

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111723\
 Data File : BM042891.D
 Acq On : 18 Nov 2023 21:33
 Operator : MA/JU
 Sample : 05370-20
 Misc :
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 GCDR4

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: BM042891.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.169	29	31	35	rBV	9374	9920	1.02%	0.103%
2	3.622	105	108	116	rBV	29345	52202	5.37%	0.543%
3	4.722	292	295	296	rBV3	1397	1515	0.16%	0.016%
4	5.687	457	459	463	rVB4	1785	1839	0.19%	0.019%
5	5.722	463	465	468	rBV3	1456	1851	0.19%	0.019%
6	6.081	521	526	538	rBV	57770	109534	11.26%	1.139%
7	6.993	673	681	694	rBV3	18797	49887	5.13%	0.519%
8	7.163	705	710	724	rBV	109869	192123	19.75%	1.998%
9	7.340	733	740	754	rBV	108321	210150	21.61%	2.185%
10	7.545	769	775	783	rVB2	27097	45596	4.69%	0.474%
11	7.810	815	820	832	rBV	112665	210496	21.64%	2.189%
12	8.540	939	944	958	rBV2	63860	137048	14.09%	1.425%
13	8.745	975	979	981	rVV3	2633	2777	0.29%	0.029%
14	9.016	1019	1025	1042	rBV	131042	261756	26.91%	2.722%
15	9.198	1055	1056	1061	rVB3	2730	2950	0.30%	0.031%
16	9.728	1140	1146	1162	rBV2	136481	285556	29.36%	2.970%
17	10.063	1201	1203	1207	rVB4	1160	1598	0.16%	0.017%
18	10.257	1229	1236	1251	rBV	124364	277461	28.53%	2.885%
19	10.628	1290	1299	1311	rBV	155246	274965	28.27%	2.859%
20	10.804	1324	1329	1342	rBV	86192	224504	23.08%	2.335%
21	10.998	1359	1362	1367	rVV6	3936	7003	0.72%	0.073%
22	11.133	1380	1385	1386	rBV4	1185	1881	0.19%	0.020%
23	11.157	1386	1389	1394	rVB7	1520	2127	0.22%	0.022%
24	11.357	1417	1423	1430	rBV2	35774	64476	6.63%	0.670%
25	11.416	1432	1433	1438	rVB3	2810	2620	0.27%	0.027%
26	11.486	1443	1445	1448	rVV4	1672	2147	0.22%	0.022%
27	11.533	1448	1453	1458	rVB6	1965	3815	0.39%	0.040%
28	11.686	1474	1479	1484	rVV6	2926	4952	0.51%	0.051%
29	11.933	1516	1521	1524	rVV5	3492	5599	0.58%	0.058%
30	12.428	1601	1605	1617	rVB	14597	29523	3.04%	0.307%
31	13.316	1751	1756	1761	rBV2	9424	16442	1.69%	0.171%
32	13.480	1780	1784	1786	rVB3	972	1512	0.16%	0.016%
33	13.892	1848	1854	1860	rBV	327010	460857	47.39%	4.793%
34	13.939	1860	1862	1867	rVV3	12958	17826	1.83%	0.185%
35	13.998	1870	1872	1875	rVB4	1673	1606	0.17%	0.017%
36	14.086	1885	1887	1889	rVB2	1866	1638	0.17%	0.017%

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Integrator: RTE

Smoothing : OFF

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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
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37	14.169	1895	1901	1913	rBV	345957	504546	51.88%	5.247%
38	14.251	1913	1915	1921	rVV4	2825	3970	0.41%	0.041%
39	14.386	1936	1938	1942	rVB4	1620	1659	0.17%	0.017%
40	14.469	1945	1952	1963	rVV	239092	358037	36.81%	3.723%
41	14.551	1963	1966	1972	rVB4	3410	5409	0.56%	0.056%
42	14.686	1984	1989	2001	rBV	138710	208016	21.39%	2.163%
43	14.792	2003	2007	2009	rVV5	2620	3775	0.39%	0.039%
44	14.857	2016	2018	2021	rBV3	1161	1723	0.18%	0.018%
45	14.974	2032	2038	2042	rVB4	4584	6382	0.66%	0.066%
46	15.104	2053	2060	2064	rBV2	13315	20475	2.11%	0.213%
47	15.151	2064	2068	2076	rVV3	37197	57900	5.95%	0.602%
48	15.210	2076	2078	2083	rVB4	4015	5564	0.57%	0.058%
49	15.268	2085	2088	2090	rBV3	1732	2149	0.22%	0.022%
50	15.404	2108	2111	2113	rBV4	1440	1850	0.19%	0.019%
51	15.463	2115	2121	2132	rBV	417292	631725	64.96%	6.569%
52	15.616	2141	2147	2161	rBV	107147	196400	20.19%	2.042%
53	15.710	2161	2163	2170	rVV5	4201	6140	0.63%	0.064%
54	15.816	2179	2181	2184	rVB2	1429	1569	0.16%	0.016%
55	15.874	2188	2191	2197	rVB3	3409	4773	0.49%	0.050%
56	15.980	2205	2209	2212	rVB5	1310	1648	0.17%	0.017%
57	16.057	2215	2222	2228	rBV4	11848	19632	2.02%	0.204%
58	16.174	2235	2242	2247	rBV3	6577	10126	1.04%	0.105%
59	16.268	2253	2258	2263	rBV	12254	18938	1.95%	0.197%
60	16.327	2263	2268	2274	rVV3	24195	39515	4.06%	0.411%
61	16.386	2274	2278	2282	rVV3	12261	19109	1.96%	0.199%
62	16.433	2282	2286	2290	rVB3	9887	14176	1.46%	0.147%
63	16.486	2290	2295	2297	rBV4	5435	7517	0.77%	0.078%
64	16.504	2297	2298	2301	rVV3	3475	3684	0.38%	0.038%
65	16.533	2301	2303	2307	rVB	6282	7292	0.75%	0.076%
66	16.586	2307	2312	2319	rVB5	14346	29221	3.00%	0.304%
67	16.663	2319	2325	2329	rBV	11700	20099	2.07%	0.209%
68	16.733	2334	2337	2344	rVV2	7693	13605	1.40%	0.141%
69	16.792	2344	2347	2350	rVV4	1606	2343	0.24%	0.024%
70	16.833	2350	2354	2355	rVV3	1745	2304	0.24%	0.024%
71	16.857	2355	2358	2363	rVV4	1805	3584	0.37%	0.037%
72	17.221	2415	2420	2431	rBV	266027	410414	42.20%	4.268%
73	17.321	2432	2437	2457	rVB	473566	721713	74.21%	7.505%
74	17.480	2462	2464	2468	rVV4	4045	6069	0.62%	0.063%
75	17.510	2468	2469	2471	rVV2	2537	1573	0.16%	0.016%
76	17.527	2471	2472	2474	rVV2	1846	1793	0.18%	0.019%

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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 >
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77	17.604	2483	2485	2490	rVV4	1830	2581	0.27%	0.027%
78	17.674	2491	2497	2501	rVV6	4464	8371	0.86%	0.087%
79	17.768	2508	2513	2522	rVV	52592	72135	7.42%	0.750%
80	17.851	2525	2527	2531	rVB4	2394	2655	0.27%	0.028%
81	17.980	2543	2549	2550	rBV3	1817	2428	0.25%	0.025%
82	18.004	2550	2553	2558	rVB2	9818	12042	1.24%	0.125%
83	18.080	2562	2566	2574	rBV3	13625	22894	2.35%	0.238%
84	18.298	2597	2603	2612	rBV	55482	86217	8.87%	0.897%
85	18.357	2612	2613	2616	rVV3	2946	3018	0.31%	0.031%
86	18.980	2716	2719	2722	rVB5	1244	1647	0.17%	0.017%
87	19.051	2725	2731	2735	rVB	20519	25184	2.59%	0.262%
88	19.192	2750	2755	2760	rBV5	5564	9505	0.98%	0.099%
89	19.256	2762	2766	2770	rBV	4219	7586	0.78%	0.079%
90	19.309	2773	2775	2778	rVB4	2294	1692	0.17%	0.018%
91	19.339	2778	2780	2782	rBV3	1475	1573	0.16%	0.016%
92	19.368	2782	2785	2789	rBV6	5491	7864	0.81%	0.082%
93	19.621	2822	2828	2842	rBV	733278	962753	98.99%	10.012%
94	19.809	2858	2860	2862	rBV3	2058	1840	0.19%	0.019%
95	20.086	2905	2907	2909	rBV2	2579	1865	0.19%	0.019%
96	21.409	3127	3132	3138	rBV	315725	455938	46.88%	4.741%
97	21.456	3138	3140	3144	rVB	35168	44125	4.54%	0.459%
98	22.939	3390	3392	3397	rVB3	19629	24804	2.55%	0.258%
99	23.615	3500	3507	3523	rBV	467179	972533	100.00%	10.114%
100	23.768	3527	3533	3549	rVB	240572	530709	54.57%	5.519%

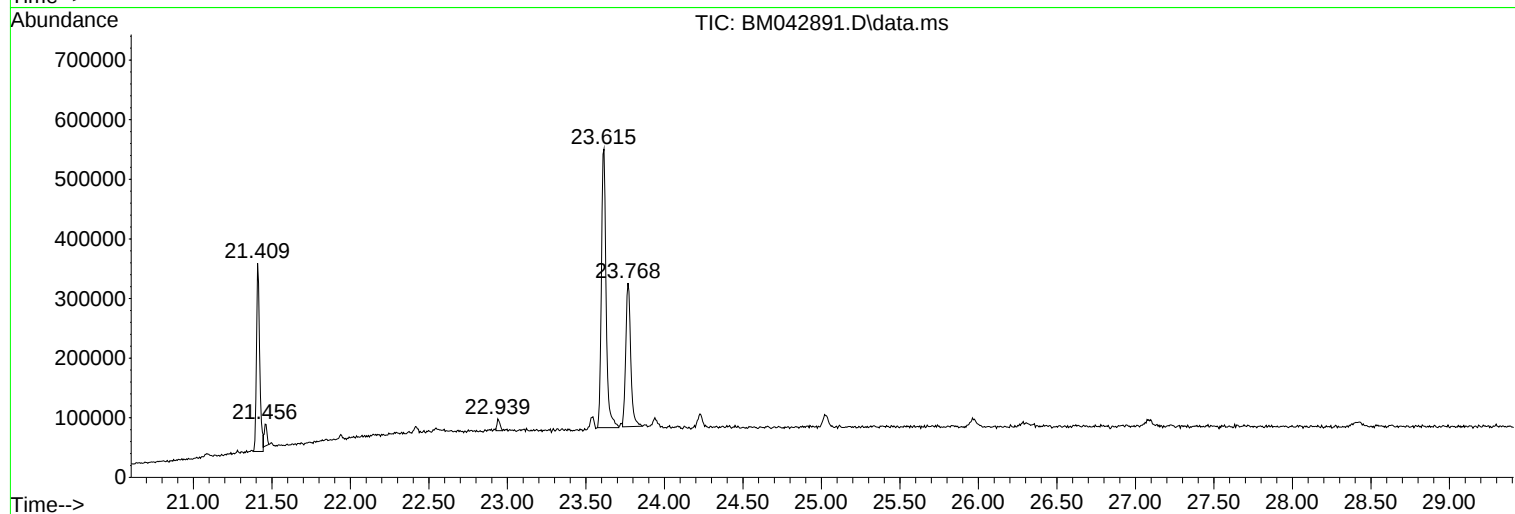
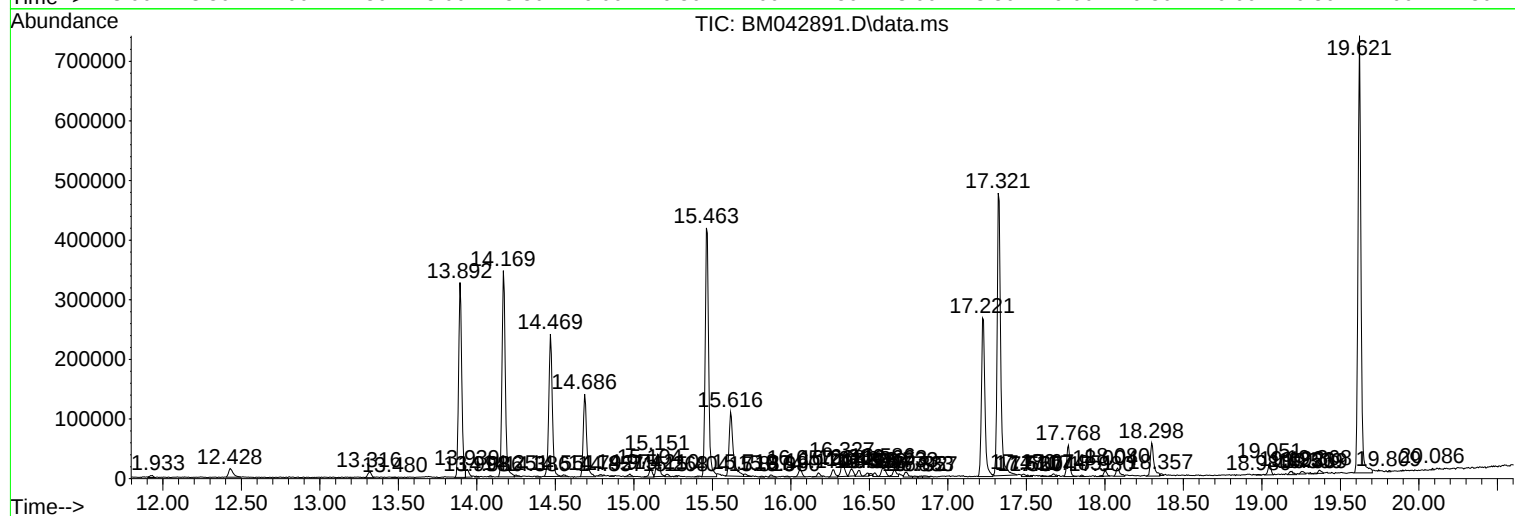
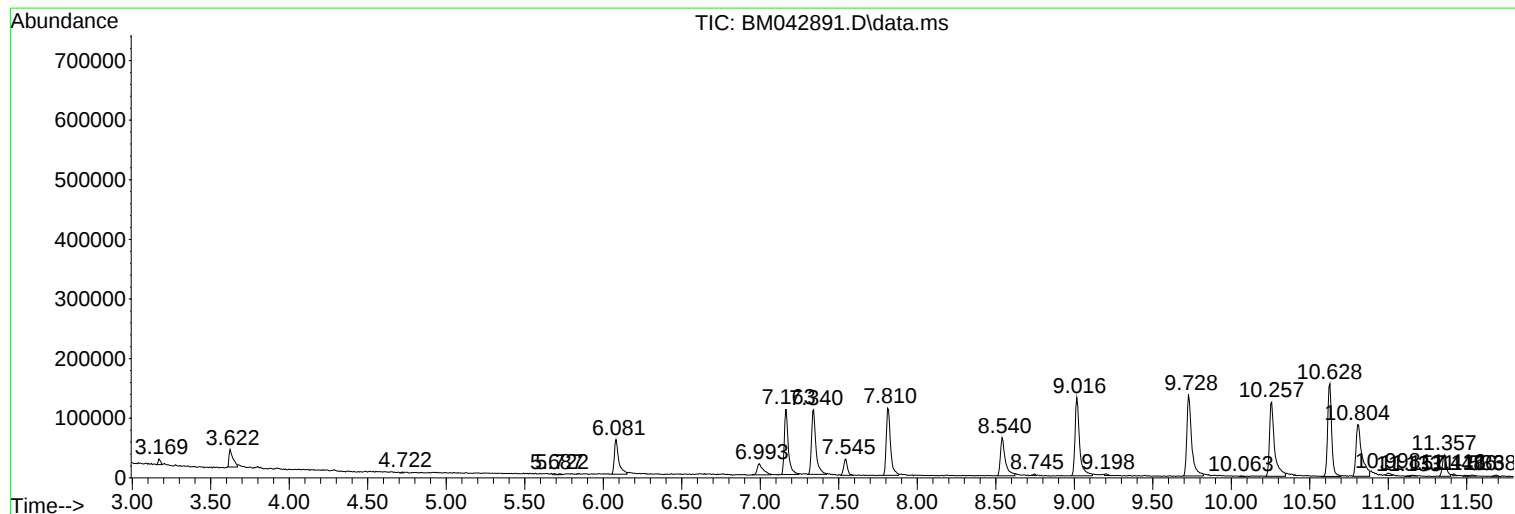
Sum of corrected areas: 9616128

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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



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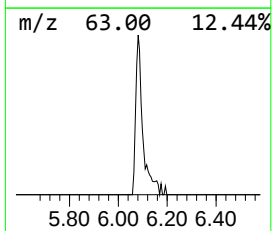
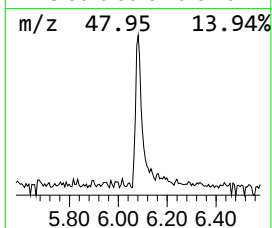
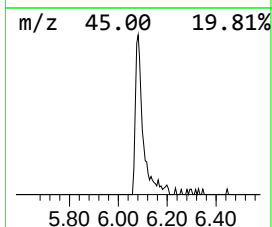
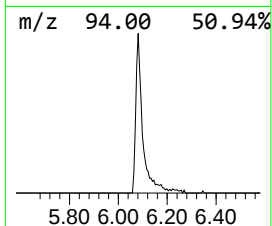
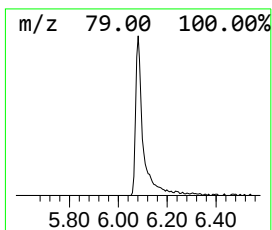
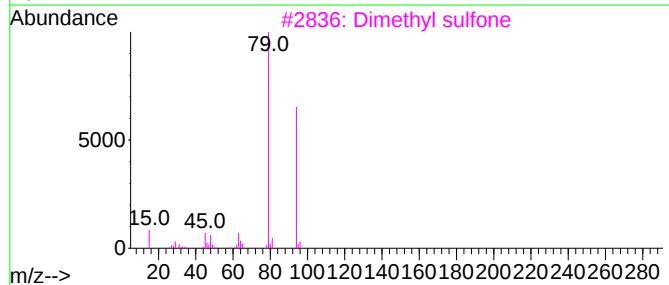
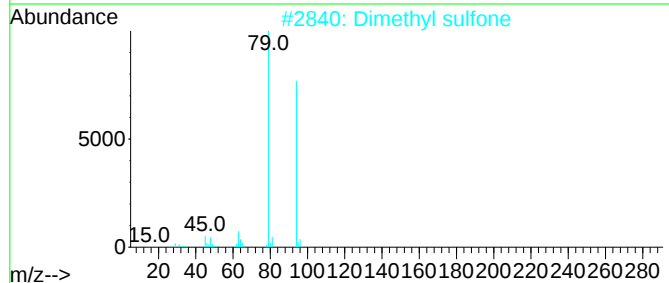
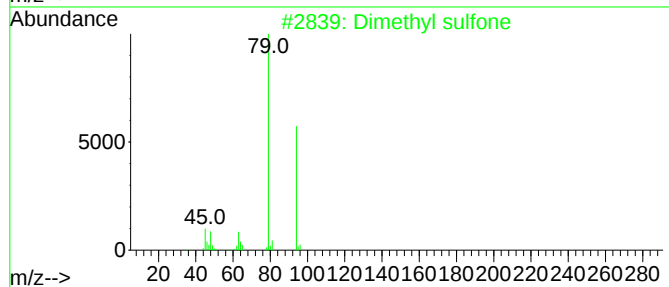
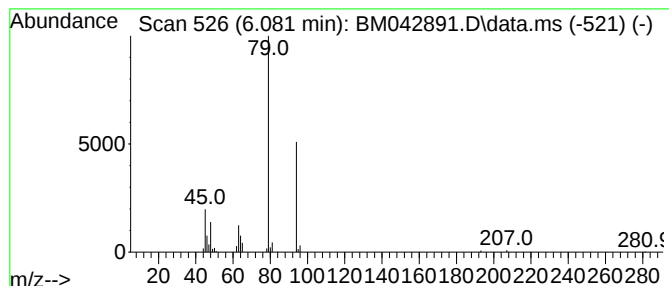
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM111323.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Dimethyl sulfone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.081	10.41 ng/ul	109534	1,4-Dichlorobenzene-d4	7.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfone	94	C2H6O2S	000067-71-0	94
2			Dimethyl sulfone	94	C2H6O2S	000067-71-0	91
3			Dimethyl sulfone	94	C2H6O2S	000067-71-0	91
4			Dimethyl sulfone	94	C2H6O2S	000067-71-0	72
5			Dimethyl sulfone	94	C2H6O2S	000067-71-0	64



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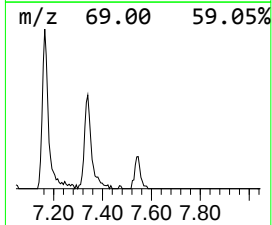
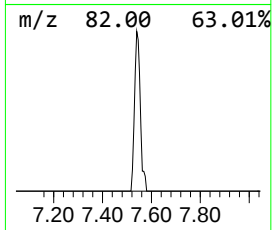
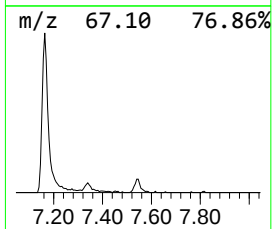
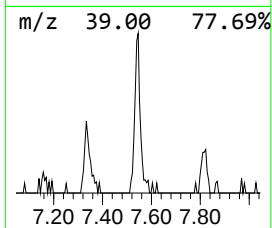
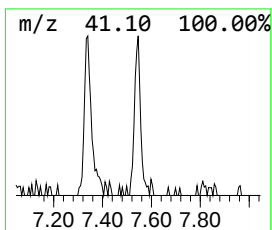
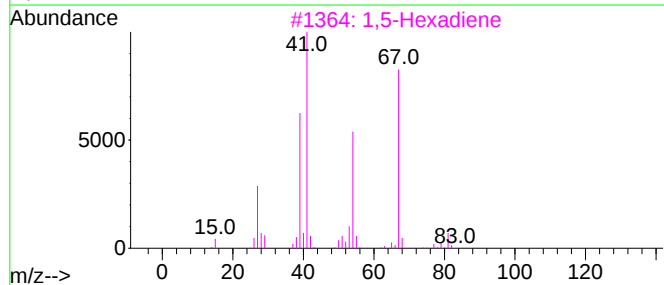
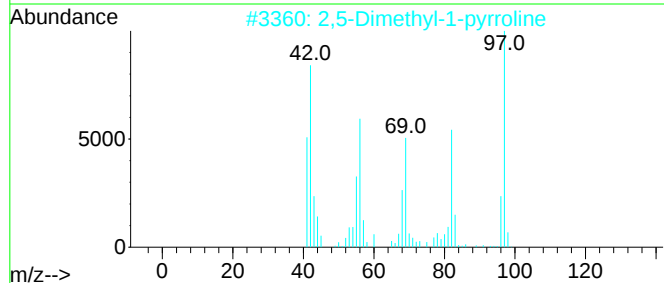
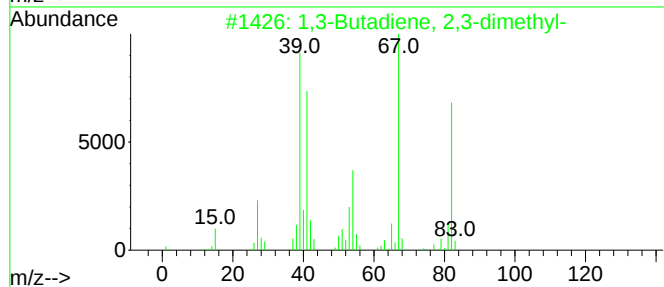
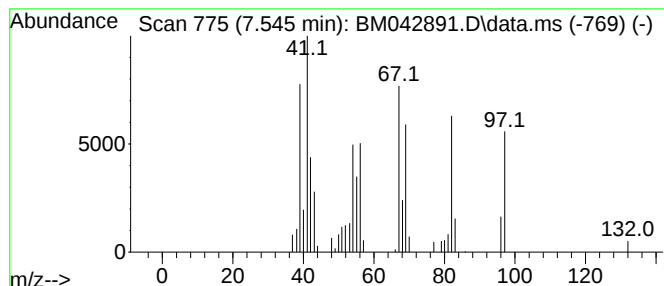
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM111323.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 1,3-Butadiene, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.545	4.33 ng/ul	45596	1,4-Dichlorobenzene-d4	7.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Butadiene, 2,3-dimethyl-	82	C6H10	000513-81-5	64
2			2,5-Dimethyl-1-pyrroline	97	C6H11N	000822-64-0	60
3			1,5-Hexadiene	82	C6H10	000592-42-7	53
4			2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	50
5			2-Cyclopenten-1-one	82	C5H6O	000930-30-3	49



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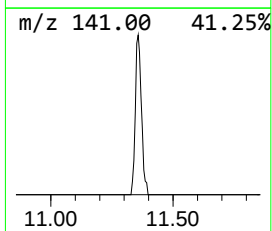
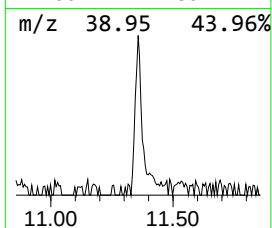
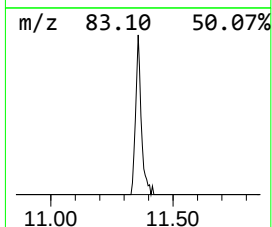
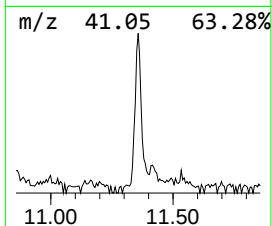
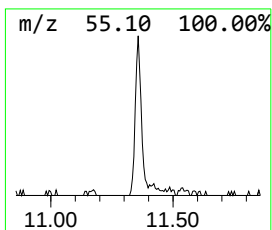
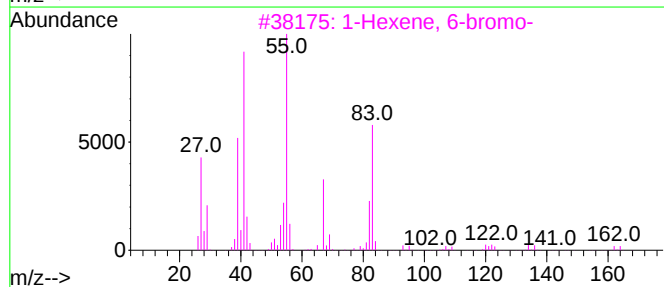
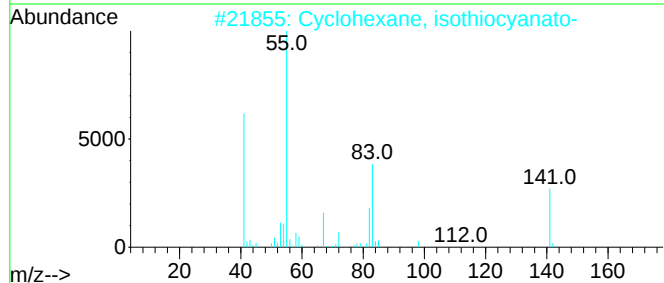
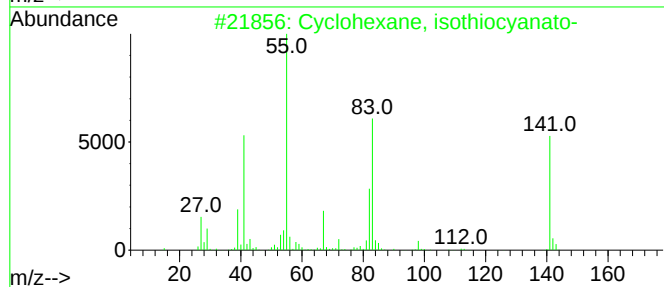
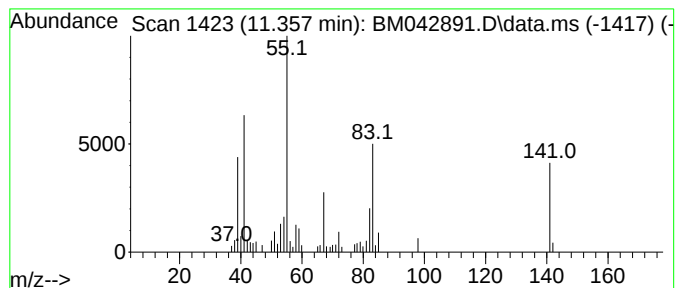
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM111323.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Cyclohexane, isothiocyanato- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.357	4.69 ng/ul	64476	Naphthalene-d8	10.628

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, isothiocyanato-	141	C7H11NS	001122-82-3	58
2			Cyclohexane, isothiocyanato-	141	C7H11NS	001122-82-3	45
3			1-Hexene, 6-bromo-	162	C6H11Br	002695-47-8	40
4			N-Ethylidenecyclohexaneamine, N-...	141	C8H15NO	003376-30-5	40
5			1-Hexene, 6-bromo-	162	C6H11Br	002695-47-8	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111723\
Data File : BM042891.D
Acq On : 18 Nov 2023 21:33
Operator : MA/JU
Sample : 05370-20
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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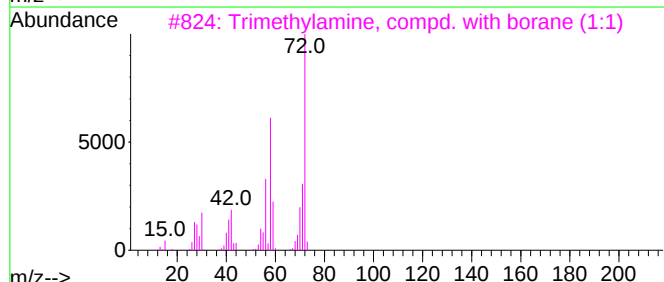
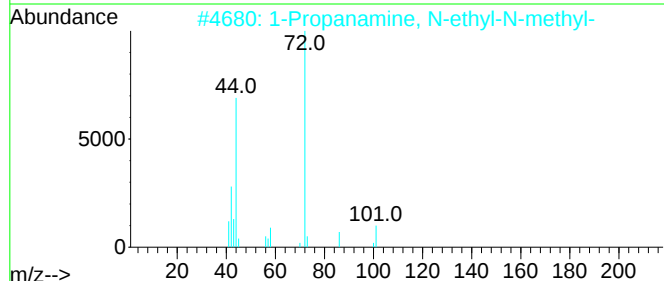
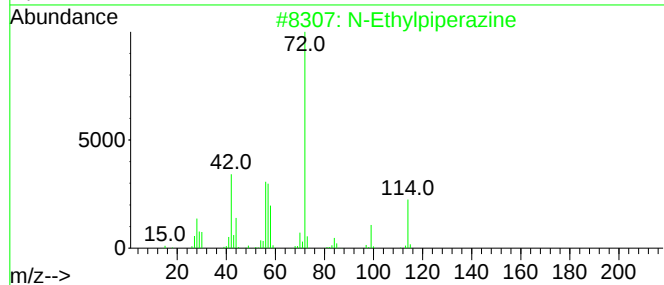
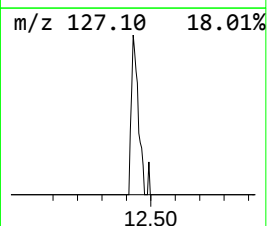
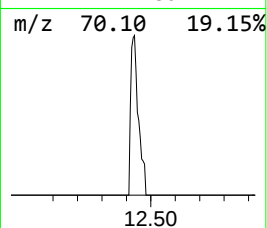
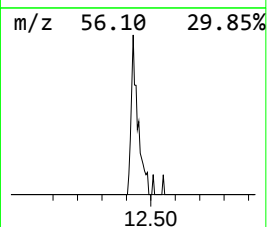
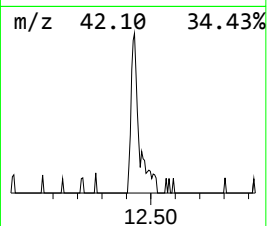
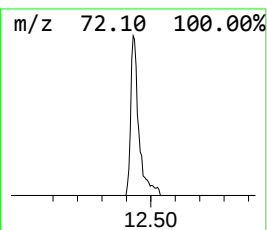
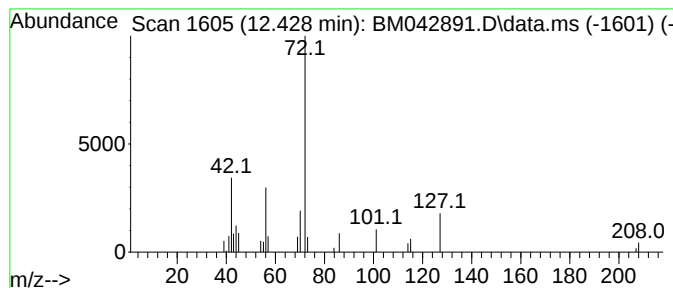
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 N-Ethylpiperazine Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.428	2.15 ng/ul	29523	Naphthalene-d8	10.628

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-Ethylpiperazine	114	C6H14N2	005308-25-8	59
2			1-Propanamine, N-ethyl-N-methyl-	101	C6H15N	004458-32-6	53
3			Trimethylamine, compd. with bora...	73	C3H12BN	000075-22-9	50
4			Acetaldehyde, methylhydrazone	72	C3H8N2	017167-73-6	47
5			1-Propanamine, N-ethyl-N-methyl-	101	C6H15N	004458-32-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111723\
Data File : BM042891.D
Acq On : 18 Nov 2023 21:33
Operator : MA/JU
Sample : 05370-20
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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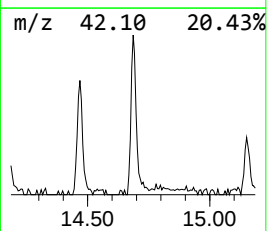
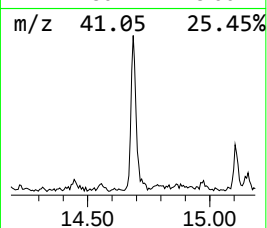
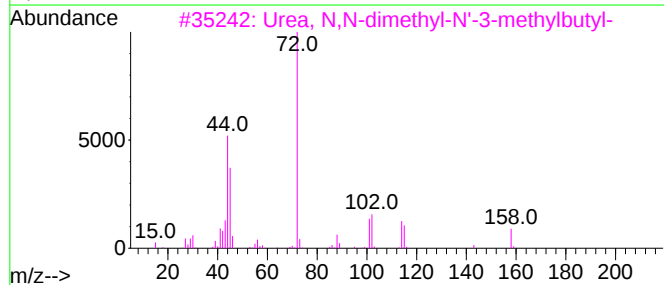
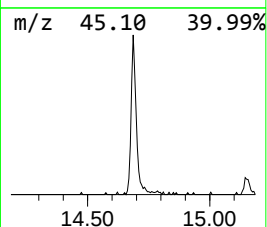
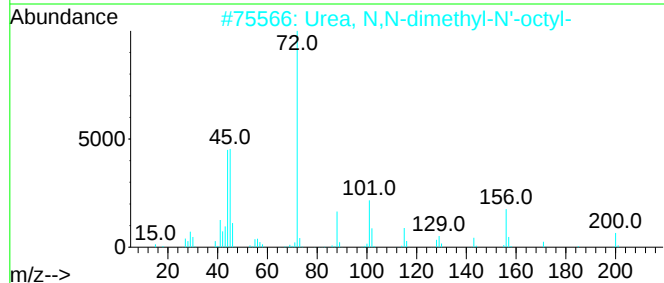
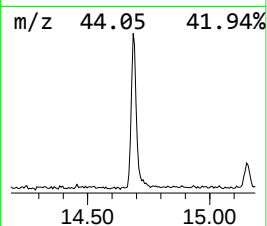
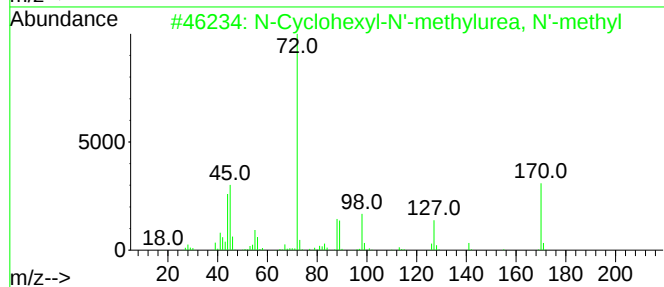
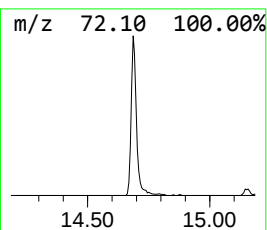
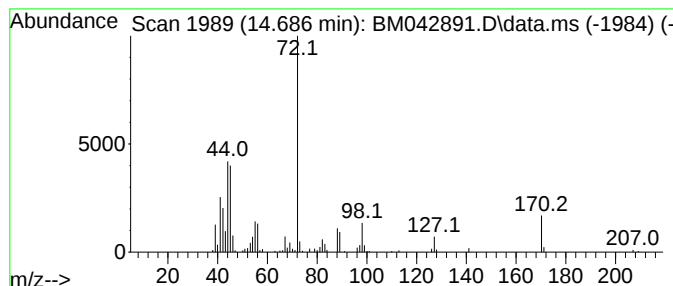
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 N-Cyclohexyl-N'-methylurea,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.686	11.62 ng/ul	208016	Acenaphthene-d10	14.469

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-Cyclohexyl-N'-methylurea, N'-m...	170	C9H18N2O	031468-12-9	94
2			Urea, N,N-dimethyl-N'-octyl-	200	C11H24N2O	1000419-88-6	59
3			Urea, N,N-dimethyl-N'-3-methylbu...	158	C8H18N2O	1000419-88-0	59
4			Urea, N,N-dimethyl-N'-pentyl-	158	C8H18N2O	1000419-88-1	59
5			Urea, N,N-dimethyl-N'-hexyl-	172	C9H20N2O	1000419-88-3	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111723\
Data File : BM042891.D
Acq On : 18 Nov 2023 21:33
Operator : MA/JU
Sample : 05370-20
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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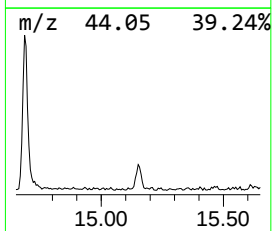
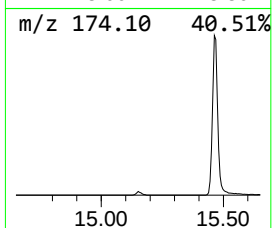
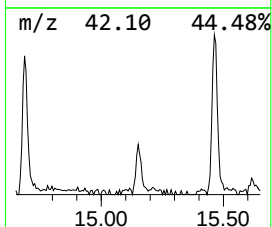
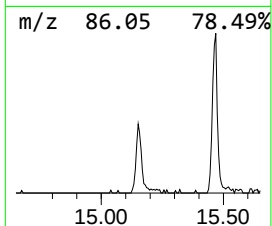
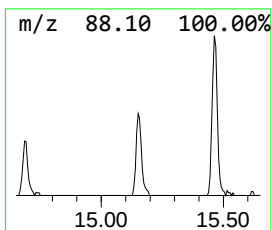
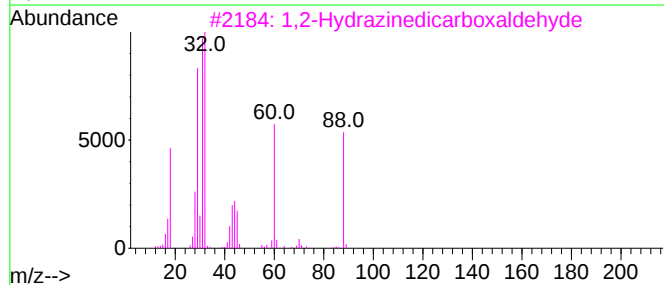
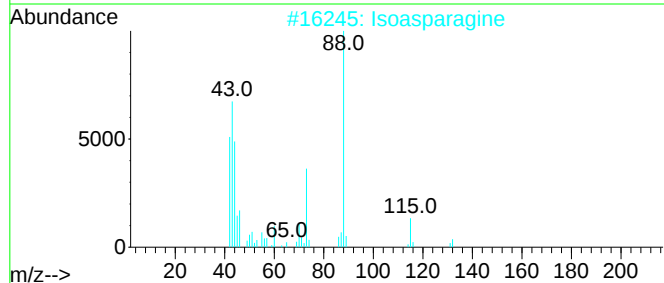
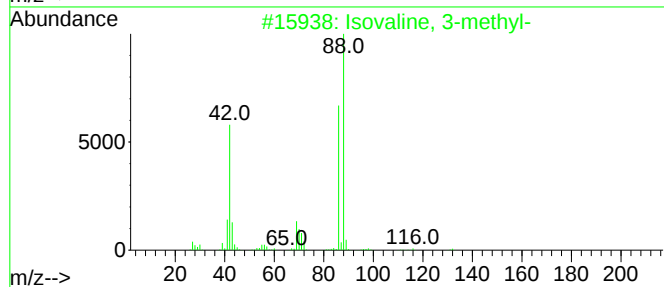
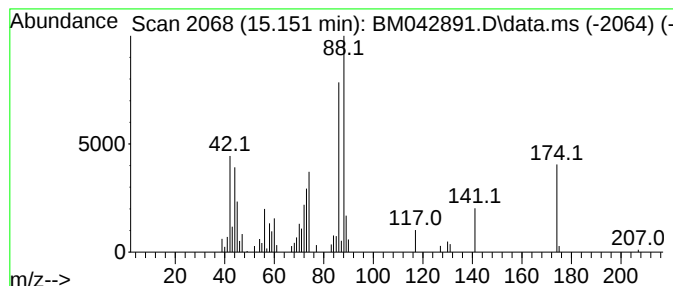
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.151	3.23 ng/ul	57900	Acenaphthene-d10	14.469

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isovaline, 3-methyl-	131	C6H13NO2	004378-19-2	43
2			Isoasparagine	132	C4H8N2O3	1010130-17-5	32
3			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	22
4			2-Propanone, methylhydrazone	86	C4H10N2	005771-02-8	22
5			1,3-Dioxol-2-one	86	C3H2O3	000872-36-6	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111723\
Data File : BM042891.D
Acq On : 18 Nov 2023 21:33
Operator : MA/JU
Sample : 05370-20
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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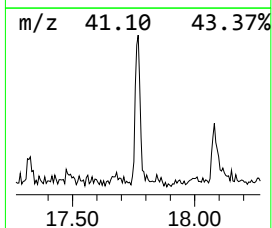
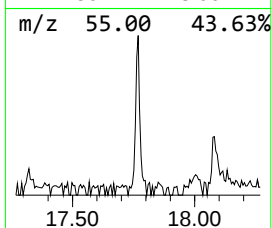
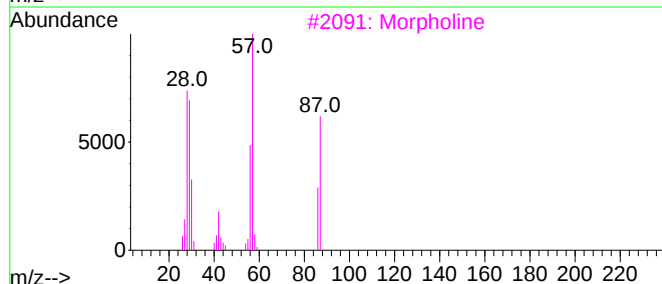
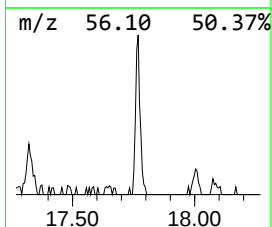
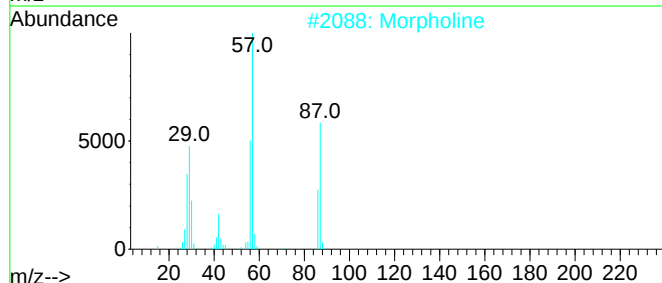
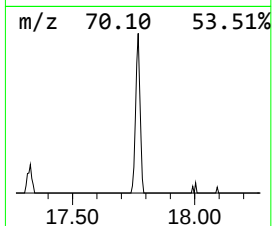
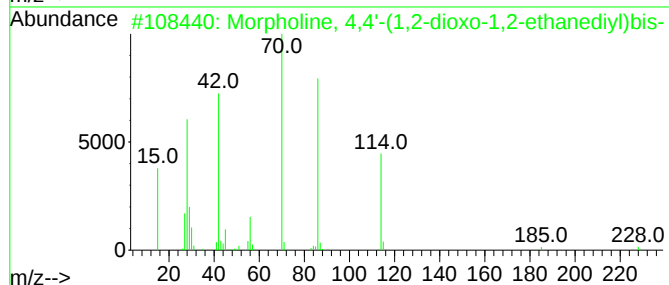
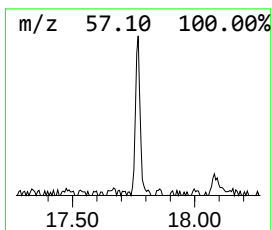
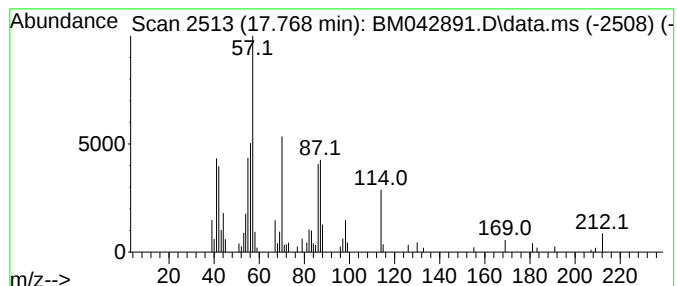
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.768	3.52 ng/ul	72135	Phenanthrene-d10	17.227

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Morpholine, 4,4'-(1,2-dioxo-1,2-...	228	C10H16N2O4	006342-79-6	43
2			Morpholine	87	C4H9NO	000110-91-8	43
3			Morpholine	87	C4H9NO	000110-91-8	43
4			Morpholine	87	C4H9NO	000110-91-8	38
5			Acetic acid, trichloro-, heptyl ...	260	C9H15Cl3O2	065611-31-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111723\
Data File : BM042891.D
Acq On : 18 Nov 2023 21:33
Operator : MA/JU
Sample : 05370-20
Misc :
ALS Vial : 47 Sample Multiplier: 1

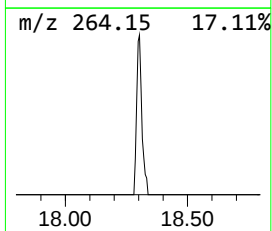
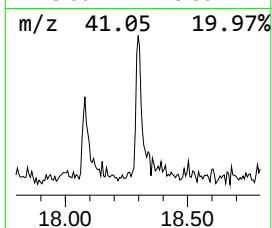
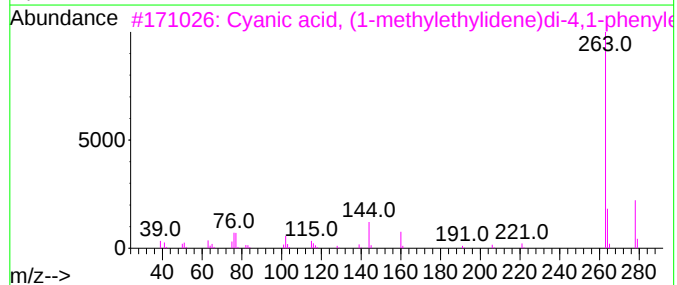
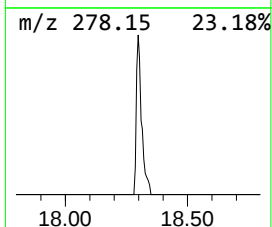
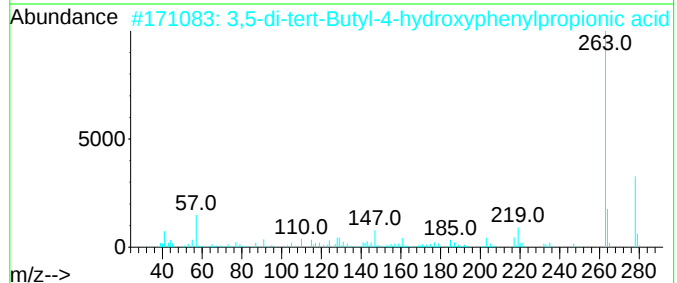
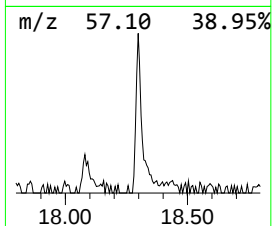
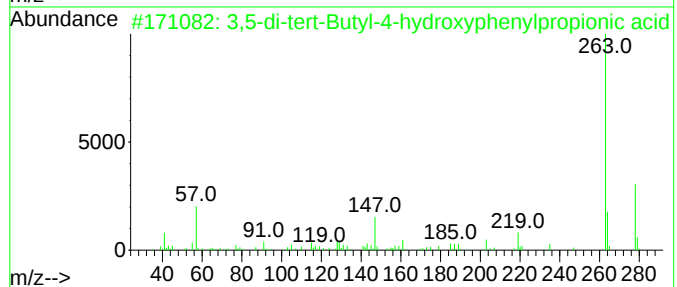
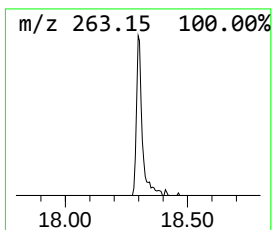
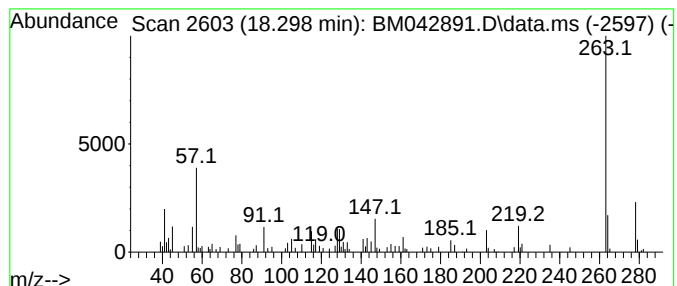
Instrument :
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.298	4.20 ng/ul	86217	Phenanthrene-d10	17.227	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-di-tert-Butyl-4-hydroxypheny...	278	C17H26O3	020170-32-5	97
2	3,5-di-tert-Butyl-4-hydroxypheny...	278	C17H26O3	020170-32-5	94
3	Cyanic acid, (1-methylethylidene...	278	C17H14N2O2	001156-51-0	58
4	Fenoxon sulfoxide	278	C10H15O5PS	006552-13-2	53
5	6,7-Dimethoxy-4(1H)-quinazolinon...	278	C13H18N2O3Si	1000479-65-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111723\
Data File : BM042891.D
Acq On : 18 Nov 2023 21:33
Operator : MA/JU
Sample : 05370-20
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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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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1,3-Butadiene, ...	7.545	4.3	ng/ul	45596	1	7.816	210496	20.0
Cyclohexane, is...	11.357	4.7	ng/ul	64476	2	10.628	274965	20.0
N-Ethylpiperazine	12.428	2.1	ng/ul	29523	2	10.628	274965	20.0
N-Cyclohexyl-N'...	14.686	11.6	ng/ul	208016	3	14.469	358037	20.0
unknown-01	15.151	3.2	ng/ul	57900	3	14.469	358037	20.0
unknown-02	17.768	3.5	ng/ul	72135	4	17.227	410414	20.0
3,5-di-tert-But...	18.298	4.2	ng/ul	86217	4	17.227	410414	20.0