

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121123\
 Data File : BF136489.D
 Acq On : 11 Dec 2023 14:27
 Operator : CG\JU
 Sample : PB157390BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB157390BL

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-BF120523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136489.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	4	9	20	rVB	39314	59779	1.33%	0.237%
2	5.446	566	571	574	rBV	3200739	3153343	70.04%	12.496%
3	6.440	734	740	743	rBV	2829323	3135591	69.65%	12.425%
4	6.793	796	800	804	rVB	775463	621016	13.79%	2.461%
5	7.357	890	896	899	rBV	1974123	1988443	44.17%	7.880%
6	8.069	1012	1017	1021	rBV	983480	853921	18.97%	3.384%
7	9.151	1195	1201	1204	rBV	4570413	4125551	91.63%	16.348%
8	9.828	1311	1316	1319	rBV	1272636	1007287	22.37%	3.992%
9	10.622	1446	1451	1454	rBV	2743608	2605126	57.86%	10.323%
10	11.322	1566	1570	1573	rBV	1212687	1090562	24.22%	4.322%
11	12.922	1837	1842	1845	rBV	4744703	4502181	100.00%	17.841%
12	13.969	2016	2020	2024	rBV	863240	796015	17.68%	3.154%
13	14.451	2098	2102	2109	rVB2	57385	61719	1.37%	0.245%
14	14.839	2163	2168	2175	rBV2	81809	101301	2.25%	0.401%
15	15.274	2237	2242	2254	rBV	83868	146136	3.25%	0.579%
16	15.451	2265	2272	2277	rBV	493368	605622	13.45%	2.400%
17	15.792	2324	2330	2337	rBV3	70423	132719	2.95%	0.526%
18	16.398	2425	2433	2442	rBV3	53303	127977	2.84%	0.507%
19	17.145	2557	2560	2574	rVB8	28444	71720	1.59%	0.284%
20	18.068	2710	2717	2726	rVB8	15731	49148	1.09%	0.195%

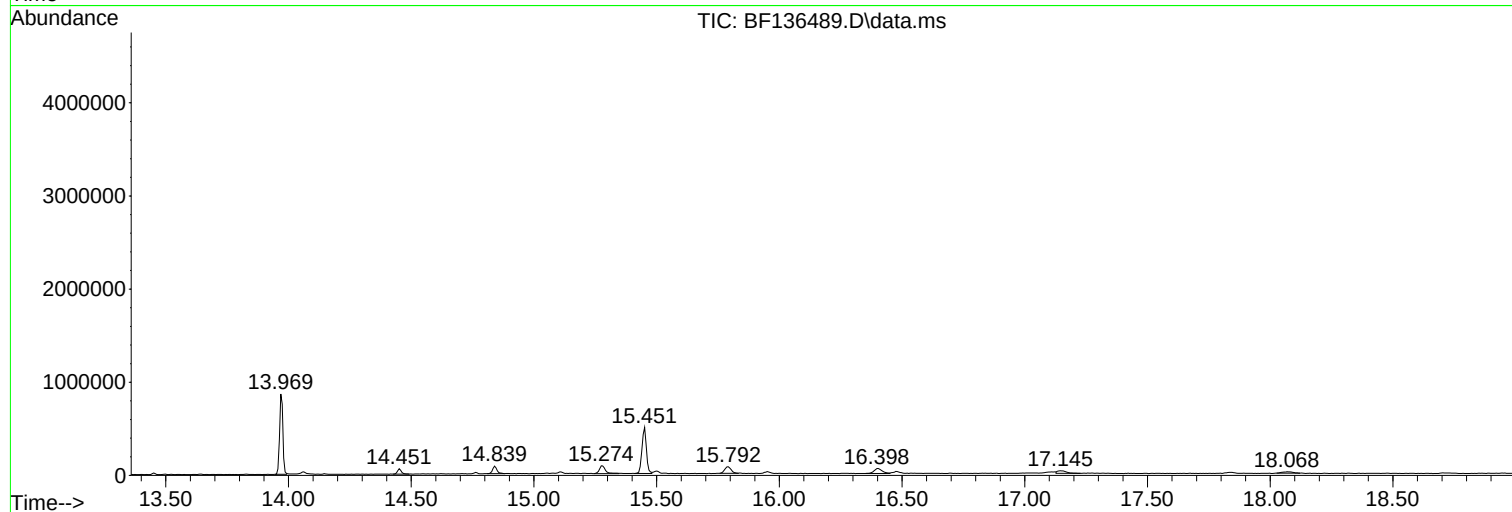
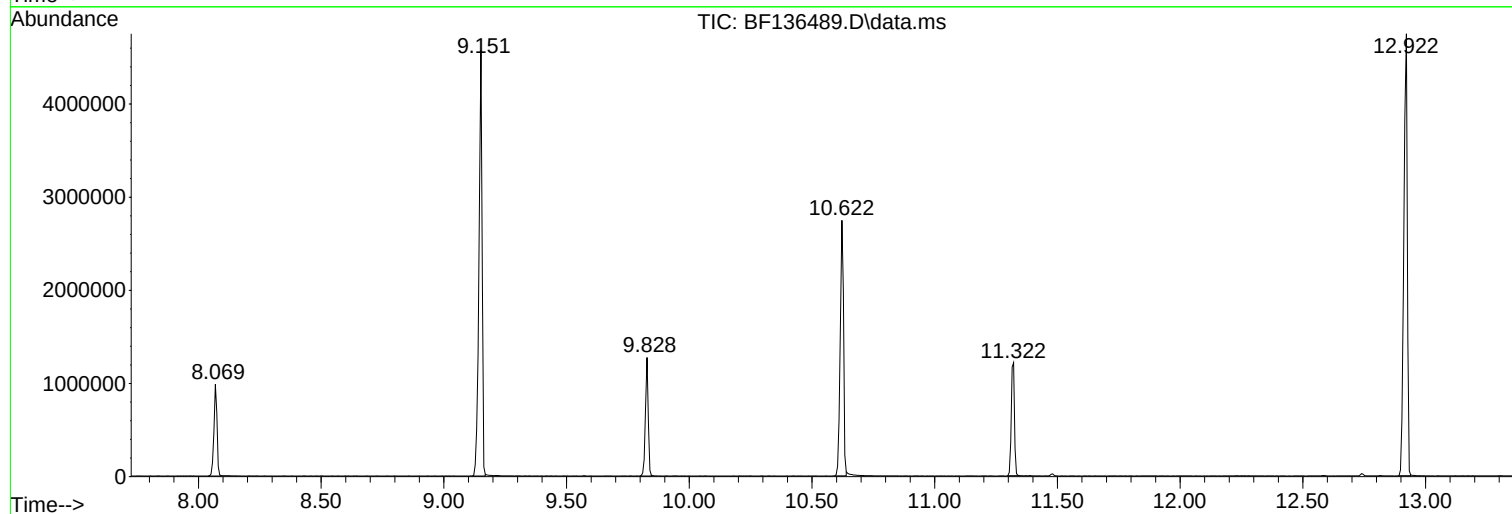
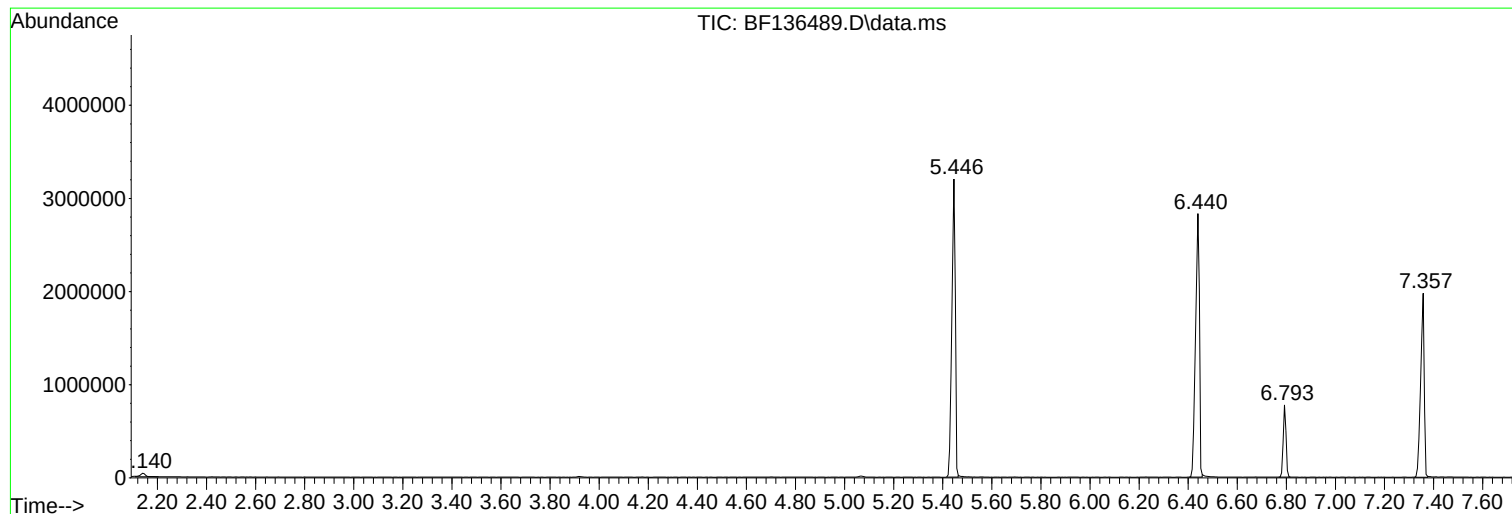
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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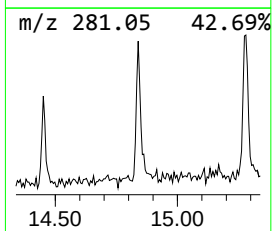
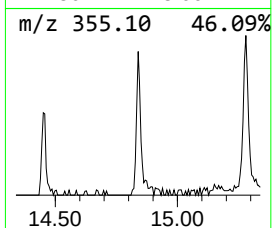
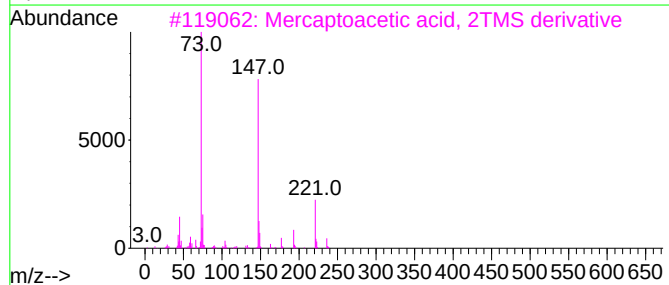
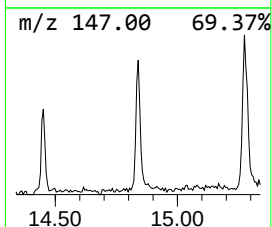
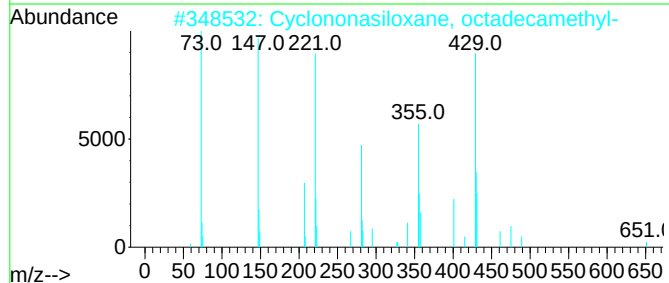
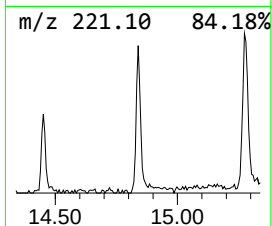
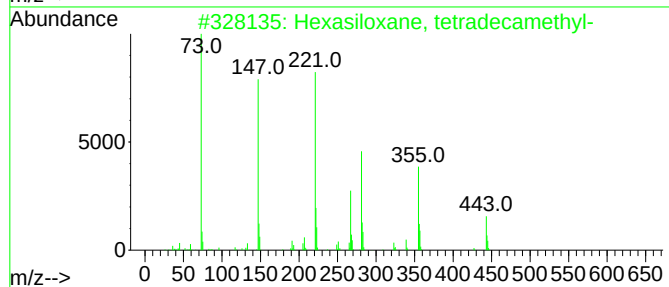
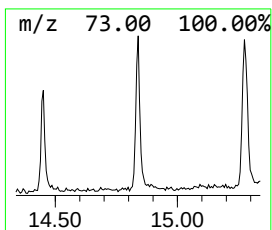
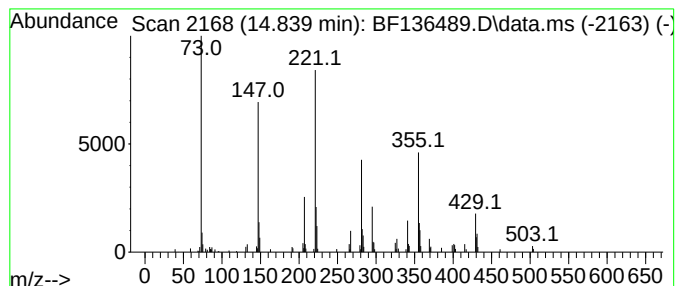
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexasiloxane, tetradecamethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	3.35 ng	101301	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	83
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	64
3			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	32
4			2-{[2-(Methoxycarbonyl)anilino]c...	371	C19H21NO5Si	1000475-02-2	30
5			Trisiloxane, octamethyl-	236	C8H24O2Si3	000107-51-7	27



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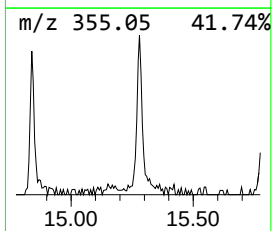
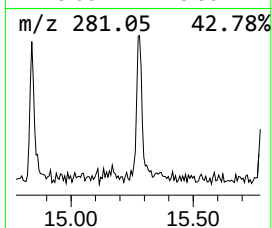
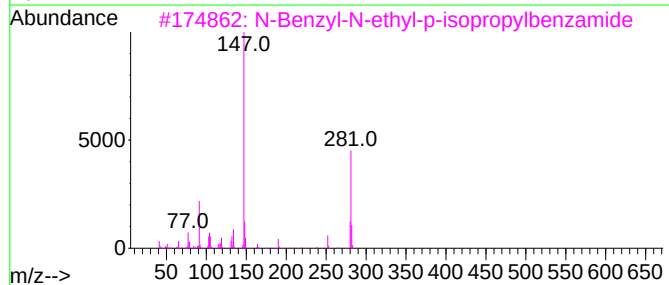
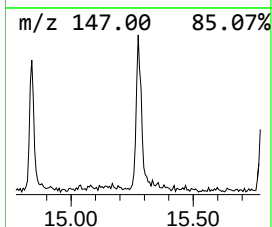
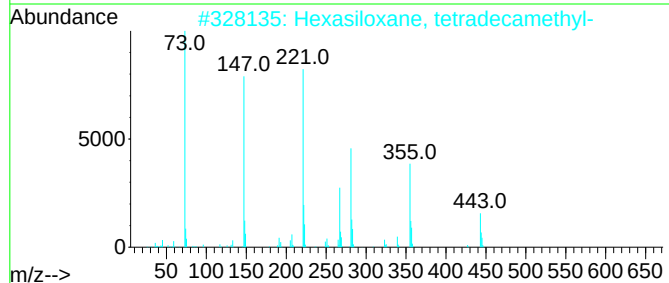
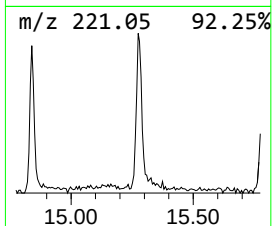
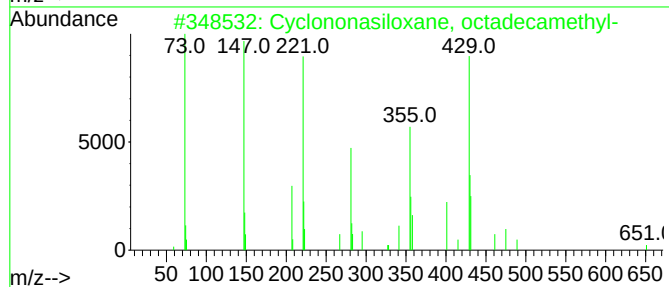
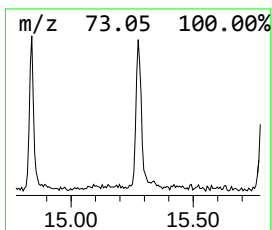
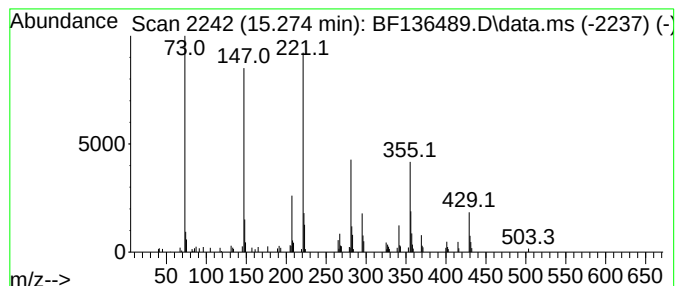
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Cyclononasiloxane, octadeca... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.274	4.83 ng	146136	Perylene-d12	15.451

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	72
3			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	38
4			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	38
5			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	35



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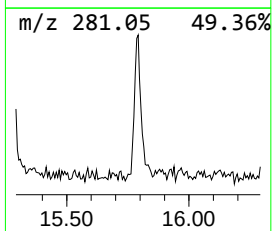
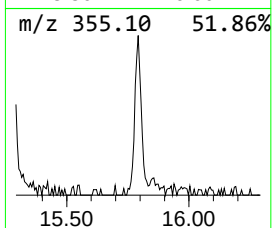
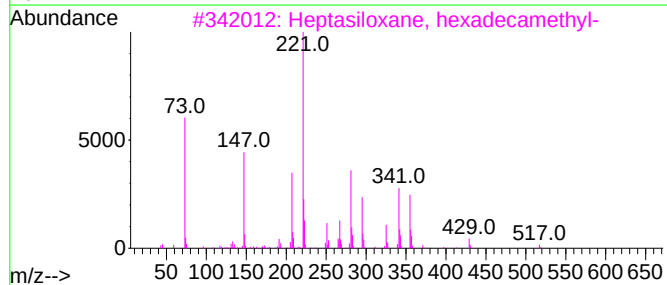
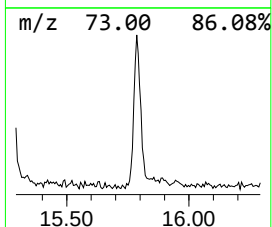
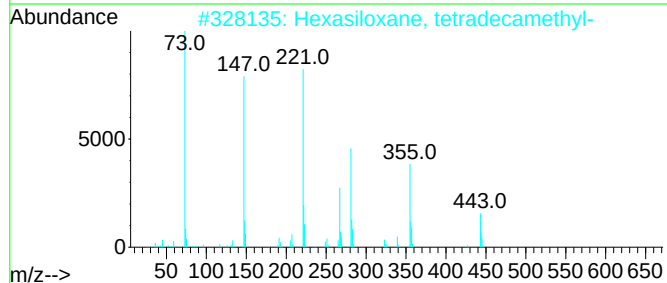
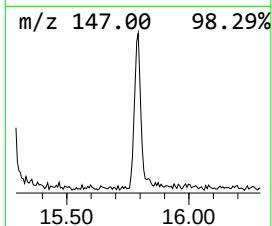
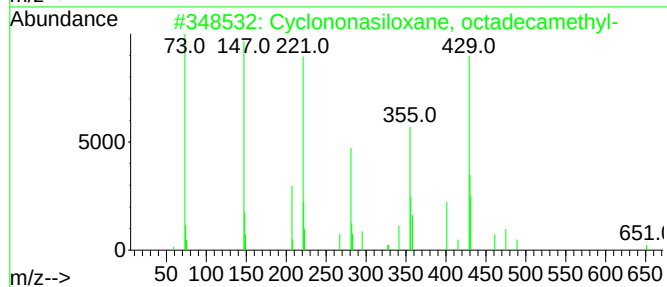
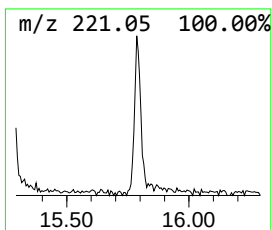
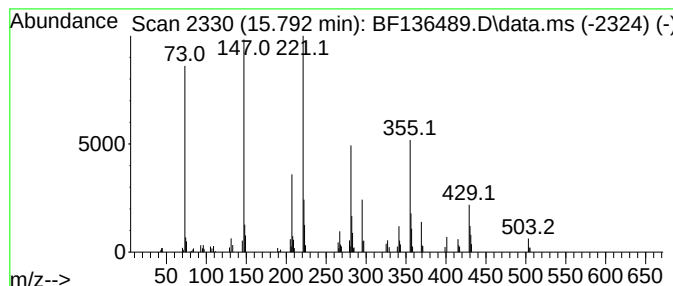
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heptasiloxane, hexadecamethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.792	4.38 ng	132719	Perylene-d12	15.451

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	74
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	64
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	43
5			1,3,5-Trisiloxane, 1,1,3,3,5,5-h...	320	C14H36O2Si3	1000458-50-5	22



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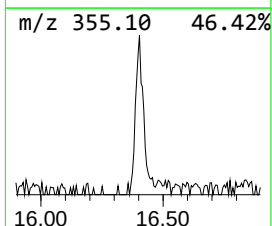
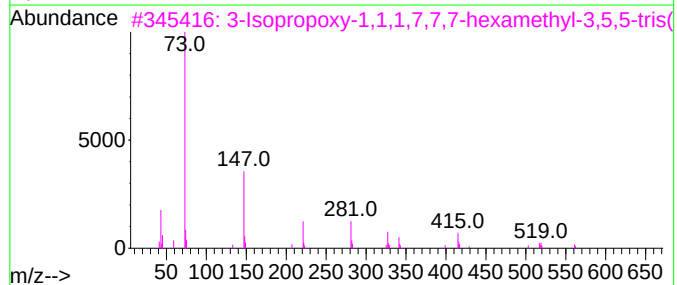
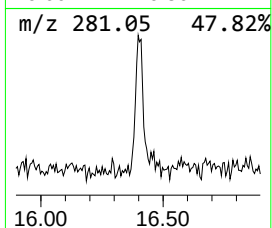
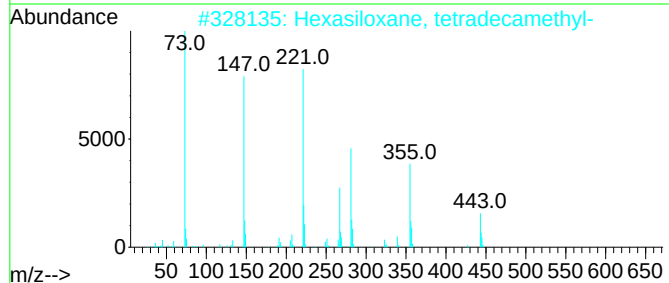
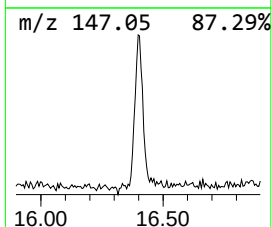
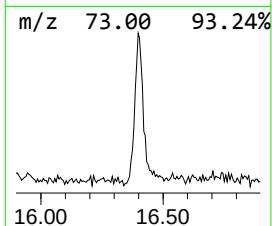
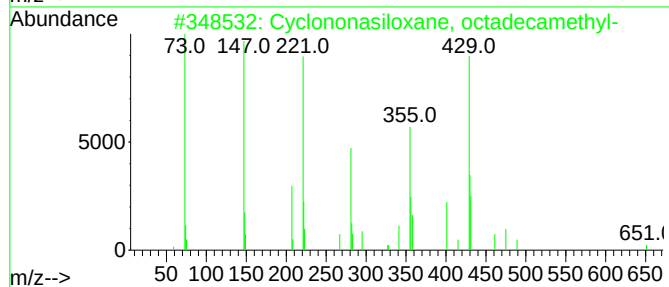
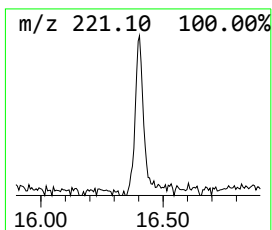
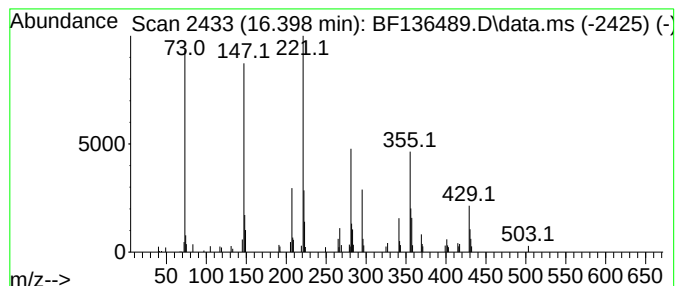
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown16.398 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.398	4.23 ng	127977	Perylene-d12	15.451

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	68
3			3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	27
4			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	25
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	22



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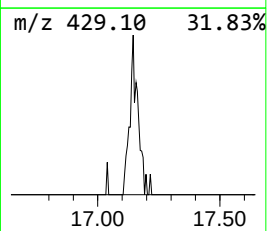
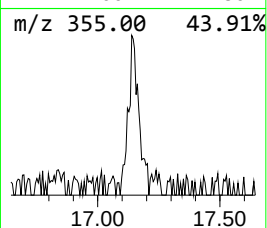
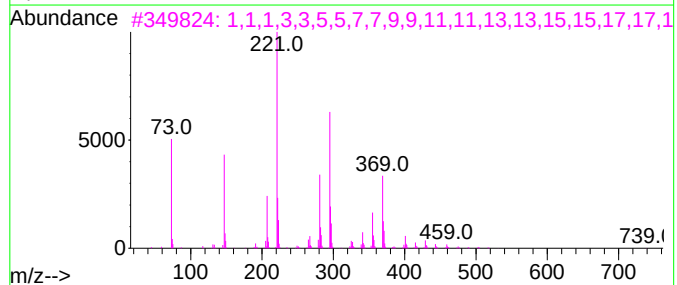
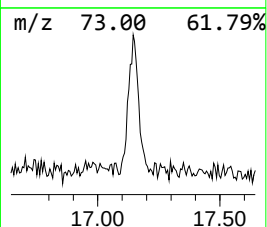
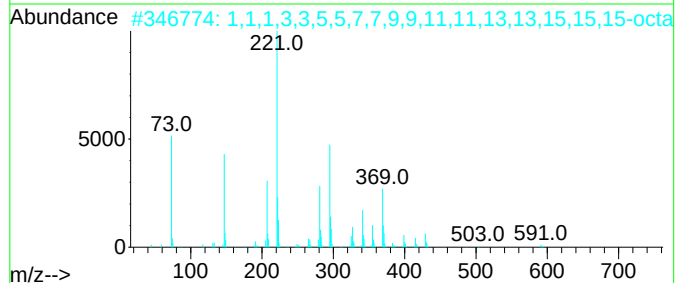
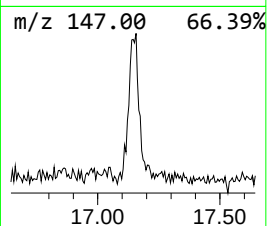
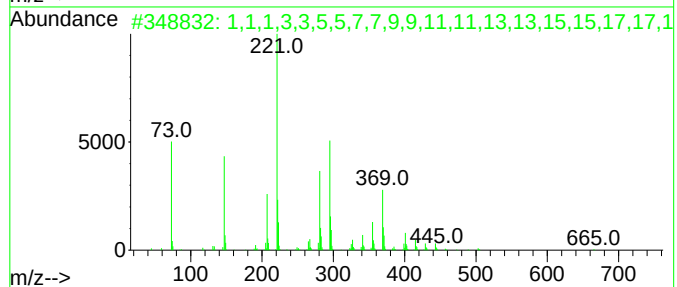
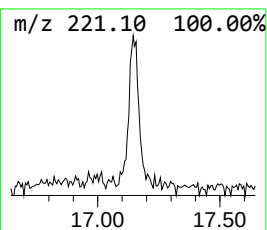
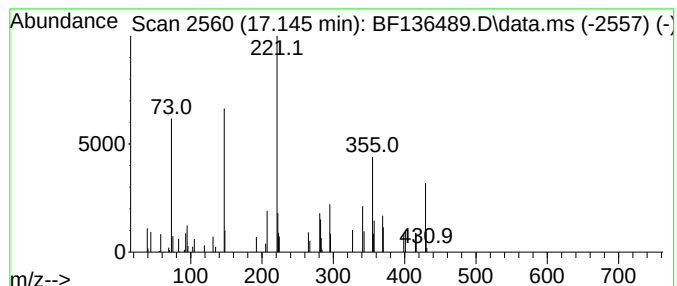
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown17.145 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.145	2.37 ng	71720	Perylene-d12	15.451

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...	680	C20H6008Si9	002652-13-3	38		
2	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H5407Si8	000556-69-4	38		
3	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H6609Si10	000556-70-7	35		
4	1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H4005Si6	038147-00-1	27		
5	benzenamine, N-[bis(2,4,6-trimet...	341	C24H28BN	1000398-20-2	27		



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexasiloxane, t...	14.839	3.4	ng	101301	6	15.451	605622	20.0
Cyclononasiloxa...	15.274	4.8	ng	146136	6	15.451	605622	20.0
Heptasiloxane, ...	15.792	4.4	ng	132719	6	15.451	605622	20.0
unknown16.398	16.398	4.2	ng	127977	6	15.451	605622	20.0
unknown17.145	17.145	2.4	ng	71720	6	15.451	605622	20.0