

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111323\
 Data File : BM042730.D
 Acq On : 14 Nov 2023 10:51
 Operator : MA/JU
 Sample : 05016-06
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 A4A88

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_M\Methods\SFAM-EPA-BM111323.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BM042730.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.622	105	108	118	rBV	112657	170612	9.86%	0.678%
2	4.910	323	327	337	rBV	107831	147344	8.52%	0.585%
3	6.998	675	682	696	rBV2	342995	646283	37.36%	2.568%
4	7.181	707	713	724	rBV	119703	199201	11.51%	0.791%
5	7.275	724	729	737	rVV	252959	388119	22.43%	1.542%
6	7.357	737	743	759	rVB	168120	286647	16.57%	1.139%
7	7.834	818	824	833	rBV	104115	179906	10.40%	0.715%
8	8.557	942	947	958	rBV	135847	253128	14.63%	1.006%
9	8.651	958	963	973	rVB	124614	197608	11.42%	0.785%
10	9.033	1022	1028	1033	rBV	125542	223881	12.94%	0.890%
11	9.081	1033	1036	1047	rVB	48863	87945	5.08%	0.349%
12	9.292	1065	1072	1085	rBV	388512	598474	34.59%	2.378%
13	9.745	1143	1149	1152	rBV	123519	217310	12.56%	0.863%
14	9.780	1152	1155	1167	rVB	97235	176879	10.22%	0.703%
15	10.275	1231	1239	1241	rBV	161212	272889	15.77%	1.084%
16	10.645	1294	1302	1307	rBV	136319	234414	13.55%	0.931%
17	10.698	1307	1311	1320	rVB	96918	169790	9.81%	0.675%
18	10.833	1327	1334	1343	rBV2	42878	107687	6.22%	0.428%
19	10.922	1343	1349	1355	rVB	218206	353204	20.42%	1.403%
20	12.174	1555	1562	1570	rBV	98484	172793	9.99%	0.687%
21	12.310	1578	1585	1600	rBV	202628	326614	18.88%	1.298%
22	12.433	1600	1606	1610	rBV2	14944	27066	1.56%	0.108%
23	12.527	1616	1622	1630	rVV	343918	549000	31.73%	2.181%
24	12.604	1630	1635	1640	rVB	163954	237253	13.71%	0.943%
25	12.663	1640	1645	1653	rVB2	88301	137386	7.94%	0.546%
26	12.927	1680	1690	1703	rBV	246062	422105	24.40%	1.677%
27	13.327	1751	1758	1762	rBV	499945	732387	42.33%	2.910%
28	13.374	1762	1766	1780	rVB	108444	183746	10.62%	0.730%
29	13.910	1852	1857	1869	rBV	295031	418296	24.18%	1.662%
30	14.110	1885	1891	1899	rBV	264916	379935	21.96%	1.510%
31	14.192	1899	1905	1908	rBV	334477	526462	30.43%	2.092%
32	14.492	1948	1956	1961	rBV	187819	277120	16.02%	1.101%
33	14.557	1961	1967	1973	rVB	129946	190869	11.03%	0.758%
34	14.663	1979	1985	1995	rBV	113799	219687	12.70%	0.873%
35	14.774	1995	2004	2016	rVV2	705126	1335075	77.17%	5.305%
36	14.892	2019	2024	2031	rVB	117215	175146	10.12%	0.696%

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37	15.486	2119	2125	2129	rBV	371748	555914	32.13%	2.209%
38	15.533	2129	2133	2144	rVV2	338921	533896	30.86%	2.121%
39	15.639	2144	2151	2169	rVB2	332630	648901	37.51%	2.578%
40	16.509	2293	2299	2307	rBV	439713	592952	34.27%	2.356%
41	16.874	2356	2361	2377	rBV	416972	635231	36.72%	2.524%
42	17.062	2387	2393	2406	rBV	512842	722219	41.75%	2.870%
43	17.245	2418	2424	2427	rBV	235939	325593	18.82%	1.294%
44	17.286	2427	2431	2436	rVV	169613	242122	14.00%	0.962%
45	17.345	2436	2441	2444	rVV	396029	595533	34.42%	2.366%
46	17.380	2444	2447	2460	rVB	267024	388553	22.46%	1.544%
47	17.668	2490	2496	2517	rBV	499517	840731	48.60%	3.340%
48	19.303	2768	2774	2782	rBV	371333	528037	30.52%	2.098%
49	19.639	2825	2831	2834	rBV	608718	868017	50.17%	3.449%
50	19.668	2834	2836	2845	rVB	435571	488557	28.24%	1.941%
51	21.409	3127	3132	3138	rBV2	738593	1338550	77.37%	5.318%
52	21.462	3138	3141	3155	rVB	251744	389985	22.54%	1.550%
53	23.062	3407	3413	3425	rBV	402054	737594	42.64%	2.931%
54	23.638	3504	3511	3516	rBV	431487	896717	51.83%	3.563%
55	23.685	3516	3519	3528	rVV	219637	416688	24.09%	1.656%
56	23.791	3531	3537	3546	rVB	227300	470197	27.18%	1.868%
57	26.268	3947	3958	3976	rBV2	495664	1730016	100.00%	6.874%

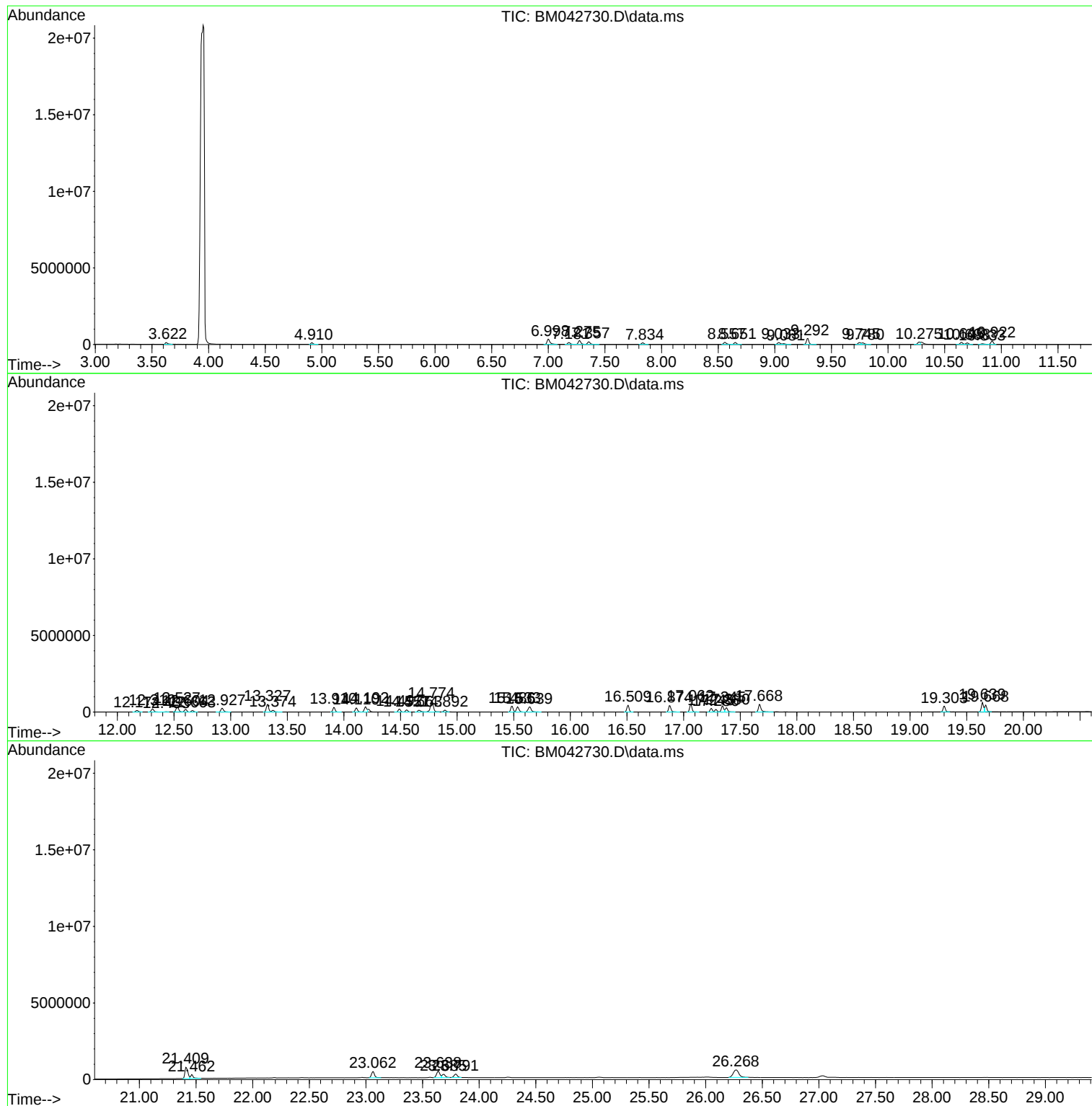
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Quant Title : SVOA CALIBRATION

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



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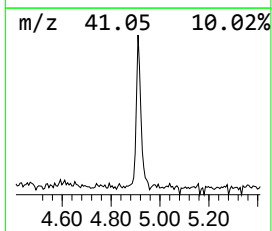
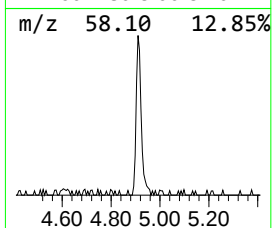
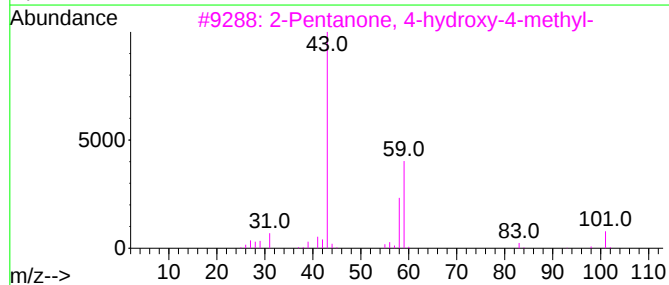
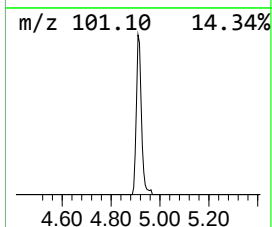
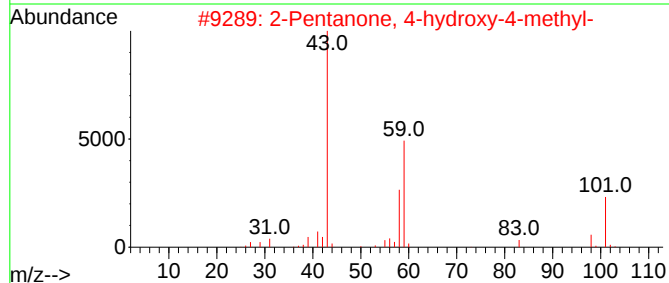
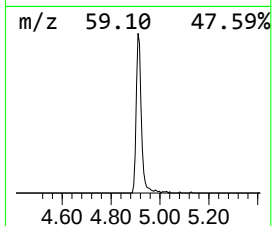
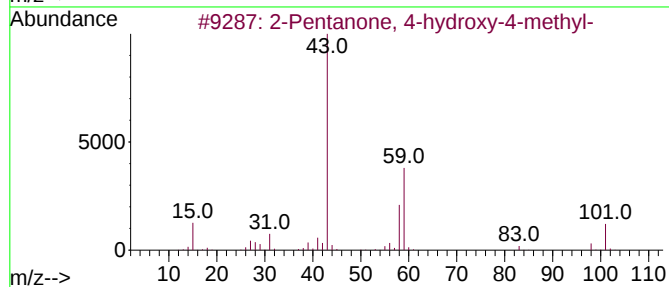
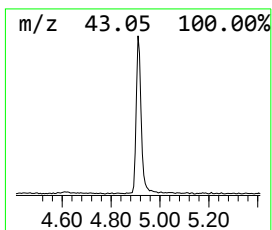
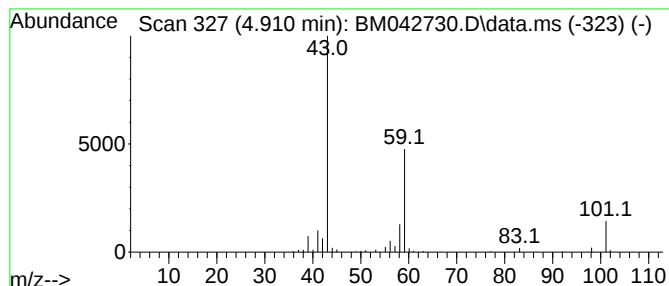
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM111323.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.910	16.38 ng/ul	147344	1,4-Dichlorobenzene-d4	7.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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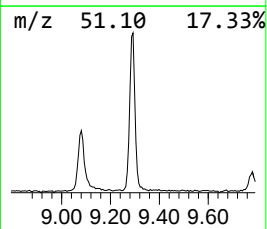
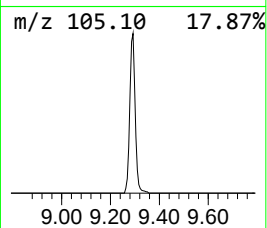
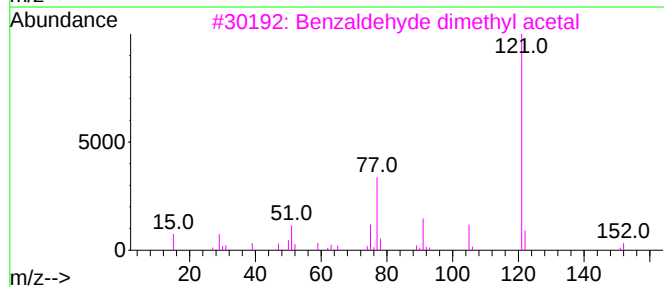
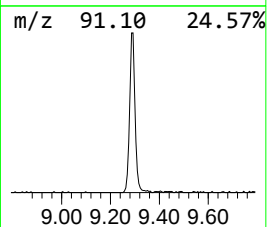
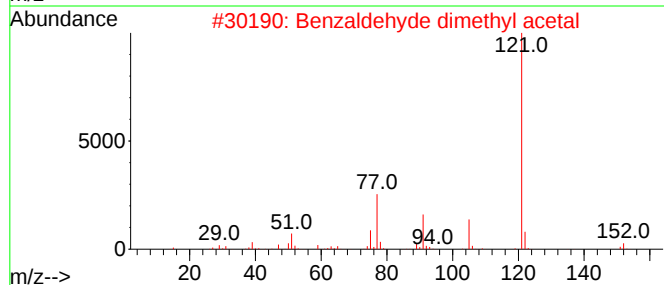
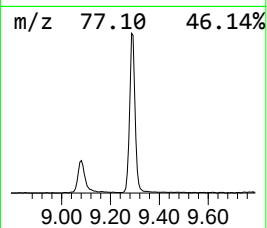
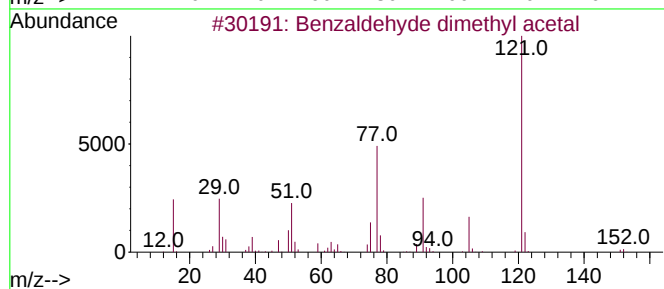
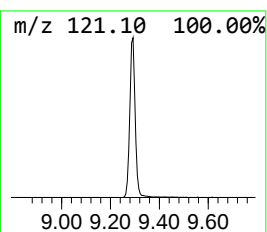
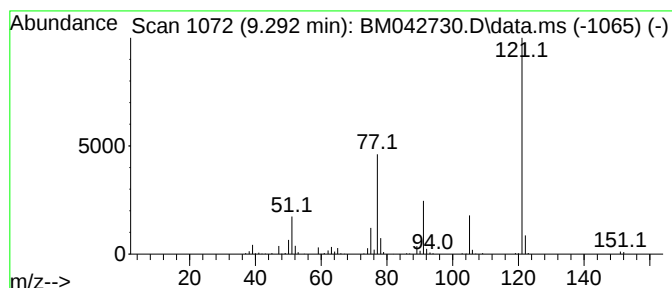
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM111323.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Benzaldehyde dimethyl acetal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.292	51.06 ng/ul	598474	Naphthalene-d8	10.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde dimethyl acetal	152	C9H12O2	001125-88-8	91
2			Benzaldehyde dimethyl acetal	152	C9H12O2	001125-88-8	91
3			Benzaldehyde dimethyl acetal	152	C9H12O2	001125-88-8	90
4			(R)-(-)-.alpha.-Methoxyphenylace...	166	C9H10O3	003966-32-3	72
5			Benzeneacetic acid, .alpha.-meth...	166	C9H10O3	007021-09-2	64



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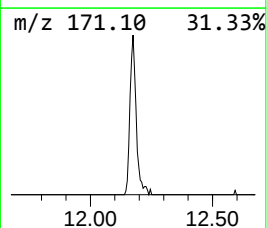
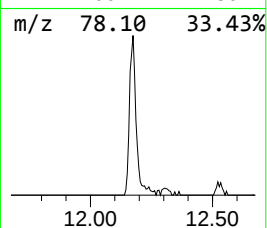
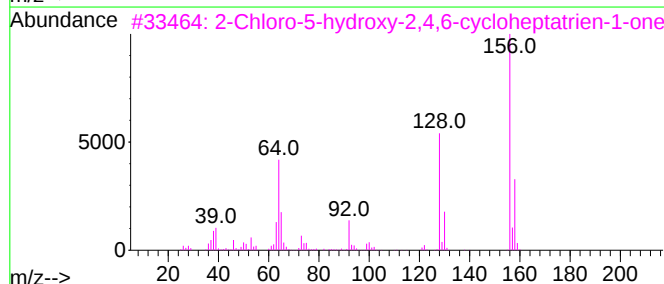
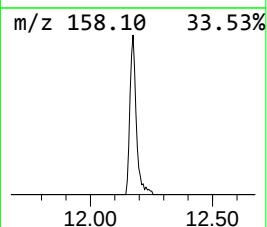
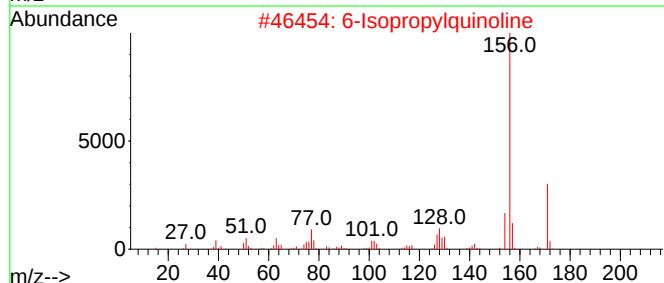
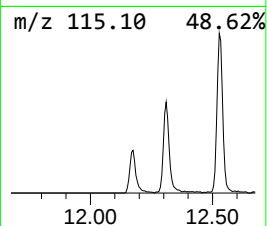
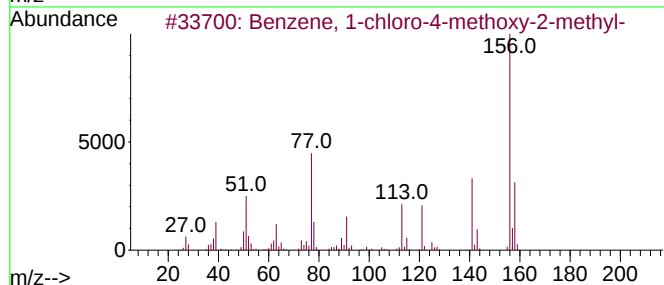
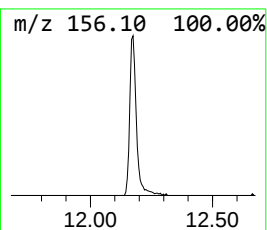
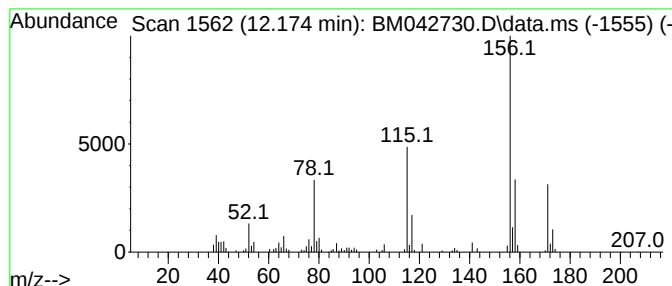
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.175	14.74 ng/ul	172793	Naphthalene-d8	10.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-chloro-4-methoxy-2-me...	156	C8H9ClO	013334-71-9	38
2			6-Isopropylquinoline	171	C12H13N	000135-79-5	38
3			2-Chloro-5-hydroxy-2,4,6-cyclohe...	156	C7H5ClO2	007009-16-7	38
4			Cyclopentanone, O-(trimethylsilyl...	171	C8H17NOSi	026208-87-7	38
5			1,2,3,4-Tetrahydropentalene, 1,1...	171	C12H13N	1000217-18-6	37



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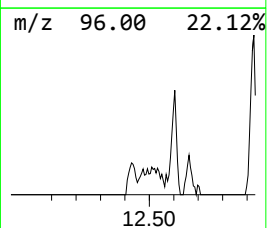
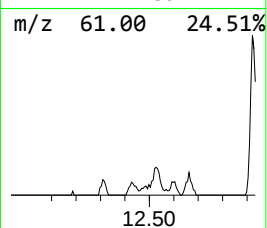
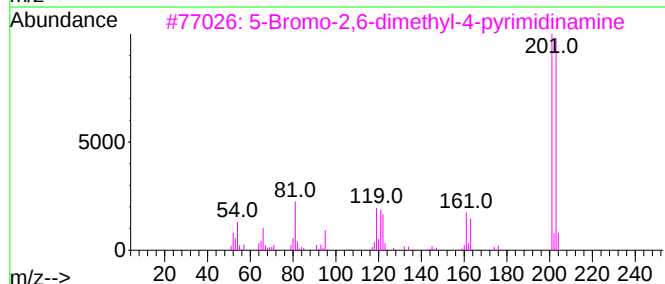
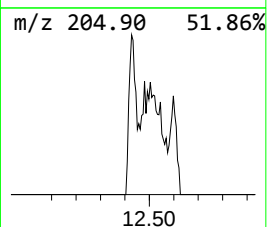
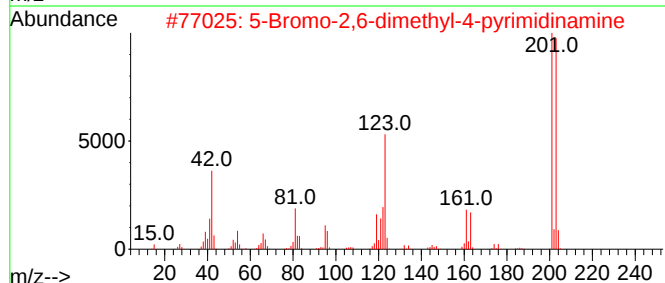
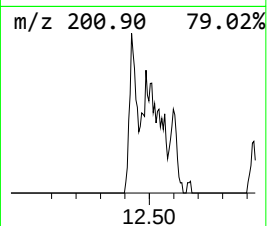
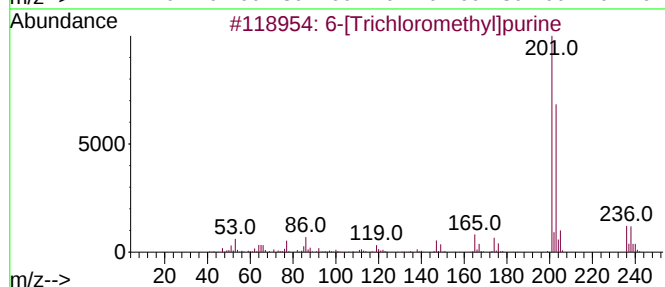
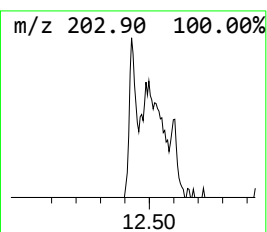
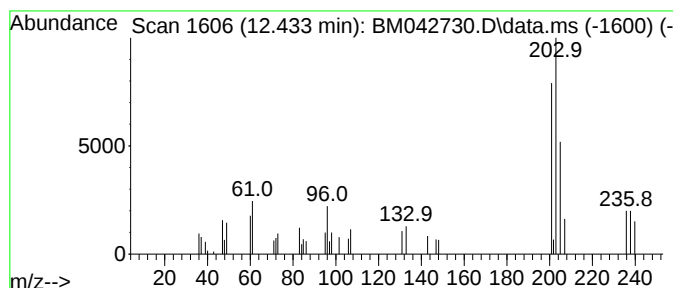
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.433	2.31 ng/ul	27066	Naphthalene-d8	10.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6	-[Trichloromethyl]purine	236	C6H3Cl3N4	002568-37-8	43	
2	5	-Bromo-2,6-dimethyl-4-pyrimidin...	201	C6H8BrN3	007752-80-9	43	
3	5	-Bromo-2,6-dimethyl-4-pyrimidin...	201	C6H8BrN3	007752-80-9	37	
4	3,4	-Dichlorophenyl thiocyanate	203	C7H3Cl2NS	003313-77-7	27	
5	3,5	-Dichlorophenyl isothiocyanate	203	C7H3Cl2NS	006590-93-8	27	



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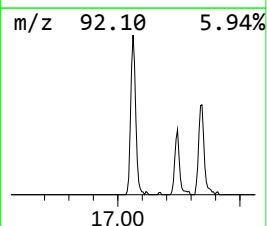
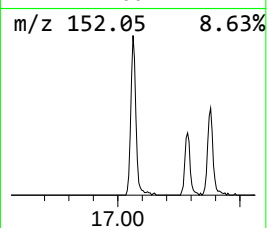
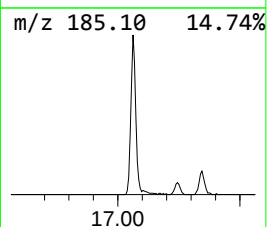
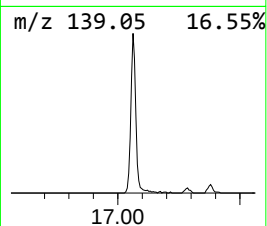
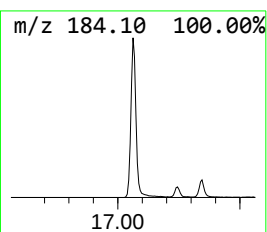
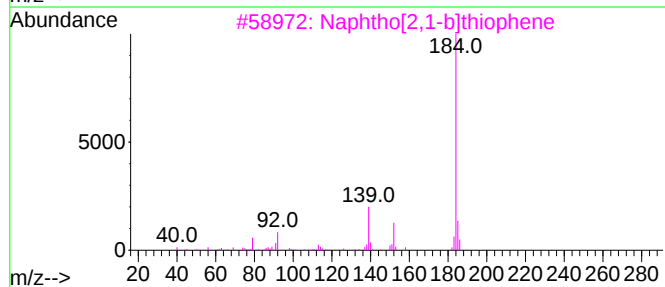
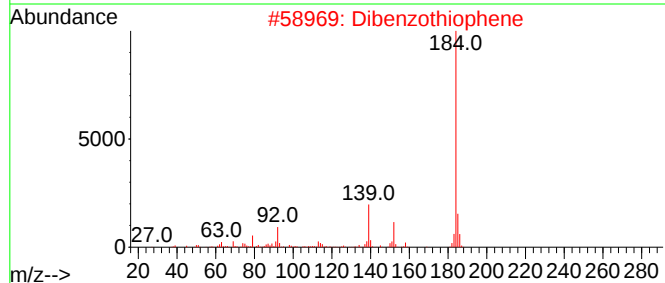
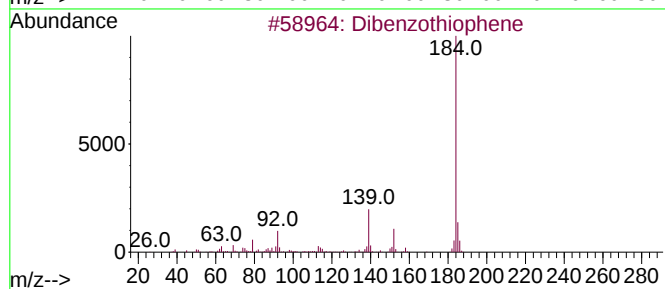
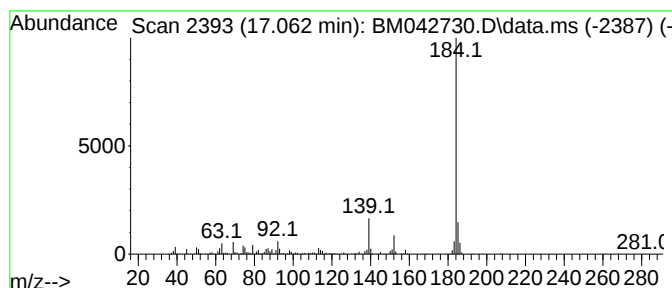
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Dibenzothiophene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.062	44.36 ng/ul	722219	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzothiophene	184	C12H8S	000132-65-0	97
2			Dibenzothiophene	184	C12H8S	000132-65-0	97
3			Naphtho[2,1-b]thiophene	184	C12H8S	000233-02-3	97
4			Naphtho[2,3-b]thiophene	184	C12H8S	000268-77-9	95
5			Naphtho[1,2-b]thiophene	184	C12H8S	000234-41-3	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111323\
Data File : BM042730.D
Acq On : 14 Nov 2023 10:51
Operator : MA/JU
Sample : 05016-06
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4A88

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM111323.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
2-Pentanone, 4-...	4.910	16.4	ng/u1	147344	1	7.839	179906	20.0
Benzaldehyde di...	9.292	51.1	ng/u1	598474	2	10.645	234414	20.0
unknown-01	12.175	14.7	ng/u1	172793	2	10.645	234414	20.0
unknown-02	12.433	2.3	ng/u1	27066	2	10.645	234414	20.0
Dibenzothiophene	17.062	44.4	ng/u1	722219	4	17.245	325593	20.0