

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
 Data File : BM042440.D
 Acq On : 25 Oct 2023 16:35
 Operator : MA/JU
 Sample : 04941-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 213

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-BM102123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042440.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.105	150	156	178	rVB	18025888	31455319	100.00%	42.766%
2	5.069	316	320	328	rVB	269587	363234	1.15%	0.494%
3	5.522	390	397	404	rBV	2245744	3305660	10.51%	4.494%
4	7.146	665	673	683	rBV	2200900	3509688	11.16%	4.772%
5	7.993	809	817	826	rBV	585156	908533	2.89%	1.235%
6	9.187	1011	1020	1033	rBV	1351568	2243207	7.13%	3.050%
7	10.810	1288	1296	1302	rBV	732368	1209727	3.85%	1.645%
8	13.257	1705	1712	1724	rBV	2531078	3555079	11.30%	4.833%
9	14.633	1939	1946	1953	rBV	1056776	1537794	4.89%	2.091%
10	16.127	2193	2200	2210	rVB	2633891	3666709	11.66%	4.985%
11	17.386	2407	2414	2418	rBV	1368757	1898628	6.04%	2.581%
12	18.233	2552	2558	2568	rBV	1957723	2986621	9.49%	4.061%
13	19.092	2699	2704	2720	rBV	970413	1738300	5.53%	2.363%
14	19.392	2747	2755	2757	rBV3	169464	336516	1.07%	0.458%
15	19.439	2759	2763	2768	rVB	389359	541134	1.72%	0.736%
16	19.509	2770	2775	2787	rBV	1645694	2393185	7.61%	3.254%
17	19.804	2821	2825	2831	rVB	357730	449736	1.43%	0.611%
18	19.998	2852	2858	2864	rBV	3818960	4639408	14.75%	6.308%
19	21.227	3061	3067	3074	rBV3	549237	946503	3.01%	1.287%
20	21.427	3098	3101	3106	rBV	510160	529320	1.68%	0.720%
21	21.562	3118	3124	3128	rBV2	1718515	2426793	7.72%	3.299%
22	21.603	3128	3131	3135	rVV	418810	490888	1.56%	0.667%
23	22.756	3323	3327	3331	rVB	316704	424763	1.35%	0.577%
24	24.021	3536	3542	3549	rVB	981221	1996201	6.35%	2.714%

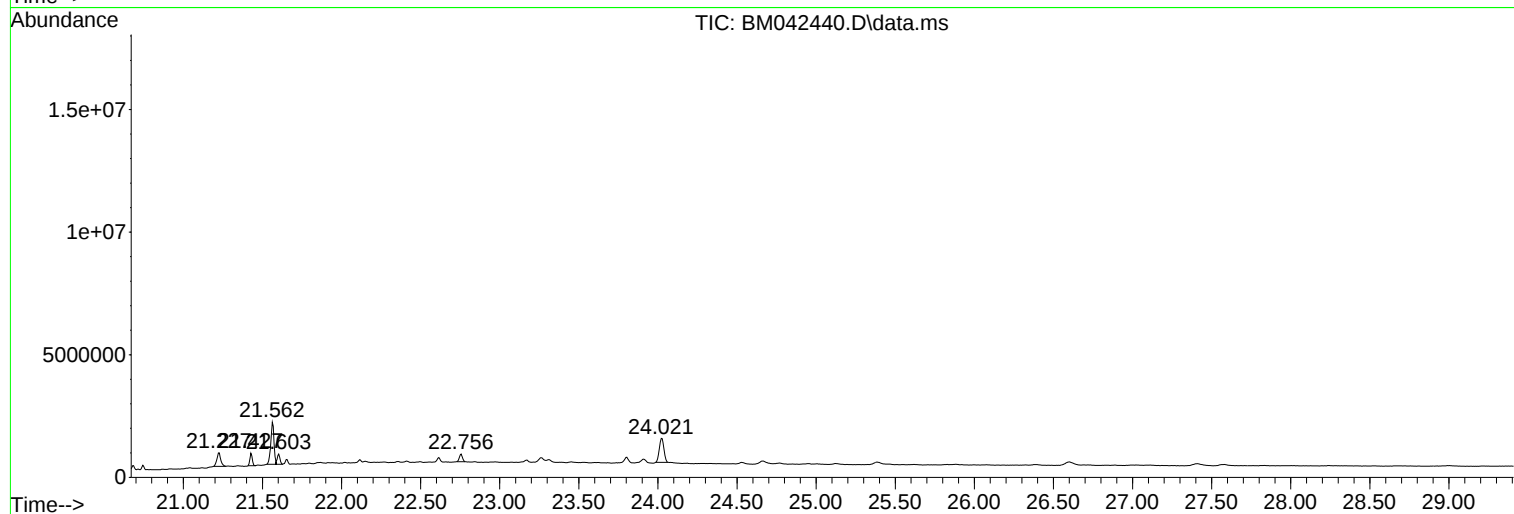
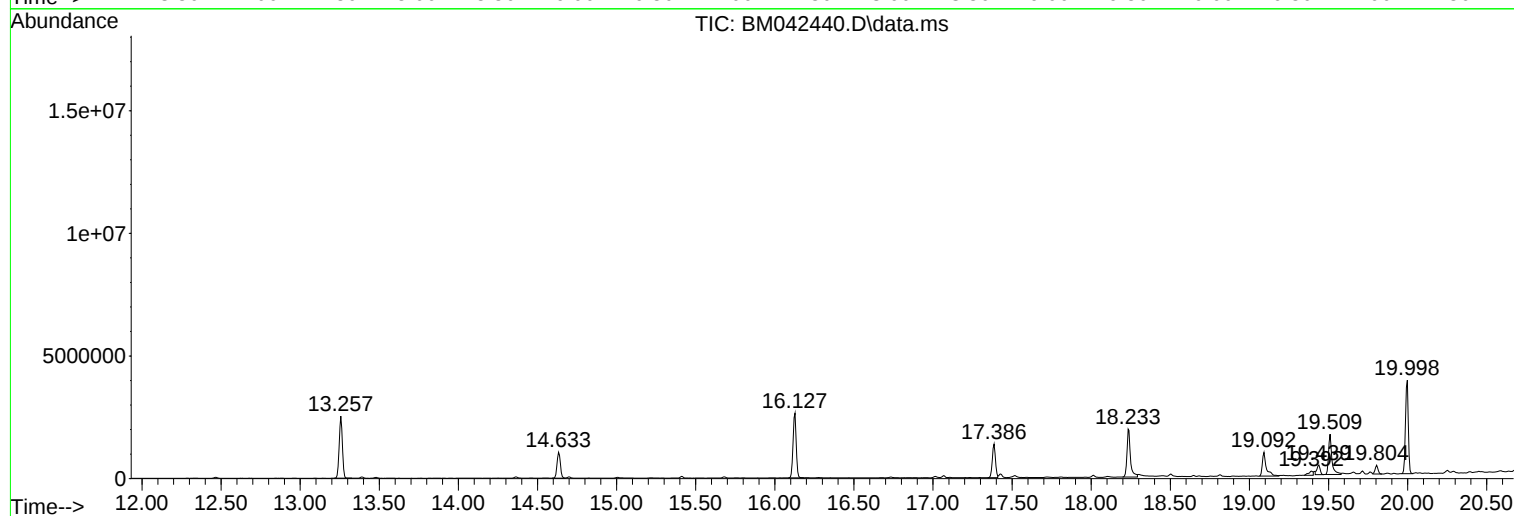
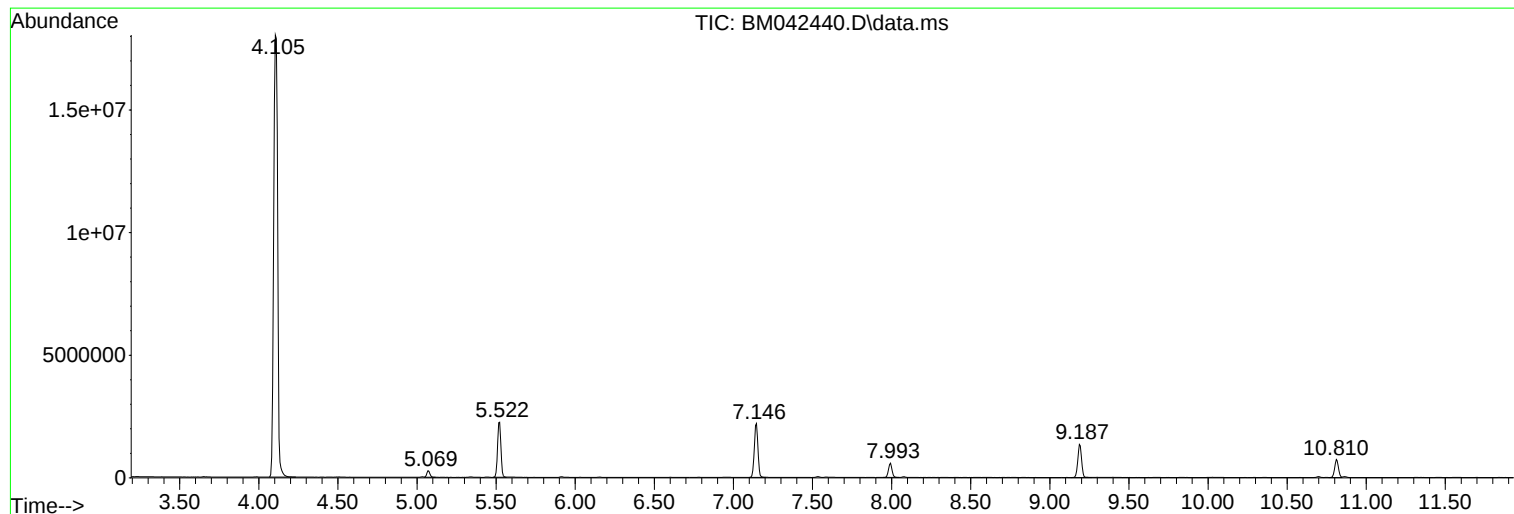
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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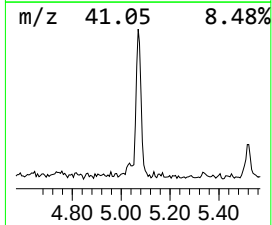
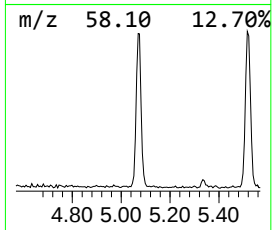
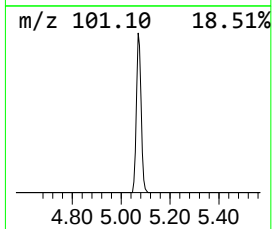
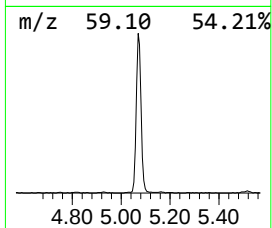
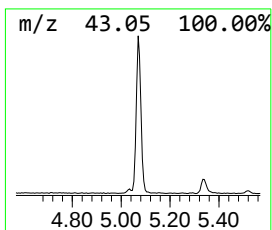
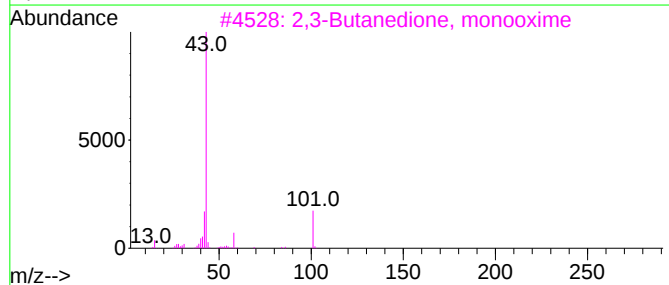
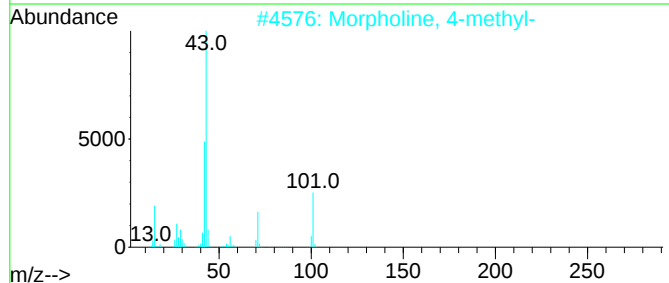
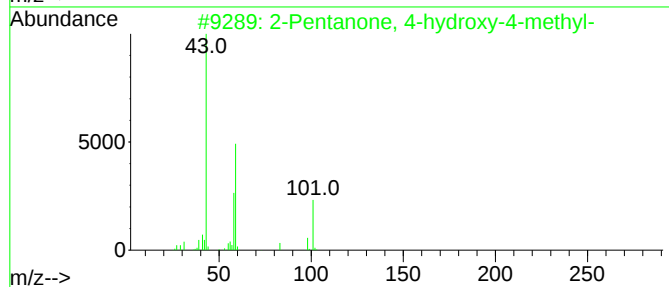
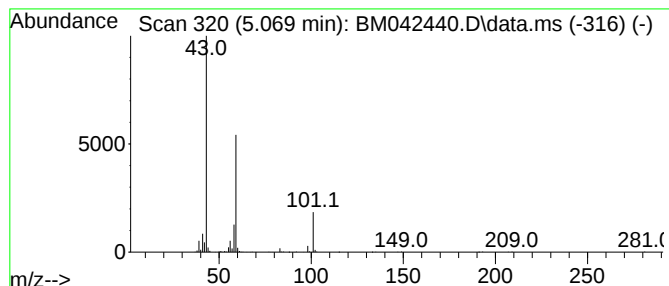
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	8.00 ng	363234	1,4-Dichlorobenzene-d4	7.992

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5		Succinic acid, isohexyl 2-methox...	260	C13H24O5	1000325-80-6	9



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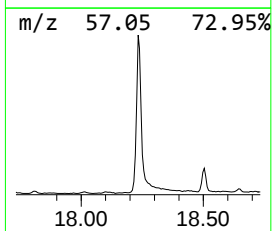
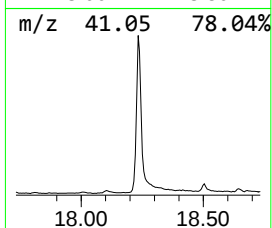
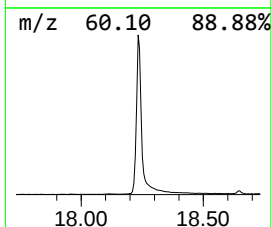
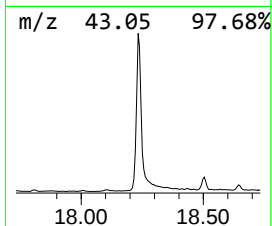
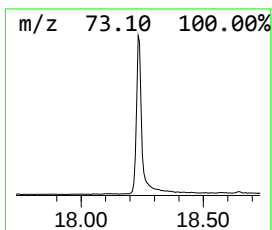
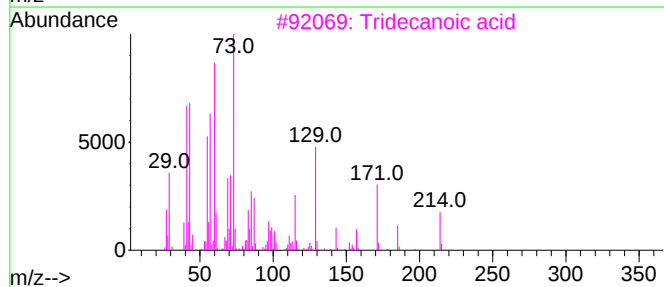
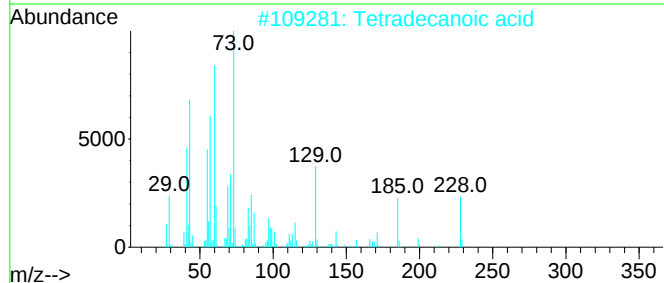
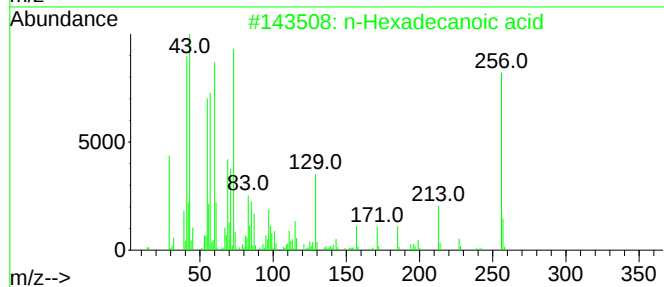
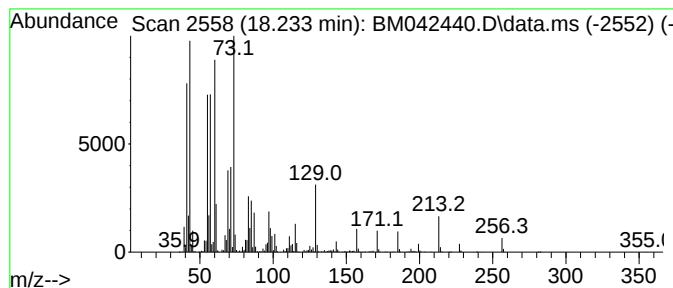
Instrument :
BNA_M
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
18.233	31.46 ng	2986620	Phenanthrene-d10	17.386	
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	95
3	Tridecanoic acid	214	C13H26O2	000638-53-9	95
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	30



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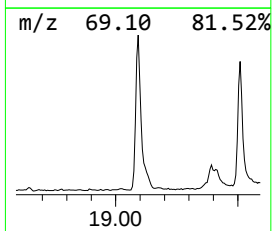
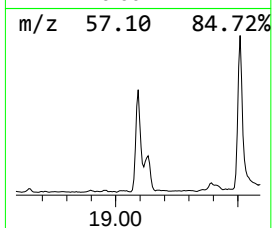
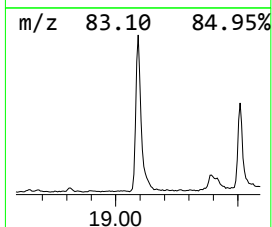
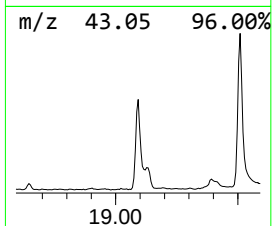
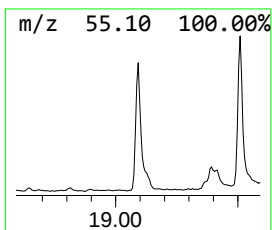
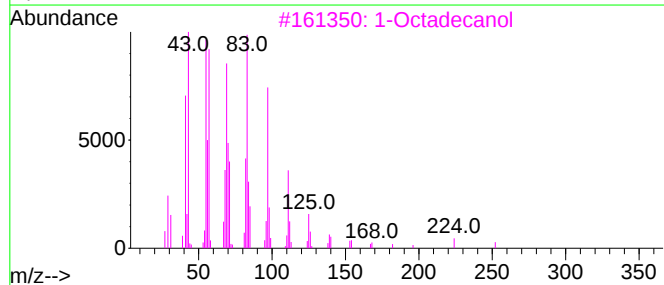
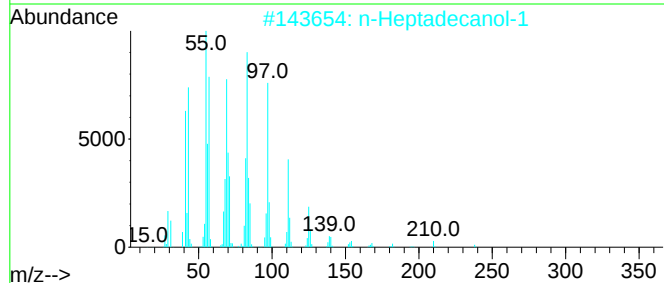
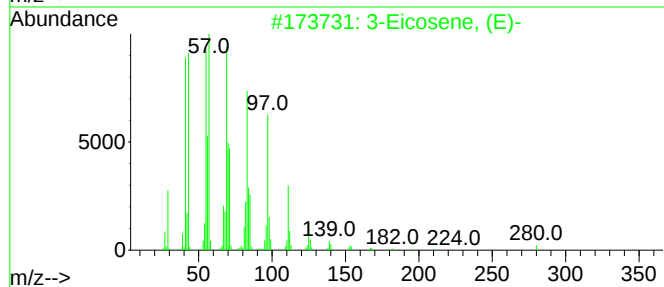
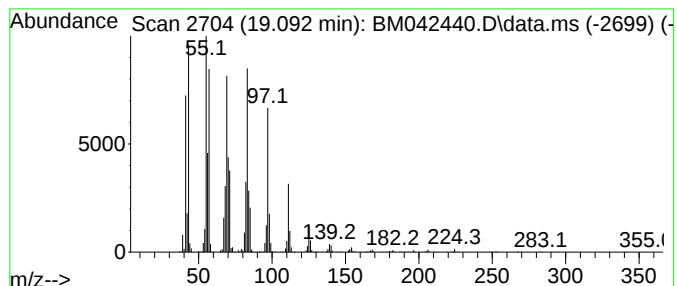
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Peak Number 4 3-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.092	18.31 ng	1738300	Phenanthrene-d10	17.386

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2		n-Heptadecanol-1	256	C17H36O	001454-85-9	94
3		1-Octadecanol	270	C18H38O	000112-92-5	94
4		9-Eicosene, (E)-	280	C20H40	074685-29-3	94
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	94



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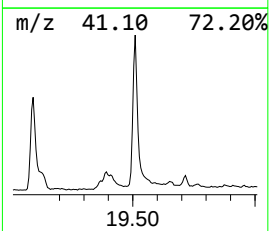
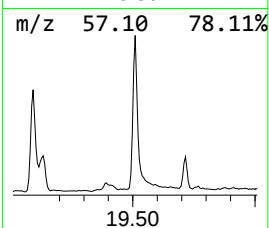
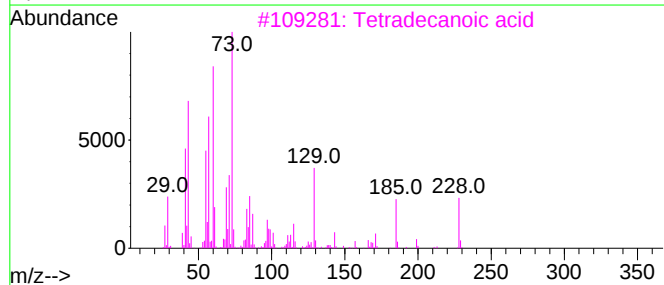
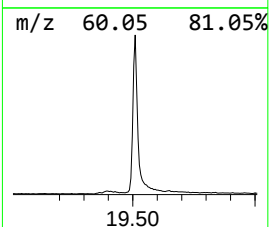
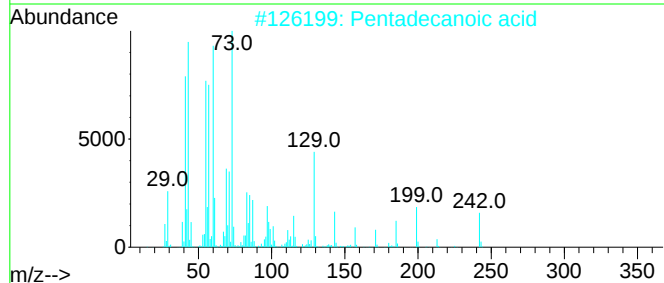
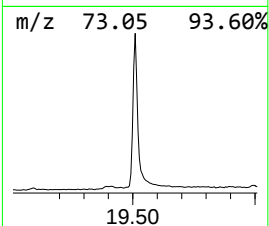
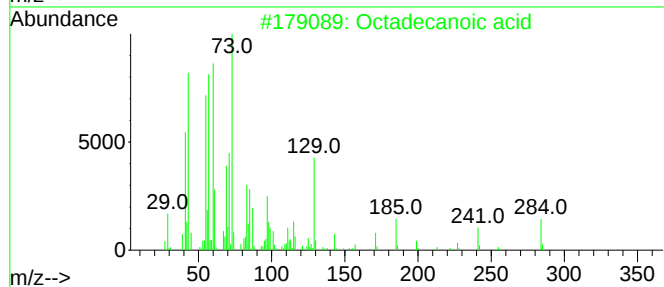
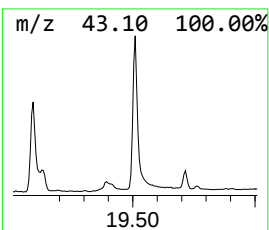
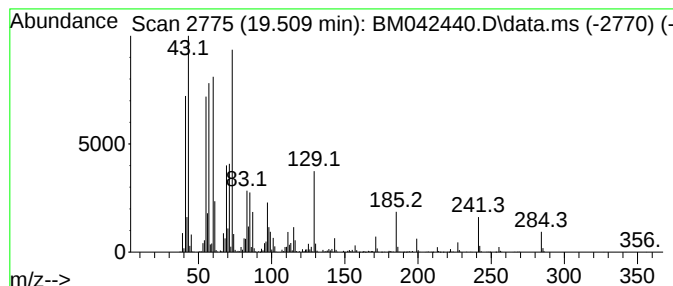
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.509	19.72 ng	2393190	Chrysene-d12	21.562

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	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			n-Decanoic acid	172	C10H20O2	000334-48-5	62
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



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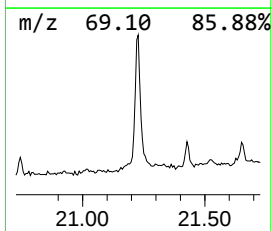
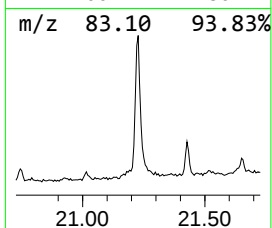
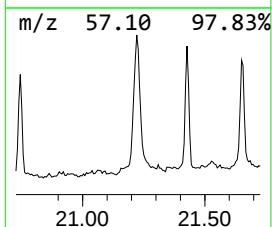
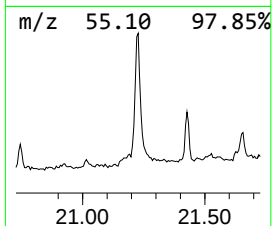
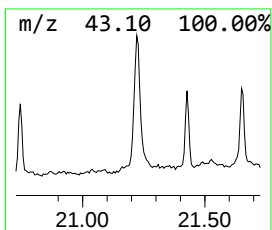
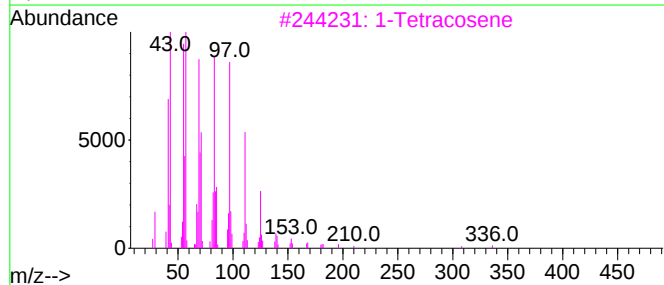
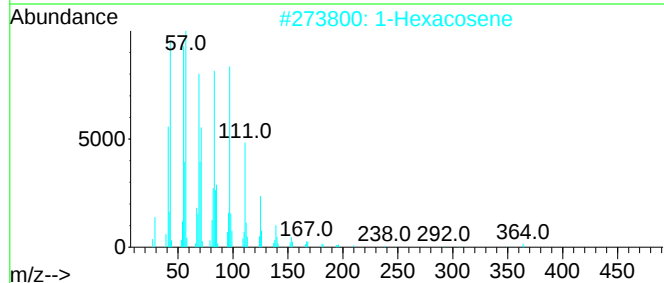
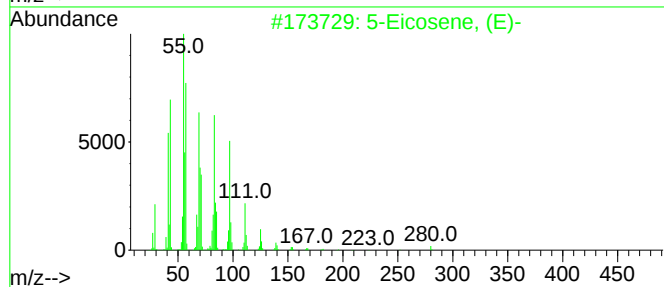
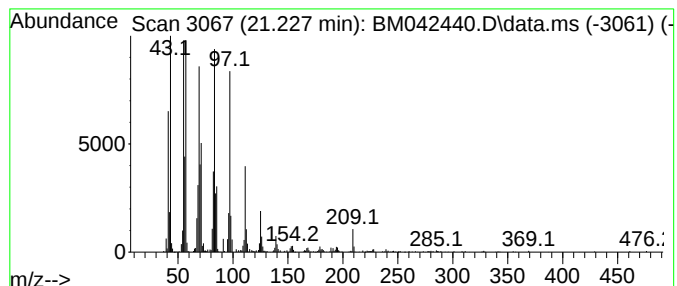
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Peak Number 6 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.227	7.80 ng	946503	Chrysene-d12	21.562

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2		1-Hexacosene	364	C26H52	018835-33-1	94
3		1-Tetracosene	336	C24H48	010192-32-2	94
4		Behenic alcohol	326	C22H46O	000661-19-8	94
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



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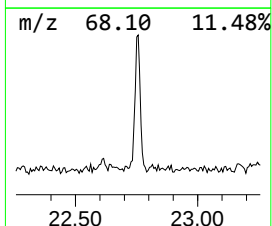
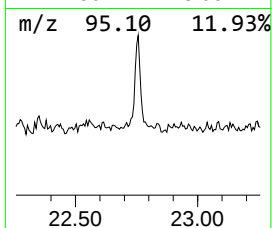
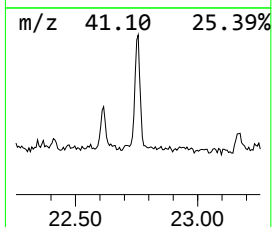
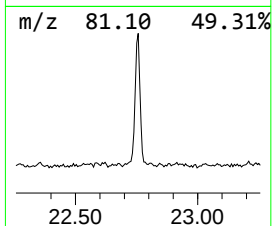
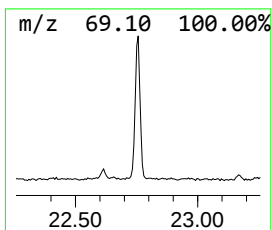
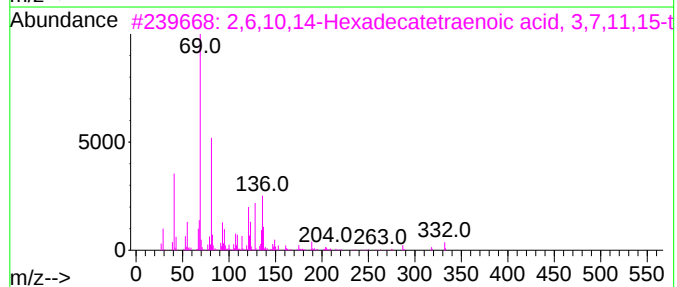
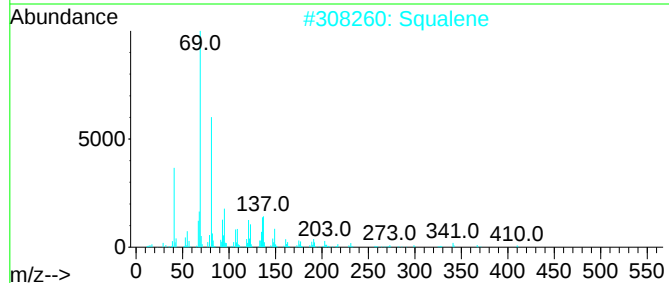
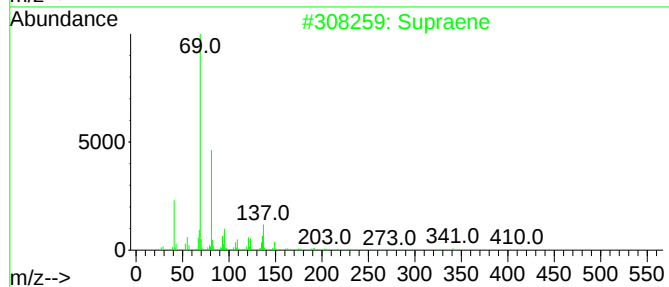
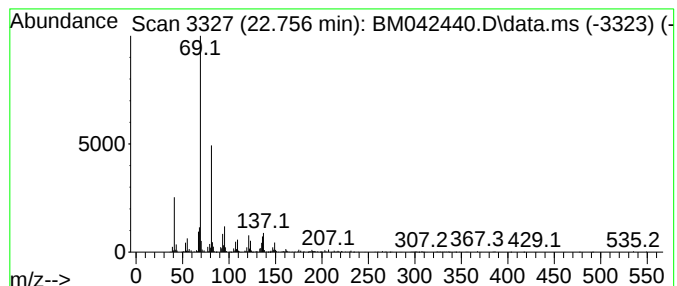
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.756	3.50 ng	424763	Chrysene-d12	21.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	90
3			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	87
4			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042440.D
Acq On : 25 Oct 2023 16:35
Operator : MA/JU
Sample : 04941-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
213

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.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
2-Pentanone, 4-...	5.069	8.0	ng	363234	1	7.992	908533	20.0
n-Hexadecanoic ...	18.233	31.5	ng	2986620	4	17.386	1898630	20.0
3-Eicosene, (E)-	19.092	18.3	ng	1738300	4	17.386	1898630	20.0
Octadecanoic acid	19.509	19.7	ng	2393190	5	21.562	2426790	20.0
5-Eicosene, (E)-	21.227	7.8	ng	946503	5	21.562	2426790	20.0
Supraene	22.756	3.5	ng	424763	5	21.562	2426790	20.0