

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012624\
 Data File : BG060444.D
 Acq On : 26 Jan 2024 16:56
 Operator : MA/JU
 Sample : P1231-06
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BH6Z9

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-BG012624.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG060444.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.360	42	46	51	rBV	31521	43118	0.63%	0.056%
2	3.402	51	53	57	rVB3	12866	15222	0.22%	0.020%
3	3.619	89	90	95	rVV4	6804	7378	0.11%	0.010%
4	3.772	112	116	131	rBV	217242	399914	5.83%	0.524%
5	4.113	169	174	176	rBV3	13181	17851	0.26%	0.023%
6	5.017	324	328	331	rBV4	6290	10260	0.15%	0.013%
7	5.458	400	403	407	rVB2	12469	16474	0.24%	0.022%
8	7.086	675	680	695	rBV	140790	278992	4.07%	0.365%
9	7.250	700	708	721	rBV	614327	1048572	15.29%	1.374%
10	7.456	737	743	755	rVV	506269	907098	13.22%	1.188%
11	7.926	816	823	831	rBV	574488	1006093	14.67%	1.318%
12	8.631	935	943	954	rBV	407817	786724	11.47%	1.031%
13	8.754	958	964	967	rVB5	9878	16399	0.24%	0.021%
14	9.024	1005	1010	1012	rBV6	6560	9730	0.14%	0.013%
15	9.083	1013	1020	1032	rBV	663978	1187584	17.31%	1.556%
16	9.242	1044	1047	1052	rBV7	5184	7379	0.11%	0.010%
17	9.806	1136	1143	1154	rBV	503365	929777	13.55%	1.218%
18	10.023	1178	1180	1184	rVB4	7995	8397	0.12%	0.011%
19	10.076	1184	1189	1190	rBV4	6819	8347	0.12%	0.011%
20	10.346	1228	1235	1247	rBV	800114	1493641	21.77%	1.957%
21	10.728	1292	1300	1312	rBV	917871	1642003	23.94%	2.151%
22	10.863	1315	1323	1339	rBV	724341	1453704	21.19%	1.904%
23	11.281	1390	1394	1398	rVB4	10126	14765	0.22%	0.019%
24	11.375	1405	1410	1421	rBV	61198	126340	1.84%	0.165%
25	11.739	1469	1472	1475	rVB4	5278	7497	0.11%	0.010%
26	12.315	1565	1570	1576	rBV3	14554	27598	0.40%	0.036%
27	12.861	1654	1663	1667	rBV5	49436	82152	1.20%	0.108%
28	12.932	1670	1675	1677	rBV6	13670	18035	0.26%	0.024%
29	13.090	1700	1702	1709	rVB5	4514	7009	0.10%	0.009%
30	13.372	1743	1750	1755	rBV7	4222	11611	0.17%	0.015%
31	13.449	1758	1763	1771	rVB5	19377	34895	0.51%	0.046%
32	13.772	1816	1818	1821	rBV4	4757	6898	0.10%	0.009%
33	13.883	1834	1837	1841	rVB4	6939	7759	0.11%	0.010%
34	13.966	1844	1851	1861	rBV	1996962	2846954	41.50%	3.729%
35	14.207	1887	1892	1894	rBV2	39110	52523	0.77%	0.069%
36	14.259	1894	1901	1917	rVB	2215745	3593499	52.39%	4.707%

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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-BG012624.MA.M
 Title : SVOA CALIBRATION

37	14.565	1940	1953	1961	rBV	1776833	2821786	41.14%	3.696%
38	14.635	1961	1965	1971	rVB2	82246	115418	1.68%	0.151%
39	14.765	1982	1987	1997	rBV3	86754	210705	3.07%	0.276%
40	14.970	2017	2022	2024	rBV6	5376	8457	0.12%	0.011%
41	15.076	2037	2040	2044	rBV5	6470	8084	0.12%	0.011%
42	15.241	2061	2068	2073	rBV3	180369	322984	4.71%	0.423%
43	15.294	2073	2077	2082	rVV2	45453	70813	1.03%	0.093%
44	15.376	2084	2091	2097	rVB	117730	172759	2.52%	0.226%
45	15.558	2114	2122	2135	rBV	3072517	4744862	69.17%	6.215%
46	15.670	2135	2141	2149	rBV	779755	1164334	16.97%	1.525%
47	15.793	2157	2162	2166	rVB7	14491	22791	0.33%	0.030%
48	15.916	2176	2183	2191	rBV	95673	154093	2.25%	0.202%
49	16.010	2196	2199	2202	rVB4	13171	13063	0.19%	0.017%
50	16.163	2221	2225	2230	rVB7	10666	12660	0.18%	0.017%
51	16.339	2250	2255	2259	rBV6	13201	21106	0.31%	0.028%
52	16.433	2268	2271	2276	rBV7	6671	11566	0.17%	0.015%
53	16.715	2317	2319	2322	rBV4	5796	7300	0.11%	0.010%
54	16.851	2338	2342	2346	rBV6	6852	12405	0.18%	0.016%
55	16.898	2346	2350	2355	rVV	48258	69580	1.01%	0.091%
56	16.974	2359	2363	2368	rVB6	9200	18832	0.27%	0.025%
57	17.103	2381	2385	2389	rVB6	7477	10121	0.15%	0.013%
58	17.256	2408	2411	2414	rBV2	32650	41852	0.61%	0.055%
59	17.309	2414	2420	2430	rVV	2451686	3590456	52.34%	4.703%
60	17.409	2430	2437	2448	rVV2	3574646	5467561	79.71%	7.162%
61	17.497	2448	2452	2457	rVB7	18428	32092	0.47%	0.042%
62	17.579	2462	2466	2471	rVB3	17923	25665	0.37%	0.034%
63	17.714	2484	2489	2492	rVB6	9740	14444	0.21%	0.019%
64	17.791	2499	2502	2508	rVB8	9884	16979	0.25%	0.022%
65	17.926	2521	2525	2527	rBV4	7700	7857	0.11%	0.010%
66	17.979	2527	2534	2544	rBV	3106210	4453416	64.92%	5.834%
67	18.102	2550	2555	2556	rBV5	27230	43761	0.64%	0.057%
68	18.196	2568	2571	2580	rVB5	45983	80897	1.18%	0.106%
69	18.272	2580	2584	2588	rVB	23766	34735	0.51%	0.045%
70	18.425	2603	2610	2630	rBV	3333664	5808732	84.68%	7.609%
71	18.789	2668	2672	2675	rVB5	25349	35433	0.52%	0.046%
72	18.936	2696	2697	2701	rBV4	10112	11829	0.17%	0.015%
73	19.265	2748	2753	2757	rVB2	59496	86252	1.26%	0.113%
74	19.336	2761	2765	2770	rVV	52272	73382	1.07%	0.096%
75	19.383	2770	2773	2777	rVB5	16910	20607	0.30%	0.027%
76	19.553	2798	2802	2803	rBV	51814	58456	0.85%	0.077%

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77	19.588	2804	2808	2811	rVV3	149085	207198	3.02%	0.271%
78	19.618	2811	2813	2819	rVB4	53125	61454	0.90%	0.080%
79	19.700	2821	2827	2838	rBV	4602351	6765408	98.63%	8.862%
80	20.023	2880	2882	2884	rBV3	7566	7683	0.11%	0.010%
81	20.482	2956	2960	2964	rBV	121693	136059	1.98%	0.178%
82	20.658	2987	2990	2996	rVB7	33739	44802	0.65%	0.059%
83	20.963	3040	3042	3043	rBV2	11581	7898	0.12%	0.010%
84	21.228	3083	3087	3090	rBV6	17696	29543	0.43%	0.039%
85	21.457	3122	3126	3128	rBV4	27088	28539	0.42%	0.037%
86	21.574	3139	3146	3164	rVB2	2419686	4160831	60.66%	5.450%
87	21.751	3174	3176	3181	rVB6	38225	43508	0.63%	0.057%
88	22.344	3274	3277	3283	rVB4	33345	51988	0.76%	0.068%
89	23.026	3390	3393	3400	rVB2	73069	120624	1.76%	0.158%
90	23.214	3419	3425	3433	rBV	78583	162638	2.37%	0.213%
91	23.813	3521	3527	3534	rVB3	93402	213415	3.11%	0.280%
92	24.095	3567	3575	3584	rBV2	395985	915220	13.34%	1.199%
93	24.518	3636	3647	3667	rBV2	2506955	6859670	100.00%	8.985%
94	24.735	3673	3684	3697	rBV	1653719	4549135	66.32%	5.959%
95	25.534	3818	3820	3821	rBV2	13758	8023	0.12%	0.011%
96	25.846	3866	3873	3880	rVB4	105886	280064	4.08%	0.367%
97	26.104	3905	3917	3931	rBV3	575997	1994970	29.08%	2.613%
98	27.162	4089	4097	4109	rVB2	100704	340878	4.97%	0.447%
99	28.930	4387	4398	4418	rVB5	275481	1322210	19.28%	1.732%

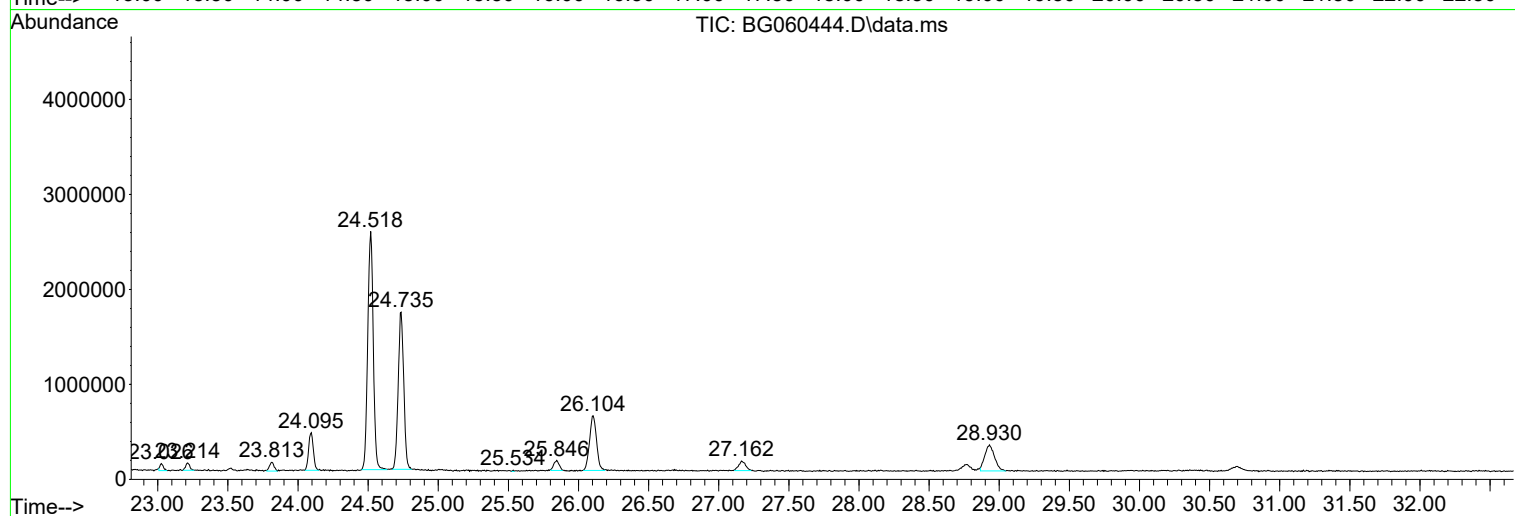
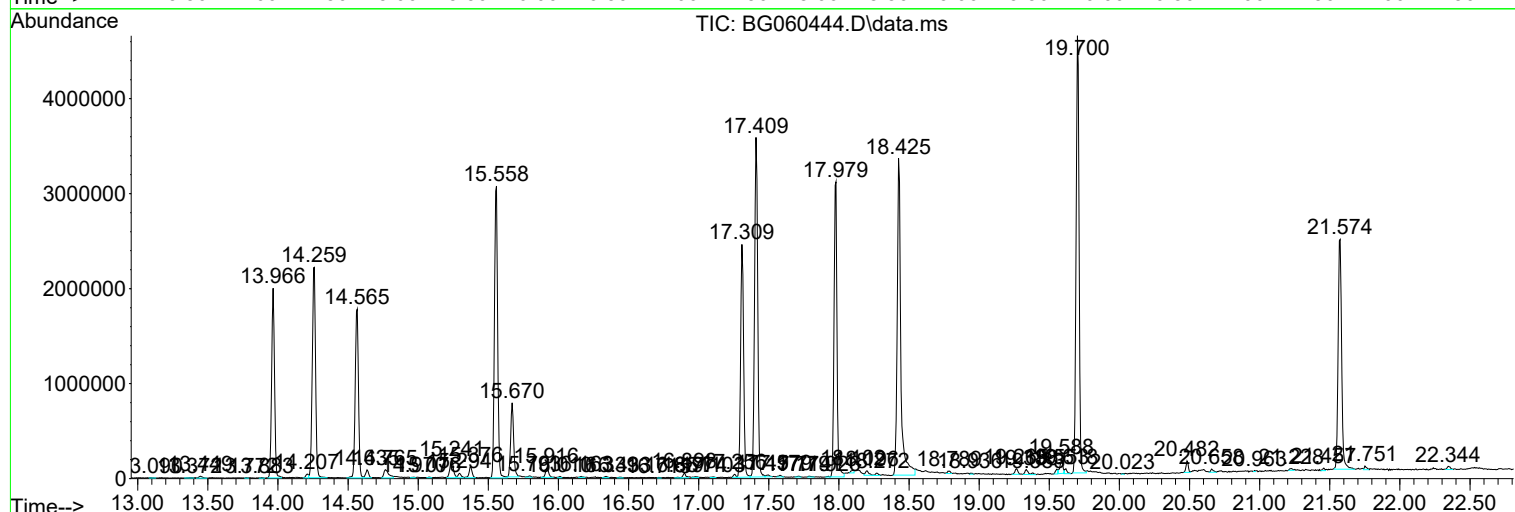
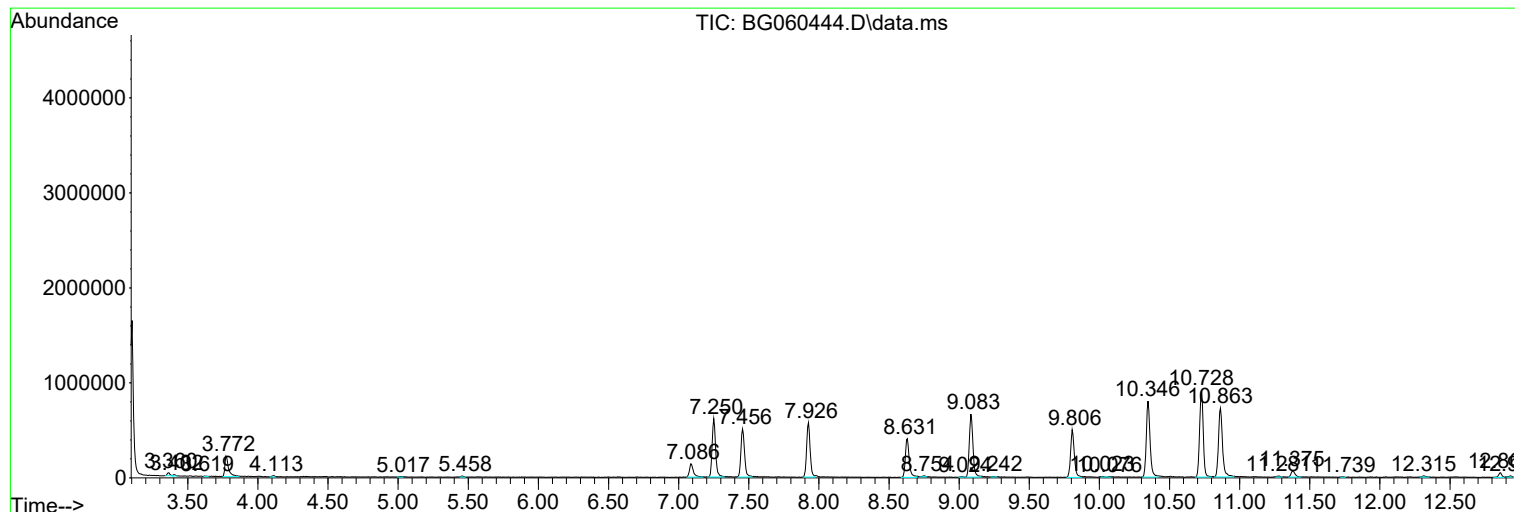
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG012624.MA.M
Quant Title : SVOA CALIBRATION

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



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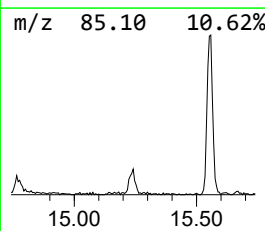
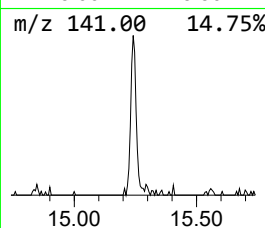
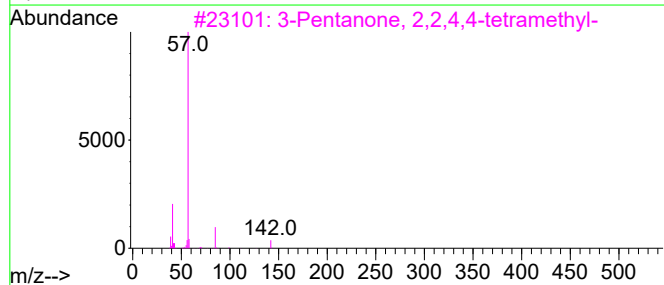
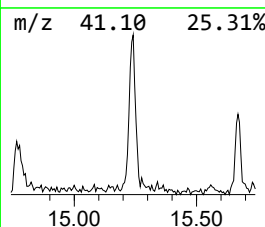
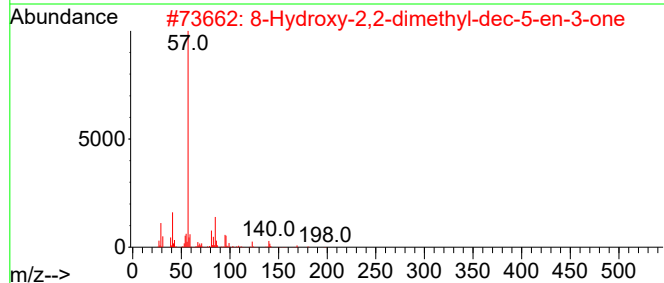
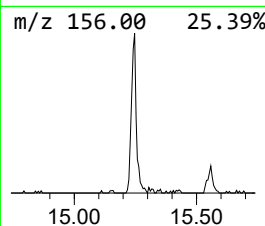
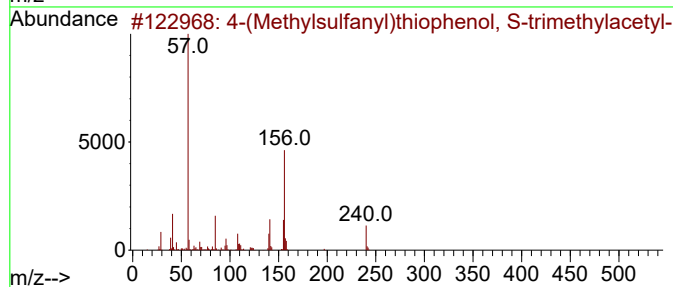
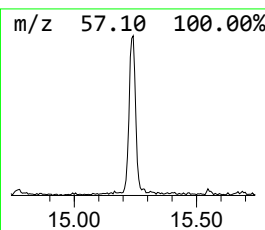
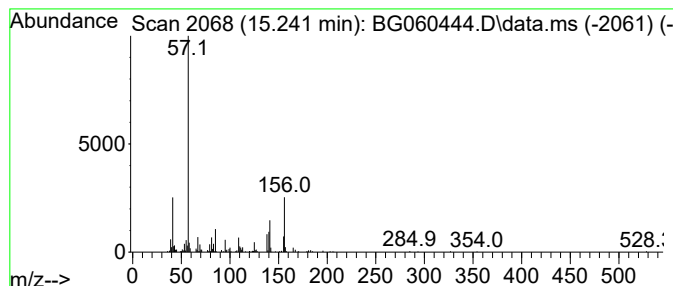
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG012624.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.241	2.29 ng/ul	322984	Acenaphthene-d10	14.565

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(Methylsulfanyl)thiophenol, S-...	240	C12H16OS2	1000469-97-3	45		
2	8-Hydroxy-2,2-dimethyl-dec-5-en-...	198	C12H22O2	1000193-60-0	25		
3	3-Pentanone, 2,2,4,4-tetramethyl-	142	C9H18O	000815-24-7	14		
4	t-Butyl n-hexyl disulfide	206	C10H22S2	064580-59-2	14		
5	7-t-Butoxybicyclo[2.2.1]heptane-...	196	C11H16O3	1000210-03-3	12		



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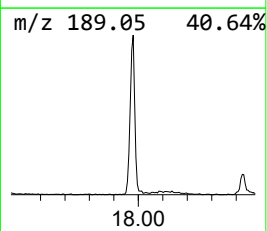
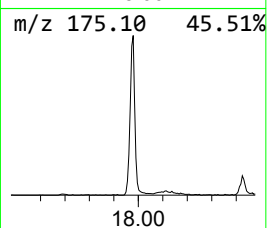
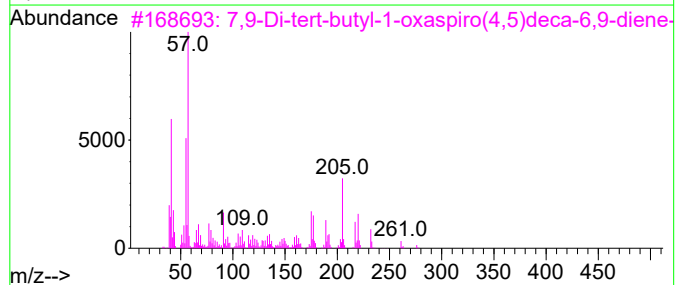
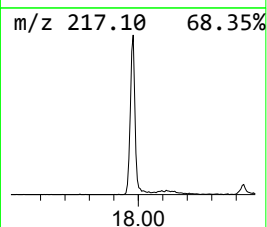
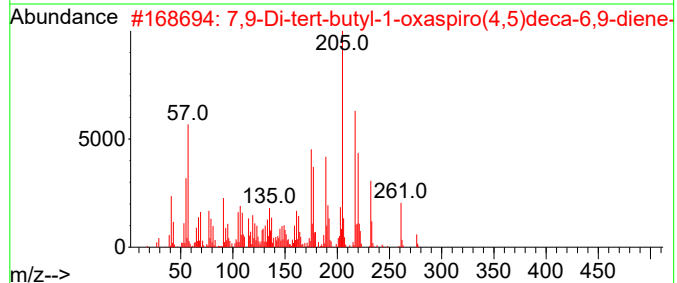
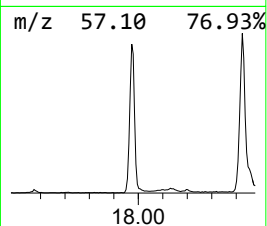
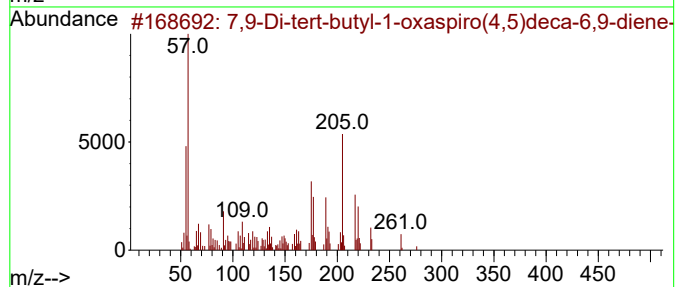
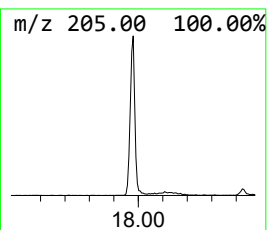
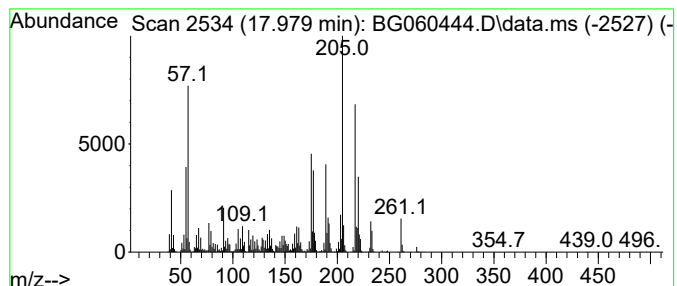
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG012624.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.979	24.81 ng/ul	4453420	Phenanthrene-d10	17.309

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	94		
2	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	94		
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	50		
4	(1R,3aR,5aR,9aS)-1,4,4,7-Tetrame...	220	C15H24O	104188-25-2	42		
5	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	42		



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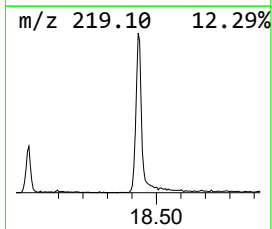
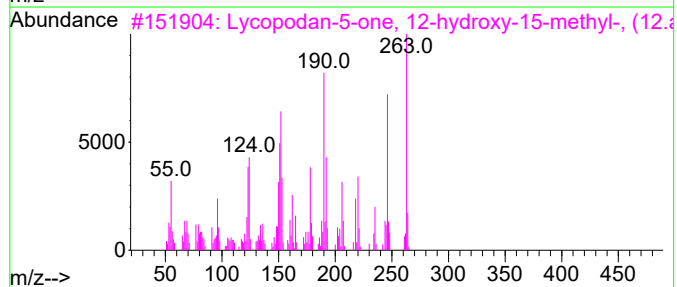
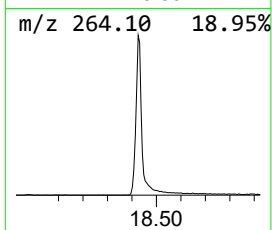
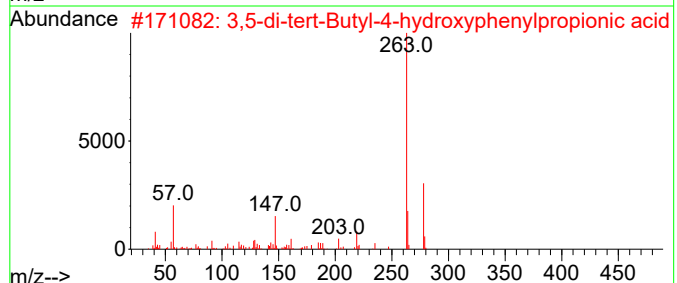
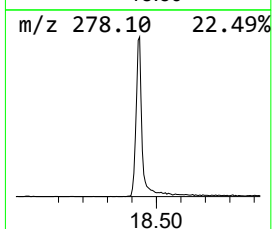
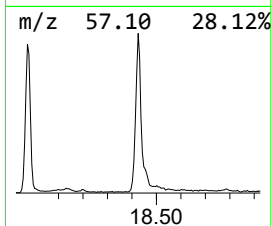
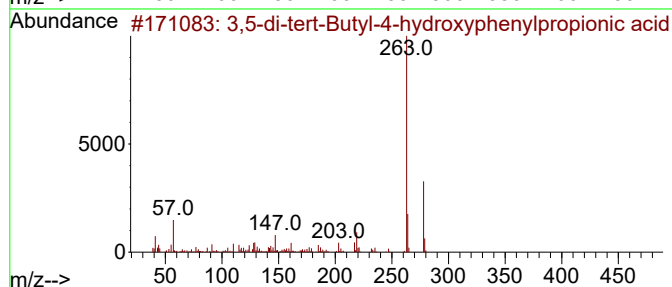
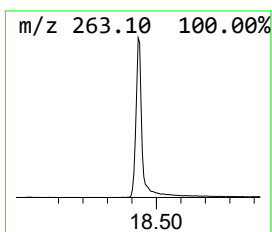
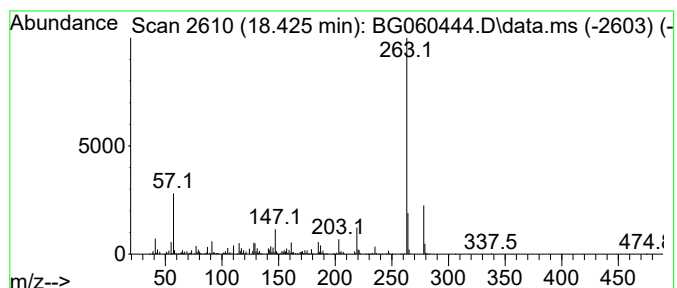
Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG012624.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.425	32.36 ng/ul	5808730	Phenanthrene-d10	17.309	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-di-tert-Butyl-4-hydroxypheny...	278	C17H26O3	020170-32-5	94
2	3,5-di-tert-Butyl-4-hydroxypheny...	278	C17H26O3	020170-32-5	93
3	Lycopodan-5-one, 12-hydroxy-15-m...	263	C16H25NO2	021061-90-5	91
4	5-(2,3-Difluorophenyl)-2-pyridin...	278	C14H16F2N2Si	1000504-49-4	74
5	1H-Isoindole-1,3(2H)-dione, 2-(2...	263	C17H13NO2	016307-59-8	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012624\
Data File : BG060444.D
Acq On : 26 Jan 2024 16:56
Operator : MA/JU
Sample : P1231-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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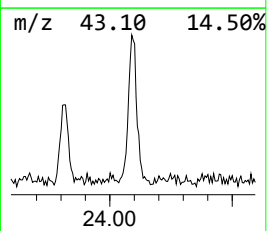
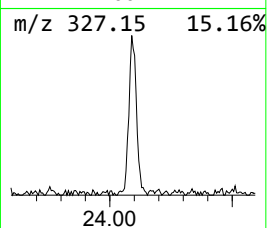
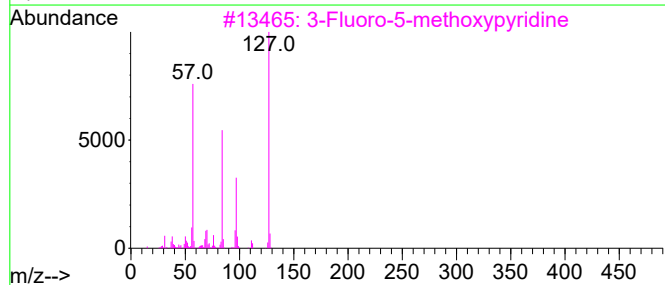
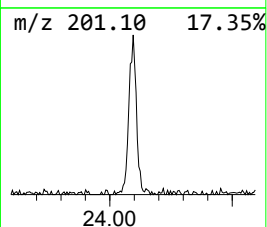
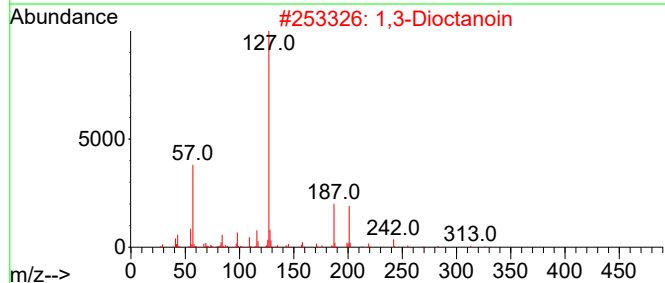
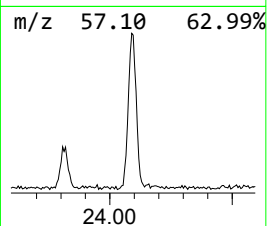
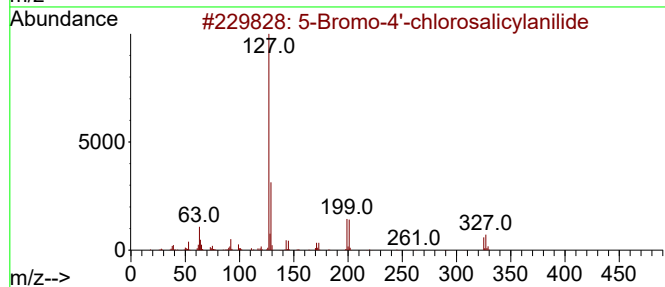
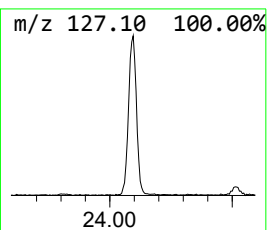
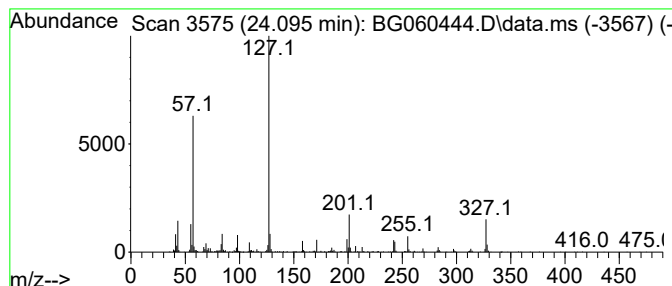
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 5-Bromo-4'-chlorosalicylani... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.095	4.02 ng/ul	915220	Perylene-d12	24.735

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Bromo-4'-chlorosalicylanilide	325	C13H9BrClNO2	003679-64-9	59
2		1,3-Dioctanoin	344	C19H36O5	001429-66-9	53
3		3-Fluoro-5-methoxypyridine	127	C6H6FNO	1060801-62-8	49
4		1,2,3,6,9-Pentaazaspiro[4.4]non-...	197	C9H19N5	1000221-38-7	49
5		Glycerol tricaprylate	470	C27H50O6	000538-23-8	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012624\
Data File : BG060444.D
Acq On : 26 Jan 2024 16:56
Operator : MA/JU
Sample : P1231-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BH6Z9

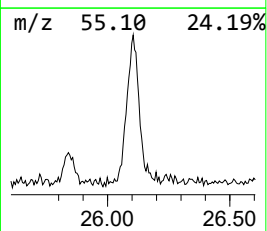
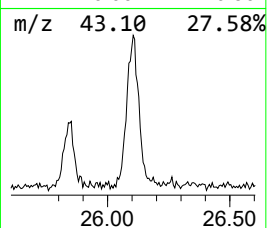
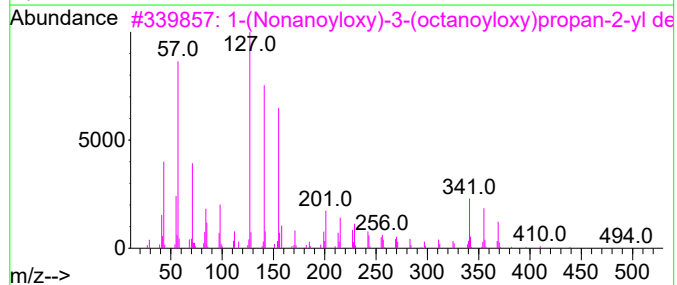
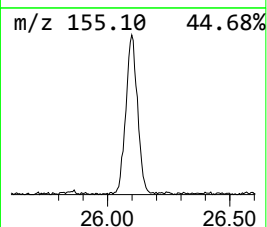
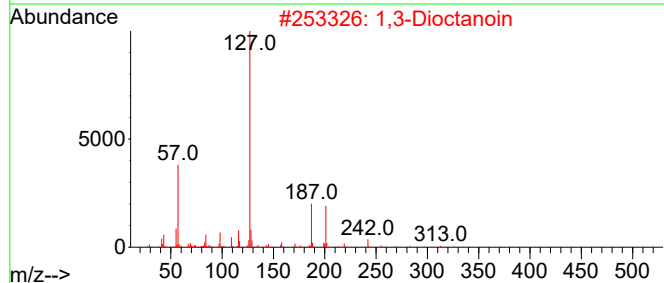
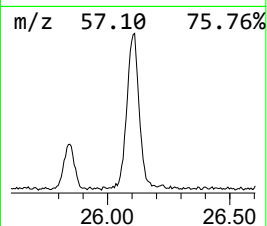
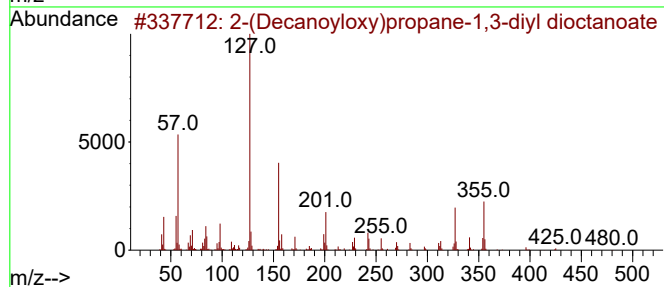
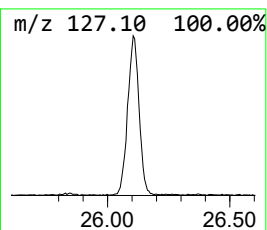
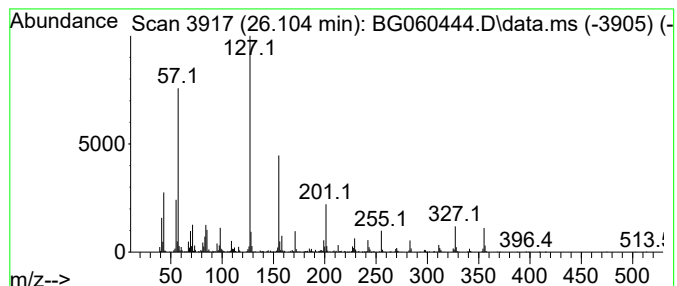
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 2-(Decanoyloxy)propane-1,3-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.104	8.77 ng/ul	1994970	Perylene-d12	24.735

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(Decanoyloxy)propane-1,3-diyl ...	498	C29H54O6	033368-87-5	64		
2	1,3-Dioctanoin	344	C19H36O5	001429-66-9	47		
3	1-(Nonanoyloxy)-3-(octanoyloxy)p...	512	C30H56O6	1000413-78-7	46		
4	Glycerol tricaprylate	470	C27H50O6	000538-23-8	43		
5	1,2-Dioctanoin	344	C19H36O5	001069-87-0	43		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012624\
Data File : BG060444.D
Acq On : 26 Jan 2024 16:56
Operator : MA/JU
Sample : P1231-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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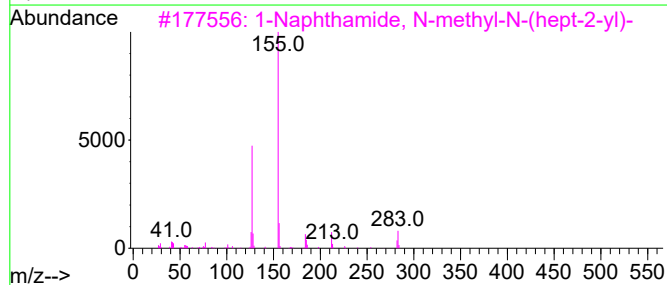
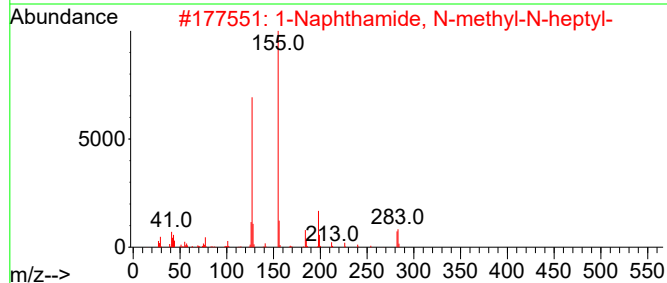
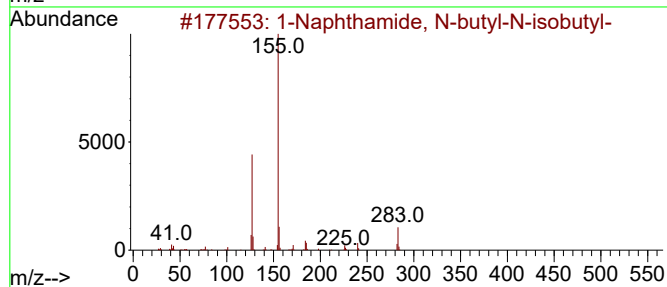
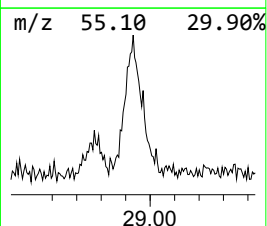
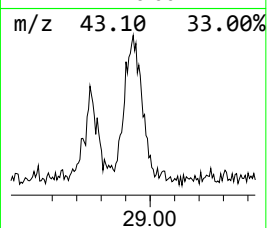
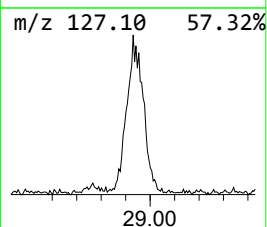
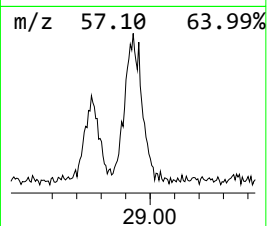
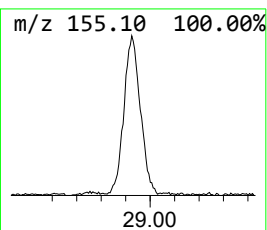
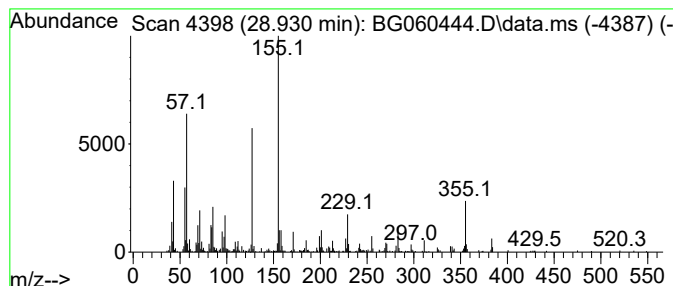
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 1-Naphthamide, N-butyl-N-is... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.930	5.81 ng/ul	1322210	Perylene-d12	24.735

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthamide, N-butyl-N-isobutyl-	283	C19H25NO	1000415-71-5	62		
2	1-Naphthamide, N-methyl-N-heptyl-	283	C19H25NO	1000421-43-6	58		
3	1-Naphthamide, N-methyl-N-(hept-...	283	C19H25NO	1000421-43-3	58		
4	1-Naphthamide, N,N-dibutyl-	283	C19H25NO	1000308-68-6	53		
5	2-[5-(3-Bromo-phenyl)-[1,3,4]oxa...	424	C20H13BrN2O2S	1000275-09-0	53		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012624\
Data File : BG060444.D
Acq On : 26 Jan 2024 16:56
Operator : MA/JU
Sample : P1231-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BH6Z9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG012624.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
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7,9-Di-tert-but...	17.979	24.8	ng/ul	4453420	4	17.309	3590460	20.0
3,5-di-tert-But...	18.425	32.4	ng/ul	5808730	4	17.309	3590460	20.0
5-Bromo-4'-chlo...	24.095	4.0	ng/ul	915220	6	24.735	4549140	20.0
2-(Decanoyloxy)...	26.104	8.8	ng/ul	1994970	6	24.735	4549140	20.0
1-Naphthamide, ...	28.930	5.8	ng/ul	1322210	6	24.735	4549140	20.0