

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051023\
 Data File : BG057386.D
 Acq On : 11 May 2023 2:29
 Operator : CG/JU
 Sample : 02591-17
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 JREF3

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: BG057386.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.652	13	19	24	rVB3	1886	2879	0.85%	0.074%
2	4.445	149	154	157	rBV	713	1109	0.33%	0.029%
3	5.379	311	313	319	rBB2	638	1003	0.30%	0.026%
4	7.506	669	675	683	rBV	34815	60051	17.75%	1.554%
5	7.670	697	703	709	rBB	25693	42707	12.63%	1.105%
6	7.893	735	741	750	rBB	35588	57433	16.98%	1.486%
7	8.363	815	821	828	rBB	55024	90037	26.62%	2.329%
8	9.068	934	941	948	rBV	38008	67815	20.05%	1.754%
9	9.198	959	963	967	rBB2	731	1018	0.30%	0.026%
10	9.538	1015	1021	1031	rVB	33959	60826	17.98%	1.574%
11	10.273	1140	1146	1154	rVB	31484	54684	16.17%	1.415%
12	10.819	1233	1239	1249	rBV2	47866	86504	25.58%	2.238%
13	11.201	1296	1304	1312	rVV	79780	137100	40.54%	3.547%
14	11.330	1319	1326	1334	rBV2	39328	70528	20.85%	1.825%
15	12.940	1593	1600	1603	rBV2	644	1033	0.31%	0.027%
16	13.832	1749	1752	1758	rVB3	1437	2045	0.60%	0.053%
17	14.232	1816	1820	1823	rBV2	1200	1387	0.41%	0.036%
18	14.361	1836	1842	1850	rBV	120793	163792	48.43%	4.238%
19	14.678	1889	1896	1903	rBV	119551	187065	55.31%	4.840%
20	14.978	1939	1947	1954	rBV	148273	225464	66.66%	5.833%
21	15.172	1974	1980	1985	rBV2	18271	34557	10.22%	0.894%
22	15.231	1985	1990	2005	rVB	48201	86990	25.72%	2.251%
23	15.959	2107	2114	2123	rVB	160669	249233	73.69%	6.448%
24	16.082	2130	2135	2144	rBV2	26912	43039	12.73%	1.113%
25	16.311	2168	2174	2179	rVB	18455	26005	7.69%	0.673%
26	16.870	2267	2269	2274	rVB3	1325	1782	0.53%	0.046%
27	17.715	2407	2413	2419	rVV	193355	290027	85.75%	7.503%
28	17.757	2419	2420	2424	rVV2	1480	1581	0.47%	0.041%
29	17.815	2424	2430	2439	rVV2	184179	267986	79.23%	6.933%
30	18.573	2555	2559	2564	rBV3	3583	6485	1.92%	0.168%
31	19.366	2690	2694	2697	rVB2	640	874	0.26%	0.023%
32	19.448	2707	2708	2711	rVB	1473	1017	0.30%	0.026%
33	19.525	2719	2721	2724	rBV2	961	764	0.23%	0.020%
34	19.648	2738	2742	2746	rVV5	2095	3539	1.05%	0.092%
35	19.719	2752	2754	2756	rVV	2237	2340	0.69%	0.061%
36	19.748	2756	2759	2764	rVB	5199	7008	2.07%	0.181%

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37	19.795	2764	2767	2769	rBV3	1161	1261	0.37%	0.033%
38	19.854	2775	2777	2780	rBV3	1525	1235	0.37%	0.032%
39	19.895	2782	2784	2786	rVV	1277	854	0.25%	0.022%
40	19.918	2786	2788	2791	rVB2	942	1057	0.31%	0.027%
41	19.995	2798	2801	2803	rVB2	893	819	0.24%	0.021%
42	20.012	2803	2804	2805	rBV	1283	815	0.24%	0.021%
43	20.083	2809	2816	2824	rVV	230141	338223	100.00%	8.750%
44	20.388	2864	2868	2870	rVB3	766	941	0.28%	0.024%
45	20.435	2875	2876	2879	rVB3	1721	1136	0.34%	0.029%
46	20.476	2879	2883	2885	rBV2	1829	2314	0.68%	0.060%
47	20.547	2892	2895	2897	rBV4	2440	2128	0.63%	0.055%
48	20.606	2901	2905	2907	rVB3	1518	1475	0.44%	0.038%
49	20.647	2911	2912	2914	rBV2	1233	960	0.28%	0.025%
50	20.729	2922	2926	2928	rBV4	1002	1453	0.43%	0.038%
51	20.747	2928	2929	2931	rVB2	1723	879	0.26%	0.023%
52	20.817	2940	2941	2943	rVB2	2040	947	0.28%	0.025%
53	20.841	2943	2945	2947	rVB3	1951	1419	0.42%	0.037%
54	20.888	2951	2953	2957	rBV3	1196	1237	0.37%	0.032%
55	20.923	2957	2959	2961	rBV2	1130	748	0.22%	0.019%
56	20.946	2961	2963	2967	rVB3	1358	1575	0.47%	0.041%
57	21.052	2977	2981	2984	rBV5	4254	6226	1.84%	0.161%
58	21.275	3012	3019	3021	rBV5	2156	4636	1.37%	0.120%
59	21.587	3068	3072	3078	rBV7	9752	23549	6.96%	0.609%
60	21.822	3110	3112	3113	rVB2	2132	1308	0.39%	0.034%
61	22.027	3139	3147	3153	rBV2	182137	316402	93.55%	8.186%
62	22.421	3212	3214	3217	rVB3	2276	2268	0.67%	0.059%
63	22.485	3224	3225	3229	rVB3	2226	1509	0.45%	0.039%
64	22.685	3257	3259	3260	rBV2	1805	987	0.29%	0.026%
65	22.803	3277	3279	3285	rVB6	6634	10317	3.05%	0.267%
66	22.950	3300	3304	3305	rBV4	2535	2887	0.85%	0.075%
67	23.543	3401	3405	3411	rVB7	6543	13450	3.98%	0.348%
68	23.654	3422	3424	3425	rBV2	1548	1398	0.41%	0.036%
69	23.772	3436	3444	3448	rBV7	7385	15674	4.63%	0.406%
70	23.936	3467	3472	3477	rBV6	4031	7430	2.20%	0.192%
71	24.418	3547	3554	3563	rVB3	29618	69512	20.55%	1.798%
72	25.053	3660	3662	3666	rBV3	2111	2319	0.69%	0.060%
73	25.164	3679	3681	3683	rVB3	2149	1315	0.39%	0.034%
74	25.288	3692	3702	3711	rBV2	104046	290469	85.88%	7.515%
75	25.452	3724	3730	3733	rBV6	4124	8564	2.53%	0.222%
76	25.528	3733	3743	3755	rVB	102990	293540	86.79%	7.594%

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77	25.652	3762	3764	3765	rBV2	1593	1030	0.30%	0.027%
78	26.457	3899	3901	3902	rBV	1329	907	0.27%	0.023%
79	26.680	3930	3939	3950	rVB4	17587	55502	16.41%	1.436%
80	26.921	3978	3980	3983	rBV4	1945	2677	0.79%	0.069%
81	27.173	4021	4023	4024	rBV	1585	1386	0.41%	0.036%
82	27.549	4085	4087	4089	rBV3	1738	2002	0.59%	0.052%
83	27.955	4154	4156	4157	rBV2	1430	1015	0.30%	0.026%
84	28.131	4183	4186	4188	rBV4	2584	3906	1.15%	0.101%
85	28.401	4230	4232	4234	rBV3	2201	2073	0.61%	0.054%
86	28.524	4251	4253	4255	rBV3	1831	1403	0.41%	0.036%
87	29.353	4392	4394	4396	rBV3	1734	1596	0.47%	0.041%
88	29.435	4406	4408	4412	rBV5	1746	2170	0.64%	0.056%
89	29.905	4486	4488	4489	rBV2	1912	1115	0.33%	0.029%
90	30.234	4543	4544	4546	rBV2	1710	928	0.27%	0.024%
91	30.304	4554	4556	4559	rVB4	2413	2206	0.65%	0.057%
92	30.334	4559	4561	4562	rBV2	1466	1040	0.31%	0.027%
93	30.680	4619	4620	4622	rBV2	1747	1381	0.41%	0.036%
94	31.191	4705	4707	4708	rBV	1980	1548	0.46%	0.040%
95	31.438	4748	4749	4751	rBV	1777	1434	0.42%	0.037%
96	31.632	4780	4782	4783	rBV2	1625	1258	0.37%	0.033%
97	32.213	4879	4881	4882	rBV2	1490	1118	0.33%	0.029%
98	32.337	4900	4902	4904	rVB3	1874	1206	0.36%	0.031%
99	32.448	4919	4921	4923	rBV2	1846	1722	0.51%	0.045%
100	32.625	4949	4951	4953	rBV3	2325	1661	0.49%	0.043%

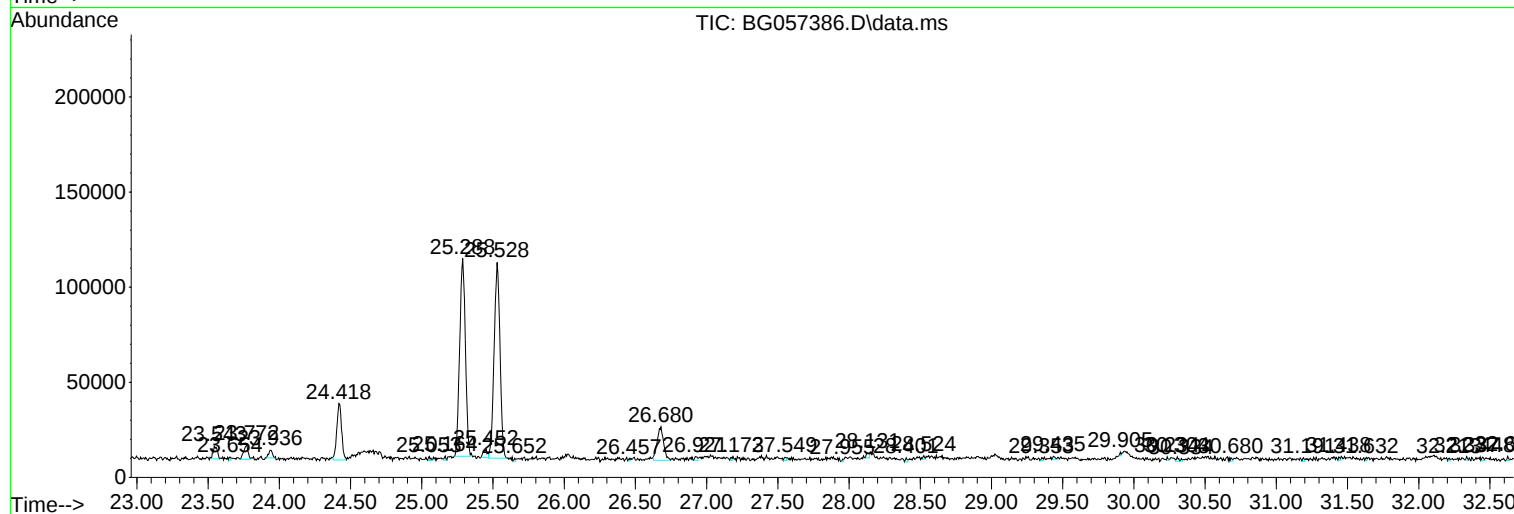
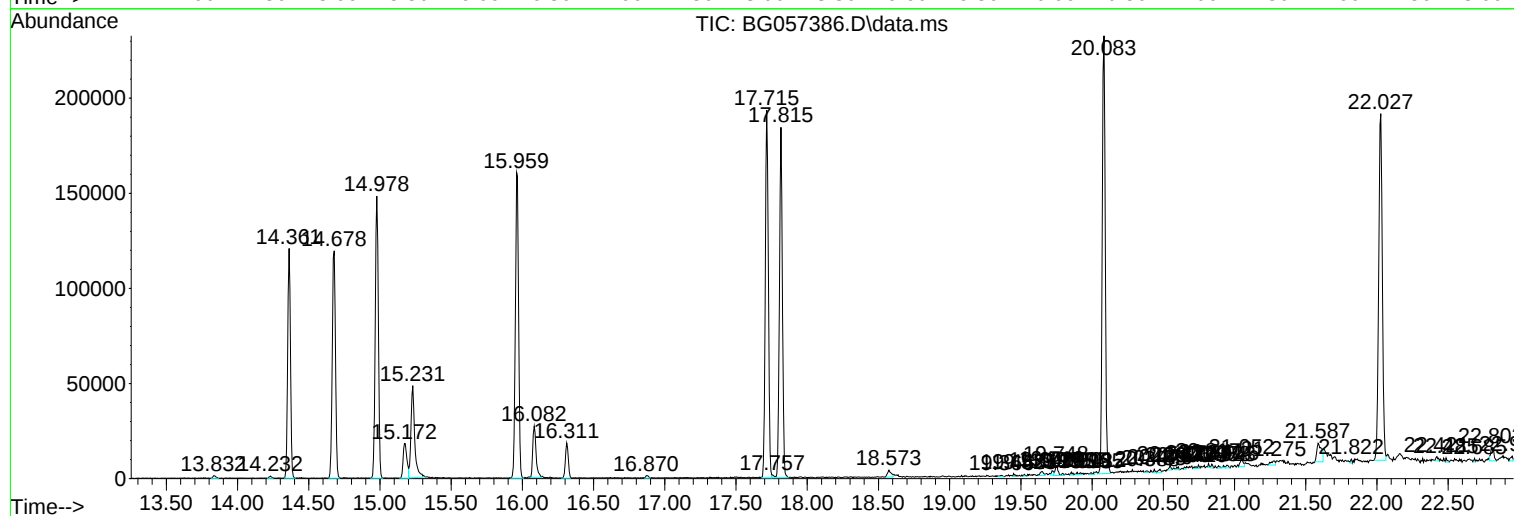
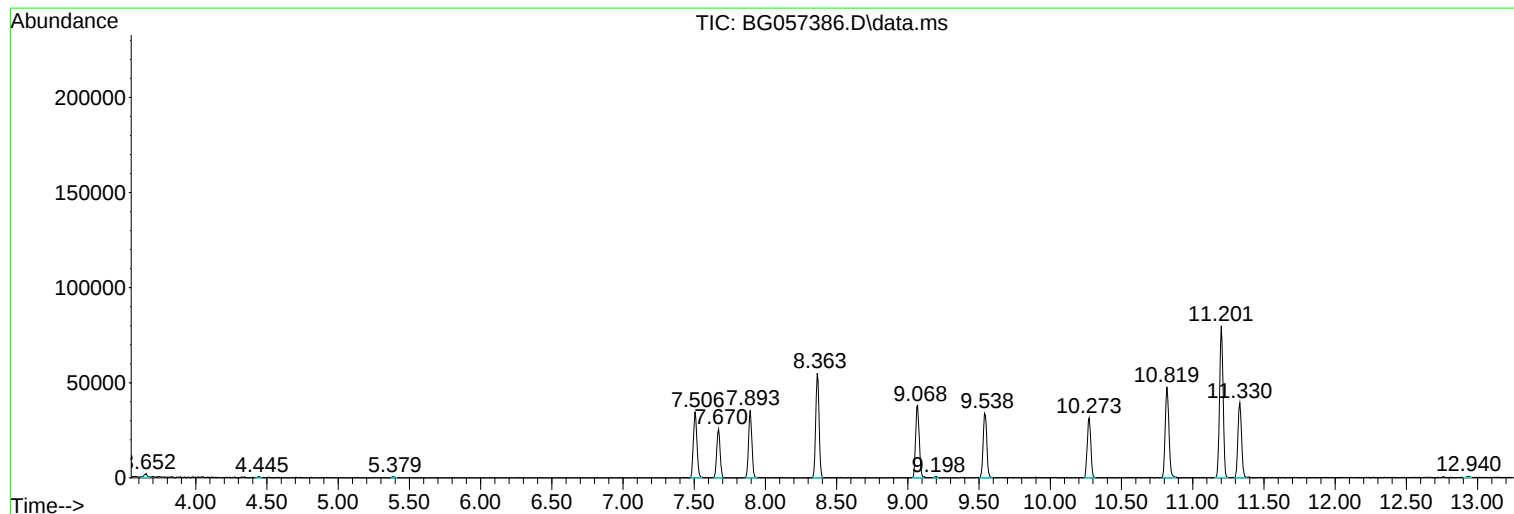
Sum of corrected areas: 3865227

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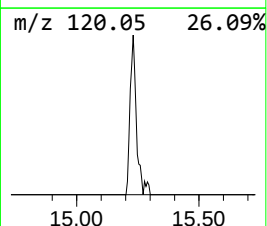
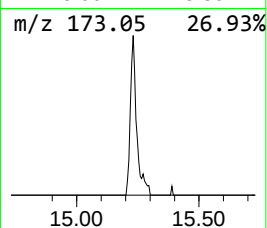
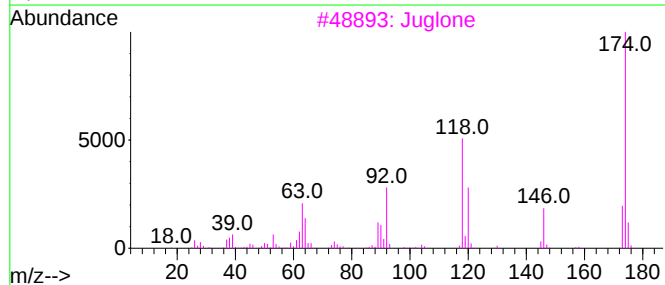
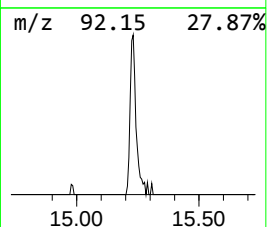
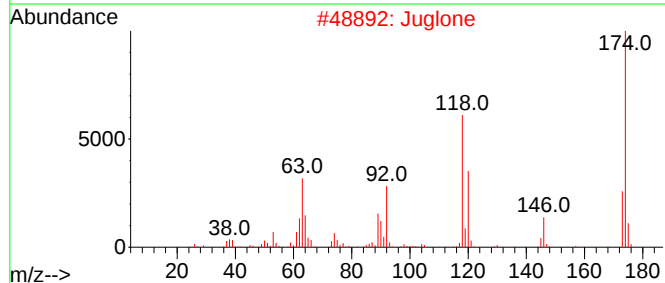
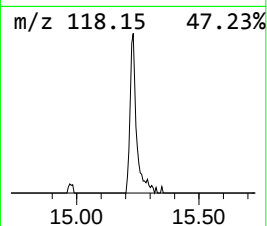
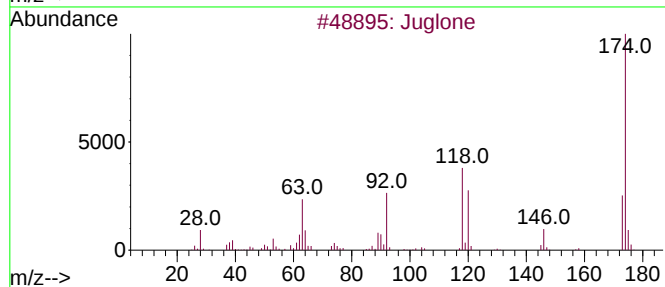
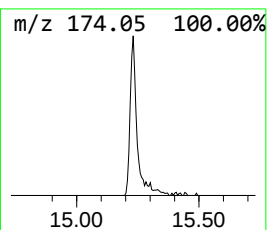
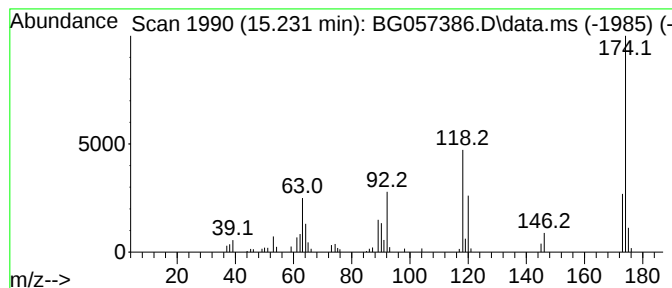
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

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.
15.231	7.72 ng/ul	86990	Acenaphthene-d10	14.978

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Juglone			174	C10H6O3	000481-39-0	98
2	Juglone			174	C10H6O3	000481-39-0	96
3	Juglone			174	C10H6O3	000481-39-0	95
4	Juglone			174	C10H6O3	000481-39-0	91
5	4H-Pyrido[1,2-a]pyrimidin-4-one,...			174	C10H10N2O	016867-28-0	43



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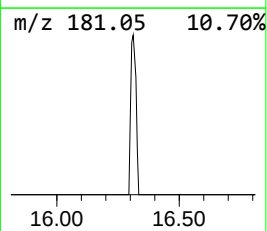
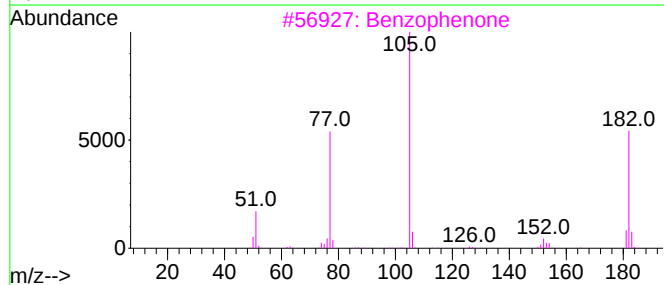
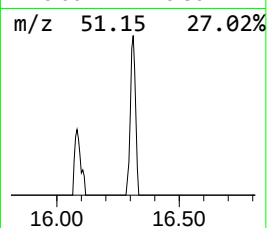
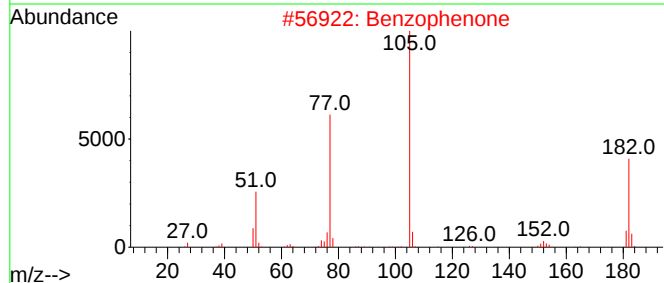
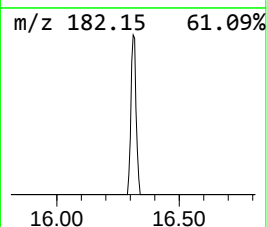
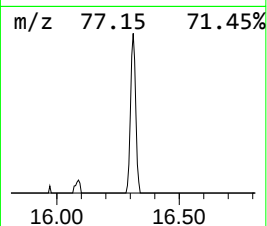
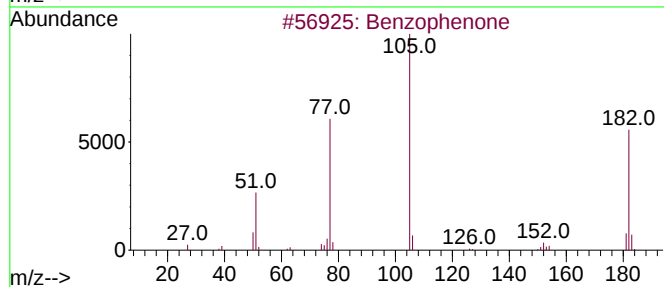
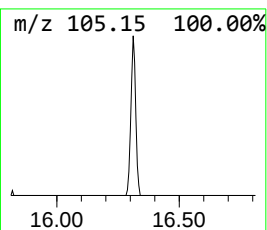
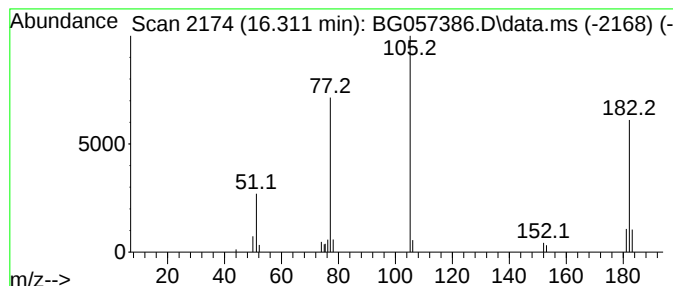
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.311	2.31 ng/ul	26005	Acenaphthene-d10	14.978

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	91
2			Benzophenone	182	C13H10O	000119-61-9	91
3			Benzophenone	182	C13H10O	000119-61-9	91
4			Benzophenone	182	C13H10O	000119-61-9	90
5			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78



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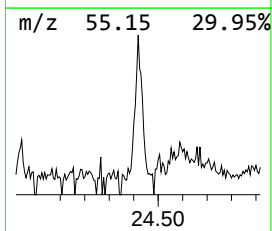
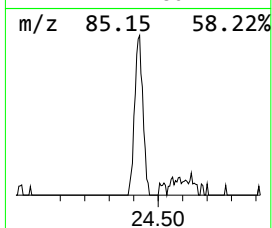
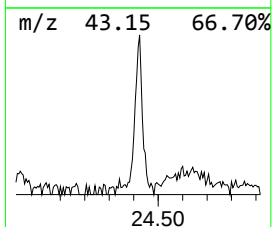
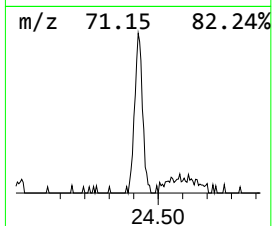
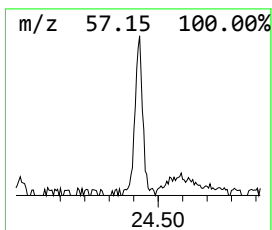
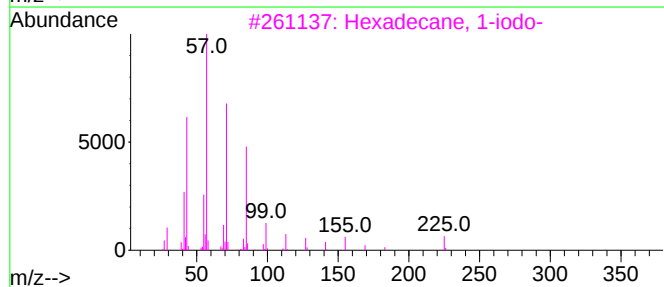
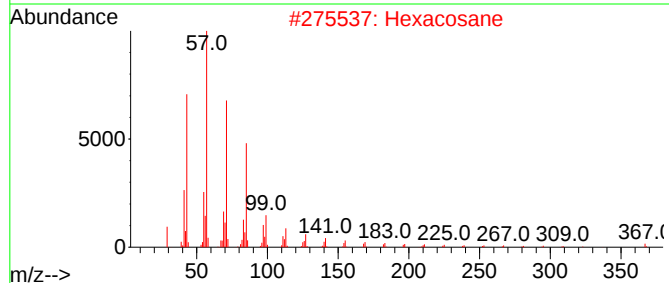
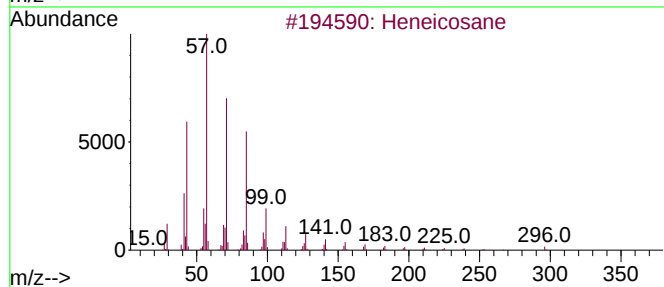
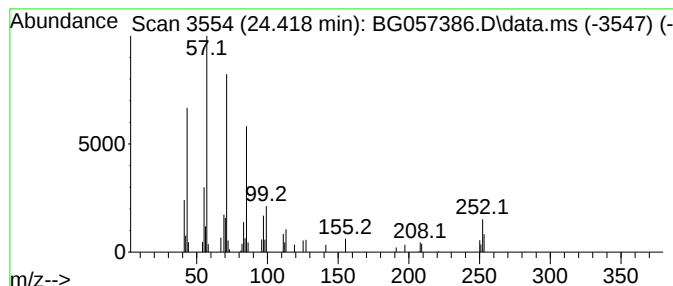
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.418	4.74 ng/ul	69512	Perylene-d12	25.528

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	80
2			Hexacosane	366	C26H54	000630-01-3	74
3			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	72
4			Hexacosane	366	C26H54	000630-01-3	72
5			Pentacosane	352	C25H52	000629-99-2	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051023\
Data File : BG057386.D
Acq On : 11 May 2023 2:29
Operator : CG/JU
Sample : 02591-17
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JREF3

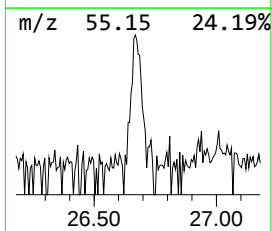
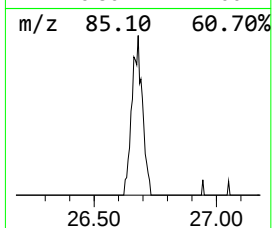
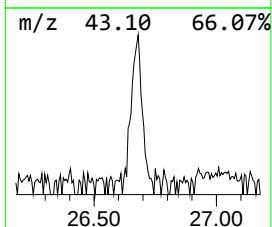
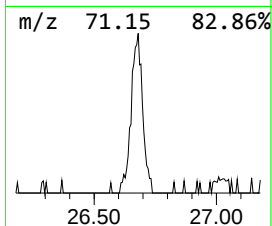
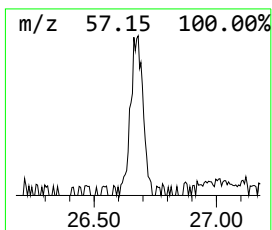
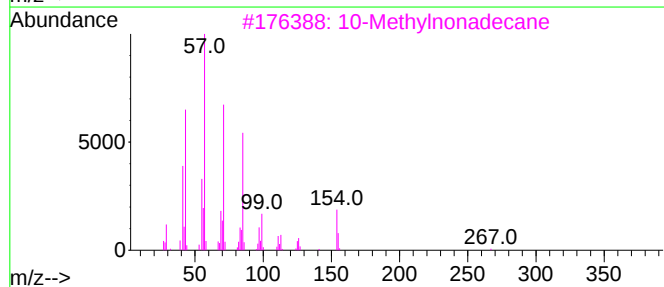
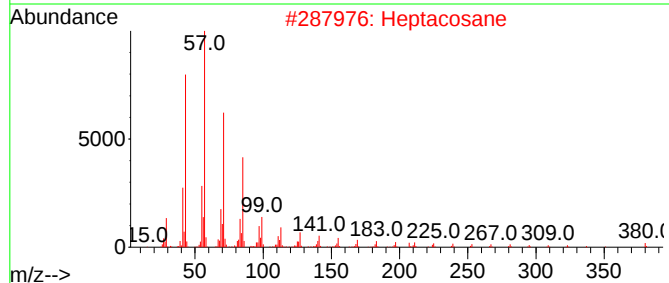
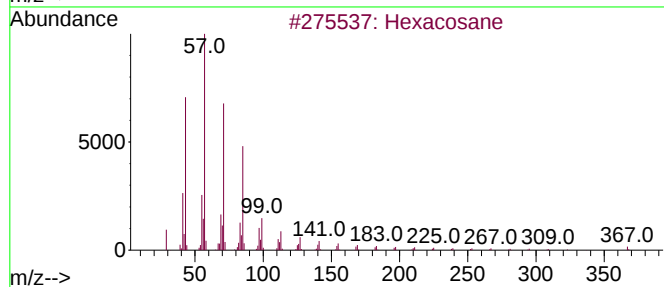
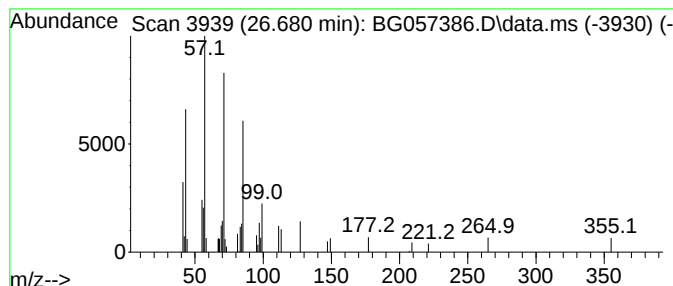
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.680	3.78 ng/ul	55502	Perylene-d12	25.528

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	90
2		Heptacosane	380	C27H56	000593-49-7	90
3		10-Methylnonadecane	282	C20H42	056862-62-5	86
4		Tetracosane	338	C24H50	000646-31-1	86
5		Octacosane	394	C28H58	000630-02-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051023\
Data File : BG057386.D
Acq On : 11 May 2023 2:29
Operator : CG/JU
Sample : 02591-17
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JREF3

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	15.231	7.7	ng/u1	86990	3	14.978	225464	20.0
Benzophenone	16.311	2.3	ng/u1	26005	3	14.978	225464	20.0
(DEL) Alkane: S...	24.418	4.7	ng/u1	69512	6	25.528	293540	20.0
(DEL) Alkane: S...	26.680	3.8	ng/u1	55502	6	25.528	293540	20.0