

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051023\
 Data File : BG057387.D
 Acq On : 11 May 2023 3:10
 Operator : CG/JU
 Sample : 02591-23
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 JREK4

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: BG057387.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.209	110	114	116	rVV	759	870	0.30%	0.030%
2	4.333	131	135	137	rVV	836	822	0.29%	0.028%
3	4.444	151	154	155	rVB	801	738	0.26%	0.025%
4	7.505	670	675	685	rBB	18129	31065	10.80%	1.066%
5	7.669	697	703	709	rVB	22354	33965	11.81%	1.166%
6	7.893	735	741	750	rBB	22196	38111	13.25%	1.308%
7	8.369	815	822	828	rVB	45815	79880	27.78%	2.742%
8	9.068	936	941	950	rBB2	19736	34216	11.90%	1.175%
9	9.197	959	963	971	rBB2	3836	6983	2.43%	0.240%
10	9.543	1015	1022	1029	rBV2	27825	49790	17.31%	1.709%
11	10.272	1139	1146	1154	rVB2	15878	27730	9.64%	0.952%
12	10.818	1233	1239	1254	rBB	26673	50945	17.71%	1.749%
13	11.200	1296	1304	1312	rBV	68947	122114	42.46%	4.192%
14	11.341	1327	1328	1332	rBV	408	531	0.18%	0.018%
15	12.087	1450	1455	1458	rBV	259	599	0.21%	0.021%
16	12.763	1566	1570	1573	rBV	571	778	0.27%	0.027%
17	14.231	1816	1820	1823	rBV2	1087	1196	0.42%	0.041%
18	14.360	1835	1842	1850	rBV	41255	54654	19.00%	1.876%
19	14.519	1865	1869	1872	rBV	396	734	0.26%	0.025%
20	14.678	1888	1896	1902	rBV	94681	147185	51.18%	5.053%
21	14.977	1940	1947	1954	rVB	131936	200962	69.88%	6.899%
22	15.230	1984	1990	1998	rBV	22658	42238	14.69%	1.450%
23	15.958	2108	2114	2123	rBV	133437	202852	70.53%	6.964%
24	16.099	2136	2138	2143	rVV	398	534	0.19%	0.018%
25	16.311	2170	2174	2179	rVB	10286	14915	5.19%	0.512%
26	17.468	2368	2371	2375	rVB	431	652	0.23%	0.022%
27	17.715	2407	2413	2423	rBV	175854	260263	90.50%	8.934%
28	17.815	2424	2430	2438	rVV2	144728	218224	75.88%	7.491%
29	17.950	2450	2453	2455	rBV	571	589	0.20%	0.020%
30	18.619	2566	2567	2570	rVV2	705	877	0.30%	0.030%
31	18.672	2574	2576	2579	rBV2	557	621	0.22%	0.021%
32	18.813	2599	2600	2602	rBV	873	542	0.19%	0.019%
33	19.365	2690	2694	2696	rVB3	1657	1577	0.55%	0.054%
34	19.401	2699	2700	2701	rBV	1010	633	0.22%	0.022%
35	19.418	2701	2703	2705	rVB2	1557	1028	0.36%	0.035%
36	19.454	2705	2709	2711	rBV3	1090	1733	0.60%	0.059%

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Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
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37	19.524	2718	2721	2722	rBV	578	577	0.20%	0.020%
38	19.542	2722	2724	2728	rBV2	767	719	0.25%	0.025%
39	19.647	2738	2742	2747	rVB4	1957	3174	1.10%	0.109%
40	19.694	2747	2750	2751	rBV	1121	1025	0.36%	0.035%
41	19.718	2751	2754	2758	rVB3	1869	2513	0.87%	0.086%
42	19.753	2758	2760	2761	rVB	1138	701	0.24%	0.024%
43	19.976	2795	2798	2799	rBV3	641	533	0.19%	0.018%
44	20.006	2801	2803	2805	rVV3	1372	1024	0.36%	0.035%
45	20.023	2805	2806	2809	rVB2	1189	863	0.30%	0.030%
46	20.082	2809	2816	2823	rBV	198073	284574	98.95%	9.769%
47	20.200	2834	2836	2839	rVB3	1759	1600	0.56%	0.055%
48	20.229	2839	2841	2842	rBV2	814	584	0.20%	0.020%
49	20.458	2878	2880	2881	rVB	1081	564	0.20%	0.019%
50	20.476	2881	2883	2886	rBV3	1029	833	0.29%	0.029%
51	20.505	2886	2888	2889	rVB	1165	676	0.24%	0.023%
52	20.552	2891	2896	2899	rBV5	3382	5100	1.77%	0.175%
53	20.599	2902	2904	2905	rVB2	901	552	0.19%	0.019%
54	20.664	2913	2915	2916	rBV	1079	717	0.25%	0.025%
55	20.717	2922	2924	2925	rBV2	853	701	0.24%	0.024%
56	20.728	2925	2926	2928	rBV2	1577	1245	0.43%	0.043%
57	20.805	2937	2939	2940	rBV	2326	1530	0.53%	0.053%
58	21.051	2979	2981	2986	rVB5	3040	4469	1.55%	0.153%
59	21.092	2986	2988	2989	rBV2	1586	1104	0.38%	0.038%
60	21.110	2989	2991	2992	rVV	1828	793	0.28%	0.027%
61	21.163	2998	3000	3001	rVB2	2282	1162	0.40%	0.040%
62	21.251	3013	3015	3019	rVB4	1801	1937	0.67%	0.066%
63	21.463	3049	3051	3054	rBV4	1243	1617	0.56%	0.056%
64	21.580	3065	3071	3076	rBV8	9286	22112	7.69%	0.759%
65	22.027	3139	3147	3155	rBV	163197	287594	100.00%	9.873%
66	22.297	3191	3193	3194	rBV2	1403	982	0.34%	0.034%
67	22.602	3243	3245	3247	rVB2	2370	1123	0.39%	0.039%
68	22.784	3274	3276	3277	rBV2	1741	1330	0.46%	0.046%
69	22.808	3277	3280	3286	rVB4	8046	12672	4.41%	0.435%
70	23.049	3319	3321	3322	rBV	1676	1387	0.48%	0.048%
71	23.219	3349	3350	3353	rBV3	1663	1257	0.44%	0.043%
72	23.366	3373	3375	3376	rVB2	1587	703	0.24%	0.024%
73	23.384	3376	3378	3380	rBV3	1518	1486	0.52%	0.051%
74	23.730	3435	3437	3438	rBV2	1559	936	0.33%	0.032%
75	23.765	3438	3443	3449	rVV7	6023	11577	4.03%	0.397%
76	23.936	3466	3472	3483	rVB4	19230	42016	14.61%	1.442%

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77	24.165	3510	3511	3512	rBV	1381	601	0.21%	0.021%
78	24.417	3549	3554	3562	rVB4	12819	26295	9.14%	0.903%
79	24.529	3567	3573	3574	rBV4	3806	6872	2.39%	0.236%
80	24.823	3621	3623	3625	rBV3	1573	1225	0.43%	0.042%
81	24.893	3632	3635	3636	rBV3	2182	2256	0.78%	0.077%
82	25.128	3673	3675	3676	rBV	1306	765	0.27%	0.026%
83	25.146	3676	3678	3679	rBV2	1714	1171	0.41%	0.040%
84	25.163	3679	3681	3682	rBV2	1800	1127	0.39%	0.039%
85	25.222	3689	3691	3692	rBV2	1817	1488	0.52%	0.051%
86	25.281	3692	3701	3713	rVB3	69931	202108	70.28%	6.938%
87	25.528	3733	3743	3757	rVB	89447	268617	93.40%	9.221%
88	26.021	3823	3827	3828	rBV4	3946	5241	1.82%	0.180%
89	26.168	3850	3852	3853	rBV2	1503	1075	0.37%	0.037%
90	26.679	3931	3939	3948	rVB5	12745	40008	13.91%	1.373%
91	27.149	4016	4019	4022	rBV4	1869	2335	0.81%	0.080%
92	28.941	4322	4324	4327	rVB3	1846	1222	0.42%	0.042%
93	29.352	4392	4394	4396	rBV3	1732	1085	0.38%	0.037%
94	29.387	4398	4400	4402	rBV3	2234	2283	0.79%	0.078%
95	30.215	4539	4541	4543	rBV2	1965	2151	0.75%	0.074%
96	31.249	4715	4717	4718	rBV	1512	1030	0.36%	0.035%
97	31.379	4737	4739	4743	rVB4	2064	1874	0.65%	0.064%
98	32.154	4870	4871	4874	rVB3	1876	1547	0.54%	0.053%
99	32.313	4896	4898	4899	rVB2	2357	1453	0.51%	0.050%
100	32.571	4940	4942	4944	rBV3	2562	2021	0.70%	0.069%

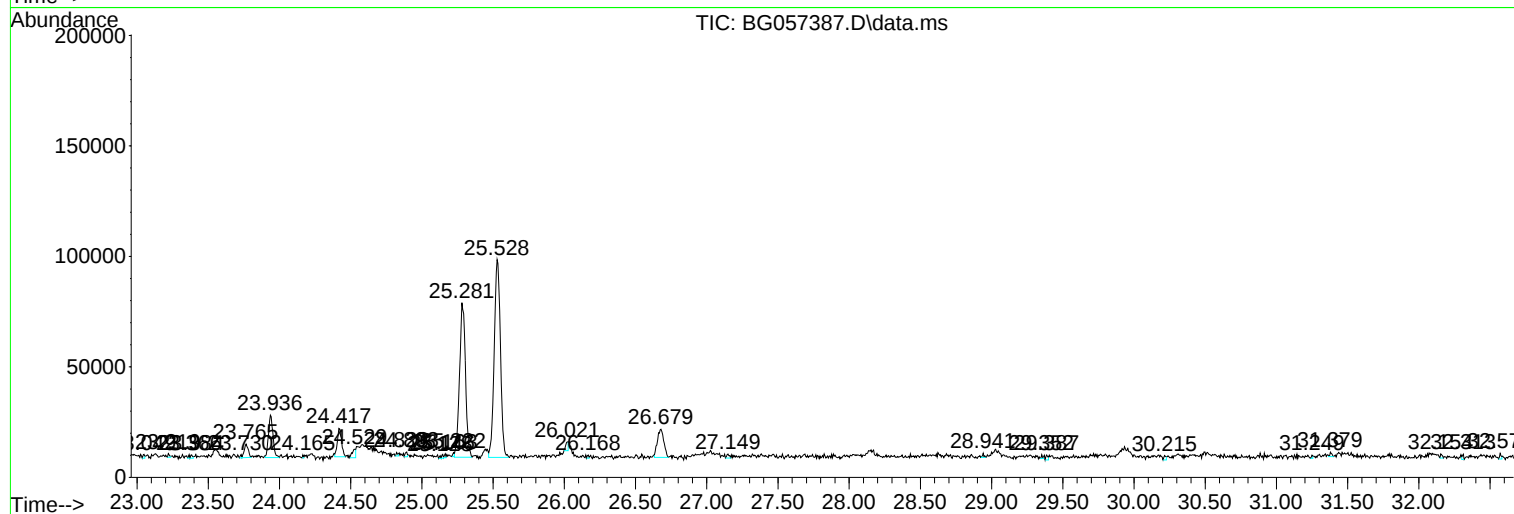
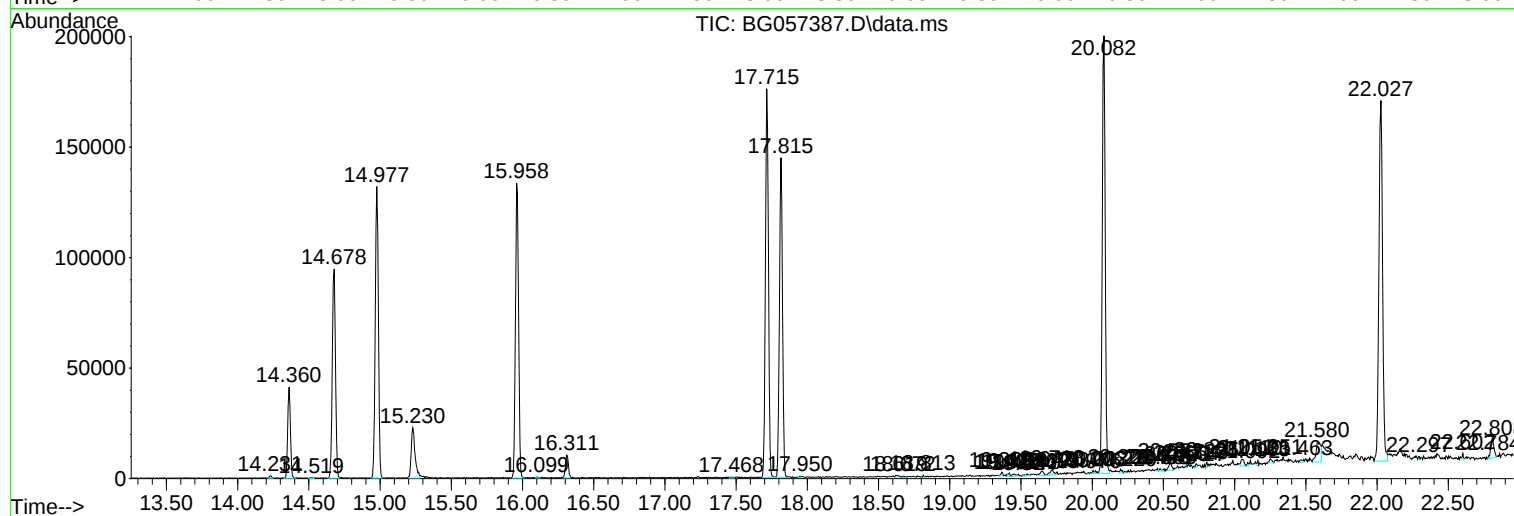
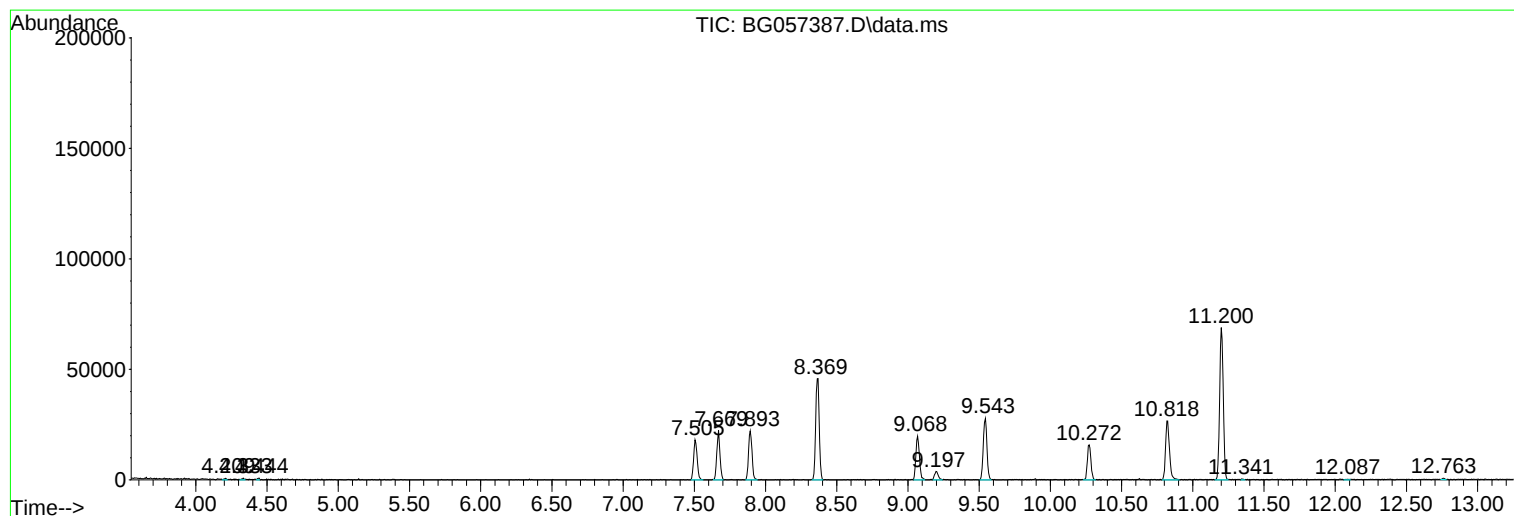
Sum of corrected areas: 2913058

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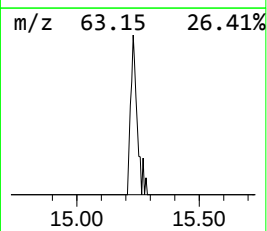
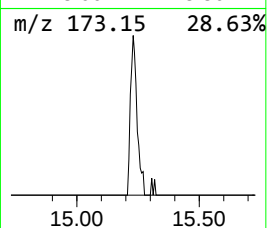
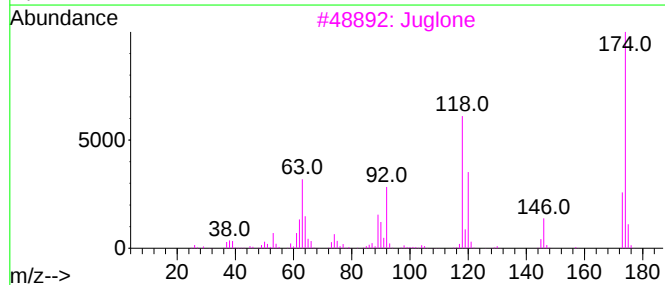
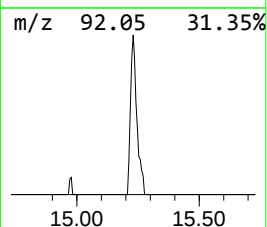
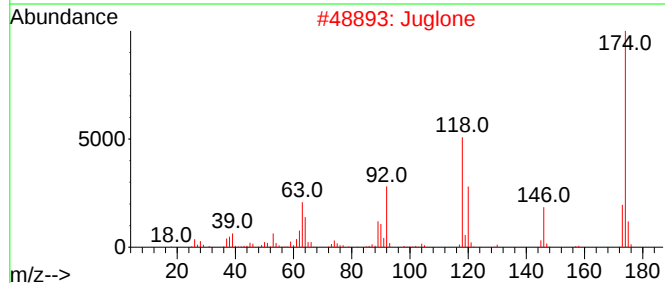
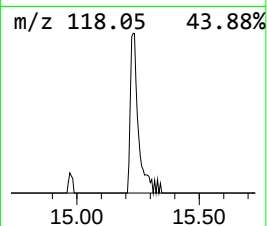
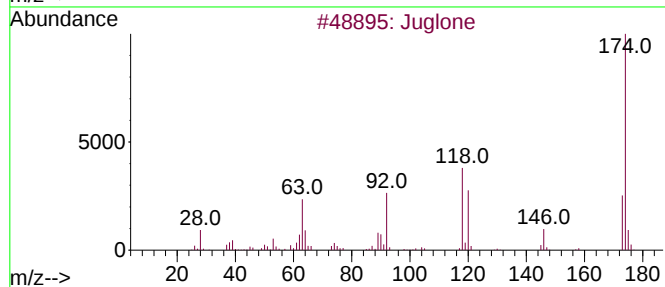
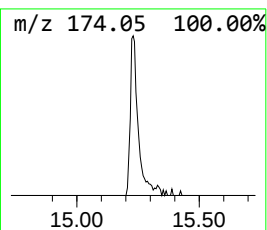
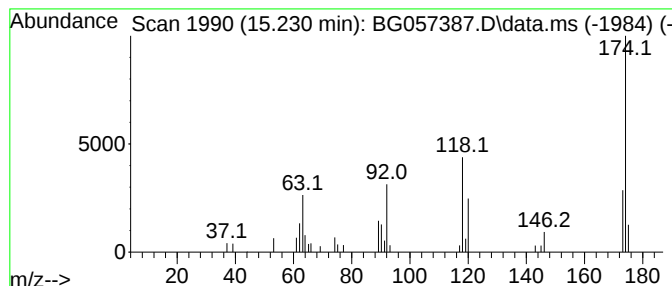
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Juglone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.230	4.20 ng/ul	42238	Acenaphthene-d10	14.977

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Juglone			174	C10H6O3	000481-39-0	96
2	Juglone			174	C10H6O3	000481-39-0	93
3	Juglone			174	C10H6O3	000481-39-0	91
4	3-(3-Methoxyphenyl)-1H-pyrazole			174	C10H10N2O	1000410-63-5	47
5	8-Quinolinol, 5-nitroso-			174	C9H6N2O2	003565-26-2	43



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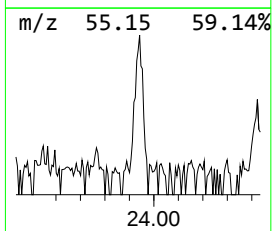
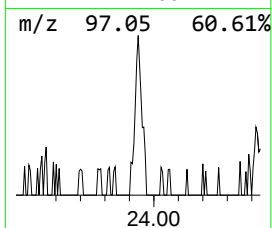
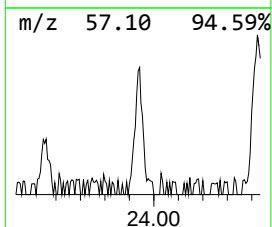
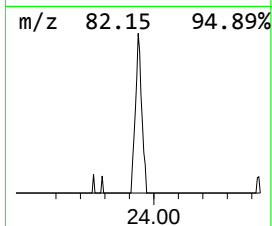
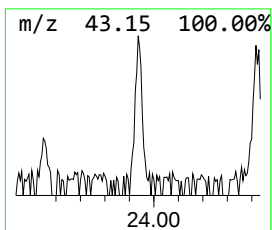
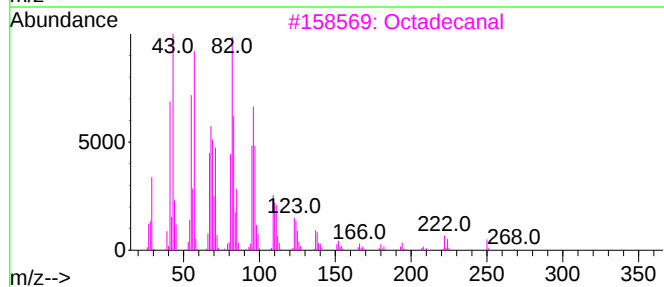
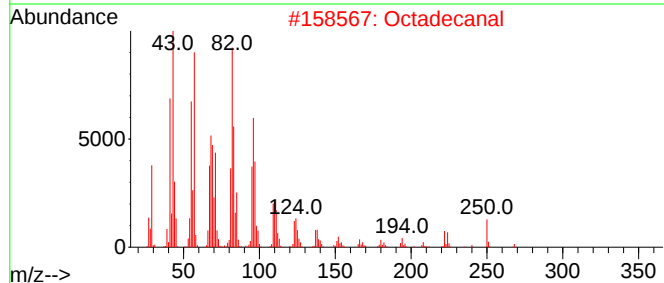
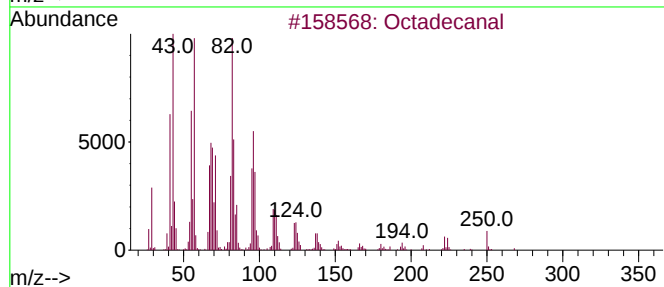
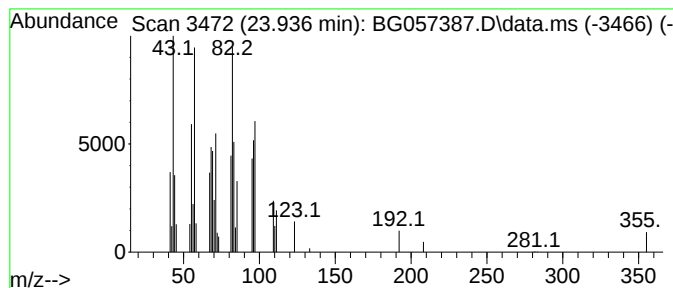
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Octadecanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.936	3.13 ng/ul	42016	Perylene-d12	25.534

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal			268	C18H36O	000638-66-4	83
2	Octadecanal			268	C18H36O	000638-66-4	80
3	Octadecanal			268	C18H36O	000638-66-4	80
4	Tetracosanal			352	C24H48O	057866-08-7	74
5	Pentadecanal-			226	C15H30O	002765-11-9	68



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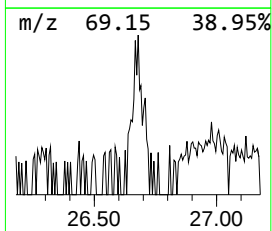
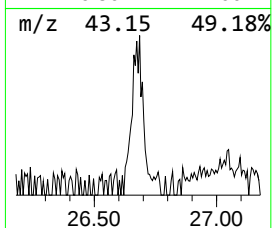
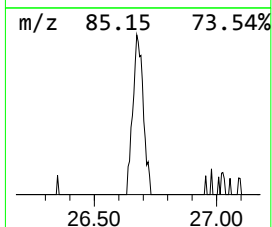
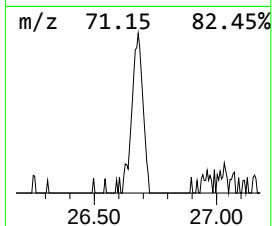
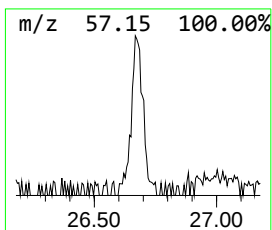
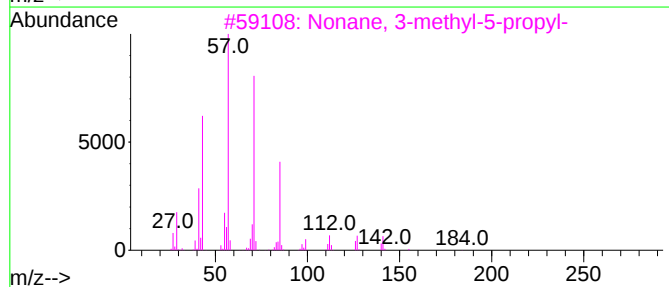
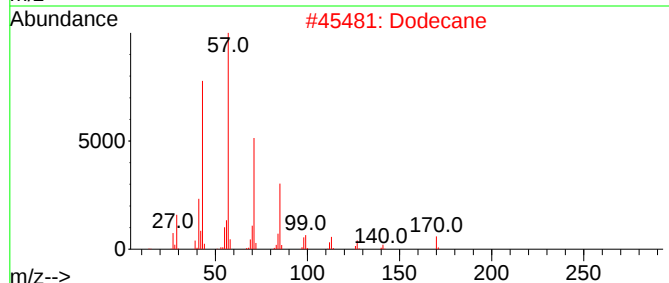
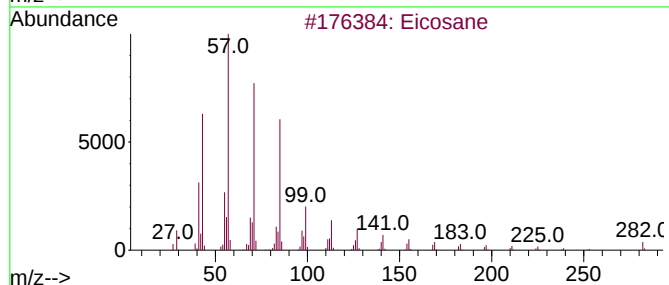
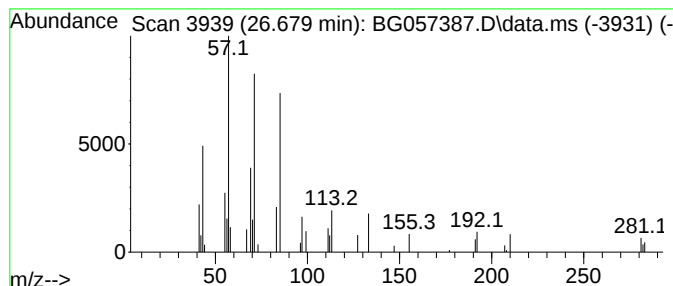
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.679	2.98 ng/ul	40008	Perylene-d12	25.534

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosane	282	C20H42	000112-95-8	64
2		Dodecane	170	C12H26	000112-40-3	43
3		Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	43
4		Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	43
5		Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051023\
Data File : BG057387.D
Acq On : 11 May 2023 3:10
Operator : CG/JU
Sample : 02591-23
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JREK4

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
Juglone	15.230	4.2	ng/ul	42238	3	14.977	200962	20.0
Octadecanal	23.936	3.1	ng/ul	42016	6	25.534	268617	20.0
(DEL) Alkane: S...	26.679	3.0	ng/ul	40008	6	25.534	268617	20.0