

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011022\
 Data File : BF126570.D
 Acq On : 10 Jan 2022 17:03
 Operator : JU/CG
 Sample : N1054-13
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220022-CAPE-4-MODIFIED-ELUTRIATE

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-BF122921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126570.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.975	487	491	498	rVB	32097	39280	1.42%	0.258%
2	5.381	556	560	564	rBV	1505276	1492097	53.92%	9.813%
3	6.398	729	733	740	rBV	1245813	1172549	42.37%	7.711%
4	6.769	792	796	799	rBV	640515	508229	18.37%	3.342%
5	7.334	886	892	895	rBV	1769880	1846156	66.72%	12.141%
6	7.957	994	998	1010	rBV	430451	359698	13.00%	2.366%
7	8.051	1010	1014	1017	rBV	864357	708389	25.60%	4.659%
8	9.134	1192	1198	1201	rBV	2919222	2767084	100.00%	18.197%
9	9.810	1308	1313	1316	rBV	818688	728779	26.34%	4.793%
10	10.598	1442	1447	1451	rBV	1640223	1591706	57.52%	10.468%
11	11.292	1561	1565	1569	rBV	756459	658841	23.81%	4.333%
12	11.692	1628	1633	1636	rBV2	43550	45020	1.63%	0.296%
13	11.833	1654	1657	1675	rBV	165707	208219	7.52%	1.369%
14	12.622	1787	1791	1800	rBV2	70654	98017	3.54%	0.645%
15	12.886	1831	1836	1839	rBV	2001308	1854192	67.01%	12.194%
16	13.792	1985	1990	2001	rBV2	97434	154140	5.57%	1.014%
17	13.939	2011	2015	2018	rVB	426139	409977	14.82%	2.696%
18	14.033	2025	2031	2038	rBV	79070	80001	2.89%	0.526%
19	14.698	2140	2144	2146	rBV	31869	32453	1.17%	0.213%
20	15.380	2255	2260	2264	rBV2	378341	451120	16.30%	2.967%

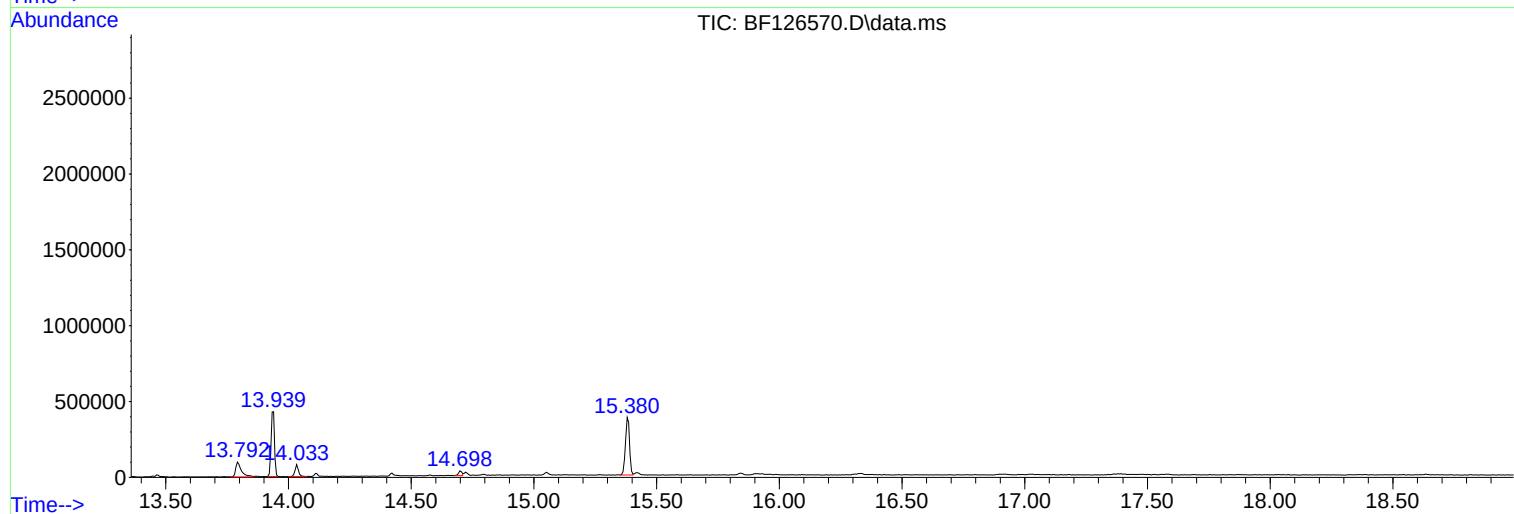
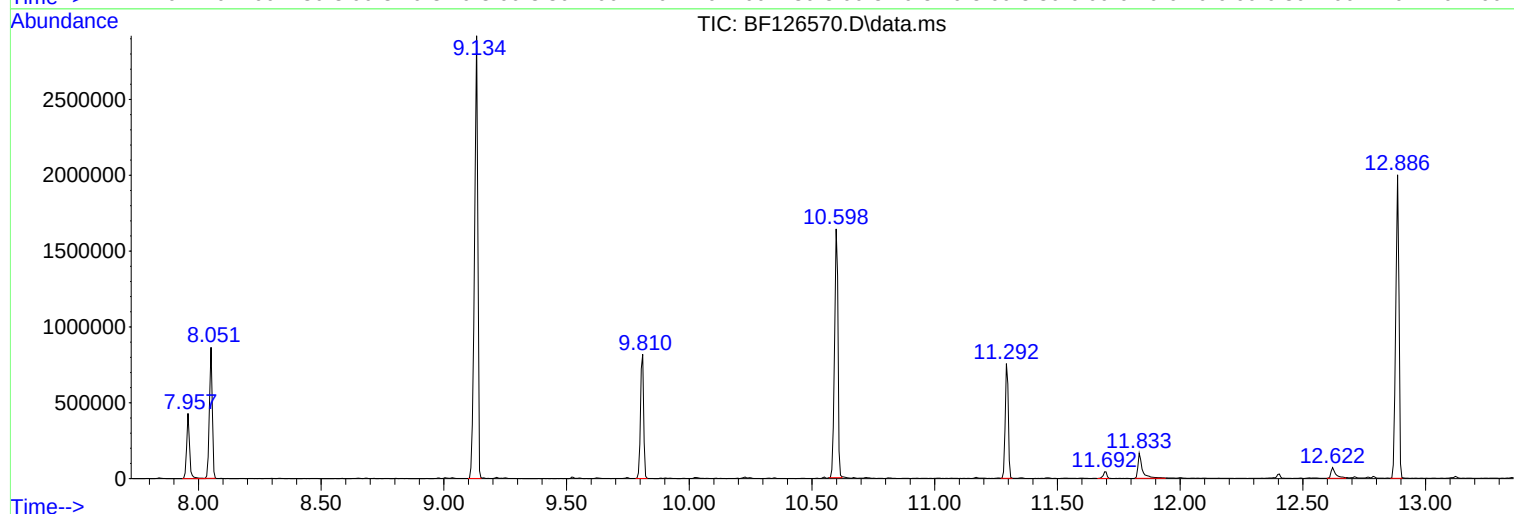
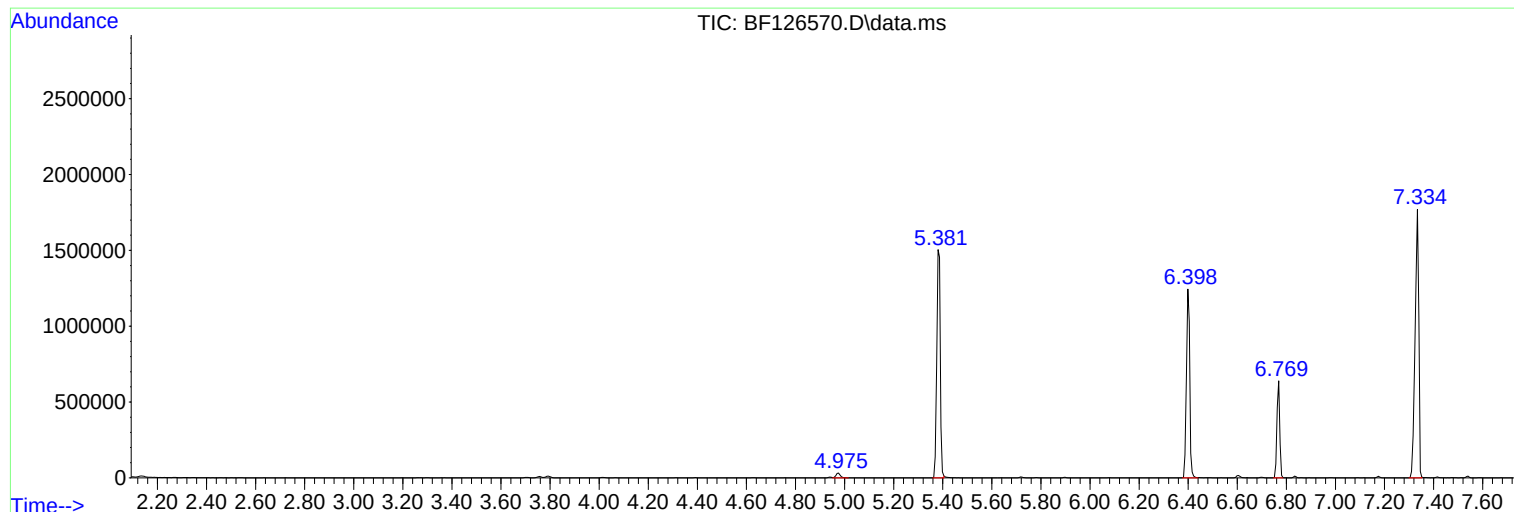
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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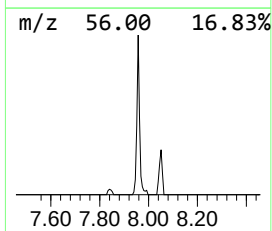
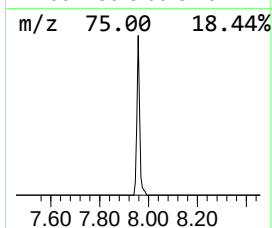
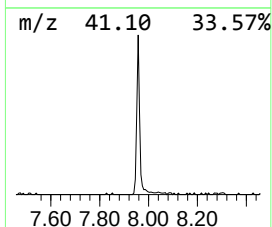
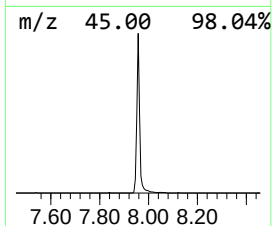
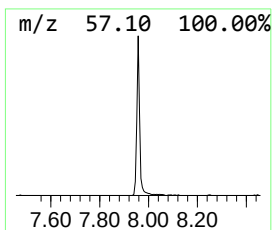
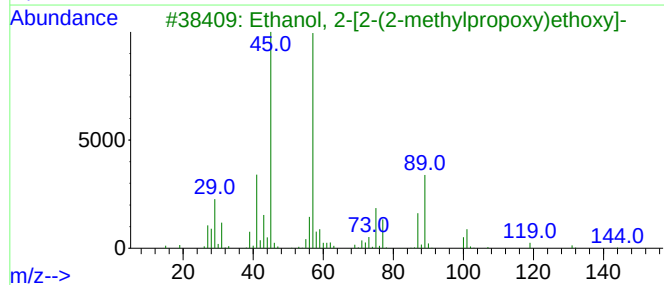
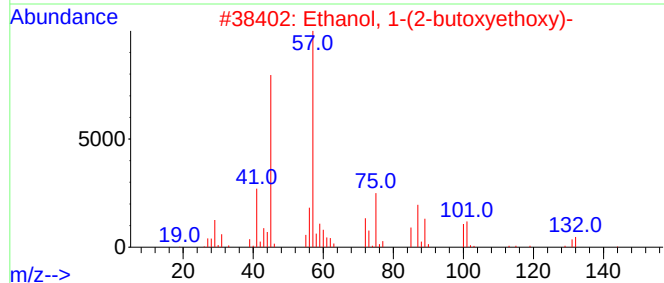
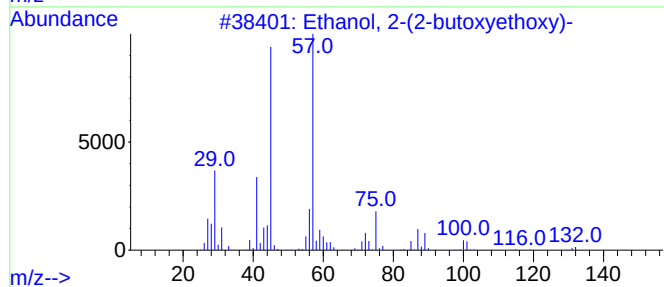
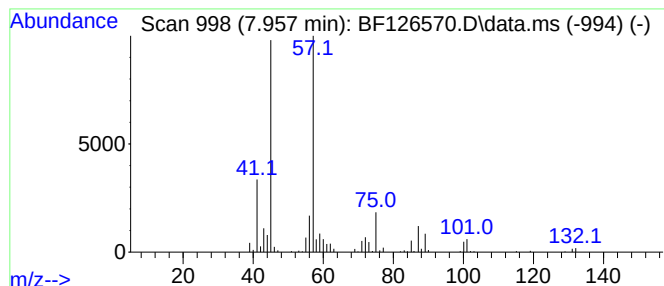
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.957	10.16 ng	359698	Naphthalene-d8	8.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53



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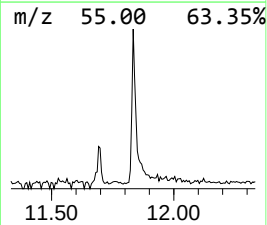
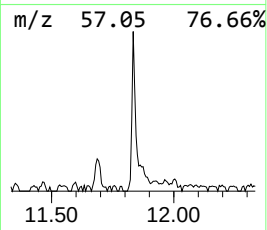
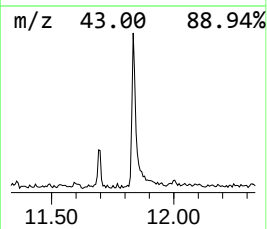
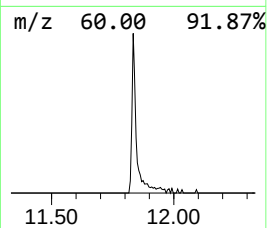
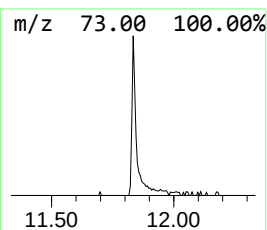
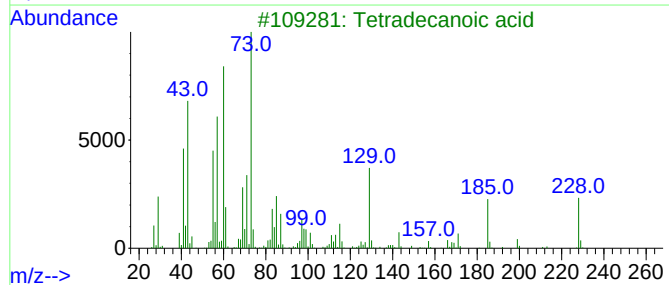
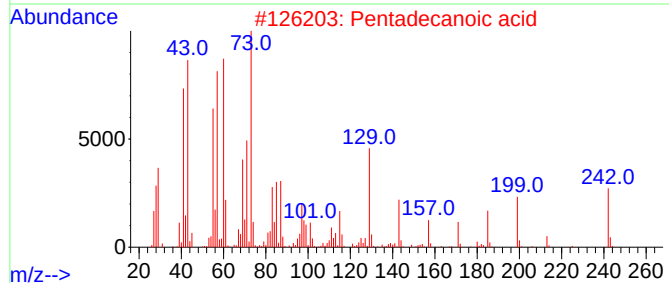
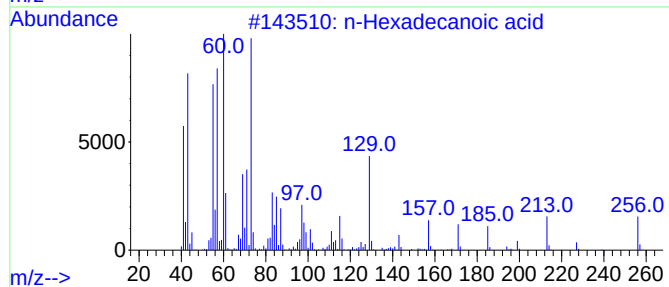
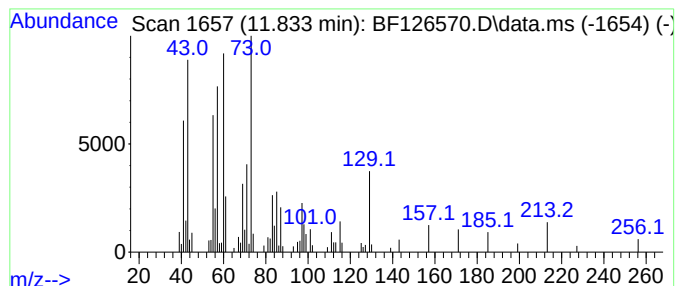
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	6.32 ng	208219	Phenanthrene-d10	11.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	25
5			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	20



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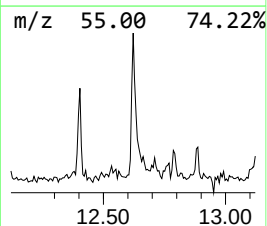
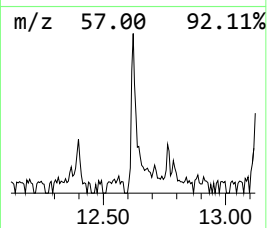
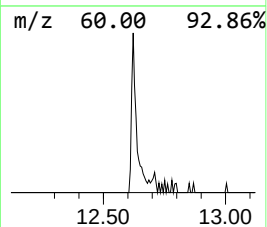
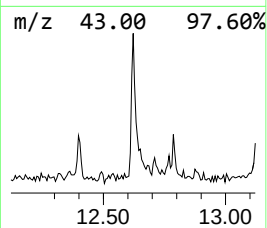
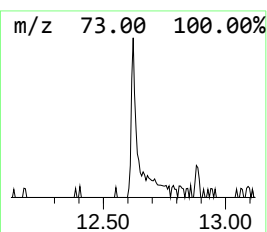
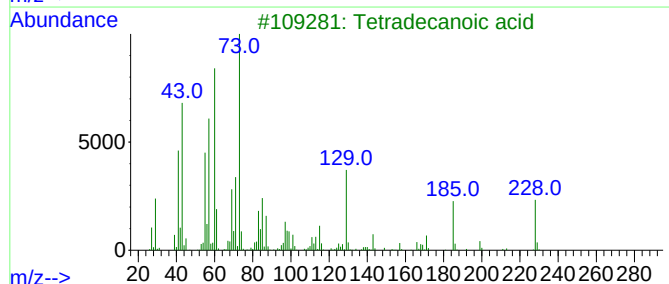
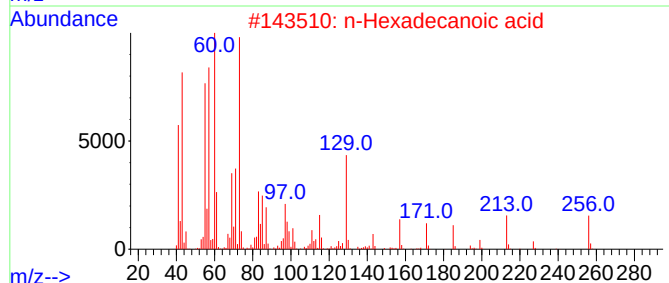
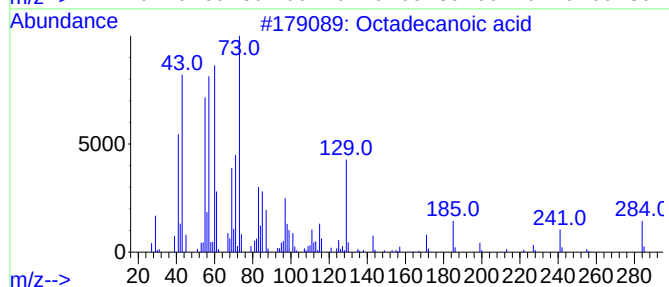
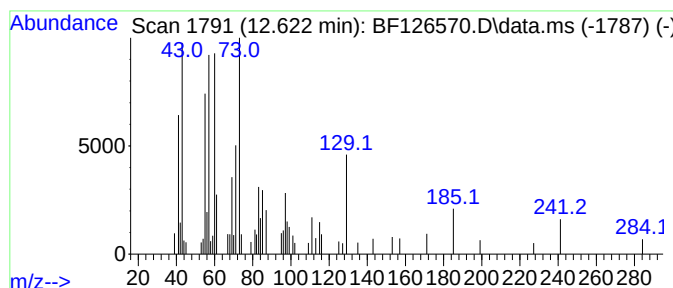
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.622	4.78 ng	98017	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	91
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64
5			Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	15



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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
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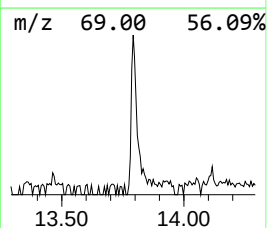
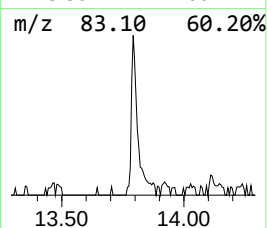
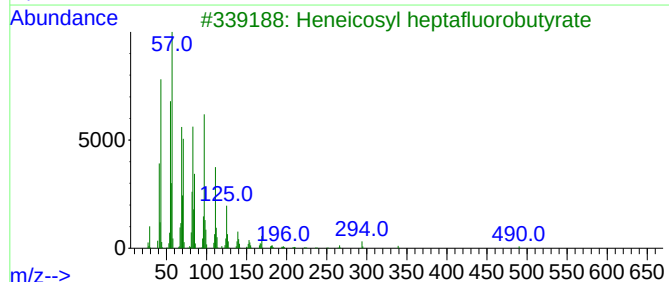
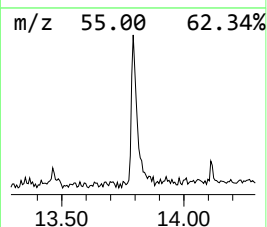
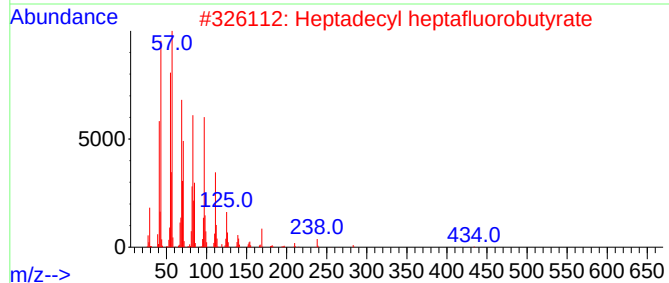
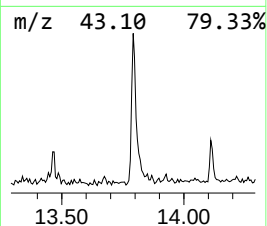
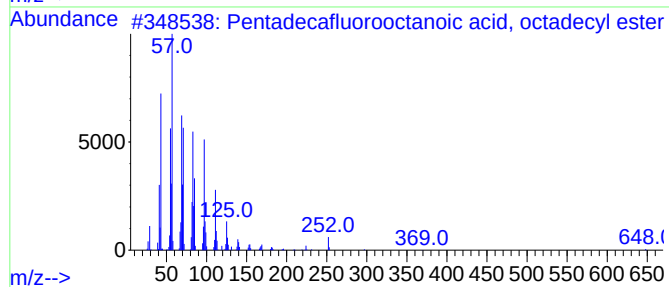
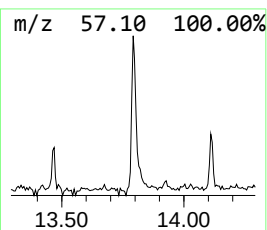
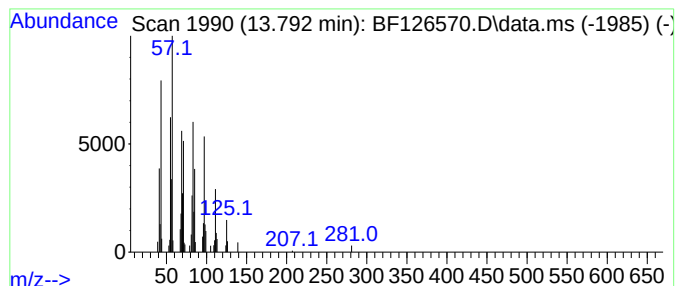
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.792	7.52 ng	154140	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
4			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
5			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91



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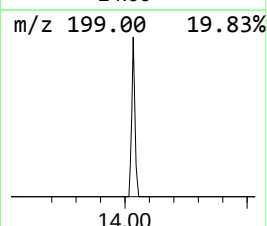
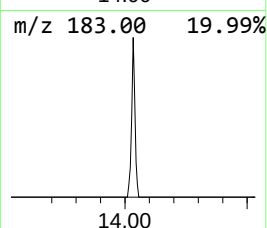
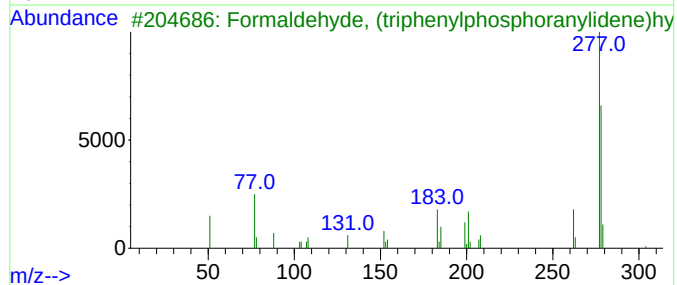
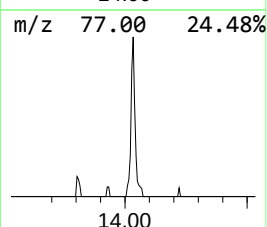
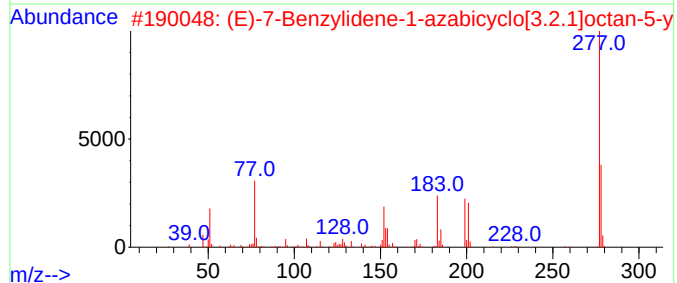
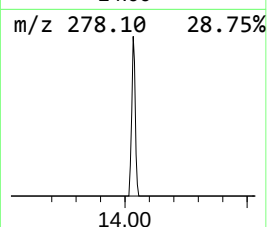
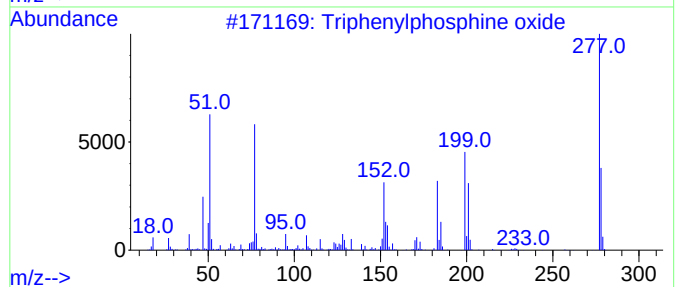
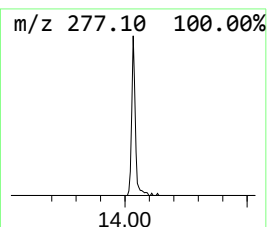
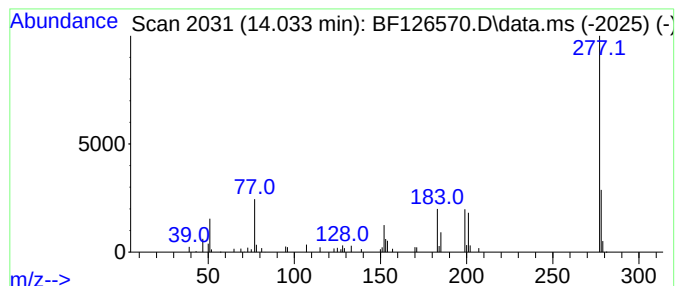
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.033	3.90 ng	80001	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	81
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	50
4			2-Propenoic acid, 2-cyano-3-(3-p...	277	C18H15NO2	1000080-00-3	47
5			3H-pyrazol-3-one, 2,4-dihydro-5-...	277	C17H15N3O	1000397-10-0	43



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-b...	7.957	10.2	ng	359698	2	8.051	708389	20.0
n-Hexadecanoic ...	11.833	6.3	ng	208219	4	11.292	658841	20.0
Octadecanoic acid	12.622	4.8	ng	98017	5	13.939	409977	20.0
Pentadecafluoro...	13.792	7.5	ng	154140	5	13.939	409977	20.0
Triphenylphosph...	14.033	3.9	ng	80001	5	13.939	409977	20.0