

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
 Data File : BM041314.D
 Acq On : 07 Aug 2023 16:12
 Operator : MA/JU
 Sample : 03903-16
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-06W

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-BM072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041314.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.363	364	370	385	rBV	1263266	1847782	17.57%	4.029%
2	6.969	637	643	661	rBV	681891	1124306	10.69%	2.451%
3	7.787	775	782	790	rBV	626210	979202	9.31%	2.135%
4	8.969	975	983	999	rBV	1997575	3210368	30.53%	7.000%
5	10.386	1215	1224	1241	rBV2	65059	167401	1.59%	0.365%
6	10.592	1252	1259	1272	rBV	835966	1419399	13.50%	3.095%
7	13.075	1674	1681	1699	rBV	5487634	7768360	73.89%	16.938%
8	14.457	1909	1916	1926	rBV	1338934	1990025	18.93%	4.339%
9	15.827	2144	2149	2161	rBV	188654	266095	2.53%	0.580%
10	15.957	2164	2171	2188	rBV	4553527	6488793	61.72%	14.148%
11	17.215	2379	2385	2397	rBV	1697245	2372906	22.57%	5.174%
12	18.115	2532	2538	2549	rBV	1084243	1629101	15.49%	3.552%
13	19.398	2751	2756	2775	rBV	790434	1227861	11.68%	2.677%
14	19.856	2828	2834	2844	rBV	8779651	10514105	100.00%	22.924%
15	21.121	3045	3049	3056	rBV	302307	432225	4.11%	0.942%
16	21.421	3095	3100	3111	rBV	1760109	2203770	20.96%	4.805%
17	22.592	3296	3299	3303	rVB	214510	252967	2.41%	0.552%
18	23.792	3497	3503	3512	rVB	1010517	1969808	18.73%	4.295%

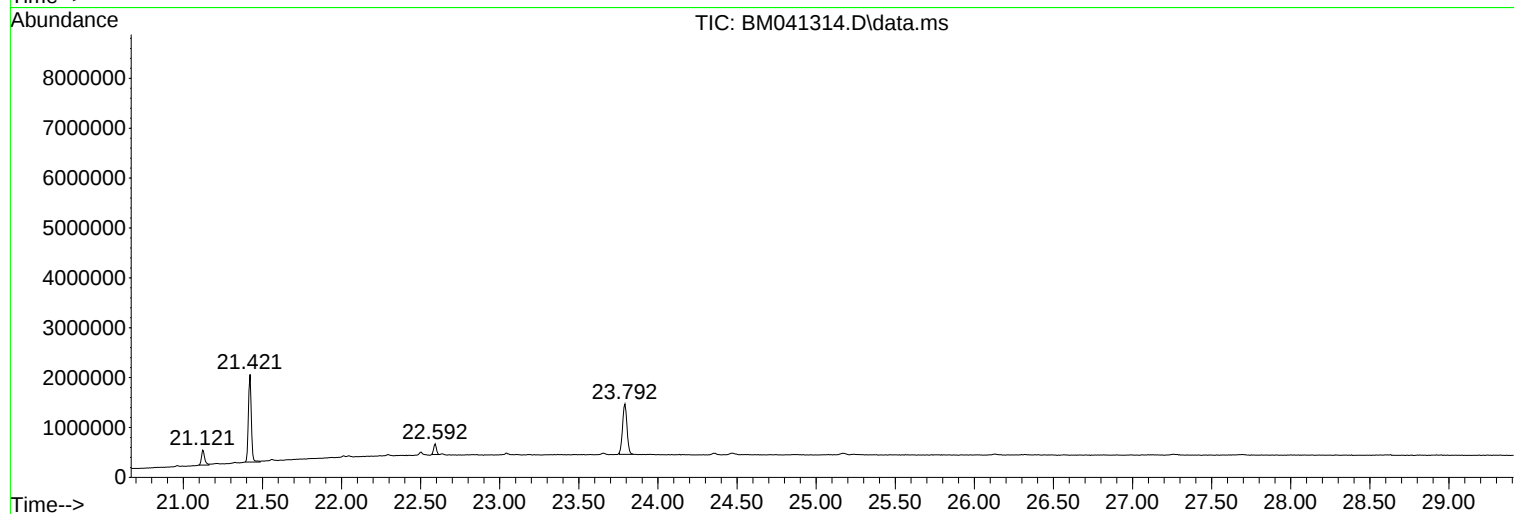
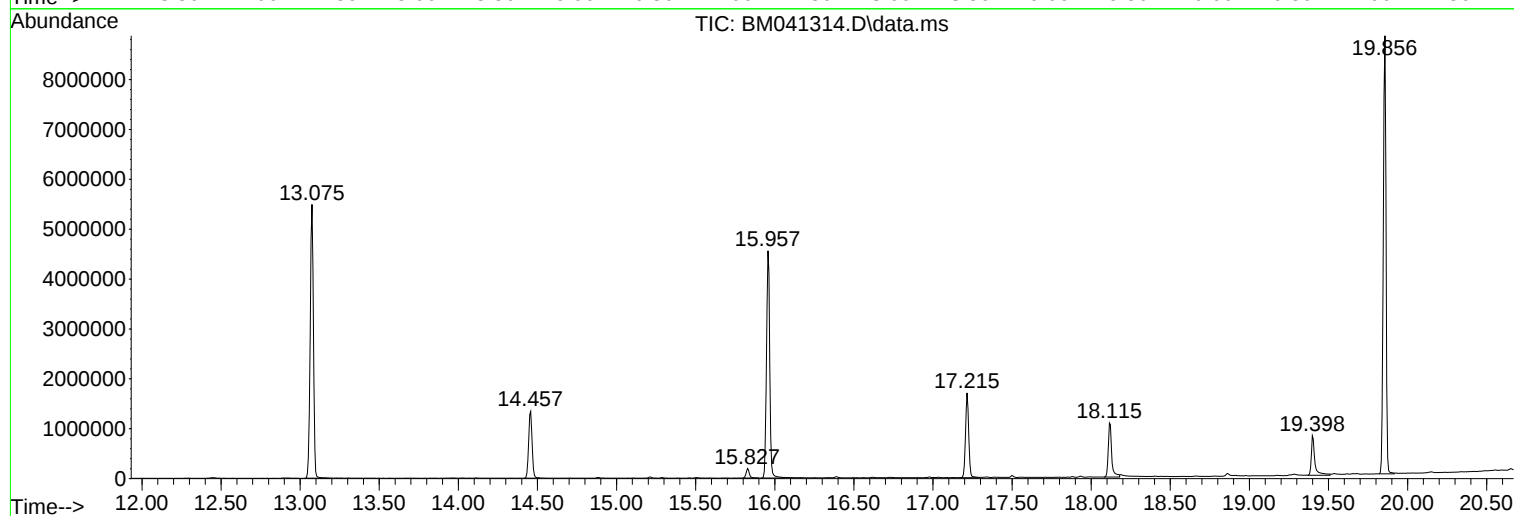
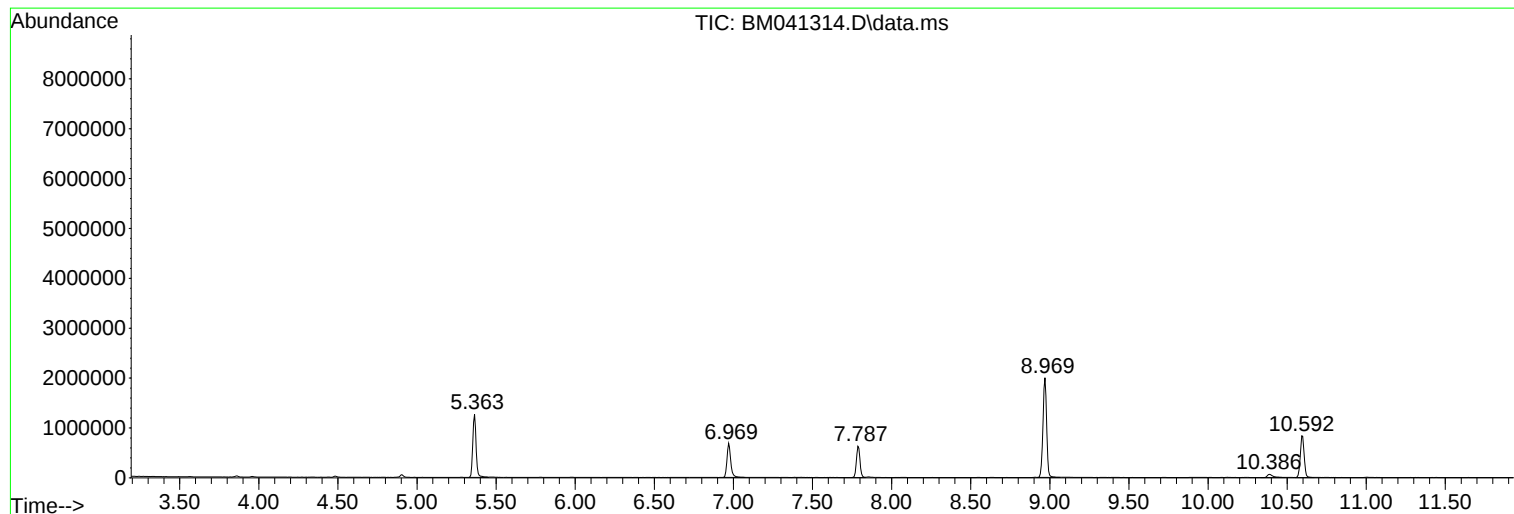
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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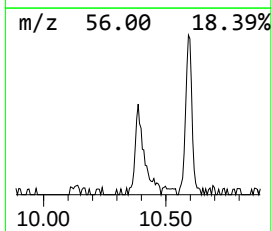
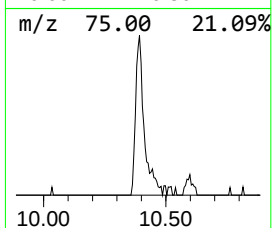
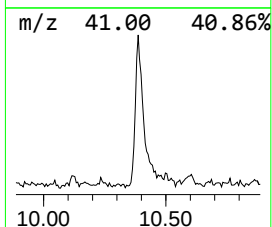
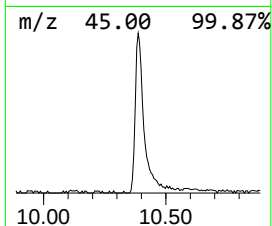
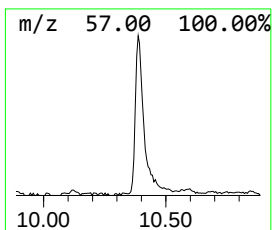
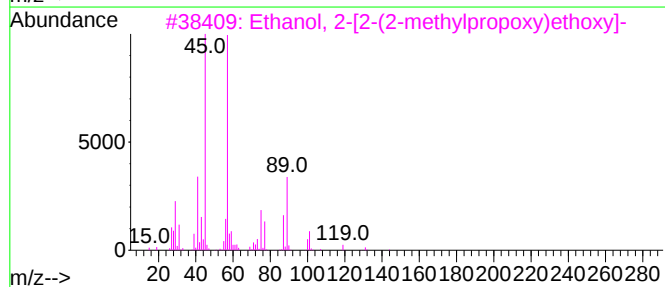
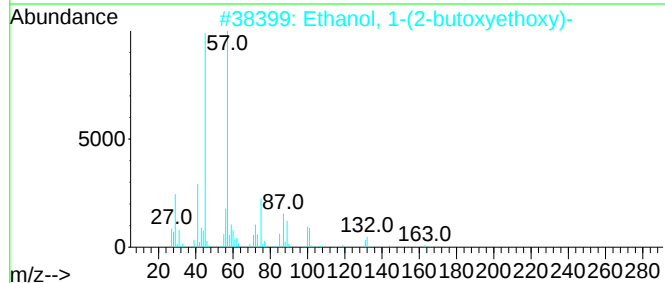
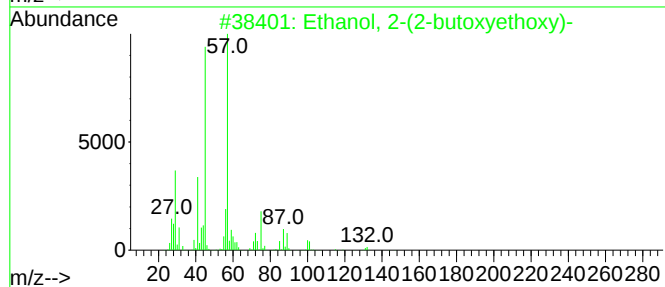
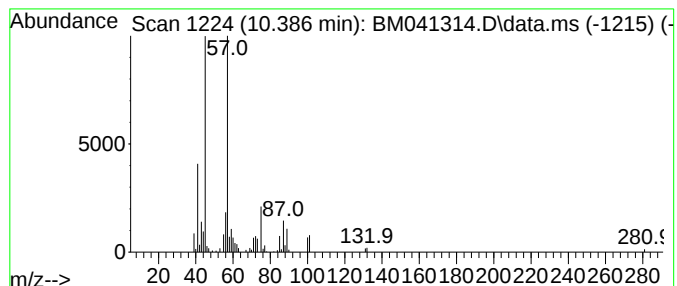
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.387	2.36 ng	167401	Naphthalene-d8	10.592

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			Tetraethylene glycol	194	C8H18O5	000112-60-7	50



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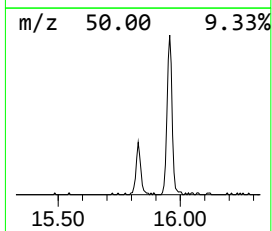
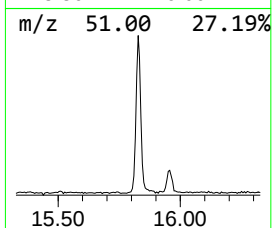
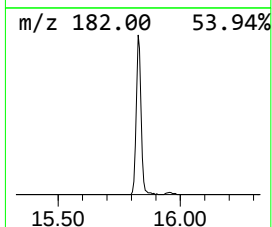
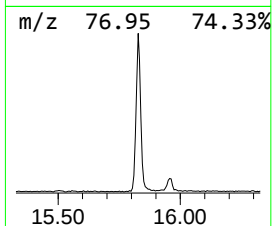
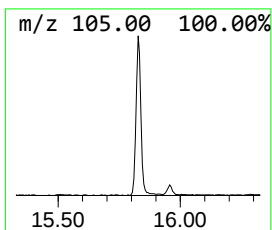
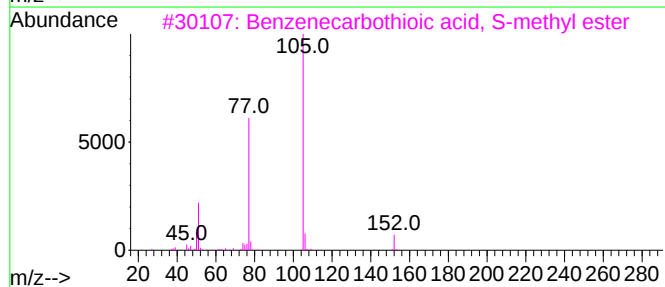
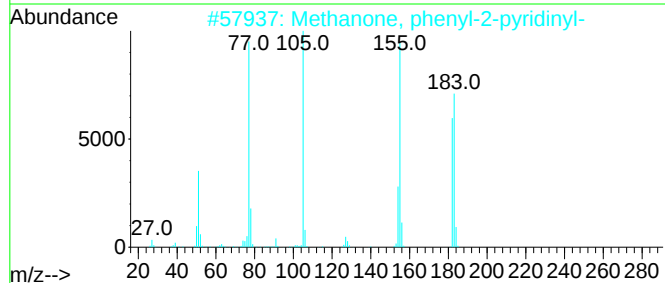
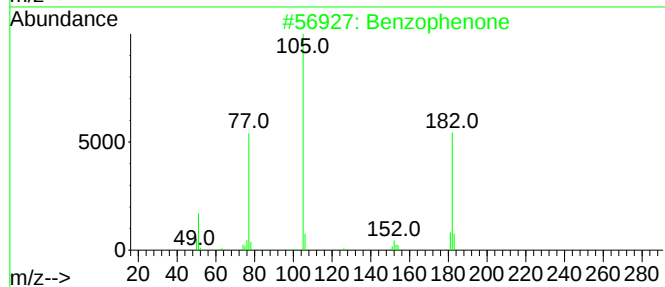
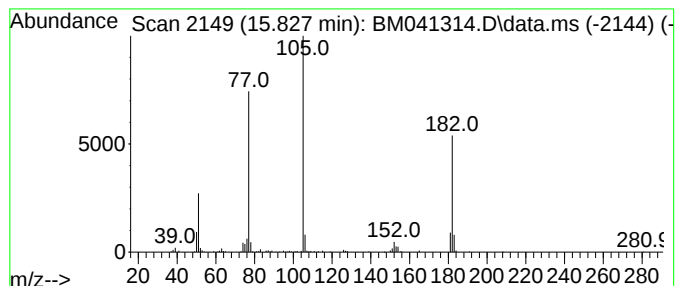
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.827	2.67 ng	266095	Acenaphthene-d10	14.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	78
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	58
4			1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	53
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	53



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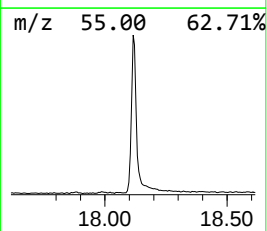
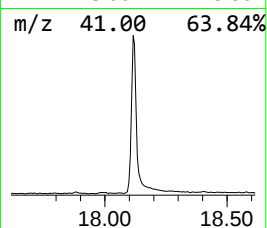
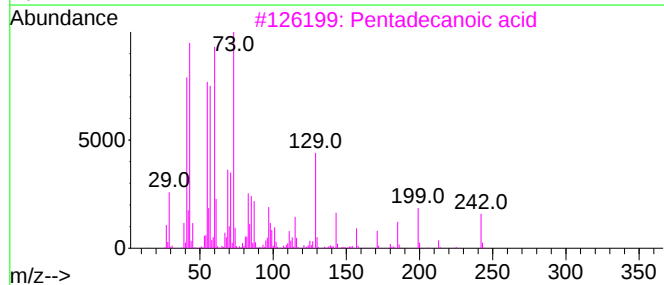
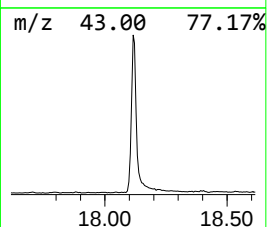
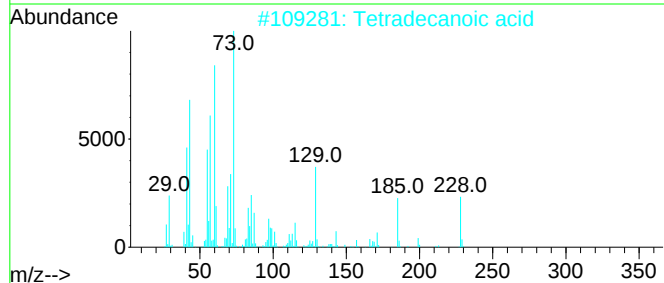
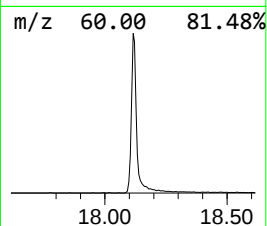
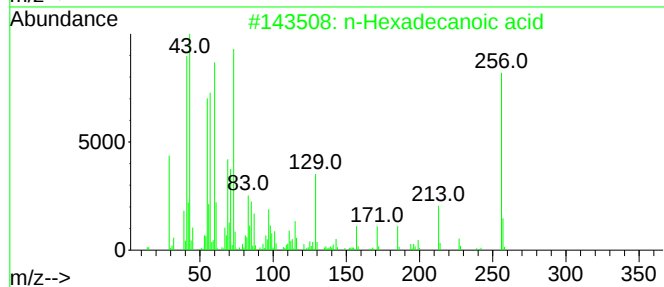
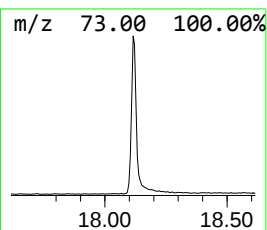
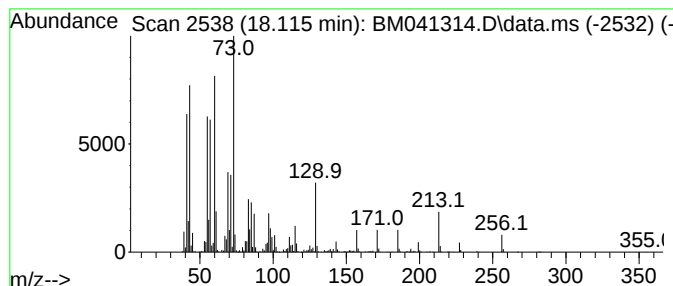
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.115	13.73 ng	1629100	Phenanthrene-d10	17.215

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	81
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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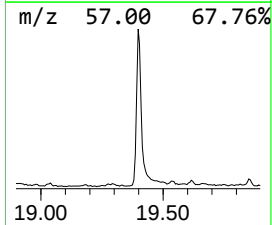
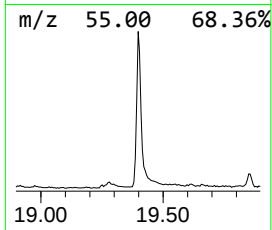
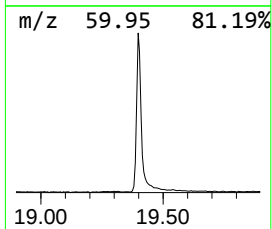
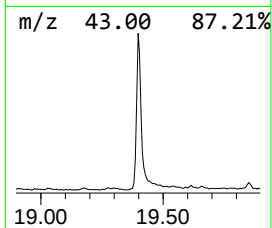
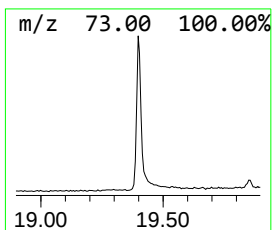
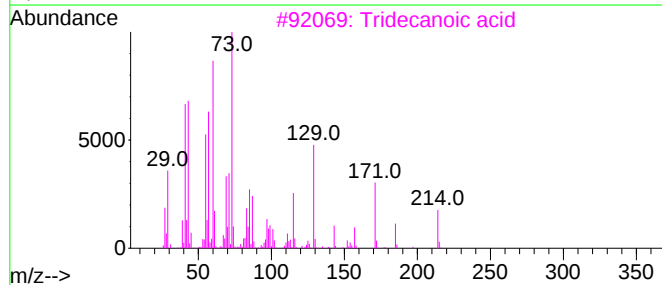
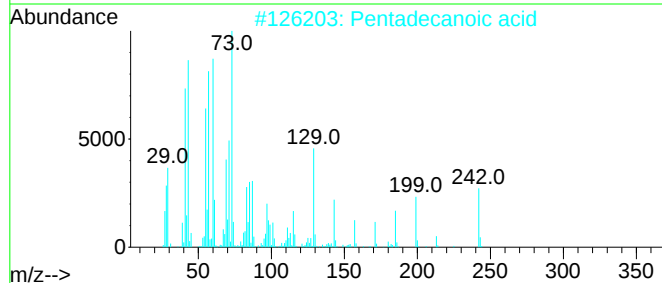
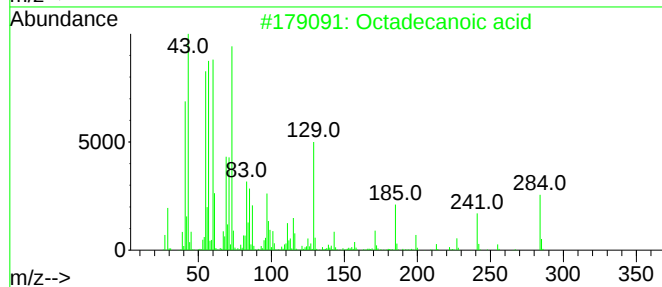
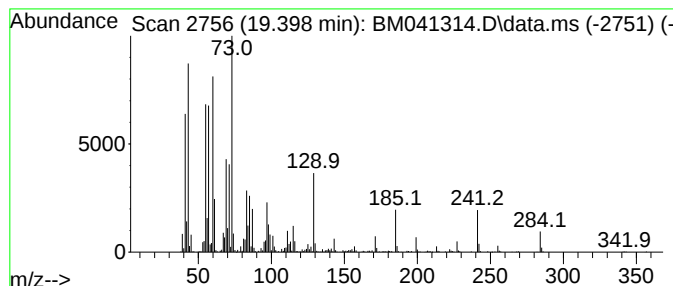
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Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.398	11.14 ng	1227860	Chrysene-d12	21.421

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	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



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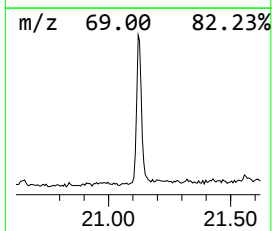
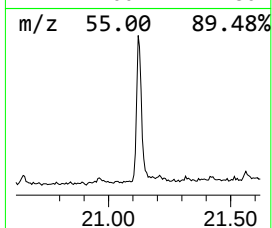
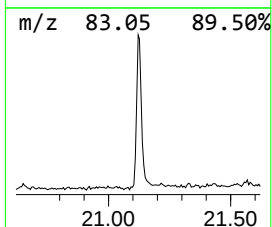
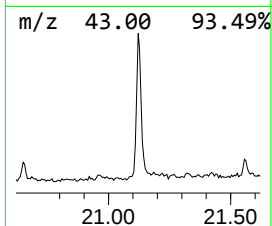
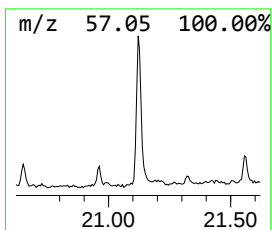
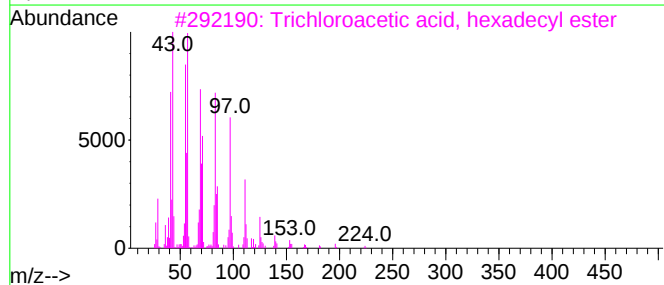
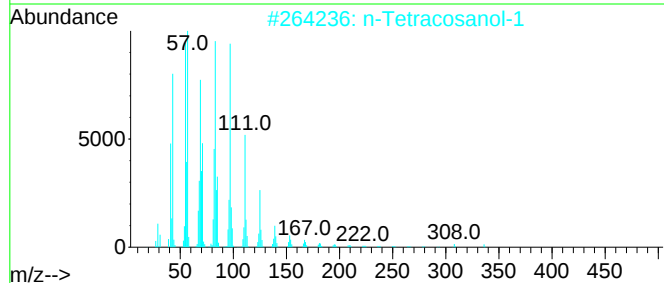
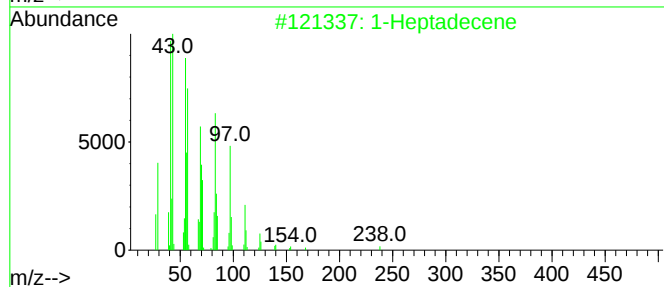
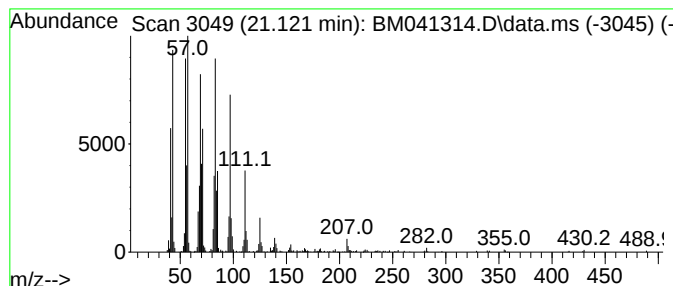
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Heptadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.121	3.92 ng	432225	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptadecene	238	C17H34	006765-39-5	95
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4			9-Eicosene, (E)-	280	C20H40	074685-29-3	93
5			E-14-Hexadecenal	238	C16H30O	330207-53-9	93



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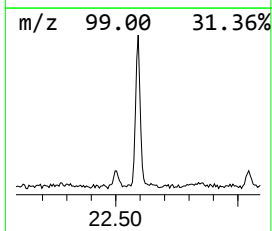
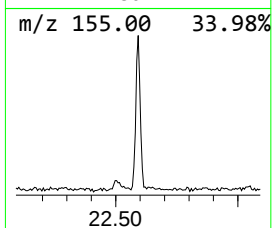
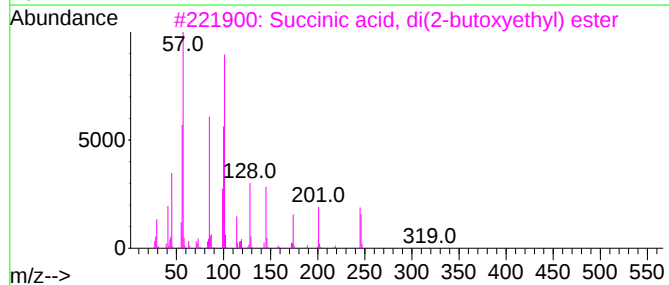
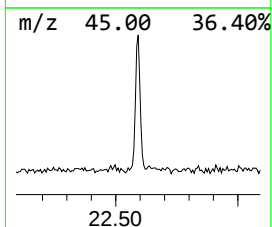
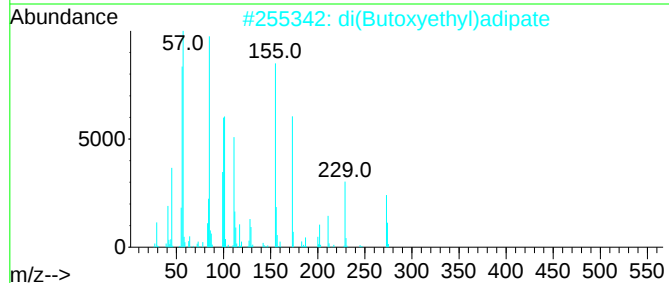
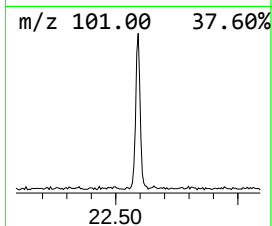
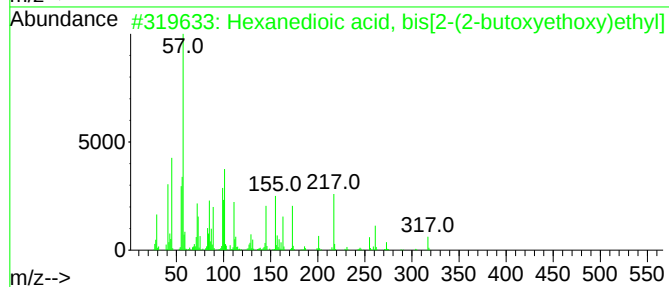
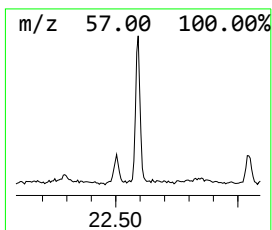
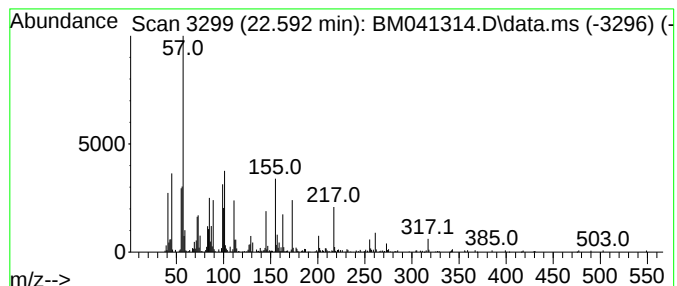
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexanedioic acid, bis[2-(2-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.592	2.30 ng	252967	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, bis[2-(2-butox...	434	C22H42O8	000141-17-3	93
2			di(Butoxyethyl)adipate	346	C18H34O6	000141-18-4	32
3			Succinic acid, di(2-butoxyethyl)...	318	C16H30O6	1010325-84-7	12
4			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	12
5			N-[1-(3-Chloroanilino)-2,2,2-tri...	376	C14H15ClF6N2O	1000224-22-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
Data File : BM041314.D
Acq On : 07 Aug 2023 16:12
Operator : MA/JU
Sample : 03903-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-06W

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.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
Ethanol, 2-(2-b...	10.387	2.4	ng	167401	2	10.592	1419400	20.0
Benzophenone	15.827	2.7	ng	266095	3	14.457	1990030	20.0
n-Hexadecanoic ...	18.115	13.7	ng	1629100	4	17.215	2372910	20.0
Octadecanoic acid	19.398	11.1	ng	1227860	5	21.421	2203770	20.0
1-Heptadecene	21.121	3.9	ng	432225	5	21.421	2203770	20.0
Hexanedioic aci...	22.592	2.3	ng	252967	5	21.421	2203770	20.0