

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
 Data File : BM042415.D
 Acq On : 24 Oct 2023 12:25
 Operator : MA/JU
 Sample : 04920-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 LSS-B1-COMP-101623

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: BM042415.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	316	321	327	rVB	213389	285435	1.25%	0.344%
2	5.522	389	397	407	rBV	2433567	3493519	15.30%	4.211%
3	7.151	666	674	683	rBV	2314741	3634507	15.92%	4.381%
4	7.993	810	817	829	rBV	500496	783627	3.43%	0.945%
5	9.192	1012	1021	1029	rBV	1450948	2298730	10.07%	2.771%
6	10.816	1289	1297	1303	rBV	642677	1054522	4.62%	1.271%
7	13.263	1706	1713	1722	rBV	3068760	4327066	18.96%	5.216%
8	14.639	1941	1947	1953	rVB	867998	1248240	5.47%	1.505%
9	15.022	2005	2012	2020	rBV	697777	1130177	4.95%	1.362%
10	16.133	2195	2201	2208	rVB	2433365	3525473	15.44%	4.250%
11	17.392	2409	2415	2426	rBV	1049880	1495735	6.55%	1.803%
12	18.262	2547	2563	2591	rVB	10005226	22826183	100.00%	27.514%
13	19.380	2748	2753	2755	rBV	1103545	1695250	7.43%	2.043%
14	19.404	2755	2757	2766	rVV2	1375419	2896395	12.69%	3.491%
15	19.527	2768	2778	2798	rVB	9912687	19571566	85.74%	23.591%
16	20.004	2854	2859	2867	rVB	4731248	5684958	24.91%	6.853%
17	20.486	2937	2941	2950	rVB	248151	452765	1.98%	0.546%
18	20.780	2988	2991	2997	rVB2	195755	281583	1.23%	0.339%
19	21.227	3062	3067	3078	rVB	749392	1226154	5.37%	1.478%
20	21.568	3121	3125	3131	rVB	1194860	1563453	6.85%	1.885%
21	21.892	3177	3180	3186	rBV	298961	432487	1.89%	0.521%
22	22.621	3299	3304	3313	rVB	371682	709467	3.11%	0.855%
23	23.427	3437	3441	3452	rVB	283488	579277	2.54%	0.698%
24	24.039	3539	3545	3561	rVB	819365	1764453	7.73%	2.127%

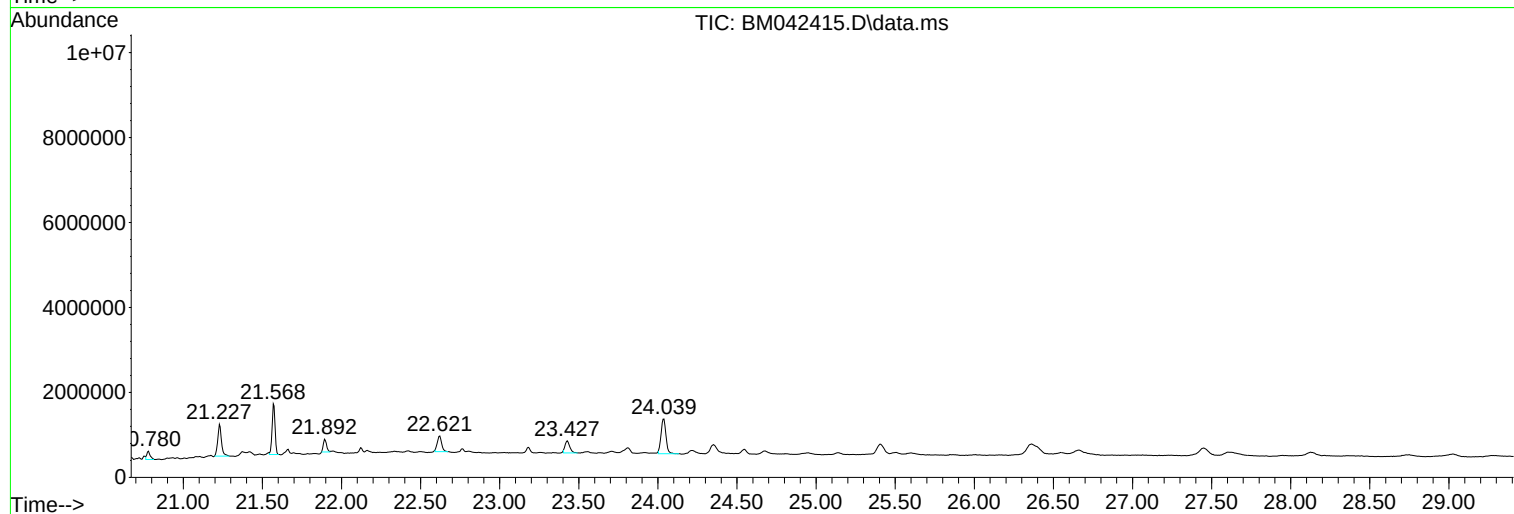
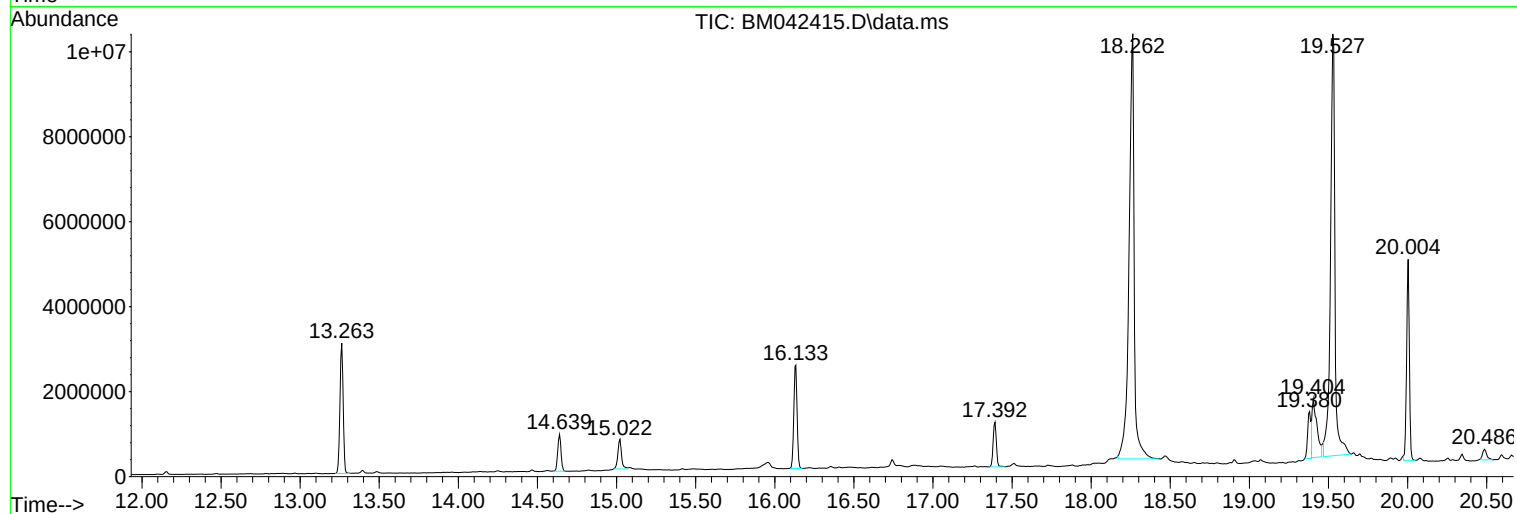
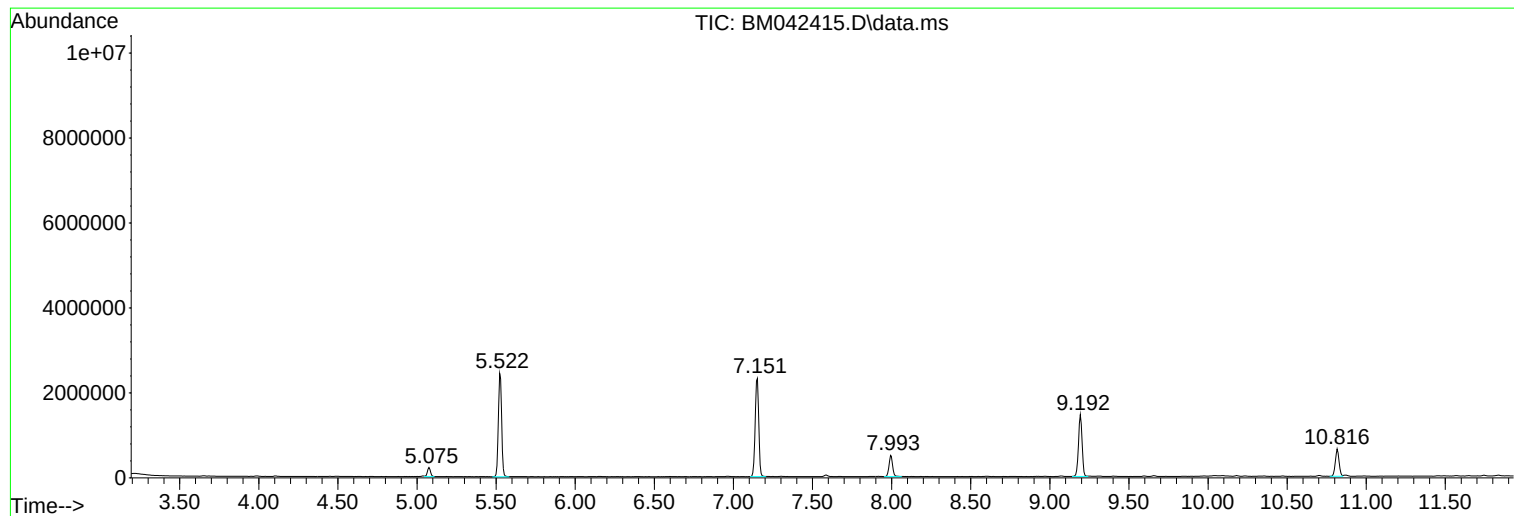
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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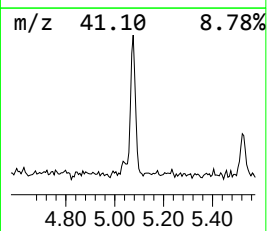
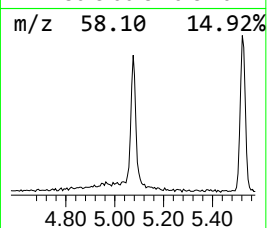
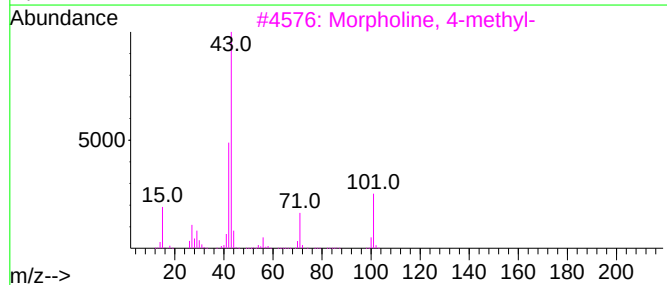
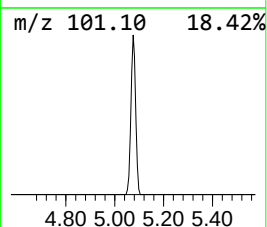
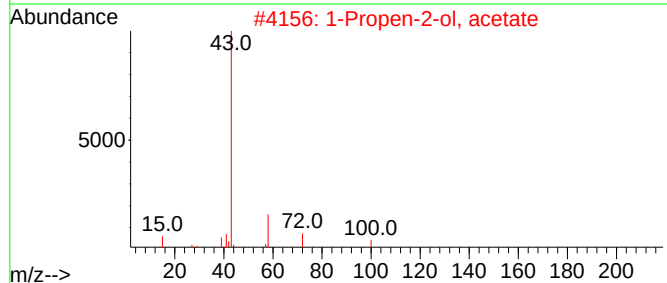
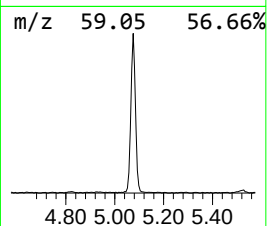
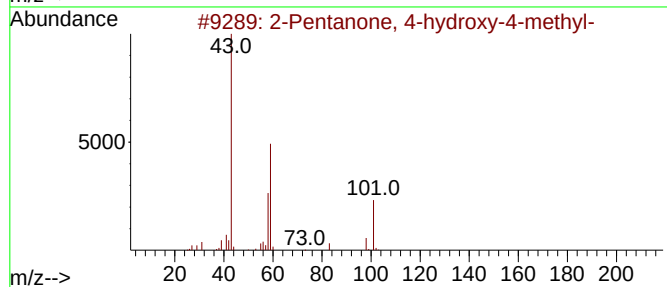
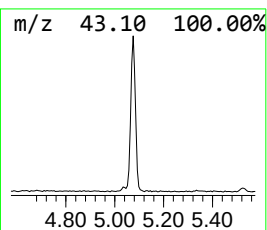
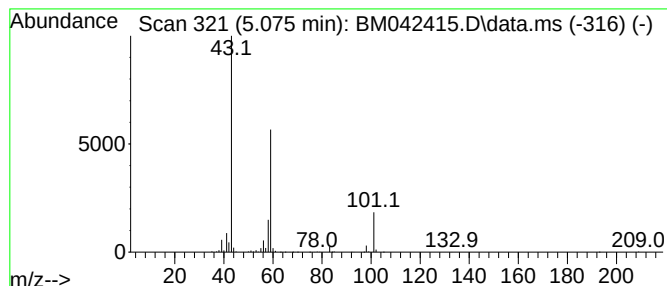
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	7.28 ng	285435	1,4-Dichlorobenzene-d4	7.993

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12	
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9	



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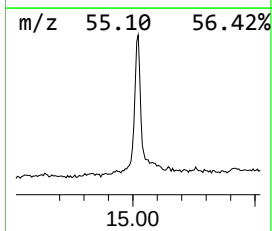
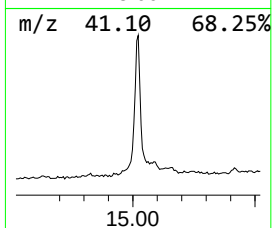
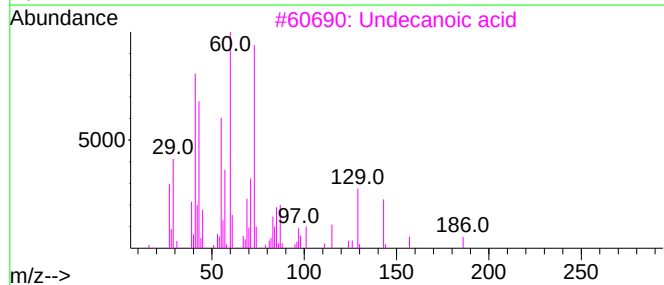
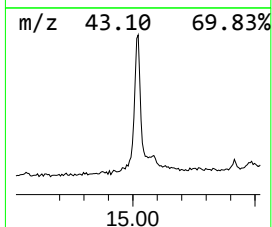
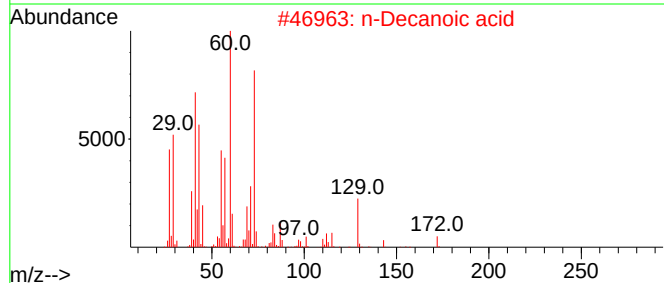
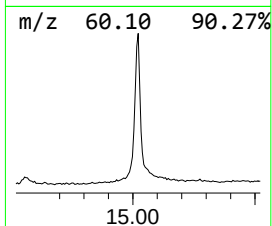
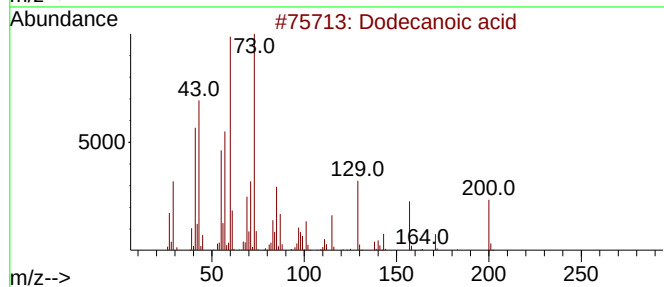
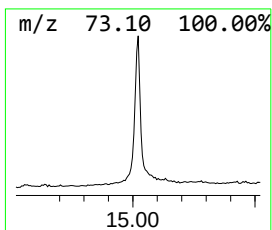
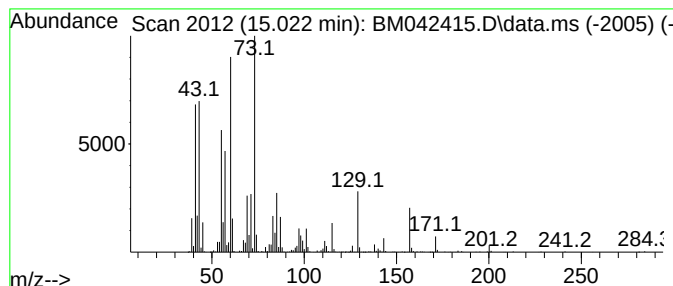
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Peak Number 2 Dodecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.022	18.11 ng	1130180	Acenaphthene-d10	14.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	93
2			n-Decanoic acid	172	C10H20O2	000334-48-5	81
3			Undecanoic acid	186	C11H22O2	000112-37-8	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	72
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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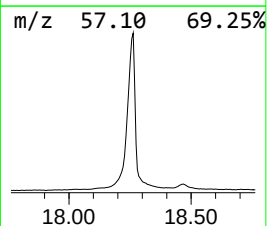
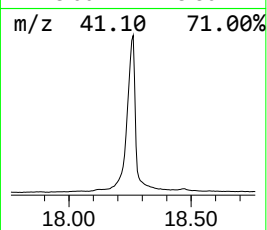
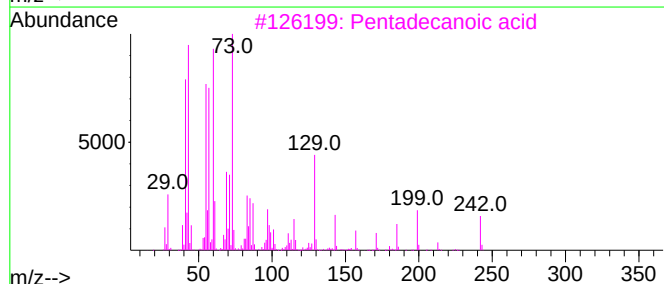
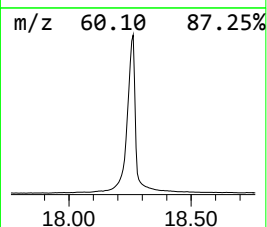
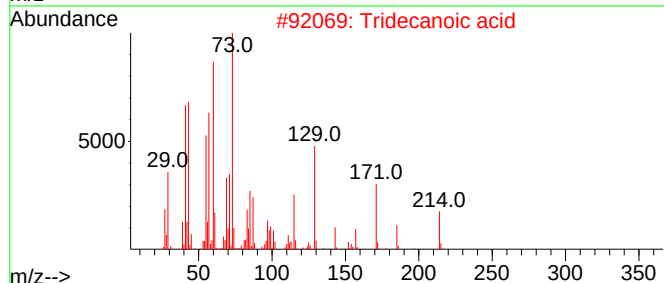
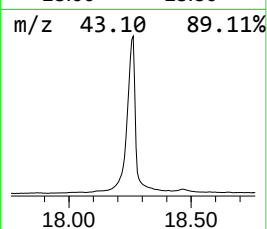
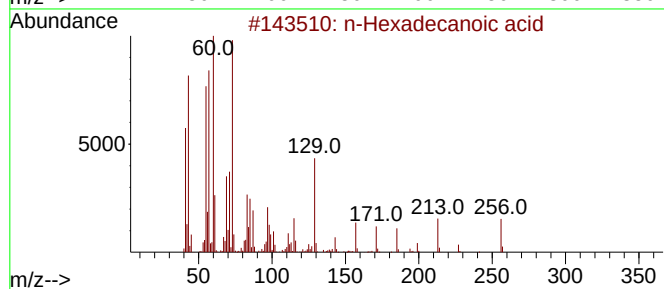
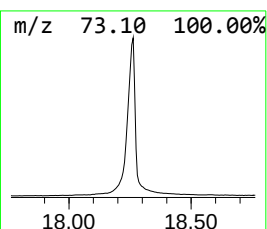
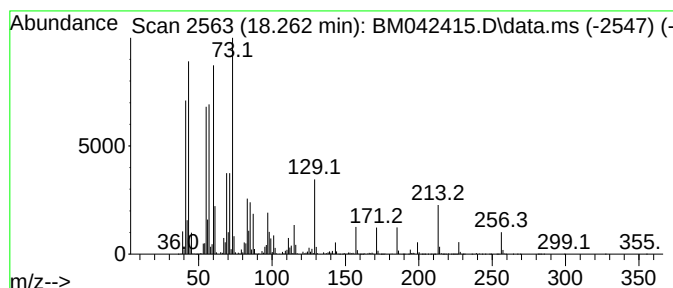
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.262	305.22 ng	22826200	Phenanthrene-d10	17.392	
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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	52



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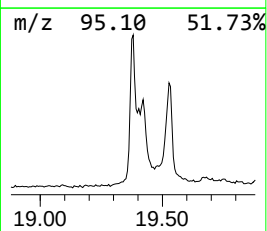
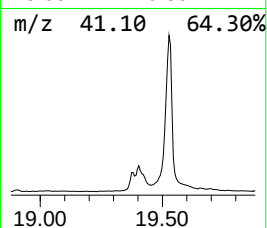
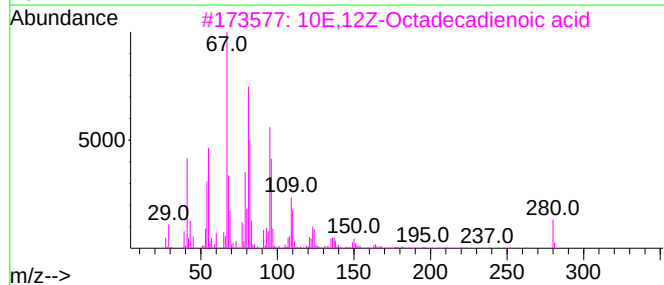
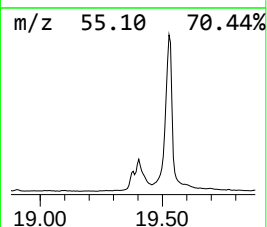
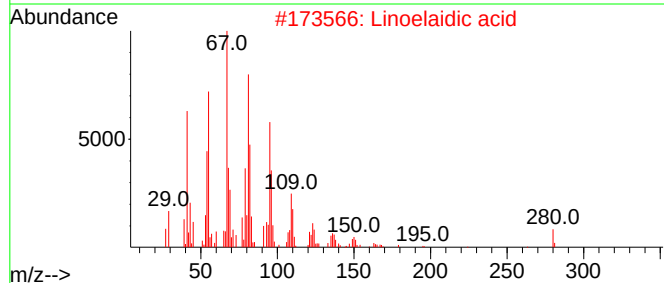
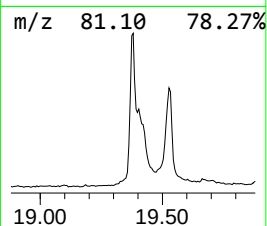
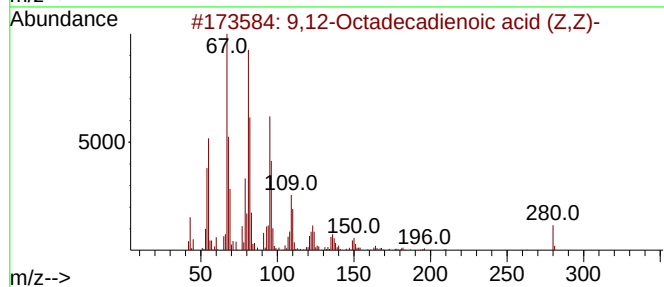
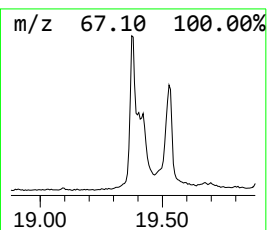
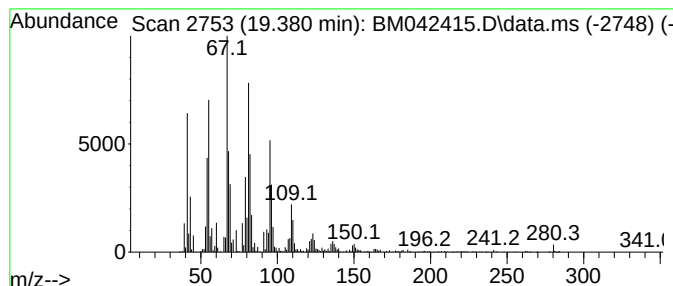
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Peak Number 4 9,12-Octadecadienoic acid (... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.380	22.67 ng	1695250	Phenanthrene-d10	17.392	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
2	Linoelaidic acid	280	C18H32O2	000506-21-8	99
3	10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	98
4	(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	97
5	5-Eicosyne	278	C20H38	074685-31-7	93



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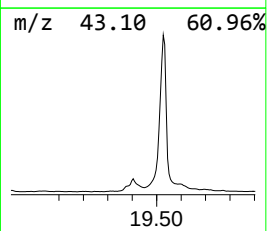
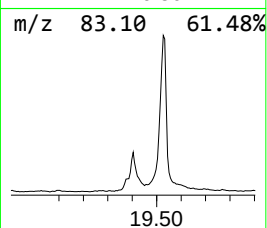
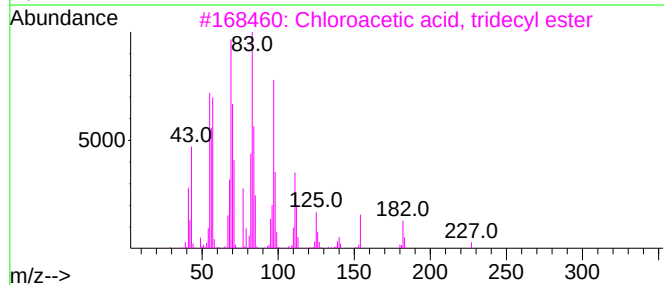
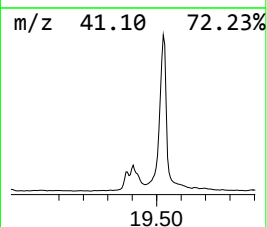
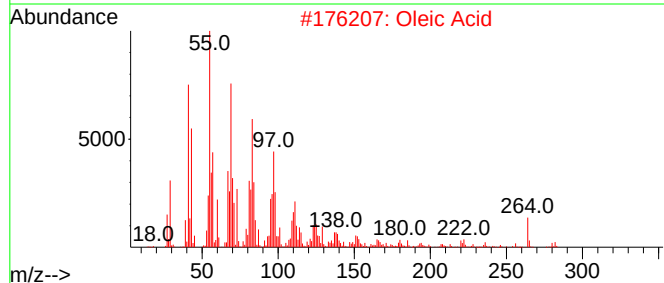
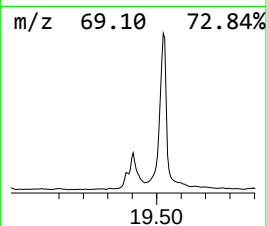
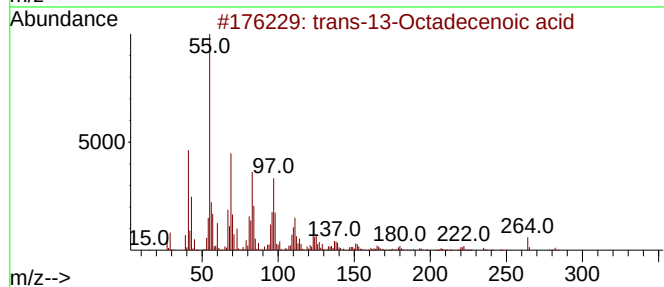
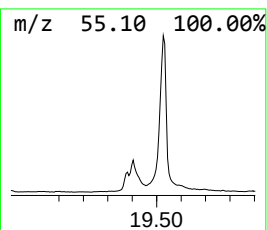
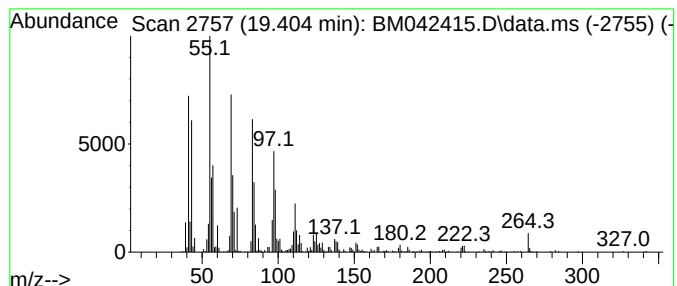
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 trans-13-Octadecenoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.404	38.73 ng	2896400	Phenanthrene-d10	17.392	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	89
2	Oleic Acid	282	C18H34O2	000112-80-1	78
3	Chloroacetic acid, tridecyl ester	276	C15H29ClO2	018277-85-5	64
4	Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	62
5	1-Hexadecanol	242	C16H34O	036653-82-4	62



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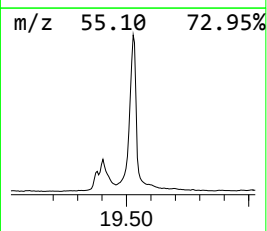
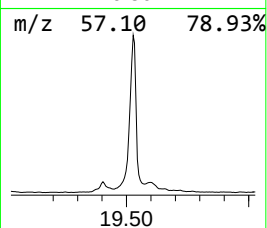
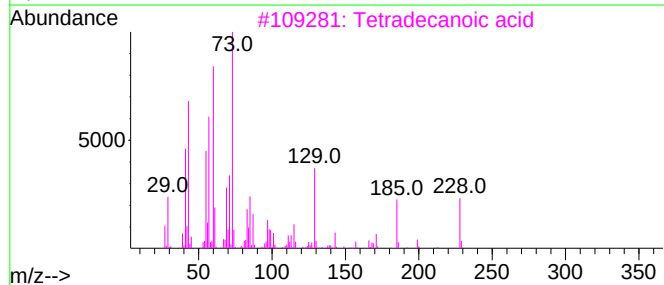
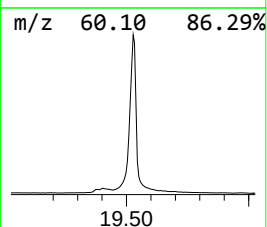
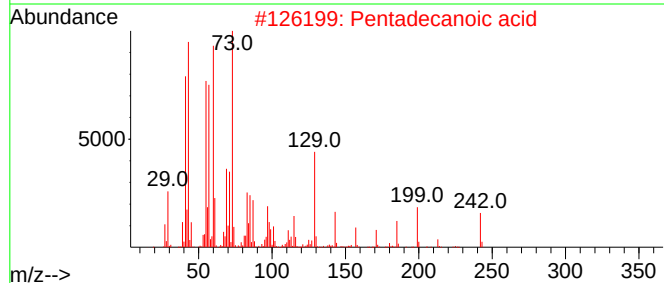
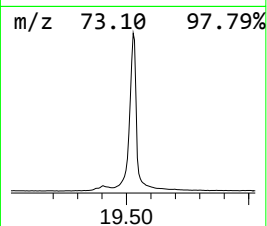
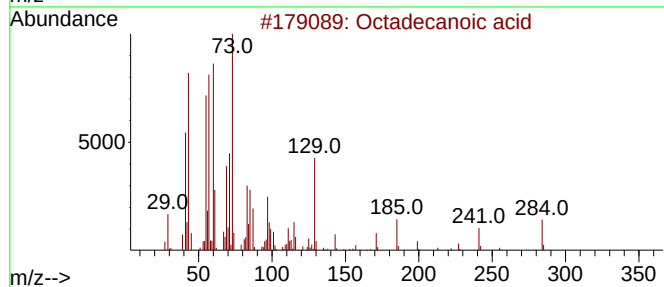
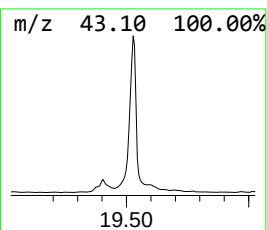
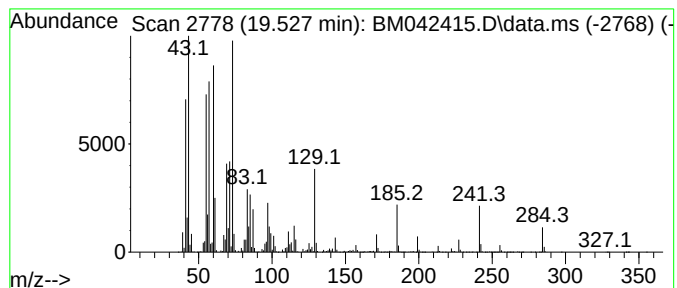
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.527	250.36 ng	19571600	Chrysene-d12	21.568

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			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
Data File : BM042415.D
Acq On : 24 Oct 2023 12:25
Operator : MA/JU
Sample : 04920-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
LSS-B1-COMP-101623

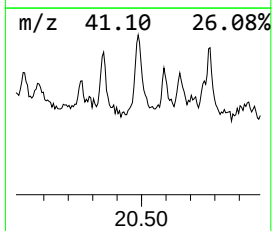
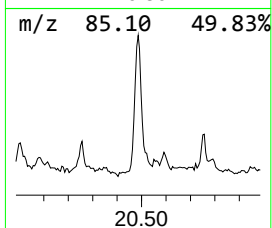
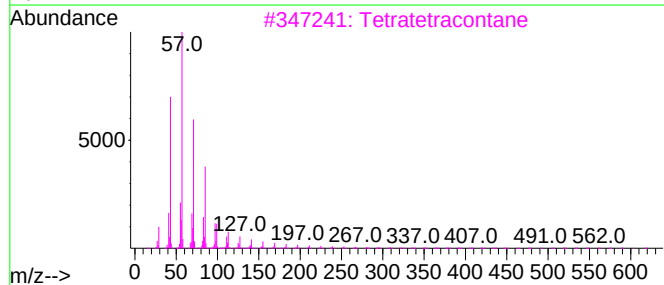
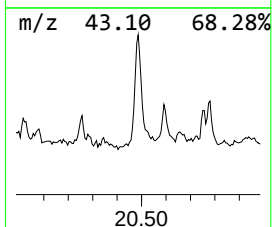
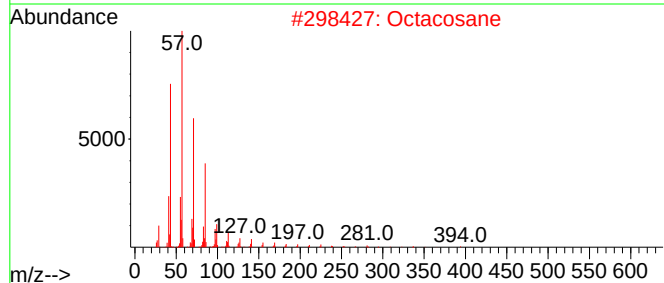
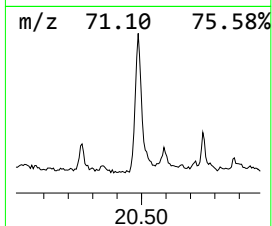
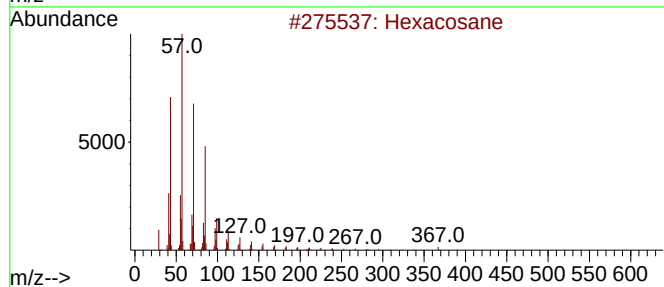
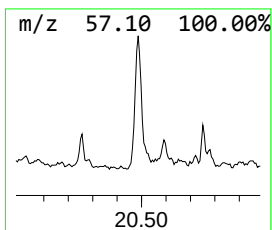
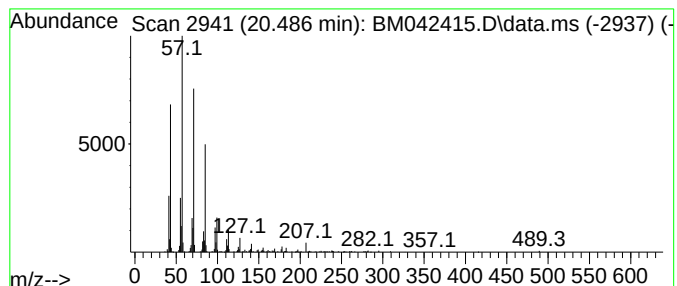
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.486	5.79 ng	452765	Chrysene-d12	21.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Tetratetracontane	619	C44H90	007098-22-8	91
4			Tetracosane	338	C24H50	000646-31-1	91
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
Data File : BM042415.D
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Operator : MA/JU
Sample : 04920-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
LSS-B1-COMP-101623

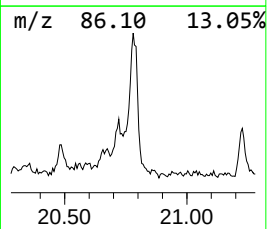
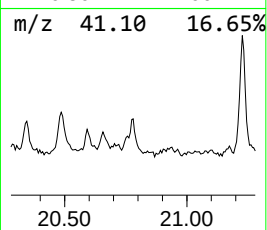
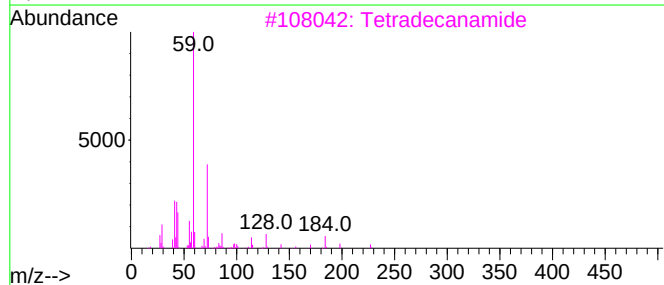
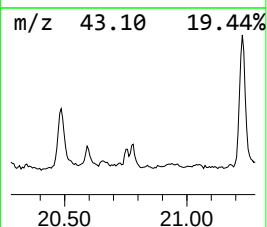
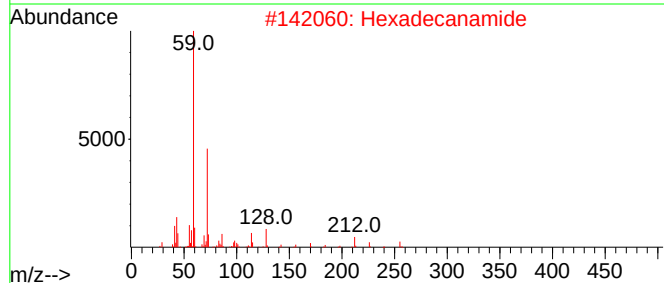
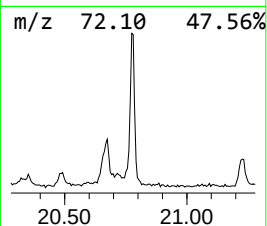
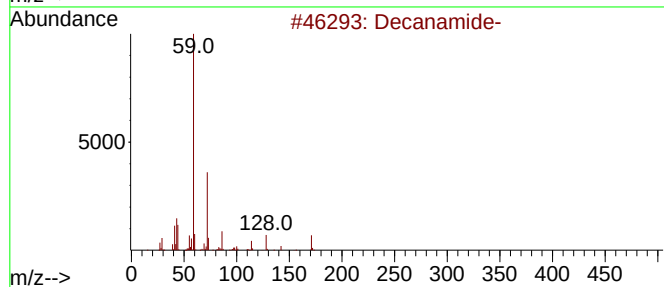
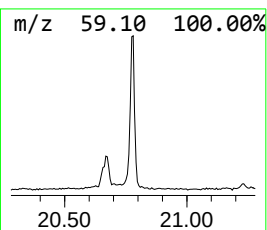
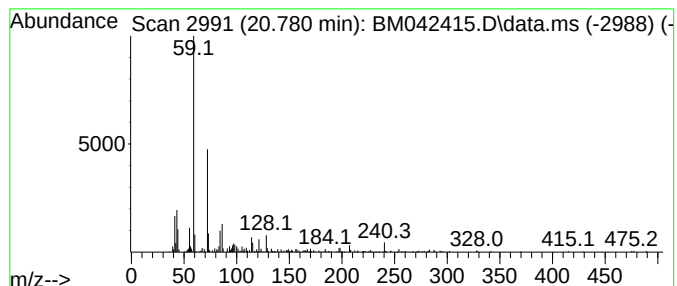
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Decanamide- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.780	3.60 ng	281583	Chrysene-d12	21.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decanamide-	171	C10H21NO	002319-29-1	83
2			Hexadecanamide	255	C16H33NO	000629-54-9	72
3			Tetradecanamide	227	C14H29NO	000638-58-4	72
4			Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	64
5			Octanamide	143	C8H17NO	000629-01-6	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
Data File : BM042415.D
Acq On : 24 Oct 2023 12:25
Operator : MA/JU
Sample : 04920-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

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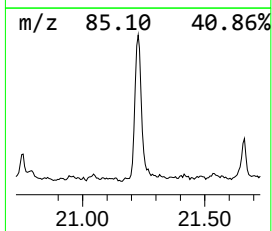
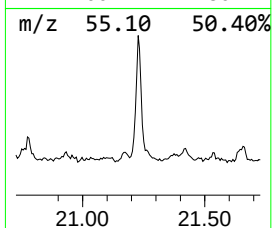
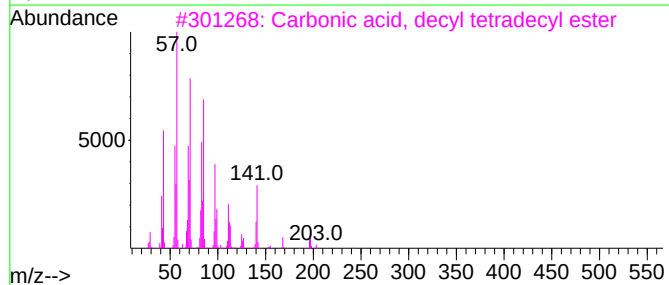
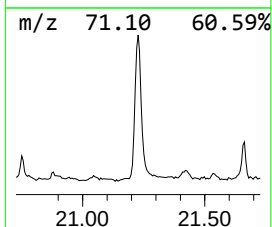
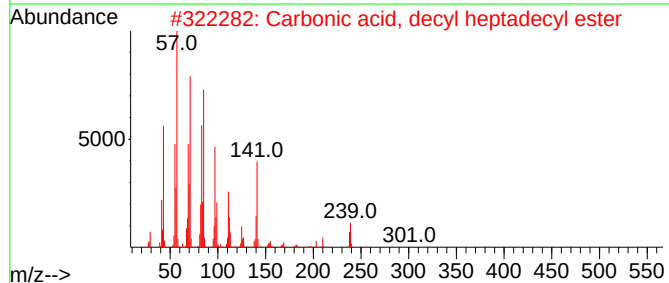
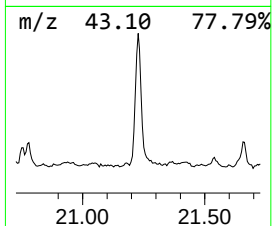
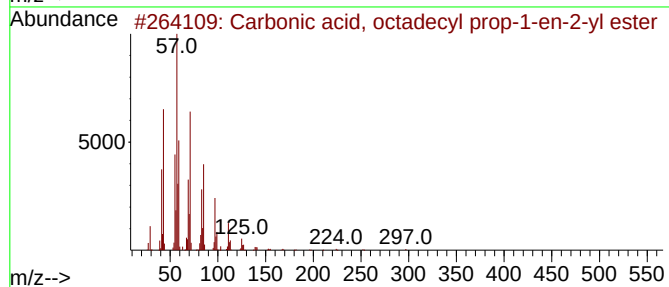
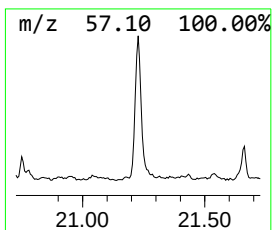
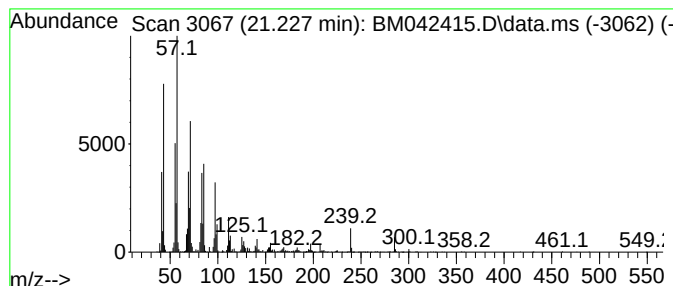
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Carbonic acid, octadecyl pr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.227	15.69 ng	1226150	Chrysene-d12	21.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
2			Carbonic acid, decyl heptadecyl ...	440	C28H56O3	1000383-16-6	91
3			Carbonic acid, decyl tetradecyl ...	398	C25H50O3	1010383-16-3	90
4			Carbonic acid, decyl octadecyl e...	454	C29H58O3	1000383-16-7	90
5			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
Data File : BM042415.D
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Operator : MA/JU
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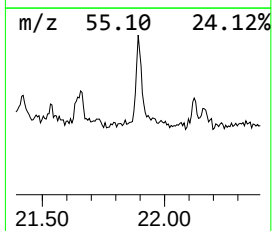
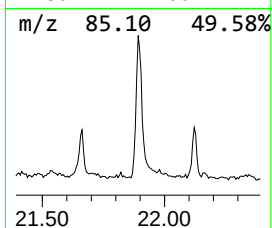
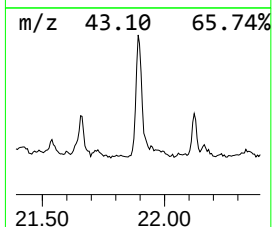
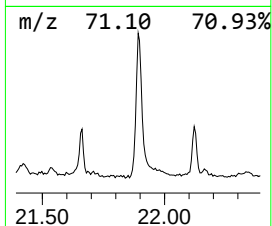
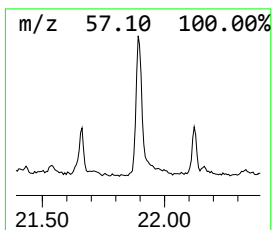
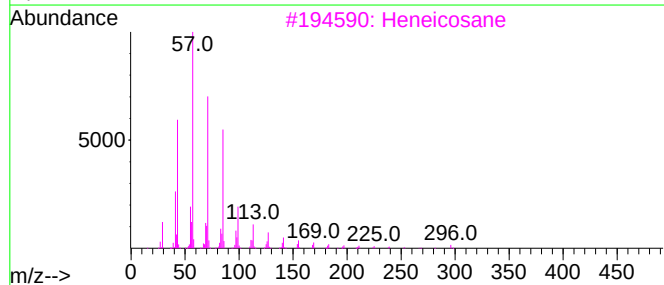
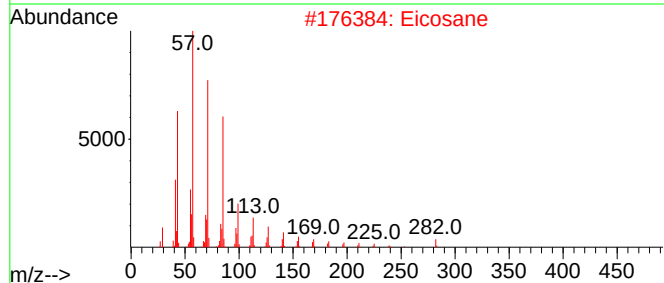
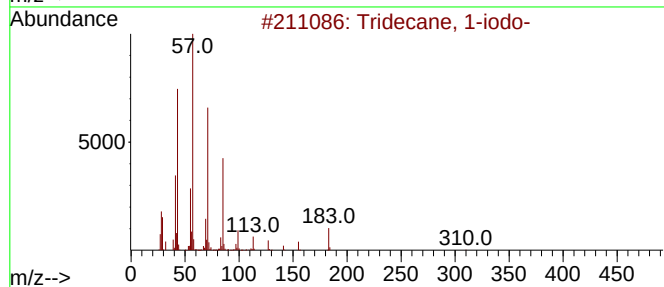
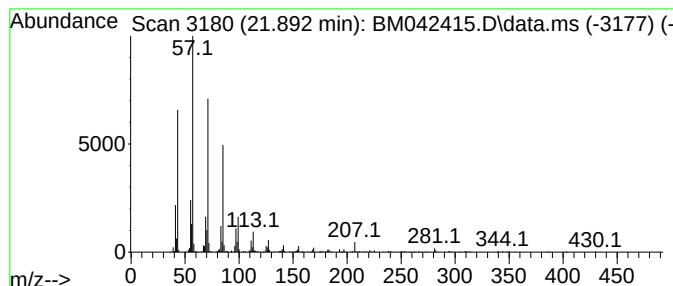
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tridecane, 1-iodo- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.892	5.53 ng	432487	Chrysene-d12	21.568	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
2	Eicosane	282	C20H42	000112-95-8	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	87
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
Data File : BM042415.D
Acq On : 24 Oct 2023 12:25
Operator : MA/JU
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ClientSampleId :
LSS-B1-COMP-101623

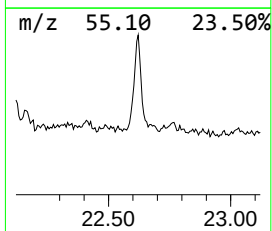
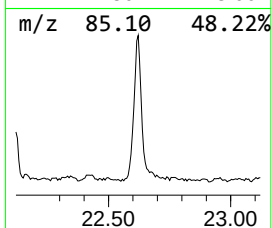
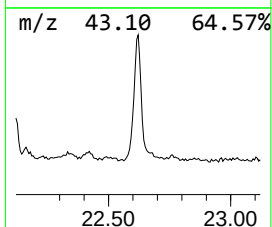
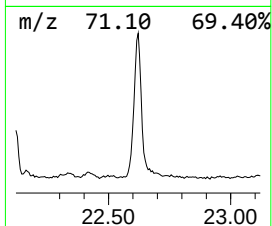
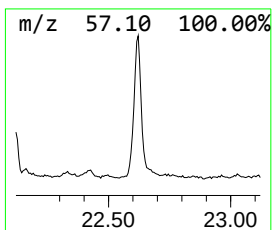
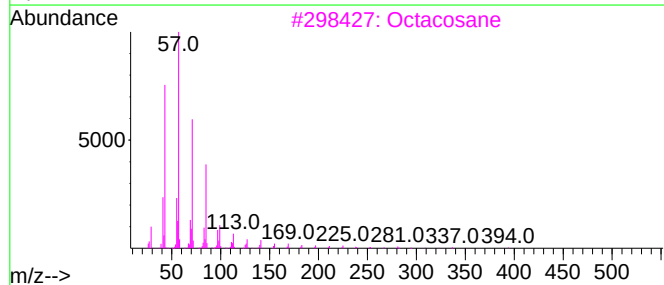
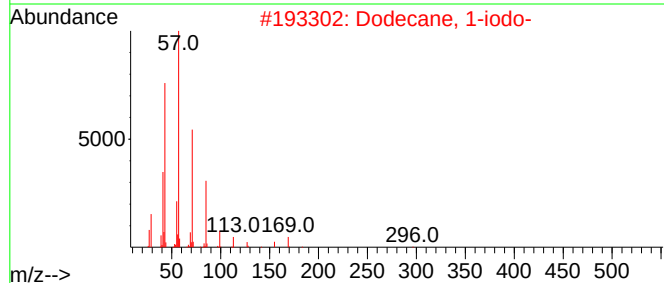
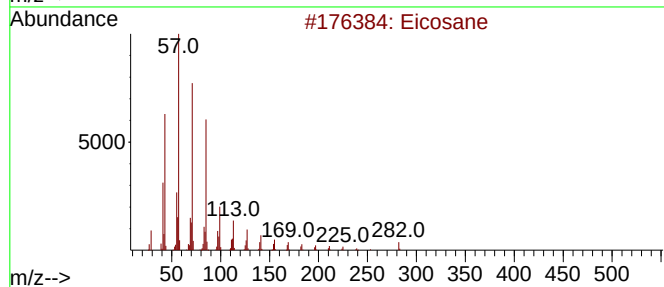
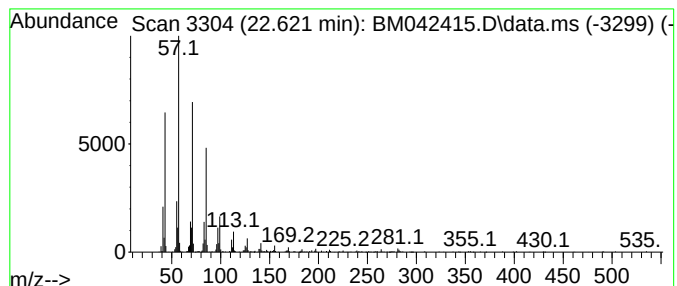
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.621	9.08 ng	709467	Chrysene-d12	21.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	91
3			Octacosane	394	C28H58	000630-02-4	90
4			Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
5			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
Data File : BM042415.D
Acq On : 24 Oct 2023 12:25
Operator : MA/JU
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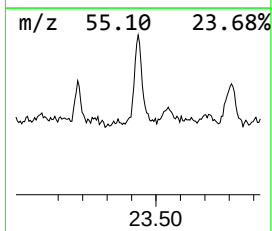
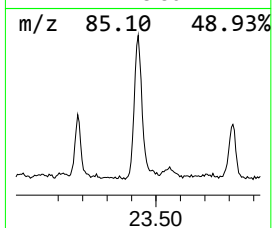
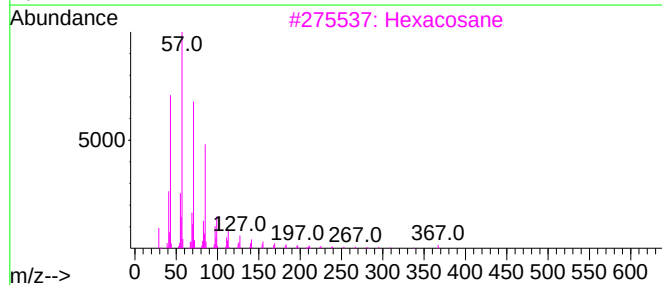
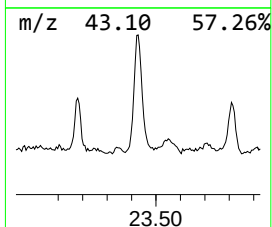
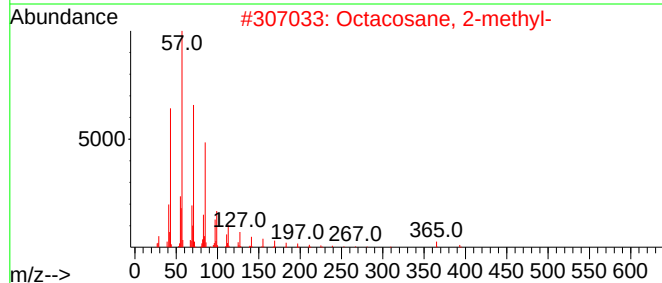
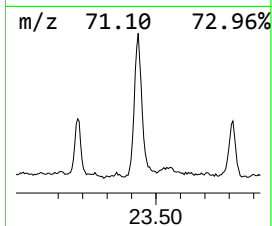
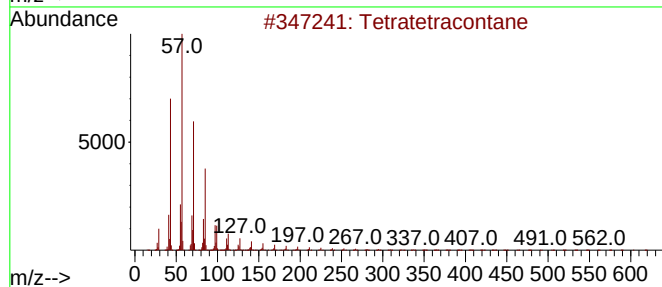
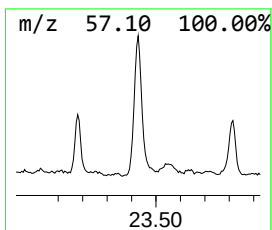
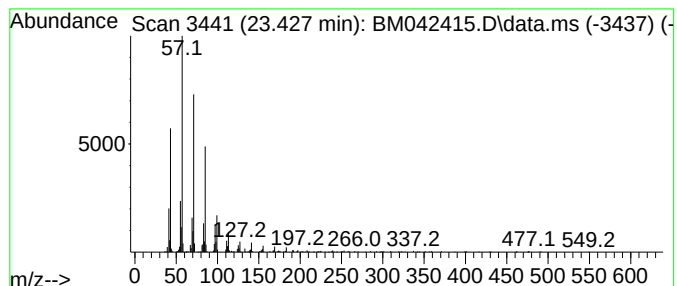
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetratetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.427	6.57 ng	579277	Perylene-d12	24.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	90
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
3			Hexacosane	366	C26H54	000630-01-3	87
4			Octacosane	394	C28H58	000630-02-4	87
5			Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
Data File : BM042415.D
Acq On : 24 Oct 2023 12:25
Operator : MA/JU
Sample : 04920-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
LSS-B1-COMP-101623

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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
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Dodecanoic acid	15.022	18.1	ng	1130180	3	14.639	1248240	20.0
n-Hexadecanoic ...	18.262	305.2	ng	22826200	4	17.392	1495740	20.0
9,12-Octadecadi...	19.380	22.7	ng	1695250	4	17.392	1495740	20.0
trans-13-Octade...	19.404	38.7	ng	2896400	4	17.392	1495740	20.0
Octadecanoic acid	19.527	250.4	ng	19571600	5	21.568	1563450	20.0
Hexacosane	20.486	5.8	ng	452765	5	21.568	1563450	20.0
Decanamide-	20.780	3.6	ng	281583	5	21.568	1563450	20.0
Carbonic acid, ...	21.227	15.7	ng	1226150	5	21.568	1563450	20.0
Tridecane, 1-iodo-	21.892	5.5	ng	432487	5	21.568	1563450	20.0
Eicosane	22.621	9.1	ng	709467	5	21.568	1563450	20.0
Tetratetracontane	23.427	6.6	ng	579277	6	24.033	1764450	20.0