

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110423\
 Data File : BF136143.D
 Acq On : 04 Nov 2023 12:57
 Operator : CG\JU
 Sample : 05243-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-7D-AT-8-8.5

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-BF103023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136144.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.063	502	506	513	rVB	41717	52287	1.50%	0.237%
2	5.451	566	572	575	rBV	2686873	2699635	77.40%	12.213%
3	6.451	736	742	745	rBV	2313984	2731852	78.32%	12.358%
4	6.645	772	775	787	rVB	70734	73406	2.10%	0.332%
5	6.816	801	804	807	rBV	712012	534515	15.32%	2.418%
6	7.381	895	900	903	rBV	1948953	1829107	52.44%	8.275%
7	8.098	1018	1022	1025	rBV	942360	722425	20.71%	3.268%
8	9.180	1202	1206	1209	rBV	4237449	3401718	97.53%	15.389%
9	9.298	1222	1226	1230	rVB	73753	65618	1.88%	0.297%
10	9.857	1317	1321	1324	rBV	1052555	834813	23.93%	3.777%
11	10.651	1451	1456	1459	rBV	2441345	2263353	64.89%	10.239%
12	11.345	1571	1574	1578	rBV	1025914	873557	25.04%	3.952%
13	11.892	1660	1667	1681	rBV	518532	599132	17.18%	2.710%
14	12.680	1797	1801	1813	rVB	135999	150727	4.32%	0.682%
15	12.951	1842	1847	1850	rBV	3615783	3487988	100.00%	15.779%
16	13.886	1999	2006	2022	rBV5	77373	299531	8.59%	1.355%
17	14.004	2022	2026	2029	rVB	561355	515815	14.79%	2.333%
18	14.186	2050	2057	2064	rBV	34759	42743	1.23%	0.193%
19	14.886	2172	2176	2180	rBV	229227	229213	6.57%	1.037%
20	15.492	2273	2279	2285	rVB	442212	546341	15.66%	2.472%
21	16.221	2394	2403	2419	rVB10	34046	151563	4.35%	0.686%

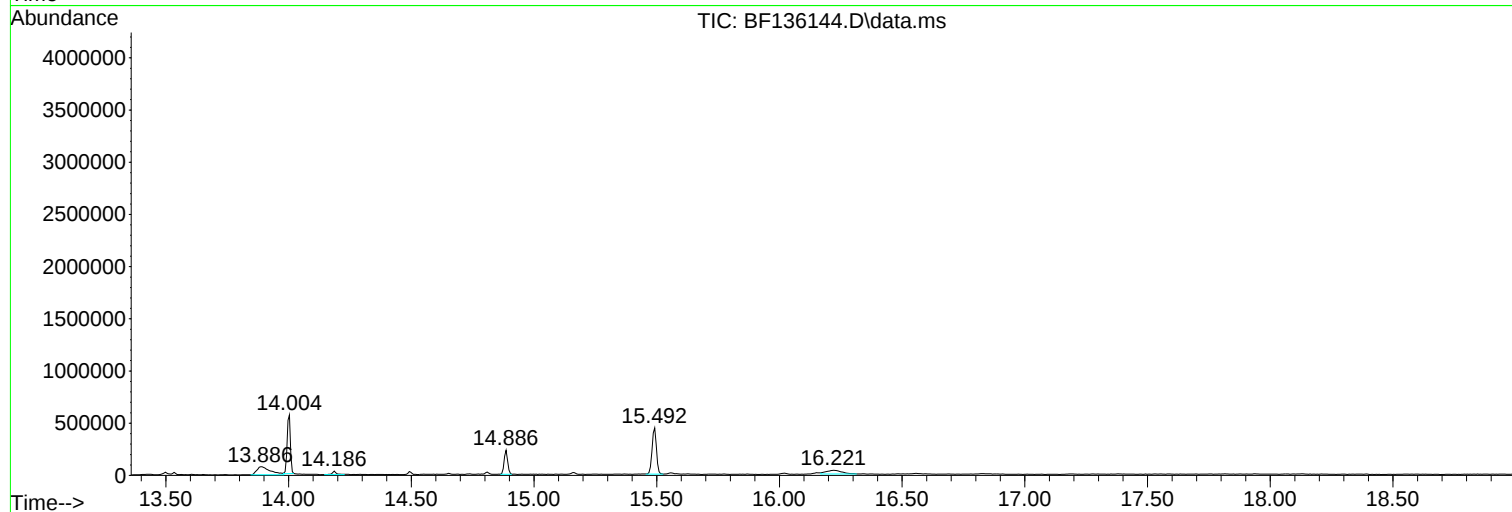
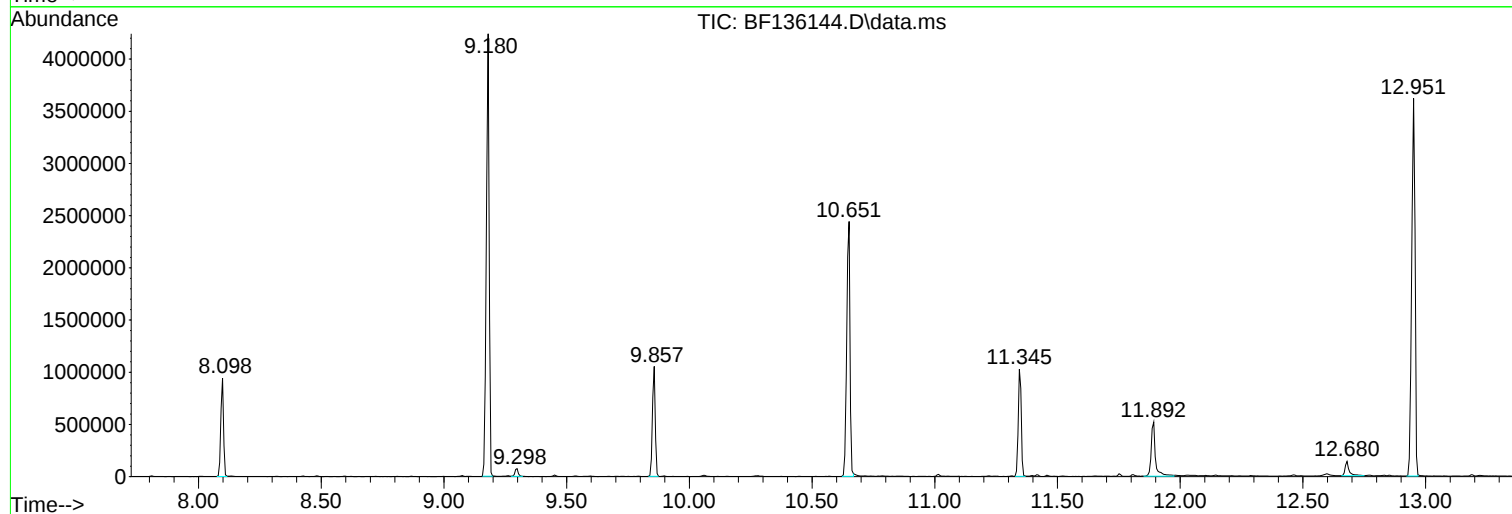
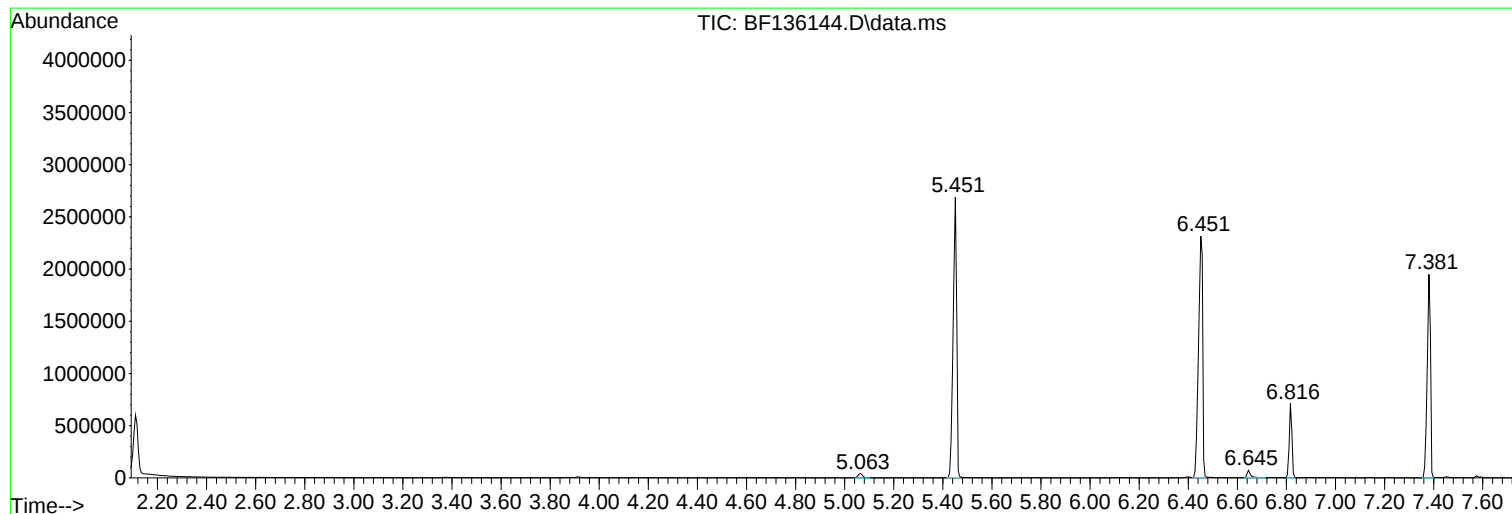
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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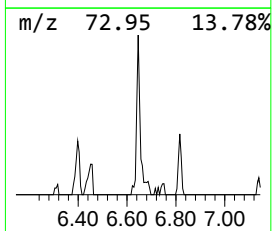
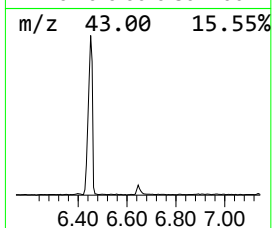
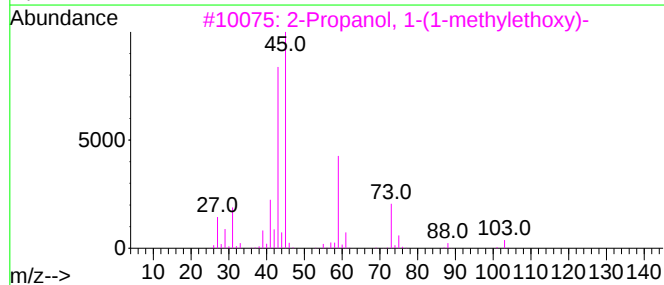
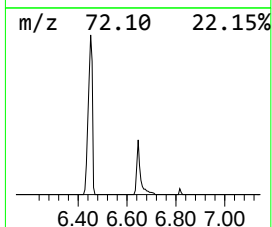
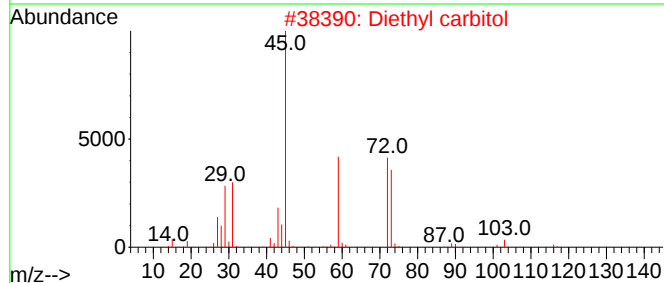
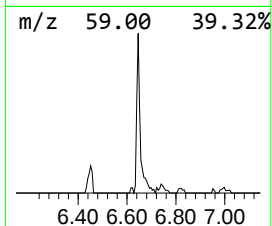
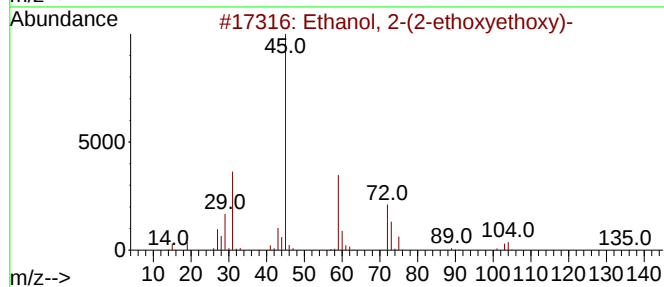
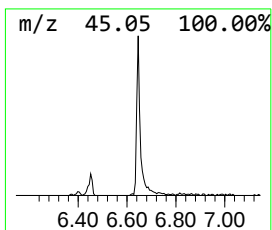
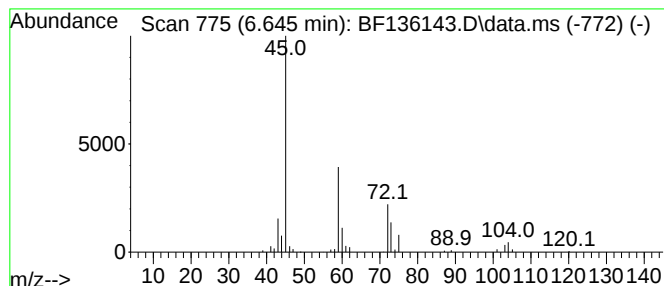
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.645	2.75 ng	73406	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Diethyl carbitol	162	C8H18O3	000112-36-7	72
3			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
4			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42
5			.beta.-Methoxyethoxymethyl chloride	124	C4H9ClO2	003970-21-6	38



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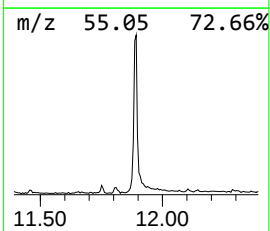
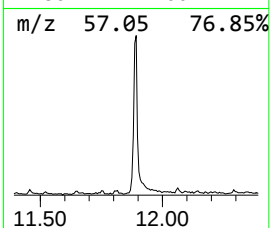
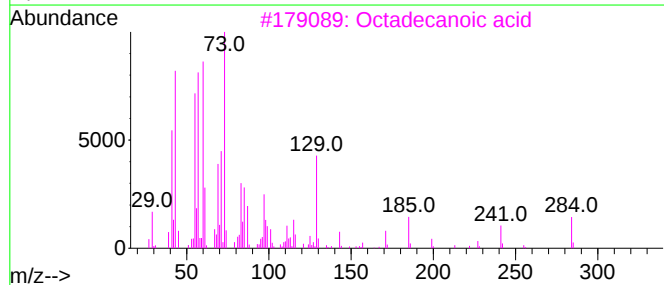
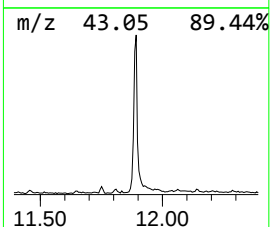
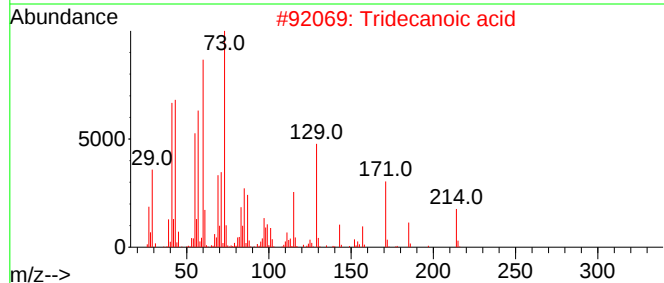
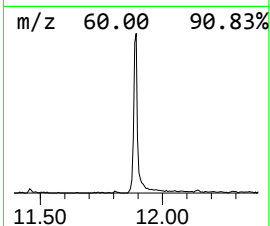
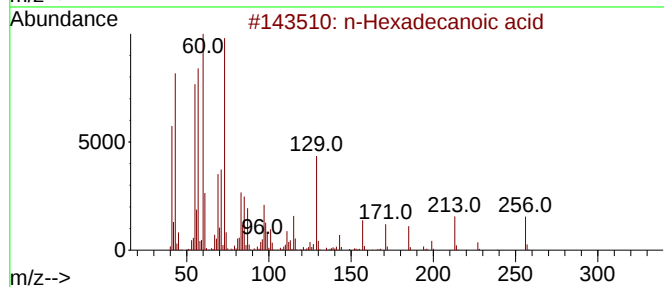
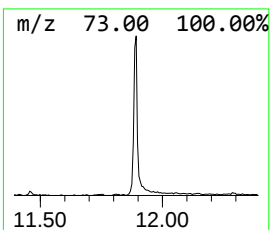
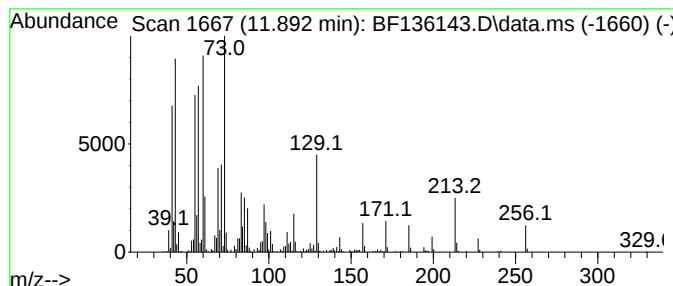
Instrument :
BNA_F
ClientSampleId :
SB-7D-AT-8-8.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.892	13.72 ng	599132	Phenanthrene-d10		11.345	
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	Octadecanoic acid		284	C18H36O2	000057-11-4	93
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	93
5	Pentadecanoic acid		242	C15H30O2	001002-84-2	93



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BNA_F
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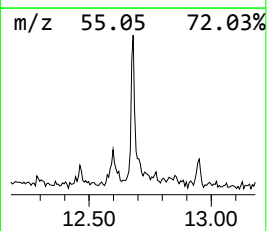
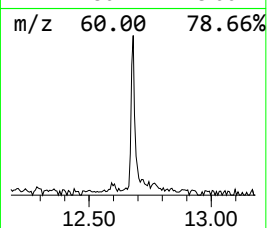
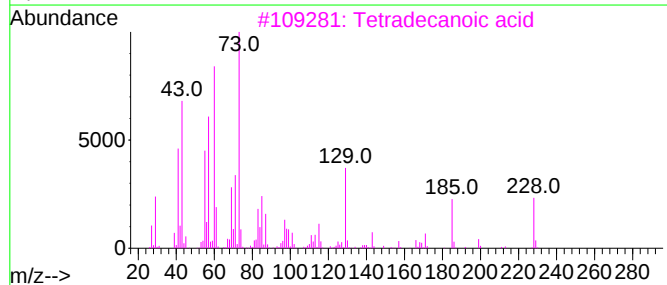
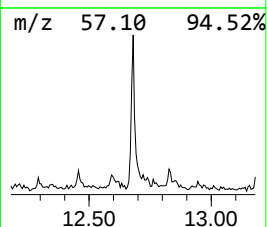
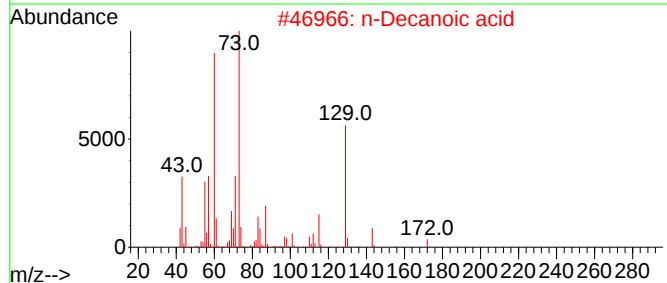
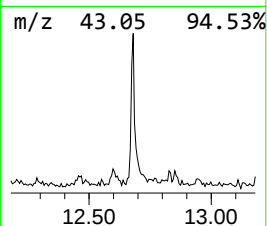
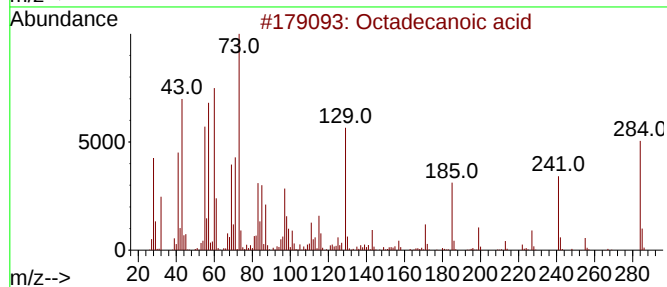
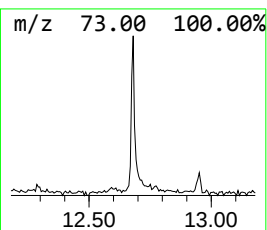
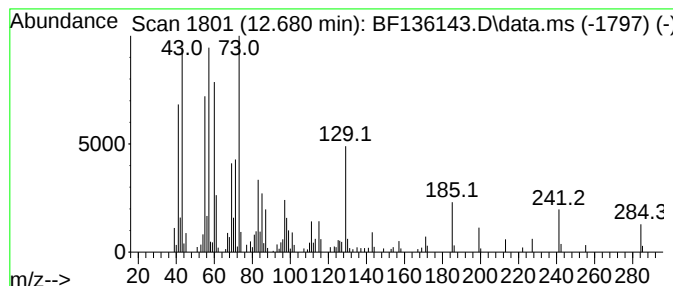
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	5.84 ng	150727	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Decanoic acid	172	C10H20O2	000334-48-5	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5			Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	30



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Sample : 05243-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-7D-AT-8-8.5

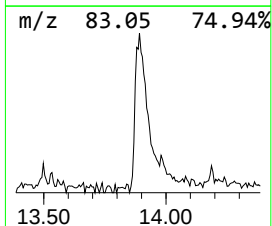
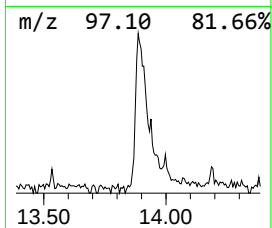
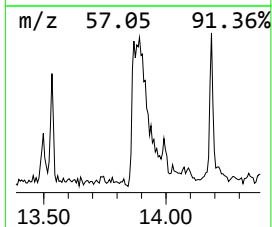
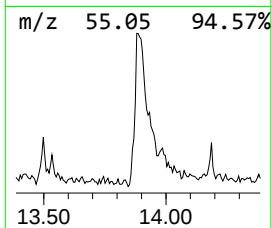
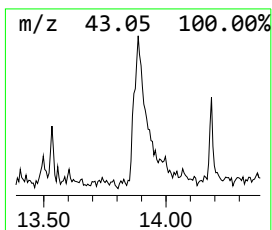
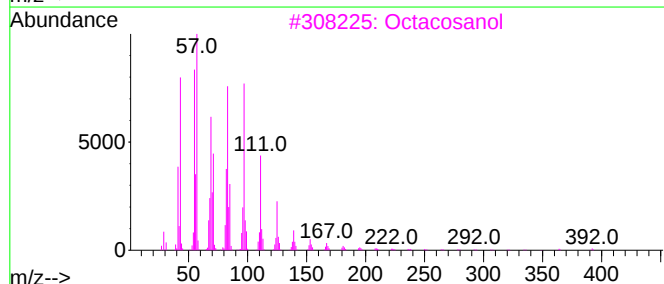
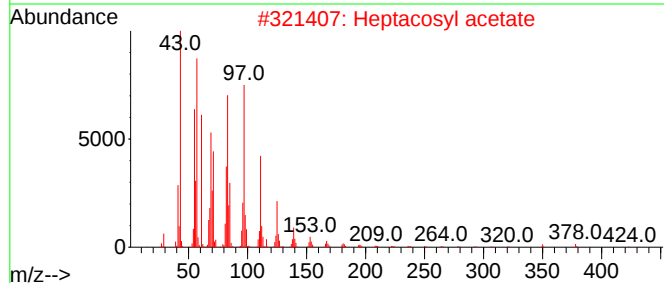
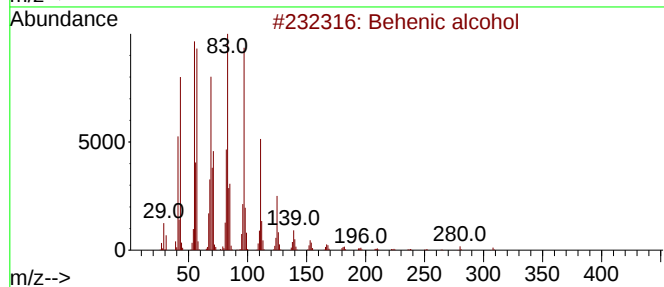
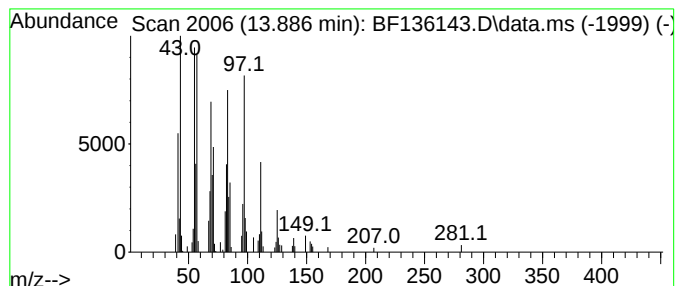
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Behenic alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	11.61 ng	299531	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	95
2			Heptacosyl acetate	438	C29H58O2	1000351-78-2	94
3			Octacosanol	410	C28H58O	000557-61-9	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5			1-Heptacosanol	396	C27H56O	002004-39-9	91



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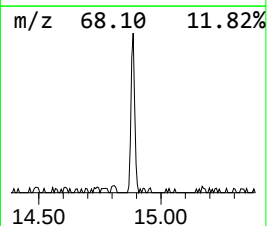
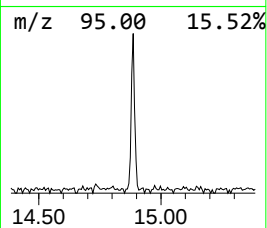
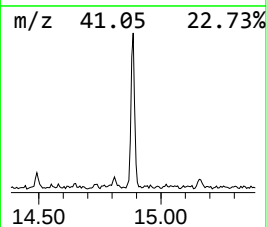
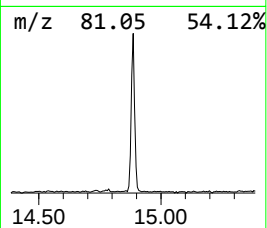
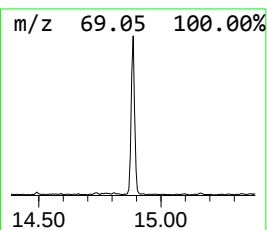
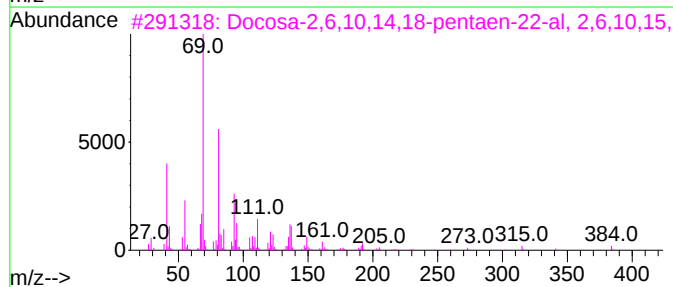
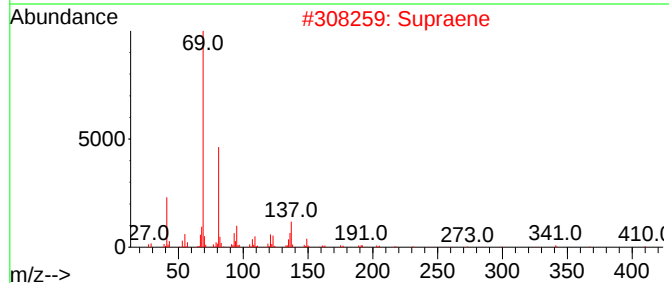
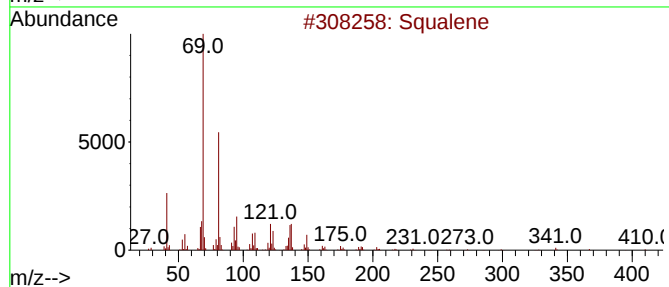
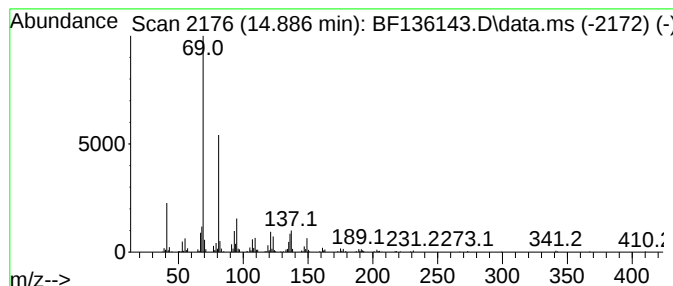
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.886	8.39 ng	229213	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	96
2			Supraene	410	C30H50	007683-64-9	93
3			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	83
5			trans-Farnesol	222	C15H26O	000106-28-5	64



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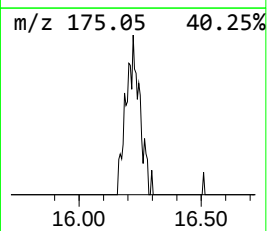
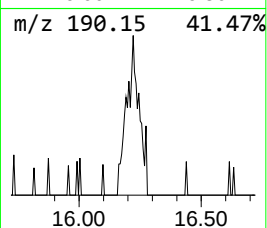
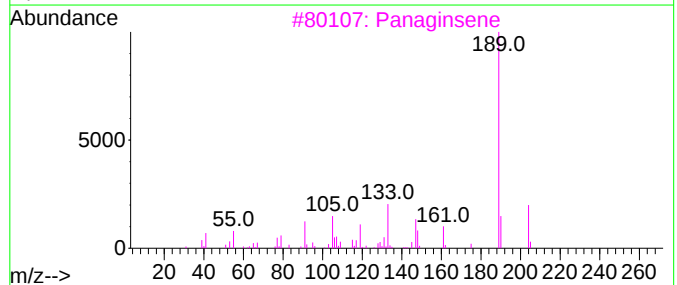
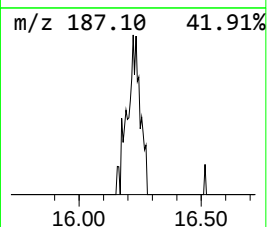
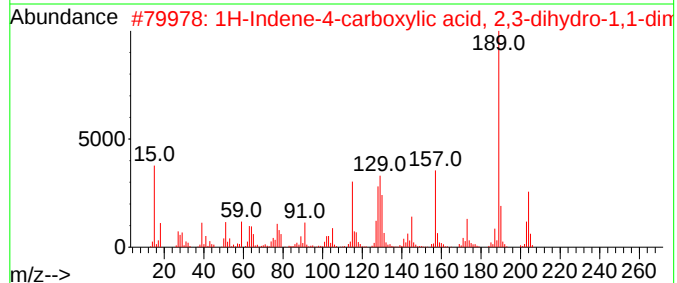
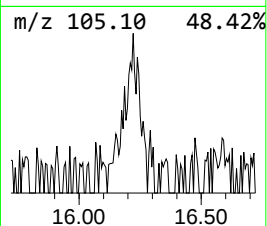
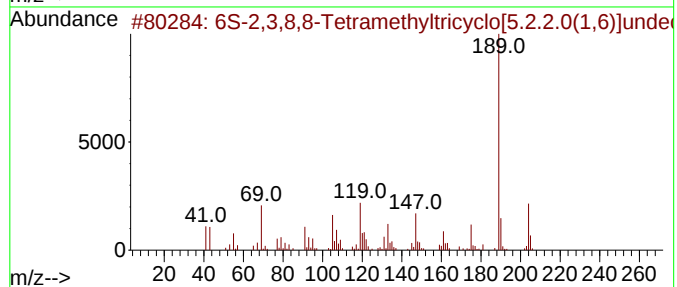
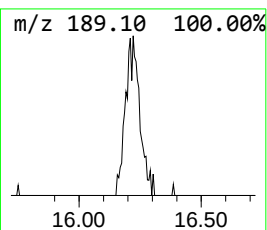
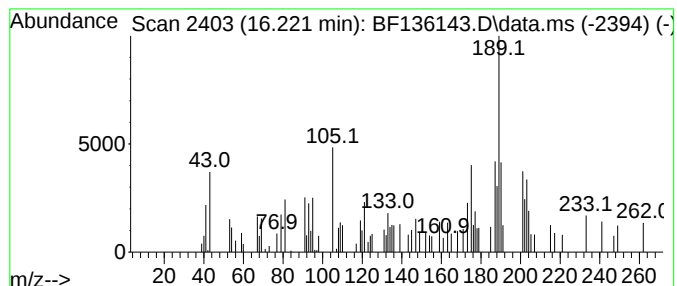
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown16.221 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.221	5.55 ng	151563	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6S-2,3,8,8-Tetramethyltricyclo[5...	204	C15H24	137235-48-4	30		
2	1H-Indene-4-carboxylic acid, 2,3...	204	C13H16O2	055591-11-2	27		
3	Panaginsene	204	C15H24	871660-96-7	25		
4	Ethanone, 1-[4-(trifluoromethoxy...	204	C9H7F3O2	085013-98-5	25		
5	(3-Aminophenyl)acetonitrile, TMS...	204	C11H16N2Si	1000474-30-8	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110423\
Data File : BF136143.D
Acq On : 04 Nov 2023 12:57
Operator : CG\JU
Sample : 05243-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-7D-AT-8-8.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.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
Ethanol, 2-(2-e...	6.645	2.8	ng	73406	1	6.816	534515	20.0
n-Hexadecanoic ...	11.892	13.7	ng	599132	4	11.345	873557	20.0
Octadecanoic acid	12.680	5.8	ng	150727	5	14.004	515815	20.0
Behenic alcohol	13.886	11.6	ng	299531	5	14.004	515815	20.0
Squalene	14.886	8.4	ng	229213	6	15.492	546341	20.0
unknown16.221	16.221	5.5	ng	151563	6	15.492	546341	20.0