

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM011422\
 Data File : BM033735.D
 Acq On : 14 Jan 2022 19:24
 Operator : CG/JU
 Sample : N1157-02 5X
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 EFF-WW

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-BM010522.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033735.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.254	809	853	856	rBV2	37555221	386866695	100.00%	74.079%
2	9.478	1015	1061	1064	rBV	1867771	11904061	3.08%	2.279%
3	9.854	1091	1125	1133	rBV	2842778	17125055	4.43%	3.279%
4	10.266	1166	1195	1202	rBV	1259230	4714647	1.22%	0.903%
5	15.089	1997	2015	2037	rBV	6463185	19009073	4.91%	3.640%
6	15.936	2150	2159	2164	rBV	15533423	20684508	5.35%	3.961%
7	16.754	2291	2298	2308	rBV	2695007	3978265	1.03%	0.762%
8	18.242	2542	2551	2572	rBV2	3211733	5562395	1.44%	1.065%
9	19.395	2737	2747	2752	rBV	2958359	4528592	1.17%	0.867%
10	20.230	2865	2889	2892	rBV3	1859272	7880799	2.04%	1.509%
11	20.324	2894	2905	2908	rBV	1925271	6241096	1.61%	1.195%
12	22.130	3208	3212	3218	rVB	3357998	4346795	1.12%	0.832%
13	23.253	3395	3403	3422	rVB	13162823	24751789	6.40%	4.740%
14	24.865	3665	3677	3679	rBV2	1546779	4641651	1.20%	0.889%

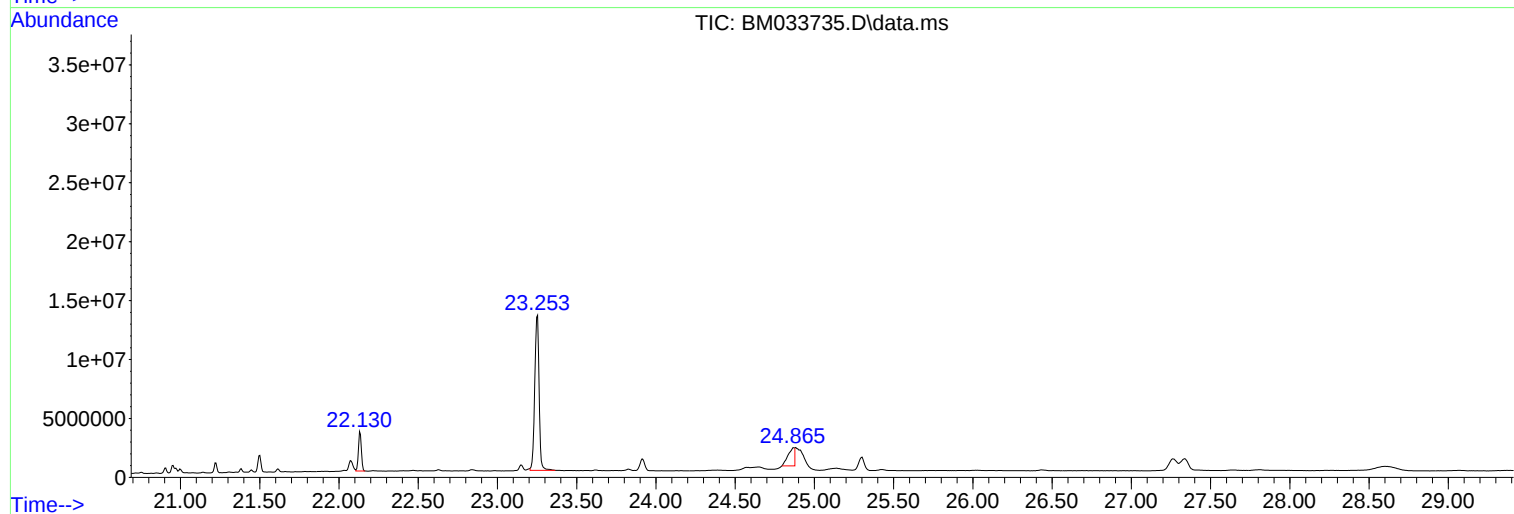
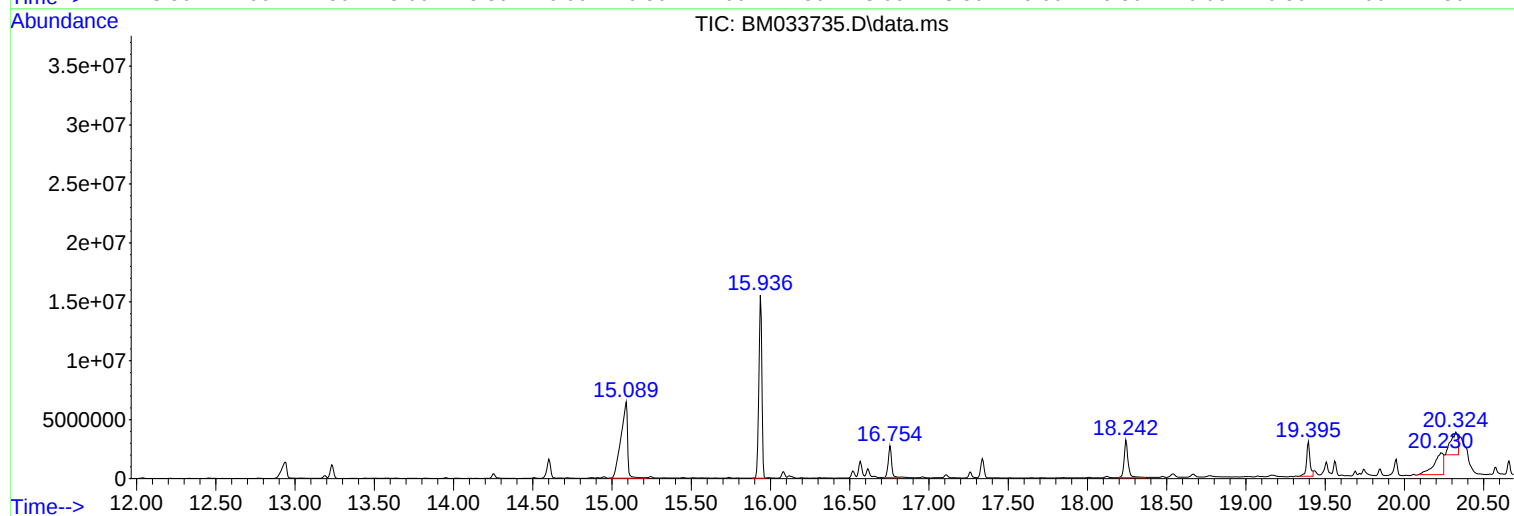
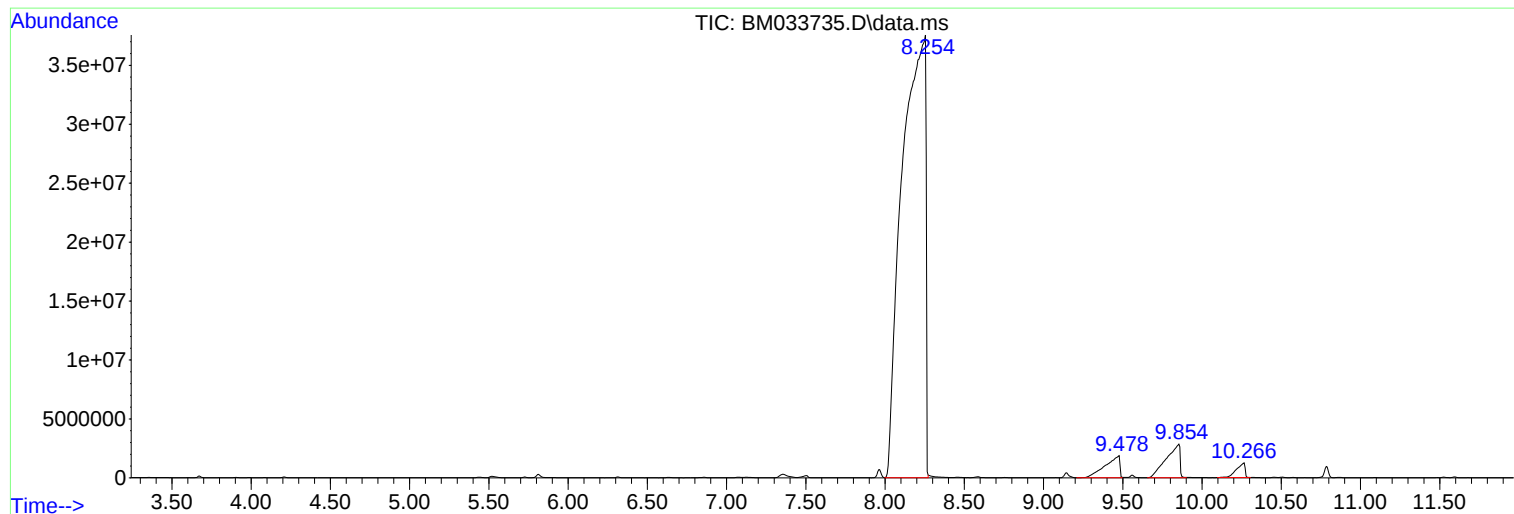
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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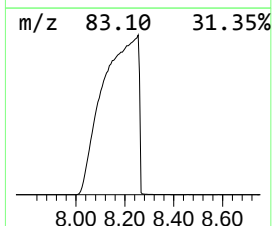
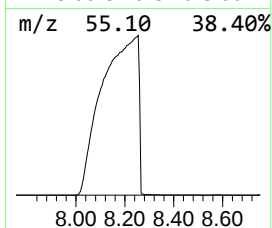
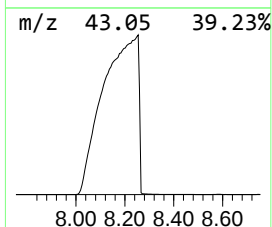
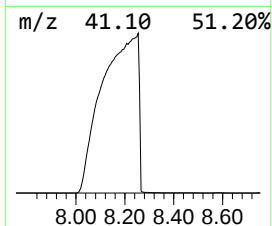
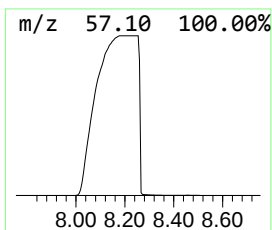
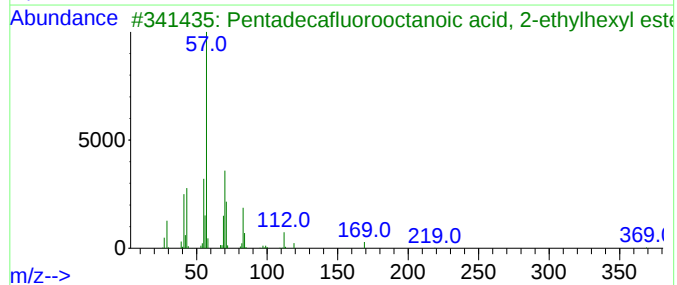
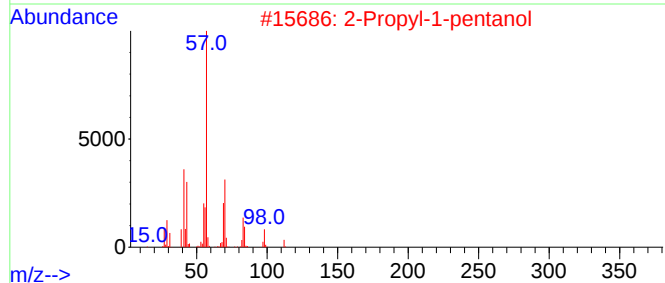
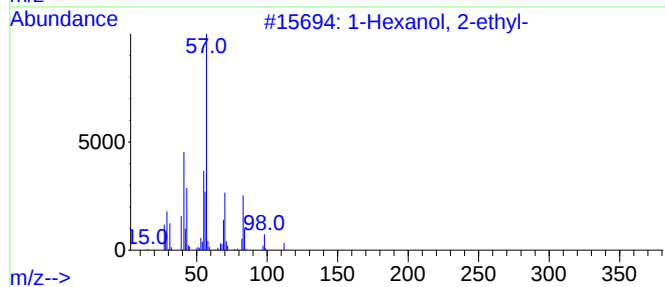
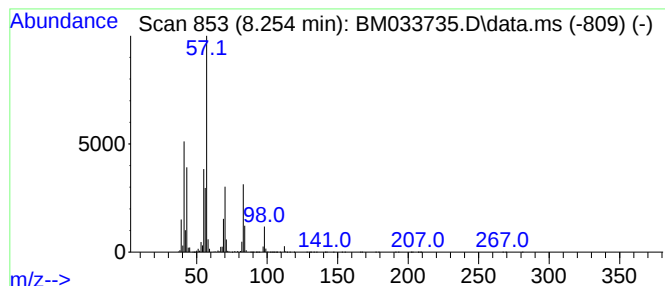
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.254	20.00 ng	386867000	1,4-Dichlorobenzene-d4	7.966

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
3			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	59
4			2-Heptenal, (E)-	112	C7H12O	018829-55-5	52
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50



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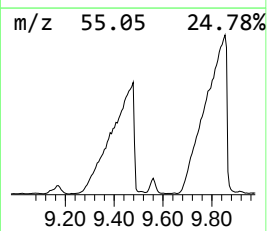
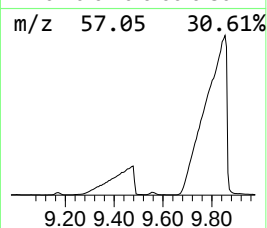
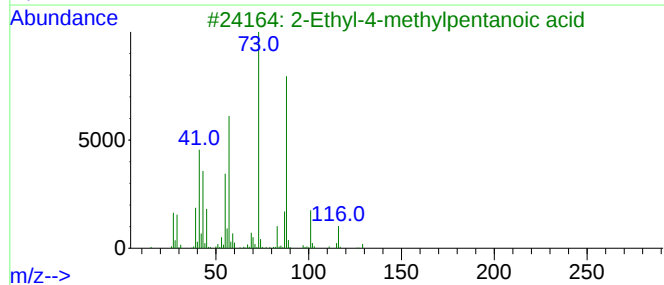
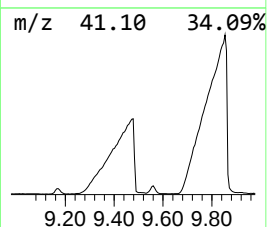
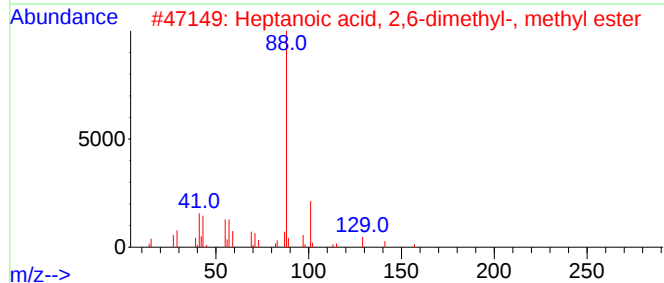
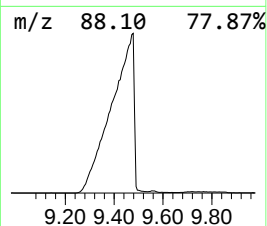
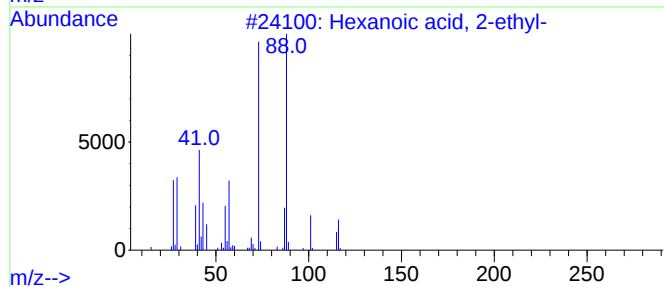
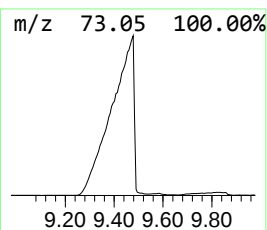
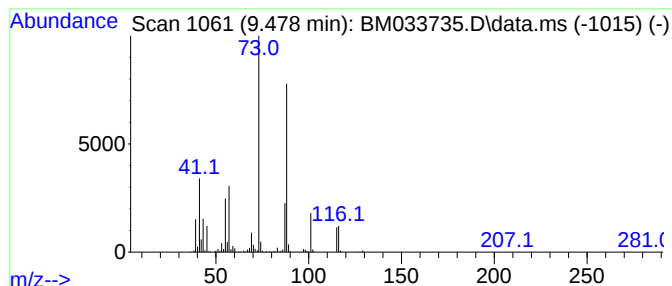
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Peak Number 2 Hexanoic acid, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.478	50.50 ng	11904100	Naphthalene-d8	10.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2			Heptanoic acid, 2,6-dimethyl-, m...	172	C10H20O2	033315-72-9	50
3			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	45
4			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	45
5			Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	40



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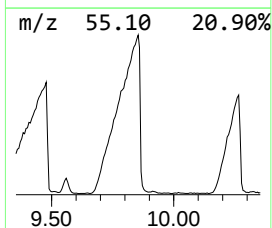
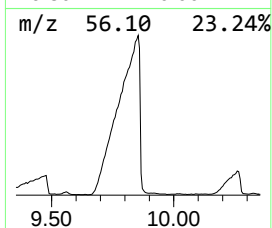
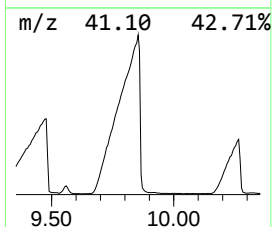
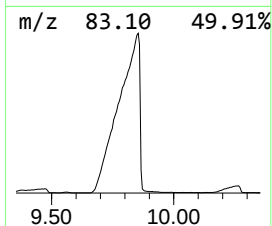
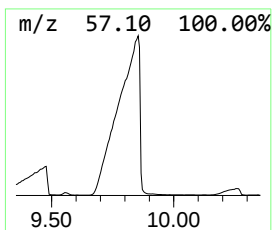
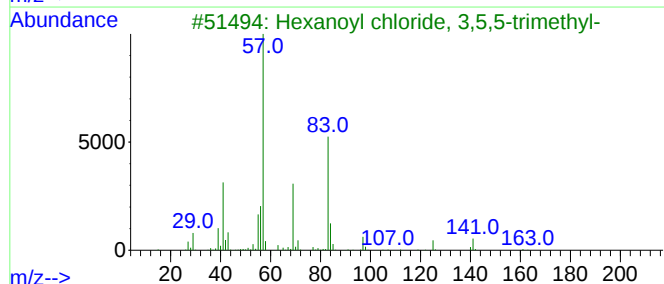
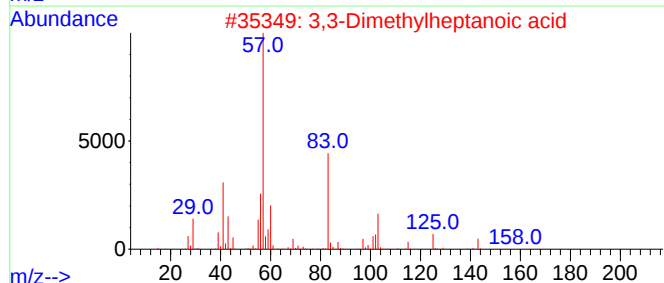
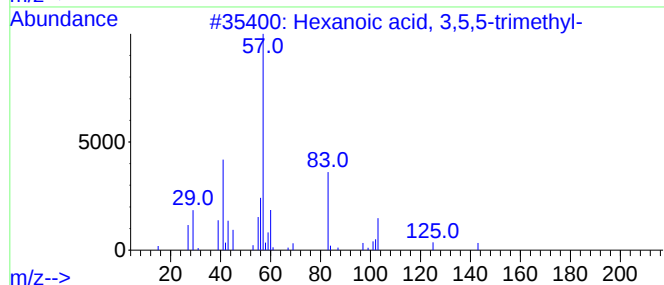
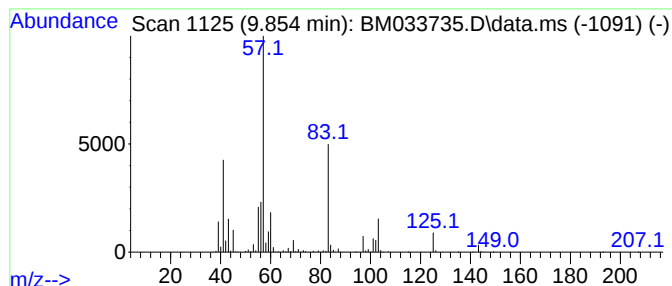
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Peak Number 3 Hexanoic acid, 3,5,5-trimet... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.854	72.65 ng	17125100	Naphthalene-d8	10.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	90
2			3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	83
3			Hexanoyl chloride, 3,5,5-trimethyl-	176	C9H17ClO	036727-29-4	53
4			4,4-Dimethyl-2-pentanol, chlorod...	228	C9H15ClF2O2	1000376-27-0	35
5			Carbonic acid, bis(1-methylpropy...	174	C9H18O3	000623-63-2	35



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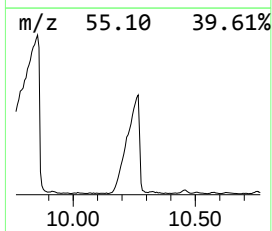
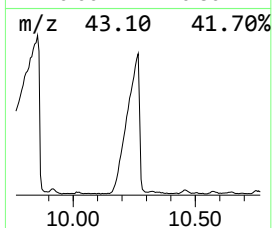
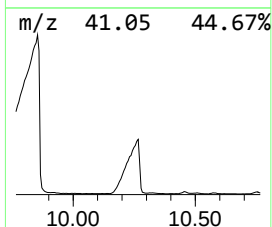
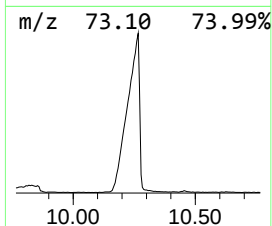
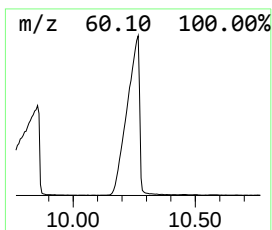
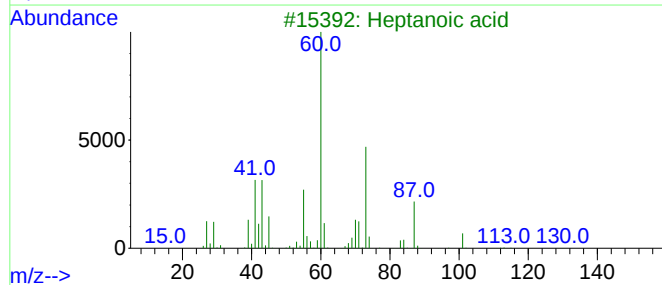
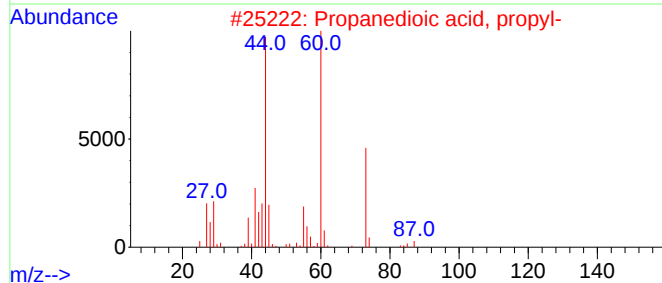
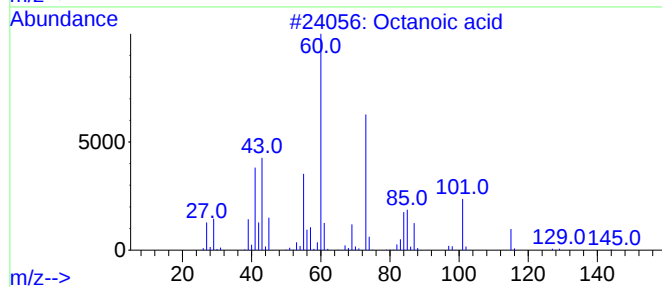
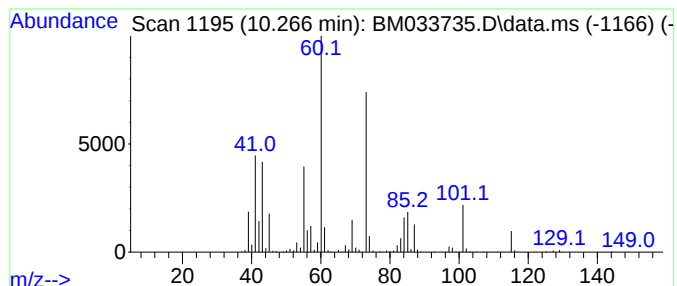
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Peak Number 4 Octanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.266	20.00 ng	4714650	Naphthalene-d8	10.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanoic acid	144	C8H16O2	000124-07-2	97
2			Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	50
3			Heptanoic acid	130	C7H14O2	000111-14-8	50
4			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	50
5			Hexanoic acid	116	C6H12O2	000142-62-1	50



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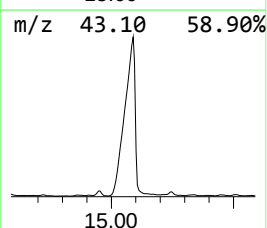
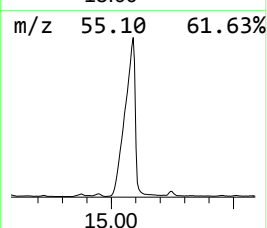
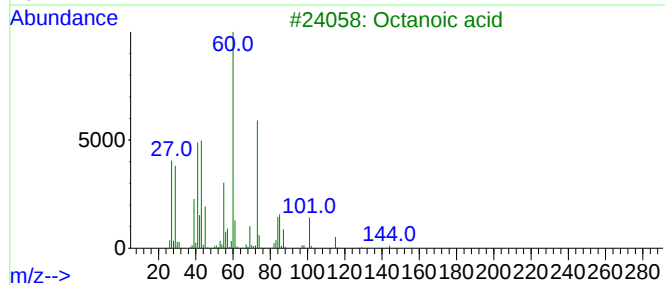
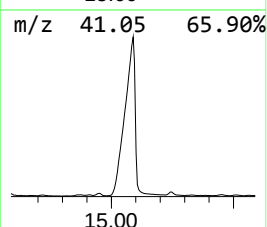
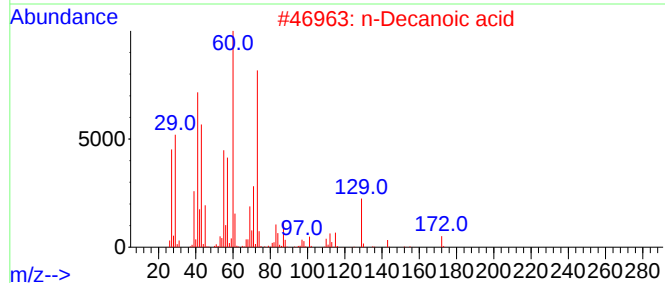
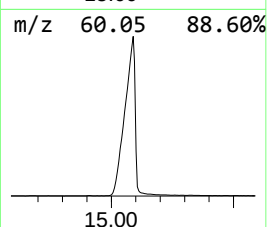
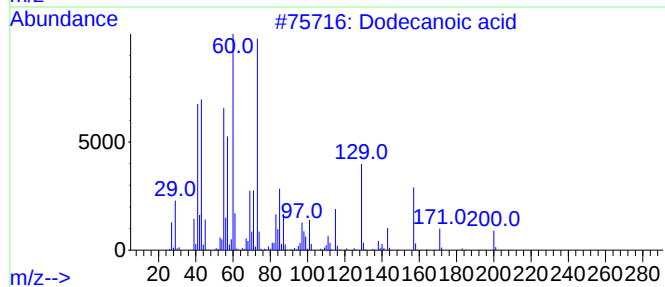
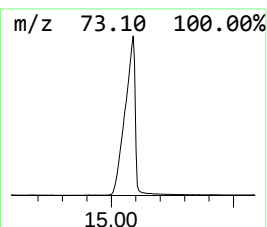
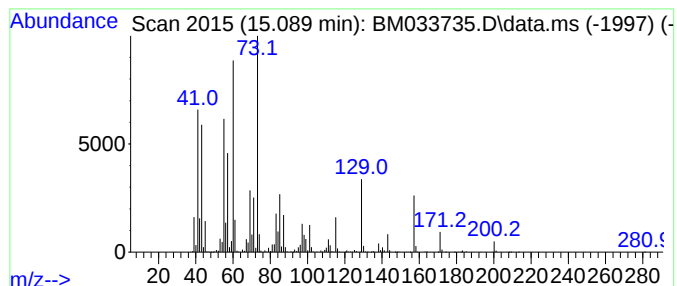
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Dodecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.089	20.00 ng	19009100	Acenaphthene-d10	14.601

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	98
2			n-Decanoic acid	172	C10H20O2	000334-48-5	53
3			Octanoic acid	144	C8H16O2	000124-07-2	49
4			Nonanoic acid	158	C9H18O2	000112-05-0	46
5			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	43



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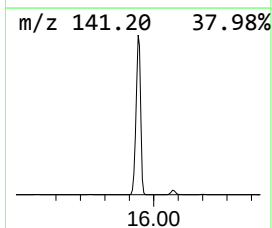
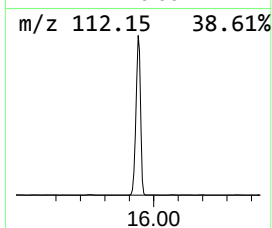
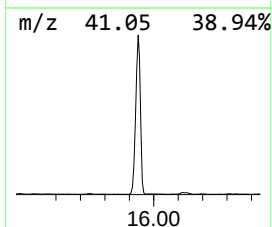
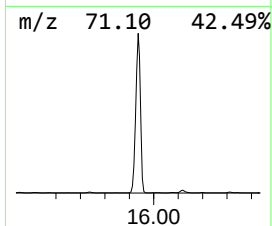
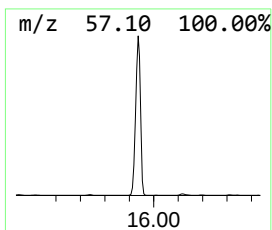
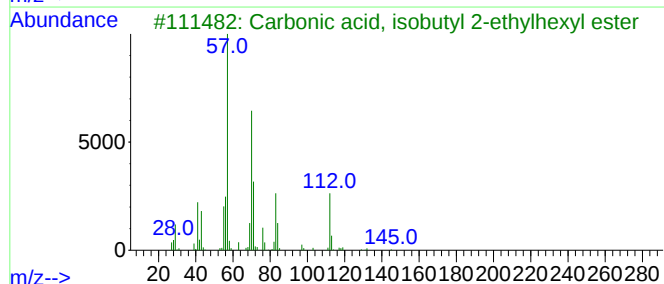
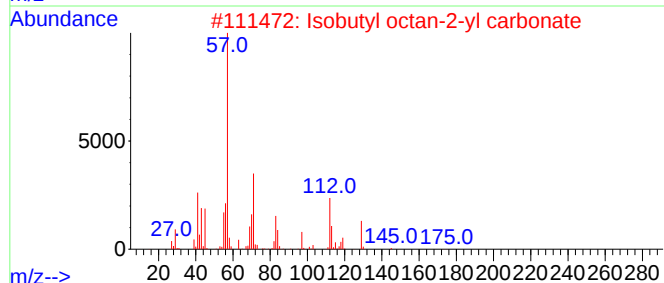
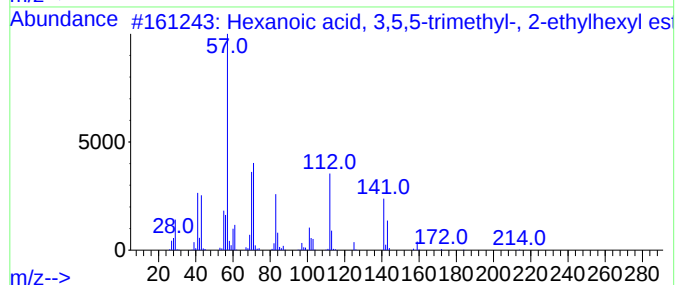
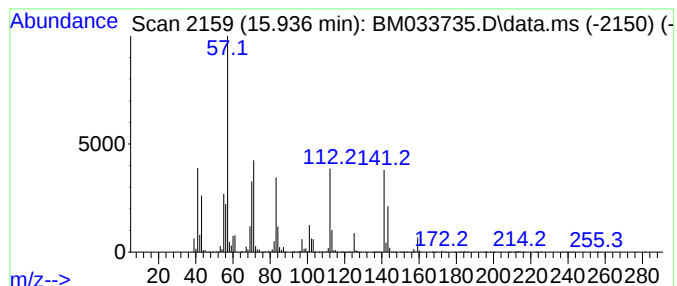
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BNA_M
ClientSampleId :
EFF-WW

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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 Hexanoic acid, 3,5,5-trimet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.936	21.76 ng	20684500	Acenaphthene-d10	14.601	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-,...	270	C17H34O2	1000406-82-2	72
2	Isobutyl octan-2-yl carbonate	230	C13H26O3	1000372-74-7	47
3	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	38
4	Octane, 4-ethyl-	142	C10H22	015869-86-0	35
5	Decanal	156	C10H20O	000112-31-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM011422\
Data File : BM033735.D
Acq On : 14 Jan 2022 19:24
Operator : CG/JU
Sample : N1157-02 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

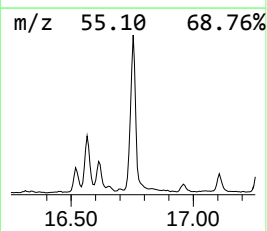
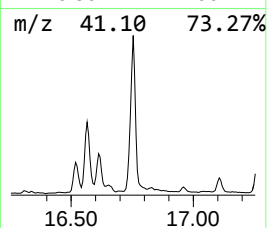
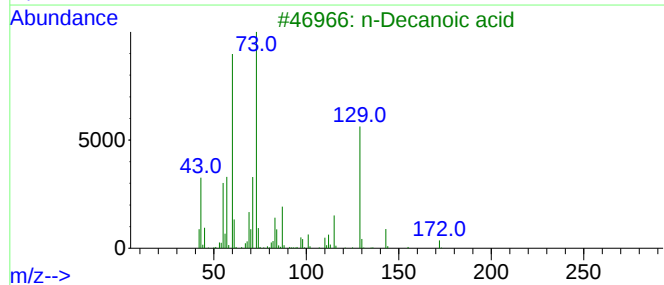
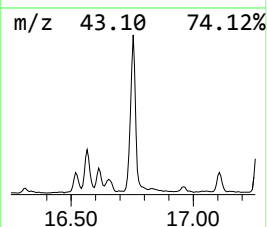
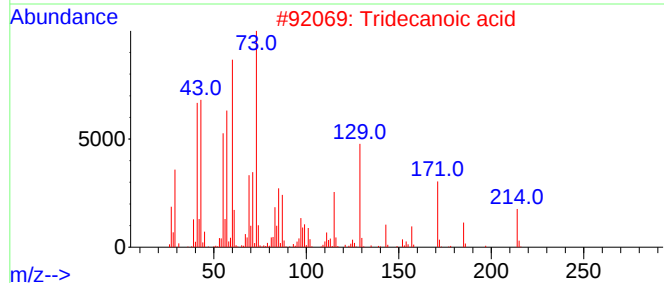
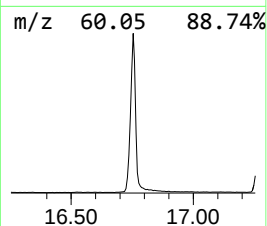
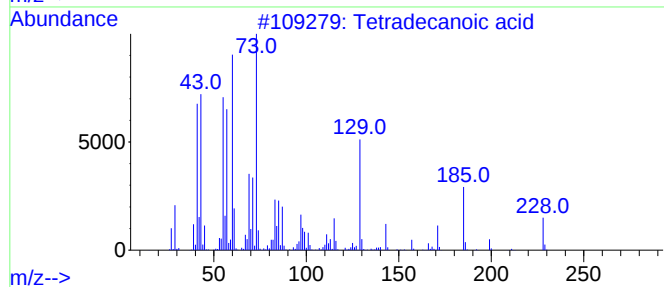
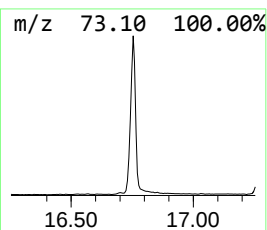
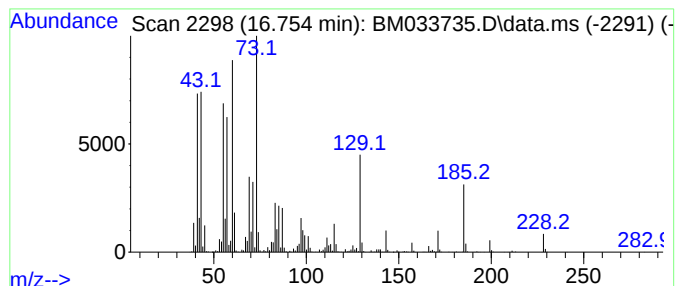
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetradecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.754	20.00 ng	3978270	Phenanthrene-d10	17.336	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	80
3	n-Decanoic acid	172	C10H20O2	000334-48-5	76
4	Undecanoic acid	186	C11H22O2	000112-37-8	70
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM011422\
Data File : BM033735.D
Acq On : 14 Jan 2022 19:24
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Sample : N1157-02 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

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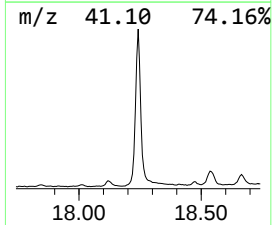
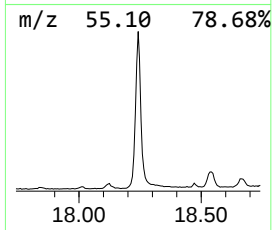
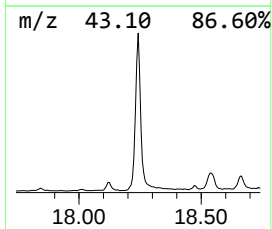
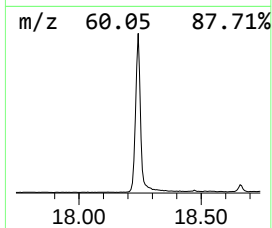
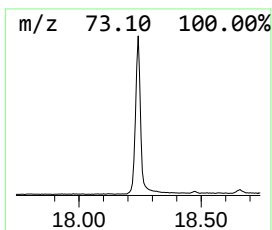
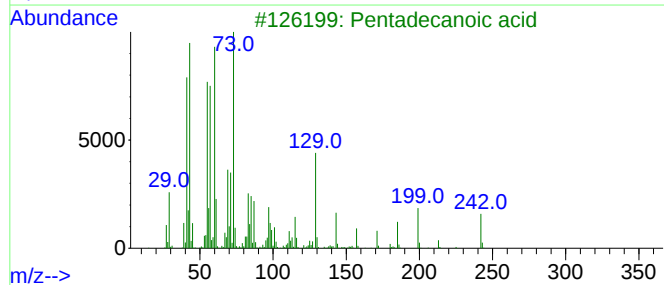
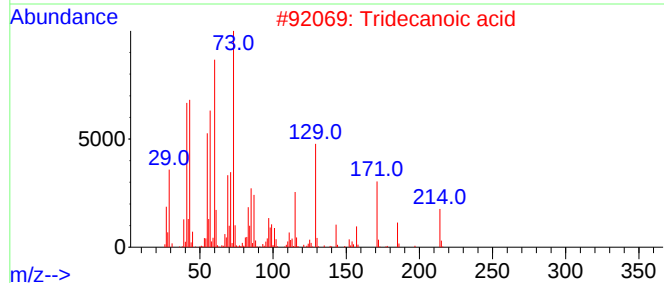
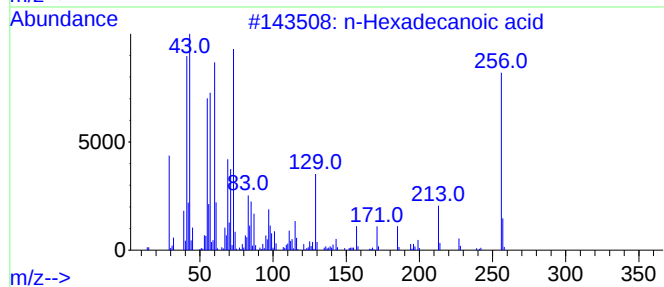
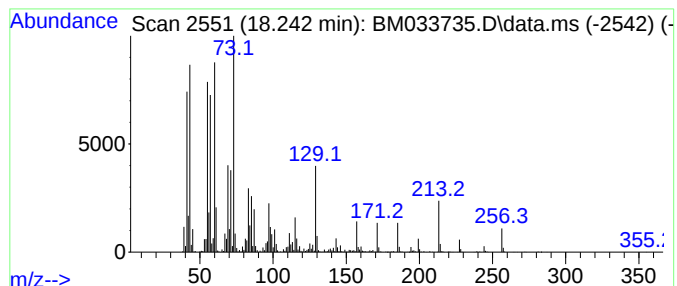
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.242	27.96 ng	5562400	Phenanthrene-d10	17.336

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	97
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM011422\
Data File : BM033735.D
Acq On : 14 Jan 2022 19:24
Operator : CG/JU
Sample : N1157-02 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

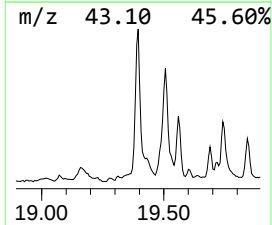
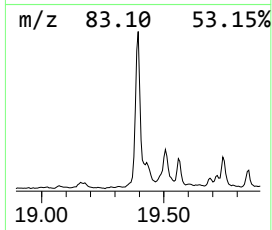
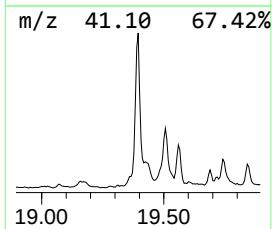
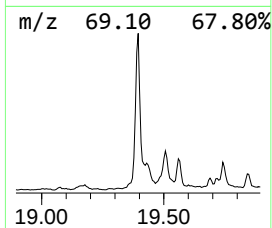
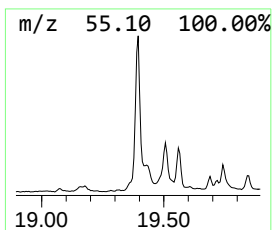
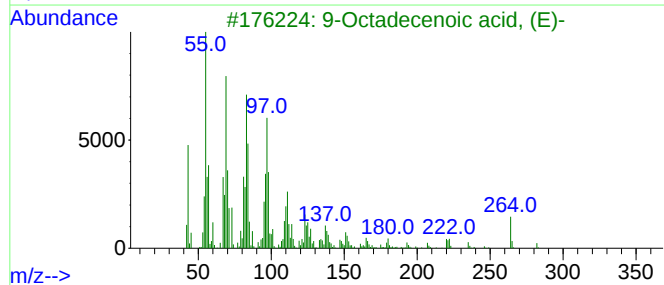
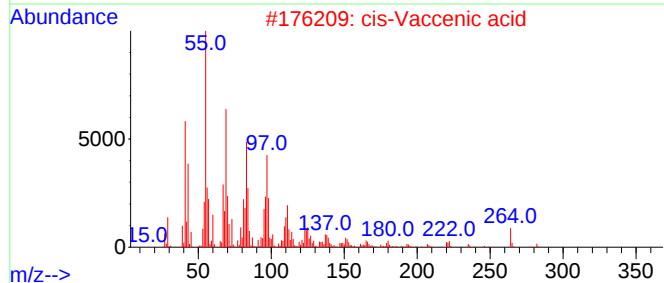
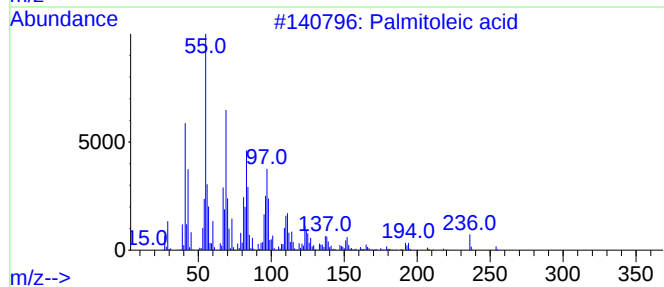
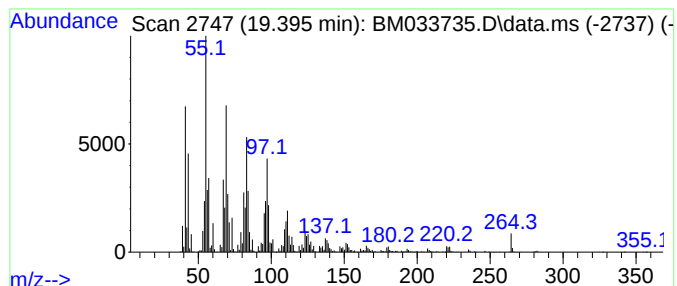
Instrument :
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ClientSampleId :
EFF-WW

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Palmitoleic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.395	22.77 ng	4528590	Phenanthrene-d10	17.336	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Palmitoleic acid	254	C16H30O2	000373-49-9	95
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	94
3	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	94
4	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	91
5	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM011422\
Data File : BM033735.D
Acq On : 14 Jan 2022 19:24
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Sample : N1157-02 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

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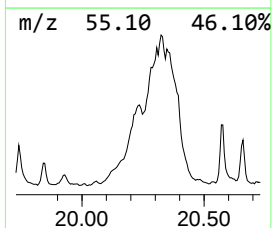
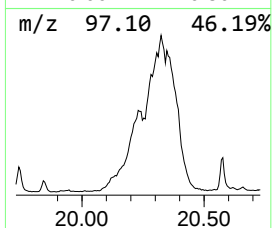
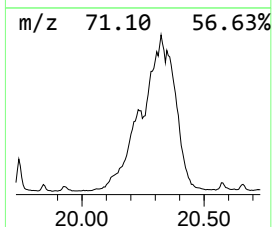
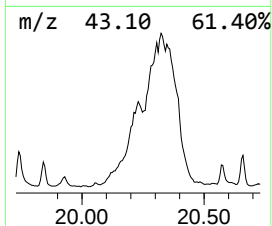
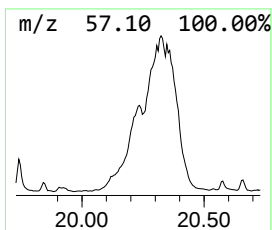
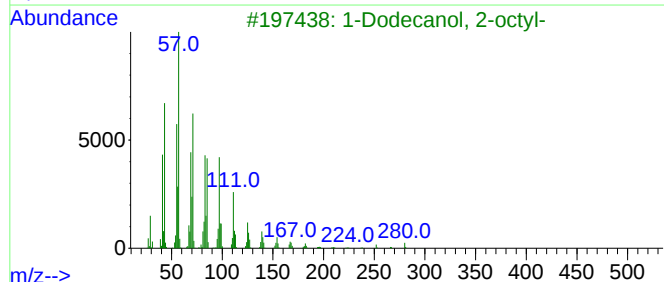
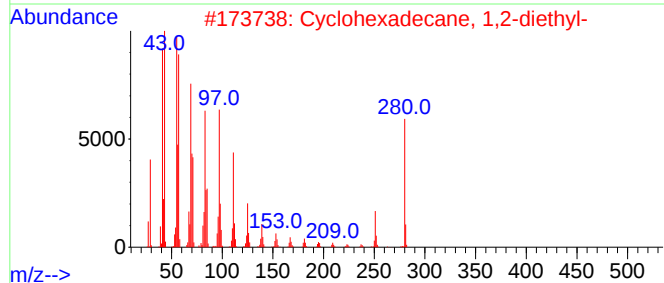
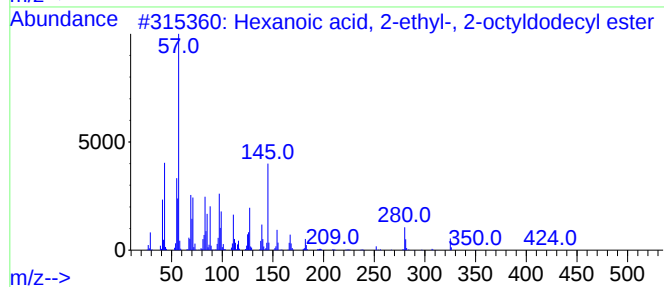
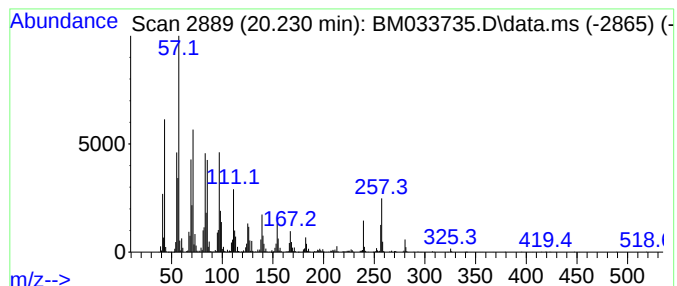
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexanoic acid, 2-ethyl-, 2-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.230	36.26 ng	7880800	Chrysene-d12	21.500

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-, 2-octyl...	424	C28H56O2	069275-04-3	91
2			Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	90
3			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	81
4			1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	81
5			Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM011422\
Data File : BM033735.D
Acq On : 14 Jan 2022 19:24
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Sample : N1157-02 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

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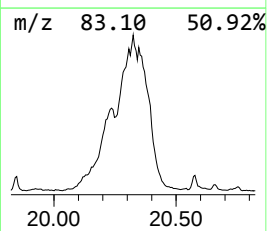
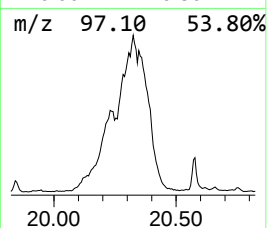
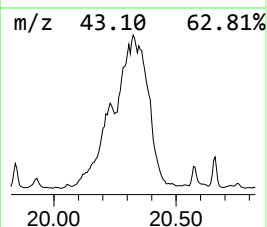
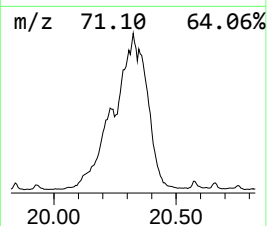
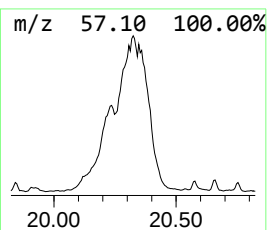
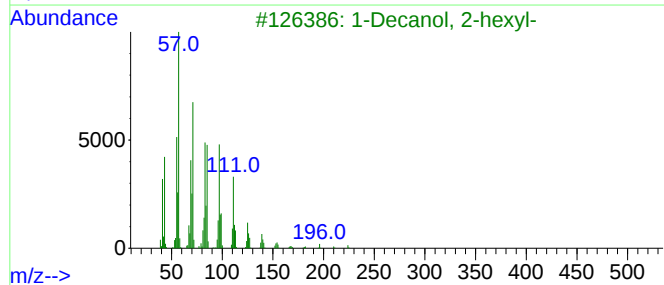
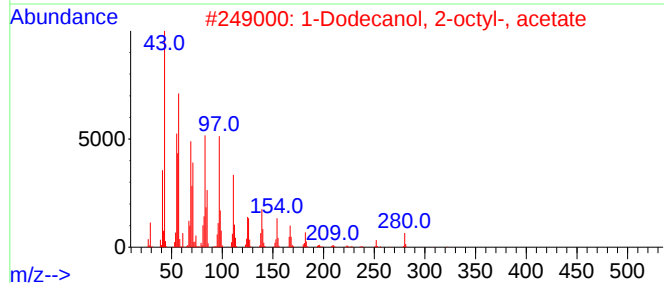
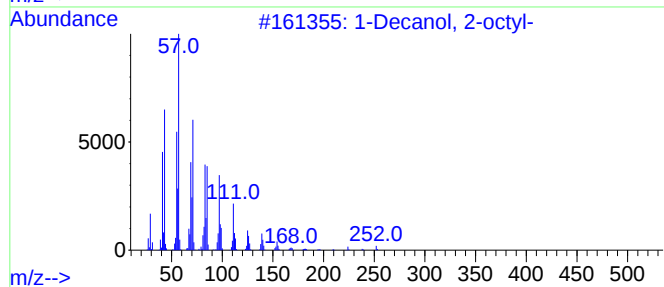
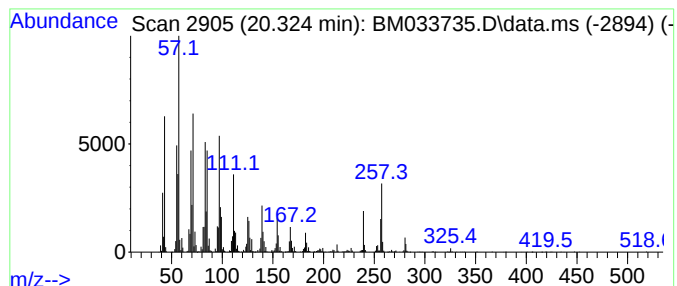
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Decanol, 2-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.324	28.72 ng	6241100	Chrysene-d12	21.500

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-octyl-		270	C18H38O	045235-48-1	83
2	1-Dodecanol, 2-octyl-, acetate		340	C22H44O2	074051-84-6	76
3	1-Decanol, 2-hexyl-		242	C16H34O	002425-77-6	76
4	2-Octyldodecyl butyrate		368	C24H48O2	1000368-55-2	76
5	1-Docosanol, methyl ether		340	C23H48O	1000333-91-9	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM011422\
Data File : BM033735.D
Acq On : 14 Jan 2022 19:24
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ALS Vial : 12 Sample Multiplier: 1

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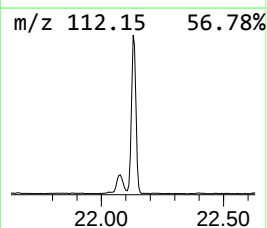
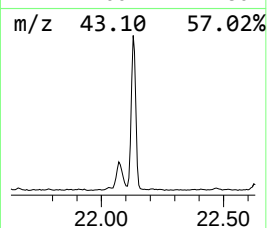
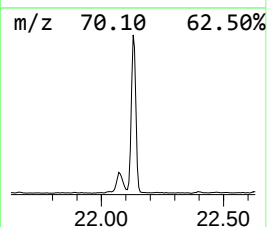
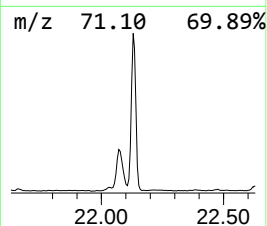
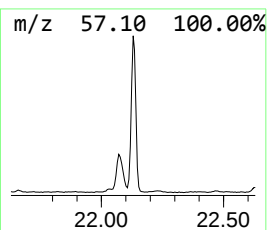
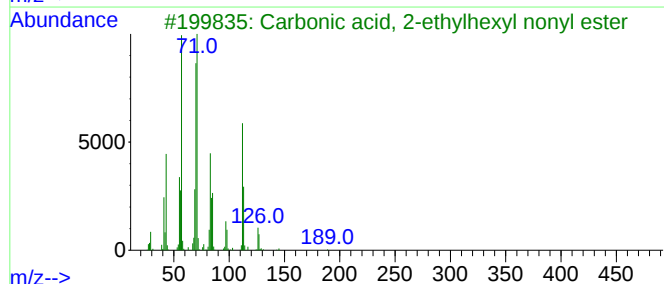
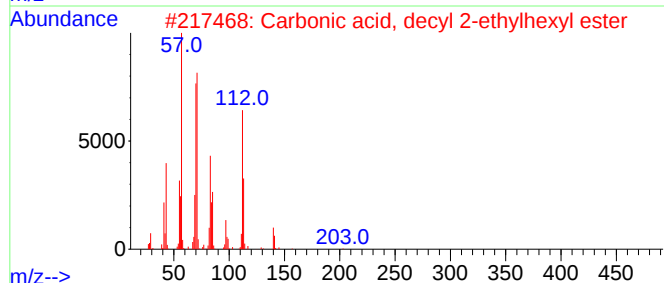
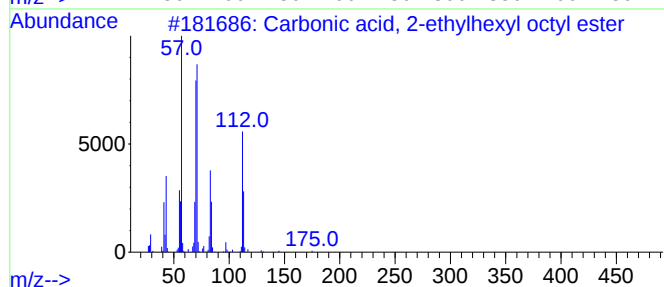
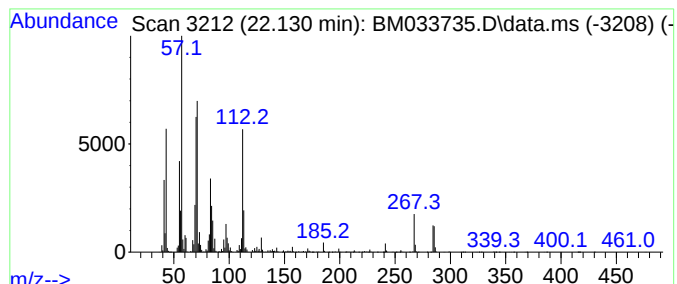
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Carbonic acid, 2-ethylhexyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.130	20.00 ng	4346800	Chrysene-d12	21.500

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, 2-ethylhexyl octy...	286	C17H34O3	1000383-13-5	68
2			Carbonic acid, decyl 2-ethylhexy...	314	C19H38O3	1000383-13-7	62
3			Carbonic acid, 2-ethylhexyl nony...	300	C18H36O3	1000383-13-6	58
4			Carbonic acid, 2-ethylhexyl unde...	328	C20H40O3	1000383-13-8	58
5			Carbonic acid, bis(2-ethylhexyl)...	286	C17H34O3	014858-73-2	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM011422\
Data File : BM033735.D
Acq On : 14 Jan 2022 19:24
Operator : CG/JU
Sample : N1157-02 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

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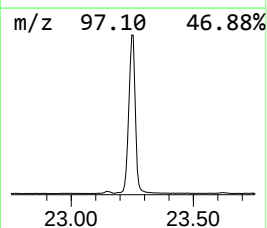
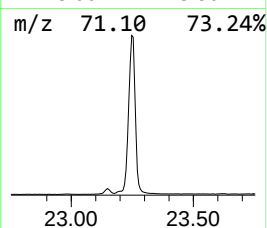
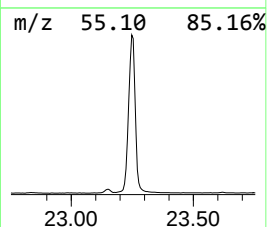
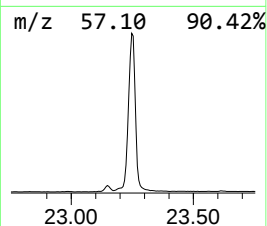
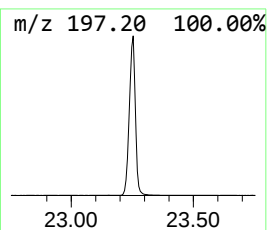
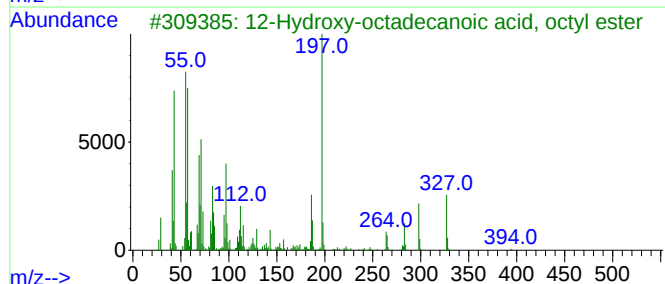
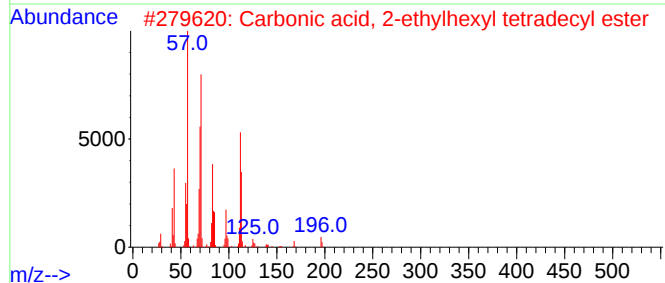
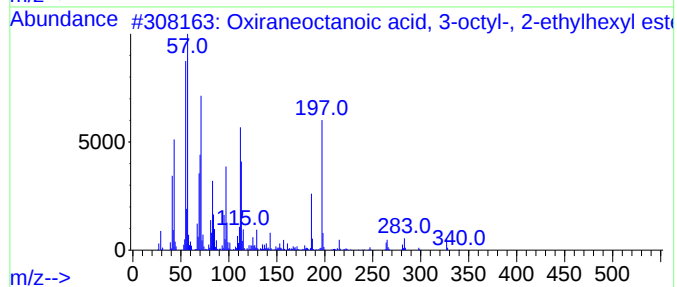
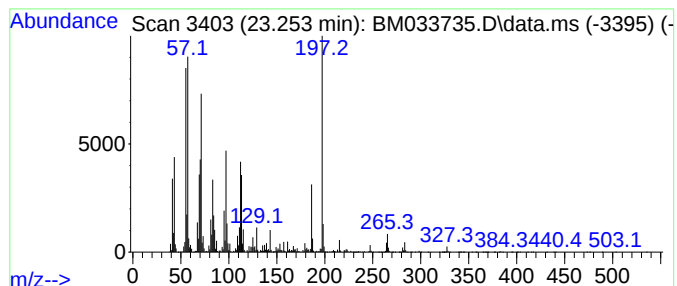
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Oxiraneoctanoic acid, 3-oct... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.253	20.00 ng	24751800	Perylene-d12	23.912

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxiraneoctanoic acid, 3-octyl-, ...	410	C26H50O3	000141-38-8	76
2			Carbonic acid, 2-ethylhexyl tetr...	370	C23H46O3	1010383-14-1	49
3			12-Hydroxy-octadecanoic acid, oc...	412	C26H52O3	074819-90-2	47
4			Carbonic acid, 2-ethylhexyl octa...	426	C27H54O3	1000383-14-5	45
5			Carbonic acid, 2-ethylhexyl hept...	412	C26H52O3	1000383-14-4	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM011422\
Data File : BM033735.D
Acq On : 14 Jan 2022 19:24
Operator : CG/JU
Sample : N1157-02 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

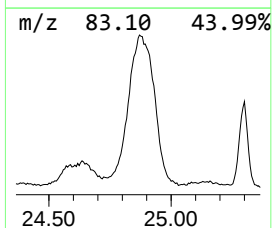
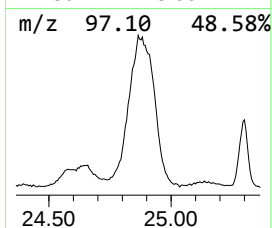
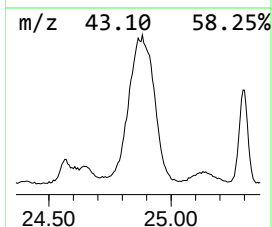
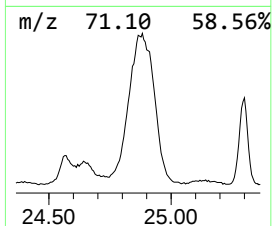
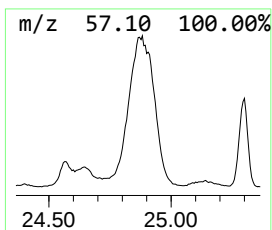
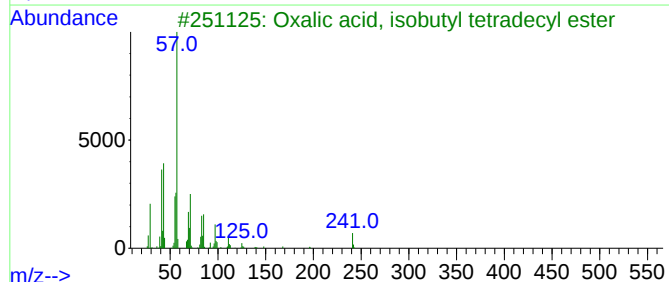
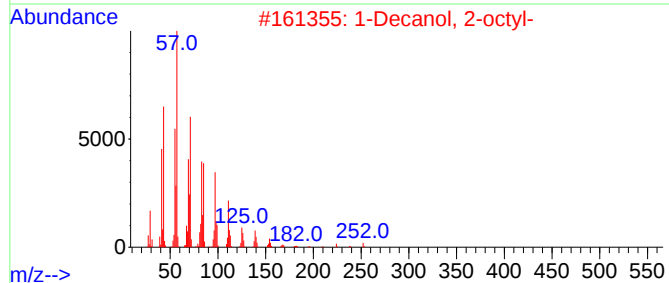
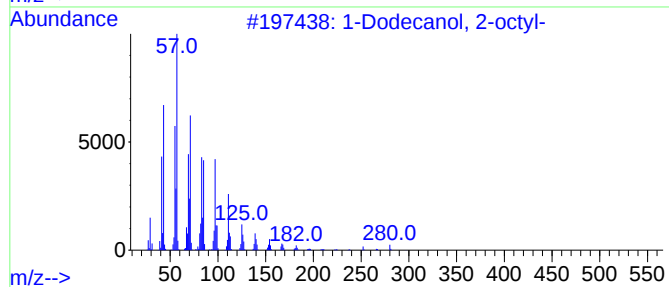
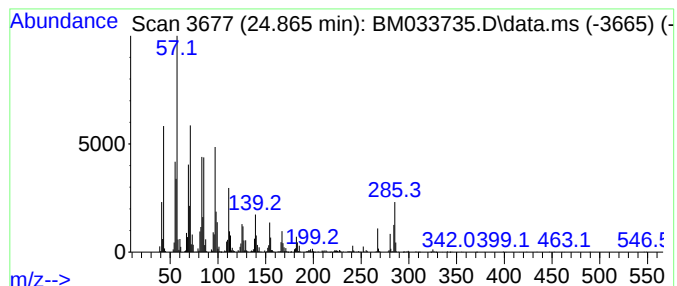
Instrument :
BNA_M
ClientSampleId :
EFF-WW

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 1-Dodecanol, 2-octyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.865	3.75 ng	4641650	Perylene-d12	23.912	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	81
2	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	76
3	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	68
4	Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	68
5	Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM011422\
Data File : BM033735.D
Acq On : 14 Jan 2022 19:24
Operator : CG/JU
Sample : N1157-02 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EFF-WW

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.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
1-Hexanol, 2-et...	8.254	20.0	ng	386867000	1	7.966	386867000	20.0
Hexanoic acid, ...	9.478	50.5	ng	11904100	2	10.783	4714650	20.0
Hexanoic acid, ...	9.854	72.7	ng	17125100	2	10.783	4714650	20.0
Octanoic acid	10.266	20.0	ng	4714650	2	10.783	4714650	20.0
Dodecanoic acid	15.089	20.0	ng	19009100	3	14.601	19009100	20.0
Hexanoic acid, ...	15.936	21.8	ng	20684500	3	14.601	19009100	20.0
Tetradecanoic acid	16.754	20.0	ng	3978270	4	17.336	3978270	20.0
n-Hexadecanoic ...	18.242	28.0	ng	5562400	4	17.336	3978270	20.0
Palmitoleic acid	19.395	22.8	ng	4528590	4	17.336	3978270	20.0
Hexanoic acid, ...	20.230	36.3	ng	7880800	5	21.500	4346800	20.0
1-Decanol, 2-oc...	20.324	28.7	ng	6241100	5	21.500	4346800	20.0
Carbonic acid, ...	22.130	20.0	ng	4346800	5	21.500	4346800	20.0
Oxiraneoctanoic...	23.253	20.0	ng	24751800	6	23.912	24751800	20.0
1-Dodecanol, 2-...	24.865	3.8	ng	4641650	6	23.912	24751800	20.0