

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110723\
 Data File : BF136177.D
 Acq On : 07 Nov 2023 15:47
 Operator : CG\JU
 Sample : PB156921BL
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB156921BL

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-BF110723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136177.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	505	508	514	rVB	29719	37645	1.20%	0.187%
2	5.457	567	573	576	rBV	2475270	2518207	80.40%	12.480%
3	6.451	736	742	745	rBV	2061583	2504493	79.96%	12.412%
4	6.816	801	804	808	rVB	714301	550560	17.58%	2.728%
5	7.381	895	900	903	rBV	1683536	1676448	53.53%	8.308%
6	8.098	1018	1022	1025	rBV	930985	722778	23.08%	3.582%
7	9.181	1201	1206	1209	rBV	3898505	3131990	100.00%	15.522%
8	9.857	1317	1321	1324	rBV	1011857	815673	26.04%	4.042%
9	10.651	1451	1456	1459	rBV	2121964	1890463	60.36%	9.369%
10	11.351	1571	1575	1578	rBV	911897	806669	25.76%	3.998%
11	12.951	1843	1847	1850	rBV	3133229	3012309	96.18%	14.929%
12	14.004	2022	2026	2030	rBV	632736	523517	16.72%	2.594%
13	14.110	2040	2044	2048	rBV2	47245	46288	1.48%	0.229%
14	14.504	2107	2111	2118	rBV	115713	125070	3.99%	0.620%
15	14.898	2173	2178	2189	rBV	148693	205416	6.56%	1.018%
16	15.351	2249	2255	2267	rBV	163819	254262	8.12%	1.260%
17	15.492	2274	2279	2288	rBV	364096	454708	14.52%	2.253%
18	15.880	2337	2345	2358	rBV2	129281	261132	8.34%	1.294%
19	16.510	2443	2452	2468	rBV3	94759	241779	7.72%	1.198%
20	17.274	2573	2582	2594	rBV4	68296	205070	6.55%	1.016%
21	18.227	2732	2744	2762	rBV5	50675	193698	6.18%	0.960%

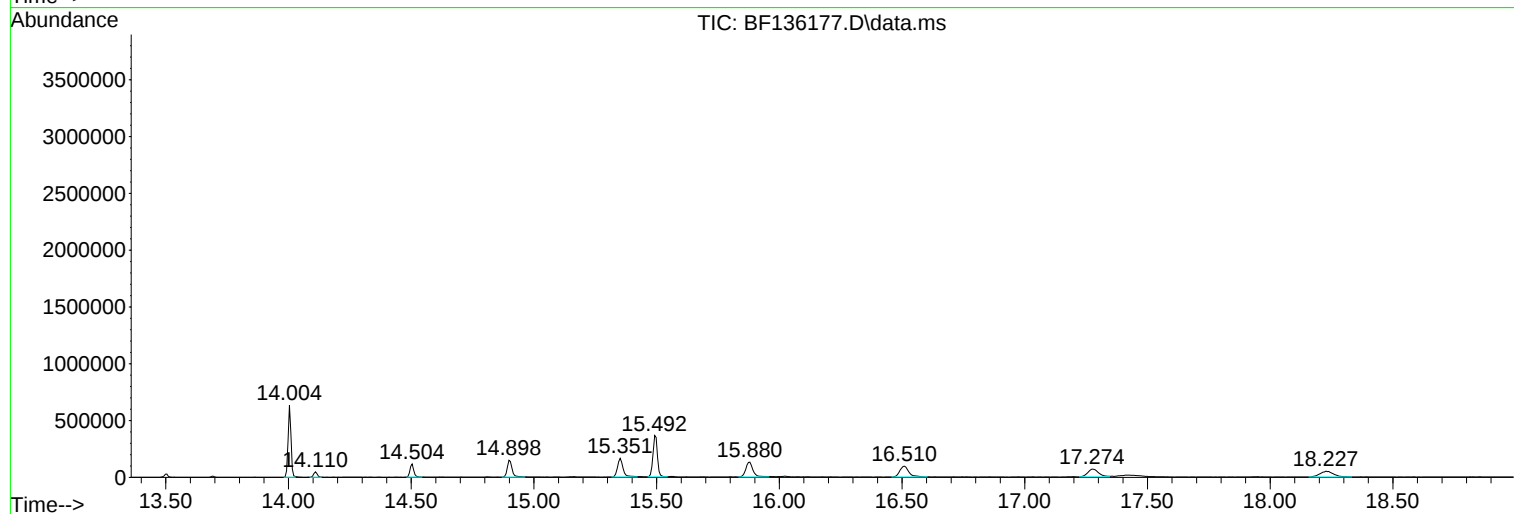
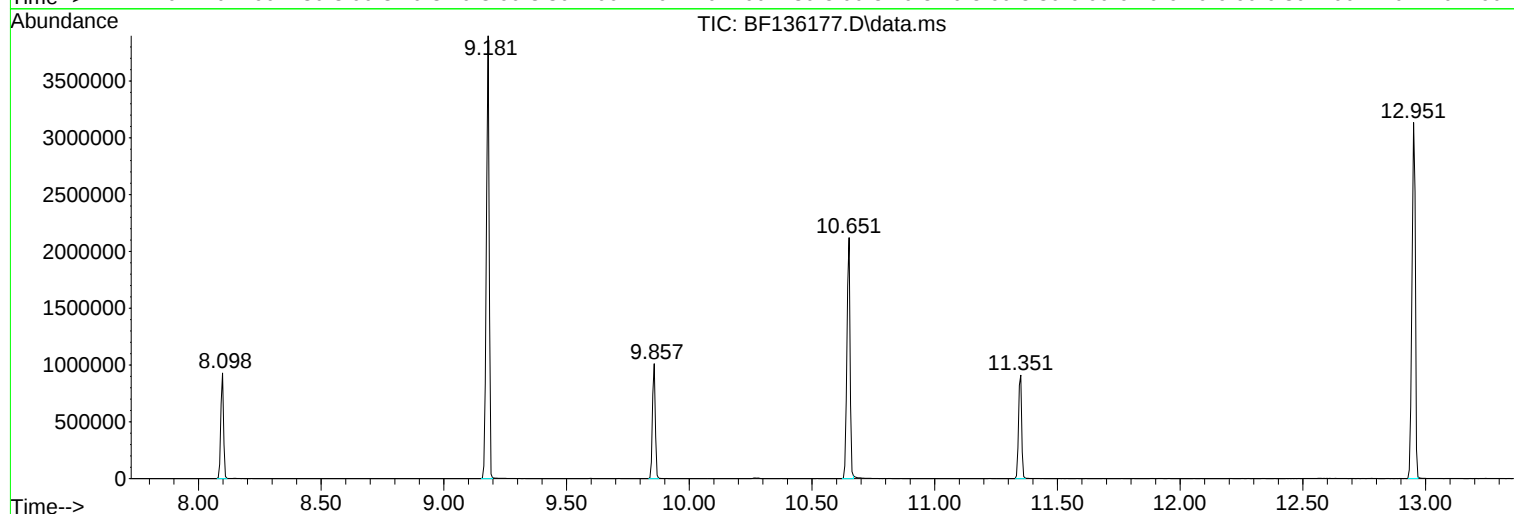
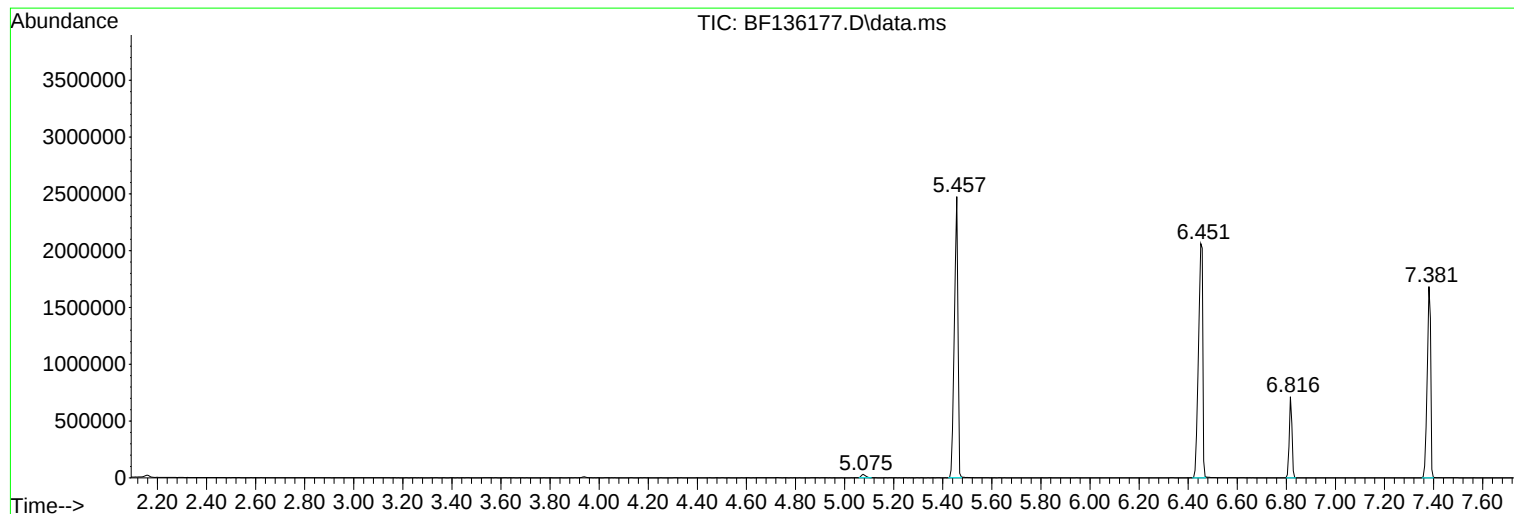
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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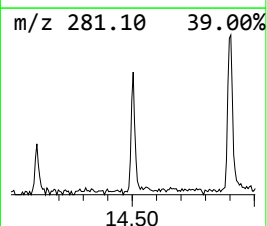
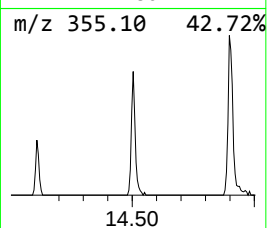
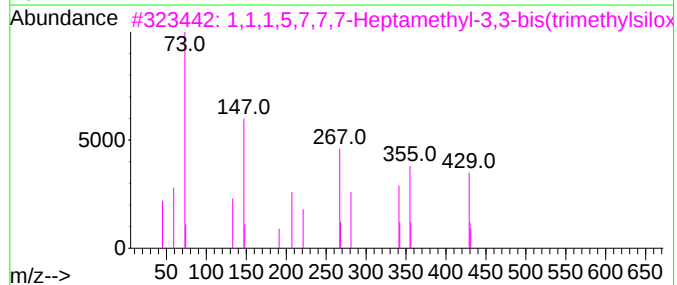
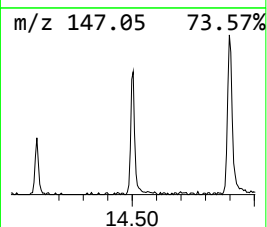
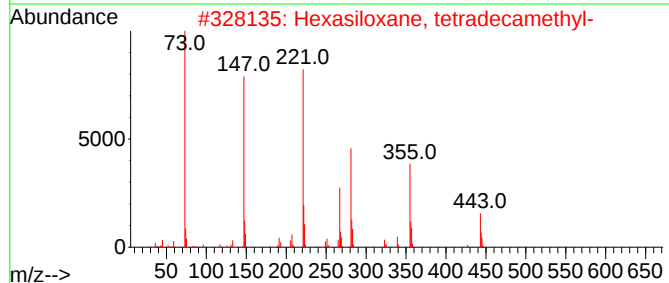
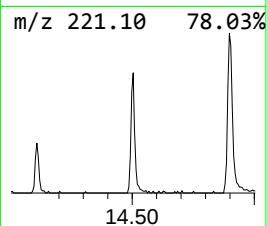
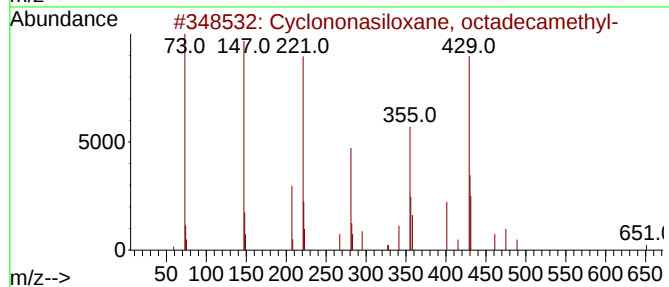
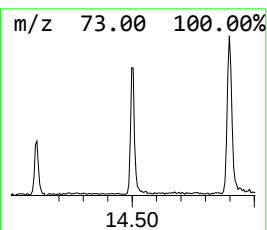
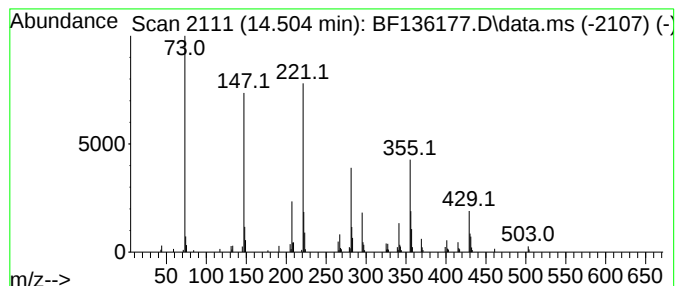
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclononasiloxane, octadeca... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.504	4.78 ng	125070	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	87
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	87
3			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	37
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	30



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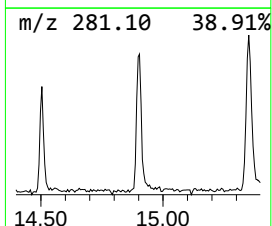
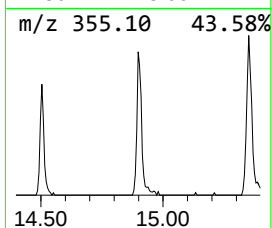
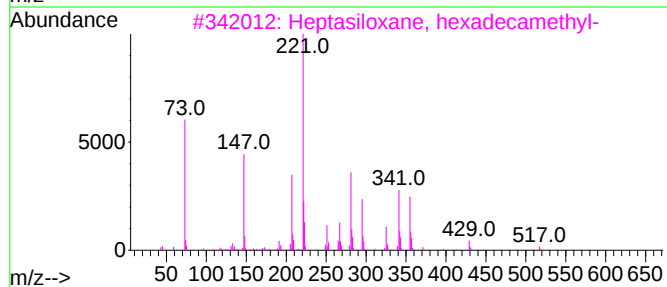
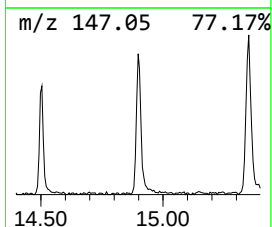
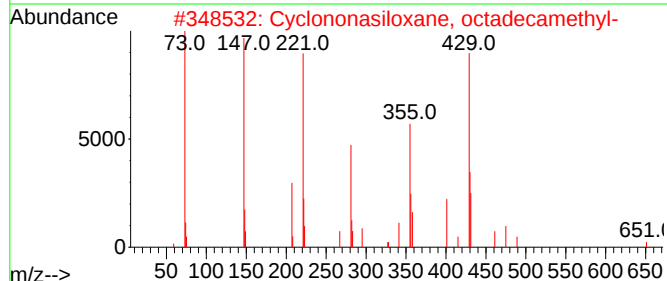
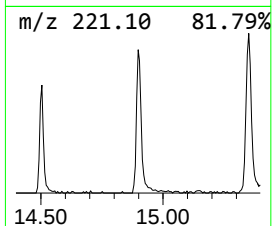
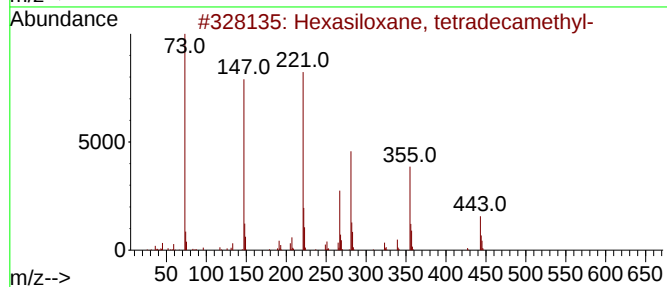
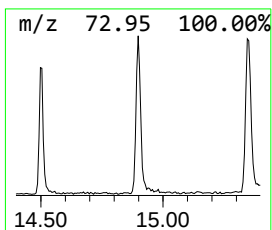
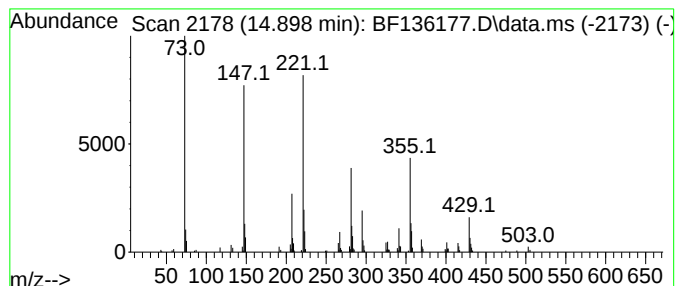
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110723.M
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Peak Number 2 Hexasiloxane, tetradecamethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	9.04 ng	205416	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	87
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	83
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	58
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	47
5			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37



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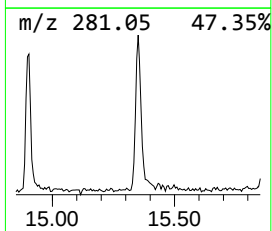
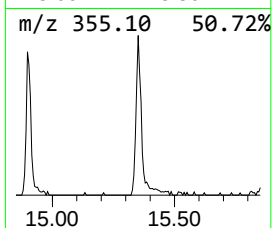
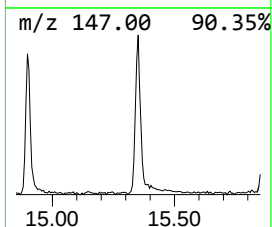
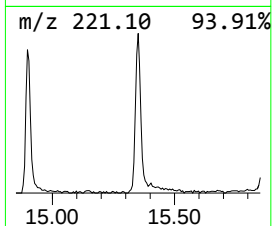
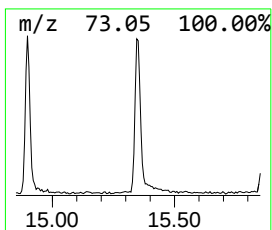
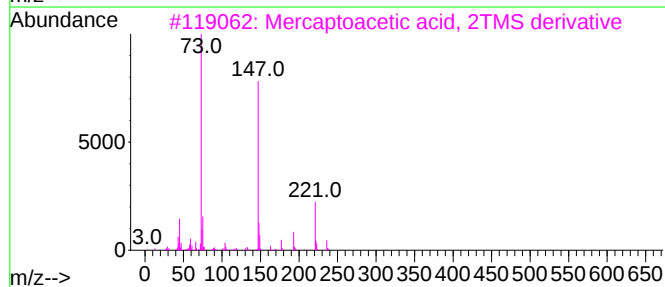
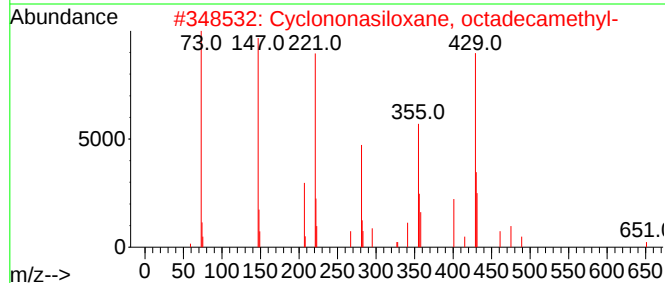
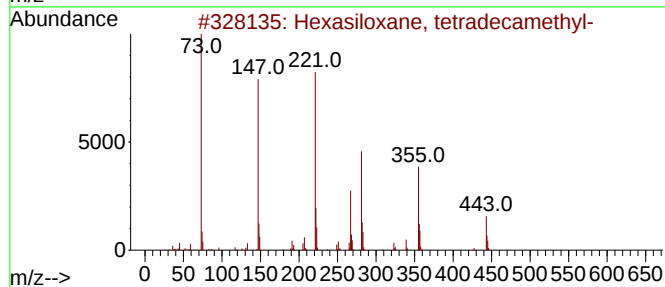
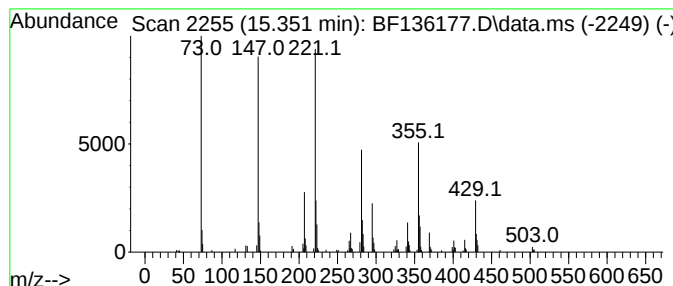
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110723.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown15.351 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.351	11.18 ng	254262	Perylene-d12	15.492	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	87
2	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	80
3	Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37
4	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	680	C20H60O8Si9	002652-13-3	37
5	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	30



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ALS Vial : 13 Sample Multiplier: 1

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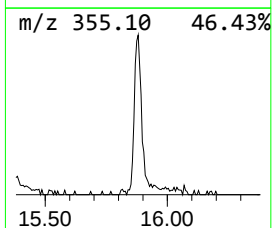
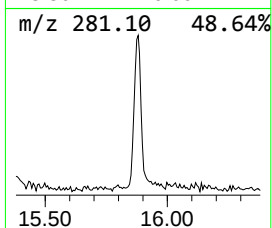
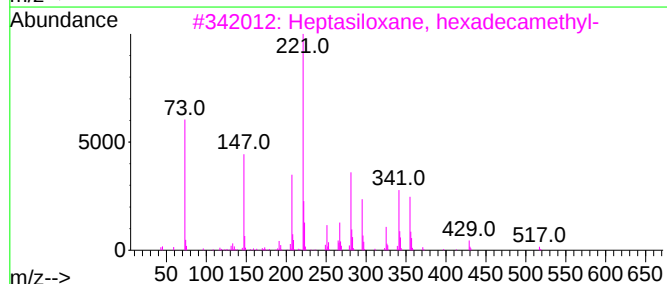
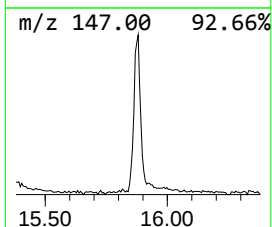
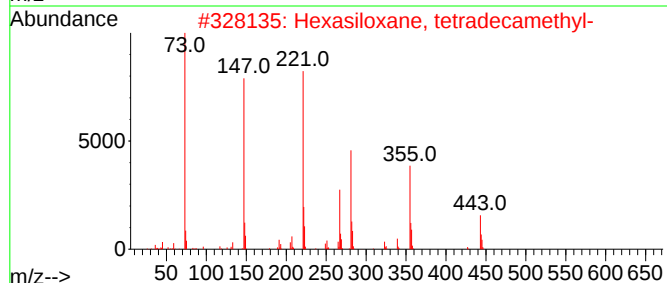
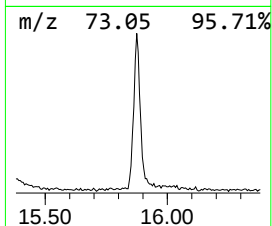
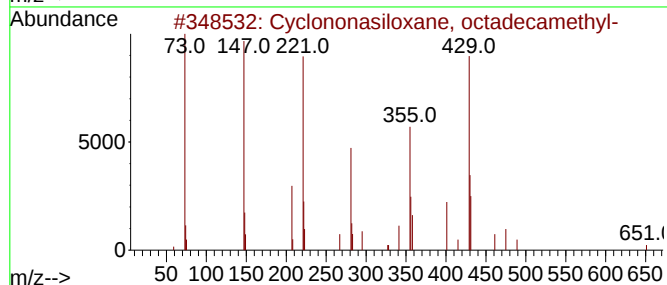
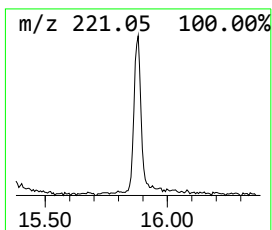
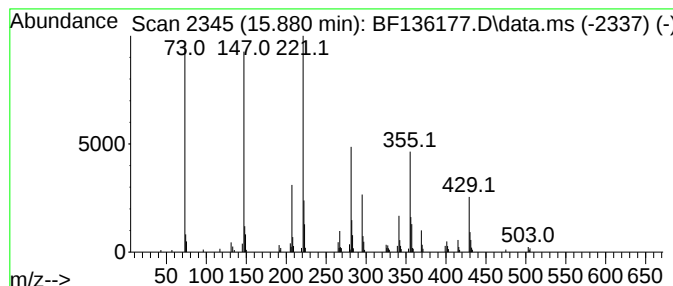
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown15.880 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.880	11.49 ng	261132	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	86
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	81
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	42
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	32
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25



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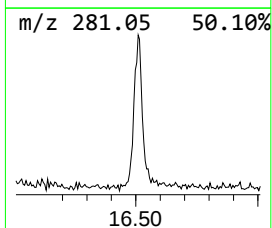
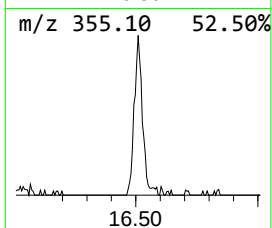
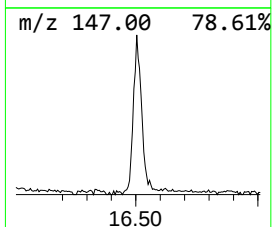
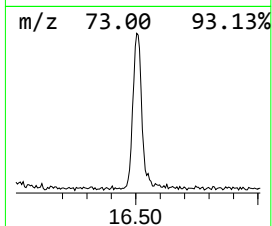
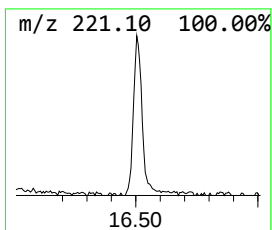
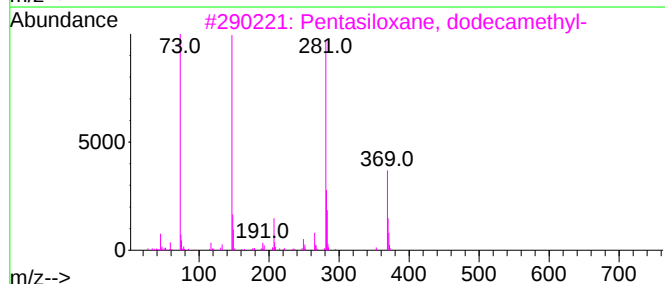
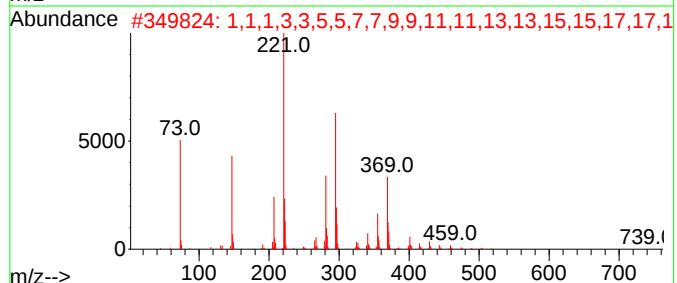
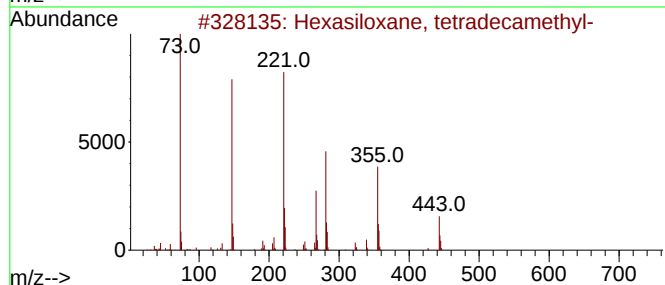
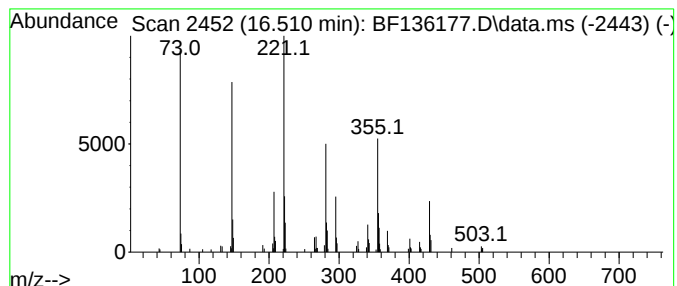
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown16.510 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.510	10.63 ng	241779	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	83
2			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	49
3			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	38
4			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	680	C20H60O8Si9	002652-13-3	38
5			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37



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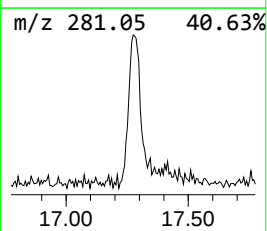
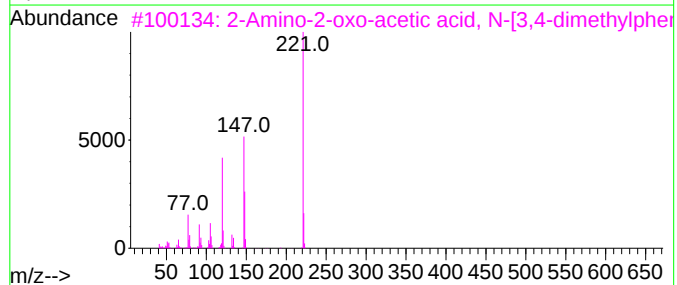
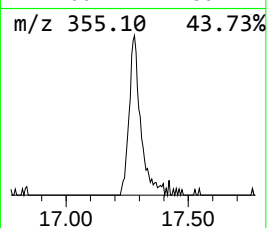
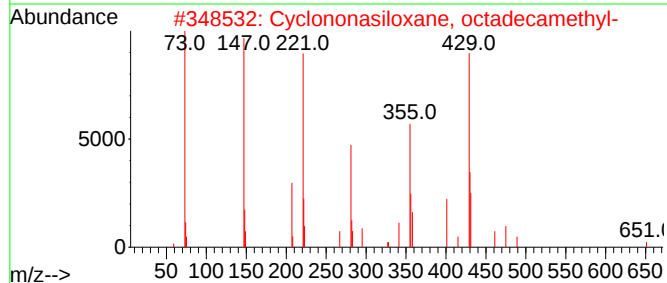
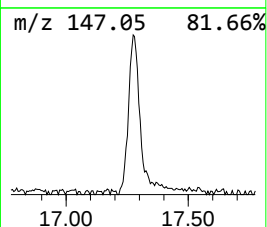
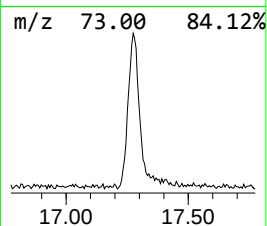
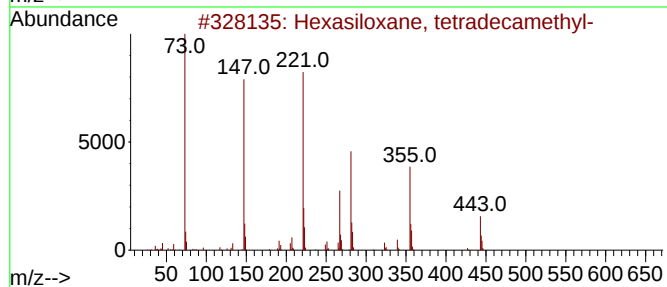
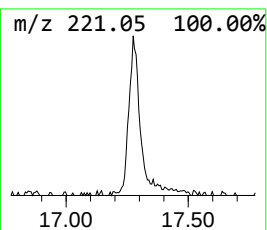
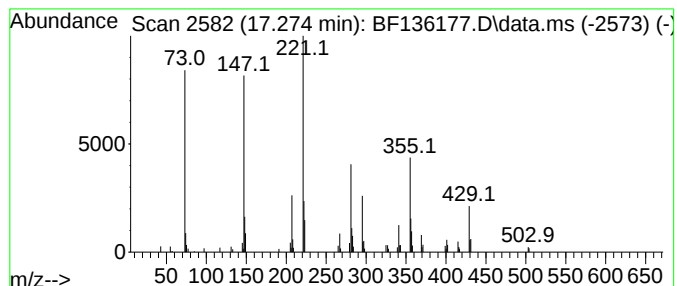
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown17.274 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.274	9.02 ng	205070	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	72
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	58
3			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	37
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110723\
Data File : BF136177.D
Acq On : 07 Nov 2023 15:47
Operator : CG\JU
Sample : PB156921BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB156921BL

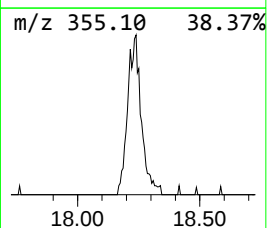
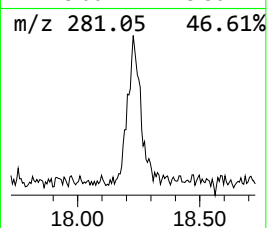
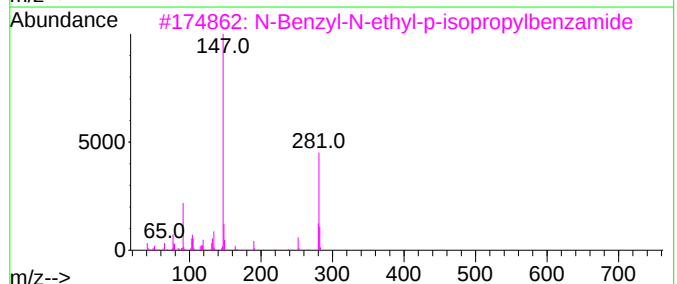
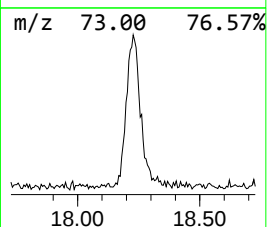
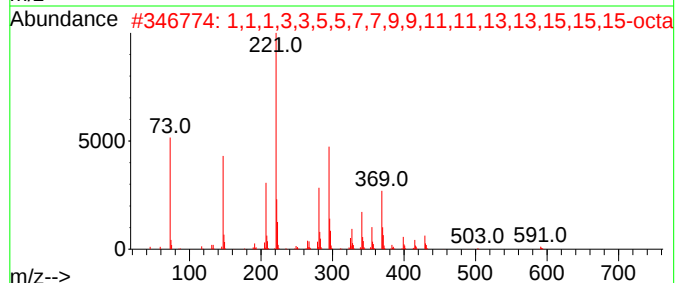
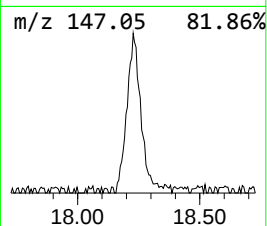
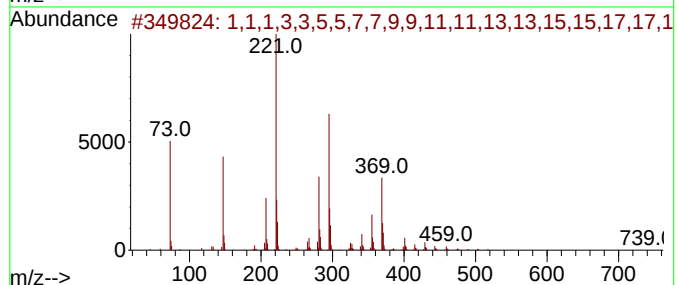
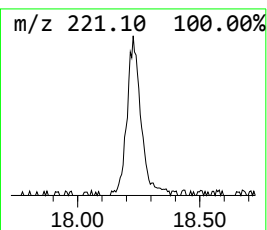
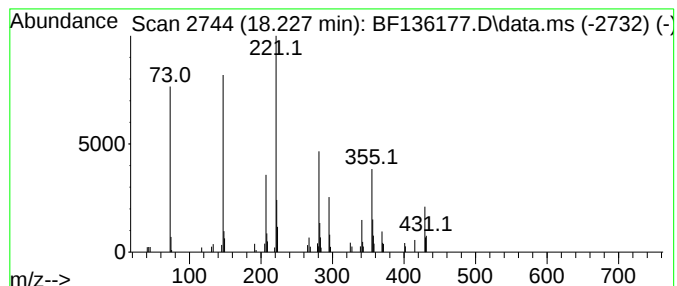
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,1,1,3,3,5,5,7,7,9,9,11,11... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.227	8.52 ng	193698	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	50		
2	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	38		
3	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25		
4	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	22		
5	3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	16		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110723\
Data File : BF136177.D
Acq On : 07 Nov 2023 15:47
Operator : CG\JU
Sample : PB156921BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB156921BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110723.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
Cyclononasiloxa...	14.504	4.8	ng	125070	5	14.004	523517	20.0
Hexasiloxane, t...	14.898	9.0	ng	205416	6	15.492	454708	20.0
unknown15.351	15.351	11.2	ng	254262	6	15.492	454708	20.0
unknown15.880	15.880	11.5	ng	261132	6	15.492	454708	20.0
unknown16.510	16.510	10.6	ng	241779	6	15.492	454708	20.0
unknown17.274	17.274	9.0	ng	205070	6	15.492	454708	20.0
1,1,1,3,3,5,5,7...	18.227	8.5	ng	193698	6	15.492	454708	20.0