

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042523\
 Data File : BM039637.D
 Acq On : 25 Apr 2023 13:05
 Operator : CG/JU
 Sample : 02433-14
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 BHE49

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-BM041823.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BM039637.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.172	18	23	31	rBV	2096024	3101494	58.39%	5.547%
2	3.237	31	34	48	rVB	368007	505246	9.51%	0.904%
3	3.507	77	80	94	rVB	23583	51614	0.97%	0.092%
4	3.631	99	101	119	rBV	225998	414618	7.81%	0.742%
5	3.854	136	139	144	rVB	22123	31548	0.59%	0.056%
6	3.954	153	156	165	rVB	22096	34185	0.64%	0.061%
7	4.066	173	175	179	rVB5	12412	15313	0.29%	0.027%
8	4.484	241	246	259	rBV	1543467	2327784	43.82%	4.163%
9	5.072	340	346	358	rBV	476688	771621	14.53%	1.380%
10	5.496	414	418	424	rVB	13279	18659	0.35%	0.033%
11	5.866	476	481	483	rBV5	9425	15515	0.29%	0.028%
12	6.313	553	557	563	rBV4	11312	18839	0.35%	0.034%
13	6.872	645	652	668	rBV	93441	242249	4.56%	0.433%
14	7.001	668	674	692	rVV	116537	294262	5.54%	0.526%
15	7.142	692	698	715	rVV	657659	1129003	21.25%	2.019%
16	7.266	717	719	726	rVV5	9356	16741	0.32%	0.030%
17	7.342	726	732	752	rVV	605901	1086249	20.45%	1.943%
18	7.478	753	755	759	rVB5	9983	11537	0.22%	0.021%
19	7.695	786	792	798	rBV9	5720	12866	0.24%	0.023%
20	7.807	805	811	819	rBV	704609	1168287	21.99%	2.089%
21	7.878	819	823	836	rVB	49280	108368	2.04%	0.194%
22	8.160	867	871	880	rVB9	7177	15256	0.29%	0.027%
23	8.548	931	937	951	rBV2	97657	255790	4.82%	0.457%
24	8.984	1004	1011	1032	rBV	723078	1392477	26.21%	2.490%
25	9.366	1071	1076	1081	rVB7	7077	13752	0.26%	0.025%
26	9.701	1126	1133	1152	rBV	597909	1182424	22.26%	2.115%
27	9.978	1172	1180	1198	rBV	171391	410319	7.72%	0.734%
28	10.254	1220	1227	1247	rBV	665384	1506602	28.36%	2.694%
29	10.407	1247	1253	1273	rVV	173131	445062	8.38%	0.796%
30	10.560	1274	1279	1282	rVV3	39138	79062	1.49%	0.141%
31	10.613	1282	1288	1310	rVB	1006626	1837009	34.58%	3.285%
32	10.795	1317	1319	1326	rVB7	5900	9159	0.17%	0.016%
33	11.295	1398	1404	1411	rVB3	11371	25523	0.48%	0.046%
34	11.442	1422	1429	1444	rBV	259956	542004	10.20%	0.969%
35	11.583	1450	1453	1459	rVB7	6426	10267	0.19%	0.018%
36	11.919	1505	1510	1521	rBV8	20830	56736	1.07%	0.101%

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37	12.130	1540	1546	1555	rBV	59022	124454	2.34%	0.223%
38	12.213	1555	1560	1568	rVB	18586	38043	0.72%	0.068%
39	12.630	1626	1631	1634	rBV7	4145	5883	0.11%	0.011%
40	12.772	1648	1655	1662	rBV7	20245	54538	1.03%	0.098%

41	12.819	1662	1663	1671	rVB8	7532	13776	0.26%	0.025%
42	12.995	1685	1693	1694	rBV8	3301	7424	0.14%	0.013%
43	13.095	1707	1710	1719	rVB3	6329	10743	0.20%	0.019%
44	13.277	1736	1741	1746	rBV7	6593	14294	0.27%	0.026%
45	13.360	1751	1755	1763	rVB2	16727	28652	0.54%	0.051%

46	13.471	1770	1774	1779	rVB4	10318	15430	0.29%	0.028%
47	13.807	1827	1831	1835	rBV7	3132	5641	0.11%	0.010%
48	13.883	1835	1844	1857	rBV	2164270	3145185	59.21%	5.625%
49	13.989	1857	1862	1871	rVB	281281	430853	8.11%	0.771%
50	14.113	1879	1883	1885	rBV5	7894	10396	0.20%	0.019%

51	14.160	1885	1891	1911	rVV	1896307	2805390	52.81%	5.017%
52	14.307	1912	1916	1920	rVB6	6228	8589	0.16%	0.015%
53	14.466	1936	1943	1960	rVB	1773421	2693467	50.71%	4.817%
54	14.654	1974	1975	1981	rVB6	4055	5392	0.10%	0.010%
55	14.701	1981	1983	1986	rBV4	5656	8685	0.16%	0.016%

56	14.771	1989	1995	1998	rBV4	28536	64736	1.22%	0.116%
57	15.030	2036	2039	2044	rVB4	7101	9746	0.18%	0.017%
58	15.101	2048	2051	2057	rVB7	8719	12160	0.23%	0.022%
59	15.154	2059	2060	2067	rBV7	4203	5790	0.11%	0.010%
60	15.460	2106	2112	2129	rBV	3000885	4486202	84.45%	8.023%

61	15.601	2131	2136	2149	rBV	603826	1025370	19.30%	1.834%
62	15.836	2170	2176	2186	rVB	114717	175443	3.30%	0.314%
63	16.136	2222	2227	2230	rBV	20729	28001	0.53%	0.050%
64	16.254	2242	2247	2250	rBV7	3962	6785	0.13%	0.012%
65	16.642	2307	2313	2315	rBV7	5560	9736	0.18%	0.017%

66	16.671	2316	2318	2323	rVB6	7366	10088	0.19%	0.018%
67	17.101	2386	2391	2395	rBV2	16174	23884	0.45%	0.043%
68	17.218	2405	2411	2422	rBV	1965143	2804914	52.80%	5.016%
69	17.318	2422	2428	2446	rVB	3074439	4422846	83.26%	7.910%
70	17.783	2504	2507	2511	rVB5	10154	14569	0.27%	0.026%

71	17.854	2517	2519	2522	rBV3	9553	10036	0.19%	0.018%
72	17.883	2522	2524	2529	rVB5	19511	22088	0.42%	0.040%
73	18.118	2559	2564	2573	rBV	101173	187666	3.53%	0.336%
74	18.624	2645	2650	2660	rBV3	49958	134779	2.54%	0.241%
75	18.971	2707	2709	2714	rVB6	12032	13678	0.26%	0.024%

76	19.183	2741	2745	2750	rBV2	39490	55461	1.04%	0.099%
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Integrator: RTE
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Sampling : 1 Min Area: 0.1 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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Title : SVOA CALIBRATION

77	19.259	2754	2758	2764	rBV	37410	70591	1.33%	0.126%
78	19.400	2778	2782	2793	rBV2	74644	133988	2.52%	0.240%
79	19.542	2803	2806	2812	rVB2	36859	45156	0.85%	0.081%
80	19.618	2813	2819	2833	rBV	3972066	5312005	100.00%	9.500%
81	21.418	3120	3125	3139	rBV	1718677	2394930	45.09%	4.283%
82	23.624	3493	3500	3517	rBV2	1780415	3712813	69.89%	6.640%
83	23.777	3520	3526	3539	rVB2	1013335	2136648	40.22%	3.821%

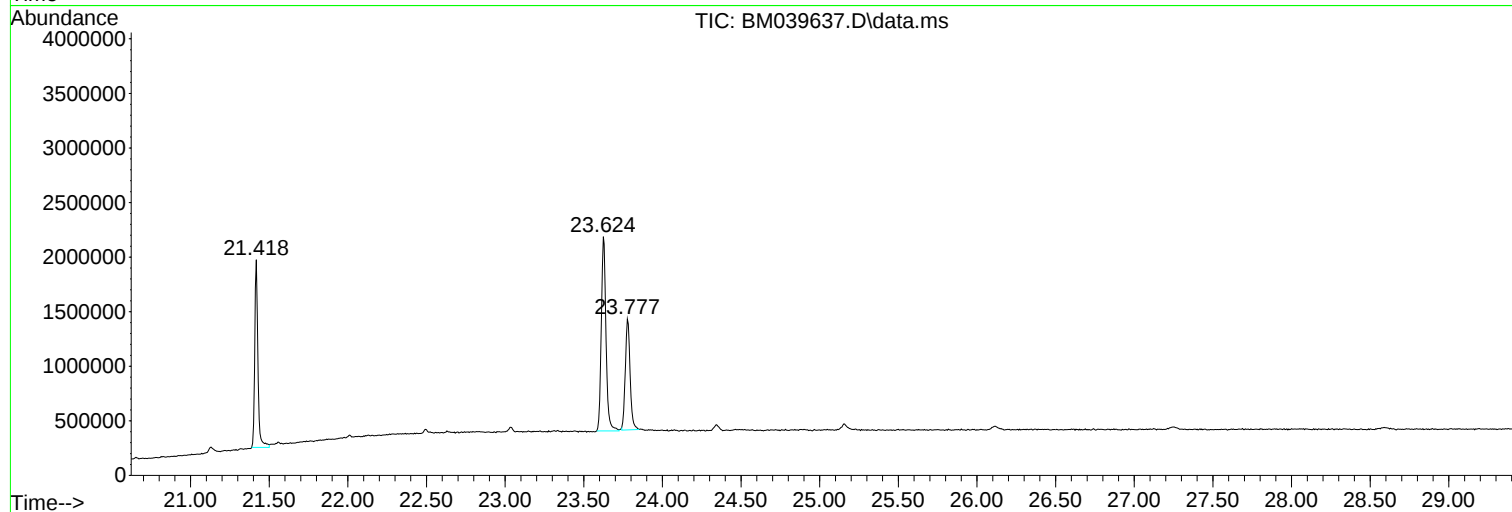
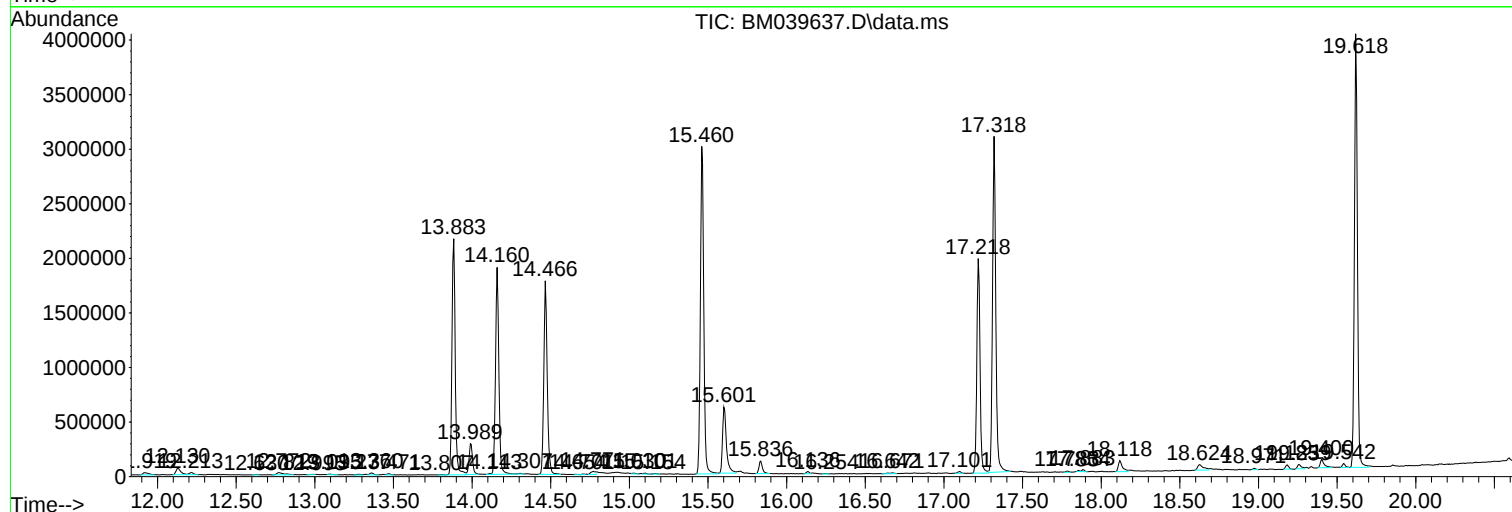
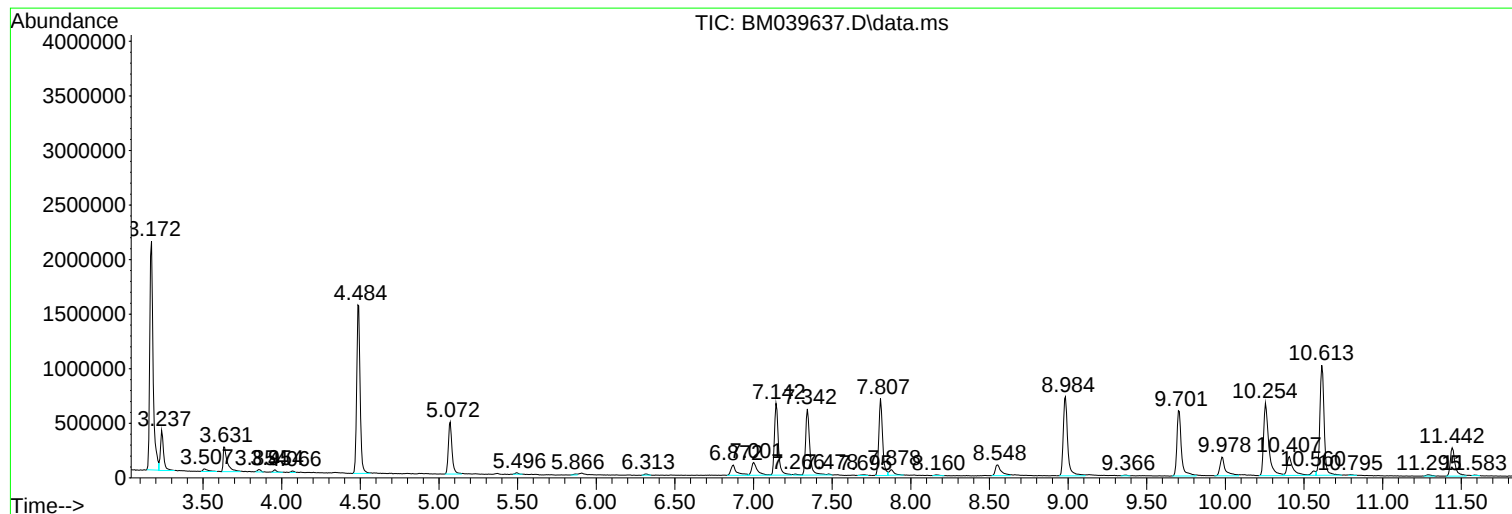
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

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



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Instrument :
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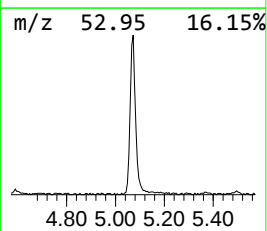
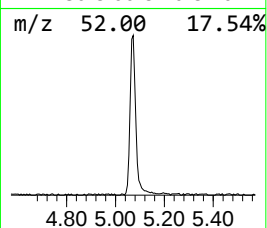
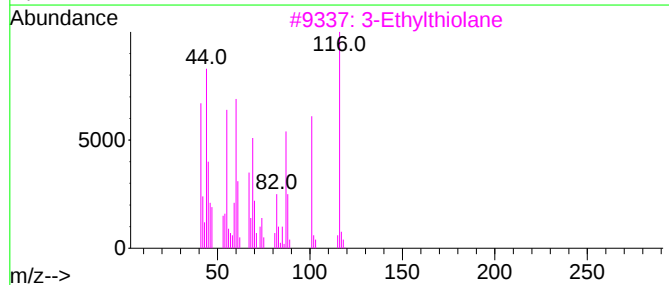
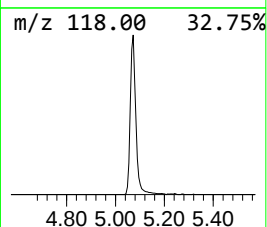
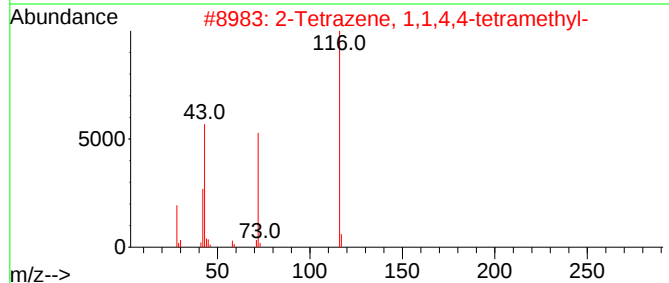
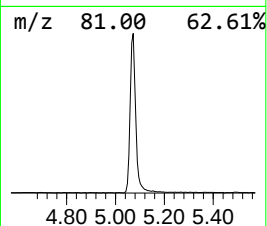
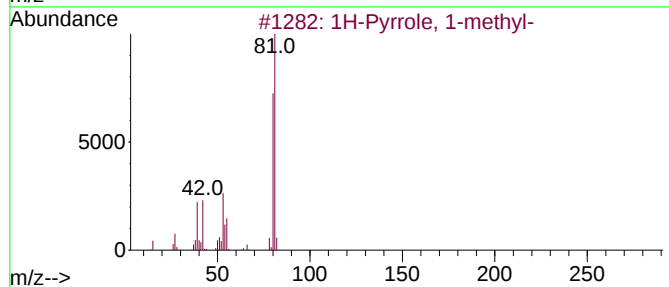
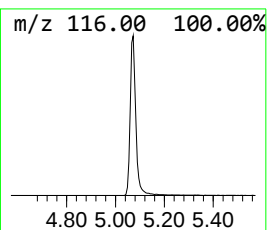
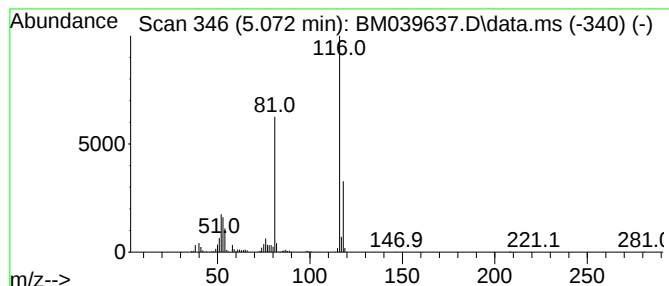
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.072	13.21 ng/ul	771621	1,4-Dichlorobenzene-d4	7.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Pyrrole, 1-methyl-	81	C5H7N	000096-54-8	10
2			2-Tetrazene, 1,1,4,4-tetramethyl-	116	C4H12N4	006130-87-6	9
3			3-Ethylthiolane	116	C6H12S	062184-67-2	9
4			4-Imidazolidinone, 2-thioxo-	116	C3H4N2OS	000503-87-7	9
5			Pyrimidine,4,6-difluoro-	116	C4H2F2N2	002802-62-2	9



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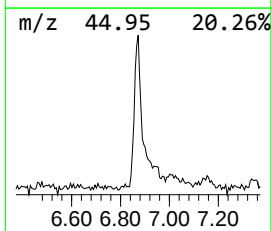
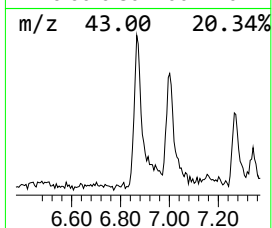
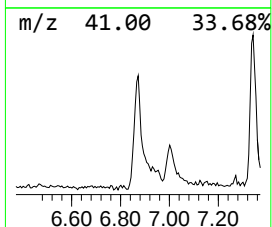
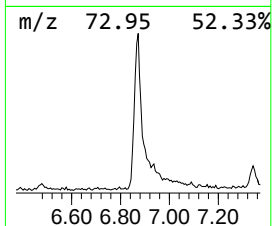
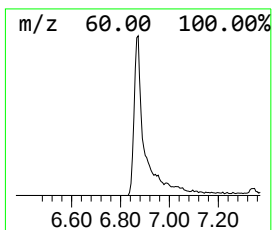
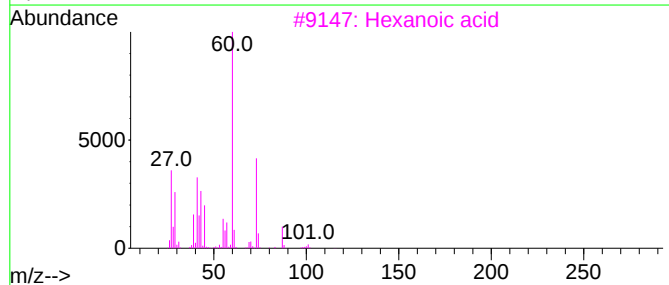
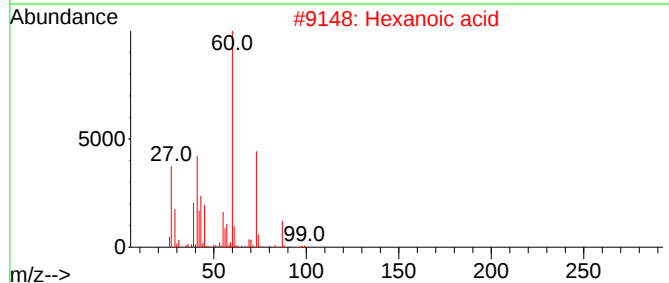
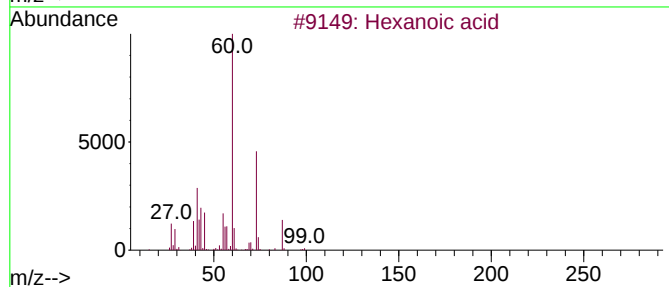
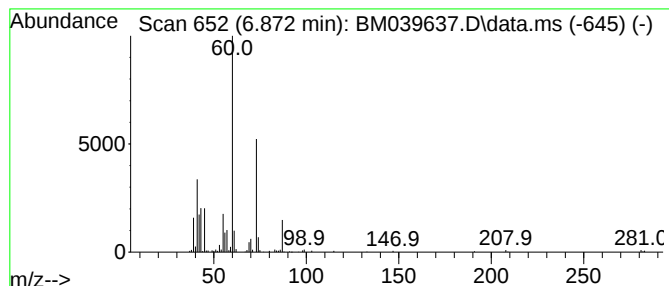
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Hexanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.872	4.15 ng/ul	242249	1,4-Dichlorobenzene-d4	7.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid	116	C6H12O2	000142-62-1	90
2			Hexanoic acid	116	C6H12O2	000142-62-1	83
3			Hexanoic acid	116	C6H12O2	000142-62-1	83
4			Hexanoic acid	116	C6H12O2	000142-62-1	72
5			Pentanoic acid	102	C5H10O2	000109-52-4	72



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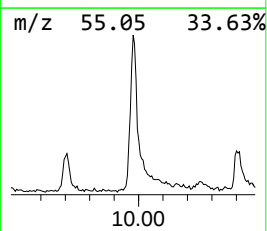
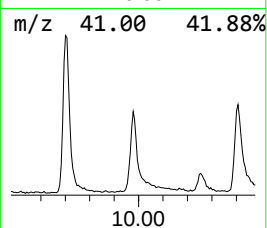
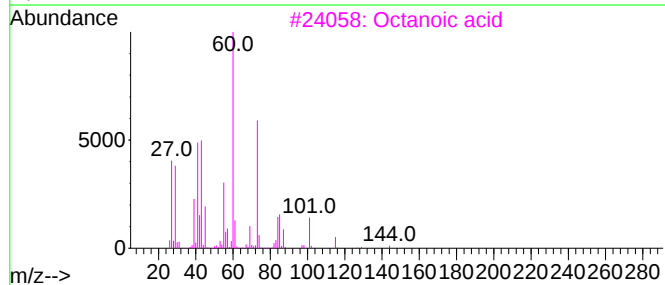
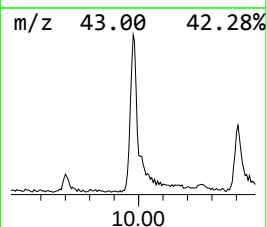
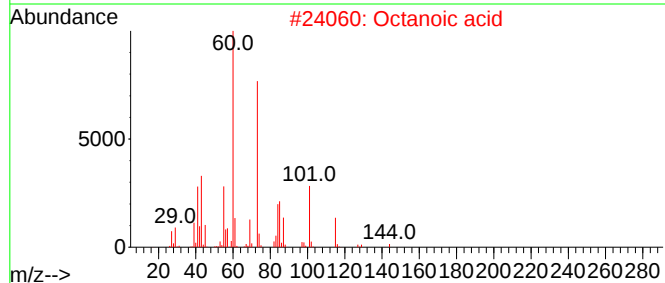
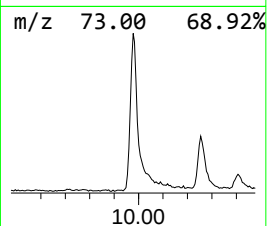
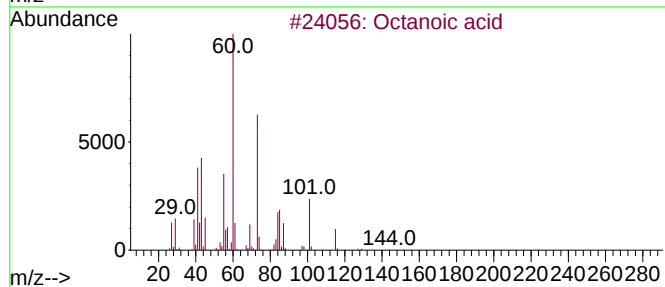
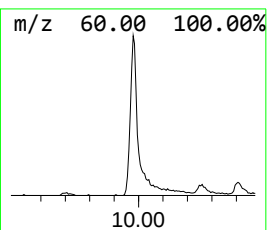
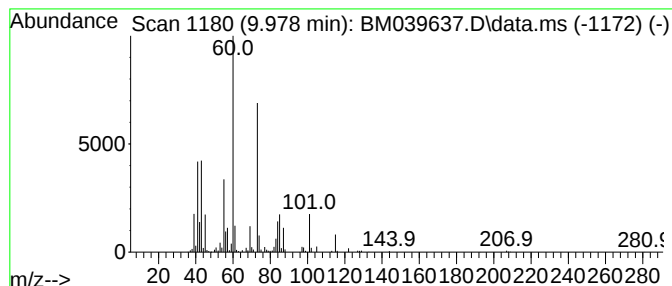
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 Octanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.978	4.47 ng/ul	410319	Naphthalene-d8	10.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid			144	C8H16O2	000124-07-2	96
2	Octanoic acid			144	C8H16O2	000124-07-2	93
3	Octanoic acid			144	C8H16O2	000124-07-2	90
4	Octanoic acid			144	C8H16O2	000124-07-2	86
5	Hexanoic acid			116	C6H12O2	000142-62-1	64



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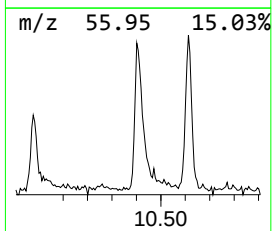
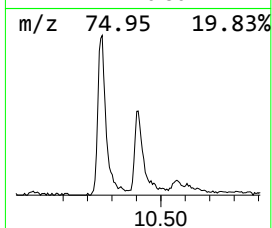
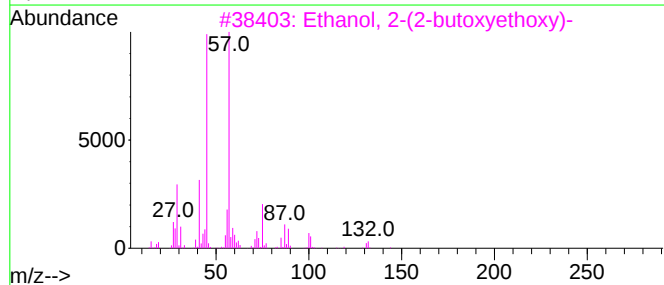
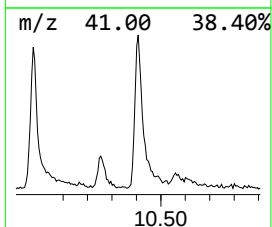
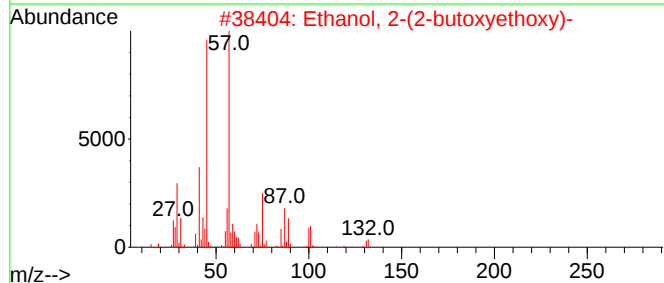
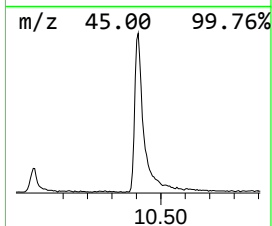
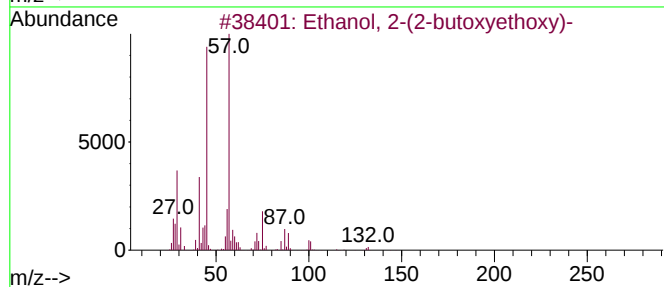
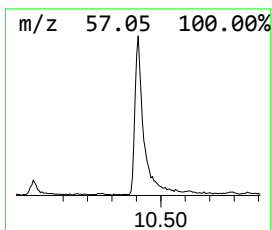
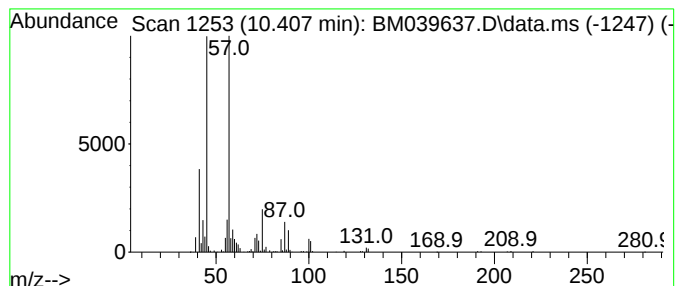
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.407	4.85 ng/ul	445062	Naphthalene-d8	10.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
4			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
5			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042523\
Data File : BM039637.D
Acq On : 25 Apr 2023 13:05
Operator : CG/JU
Sample : 02433-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BHE49

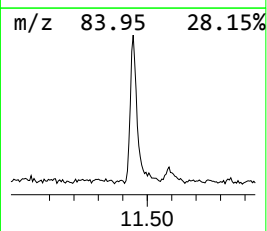
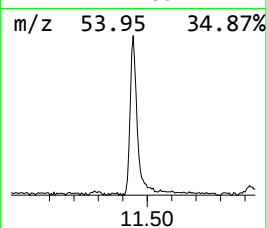
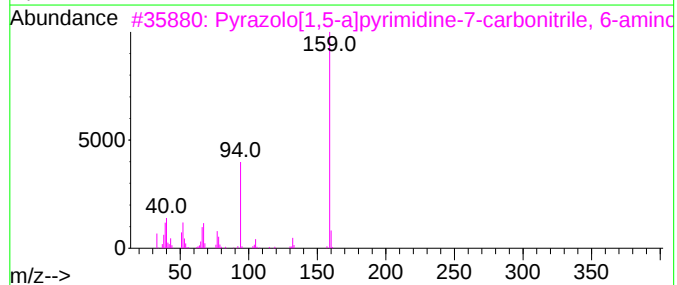
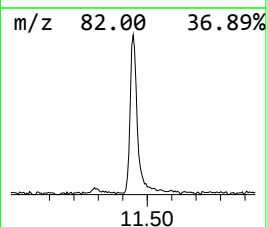
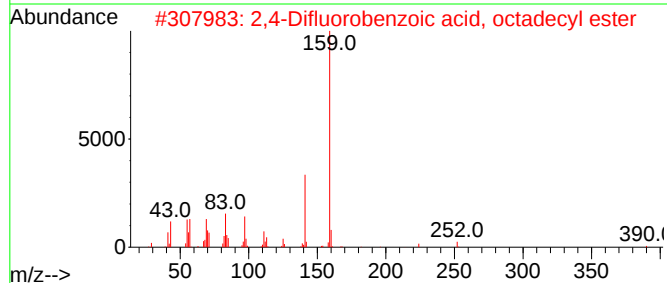
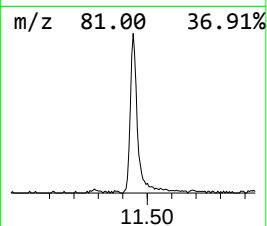
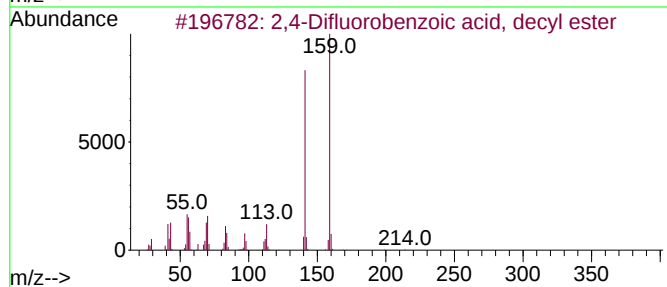
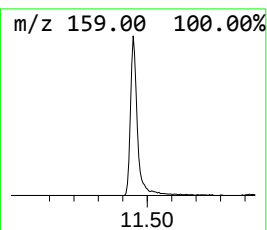
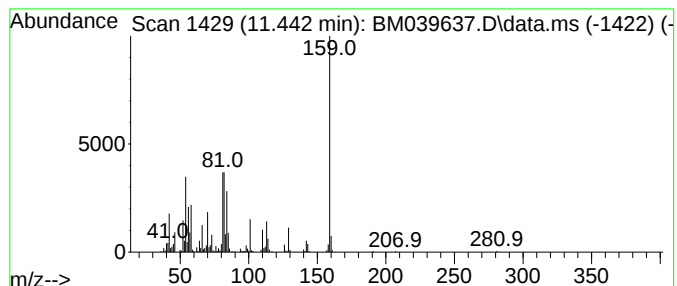
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.442	5.90 ng/ul	542004	Naphthalene-d8	10.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Difluorobenzoic acid, decyl ...	298	C17H24F2O2	1000338-78-8	37
2			2,4-Difluorobenzoic acid, octade...	410	C25H40F2O2	1000338-79-6	35
3			Pyrazolo[1,5-a]pyrimidine-7-carb...	159	C7H5N5	1000267-04-4	35
4			2,5-Difluorobenzoic acid, octyl ...	270	C15H20F2O2	1000338-80-7	35
5			7-Aminopyrazolo[1,5-a]pyrimidine...	159	C7H5N5	089975-57-5	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042523\
Data File : BM039637.D
Acq On : 25 Apr 2023 13:05
Operator : CG/JU
Sample : 02433-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BHE49

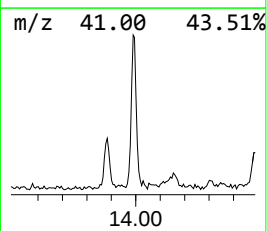
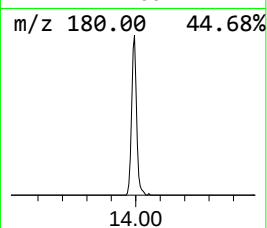
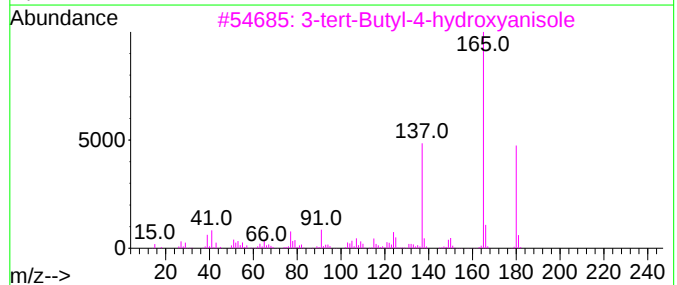
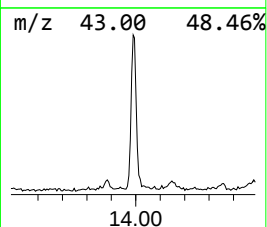
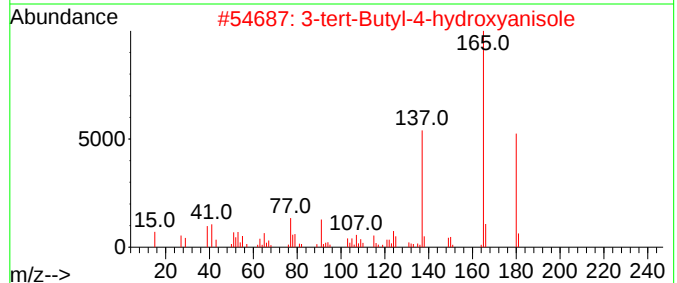
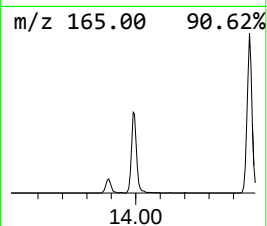
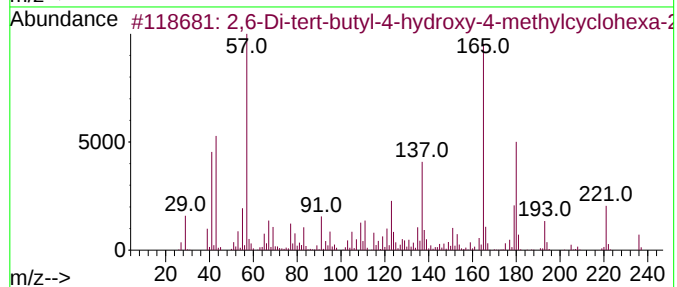
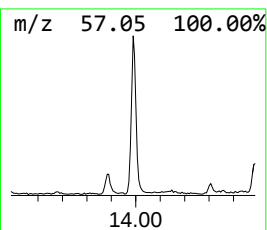
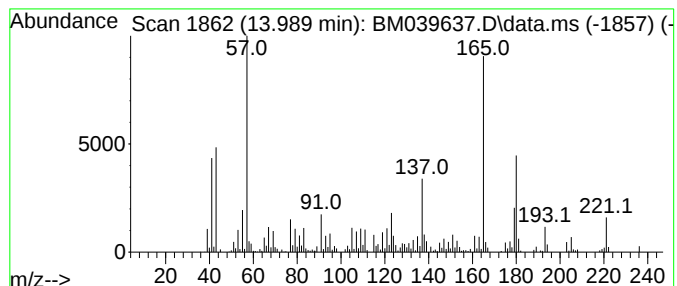
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 7 2,6-Di-tert-butyl-4-hydroxy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.989	3.20 ng/ul	430853	Acenaphthene-d10	14.466

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,6-Di-tert-butyl-4-hydroxy-4-me...	236	C15H24O2	010396-80-2	91
2			3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	64
3			3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	58
4			Furan, 2,5-dihydro-2,2-dimethyl-...	180	C12H20O	077822-53-8	53
5			Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042523\
Data File : BM039637.D
Acq On : 25 Apr 2023 13:05
Operator : CG/JU
Sample : 02433-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BHE49

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.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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Hexanoic acid	6.872	4.2	ng/ul	242249	1	7.807	1168290	20.0
Octanoic acid	9.978	4.5	ng/ul	410319	2	10.613	1837010	20.0
Ethanol, 2-(2-b...	10.407	4.8	ng/ul	445062	2	10.613	1837010	20.0
unknown-02	11.442	5.9	ng/ul	542004	2	10.613	1837010	20.0
2,6-Di-tert-but...	13.989	3.2	ng/ul	430853	3	14.466	2693470	20.0