

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051023\
 Data File : BG057383.D
 Acq On : 11 May 2023 00:26
 Operator : CG/JU
 Sample : 02591-14
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 JREF0

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: BG057383.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.642	16	18	23	rBV2	1327	1623	0.48%	0.042%
2	3.942	66	69	76	rVB2	822	1383	0.41%	0.036%
3	4.341	135	137	140	rVV	1004	913	0.27%	0.024%
4	7.508	670	676	687	rBB2	31500	57745	17.02%	1.501%
5	7.666	698	703	711	rBB	25904	43985	12.97%	1.143%
6	7.895	735	742	749	rBB	33320	57303	16.89%	1.489%
7	8.365	815	822	829	rBB	59608	97580	28.77%	2.536%
8	9.064	935	941	951	rBV2	41635	71725	21.14%	1.864%
9	9.540	1016	1022	1031	rBB	35038	62215	18.34%	1.617%
10	10.275	1141	1147	1154	rBV	29907	53560	15.79%	1.392%
11	10.815	1233	1239	1250	rBV	44558	81804	24.12%	2.126%
12	11.203	1297	1305	1312	rBV	85620	148229	43.70%	3.852%
13	11.332	1320	1327	1338	rBV3	16698	30302	8.93%	0.788%
14	12.765	1566	1571	1573	rVV2	738	920	0.27%	0.024%
15	14.363	1836	1843	1850	rVB	99437	141515	41.72%	3.678%
16	14.675	1889	1896	1904	rVB	113420	172997	51.00%	4.496%
17	14.980	1940	1948	1954	rBV	155061	241333	71.15%	6.272%
18	15.180	1977	1982	1992	rBV2	13777	28448	8.39%	0.739%
19	15.961	2109	2115	2123	rVB	158856	227850	67.17%	5.922%
20	16.084	2131	2136	2145	rBV2	20376	34772	10.25%	0.904%
21	16.313	2170	2175	2180	rBV	16644	22720	6.70%	0.590%
22	17.717	2406	2414	2422	rBV	214052	318763	93.97%	8.284%
23	17.817	2424	2431	2440	rVV2	162831	251693	74.20%	6.541%
24	18.522	2546	2551	2553	rBV3	805	1228	0.36%	0.032%
25	18.569	2554	2559	2567	rVV6	4482	11883	3.50%	0.309%
26	18.634	2567	2570	2573	rVV3	2402	3363	0.99%	0.087%
27	19.456	2705	2710	2713	rBV3	1291	2311	0.68%	0.060%
28	19.550	2724	2726	2729	rBV3	1305	1685	0.50%	0.044%
29	19.644	2740	2742	2746	rVB3	2104	1984	0.58%	0.052%
30	19.715	2751	2754	2758	rBV4	3110	4003	1.18%	0.104%
31	19.762	2760	2762	2765	rBV3	1108	994	0.29%	0.026%
32	19.826	2770	2773	2774	rBV2	1202	1141	0.34%	0.030%
33	19.844	2774	2776	2779	rBV4	1524	1759	0.52%	0.046%
34	20.020	2803	2806	2809	rBV4	1673	2313	0.68%	0.060%
35	20.079	2809	2816	2824	rVV	223239	316639	93.35%	8.229%
36	20.191	2832	2835	2838	rBV2	1517	2220	0.65%	0.058%

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Start Thrs: 0.2

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Filtering: 5

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Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
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37	20.332	2858	2859	2863	rBV2	1583	1773	0.52%	0.046%
38	20.420	2869	2874	2875	rBV4	1294	1819	0.54%	0.047%
39	20.478	2880	2884	2885	rBV3	1182	1064	0.31%	0.028%
40	20.549	2890	2896	2901	rBV5	5470	8708	2.57%	0.226%
41	20.584	2901	2902	2904	rBV2	1422	1217	0.36%	0.032%
42	20.678	2916	2918	2919	rBV2	2157	1058	0.31%	0.027%
43	20.690	2919	2920	2921	rBV	1657	999	0.29%	0.026%
44	20.731	2924	2927	2928	rVV2	1439	1642	0.48%	0.043%
45	20.749	2928	2930	2932	rVB3	1366	1244	0.37%	0.032%
46	20.807	2939	2940	2942	rBV2	1523	903	0.27%	0.023%
47	20.890	2952	2954	2956	rBV2	1242	1214	0.36%	0.032%
48	20.990	2968	2971	2972	rBV3	1430	1358	0.40%	0.035%
49	21.048	2976	2981	2985	rBV5	6874	10519	3.10%	0.273%
50	21.089	2985	2988	2990	rVB3	1581	1811	0.53%	0.047%
51	21.177	3001	3003	3004	rBV	1938	1826	0.54%	0.047%
52	21.254	3014	3016	3018	rVB3	2165	1924	0.57%	0.050%
53	21.536	3062	3064	3066	rBV3	1837	1463	0.43%	0.038%
54	21.589	3068	3073	3084	rBV6	15799	49070	14.47%	1.275%
55	21.847	3115	3117	3125	rVB5	5355	6572	1.94%	0.171%
56	22.023	3141	3147	3159	rVB2	196490	339210	100.00%	8.816%
57	22.159	3167	3170	3173	rBV5	4527	5412	1.60%	0.141%
58	22.440	3216	3218	3219	rBV2	1664	1225	0.36%	0.032%
59	22.675	3256	3258	3260	rBV2	1718	1537	0.45%	0.040%
60	22.811	3276	3281	3286	rBV3	7893	11997	3.54%	0.312%
61	23.122	3332	3334	3335	rBV	1731	919	0.27%	0.024%
62	23.492	3395	3397	3399	rBV2	1899	1681	0.50%	0.044%
63	23.551	3404	3407	3415	rVB5	7636	14263	4.20%	0.371%
64	23.768	3437	3444	3450	rBV	31857	64491	19.01%	1.676%
65	23.938	3466	3473	3479	rBV3	26665	49864	14.70%	1.296%
66	24.256	3525	3527	3528	rBV	2481	1419	0.42%	0.037%
67	24.420	3549	3555	3562	rVB4	17917	40811	12.03%	1.061%
68	24.502	3565	3569	3570	rBV4	4649	5317	1.57%	0.138%
69	24.732	3606	3608	3614	rBV6	1827	3173	0.94%	0.082%
70	25.166	3680	3682	3683	rBV2	1569	999	0.29%	0.026%
71	25.290	3692	3703	3713	rBV	97853	279089	82.28%	7.253%
72	25.442	3727	3729	3734	rBV5	3590	6156	1.81%	0.160%
73	25.530	3734	3744	3755	rVV	106972	317599	93.63%	8.254%
74	25.619	3757	3759	3762	rBV4	1859	996	0.29%	0.026%
75	25.730	3776	3778	3779	rBV	1495	976	0.29%	0.025%
76	26.018	3823	3827	3828	rBV2	3518	4109	1.21%	0.107%

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77	26.359	3883	3885	3892	rBV6	1615	2890	0.85%	0.075%
78	26.482	3904	3906	3907	rBV2	1854	1360	0.40%	0.035%
79	26.600	3924	3926	3927	rVB	2078	1226	0.36%	0.032%
80	26.682	3932	3940	3947	rVB6	12774	37772	11.14%	0.982%
81	27.351	4051	4054	4056	rVV3	1814	2045	0.60%	0.053%
82	27.375	4056	4058	4062	rVB5	3064	2664	0.79%	0.069%
83	27.639	4101	4103	4105	rBV3	1955	1049	0.31%	0.027%
84	28.139	4181	4188	4189	rBV6	3517	6401	1.89%	0.166%
85	28.479	4240	4246	4248	rBV5	3021	6201	1.83%	0.161%
86	29.472	4413	4415	4418	rVB5	1814	1954	0.58%	0.051%
87	29.760	4460	4464	4465	rBV3	2013	2170	0.64%	0.056%
88	29.807	4470	4472	4473	rBV2	1642	1084	0.32%	0.028%
89	29.895	4485	4487	4488	rBV2	2105	1769	0.52%	0.046%
90	29.930	4488	4493	4497	rVV7	4341	10020	2.95%	0.260%
91	30.283	4551	4553	4554	rVB2	2202	991	0.29%	0.026%
92	30.336	4560	4562	4564	rBV3	1992	1815	0.54%	0.047%
93	30.436	4577	4579	4581	rBV3	2144	2157	0.64%	0.056%
94	31.323	4728	4730	4732	rBV3	2091	1689	0.50%	0.044%
95	31.810	4809	4813	4814	rBV4	1506	1724	0.51%	0.045%
96	32.092	4858	4861	4865	rBV6	2760	4834	1.43%	0.126%
97	32.327	4899	4901	4904	rBV3	1857	1850	0.55%	0.048%
98	32.439	4918	4920	4923	rBV4	2004	2847	0.84%	0.074%
99	32.603	4945	4948	4950	rVB4	1926	1958	0.58%	0.051%
100	32.621	4950	4951	4952	rBV	2088	948	0.28%	0.025%

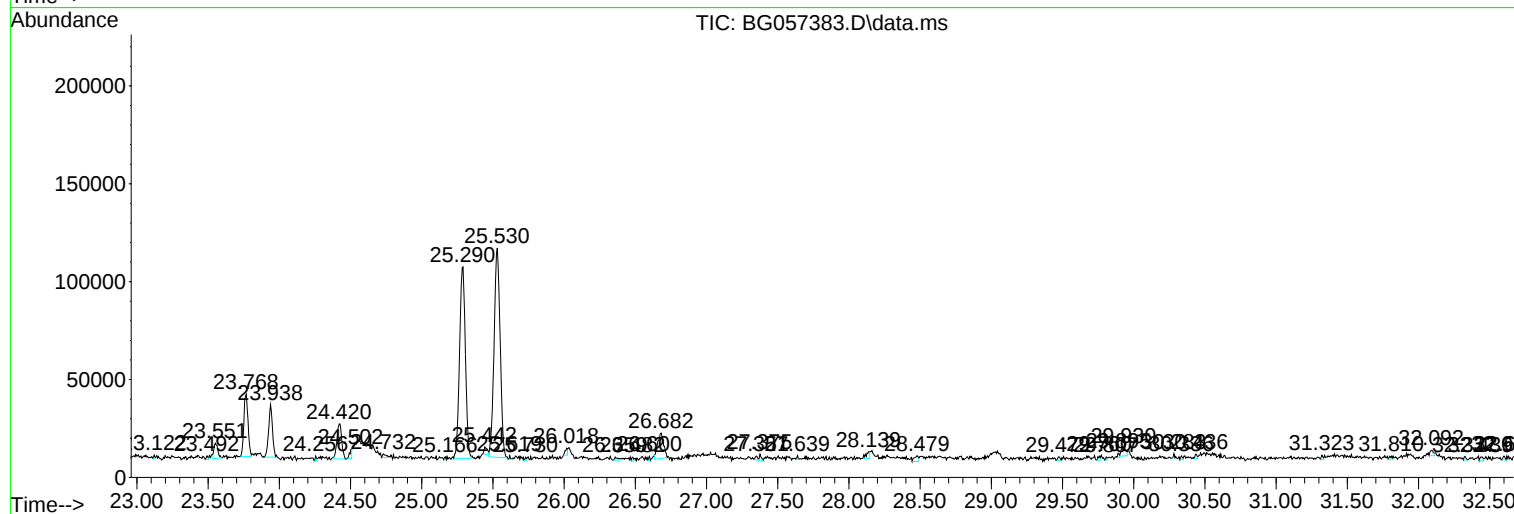
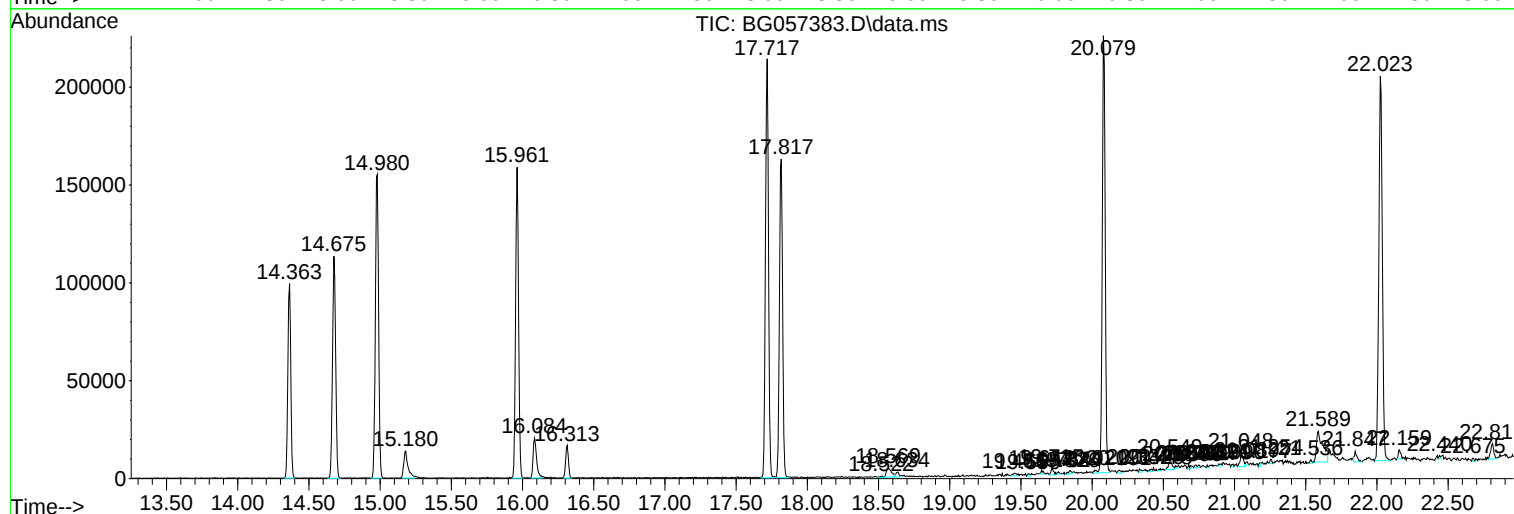
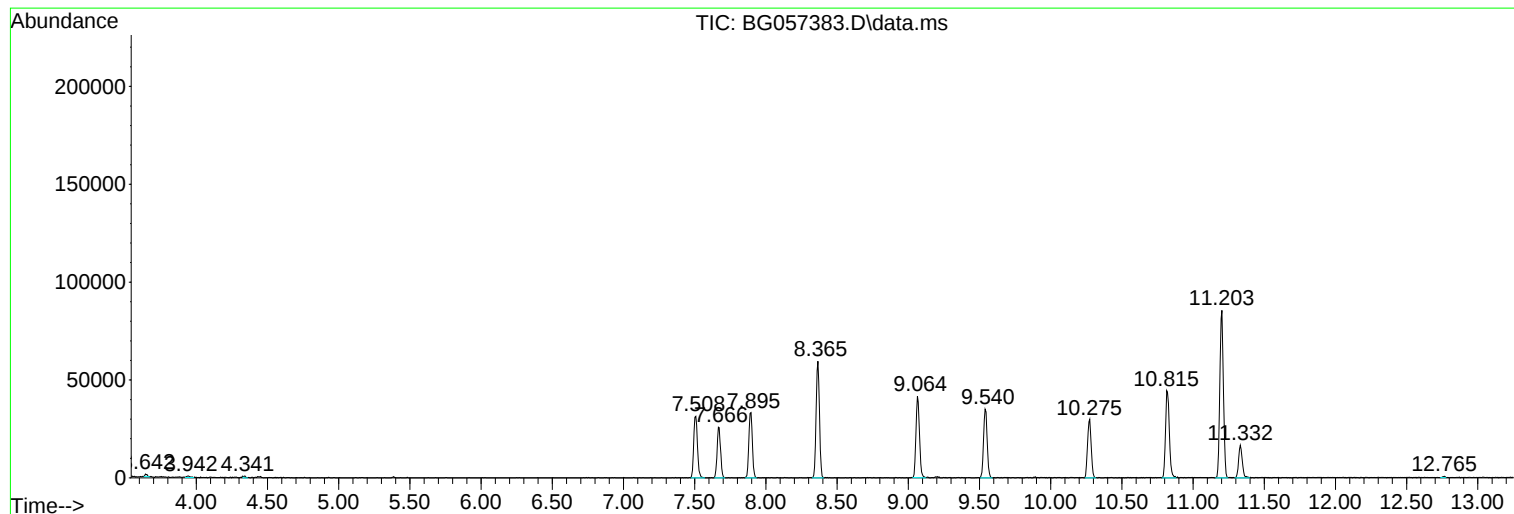
Sum of corrected areas: 3847746

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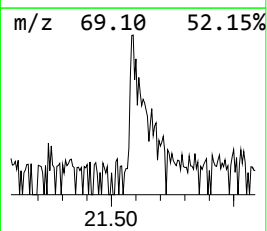
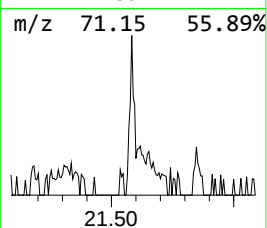
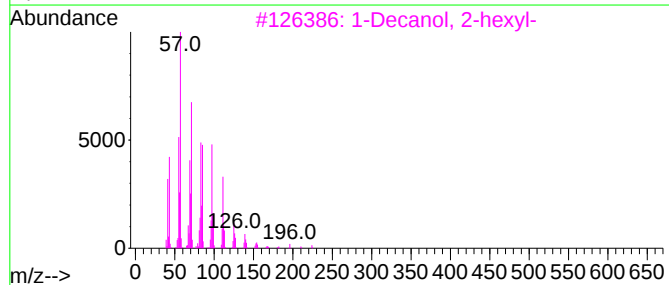
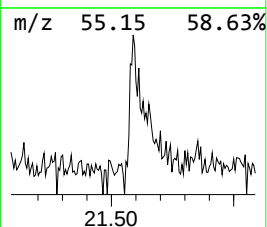
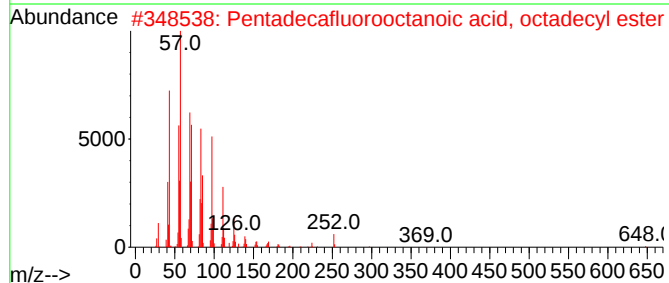
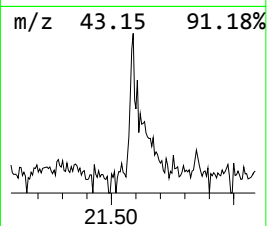
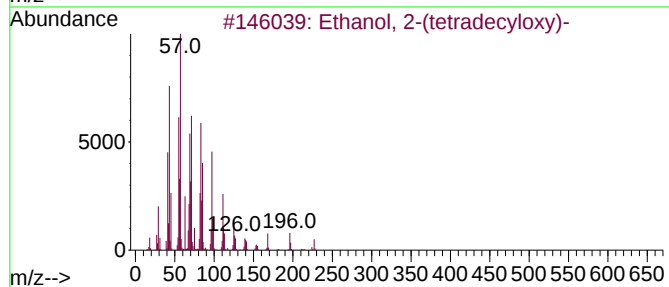
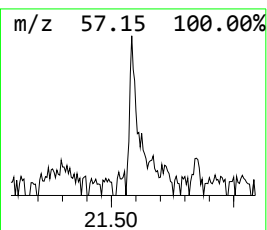
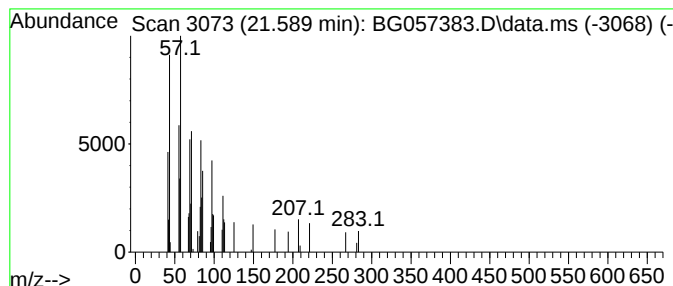
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Ethanol, 2-(tetradecyloxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.589	2.89 ng/ul	49070	Chrysene-d12	22.023

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	81
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	74
3			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	74
4			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	72
5			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	72



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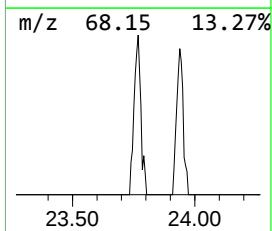
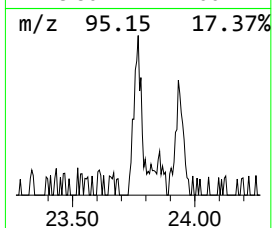
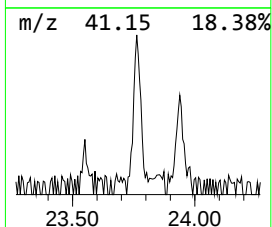
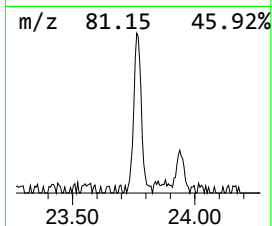
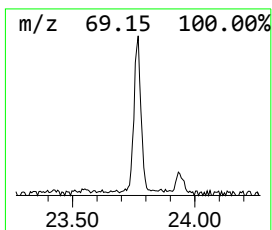
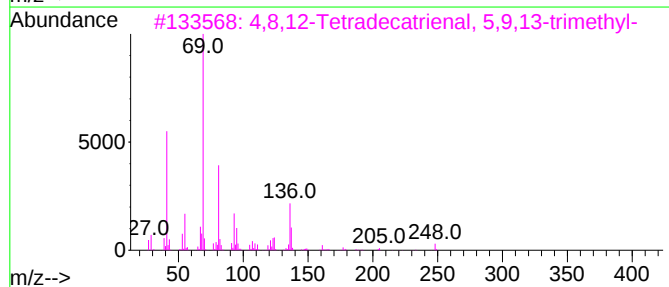
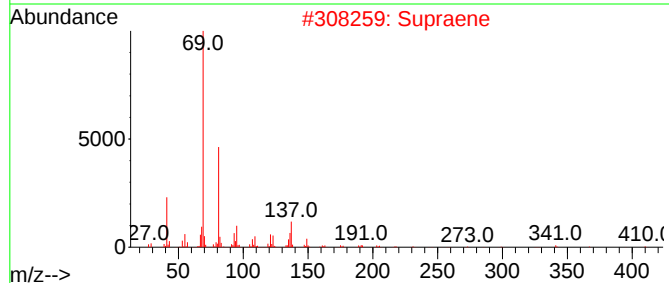
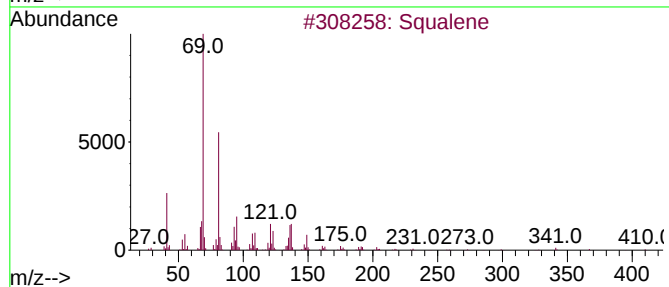
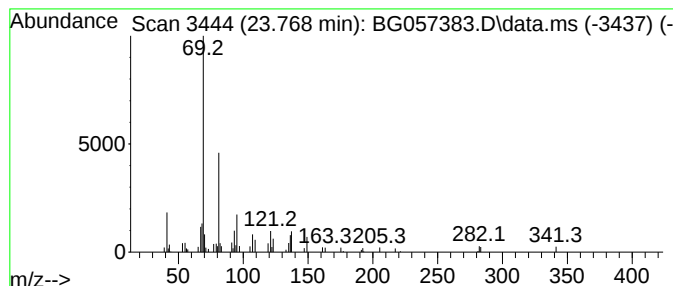
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Squalene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.768	3.80 ng/ul	64491	Chrysene-d12	22.023

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			Supraene	410	C30H50	007683-64-9	86
3			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5			(3E,7E)-4,8,12-Trimethyltrideca-	218	C16H26	062235-06-7	64



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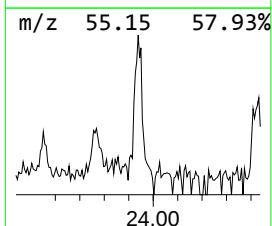
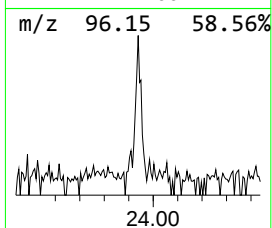
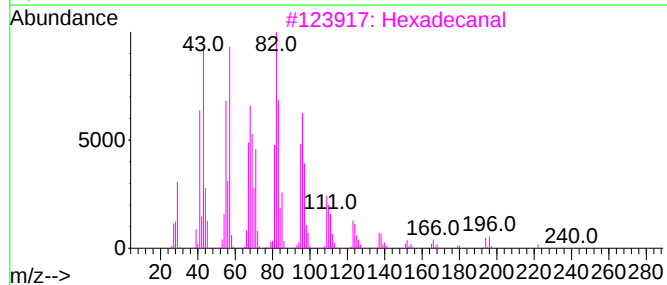
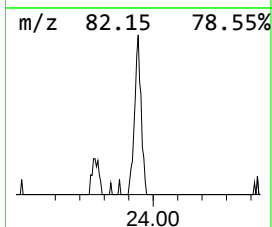
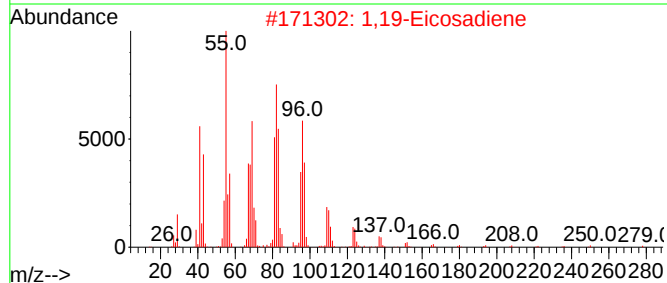
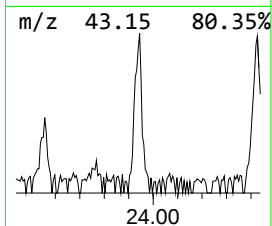
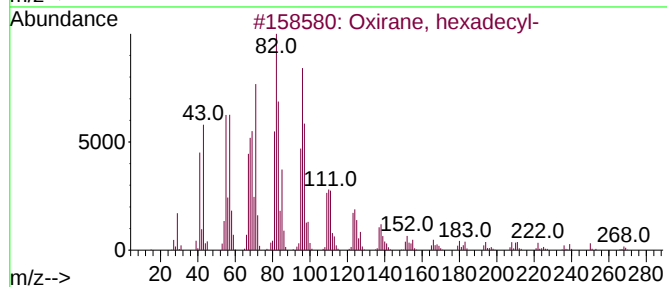
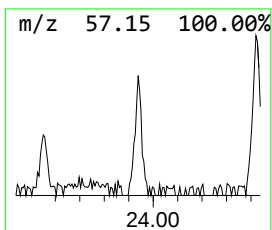
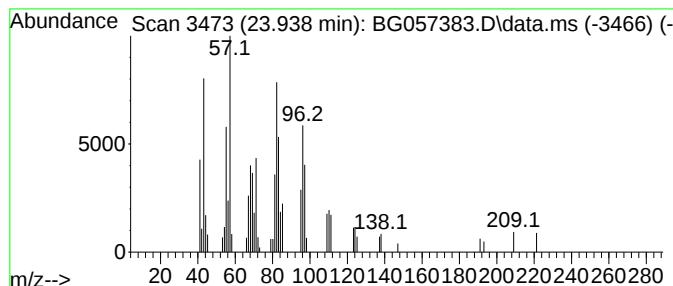
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Oxirane, hexadecyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.939	3.14 ng/ul	49864	Perylene-d12	25.525

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-		268	C18H36O	007390-81-0	87	
2	1,19-Eicosadiene		278	C20H38	014811-95-1	64	
3	Hexadecanal		240	C16H32O	000629-80-1	64	
4	Oxirane, dodecyl-		212	C14H28O	003234-28-4	52	
5	1,16-Hexadecanediol		258	C16H34O2	007735-42-4	50	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051023\
Data File : BG057383.D
Acq On : 11 May 2023 00:26
Operator : CG/JU
Sample : 02591-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JREF0

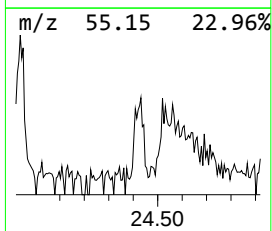
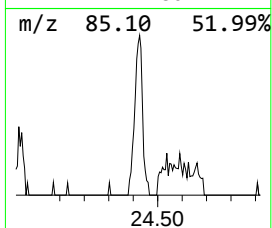
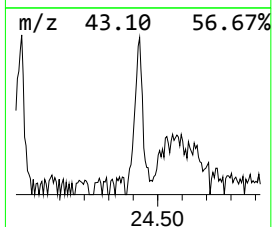
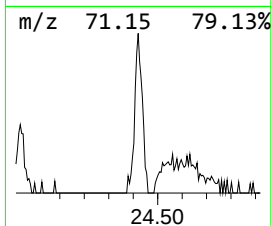
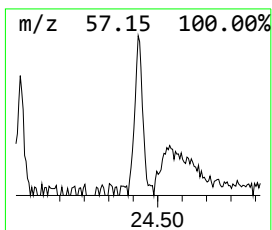
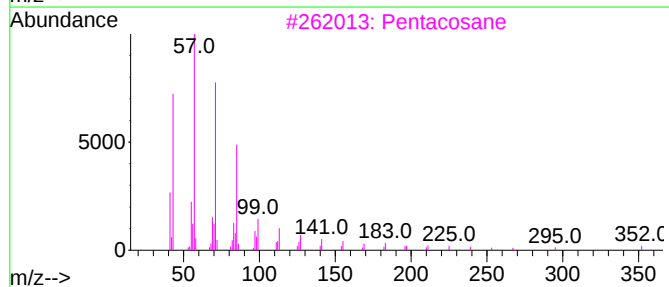
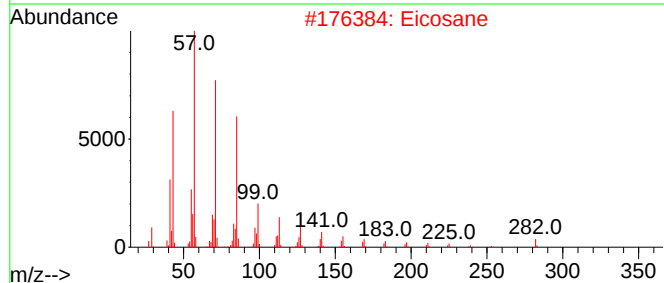
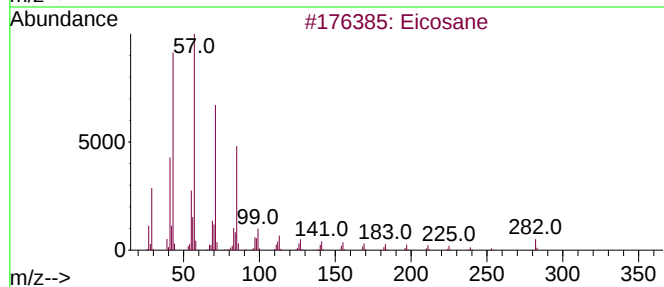
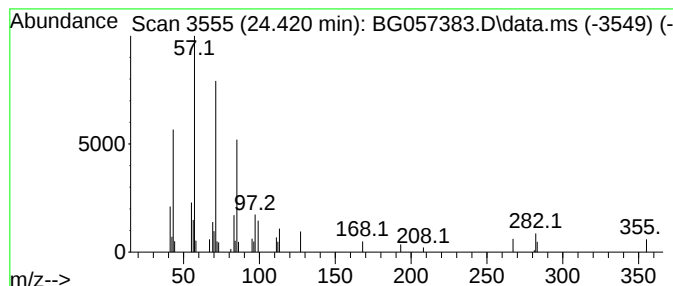
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.420	2.57 ng/ul	40811	Perylene-d12	25.525

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	90
2			Eicosane	282	C20H42	000112-95-8	87
3			Pentacosane	352	C25H52	000629-99-2	86
4			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	86
5			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051023\
Data File : BG057383.D
Acq On : 11 May 2023 00:26
Operator : CG/JU
Sample : 02591-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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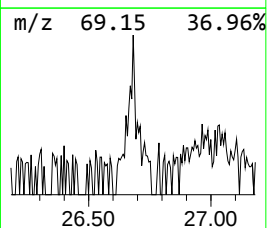
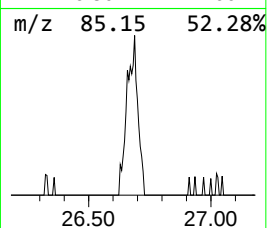
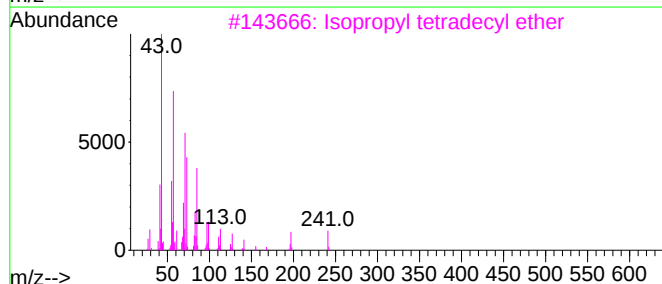
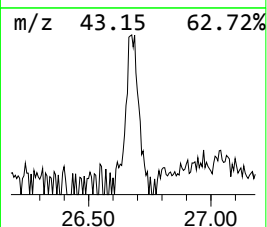
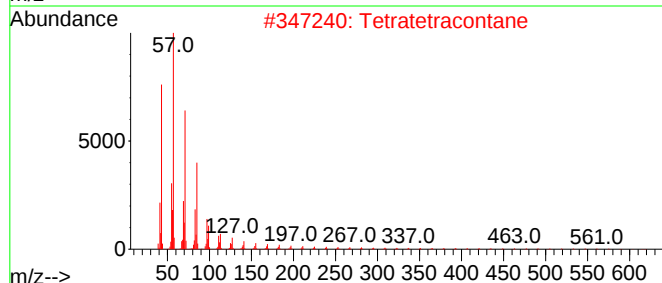
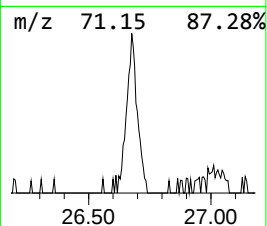
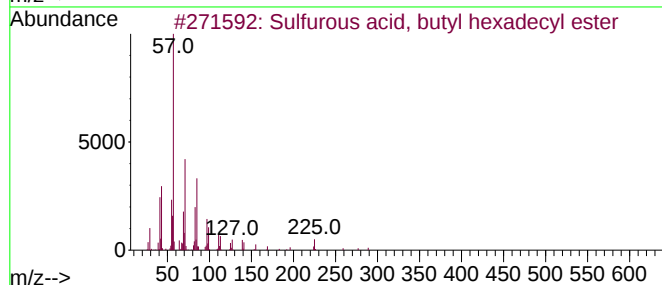
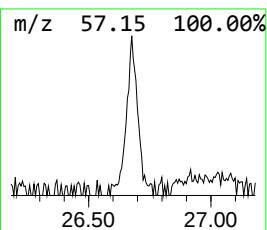
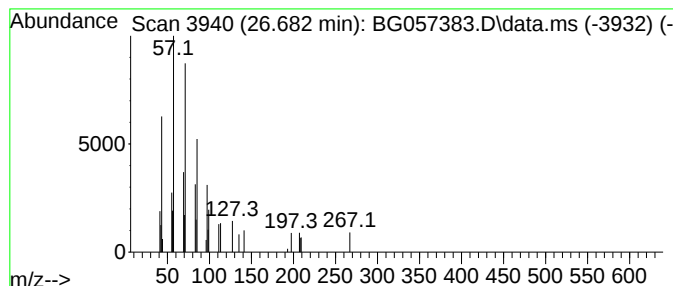
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Sulfurous acid, butyl hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.682	2.38 ng/ul	37772	Perylene-d12	25.525

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	86
2			Tetratetracontane	619	C44H90	007098-22-8	86
3			Isopropyl tetradecyl ether	256	C17H36O	1000406-34-0	80
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	78
5			Tritetracontane	605	C43H88	007098-21-7	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051023\
Data File : BG057383.D
Acq On : 11 May 2023 00:26
Operator : CG/JU
Sample : 02591-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JREF0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.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
Ethanol, 2-(tet...	21.589	2.9	ng/u1	49070	5	22.023	339210	20.0
Squalene	23.768	3.8	ng/u1	64491	5	22.023	339210	20.0
Oxirane, hexade...	23.939	3.1	ng/u1	49864	6	25.525	317599	20.0
(DEL) Alkane: S...	24.420	2.6	ng/u1	40811	6	25.525	317599	20.0
Sulfurous acid,...	26.682	2.4	ng/u1	37772	6	25.525	317599	20.0