

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011722\
 Data File : BG052048.D
 Acq On : 18 Jan 2022 11:44
 Operator : CG/JU
 Sample : N1169-16
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BGLY3

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-BG010622.M
 Title : SVOA CALIBRATION

Signal : TIC: BG052048.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.567	9	13	22	rBV2	7459	12373	1.19%	0.117%
2	3.849	59	61	63	rBV3	1704	2008	0.19%	0.019%
3	3.996	82	86	101	rBV	107260	178770	17.19%	1.696%
4	4.255	125	130	134	rVB4	1868	2888	0.28%	0.027%
5	5.277	301	304	309	rBV3	1976	2988	0.29%	0.028%
6	7.380	656	662	673	rBV	148286	268437	25.81%	2.546%
7	7.550	683	691	697	rBV	101770	168435	16.20%	1.598%
8	7.768	722	728	737	rBV	135211	230996	22.21%	2.191%
9	8.243	802	809	817	rBV	83201	138806	13.35%	1.317%
10	8.943	921	928	936	rBV	176546	312418	30.04%	2.964%
11	9.412	1000	1008	1018	rBV	138925	252189	24.25%	2.392%
12	10.147	1126	1133	1143	rVB2	126220	225796	21.71%	2.142%
13	10.693	1220	1226	1236	rVB	184084	328483	31.59%	3.116%
14	10.834	1244	1250	1253	rBV2	2081	3063	0.29%	0.029%
15	11.081	1285	1292	1301	rBV	116314	210271	20.22%	1.995%
16	11.204	1307	1313	1325	rVB	173709	323551	31.11%	3.069%
17	12.661	1556	1561	1569	rVB2	2938	5445	0.52%	0.052%
18	13.701	1733	1738	1745	rVB3	4370	6274	0.60%	0.060%
19	14.118	1805	1809	1816	rBV3	10457	17130	1.65%	0.162%
20	14.277	1830	1836	1842	rBV	388217	539360	51.87%	5.116%
21	14.506	1871	1875	1876	rBV2	2257	2432	0.23%	0.023%
22	14.582	1881	1888	1896	rVB	404100	643187	61.85%	6.101%
23	14.764	1916	1919	1922	rVB2	3260	3311	0.32%	0.031%
24	14.887	1934	1940	1947	rVB2	212191	336351	32.34%	3.191%
25	15.064	1964	1970	1976	rBV	164167	280687	26.99%	2.663%
26	15.128	1976	1981	1992	rVB	136729	231246	22.24%	2.194%
27	15.281	2005	2007	2010	rVB3	2739	2486	0.24%	0.024%
28	15.516	2042	2047	2050	rBV	3551	4048	0.39%	0.038%
29	15.669	2067	2073	2077	rBV4	2552	5837	0.56%	0.055%
30	15.710	2077	2080	2087	rVB4	4642	6296	0.61%	0.060%
31	15.880	2103	2109	2120	rVB	534990	820903	78.94%	7.787%
32	15.980	2120	2126	2137	rBV	164873	257581	24.77%	2.443%
33	16.115	2147	2149	2153	rVB3	3867	4726	0.45%	0.045%
34	16.268	2172	2175	2178	rBV2	1708	1867	0.18%	0.018%
35	16.409	2195	2199	2202	rBV2	1087	1628	0.16%	0.015%
36	16.509	2210	2216	2220	rBV3	5415	8562	0.82%	0.081%

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011722\
 Data File : BG052048.D
 Acq On : 18 Jan 2022 11:44
 Operator : CG/JU
 Sample : N1169-16
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BGLY3

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-BG010622.M
 Title : SVOA CALIBRATION

37	16.544	2220	2222	2225	rVV3	2460	2608	0.25%	0.025%
38	16.579	2225	2228	2229	rVV3	1683	1623	0.16%	0.015%
39	16.662	2240	2242	2245	rVB3	1442	1566	0.15%	0.015%
40	16.756	2255	2258	2263	rVB4	2379	3274	0.31%	0.031%
41	16.920	2283	2286	2287	rBV2	1396	1679	0.16%	0.016%
42	16.979	2294	2296	2300	rBV3	2102	1791	0.17%	0.017%
43	17.084	2312	2314	2320	rVB4	2429	3481	0.33%	0.033%
44	17.149	2320	2325	2329	rBV2	1588	3133	0.30%	0.030%
45	17.366	2357	2362	2369	rVV4	2999	4967	0.48%	0.047%
46	17.425	2369	2372	2377	rVB6	2721	4360	0.42%	0.041%
47	17.525	2386	2389	2393	rVB3	4740	5920	0.57%	0.056%
48	17.637	2399	2408	2415	rBV	306765	455800	43.83%	4.324%
49	17.737	2418	2425	2434	rVV	613263	915711	88.06%	8.686%
50	17.807	2434	2437	2441	rVB4	8816	11054	1.06%	0.105%
51	17.895	2450	2452	2456	rVB2	2762	2903	0.28%	0.028%
52	18.042	2475	2477	2480	rVB3	2082	1519	0.15%	0.014%
53	18.283	2515	2518	2523	rBV4	3276	3918	0.38%	0.037%
54	18.394	2533	2537	2538	rBV3	1402	2025	0.19%	0.019%
55	18.418	2538	2541	2546	rVB3	2093	3407	0.33%	0.032%
56	18.459	2546	2548	2551	rBV2	1549	1910	0.18%	0.018%
57	18.506	2551	2556	2561	rBV2	36087	49146	4.73%	0.466%
58	18.577	2566	2568	2572	rVB	5551	7419	0.71%	0.070%
59	18.759	2598	2599	2602	rVB2	2279	1660	0.16%	0.016%
60	18.794	2602	2605	2607	rBV2	2215	2488	0.24%	0.024%
61	18.929	2626	2628	2630	rVB2	2142	1749	0.17%	0.017%
62	19.029	2642	2645	2648	rVB4	2081	2494	0.24%	0.024%
63	19.111	2657	2659	2662	rVB3	1810	1967	0.19%	0.019%
64	19.281	2684	2688	2690	rBV4	2988	4453	0.43%	0.042%
65	19.364	2699	2702	2706	rBV3	3511	4612	0.44%	0.044%
66	19.581	2736	2739	2741	rBV3	6390	8343	0.80%	0.079%
67	19.652	2747	2751	2759	rBV	8661	14120	1.36%	0.134%
68	19.763	2768	2770	2775	rBV3	2739	4019	0.39%	0.038%
69	20.016	2807	2813	2819	rBV	746465	1039906	100.00%	9.865%
70	20.145	2834	2835	2840	rVB5	1579	1635	0.16%	0.016%
71	20.357	2869	2871	2873	rBV3	2013	2094	0.20%	0.020%
72	20.521	2897	2899	2904	rVB5	4691	4646	0.45%	0.044%
73	20.903	2962	2964	2970	rVB6	6384	8042	0.77%	0.076%
74	21.414	3050	3051	3053	rBV	2513	2003	0.19%	0.019%
75	21.555	3070	3075	3087	rBV3	63205	153833	14.79%	1.459%
76	21.960	3137	3144	3150	rVB2	274914	466061	44.82%	4.421%

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011722\
Data File : BG052048.D
Acq On : 18 Jan 2022 11:44
Operator : CG/JU
Sample : N1169-16
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BGLY3

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-BG010622.M
Title : SVOA CALIBRATION

77	23.764	3445	3451	3457	rBV6	6149	15368	1.48%	0.146%
78	25.209	3685	3697	3710	rVB2	338136	990563	95.26%	9.397%
79	25.450	3728	3738	3751	rVB2	150319	471384	45.33%	4.472%
80	25.655	3771	3773	3776	rBV4	3777	3271	0.31%	0.031%
81	26.119	3850	3852	3854	rVB3	3082	1870	0.18%	0.018%
82	26.701	3950	3951	3952	rBV	4582	2763	0.27%	0.026%
83	31.259	4725	4727	4728	rBV2	3414	2397	0.23%	0.023%

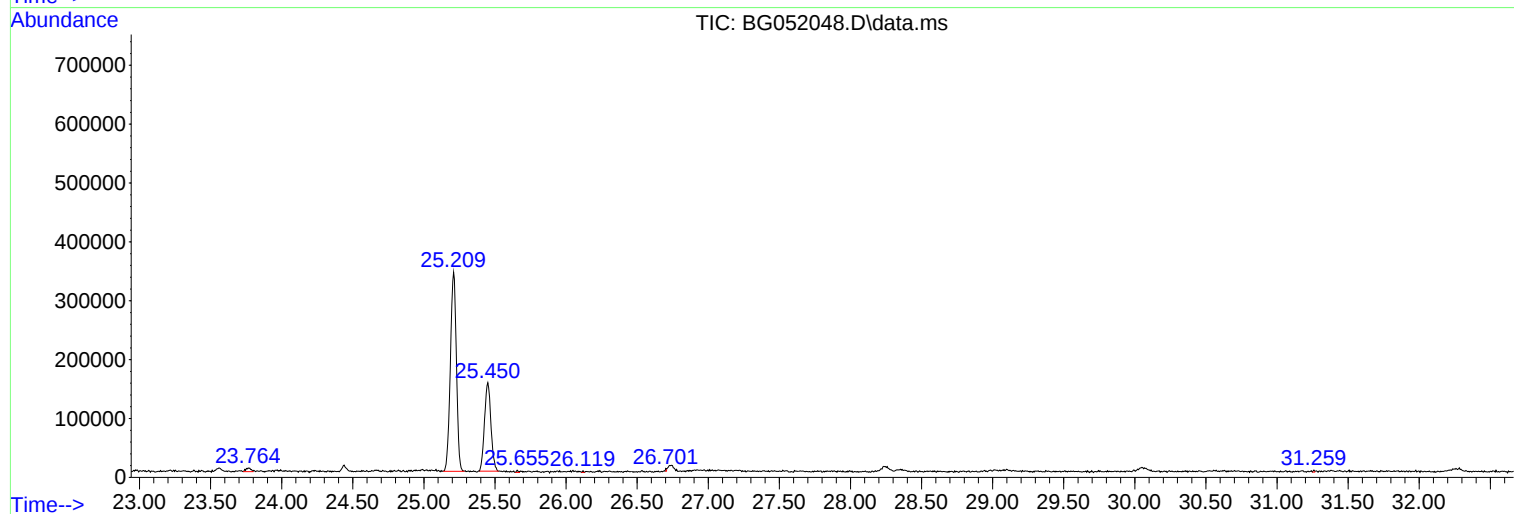
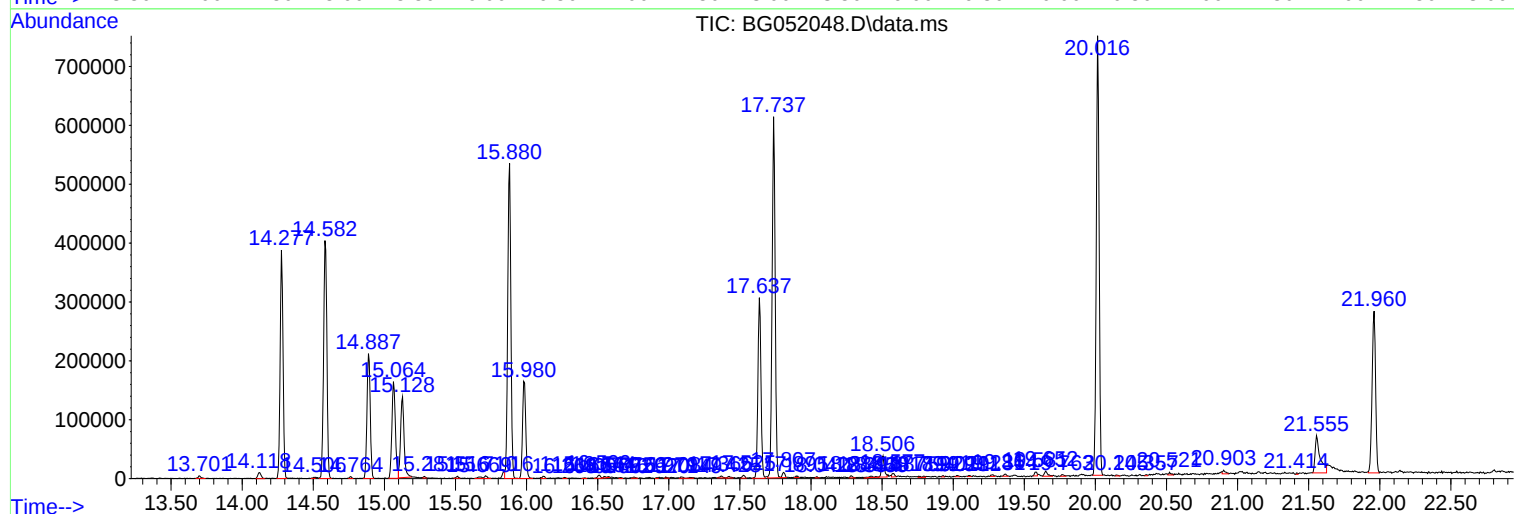
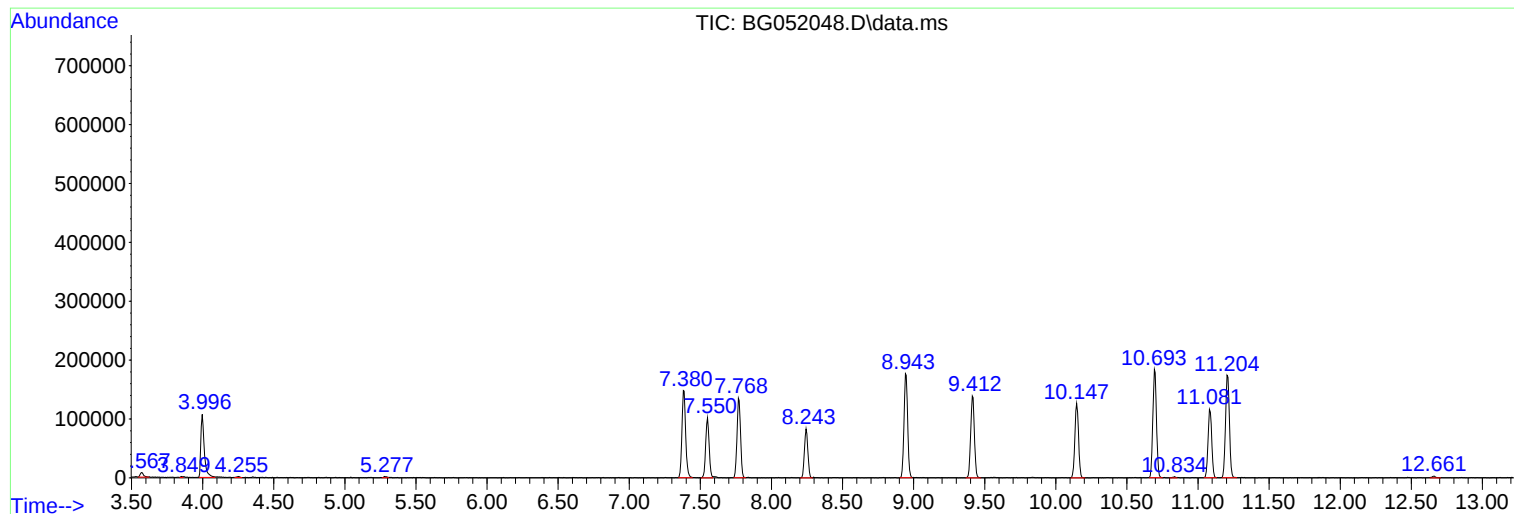
Sum of corrected areas: 10541784

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011722\
Data File : BG052048.D
Acq On : 18 Jan 2022 11:44
Operator : CG/JU
Sample : N1169-16
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BGLY3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010622.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011722\
Data File : BG052048.D
Acq On : 18 Jan 2022 11:44
Operator : CG/JU
Sample : N1169-16
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BGLY3

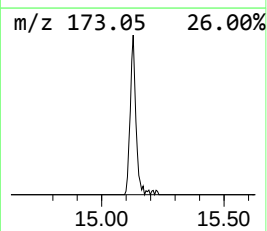
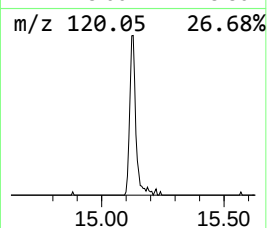
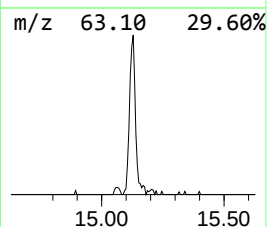
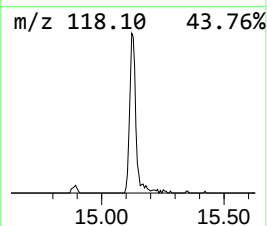
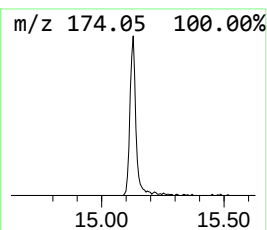
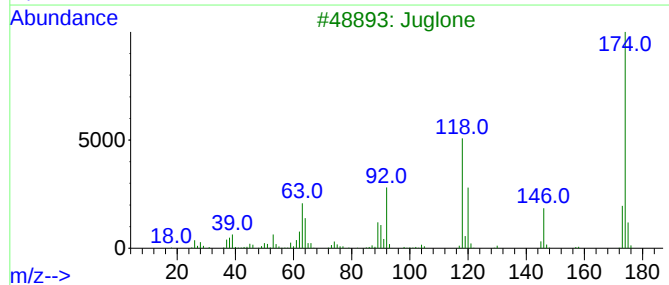
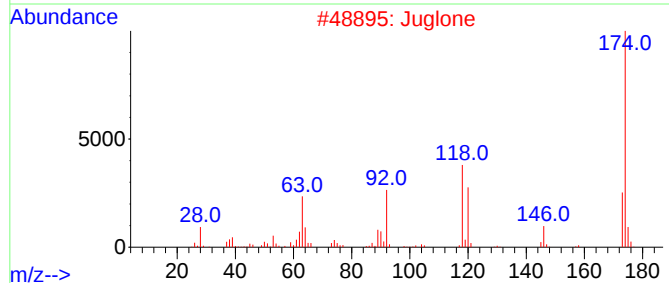
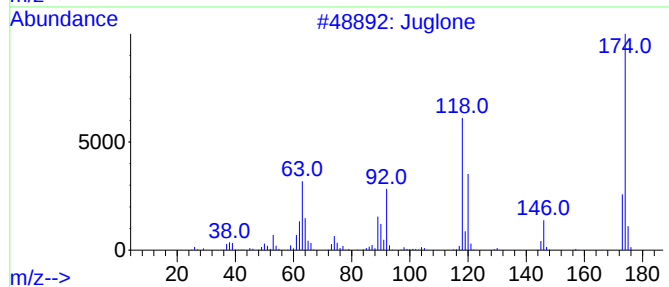
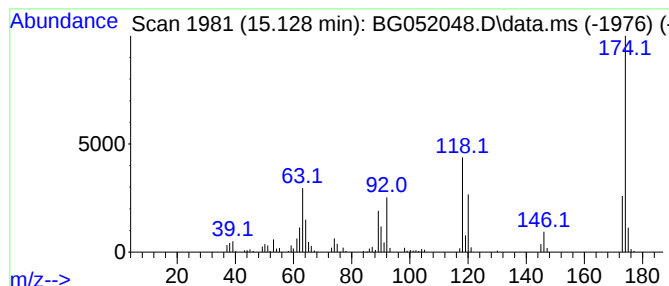
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010622.M
Quant Title : SVOA CALIBRATION

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.
15.128	13.75 ng/ul	231246	Acenaphthene-d10	14.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Juglone			174	C10H6O3	000481-39-0	98
2	Juglone			174	C10H6O3	000481-39-0	94
3	Juglone			174	C10H6O3	000481-39-0	91
4	Juglone			174	C10H6O3	000481-39-0	59
5	1-Methyl-5-(4-methylphenyl)tetra...			174	C9H10N4	068826-33-5	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011722\
Data File : BG052048.D
Acq On : 18 Jan 2022 11:44
Operator : CG/JU
Sample : N1169-16
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BGLY3

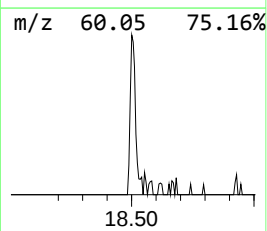
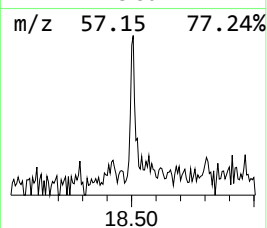
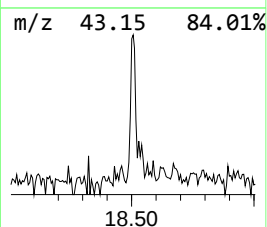
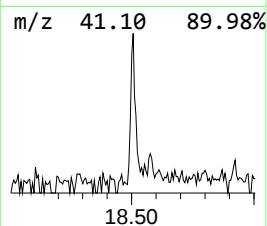
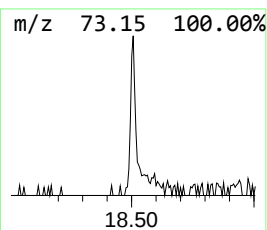
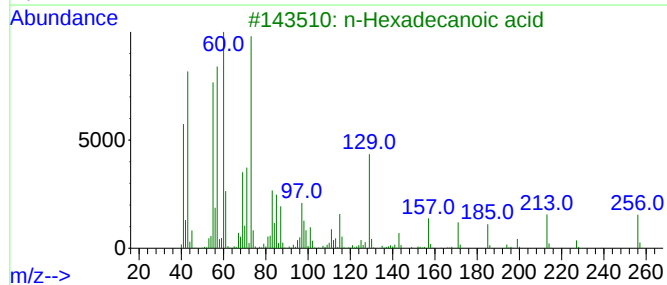
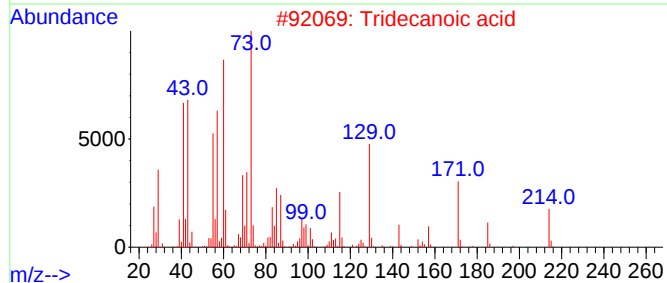
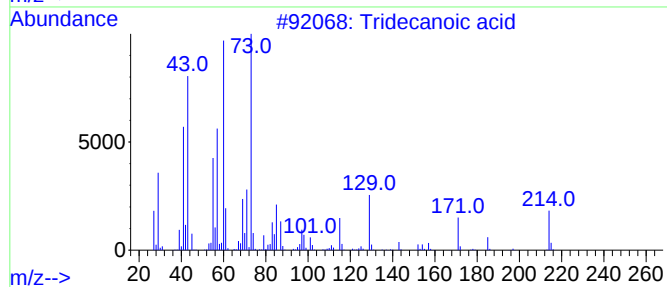
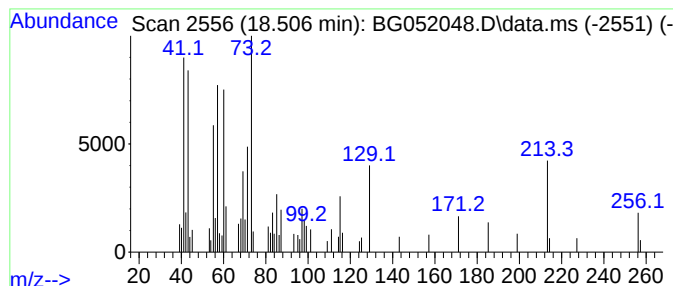
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010622.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.506	2.16 ng/ul	49146	Phenanthrene-d10	17.637

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	93
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5			Tridecanoic acid	214	C13H26O2	000638-53-9	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011722\
Data File : BG052048.D
Acq On : 18 Jan 2022 11:44
Operator : CG/JU
Sample : N1169-16
Misc :
ALS Vial : 34 Sample Multiplier: 1

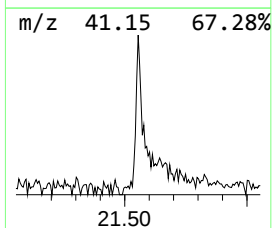
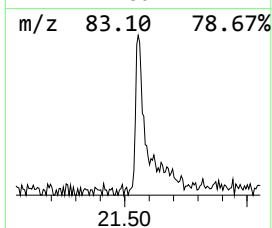
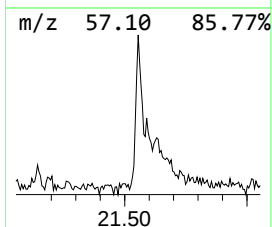
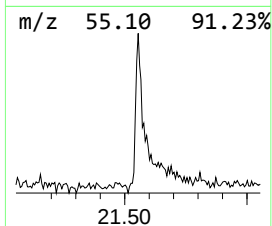
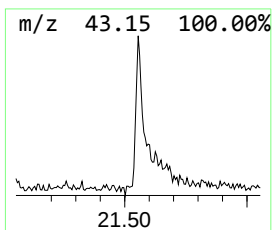
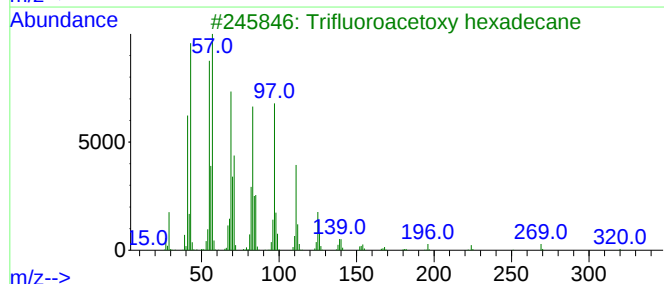
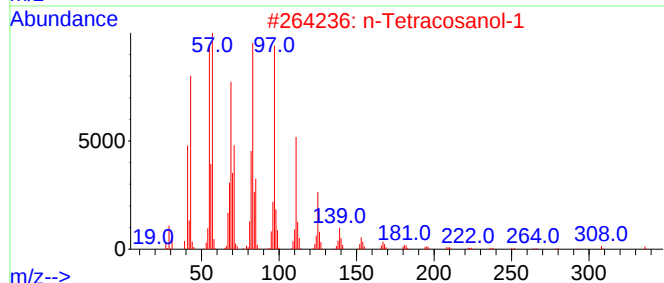
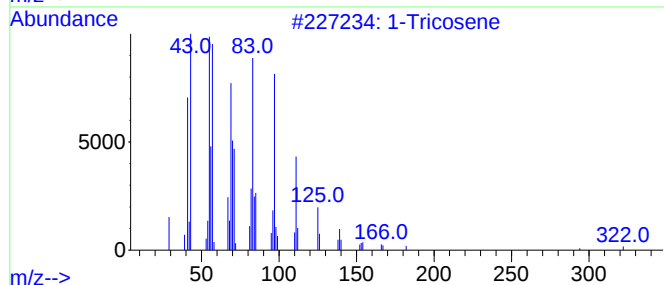
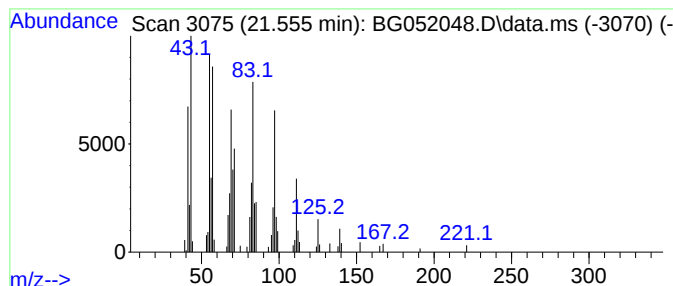
Instrument :
BNA_G
ClientSampleId :
BGLY3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010622.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 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.555	6.60 ng/ul	153833	Chrysene-d12		21.960	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Tricosene		322	C23H46	018835-32-0	95
2	n-Tetracosanol-1		354	C24H50O	000506-51-4	94
3	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	91
4	Pentafluoropropionic acid, penta...		374	C18H31F5O2	959092-08-1	91
5	1-Hexacosanol		382	C26H54O	000506-52-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011722\
Data File : BG052048.D
Acq On : 18 Jan 2022 11:44
Operator : CG/JU
Sample : N1169-16
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BGLY3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010622.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	15.128	13.8	ng/ul	231246	3	14.887	336351	20.0
Tridecanoic acid	18.506	2.2	ng/ul	49146	4	17.637	455800	20.0
(DEL) Alkane: S...	21.555	6.6	ng/ul	153833	5	21.960	466061	20.0