

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050823\
 Data File : BG057336.D
 Acq On : 8 May 2023 18:48
 Operator : CG/JU
 Sample : PB152657BL
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SBLK657

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_G\Methods\SFAM-EPA-BG042823.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG057336.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.649	17	19	25	rVB5	4839	6775	1.24%	0.110%
2	3.749	34	36	39	rBV4	1068	1086	0.20%	0.018%
3	4.043	85	86	89	rVB2	1382	839	0.15%	0.014%
4	4.101	93	96	104	rVV	16530	28319	5.19%	0.461%
5	4.454	151	156	159	rBV6	1106	1709	0.31%	0.028%
6	4.530	167	169	176	rVB4	641	1045	0.19%	0.017%
7	4.607	180	182	185	rBV3	542	677	0.12%	0.011%
8	5.388	310	315	318	rVB4	427	726	0.13%	0.012%
9	5.435	322	323	328	rBV3	764	979	0.18%	0.016%
10	6.292	468	469	473	rVB2	599	649	0.12%	0.011%
11	6.357	476	480	483	rBV	596	940	0.17%	0.015%
12	6.457	494	497	502	rVB	527	770	0.14%	0.013%
13	6.498	502	504	507	rBV	590	626	0.11%	0.010%
14	6.845	561	563	568	rVB	656	668	0.12%	0.011%
15	7.003	587	590	593	rVB	716	860	0.16%	0.014%
16	7.508	669	676	687	rBV	62929	115258	21.13%	1.878%
17	7.585	687	689	692	rVV	680	732	0.13%	0.012%
18	7.679	698	705	714	rBB	46241	78784	14.44%	1.283%
19	7.832	727	731	734	rBB	467	624	0.11%	0.010%
20	7.896	734	742	750	rBV	59336	107459	19.70%	1.751%
21	8.372	817	823	832	rBB	61909	107125	19.64%	1.745%
22	9.071	935	942	956	rBV	76345	142125	26.05%	2.315%
23	9.553	1016	1024	1031	rBV	61937	111766	20.49%	1.821%
24	10.281	1142	1148	1155	rVV	57544	101323	18.57%	1.651%
25	10.828	1235	1241	1251	rBV	85149	151095	27.70%	2.461%
26	11.209	1299	1306	1317	rBV	92047	166661	30.55%	2.715%
27	11.339	1322	1328	1339	rVV	39379	69651	12.77%	1.135%
28	12.772	1568	1572	1577	rVB2	1146	1607	0.29%	0.026%
29	13.847	1751	1755	1760	rBV3	1147	1576	0.29%	0.026%
30	14.370	1837	1844	1851	rBV	185257	263259	48.26%	4.289%
31	14.687	1891	1898	1905	rBV	205277	313645	57.49%	5.109%
32	14.987	1940	1949	1958	rBV	184568	279464	51.23%	4.553%
33	15.175	1976	1981	1997	rBV	49118	98833	18.12%	1.610%
34	15.974	2110	2117	2124	rVB	271527	403984	74.05%	6.581%
35	16.091	2131	2137	2149	rBV	60189	97185	17.81%	1.583%
36	17.724	2408	2415	2426	rBV	239687	367157	67.30%	5.981%

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37	17.824	2426	2432	2442	rVB2	308238	457599	83.88%	7.455%
38	18.012	2463	2464	2468	rVB2	564	612	0.11%	0.010%
39	18.928	2618	2620	2626	rVB2	579	781	0.14%	0.013%
40	19.310	2684	2685	2688	rBV2	798	634	0.12%	0.010%
41	19.627	2736	2739	2740	rBV2	723	727	0.13%	0.012%
42	19.657	2740	2744	2751	rVB4	3720	5937	1.09%	0.097%
43	19.704	2751	2752	2754	rBV2	869	824	0.15%	0.013%
44	19.727	2754	2756	2760	rVB4	3395	4263	0.78%	0.069%
45	19.774	2760	2764	2766	rBV3	1066	1133	0.21%	0.018%
46	19.862	2776	2779	2782	rVV3	948	1236	0.23%	0.020%
47	19.909	2783	2787	2790	rVV3	1318	1920	0.35%	0.031%
48	19.956	2792	2795	2799	rVV5	2263	3093	0.57%	0.050%
49	19.992	2799	2801	2804	rVV3	811	690	0.13%	0.011%
50	20.039	2808	2809	2812	rBV	828	1005	0.18%	0.016%
51	20.091	2812	2818	2825	rBV	394953	545553	100.00%	8.887%
52	20.326	2856	2858	2860	rBV2	1292	1125	0.21%	0.018%
53	20.567	2897	2899	2900	rBV2	969	647	0.12%	0.011%
54	20.638	2910	2911	2913	rBV2	1240	1167	0.21%	0.019%
55	20.691	2918	2920	2921	rVV2	1015	623	0.11%	0.010%
56	20.838	2943	2945	2946	rBV2	1214	949	0.17%	0.015%
57	20.914	2955	2958	2960	rBV4	1259	1824	0.33%	0.030%
58	20.961	2964	2966	2967	rVV2	1456	1401	0.26%	0.023%
59	20.990	2969	2971	2975	rBV5	1696	2691	0.49%	0.044%
60	21.061	2982	2983	2986	rBV3	1998	1598	0.29%	0.026%
61	21.143	2995	2997	3000	rBV3	1324	1120	0.21%	0.018%
62	21.942	3129	3133	3137	rVB4	5287	7930	1.45%	0.129%
63	22.042	3143	3150	3157	rVB2	220857	389352	71.37%	6.343%
64	22.735	3264	3268	3275	rVB4	14422	23659	4.34%	0.385%
65	23.563	3407	3409	3411	rBV3	2378	1923	0.35%	0.031%
66	23.663	3419	3426	3433	rVB2	30280	63298	11.60%	1.031%
67	24.068	3493	3495	3497	rVB3	2517	1774	0.33%	0.029%
68	24.092	3497	3499	3500	rBV	1933	1645	0.30%	0.027%
69	24.168	3510	3512	3514	rBV3	2197	2209	0.40%	0.036%
70	24.433	3555	3557	3559	rBV3	2650	3304	0.61%	0.054%
71	24.779	3607	3616	3625	rBV3	40772	119795	21.96%	1.952%
72	24.879	3632	3633	3634	rBV	2939	1061	0.19%	0.017%
73	25.314	3696	3707	3717	rBV2	171915	488404	89.52%	7.956%
74	25.472	3732	3734	3738	rBV4	2720	3682	0.67%	0.060%
75	25.555	3739	3748	3759	rVB	121603	361983	66.35%	5.897%
76	25.889	3803	3805	3806	rBV2	1840	1212	0.22%	0.020%

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77	25.954	3814	3816	3819	rVB3	2292	1966	0.36%	0.032%
78	25.995	3821	3823	3824	rVV2	2191	1245	0.23%	0.020%
79	26.154	3840	3850	3863	rVB5	51741	180443	33.08%	2.940%
80	26.359	3883	3885	3888	rBV5	2143	1387	0.25%	0.023%
81	27.264	4037	4039	4042	rBV4	2192	2386	0.44%	0.039%
82	27.881	4131	4144	4160	rVB3	56148	241988	44.36%	3.942%
83	28.363	4224	4226	4227	rBV2	2049	1695	0.31%	0.028%
84	28.445	4238	4240	4241	rBV	1821	1737	0.32%	0.028%
85	28.609	4266	4268	4269	rVB2	2150	1098	0.20%	0.018%
86	28.809	4300	4302	4303	rVB2	2415	1310	0.24%	0.021%
87	29.308	4385	4387	4388	rBV2	2497	1901	0.35%	0.031%
88	29.731	4457	4459	4462	rVB3	2442	2060	0.38%	0.034%
89	30.037	4499	4511	4514	rBV4	43921	141583	25.95%	2.306%
90	30.889	4654	4656	4661	rBV5	2120	3037	0.56%	0.049%
91	30.930	4661	4663	4664	rBV2	1805	1495	0.27%	0.024%
92	30.983	4670	4672	4674	rBV3	1419	947	0.17%	0.015%
93	31.006	4674	4676	4677	rBV	1757	1124	0.21%	0.018%
94	31.887	4825	4826	4830	rBV4	3131	3069	0.56%	0.050%
95	32.022	4844	4849	4851	rBV5	2109	4279	0.78%	0.070%
96	32.081	4858	4859	4862	rBV3	1820	1197	0.22%	0.019%
97	32.122	4862	4866	4867	rBV4	2886	3354	0.61%	0.055%
98	32.181	4875	4876	4877	rVB	2599	916	0.17%	0.015%
99	32.199	4877	4879	4881	rBV3	1749	1046	0.19%	0.017%
100	32.363	4905	4907	4908	rBV2	1956	894	0.16%	0.015%

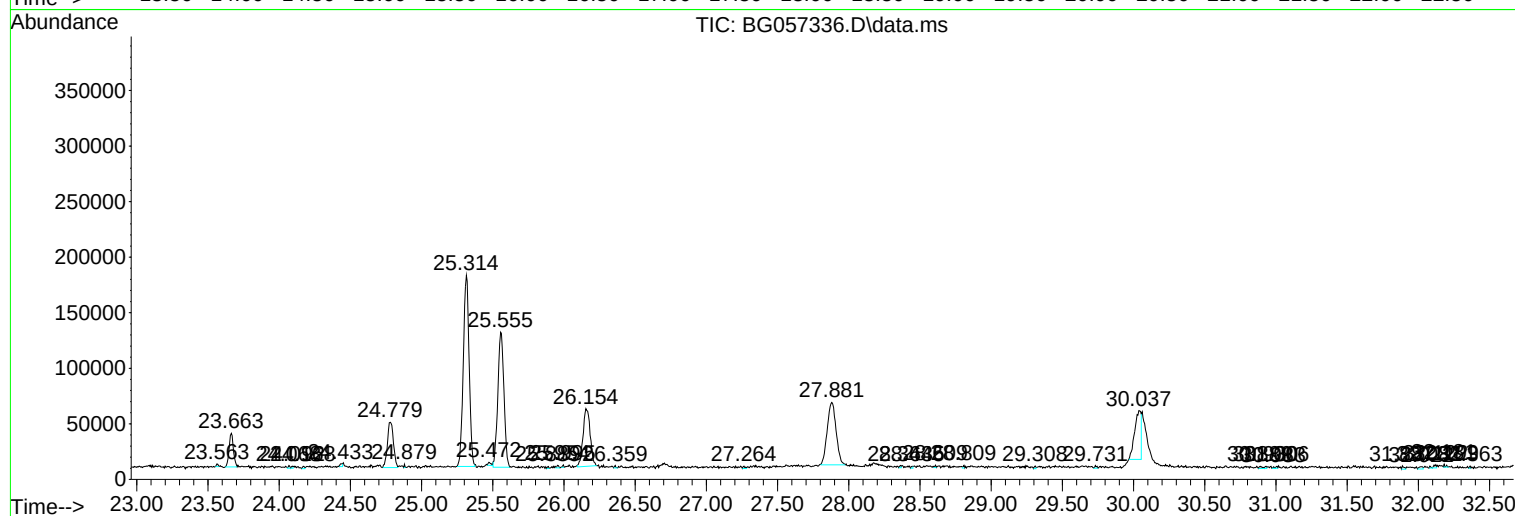
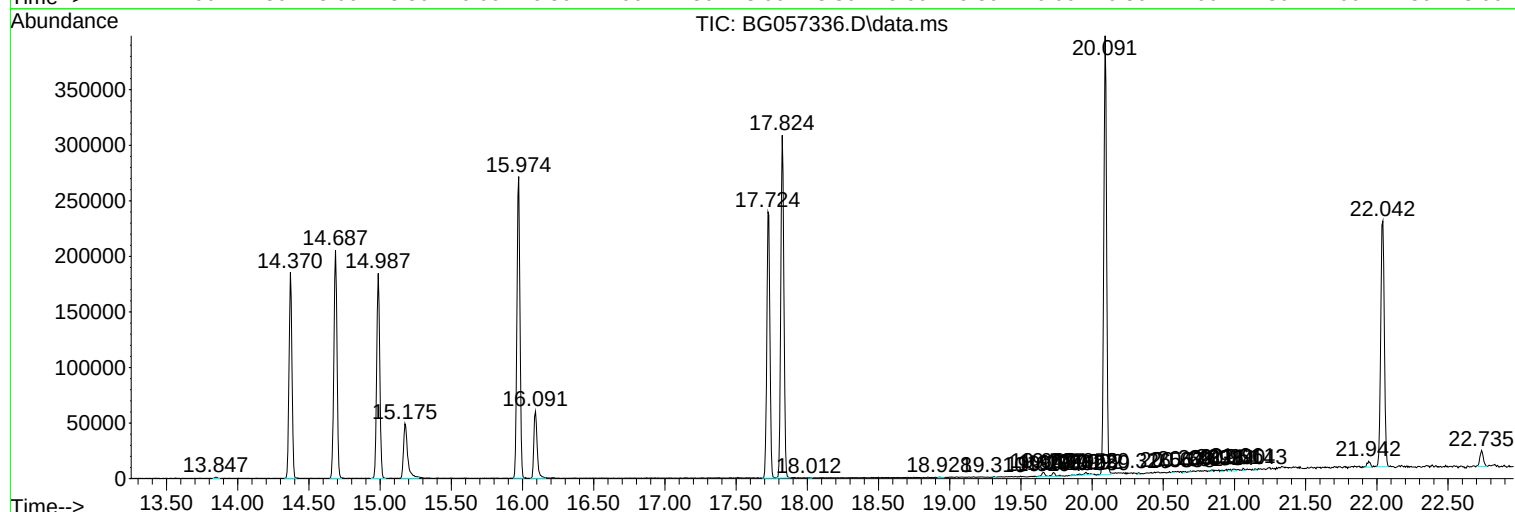
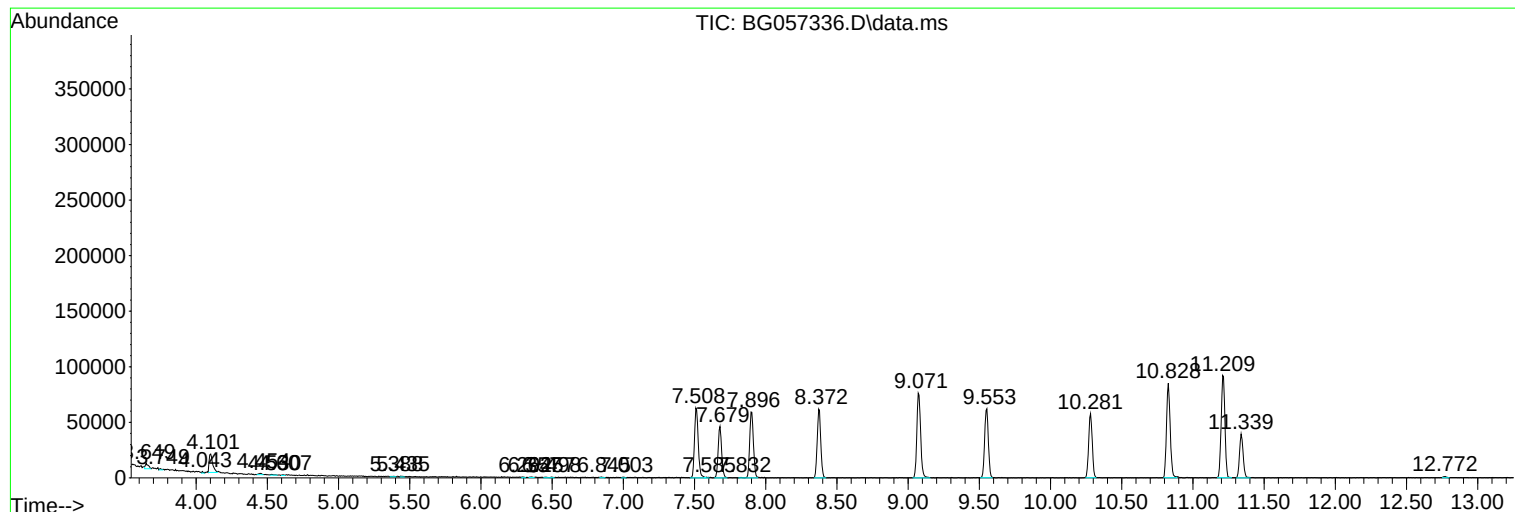
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

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



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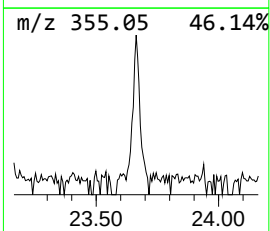
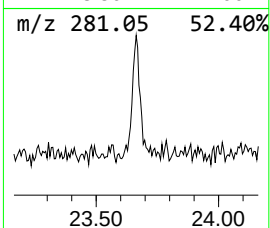
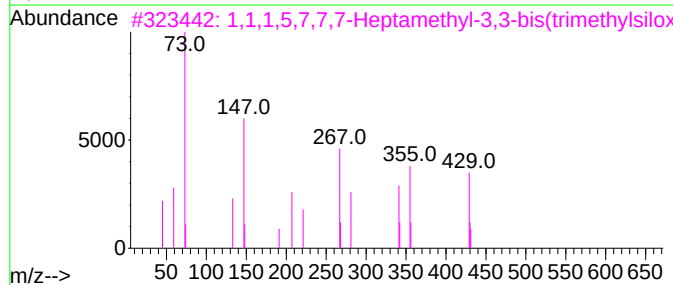
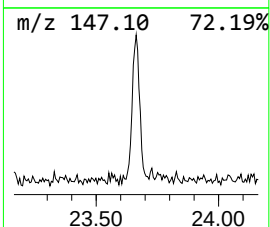
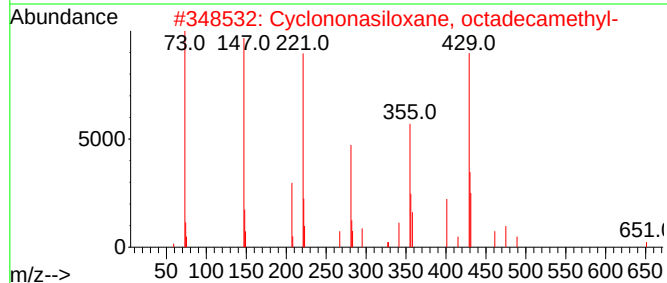
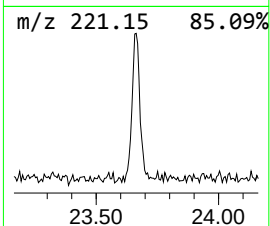
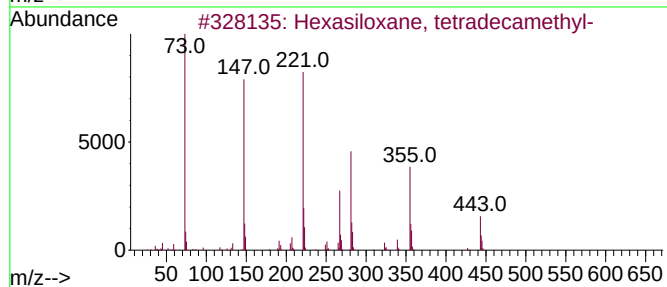
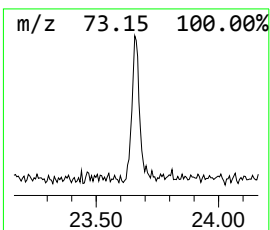
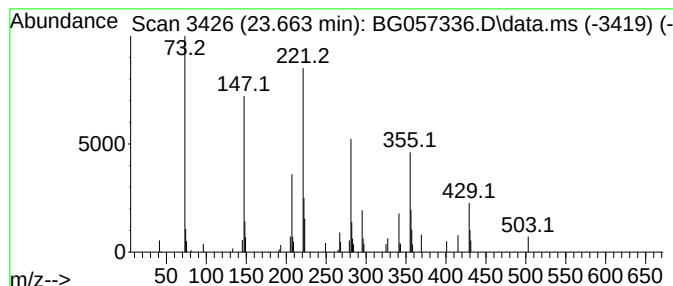
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Hexasiloxane, tetradecamethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.663	3.25 ng/ul	63298	Chrysene-d12	22.042

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	37
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	25
5			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	25



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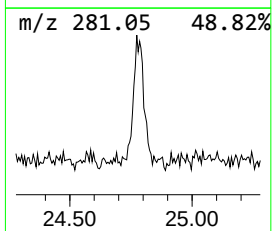
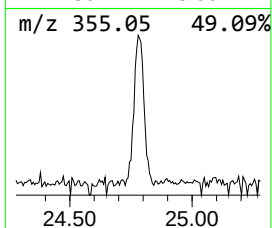
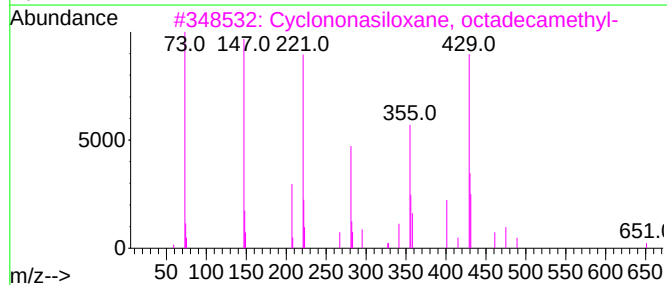
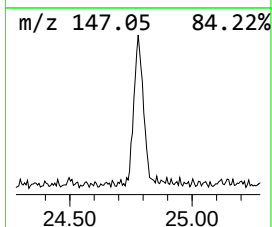
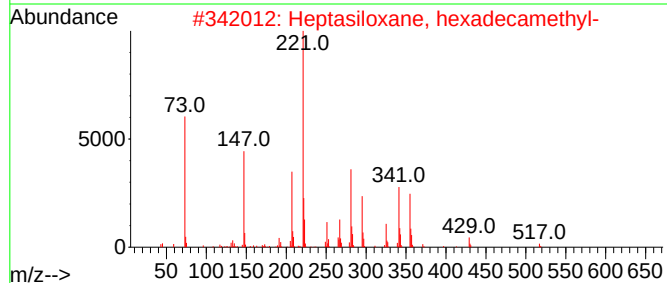
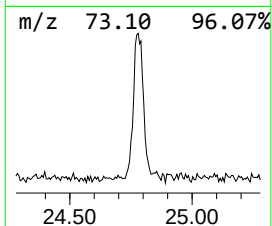
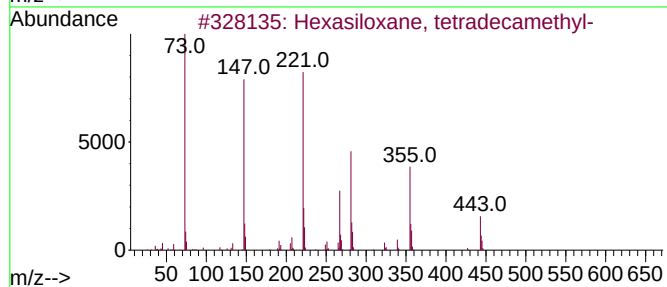
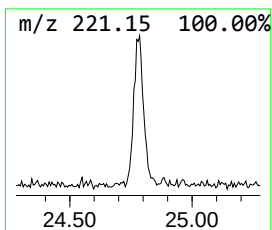
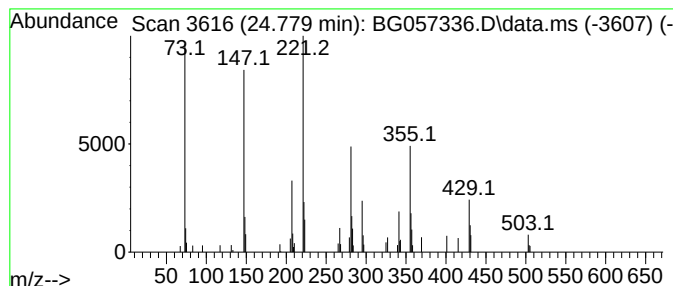
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 Heptasiloxane, hexadecamethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.779	6.62 ng/ul	119795	Perylene-d12	25.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	74
2			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	58
3			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	40
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37
5			2,3-Dimercaptobutane-1,4-diol, 4TMS	442	C16H42O2S2Si4	959295-06-8	35



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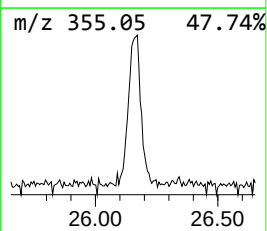
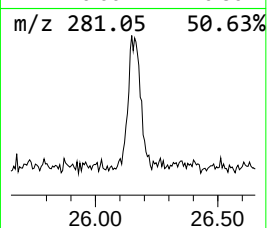
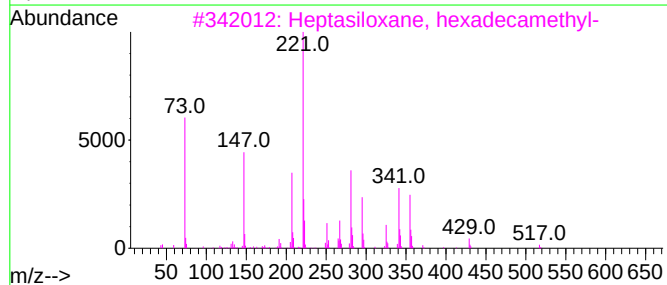
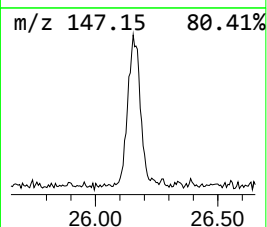
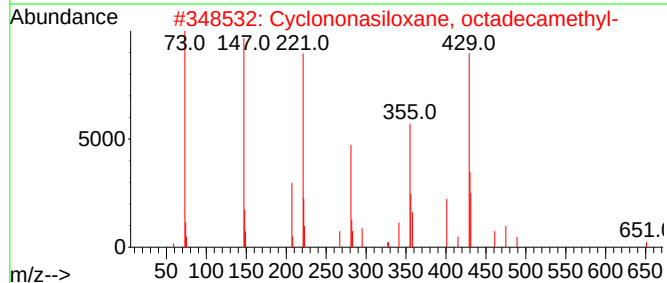
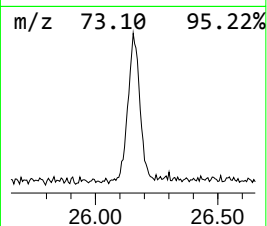
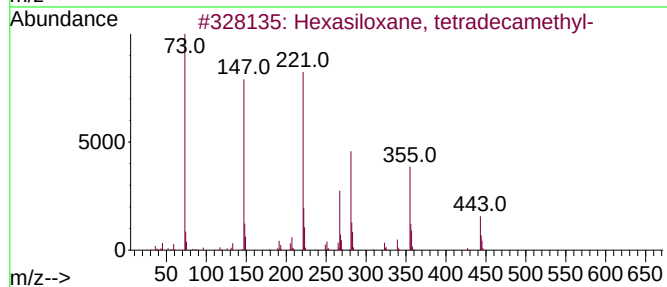
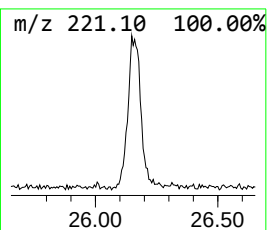
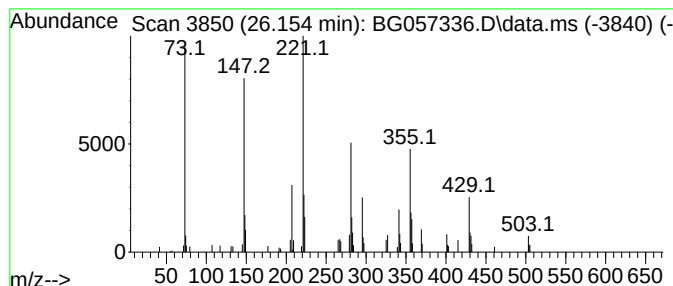
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Cyclononasiloxane, octadeca... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.154	9.97 ng/ul	180443	Perylene-d12	25.555

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	72
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	47
4			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	38
5			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050823\
Data File : BG057336.D
Acq On : 8 May 2023 18:48
Operator : CG/JU
Sample : PB152657BL
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SBLK657

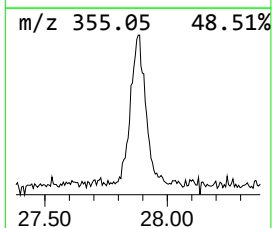
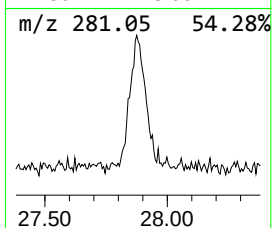
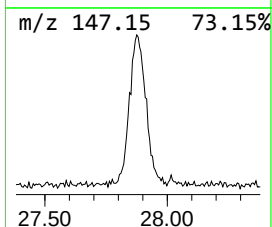
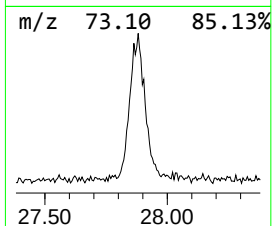
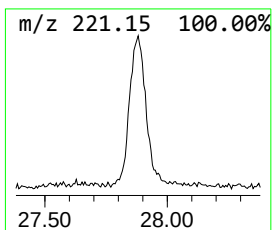
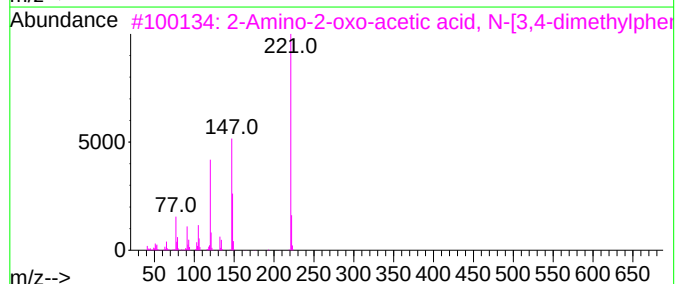
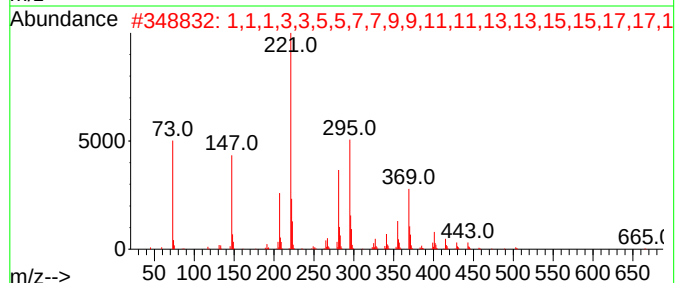
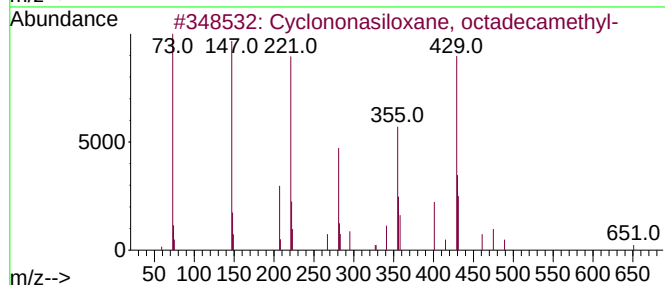
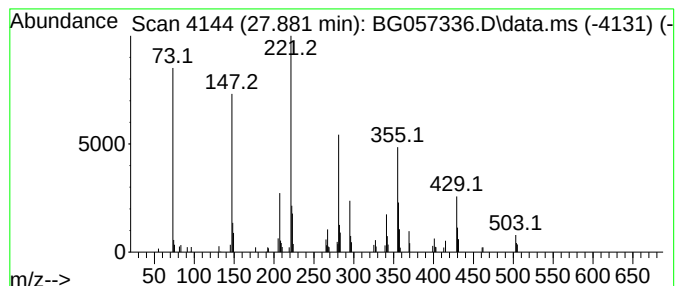
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.881	13.37 ng/ul	241988	Perylene-d12	25.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	59
2			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	680	C20H60O8Si9	002652-13-3	38
3			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	38
4			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	32
5			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050823\
Data File : BG057336.D
Acq On : 8 May 2023 18:48
Operator : CG/JU
Sample : PB152657BL
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SBLK657

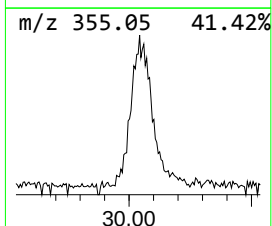
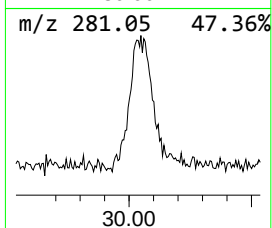
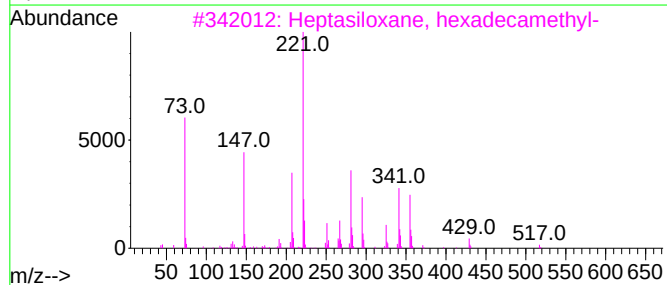
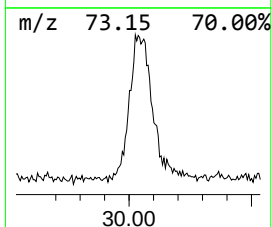
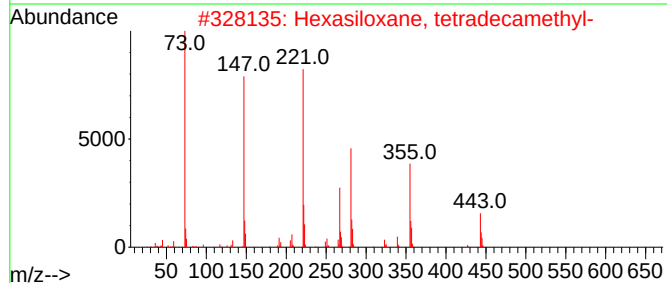
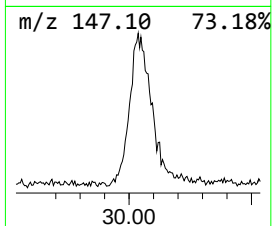
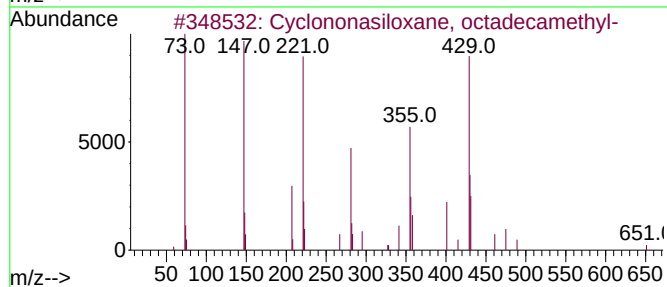
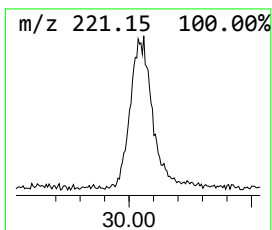
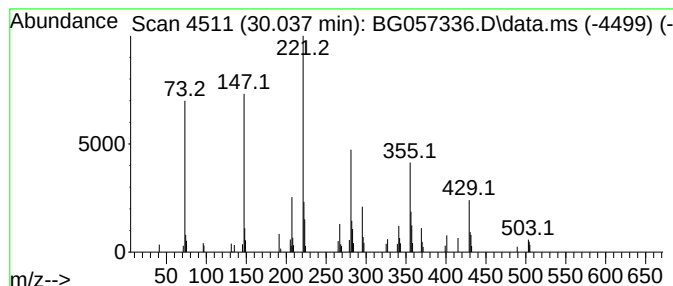
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Quant Title : SVOA CALIBRATION

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.
30.037	7.82 ng/ul	141583	Perylene-d12	25.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	53
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	50
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	46
4			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	37
5			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050823\
Data File : BG057336.D
Acq On : 8 May 2023 18:48
Operator : CG/JU
Sample : PB152657BL
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SBLK657

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

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...	23.663	3.3	ng/ul	63298	5	22.042	389352	20.0
Heptasiloxane, ...	24.779	6.6	ng/ul	119795	6	25.555	361983	20.0
Cyclononasiloxa...	26.154	10.0	ng/ul	180443	6	25.555	361983	20.0
unknown-01	27.881	13.4	ng/ul	241988	6	25.555	361983	20.0
unknown-02	30.037	7.8	ng/ul	141583	6	25.555	361983	20.0