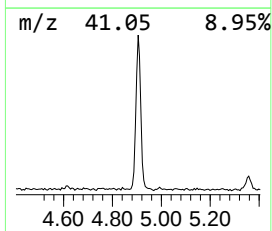
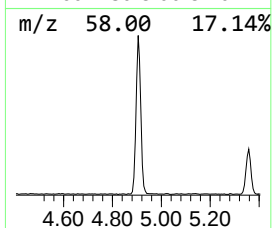
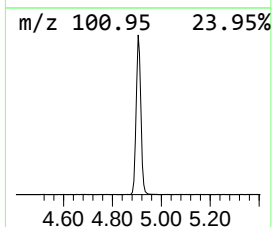
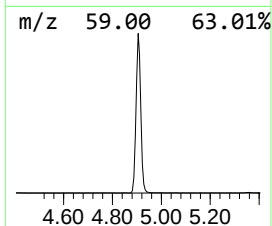
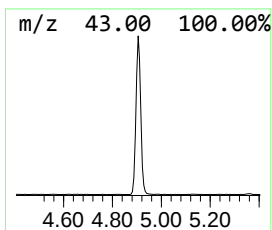
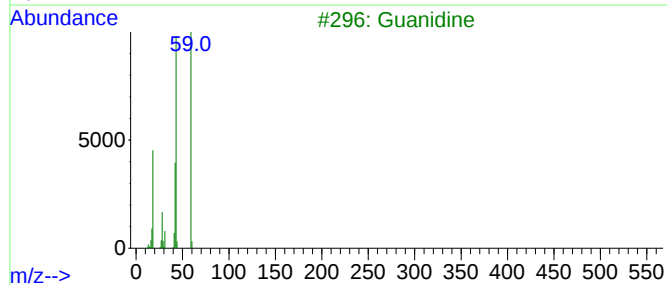
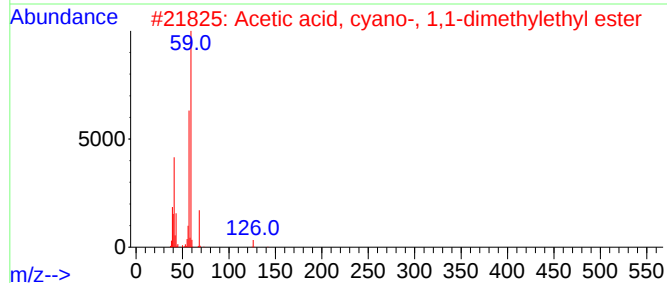
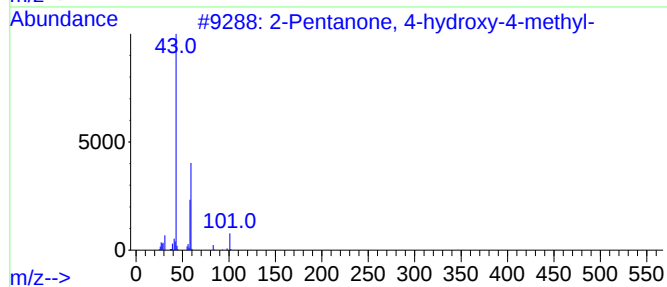
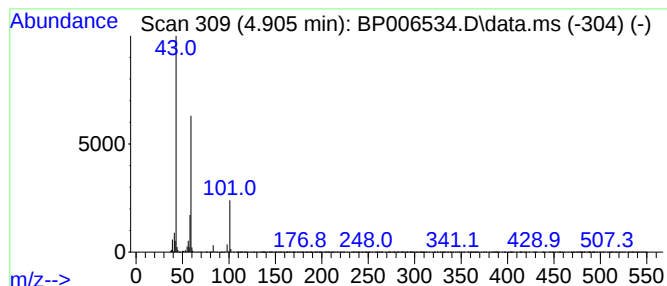
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.905	22.23 ng	1505670	1,4-Dichlorobenzene-d4	7.758

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
3	Guanidine	59	CH5N3	000113-00-8	9		
4	Acetone	58	C3H6O	000067-64-1	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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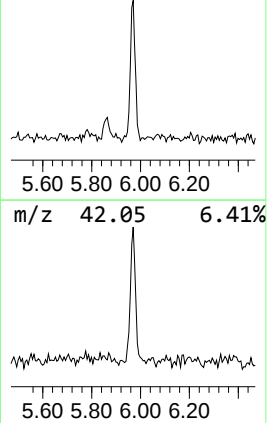
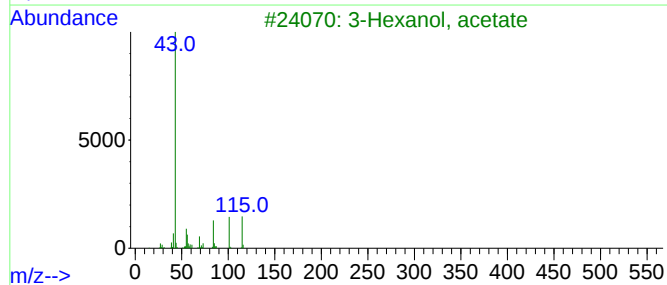
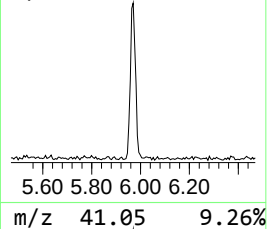
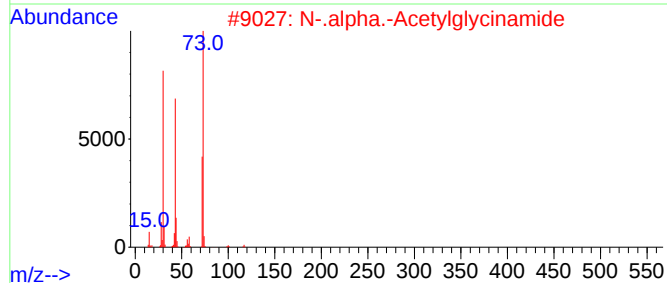
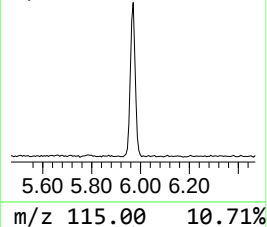
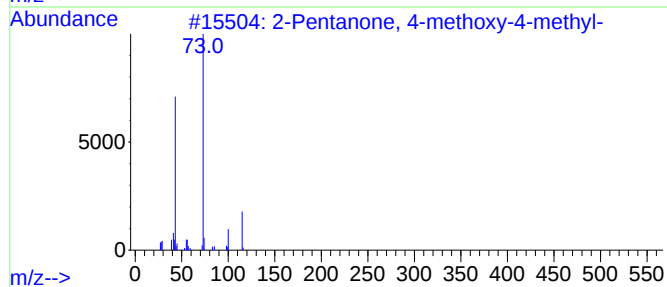
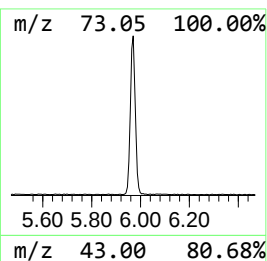
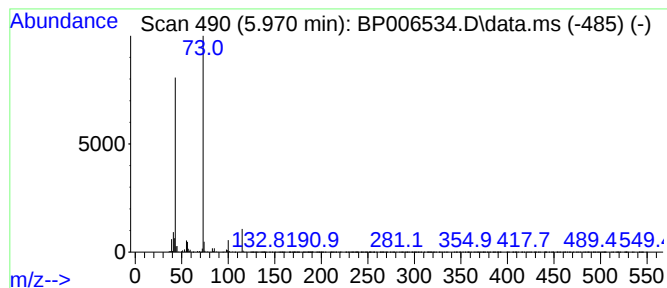
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.970	4.62 ng	312783	1,4-Dichlorobenzene-d4	7.758

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			3-Hexanol, acetate	144	C8H16O2	040780-64-1	23
4			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
5			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9



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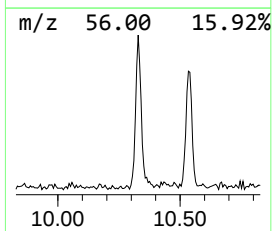
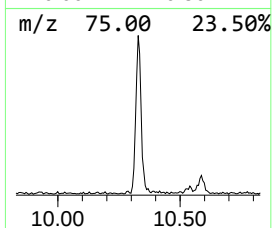
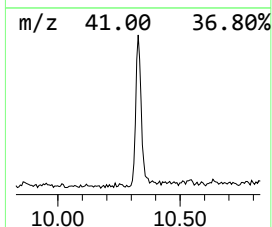
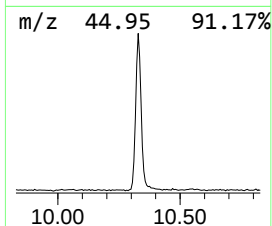
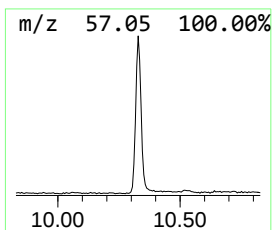
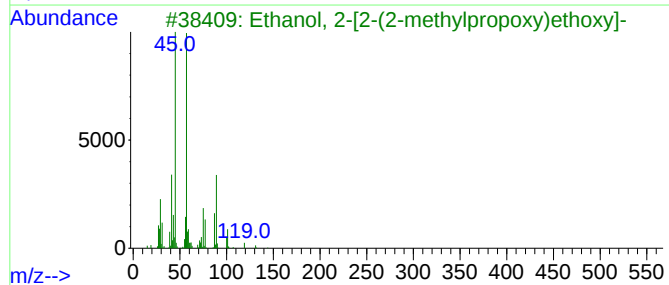
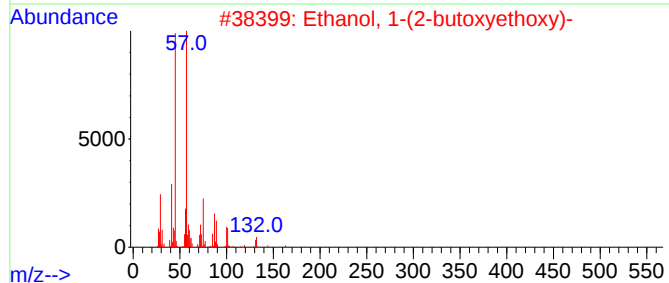
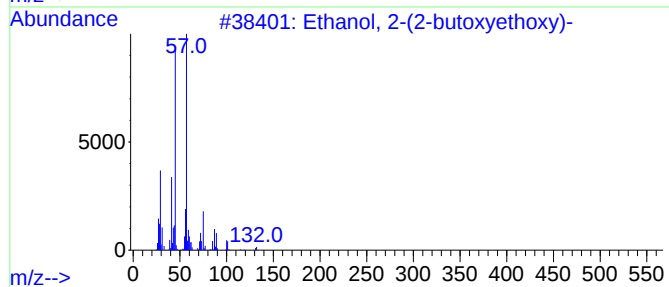
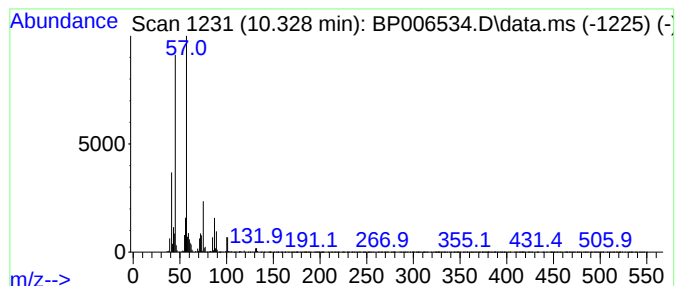
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.328	3.60 ng	355718	Naphthalene-d8	10.540

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	64
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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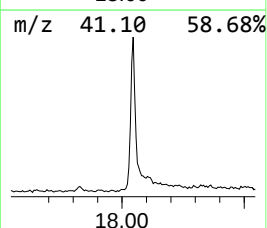
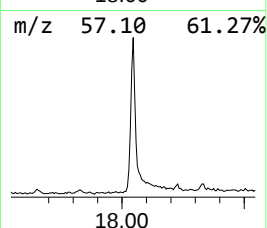
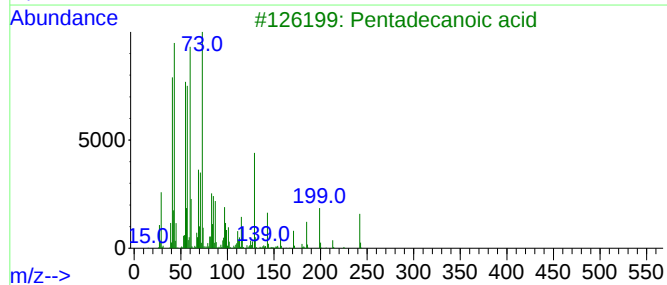
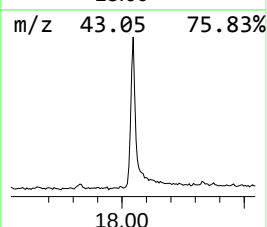
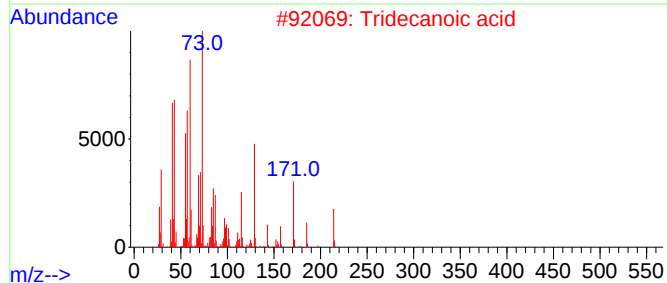
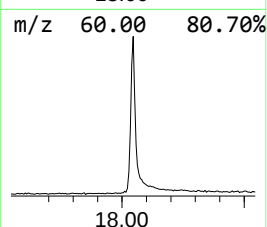
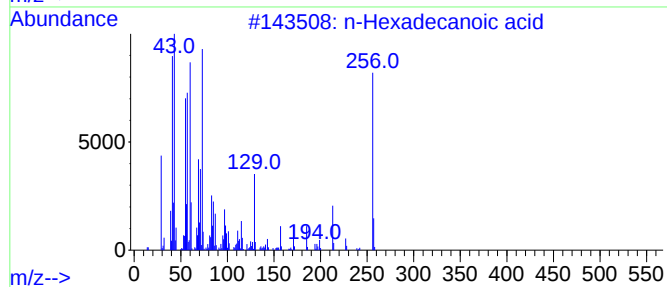
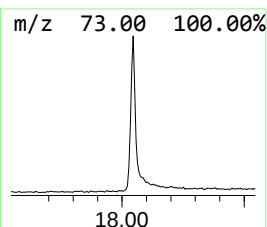
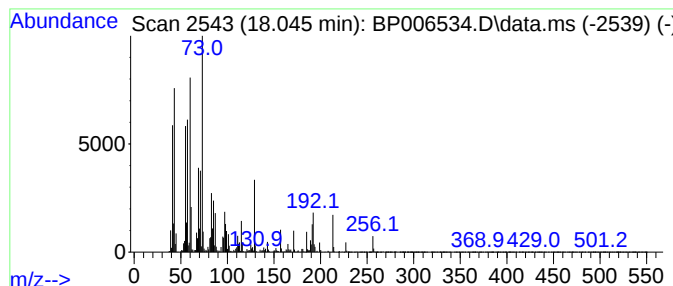
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.045	8.29 ng	1194870	Phenanthrene-d10	17.134

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5			Dodecanoic acid	200	C12H24O2	000143-07-7	58



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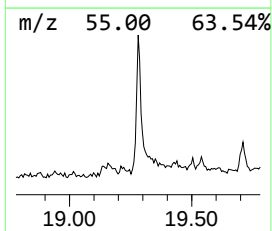
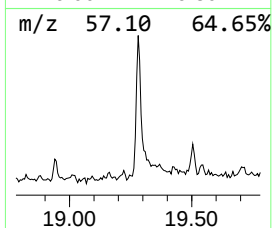
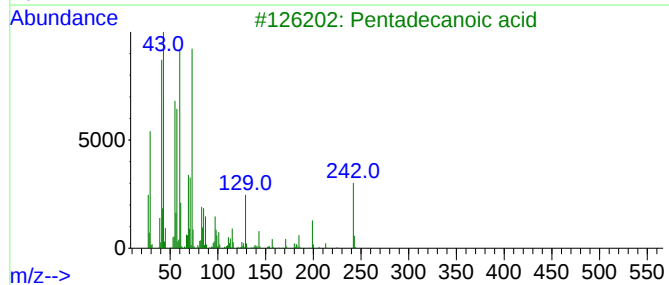
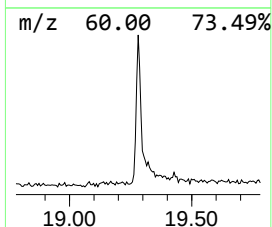
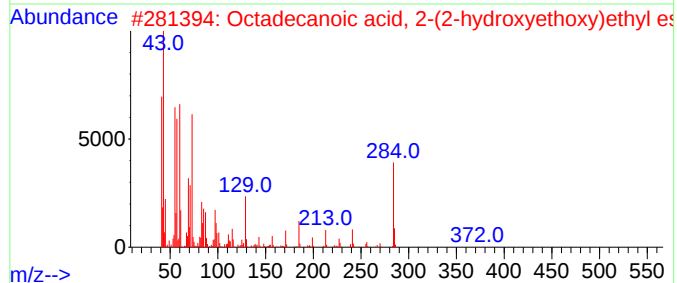
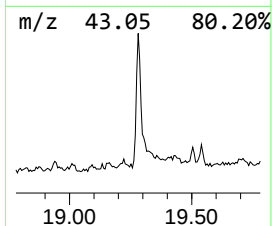
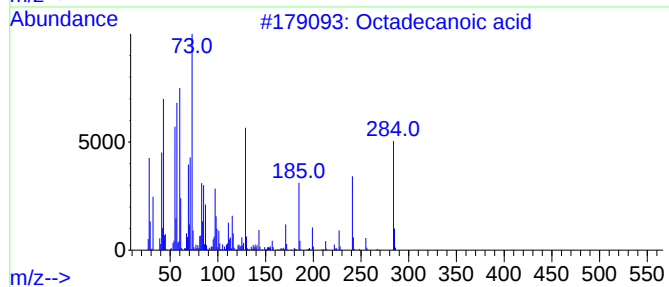
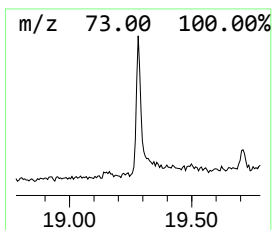
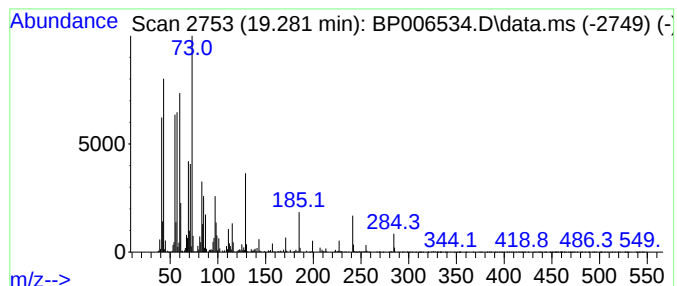
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.281	2.35 ng	446870	Chrysene-d12	21.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	78
4			n-Decanoic acid	172	C10H20O2	000334-48-5	62
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006534.D
Acq On : 06 Aug 2021 12:04
Operator : CG/JU
Sample : M3271-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-4

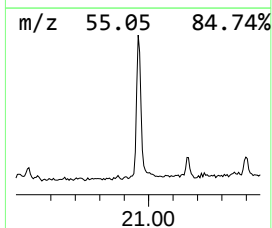
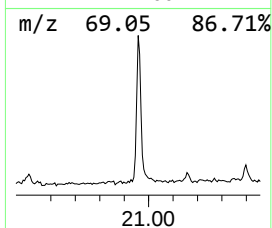
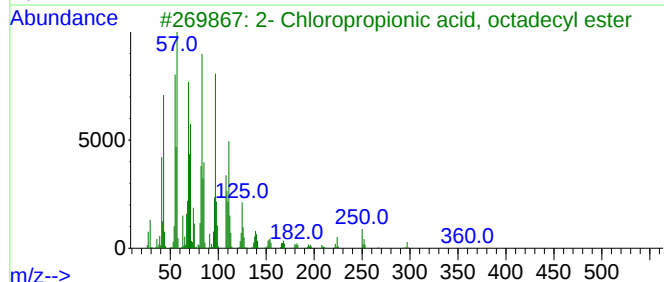
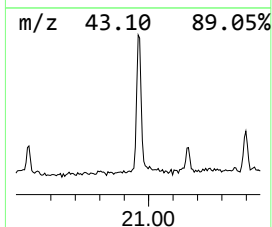
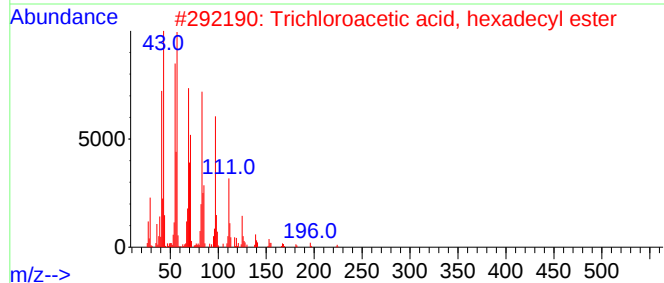
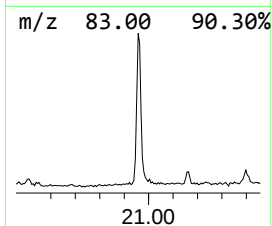
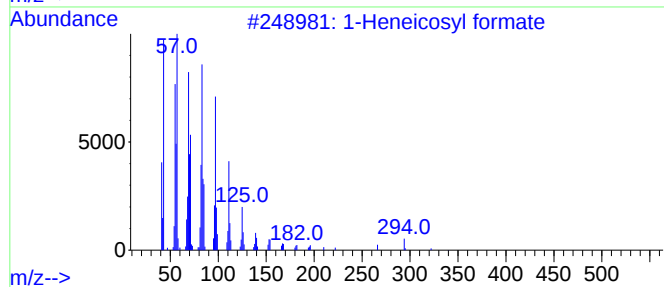
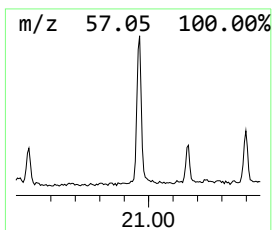
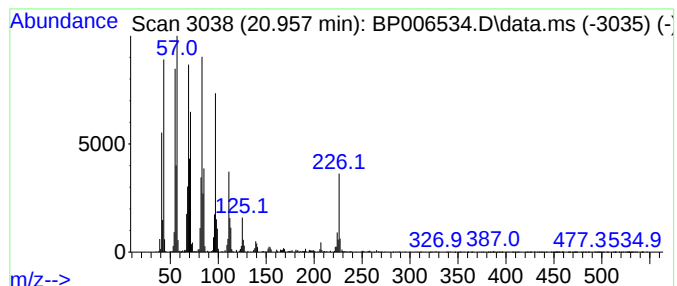
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heneicosyl formate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.957	4.06 ng	771288	Chrysene-d12	21.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
3			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90
4			Cyclohexadecane	224	C16H32	000295-65-8	90
5			Octacosanol	410	C28H58O	000557-61-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006534.D
Acq On : 06 Aug 2021 12:04
Operator : CG/JU
Sample : M3271-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-4

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	22.2	ng	1505670	1	7.758	1354340	20.0
2-Pentanone, 4-...	5.970	4.6	ng	312783	1	7.758	1354340	20.0
Ethanol, 2-(2-b...	10.328	3.6	ng	355718	2	10.540	1977410	20.0
n-Hexadecanoic ...	18.045	8.3	ng	1194870	4	17.134	2882820	20.0
Octadecanoic acid	19.281	2.4	ng	446870	5	21.233	3800580	20.0
1-Heneicosyl fo...	20.957	4.1	ng	771288	5	21.233	3800580	20.0