

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110123\
 Data File : BM042549.D
 Acq On : 01 Nov 2023 20:49
 Operator : MA/JU
 Sample : 05083-01 5X
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SU-04-10252023

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-BM103023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042549.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.463	381	387	400	rBV	184080	281518	12.76%	2.544%
2	7.092	655	664	675	rBV	173674	295228	13.39%	2.668%
3	7.922	799	805	816	rBV	282197	481449	21.83%	4.350%
4	9.122	1004	1009	1018	rBV	104380	178103	8.08%	1.609%
5	10.745	1278	1285	1291	rBV	349460	582789	26.42%	5.266%
6	12.080	1505	1512	1520	rBV2	17112	25939	1.18%	0.234%
7	13.192	1696	1701	1714	rBV	283050	425274	19.28%	3.843%
8	13.327	1714	1724	1728	rBV	28983	44839	2.03%	0.405%
9	13.421	1733	1740	1747	rBV	111593	172876	7.84%	1.562%
10	14.398	1902	1906	1911	rBV	40477	47442	2.15%	0.429%
11	14.574	1930	1936	1943	rBV	527558	735836	33.36%	6.649%
12	15.351	2063	2068	2072	rBV	47701	58861	2.67%	0.532%
13	15.745	2130	2135	2141	rBV2	18450	32530	1.47%	0.294%
14	16.068	2184	2190	2200	rBV	218848	317321	14.39%	2.867%
15	16.215	2210	2215	2223	rBV	60620	88037	3.99%	0.796%
16	17.009	2345	2350	2353	rBV	51345	66018	2.99%	0.597%
17	17.045	2353	2356	2362	rVB	19777	29923	1.36%	0.270%
18	17.327	2398	2404	2409	rBV	622079	857086	38.86%	7.745%
19	17.368	2409	2411	2416	rVB	29274	36195	1.64%	0.327%
20	17.745	2471	2475	2480	rBV	51886	67175	3.05%	0.607%
21	17.945	2504	2509	2514	rBV	349011	412899	18.72%	3.731%
22	18.174	2544	2548	2556	rBV	151246	240545	10.91%	2.174%
23	18.445	2590	2594	2599	rBV	51179	67263	3.05%	0.608%
24	18.574	2613	2616	2622	rVB3	31387	39623	1.80%	0.358%
25	19.092	2699	2704	2707	rBV	1915223	2205465	100.00%	19.929%
26	19.121	2707	2709	2720	rVB2	940665	1189198	53.92%	10.746%
27	19.250	2727	2731	2735	rBV	205431	233660	10.59%	2.111%
28	19.315	2739	2742	2744	rBV	96797	118744	5.38%	1.073%
29	19.339	2744	2746	2750	rVB2	104157	121185	5.49%	1.095%
30	19.456	2762	2766	2772	rBV	112910	182264	8.26%	1.647%
31	19.939	2844	2848	2855	rBV	464769	606102	27.48%	5.477%
32	21.509	3112	3115	3120	rVB	683598	825216	37.42%	7.457%

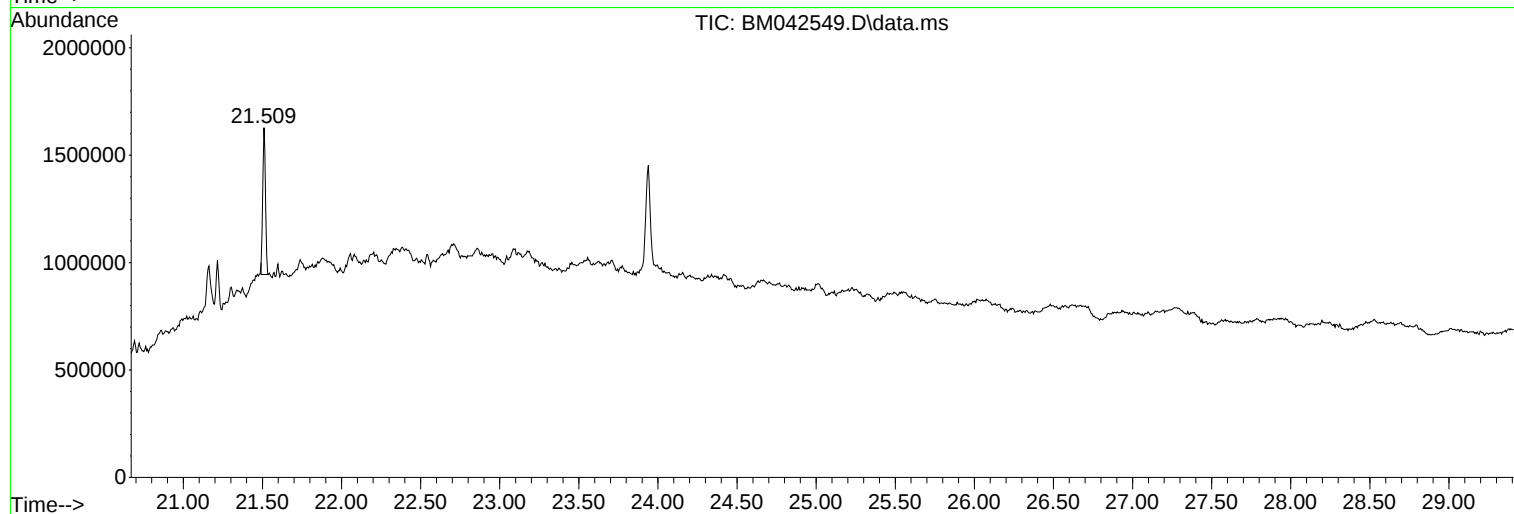
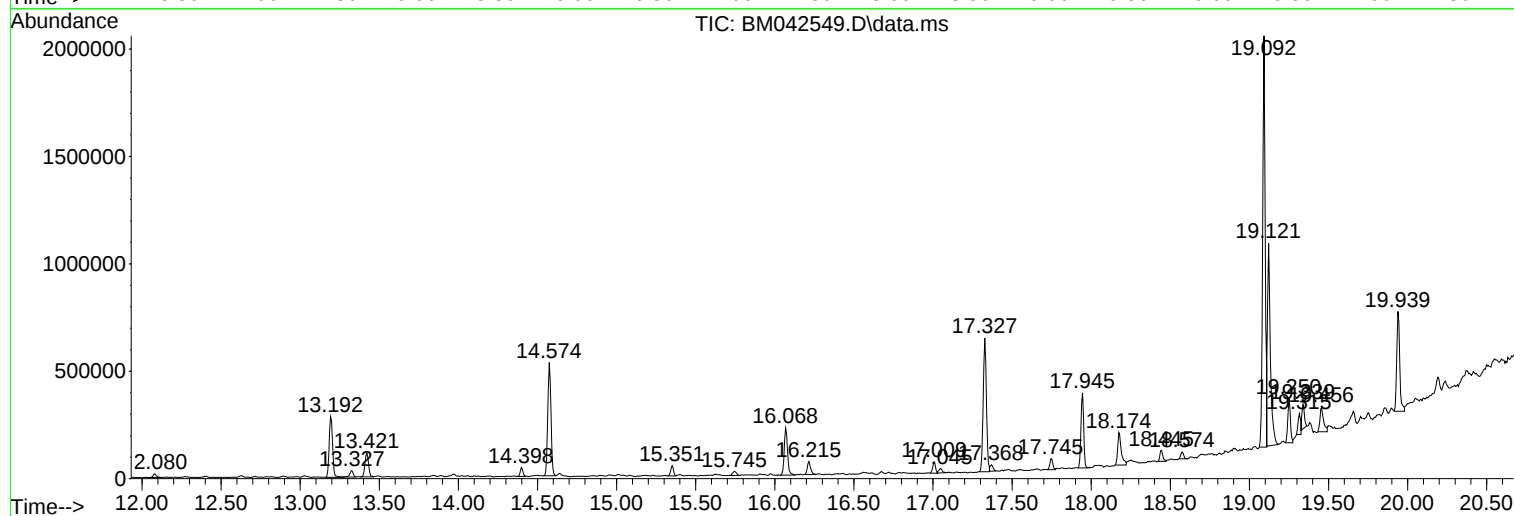
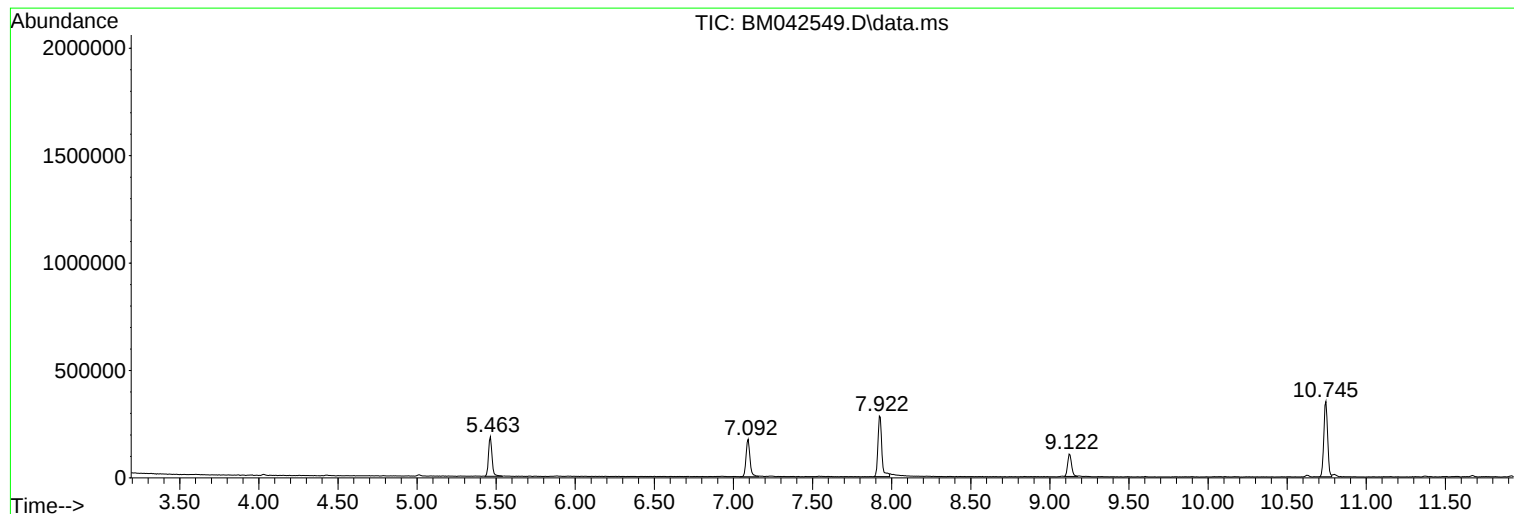
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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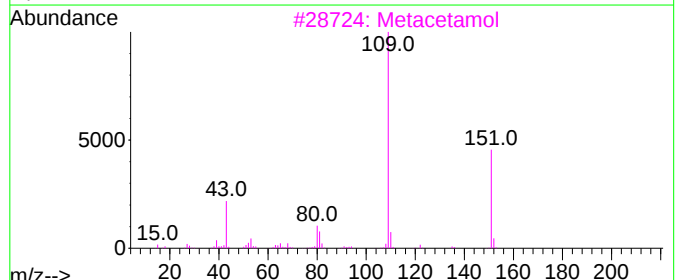
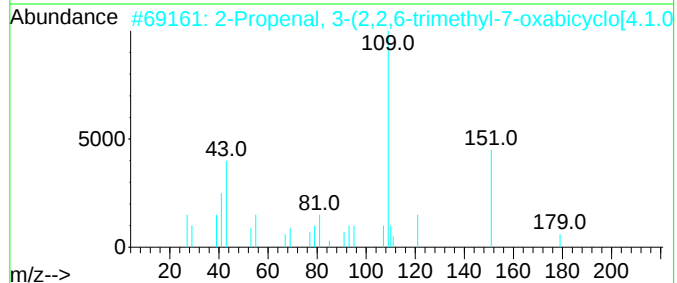
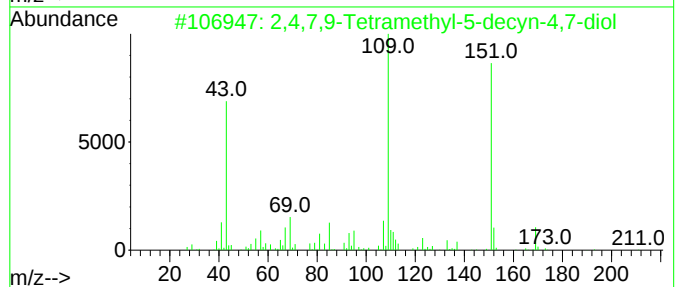
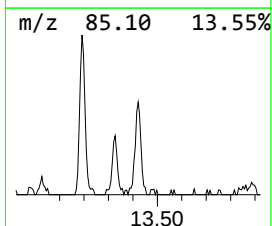
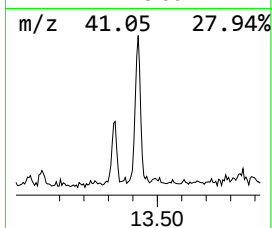
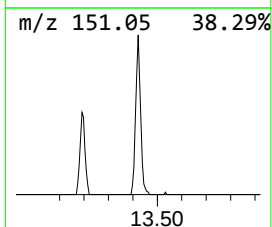
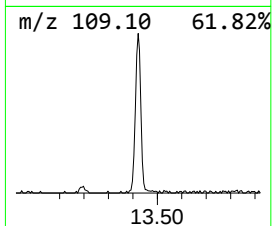
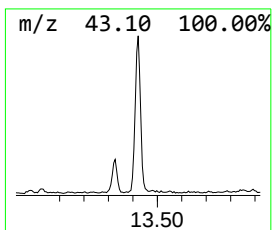
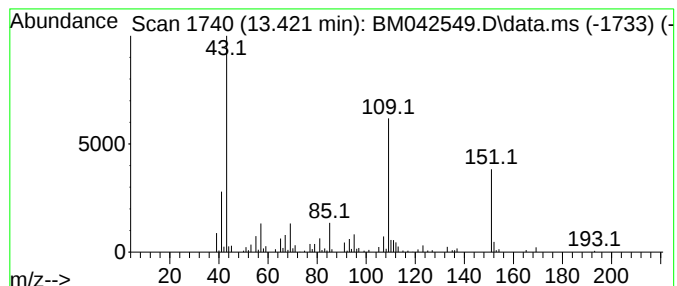
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.421	4.70 ng	172876	Acenaphthene-d10	14.574

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90	
2	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	59	
3	Metacetamol	151	C8H9NO2	000621-42-1	58	
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53	
5	Acetaminophen	151	C8H9NO2	000103-90-2	53	



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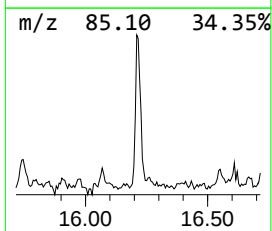
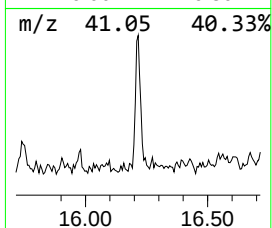
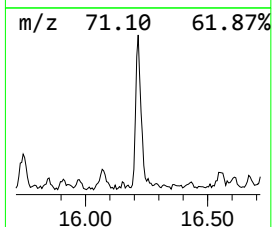
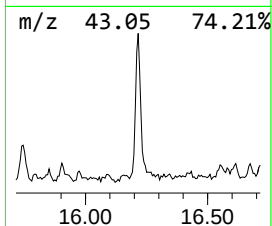
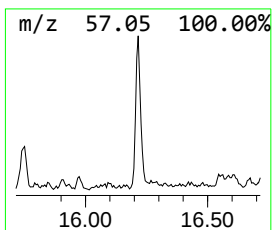
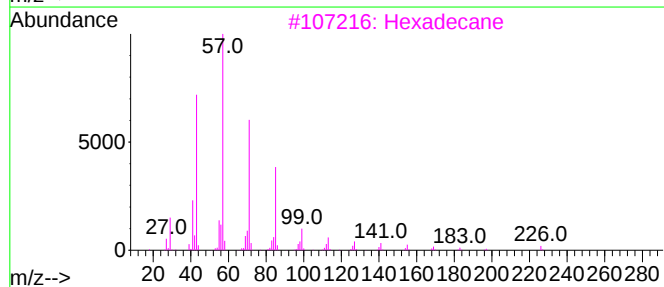
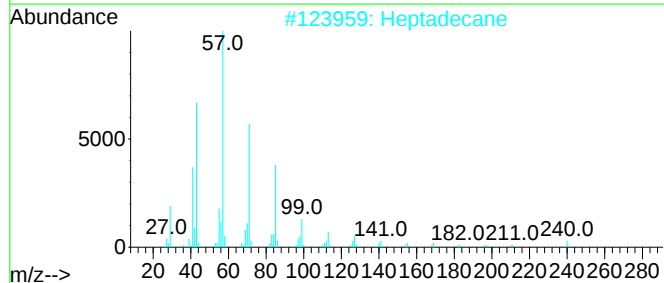
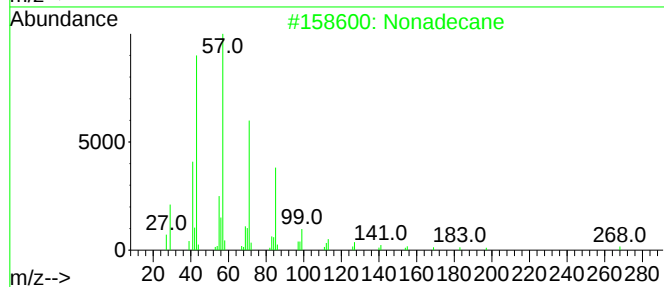
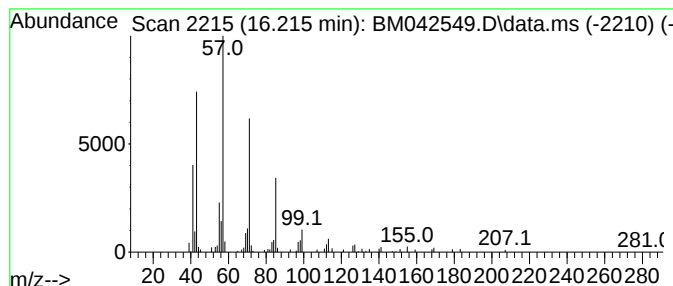
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.215	2.05 ng	88037	Phenanthrene-d10	17.327

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	91
2			Heptadecane	240	C17H36	000629-78-7	91
3			Hexadecane	226	C16H34	000544-76-3	91
4			Tetradecane	198	C14H30	000629-59-4	91
5			Heptacosane	380	C27H56	000593-49-7	90



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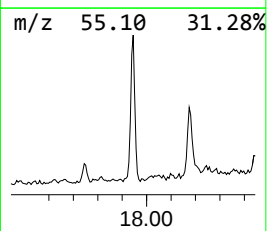
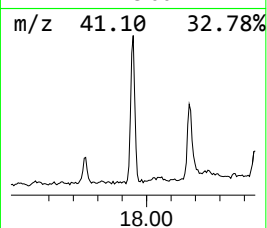
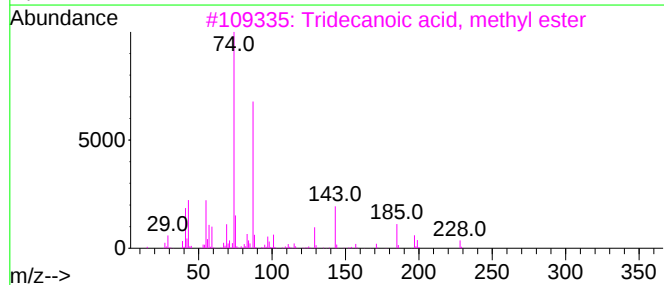
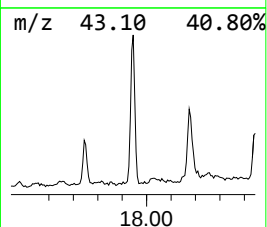
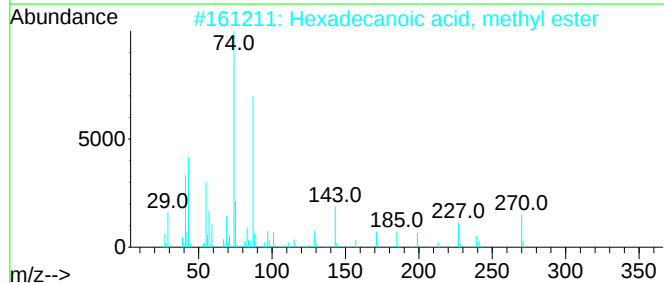
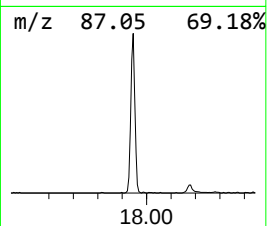
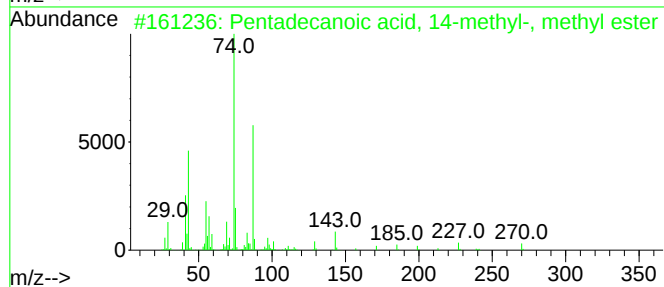
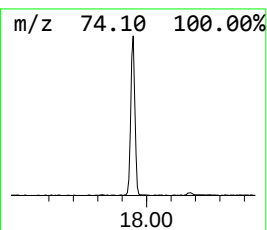
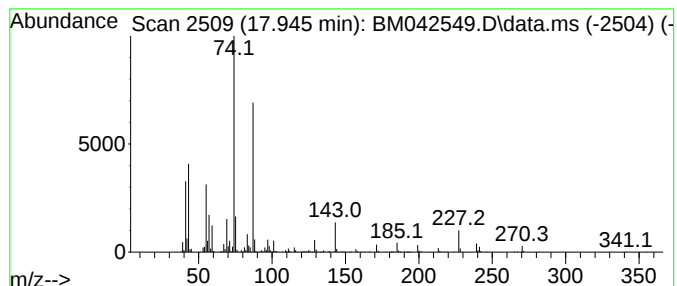
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Pentadecanoic acid, 14-meth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.945	9.63 ng	412899	Phenanthrene-d10	17.327	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	97
2	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	90
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86



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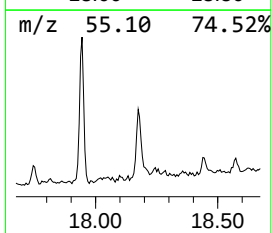
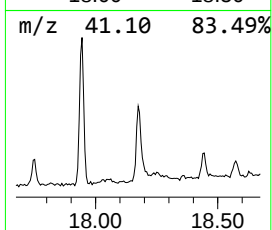
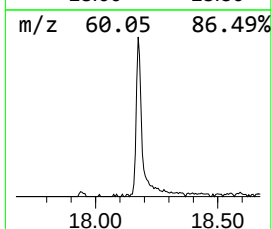
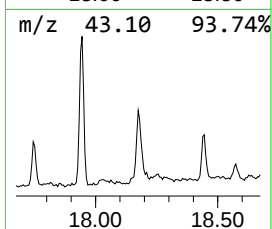
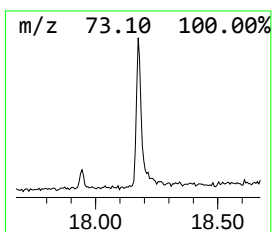
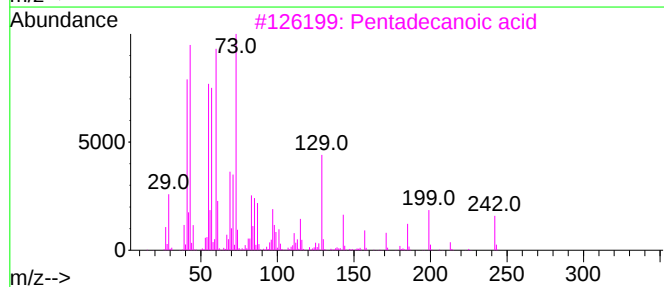
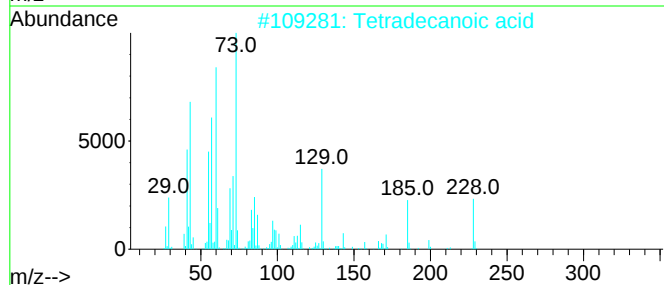
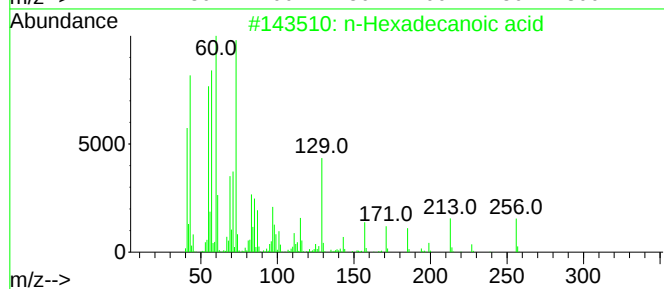
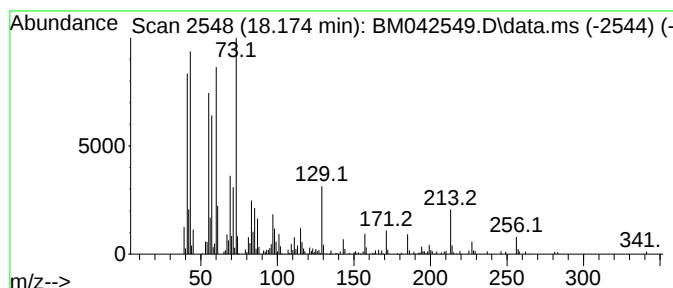
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.174	5.61 ng	240545	Phenanthrene-d10	17.327	
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	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64



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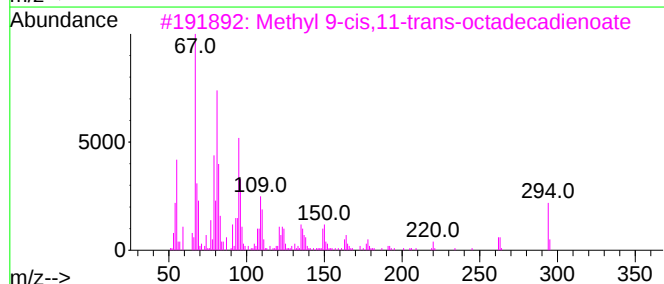
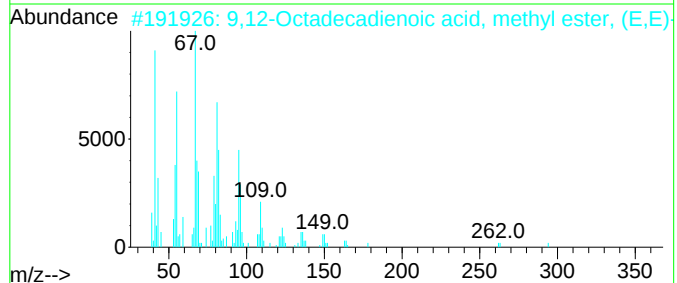
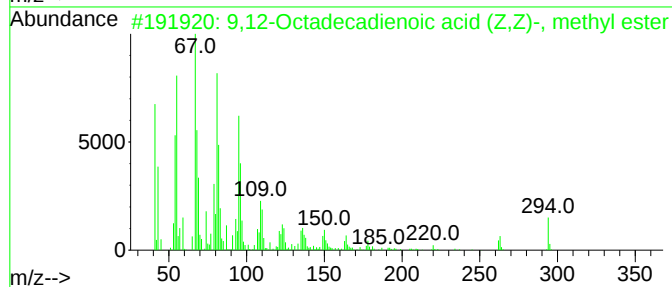
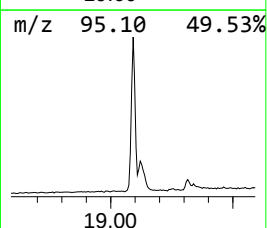
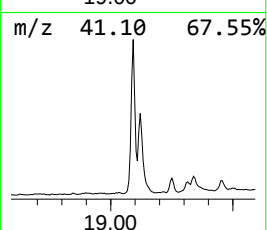
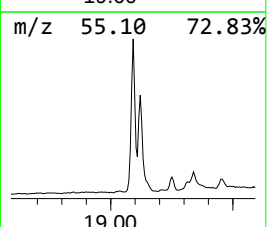
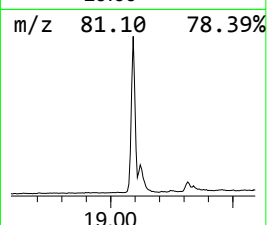
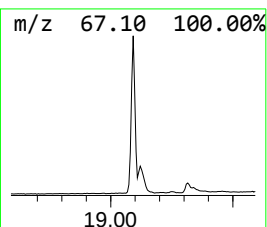
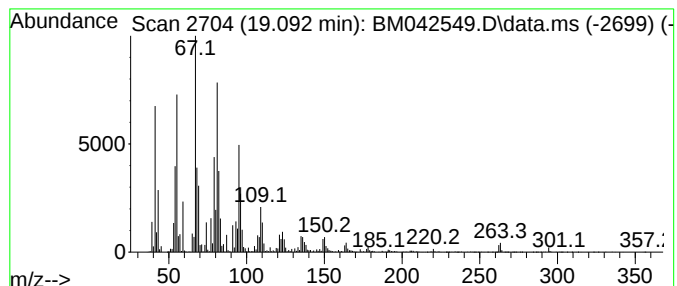
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Peak Number 5 9,12-Octadecadienoic acid (... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.092	51.46 ng	2205470	Phenanthrene-d10	17.327	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
3	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
5	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98



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Misc :
ALS Vial : 18 Sample Multiplier: 1

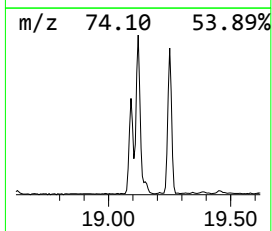
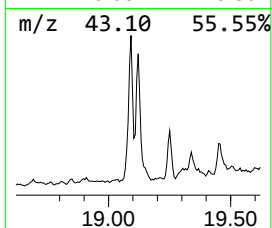
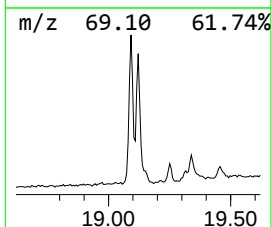
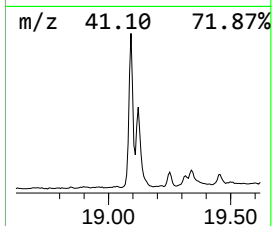
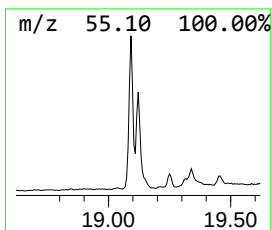
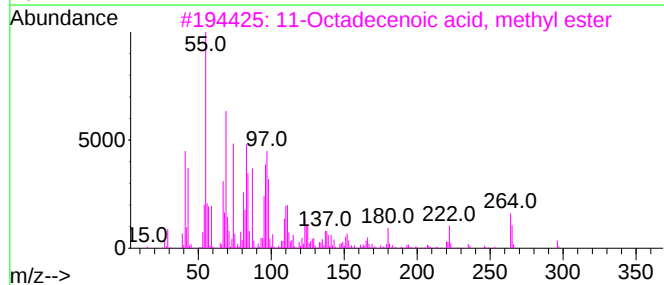
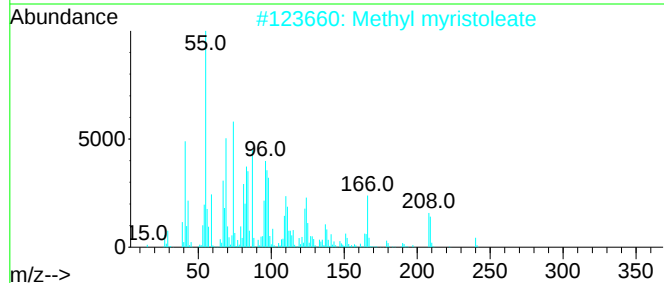
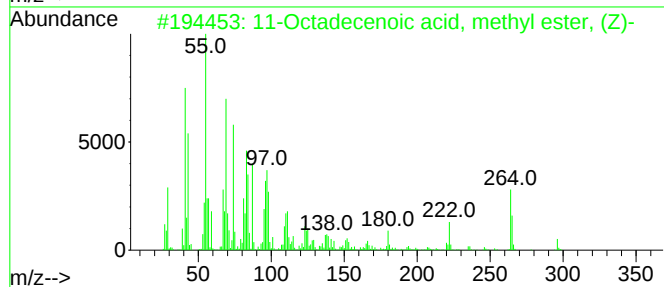
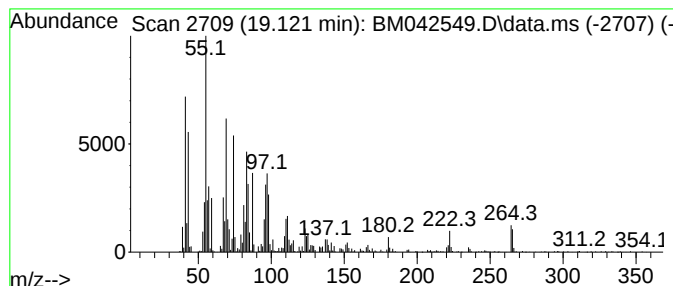
Instrument :
BNA_M
ClientSampleId :
SU-04-10252023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 11-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.121	27.75 ng	1189200	Phenanthrene-d10	17.327	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	94
2	Methyl myristoleate	240	C15H28O2	056219-06-8	91
3	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	91
4	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	91
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110123\
Data File : BM042549.D
Acq On : 01 Nov 2023 20:49
Operator : MA/JU
Sample : 05083-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SU-04-10252023

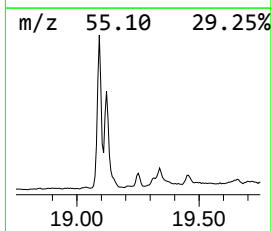
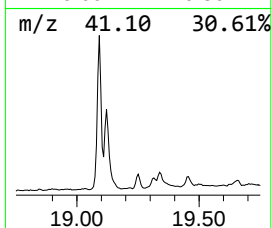
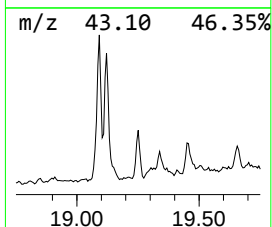
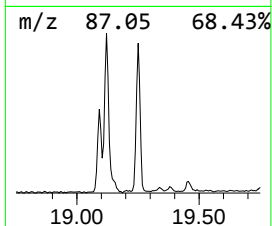
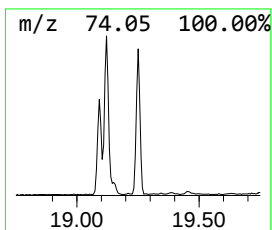
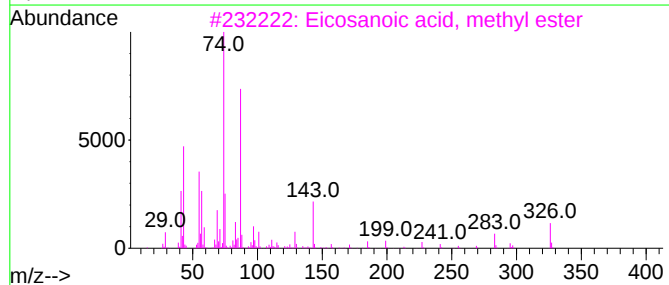
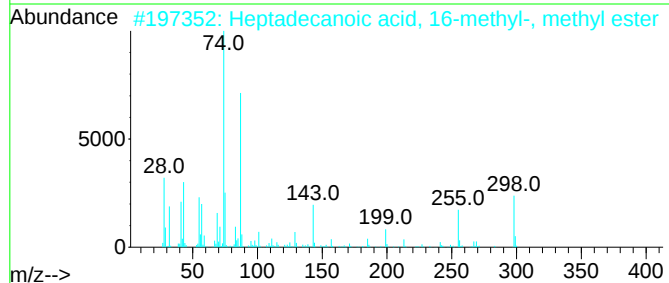
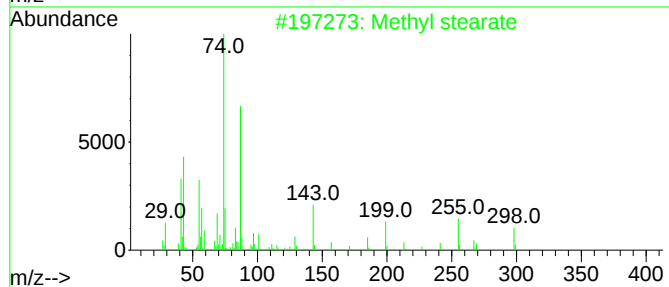
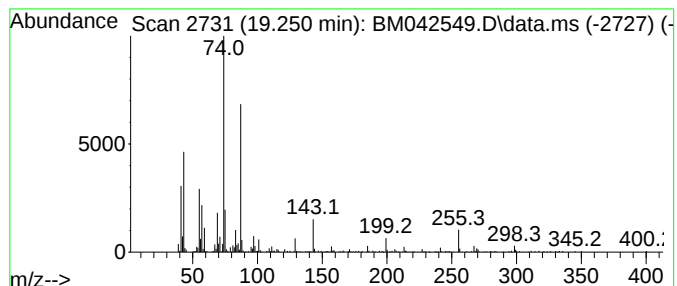
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Methyl stearate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.250	5.45 ng	233660	Phenanthrene-d10	17.327

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	97
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	97
3			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	93
4			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110123\
Data File : BM042549.D
Acq On : 01 Nov 2023 20:49
Operator : MA/JU
Sample : 05083-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SU-04-10252023

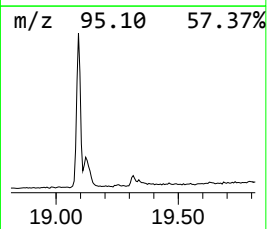
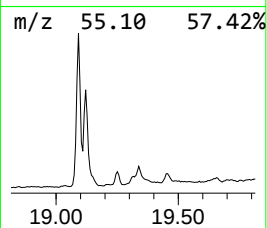
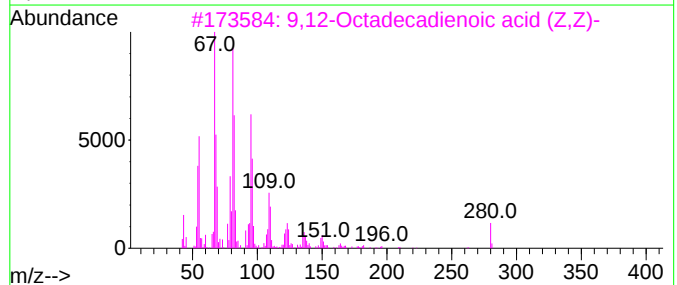
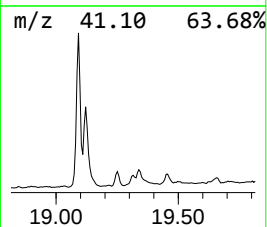
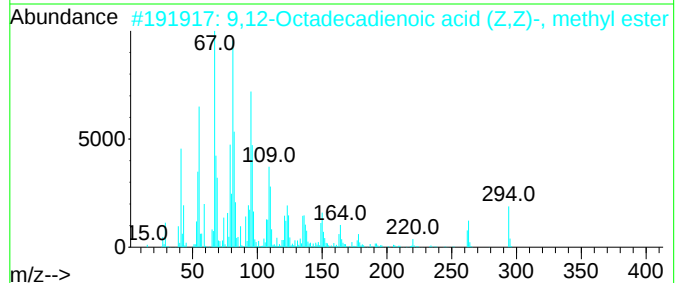
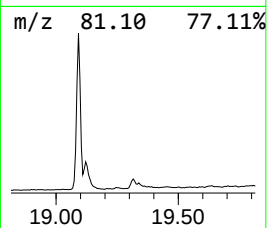
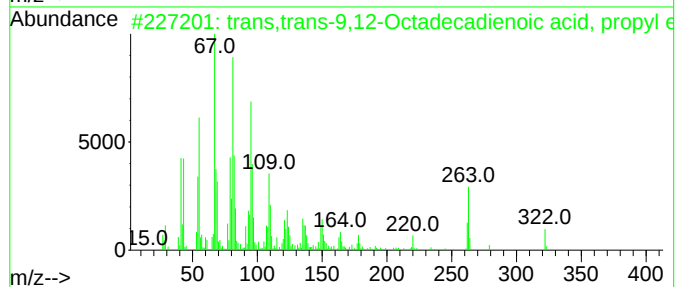
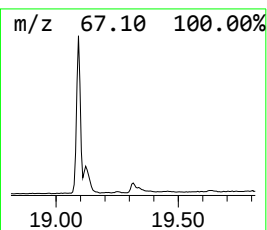
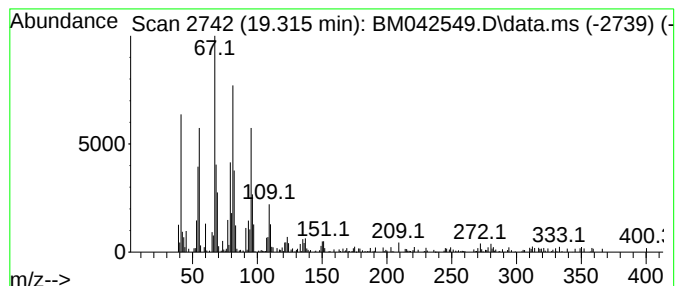
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 trans,trans-9,12-Octadecadi... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.315	2.77 ng	118744	Phenanthrene-d10	17.327

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans,trans-9,12-Octadecadienoic...	322	C21H38O2	1000405-14-9	97
2			9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	95
3			9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	93
4			10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	93
5			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110123\
Data File : BM042549.D
Acq On : 01 Nov 2023 20:49
Operator : MA/JU
Sample : 05083-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

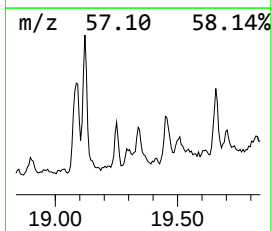
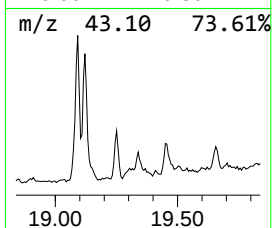
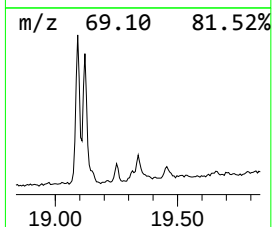
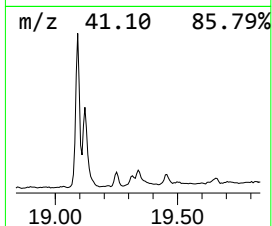
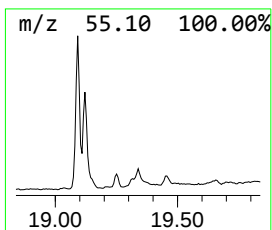
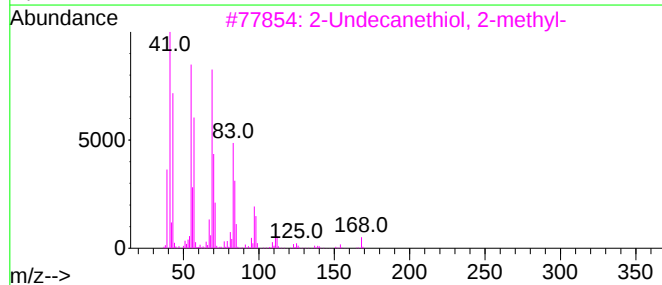
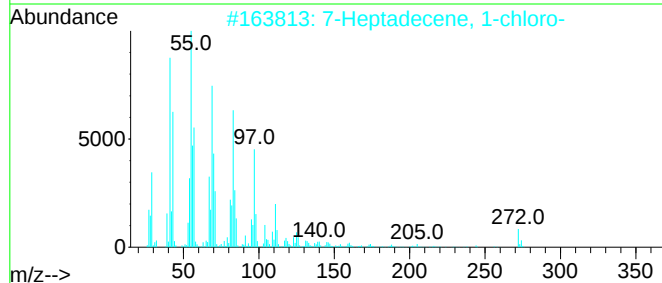
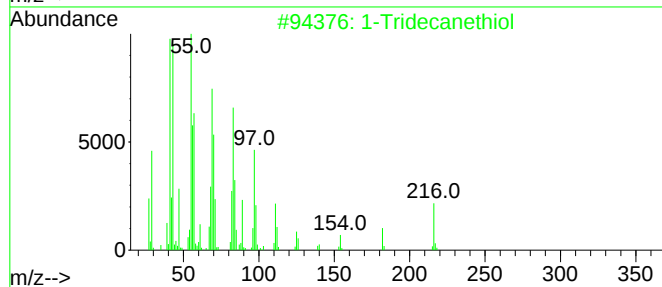
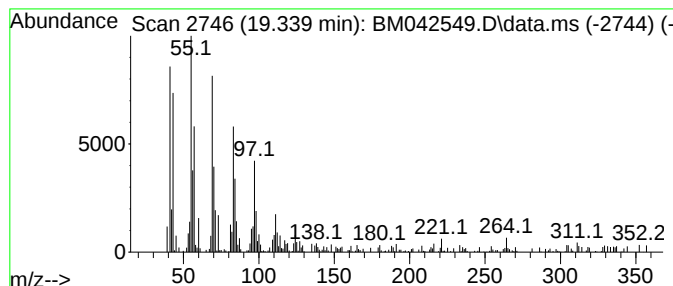
Instrument :
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ClientSampleId :
SU-04-10252023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Tridecanethiol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.339	2.83 ng	121185	Phenanthrene-d10	17.327	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tridecanethiol	216	C13H28S	019484-26-5	89
2	7-Heptadecene, 1-chloro-	272	C17H33Cl	056554-78-0	80
3	2-Undecanethiol, 2-methyl-	202	C12H26S	010059-13-9	72
4	7-Tetradecene	196	C14H28	010374-74-0	72
5	n-Pentadecanol	228	C15H32O	000629-76-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110123\
Data File : BM042549.D
Acq On : 01 Nov 2023 20:49
Operator : MA/JU
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Misc :
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Instrument :
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ClientSampleId :
SU-04-10252023

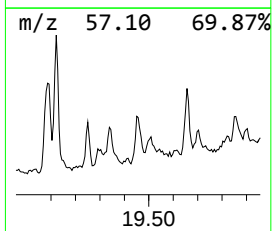
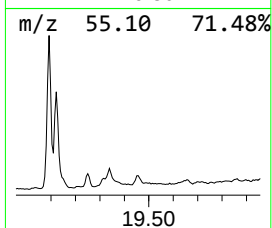
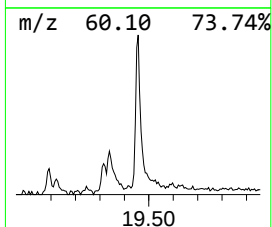
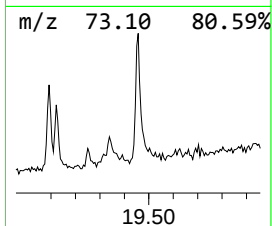
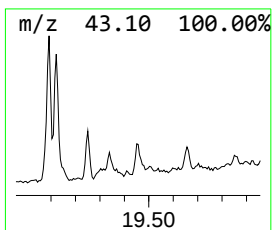
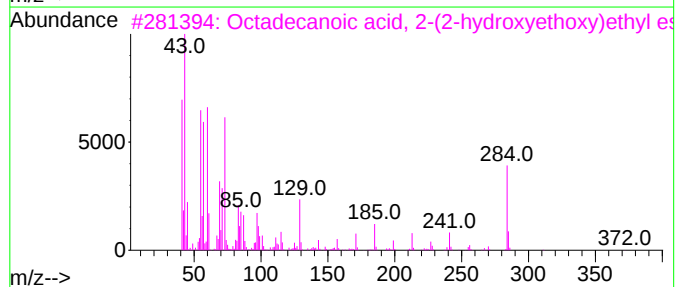
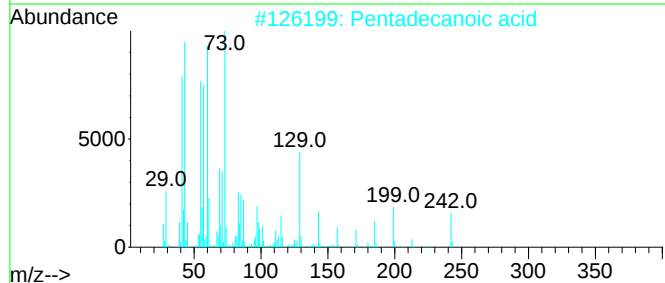
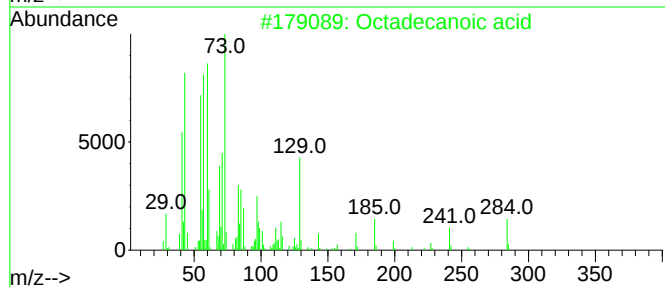
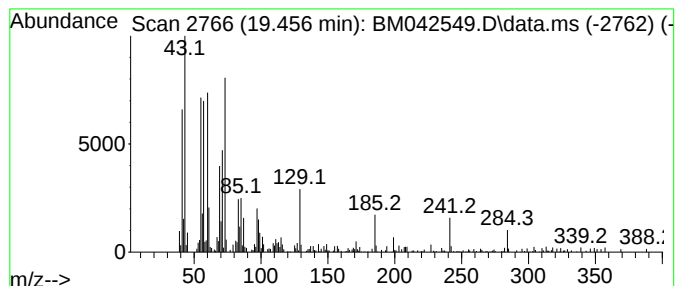
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.456	4.42 ng	182264	Chrysene-d12	21.509

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			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5			Tricosanoic acid	354	C23H46O2	002433-96-7	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110123\
Data File : BM042549.D
Acq On : 01 Nov 2023 20:49
Operator : MA/JU
Sample : 05083-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SU-04-10252023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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
2,4,7,9-Tetrame...	13.421	4.7	ng	172876	3	14.574	735836	20.0
Nonadecane	16.215	2.0	ng	88037	4	17.327	857086	20.0
Pentadecanoic a...	17.945	9.6	ng	412899	4	17.327	857086	20.0
n-Hexadecanoic ...	18.174	5.6	ng	240545	4	17.327	857086	20.0
9,12-Octadecadi...	19.092	51.5	ng	2205470	4	17.327	857086	20.0
11-Octadecenoic...	19.121	27.8	ng	1189200	4	17.327	857086	20.0
Methyl stearate	19.250	5.5	ng	233660	4	17.327	857086	20.0
trans,trans-9,1...	19.315	2.8	ng	118744	4	17.327	857086	20.0
1-Tridecanethiol	19.339	2.8	ng	121185	4	17.327	857086	20.0
Octadecanoic acid	19.456	4.4	ng	182264	5	21.509	825216	20.0