

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061125\
 Data File : BF142732.D
 Acq On : 11 Jun 2025 13:52
 Operator : RC/JU
 Sample : Q2264-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EF-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_F\Methods\8270-BF061125.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142732.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.534	44	58	64	rBV	903285	1890197	1.74%	1.112%
2	7.175	803	847	853	rBV	9783822	108857761	100.00%	64.059%
3	10.257	1345	1371	1379	rBV	3431548	16597652	15.25%	9.767%
4	10.957	1482	1490	1491	rBV	1095421	1349793	1.24%	0.794%
5	10.980	1491	1494	1497	rVV	2406488	3665687	3.37%	2.157%
6	11.010	1497	1499	1508	rVV	1476414	2113058	1.94%	1.243%
7	11.104	1508	1515	1521	rVV	899582	1533946	1.41%	0.903%
8	11.957	1654	1660	1663	rVV	1017242	1655613	1.52%	0.974%
9	11.998	1663	1667	1679	rVB	990868	1696019	1.56%	0.998%
10	12.510	1748	1754	1760	rBV	3182529	4400702	4.04%	2.590%
11	12.669	1773	1781	1788	rBV	1400430	2542725	2.34%	1.496%
12	13.010	1834	1839	1844	rBV	1045337	1326822	1.22%	0.781%
13	13.910	1987	1992	1999	rBV	1034146	1383096	1.27%	0.814%
14	14.539	2094	2099	2104	rVV	2772526	3887992	3.57%	2.288%
15	15.257	2210	2221	2233	rVB	6092391	15691574	14.41%	9.234%
16	16.486	2421	2430	2436	rBV	644778	1339724	1.23%	0.788%

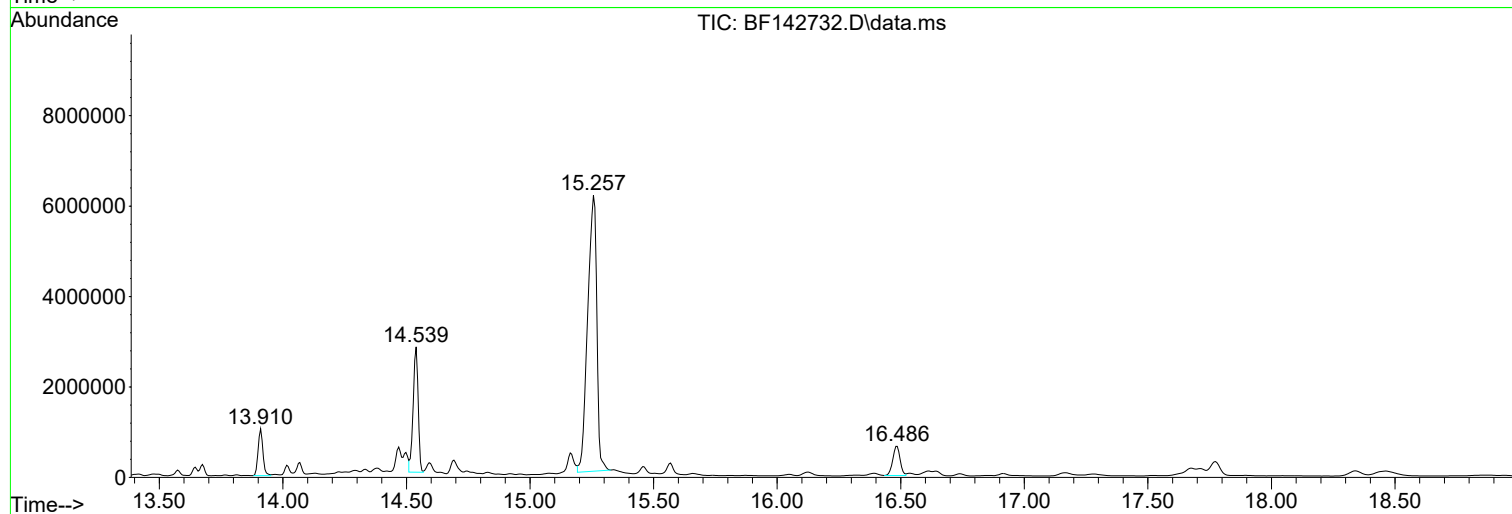
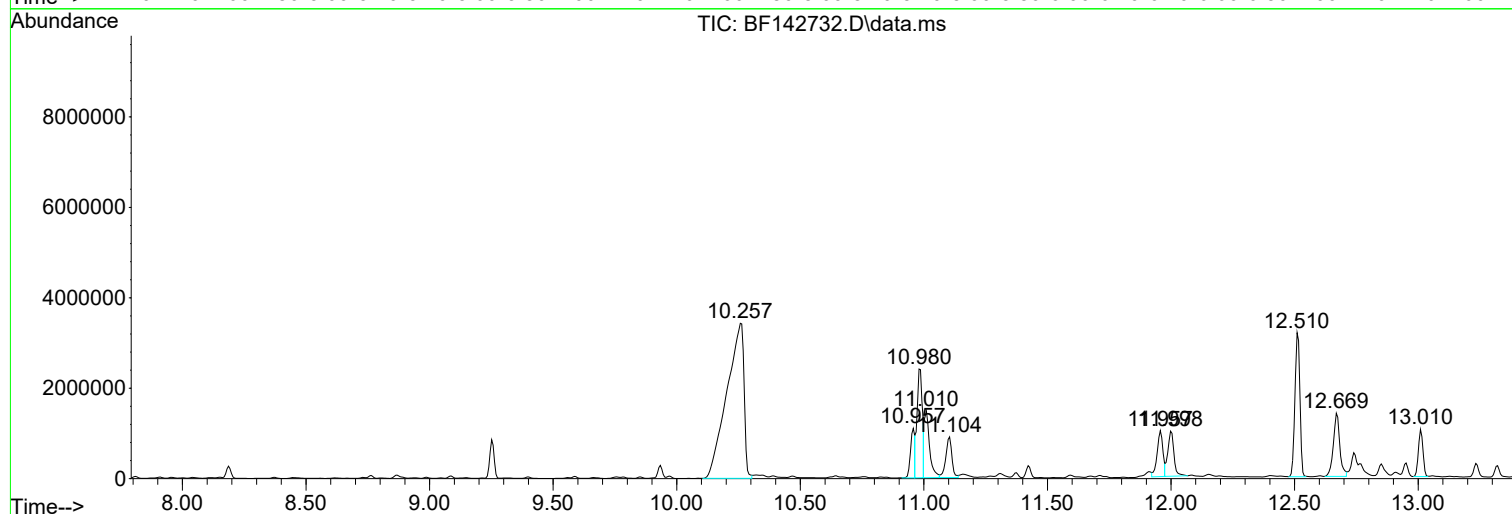
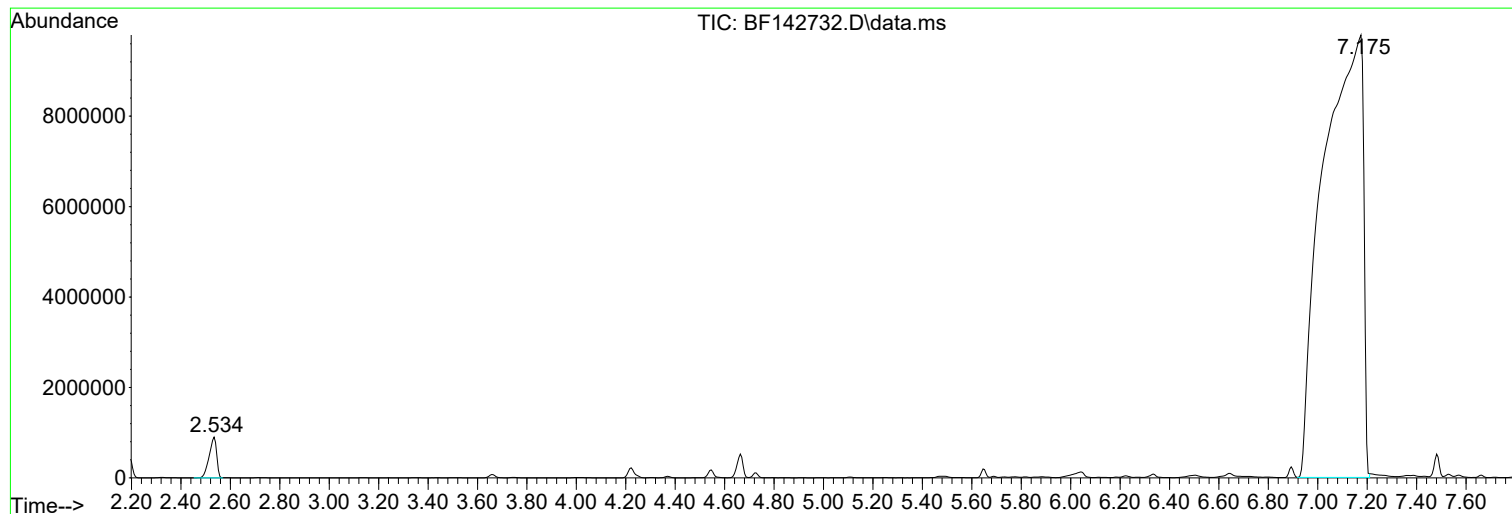
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061125.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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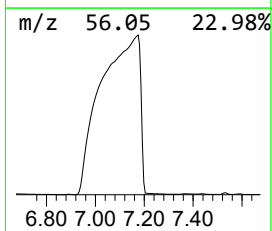
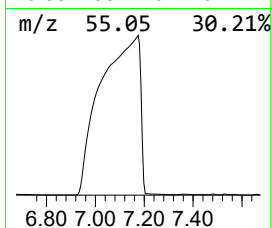
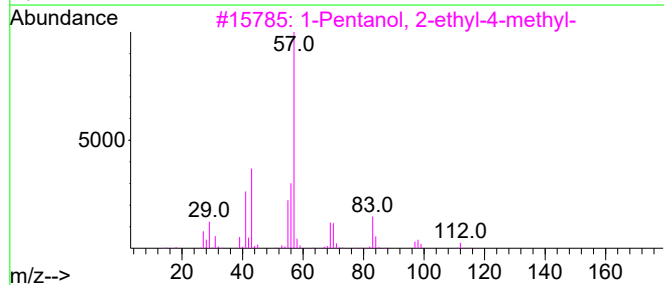
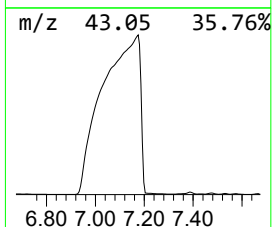
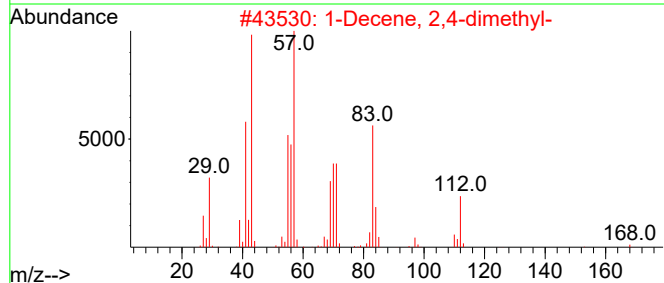
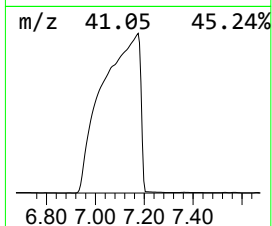
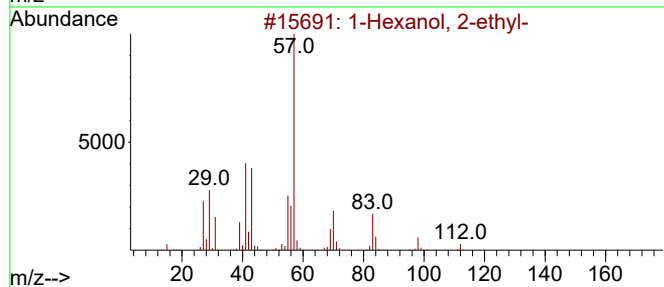
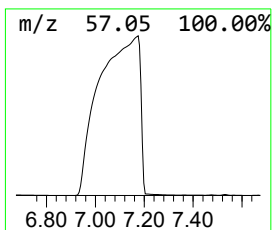
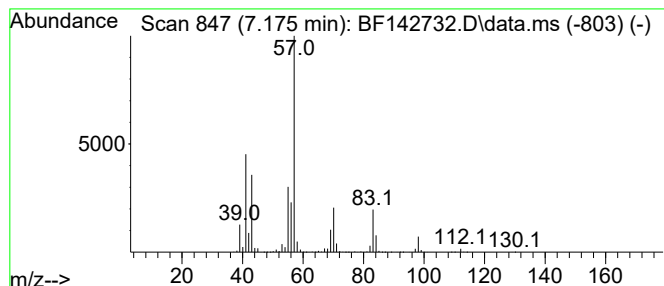
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061125.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
7.175	20.00 ng	108858000	1,4-Dichlorobenzene-d4	6.892

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2		1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	53
3		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
4		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	45



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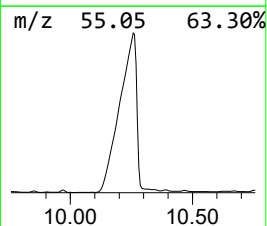
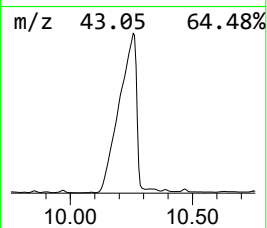
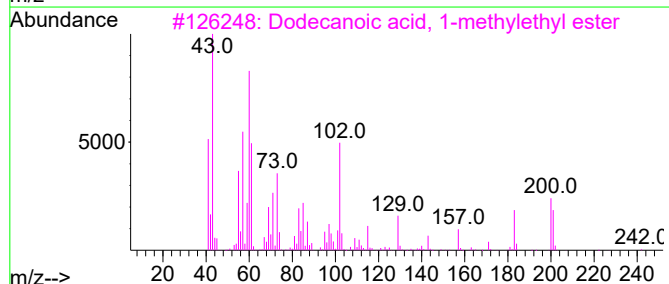
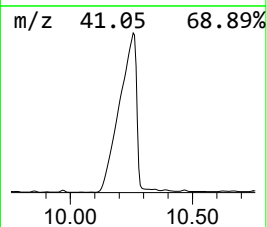
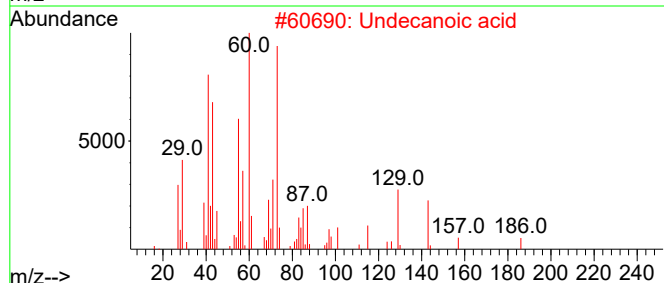
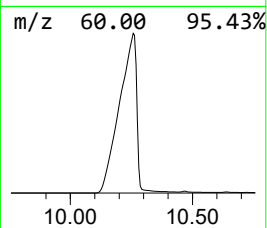
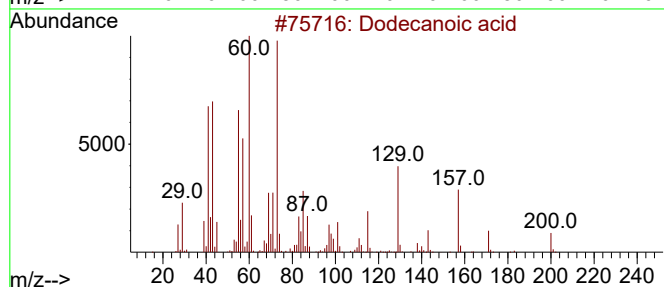
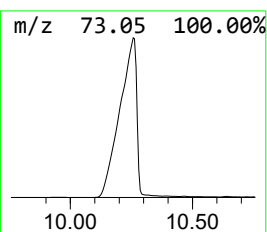
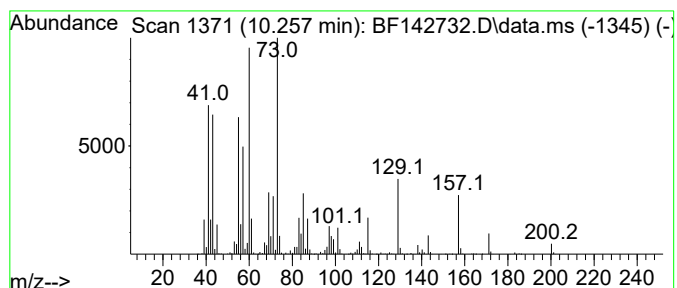
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Dodecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.257	20.00 ng	16597700	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	98
2			Undecanoic acid	186	C11H22O2	000112-37-8	64
3			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	59
4			Nonanoic acid	158	C9H18O2	000112-05-0	58
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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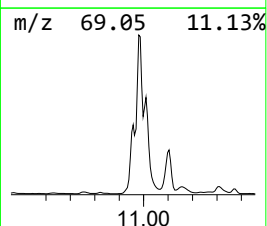
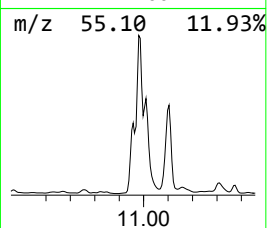
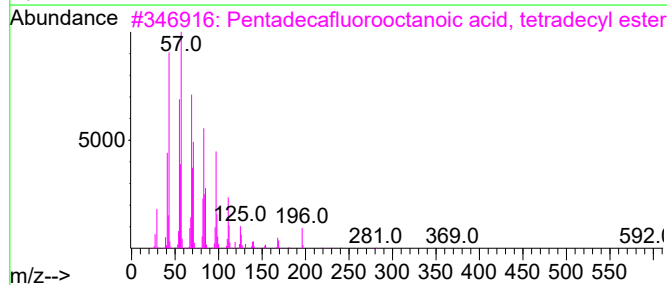
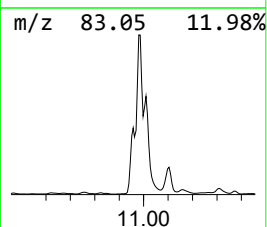
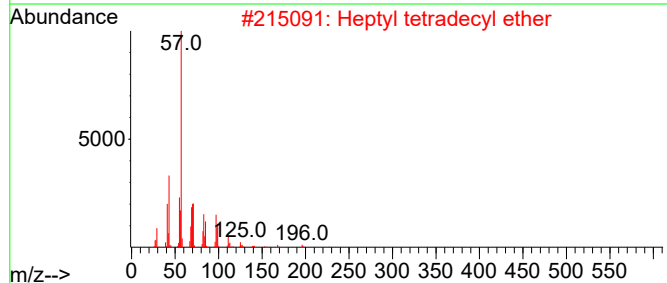
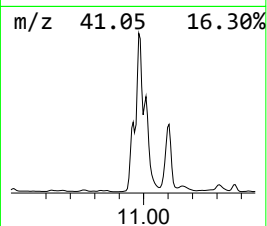
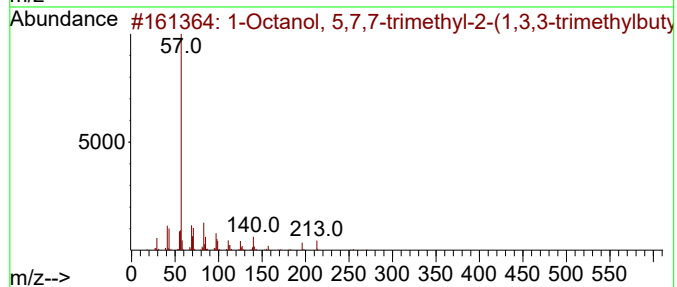
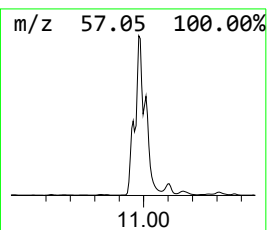
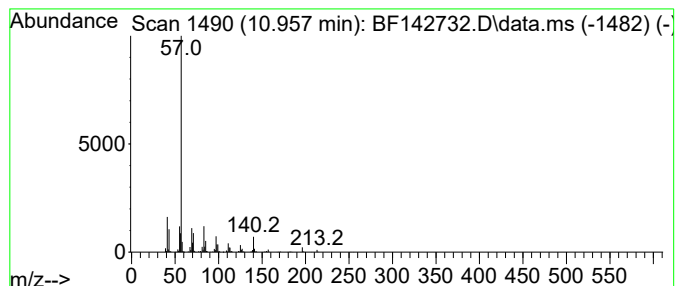
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Octanol, 5,7,7-trimethyl-... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.957	17.60 ng	1349790	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 5,7,7-trimethyl-2-(1,...	270	C18H38O	036400-98-3	80		
2	Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	78		
3	Pentadecafluorooctanoic acid, te...	610	C22H29F15O2	1000406-04-4	53		
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	50		
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	50		



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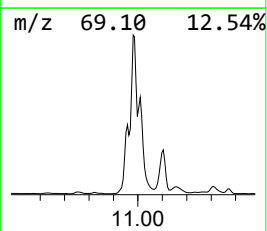
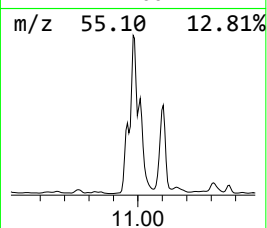
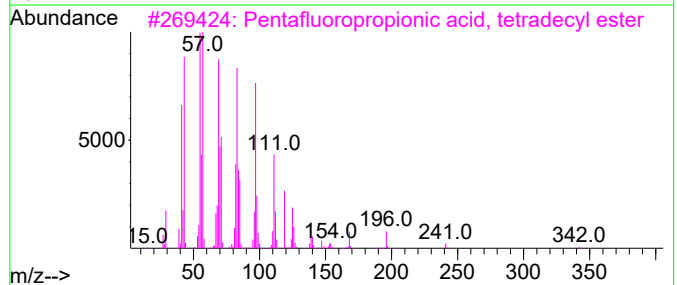
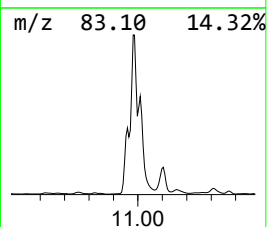
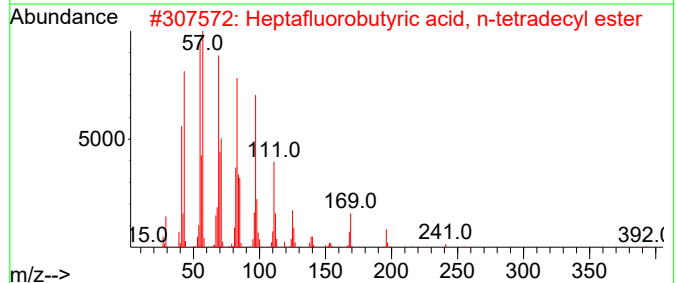
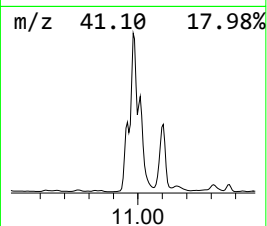
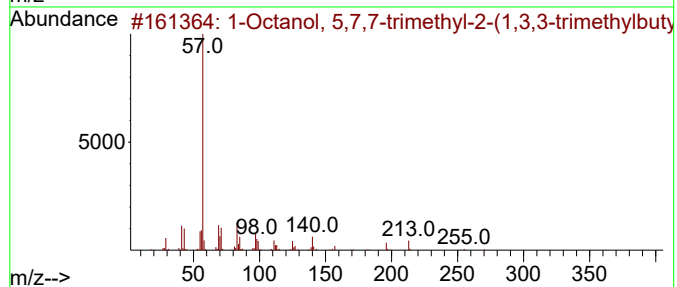
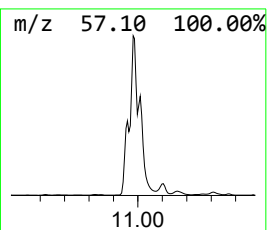
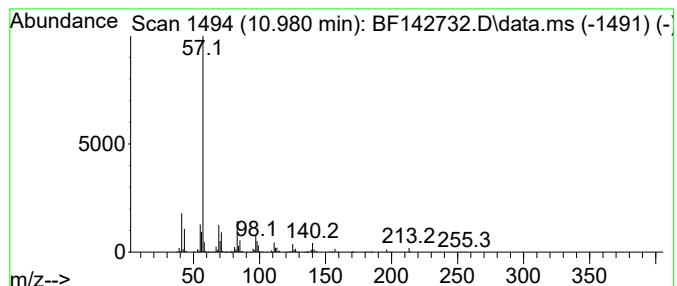
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Heptafluorobutyric acid, n-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.980	47.79 ng	3665690	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 5,7,7-trimethyl-2-(1,...	270	C18H38O	036400-98-3	90		
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	64		
3	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	64		
4	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	53		
5	1-Dodecanol, 3,7,11-trimethyl-	228	C15H32O	006750-34-1	53		



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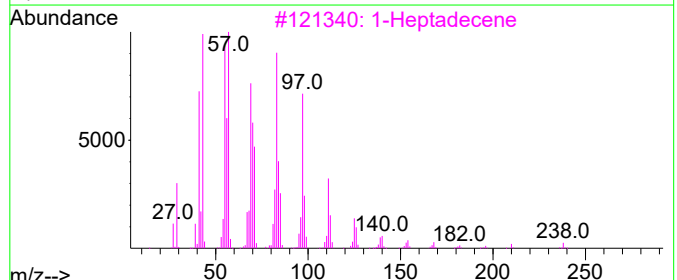
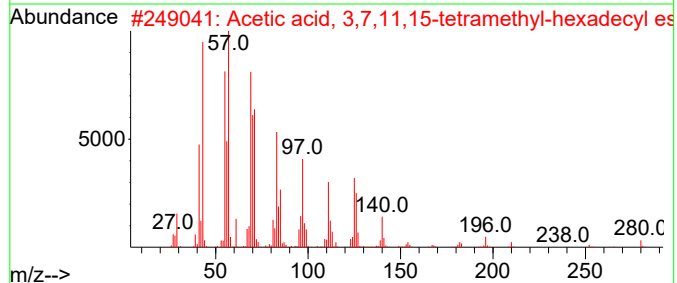
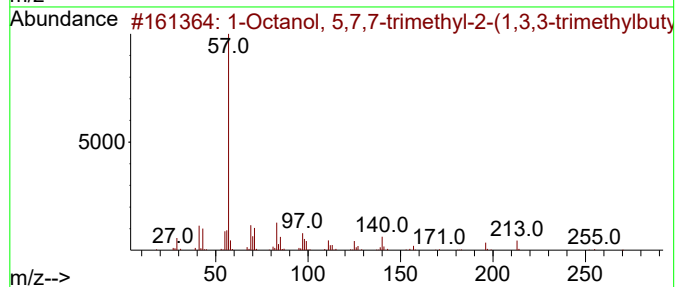
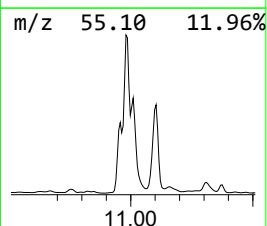
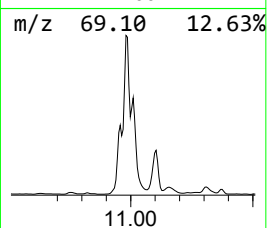
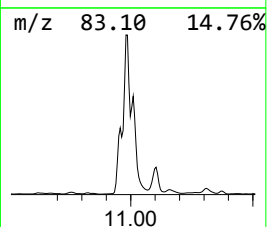
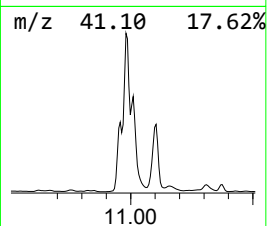
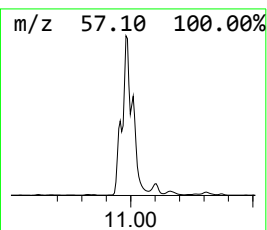
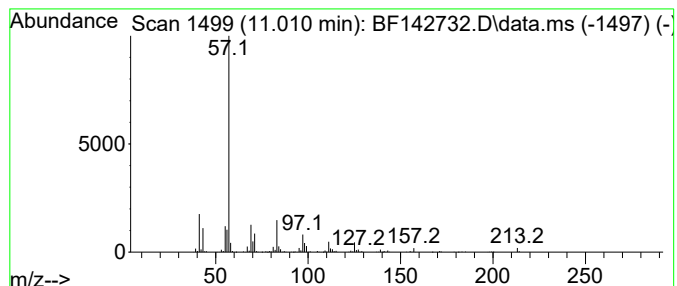
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Acetic acid, 3,7,11,15-tetr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.010	27.55 ng	2113060	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 5,7,7-trimethyl-2-(1,...	270	C18H38O	036400-98-3	64		
2	Acetic acid, 3,7,11,15-tetrameth...	340	C22H44O2	1000193-63-0	59		
3	1-Heptadecene	238	C17H34	006765-39-5	59		
4	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	53		
5	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	53		



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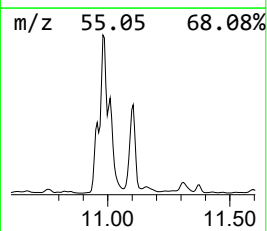
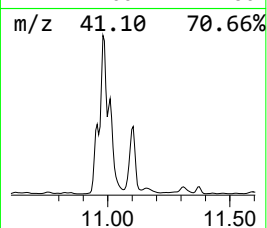
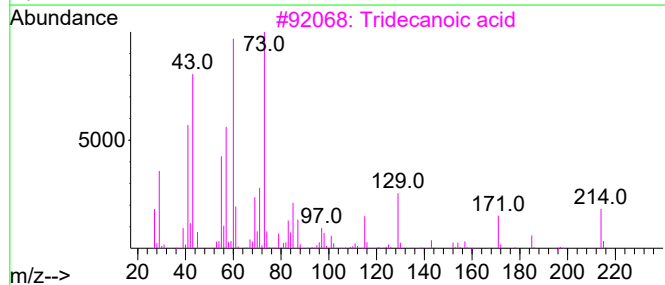
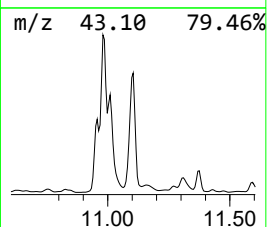
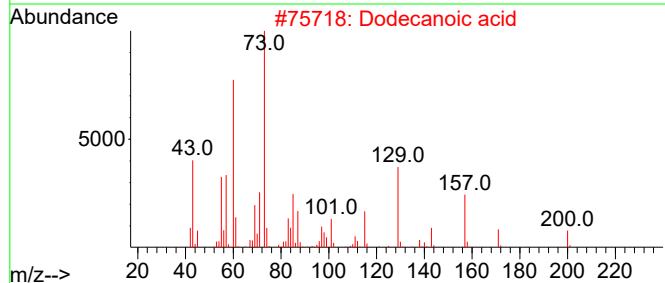
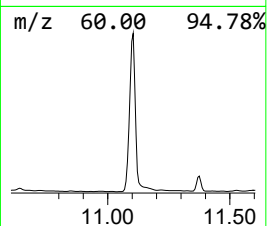
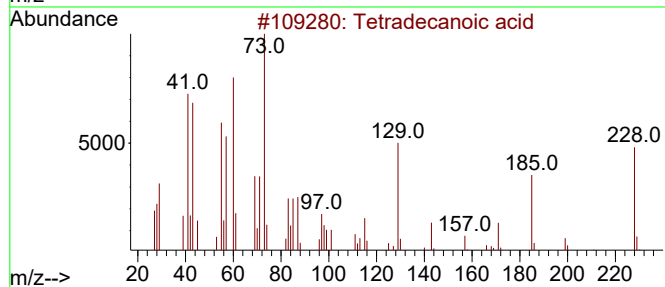
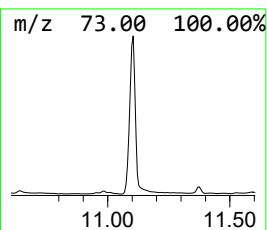
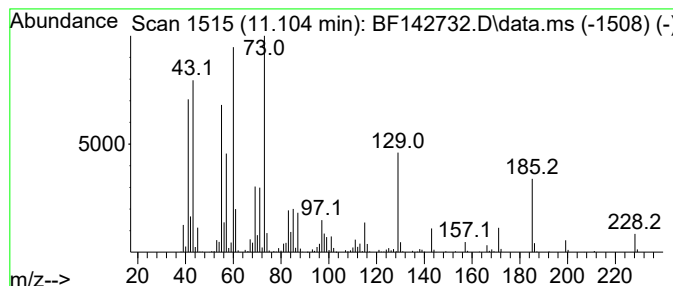
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ClientSampleId :
EF-WW

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061125.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetradecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.104	20.00 ng	1533950	Phenanthrene-d10		11.422	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tetradecanoic acid		228	C14H28O2	000544-63-8	94
2	Dodecanoic acid		200	C12H24O2	000143-07-7	72
3	Tridecanoic acid		214	C13H26O2	000638-53-9	72
4	Undecanoic acid		186	C11H22O2	000112-37-8	64
5	n-Decanoic acid		172	C10H20O2	000334-48-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061125\
Data File : BF142732.D
Acq On : 11 Jun 2025 13:52
Operator : RC/JU
Sample : Q2264-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EF-WW

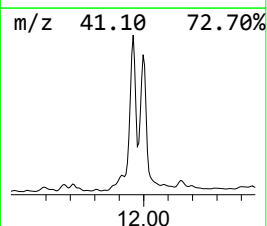
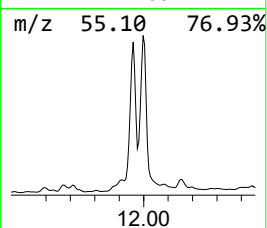
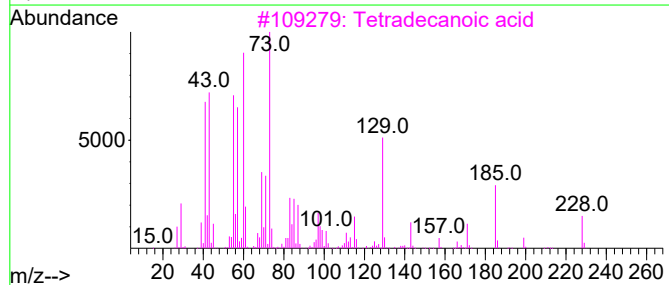
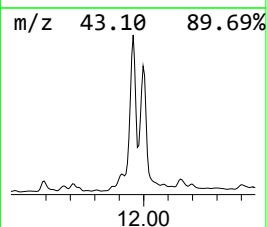
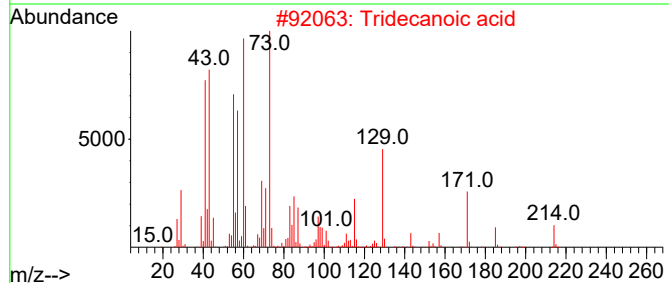
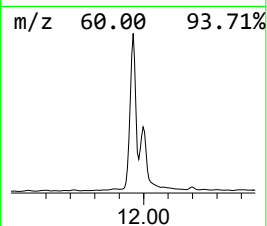
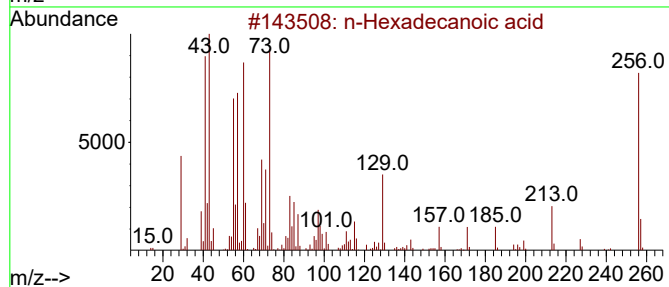
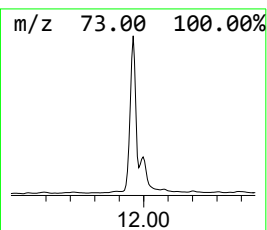
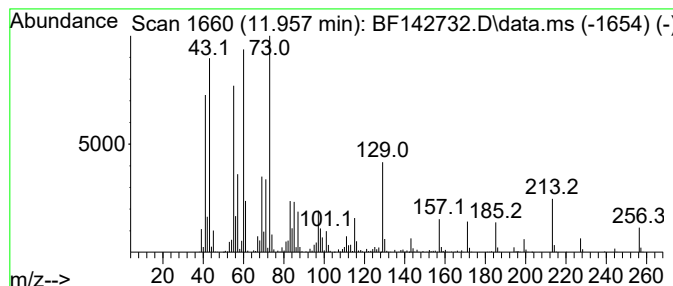
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	21.59 ng	1655610	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061125\
Data File : BF142732.D
Acq On : 11 Jun 2025 13:52
Operator : RC/JU
Sample : Q2264-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

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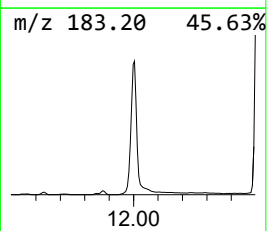
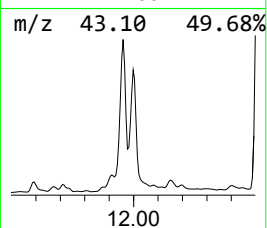
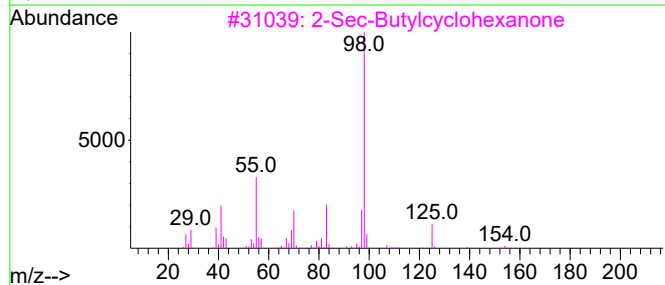
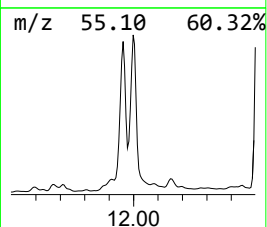
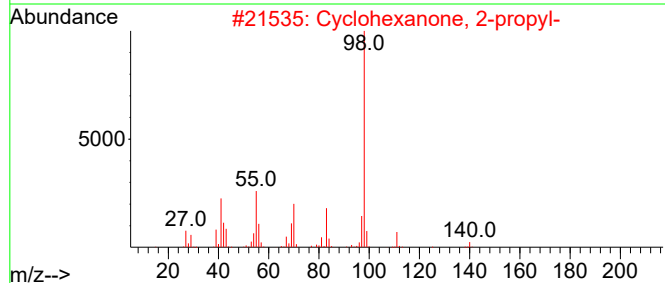
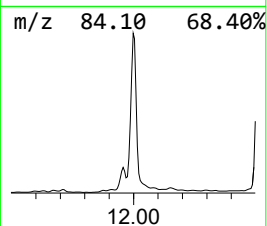
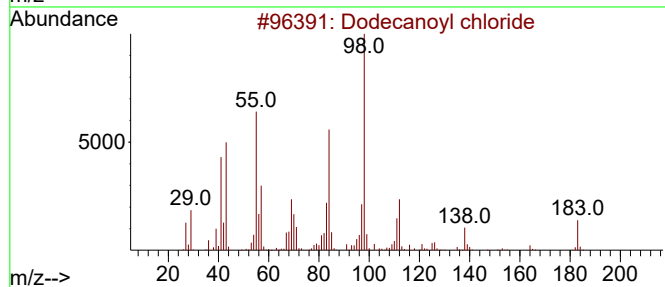
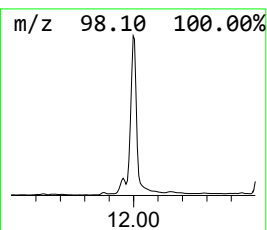
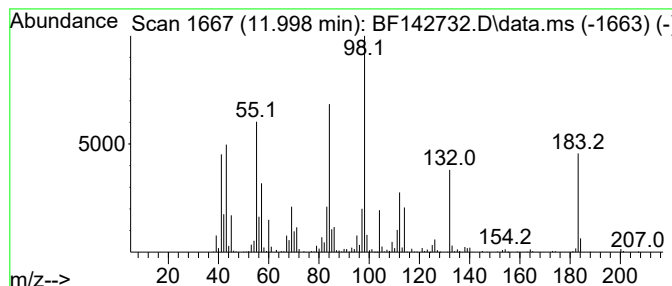
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown11.998 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.998	22.11 ng	1696020	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoyl chloride	218	C12H23ClO	000112-16-3	49
2			Cyclohexanone, 2-propyl-	140	C9H16O	000094-65-5	38
3			2-Sec-Butylcyclohexanone	154	C10H18O	014765-30-1	25
4			Cyclohexanone, 2-isobutyl-	154	C10H18O	004668-64-8	25
5			Methyl 5-piperidino-4-ketocaproate	213	C11H19NO3	018904-36-4	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061125\
Data File : BF142732.D
Acq On : 11 Jun 2025 13:52
Operator : RC/JU
Sample : Q2264-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

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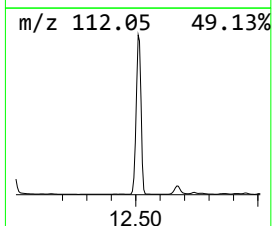
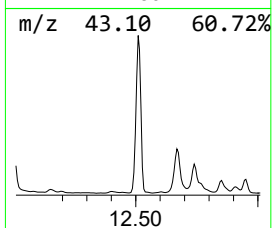
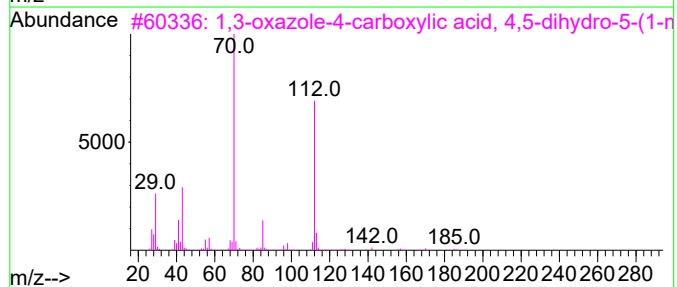
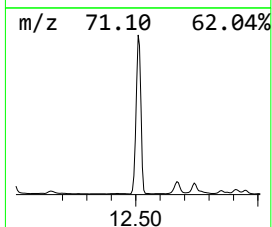
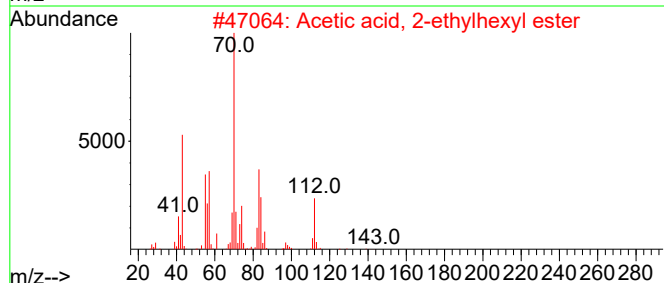
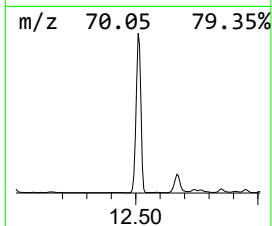
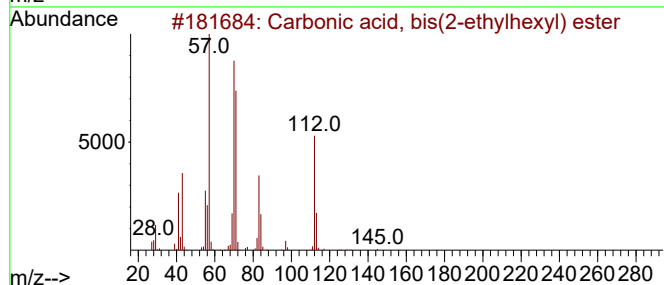
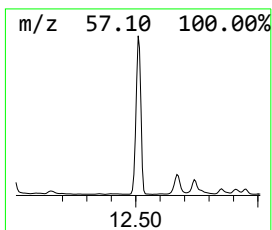
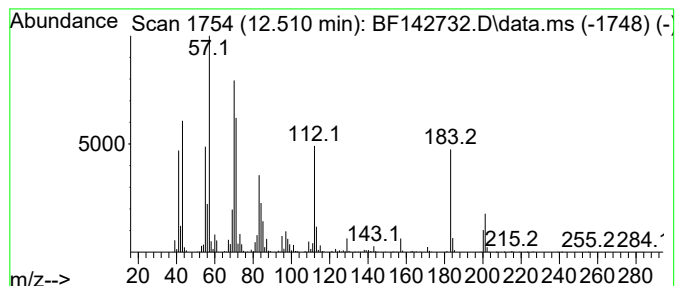
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Carbonic acid, bis(2-ethylh... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.510	57.38 ng	4400700	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, bis(2-ethylhexyl)...	286	C17H34O3	014858-73-2	52
2			Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	47
3			1,3-oxazole-4-carboxylic acid, 4...	185	C9H15NO3	1000197-69-0	43
4			Carbonic acid, decyl 2-ethylhexy...	314	C19H38O3	1000383-13-7	38
5			Heptane, 3-ethyl-4-methyl-	142	C10H22	052896-91-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061125\
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Sample : Q2264-04
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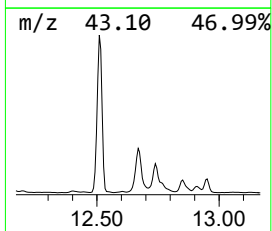
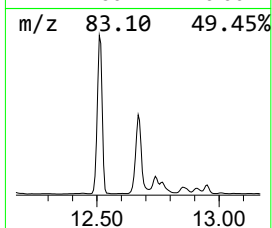
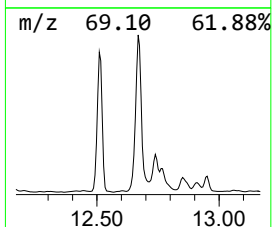
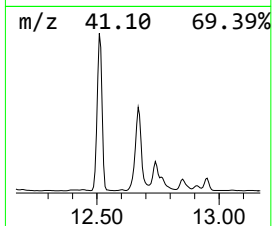
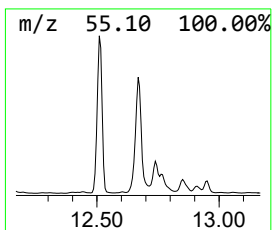
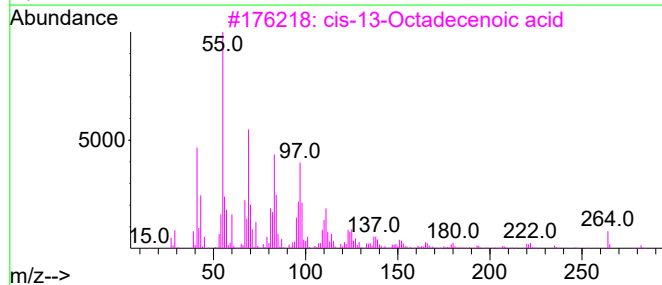
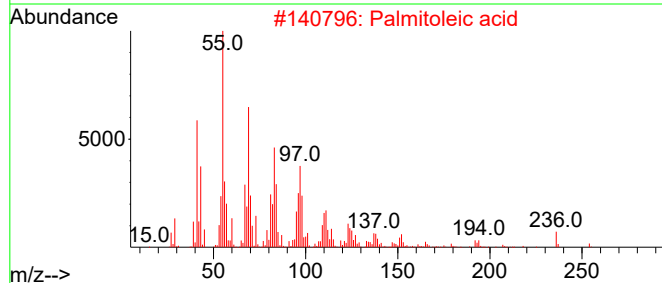
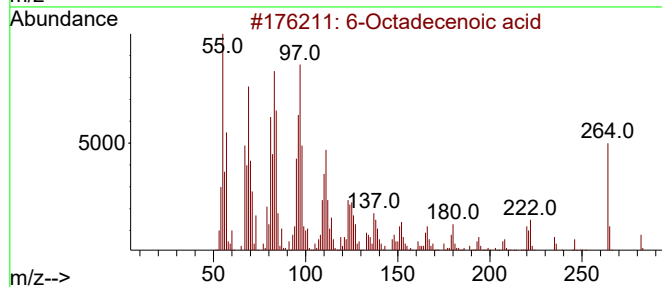
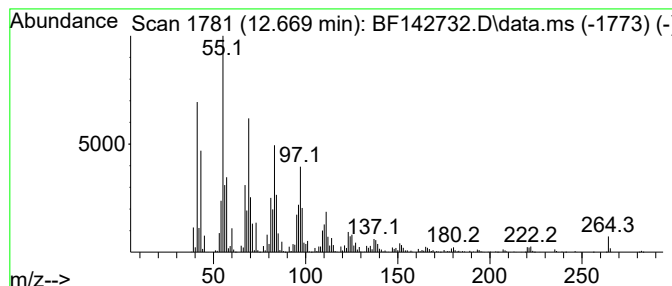
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 6-Octadecenoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.669	33.15 ng	2542730	Phenanthrene-d10	11.422	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid	282	C18H34O2	1000336-66-8	98
2	Palmitoleic acid	254	C16H30O2	000373-49-9	95
3	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	94
4	cis-Vaccenic acid	282	C18H34O2	000506-17-2	94
5	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061125\
Data File : BF142732.D
Acq On : 11 Jun 2025 13:52
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Sample : Q2264-04
Misc :
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Instrument :
BNA_F
ClientSampleId :
EF-WW

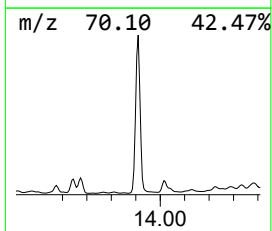
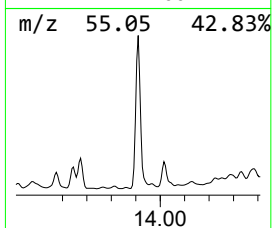
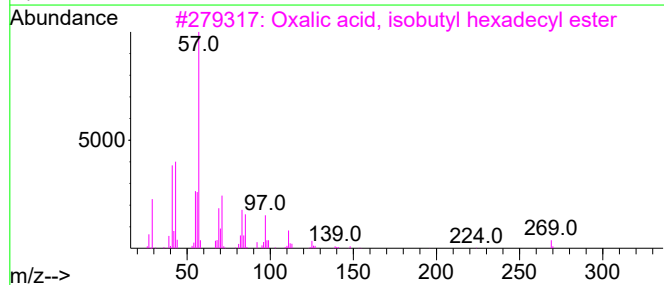
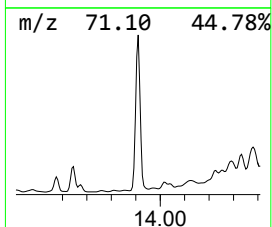
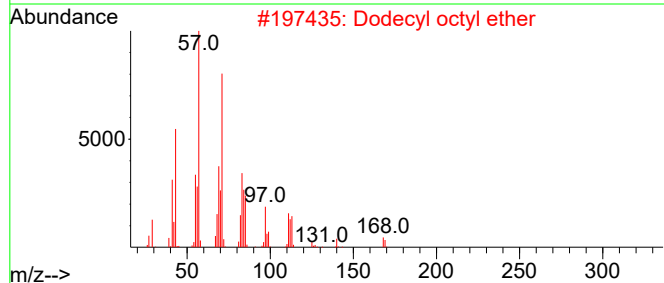
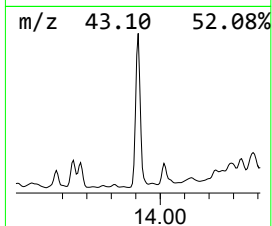
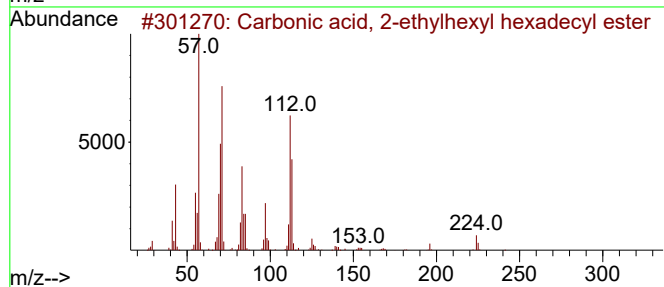
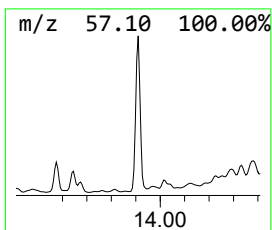
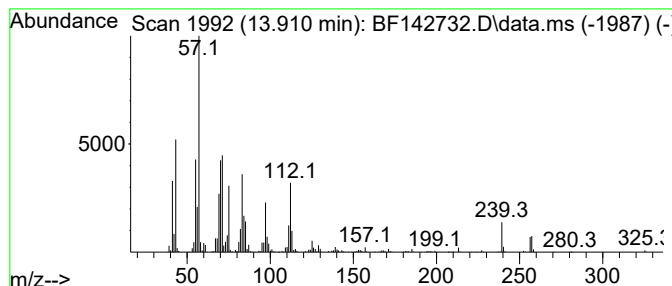
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Carbonic acid, 2-ethylhexyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	20.00 ng	1383100	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, 2-ethylhexyl hexa...	398	C25H50O3	1000383-14-3	58
2			Dodecyl octyl ether	298	C20H42O	1000406-38-4	49
3			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	49
4			1-Undecene, 8-methyl-	168	C12H24	074630-40-3	43
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061125\
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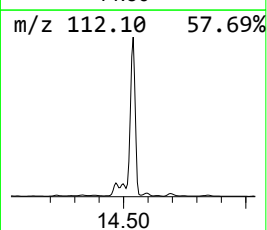
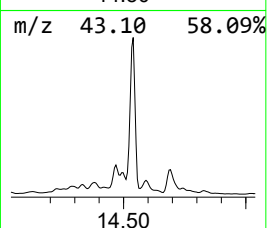
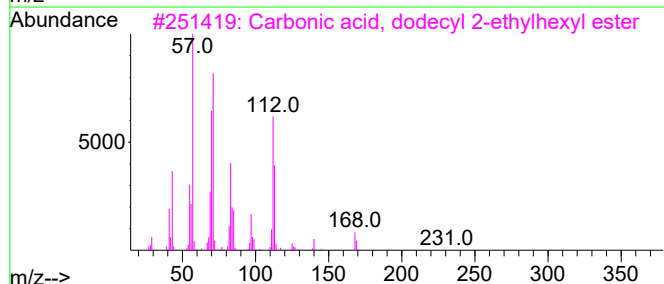
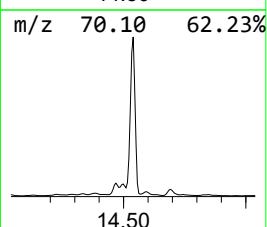
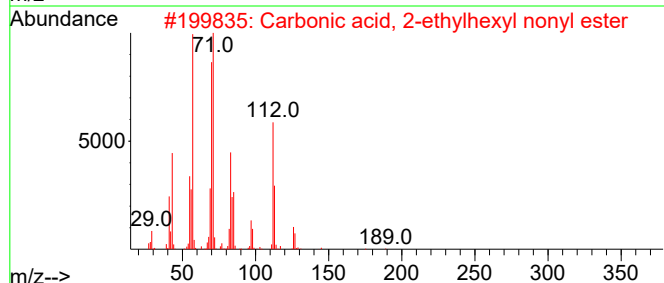
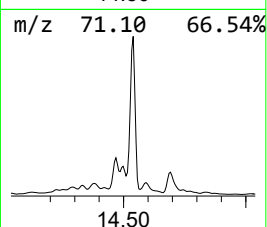
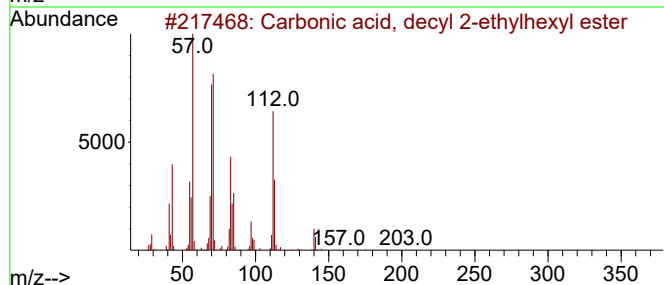
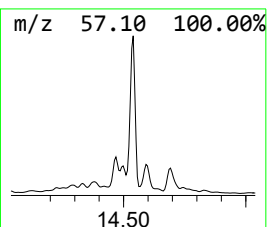
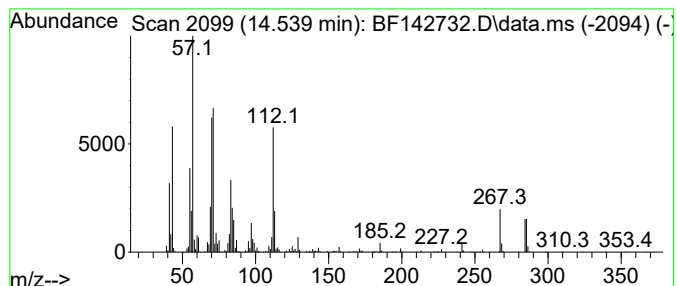
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Carbonic acid, decyl 2-ethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.539	56.22 ng	3887990	Chrysene-d12	14.068	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, decyl 2-ethylhexy...	314	C19H38O3	1000383-13-7	60
2	Carbonic acid, 2-ethylhexyl nony...	300	C18H36O3	1000383-13-6	58
3	Carbonic acid, dodecyl 2-ethylhe...	342	C21H42O3	1000383-13-9	58
4	Carbonic acid, 2-ethylhexyl octy...	286	C17H34O3	1000383-13-5	52
5	2-Ethylhexyl stearate	396	C26H52O2	022047-49-0	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061125\
Data File : BF142732.D
Acq On : 11 Jun 2025 13:52
Operator : RC/JU
Sample : Q2264-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EF-WW

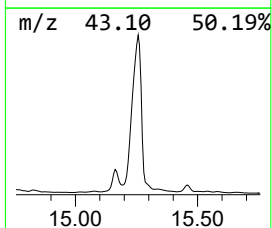
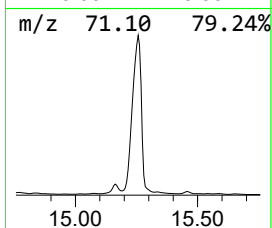
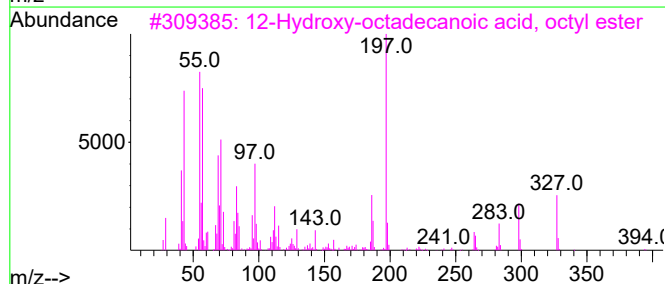
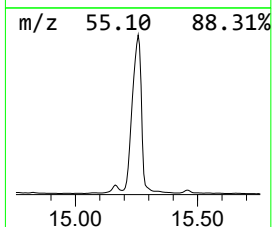
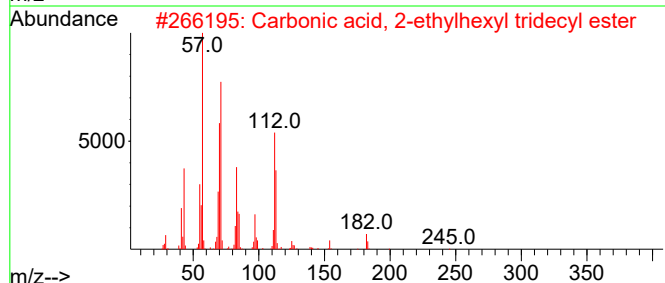
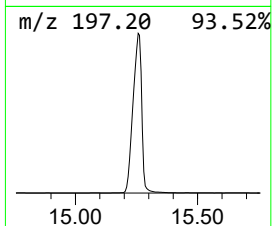
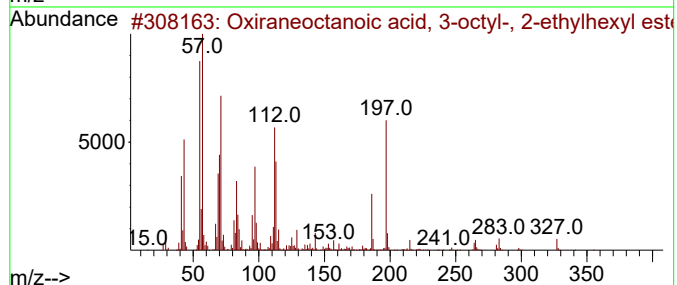
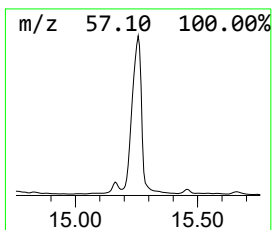
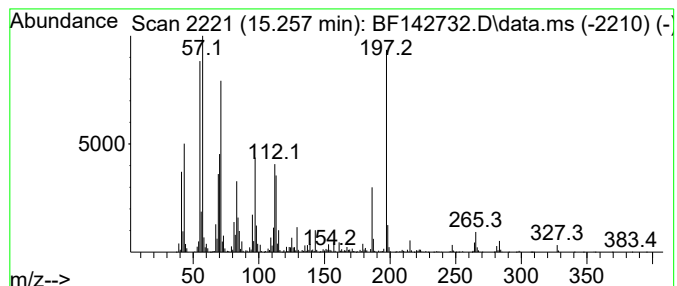
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061125.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Oxiraneoctanoic acid, 3-oct... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.257	20.00 ng	15691600	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxiraneoctanoic acid, 3-octyl-, ...	410	C26H50O3	000141-38-8	62
2			Carbonic acid, 2-ethylhexyl trid...	356	C22H44O3	1000383-14-0	46
3			12-Hydroxy-octadecanoic acid, oc...	412	C26H52O3	074819-90-2	43
4			Propanoic acid, 3-mercapto-, 2-e...	218	C11H22O2S	050448-95-8	38
5			Carbonic acid, 2-ethylhexyl tetr...	370	C23H46O3	1010383-14-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061125\
Data File : BF142732.D
Acq On : 11 Jun 2025 13:52
Operator : RC/JU
Sample : Q2264-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EF-WW

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061125.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...	7.175	20.0	ng	108858000	1	6.892	108858000	20.0
Dodecanoic acid	10.257	20.0	ng	16597700	3	9.933	16597700	20.0
1-Octanol, 5,7,...	10.957	17.6	ng	1349790	4	11.422	1533950	20.0
Heptafluorobuty...	10.980	47.8	ng	3665690	4	11.422	1533950	20.0
Acetic acid, 3,...	11.010	27.6	ng	2113060	4	11.422	1533950	20.0
Tetradecanoic acid	11.104	20.0	ng	1533950	4	11.422	1533950	20.0
n-Hexadecanoic ...	11.957	21.6	ng	1655610	4	11.422	1533950	20.0
unknown11.998	11.998	22.1	ng	1696020	4	11.422	1533950	20.0
Carbonic acid, ...	12.510	57.4	ng	4400700	4	11.422	1533950	20.0
6-Octadecenoic ...	12.669	33.1	ng	2542730	4	11.422	1533950	20.0
Carbonic acid, ...	13.910	20.0	ng	1383100	5	14.068	1383100	20.0
Carbonic acid, ...	14.539	56.2	ng	3887990	5	14.068	1383100	20.0
Oxiraneoctanoic...	15.257	20.0	ng	15691600	6	15.568	15691600	20.0