

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112322\
 Data File : BP012708.D
 Acq On : 23 Nov 2022 13:49
 Operator : CG/JU
 Sample : N5742-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 MW-42

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-BP112222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP012708.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.064	7	13	21	rBV2	317279	587674	2.04%	0.462%
2	3.140	21	26	45	rVB	7560333	9634836	33.52%	7.576%
3	5.111	355	361	369	rBV	264033	385740	1.34%	0.303%
4	5.575	433	440	452	rBV	3296701	4750577	16.53%	3.735%
5	7.175	705	712	721	rBV	2461922	3831507	13.33%	3.013%
6	8.034	848	858	864	rBV	1544119	2470548	8.59%	1.943%
7	9.199	1048	1056	1065	rBV	3701544	5875306	20.44%	4.620%
8	10.852	1330	1337	1343	rBV	1892062	3188415	11.09%	2.507%
9	13.298	1745	1753	1761	rBV	8871594	13382647	46.56%	10.522%
10	14.669	1977	1986	1995	rBV	2547339	3817637	13.28%	3.002%
11	16.157	2232	2239	2252	rBV	6476659	9494118	33.03%	7.465%
12	17.422	2448	2454	2463	rVB	2905214	4144209	14.42%	3.258%
13	18.310	2598	2605	2643	rBV	6553875	12199661	42.44%	9.592%
14	19.416	2785	2793	2805	rBV3	478937	1496759	5.21%	1.177%
15	19.551	2808	2816	2853	rVV	15386571	28744322	100.00%	22.601%
16	19.975	2883	2888	2893	rVB	9427757	11318423	39.38%	8.899%
17	21.210	3094	3098	3109	rBV	503703	743221	2.59%	0.584%
18	21.510	3144	3149	3155	rVB	3931283	5044949	17.55%	3.967%
19	24.033	3571	3578	3591	rVB2	2848540	6072790	21.13%	4.775%

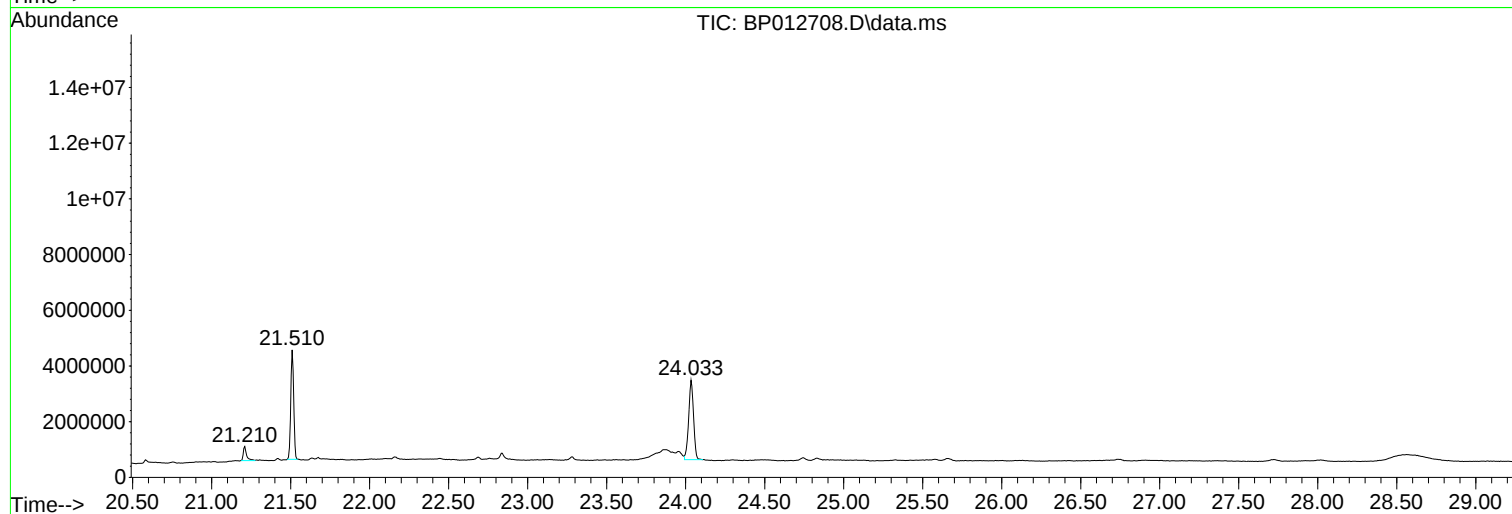
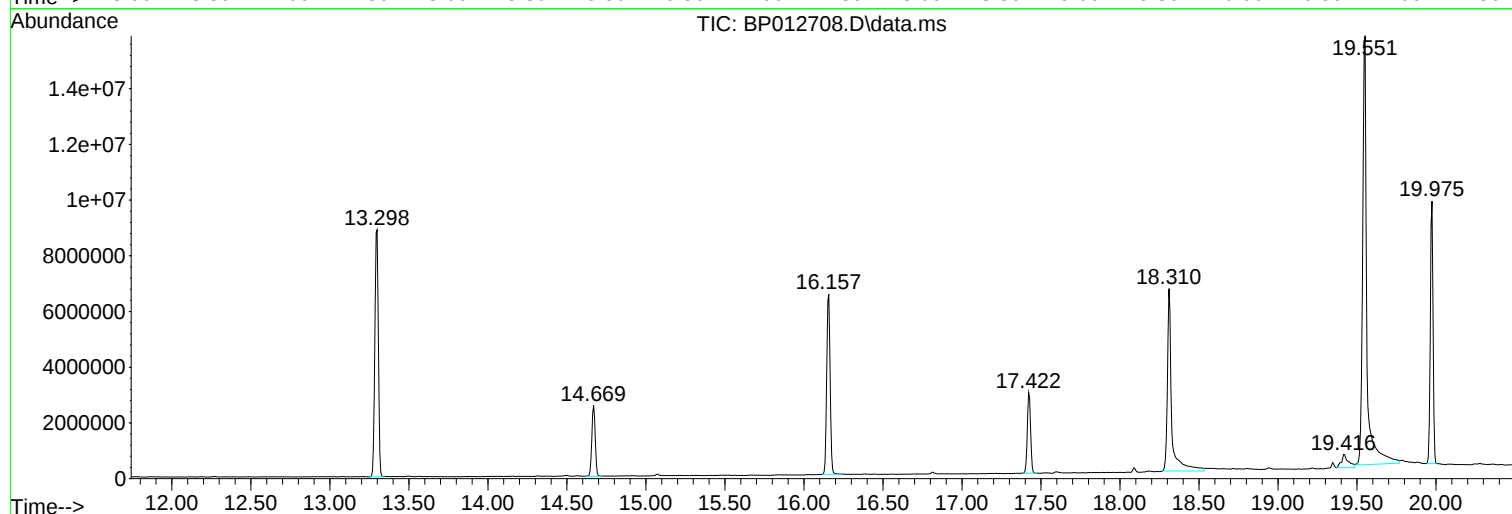
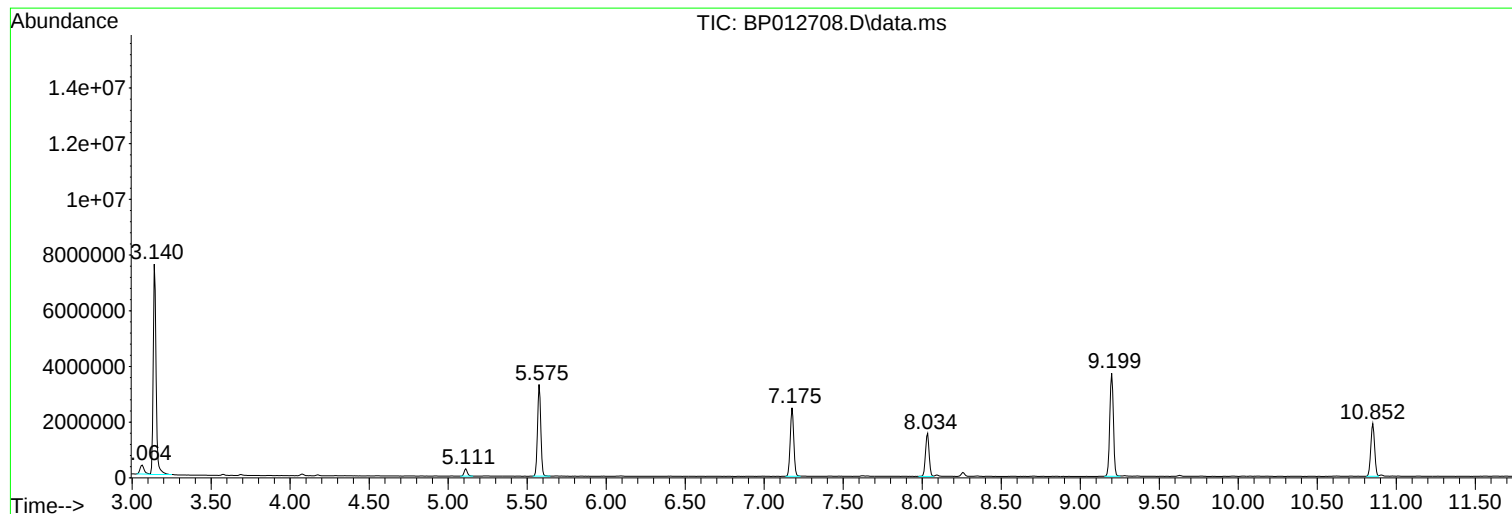
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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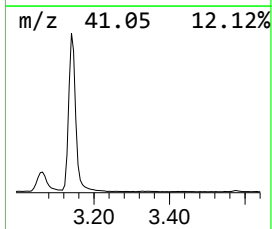
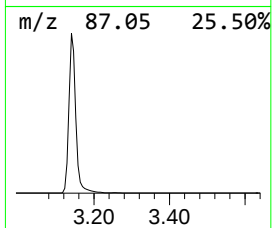
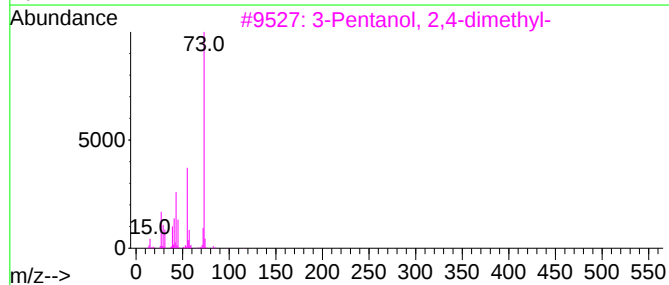
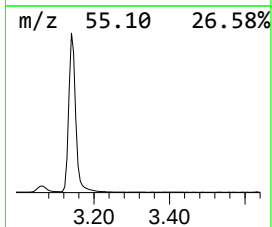
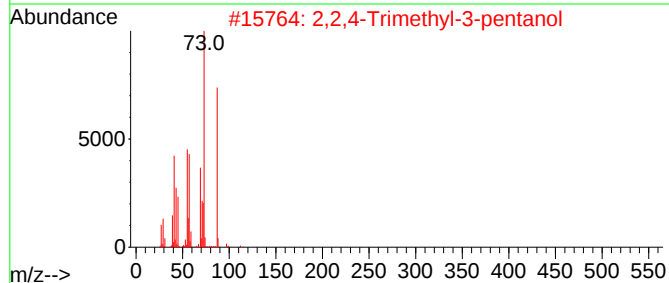
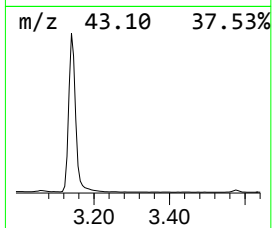
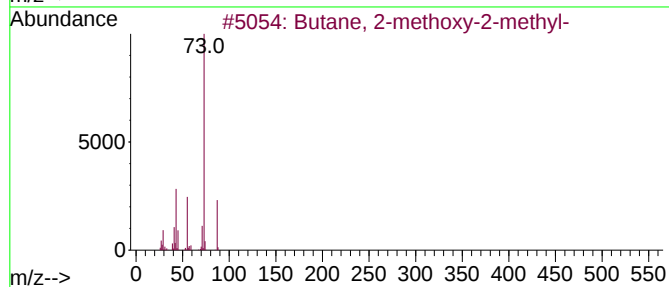
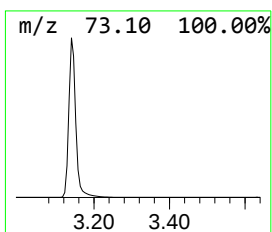
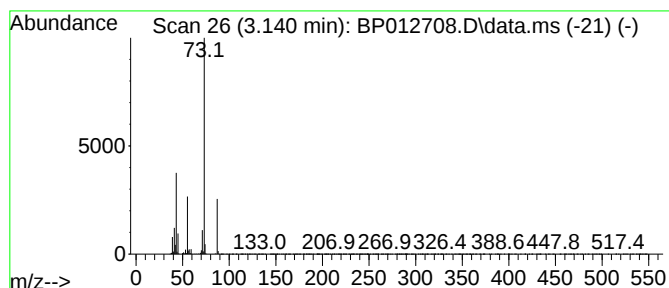
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.140	78.00 ng	9634840	1,4-Dichlorobenzene-d4	8.034

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22



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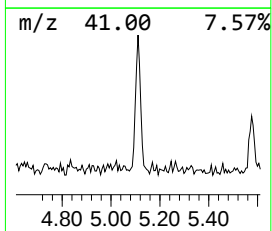
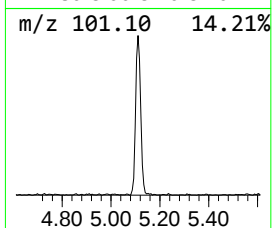
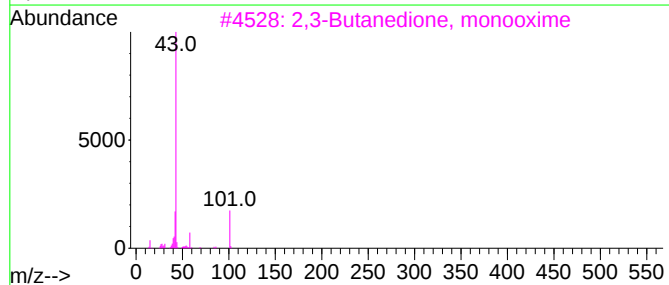
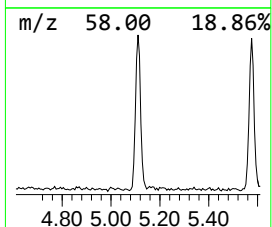
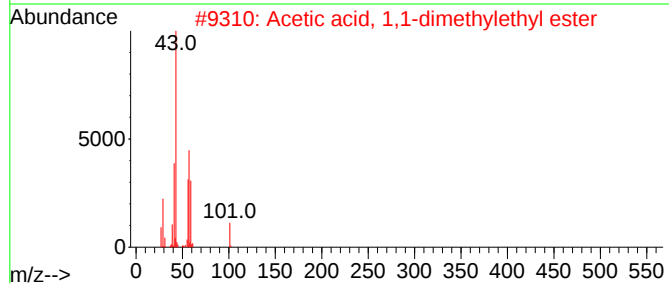
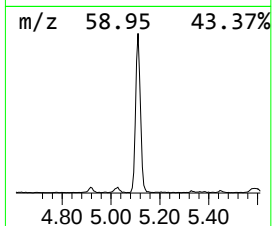
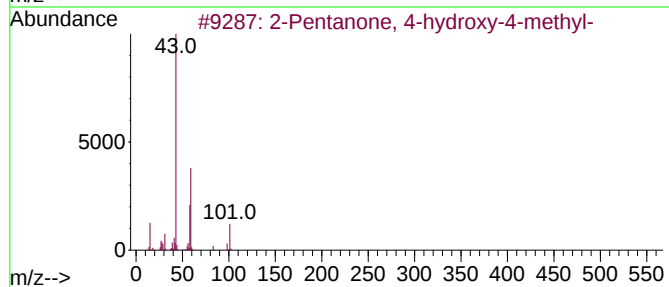
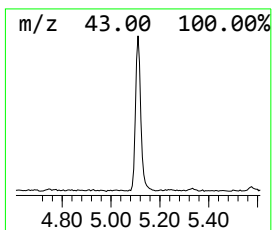
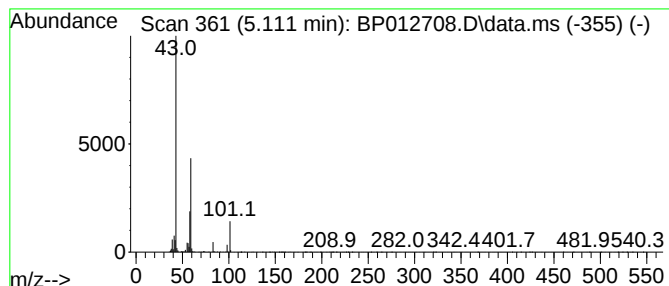
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.111	3.12 ng	385740	1,4-Dichlorobenzene-d4	8.034

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Acetone	58	C3H6O	000067-64-1	10



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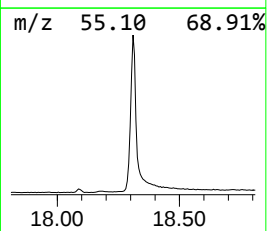
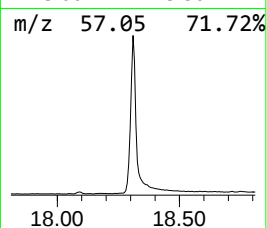
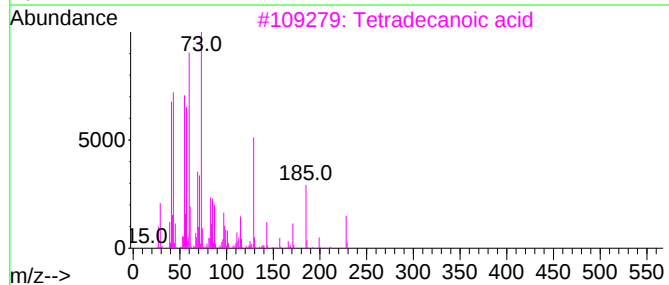
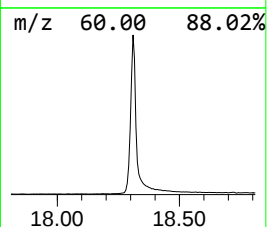
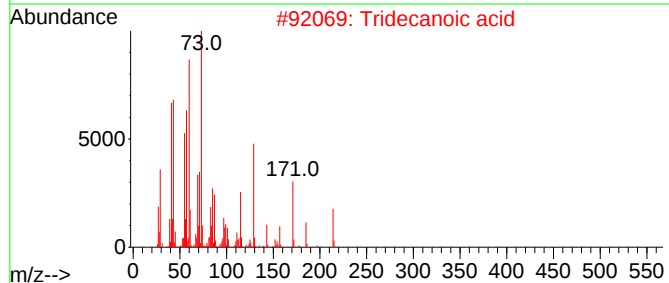
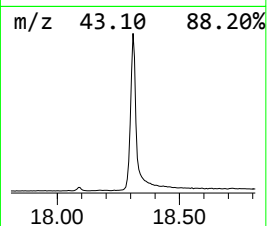
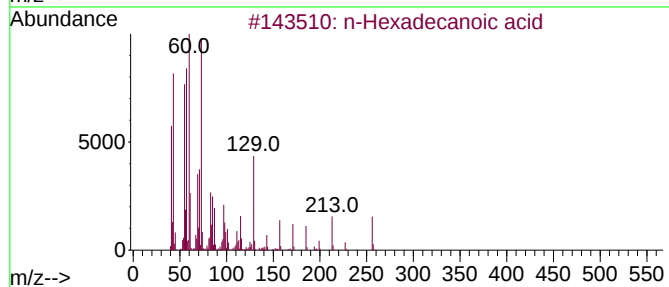
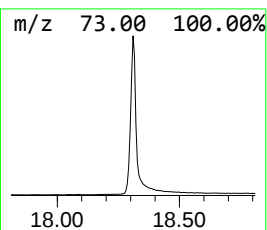
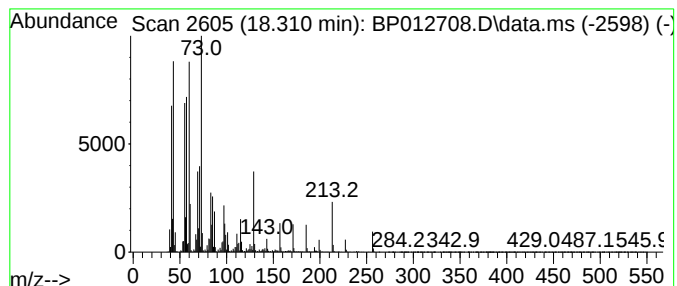
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.310	58.88 ng	12199700	Phenanthrene-d10		17.422	
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	Tetradecanoic acid		228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	91
5	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	55



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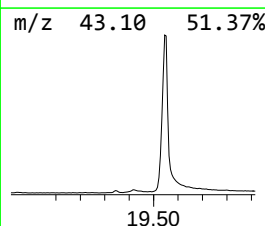
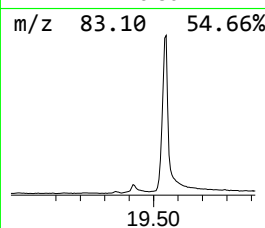
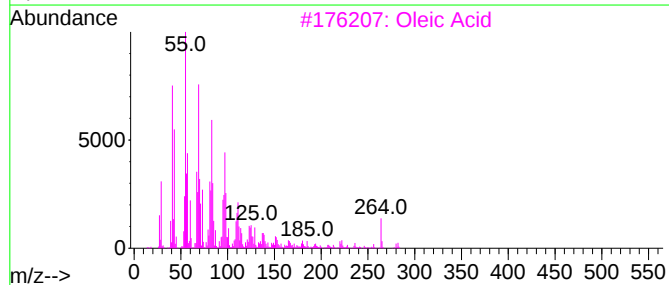
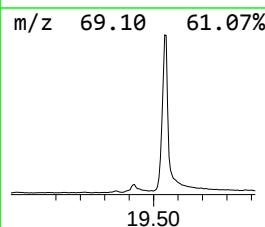
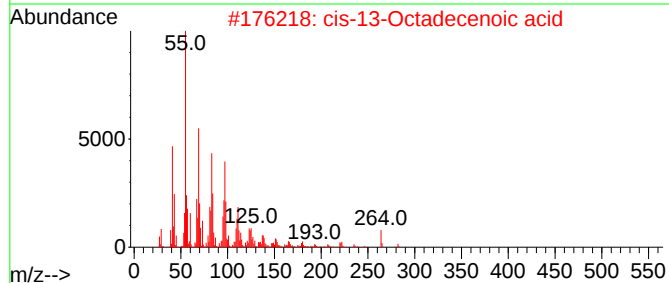
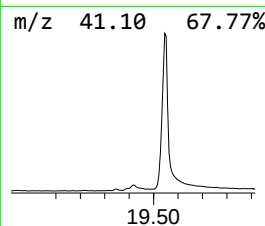
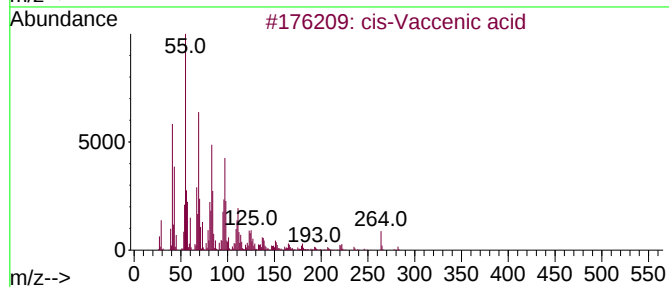
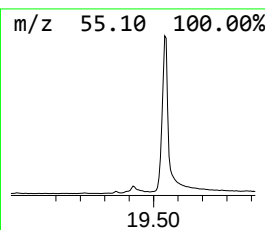
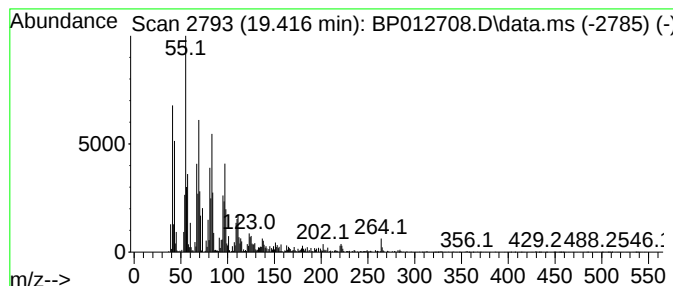
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Peak Number 5 cis-Vaccenic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.416	7.22 ng	1496760	Phenanthrene-d10	17.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	98
2			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	97
3			Oleic Acid	282	C18H34O2	000112-80-1	95
4			9-Octadecenoic acid	282	C18H34O2	002027-47-6	90
5			9-Octadecenoic acid (Z)-, 2,3-di...	356	C21H40O4	000111-03-5	86



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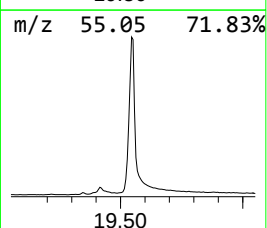
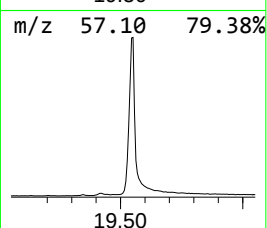
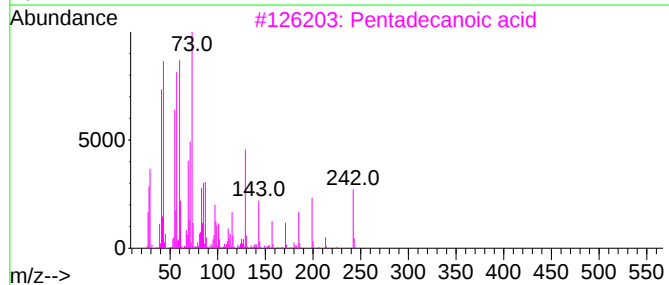
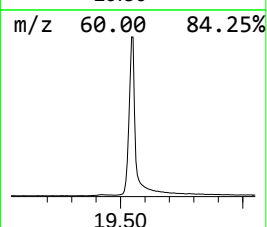
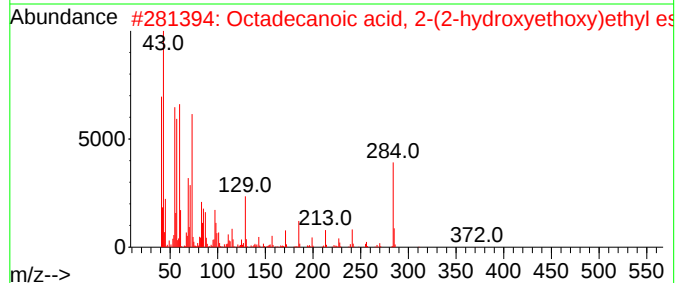
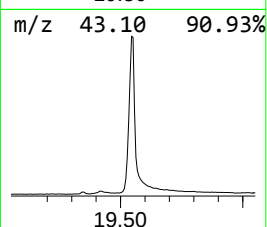
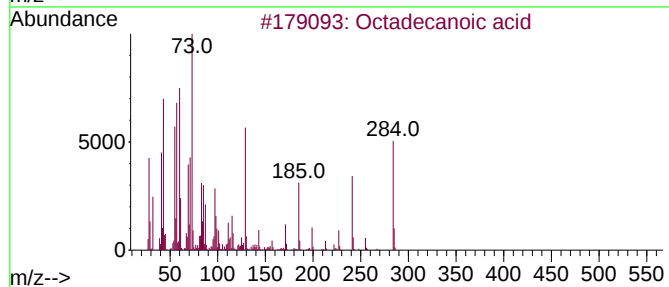
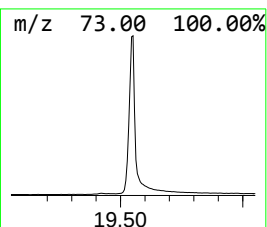
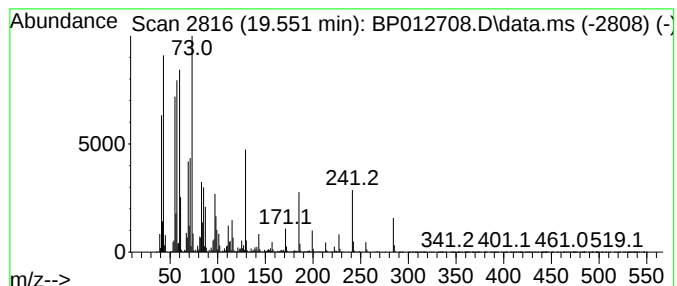
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.551	113.95 ng	28744300	Chrysene-d12	21.510

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	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Undecanoic acid	186	C11H22O2	000112-37-8	74



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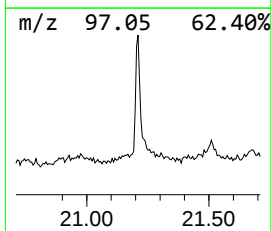
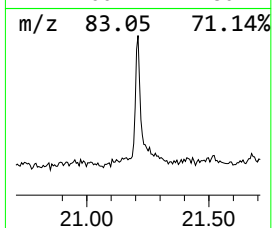
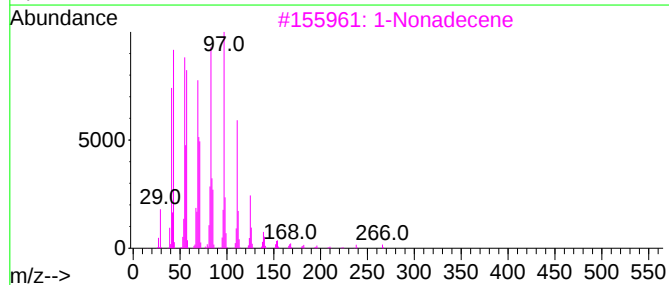
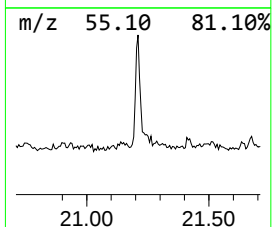
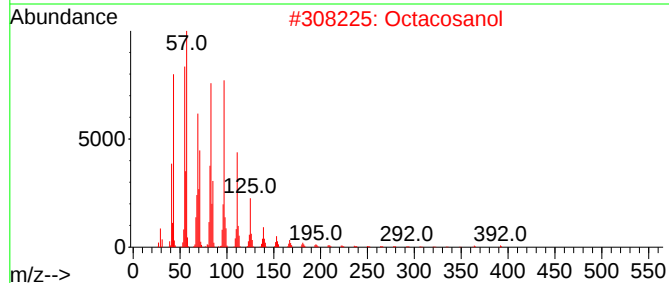
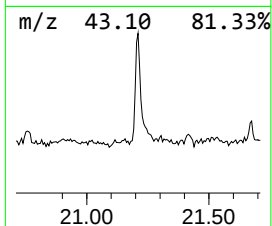
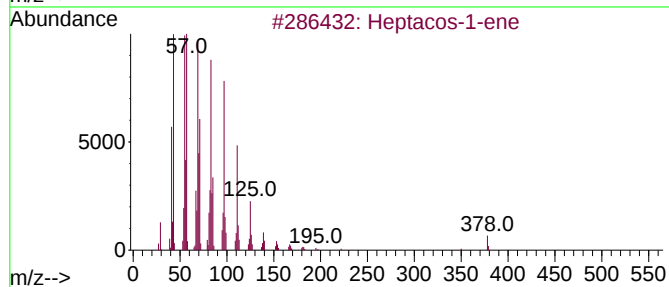
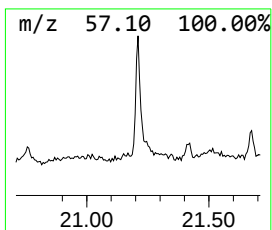
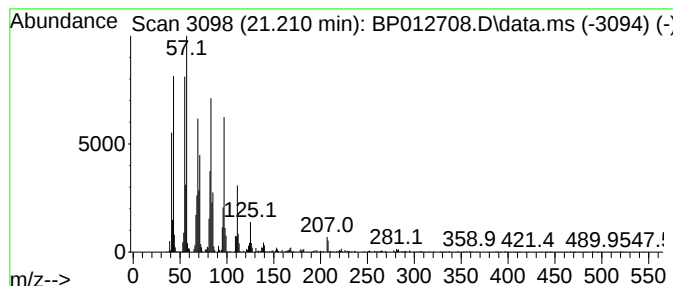
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacos-1-ene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.210	2.95 ng	743221	Chrysene-d12	21.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacos-1-ene	378	C27H54	015306-27-1	94
2			Octacosanol	410	C28H58O	000557-61-9	94
3			1-Nonadecene	266	C19H38	018435-45-5	93
4			1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112322\
Data File : BP012708.D
Acq On : 23 Nov 2022 13:49
Operator : CG/JU
Sample : N5742-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-42

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112222.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...	3.140	78.0	ng	9634840	1	8.034	2470550	20.0
2-Pentanone, 4-...	5.111	3.1	ng	385740	1	8.034	2470550	20.0
n-Hexadecanoic ...	18.310	58.9	ng	12199700	4	17.422	4144210	20.0
cis-Vaccenic acid	19.416	7.2	ng	1496760	4	17.422	4144210	20.0
Octadecanoic acid	19.551	114.0	ng	28744300	5	21.510	5044950	20.0
Heptacos-1-ene	21.210	3.0	ng	743221	5	21.510	5044950	20.0