

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
 Data File : BM037726.D
 Acq On : 26 Nov 2022 10:36
 Operator : CG/JU
 Sample : N5592-06
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 H0AB1

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-BM112322.M
 Title : SVOA CALIBRATION

Signal : TIC: BM037726.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.434	5	8	12	rVV	46555	53639	0.62%	0.067%
2	3.469	12	14	20	rVB	41818	55041	0.63%	0.069%
3	3.875	80	83	100	rBV	315657	562560	6.46%	0.707%
4	4.110	120	123	130	rVB2	27852	43225	0.50%	0.054%
5	4.216	136	141	145	rVB4	17623	30163	0.35%	0.038%
6	4.604	204	207	210	rVB5	9383	11462	0.13%	0.014%
7	4.669	216	218	224	rVB7	11174	16241	0.19%	0.020%
8	4.763	228	234	243	rVB	360033	550880	6.33%	0.692%
9	6.357	501	505	509	rBV4	5189	10301	0.12%	0.013%
10	7.069	623	626	634	rBV9	5986	11418	0.13%	0.014%
11	7.257	651	658	667	rVB	342853	534324	6.14%	0.671%
12	7.428	681	687	698	rBV	1015414	1582730	18.18%	1.988%
13	7.634	715	722	732	rBV	1005037	1546058	17.76%	1.942%
14	7.716	732	736	741	rVB7	7481	13102	0.15%	0.016%
15	8.110	795	803	814	rBV	842811	1344146	15.44%	1.688%
16	8.816	915	923	931	rBV	920879	1450394	16.66%	1.822%
17	9.281	994	1002	1012	rBV	1358209	2170597	24.94%	2.726%
18	9.616	1055	1059	1065	rBV5	11419	22002	0.25%	0.028%
19	10.004	1117	1125	1134	rBV	993287	1658567	19.05%	2.083%
20	10.216	1156	1161	1167	rBV8	7641	15913	0.18%	0.020%
21	10.486	1201	1207	1209	rBV5	7092	11456	0.13%	0.014%
22	10.545	1209	1217	1228	rVV	1480775	2402322	27.60%	3.017%
23	10.710	1238	1245	1248	rBV8	6031	11220	0.13%	0.014%
24	10.857	1266	1270	1276	rBV4	23956	44905	0.52%	0.056%
25	10.933	1276	1283	1290	rVV	1270820	2087298	23.98%	2.622%
26	10.986	1290	1292	1297	rVB5	9872	15199	0.17%	0.019%
27	11.063	1297	1305	1313	rBV	1161153	1931716	22.19%	2.426%
28	11.180	1322	1325	1332	rVB8	6087	11452	0.13%	0.014%
29	11.592	1388	1395	1399	rBV9	4913	10444	0.12%	0.013%
30	11.704	1408	1414	1418	rBV7	12412	23980	0.28%	0.030%
31	12.169	1488	1493	1498	rVB6	8833	16491	0.19%	0.021%
32	12.404	1530	1533	1540	rBV8	8736	18226	0.21%	0.023%
33	12.469	1540	1544	1546	rVV4	11159	17260	0.20%	0.022%
34	12.504	1546	1550	1555	rVB2	25045	39736	0.46%	0.050%
35	12.721	1584	1587	1593	rVB8	8147	12981	0.15%	0.016%
36	13.004	1631	1635	1645	rVB8	5392	10454	0.12%	0.013%

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37	13.104	1647	1652	1654	rBV6	7767	12159	0.14%	0.015%
38	13.345	1691	1693	1700	rVB7	10153	19858	0.23%	0.025%
39	13.474	1711	1715	1721	rVB8	7255	12381	0.14%	0.016%
40	13.627	1736	1741	1746	rBV3	19665	34044	0.39%	0.043%

41	13.716	1748	1756	1765	rVB3	10300	26689	0.31%	0.034%
42	13.933	1787	1793	1794	rBV5	5684	10548	0.12%	0.013%
43	14.139	1821	1828	1834	rBV	3206344	4422343	50.81%	5.554%
44	14.433	1871	1878	1887	rBV	3463487	4842220	55.63%	6.082%
45	14.498	1887	1889	1894	rVV6	8124	14060	0.16%	0.018%

46	14.545	1894	1897	1900	rVB5	7444	9724	0.11%	0.012%
47	14.615	1905	1909	1912	rBV3	14487	23271	0.27%	0.029%
48	14.657	1912	1916	1921	rVB2	91292	119899	1.38%	0.151%
49	14.733	1923	1929	1937	rVB	1946983	2840334	32.63%	3.567%
50	14.810	1937	1942	1946	rBV7	9314	16271	0.19%	0.020%

51	14.910	1953	1959	1967	rBV	456065	683908	7.86%	0.859%
52	15.133	1993	1997	2003	rVB7	29280	48145	0.55%	0.060%
53	15.198	2003	2008	2013	rBV9	10984	19417	0.22%	0.024%
54	15.333	2028	2031	2036	rBV7	8028	11967	0.14%	0.015%
55	15.462	2050	2053	2057	rBV	25738	37887	0.44%	0.048%

56	15.539	2061	2066	2068	rVV2	32312	51864	0.60%	0.065%
57	15.562	2068	2070	2074	rVB	28350	28397	0.33%	0.036%
58	15.627	2078	2081	2084	rVB4	11325	13823	0.16%	0.017%
59	15.721	2089	2097	2109	rBV	4497640	6246930	71.77%	7.846%
60	15.827	2109	2115	2127	rBV	1799528	2439523	28.03%	3.064%

61	15.957	2132	2137	2144	rVB6	34599	75804	0.87%	0.095%
62	16.221	2178	2182	2187	rVB	102150	142980	1.64%	0.180%
63	16.298	2192	2195	2199	rVB5	18165	24344	0.28%	0.031%
64	16.392	2206	2211	2220	rBV2	225259	400621	4.60%	0.503%
65	16.733	2264	2269	2273	rBV	54150	75316	0.87%	0.095%

66	16.933	2299	2303	2305	rBV5	15723	21858	0.25%	0.027%
67	17.209	2347	2350	2354	rVB2	34764	39959	0.46%	0.050%
68	17.256	2356	2358	2363	rVB5	17574	23508	0.27%	0.030%
69	17.468	2388	2394	2400	rBV	2335334	3307281	38.00%	4.154%
70	17.574	2405	2412	2419	rBV	5258007	7499279	86.16%	9.419%

71	17.951	2473	2476	2480	rBV	30542	36738	0.42%	0.046%
72	17.998	2482	2484	2490	rVB6	15686	22759	0.26%	0.029%
73	18.127	2502	2506	2511	rVB	52796	66756	0.77%	0.084%
74	18.345	2539	2543	2553	rBV	273662	420442	4.83%	0.528%
75	18.421	2553	2556	2565	rVB4	52907	101874	1.17%	0.128%

76	18.639	2590	2593	2598	rBV2	27535	34962	0.40%	0.044%
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77	19.262	2696	2699	2701	rBV2	38140	43420	0.50%	0.055%
78	19.415	2721	2725	2730	rBV2	80461	106886	1.23%	0.134%
79	19.486	2732	2737	2743	rBV	83873	156711	1.80%	0.197%
80	19.550	2743	2748	2753	rVV	1640875	1704357	19.58%	2.141%
81	19.609	2754	2758	2764	rBV2	250687	331734	3.81%	0.417%
82	19.850	2793	2799	2809	rBV	6809078	8704115	100.00%	10.932%
83	20.821	2961	2964	2967	rBV2	84868	92188	1.06%	0.116%
84	21.321	3047	3049	3054	rVB	89279	91875	1.06%	0.115%
85	21.633	3097	3102	3108	rBV	2813230	3582942	41.16%	4.500%
86	23.968	3491	3499	3510	rVB2	4008374	8369551	96.16%	10.512%
87	24.127	3519	3526	3534	rVB2	1586860	3233904	37.15%	4.062%
88	24.738	3627	3630	3638	rVB	302205	574754	6.60%	0.722%

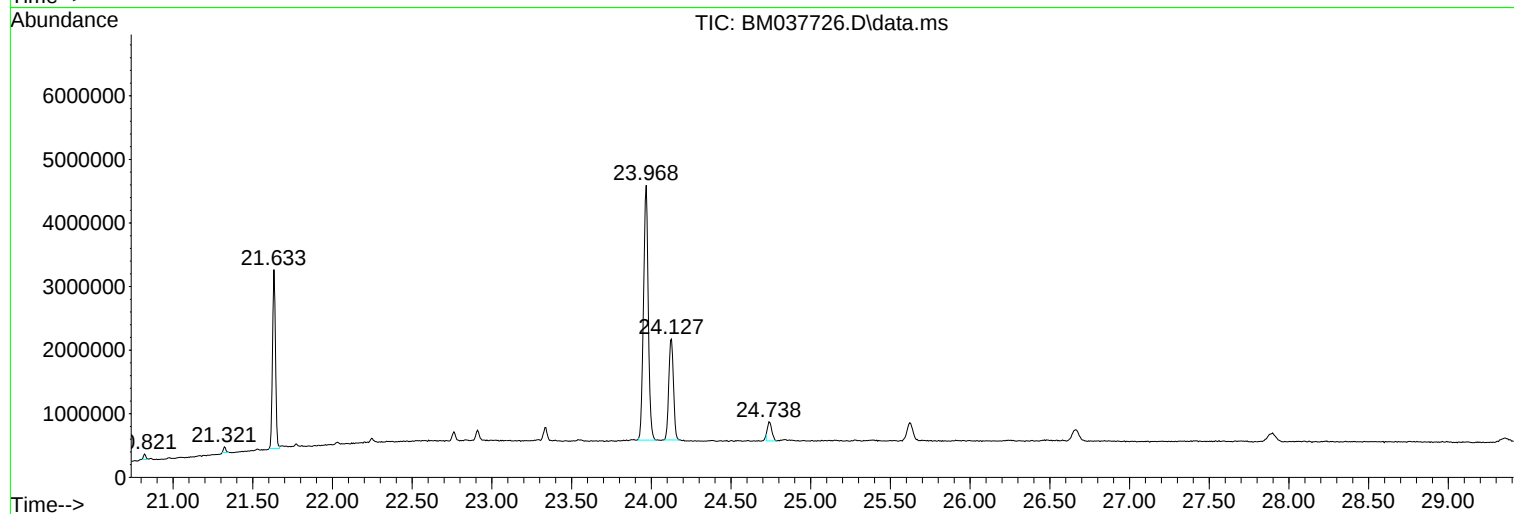
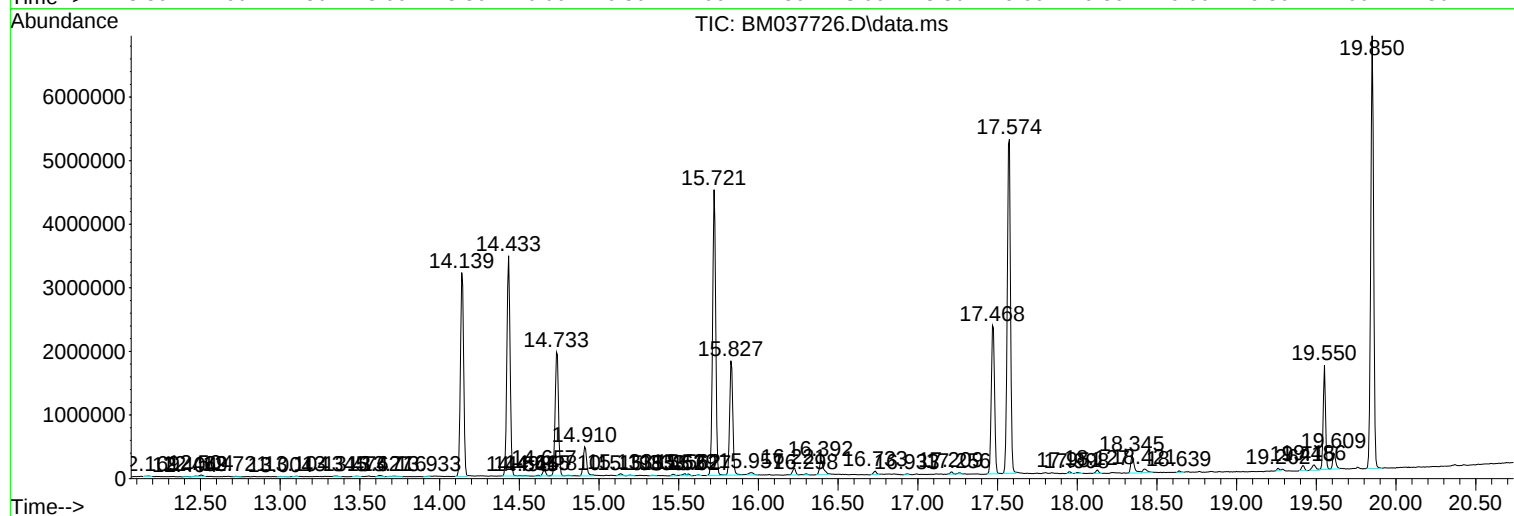
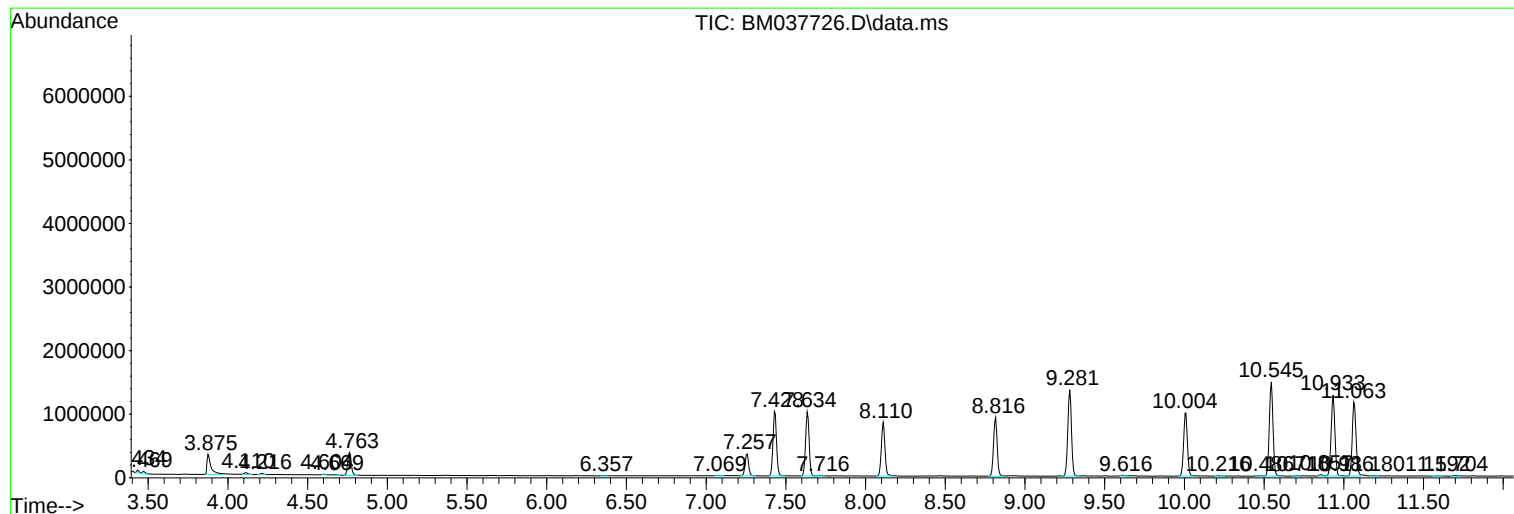
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

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



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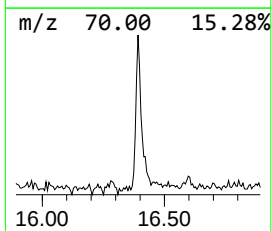
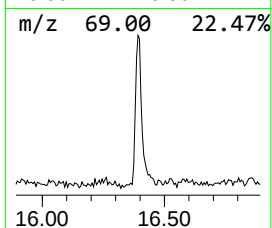
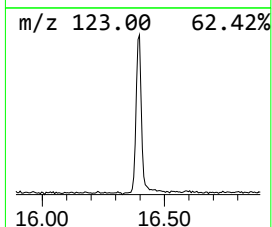
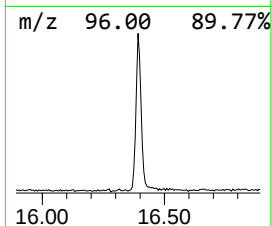
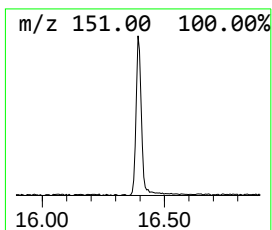
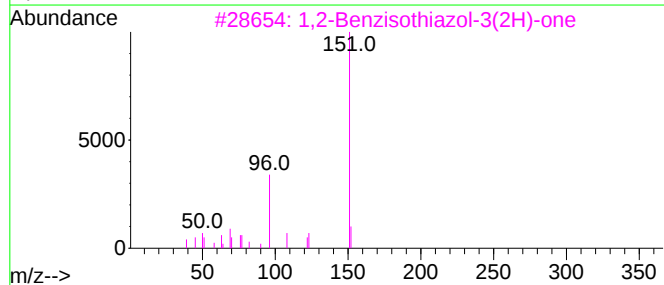
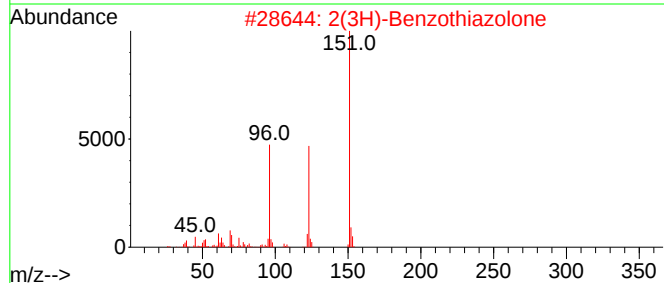
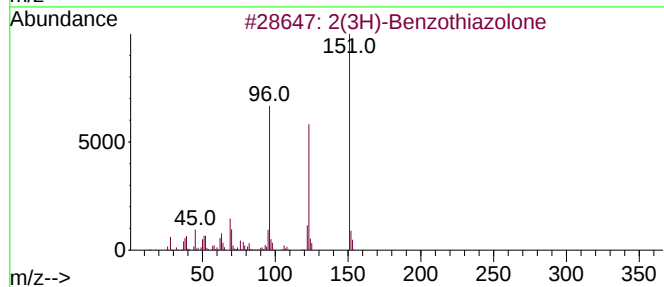
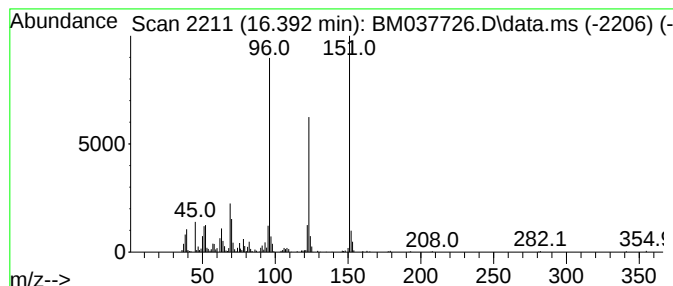
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 2(3H)-Benzothiazolone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.392	2.42 ng/ul	400621	Phenanthrene-d10	17.468

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	94
2		2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	81
3		1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	64
4		Thieno[3,2-b]pyridin-7-ol	151	C7H5NOS	107818-20-2	52
5		1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	46



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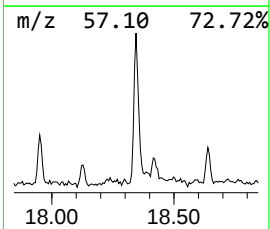
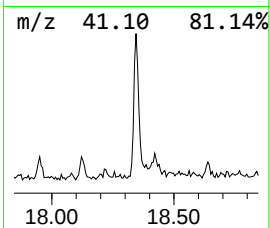
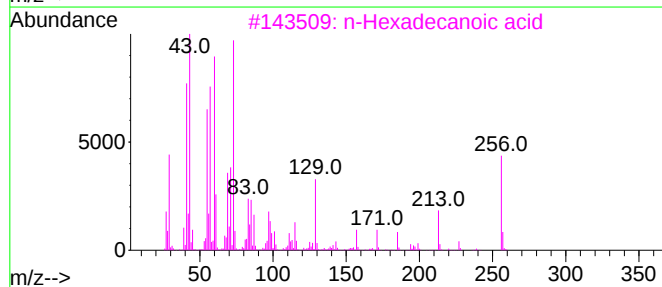
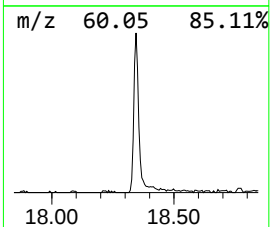
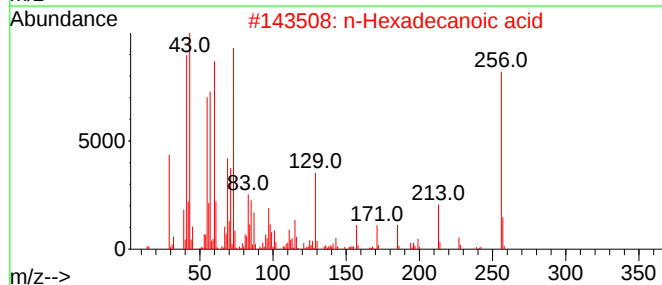
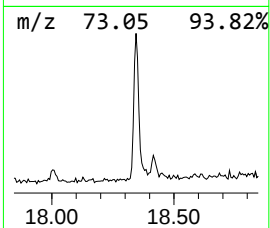
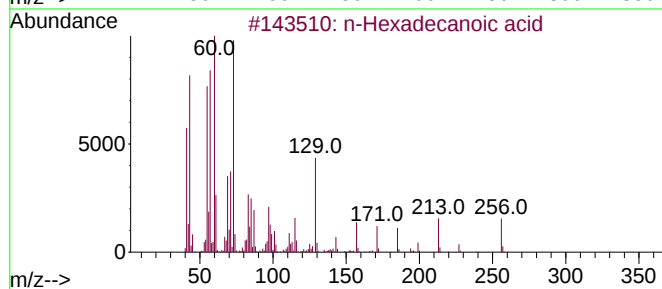
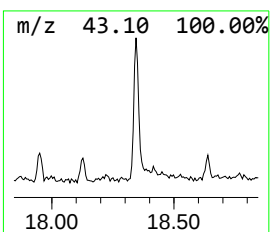
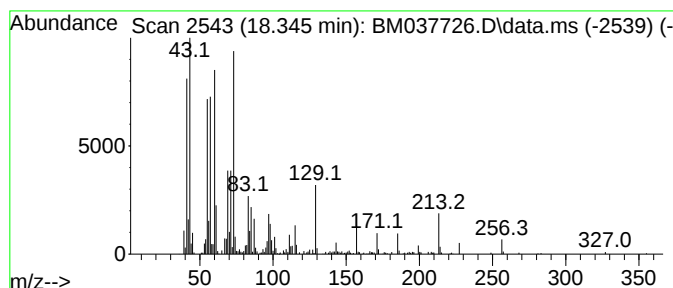
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.345	2.54 ng/ul	420442	Phenanthrene-d10	17.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
4			Tridecanoic acid	214	C13H26O2	000638-53-9	93
5			Tridecanoic acid	214	C13H26O2	000638-53-9	87



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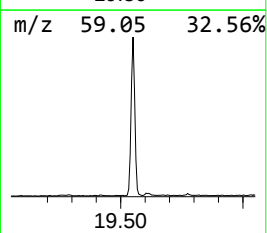
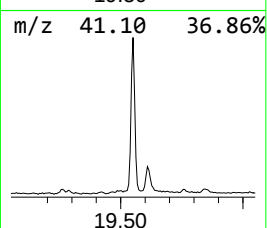
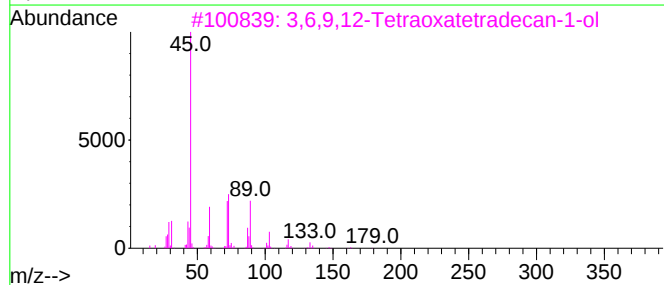
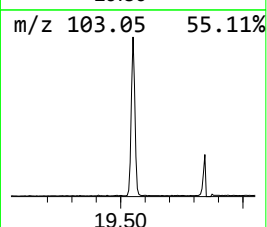
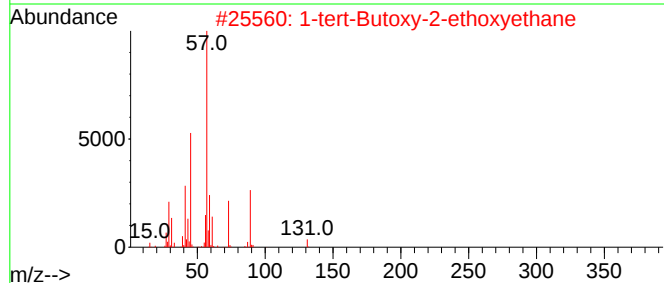
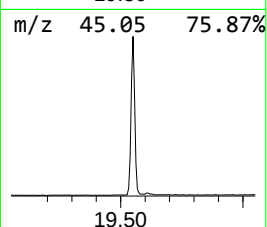
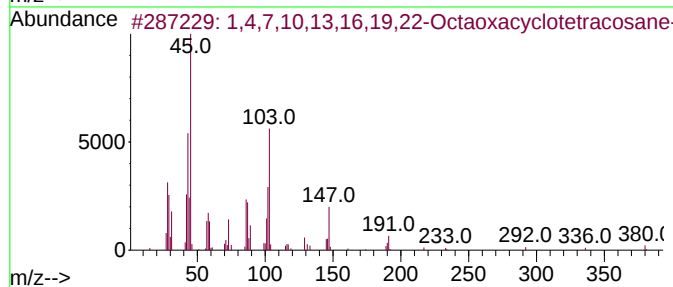
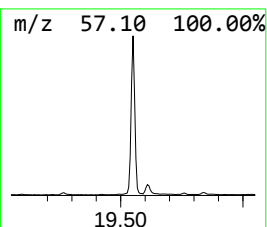
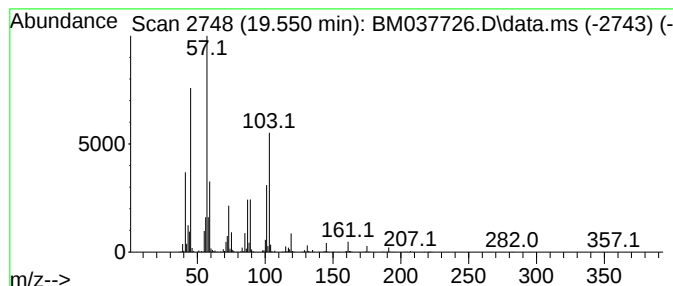
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 1,4,7,10,13,16,19,22-Octaox... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.550	10.31 ng/ul	1704360	Phenanthrene-d10	17.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4,7,10,13,16,19,22-Octaoxacycl...	380	C16H28O10	1000221-60-1	53		
2	1-tert-Butoxy-2-ethoxyethane	146	C8H18O2	051422-54-9	50		
3	3,6,9,12-Tetraoxatetradecan-1-ol	222	C10H22O5	005650-20-4	43		
4	2-[2-[2-[2-[2-[2-[2-[2-[2-...	546	C24H50O13	1000352-12-7	38		
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	38		



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Instrument :
BNA_M
ClientSampleId :
H0AB1

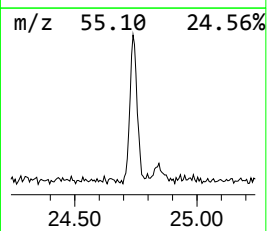
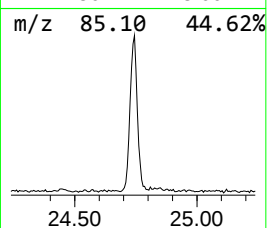
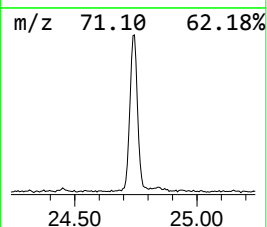
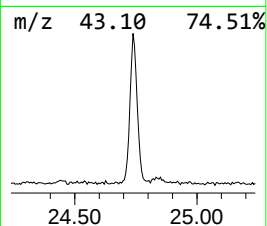
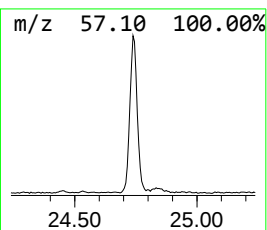
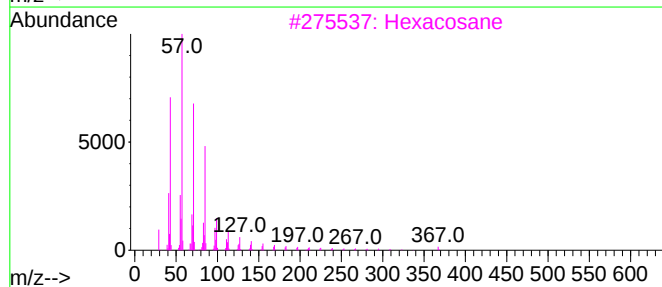
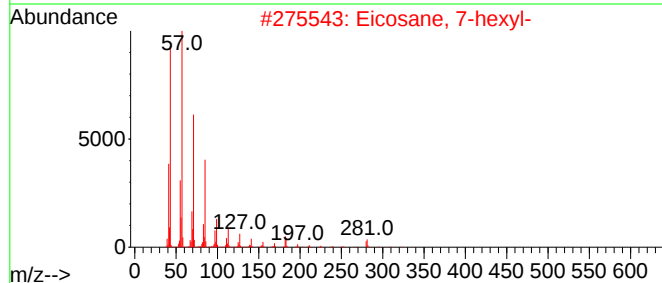
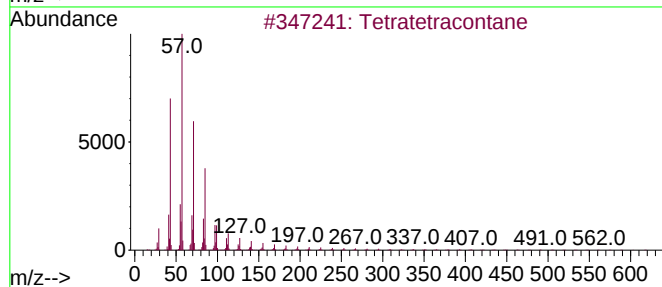
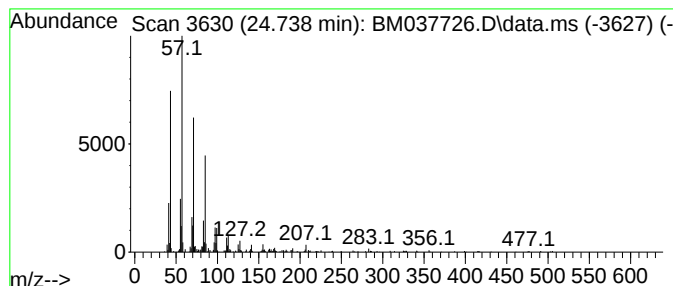
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.738	3.55 ng/ul	574754	Perylene-d12	24.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	87
2			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87
3			Hexacosane	366	C26H54	000630-01-3	87
4			Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	86
5			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037726.D
Acq On : 26 Nov 2022 10:36
Operator : CG/JU
Sample : N5592-06
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
H0AB1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.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(3H)-Benzothia...	16.392	2.4	ng/u1	400621	4	17.468	3307280	20.0
n-Hexadecanoic ...	18.345	2.5	ng/u1	420442	4	17.468	3307280	20.0
1,4,7,10,13,16,...	19.550	10.3	ng/u1	1704360	4	17.468	3307280	20.0
(DEL) Alkane: S...	24.738	3.5	ng/u1	574754	6	24.127	3233900	20.0