

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
 Data File : BF126078.D
 Acq On : 9 Nov 2021 12:41
 Operator : JU/CG
 Sample : M4540-07
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-4

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-BF110321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126078.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	4	13	18	rBV	1951257	2579709	44.75%	6.311%
2	5.081	505	509	516	rVB	62597	76283	1.32%	0.187%
3	5.475	570	576	579	rBV	4881976	4531391	78.60%	11.086%
4	6.481	741	747	750	rBV	4678311	4750694	82.41%	11.623%
5	6.851	806	810	813	rBV	1322979	998018	17.31%	2.442%
6	7.410	900	905	909	rBV	2968941	3140498	54.48%	7.683%
7	8.034	1007	1011	1021	rBV	418564	452698	7.85%	1.108%
8	8.134	1023	1028	1031	rBV	1500606	1276632	22.14%	3.123%
9	9.210	1206	1211	1214	rBV	6591222	5764907	100.00%	14.104%
10	9.886	1321	1326	1335	rVB	1879581	1570073	27.24%	3.841%
11	10.675	1455	1460	1463	rBV	4695540	3827030	66.38%	9.363%
12	11.369	1574	1578	1582	rBV	1736800	1571754	27.26%	3.845%
13	11.439	1585	1590	1593	rVB2	110387	102961	1.79%	0.252%
14	11.898	1662	1668	1672	rBV	145685	149268	2.59%	0.365%
15	12.039	1688	1692	1695	rBV	94901	124701	2.16%	0.305%
16	12.069	1695	1697	1706	rVB5	81510	127151	2.21%	0.311%
17	12.957	1844	1848	1851	rBV	6056356	5068125	87.91%	12.400%
18	13.863	1998	2002	2014	rBV2	402395	890164	15.44%	2.178%
19	14.010	2023	2027	2033	rVB	1035548	1025644	17.79%	2.509%
20	14.498	2105	2110	2115	rBV3	78610	138454	2.40%	0.339%
21	14.568	2117	2122	2128	rVB	109082	197065	3.42%	0.482%
22	14.868	2170	2173	2179	rVB	83702	98256	1.70%	0.240%
23	15.133	2214	2218	2221	rBV	152136	175804	3.05%	0.430%
24	15.233	2229	2235	2242	rVB2	108205	232198	4.03%	0.568%
25	15.474	2271	2276	2280	rBV	774968	946544	16.42%	2.316%
26	15.515	2280	2283	2287	rVB3	52774	66630	1.16%	0.163%
27	15.598	2292	2297	2309	rVB3	67322	213814	3.71%	0.523%
28	15.715	2314	2317	2322	rVB6	46038	65721	1.14%	0.161%
29	15.951	2353	2357	2361	rBV	130787	221035	3.83%	0.541%
30	16.010	2364	2367	2374	rVB4	111802	213345	3.70%	0.522%
31	16.327	2417	2421	2433	rVB9	69590	203824	3.54%	0.499%
32	17.539	2625	2627	2636	rVB10	37340	72979	1.27%	0.179%

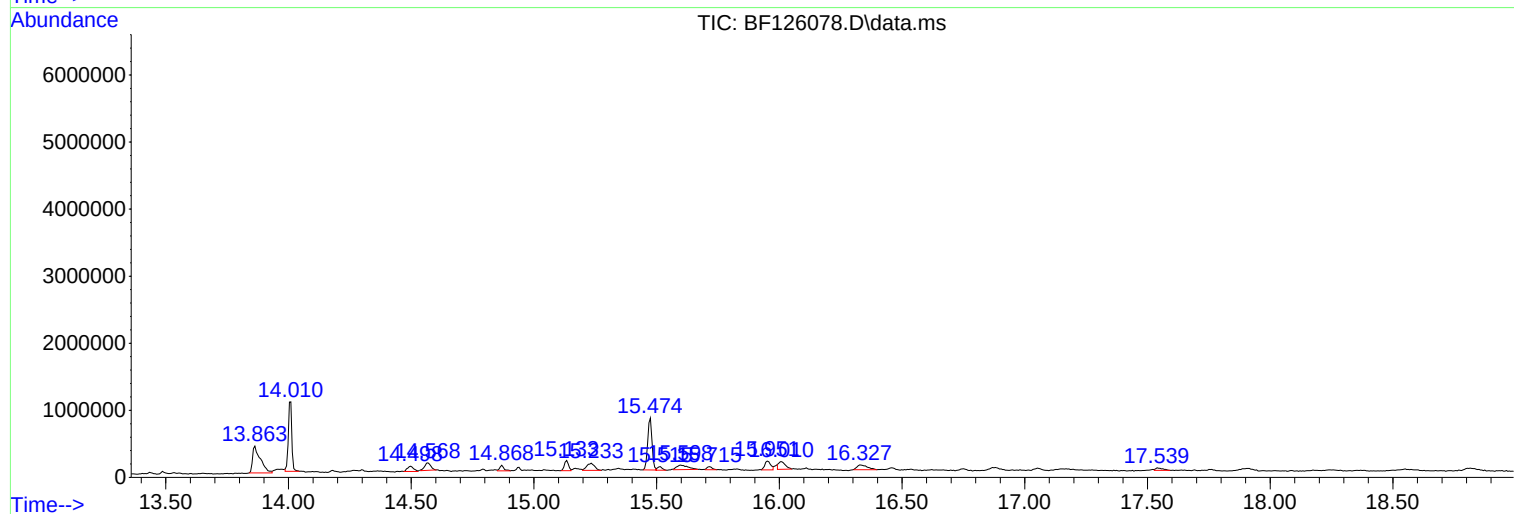
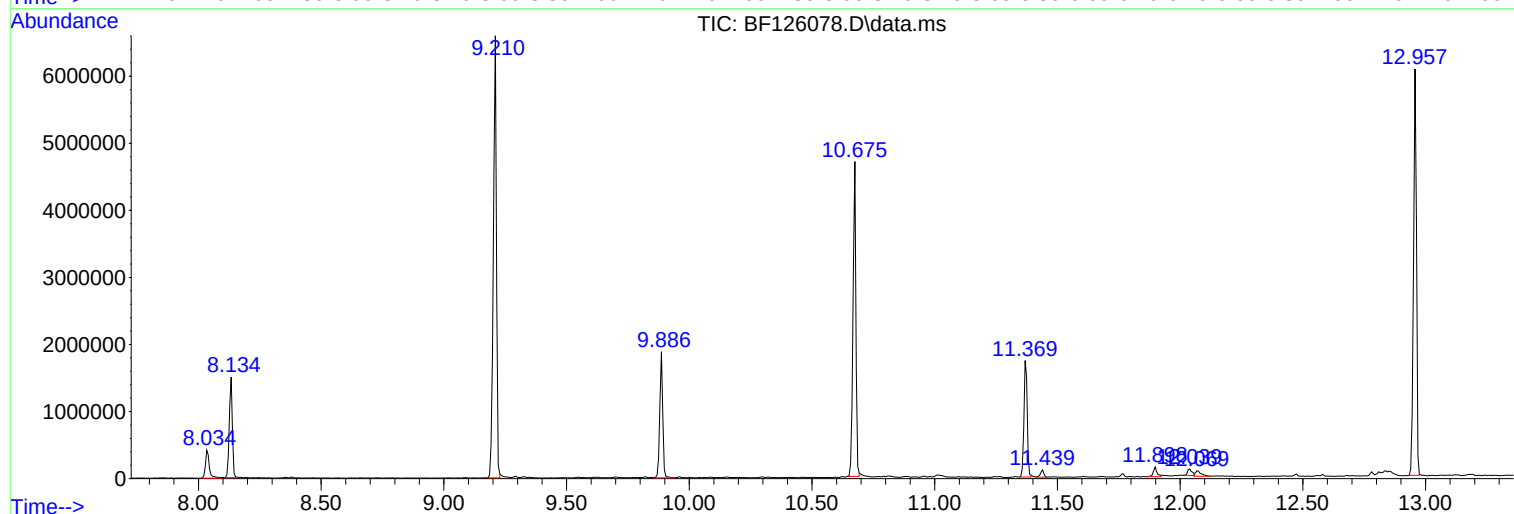
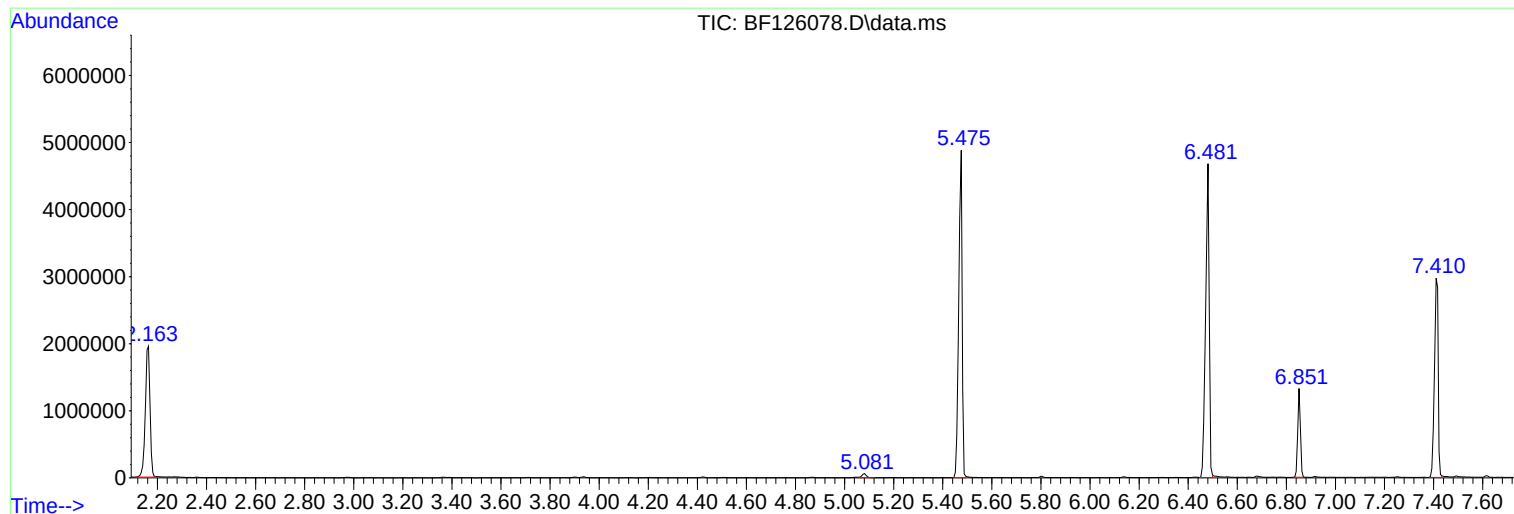
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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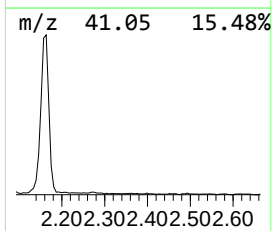
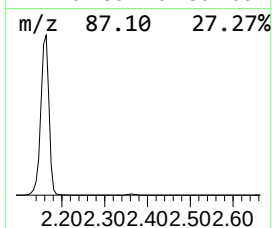
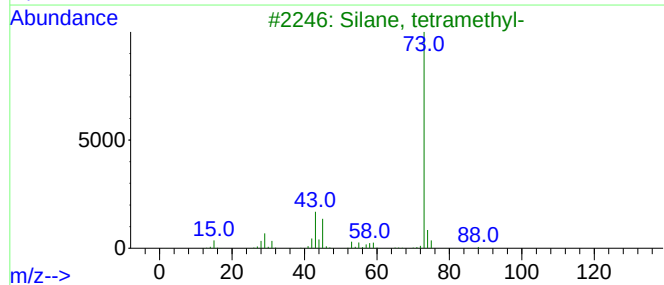
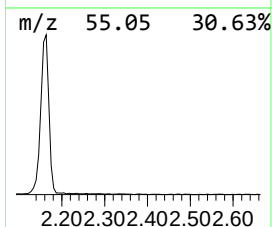
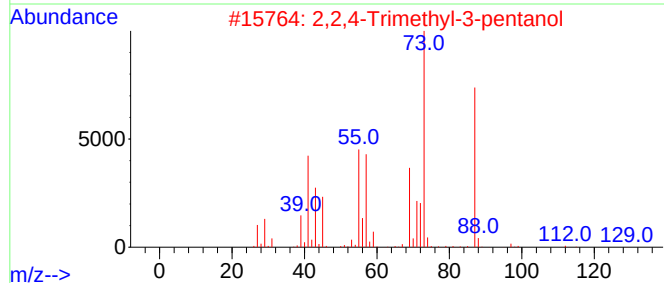
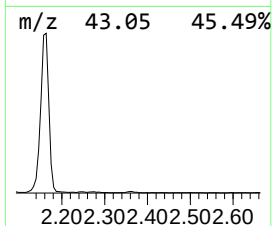
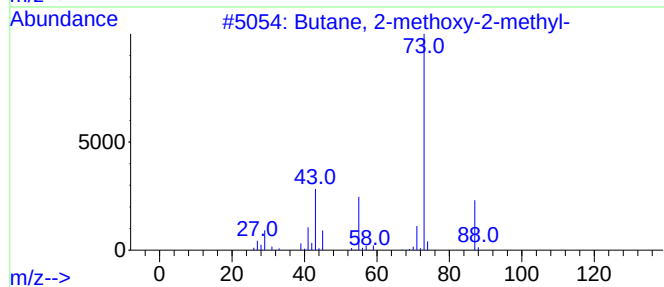
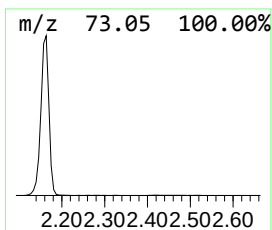
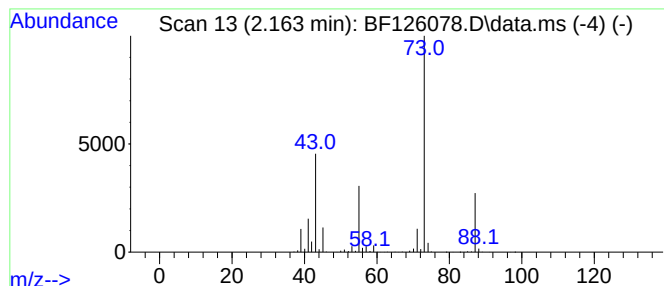
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	51.70 ng	2579710	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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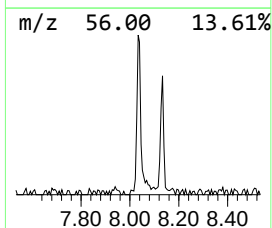
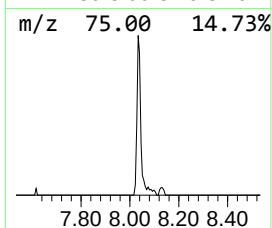
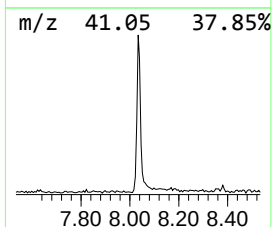
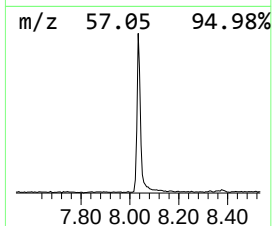
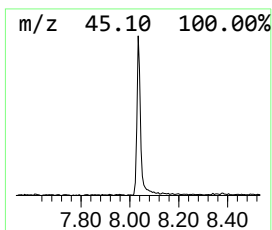
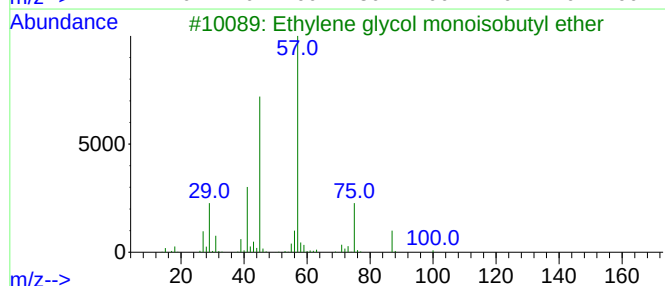
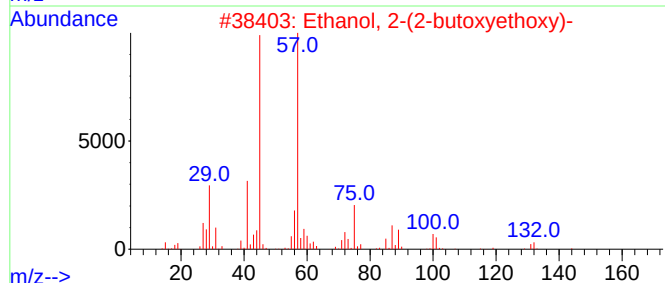
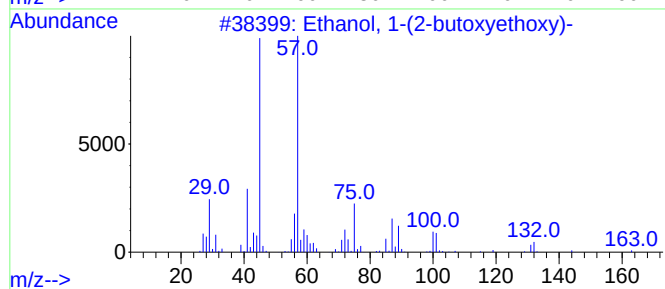
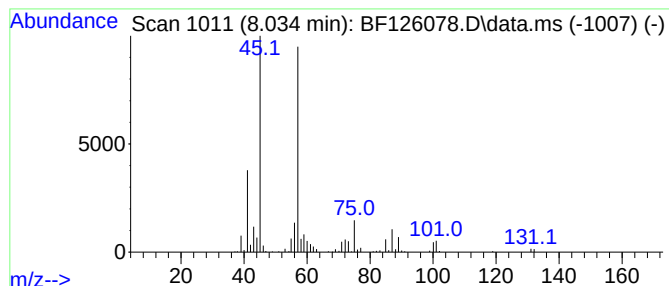
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.034	7.09 ng	452698	Naphthalene-d8	8.134

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53



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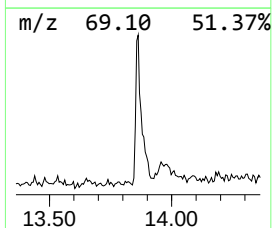
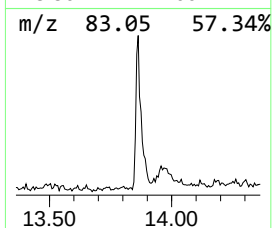
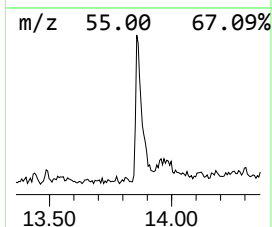
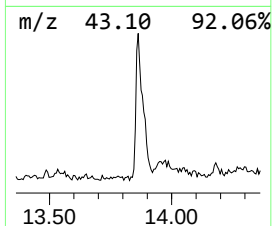
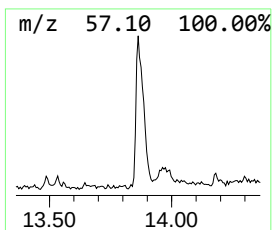
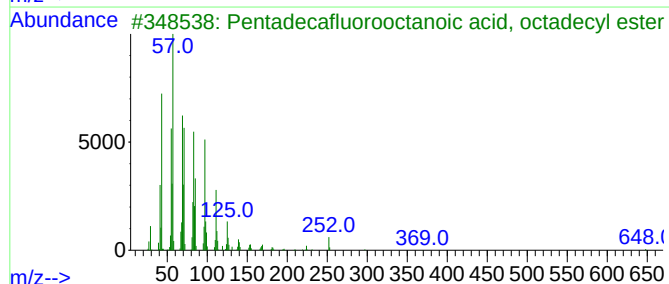
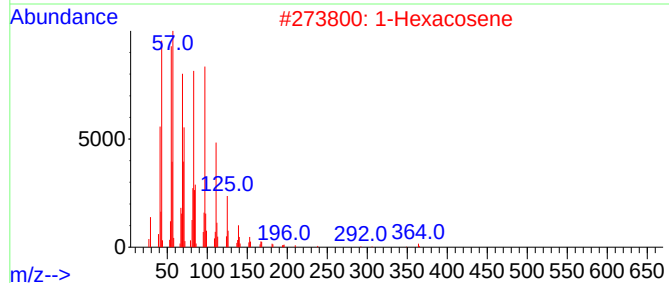
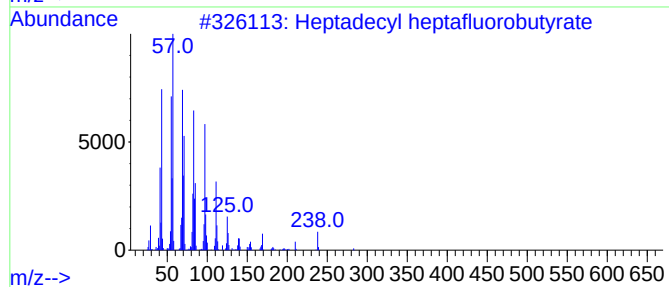
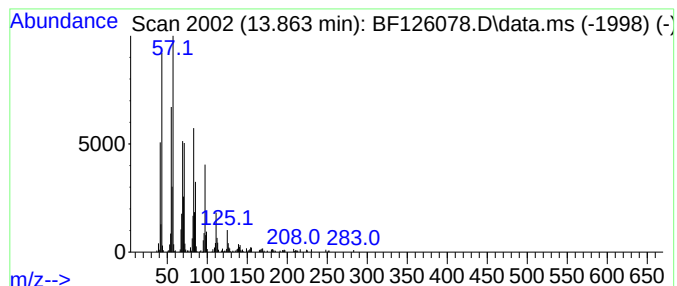
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Heptadecyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	17.36 ng	890164	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2			1-Hexacosene	364	C26H52	018835-33-1	90
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
4			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	87
5			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	87



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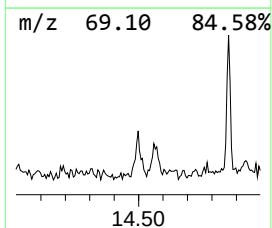
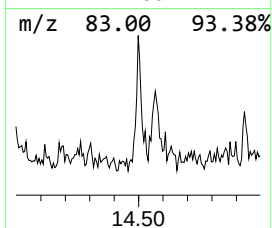
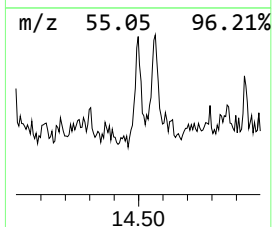
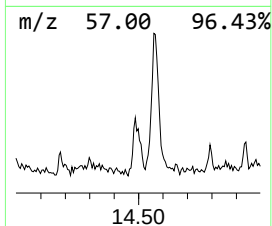
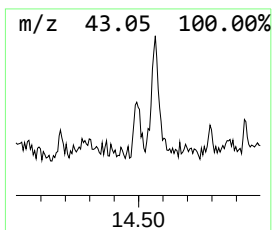
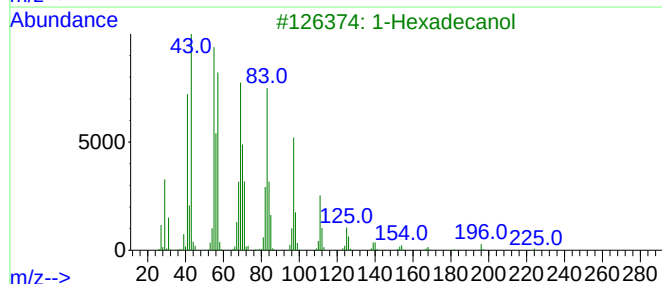
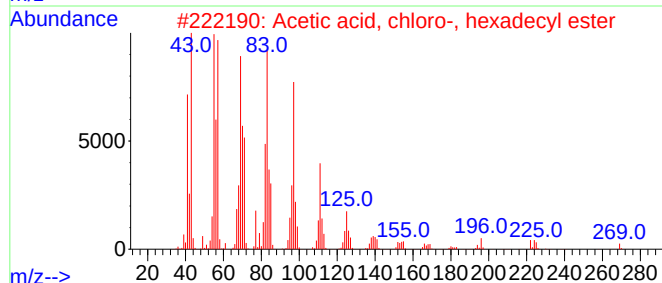
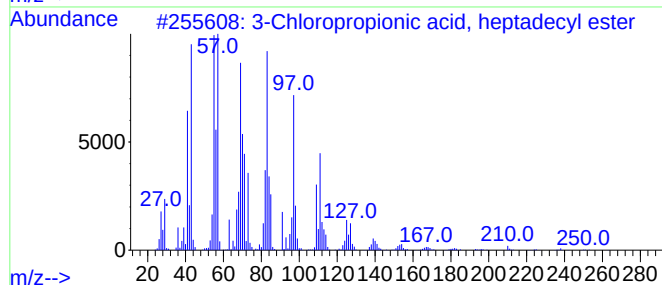
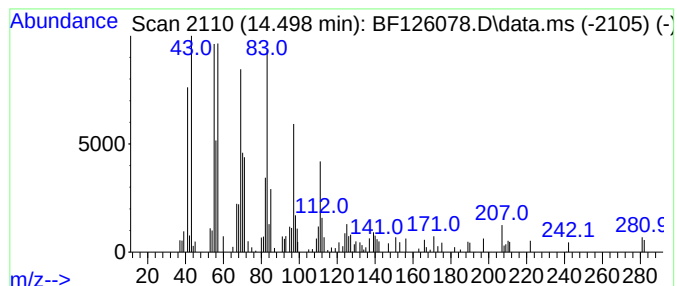
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Peak Number 4 3-Chloropropionic acid, hep... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.498	2.70 ng	138454	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
2			Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	91
3			1-Hexadecanol	242	C16H34O	036653-82-4	90
4			3-Eicosene, (E)-	280	C20H40	074685-33-9	90
5			11-Tricosene	322	C23H46	052078-56-5	87



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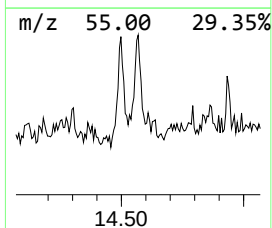
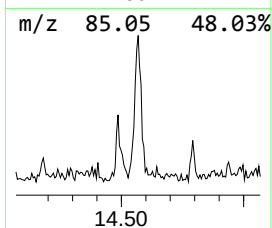
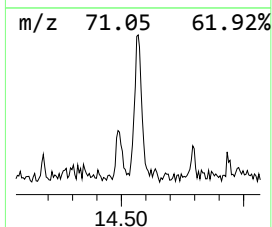
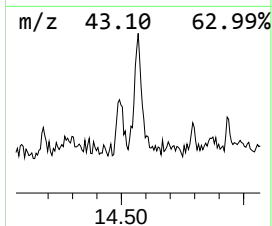
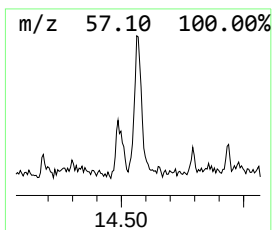
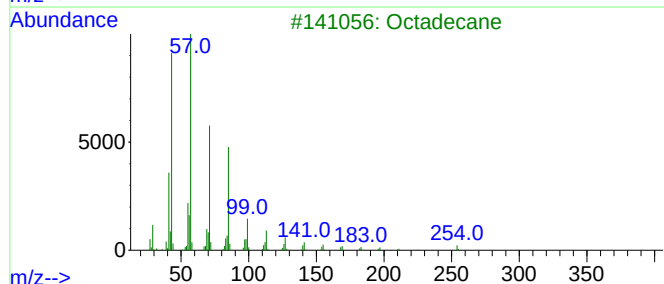
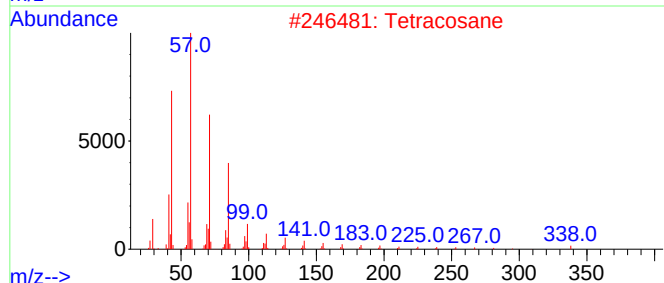
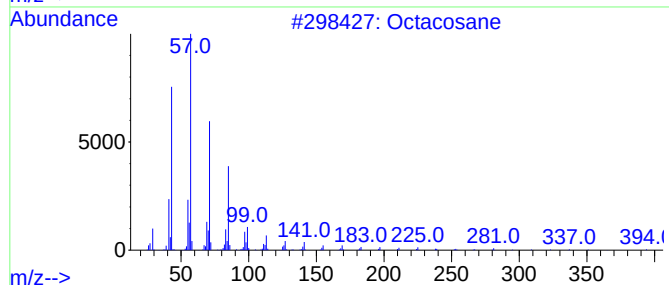
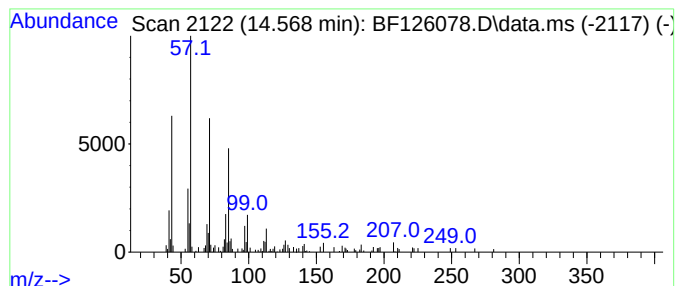
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Peak Number 5 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.569	3.84 ng	197065	Chrysene-d12	14.010	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Tetracosane	338	C24H50	000646-31-1	87
3	Octadecane	254	C18H38	000593-45-3	86
4	Docosane	310	C22H46	000629-97-0	86
5	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	86



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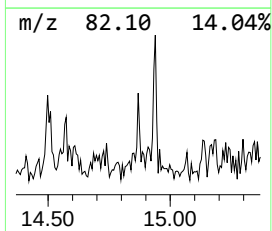
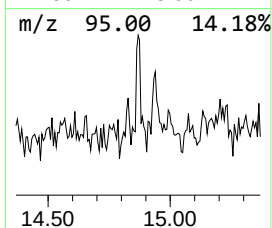
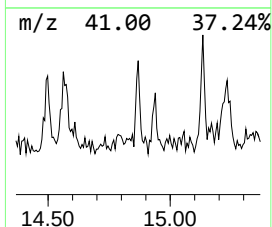
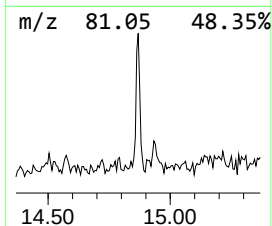
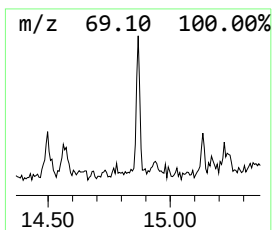
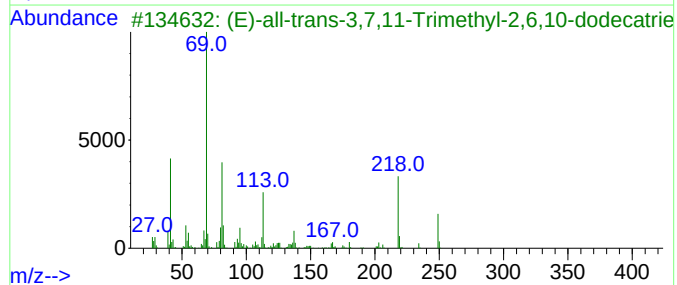
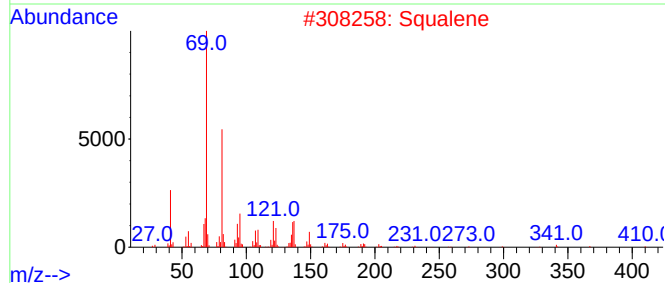
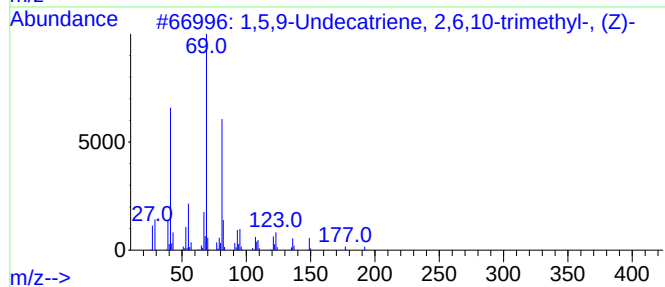
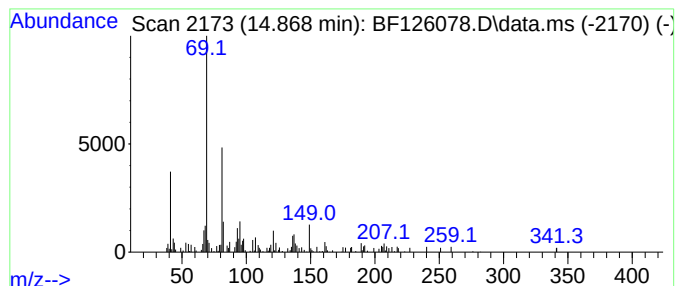
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.868	2.08 ng	98256	Perylene-d12	15.474	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
2	Squalene	410	C30H50	000111-02-4	72
3	(E)-all-trans-3,7,11-Trimethyl-2...	249	C16H27NO	1010161-37-4	53
4	1,6,10,14-Hexadecatetraen-3-ol, ...	290	C20H34O	001113-21-9	53
5	1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
Data File : BF126078.D
Acq On : 9 Nov 2021 12:41
Operator : JU/CG
Sample : M4540-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

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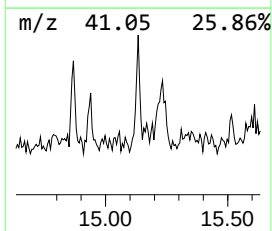
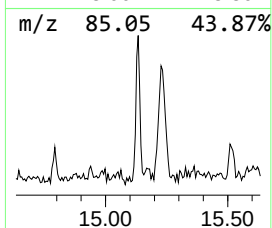
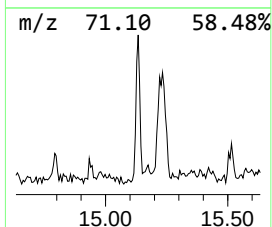
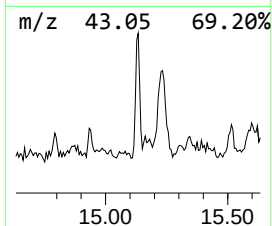
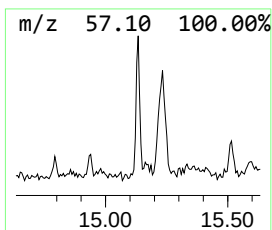
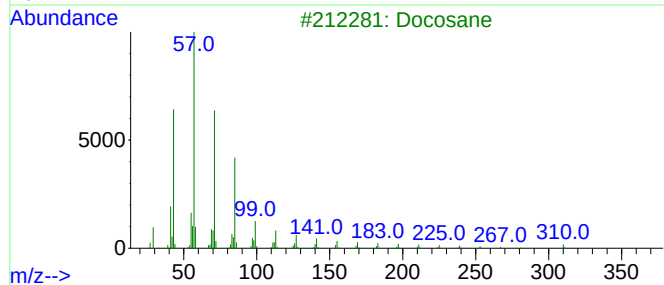
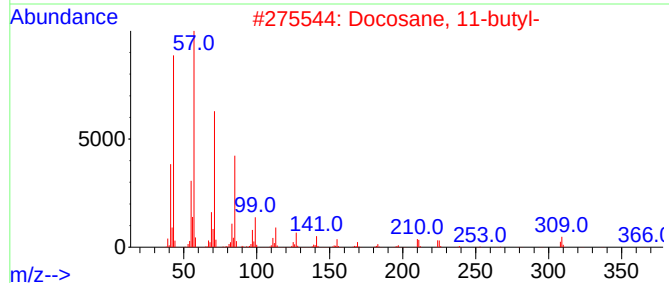
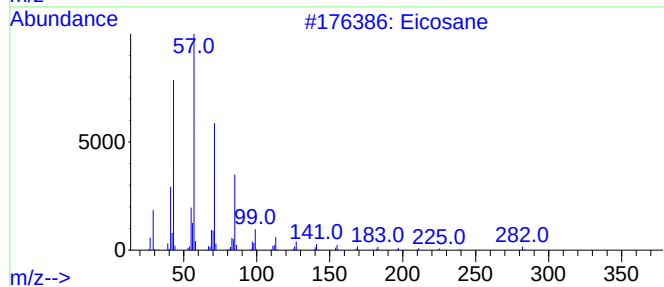
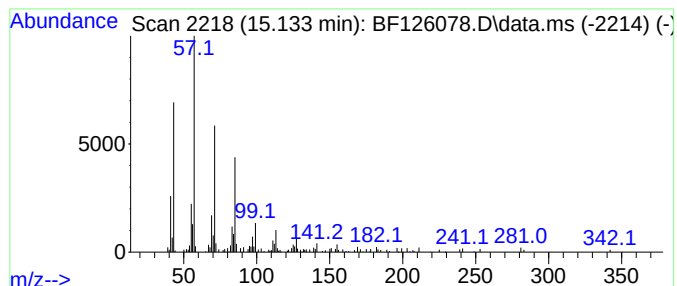
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	3.71 ng	175804	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	90
2	Docosane, 11-butyl-			366	C26H54	013475-76-8	90
3	Docosane			310	C22H46	000629-97-0	87
4	Heptadecane, 9-octyl-			352	C25H52	007225-64-1	87
5	Tetracosane			338	C24H50	000646-31-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
Data File : BF126078.D
Acq On : 9 Nov 2021 12:41
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Sample : M4540-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

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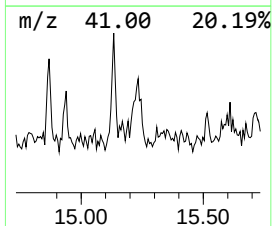
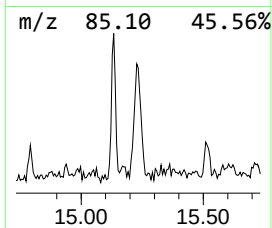
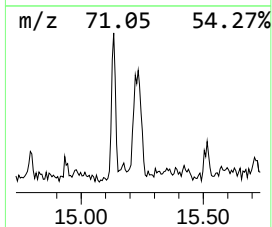
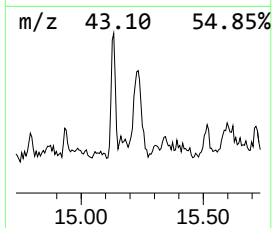
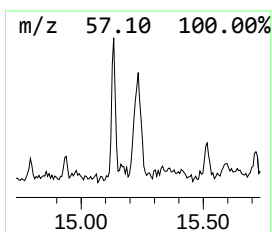
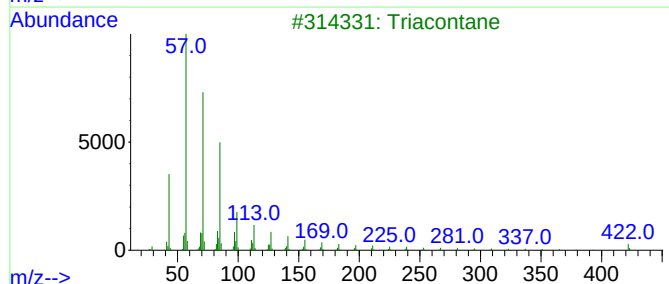
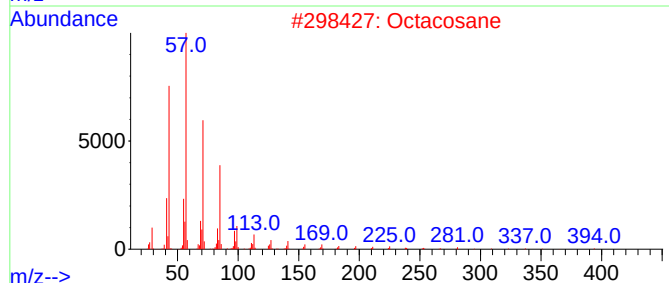
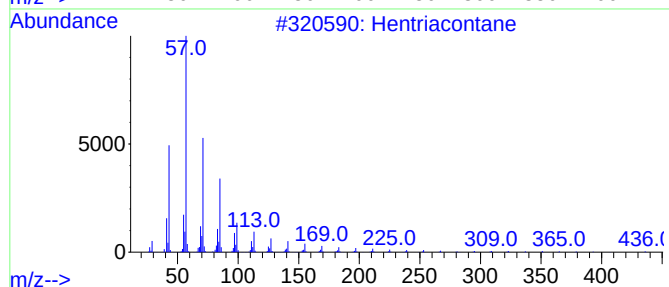
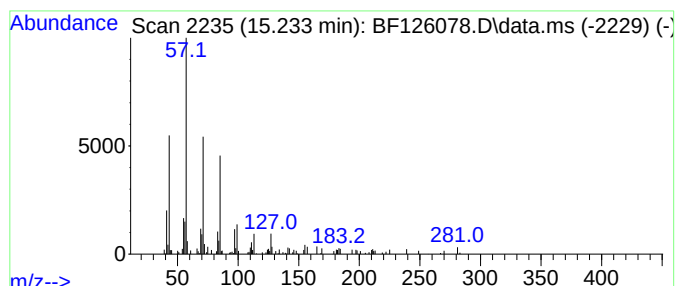
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hentriacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.233	4.91 ng	232198	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Octacosane	394	C28H58	000630-02-4	91
3			triacontane	422	C30H62	000638-68-6	91
4			Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1010115-66-1	91
5			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
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Acq On : 9 Nov 2021 12:41
Operator : JU/CG
Sample : M4540-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

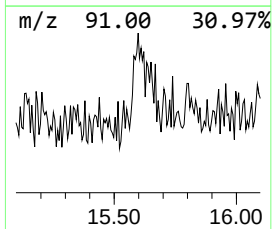
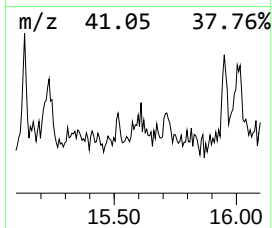
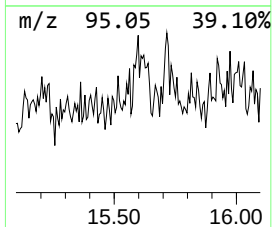
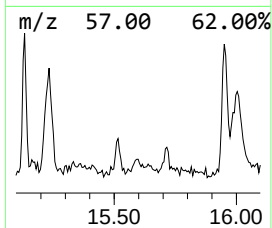
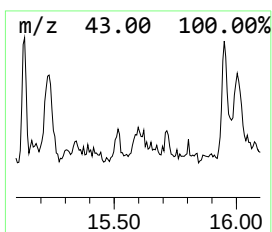
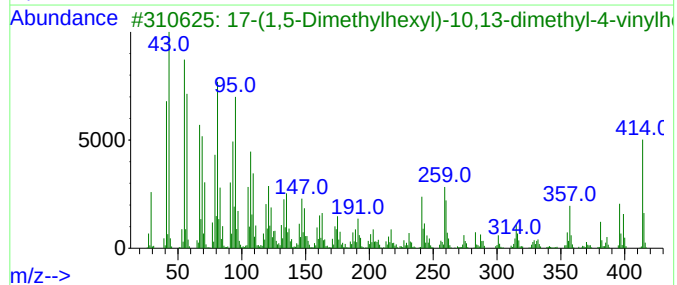
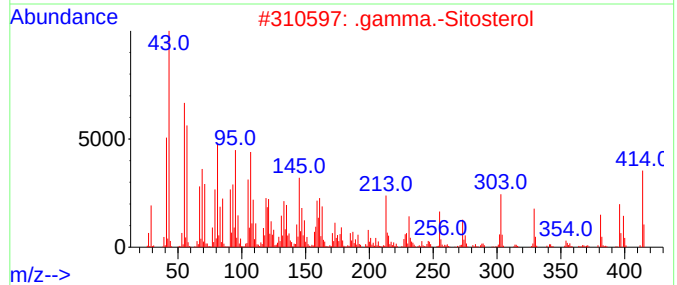
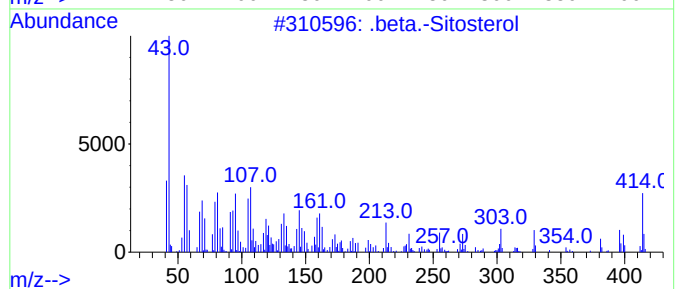
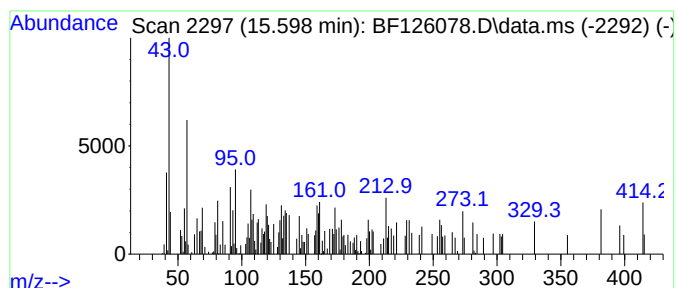
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 .beta.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.598	4.52 ng	213814	Perylene-d12	15.474	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	58
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	58
3	17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	32
4	22,26-Oxido-4,17-cholestadien-3...	414	C27H42O3	1000252-80-4	30
5	Stigmastan-7-one	414	C29H50O	055331-88-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
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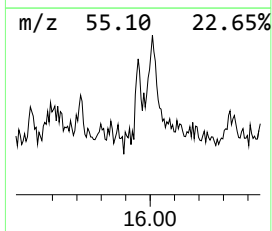
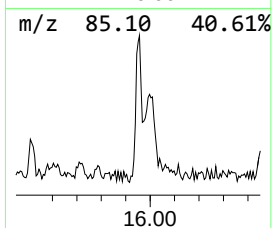
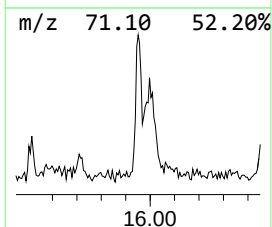
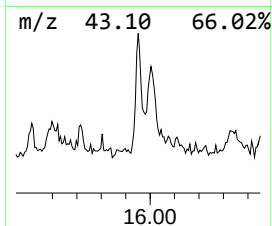
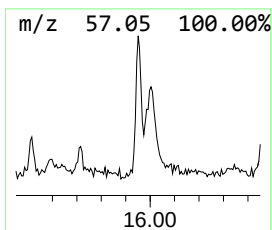
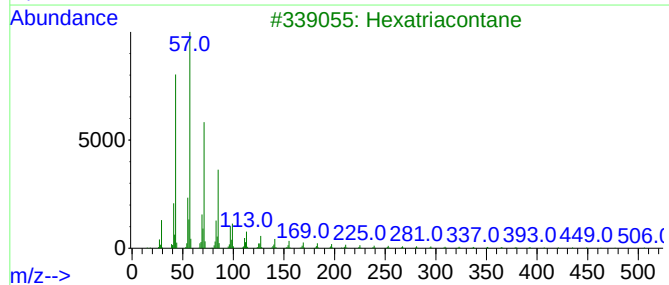
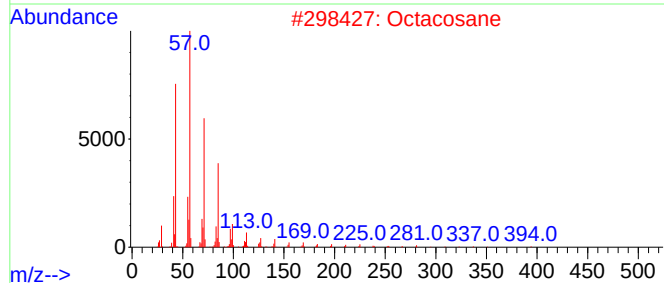
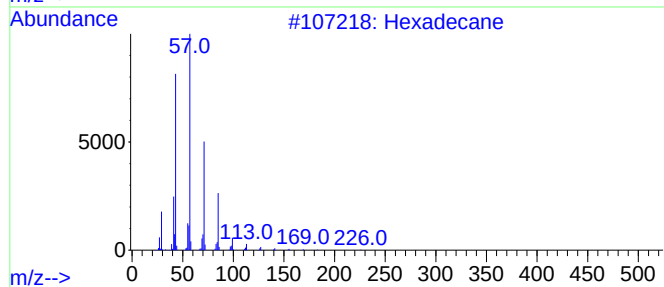
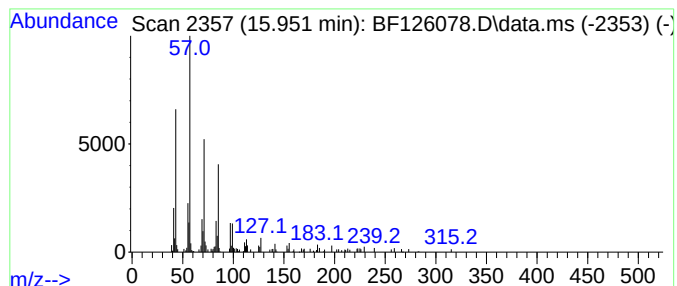
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	4.67 ng	221035	Perylene-d12	15.474

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane	226	C16H34	000544-76-3	94
2		Octacosane	394	C28H58	000630-02-4	90
3		Hexatriacontane	507	C36H74	000630-06-8	90
4		Hentriacontane	437	C31H64	000630-04-6	90
5		Octacosane, 2-methyl-	408	C29H60	001560-98-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
Data File : BF126078.D
Acq On : 9 Nov 2021 12:41
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Sample : M4540-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

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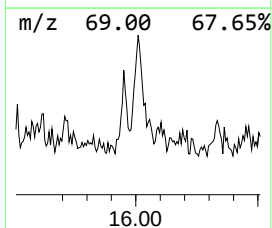
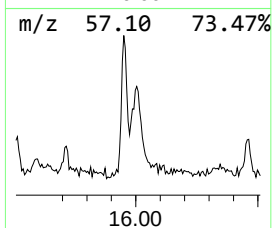
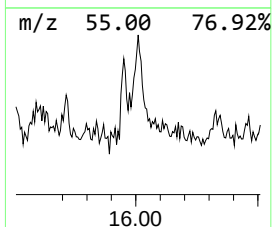
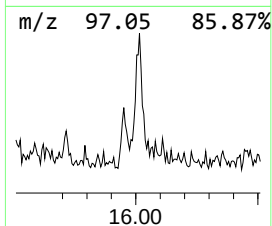
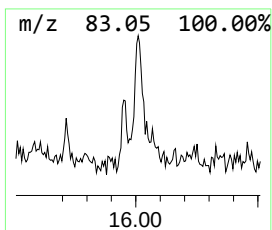
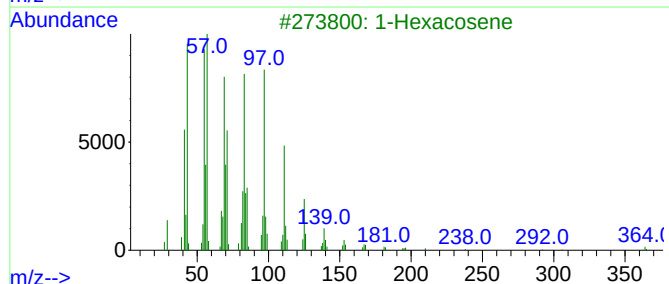
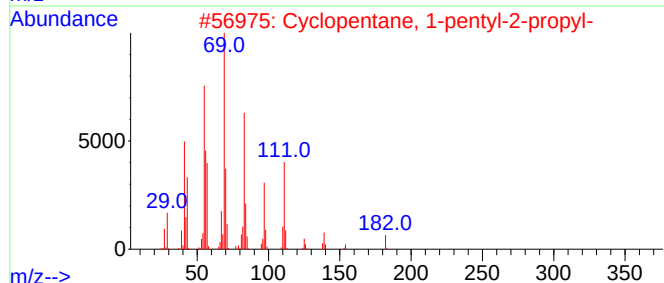
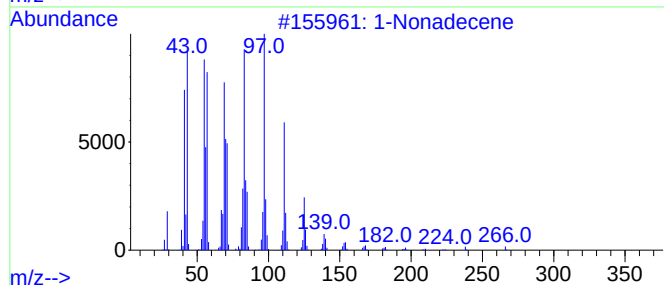
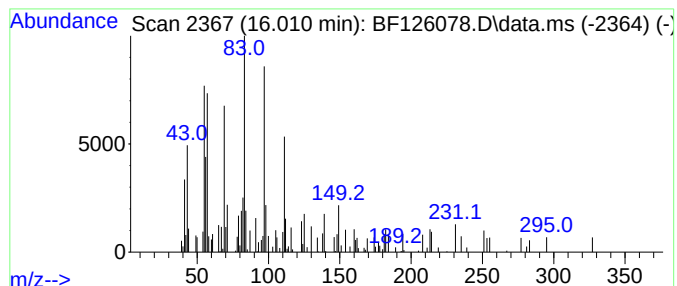
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Nonadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.010	4.51 ng	213345	Perylene-d12	15.474

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene		266	C19H38	018435-45-5	64
2	Cyclopentane, 1-pentyl-2-propyl-		182	C13H26	062199-51-3	45
3	1-Hexacosene		364	C26H52	018835-33-1	43
4	Cyclohexane, 1,2,4,5-tetraethyl-...		196	C14H28	061142-24-3	43
5	3-Heptene, 4-propyl-		140	C10H20	004485-13-6	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
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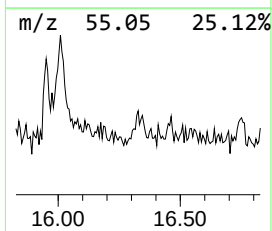
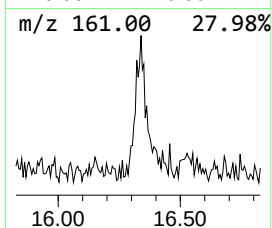
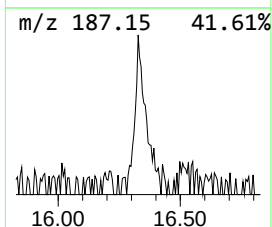
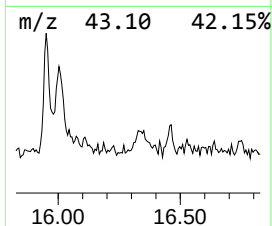
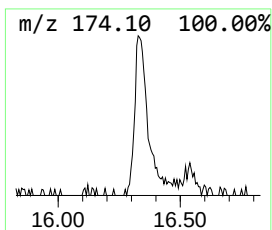
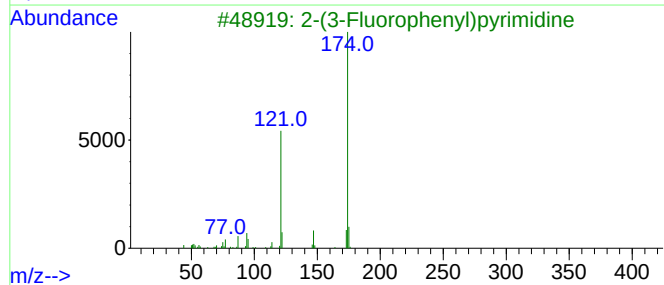
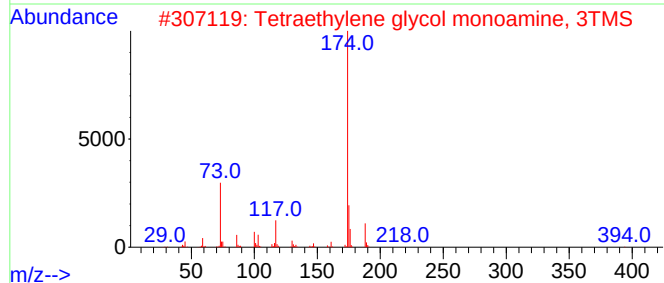
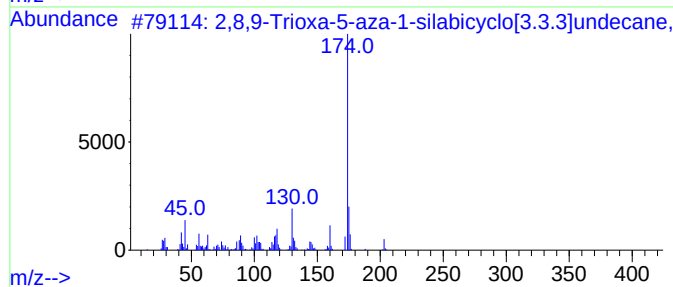
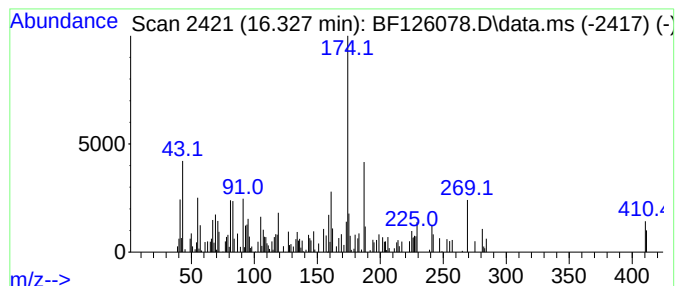
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.327 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.327	4.31 ng	203824	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,8,9-Trioxa-5-aza-1-silabicyclo...	203	C8H17N03Si	002097-16-7	38		
2	Tetraethylene glycol monoamine, ...	409	C17H43N04Si3	1010499-42-2	35		
3	2-(3-Fluorophenyl)pyrimidine	174	C10H7FN2	068049-16-1	30		
4	3-[(2-Aminoethyl)sulfanyl]-2-met...	379	C15H37N02SSi3	1000501-00-8	27		
5	2,2,4-Trimethyl-1,2-dihydro-quin...	189	C12H15NO	117330-56-0	27		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
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 Acq On : 9 Nov 2021 12:41
 Operator : JU/CG
 Sample : M4540-07
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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
Butane, 2-metho...	2.163	51.7	ng	2579710	1	6.851	998018	20.0
Ethanol, 1-(2-b...	8.034	7.1	ng	452698	2	8.134	1276630	20.0
Heptadecyl hept...	13.863	17.4	ng	890164	5	14.010	1025640	20.0
3-Chloropropion...	14.498	2.7	ng	138454	5	14.010	1025640	20.0
Octacosane	14.569	3.8	ng	197065	5	14.010	1025640	20.0
1,5,9-Undecatri...	14.868	2.1	ng	98256	6	15.474	946544	20.0
Eicosane	15.133	3.7	ng	175804	6	15.474	946544	20.0
Hentriacontane	15.233	4.9	ng	232198	6	15.474	946544	20.0
.beta.-Sitosterol	15.598	4.5	ng	213814	6	15.474	946544	20.0
Hexadecane	15.951	4.7	ng	221035	6	15.474	946544	20.0
1-Nonadecene	16.010	4.5	ng	213345	6	15.474	946544	20.0
unknown16.327	16.327	4.3	ng	203824	6	15.474	946544	20.0