

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010722\
 Data File : BM033684.D
 Acq On : 08 Jan 2022 00:16
 Operator : CG/JU
 Sample : N1071-02
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 FM-E1-01-4.5

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-BM010522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033684.D\data.ms

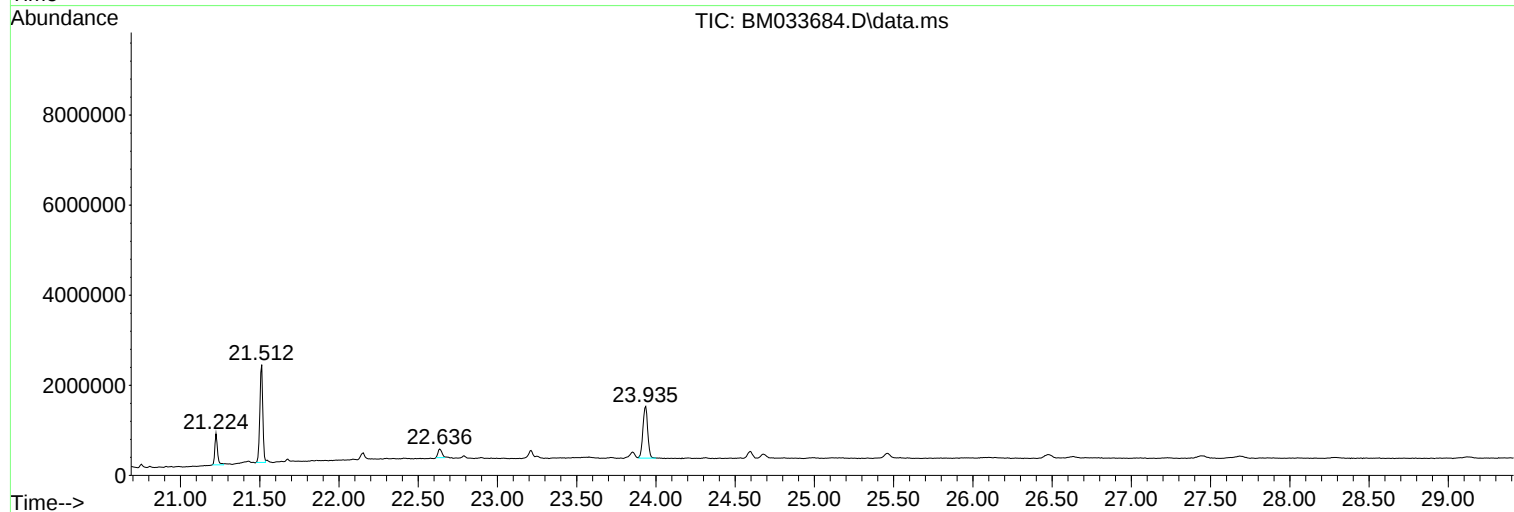
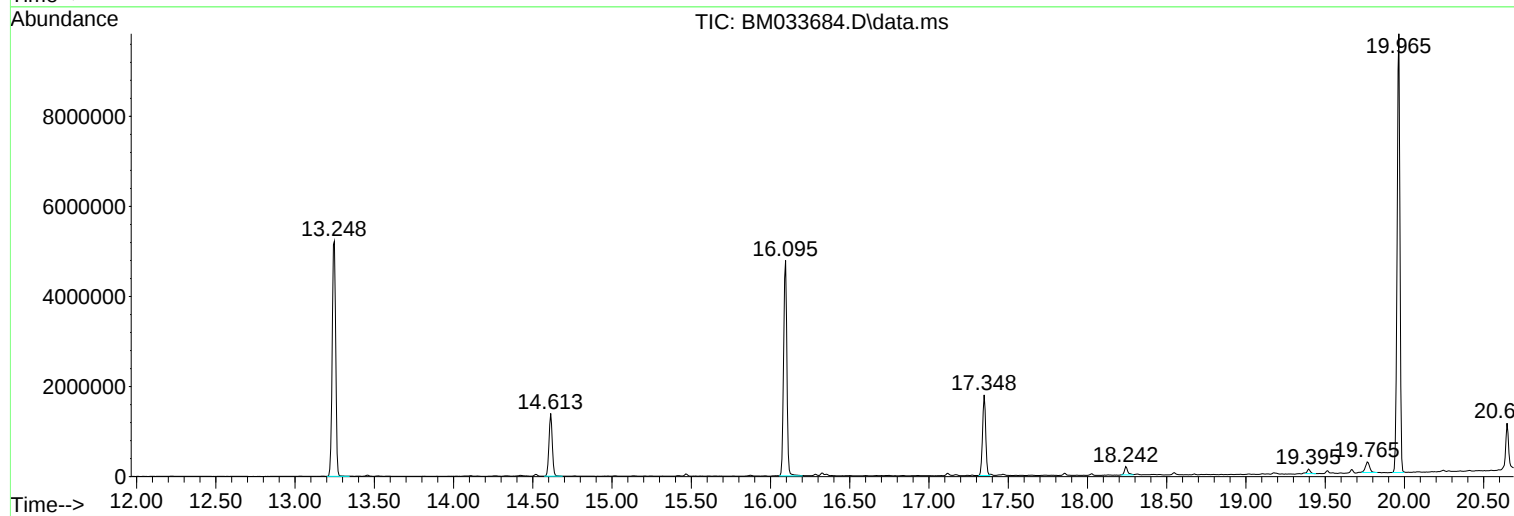
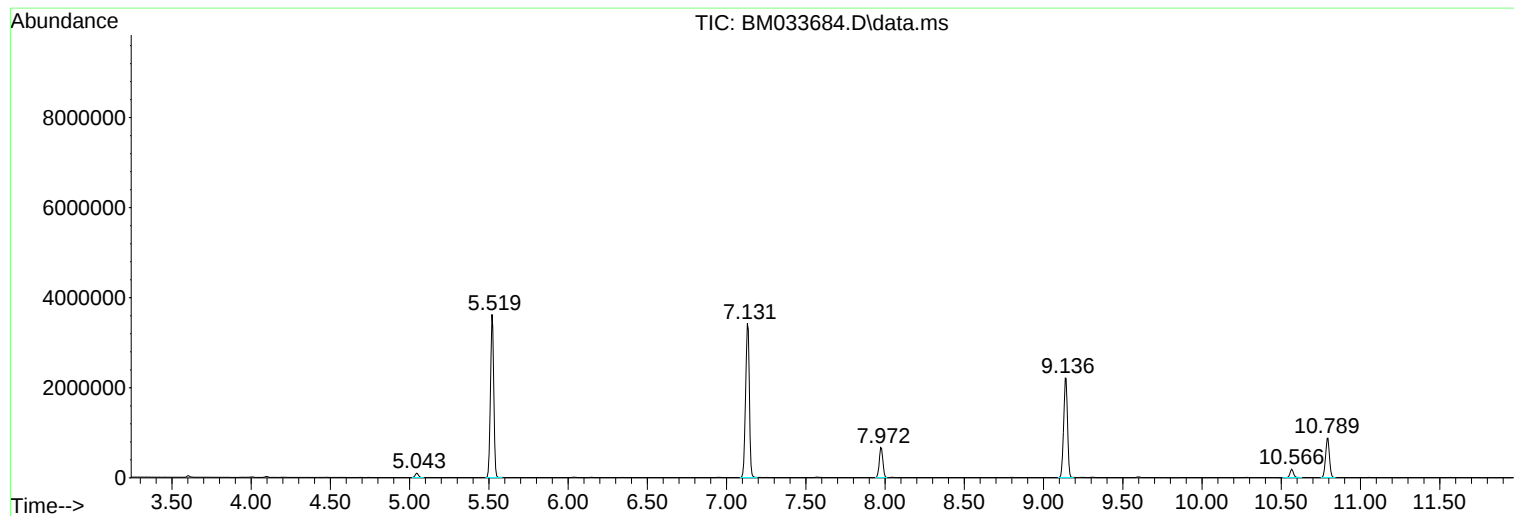
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.043	302	307	315	rVB2	94296	144110	1.17%	0.249%
2	5.519	381	388	399	rBV	3624246	5236907	42.64%	9.047%
3	7.131	654	662	673	rBV	3424132	5607614	45.65%	9.687%
4	7.972	799	805	812	rBV	668323	1050236	8.55%	1.814%
5	9.136	995	1003	1012	rBV	2211450	3755159	30.57%	

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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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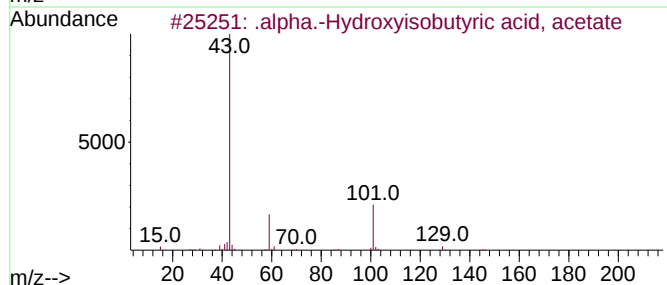
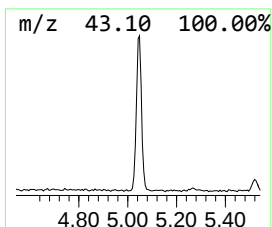
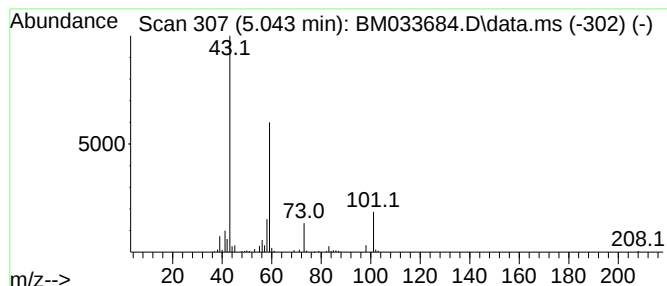
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Peak Number 1 .alpha.-Hydroxyisobutyric a... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.043	2.74 ng	144110	1,4-Dichlorobenzene-d4	7.972

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.alpha.-Hydroxyisobutyric acid, ...	146	C6H10O4	1000374-31-3	53
2			Dimethadione	129	C5H7NO3	000695-53-4	42
3			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
4			.alpha.-D-Galactopyranoside, met...	249	C10H19NO6	017296-07-0	39
5			DL-Lactamide, N,O-dimethyl-	117	C5H11NO2	1000452-56-3	32



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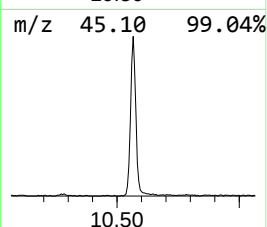
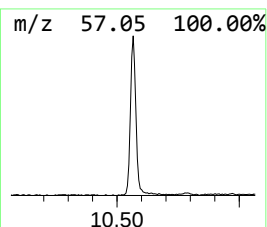
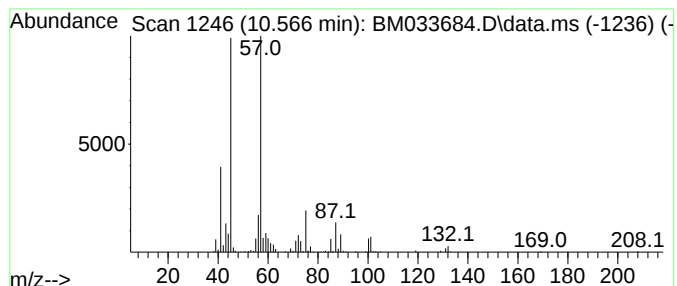
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.566	3.93 ng	293613	Naphthalene-d8	10.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	52
5			Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	50



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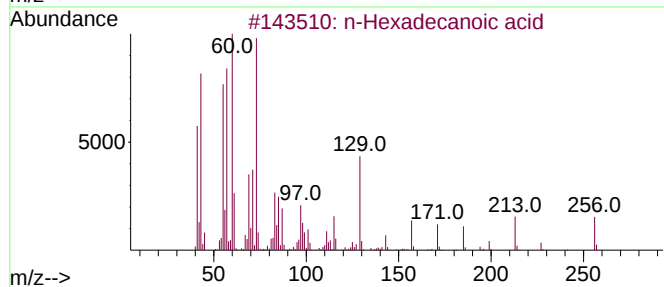
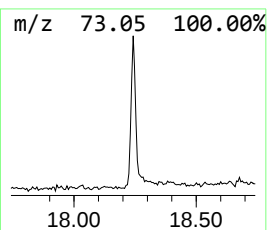
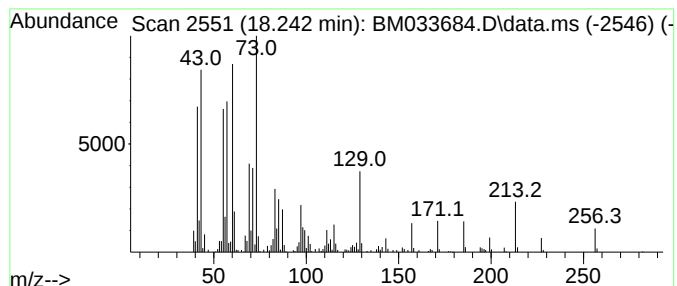
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.242	2.22 ng	274526	Phenanthrene-d10	17.348

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	64



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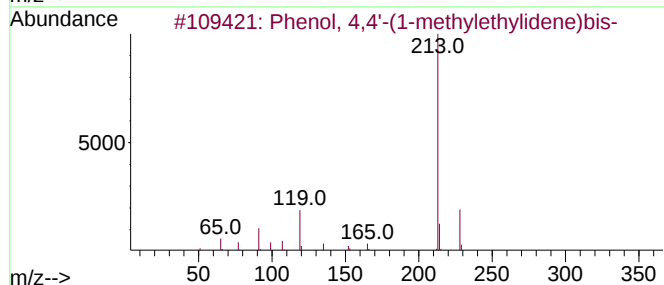
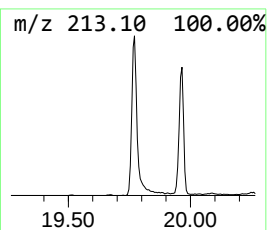
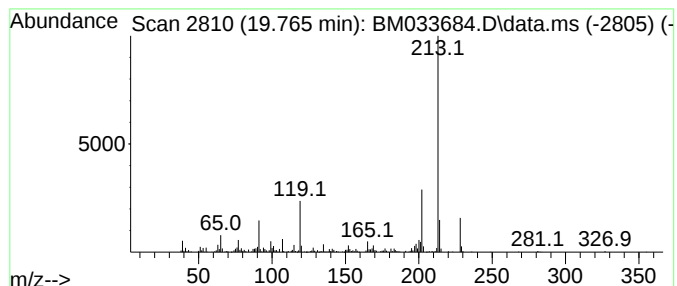
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phenol, 4,4'-(1-methylethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.765	3.02 ng	423922	Chrysene-d12	21.512

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	97
2			3,4'-Isopropylidenediphenol	228	C15H16O2	046765-25-7	70
3			2,2-Bis-(4-hydroxyphenyl)-butane	242	C16H18O2	000077-40-7	58
4			3,4,6-Trichloro-guaiacol	226	C7H5Cl3O2	060712-44-9	53
5			Diphenolic acid	286	C17H18O4	000126-00-1	50



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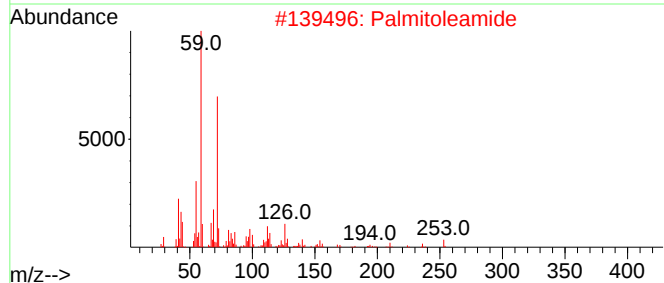
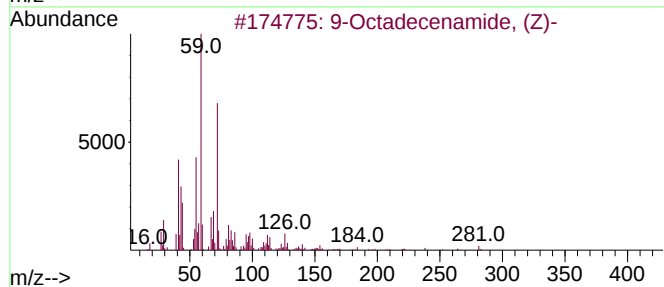
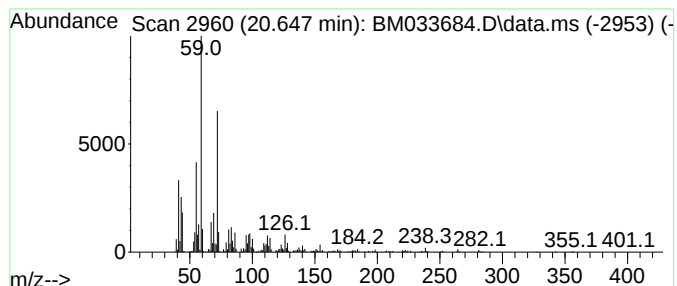
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.647	10.18 ng	1431410	Chrysene-d12	21.512

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2			Palmitoleamide	253	C16H31NO	106010-22-4	80
3			Tetradecanamide	227	C14H29NO	000638-58-4	72
4			Octadecanamide	283	C18H37NO	000124-26-5	59
5			Octanamide	143	C8H17NO	000629-01-6	59



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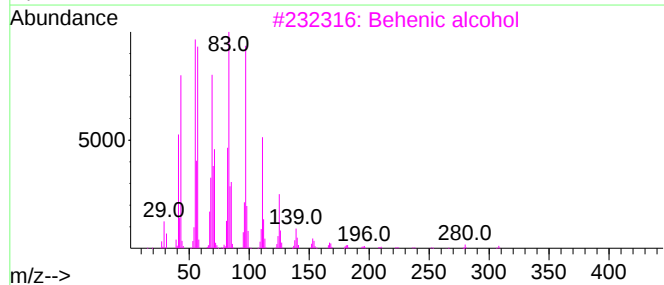
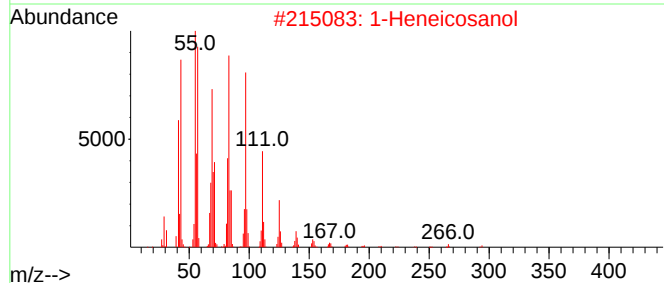
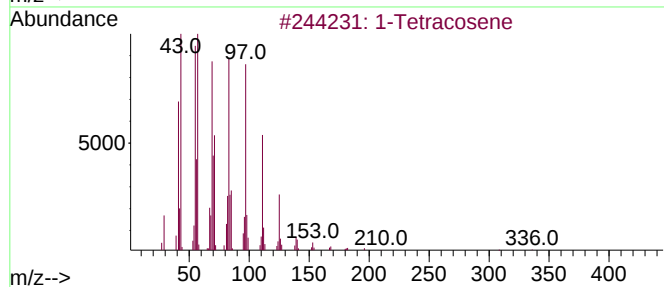
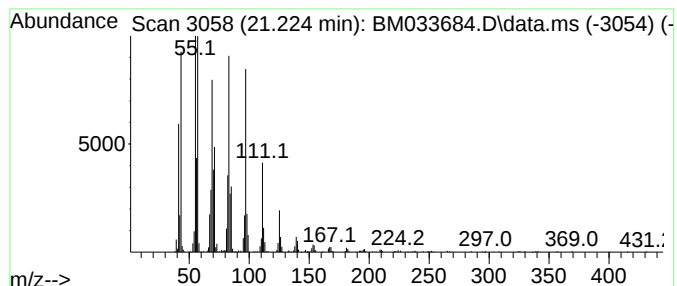
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Tetracosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.224	5.72 ng	804043	Chrysene-d12	21.512	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	Pentacos-1-ene	350	C25H50	016980-85-1	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



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Misc :
ALS Vial : 19 Sample Multiplier: 1

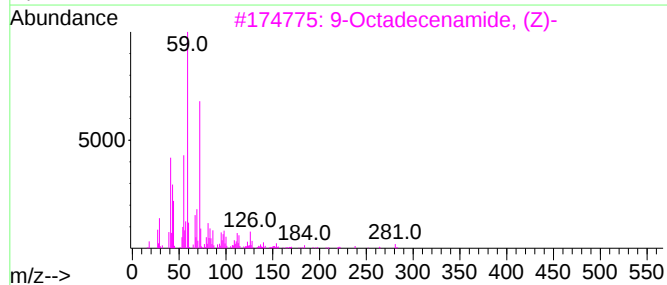
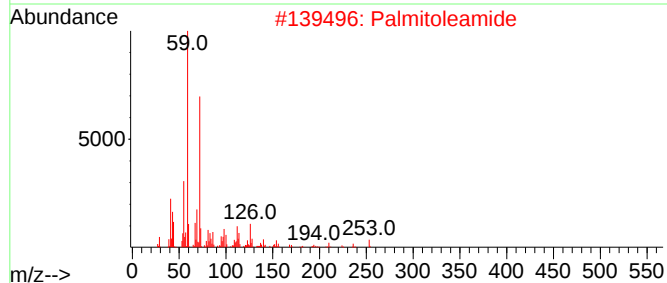
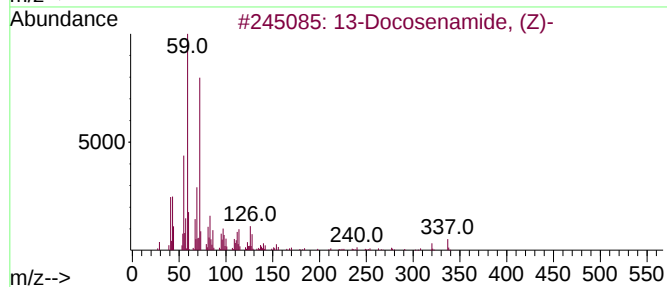
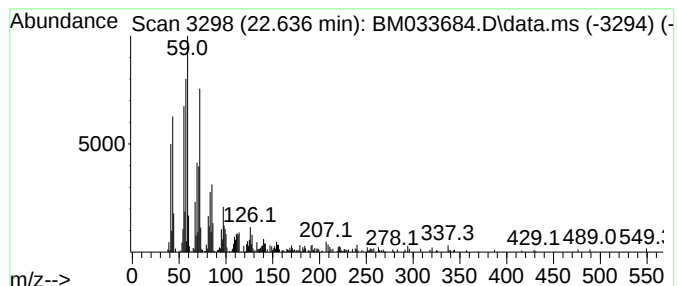
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.636	2.36 ng	331966	Chrysene-d12	21.512	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	97
2	Palmitoleamide	253	C16H31NO	106010-22-4	64
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	58
4	Dodecanamide	199	C12H25NO	001120-16-7	41
5	3-Hexadecanone	240	C16H32O	018787-64-9	38



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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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Ethanol, 2-(2-b...	10.566	3.9	ng	293613	2	10.795	1492350	20.0
n-Hexadecanoic ...	18.242	2.2	ng	274526	4	17.348	2468150	20.0
Phenol, 4,4'-(1...	19.765	3.0	ng	423922	5	21.512	2811730	20.0
9-Octadecenamid...	20.647	10.2	ng	1431410	5	21.512	2811730	20.0
1-Tetracosene	21.224	5.7	ng	804043	5	21.512	2811730	20.0
13-Docosenamide...	22.636	2.4	ng	331966	5	21.512	2811730	20.0