

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020122\
 Data File : BG052228.D
 Acq On : 1 Feb 2022 14:01
 Operator : CG/JU
 Sample : N1318-05
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 P031-TW001-B-01

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-BG013122.M
 Title : SVOA CALIBRATION

Signal : TIC: BG052228.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.564	9	13	19	rVB4	7622	13036	1.30%	0.130%
2	3.998	84	87	97	rBV2	14253	26755	2.66%	0.268%
3	4.345	142	146	150	rBV3	2635	3839	0.38%	0.038%
4	7.376	655	662	672	rBV3	39347	71322	7.09%	0.714%
5	7.540	683	690	698	rBV	109090	181653	18.05%	1.817%
6	7.764	721	728	736	rVB	111938	197306	19.60%	1.974%
7	8.234	802	808	815	rBV	112413	184038	18.29%	1.841%
8	8.939	921	928	937	rVB	94863	163932	16.29%	1.640%
9	9.403	1000	1007	1017	rVB	143945	252644	25.10%	2.528%
10	9.826	1073	1079	1082	rVB3	4661	6711	0.67%	0.067%
11	10.137	1125	1132	1139	rBV2	117356	206576	20.53%	2.067%
12	10.689	1218	1226	1236	rBV	155171	278639	27.69%	2.788%
13	11.071	1285	1291	1304	rVB	150811	270254	26.85%	2.704%
14	11.200	1304	1313	1320	rBV	119954	224870	22.34%	2.250%
15	12.469	1525	1529	1536	rBV2	1193	2110	0.21%	0.021%
16	12.645	1555	1559	1564	rVB4	2569	4636	0.46%	0.046%
17	13.480	1696	1701	1705	rBV3	1811	2495	0.25%	0.025%
18	13.691	1732	1737	1740	rBV3	4117	5823	0.58%	0.058%
19	14.267	1828	1835	1843	rBV	350263	492391	48.92%	4.926%
20	14.496	1870	1874	1877	rBV4	1801	2068	0.21%	0.021%
21	14.572	1880	1887	1895	rVV	385315	586997	58.32%	5.873%
22	14.743	1914	1916	1922	rVB4	1953	2949	0.29%	0.030%
23	14.878	1933	1939	1948	rVB	255182	395121	39.26%	3.953%
24	15.066	1964	1971	1984	rBV3	23688	50160	4.98%	0.502%
25	15.500	2041	2045	2052	rBV4	1870	3394	0.34%	0.034%
26	15.653	2066	2071	2076	rBV2	3303	5573	0.55%	0.056%
27	15.694	2076	2078	2083	rVB4	1993	2391	0.24%	0.024%
28	15.865	2100	2107	2119	rBV	488935	742039	73.73%	7.424%
29	15.976	2119	2126	2134	rBV	145263	223508	22.21%	2.236%
30	16.105	2145	2148	2152	rVB3	3395	4048	0.40%	0.040%
31	16.258	2171	2174	2177	rVB3	1553	1598	0.16%	0.016%
32	16.446	2201	2206	2207	rBV2	902	1379	0.14%	0.014%
33	16.499	2213	2215	2218	rBV2	1437	1793	0.18%	0.018%
34	16.534	2218	2221	2223	rBV2	2311	2231	0.22%	0.022%
35	16.558	2223	2225	2227	rBV2	2009	1600	0.16%	0.016%
36	16.746	2254	2257	2259	rBV2	1939	2019	0.20%	0.020%

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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-BG013122.M
 Title : SVOA CALIBRATION

37	16.822	2267	2270	2273	rBV2	905	1399	0.14%	0.014%
38	16.904	2281	2284	2285	rBV2	1638	1394	0.14%	0.014%
39	17.063	2308	2311	2312	rBV	1277	1344	0.13%	0.013%
40	17.081	2312	2314	2317	rVB2	1498	1751	0.17%	0.018%

41	17.357	2358	2361	2365	rBV4	3152	3950	0.39%	0.040%
42	17.409	2367	2370	2375	rVB3	3069	3867	0.38%	0.039%
43	17.509	2384	2387	2394	rVB5	3700	5478	0.54%	0.055%
44	17.627	2398	2407	2413	rBV	336076	510179	50.69%	5.104%
45	17.721	2415	2423	2432	rVV	551690	860040	85.45%	8.605%

46	17.897	2450	2453	2454	rBV3	1317	1361	0.14%	0.014%
47	18.003	2469	2471	2474	rBV3	2005	2243	0.22%	0.022%
48	18.097	2482	2487	2489	rBV4	2404	3428	0.34%	0.034%
49	18.203	2503	2505	2511	rVB5	2352	4408	0.44%	0.044%
50	18.261	2513	2515	2516	rBV	2787	2195	0.22%	0.022%

51	18.320	2524	2525	2528	rVB3	1622	1322	0.13%	0.013%
52	18.449	2546	2547	2549	rVB2	2575	1525	0.15%	0.015%
53	18.696	2587	2589	2592	rVB3	2221	1812	0.18%	0.018%
54	18.902	2622	2624	2627	rBV4	1820	2702	0.27%	0.027%
55	19.195	2673	2674	2676	rBV2	2133	1863	0.19%	0.019%

56	19.342	2697	2699	2704	rBV6	3293	4753	0.47%	0.048%
57	19.571	2734	2738	2745	rVV8	6304	12846	1.28%	0.129%
58	19.642	2746	2750	2754	rVB3	9129	13771	1.37%	0.138%
59	19.877	2787	2790	2791	rBV3	3321	3580	0.36%	0.036%
60	20.000	2805	2811	2821	rVB	689864	1006450	100.00%	10.069%

61	20.400	2877	2879	2882	rVB4	2524	2218	0.22%	0.022%
62	21.005	2980	2982	2984	rBV3	2787	1764	0.18%	0.018%
63	21.234	3015	3021	3023	rBV5	3873	6981	0.69%	0.070%
64	21.798	3113	3117	3121	rBV	30231	40247	4.00%	0.403%
65	21.939	3134	3141	3149	rBV	319848	537498	53.41%	5.378%

66	22.743	3276	3278	3288	rVB8	12180	27458	2.73%	0.275%
67	23.178	3346	3352	3359	rBV3	69434	128222	12.74%	1.283%
68	23.531	3408	3412	3416	rVB6	9151	14548	1.45%	0.146%
69	23.701	3436	3441	3449	rBV3	22481	50395	5.01%	0.504%
70	24.400	3555	3560	3567	rVB6	11451	26604	2.64%	0.266%

71	24.858	3629	3638	3649	rVB4	40676	116128	11.54%	1.162%
72	25.175	3681	3692	3709	rVB2	323923	953953	94.78%	9.544%
73	25.416	3722	3733	3746	rBV2	177317	559391	55.58%	5.597%
74	26.280	3870	3880	3891	rBV4	55639	188957	18.77%	1.890%
75	28.066	4173	4184	4198	rBV5	69302	267465	26.58%	2.676%

76	29.211	4377	4379	4380	rBV2	3365	1782	0.18%	0.018%
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ClientSampleId :
P031-TW001-B-01

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-BG013122.M
Title : SVOA CALIBRATION

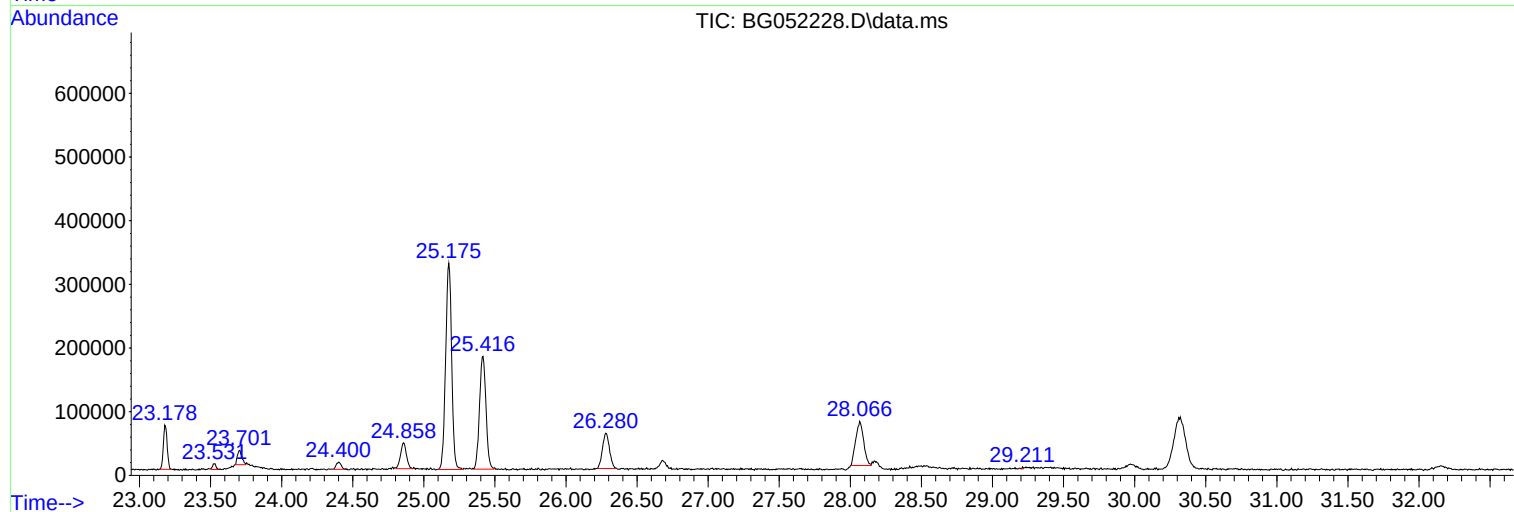
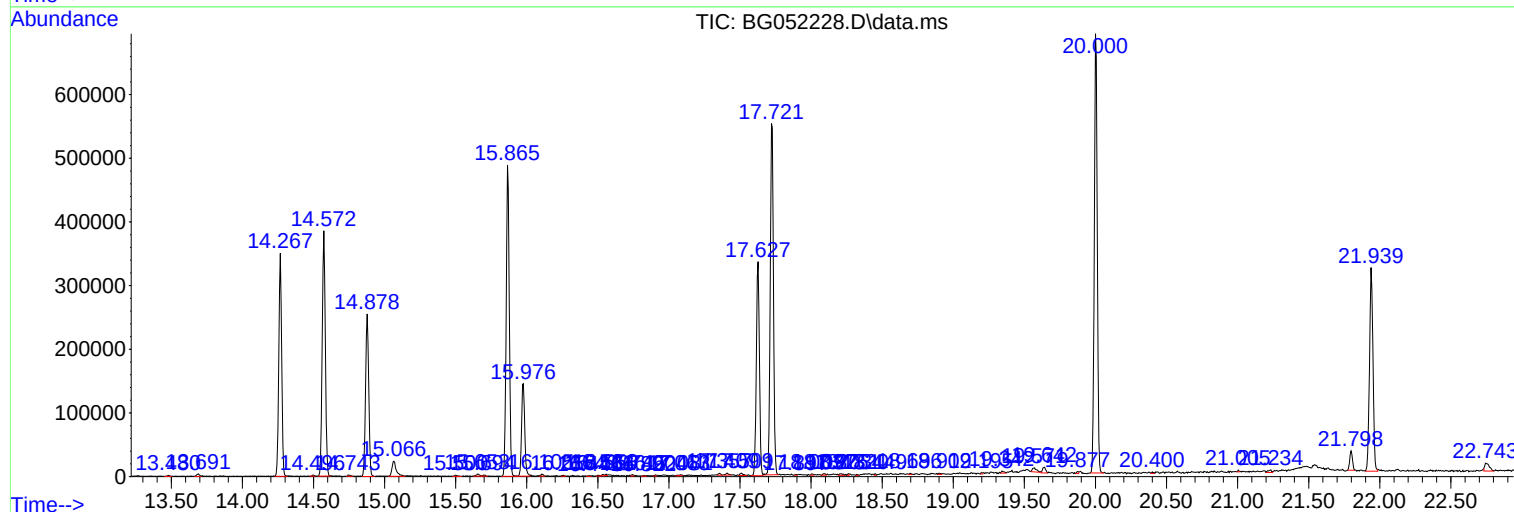
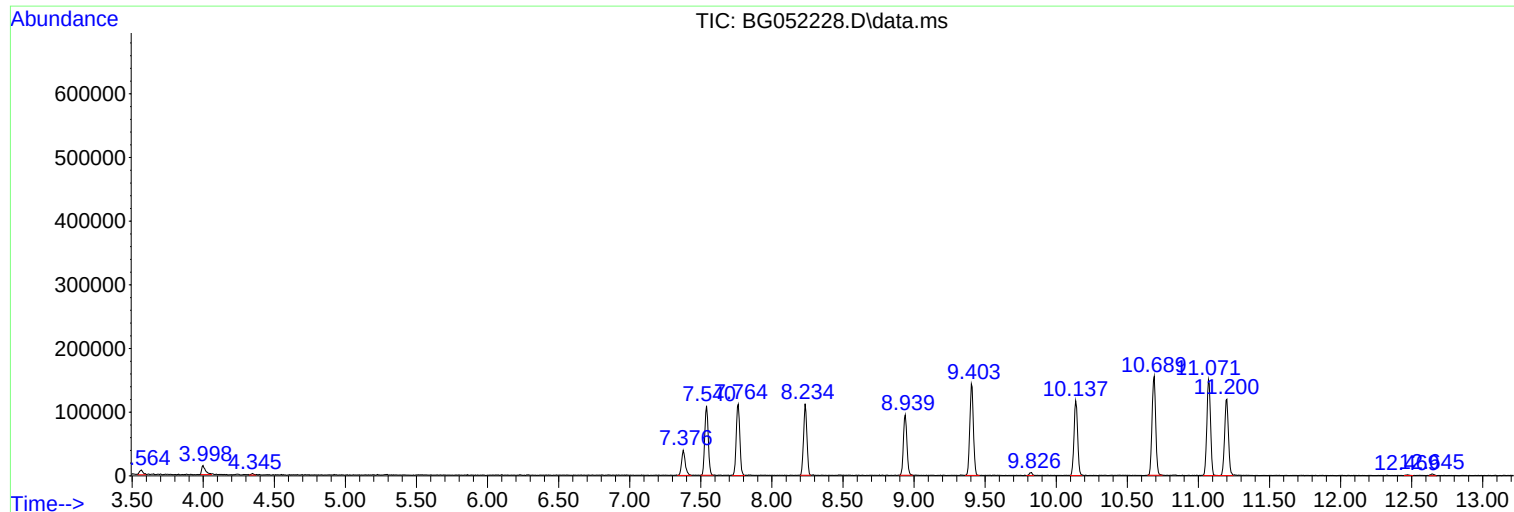
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Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020122\
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Misc :
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Instrument :
BNA_G
ClientSampleId :
P031-TW001-B-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG013122.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020122\
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Acq On : 1 Feb 2022 14:01
Operator : CG/JU
Sample : N1318-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P031-TW001-B-01

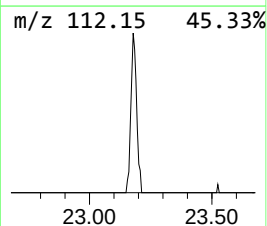
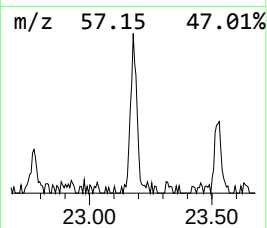
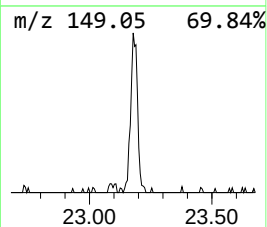
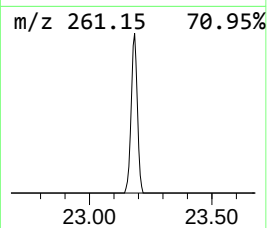
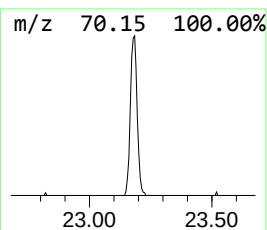
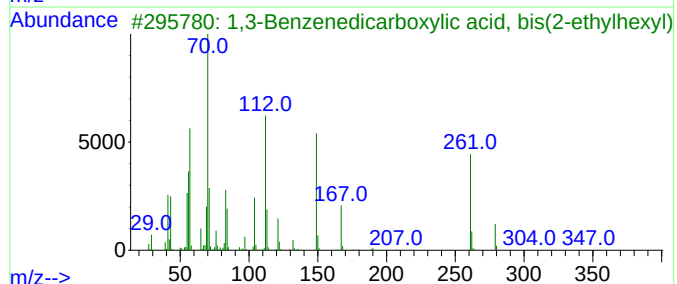
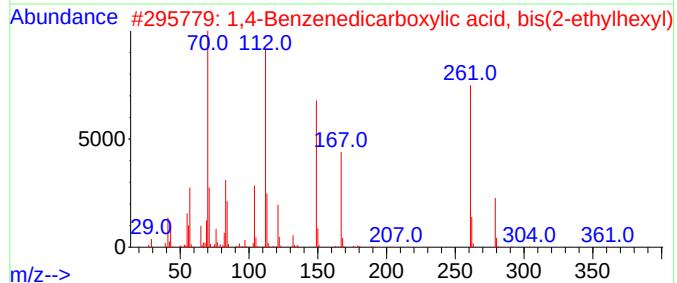
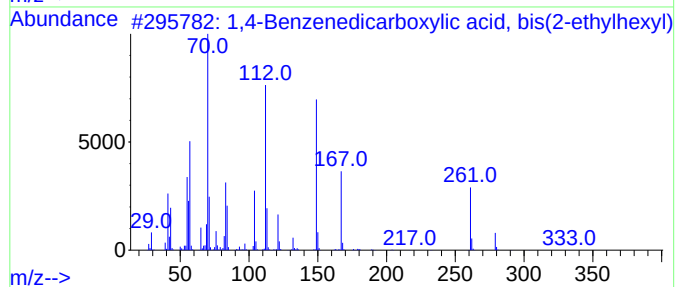
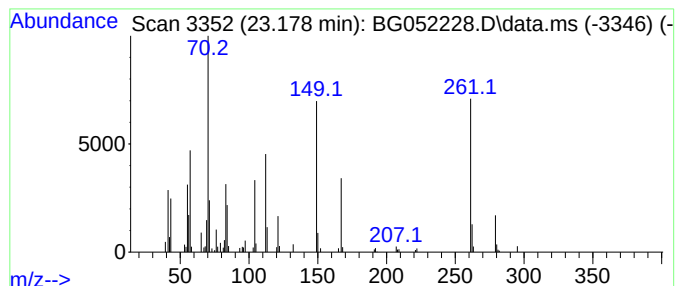
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG013122.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 1,4-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.178	4.77 ng/ul	128222	Chrysene-d12	21.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	87		
2	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	72		
3	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	72		
4	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	59		
5	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	50		



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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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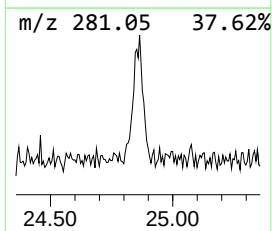
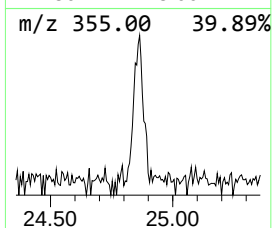
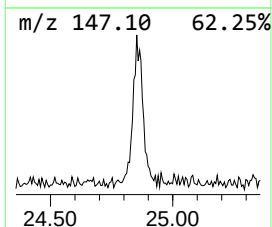
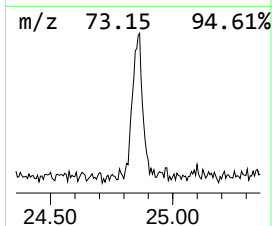
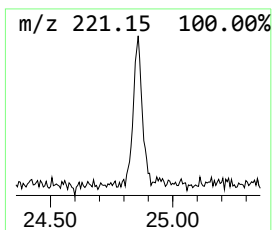
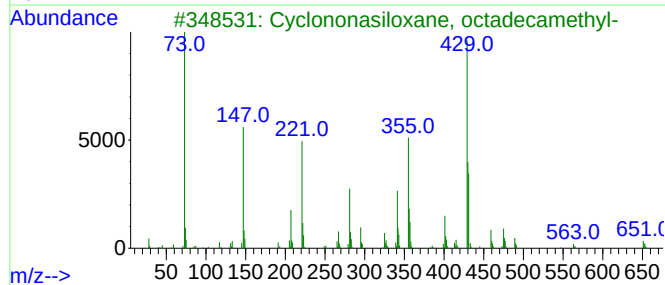
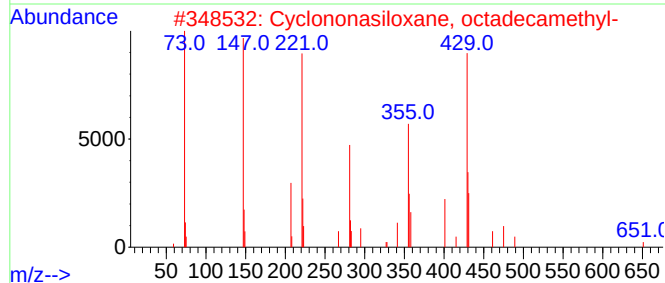
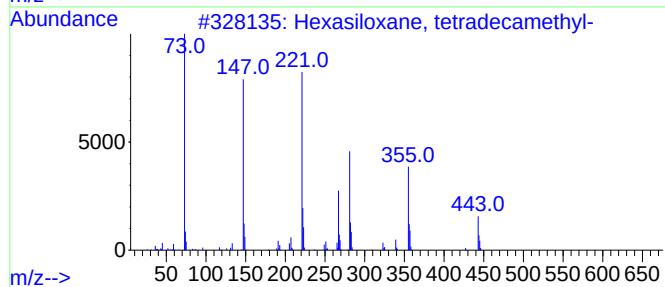
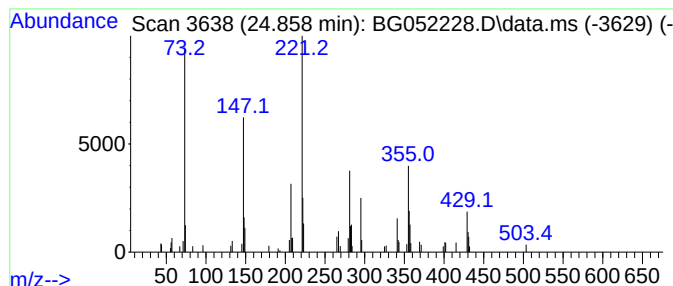
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG013122.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.858	4.15 ng/ul	116128	Perylene-d12	25.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	47
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	40
3			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	40
4			3,6-Dioxo-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
5			2,3-Dimercaptobutane-1,4-diol, 4TMS	442	C16H42O2S2Si4	959295-06-8	32



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ClientSampleId :
P031-TW001-B-01

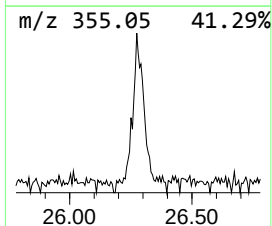
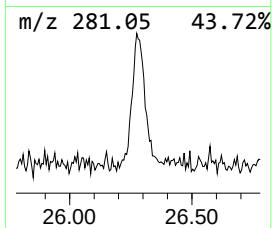
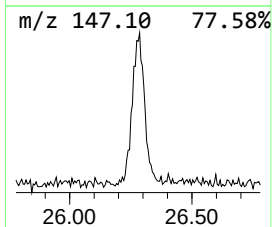
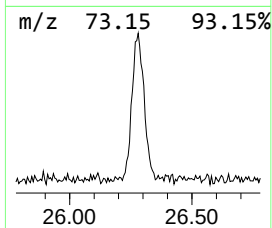
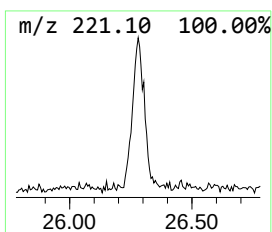
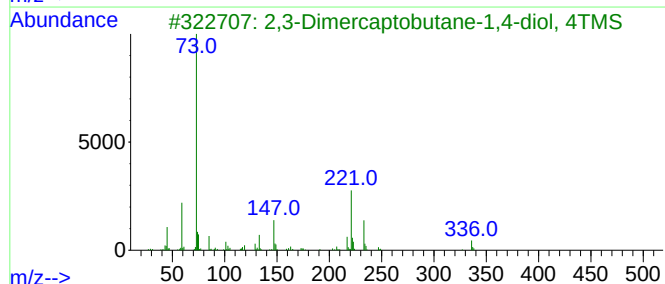
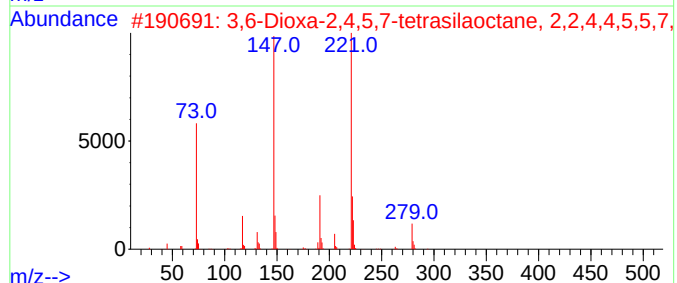
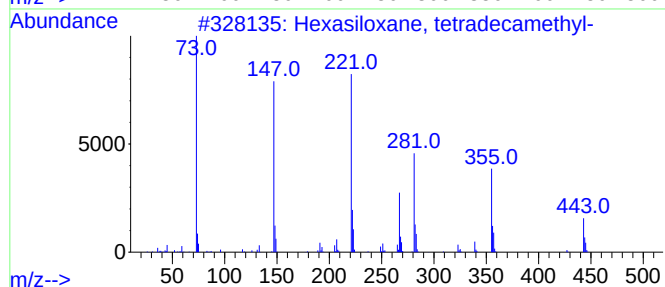
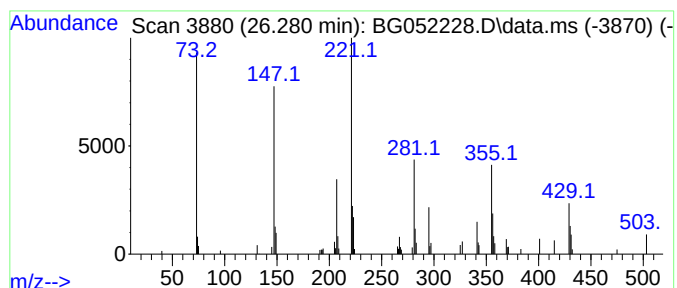
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG013122.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.280	6.76 ng/ul	188957	Perylene-d12	25.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	64
2			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
3			2,3-Dimercaptobutane-1,4-diol, 4TMS	442	C16H42O5S2Si4	959295-06-8	27
4			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	25
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	22



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P031-TW001-B-01

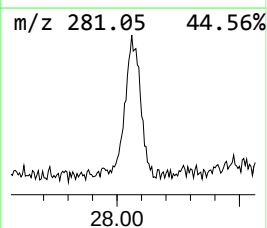
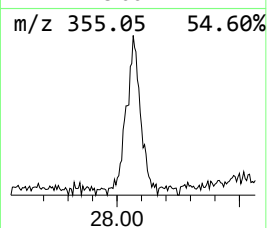
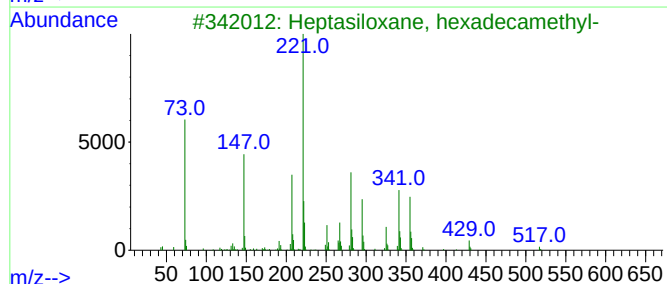
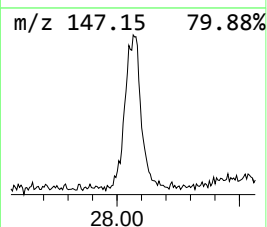
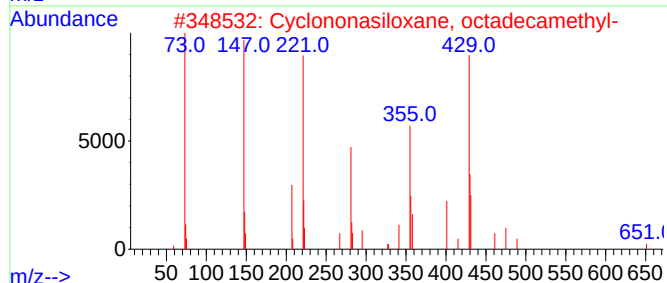
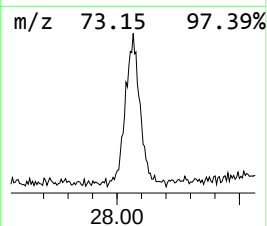
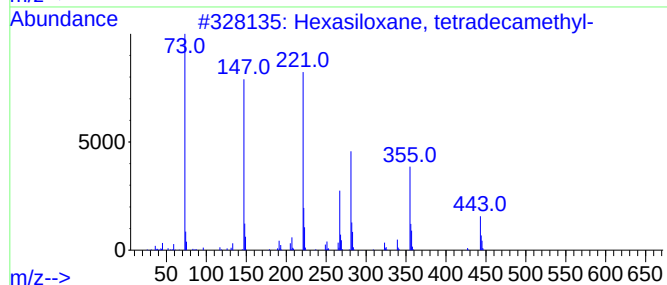
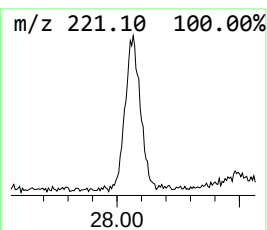
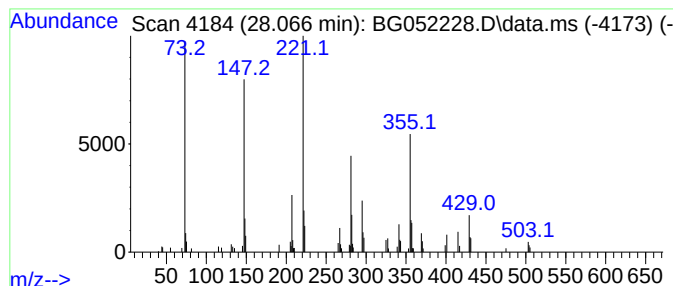
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG013122.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 Hexasiloxane, tetradecamethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.066	9.56 ng/ul	267465	Perylene-d12	25.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	80
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	62
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	50
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
5			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020122\
Data File : BG052228.D
Acq On : 1 Feb 2022 14:01
Operator : CG/JU
Sample : N1318-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P031-TW001-B-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG013122.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
1,4-Benzenedica...	23.178	4.8	ng/u1	128222	5	21.939	537498	20.0
unknown-01	24.858	4.2	ng/u1	116128	6	25.410	559391	20.0
unknown-02	26.280	6.8	ng/u1	188957	6	25.410	559391	20.0
Hexasiloxane, t...	28.066	9.6	ng/u1	267465	6	25.410	559391	20.0