

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080223\
 Data File : BM041247.D
 Acq On : 02 Aug 2023 16:30
 Operator : MA/JU
 Sample : 03810-08
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 B-P1A

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: BM041247.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	363	371	387	rBV	2245077	3317956	40.48%	5.764%
2	6.981	637	645	659	rBV	2369656	3786326	46.20%	6.578%
3	7.798	777	784	791	rBV	709440	1103804	13.47%	1.917%
4	8.975	976	984	1001	rBV	1498210	2434082	29.70%	4.228%
5	10.604	1253	1261	1270	rBV	1052796	1689937	20.62%	2.936%
6	11.839	1465	1471	1478	rBV	130800	205112	2.50%	0.356%
7	13.080	1675	1682	1695	rBV	4150630	5794189	70.69%	10.066%
8	14.463	1910	1917	1924	rBV	1709762	2444359	29.82%	4.246%
9	15.969	2166	2173	2181	rBV	3862510	5434666	66.31%	9.441%
10	16.627	2281	2285	2291	rBV3	63136	121111	1.48%	0.210%
11	17.121	2365	2369	2377	rBV	89921	148556	1.81%	0.258%
12	17.227	2381	2387	2396	rVB	2129680	3107270	37.91%	5.398%
13	18.010	2514	2520	2525	rBV4	89973	197392	2.41%	0.343%
14	18.062	2526	2529	2534	rVV2	74240	104821	1.28%	0.182%
15	18.127	2535	2540	2557	rBV	2152707	3132375	38.22%	5.441%
16	18.421	2585	2590	2596	rBV3	101122	208201	2.54%	0.362%
17	18.562	2610	2614	2620	rBV	99052	167777	2.05%	0.291%
18	19.039	2693	2695	2699	rBV	77389	89127	1.09%	0.155%
19	19.292	2730	2738	2749	rBV	825983	1789958	21.84%	3.109%
20	19.409	2754	2758	2767	rBV	1083297	1479634	18.05%	2.570%
21	19.862	2830	2835	2842	rVB	6832805	8196062	100.00%	14.238%
22	21.133	3047	3051	3059	rVB	728701	1102438	13.45%	1.915%
23	21.333	3081	3085	3090	rVB	1107628	1196929	14.60%	2.079%
24	21.427	3097	3101	3106	rBV	2102934	2498387	30.48%	4.340%
25	22.021	3197	3202	3206	rBV	4238602	5258270	64.16%	9.135%
26	23.803	3499	3505	3521	rVB	1229561	2556023	31.19%	4.440%

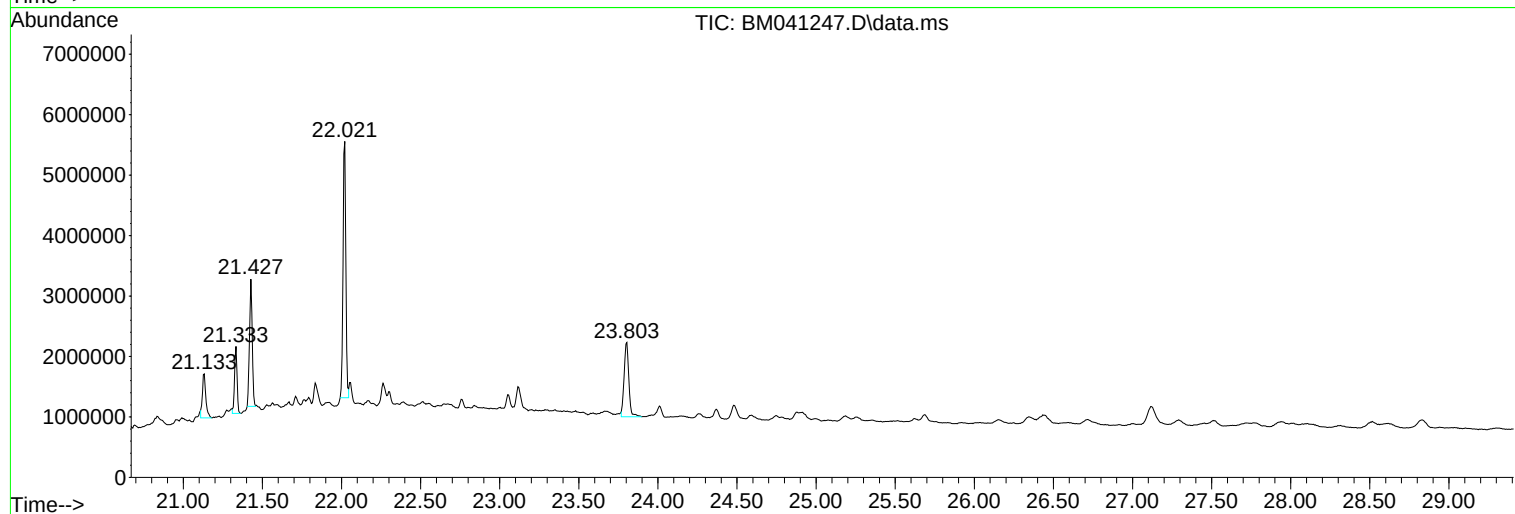
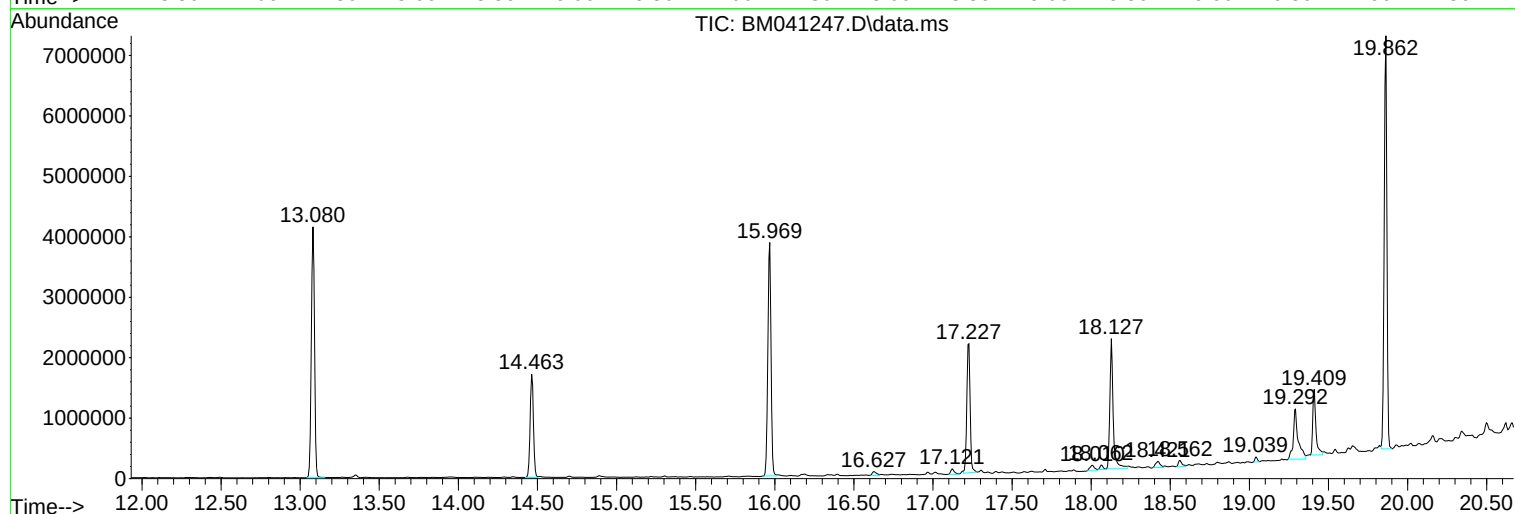
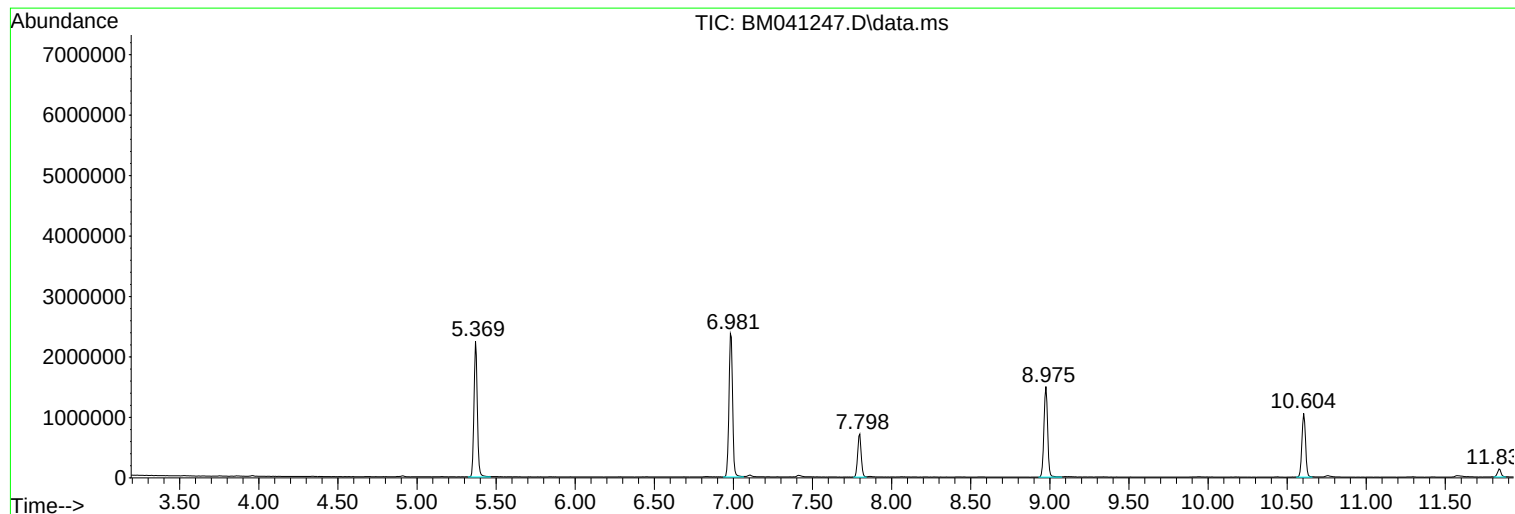
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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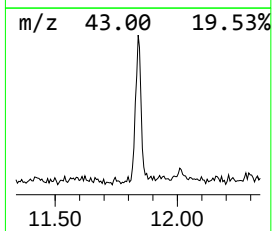
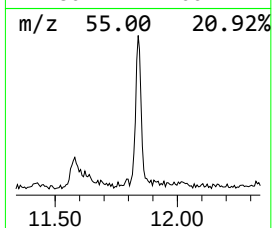
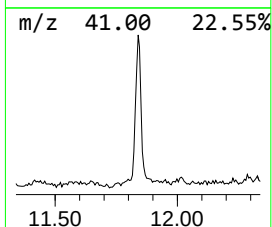
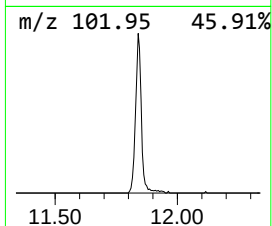
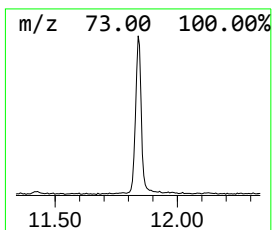
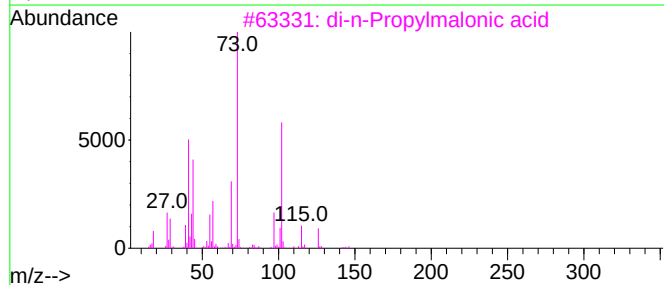
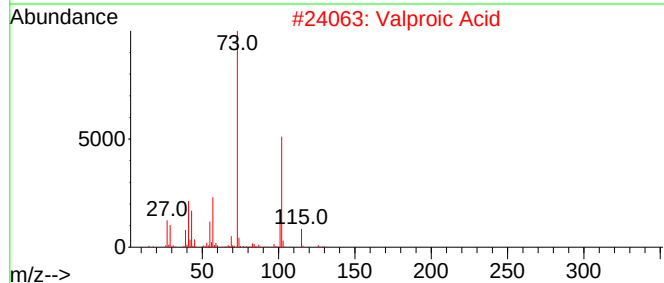
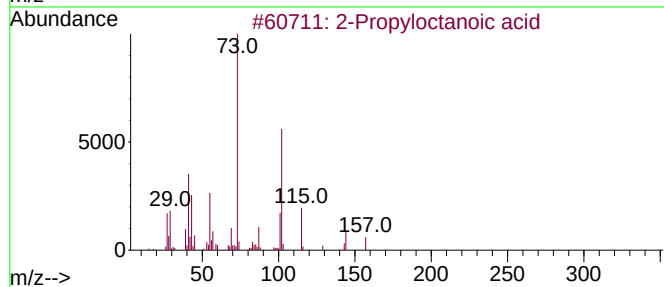
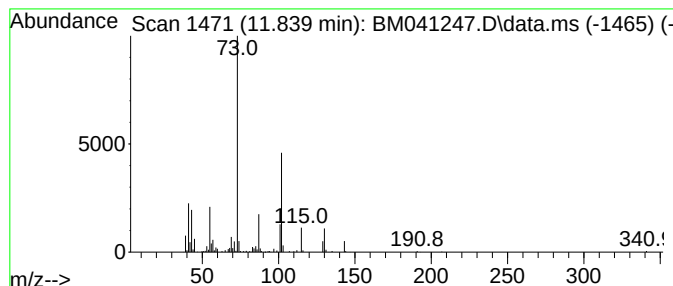
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 1 2-Propyloctanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	2.43 ng	205112	Naphthalene-d8	10.604

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propyloctanoic acid	186	C11H22O2	031080-41-8	53
2		Valproic Acid	144	C8H16O2	000099-66-1	53
3		di-n-Propylmalonic acid	188	C9H16O4	001636-27-7	28
4		Triethylmethylsilane	130	C7H18Si	1000423-80-6	27
5		Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	17



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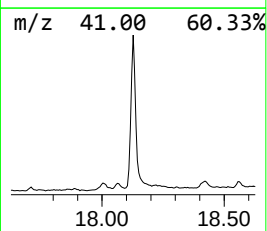
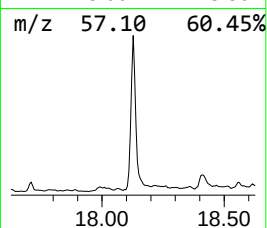
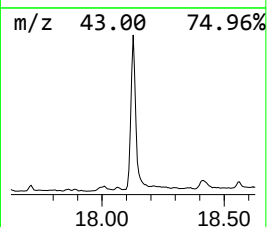
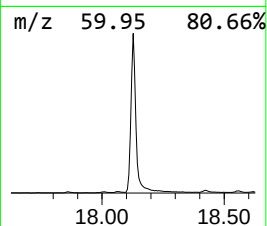
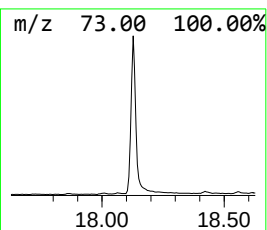
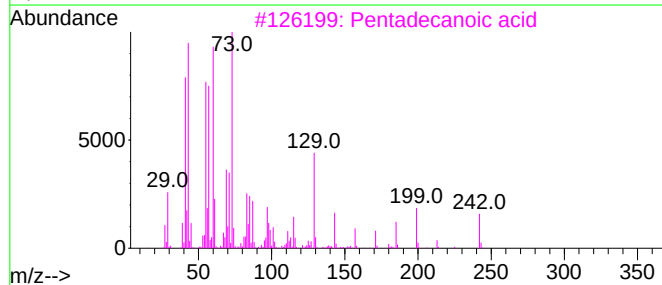
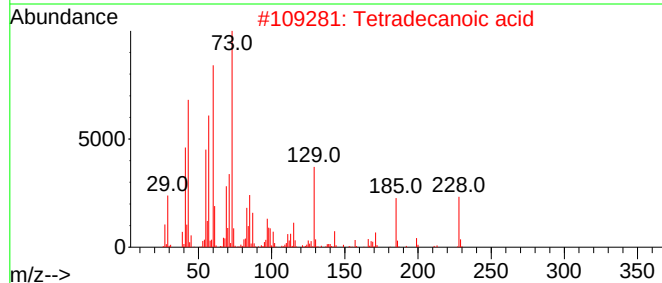
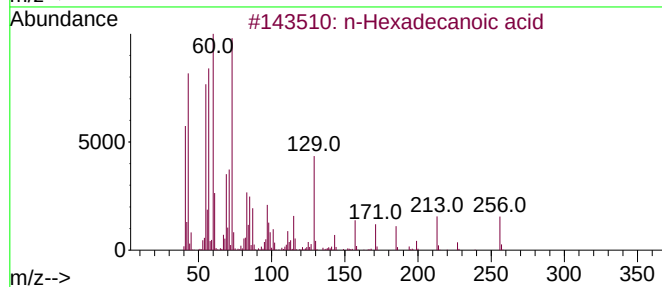
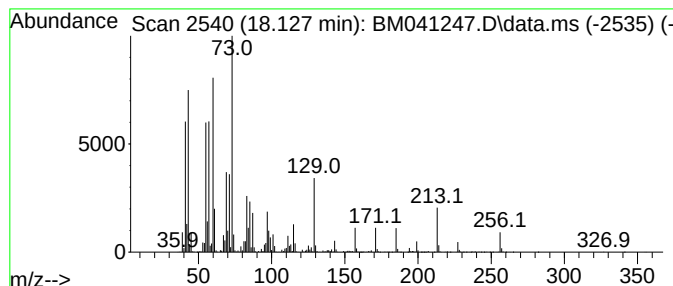
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.127	20.16 ng	3132380	Phenanthrene-d10	17.227

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			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tridecanoic acid	214	C13H26O2	000638-53-9	70
5			Undecanoic acid	186	C11H22O2	000112-37-8	53



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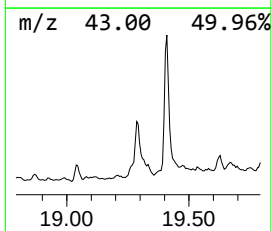
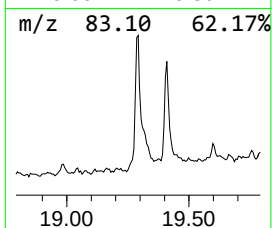
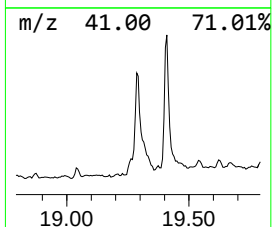
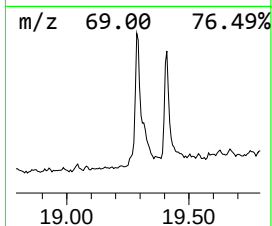
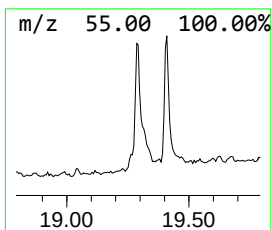
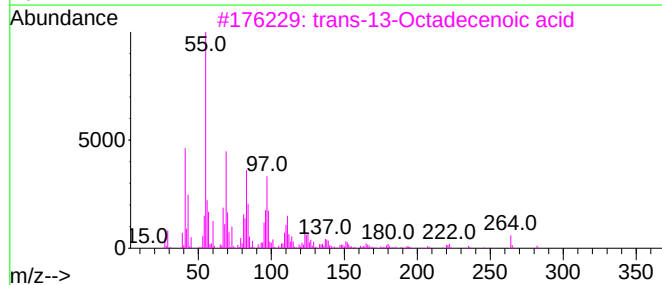
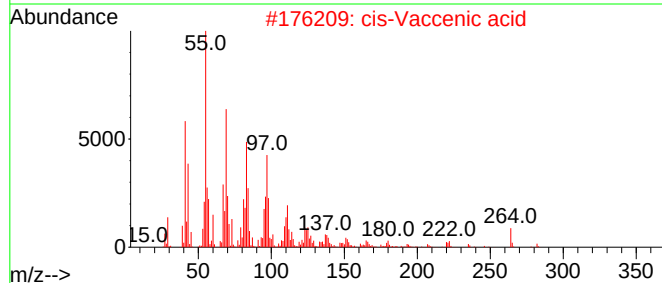
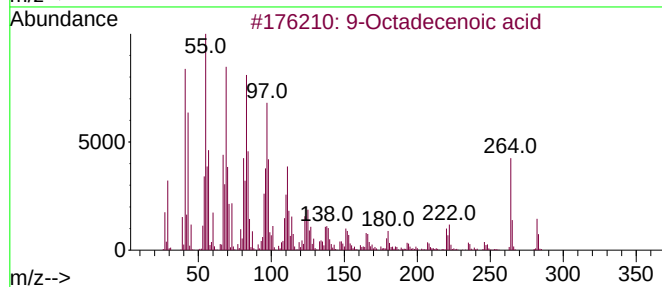
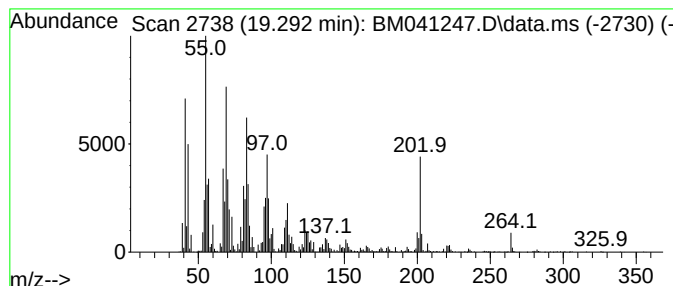
Instrument :
BNA_M
ClientSampleId :
B-P1A

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

Peak Number 3 9-Octadecenoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.292	11.52 ng	1789960	Phenanthrene-d10	17.227	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid	282	C18H34O2	002027-47-6	99
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	97
3	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	95
4	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	90
5	Oleic Acid	282	C18H34O2	000112-80-1	90



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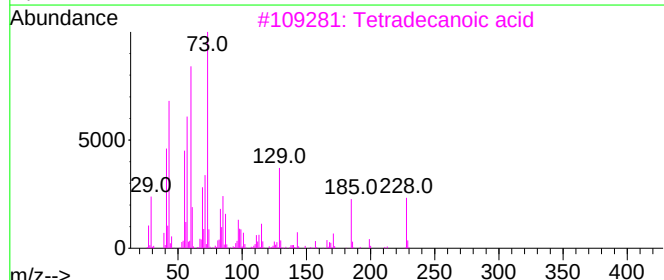
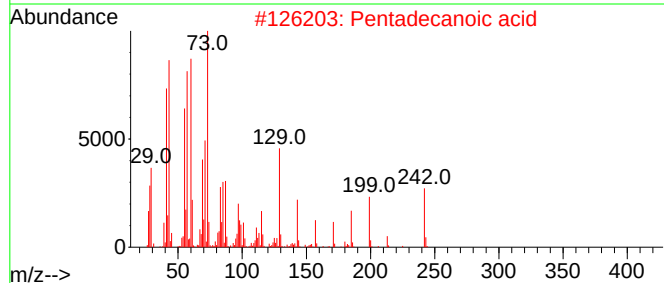
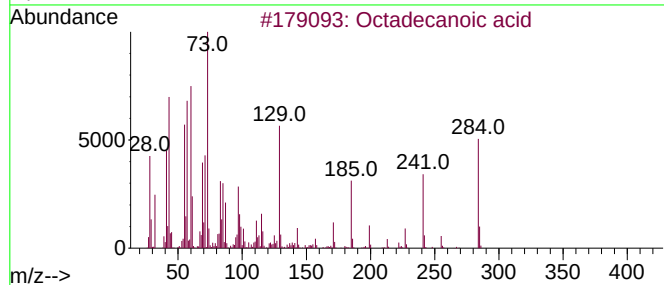
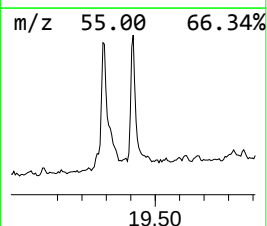
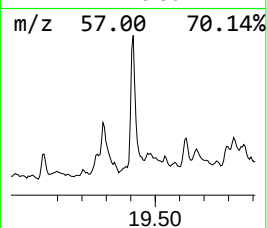
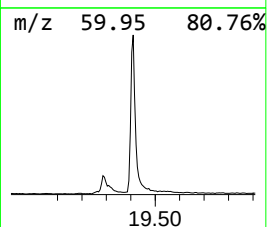
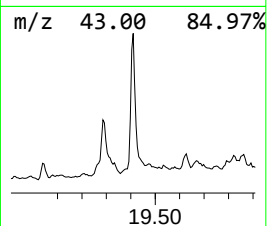
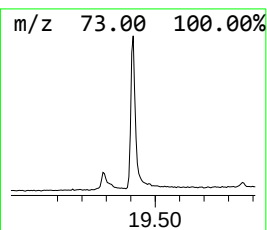
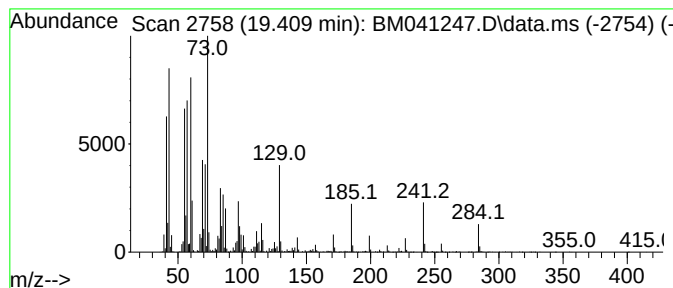
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.410	11.84 ng	1479630	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			n-Decanoic acid	172	C10H20O2	000334-48-5	62
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	25



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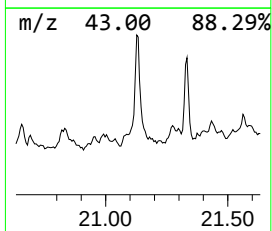
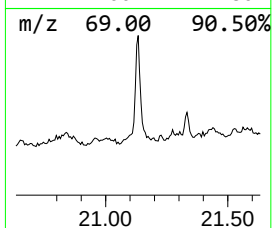
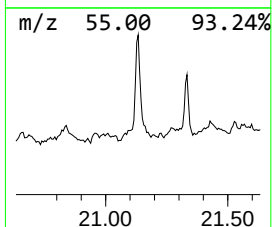
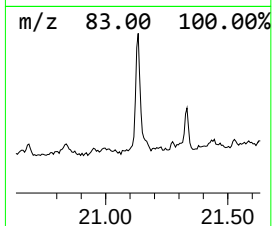
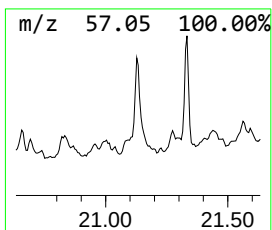
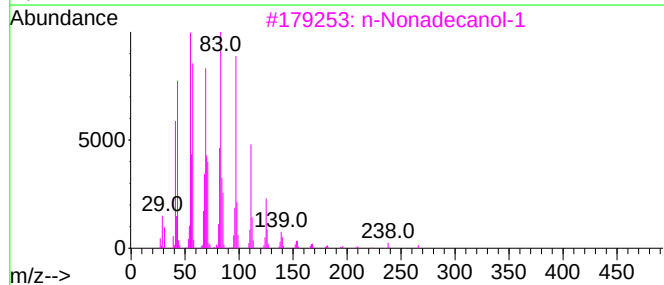
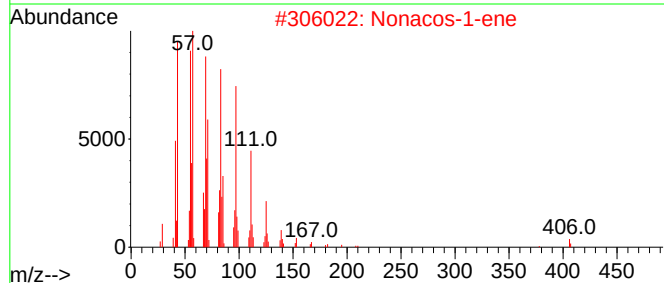
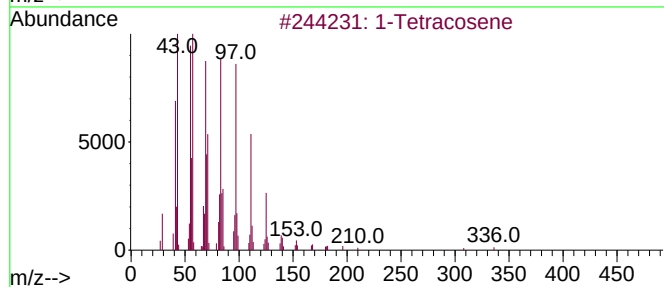
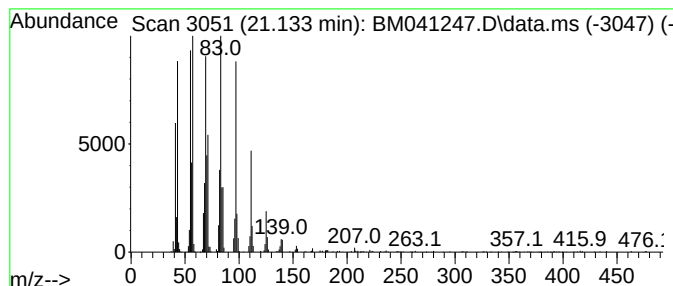
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Peak Number 5 1-Tetracosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.133	8.83 ng	1102440	Chrysene-d12	21.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetracosene	336	C24H48	010192-32-2	94
2			Nonacos-1-ene	406	C29H58	018835-35-3	94
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4			Pentacos-1-ene	350	C25H50	016980-85-1	94
5			E-14-Hexadecenal	238	C16H30O	330207-53-9	93



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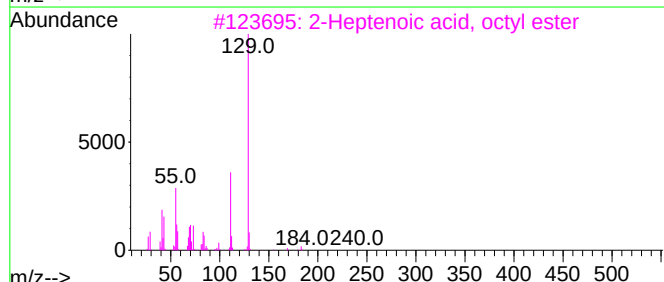
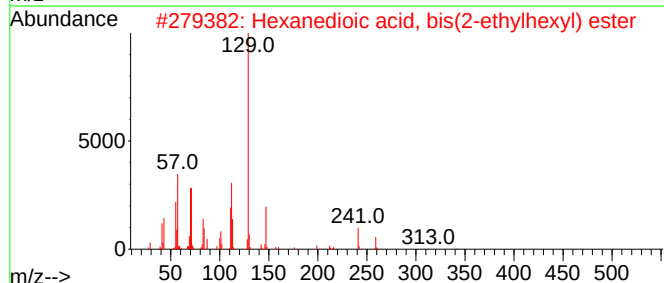
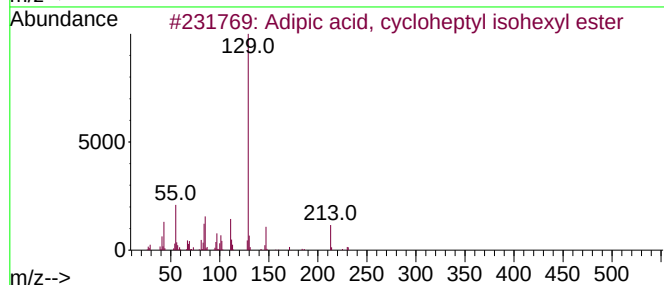
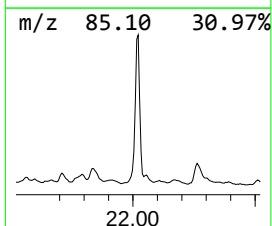
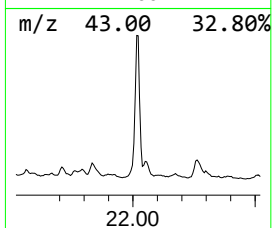
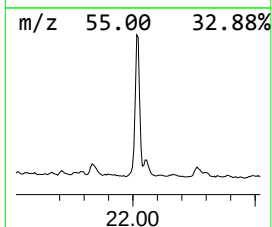
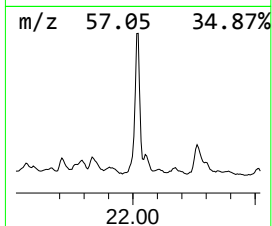
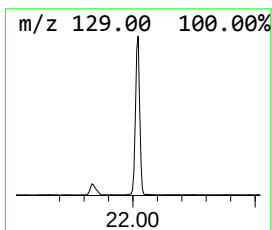
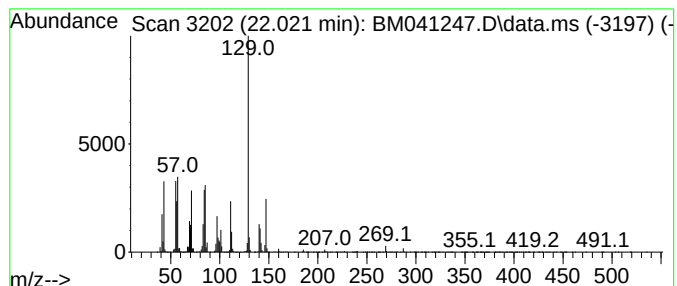
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Adipic acid, cycloheptyl is... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.021	42.09 ng	5258270	Chrysene-d12	21.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adipic acid, cycloheptyl isohexy...	326	C19H34O4	1000324-71-8	64
2			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	50
3			2-Heptenoic acid, octyl ester	240	C15H28O2	1000406-09-4	50
4			Hexanedioic acid, bis(1,3-dimeth...	314	C18H34O4	055125-22-9	50
5			Succinic acid, ethyl 6-ethyloct-...	286	C16H30O4	1000324-92-1	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080223\
Data File : BM041247.D
Acq On : 02 Aug 2023 16:30
Operator : MA/JU
Sample : 03810-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P1A

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
2-Propyloctanoi...	11.839	2.4	ng	205112	2	10.604	1689940	20.0
n-Hexadecanoic ...	18.127	20.2	ng	3132380	4	17.227	3107270	20.0
9-Octadecenoic ...	19.292	11.5	ng	1789960	4	17.227	3107270	20.0
Octadecanoic acid	19.410	11.8	ng	1479630	5	21.427	2498390	20.0
1-Tetracosene	21.133	8.8	ng	1102440	5	21.427	2498390	20.0
Adipic acid, cy...	22.021	42.1	ng	5258270	5	21.427	2498390	20.0