

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071323\
 Data File : BG058265.D
 Acq On : 15 Jul 2023 17:25
 Operator : CG/JU
 Sample : 03457-02
 Misc :
 ALS Vial : 76 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C0C52

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-BG070123.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG058265.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.751	109	113	124	rVB	47234	79831	5.51%	0.527%
2	3.992	150	154	158	rVB5	4901	6978	0.48%	0.046%
3	4.086	168	170	175	rVB4	3293	3271	0.23%	0.022%
4	5.003	321	326	331	rVB4	3967	7389	0.51%	0.049%
5	6.636	600	604	607	rVB3	1212	1582	0.11%	0.010%
6	7.065	671	677	684	rBV	33092	56294	3.89%	0.372%
7	7.230	698	705	719	rBV	127902	218286	15.06%	1.442%
8	7.435	733	740	749	rBV	126073	219898	15.18%	1.453%
9	7.512	752	753	760	rVB3	1619	2354	0.16%	0.016%
10	7.899	813	819	827	rVV	149404	254497	17.56%	1.681%
11	8.604	933	939	953	rVV	99607	183931	12.69%	1.215%
12	9.063	1009	1017	1031	rBV	155259	294439	20.32%	1.945%
13	9.785	1131	1140	1149	rBV	120935	225002	15.53%	1.486%
14	10.326	1224	1232	1241	rBV	188564	354378	24.46%	2.341%
15	10.702	1289	1296	1305	rBV	246865	437462	30.19%	2.890%
16	10.837	1312	1319	1336	rBV	185907	362194	25.00%	2.393%
17	11.507	1426	1433	1435	rBV	1087	1504	0.10%	0.010%
18	11.630	1449	1454	1455	rBV3	1928	2709	0.19%	0.018%
19	12.218	1547	1554	1561	rBV	48659	79589	5.49%	0.526%
20	12.282	1563	1565	1574	rVB2	5061	8179	0.56%	0.054%
21	13.422	1755	1759	1764	rVB2	6226	9615	0.66%	0.064%
22	13.939	1841	1847	1856	rBV	409541	610100	42.11%	4.031%
23	14.233	1889	1897	1910	rVV	476562	774735	53.47%	5.118%
24	14.539	1942	1949	1958	rBV	434080	679588	46.90%	4.490%
25	14.744	1980	1984	1994	rBV4	15992	40355	2.79%	0.267%
26	14.944	2014	2018	2026	rBV3	14263	21941	1.51%	0.145%
27	15.185	2056	2059	2062	rVB2	1748	1991	0.14%	0.013%
28	15.320	2078	2082	2083	rBV	1633	1703	0.12%	0.011%
29	15.344	2085	2086	2090	rVB	2146	2011	0.14%	0.013%
30	15.532	2111	2118	2129	rBV	634522	991321	68.41%	6.549%
31	15.649	2132	2138	2146	rBV	152160	231268	15.96%	1.528%
32	15.761	2155	2157	2159	rBV3	2443	2696	0.19%	0.018%
33	15.955	2184	2190	2193	rVB2	769	1471	0.10%	0.010%
34	17.024	2370	2372	2378	rBV3	5739	7614	0.53%	0.050%
35	17.077	2378	2381	2383	rVB3	1862	2188	0.15%	0.014%
36	17.130	2389	2390	2394	rVB2	1534	1592	0.11%	0.011%

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37	17.282	2410	2416	2425	rBV	580779	871448	60.14%	5.757%
38	17.382	2426	2433	2442	rBV	715643	1114232	76.90%	7.361%
39	17.559	2460	2463	2467	rVB3	1781	2551	0.18%	0.017%
40	17.688	2482	2485	2490	rBV5	1691	1946	0.13%	0.013%
41	17.946	2524	2529	2532	rBV3	3235	4602	0.32%	0.030%
42	18.164	2561	2566	2574	rBV3	25052	44158	3.05%	0.292%
43	18.240	2577	2579	2584	rVB3	4295	4434	0.31%	0.029%
44	18.892	2689	2690	2695	rVV4	1543	2101	0.14%	0.014%
45	19.104	2725	2726	2730	rVB2	1318	1486	0.10%	0.010%
46	19.168	2735	2737	2741	rVB4	1598	1505	0.10%	0.010%
47	19.233	2741	2748	2754	rBV3	11067	18814	1.30%	0.124%
48	19.310	2754	2761	2764	rBV	13701	23651	1.63%	0.156%
49	19.439	2779	2783	2790	rBV4	13317	24350	1.68%	0.161%
50	19.586	2804	2808	2813	rVB5	8095	9888	0.68%	0.065%
51	19.668	2816	2822	2837	rBV	869819	1355084	93.52%	8.952%
52	19.973	2872	2874	2876	rVB3	1770	1652	0.11%	0.011%
53	20.026	2882	2883	2886	rBV2	2105	1729	0.12%	0.011%
54	20.103	2894	2896	2899	rBV4	1829	2055	0.14%	0.014%
55	20.414	2946	2949	2951	rBV4	2188	2937	0.20%	0.019%
56	20.438	2951	2953	2956	rVB4	1879	2190	0.15%	0.014%
57	20.502	2962	2964	2968	rVB4	2947	2948	0.20%	0.019%
58	20.584	2974	2978	2980	rVV4	5042	5929	0.41%	0.039%
59	20.626	2982	2985	2990	rVB4	8309	9675	0.67%	0.064%
60	20.867	3023	3026	3031	rVV3	11492	12940	0.89%	0.085%
61	20.925	3034	3036	3037	rVB2	3227	1490	0.10%	0.010%
62	21.137	3070	3072	3077	rBV6	3622	7048	0.49%	0.047%
63	21.419	3116	3120	3124	rVB2	11761	17126	1.18%	0.113%
64	21.530	3132	3139	3151	rBV	567405	994066	68.60%	6.567%
65	21.713	3167	3170	3174	rVB3	8921	11224	0.77%	0.074%
66	22.241	3254	3260	3265	rBV2	52654	91298	6.30%	0.603%
67	22.300	3267	3270	3276	rVB5	14841	25384	1.75%	0.168%
68	22.447	3294	3295	3298	rVB3	4463	2224	0.15%	0.015%
69	22.882	3367	3369	3370	rBV2	3204	1876	0.13%	0.012%
70	22.970	3378	3384	3391	rVB3	28145	62094	4.29%	0.410%
71	23.076	3395	3402	3412	rBV2	67168	153902	10.62%	1.017%
72	23.481	3469	3471	3473	rBV2	2700	2044	0.14%	0.014%
73	23.751	3510	3517	3525	rVB3	35863	80582	5.56%	0.532%
74	24.080	3565	3573	3584	rBV2	75331	198694	13.71%	1.313%
75	24.456	3626	3637	3655	rBV2	503310	1448993	100.00%	9.573%
76	24.674	3663	3674	3690	rBV	410050	1176968	81.23%	7.775%

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77	25.150	3753	3755	3756	rBV	3231	1547	0.11%	0.010%
78	25.302	3772	3781	3797	rBV3	68841	234580	16.19%	1.550%
79	25.761	3850	3859	3868	rBV2	58689	171728	11.85%	1.134%
80	26.019	3897	3903	3916	rVB	16678	51365	3.54%	0.339%
81	26.836	4031	4042	4056	rBV4	48711	214069	14.77%	1.414%
82	27.000	4068	4070	4071	rBV2	4093	2327	0.16%	0.015%
83	27.071	4073	4082	4096	rVB3	58809	213715	14.75%	1.412%
84	28.646	4341	4350	4351	rBV	41667	89730	6.19%	0.593%
85	30.303	4630	4632	4634	rBV3	3290	4105	0.28%	0.027%
86	30.555	4666	4675	4690	rVB4	36151	170469	11.76%	1.126%
87	31.666	4860	4864	4867	rBV5	3708	5981	0.41%	0.040%

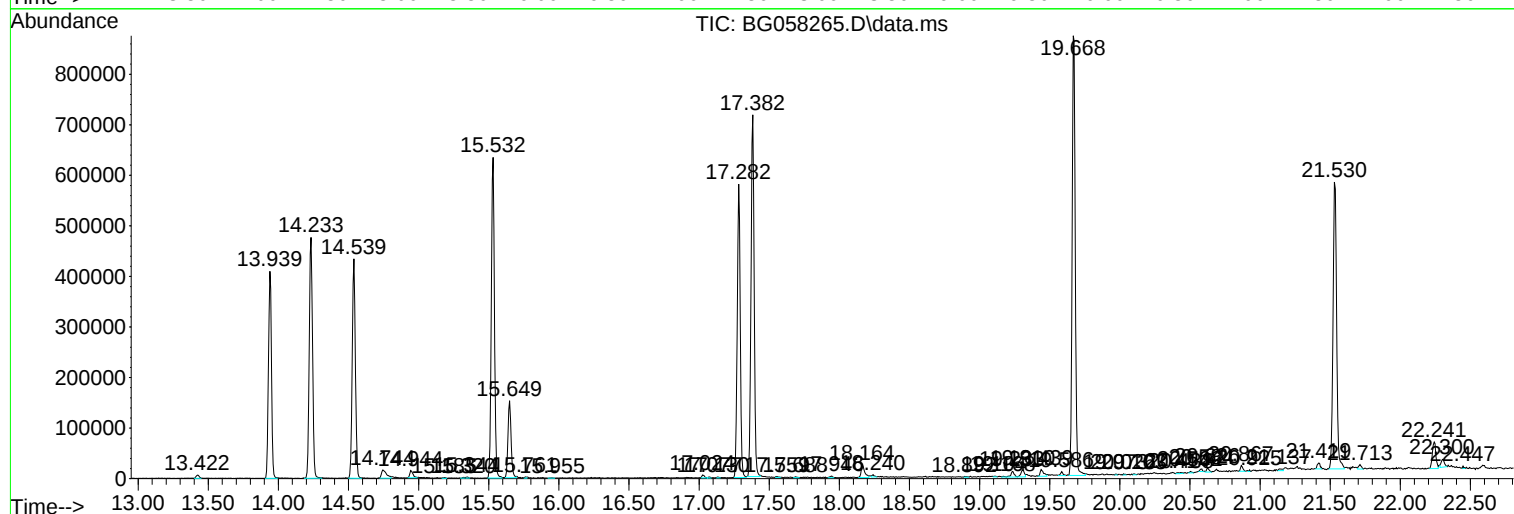
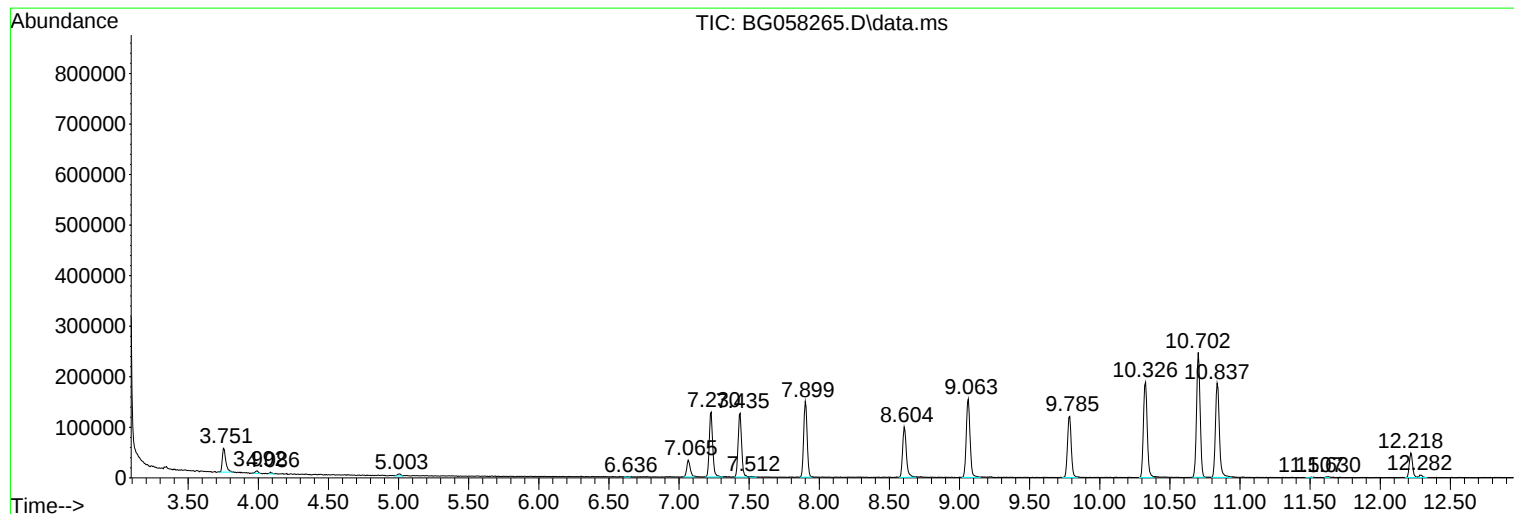
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

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



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ALS Vial : 76 Sample Multiplier: 1

Instrument :
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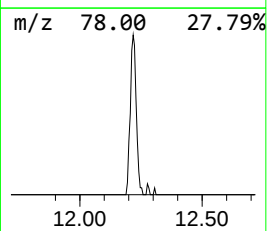
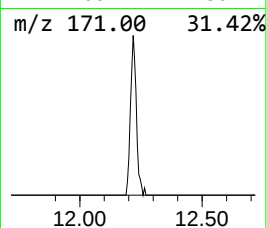
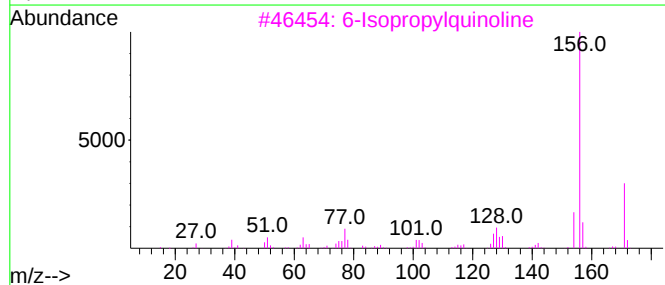
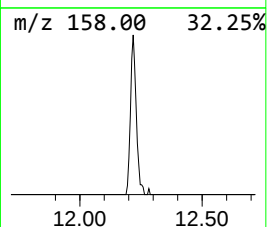
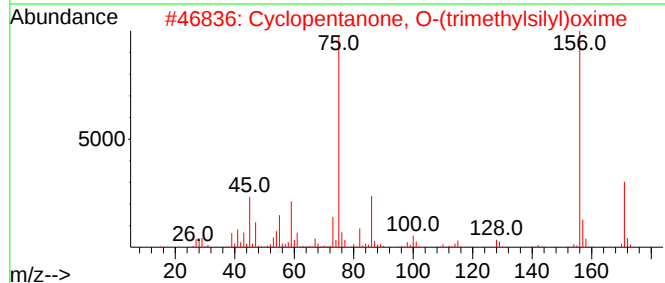
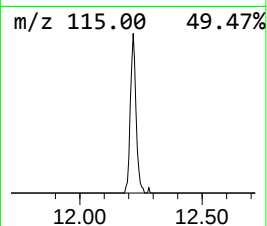
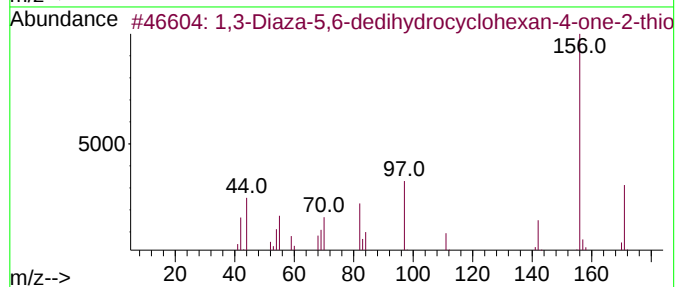
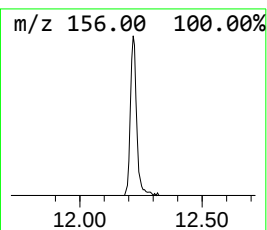
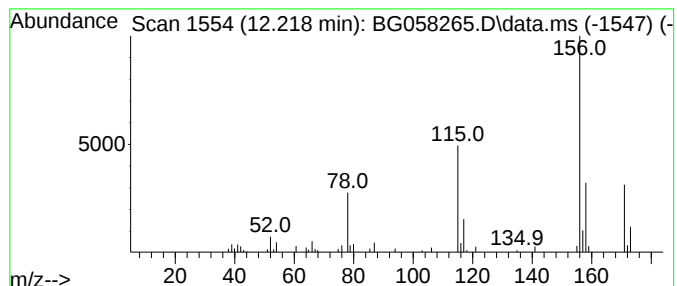
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.218	3.64 ng/ul	79589	Naphthalene-d8	10.702

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Diaza-5,6-dedihydrocyclohexa...	171	C6H9N3OS	021263-85-4	38
2			Cyclopentanone, O-(trimethylsilyl...	171	C8H17NOSi	026208-87-7	38
3			6-Isopropylquinoline	171	C12H13N	000135-79-5	38
4			1,2,3,4-Tetrahydropentalene, 1,1...	171	C12H13N	1000217-18-6	37
5			Tebuthiuron	228	C9H16N4OS	034014-18-1	37



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Misc :
ALS Vial : 76 Sample Multiplier: 1

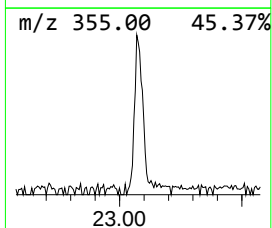
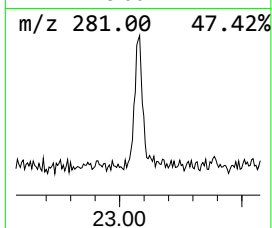
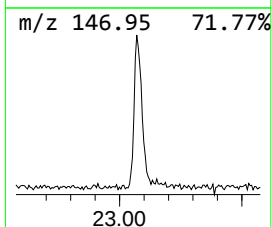
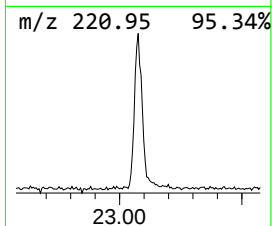
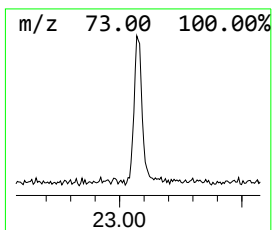
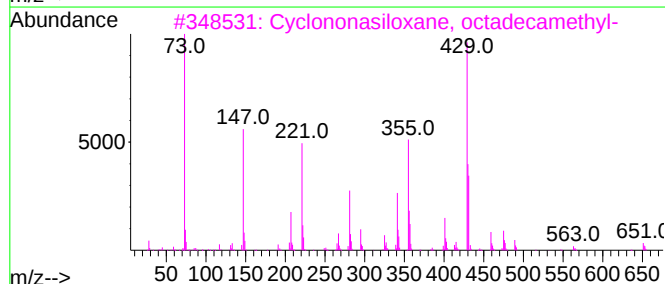
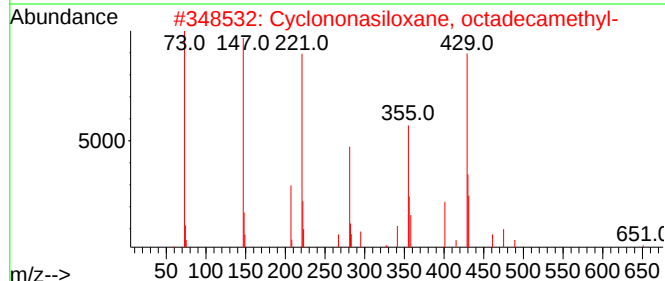
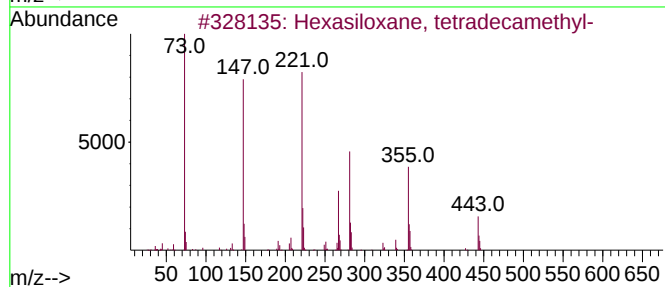
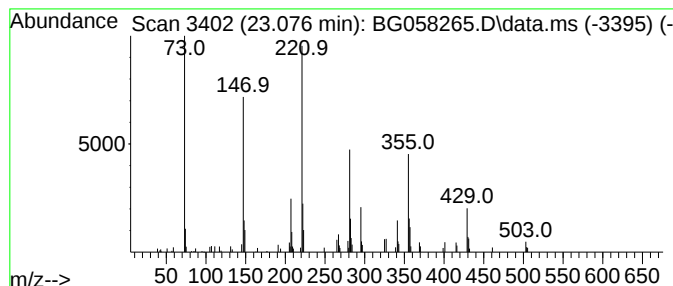
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Hexasiloxane, tetradecamethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.076	3.10 ng/ul	153902	Chrysene-d12	21.536	
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	59
3	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	32
4	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	32
5	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	30



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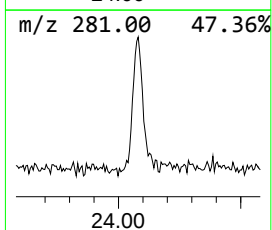
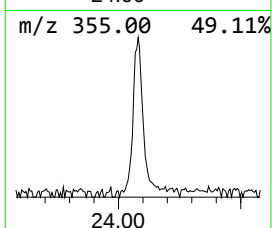
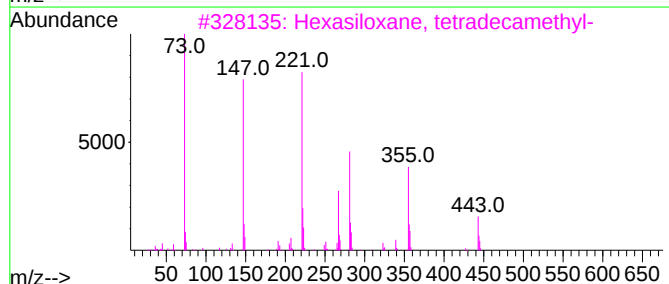
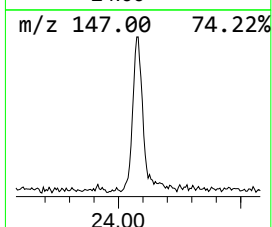
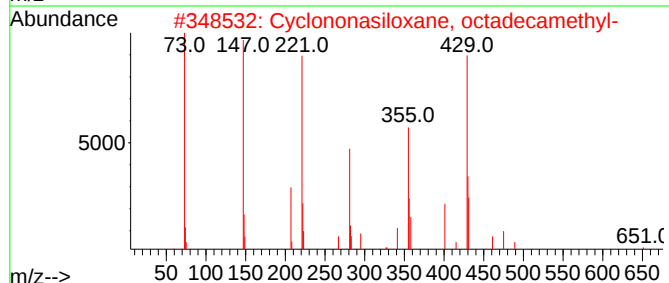
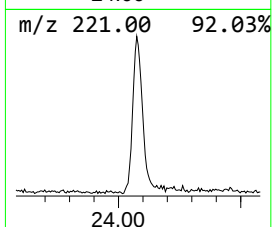
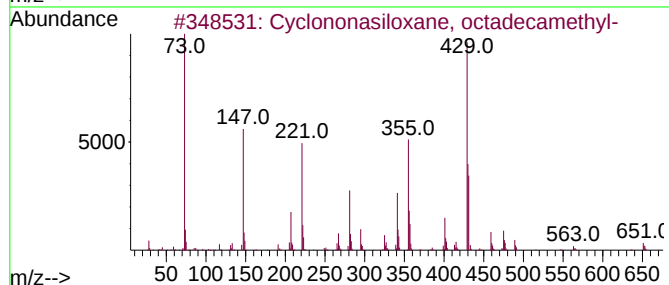
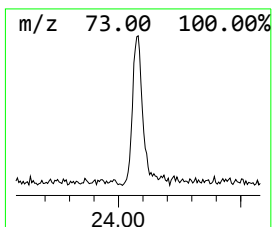
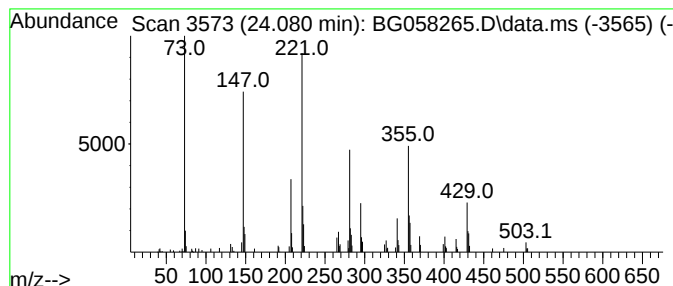
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Cyclononasiloxane, octadeca... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.080	3.38 ng/ul	198694	Perylene-d12	24.674

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	80
2		Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	53
3		Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	50
4		2,3-Dimercaptobutane-1,4-diol, 4TMS	442	C16H42O2S2Si4	959295-06-8	37
5		3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	27



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ClientSampleId :
C0C52

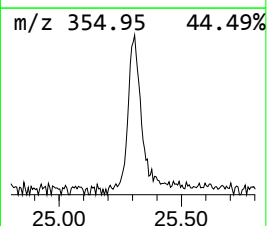
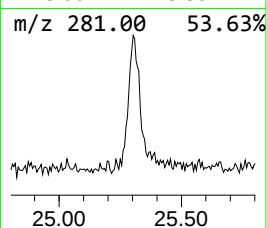
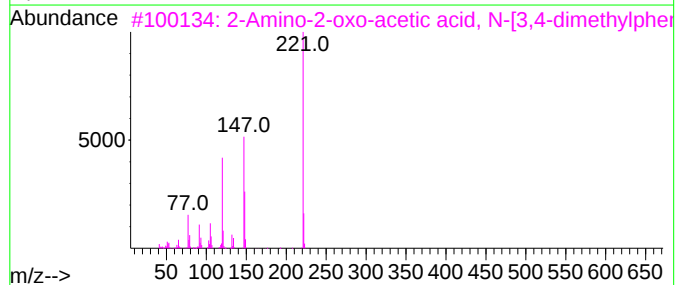
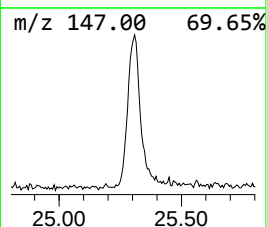
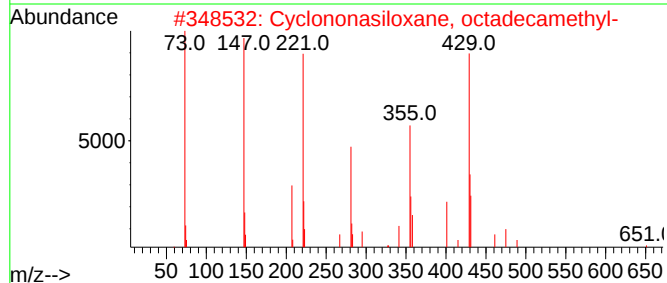
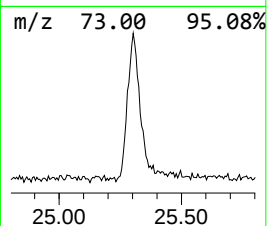
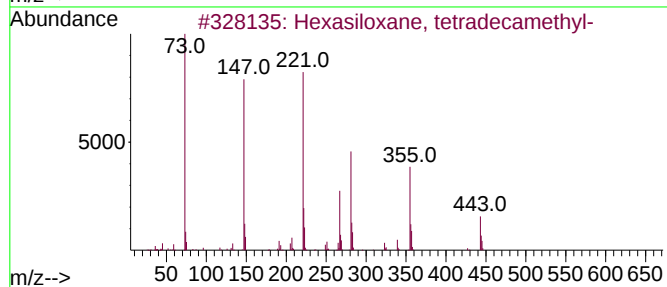
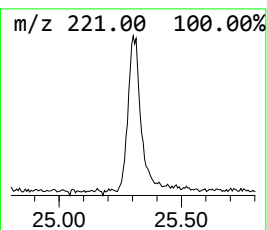
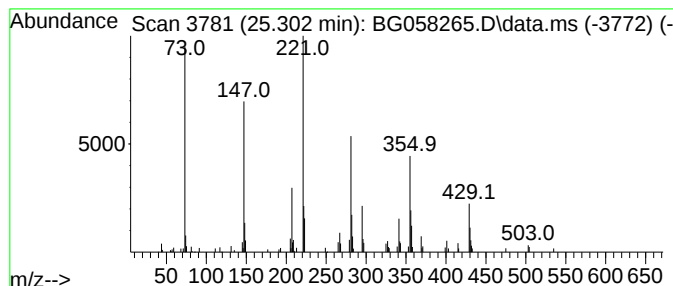
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.302	3.99 ng/ul	234580	Perylene-d12	24.674

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	38
3			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	35
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	32
5			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071323\
Data File : BG058265.D
Acq On : 15 Jul 2023 17:25
Operator : CG/JU
Sample : 03457-02
Misc :
ALS Vial : 76 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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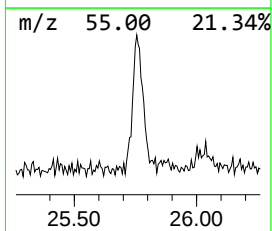
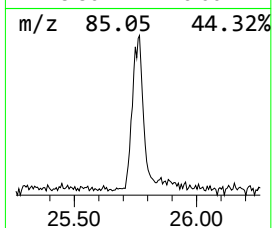
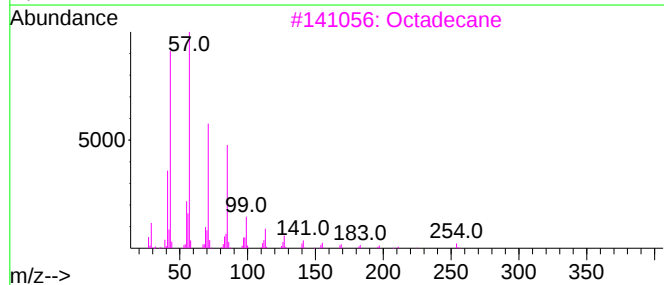
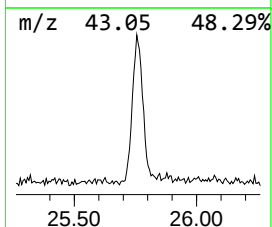
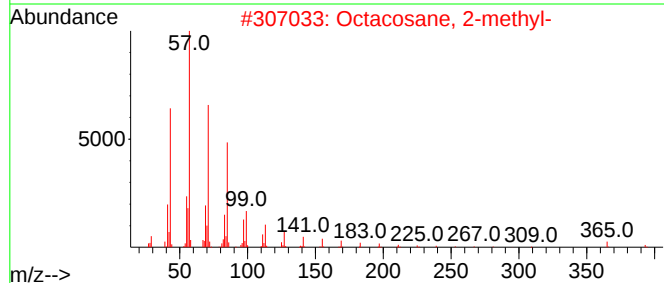
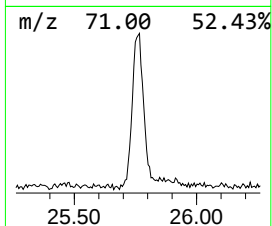
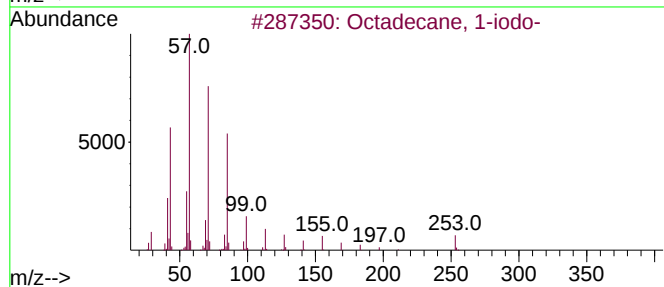
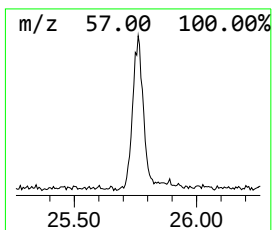
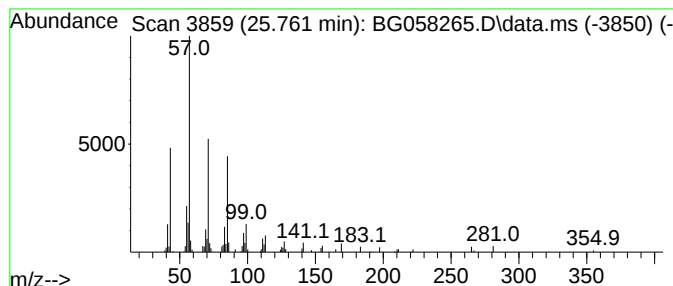
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Octadecane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.761	2.92 ng/ul	171728	Perylene-d12	24.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
3			Octadecane	254	C18H38	000593-45-3	87
4			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
5			triacontane	422	C30H62	000638-68-6	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071323\
Data File : BG058265.D
Acq On : 15 Jul 2023 17:25
Operator : CG/JU
Sample : 03457-02
Misc :
ALS Vial : 76 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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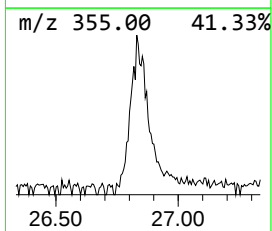
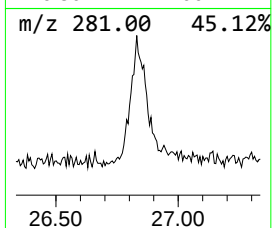
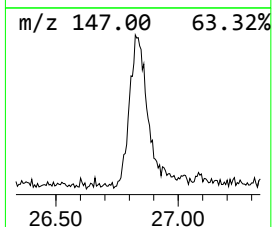
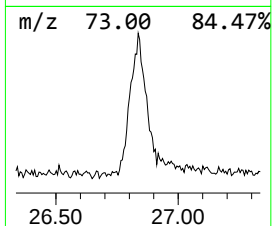
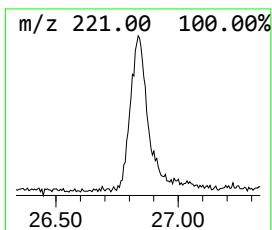
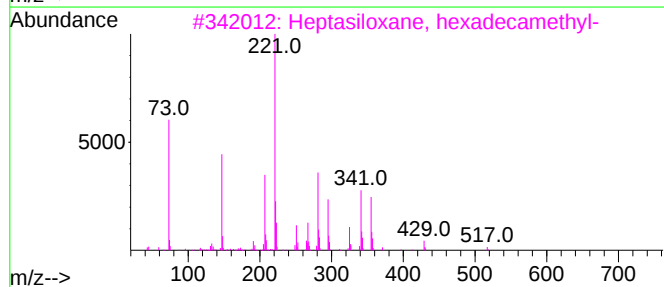
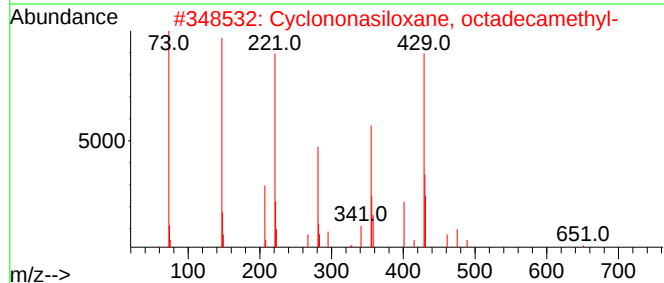
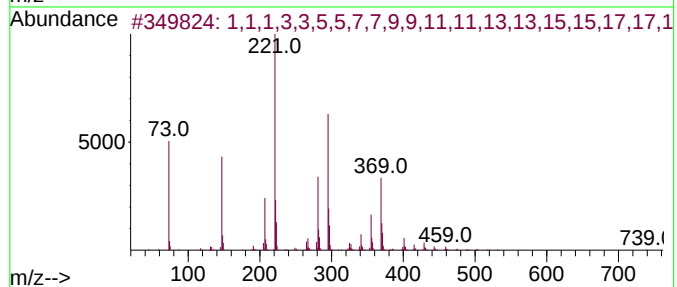
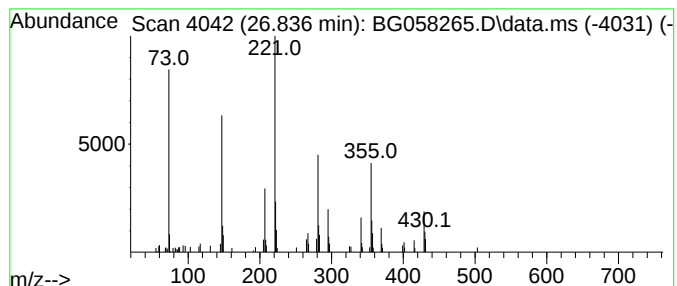
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 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.
26.836	3.64 ng/ul	214069	Perylene-d12	24.674

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...		754	C22H66O9Si10	000556-70-7	59
2	Cyclononasiloxane, octadecamethyl-		666	C18H54O9Si9	000556-71-8	47
3	Heptasiloxane, hexadecamethyl-		532	C16H48O6Si7	000541-01-5	40
4	2,6-Dimethyl-3,4-bis(trimethylsi...		311	C15H29N02Si2	1000079-52-1	38
5	Hexasiloxane, tetradecamethyl-		458	C14H42O5Si6	000107-52-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071323\
Data File : BG058265.D
Acq On : 15 Jul 2023 17:25
Operator : CG/JU
Sample : 03457-02
Misc :
ALS Vial : 76 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0C52

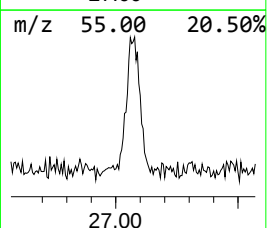
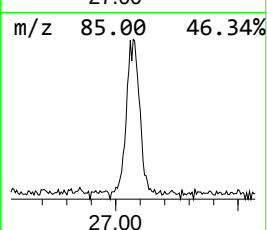
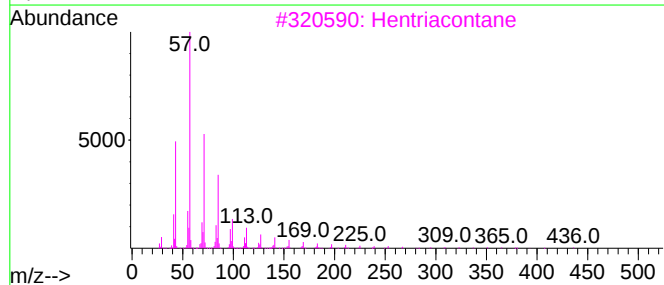
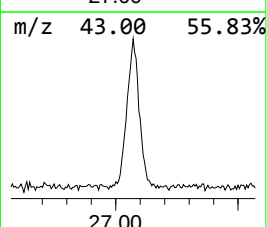
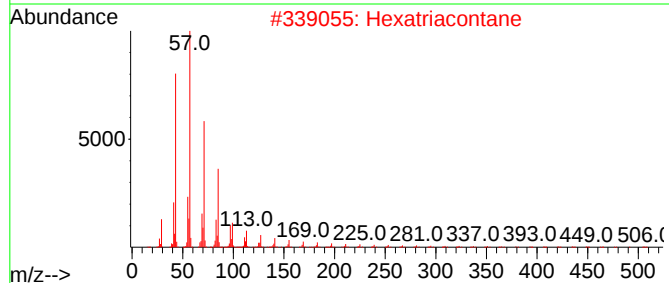
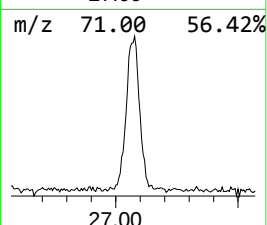
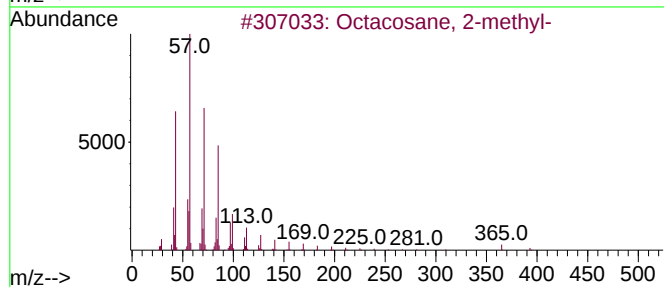
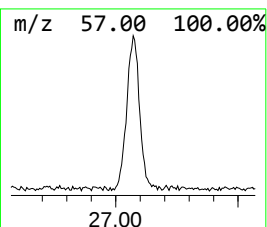
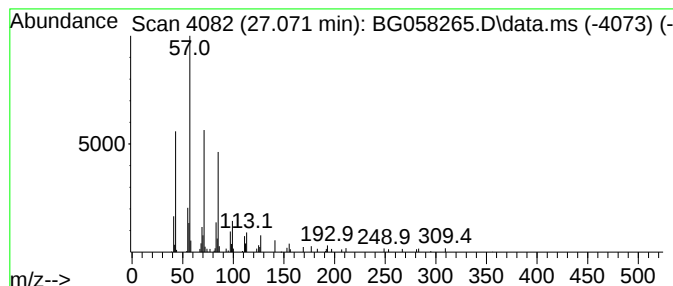
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.071	3.63 ng/ul	213715	Perylene-d12	24.674

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
2		Hexatriacontane	507	C36H74	000630-06-8	87
3		Hentriacontane	437	C31H64	000630-04-6	87
4		4-Methylheneicosane	310	C22H46	025117-29-7	87
5		Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071323\
Data File : BG058265.D
Acq On : 15 Jul 2023 17:25
Operator : CG/JU
Sample : 03457-02
Misc :
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Instrument :
BNA_G
ClientSampleId :
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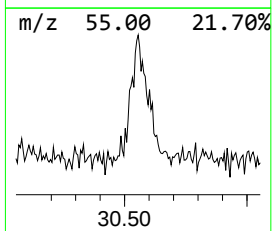
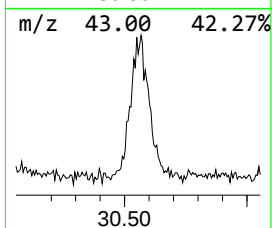
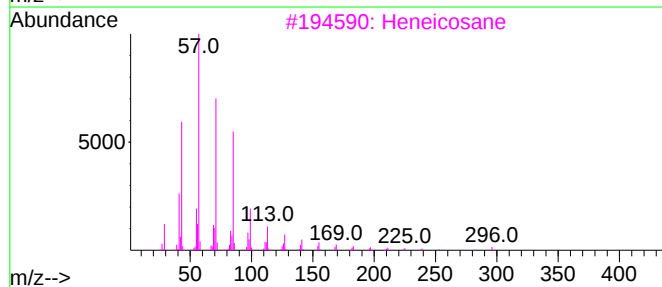
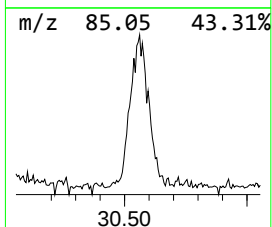
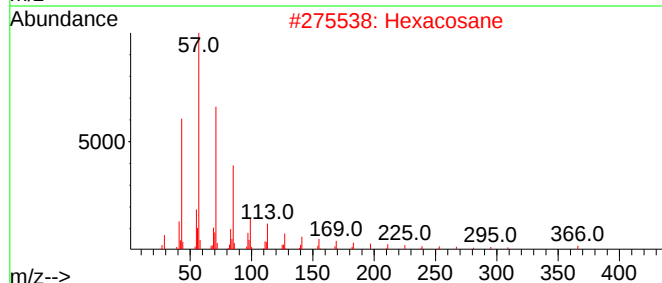
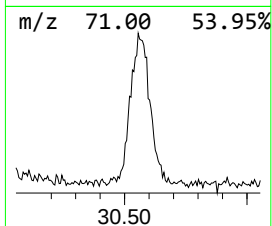
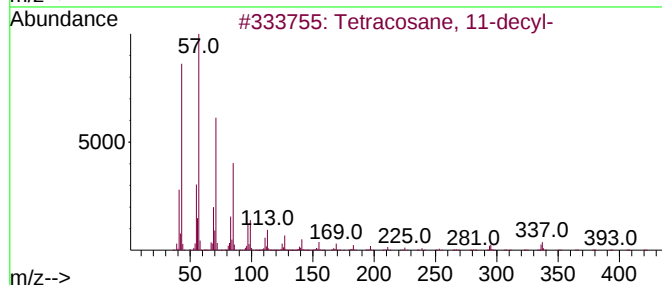
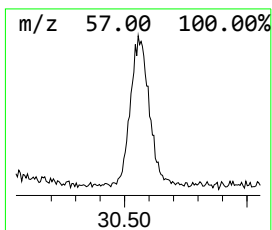
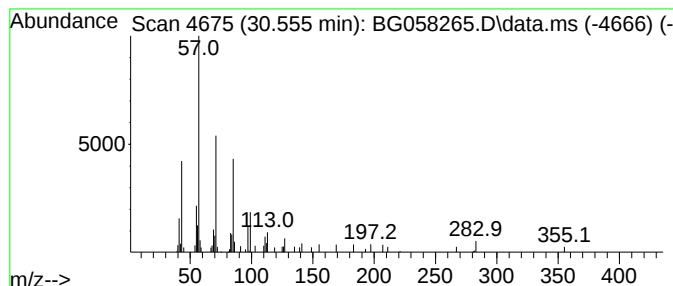
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.555	2.90 ng/ul	170469	Perylene-d12	24.674

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane, 11-decyl-	479	C34H70	055429-84-0	86
2		Hexacosane	366	C26H54	000630-01-3	83
3		Heneicosane	296	C21H44	000629-94-7	83
4		2-Bromotetradecane	276	C14H29Br	074036-95-6	80
5		Octadecane	254	C18H38	000593-45-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071323\
Data File : BG058265.D
Acq On : 15 Jul 2023 17:25
Operator : CG/JU
Sample : 03457-02
Misc :
ALS Vial : 76 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0C52

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST0.L
TIC Integration Parameters: LSCINT.P

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					#	RT	Resp	Conc
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Hexasiloxane, t...	23.076	3.1	ng/ul	153902	5	21.536	994066	20.0
Cyclononasiloxa...	24.080	3.4	ng/ul	198694	6	24.674	1176970	20.0
unknown-02	25.302	4.0	ng/ul	234580	6	24.674	1176970	20.0
Octadecane, 1-i...	25.761	2.9	ng/ul	171728	6	24.674	1176970	20.0
1,1,1,3,3,5,5,7...	26.836	3.6	ng/ul	214069	6	24.674	1176970	20.0
(DEL) Alkane: S...	27.071	3.6	ng/ul	213715	6	24.674	1176970	20.0
(DEL) Alkane: S...	30.555	2.9	ng/ul	170469	6	24.674	1176970	20.0