

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
 Data File : BF137336.D
 Acq On : 08 Feb 2024 14:27
 Operator : CG\JU
 Sample : P1371-03
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T180-AOP

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-BF013024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137336.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.404	561	564	578	rBV	453138	499709	28.95%	5.849%
2	6.410	732	735	752	rBV	247009	289278	16.76%	3.386%
3	6.787	795	799	816	rBV	190575	214719	12.44%	2.513%
4	7.345	890	894	908	rBV	974607	855442	49.56%	10.012%
5	8.063	1013	1016	1035	rVB	324669	291655	16.90%	3.414%
6	9.139	1196	1199	1202	rBV	2116315	1676071	97.10%	19.617%
7	9.816	1311	1314	1323	rBV	439824	350463	20.30%	4.102%
8	10.610	1445	1449	1463	rBV	1237597	1111800	64.41%	13.013%
9	11.310	1564	1568	1585	rBV	386379	353917	20.50%	4.142%
10	12.910	1836	1840	1843	rBV	2068368	1726139	100.00%	20.203%
11	13.963	2015	2019	2028	rBV	328009	314070	18.19%	3.676%
12	14.069	2034	2037	2044	rVB2	25992	26330	1.53%	0.308%
13	14.457	2098	2103	2110	rBV2	58665	74546	4.32%	0.872%
14	14.857	2166	2171	2176	rBV	61913	84965	4.92%	0.994%
15	15.298	2241	2246	2253	rBV	64279	96929	5.62%	1.134%
16	15.439	2266	2270	2278	rBV	195615	251226	14.55%	2.940%
17	15.821	2328	2335	2346	rBV2	50332	98679	5.72%	1.155%
18	16.445	2429	2441	2448	rBV	38773	97309	5.64%	1.139%
19	17.198	2560	2569	2580	rBV4	24371	75365	4.37%	0.882%
20	18.139	2717	2729	2737	rBV6	15997	55410	3.21%	0.649%

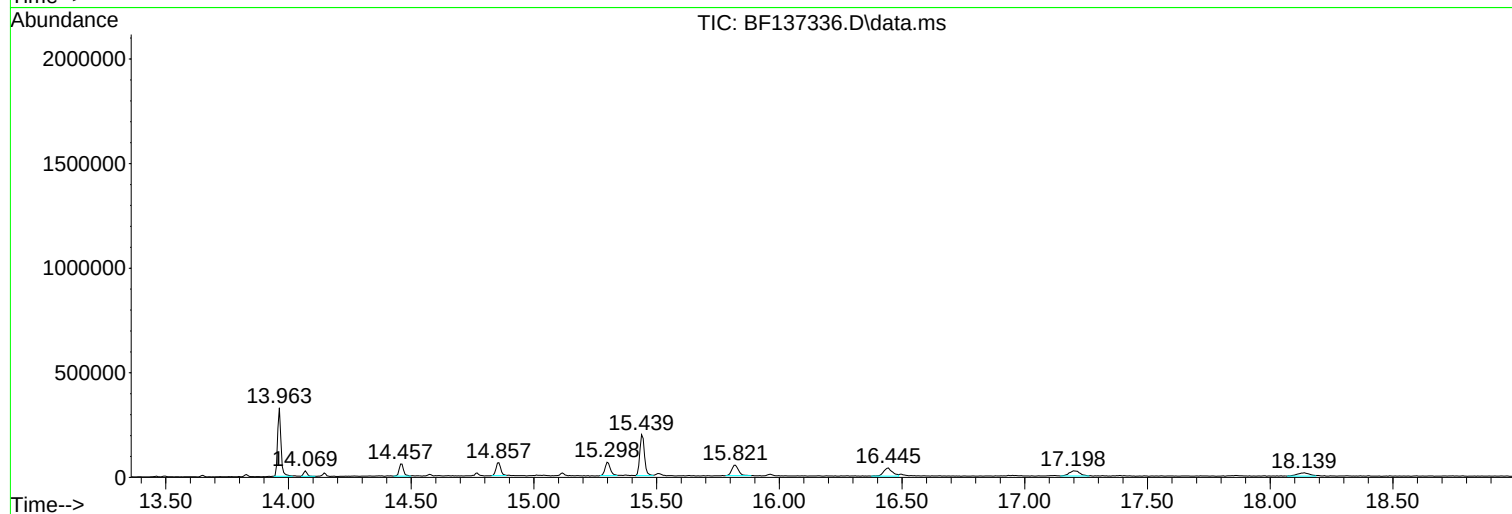
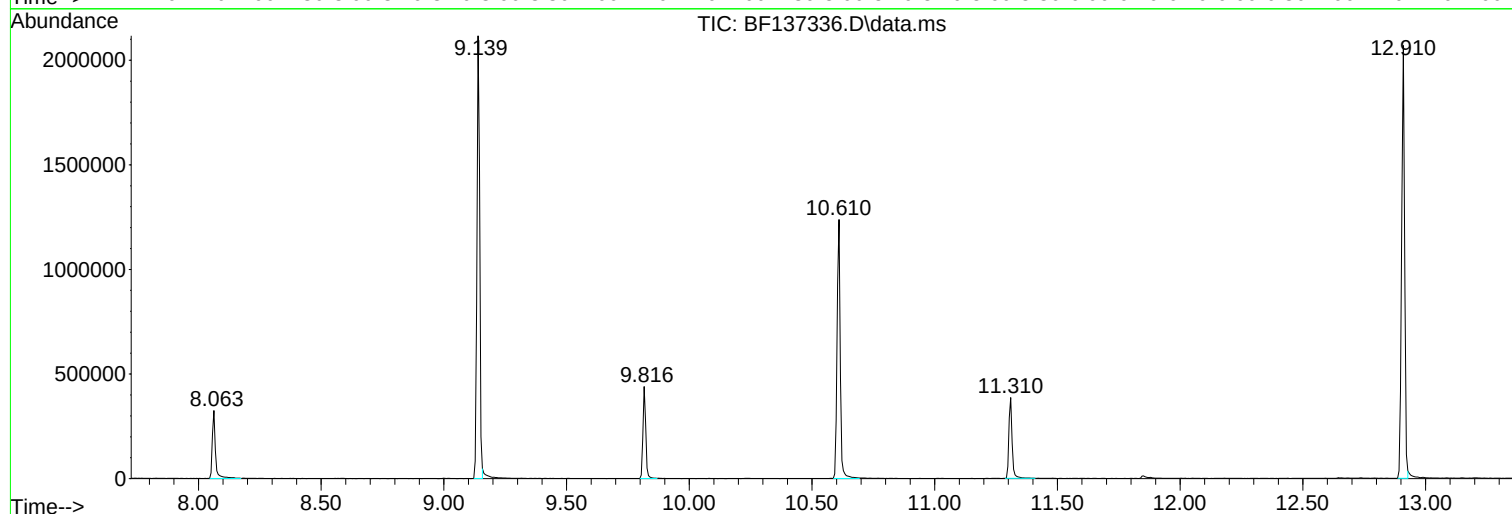
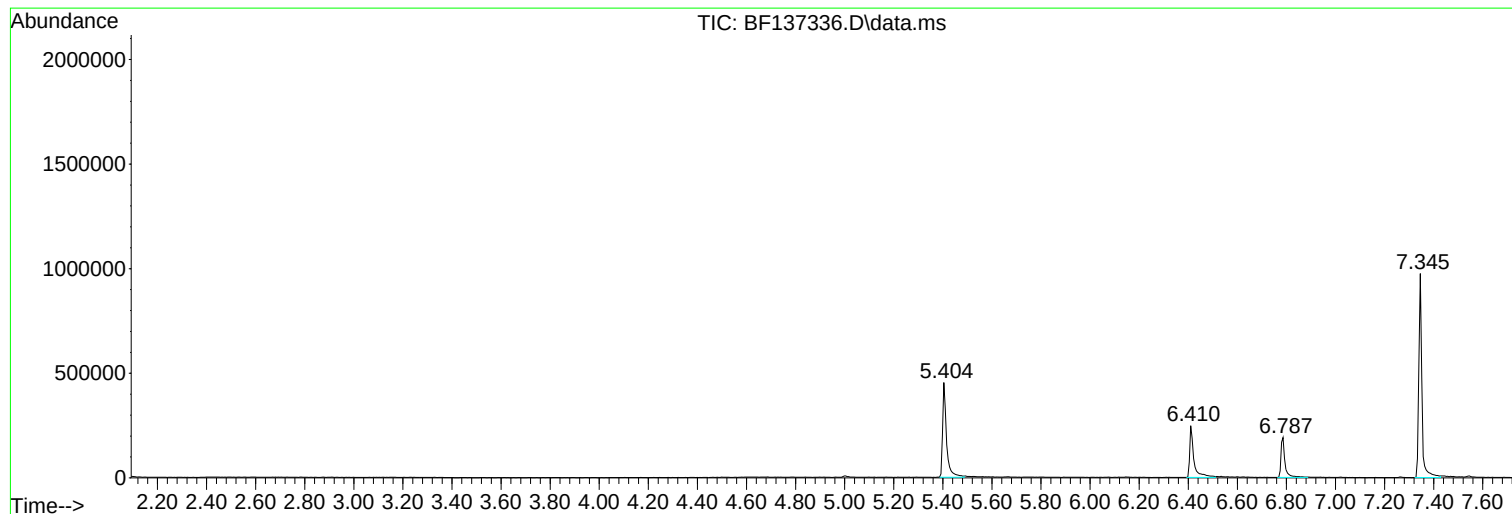
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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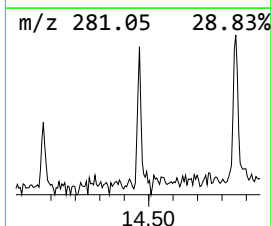
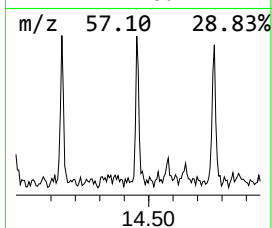
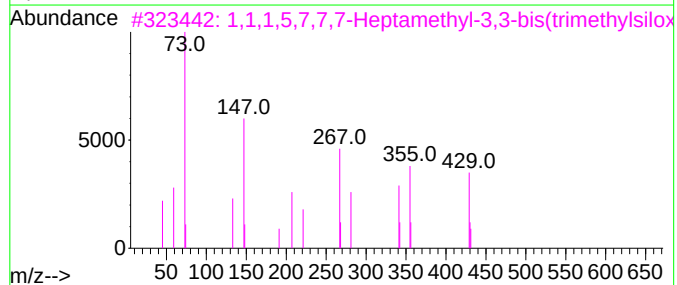
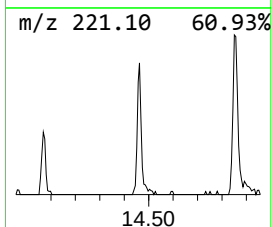
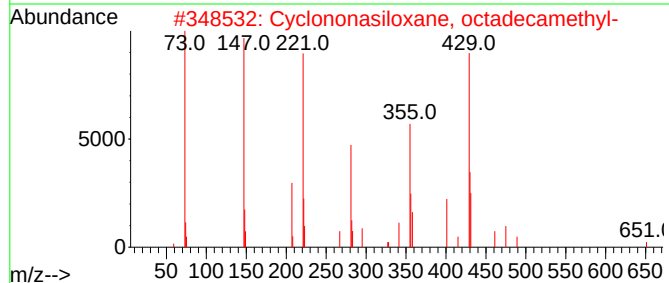
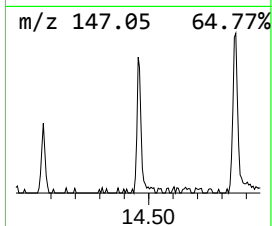
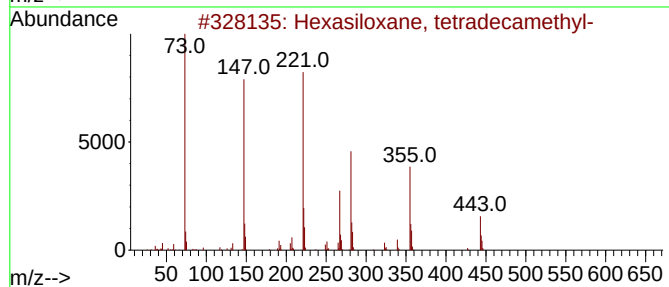
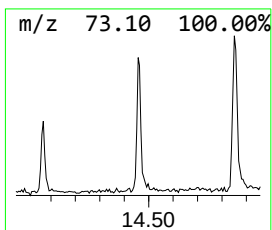
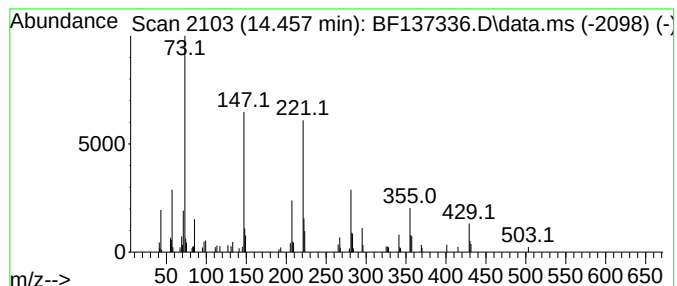
Instrument :
BNA_F
ClientSampleId :
T180-AOP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexasiloxane, tetradecamethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.457	4.75 ng	74546	Chrysene-d12	13.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	64
2	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	50
3	1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	47
4	2,6-Dimethyl-3,4-bis(trimethylsi...	311	C15H29N02Si2	1000079-52-1	38
5	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38



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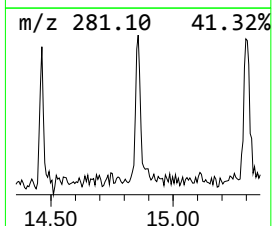
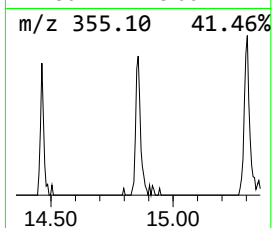
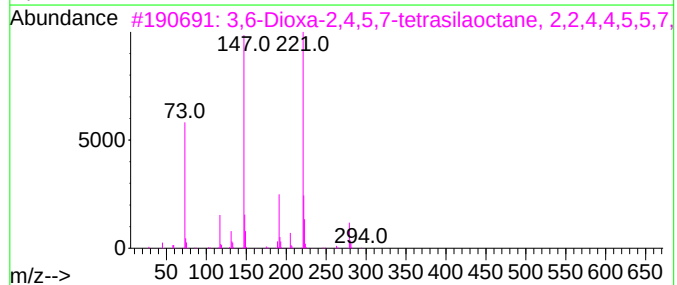
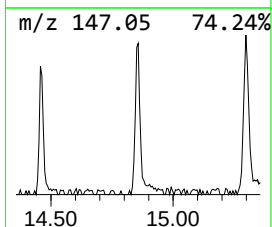
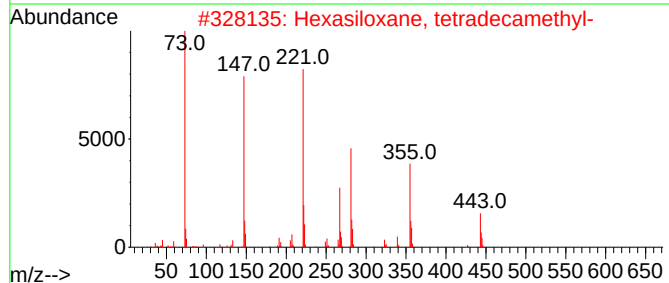
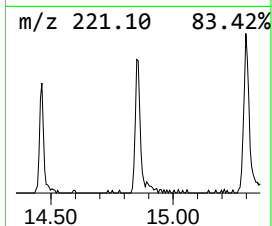
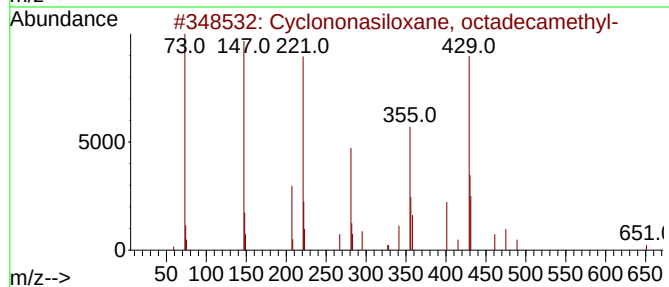
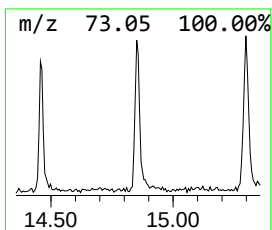
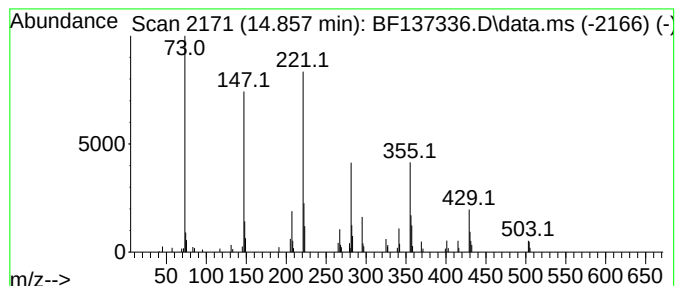
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Cyclononasiloxane, octadeca... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.857	6.76 ng	84965	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	74
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	72
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
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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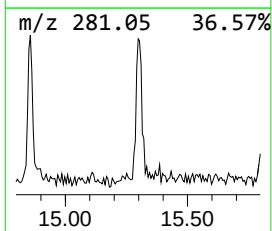
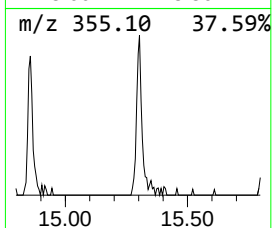
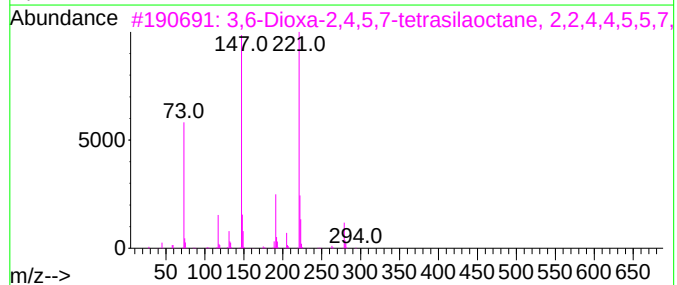
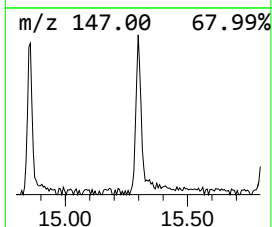
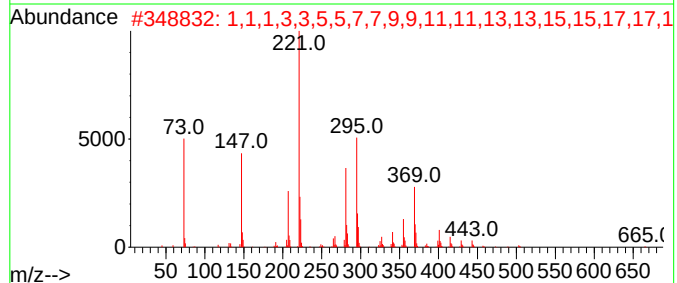
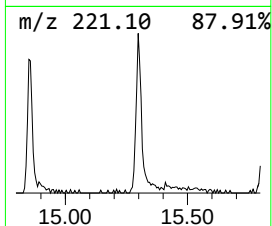
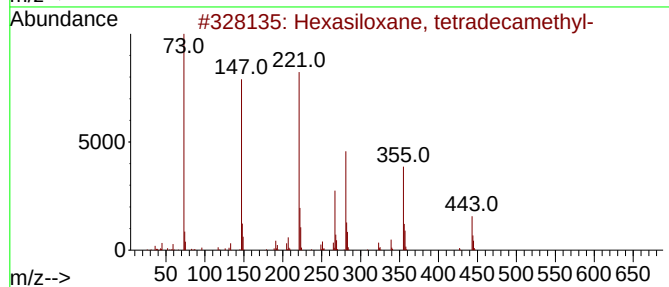
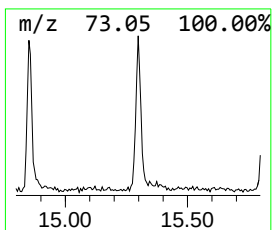
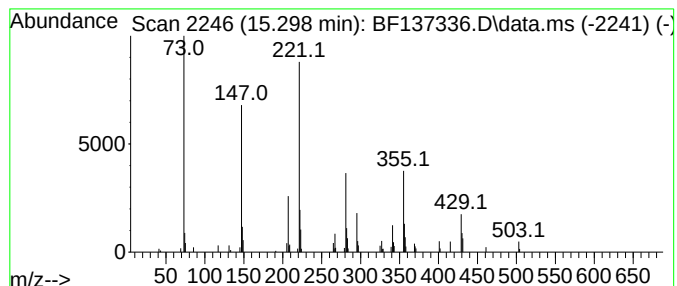
Instrument :
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ClientSampleId :
T180-AOP

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

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
15.298	7.72 ng	96929	Perylene-d12			15.439
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexasiloxane, tetradecamethyl-		458	C14H42O5Si6	000107-52-8	87
2	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...		680	C20H60O8Si9	002652-13-3	50
3	3,6-Dioxa-2,4,5,7-tetrasilaoctan...		294	C10H30O2Si4	004342-25-0	40
4	2-Amino-2-oxo-acetic acid, N-[3,...		221	C12H15NO3	024451-17-0	40
5	Mercaptoacetic acid, 2TMS deriva...		236	C8H20O2SSi2	006398-62-5	38



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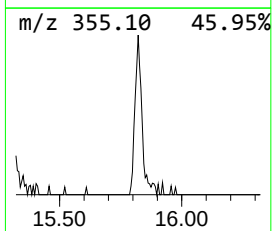
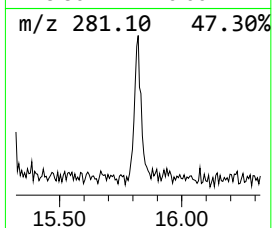
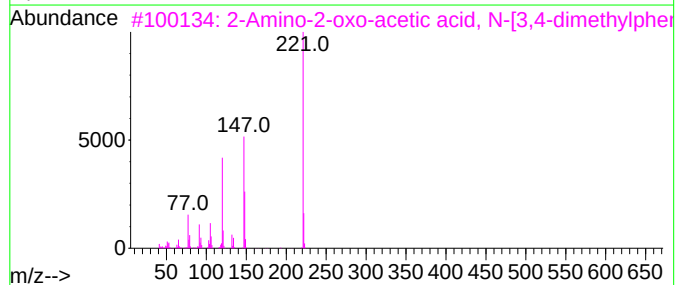
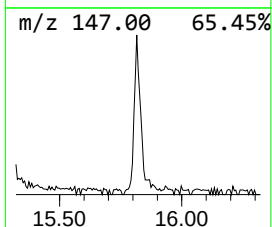
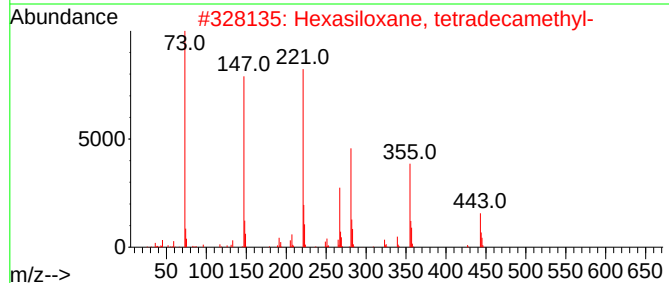
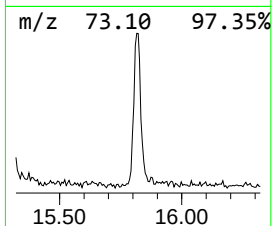
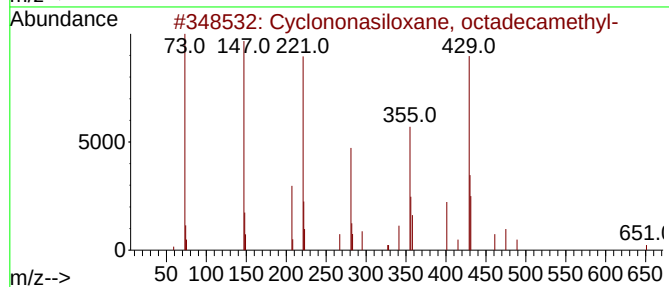
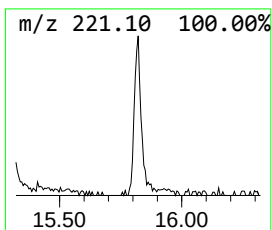
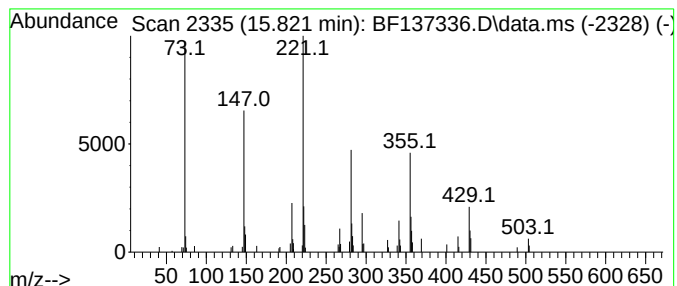
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown45.821 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.821	7.86 ng	98679	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	50
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	50
3			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	38
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	32
5			2-Methyl-6-tert-butylphenol, TBD...	278	C17H30OSi	1000467-05-0	27



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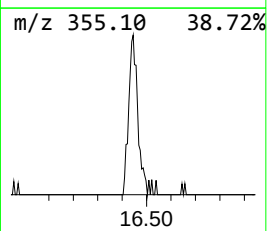
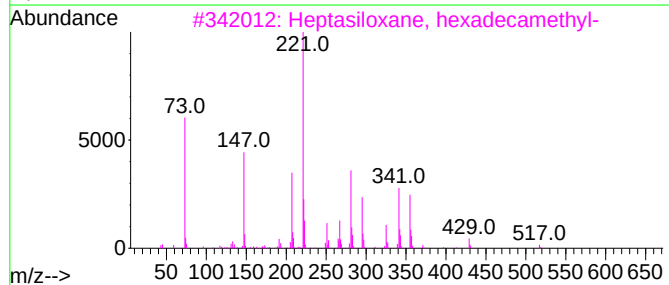
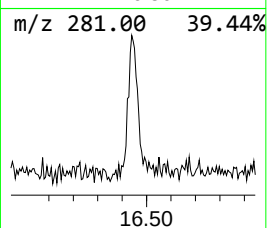
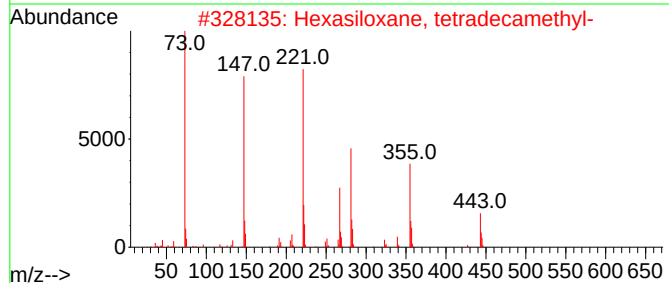
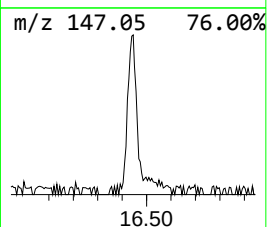
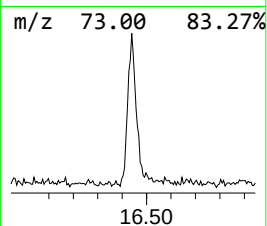
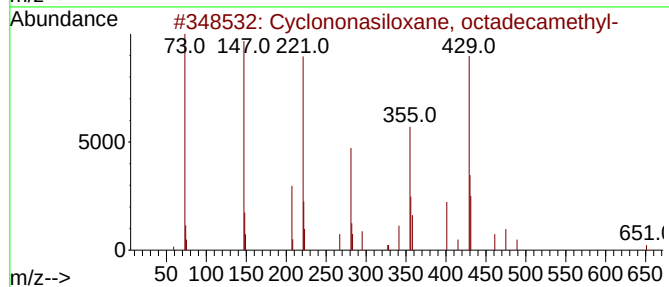
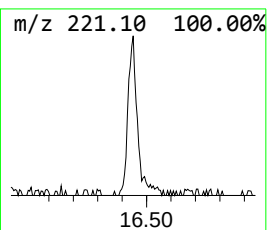
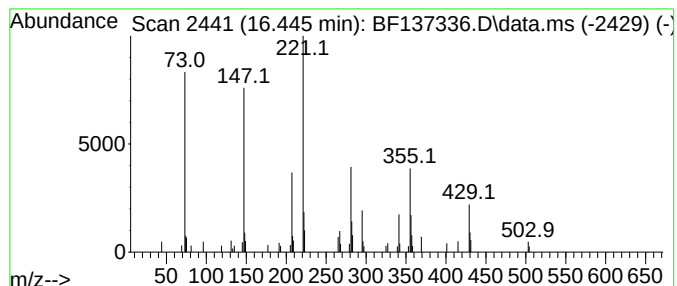
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown16.445 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.445	7.75 ng	97309	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	78
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	50
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	38
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	32
5			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	32



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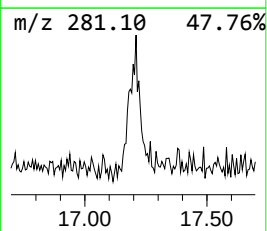
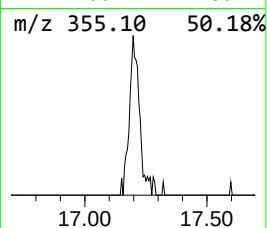
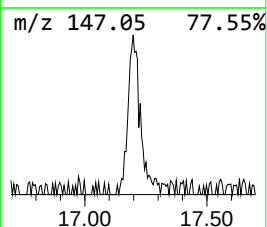
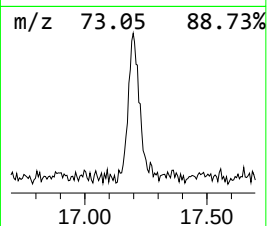
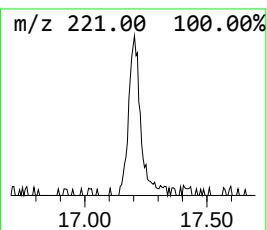
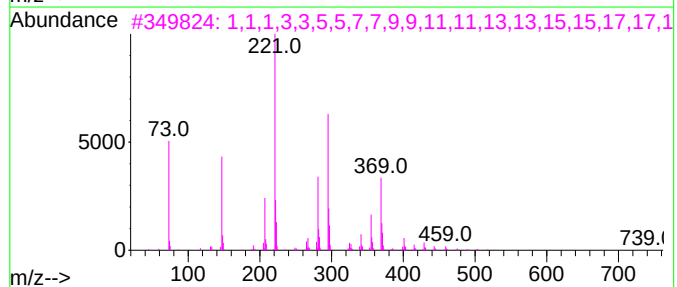
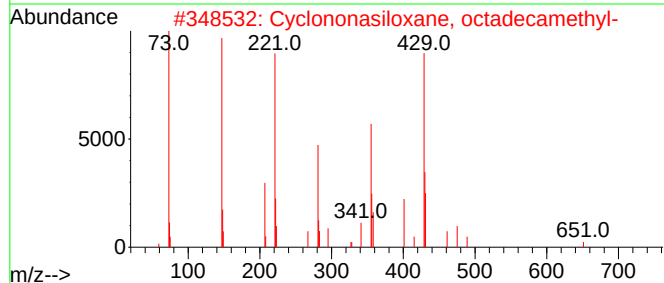
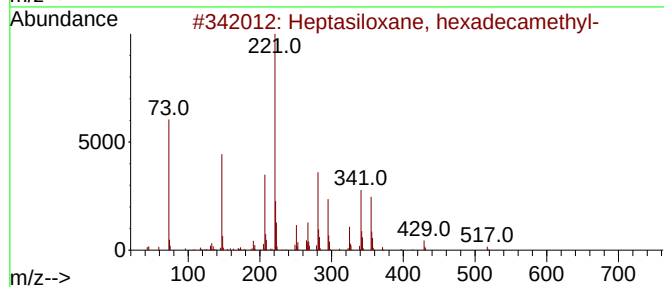
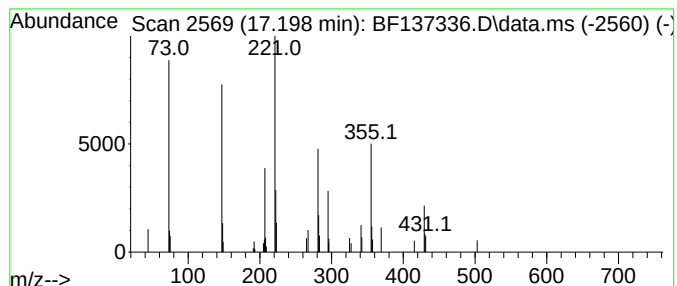
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptasiloxane, hexadecamethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.198	6.00 ng	75365	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	64
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	64
3			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	47
4			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	45
5			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	680	C20H60O8Si9	002652-13-3	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137336.D
Acq On : 08 Feb 2024 14:27
Operator : CG\JU
Sample : P1371-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T180-AOP

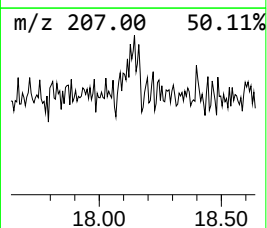
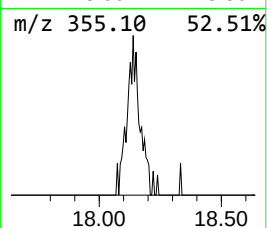
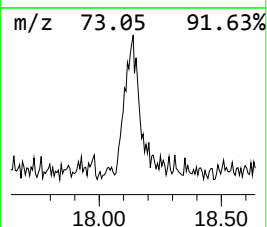
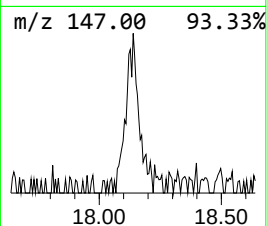
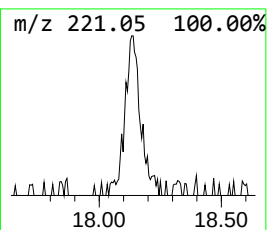
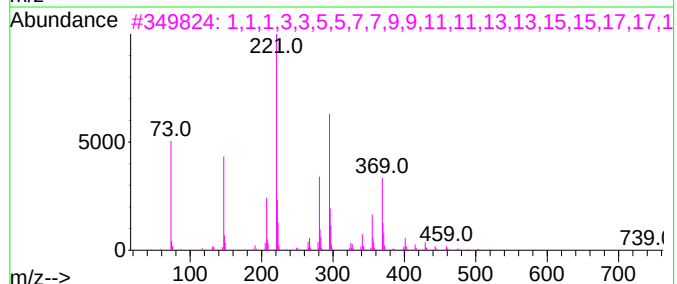
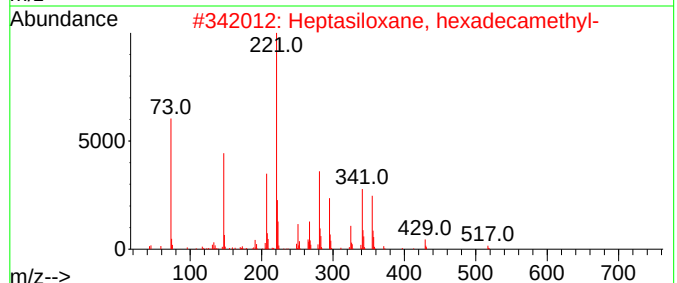
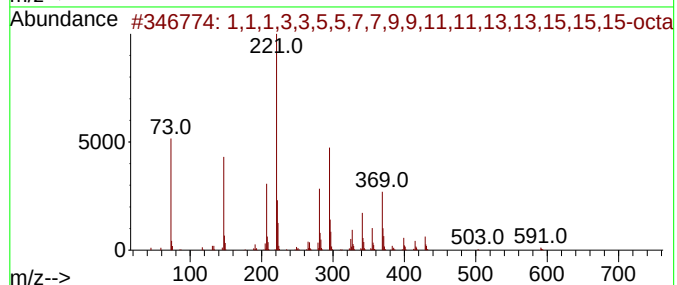
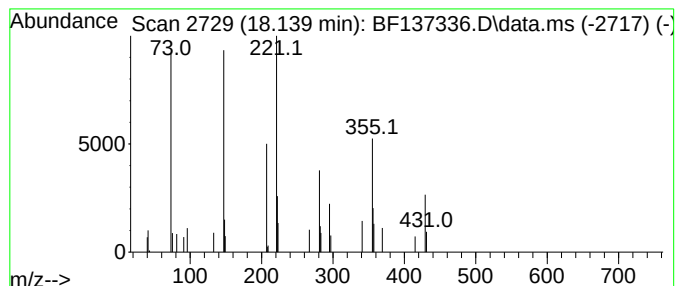
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown18.139 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.139	4.41 ng	55410	Perylene-d12	15.439

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...	606	C18H5407Si8	000556-69-4	53		
2	Heptasiloxane, hexadecamethyl-	532	C16H4806Si7	000541-01-5	38		
3	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H6609Si10	000556-70-7	37		
4	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	680	C20H6008Si9	002652-13-3	37		
5	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H3002Si4	004342-25-0	32		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137336.D
Acq On : 08 Feb 2024 14:27
Operator : CG\JU
Sample : P1371-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T180-AOP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.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
Hexasiloxane, t...	14.457	4.8	ng	74546	5	13.963	314070	20.0
Cyclononasiloxa...	14.857	6.8	ng	84965	6	15.439	251226	20.0
1,1,1,3,3,5,5,7...	15.298	7.7	ng	96929	6	15.439	251226	20.0
unknown45.821	15.821	7.9	ng	98679	6	15.439	251226	20.0
unknown16.445	16.445	7.8	ng	97309	6	15.439	251226	20.0
Heptasiloxane, ...	17.198	6.0	ng	75365	6	15.439	251226	20.0
unknown18.139	18.139	4.4	ng	55410	6	15.439	251226	20.0