

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP113021\
 Data File : BP008159.D
 Acq On : 30 Nov 2021 15:34
 Operator : CG/JU
 Sample : M4848-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 PSC124019

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-BP112521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008159.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.076	13	15	43	rVB	60894	153904	3.98%	0.554%
2	4.928	324	330	338	rBV	234721	325818	8.42%	1.174%
3	5.393	402	409	420	rBV	1807197	2576443	66.55%	9.282%
4	6.987	671	680	695	rBV	1662975	2739462	70.76%	9.869%
5	7.805	811	819	826	rBV	414602	646052	16.69%	2.328%
6	8.963	1007	1016	1028	rBV	1029100	1702813	43.99%	6.135%
7	10.393	1252	1259	1269	rBV2	69833	146312	3.78%	0.527%
8	10.599	1285	1294	1302	rBV	490448	838400	21.66%	3.020%
9	13.069	1707	1714	1724	rBV	2006340	2950375	76.21%	10.629%
10	13.287	1745	1751	1758	rBV2	25653	53866	1.39%	0.194%
11	14.116	1885	1892	1898	rBV2	35387	73356	1.89%	0.264%
12	14.310	1918	1925	1938	rBV	72948	224282	5.79%	0.808%
13	14.451	1942	1949	1955	rVV	736939	1068221	27.59%	3.848%
14	15.263	2082	2087	2093	rVB3	33448	60000	1.55%	0.216%
15	15.945	2193	2203	2211	rBV	1764409	2545171	65.75%	9.169%
16	16.010	2211	2214	2223	rVB9	19243	42662	1.10%	0.154%
17	17.140	2401	2406	2411	rBV	57848	69851	1.80%	0.252%
18	17.210	2411	2418	2422	rBV	846835	1207633	31.20%	4.351%
19	17.251	2422	2425	2430	rVB	107423	142701	3.69%	0.514%
20	17.340	2436	2440	2446	rVB2	39195	64841	1.67%	0.234%
21	17.510	2464	2469	2478	rVB3	18080	45013	1.16%	0.162%
22	18.110	2567	2571	2579	rVB2	167089	269688	6.97%	0.972%
23	18.269	2593	2598	2602	rBV4	37473	67212	1.74%	0.242%
24	19.228	2756	2761	2767	rBV	215604	278993	7.21%	1.005%
25	19.345	2778	2781	2785	rVB3	42633	48278	1.25%	0.174%
26	19.581	2817	2821	2830	rVB	183062	251103	6.49%	0.905%
27	19.781	2849	2855	2860	rBV	3194248	3871218	100.00%	13.947%
28	20.563	2984	2988	2996	rVB2	74733	122484	3.16%	0.441%
29	21.028	3063	3067	3073	rBV2	217663	310854	8.03%	1.120%
30	21.086	3075	3077	3084	rVB2	66186	82105	2.12%	0.296%
31	21.222	3097	3100	3105	rVB	284780	332610	8.59%	1.198%
32	21.310	3109	3115	3119	rBV	827833	1145144	29.58%	4.126%
33	21.428	3130	3135	3149	rBV	1223874	1959871	50.63%	7.061%
34	21.569	3155	3159	3168	rVB2	170905	343832	8.88%	1.239%
35	23.704	3516	3522	3529	rVB2	495999	996667	25.75%	3.591%

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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-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

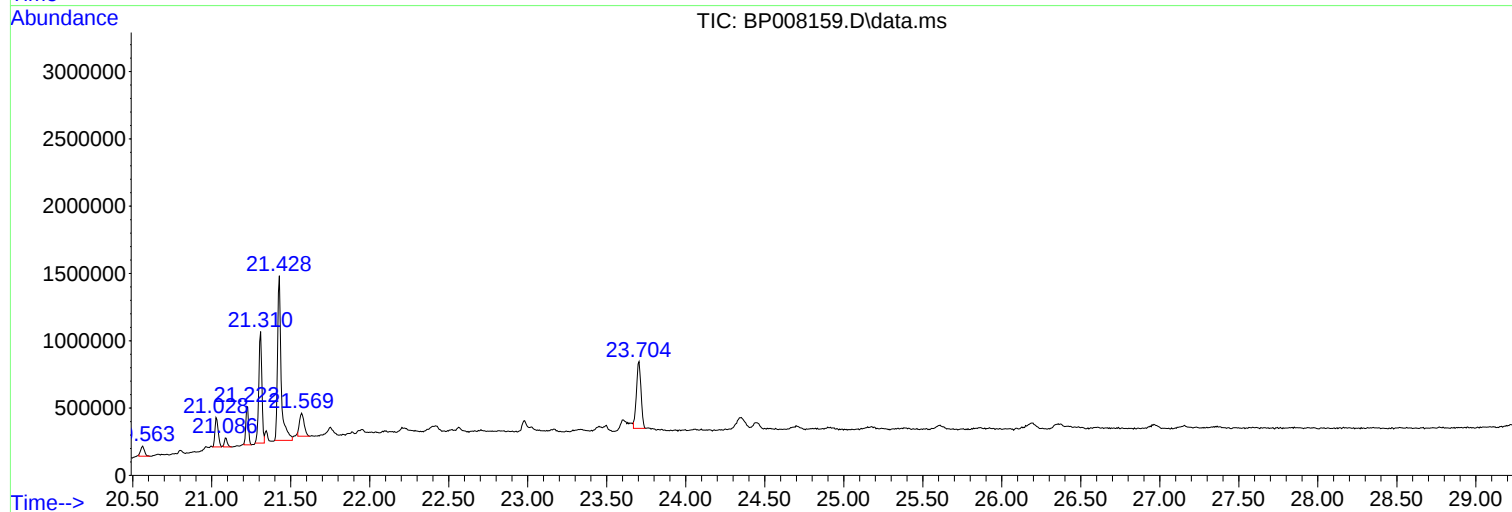
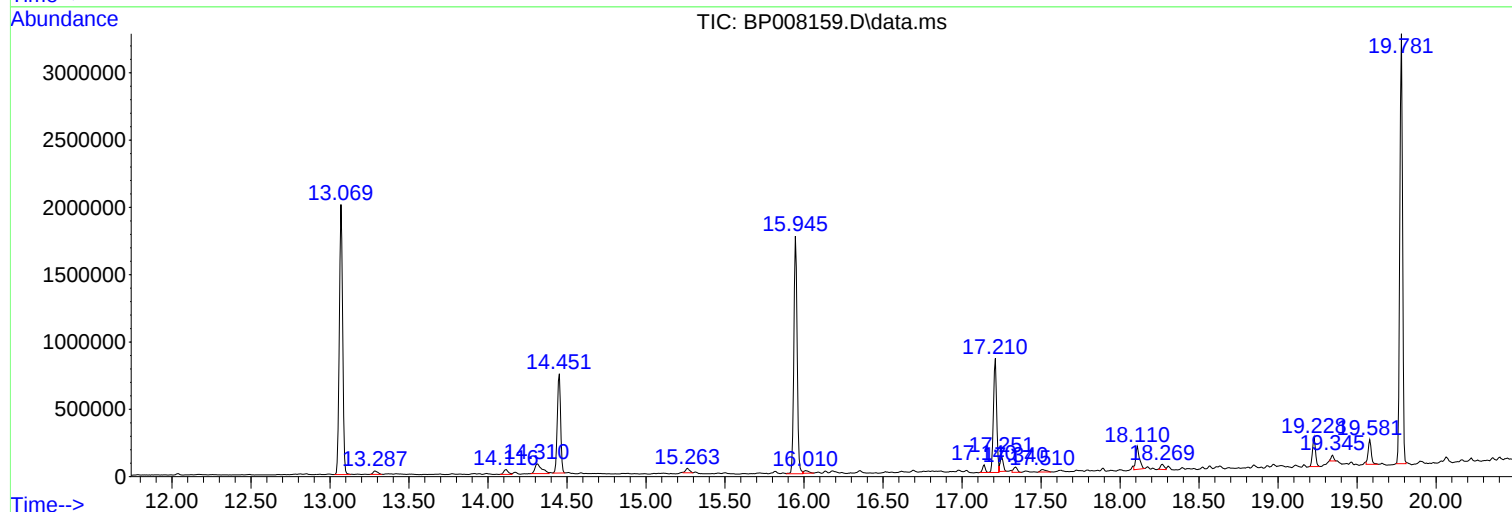
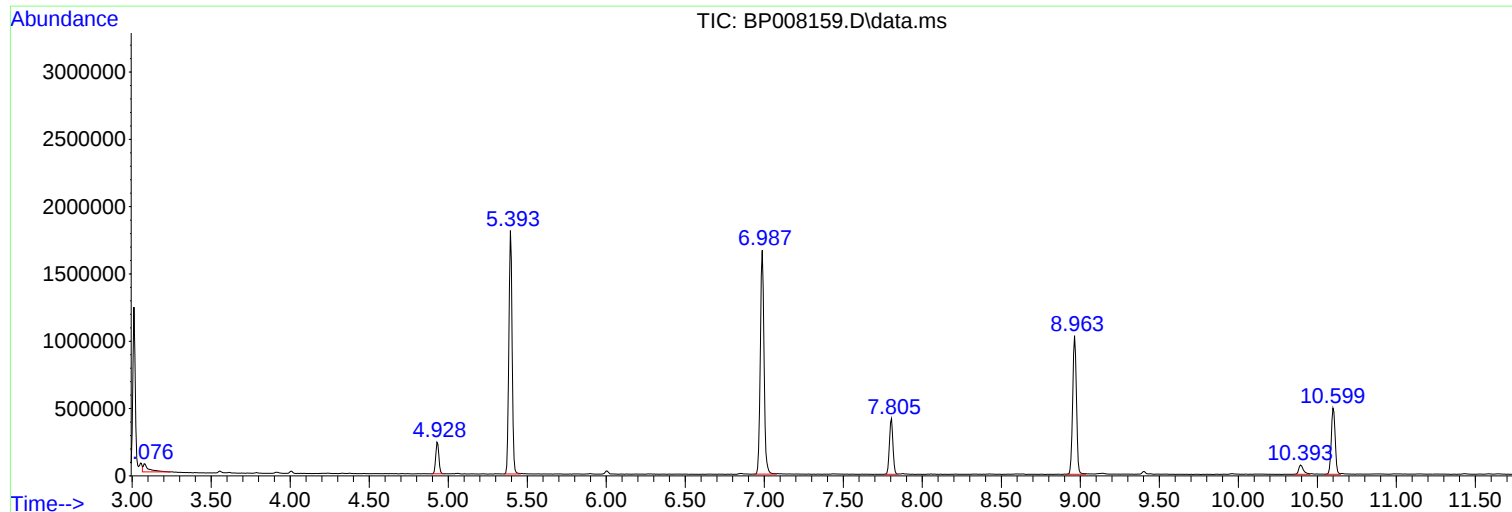
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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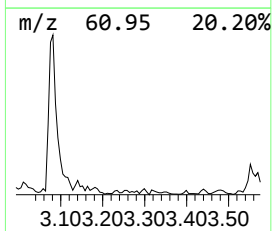
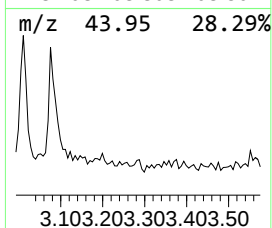
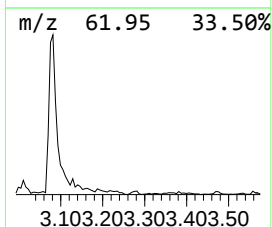
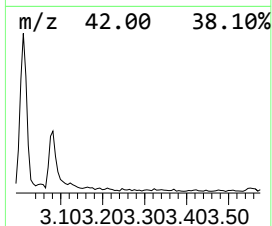
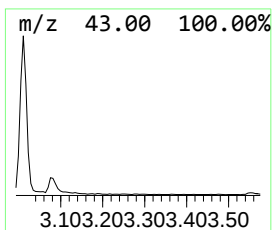
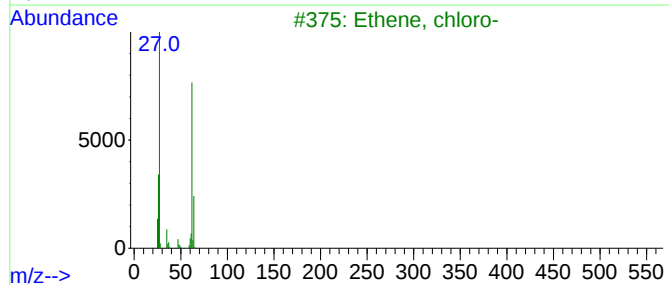
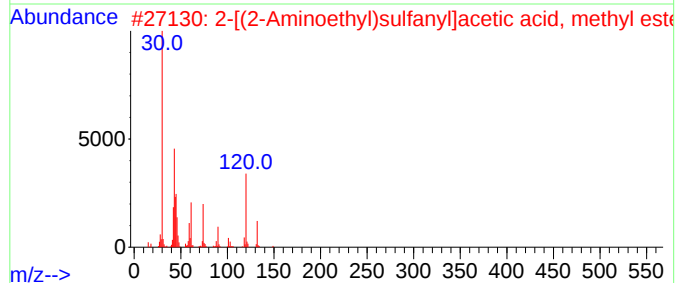
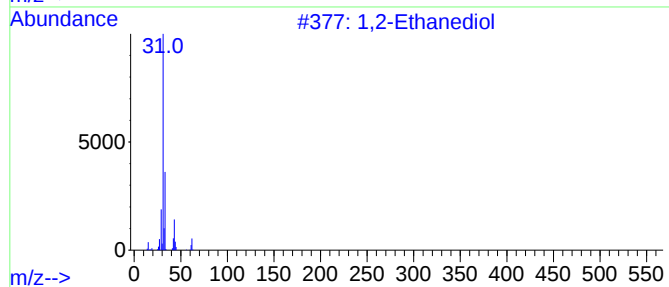
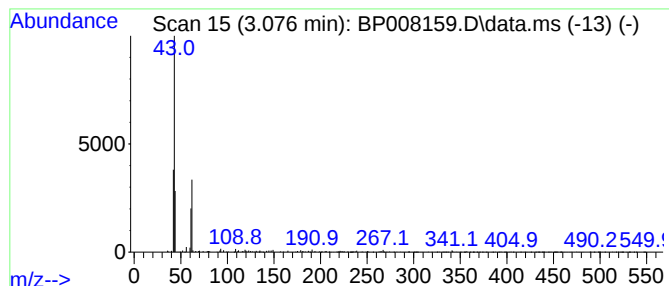
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.076 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.076	4.76 ng	153904	1,4-Dichlorobenzene-d4	7.805

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Ethanediol	62	C2H6O2	000107-21-1	7
2			2-[(2-Aminoethyl)sulfanyl]acetic...	149	C5H11NO2S	366446-58-4	5
3			Ethene, chloro-	62	C2H3Cl	000075-01-4	5
4			Ethanamine, 2-(methylthio)-	91	C3H9NS	018542-42-2	4
5			Peroxide, dimethyl	62	C2H6O2	000690-02-8	4



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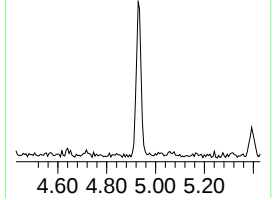
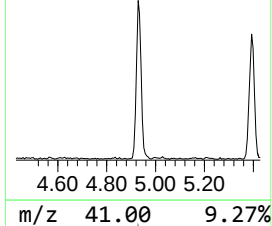
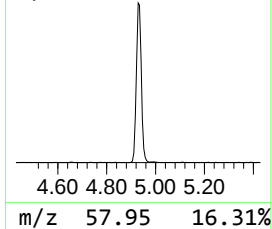
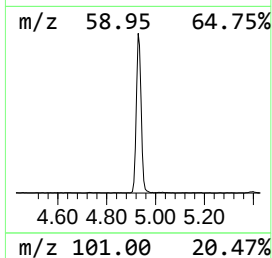
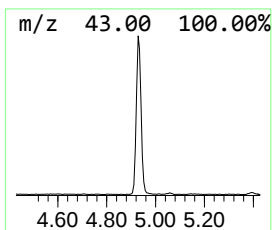
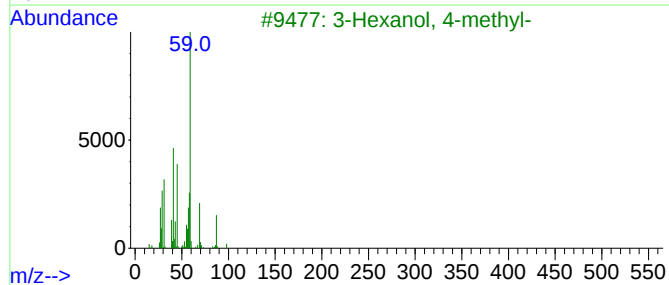
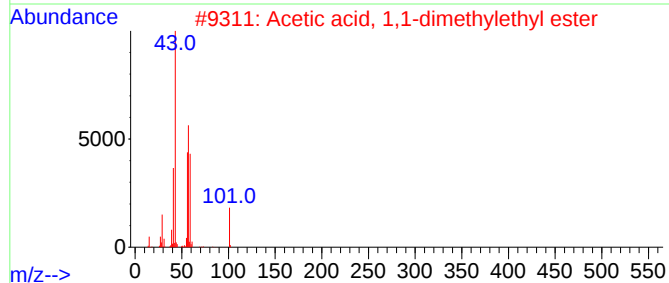
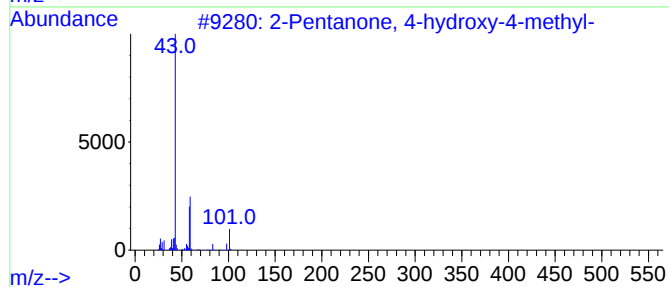
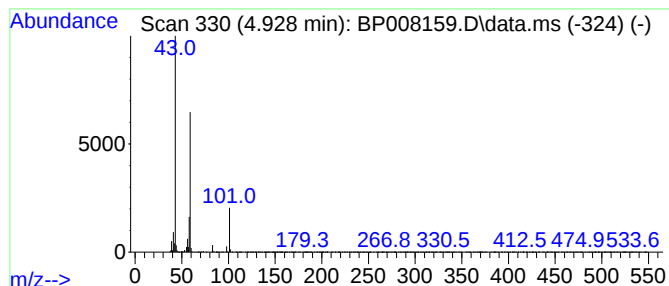
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.928	10.09 ng	325818	1,4-Dichlorobenzene-d4			7.805
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	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	28
4	3-Hexanol		102	C6H14O	000623-37-0	28
5	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	17



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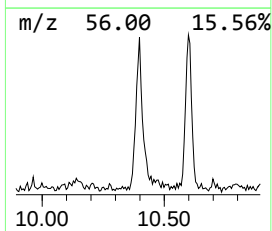
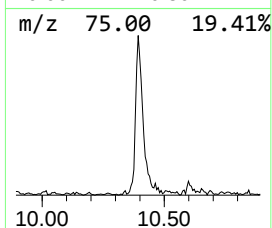
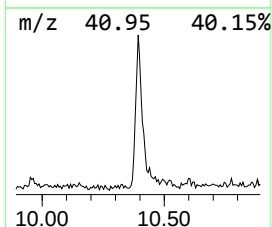
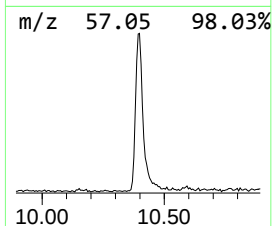
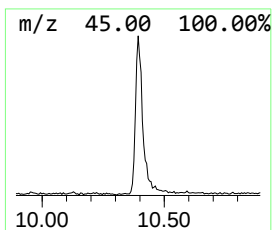
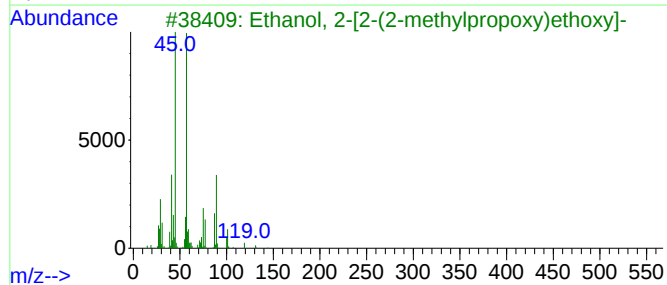
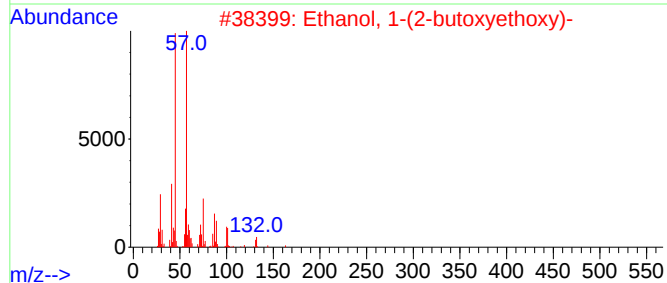
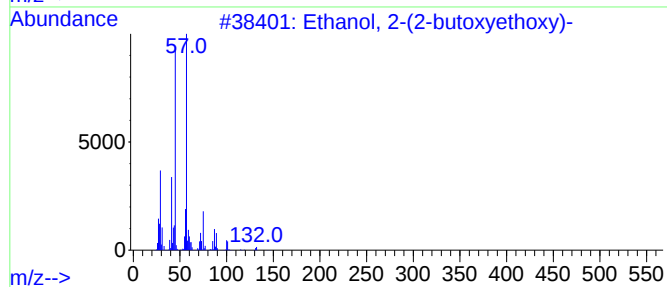
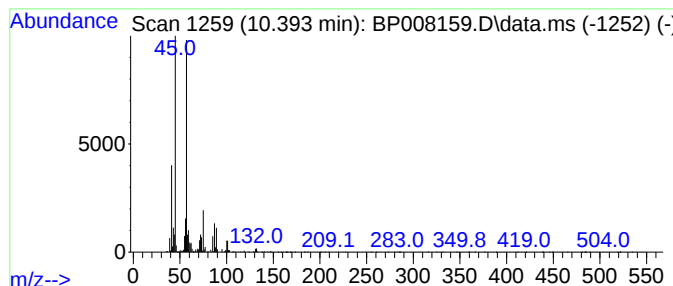
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.393	3.49 ng	146312	Naphthalene-d8	10.599

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	56
4			Tetraethylene glycol	194	C8H18O5	000112-60-7	50
5			DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	47



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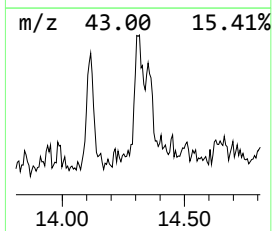
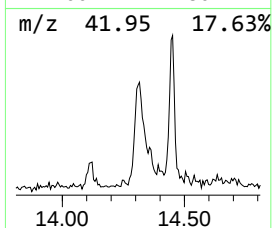
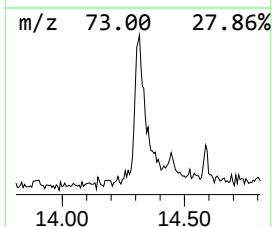
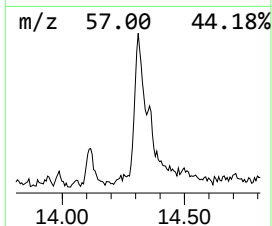
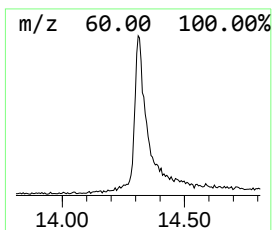
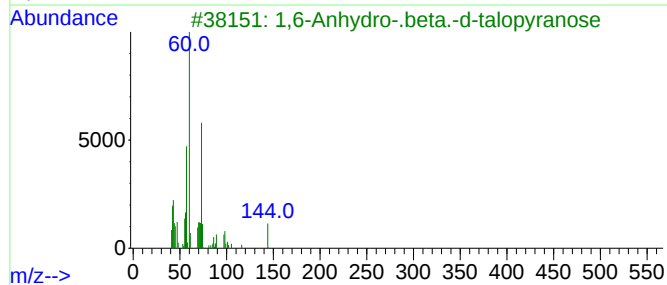
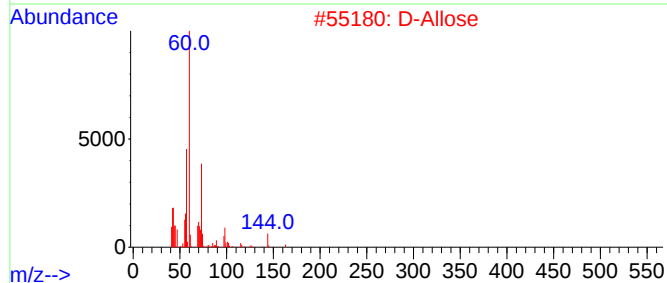
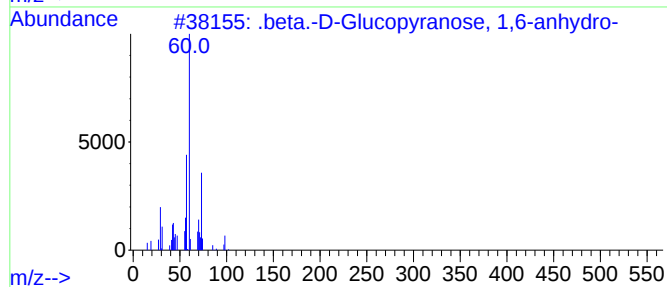
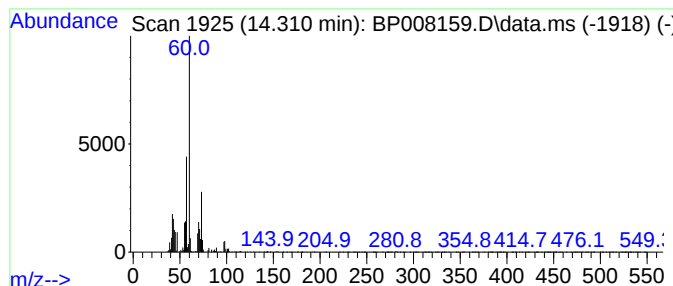
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 .beta.-D-Glucopyranose, 1,6... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.310	4.20 ng	224282	Acenaphthene-d10	14.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	80
2			D-Allose	180	C6H12O6	002595-97-3	53
3			1,6-Anhydro-.beta.-d-talopyranose	162	C6H10O5	1000133-05-8	47
4			Butanoic acid	88	C4H8O2	000107-92-6	42
5			Pentanoic acid	102	C5H10O2	000109-52-4	42



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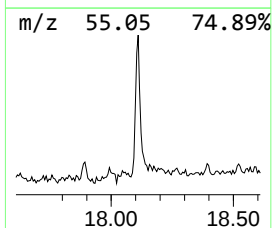
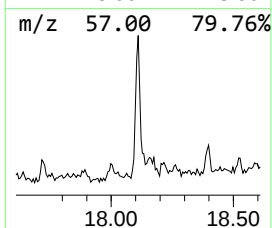
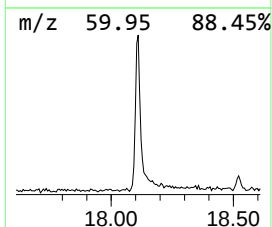
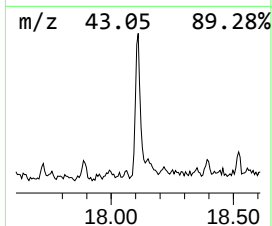
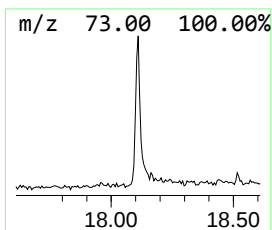
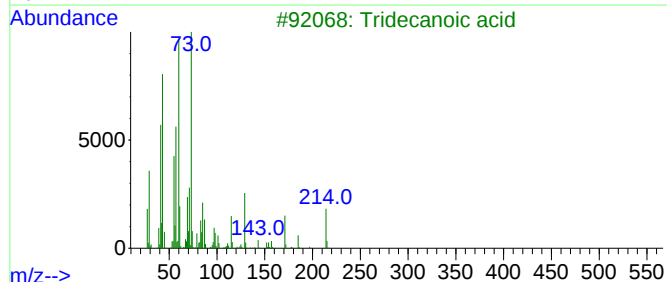
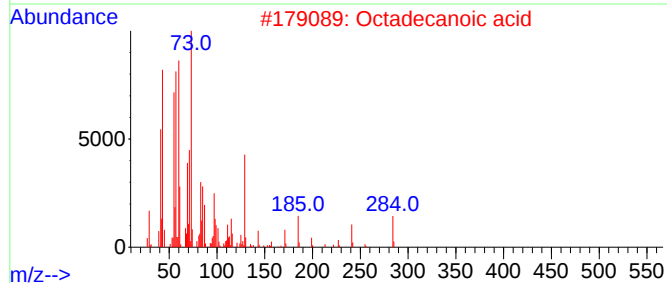
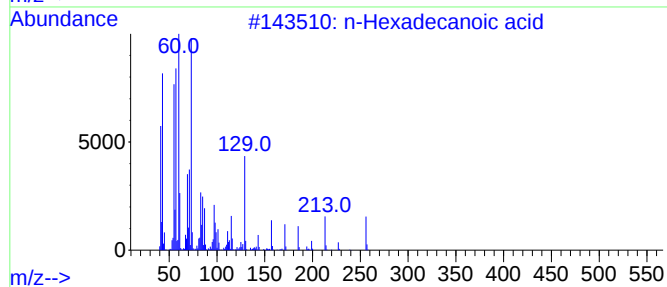
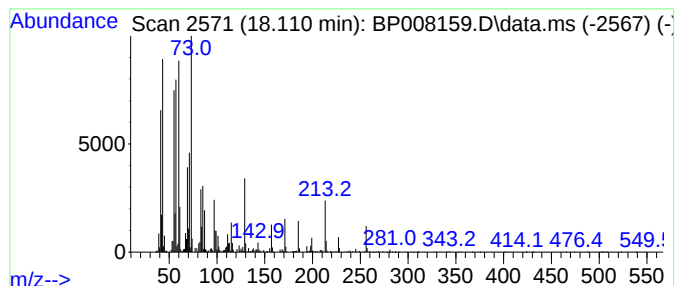
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TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.110	4.47 ng	269688	Phenanthrene-d10		17.210	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Octadecanoic acid		284	C18H36O2	000057-11-4	91
3	Tridecanoic acid		214	C13H26O2	000638-53-9	89
4	Dodecanoic acid		200	C12H24O2	000143-07-7	80
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP113021\
Data File : BP008159.D
Acq On : 30 Nov 2021 15:34
Operator : CG/JU
Sample : M4848-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PSC124019

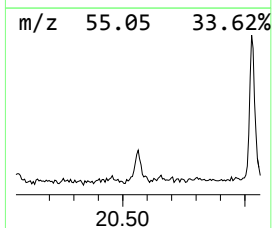
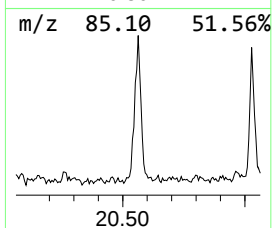
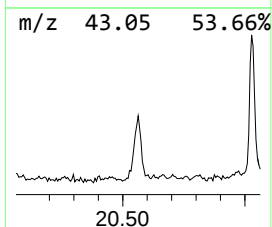
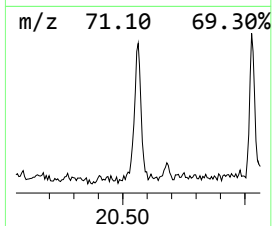
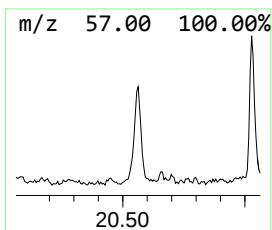
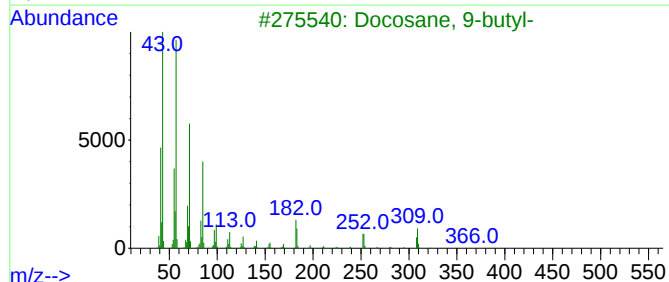
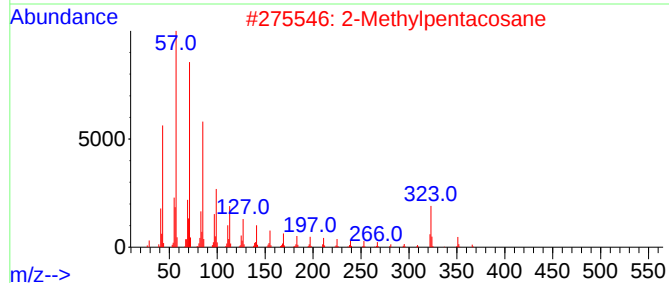
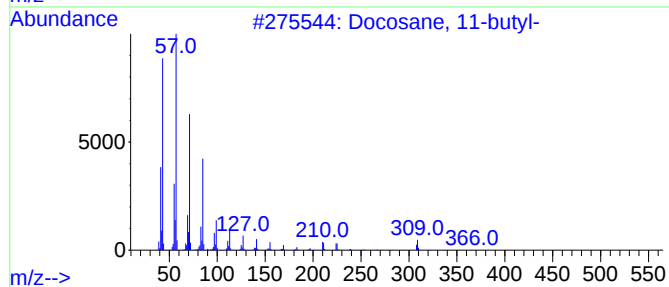
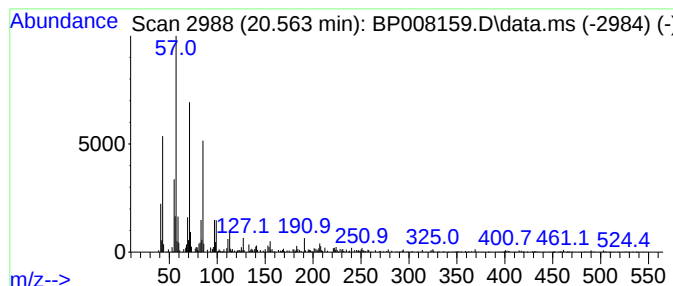
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Docosane, 11-butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.563	2.14 ng	122484	Chrysene-d12	21.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane, 11-butyl-	366	C26H54	013475-76-8	90
2			2-Methylpentacosane	366	C26H54	000629-87-8	81
3			Docosane, 9-butyl-	366	C26H54	055282-14-9	81
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	74
5			Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP113021\
Data File : BP008159.D
Acq On : 30 Nov 2021 15:34
Operator : CG/JU
Sample : M4848-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PSC124019

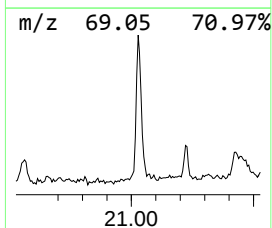
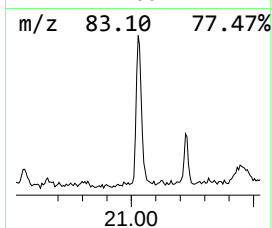
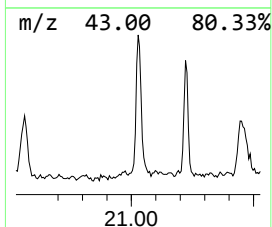
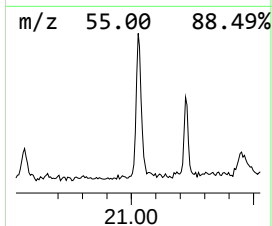
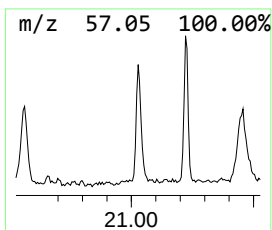
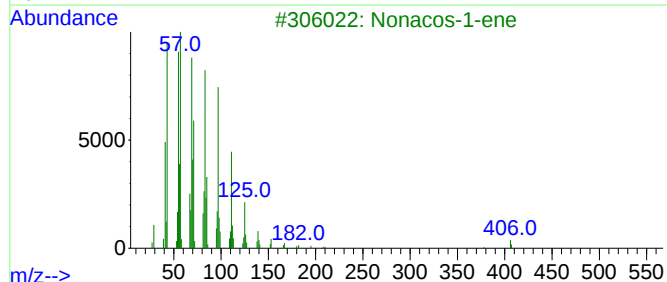
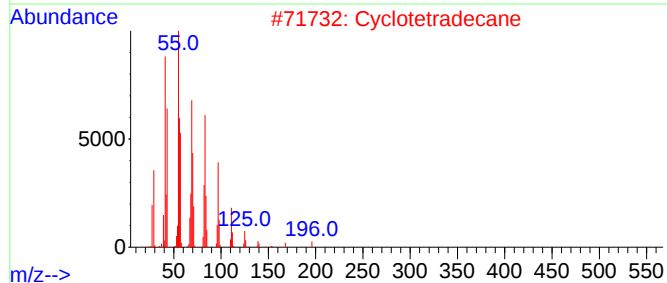
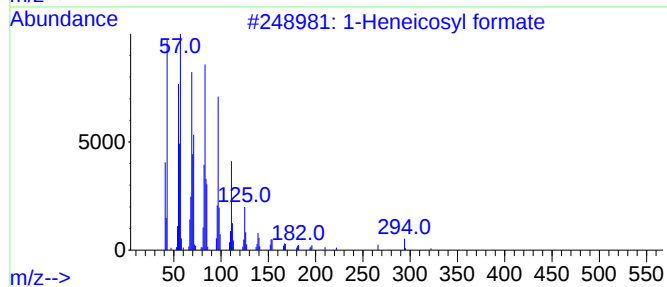
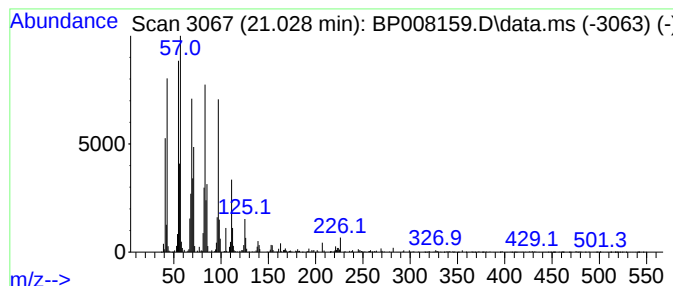
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosyl formate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.028	5.43 ng	310854	Chrysene-d12	21.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2			Cyclotetradecane	196	C14H28	000295-17-0	95
3			Nonacos-1-ene	406	C29H58	018835-35-3	94
4			Pentacos-1-ene	350	C25H50	016980-85-1	94
5			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP113021\
Data File : BP008159.D
Acq On : 30 Nov 2021 15:34
Operator : CG/JU
Sample : M4848-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PSC124019

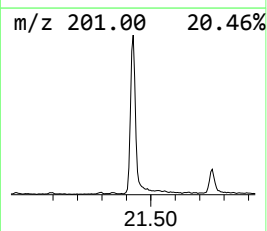
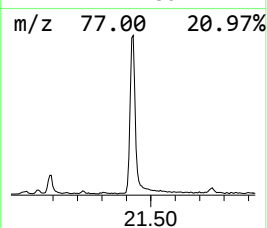
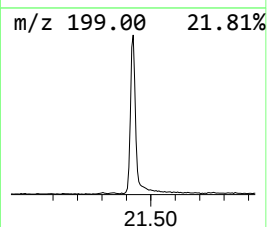
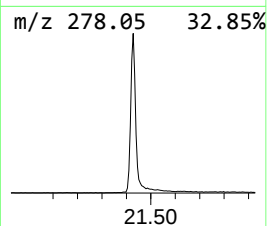
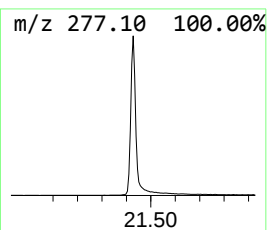
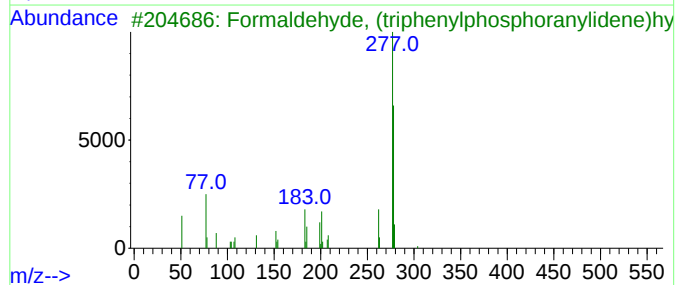
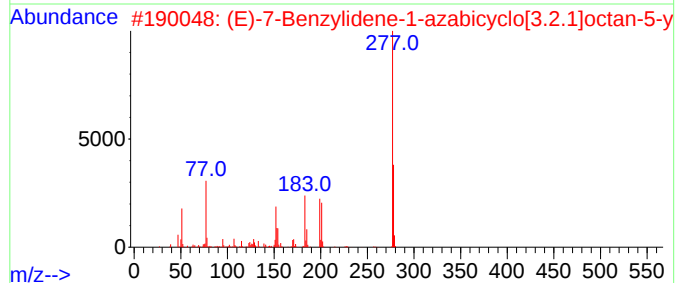
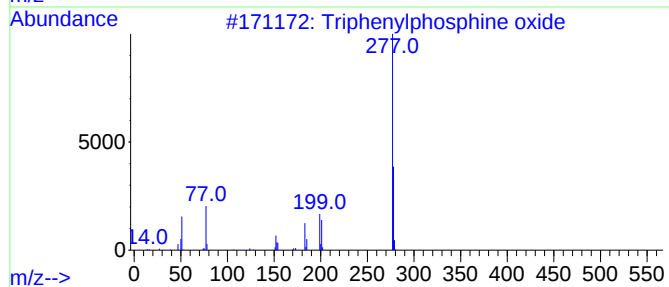
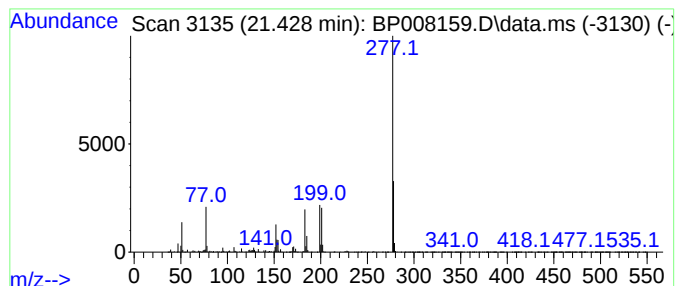
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.427	34.23 ng	1959870	Chrysene-d12	21.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	83
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	42
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	23
5			Oxoprophines	277	C17H11NO3	1000128-51-1	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP113021\
Data File : BP008159.D
Acq On : 30 Nov 2021 15:34
Operator : CG/JU
Sample : M4848-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PSC124019

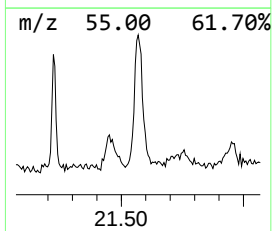
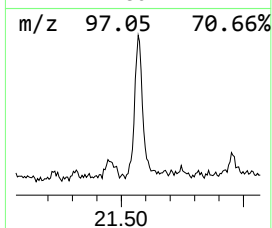
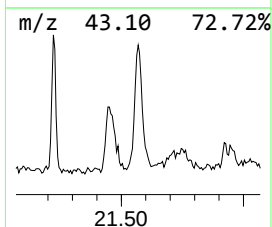
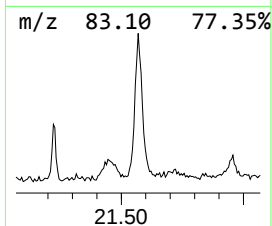
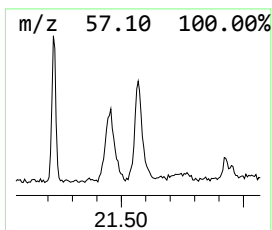
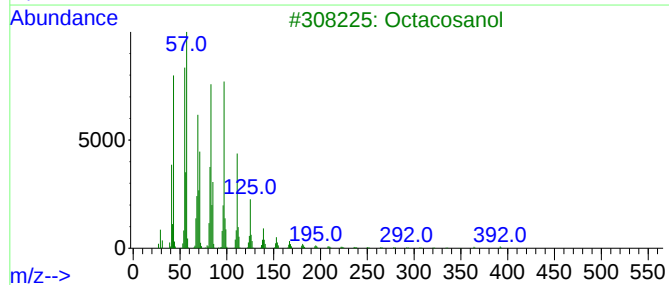
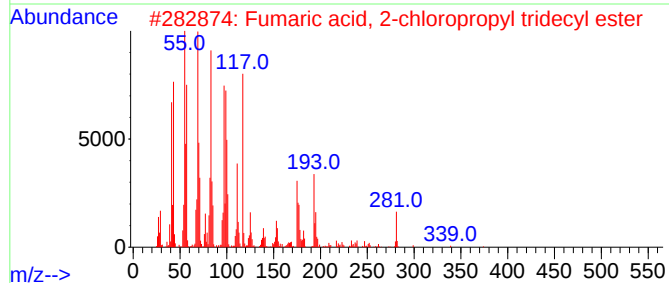
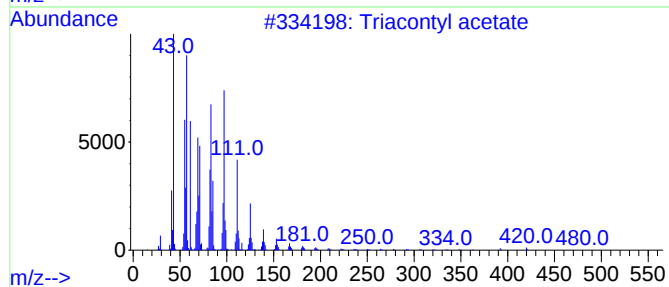
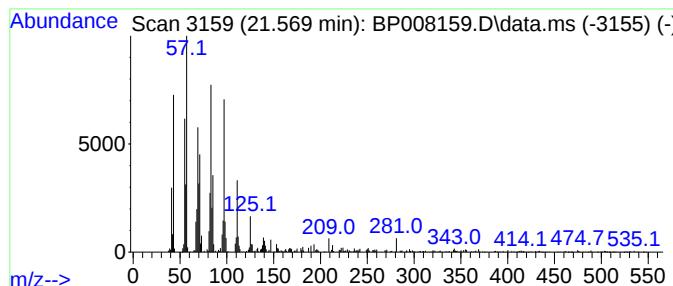
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triacetyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.569	6.01 ng	343832	Chrysene-d12	21.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacetyl acetate	480	C32H64O2	041755-58-2	98
2			Fumaric acid, 2-chloropropyl tri...	374	C20H35ClO4	1010348-57-1	95
3			Octacosanol	410	C28H58O	000557-61-9	94
4			Octacosyl acetate	452	C30H60O2	018206-97-8	93
5			1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP113021\
Data File : BP008159.D
Acq On : 30 Nov 2021 15:34
Operator : CG/JU
Sample : M4848-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PSC124019

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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
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2-Pentanone, 4-...	4.928	10.1	ng	325818	1	7.805	646052	20.0
Ethanol, 2-(2-b...	10.393	3.5	ng	146312	2	10.599	838400	20.0
.beta.-D-Glucop...	14.310	4.2	ng	224282	3	14.451	1068220	20.0
n-Hexadecanoic ...	18.110	4.5	ng	269688	4	17.210	1207630	20.0
Docosane, 11-bu...	20.563	2.1	ng	122484	5	21.310	1145140	20.0
1-Heneicosyl fo...	21.028	5.4	ng	310854	5	21.310	1145140	20.0
Triphenylphosph...	21.427	34.2	ng	1959870	5	21.310	1145140	20.0
Triacetyl acetate	21.569	6.0	ng	343832	5	21.310	1145140	20.0