

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
 Data File : BF126089.D
 Acq On : 9 Nov 2021 19:17
 Operator : JU/CG
 Sample : M4523-02
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VWE-B4-110421-10-20

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: BF126089.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	9	22	rVB	1586779	1931035	35.48%	5.023%
2	5.469	570	575	578	rBV	4423364	4013196	73.73%	10.439%
3	6.481	741	747	750	rBV	4211758	4285664	78.74%	11.148%
4	6.851	806	810	813	rBV	1397118	1077866	19.80%	2.804%
5	7.410	895	905	908	rBV	2842430	2854418	52.44%	7.425%
6	8.034	1008	1011	1023	rBV	368670	357818	6.57%	0.931%
7	8.134	1023	1028	1031	rBV	1696257	1416984	26.03%	3.686%
8	9.210	1206	1211	1214	rBV	6624347	5443033	100.00%	14.158%
9	9.292	1221	1225	1228	rBV2	64719	74661	1.37%	0.194%
10	9.610	1274	1279	1281	rBV2	76662	89909	1.65%	0.234%
11	9.886	1320	1326	1329	rBV	1996503	1628433	29.92%	4.236%
12	9.916	1329	1331	1336	rVB	79075	77725	1.43%	0.202%
13	10.428	1415	1418	1425	rBV	82482	97384	1.79%	0.253%
14	10.675	1455	1460	1463	rBV	3737316	3367524	61.87%	8.759%
15	10.804	1477	1482	1489	rVB	110733	168510	3.10%	0.438%
16	11.269	1558	1561	1566	rVB2	80710	88245	1.62%	0.230%
17	11.369	1574	1578	1580	rBV	1825105	1500646	27.57%	3.903%
18	11.392	1580	1582	1585	rVV	601783	453904	8.34%	1.181%
19	11.439	1588	1590	1594	rVB	141730	132879	2.44%	0.346%
20	11.598	1613	1617	1619	rBV2	56302	70292	1.29%	0.183%
21	11.869	1658	1663	1666	rBV	74519	92162	1.69%	0.240%
22	11.898	1666	1668	1670	rVB	119509	88932	1.63%	0.231%
23	11.980	1679	1682	1685	rBV2	97044	113506	2.09%	0.295%
24	12.592	1783	1786	1789	rBV	524540	409901	7.53%	1.066%
25	12.810	1818	1823	1826	rBV	408781	384291	7.06%	1.000%
26	12.957	1844	1848	1851	rBV	5298531	4197751	77.12%	10.919%
27	13.857	1998	2001	2008	rVB2	278854	343658	6.31%	0.894%
28	14.004	2021	2026	2029	rBV2	1128221	1250235	22.97%	3.252%
29	14.027	2029	2030	2035	rVB	169794	134527	2.47%	0.350%
30	14.492	2105	2109	2113	rBV4	103700	195237	3.59%	0.508%
31	14.974	2188	2191	2196	rBV6	74082	103430	1.90%	0.269%
32	15.045	2199	2203	2205	rBV	124236	179573	3.30%	0.467%
33	15.127	2214	2217	2220	rBV2	87825	100367	1.84%	0.261%
34	15.345	2251	2254	2260	rVB	90706	127434	2.34%	0.331%
35	15.404	2261	2264	2268	rVB	114180	119225	2.19%	0.310%
36	15.474	2271	2276	2280	rBV	798432	984558	18.09%	2.561%

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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

37	15.710	2312	2316	2320	rBV6	77149	123141	2.26%	0.320%
38	15.951	2353	2357	2361	rBV2	75515	106917	1.96%	0.278%
39	16.009	2363	2367	2375	rVB4	72374	149104	2.74%	0.388%
40	16.921	2518	2522	2530	rVB4	51034	110970	2.04%	0.289%

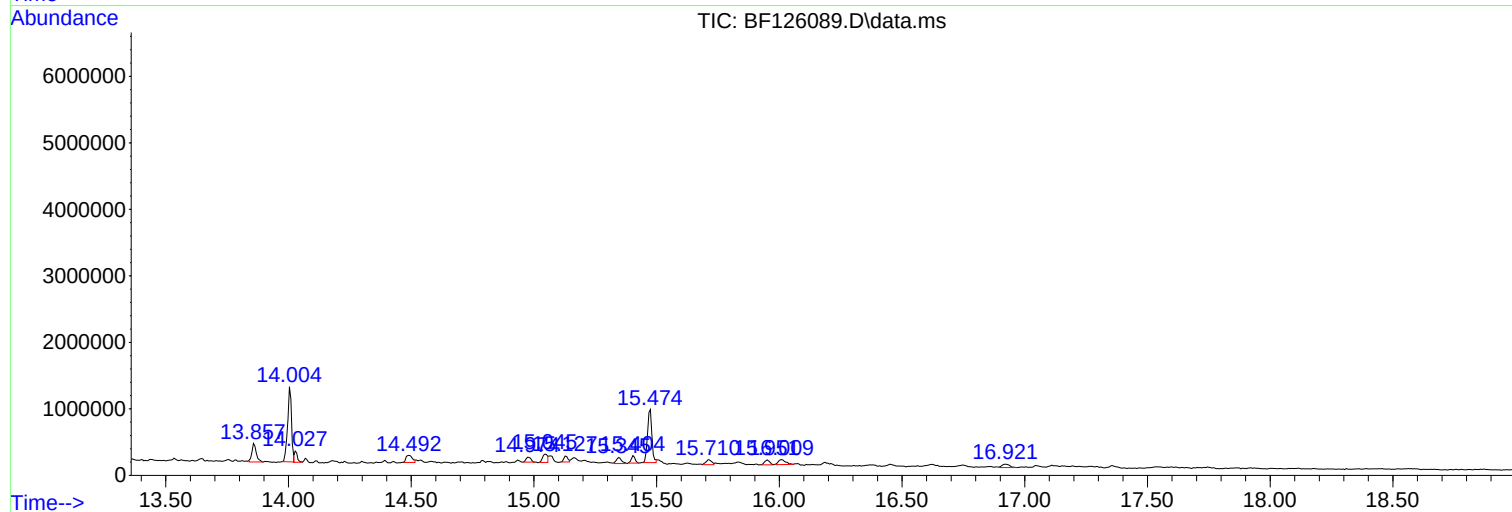
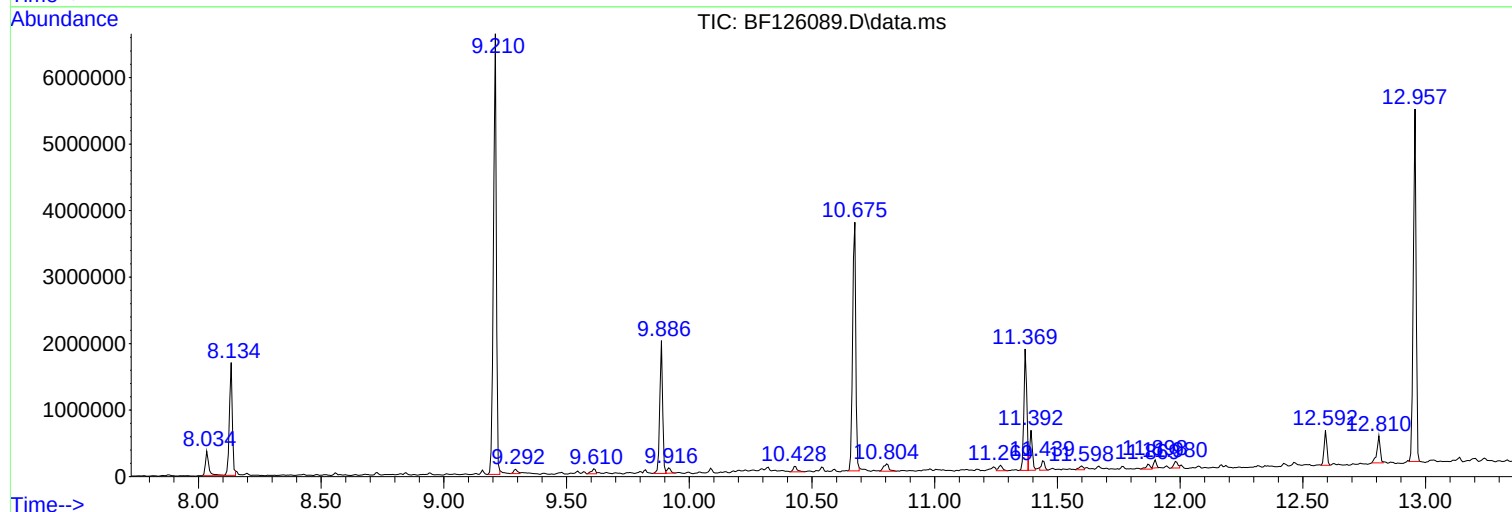
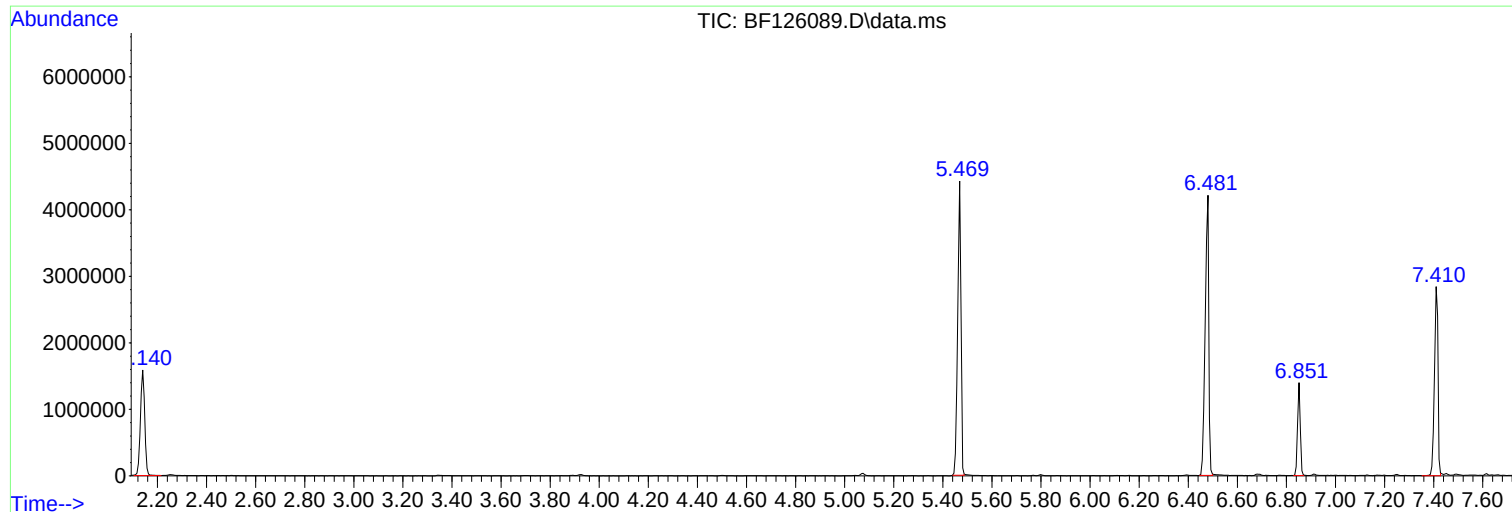
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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VWE-B4-110421-10-20

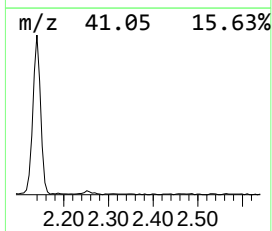
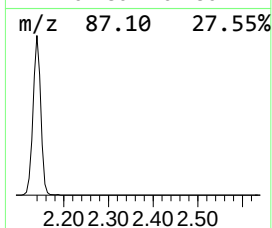
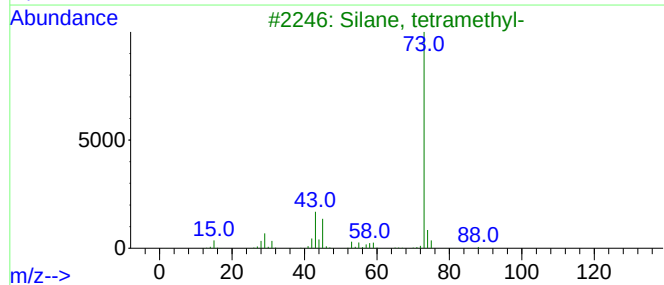
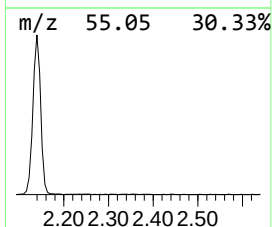
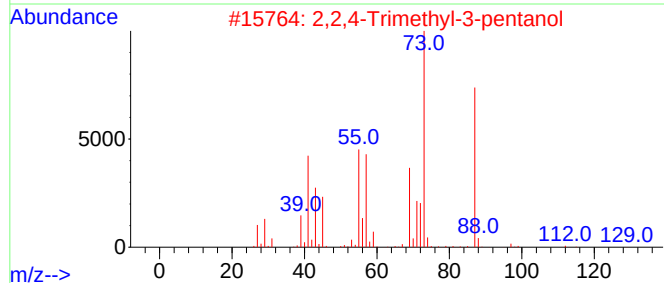
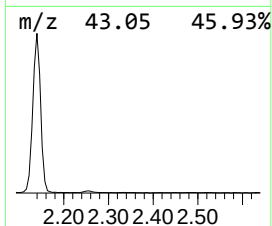
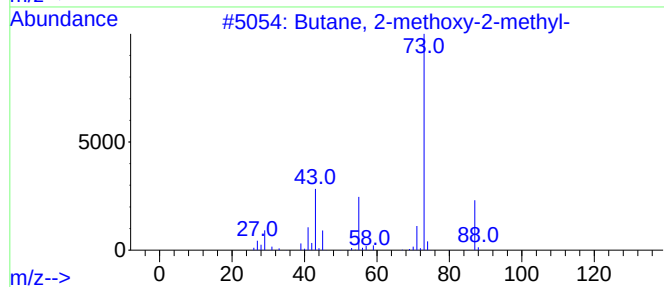
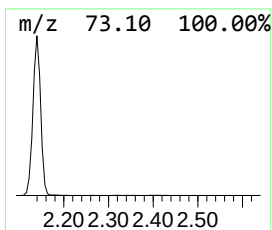
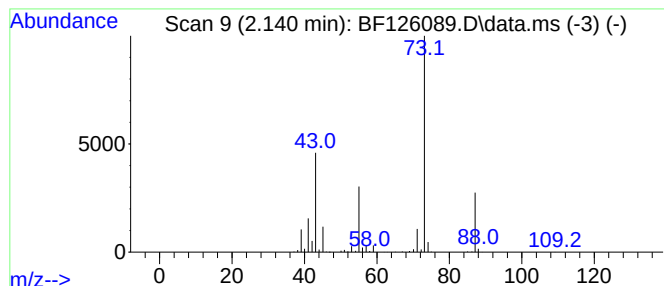
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.140	35.83 ng	1931040	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			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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Instrument :
BNA_F
ClientSampleId :
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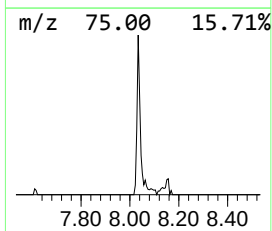
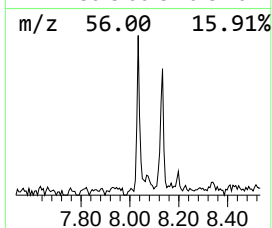
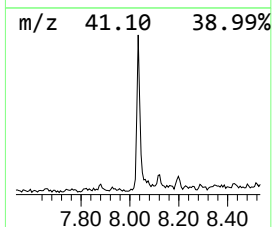
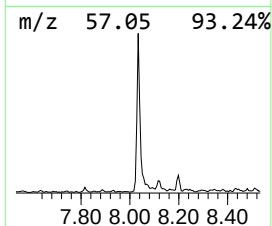
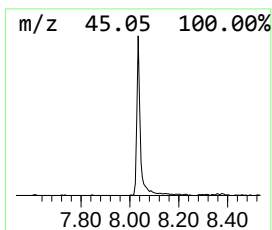
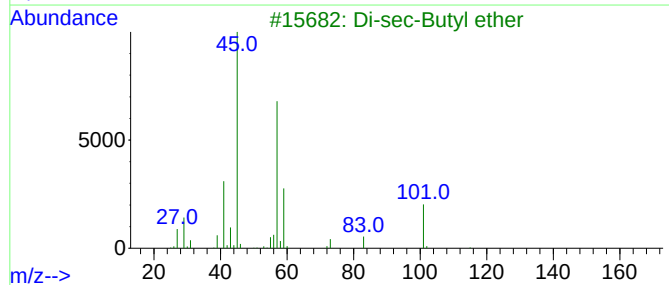
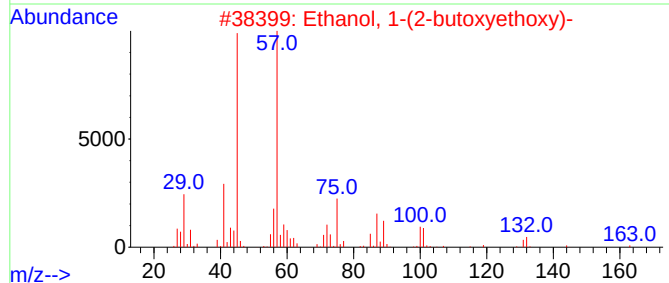
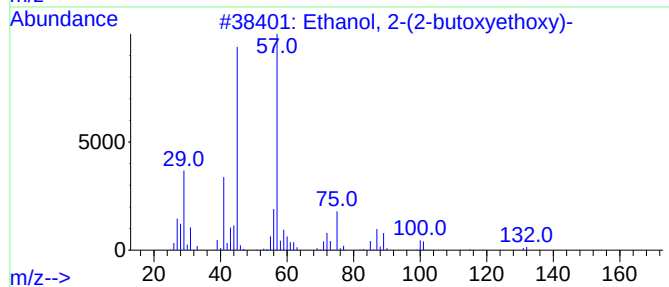
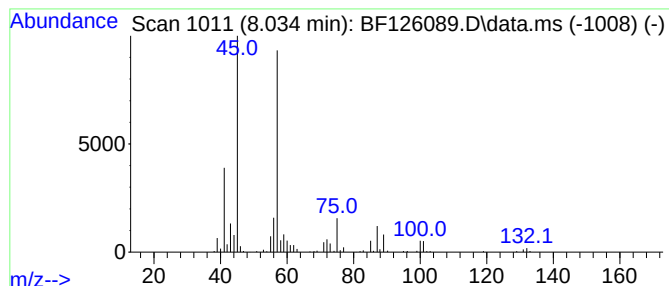
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.034	5.05 ng	357818	Naphthalene-d8	8.134

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			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5			Butyl lactate	146	C7H14O3	000138-22-7	50



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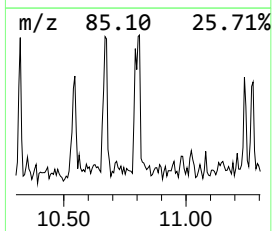
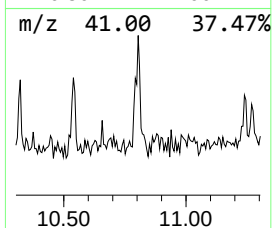
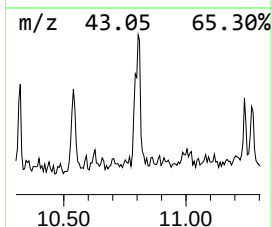
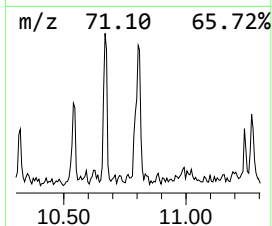
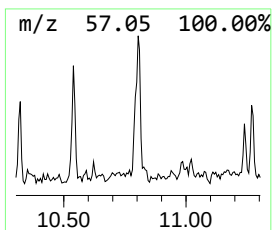
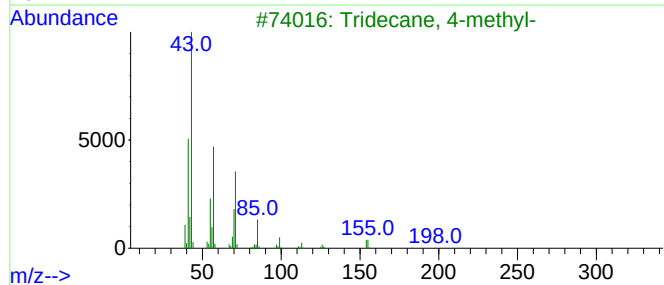
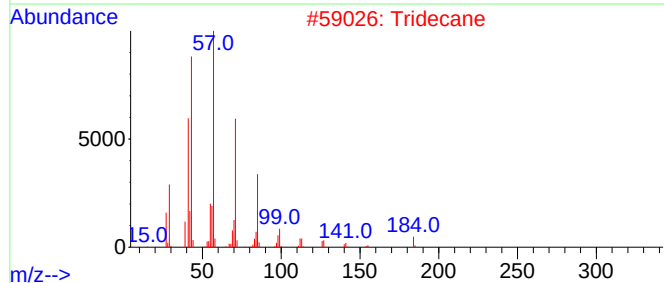
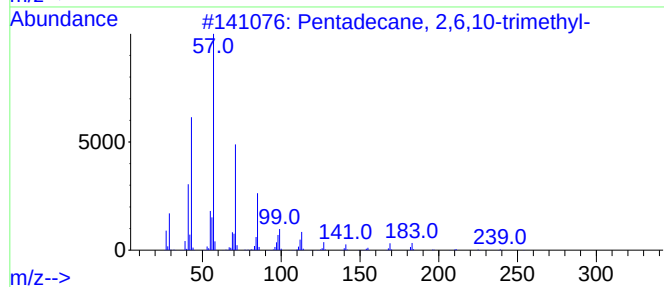
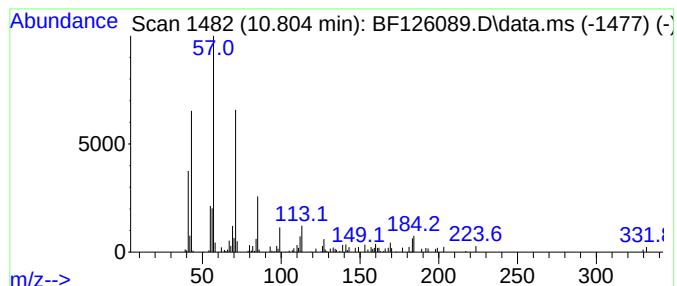
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentadecane, 2,6,10-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.804	2.25 ng	168510	Phenanthrene-d10		11.369	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-		254	C18H38	003892-00-0	86
2	Tridecane		184	C13H28	000629-50-5	80
3	Tridecane, 4-methyl-		198	C14H30	026730-12-1	72
4	Dodecane, 2,6,11-trimethyl-		212	C15H32	031295-56-4	72
5	Dodecane, 2,7,10-trimethyl-		212	C15H32	074645-98-0	72



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Instrument :
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ClientSampleId :
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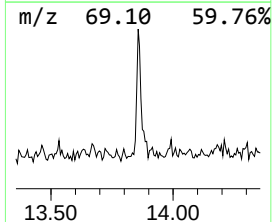
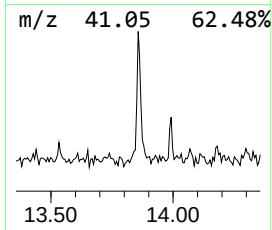
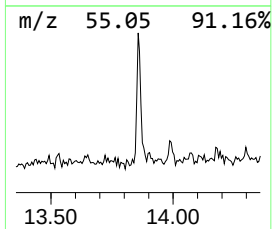
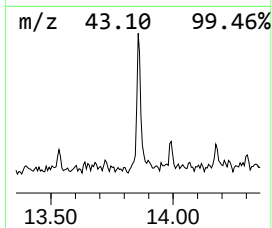
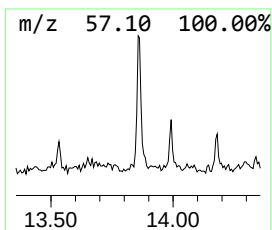
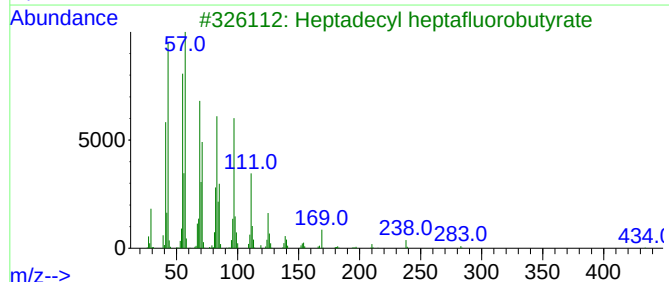
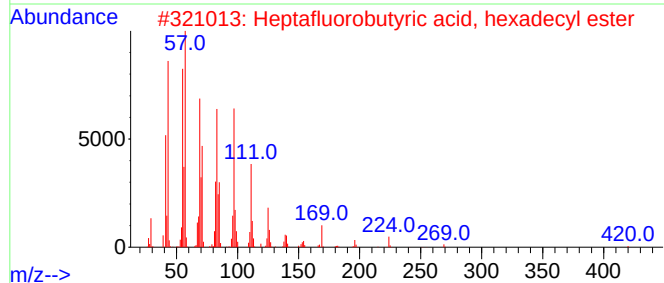
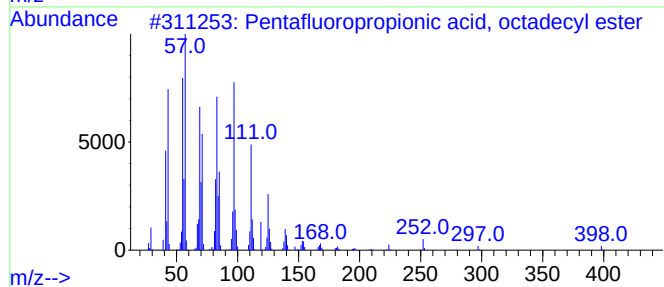
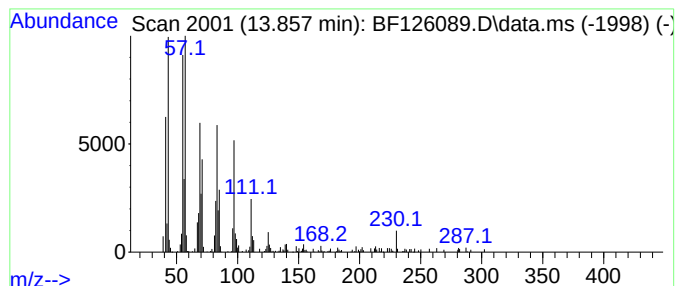
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Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	5.50 ng	343658	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
2			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
4			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91



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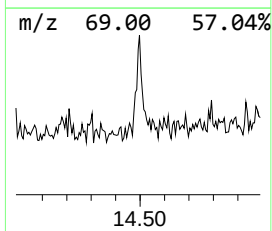
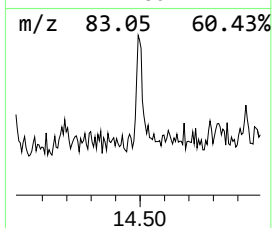
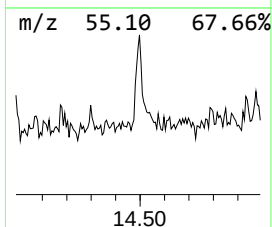
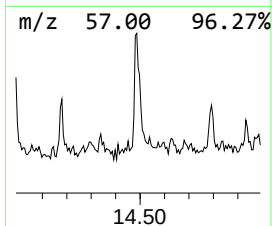
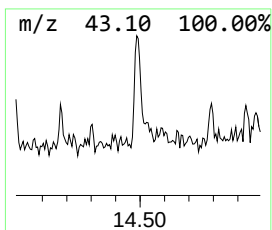
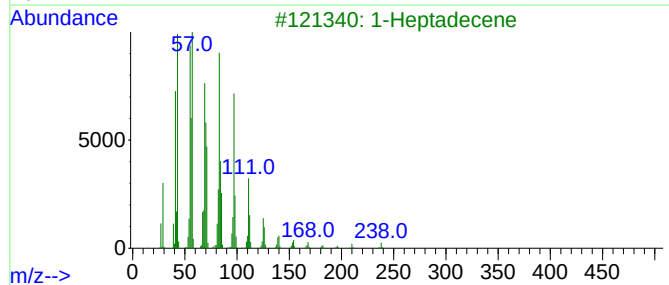
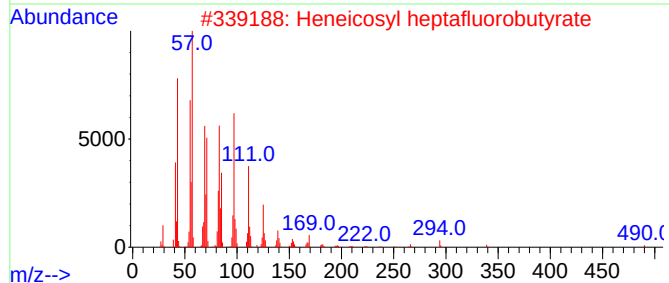
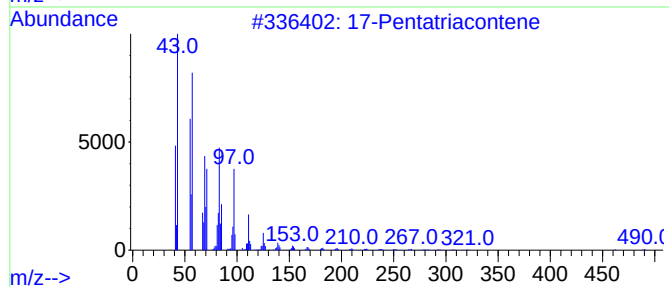
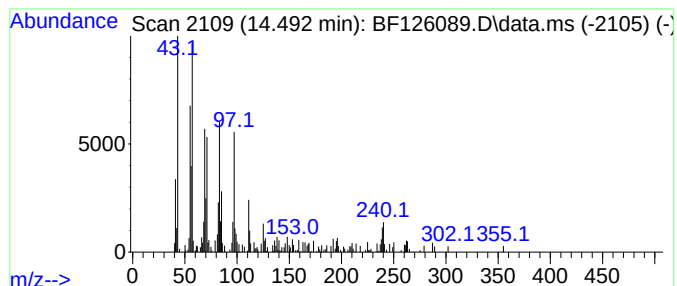
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 17-Pentatriacontene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.492	3.12 ng	195237	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	81
2			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	81
3			1-Heptadecene	238	C17H34	006765-39-5	76
4			3-Heptadecene, (Z)-	238	C17H34	1000141-67-3	76
5			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
Data File : BF126089.D
Acq On : 9 Nov 2021 19:17
Operator : JU/CG
Sample : M4523-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VWE-B4-110421-10-20

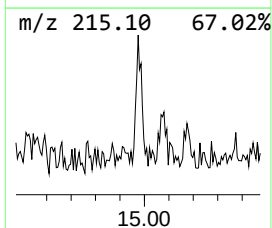
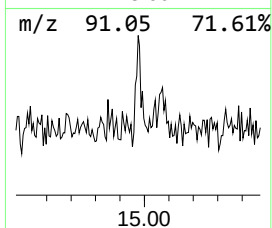
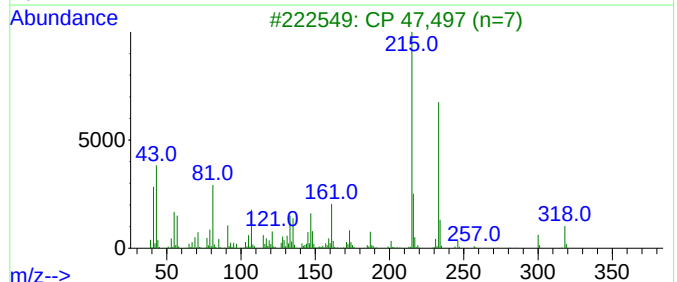
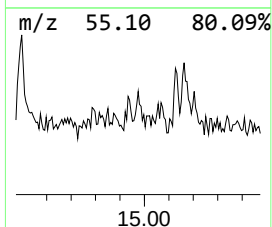
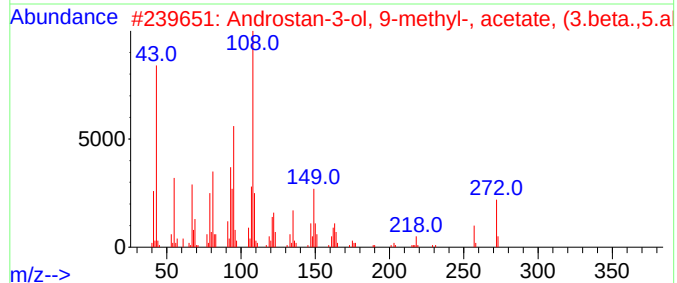
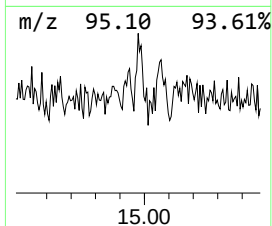
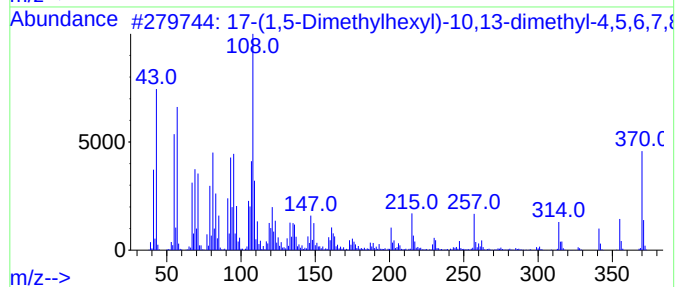
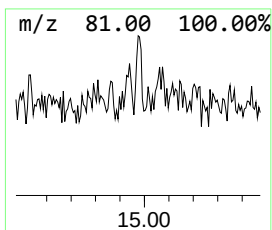
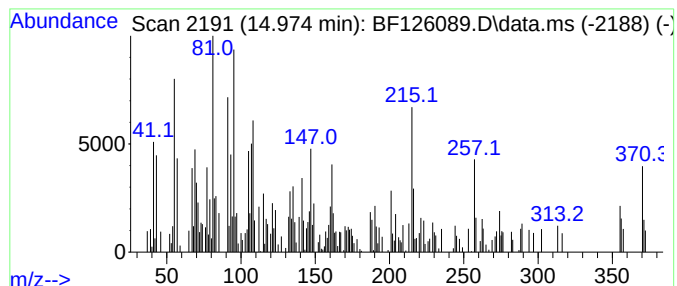
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.974 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.974	2.10 ng	103430	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-(1,5-Dimethylhexyl)-10,13-dim...	370	C27H46	1000210-50-1	41		
2	Androstan-3-ol, 9-methyl-, aceta...	332	C22H36O2	054550-12-8	22		
3	CP 47,497 (n=7)	318	C21H34O2	070434-82-1	22		
4	Benzo[e]pyrene, 8b,9,10,11,12,12...	258	C20H18	086439-17-0	22		
5	Longifolene	204	C15H24	000475-20-7	20		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
Data File : BF126089.D
Acq On : 9 Nov 2021 19:17
Operator : JU/CG
Sample : M4523-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VWE-B4-110421-10-20

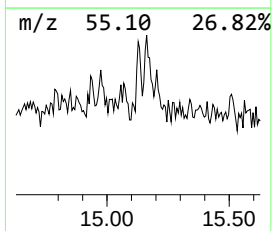
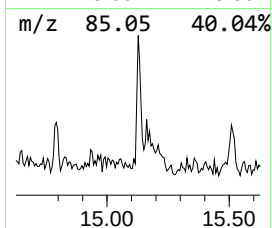
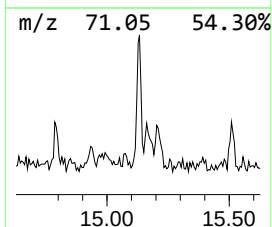
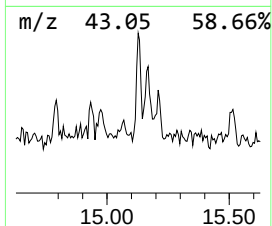
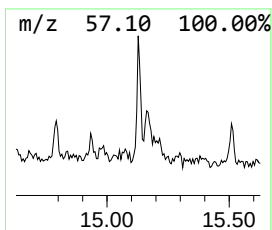
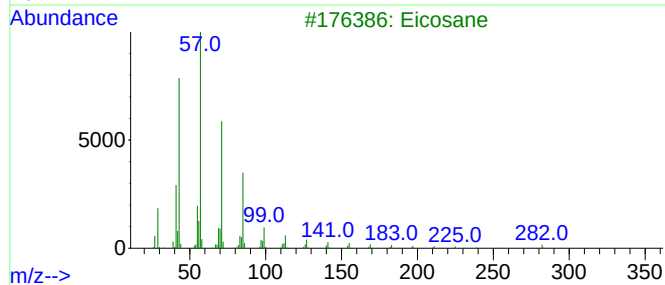
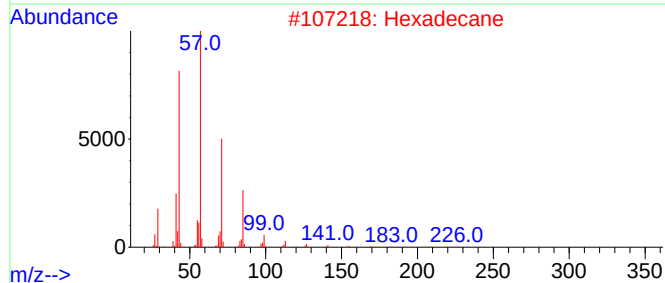
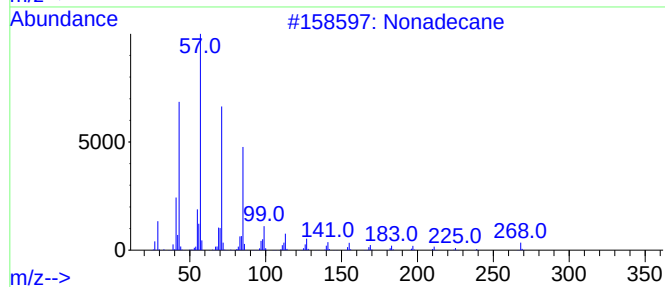
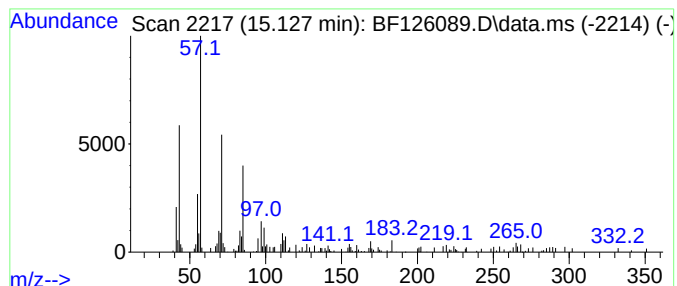
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	2.04 ng	100367	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	91
2			Hexadecane	226	C16H34	000544-76-3	90
3			Eicosane	282	C20H42	000112-95-8	81
4			1-Iodoundecane	282	C11H23I	004282-44-4	74
5			Tetracosane	338	C24H50	000646-31-1	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
Data File : BF126089.D
Acq On : 9 Nov 2021 19:17
Operator : JU/CG
Sample : M4523-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

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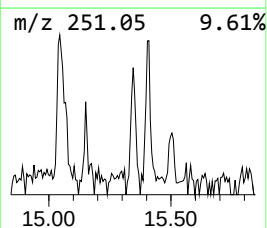
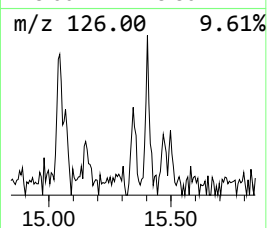
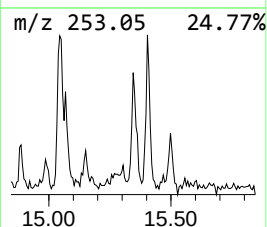
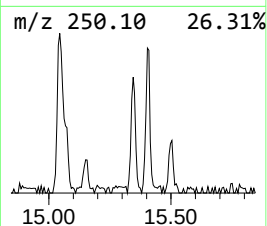
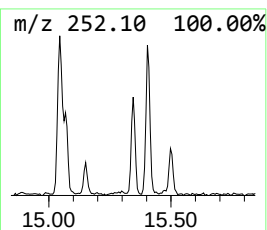
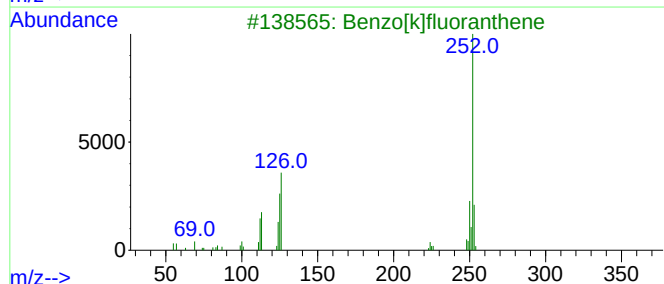
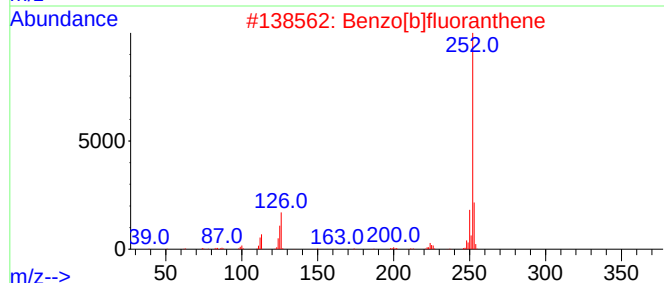
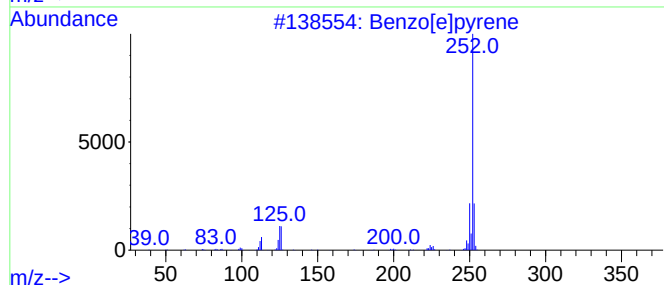
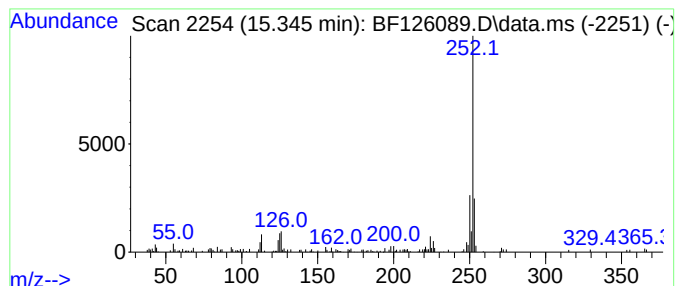
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.345	2.59 ng	127434	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4			Benzo[a]pyrene	252	C20H12	000050-32-8	93
5			(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
Data File : BF126089.D
Acq On : 9 Nov 2021 19:17
Operator : JU/CG
Sample : M4523-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VWE-B4-110421-10-20

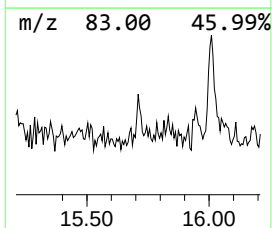
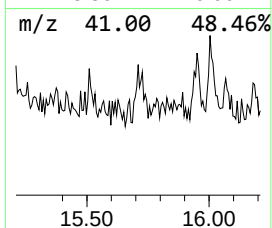
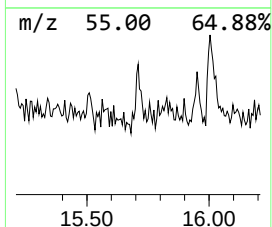
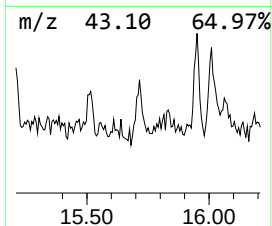
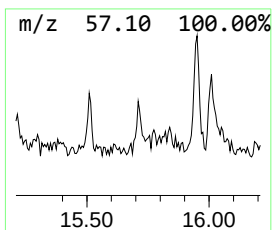
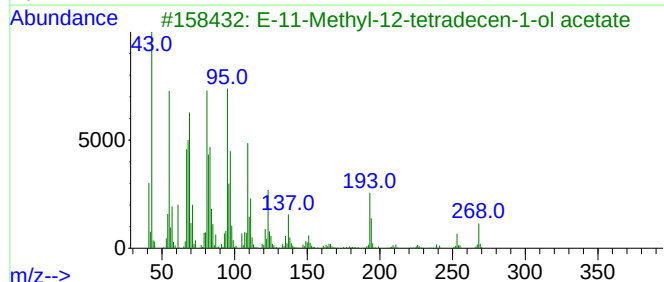
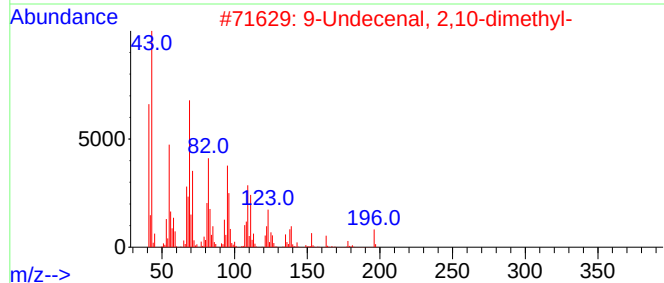
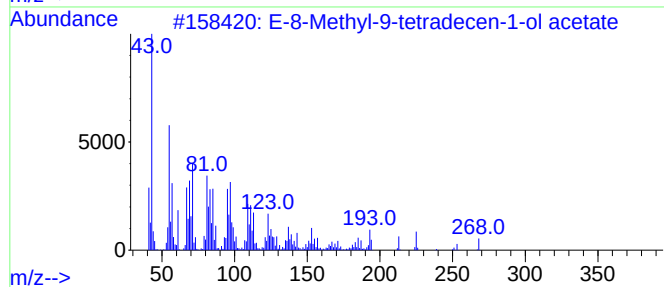
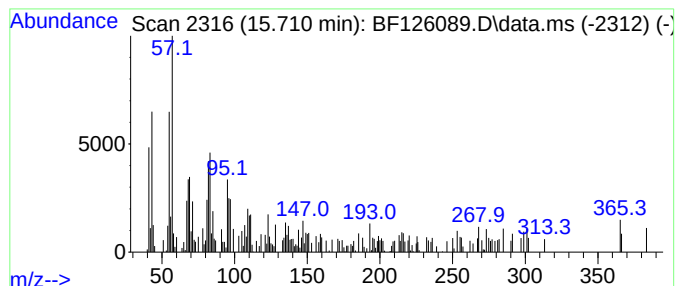
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 E-8-Methyl-9-tetradecen-1-o... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.710	2.50 ng	123141	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-8-Methyl-9-tetradecen-1-ol	ace...	268	C17H32O2	1000130-81-4	58	
2	9-Undecenal, 2,10-dimethyl-		196	C13H24O	1000131-85-9	48	
3	E-11-Methyl-12-tetradecen-1-ol	a...	268	C17H32O2	1000130-80-7	43	
4	Heptadecanal		254	C17H34O	1000376-70-0	38	
5	2-Nonen-1-ol		142	C9H18O	022104-79-6	35	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
Data File : BF126089.D
Acq On : 9 Nov 2021 19:17
Operator : JU/CG
Sample : M4523-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VWE-B4-110421-10-20

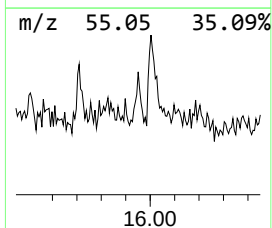
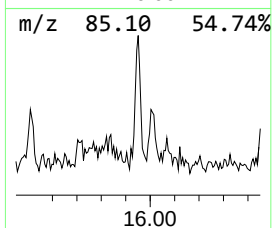
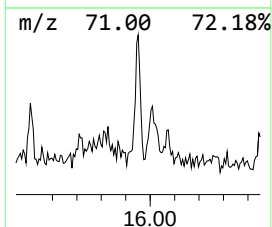
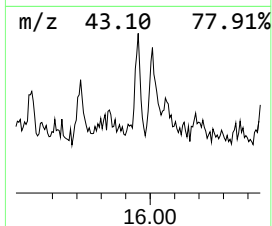
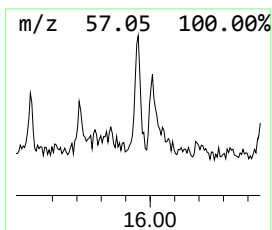
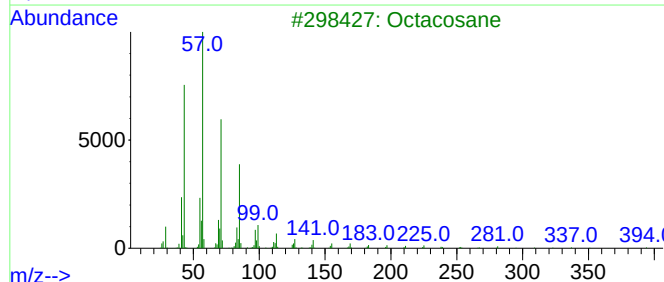
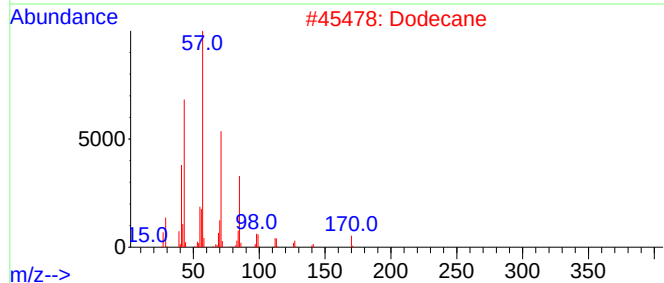
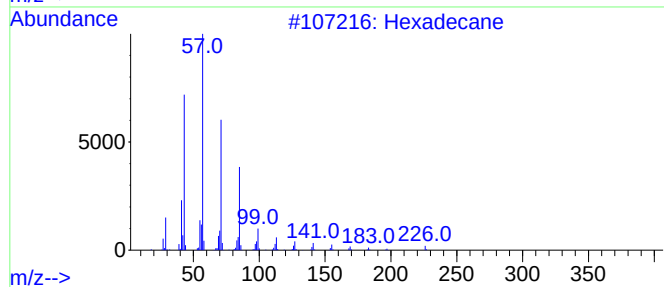
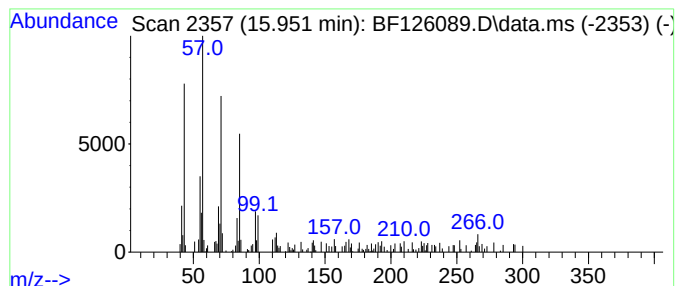
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	2.17 ng	106917	Perylene-d12	15.474

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane	226	C16H34	000544-76-3	58
2		Dodecane	170	C12H26	000112-40-3	58
3		Octacosane	394	C28H58	000630-02-4	52
4		Heptacosane	380	C27H56	000593-49-7	52
5		Hentriacontane	437	C31H64	000630-04-6	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
Data File : BF126089.D
Acq On : 9 Nov 2021 19:17
Operator : JU/CG
Sample : M4523-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VWE-B4-110421-10-20

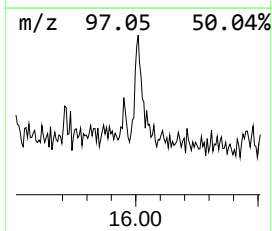
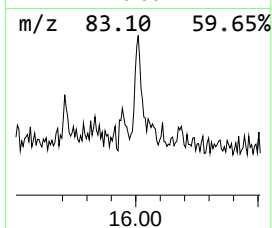
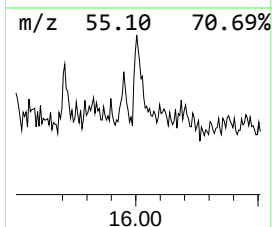
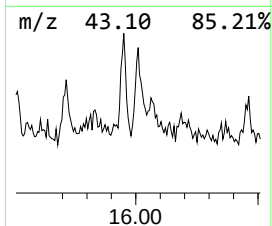
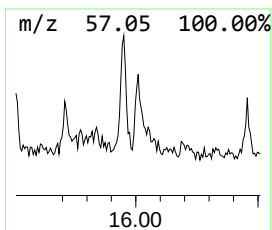
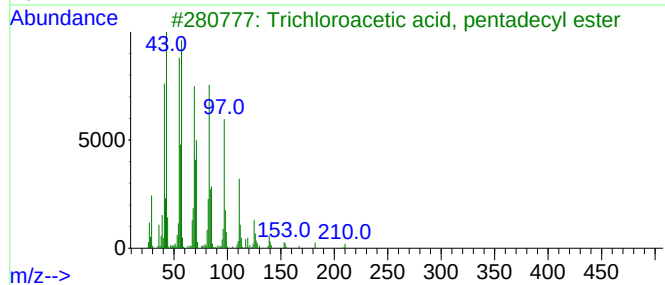
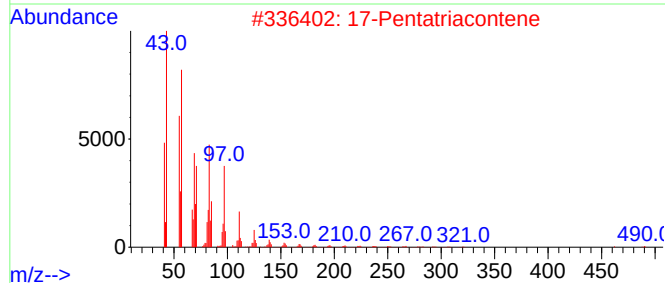
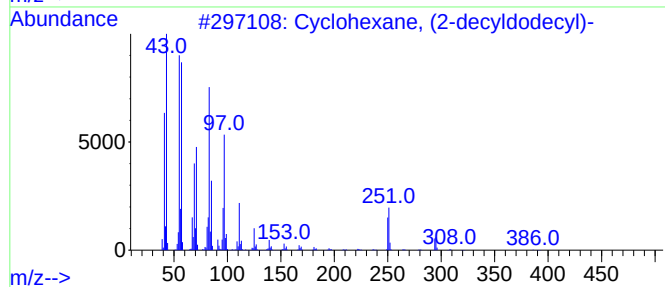
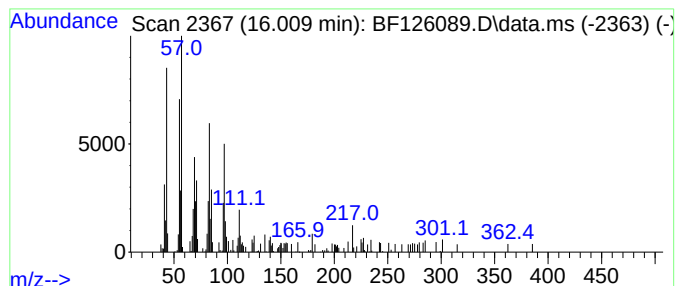
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Cyclohexane, (2-decyldodecyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.009	3.03 ng	149104	Perylene-d12	15.474

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, (2-decyldodecyl)-	392	C28H56	006704-00-3	72
2		17-Pentatriacontene	491	C35H70	006971-40-0	64
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	64
4		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	62
5		Cyclotetracosane	336	C24H48	000297-03-0	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110921\
Data File : BF126089.D
Acq On : 9 Nov 2021 19:17
Operator : JU/CG
Sample : M4523-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VWE-B4-110421-10-20

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
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Ethanol, 2-(2-b...	8.034	5.0	ng	357818	2	8.134	1416980	20.0
Pentadecane, 2,...	10.804	2.3	ng	168510	4	11.369	1500650	20.0
Pentafluoroprop...	13.857	5.5	ng	343658	5	14.004	1250240	20.0
17-Pentatriacon...	14.492	3.1	ng	195237	5	14.004	1250240	20.0
unknown14.974	14.974	2.1	ng	103430	6	15.474	984558	20.0
Nonadecane	15.127	2.0	ng	100367	6	15.474	984558	20.0
Benzo[e]pyrene	15.345	2.6	ng	127434	6	15.474	984558	20.0
E-8-Methyl-9-te...	15.710	2.5	ng	123141	6	15.474	984558	20.0
Hexadecane	15.951	2.2	ng	106917	6	15.474	984558	20.0
Cyclohexane, (2...	16.009	3.0	ng	149104	6	15.474	984558	20.0