

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
 Data File : BM043397.D
 Acq On : 18 Dec 2023 17:31
 Operator : MA/JU
 Sample : 05830-04DL 5X
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 H0AB4DL

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_M\Methods\SFAM-EPA-BM121523.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BM043397.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.352	23	28	36	rBV	1234885	1714790	10.23%	2.838%
2	3.422	36	40	52	rVB	539360	723793	4.32%	1.198%
3	3.822	105	108	119	rBV	64131	113268	0.68%	0.187%
4	4.140	158	162	167	rBV2	21381	31543	0.19%	0.052%
5	4.669	246	252	266	rBV	11470533	16767717	100.00%	27.747%
6	7.151	668	674	682	rVB	70730	117287	0.70%	0.194%
7	7.328	698	704	712	rBV	326240	540307	3.22%	0.894%
8	7.516	730	736	744	rBV	286153	474727	2.83%	0.786%
9	7.993	810	817	827	rBV	1284322	2049105	12.22%	3.391%
10	8.704	931	938	945	rBV	205135	344479	2.05%	0.570%
11	9.163	1008	1016	1025	rBV	379094	645619	3.85%	1.068%
12	9.887	1130	1139	1150	rBV	261505	461677	2.75%	0.764%
13	10.422	1222	1230	1239	rBV	385656	668411	3.99%	1.106%
14	10.798	1287	1294	1302	rBV	1661791	2884434	17.20%	4.773%
15	10.945	1312	1319	1337	rBV	402651	726471	4.33%	1.202%
16	13.522	1752	1757	1765	rVB	28928	52626	0.31%	0.087%
17	14.039	1838	1845	1857	rBV	739323	1054008	6.29%	1.744%
18	14.316	1884	1892	1903	rBV	827013	1267936	7.56%	2.098%
19	14.622	1937	1944	1958	rBV	2186415	3184421	18.99%	5.270%
20	14.827	1972	1979	1989	rBV4	35734	83035	0.50%	0.137%
21	15.616	2105	2113	2121	rBV	990617	1491855	8.90%	2.469%
22	15.733	2127	2133	2139	rBV	216556	309790	1.85%	0.513%
23	17.363	2403	2410	2420	rBV	2105467	3138893	18.72%	5.194%
24	17.463	2421	2427	2440	rVV2	976176	1453038	8.67%	2.404%
25	18.262	2557	2563	2568	rBV4	49976	80208	0.48%	0.133%
26	18.345	2573	2577	2583	rBV2	34150	49889	0.30%	0.083%
27	19.539	2777	2780	2784	rBV5	19499	23952	0.14%	0.040%
28	19.692	2802	2806	2810	rBV	59716	71290	0.43%	0.118%
29	19.751	2810	2816	2822	rVV	1035990	1425551	8.50%	2.359%
30	20.756	2981	2987	2991	rBV2	113054	190721	1.14%	0.316%
31	21.262	3070	3073	3077	rBV4	55632	69235	0.41%	0.115%
32	21.539	3115	3120	3131	rBV2	2109612	2936516	17.51%	4.859%
33	22.139	3217	3222	3226	rBV	382983	562331	3.35%	0.931%
34	22.692	3313	3316	3321	rVB	154622	202536	1.21%	0.335%
35	22.762	3324	3328	3336	rVB	618037	1028496	6.13%	1.702%
36	23.256	3409	3412	3419	rVB	217519	334798	2.00%	0.554%

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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_M\Methods\SFAM-EPA-BM121523.MA.M
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37	23.474	3444	3449	3458	rVB	769309	1486162	8.86%	2.459%
38	23.803	3500	3505	3515	rVB2	698859	1345937	8.03%	2.227%
39	23.903	3518	3522	3526	rVV	290438	530764	3.17%	0.878%
40	23.962	3526	3532	3543	rVB	1418472	2900206	17.30%	4.799%
41	24.309	3584	3591	3600	rVB2	747026	1758718	10.49%	2.910%
42	24.650	3645	3649	3658	rVB	284795	563382	3.36%	0.932%
43	25.303	3753	3760	3771	rVB	690353	1992560	11.88%	3.297%
44	26.521	3958	3967	3986	rVB2	615475	2577478	15.37%	4.265%

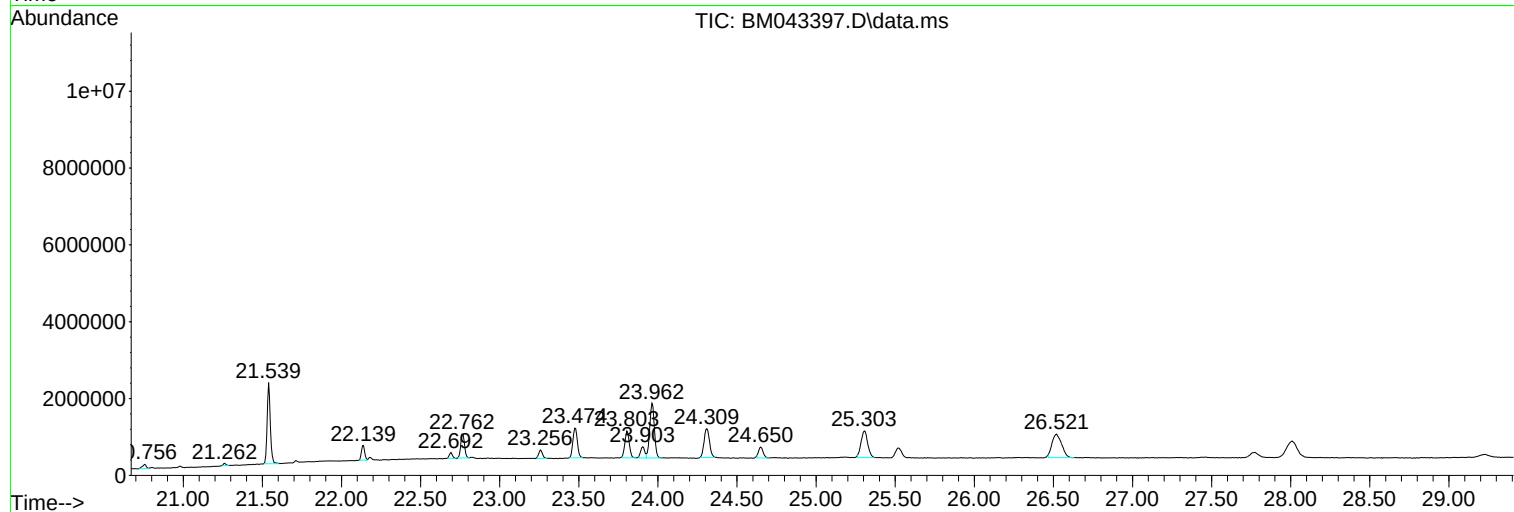
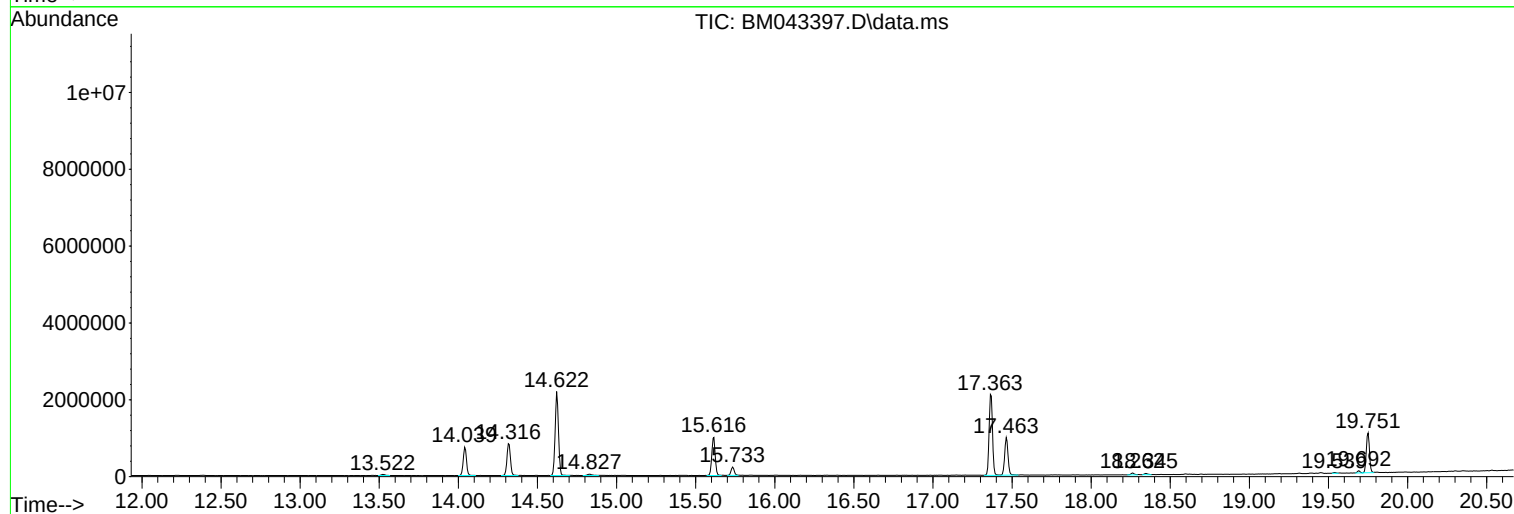
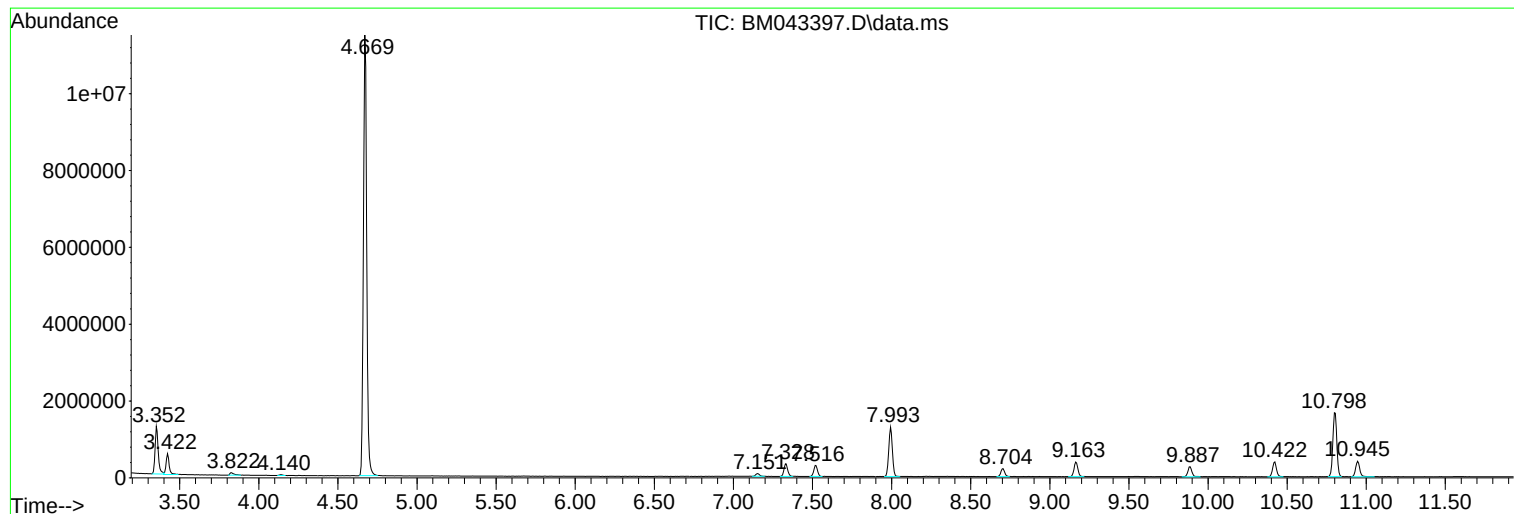
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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



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Instrument :
BNA_M
ClientSampleId :
H0AB4DL

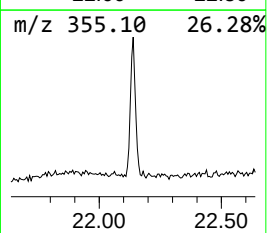
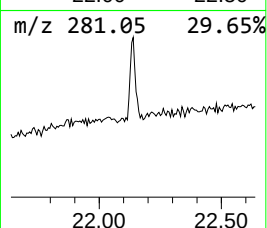
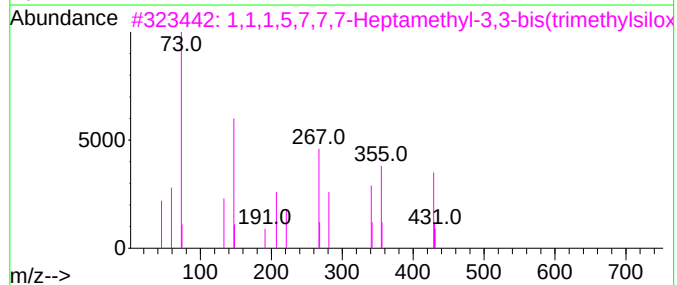
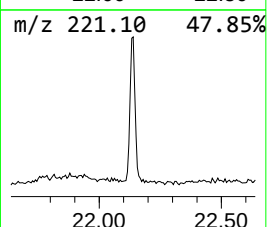
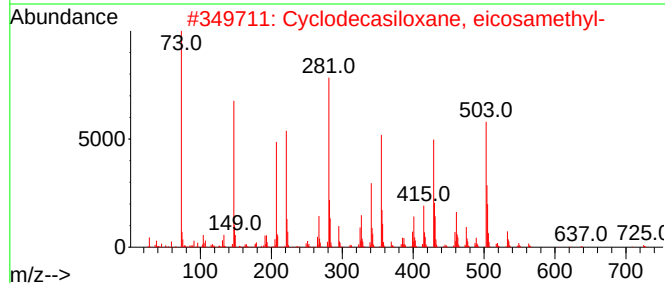
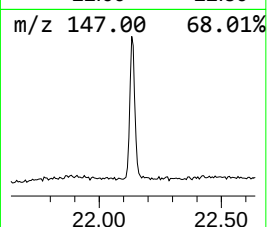
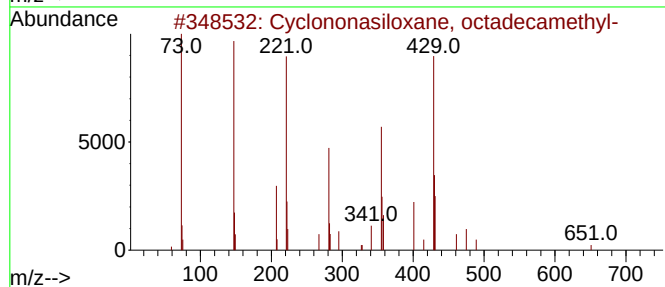
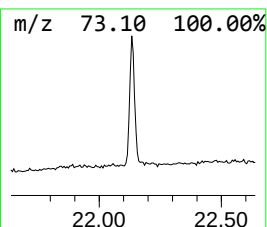
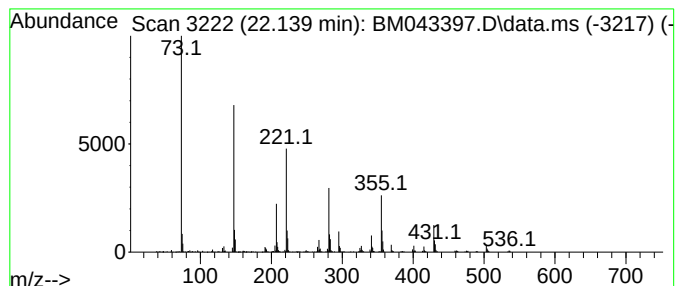
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Cyclononasiloxane, octadeca... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.139	3.83 ng/ul	562331	Chrysene-d12	21.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	90
2			Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	50
3			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	50
4			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	45
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	27



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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
H0AB4DL

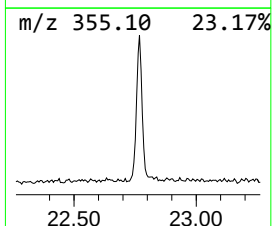
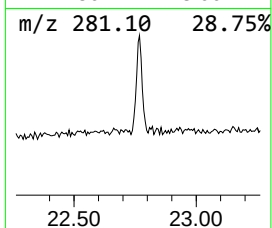
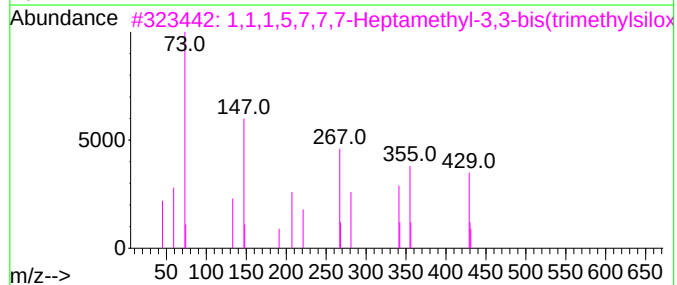
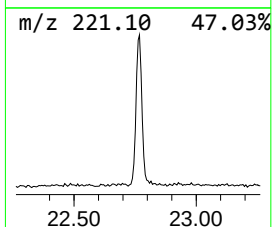
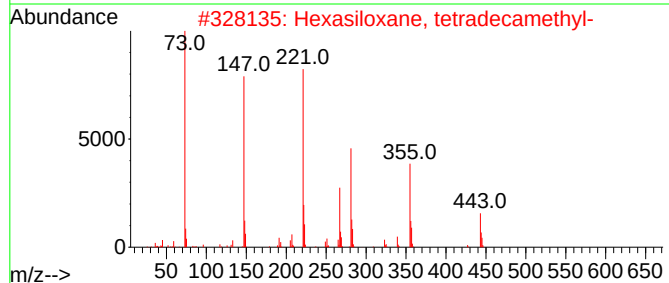
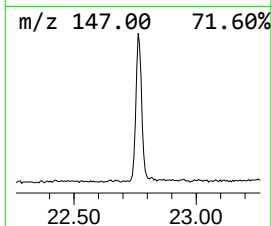
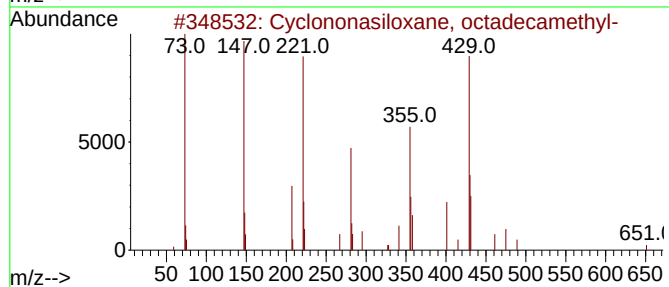
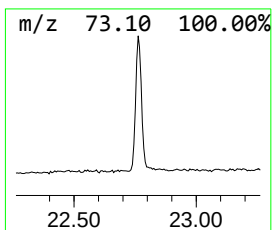
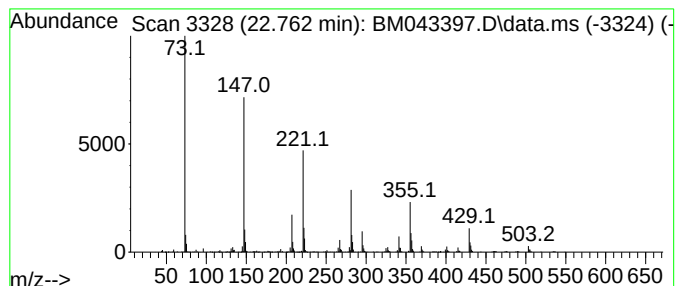
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.762	7.09 ng/ul	1028500	Perylene-d12	23.962

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	38
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	38
3			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	33
4			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	32
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	27



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ALS Vial : 15 Sample Multiplier: 1

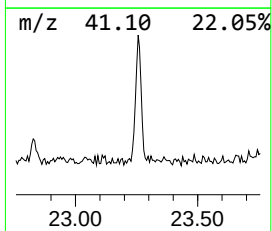
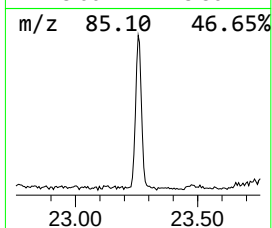
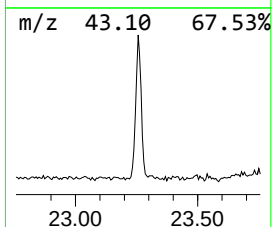
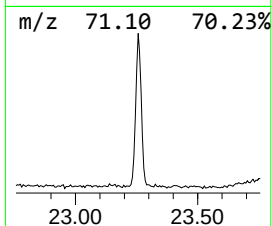
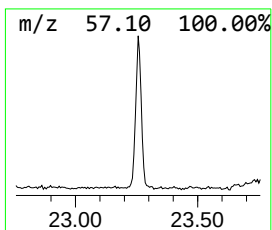
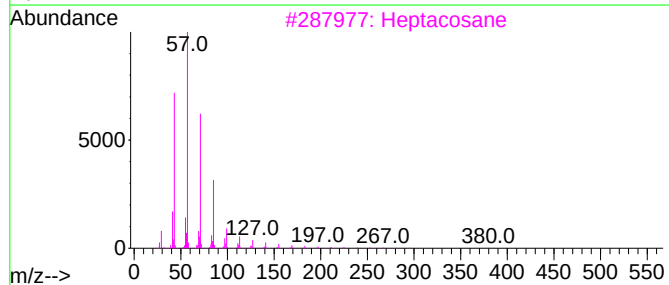
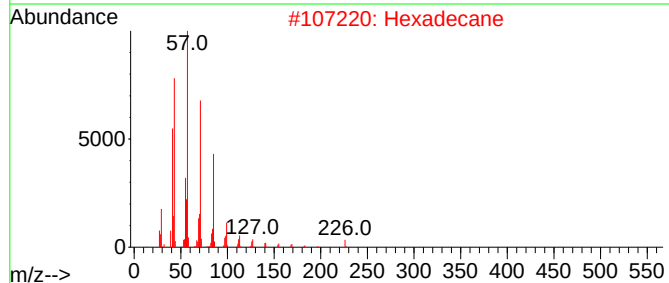
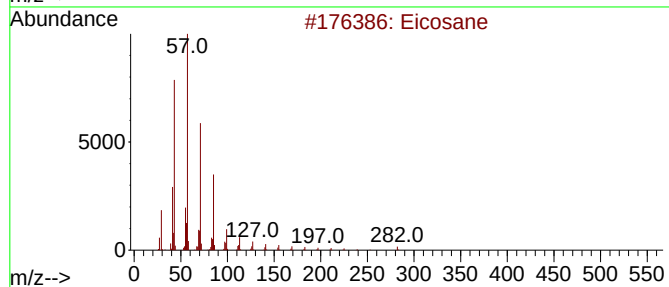
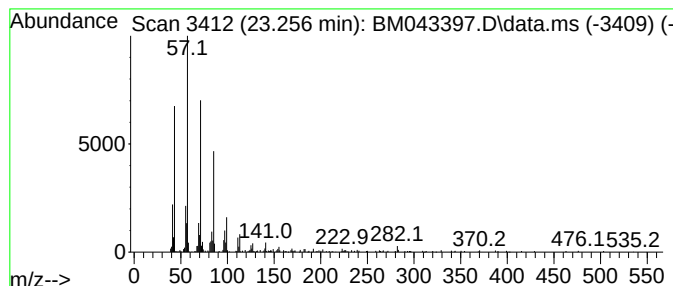
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.256	2.31 ng/ul	334798	Perylene-d12	23.962	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heptacosane	380	C27H56	000593-49-7	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86



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Misc :
ALS Vial : 15 Sample Multiplier: 1

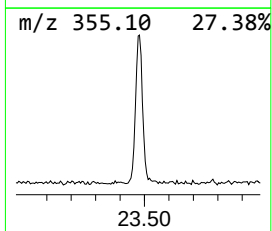
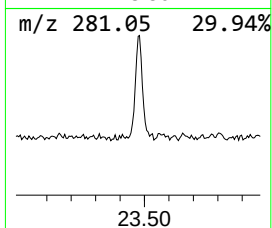
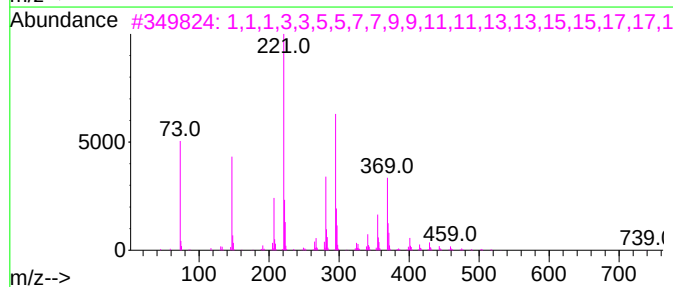
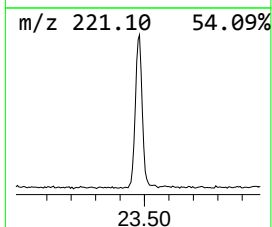
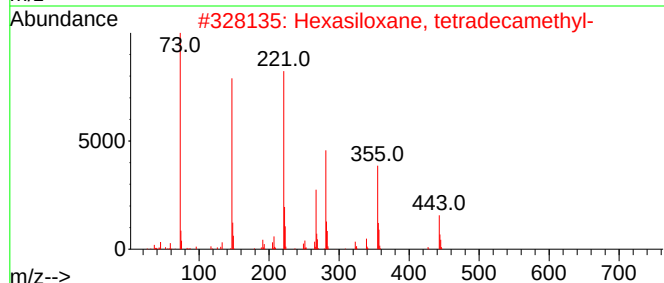
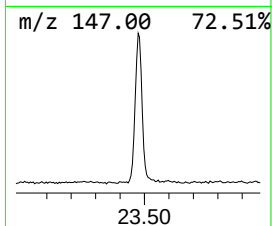
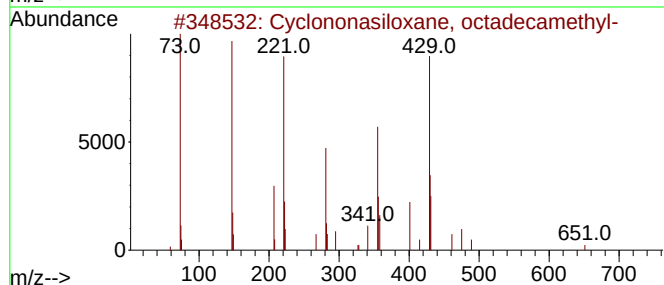
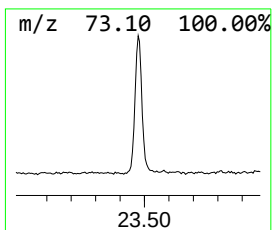
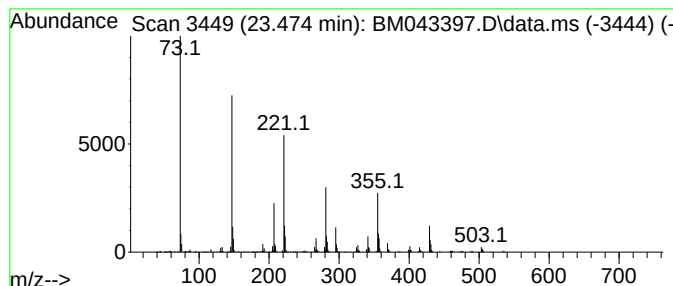
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 Hexasiloxane, tetradecamethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
23.474	10.25 ng/ul	1486160	Perylene-d12		23.962	
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	72
3	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...		754	C22H66O9Si10	000556-70-7	38
4	N-Benzyl-N-ethyl-p-isopropylbenz...		281	C19H23NO	015089-22-2	30
5	Pentasiloxane, dodecamethyl-		384	C12H36O4Si5	000141-63-9	27



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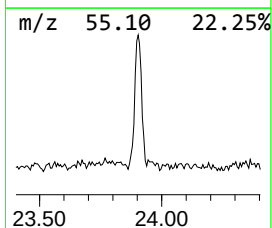
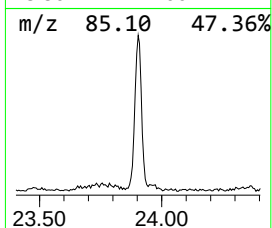
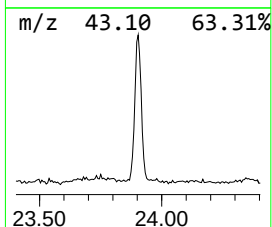
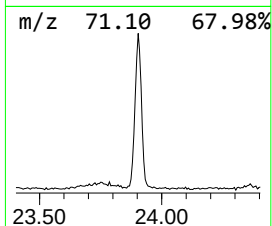
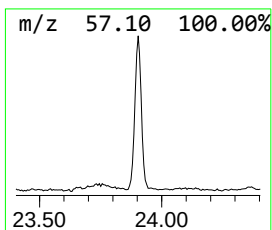
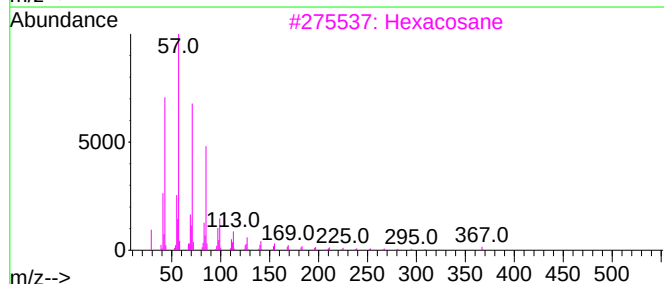
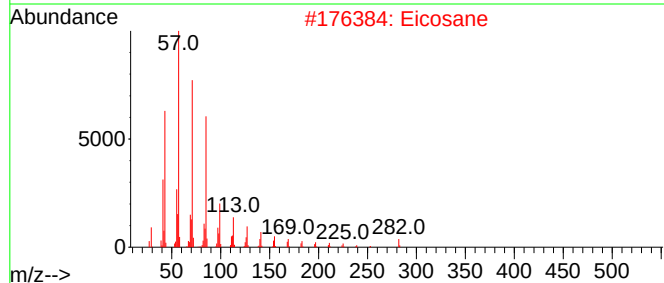
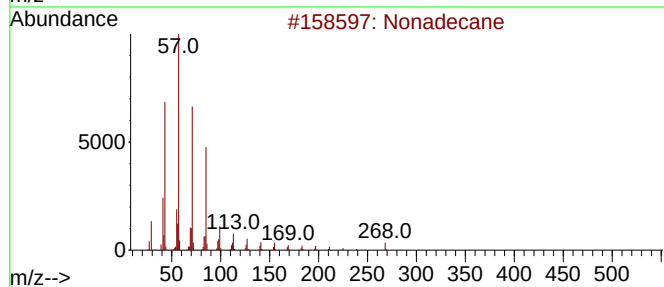
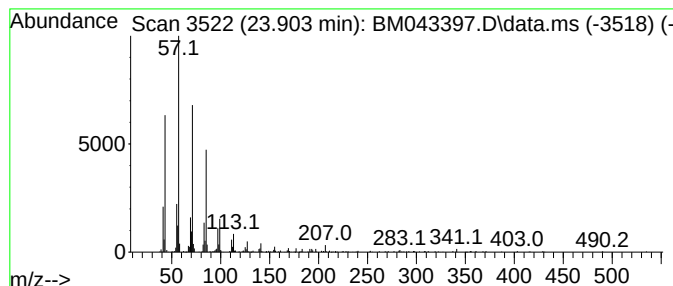
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.903	3.66 ng/ul	530764	Perylene-d12	23.962

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	93
2			Eicosane	282	C20H42	000112-95-8	91
3			Hexacosane	366	C26H54	000630-01-3	90
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043397.D
Acq On : 18 Dec 2023 17:31
Operator : MA/JU
Sample : 05830-04DL 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

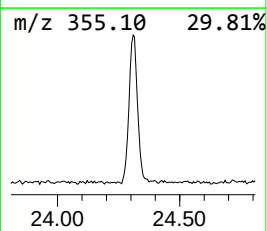
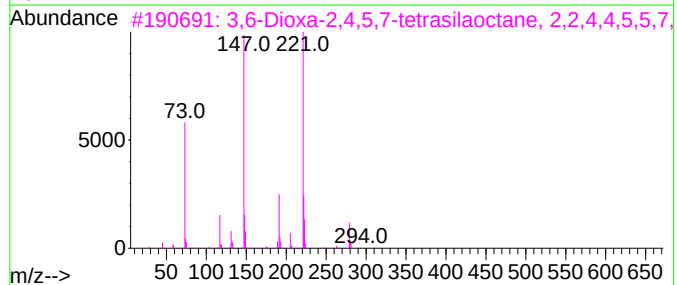
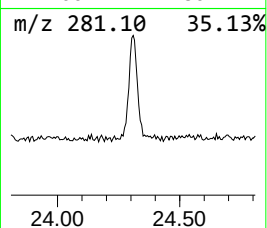
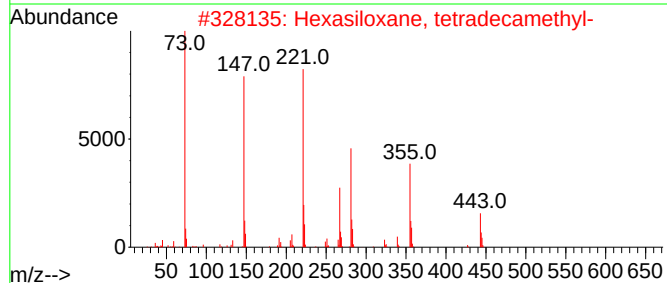
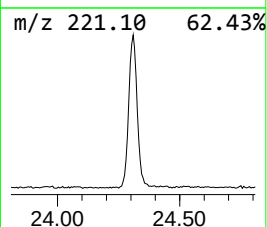
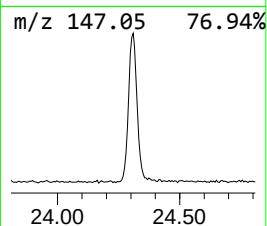
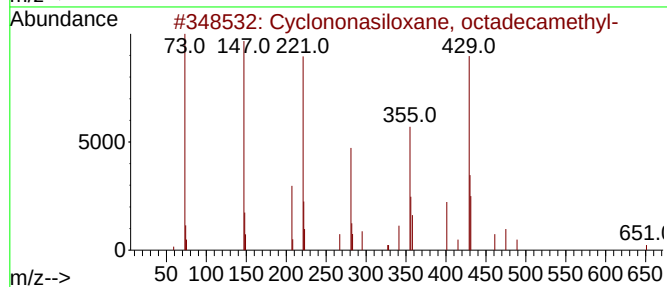
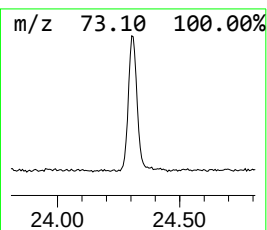
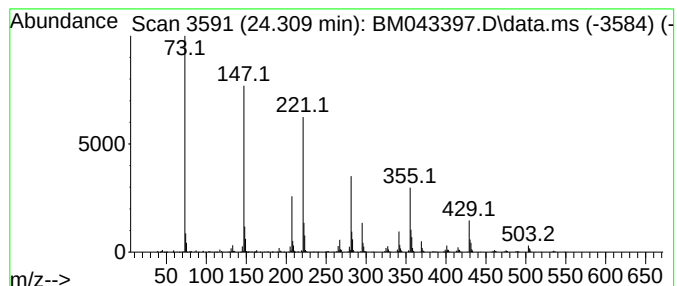
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 8 3,6-Dioxa-2,4,5,7-tetrasila... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.309	12.13 ng/ul	1758720	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	87
3	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	50
4	Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	47
5	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043397.D
Acq On : 18 Dec 2023 17:31
Operator : MA/JU
Sample : 05830-04DL 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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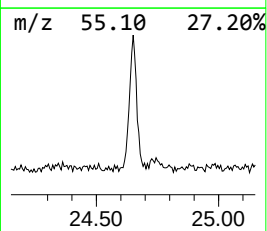
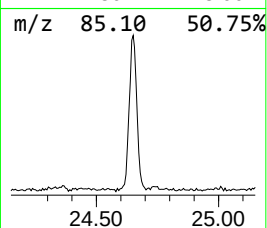
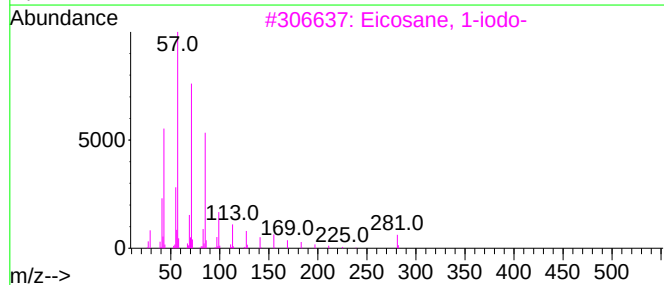
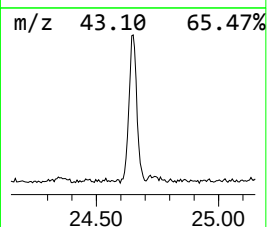
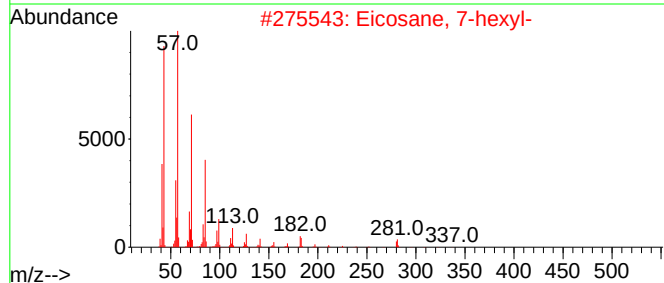
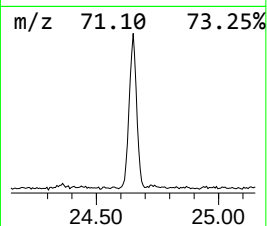
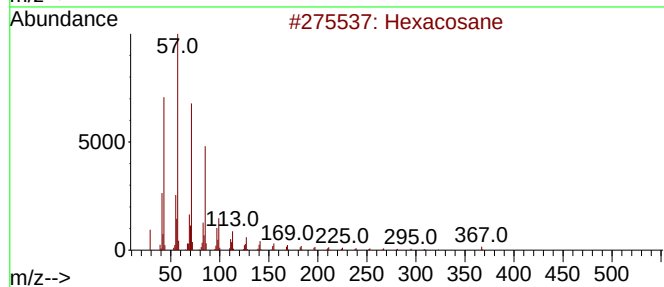
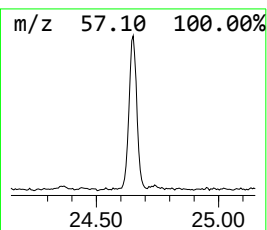
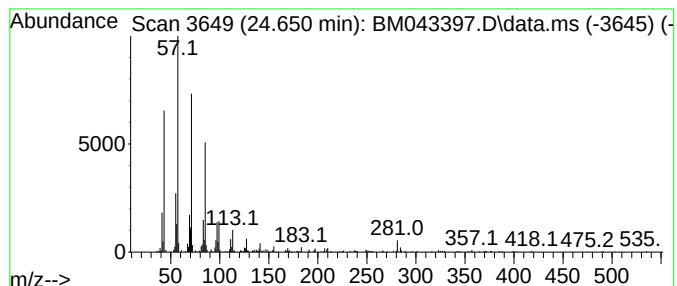
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.650	3.89 ng/ul	563382	Perylene-d12	23.962

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	90
2			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
3			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87
4			Tetratetracontane	619	C44H90	007098-22-8	87
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043397.D
Acq On : 18 Dec 2023 17:31
Operator : MA/JU
Sample : 05830-04DL 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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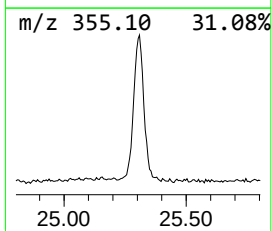
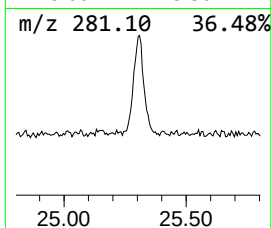
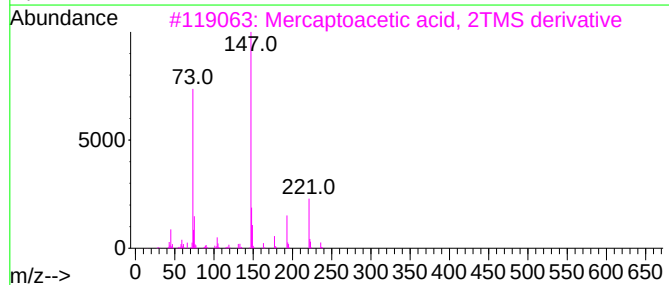
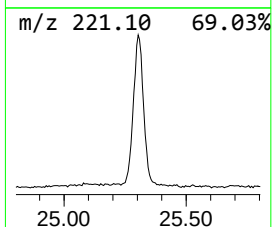
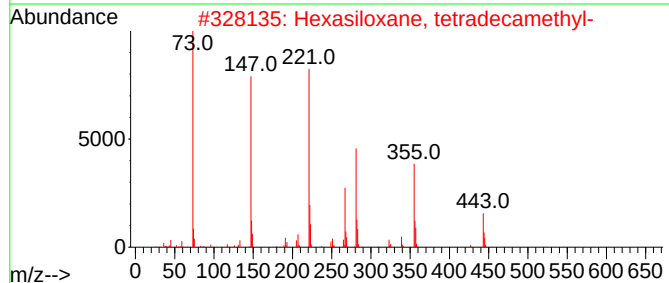
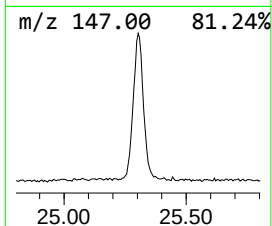
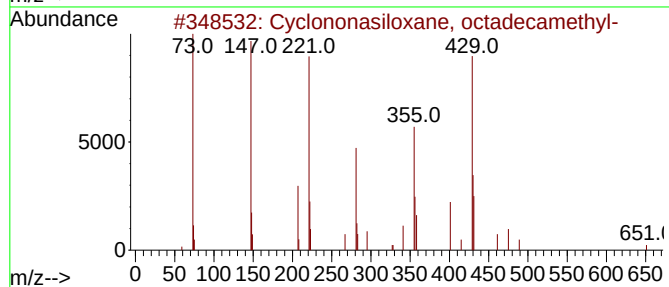
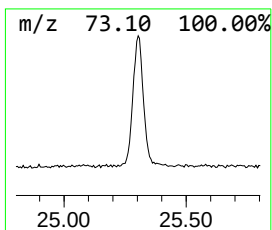
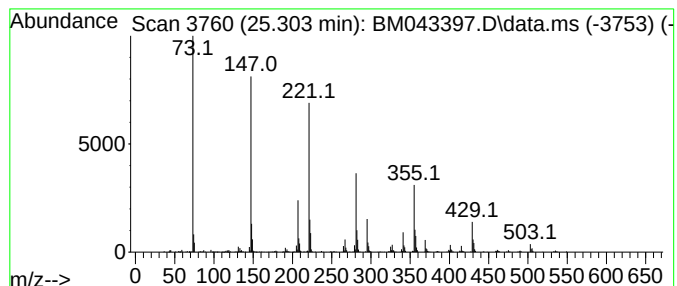
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.303	13.74 ng/ul	1992560	Perylene-d12	23.962

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	91
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	83
3			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	47
4			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	43
5			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043397.D
Acq On : 18 Dec 2023 17:31
Operator : MA/JU
Sample : 05830-04DL 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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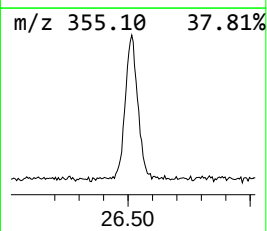
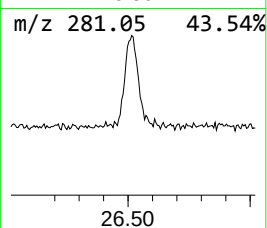
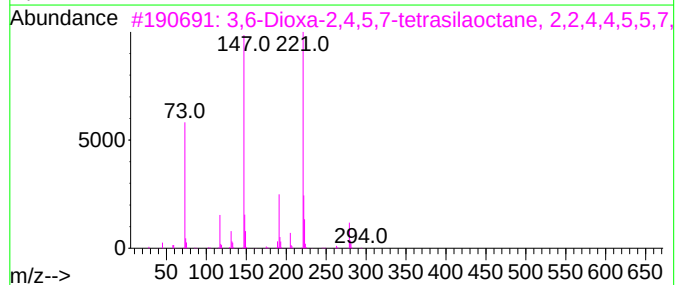
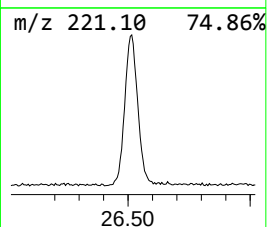
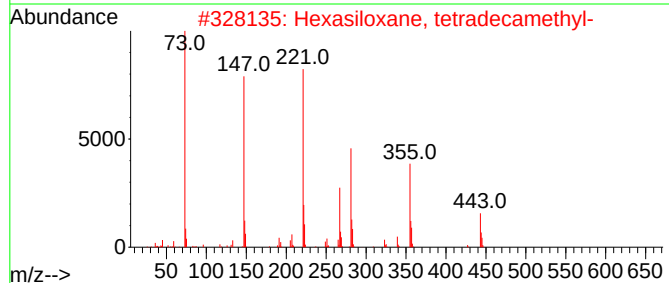
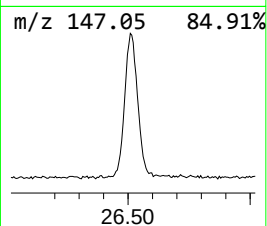
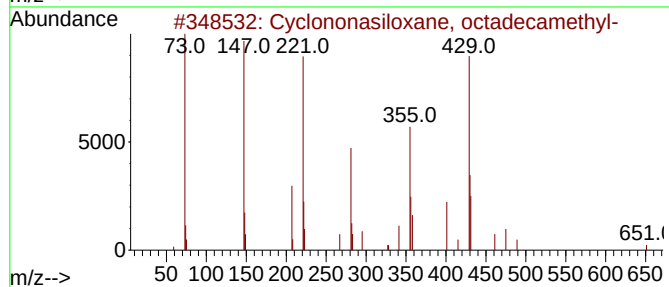
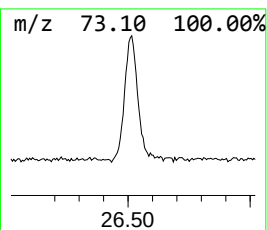
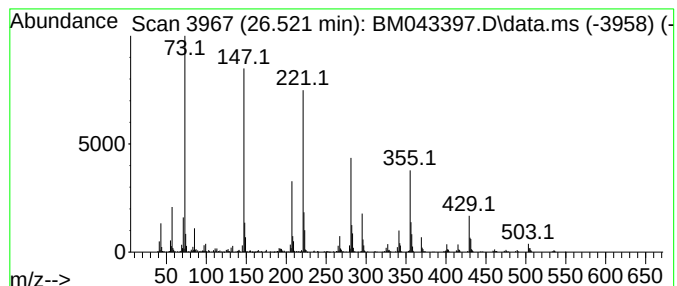
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Quant Title : SVOA CALIBRATION

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

Peak Number 11 unknown-03 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.521	17.77 ng/ul	2577480	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	87
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	58
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	38
5			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043397.D
Acq On : 18 Dec 2023 17:31
Operator : MA/JU
Sample : 05830-04DL 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.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...	22.139	3.8	ng/ul	562331	5	21.539	2936520	20.0
unknown-01	22.762	7.1	ng/ul	1028500	6	23.962	2900210	20.0
(DEL) Alkane: S...	23.256	2.3	ng/ul	334798	6	23.962	2900210	20.0
Hexasiloxane, t...	23.474	10.3	ng/ul	1486160	6	23.962	2900210	20.0
(DEL) Alkane: S...	23.903	3.7	ng/ul	530764	6	23.962	2900210	20.0
3,6-Dioxa-2,4,5...	24.309	12.1	ng/ul	1758720	6	23.962	2900210	20.0
(DEL) Alkane: S...	24.650	3.9	ng/ul	563382	6	23.962	2900210	20.0
unknown-02	25.303	13.7	ng/ul	1992560	6	23.962	2900210	20.0
unknown-03	26.521	17.8	ng/ul	2577480	6	23.962	2900210	20.0