

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080322\
 Data File : BM036078.D
 Acq On : 03 Aug 2022 15:09
 Operator : CG/JU
 Sample : N3998-07
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-7

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_M\Methods\8270-BM080122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036078.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.428	391	398	415	rBV	4925817	7128749	45.73%	7.956%
2	7.040	664	672	685	rVB	4719080	7539136	48.36%	8.414%
3	7.863	805	812	818	rBV	1013605	1550208	9.94%	1.730%
4	7.928	818	823	832	rBV	150473	257215	1.65%	0.287%
5	9.034	1003	1011	1025	rBV	2906375	4709762	30.21%	5.256%
6	10.669	1279	1289	1297	rBV	1483227	2443638	15.67%	2.727%
7	13.133	1700	1708	1715	rBV	7442047	10651465	68.32%	11.887%
8	13.727	1801	1809	1817	rBV	1925751	2600499	16.68%	2.902%
9	14.504	1934	1941	1947	rBV	2361792	3305176	21.20%	3.689%
10	15.992	2186	2194	2208	rBV	6721423	9768937	62.66%	10.902%
11	17.245	2400	2407	2417	rBV	2950644	4097530	26.28%	4.573%
12	18.145	2554	2560	2570	rBV	2016297	2955214	18.96%	3.298%
13	19.174	2731	2735	2741	rBV	339935	451290	2.89%	0.504%
14	19.304	2753	2757	2768	rVB	227890	409922	2.63%	0.457%
15	19.427	2772	2778	2795	rBV	2184504	3416124	21.91%	3.812%
16	19.868	2848	2853	2859	rBV	12306736	15590191	100.00%	17.398%
17	21.139	3065	3069	3079	rBV	1359983	1903571	12.21%	2.124%
18	21.427	3113	3118	3124	rBV	4073902	5005572	32.11%	5.586%
19	21.833	3184	3187	3194	rBV	290046	363202	2.33%	0.405%
20	23.791	3513	3520	3533	rVB2	2734750	5459318	35.02%	6.093%

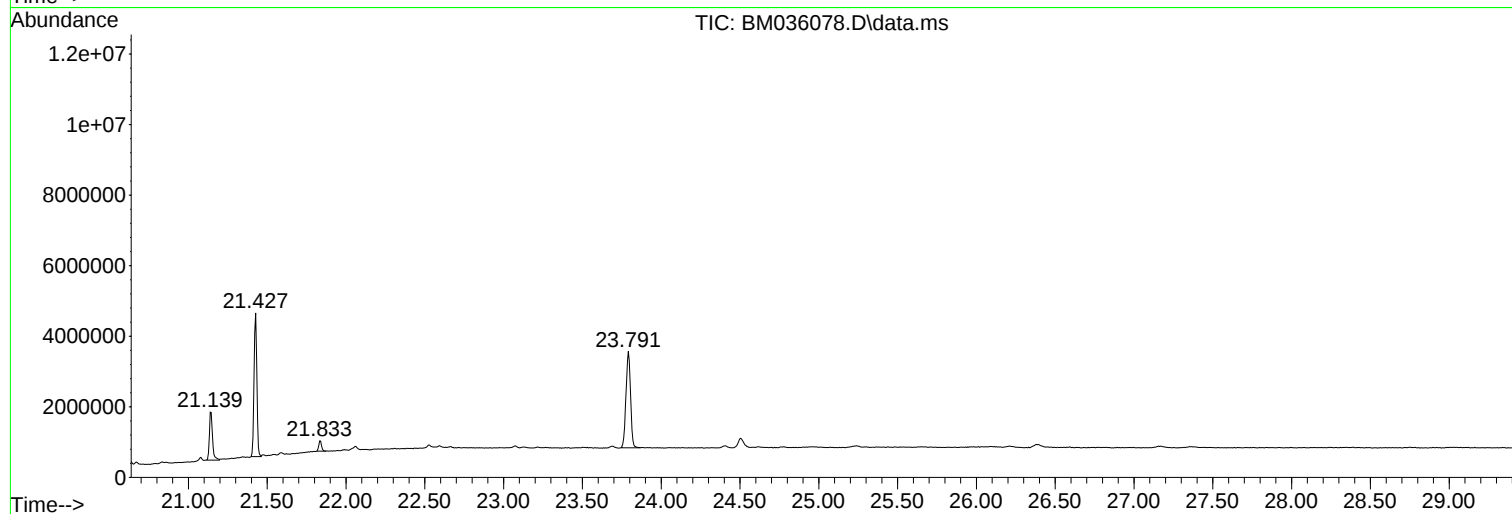
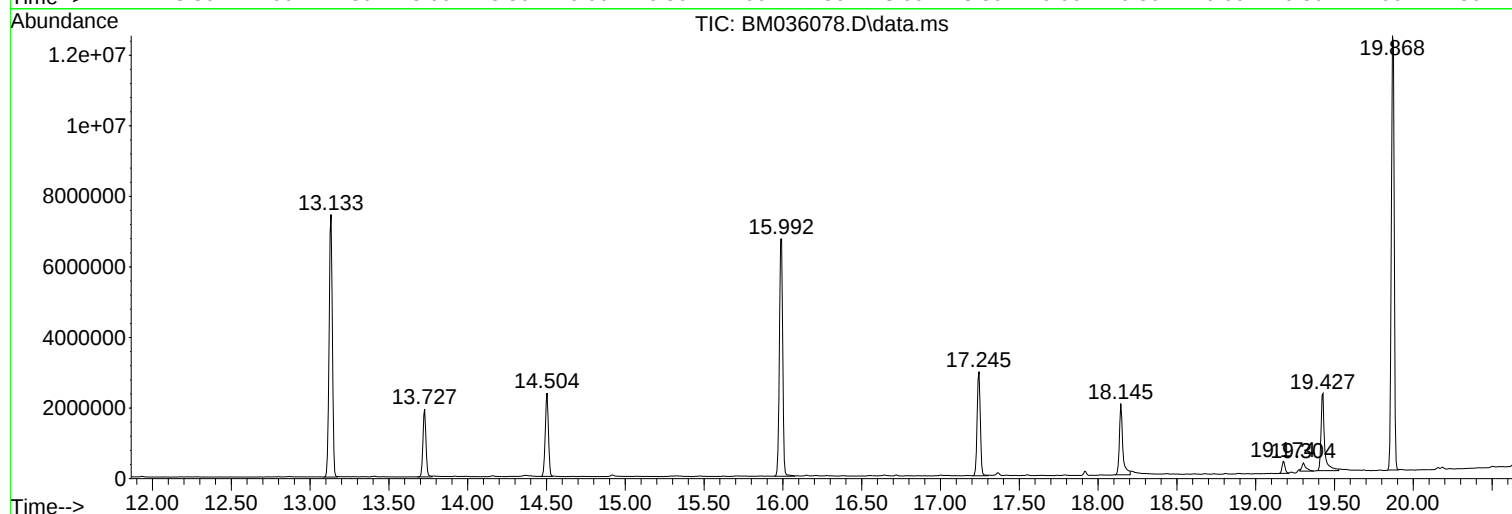
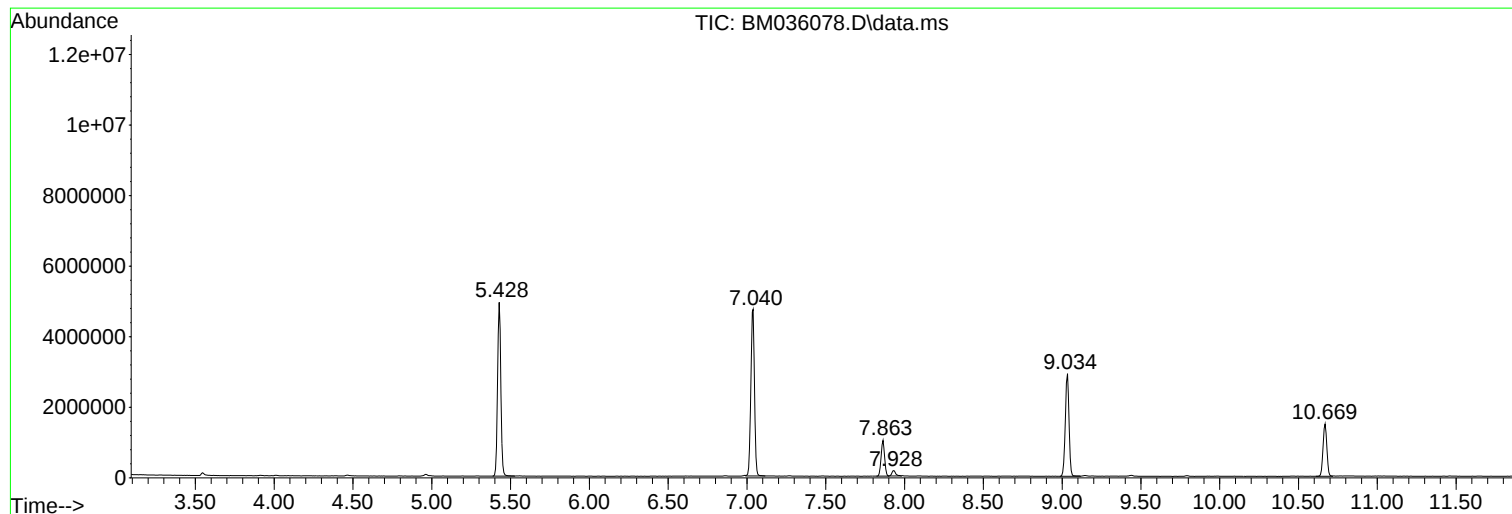
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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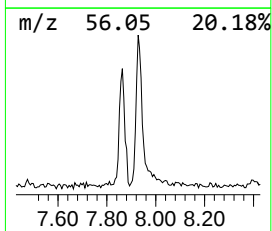
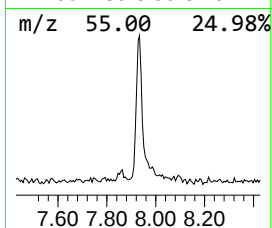
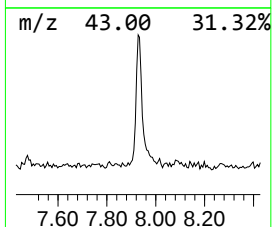
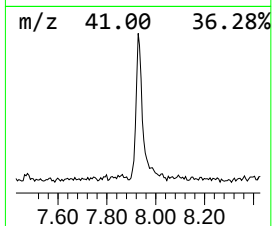
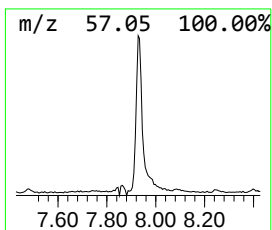
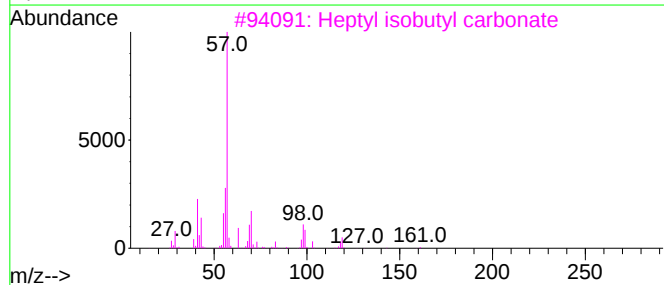
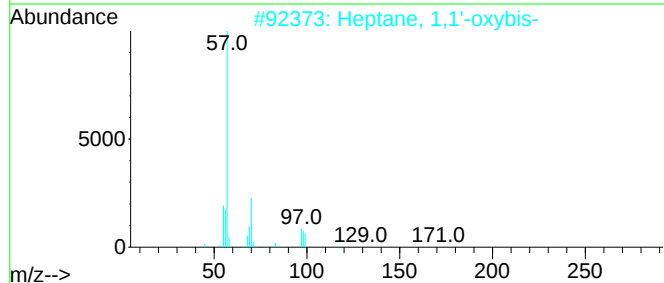
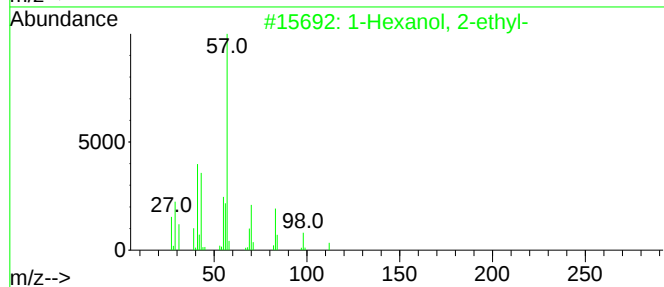
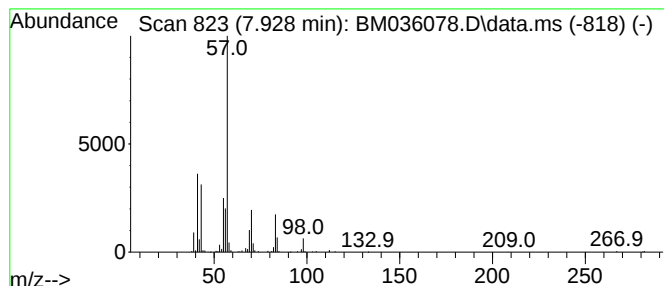
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.928	3.32 ng	257215	1,4-Dichlorobenzene-d4	7.863

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
3		Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	53
4		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5		Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	50



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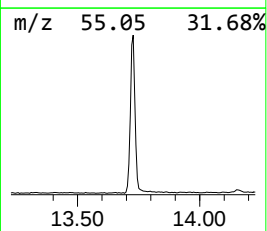
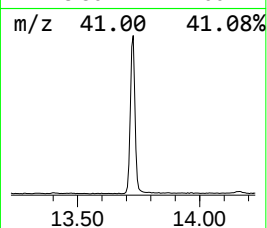
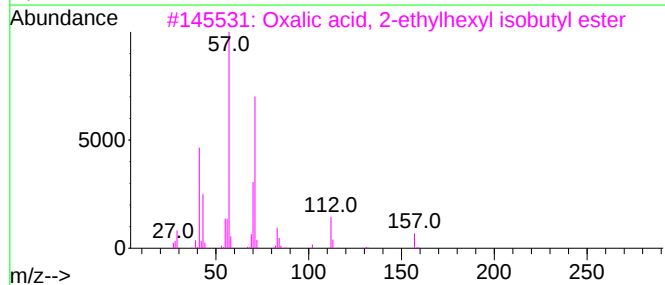
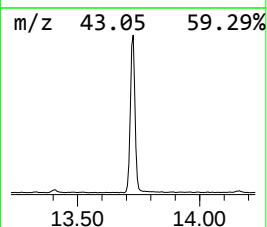
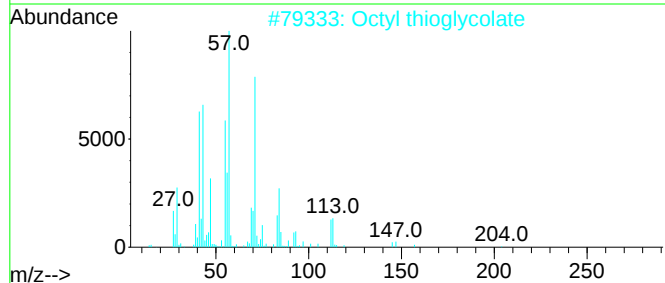
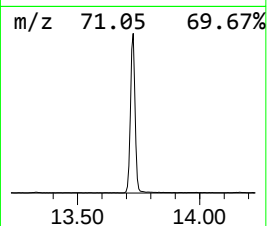
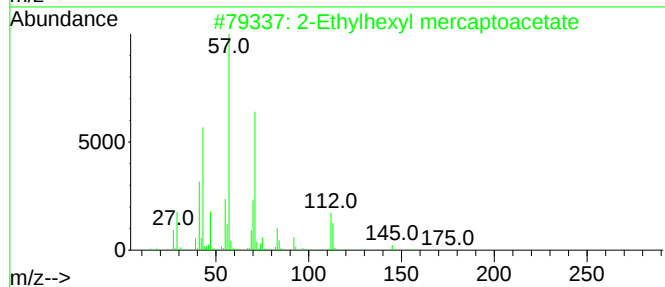
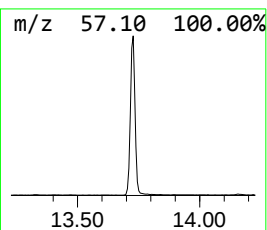
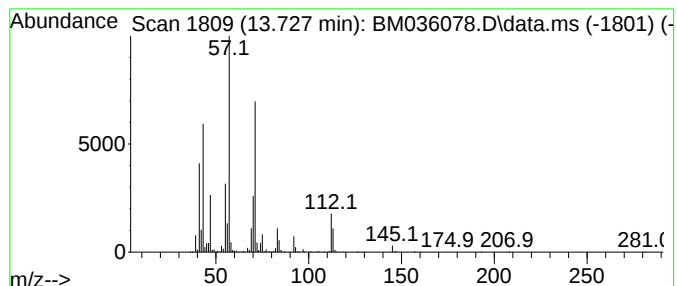
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Ethylhexyl mercaptoacetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.727	15.74 ng	2600500	Acenaphthene-d10	14.504	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	87
2	Octyl thioglycolate	204	C10H20O2S	007664-80-4	59
3	Oxalic acid, 2-ethylhexyl isobut...	258	C14H26O4	1010309-38-5	58
4	Oxalic acid, bis(2-ethylhexyl) e...	314	C18H34O4	1000309-39-0	53
5	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	50



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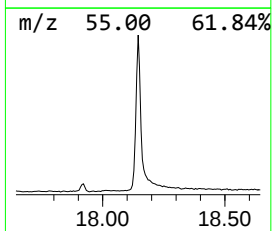
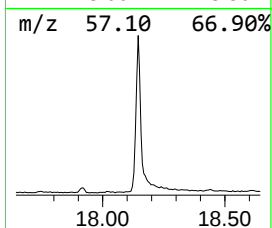
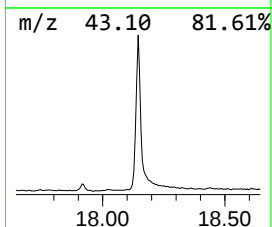
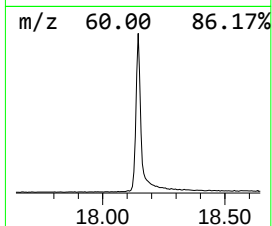
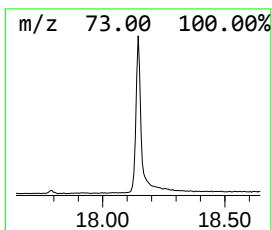
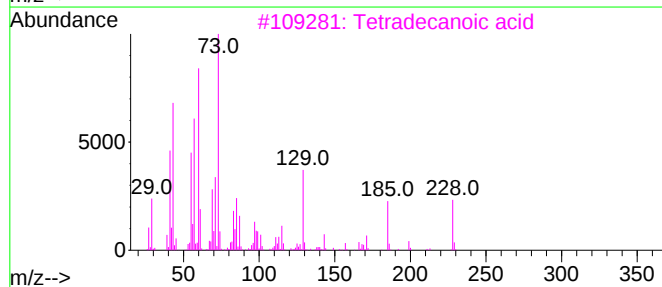
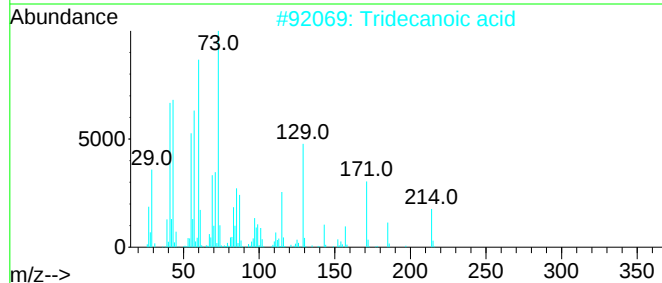
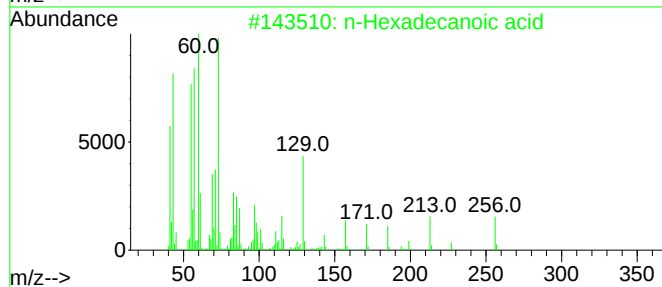
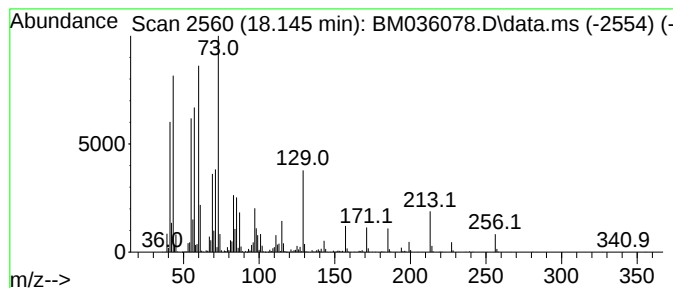
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.145	14.42 ng	2955210	Phenanthrene-d10	17.245

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	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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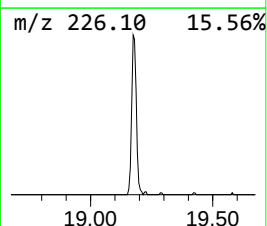
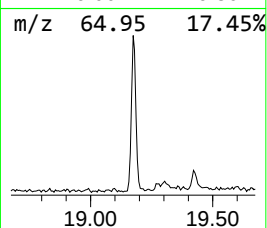
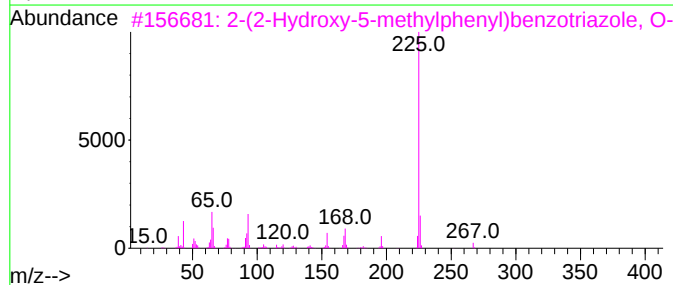
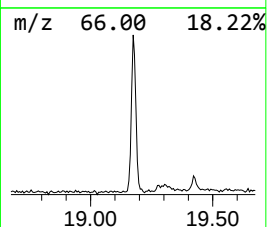
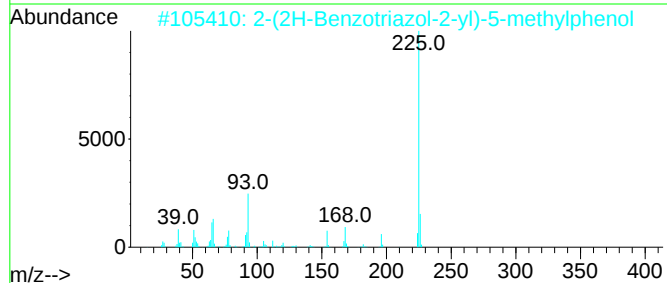
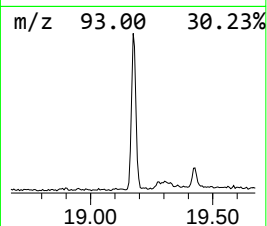
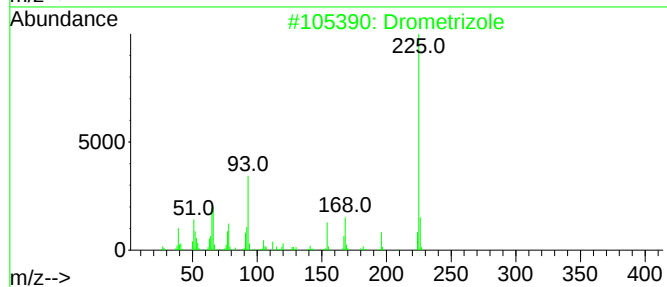
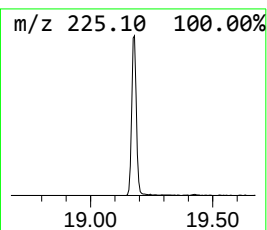
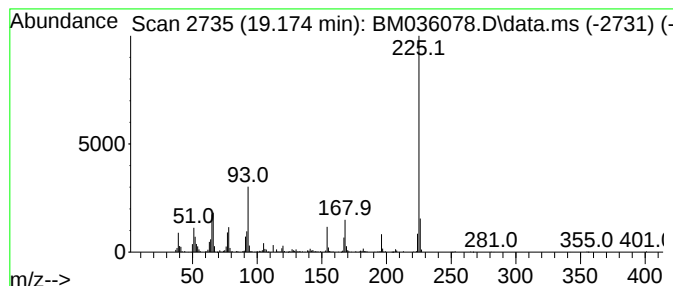
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Drometrizole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.174	2.20 ng	451290	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Drometrizole	225	C13H11N3O	002440-22-4	99
2			2-(2H-Benzotriazol-2-yl)-5-methy...	225	C13H11N3O	004998-48-5	96
3			2-(2-Hydroxy-5-methylphenyl)benz...	267	C15H13N3O2	1000384-15-2	87
4			2H-Benzotriazole, 2-(2-butoxy-5-...	281	C17H19N3O	1000262-87-5	72
5			4,5-Diamino-2-phenyl(2H)benzotri...	225	C12H11N5	166766-26-3	50



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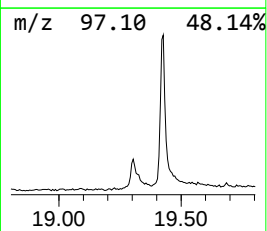
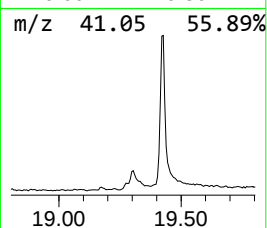
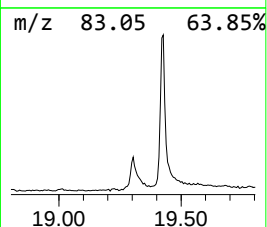
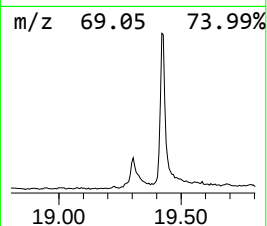
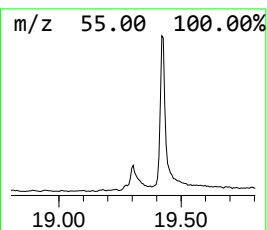
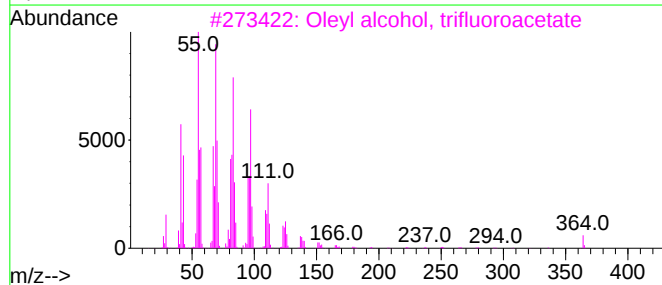
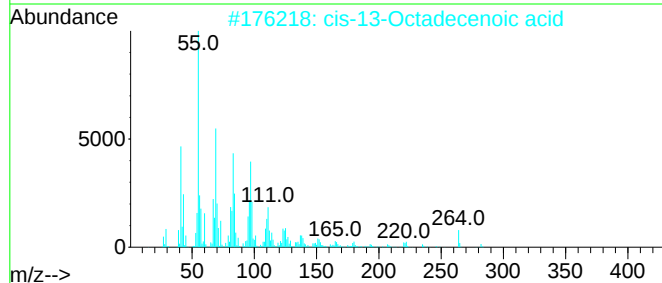
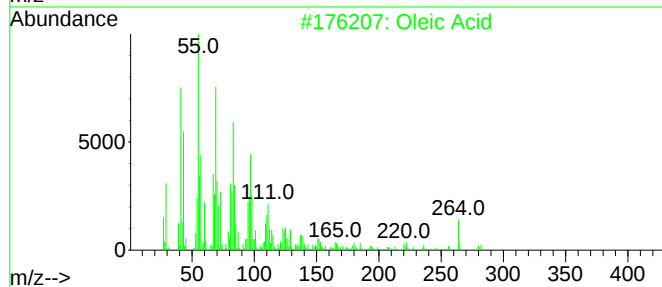
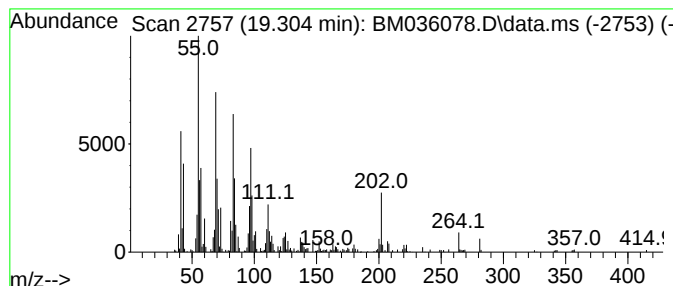
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Oleic Acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.304	2.00 ng	409922	Phenanthrene-d10		17.245	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Oleic Acid		282	C18H34O2	000112-80-1	93
2	cis-13-Octadecenoic acid		282	C18H34O2	013126-39-1	78
3	Oleyl alcohol, trifluoroacetate		364	C20H35F3O2	1000352-68-4	72
4	9-Octadecenoic acid, (E)-		282	C18H34O2	000112-79-8	68
5	trans-13-Octadecenoic acid		282	C18H34O2	000693-71-0	53



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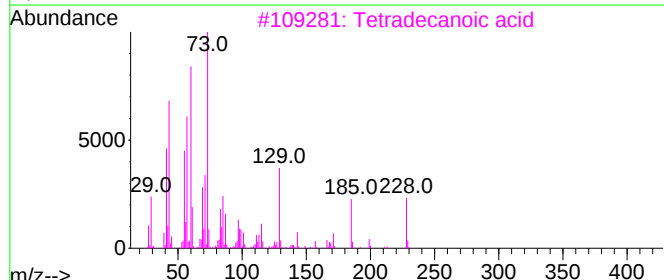
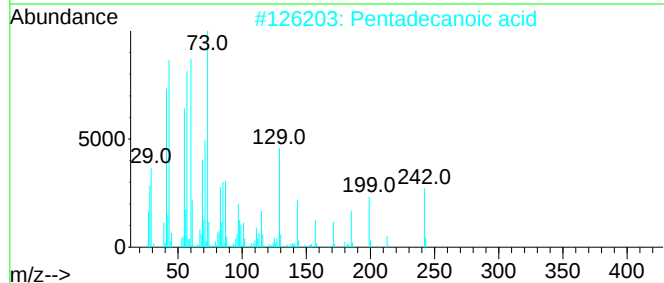
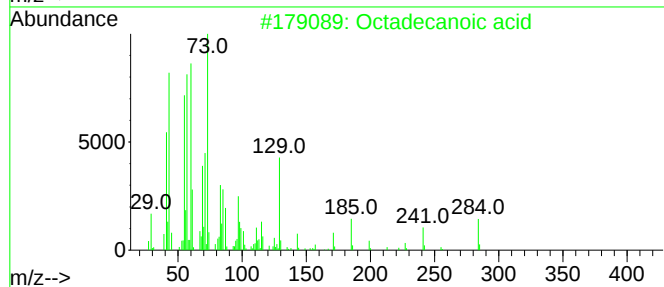
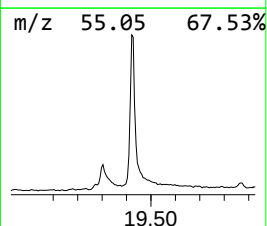
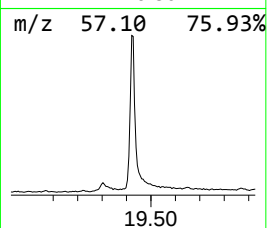
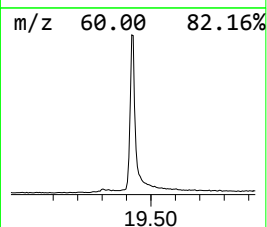
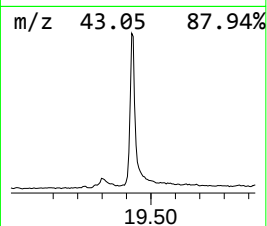
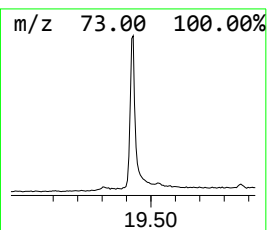
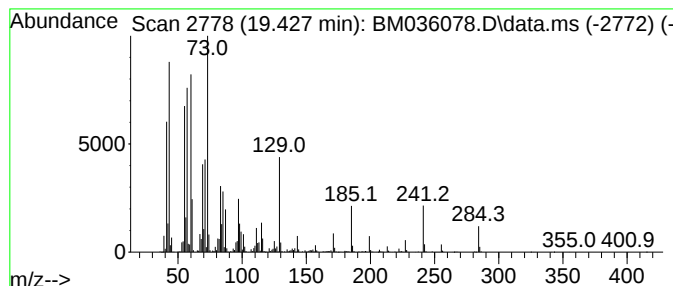
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.427	13.65 ng	3416120	Chrysene-d12	21.427

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	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080322\
Data File : BM036078.D
Acq On : 03 Aug 2022 15:09
Operator : CG/JU
Sample : N3998-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-7

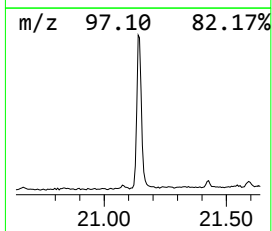
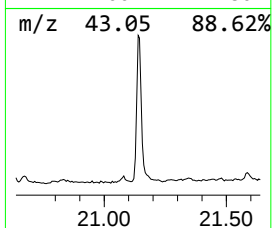
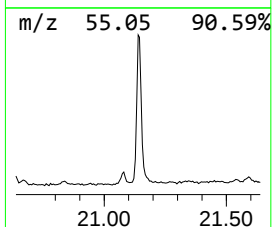
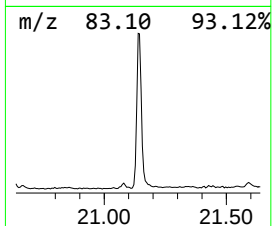
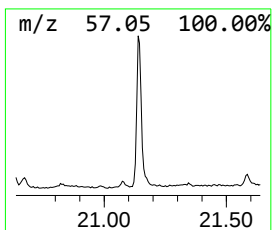
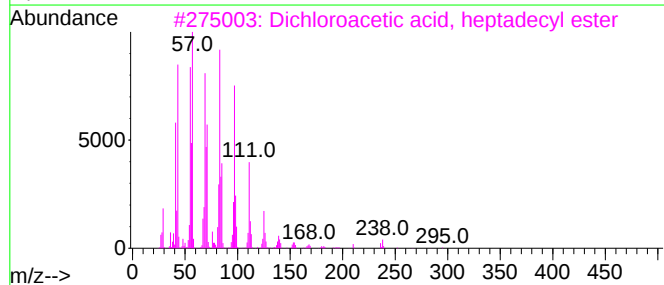
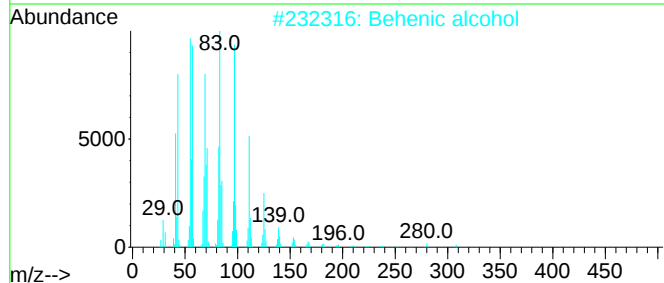
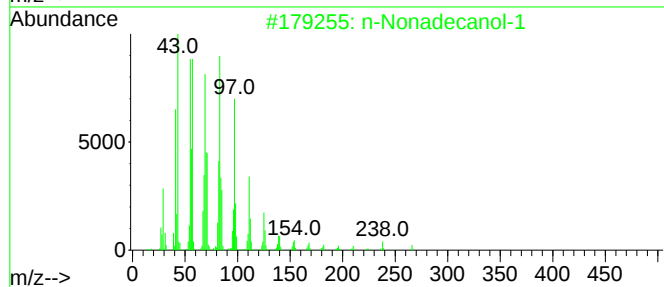
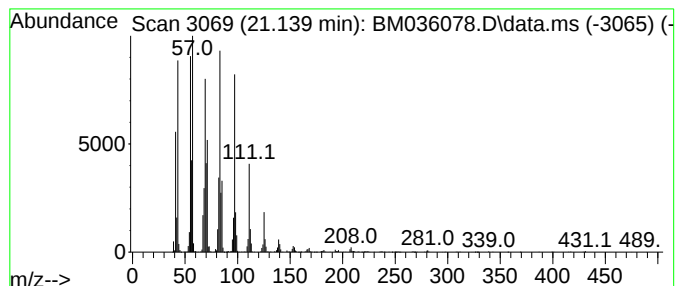
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.139	7.61 ng	1903570	Chrysene-d12	21.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4			Pentacos-1-ene	350	C25H50	016980-85-1	94
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080322\
Data File : BM036078.D
Acq On : 03 Aug 2022 15:09
Operator : CG/JU
Sample : N3998-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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
1-Hexanol, 2-et...	7.928	3.3	ng	257215	1	7.863	1550210	20.0
2-Ethylhexyl me...	13.727	15.7	ng	2600500	3	14.504	3305180	20.0
n-Hexadecanoic ...	18.145	14.4	ng	2955210	4	17.245	4097530	20.0
Drometrizole	19.174	2.2	ng	451290	4	17.245	4097530	20.0
Oleic Acid	19.304	2.0	ng	409922	4	17.245	4097530	20.0
Octadecanoic acid	19.427	13.7	ng	3416120	5	21.427	5005570	20.0
n-Nonadecanol-1	21.139	7.6	ng	1903570	5	21.427	5005570	20.0