

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011022\
 Data File : BF126571.D
 Acq On : 10 Jan 2022 17:29
 Operator : JU/CG
 Sample : N1054-14
 Misc :
 ALS Vial : 14 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: BF126571.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.981	488	492	500	rVB	61337	78013	2.45%	0.420%
2	5.387	557	561	565	rBV	1866396	1889087	59.31%	10.167%
3	6.404	729	734	737	rBV	1620627	1543692	48.46%	8.308%
4	6.769	792	796	799	rBV	656042	547331	17.18%	2.946%
5	7.333	886	892	895	rBV	1876710	2066739	64.88%	11.123%
6	7.957	994	998	1009	rBV	242954	219424	6.89%	1.181%
7	8.051	1009	1014	1017	rVV	899011	771334	24.22%	4.151%
8	8.328	1058	1061	1068	rVB	71581	58076	1.82%	0.313%
9	9.133	1192	1198	1201	rBV	3141110	3185306	100.00%	17.143%
10	9.527	1260	1265	1268	rBV	284892	249116	7.82%	1.341%
11	9.810	1306	1313	1316	rBV	895785	826027	25.93%	4.446%
12	10.604	1441	1448	1451	rBV	1981095	2074683	65.13%	11.166%
13	11.292	1561	1565	1569	rBV	892760	757790	23.79%	4.078%
14	11.692	1625	1633	1637	rBV2	49751	52574	1.65%	0.283%
15	11.833	1653	1657	1671	rBV2	298667	361722	11.36%	1.947%
16	12.404	1751	1754	1757	rVB	41142	34003	1.07%	0.183%
17	12.621	1787	1791	1803	rBV	182500	230386	7.23%	1.240%
18	12.886	1831	1836	1840	rBV	2218727	2399572	75.33%	12.914%
19	13.792	1985	1990	2000	rBV2	81058	140653	4.42%	0.757%
20	13.939	2011	2015	2018	rBV	497521	468599	14.71%	2.522%
21	14.033	2026	2031	2036	rBV	73457	73478	2.31%	0.395%
22	14.268	2067	2071	2075	rBV	45225	40473	1.27%	0.218%
23	14.704	2142	2145	2147	rBV	45085	46119	1.45%	0.248%
24	15.380	2255	2260	2265	rBV	382616	466297	14.64%	2.510%

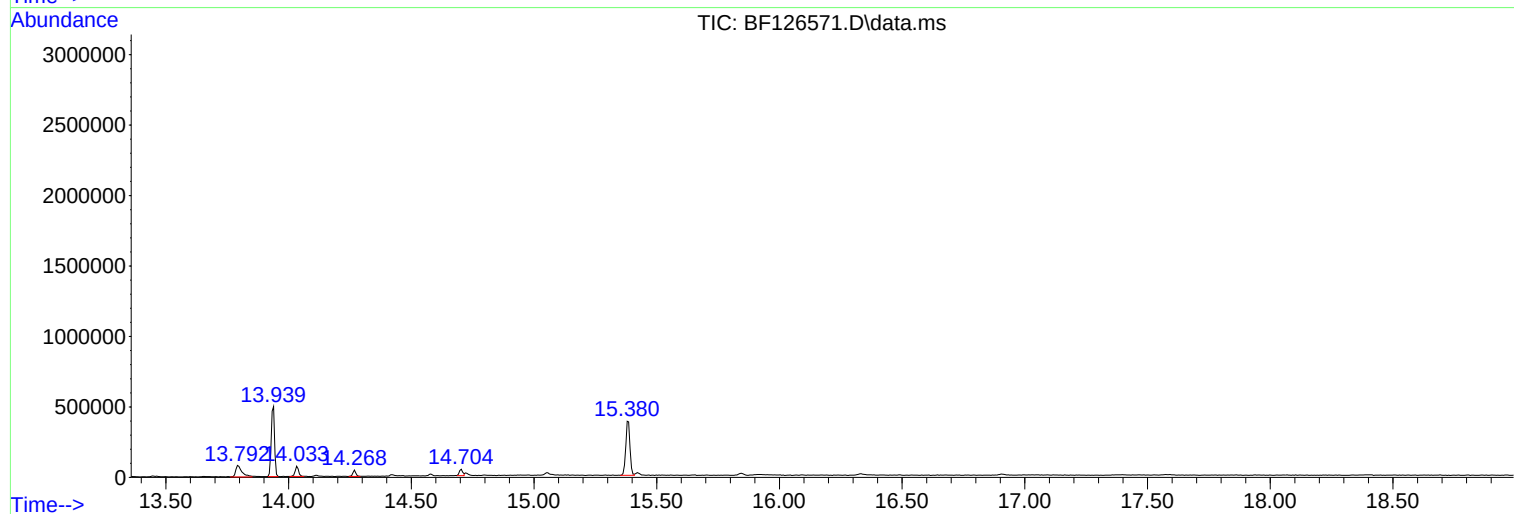
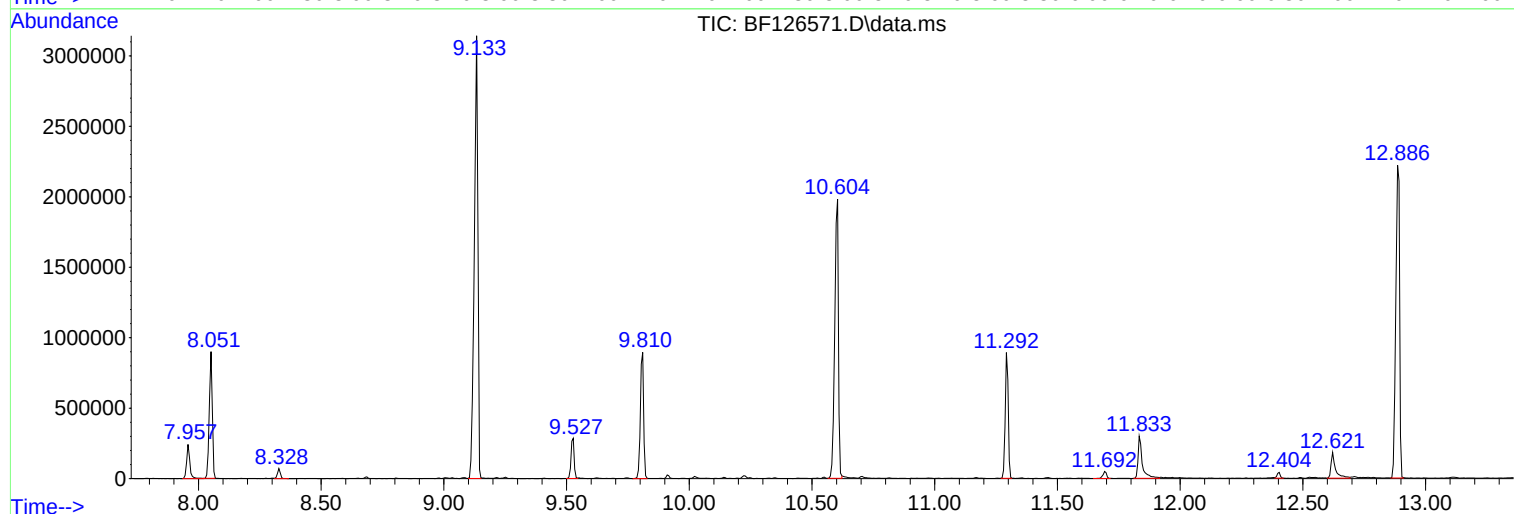
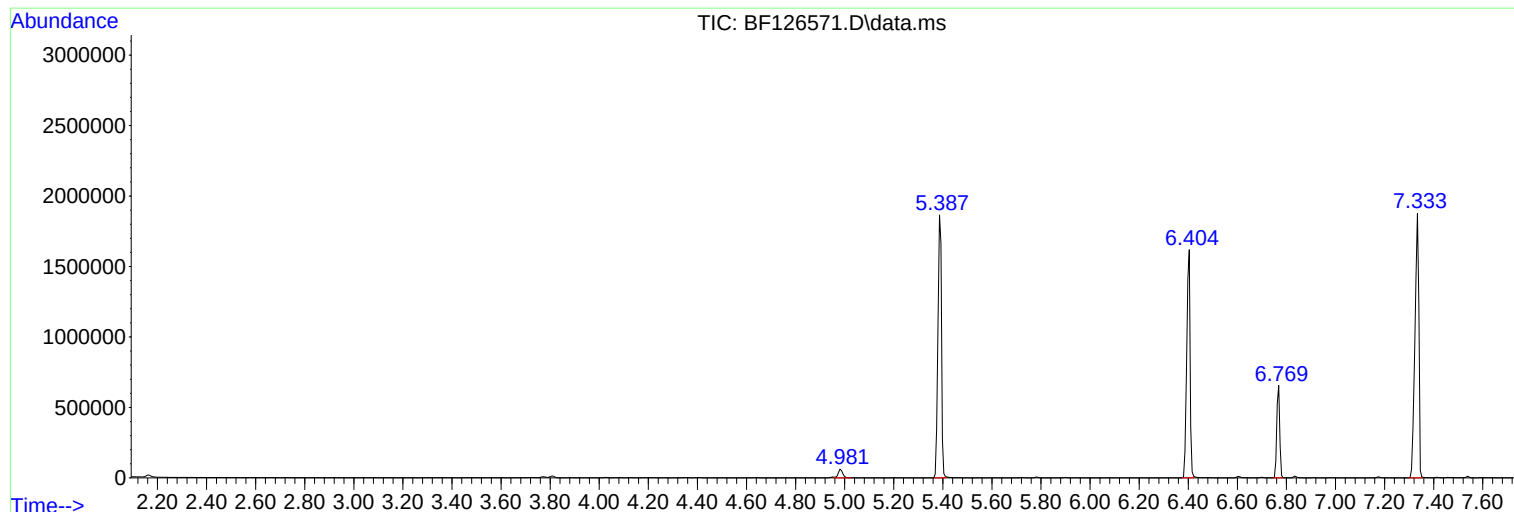
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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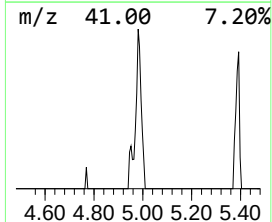
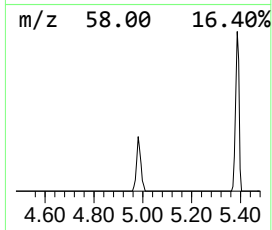
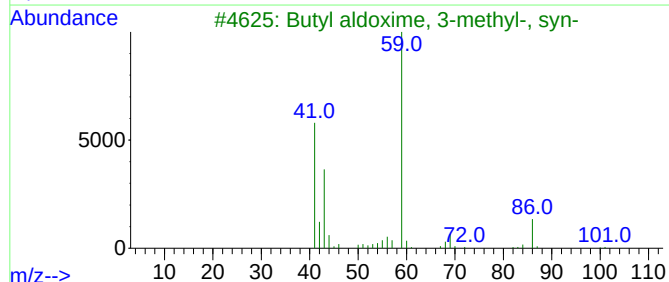
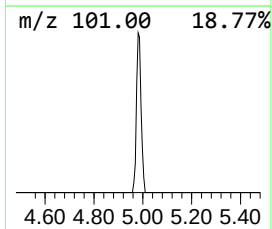
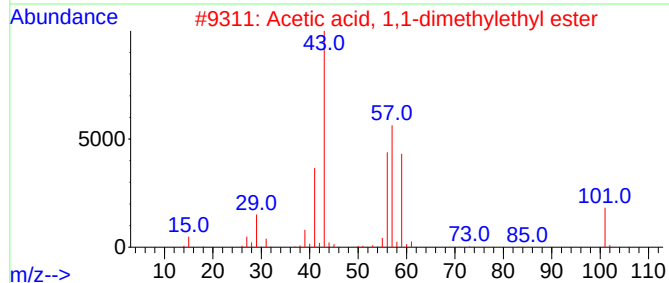
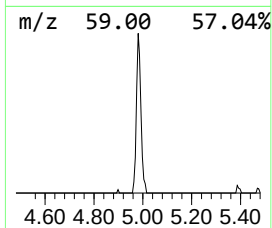
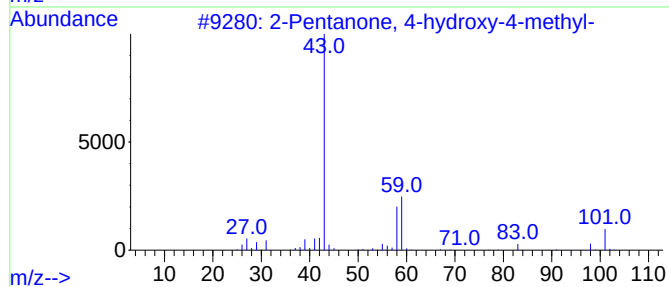
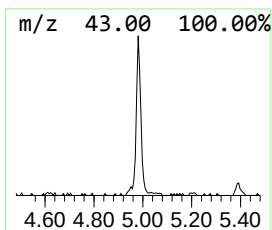
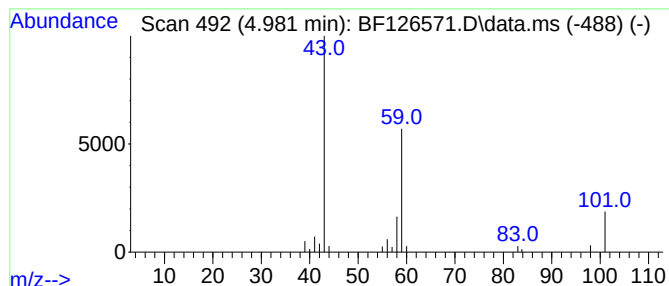
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.981	2.85 ng	78013	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Guanidine	59	CH5N3	000113-00-8	9		



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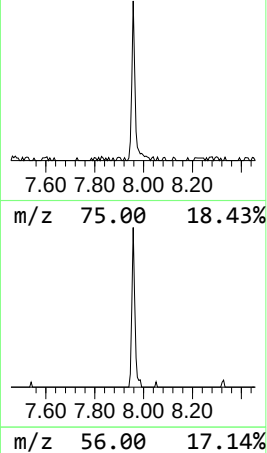
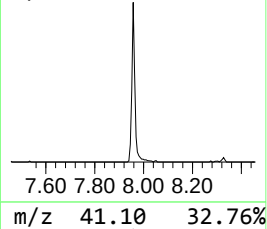
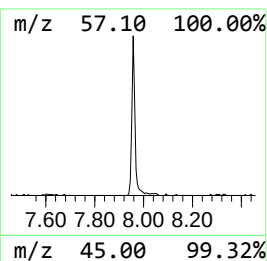
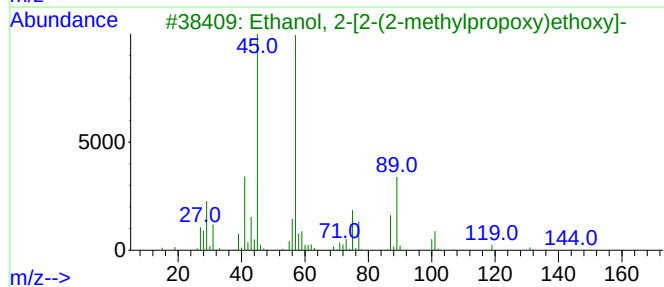
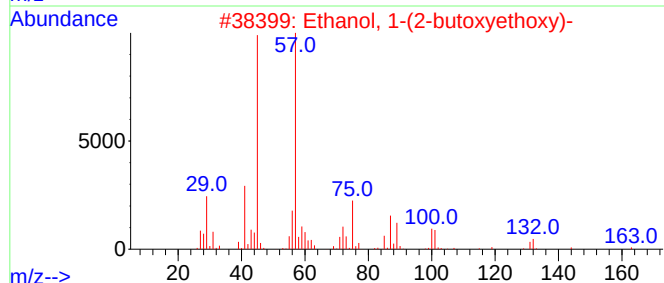
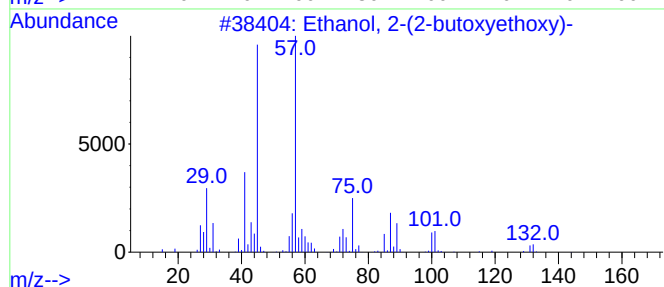
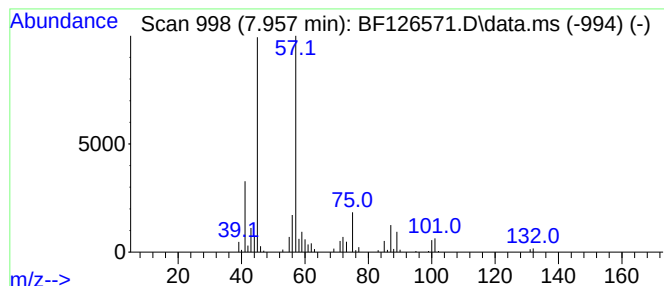
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.957	5.69 ng	219424	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	59
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53



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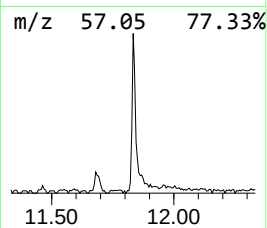
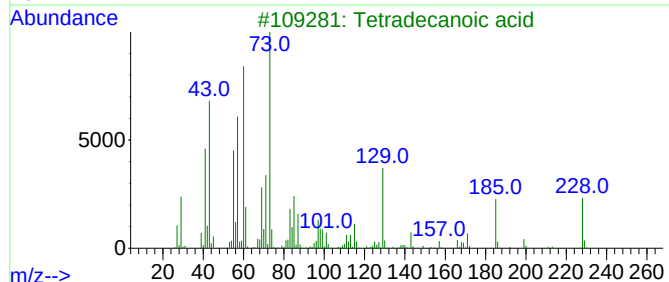
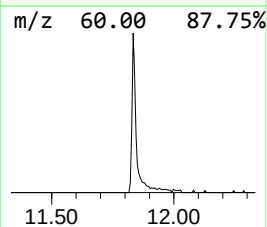
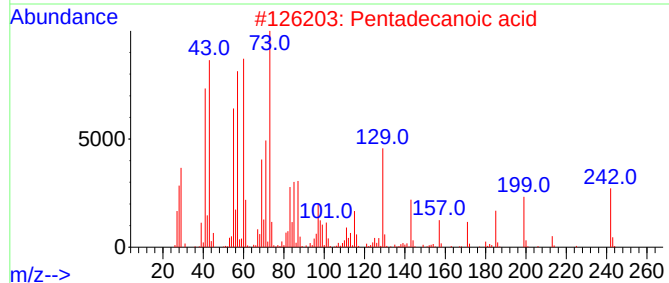
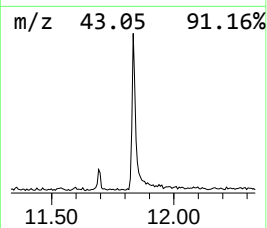
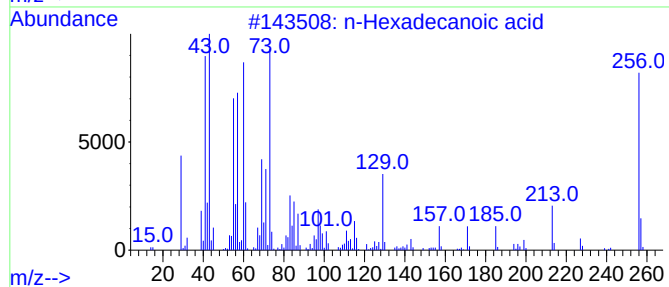
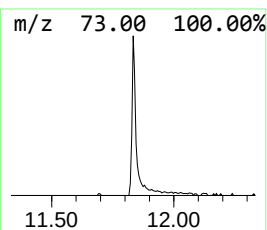
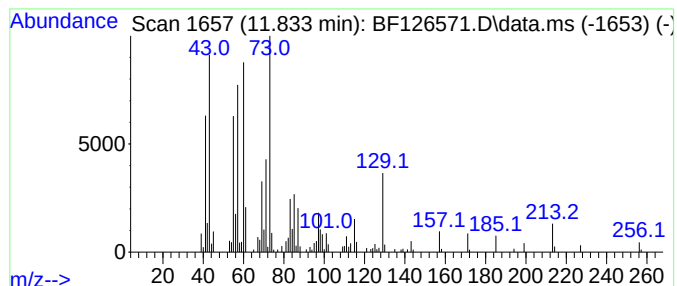
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	9.55 ng	361722	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	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	81
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



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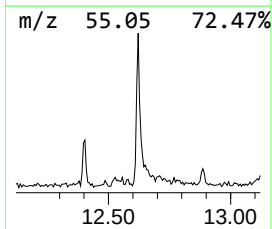
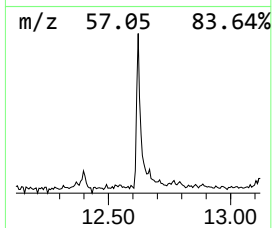
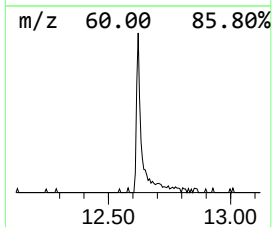
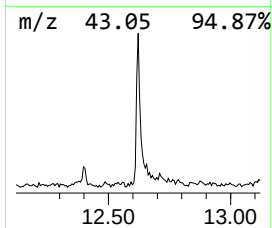
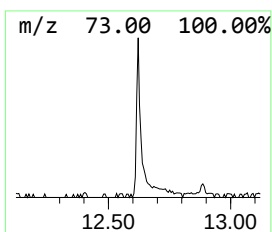
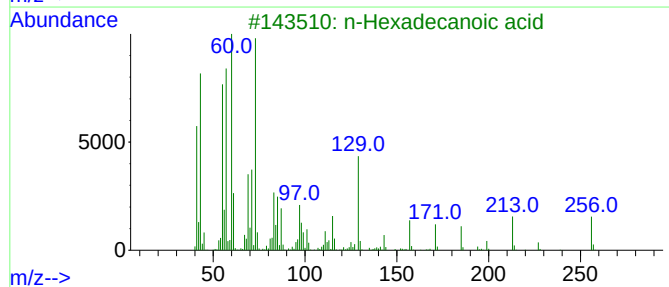
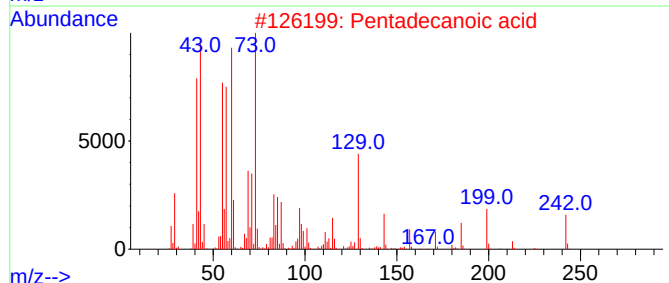
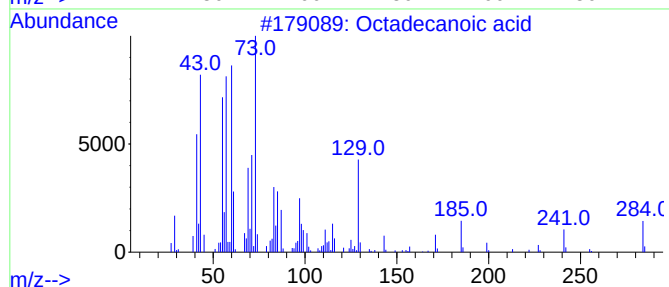
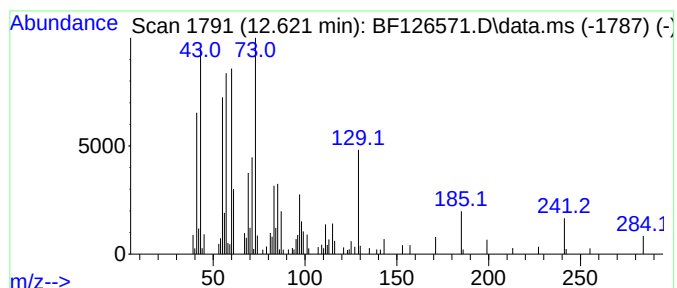
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Peak Number 4 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.621	9.83 ng	230386	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	38



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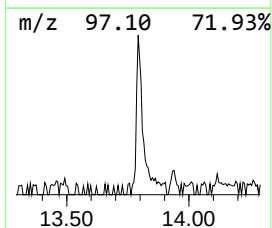
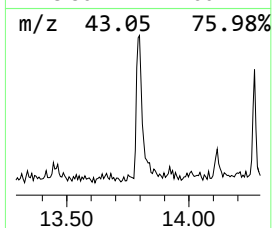
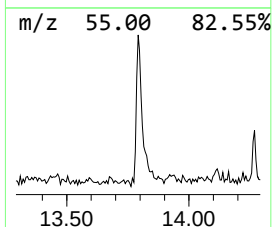
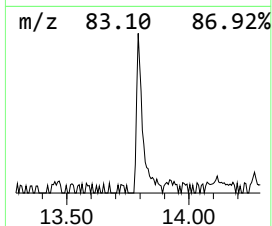
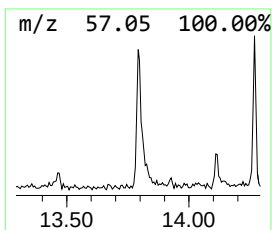
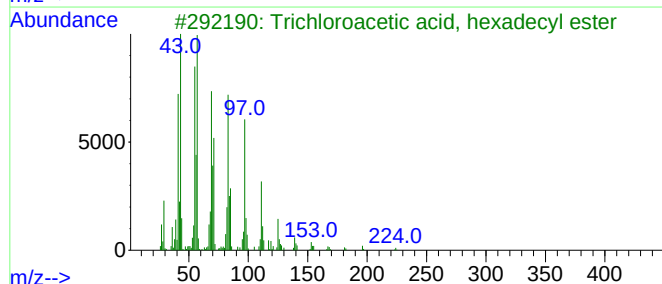
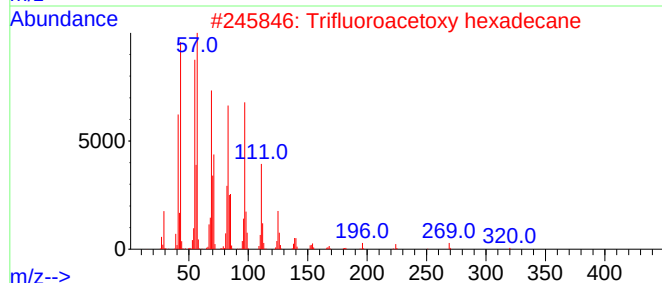
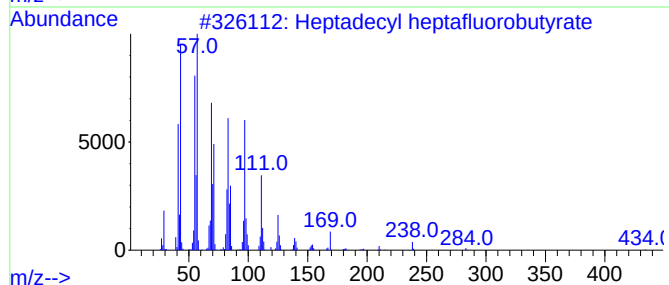
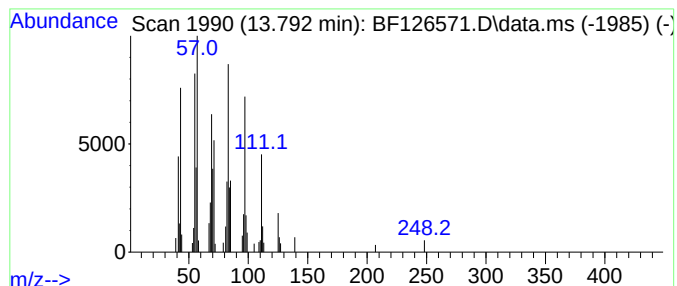
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.792	6.00 ng	140653	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4			5-Eicosene, (E)-	280	C20H40	074685-30-6	91
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91



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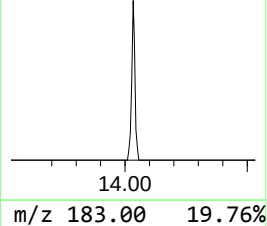
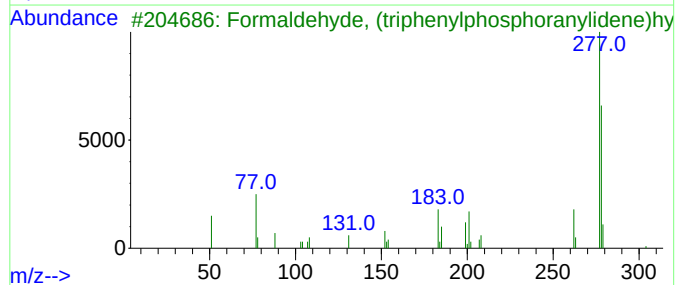
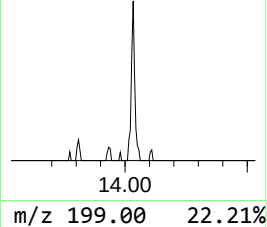
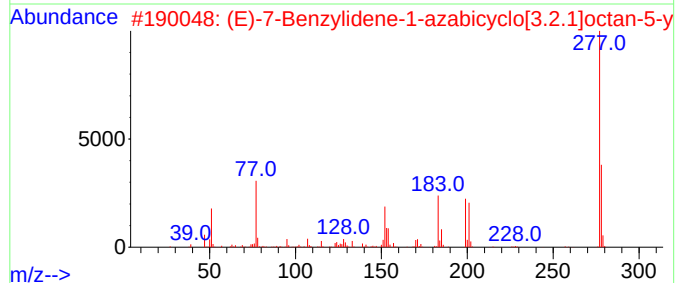
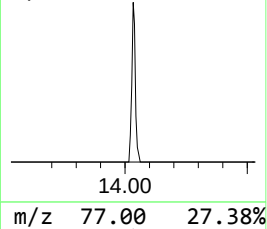
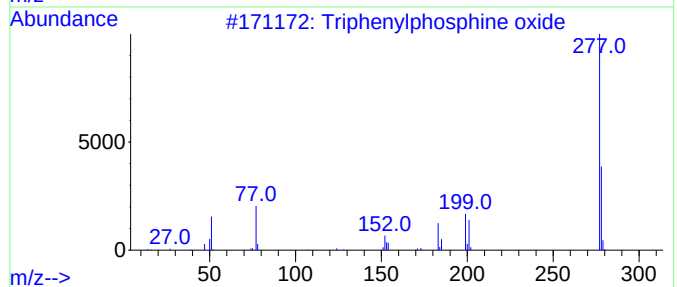
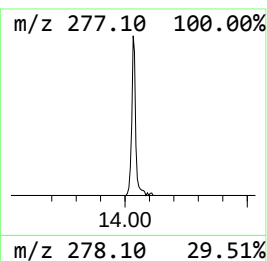
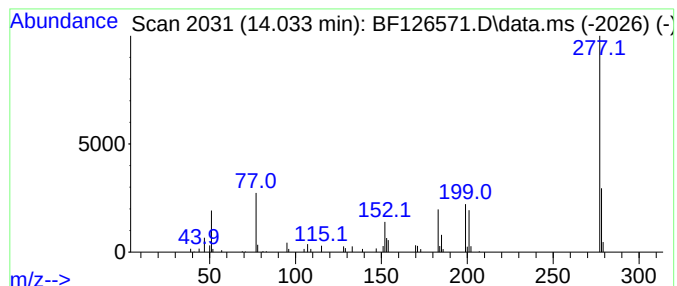
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.033	3.14 ng	73478	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	64
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	45
4			2-Propenoic acid, 2-cyano-3-(3-p...]	277	C18H15NO2	1000080-00-3	43
5			Cobalt,(.eta.<5>-2,4-cyclopentad...]	277	C16H15BCo	036682-12-9	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011022\
Data File : BF126571.D
Acq On : 10 Jan 2022 17:29
Operator : JU/CG
Sample : N1054-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

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

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.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
2-Pentanone, 4-...	4.981	2.9	ng	78013	1	6.769	547331	20.0
Ethanol, 2-(2-b...	7.957	5.7	ng	219424	2	8.051	771334	20.0
n-Hexadecanoic ...	11.833	9.6	ng	361722	4	11.292	757790	20.0
Octadecanoic acid	12.621	9.8	ng	230386	5	13.939	468599	20.0
Heptadecyl hept...	13.792	6.0	ng	140653	5	13.939	468599	20.0
Triphenylphosph...	14.033	3.1	ng	73478	5	13.939	468599	20.0