

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040725\
 Data File : BM049837.D
 Acq On : 07 Apr 2025 13:24
 Operator : RC/JU
 Sample : Q1675-20
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 K2

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-BM031325.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM049837.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.369	398	405	412	rBV	4500040	6437207	8.45%	2.965%
2	6.957	667	675	689	rBV	4121157	6386945	8.39%	2.941%
3	7.786	806	816	823	rBV	1291034	2049292	2.69%	0.944%
4	8.939	1000	1012	1022	rBV	2355483	3887748	5.11%	1.790%
5	10.580	1283	1291	1297	rBV	1559935	2608692	3.43%	1.201%
6	13.045	1703	1710	1717	rBV	6839943	9735563	12.79%	4.484%
7	14.427	1935	1945	1952	rBV	2518120	3617025	4.75%	1.666%
8	15.786	2170	2176	2183	rBV	1692409	2318142	3.04%	1.068%
9	15.915	2192	2198	2206	rBV	6833208	9293413	12.21%	4.280%
10	17.168	2406	2411	2417	rVB2	2869114	3919079	5.15%	1.805%
11	17.845	2522	2526	2532	rBV	925610	1241567	1.63%	0.572%
12	18.103	2554	2570	2604	rVB	21947389	61741497	81.09%	28.434%
13	18.621	2655	2658	2666	rVB	920189	1195613	1.57%	0.551%
14	19.156	2745	2749	2753	rBV	2608293	3116797	4.09%	1.435%
15	19.209	2754	2758	2760	rBV	1370954	1897046	2.49%	0.874%
16	19.239	2760	2763	2769	rVB2	1008723	1680968	2.21%	0.774%
17	19.380	2774	2787	2840	rVB	26316055	76135500	100.00%	35.063%
18	19.797	2852	2858	2870	rVB	11488751	14870449	19.53%	6.848%
19	21.091	3074	3078	3086	rVB	646807	928462	1.22%	0.428%
20	21.403	3127	3131	3137	rBV	2917365	4080261	5.36%	1.879%

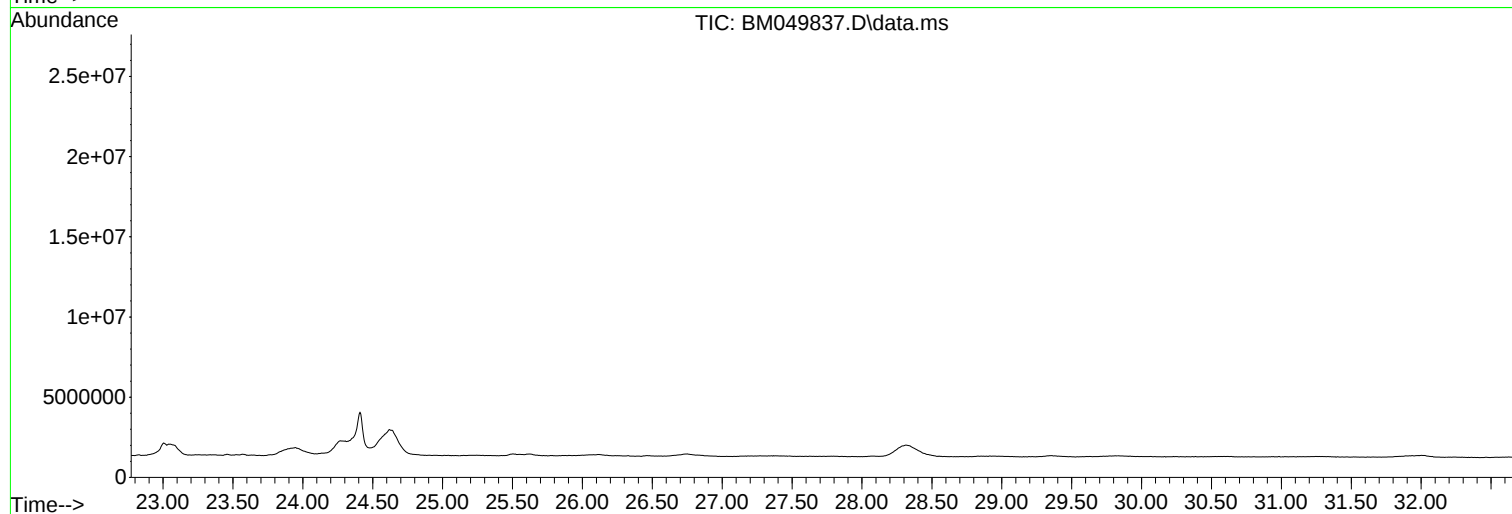
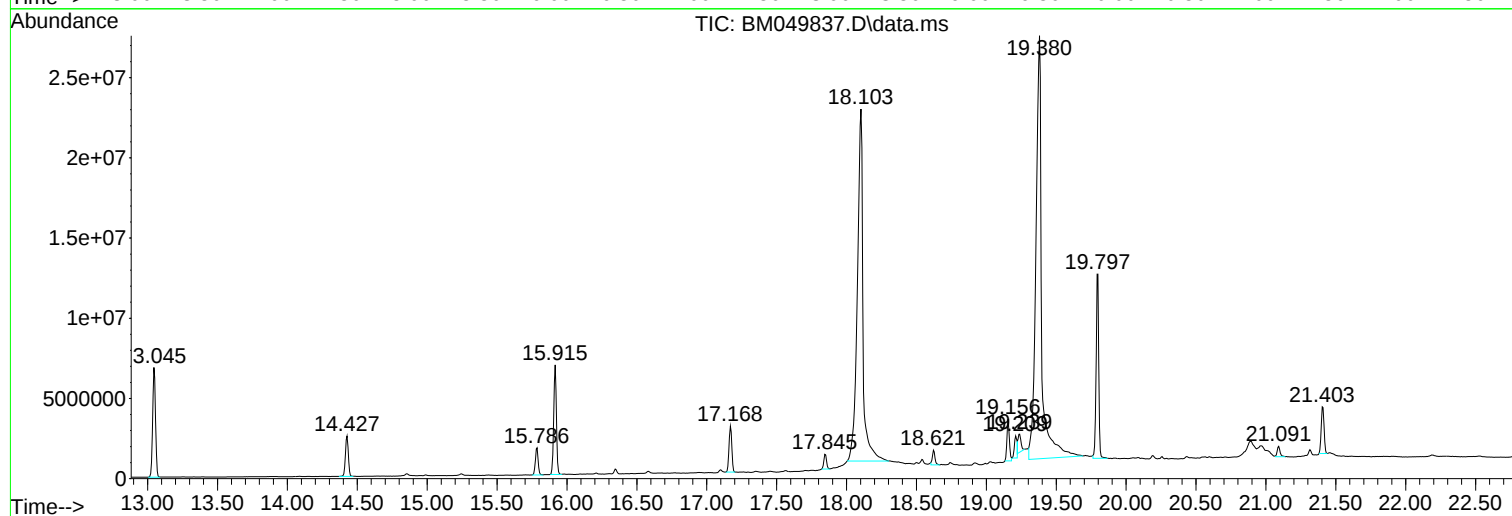
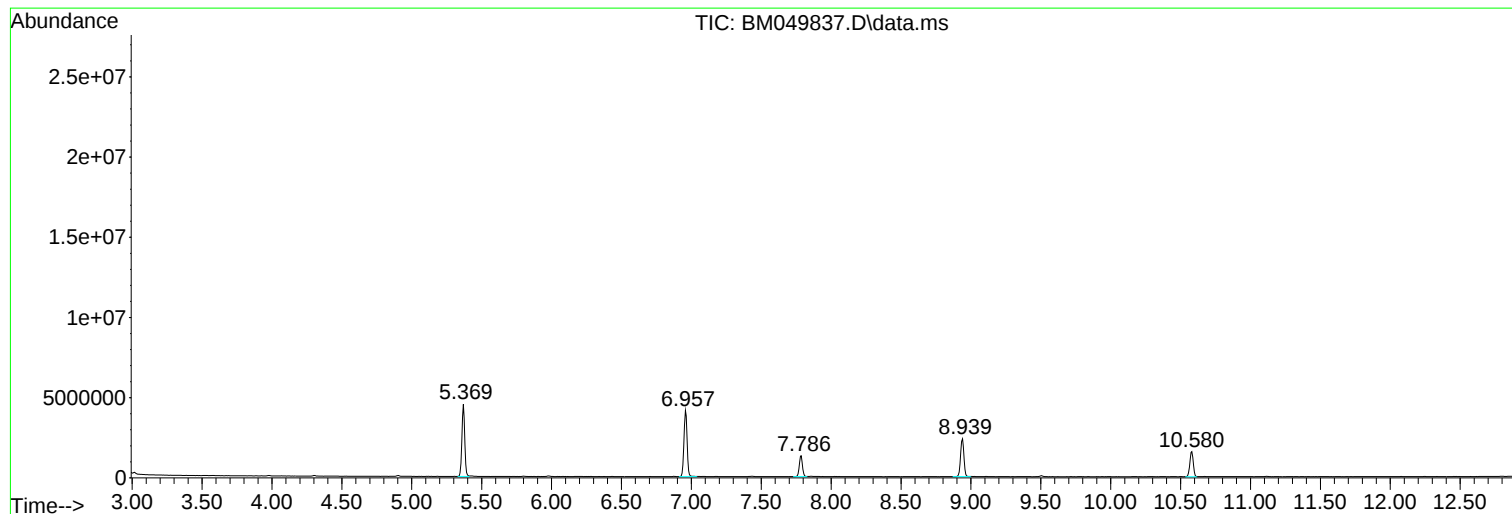
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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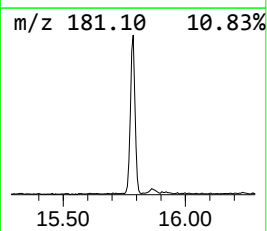
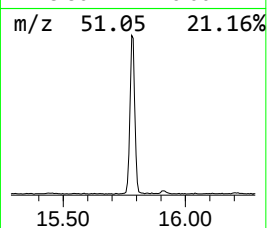
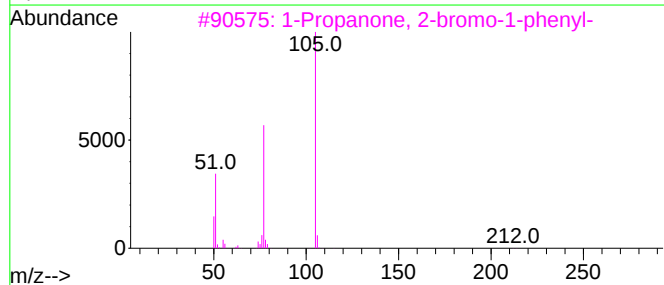
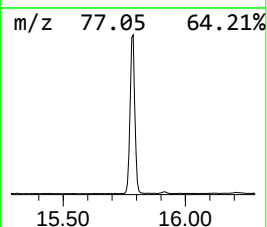
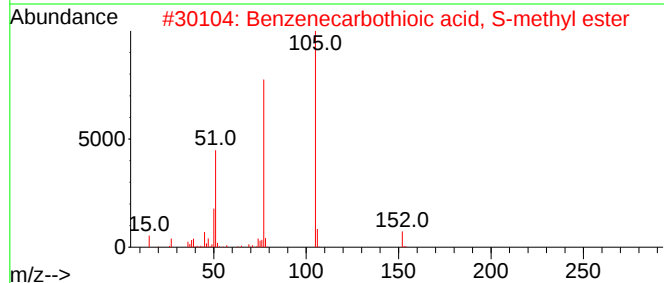
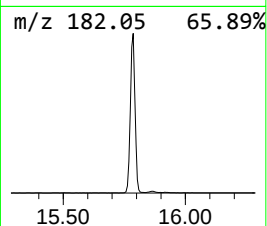
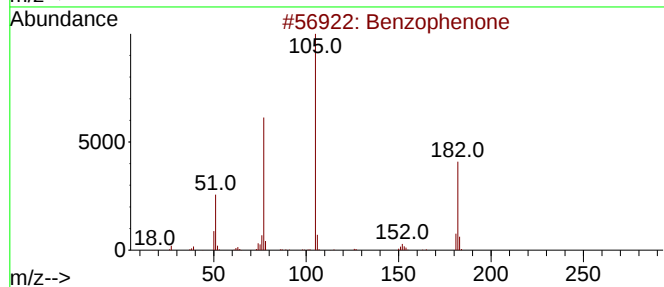
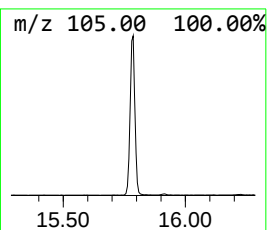
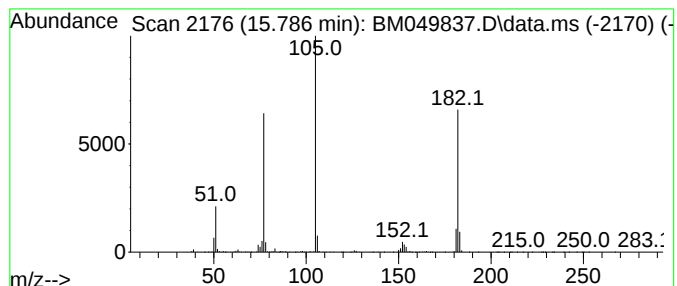
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.786	12.82 ng	2318140	Acenaphthene-d10	14.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
3			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	43
4			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	43
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	43



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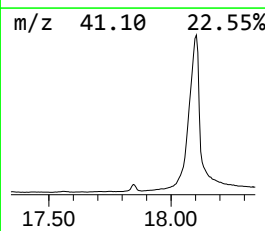
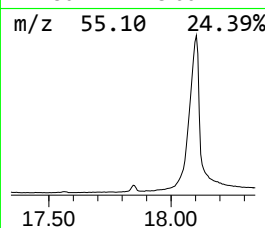
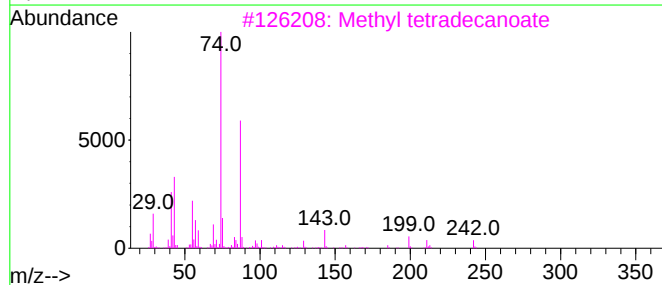
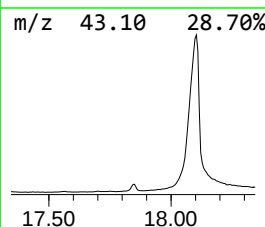
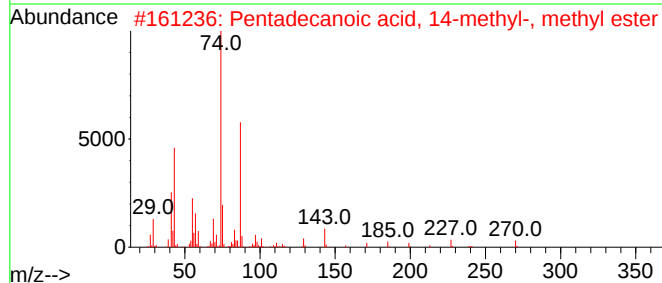
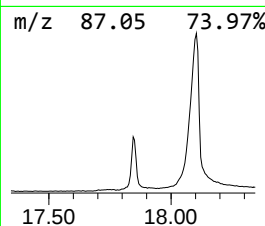
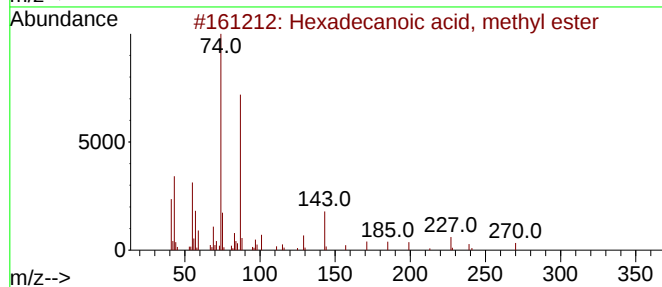
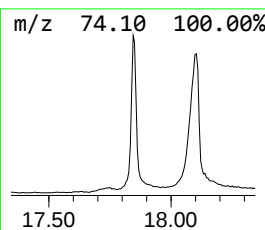
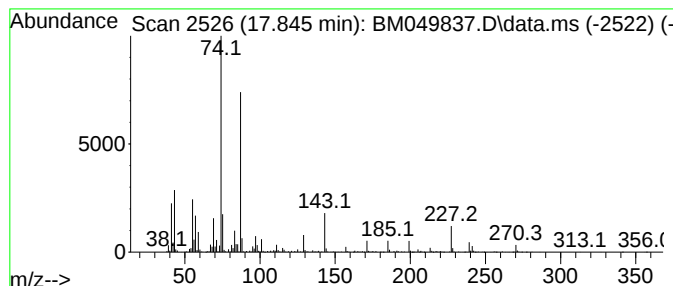
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.845	6.34 ng	1241570	Phenanthrene-d10	17.168

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
4			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
5			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87



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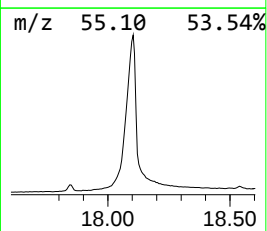
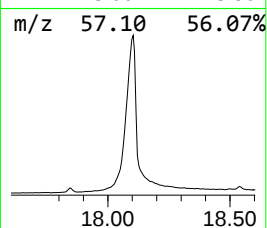
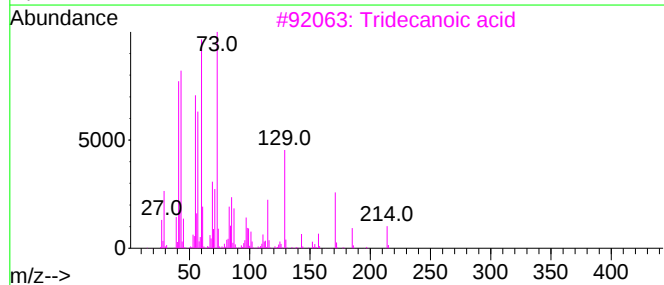
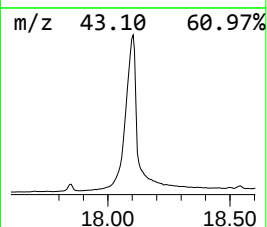
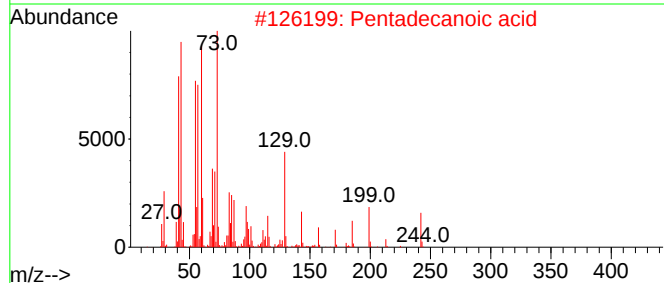
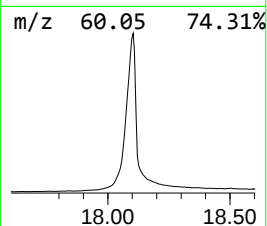
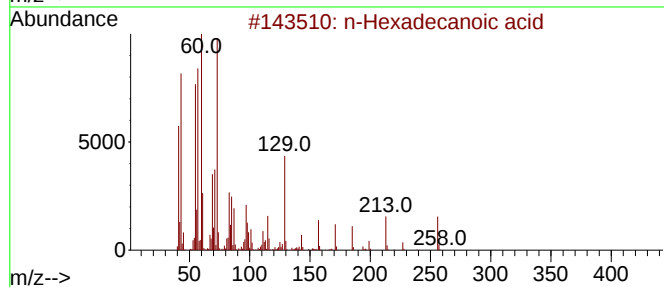
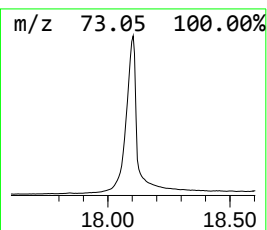
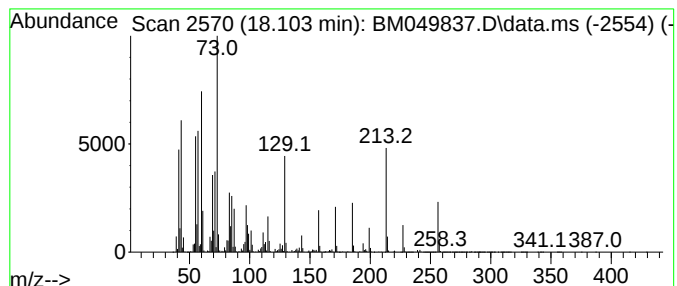
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.104	315.08 ng	61741500	Phenanthrene-d10	17.168

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			n-Decanoic acid	172	C10H20O2	000334-48-5	60
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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ALS Vial : 6 Sample Multiplier: 1

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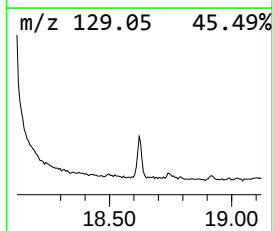
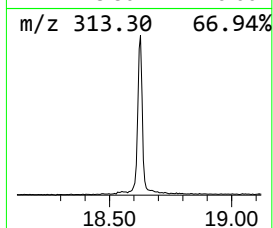
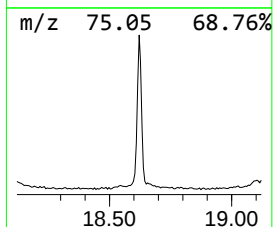
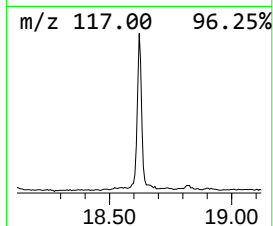
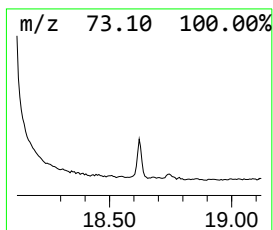
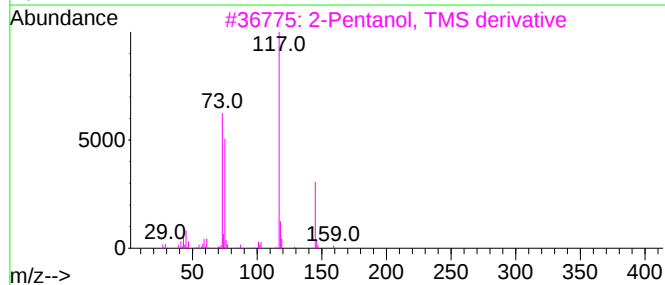
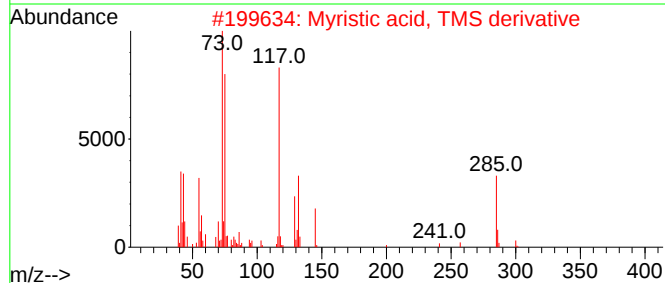
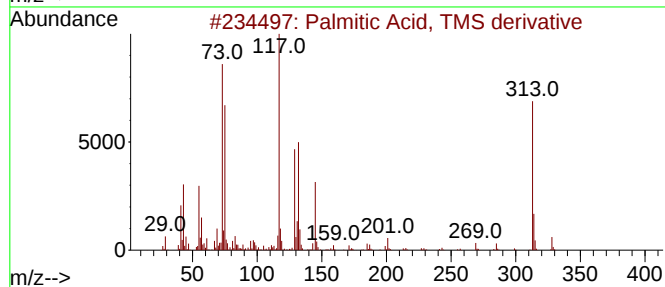
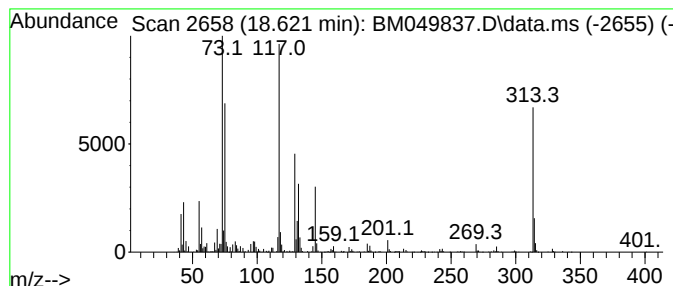
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Palmitic Acid, TMS derivative Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.621	6.10 ng	1195610	Phenanthrene-d10	17.168

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Palmitic Acid, TMS derivative	328	C19H40O2Si	055520-89-3	87
2			Myristic acid, TMS derivative	300	C17H36O2Si	018603-17-3	58
3			2-Pentanol, TMS derivative	160	C8H20O2Si	001825-67-8	41
4			2-(3,3,5-Trimethylcyclohexyl)ace...	256	C14H28O2Si	1000505-45-6	38
5			Indan, 1-methyl-	132	C10H12	000767-58-8	30



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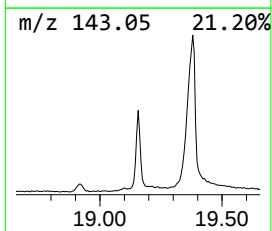
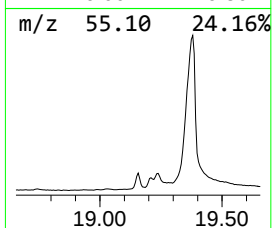
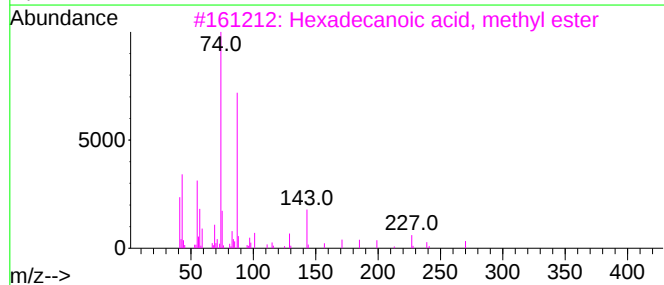
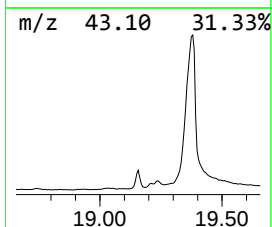
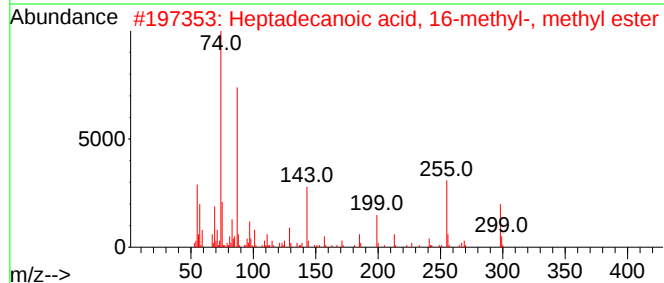
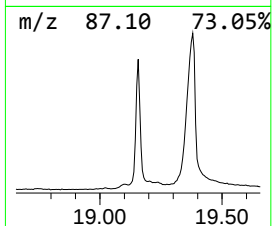
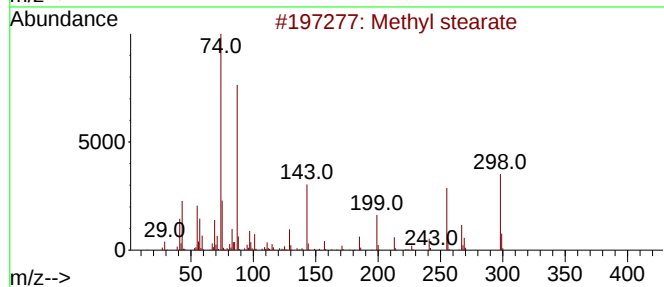
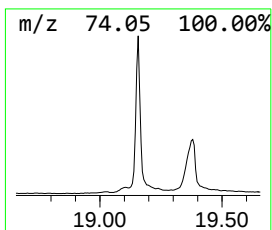
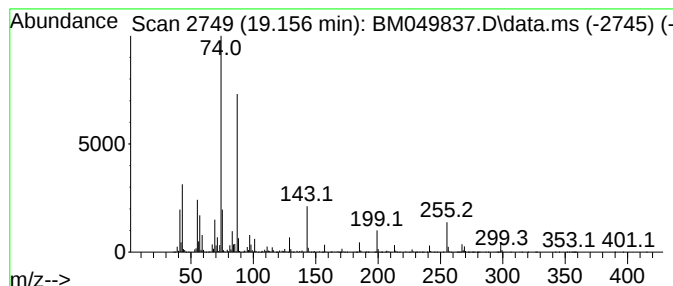
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Methyl stearate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.156	15.91 ng	3116800	Phenanthrene-d10	17.168

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	94
3			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87



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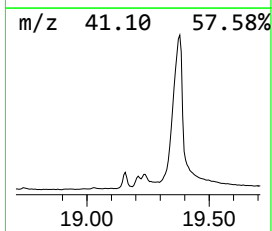
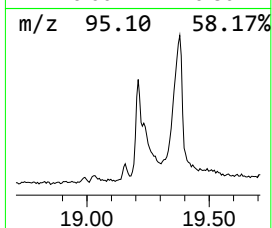
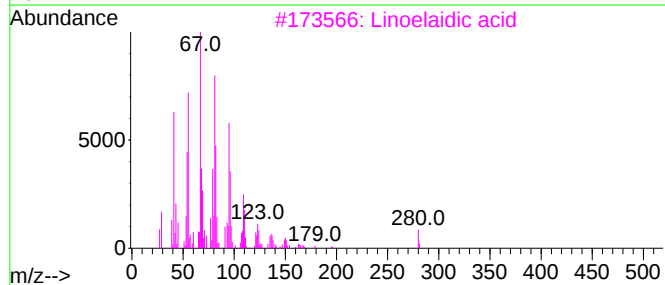
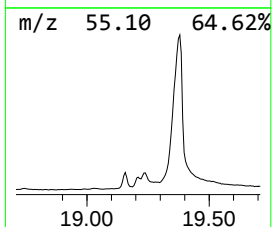
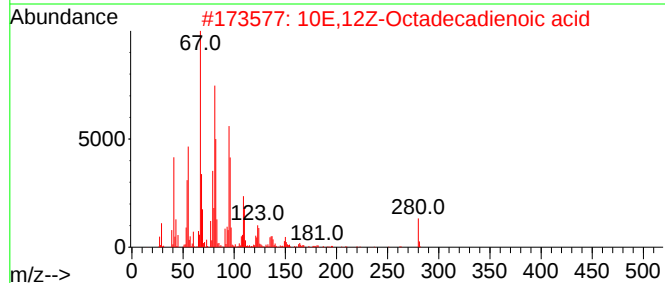
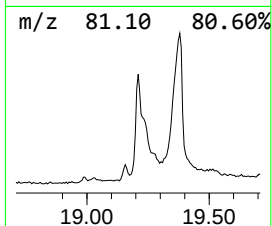
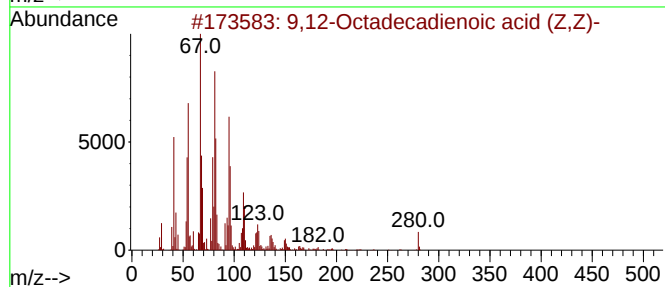
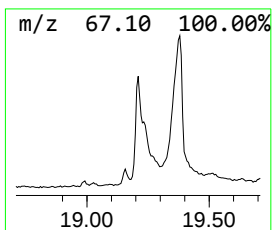
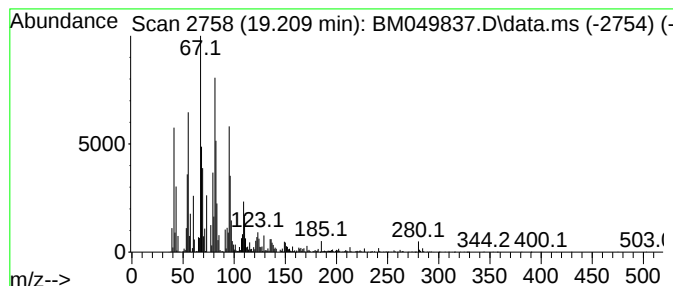
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9,12-Octadecadienoic acid (... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.209	9.68 ng	1897050	Phenanthrene-d10	17.168

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
2		10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	99
3		Linoleic acid	280	C18H32O2	000506-21-8	99
4		(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	96
5		cis-9-Tetradecen-1-ol	212	C14H28O	035153-15-2	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040725\
Data File : BM049837.D
Acq On : 07 Apr 2025 13:24
Operator : RC/JU
Sample : Q1675-20
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
K2

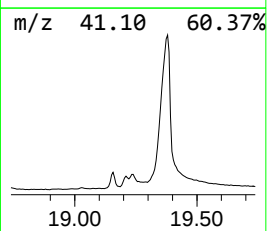
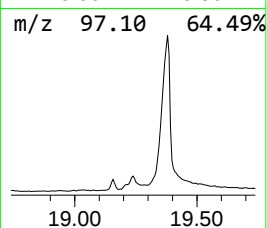
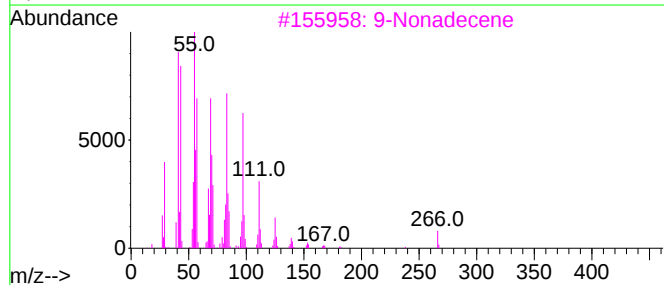
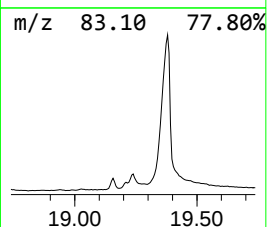
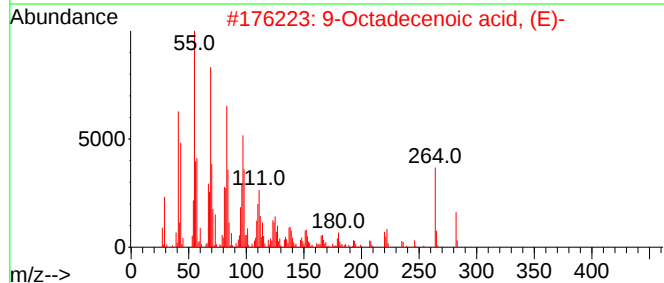
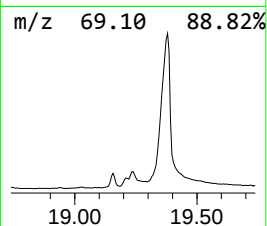
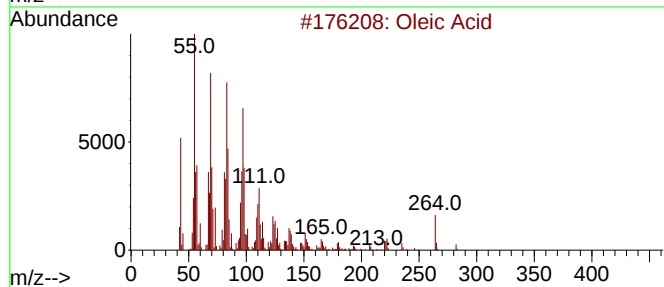
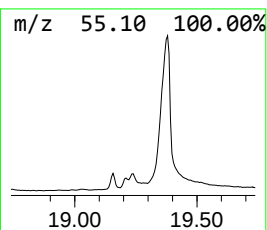
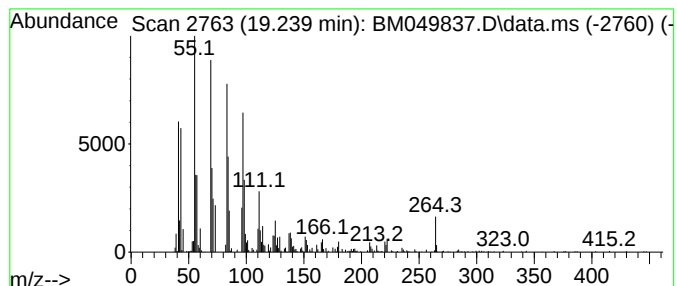
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oleic Acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.239	8.58 ng	1680970	Phenanthrene-d10	17.168

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oleic Acid	282	C18H34O2	000112-80-1	80
2			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	80
3			9-Nonadecene	266	C19H38	031035-07-1	70
4			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	58
5			1-Octadecanol	270	C18H38O	000112-92-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040725\
Data File : BM049837.D
Acq On : 07 Apr 2025 13:24
Operator : RC/JU
Sample : Q1675-20
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
K2

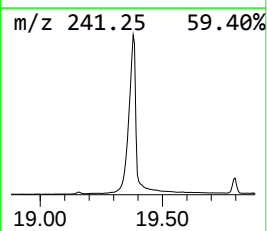
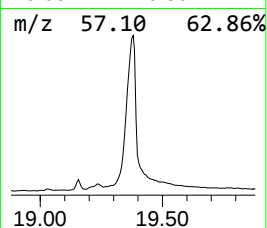
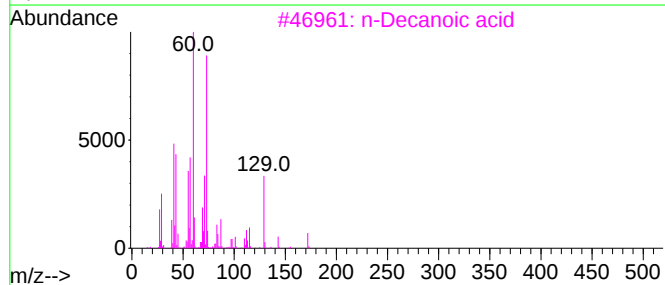
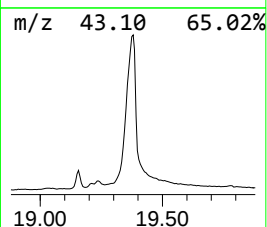
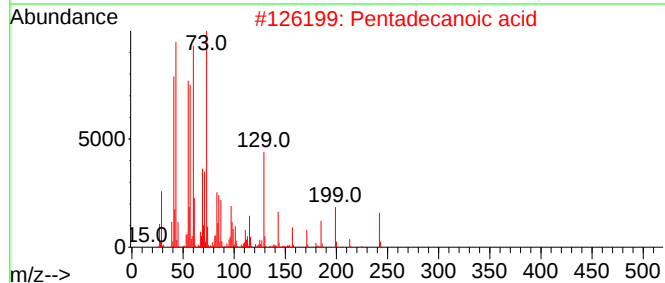
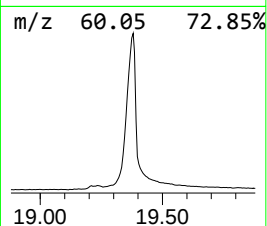
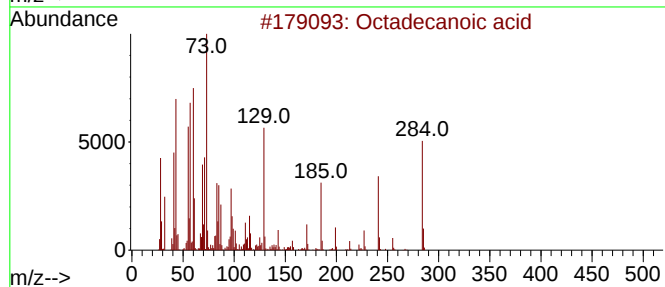
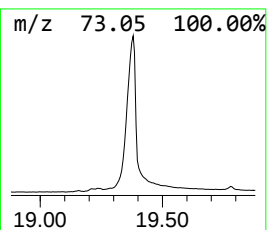
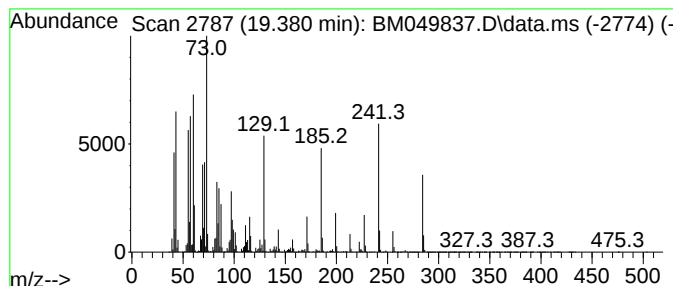
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.380	373.19 ng	76135500	Chrysene-d12	21.403

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	78
3			n-Decanoic acid	172	C10H20O2	000334-48-5	70
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	47
5			Undecanoic acid	186	C11H22O2	000112-37-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040725\
Data File : BM049837.D
Acq On : 07 Apr 2025 13:24
Operator : RC/JU
Sample : Q1675-20
Misc :
ALS Vial : 6 Sample Multiplier: 1

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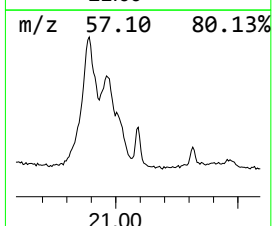
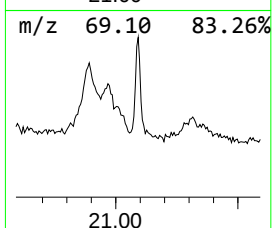
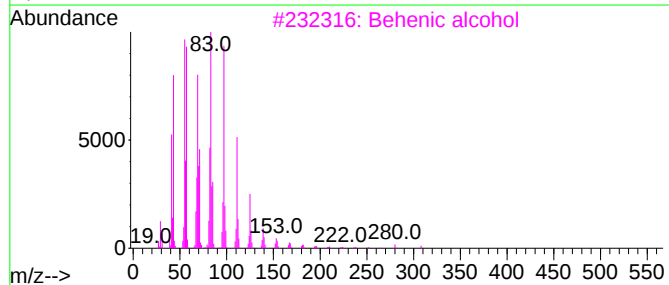
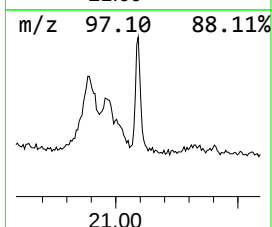
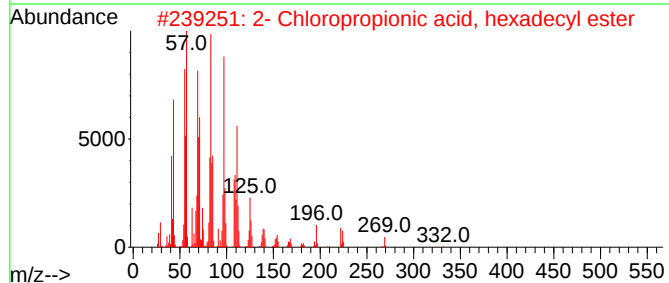
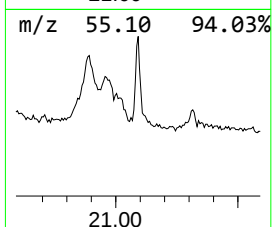
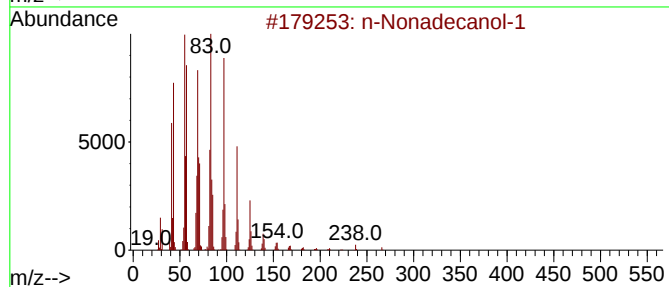
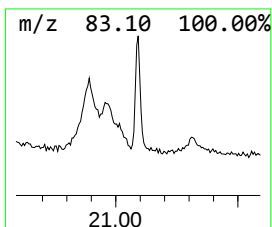
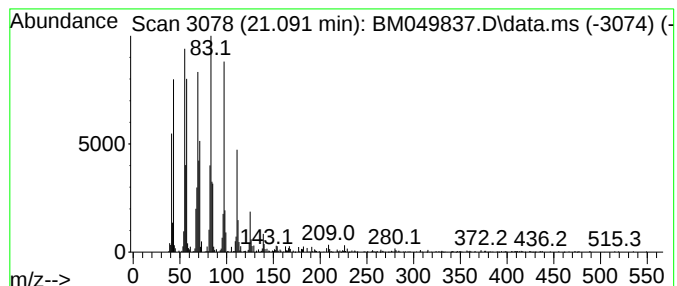
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Nonadecanol-1 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	4.55 ng	928462	Chrysene-d12	21.403

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2		2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	94
3		Behenic alcohol	326	C22H46O	000661-19-8	94
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	92
5		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040725\
Data File : BM049837.D
Acq On : 07 Apr 2025 13:24
Operator : RC/JU
Sample : Q1675-20
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
K2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.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
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Hexadecanoic ac...	17.845	6.3	ng	1241570	4	17.168	3919080	20.0
n-Hexadecanoic ...	18.104	315.1	ng	61741500	4	17.168	3919080	20.0
Palmitic Acid, ...	18.621	6.1	ng	1195610	4	17.168	3919080	20.0
Methyl stearate	19.156	15.9	ng	3116800	4	17.168	3919080	20.0
9,12-Octadecadi...	19.209	9.7	ng	1897050	4	17.168	3919080	20.0
Oleic Acid	19.239	8.6	ng	1680970	4	17.168	3919080	20.0
Octadecanoic acid	19.380	373.2	ng	76135500	5	21.403	4080260	20.0
n-Nonadecanol-1	21.092	4.5	ng	928462	5	21.403	4080260	20.0