

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
 Data File : BM041309.D
 Acq On : 07 Aug 2023 13:06
 Operator : MA/JU
 Sample : 03903-02
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-02

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: BM041309.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.904	284	292	302	rBV	42040	67080	1.20%	0.162%
2	5.363	363	370	385	rBV	1696152	2447697	43.75%	5.904%
3	6.969	636	643	659	rBV	1630915	2607704	46.61%	6.290%
4	7.410	712	718	731	rBV2	25378	62657	1.12%	0.151%
5	7.787	775	782	789	rBV	460988	714334	12.77%	1.723%
6	8.963	975	982	998	rBV	967117	1622413	29.00%	3.914%
7	10.592	1252	1259	1271	rBV	611319	1029903	18.41%	2.484%
8	13.074	1673	1681	1690	rBV	2496397	3714989	66.40%	8.961%
9	13.339	1720	1726	1734	rVB	185809	284279	5.08%	0.686%
10	14.457	1909	1916	1928	rBV	1019611	1487846	26.59%	3.589%
11	14.880	1982	1988	1998	rBV	91296	172784	3.09%	0.417%
12	15.292	2040	2058	2082	rBV3	116427	701670	12.54%	1.693%
13	15.957	2164	2171	2190	rBV	2476635	3511701	62.76%	8.471%
14	16.615	2275	2283	2292	rBV	157619	256524	4.58%	0.619%
15	17.215	2379	2385	2391	rVB	1389376	1837442	32.84%	4.432%
16	17.339	2402	2406	2410	rVB	47149	63587	1.14%	0.153%
17	17.386	2410	2414	2428	rVB	85392	142129	2.54%	0.343%
18	17.880	2487	2498	2510	rBV4	86708	293017	5.24%	0.707%
19	17.986	2512	2516	2526	rBV	154560	283840	5.07%	0.685%
20	18.121	2532	2539	2561	rBV	3004912	4808758	85.94%	11.600%
21	19.062	2696	2699	2704	rVB3	58611	65768	1.18%	0.159%
22	19.280	2729	2736	2748	rVB3	92630	228261	4.08%	0.551%
23	19.398	2752	2756	2777	rVV	1401306	2150370	38.43%	5.187%
24	19.856	2828	2834	2839	rBV	4515264	5595208	100.00%	13.497%
25	21.127	3046	3050	3056	rBV	268976	373602	6.68%	0.901%
26	21.421	3095	3100	3111	rBV	1443700	1828525	32.68%	4.411%
27	22.321	3249	3253	3268	rVB	1007359	1514176	27.06%	3.653%
28	22.638	3302	3307	3315	rVB	1387978	1994070	35.64%	4.810%
29	23.791	3497	3503	3513	rVB	816352	1595046	28.51%	3.848%

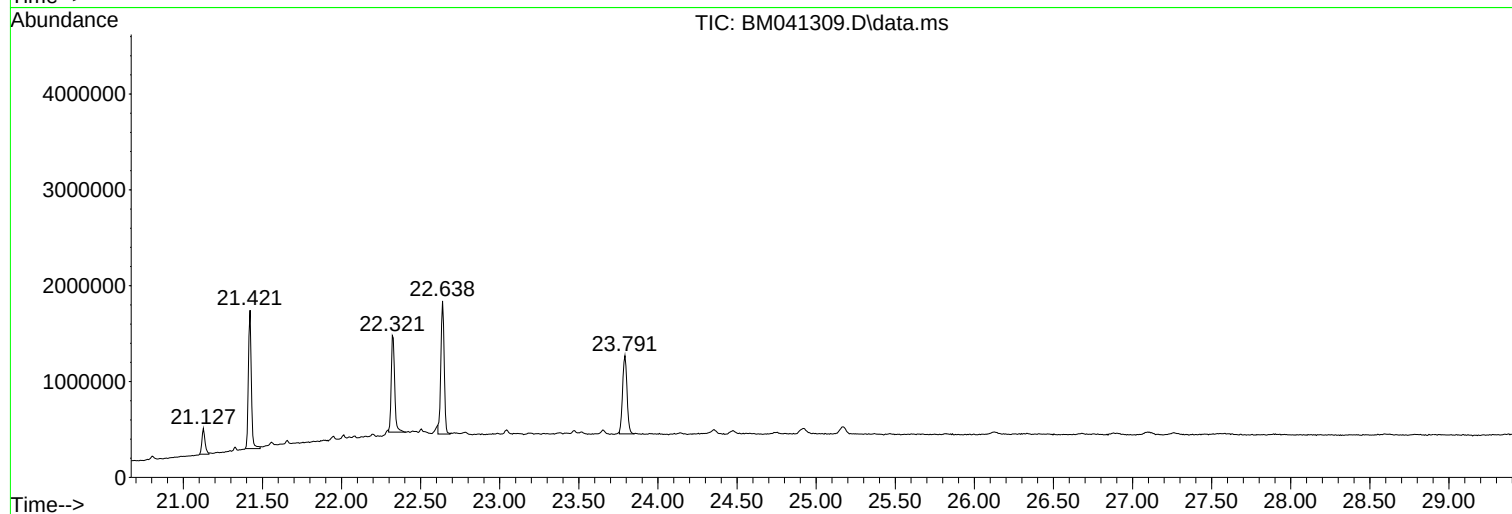
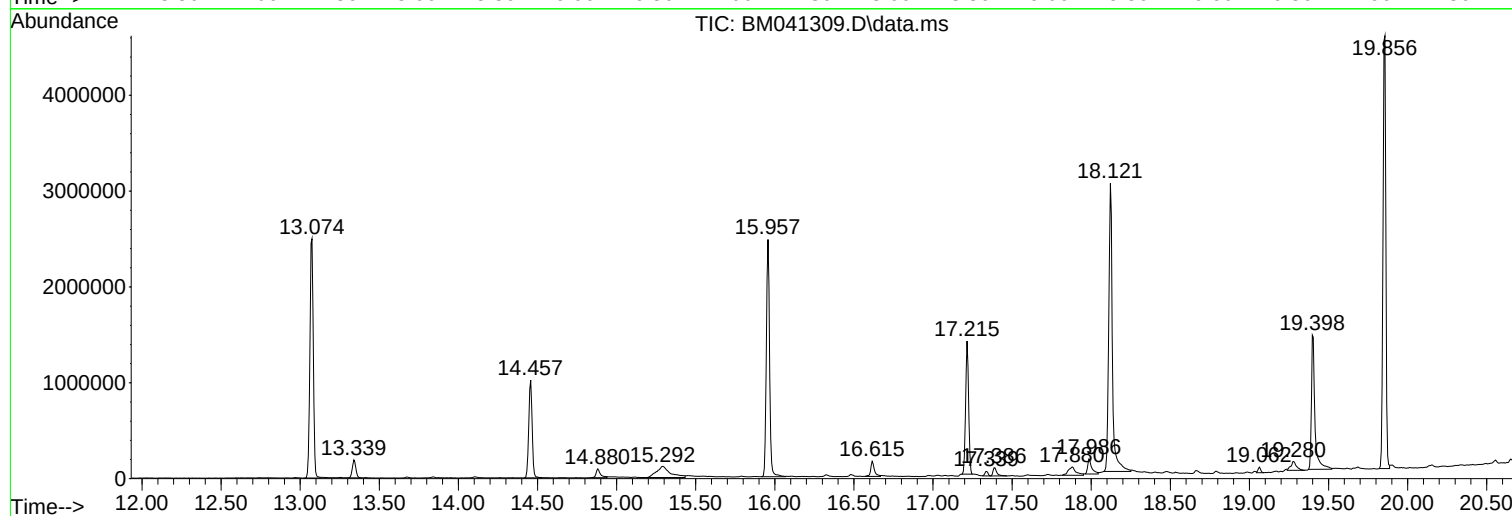
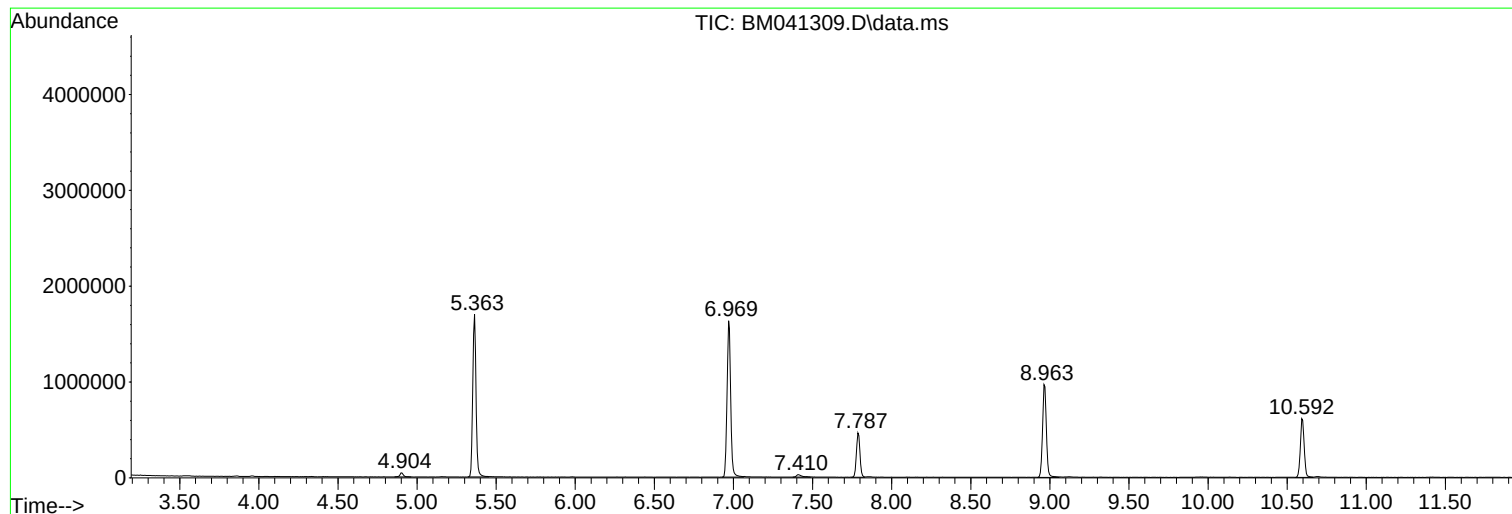
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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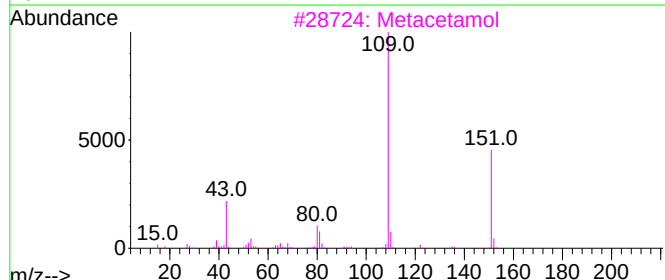
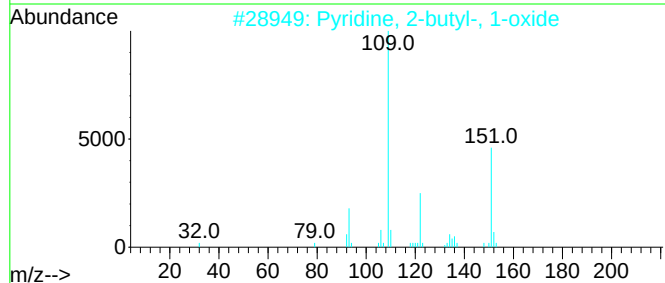
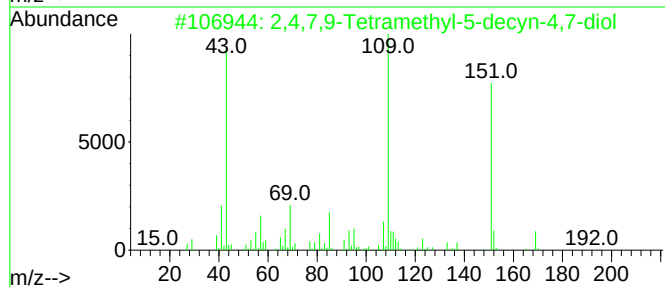
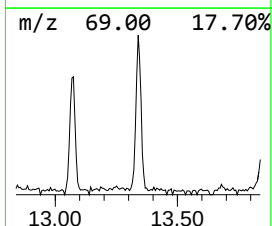
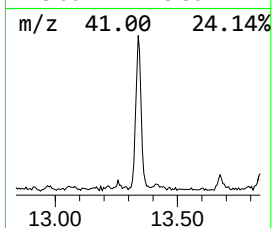
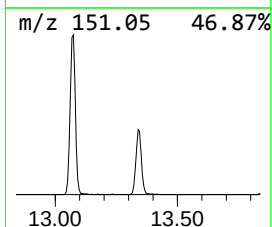
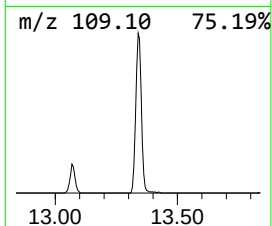
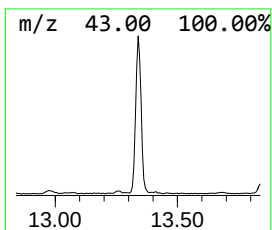
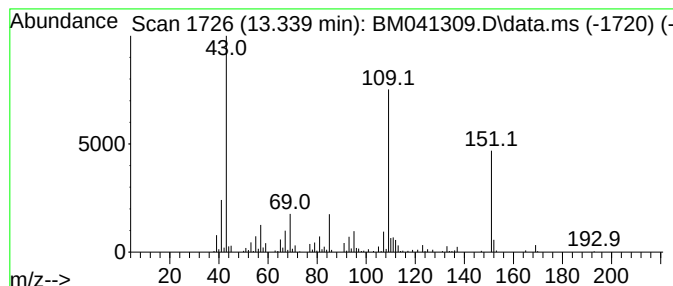
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.339	3.82 ng	284279	Acenaphthene-d10	14.457

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2		000126-86-3	91
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO		031396-32-4	59
3	Metacetamol	151	C8H9NO2		000621-42-1	58
4	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2		055759-91-6	56
5	Diacetamate	193	C10H11NO3		002623-33-8	53



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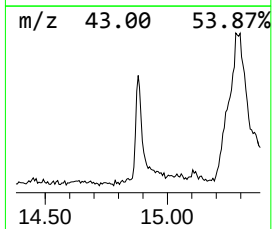
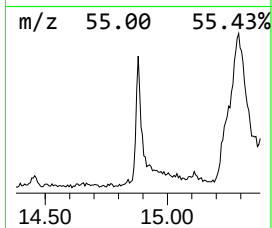
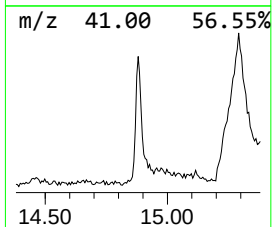
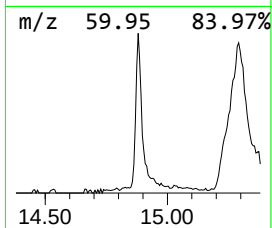
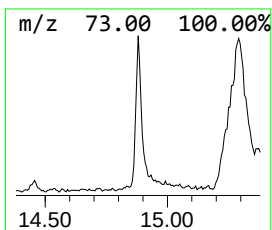
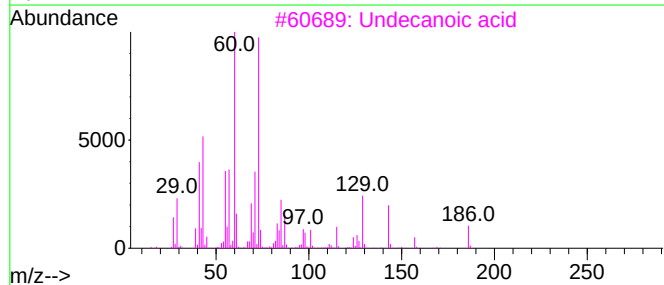
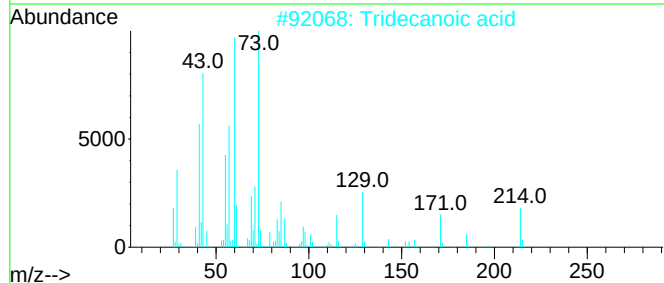
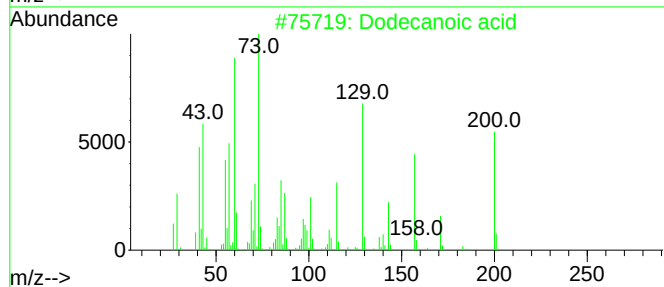
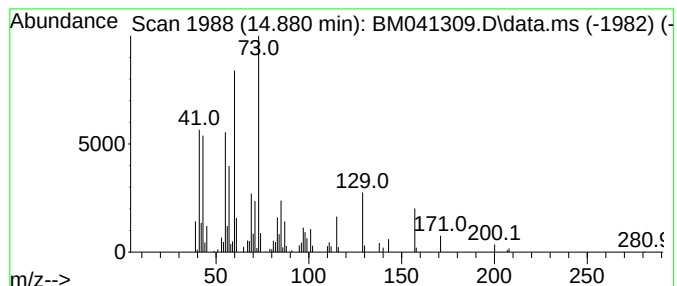
Instrument :
BNA_M
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Dodecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.880	2.32 ng	172784	Acenaphthene-d10	14.457	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	80
3	Undecanoic acid	186	C11H22O2	000112-37-8	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Nonanoic acid	158	C9H18O2	000112-05-0	53



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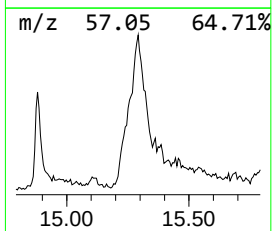
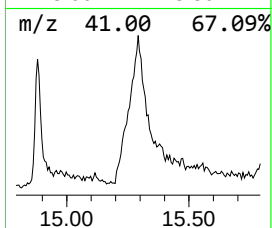
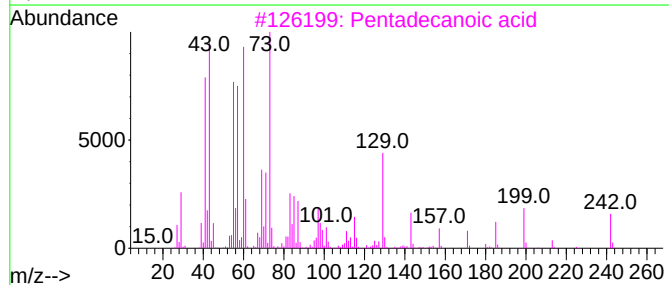
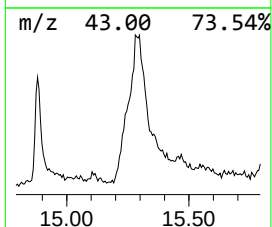
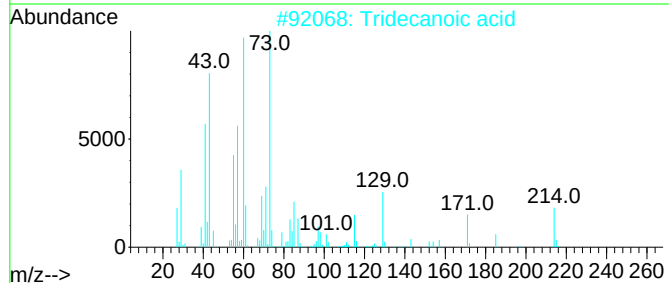
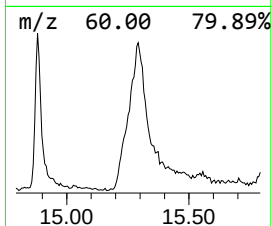
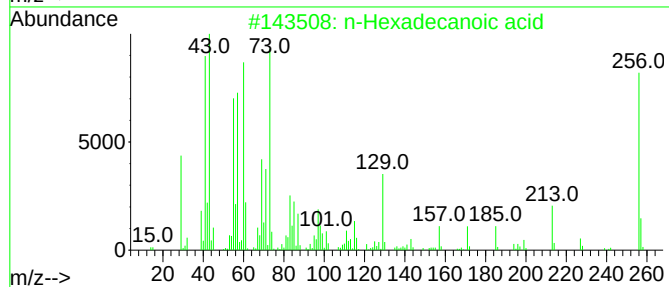
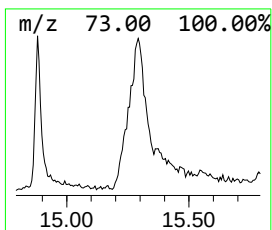
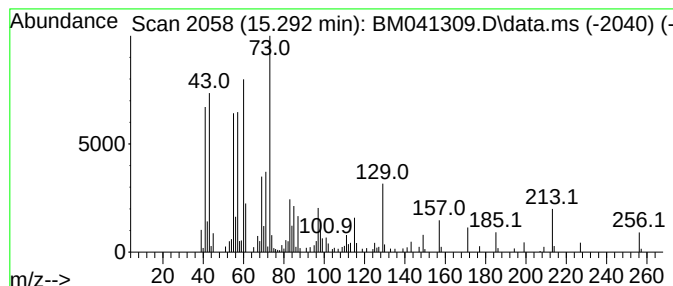
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.292	9.43 ng	701670	Acenaphthene-d10	14.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	76
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5			Undecanoic acid	186	C11H22O2	000112-37-8	50



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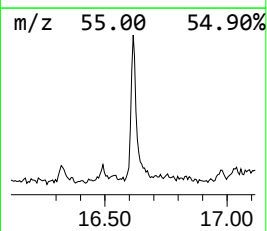
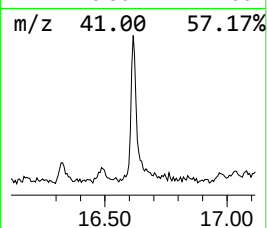
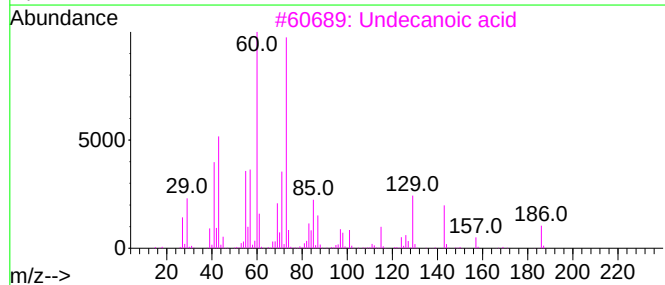
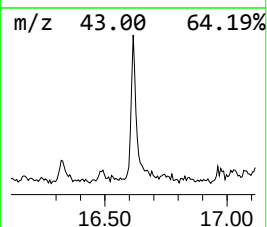
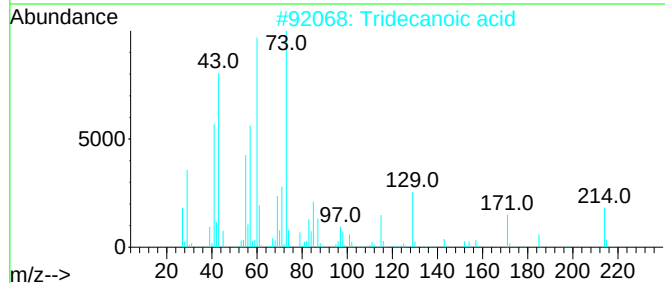
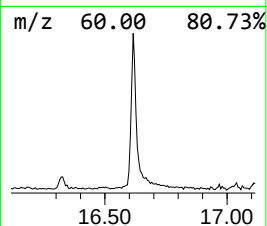
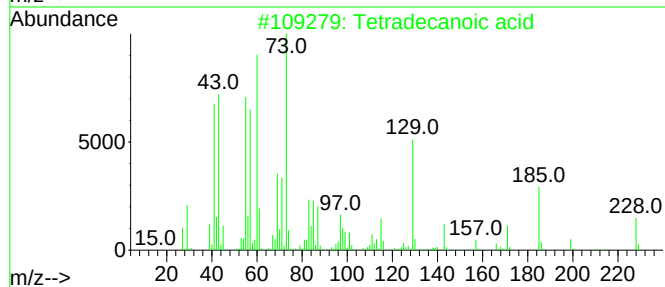
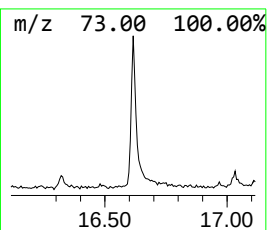
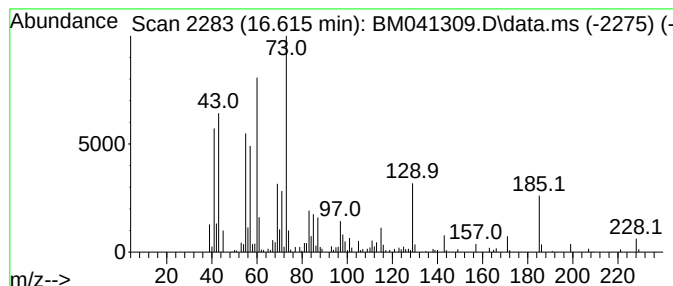
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Tetradecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.615	2.79 ng	256524	Phenanthrene-d10	17.215

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	97
2			Tridecanoic acid	214	C13H26O2	000638-53-9	72
3			Undecanoic acid	186	C11H22O2	000112-37-8	64
4			Dodecanoic acid	200	C12H24O2	000143-07-7	53
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



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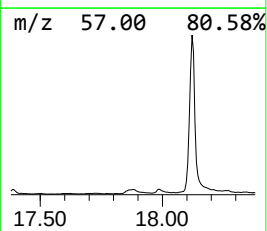
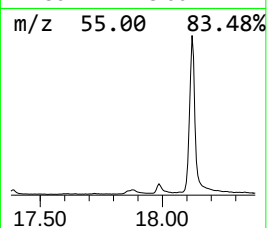
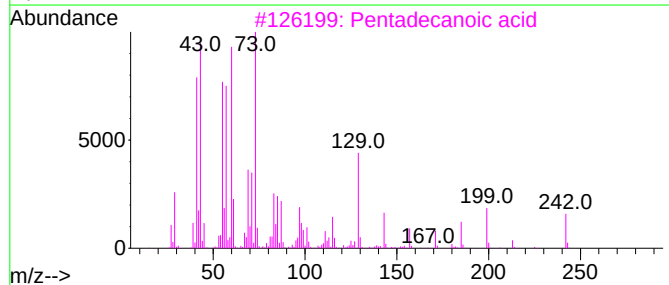
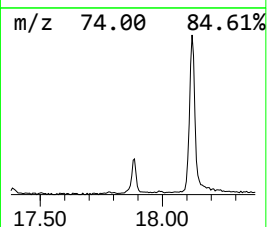
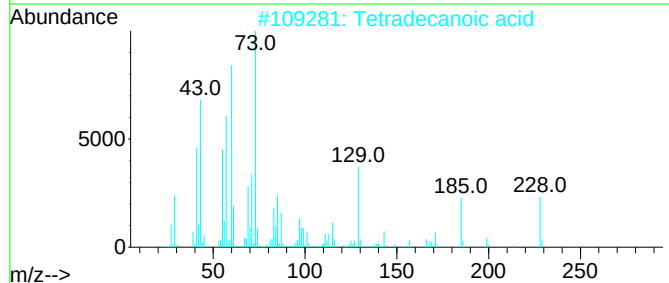
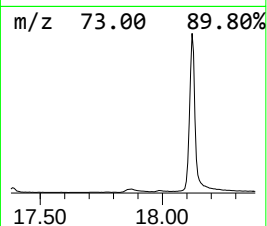
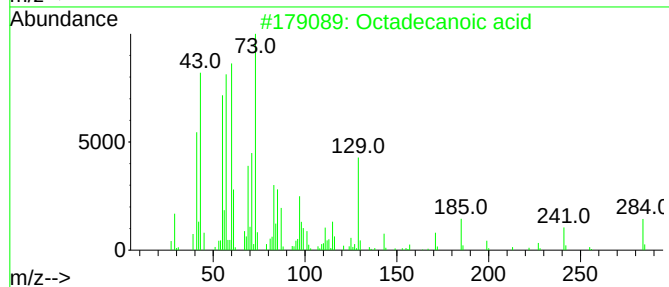
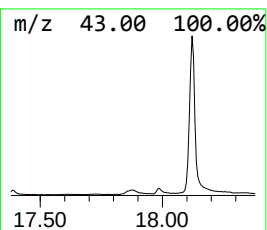
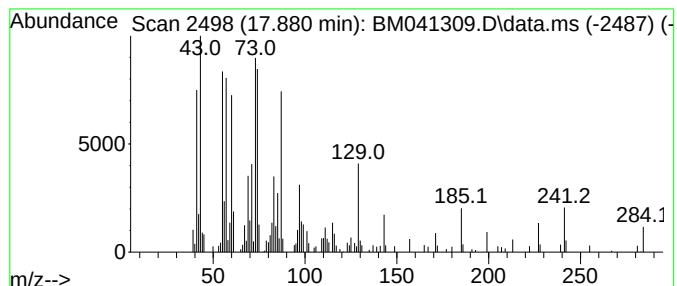
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.880	3.19 ng	293017	Phenanthrene-d10	17.215

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	94
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	66
4			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	50
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	50



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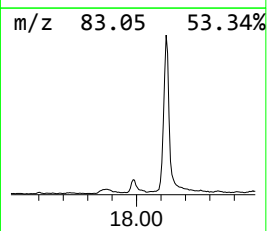
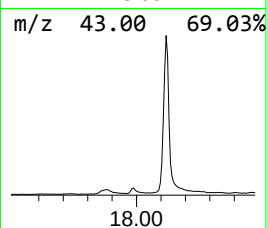
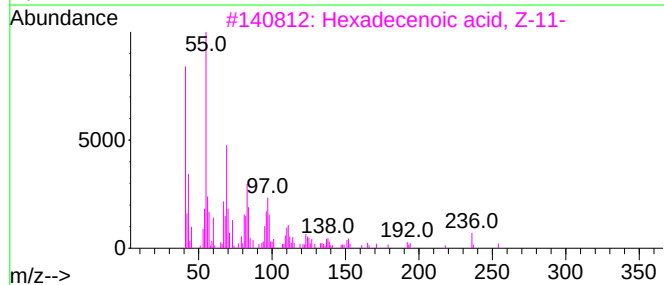
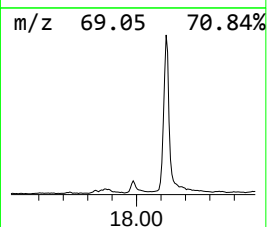
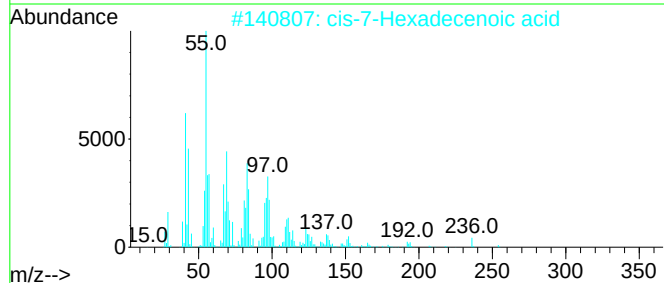
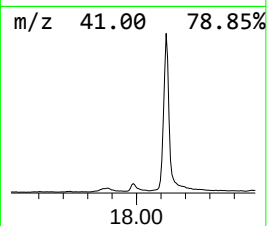
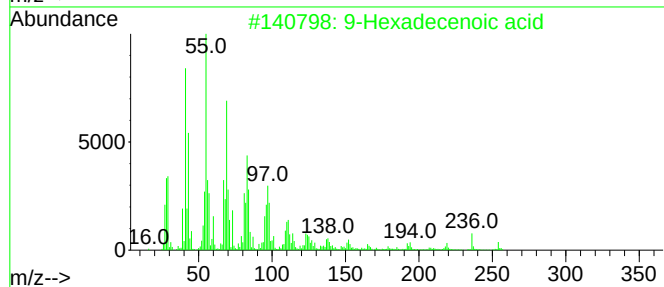
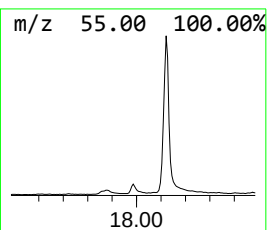
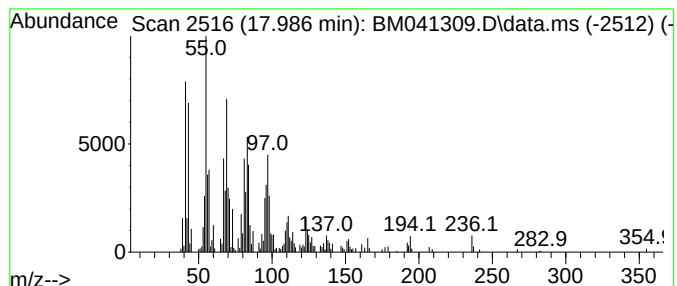
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Hexadecenoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.986	3.09 ng	283840	Phenanthrene-d10	17.215

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Hexadecenoic acid	254	C16H30O2	002091-29-4	87
2			cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	87
3			Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	83
4			Palmitoleic acid	254	C16H30O2	000373-49-9	81
5			9-Eicosenoic acid, (Z)-	310	C20H38O2	029204-02-2	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
Data File : BM041309.D
Acq On : 07 Aug 2023 13:06
Operator : MA/JU
Sample : 03903-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-02

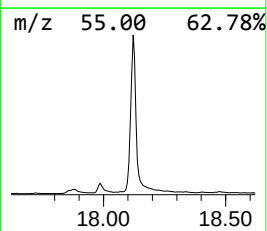
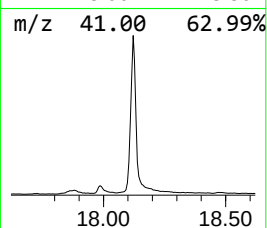
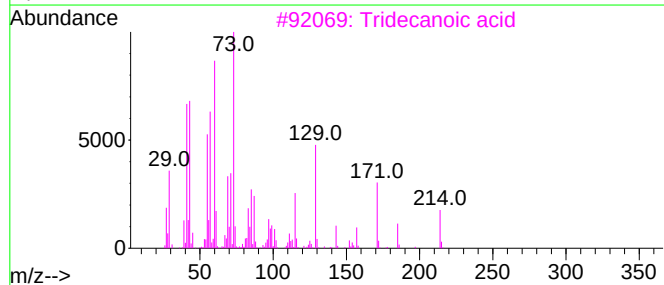
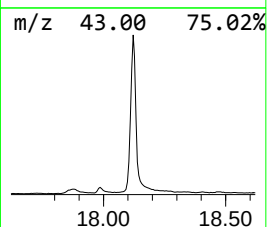
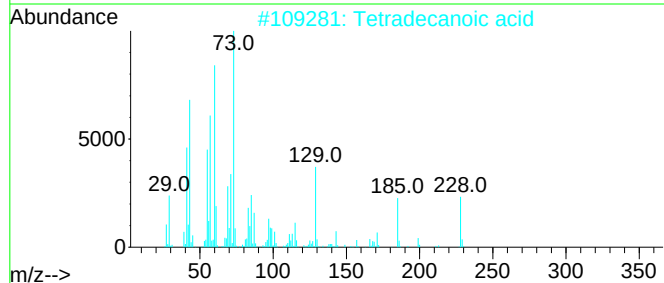
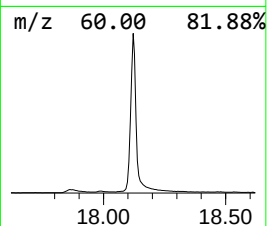
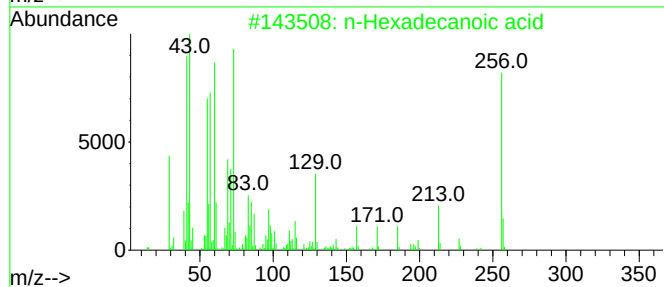
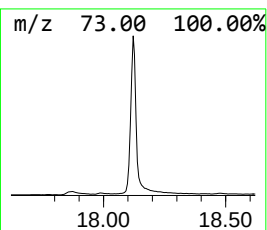
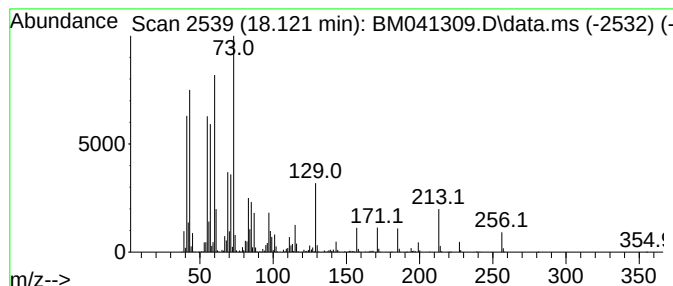
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tridecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.121	52.34 ng	4808760	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	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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
Data File : BM041309.D
Acq On : 07 Aug 2023 13:06
Operator : MA/JU
Sample : 03903-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

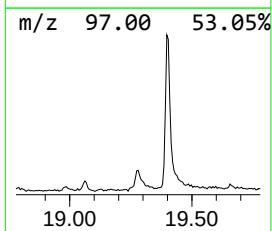
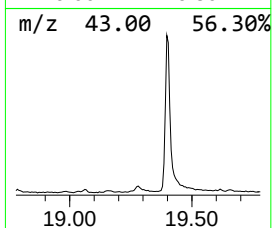
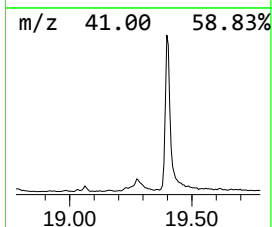
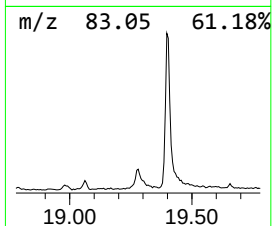
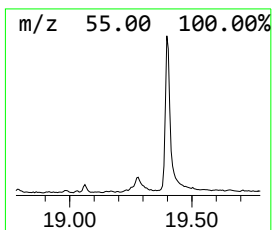
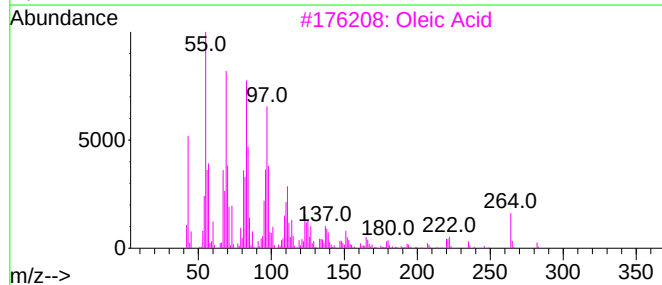
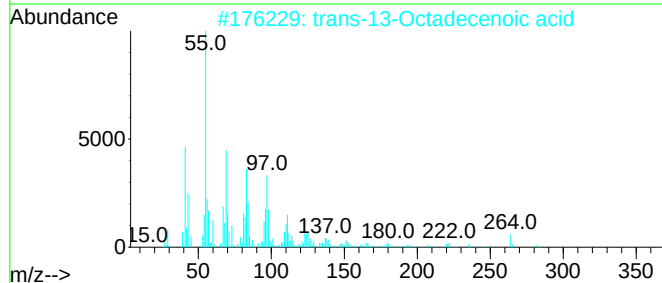
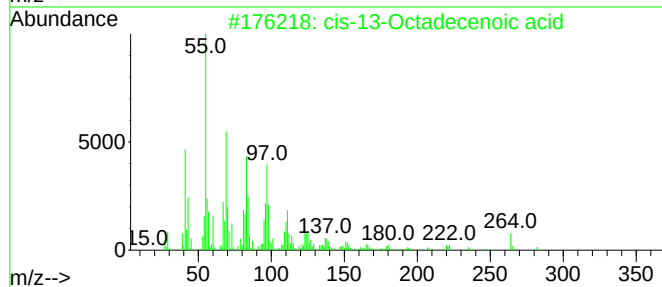
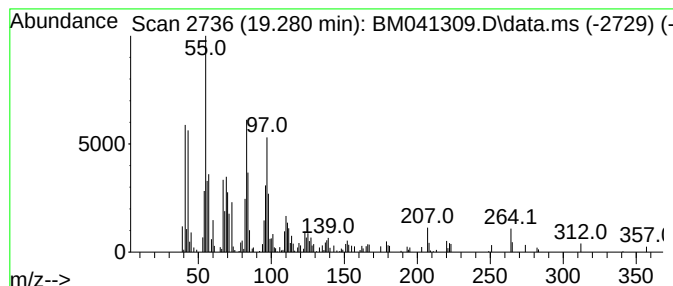
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 cis-13-Octadecenoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.280	2.48 ng	228261	Phenanthrene-d10	17.215	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	95
2	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	93
3	Oleic Acid	282	C18H34O2	000112-80-1	93
4	cis-Vaccenic acid	282	C18H34O2	000506-17-2	91
5	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
Data File : BM041309.D
Acq On : 07 Aug 2023 13:06
Operator : MA/JU
Sample : 03903-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

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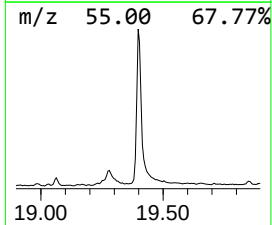
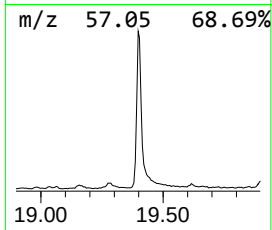
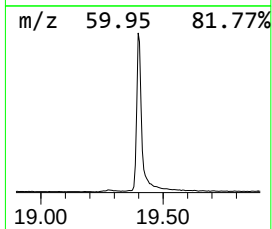
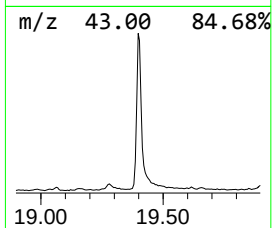
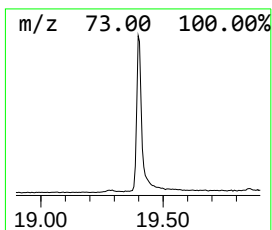
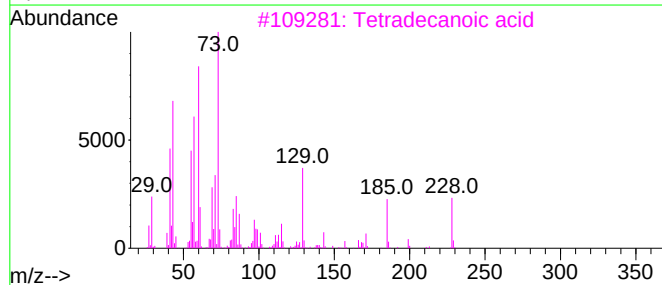
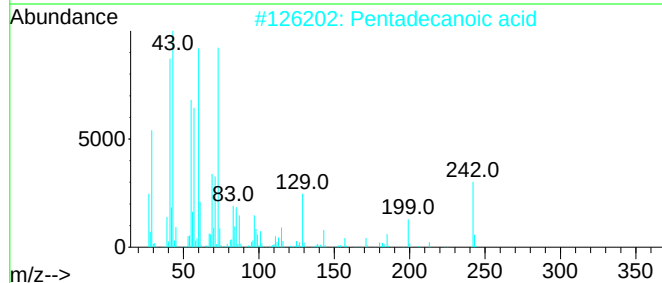
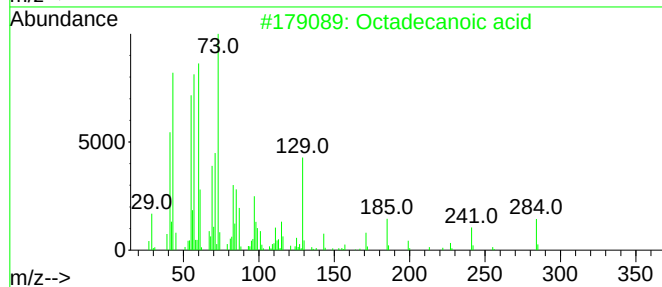
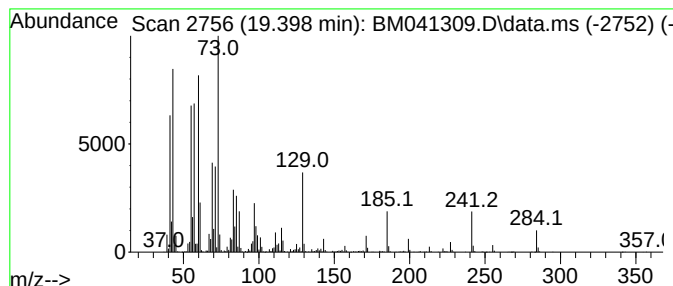
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.398	23.52 ng	2150370	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	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
Data File : BM041309.D
Acq On : 07 Aug 2023 13:06
Operator : MA/JU
Sample : 03903-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-02

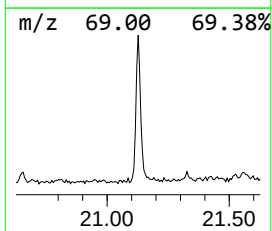
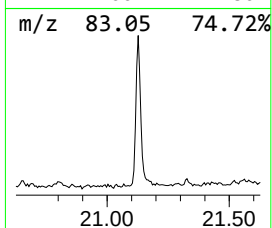
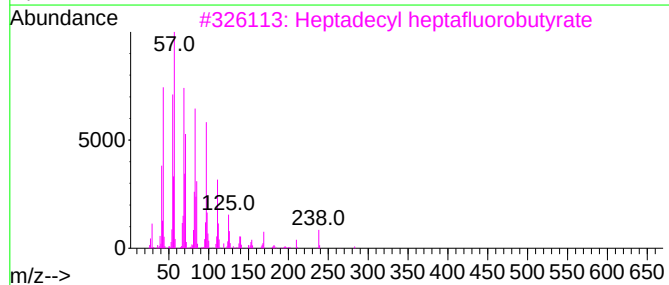
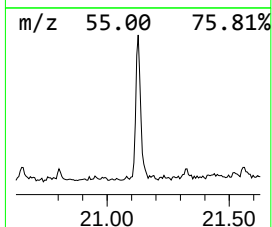
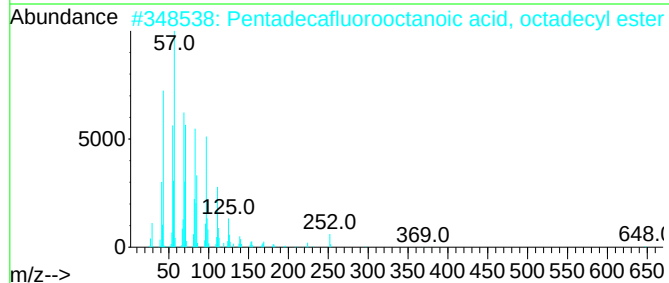
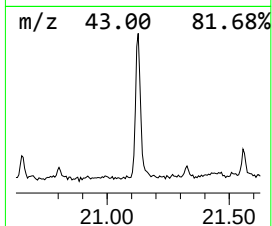
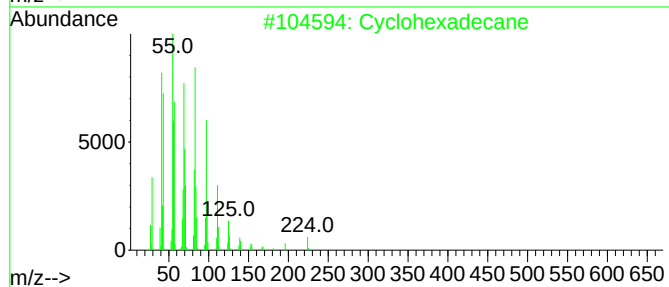
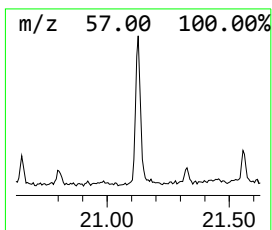
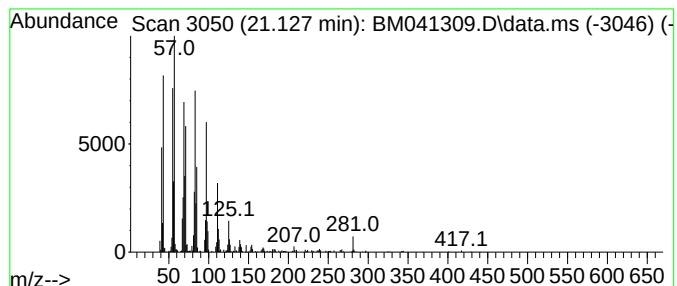
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclohexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	4.09 ng	373602	Chrysene-d12	21.421

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexadecane	224	C16H32	000295-65-8	94
2		Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
4		Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	91
5		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
Data File : BM041309.D
Acq On : 07 Aug 2023 13:06
Operator : MA/JU
Sample : 03903-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

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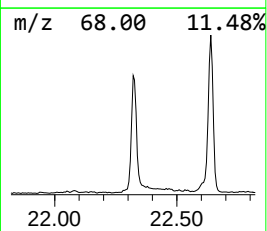
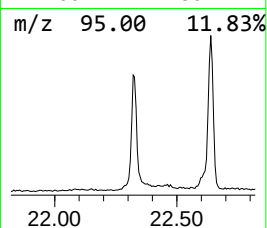
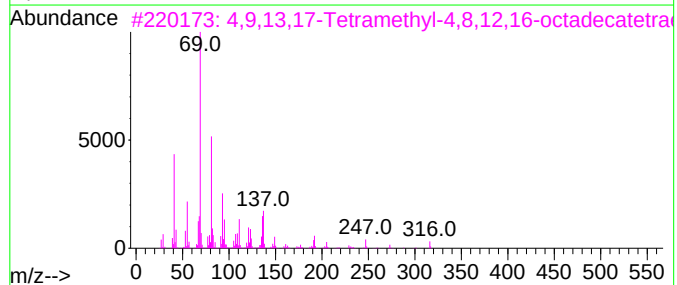
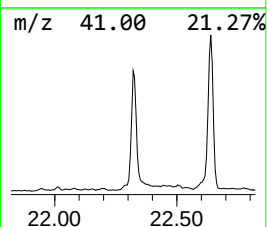
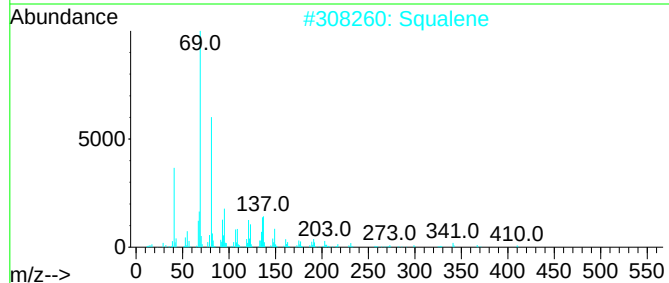
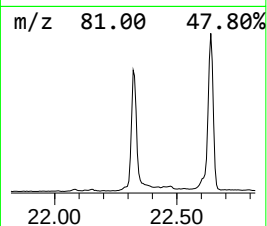
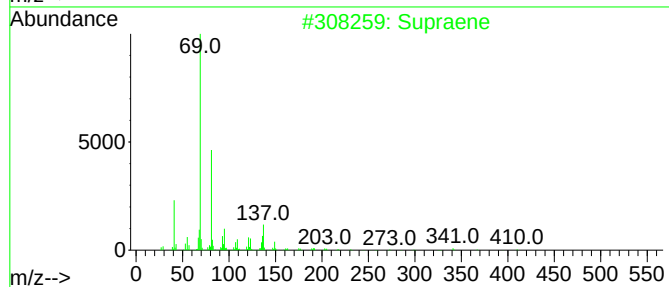
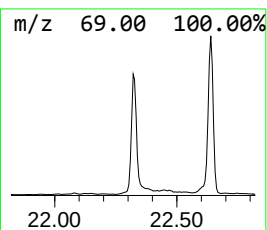
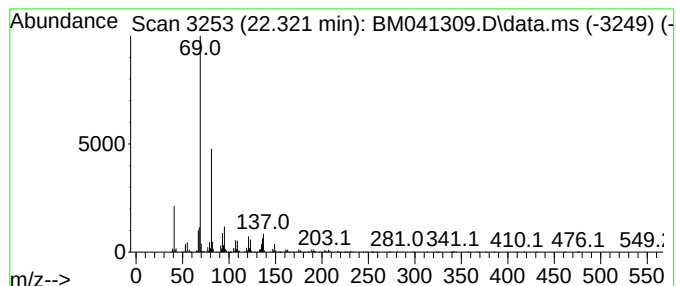
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.321	16.56 ng	1514180	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	83
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4			Farnesol isomer a	222	C15H26O	1000108-92-4	72
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
Data File : BM041309.D
Acq On : 07 Aug 2023 13:06
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Sample : 03903-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

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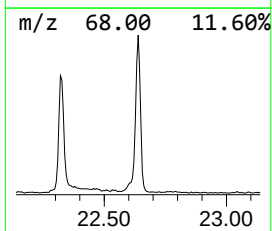
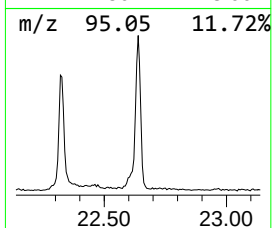
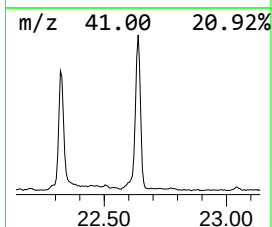
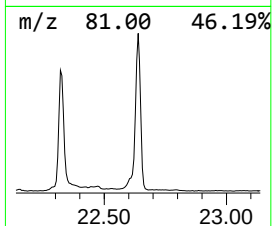
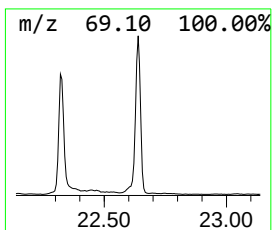
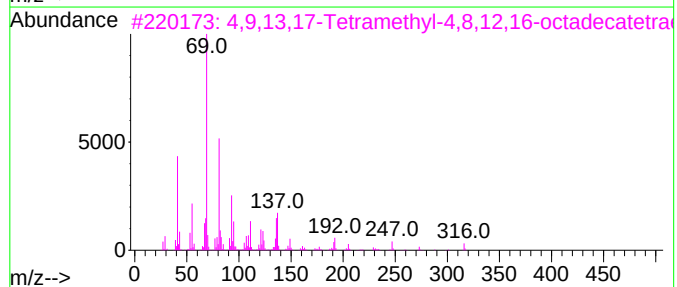
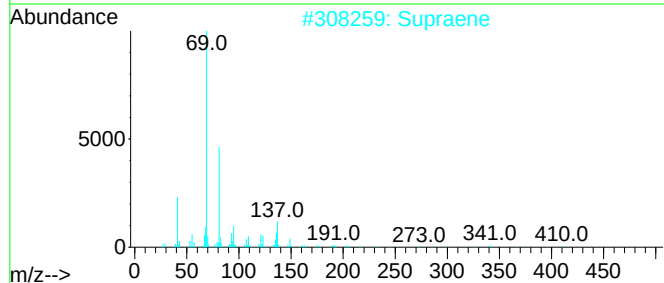
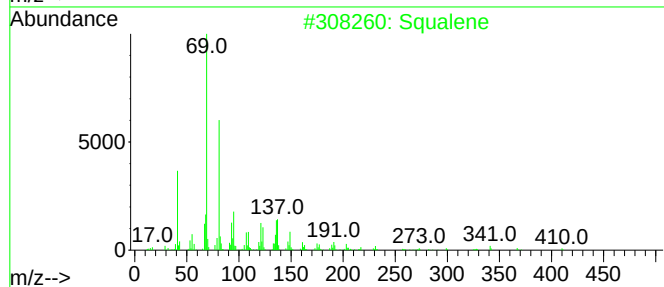
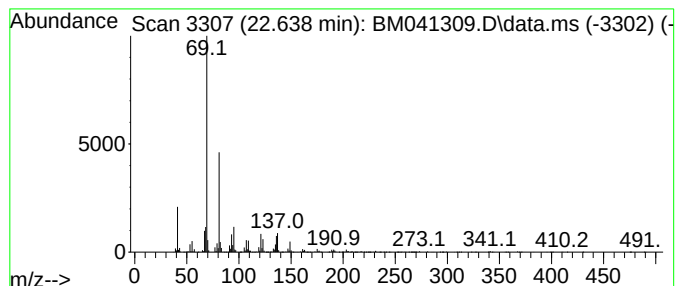
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.639	25.00 ng	1994070	Perylene-d12	23.791

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	95
2			Supraene	410	C30H50	007683-64-9	91
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4			2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	64
5			4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
Data File : BM041309.D
Acq On : 07 Aug 2023 13:06
Operator : MA/JU
Sample : 03903-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-02

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
2,4,7,9-Tetrame...	13.339	3.8	ng	284279	3	14.457	1487850	20.0
Dodecanoic acid	14.880	2.3	ng	172784	3	14.457	1487850	20.0
n-Hexadecanoic ...	15.292	9.4	ng	701670	3	14.457	1487850	20.0
Tetradecanoic acid	16.615	2.8	ng	256524	4	17.215	1837440	20.0
Octadecanoic acid	17.880	3.2	ng	293017	4	17.215	1837440	20.0
9-Hexadecenoic ...	17.986	3.1	ng	283840	4	17.215	1837440	20.0
Tridecanoic acid	18.121	52.3	ng	4808760	4	17.215	1837440	20.0
cis-13-Octadece...	19.280	2.5	ng	228261	4	17.215	1837440	20.0
Pentadecanoic acid	19.398	23.5	ng	2150370	5	21.421	1828530	20.0
Cyclohexadecane	21.127	4.1	ng	373602	5	21.421	1828530	20.0
Supraene	22.321	16.6	ng	1514180	5	21.421	1828530	20.0
Squalene	22.639	25.0	ng	1994070	6	23.791	1595050	20.0