

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080323\
 Data File : BM041268.D
 Acq On : 03 Aug 2023 19:00
 Operator : MA/JU
 Sample : 03756-24
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 415/417-TP-1-4-CS-1

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: BM041268.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.369	365	371	386	rBV	1488894	2155592	31.98%	5.818%
2	6.981	637	645	660	rBV	1479560	2416241	35.85%	6.522%
3	7.793	777	783	792	rBV	509514	811327	12.04%	2.190%
4	8.969	976	983	995	rBV	861762	1456311	21.61%	3.931%
5	10.604	1253	1261	1274	rBV	765563	1266856	18.80%	3.419%
6	13.080	1675	1682	1692	rBV	2816685	3951103	58.62%	10.664%
7	14.463	1910	1917	1931	rBV	1374556	1974260	29.29%	5.329%
8	15.963	2165	2172	2190	rBV	2519004	3615483	53.64%	9.759%
9	16.621	2279	2284	2290	rBV	85492	130305	1.93%	0.352%
10	17.221	2380	2386	2392	rBV	1779422	2413525	35.81%	6.514%
11	17.392	2411	2415	2430	rVB	64528	110570	1.64%	0.298%
12	17.992	2513	2517	2525	rBV	160110	271291	4.03%	0.732%
13	18.127	2534	2540	2550	rBV	1446759	2163136	32.10%	5.839%
14	19.286	2730	2737	2749	rBV2	126871	328760	4.88%	0.887%
15	19.404	2753	2757	2772	rBV	446999	726074	10.77%	1.960%
16	19.856	2829	2834	2842	rBV	5517382	6739733	100.00%	18.191%
17	21.127	3046	3050	3059	rBV	444950	582015	8.64%	1.571%
18	21.427	3096	3101	3106	rBV	2050164	2569146	38.12%	6.934%
19	22.644	3303	3308	3314	rVB	806846	1114021	16.53%	3.007%
20	23.797	3498	3504	3515	rVB	1169708	2253684	33.44%	6.083%

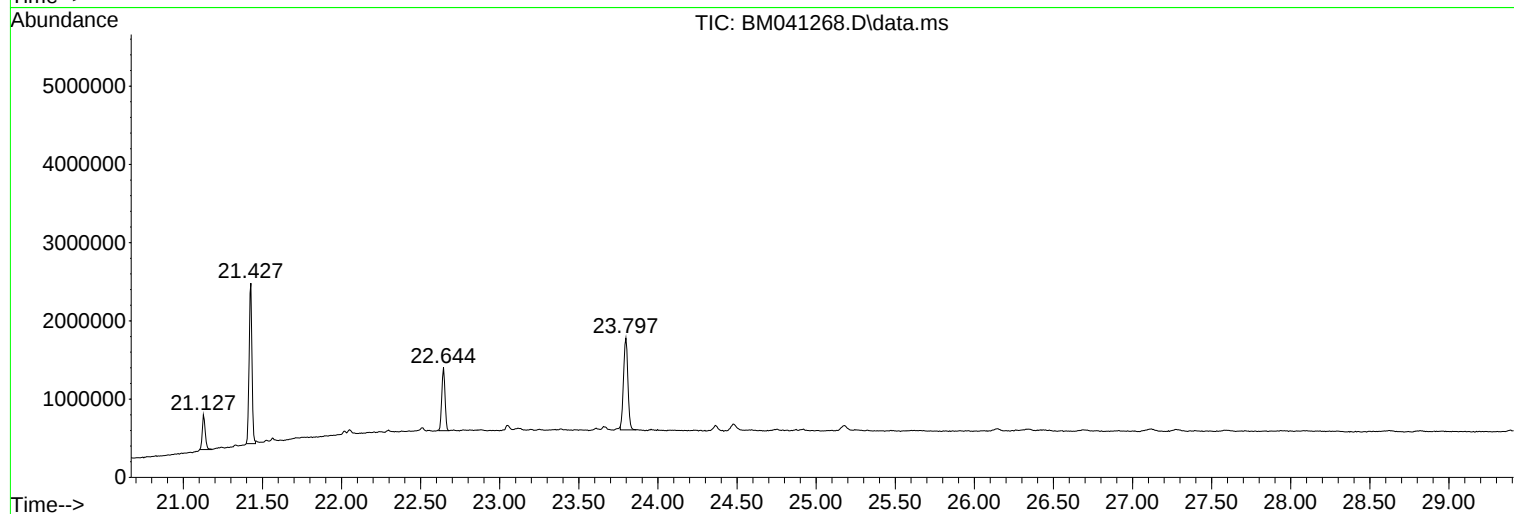
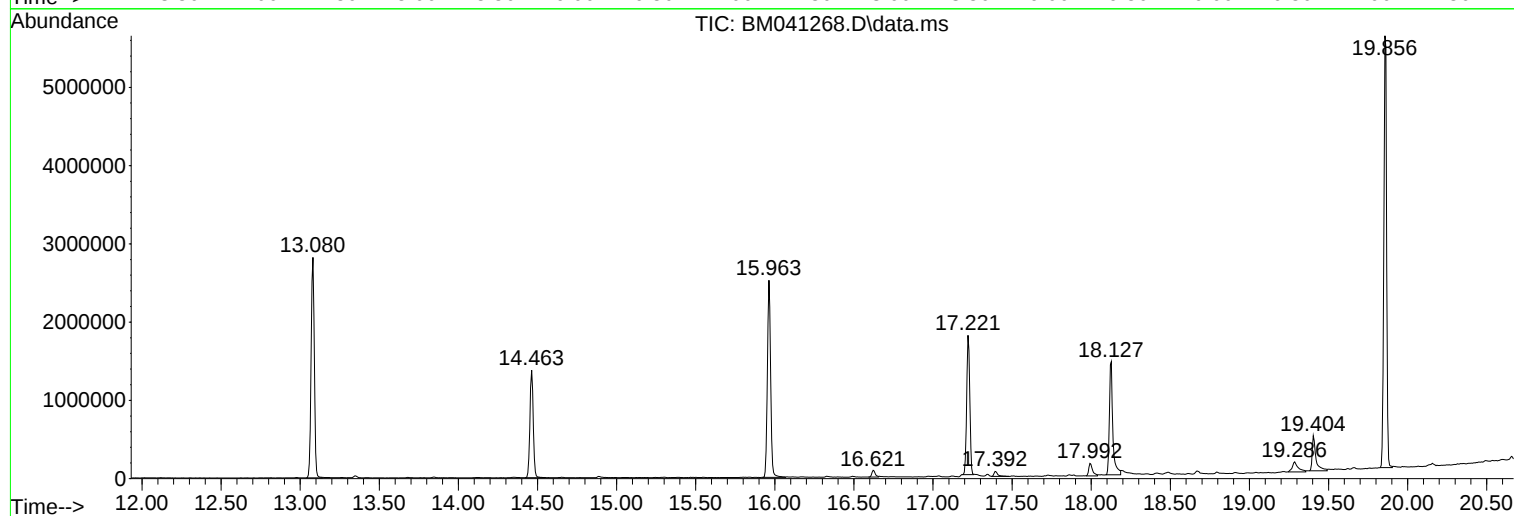
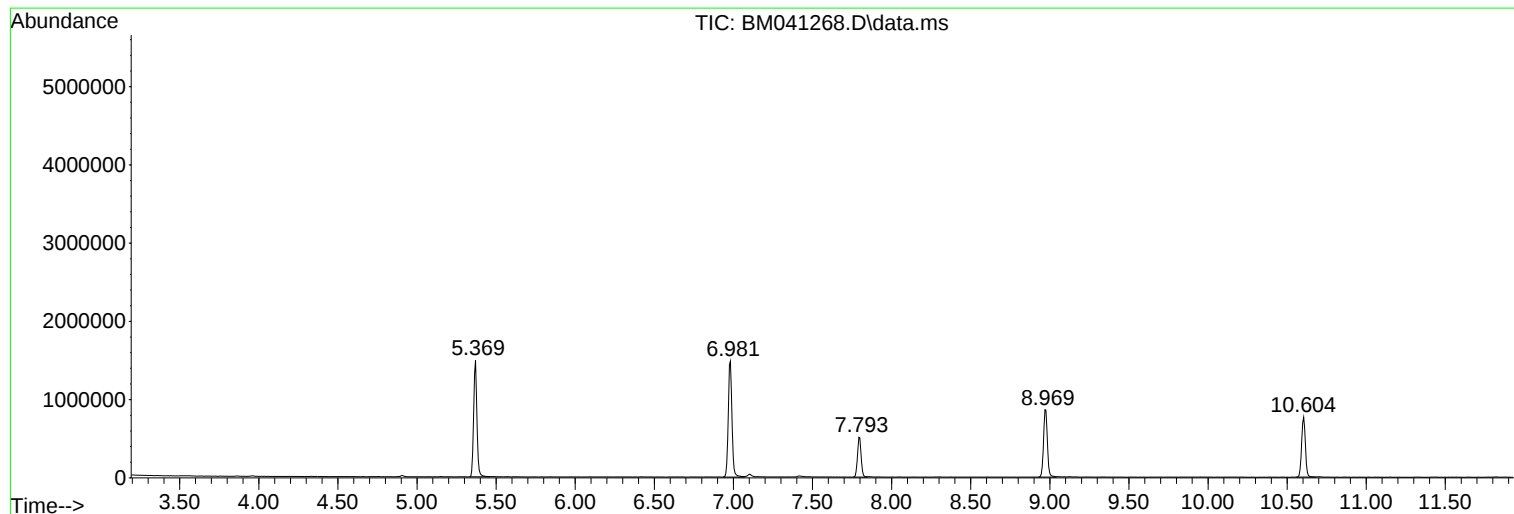
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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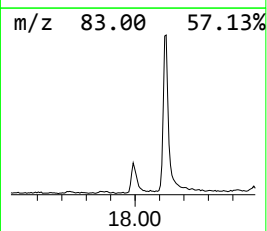
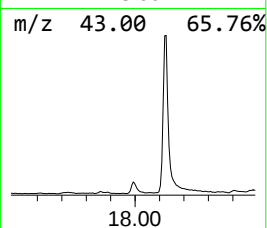
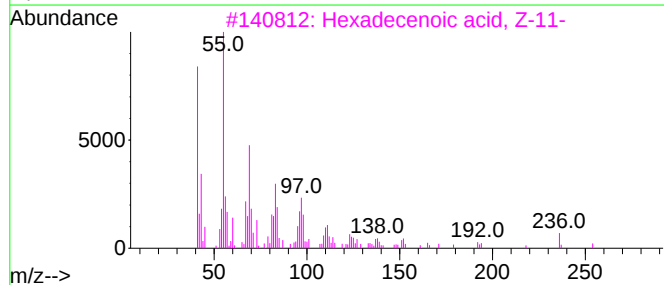
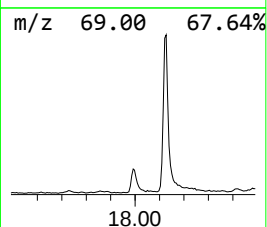
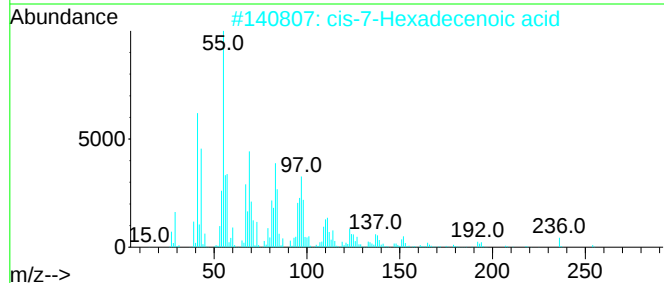
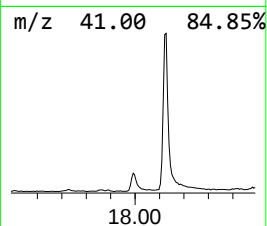
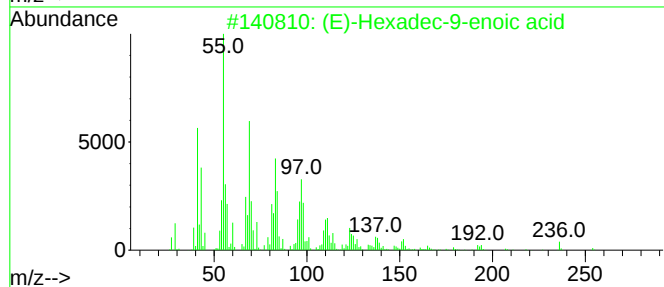
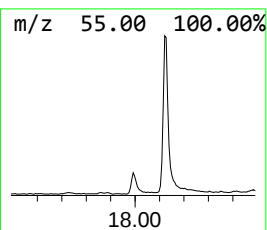
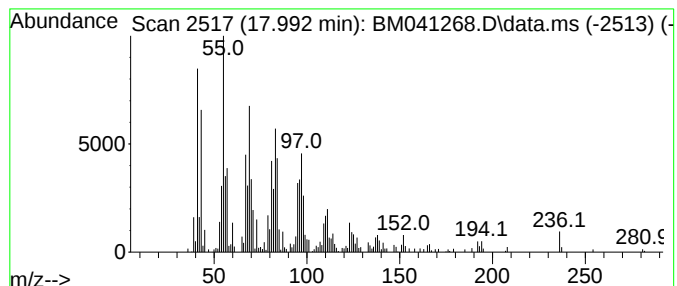
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 (E)-Hexadec-9-enoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.992	2.25 ng	271291	Phenanthrene-d10	17.221

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	99
2		cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	98
3		Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	97
4		Palmitoleic acid	254	C16H30O2	000373-49-9	96
5		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	91



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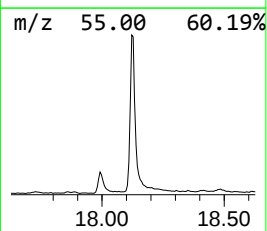
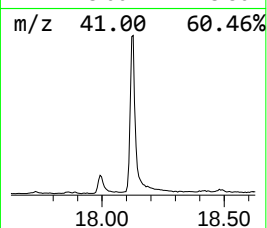
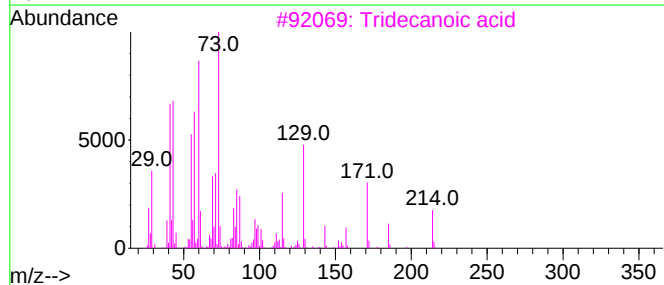
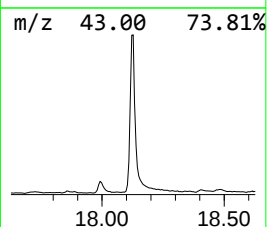
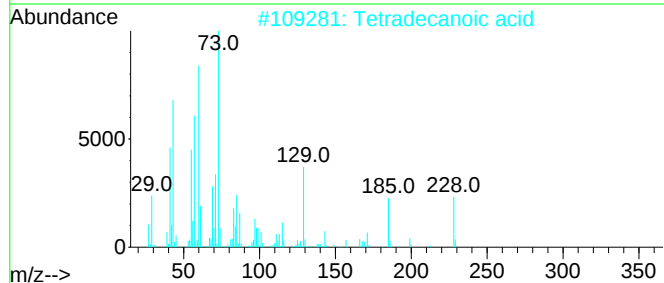
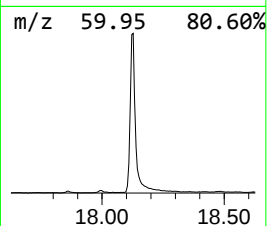
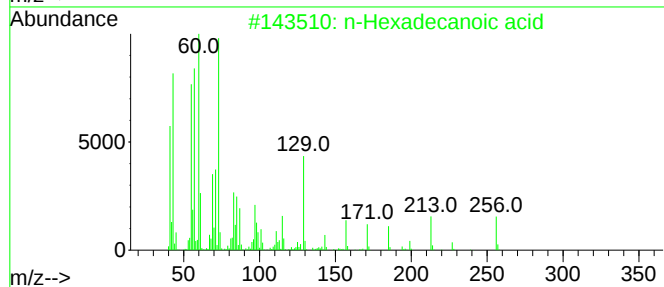
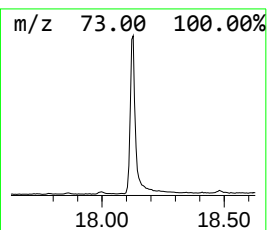
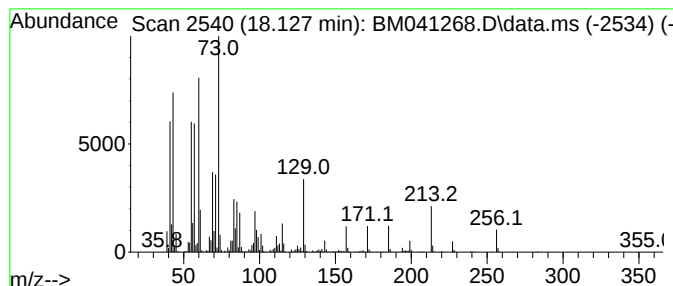
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.127	17.93 ng	2163140	Phenanthrene-d10	17.221

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	94		
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93		
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81		
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47		



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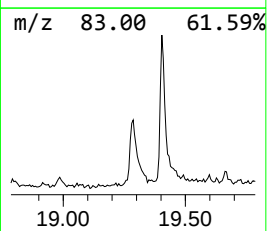
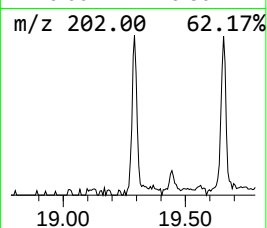
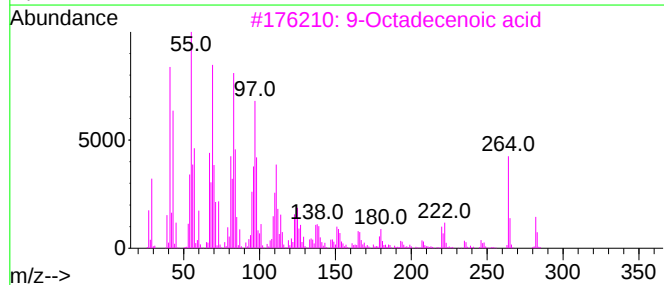
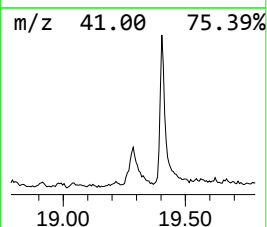
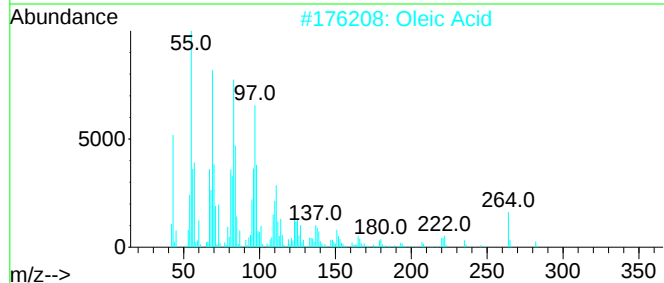
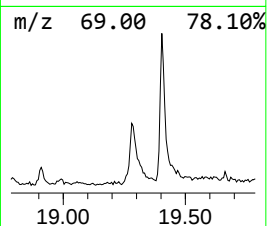
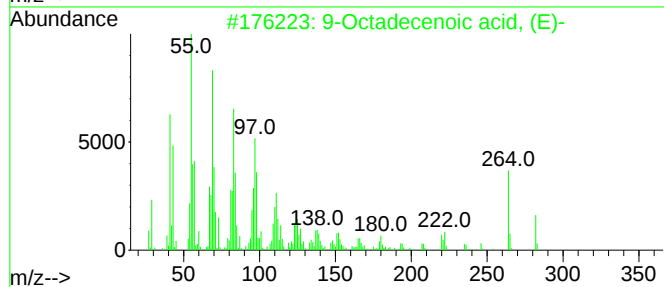
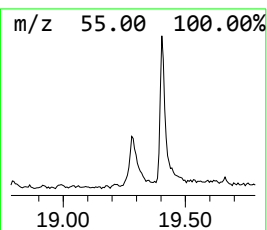
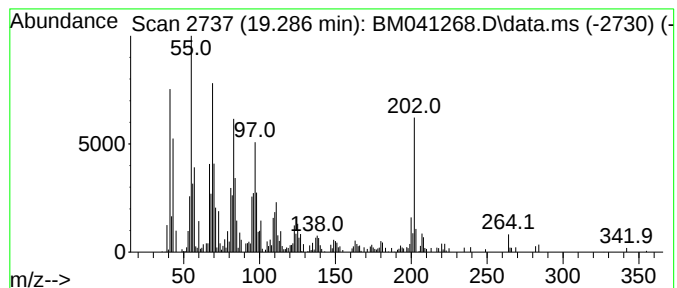
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TIC Integration Parameters: LSCINT.P

Peak Number 3 9-Octadecenoic acid, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.286	2.72 ng	328760	Phenanthrene-d10	17.221

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	99
2			Oleic Acid	282	C18H34O2	000112-80-1	99
3			9-Octadecenoic acid	282	C18H34O2	002027-47-6	99
4			6-Octadecenoic acid	282	C18H34O2	1000336-66-8	97
5			cis-Vaccenic acid	282	C18H34O2	000506-17-2	97



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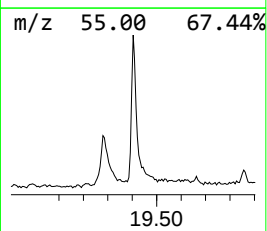
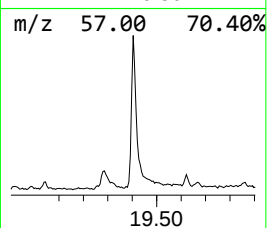
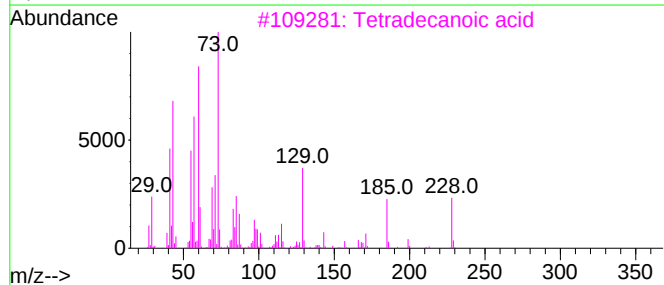
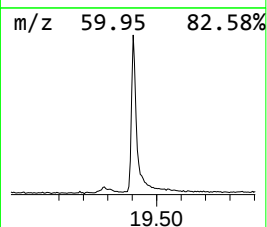
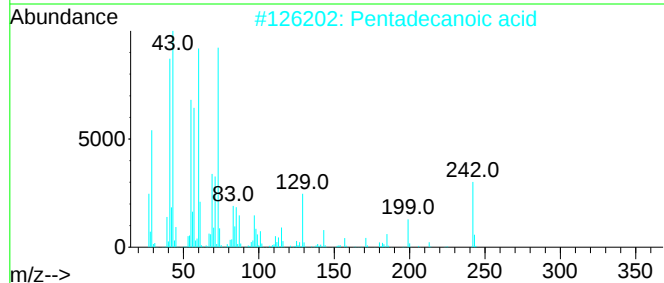
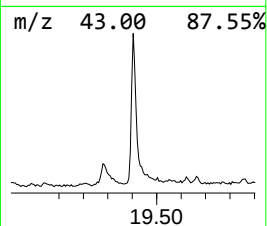
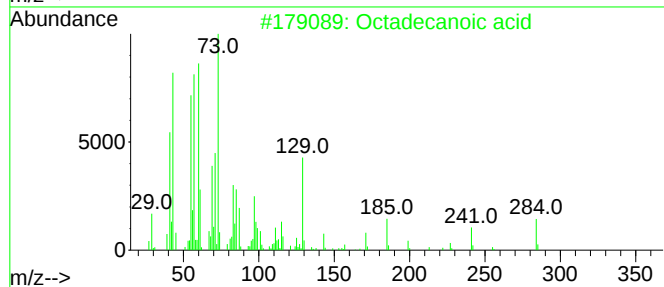
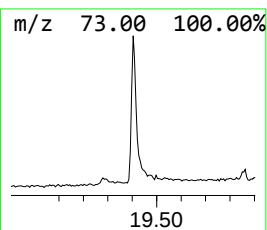
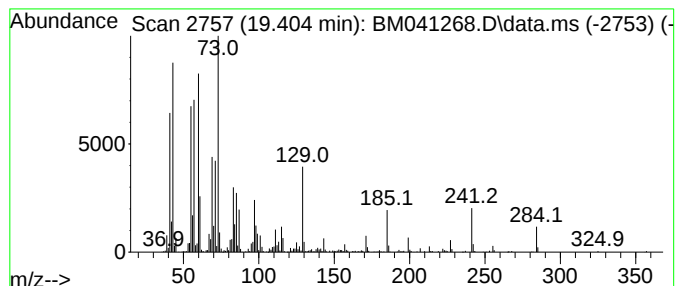
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.404	5.65 ng	726074	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	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	74



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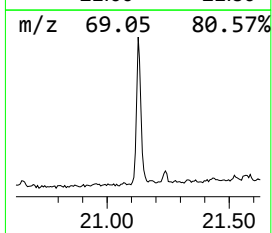
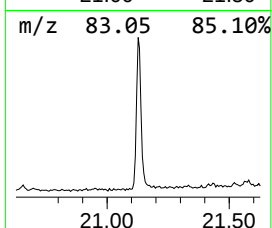
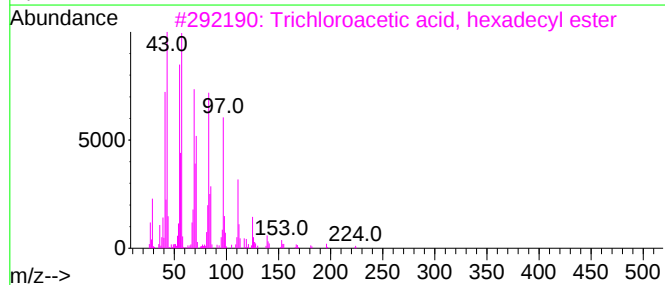
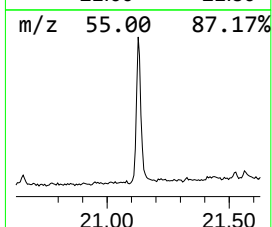
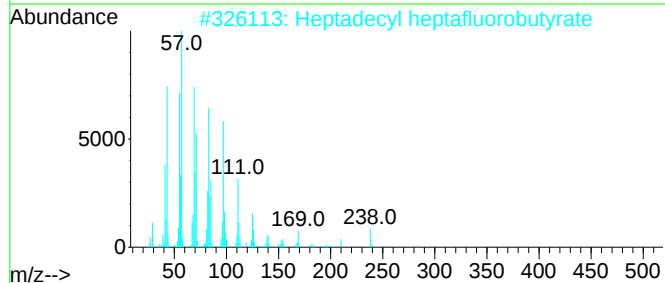
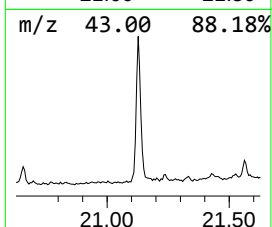
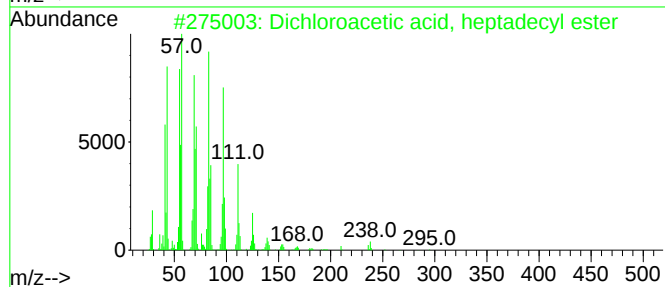
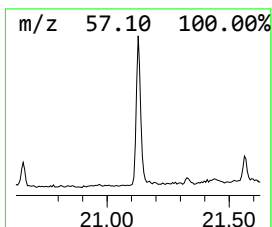
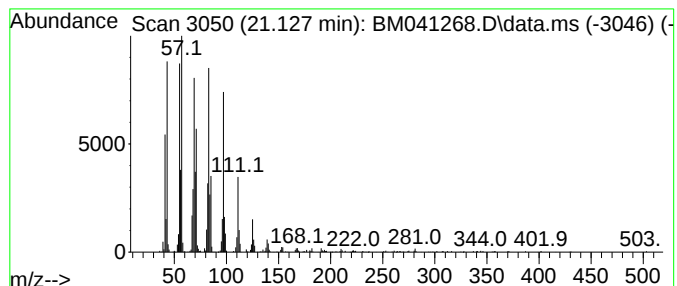
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	4.53 ng	582015	Chrysene-d12	21.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91



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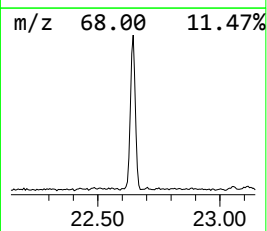
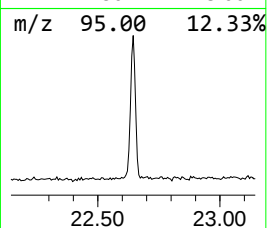
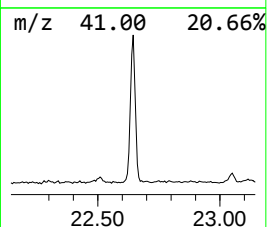
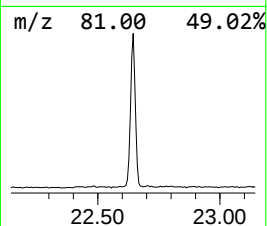
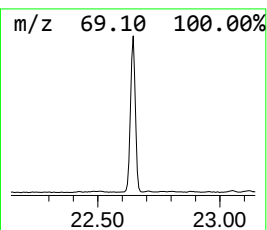
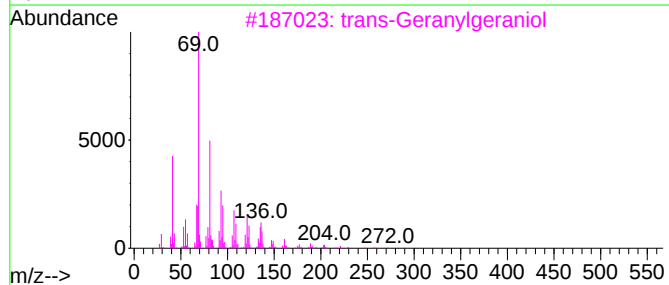
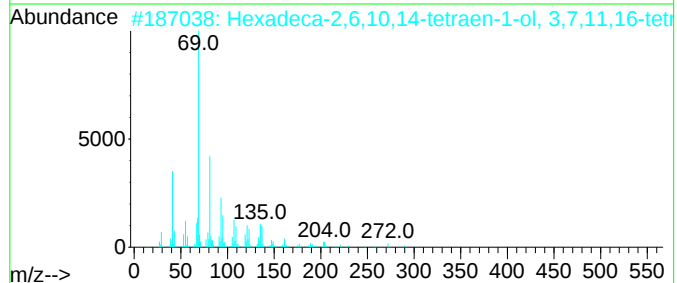
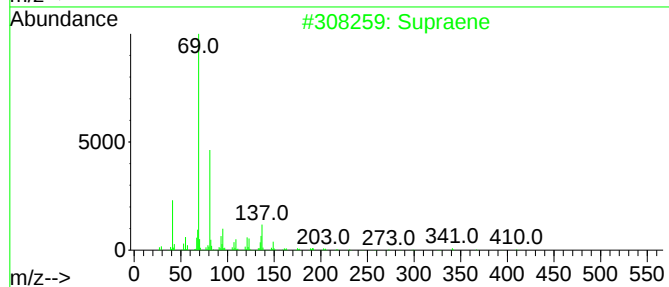
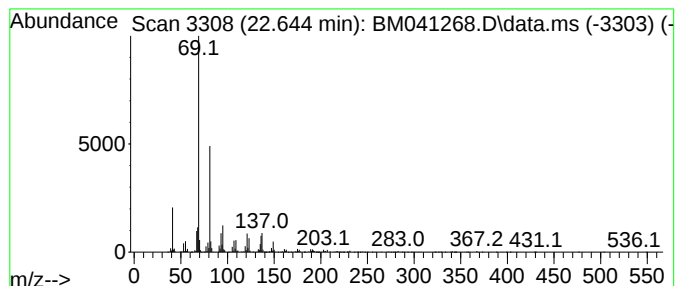
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.645	9.89 ng	1114020	Perylene-d12	23.797

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	80
3			trans-Geranylgeraniol	290	C20H34O	024034-73-9	78
4			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58
5			4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080323\
Data File : BM041268.D
Acq On : 03 Aug 2023 19:00
Operator : MA/JU
Sample : 03756-24
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
415/417-TP-1-4-CS-1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(E)-Hexadec-9-e...	17.992	2.3	ng	271291	4	17.221	2413530	20.0
n-Hexadecanoic ...	18.127	17.9	ng	2163140	4	17.221	2413530	20.0
9-Octadecenoic ...	19.286	2.7	ng	328760	4	17.221	2413530	20.0
Octadecanoic acid	19.404	5.7	ng	726074	5	21.427	2569150	20.0
Dichloroacetic ...	21.127	4.5	ng	582015	5	21.427	2569150	20.0
Supraene	22.645	9.9	ng	1114020	6	23.797	2253680	20.0