

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN111522\
 Data File : BN022654.D
 Acq On : 15 Nov 2022 18:13
 Operator : CG/JU
 Sample : PB149003BL
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 SBLK003

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0.1 % 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_N\Methods\SFAM-EPA-BN111522.M
 Title : SVOA CALIBRATION

Signal : TIC: BN022654.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.187	31	34	45	rVB	21484	32185	1.50%	0.120%
2	3.628	106	109	136	rBV	242211	402555	18.72%	1.498%
3	3.958	160	165	173	rVB	5044	9073	0.42%	0.034%
4	5.893	491	494	498	rVB6	1559	2461	0.11%	0.009%
5	7.052	684	691	700	rBV	325573	514987	23.95%	1.916%
6	7.210	711	718	729	rVB	251371	402835	18.73%	1.499%
7	7.405	744	751	763	rBV	327932	515681	23.98%	1.919%
8	7.875	825	831	841	rVB	268745	421017	19.58%	1.567%
9	8.610	949	956	971	rBV	393189	641045	29.81%	2.386%
10	9.057	1024	1032	1046	rBV	318207	517808	24.08%	1.927%
11	9.787	1149	1156	1165	rBV	263768	442373	20.57%	1.646%
12	10.334	1241	1249	1263	rBV	366453	631171	29.35%	2.349%
13	10.704	1304	1312	1321	rBV	378016	629450	29.27%	2.342%
14	10.851	1329	1337	1349	rBV	320186	566220	26.33%	2.107%
15	12.310	1578	1585	1591	rBV2	4681	9595	0.45%	0.036%
16	13.975	1862	1868	1884	rVB	753312	1052659	48.95%	3.917%
17	14.251	1906	1915	1929	rBV	790100	1162697	54.07%	4.327%
18	14.557	1961	1967	1975	rBV	583091	880084	40.93%	3.275%
19	14.792	2001	2007	2026	rBV	354854	575342	26.76%	2.141%
20	15.557	2130	2137	2144	rBV	1063980	1473395	68.52%	5.483%
21	15.610	2144	2146	2151	rVB4	1996	2784	0.13%	0.010%
22	15.687	2153	2159	2173	rBV	405122	566168	26.33%	2.107%
23	15.798	2175	2178	2180	rVV2	3355	3484	0.16%	0.013%
24	17.322	2429	2437	2444	rBV	750063	1075243	50.00%	4.001%
25	17.422	2447	2454	2465	rVV	1147701	1664596	77.41%	6.195%
26	17.704	2497	2502	2503	rBV3	1957	2330	0.11%	0.009%
27	17.845	2524	2526	2531	rBV5	1687	2519	0.12%	0.009%
28	18.216	2585	2589	2595	rBV4	11942	17618	0.82%	0.066%
29	18.292	2600	2602	2608	rVB4	2931	4130	0.19%	0.015%
30	18.792	2684	2687	2691	rVB5	1492	2164	0.10%	0.008%
31	19.286	2767	2771	2775	rBV2	13972	17602	0.82%	0.066%
32	19.357	2780	2783	2787	rVV	10935	13376	0.62%	0.050%
33	19.504	2804	2808	2813	rBV4	10979	17076	0.79%	0.064%
34	19.727	2840	2846	2854	rBV	1412669	1879365	87.40%	6.994%
35	21.527	3145	3152	3163	rVB	939491	1265763	58.87%	4.710%
36	22.069	3241	3244	3250	rVB	72338	100502	4.67%	0.374%

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37	22.686	3344	3349	3356	rVB2	154598	265076	12.33%	0.986%
38	23.204	3433	3437	3442	rVB2	52249	80593	3.75%	0.300%
39	23.374	3461	3466	3478	rVB2	250300	463073	21.54%	1.723%
40	23.804	3532	3539	3552	rVB	1029054	2150281	100.00%	8.002%
41	23.963	3559	3566	3576	rVB2	604439	1233409	57.36%	4.590%
42	24.180	3597	3603	3612	rVB2	312630	702884	32.69%	2.616%
43	24.574	3666	3670	3679	rVB2	85657	183123	8.52%	0.681%
44	25.145	3759	3767	3780	rVB2	384445	1080511	50.25%	4.021%
45	26.315	3956	3966	3980	rVB3	410917	1424952	66.27%	5.303%
46	27.745	4200	4209	4226	rVB2	442828	1770878	82.36%	6.590%

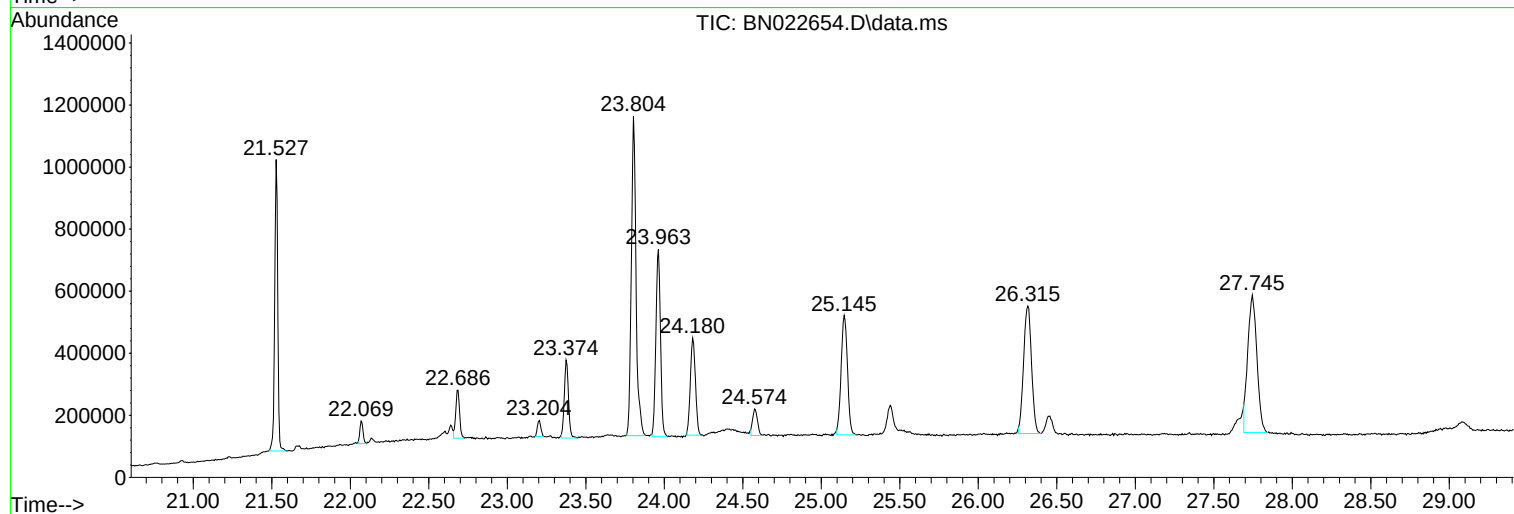
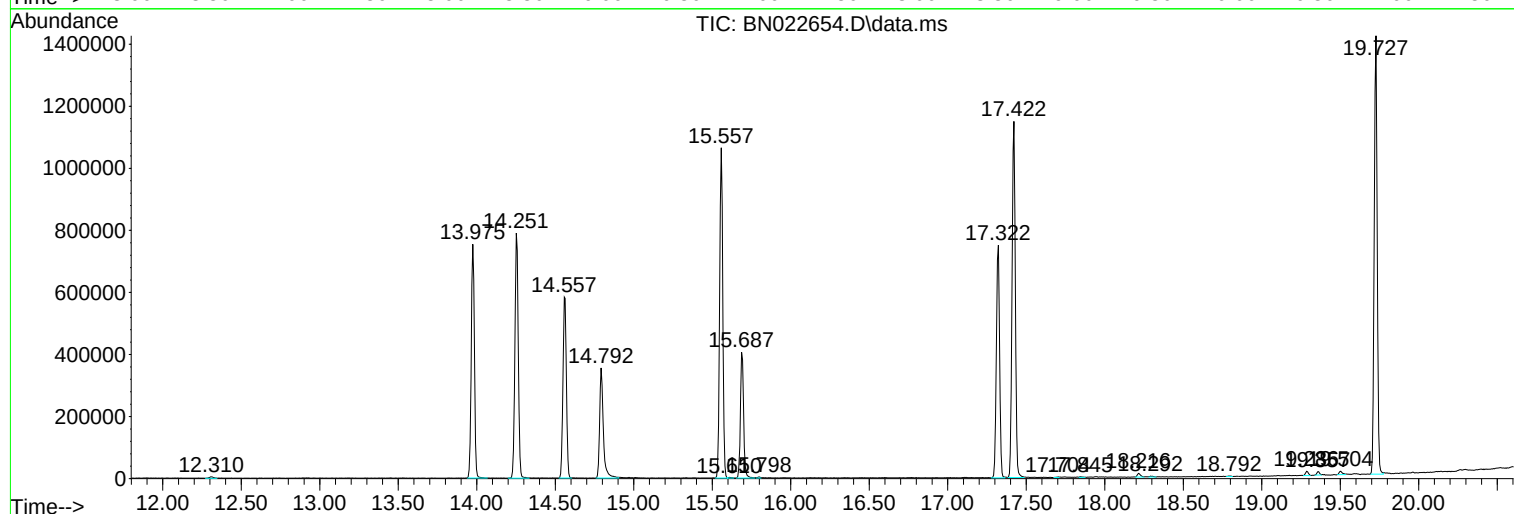
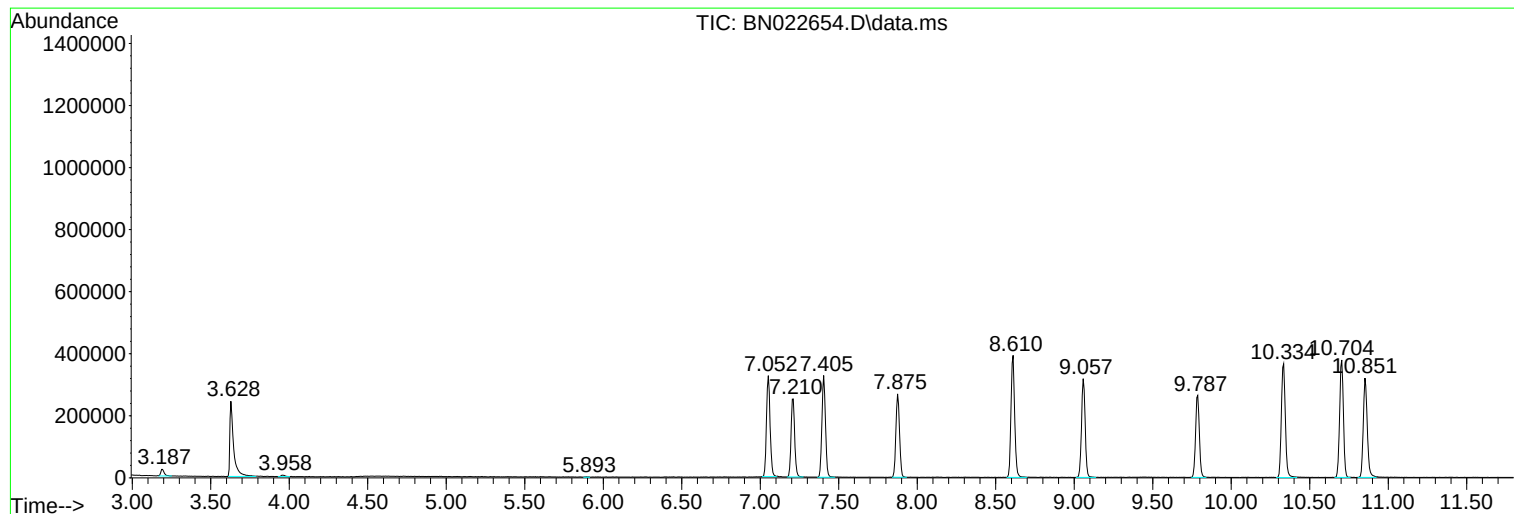
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

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



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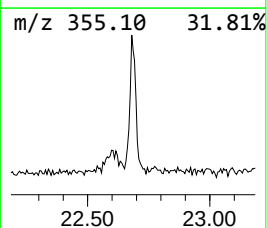
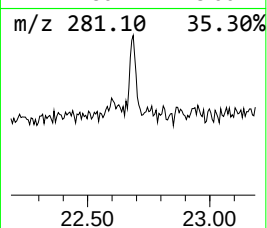
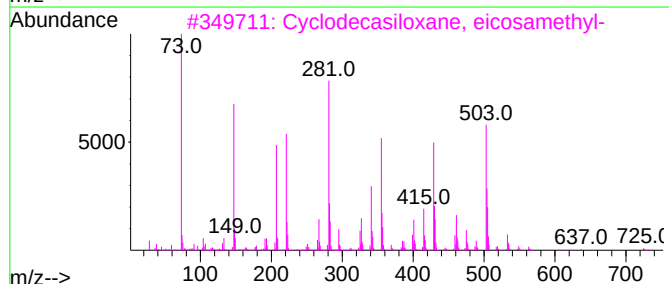
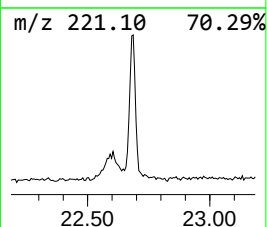
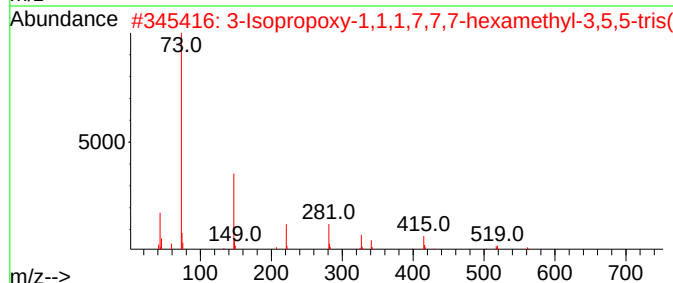
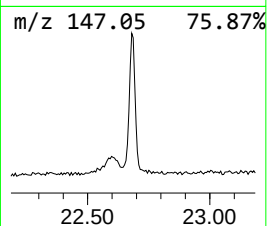
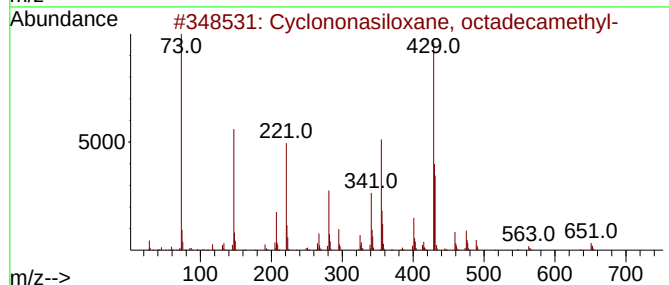
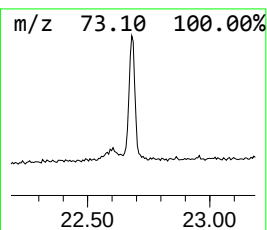
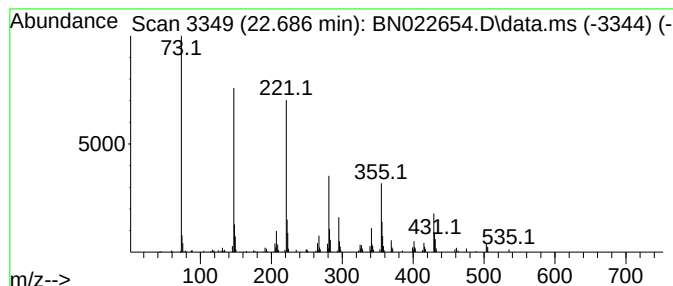
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Quant Title : SVOA CALIBRATION

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

Peak Number 1 Cyclononasiloxane, octadeca... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.686	4.19 ng/ul	265076	Chrysene-d12	21.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	86
2			3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	50
3			Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	38
4			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	38
5			N-[4-(Aminosulfonyl)phenyl]propa...	444	C18H36N2O3SSi3	1000500-82-8	32



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Instrument :
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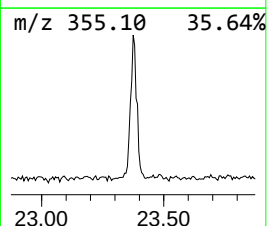
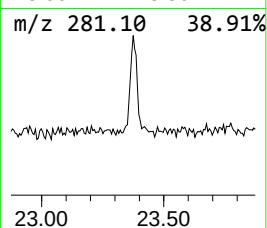
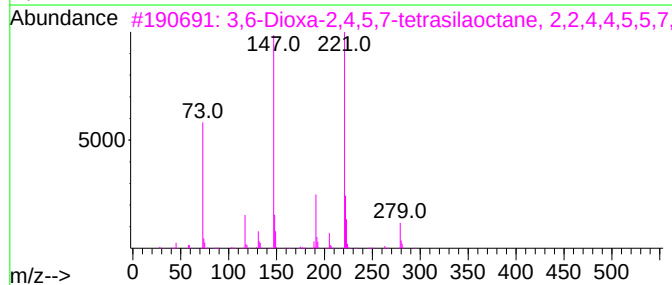
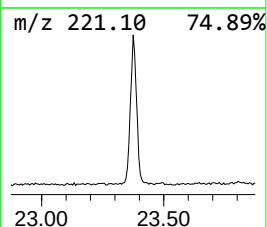
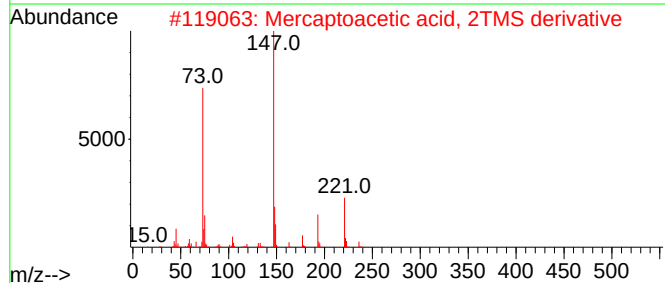
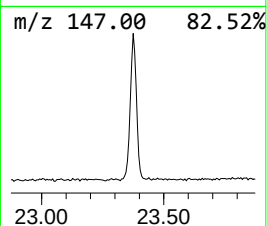
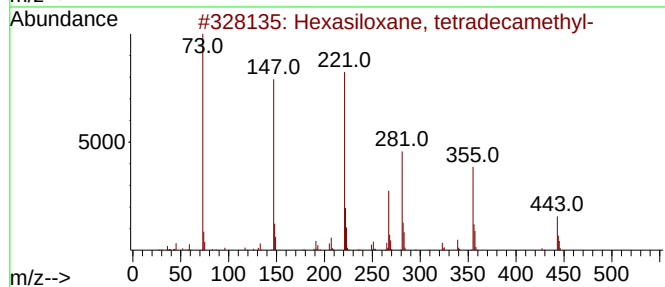
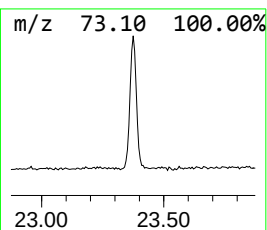
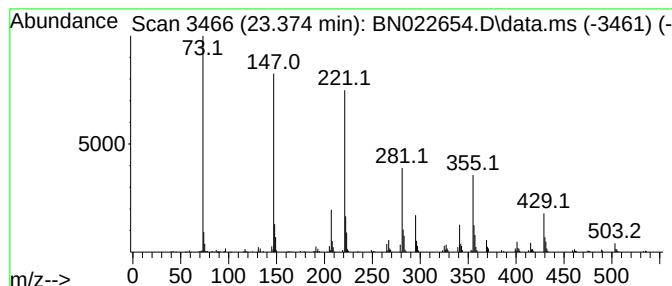
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Hexasiloxane, tetradecamethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.374	7.51 ng/ul	463073	Perylene-d12	23.962

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	87
2			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	47
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	40
4			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	38
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	38



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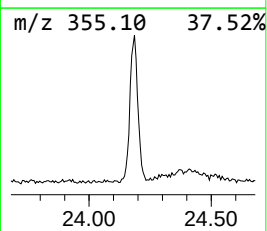
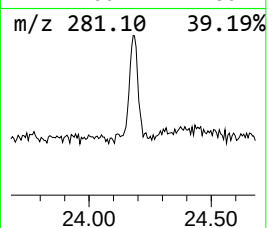
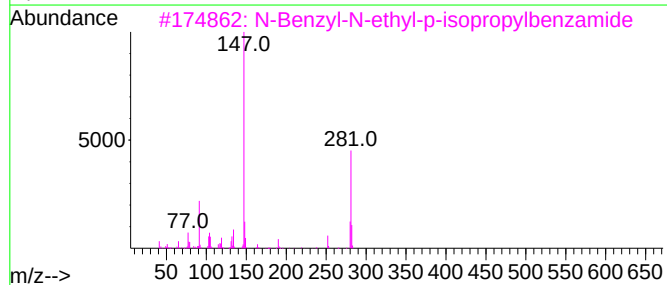
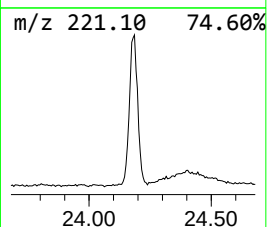
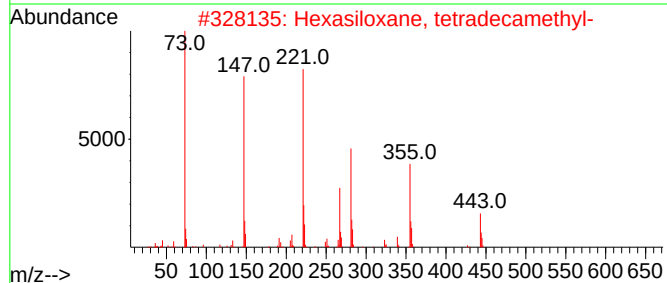
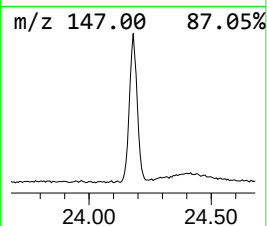
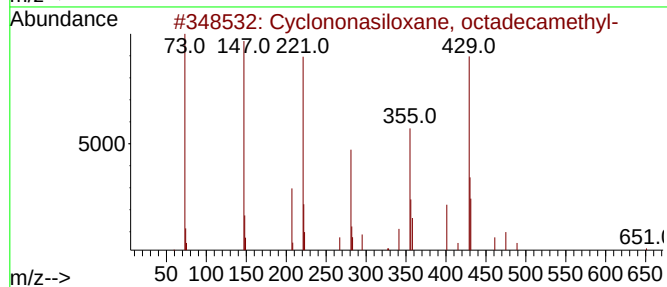
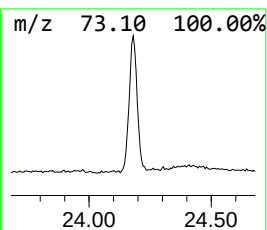
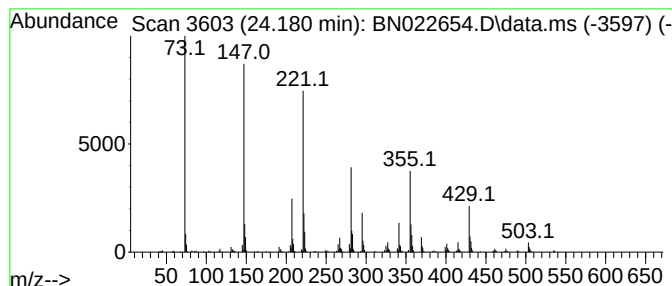
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.180	11.40 ng/ul	702884	Perylene-d12	23.962

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	90
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	83
3			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	38
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	38
5			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	35



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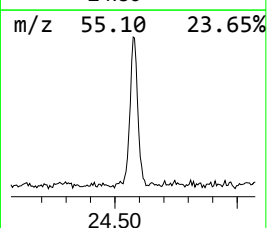
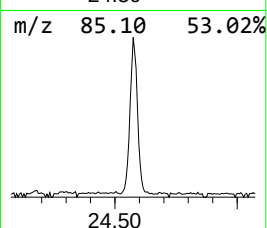
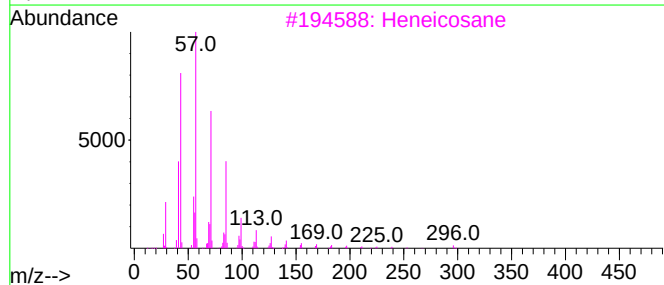
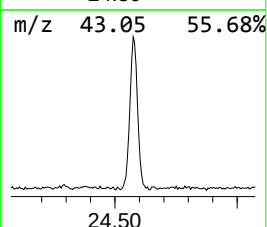
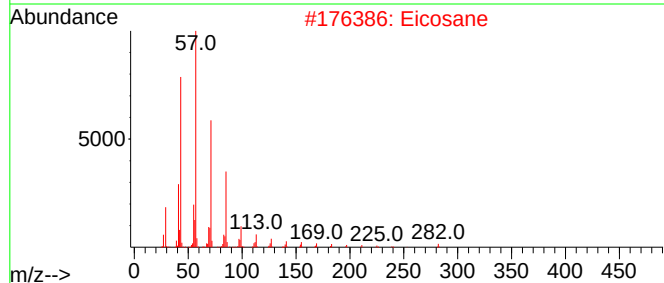
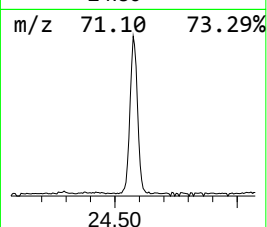
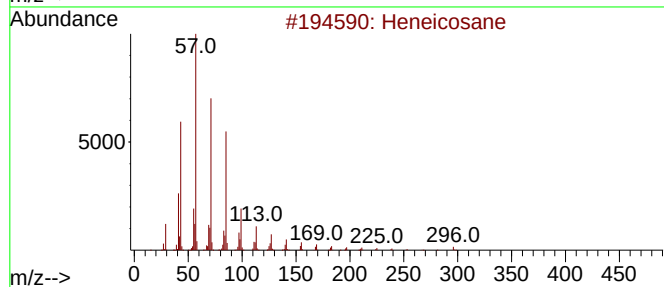
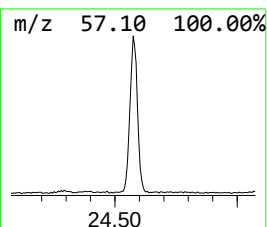
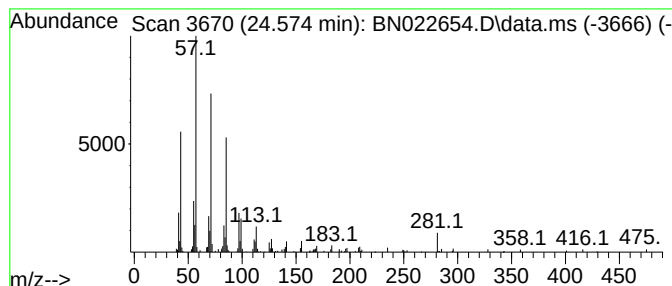
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.574	2.97 ng/ul	183123	Perylene-d12	23.962

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	98
2		Eicosane	282	C20H42	000112-95-8	95
3		Heneicosane	296	C21H44	000629-94-7	93
4		Heptacosane	380	C27H56	000593-49-7	91
5		Docosane, 1-iodo-	436	C22H45I	1000406-31-9	90



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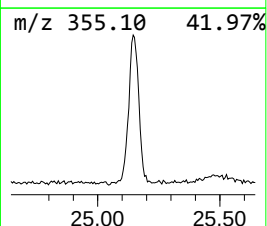
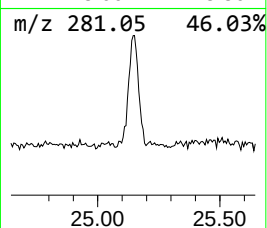
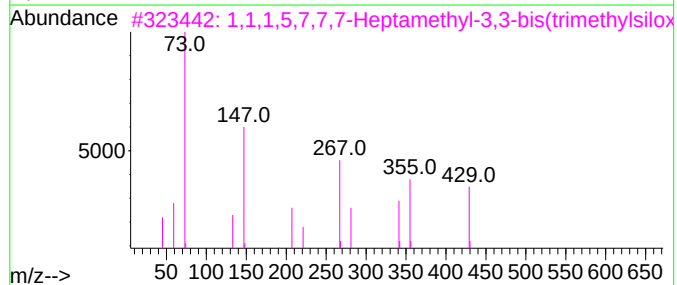
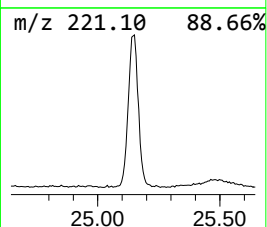
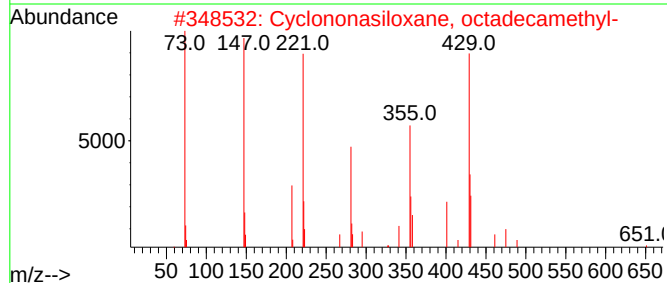
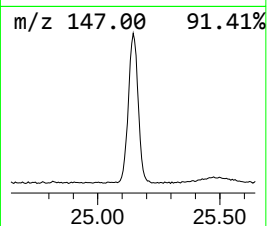
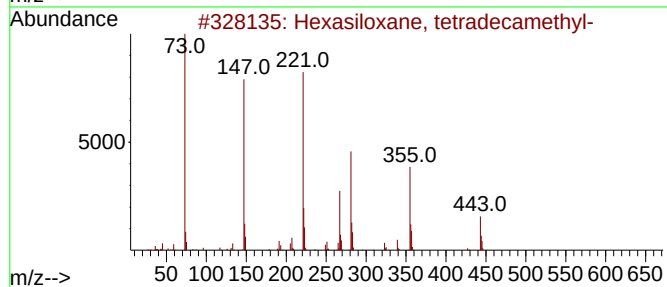
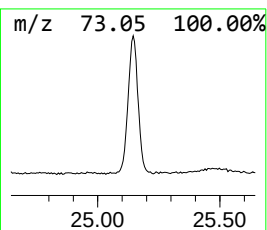
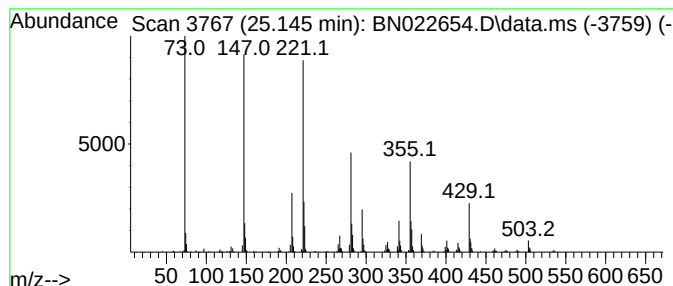
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.145	17.52 ng/ul	1080510	Perylene-d12	23.962

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	81
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	78
3			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	40
4			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	38
5			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN111522\
Data File : BN022654.D
Acq On : 15 Nov 2022 18:13
Operator : CG/JU
Sample : PB149003BL
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SBLK003

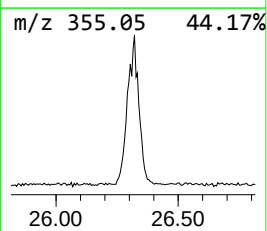
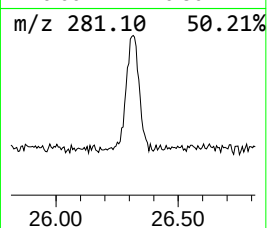
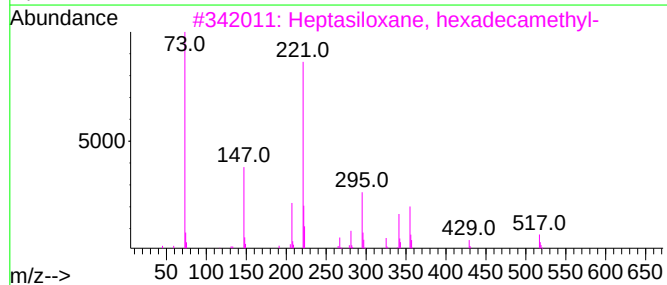
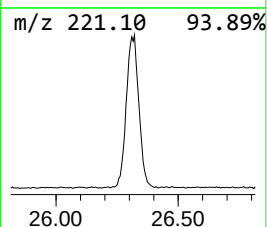
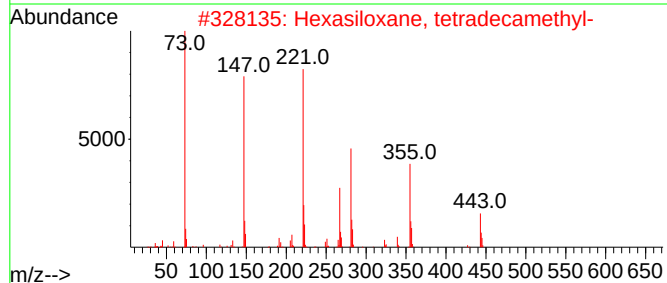
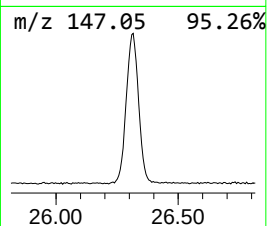
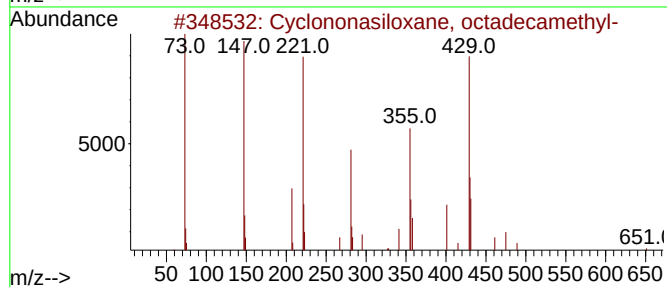
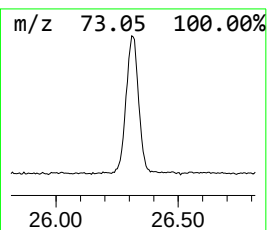
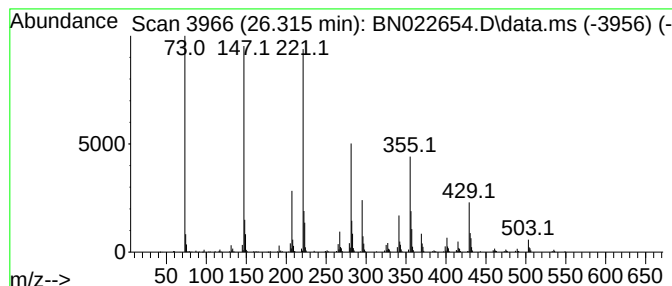
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 unknown-03 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.315	23.11 ng/ul	1424950	Perylene-d12	23.962

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			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	43
4			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	37
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN111522\
Data File : BN022654.D
Acq On : 15 Nov 2022 18:13
Operator : CG/JU
Sample : PB149003BL
Misc :
ALS Vial : 12 Sample Multiplier: 1

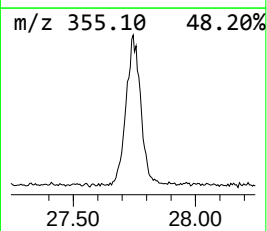
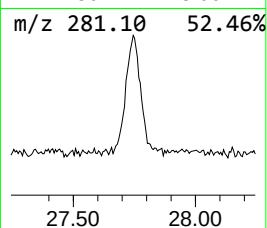
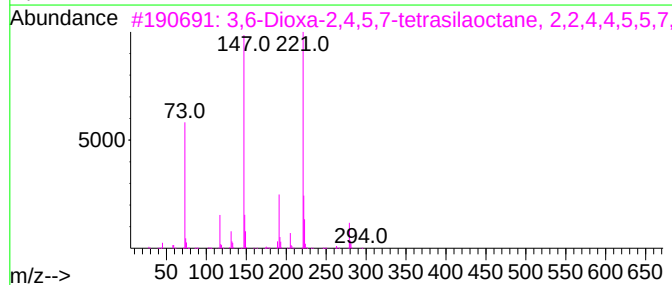
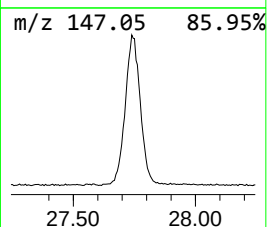
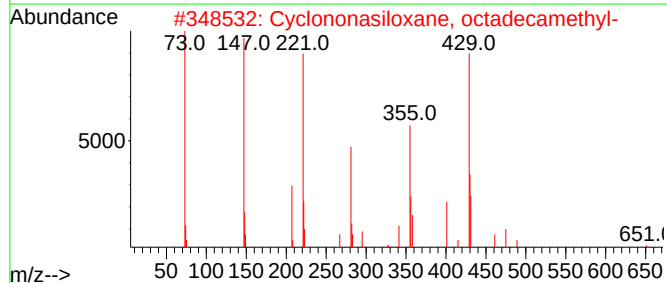
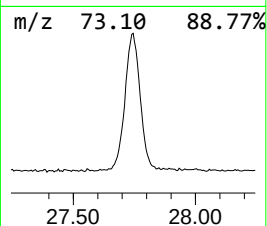
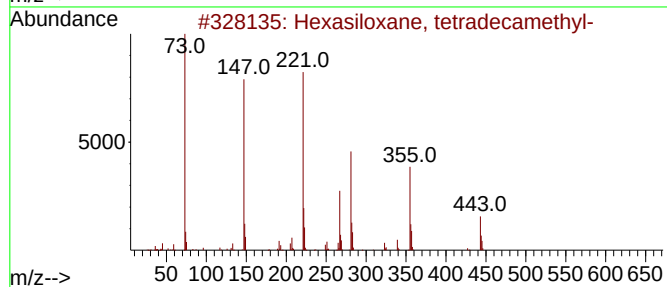
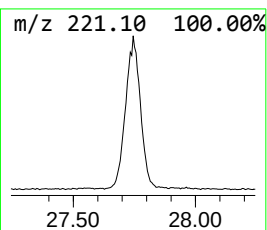
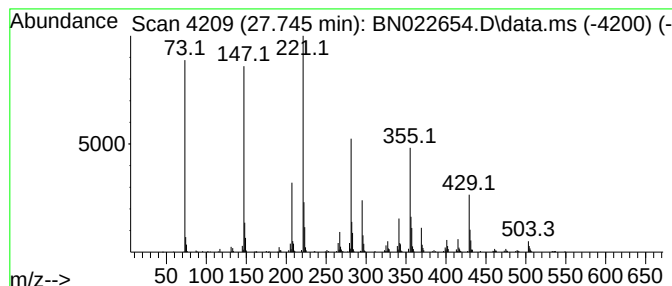
Instrument :
BNA_N
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

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

Peak Number 7 3,6-Dioxa-2,4,5,7-tetrasil... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
27.745	28.72 ng/ul	1770880	Perylene-d12			23.962
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexasiloxane, tetradecamethyl-		458	C14H42O5Si6	000107-52-8	81
2	Cyclononasiloxane, octadecamethyl-		666	C18H54O9Si9	000556-71-8	64
3	3,6-Dioxa-2,4,5,7-tetrasilaoctan...		294	C10H30O2Si4	004342-25-0	55
4	Heptasiloxane, hexadecamethyl-		532	C16H48O6Si7	000541-01-5	52
5	Cyclodecasiloxane, eicosamethyl-		740	C20H60O10Si10	018772-36-6	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN111522\
Data File : BN022654.D
Acq On : 15 Nov 2022 18:13
Operator : CG/JU
Sample : PB149003BL
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SBLK003

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA 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...	22.686	4.2	ng/u1	265076	5	21.527	1265760	20.0
Hexasiloxane, t...	23.374	7.5	ng/u1	463073	6	23.962	1233410	20.0
unknown-01	24.180	11.4	ng/u1	702884	6	23.962	1233410	20.0
(DEL) Alkane: S...	24.574	3.0	ng/u1	183123	6	23.962	1233410	20.0
unknown-02	25.145	17.5	ng/u1	1080510	6	23.962	1233410	20.0
unknown-03	26.315	23.1	ng/u1	1424950	6	23.962	1233410	20.0
3,6-Dioxa-2,4,5...	27.745	28.7	ng/u1	1770880	6	23.962	1233410	20.0