

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
 Data File : BM043406.D
 Acq On : 18 Dec 2023 22:58
 Operator : MA/JU
 Sample : 05807-06
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 C0AX8

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-BM121523.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BM043406.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.387	30	34	39	rBV	168622	203946	1.91%	0.141%
2	3.693	79	86	99	rVB2	162389	369714	3.45%	0.256%
3	3.810	102	106	125	rBV	2194215	3425241	32.00%	2.370%
4	4.075	137	151	158	rBV	474265	1325912	12.39%	0.917%
5	4.134	159	161	167	rVB	34584	48792	0.46%	0.034%
6	4.822	272	278	286	rVB	83842	129991	1.21%	0.090%
7	4.957	296	301	310	rVB	59980	90565	0.85%	0.063%
8	5.075	317	321	330	rVB	20172	37698	0.35%	0.026%
9	5.287	350	357	365	rBV	1526633	2333228	21.80%	1.614%
10	5.416	375	379	385	rVB4	16120	27374	0.26%	0.019%
11	6.063	484	489	498	rBV	73818	120757	1.13%	0.084%
12	6.981	639	645	654	rVB	33445	59985	0.56%	0.042%
13	7.151	667	674	690	rVB	2948514	4828625	45.11%	3.341%
14	7.334	698	705	718	rVB	2304837	3712277	34.68%	2.569%
15	7.522	729	737	747	rBV	2850471	4547889	42.49%	3.147%
16	7.616	749	753	760	rVV3	21457	44262	0.41%	0.031%
17	7.992	809	817	838	rBV	1988570	3397588	31.74%	2.351%
18	8.704	930	938	945	rBV	3665949	5890115	55.03%	4.075%
19	9.169	1009	1017	1029	rBV	2800597	4725889	44.15%	3.270%
20	9.257	1030	1032	1039	rVV7	7531	11663	0.11%	0.008%
21	9.322	1039	1043	1048	rVV7	10966	18335	0.17%	0.013%
22	9.539	1075	1080	1088	rVB2	18283	37962	0.35%	0.026%
23	9.734	1105	1113	1120	rBV	113845	186013	1.74%	0.129%
24	9.886	1130	1139	1153	rBV	2388723	3977169	37.16%	2.752%
25	10.110	1172	1177	1184	rVB10	8891	18395	0.17%	0.013%
26	10.328	1209	1214	1220	rVB8	8587	16753	0.16%	0.012%
27	10.422	1220	1230	1244	rBV	3393018	5716109	53.41%	3.955%
28	10.804	1285	1295	1304	rBV	2618132	4544086	42.46%	3.144%
29	10.945	1311	1319	1335	rBV	3588760	6069512	56.71%	4.200%
30	11.351	1381	1388	1395	rBV3	39485	93650	0.87%	0.065%
31	11.551	1415	1422	1435	rBV	159694	316203	2.95%	0.219%
32	11.710	1442	1449	1454	rBV	6410	14565	0.14%	0.010%
33	12.216	1528	1535	1543	rVB2	45227	71726	0.67%	0.050%
34	12.380	1558	1563	1569	rVV	61719	106162	0.99%	0.073%
35	12.592	1594	1599	1605	rVB9	7465	13457	0.13%	0.009%
36	13.022	1668	1672	1680	rVV9	12057	22092	0.21%	0.015%

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37	13.110	1684	1687	1690	rVB4	10944	15422	0.14%	0.011%
38	13.157	1693	1695	1701	rVB4	10561	11467	0.11%	0.008%
39	13.451	1737	1745	1749	rBV	60418	94089	0.88%	0.065%
40	13.527	1752	1758	1763	rVV2	28710	50003	0.47%	0.035%
41	13.845	1804	1812	1817	rBV2	35186	54082	0.51%	0.037%
42	13.951	1826	1830	1834	rBV6	9070	15936	0.15%	0.011%
43	14.045	1837	1846	1855	rBV	5452778	7476495	69.85%	5.173%
44	14.274	1881	1885	1886	rBV4	10909	15681	0.15%	0.011%
45	14.321	1886	1893	1903	rVB	6422783	9572665	89.44%	6.623%
46	14.516	1923	1926	1932	rVB3	11031	18055	0.17%	0.012%
47	14.621	1936	1944	1953	rBV	3526032	5179147	48.39%	3.584%
48	14.821	1971	1978	1993	rBV	2568601	3986570	37.25%	2.758%
49	15.045	2010	2016	2026	rVB5	45112	100337	0.94%	0.069%
50	15.133	2028	2031	2036	rVB7	6921	11041	0.10%	0.008%
51	15.415	2073	2079	2080	rBV5	8064	11123	0.10%	0.008%
52	15.468	2084	2088	2095	rVB9	10766	20601	0.19%	0.014%
53	15.615	2103	2113	2125	rBV	7764841	10703103	100.00%	7.406%
54	15.733	2125	2133	2145	rBV	2068072	2913288	27.22%	2.016%
55	15.851	2148	2153	2160	rVB6	35433	67652	0.63%	0.047%
56	15.951	2165	2170	2174	rBV8	8458	16774	0.16%	0.012%
57	16.327	2229	2234	2237	rBV3	18241	30333	0.28%	0.021%
58	16.398	2241	2246	2250	rVB4	28468	42281	0.40%	0.029%
59	16.474	2256	2259	2263	rVB3	10538	12780	0.12%	0.009%
60	16.557	2268	2273	2278	rVV6	15855	23710	0.22%	0.016%
61	16.768	2304	2309	2312	rBV4	23727	36185	0.34%	0.025%
62	16.833	2317	2320	2325	rVB7	6474	11745	0.11%	0.008%
63	17.045	2350	2356	2359	rBV7	10151	17747	0.17%	0.012%
64	17.127	2365	2370	2371	rBV3	11385	15358	0.14%	0.011%
65	17.368	2404	2411	2421	rBV	3406888	4936747	46.12%	3.416%
66	17.468	2421	2428	2437	rBV	6979612	9992832	93.36%	6.914%
67	17.562	2437	2444	2448	rVV3	69504	109613	1.02%	0.076%
68	17.621	2451	2454	2458	rVB4	13853	19906	0.19%	0.014%
69	17.751	2472	2476	2484	rVB5	44657	67675	0.63%	0.047%
70	17.862	2491	2495	2500	rBV8	8011	13903	0.13%	0.010%
71	18.039	2521	2525	2528	rVB6	13966	16952	0.16%	0.012%
72	18.133	2536	2541	2546	rBV9	11750	21952	0.21%	0.015%
73	18.268	2558	2564	2581	rBV	703767	1238411	11.57%	0.857%
74	18.598	2616	2620	2623	rBV4	17975	23854	0.22%	0.017%
75	18.692	2633	2636	2641	rVB2	58802	73699	0.69%	0.051%
76	19.062	2696	2699	2702	rBV4	12239	15511	0.14%	0.011%

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77	19.315	2738	2742	2747	rVB	78359	109439	1.02%	0.076%
78	19.386	2750	2754	2758	rBV2	99712	158272	1.48%	0.110%
79	19.539	2776	2780	2789	rBV	148175	230872	2.16%	0.160%
80	19.751	2810	2816	2823	rBV	7249378	9606133	89.75%	6.647%
81	20.268	2901	2904	2908	rBV3	86285	120910	1.13%	0.084%
82	21.256	3068	3072	3083	rBV	1380392	1901446	17.77%	1.316%
83	21.539	3115	3120	3129	rBV	3245086	4154804	38.82%	2.875%
84	22.827	3336	3339	3344	rVB	330043	463457	4.33%	0.321%
85	23.815	3498	3507	3517	rBV	4694911	9345699	87.32%	6.466%
86	23.968	3526	3533	3544	rVB	2145325	4331727	40.47%	2.997%
87	24.738	3661	3664	3673	rVB2	246492	495902	4.63%	0.343%

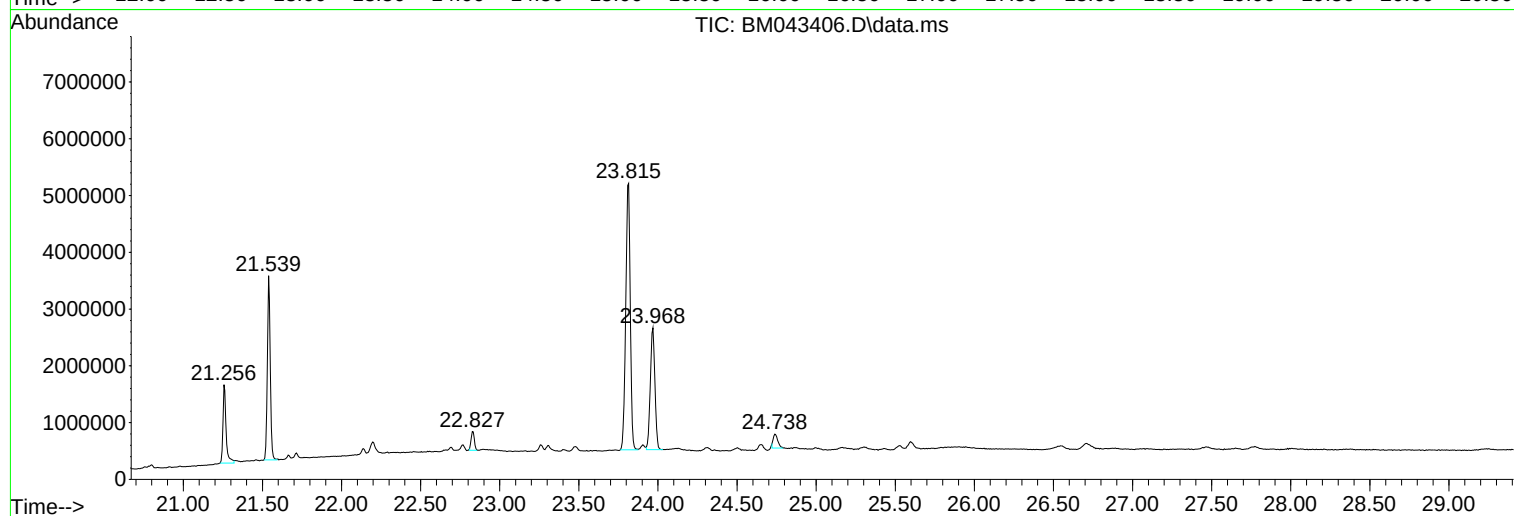
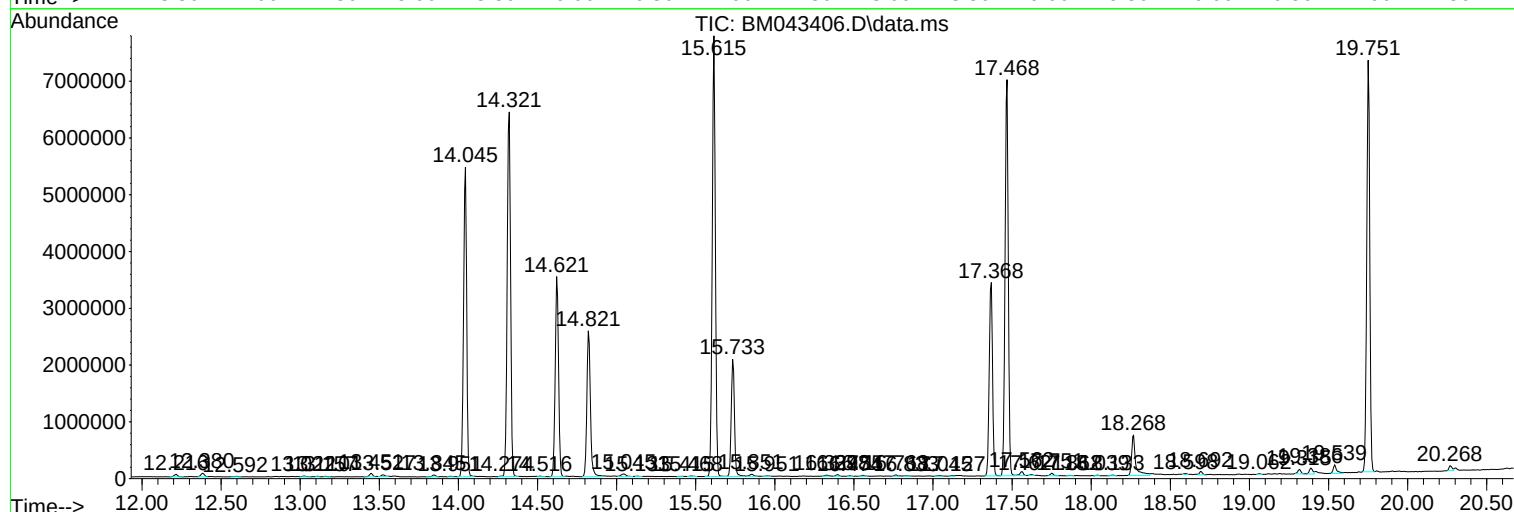
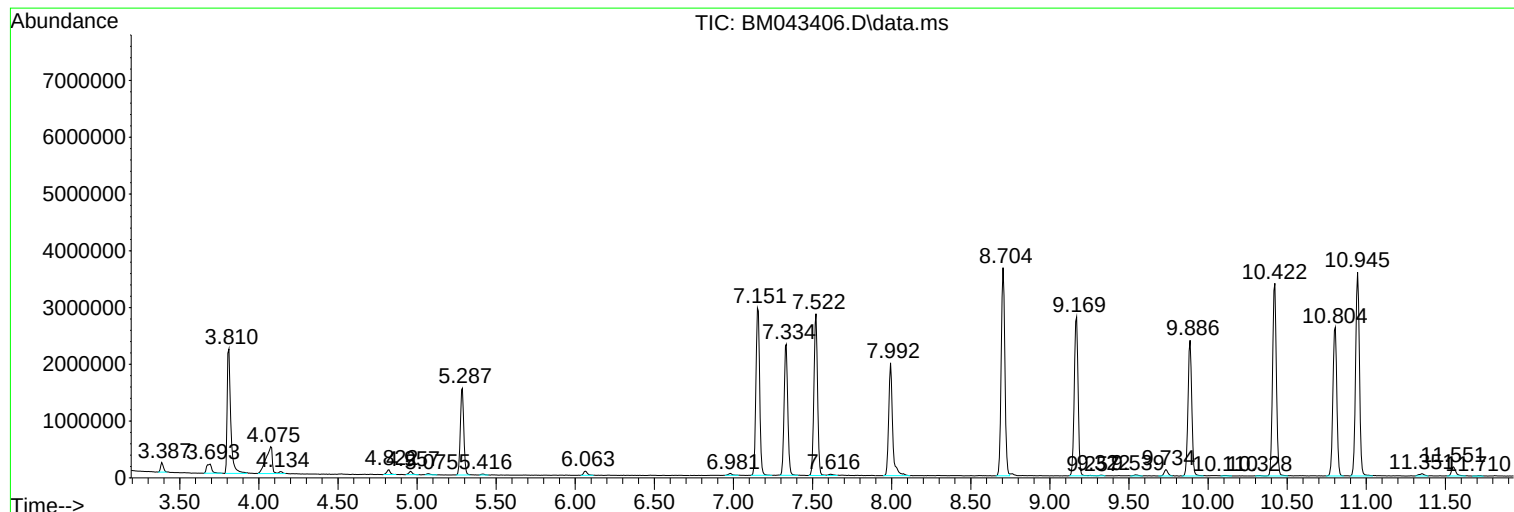
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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



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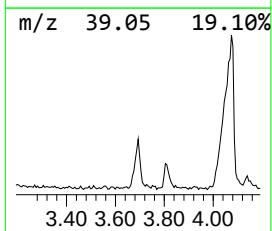
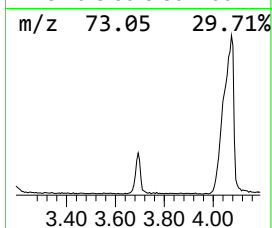
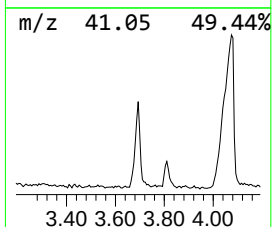
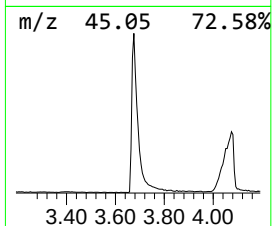
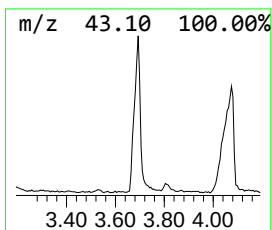
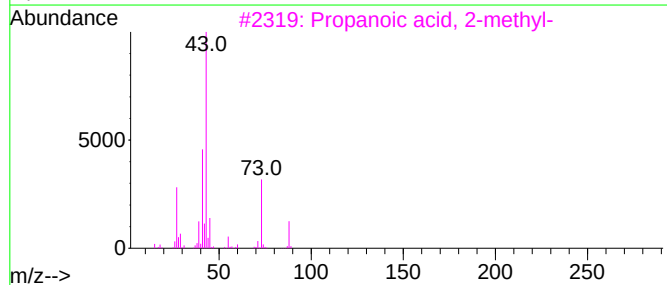
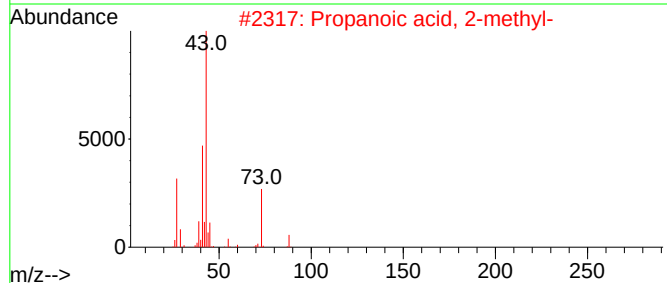
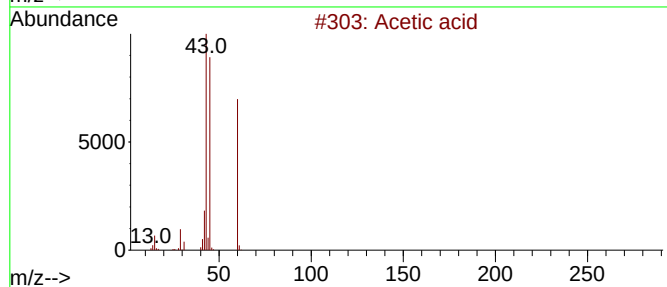
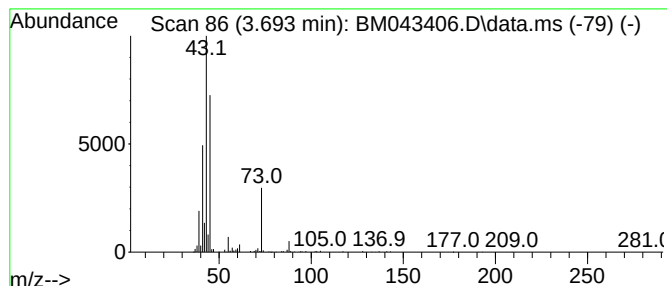
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Acetic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.693	2.18 ng/ul	369714	1,4-Dichlorobenzene-d4	7.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid	60	C2H4O2	000064-19-7	50
2			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	49
3			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	47
4			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	37
5			Sulfurous acid, bis(1-methylethy...	166	C6H14O3S	004773-13-1	36



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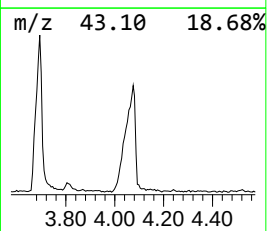
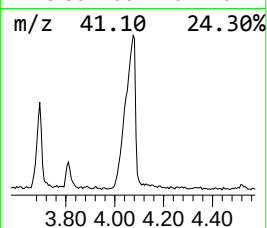
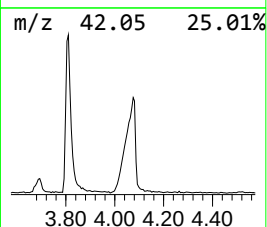
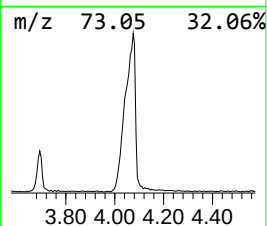
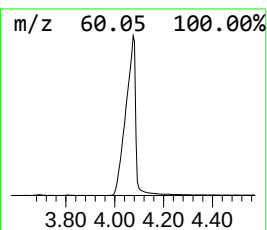
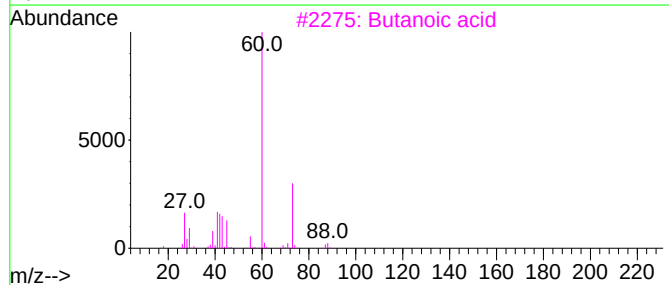
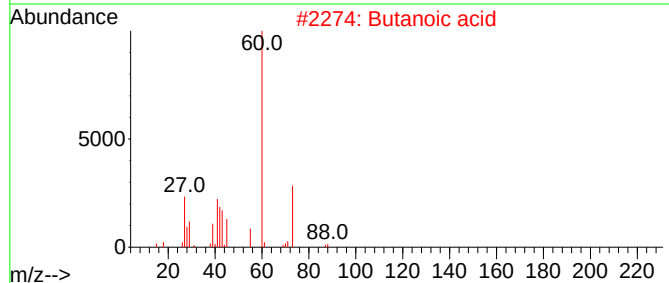
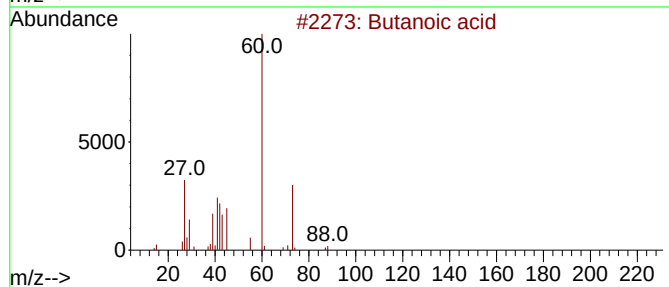
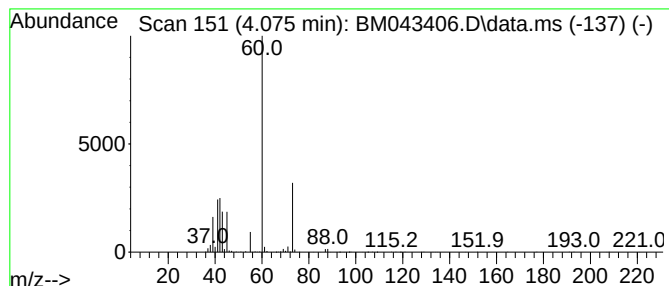
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Butanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.075	7.81 ng/ul	1325910	1,4-Dichlorobenzene-d4	7.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid	88	C4H8O2	000107-92-6	91
2			Butanoic acid	88	C4H8O2	000107-92-6	91
3			Butanoic acid	88	C4H8O2	000107-92-6	86
4			Butanoic acid	88	C4H8O2	000107-92-6	80
5			Pentanoic acid	102	C5H10O2	000109-52-4	40



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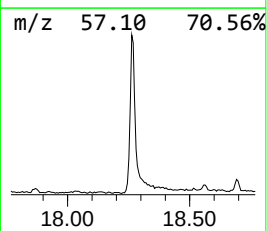
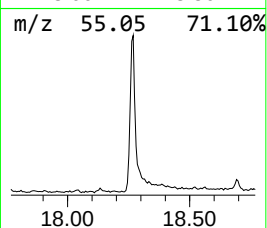
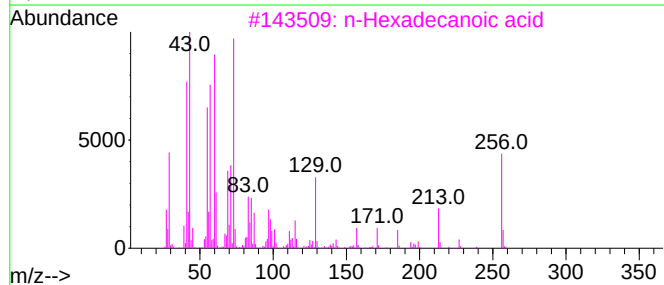
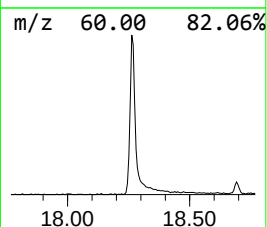
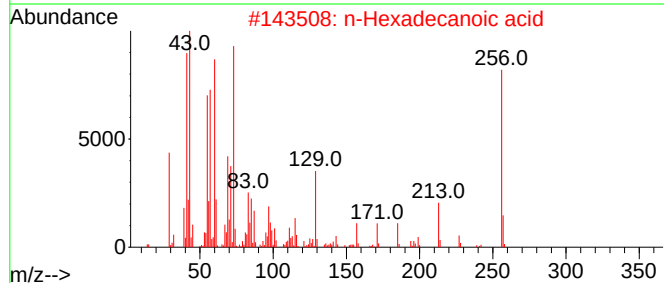
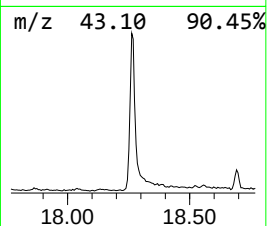
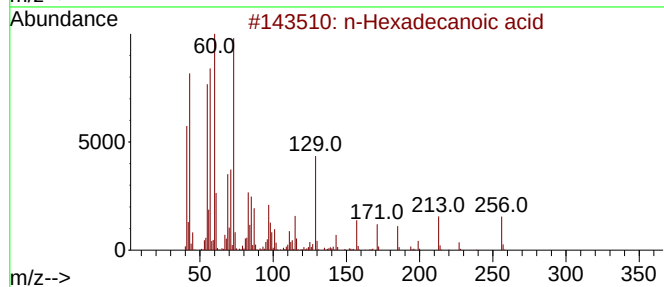
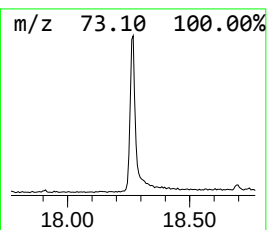
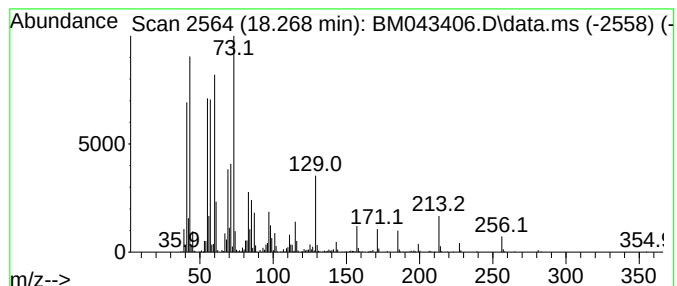
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.268	5.02 ng/ul	1238410	Phenanthrene-d10	17.368

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	99
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5			Tridecanoic acid	214	C13H26O2	000638-53-9	92



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C0AX8

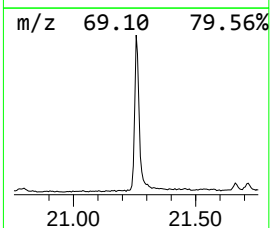
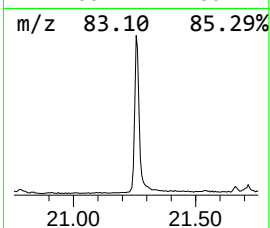
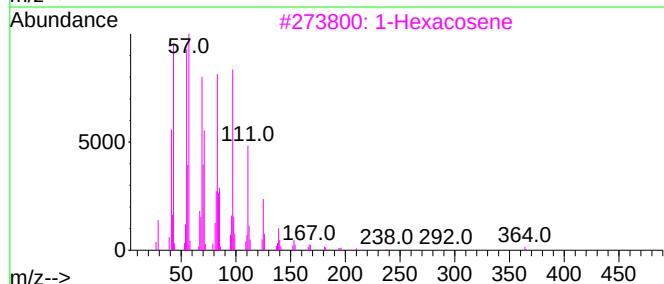
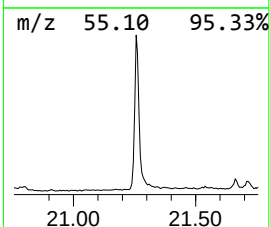
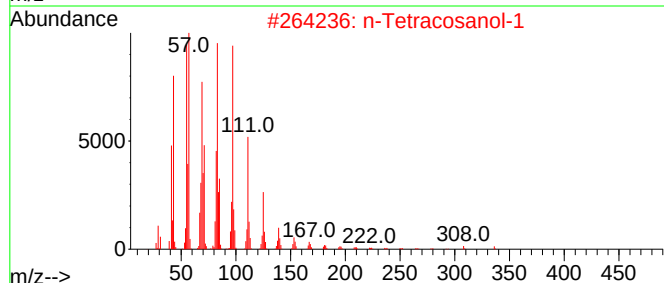
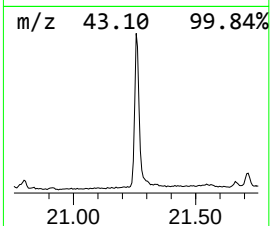
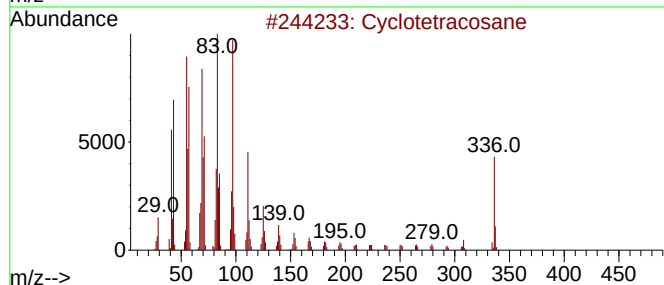
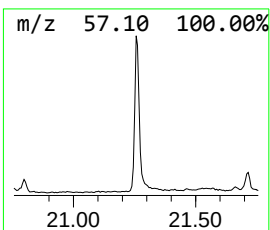
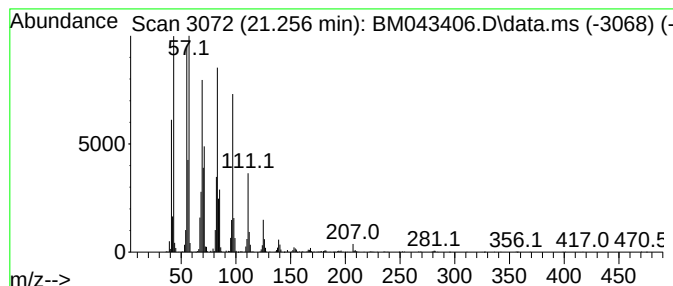
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Cyclic21.256 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.256	9.15 ng/ul	1901450	Chrysene-d12	21.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	96
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			1-Hexacosene	364	C26H52	018835-33-1	94
4			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
5			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043406.D
Acq On : 18 Dec 2023 22:58
Operator : MA/JU
Sample : 05807-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX8

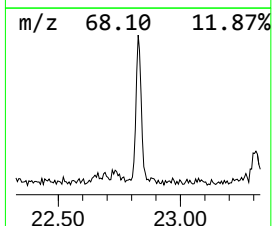
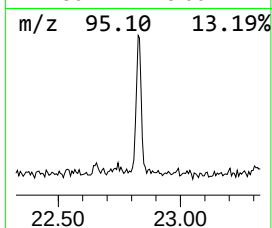
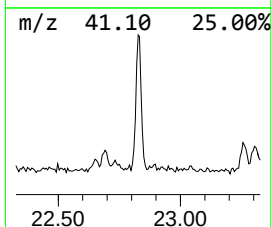
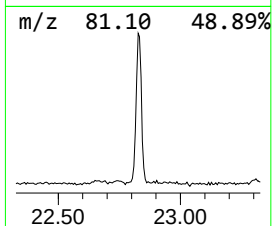
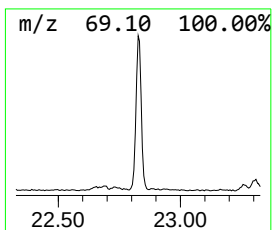
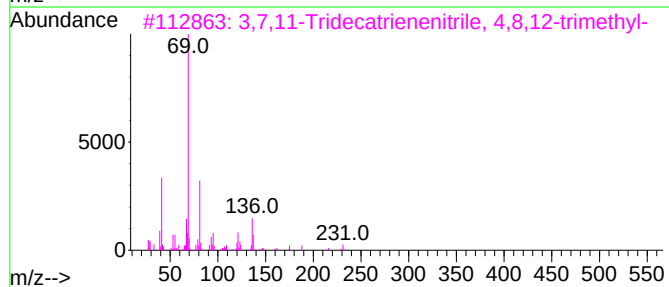
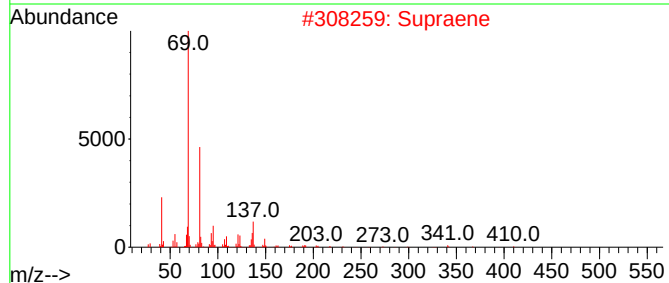
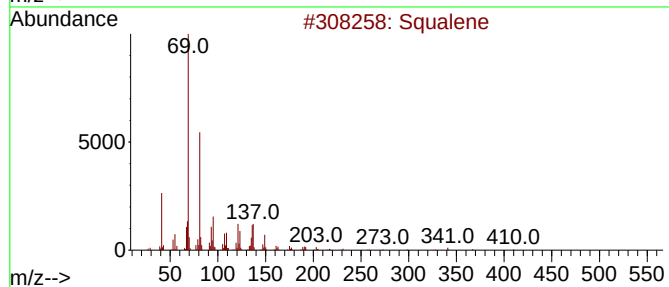
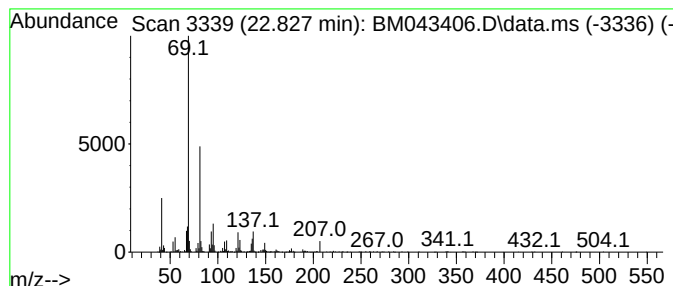
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.827	2.14 ng/ul	463457	Perylene-d12	23.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	90
2			Supraene	410	C30H50	007683-64-9	87
3			3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	72
4			2,6,10-Dodecatrienoic acid, 3,7,...	250	C16H26O2	004176-79-8	72
5			2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043406.D
Acq On : 18 Dec 2023 22:58
Operator : MA/JU
Sample : 05807-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

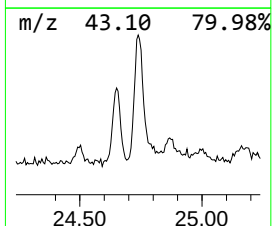
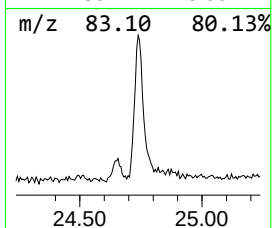
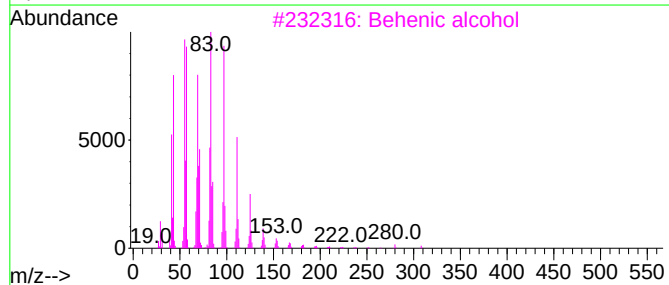
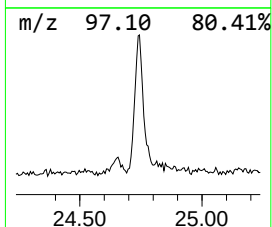
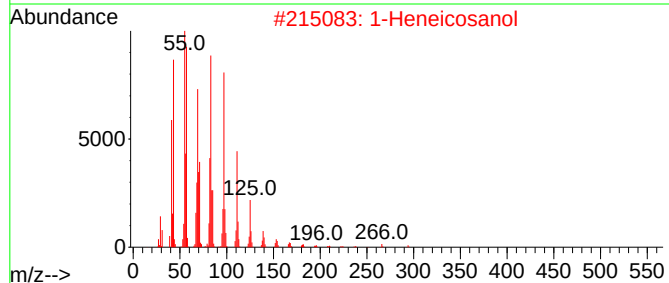
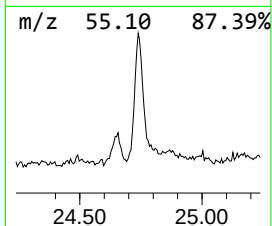
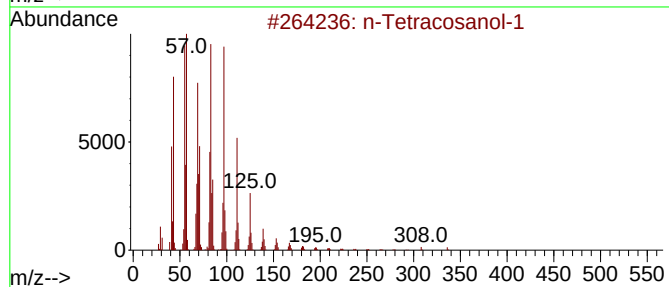
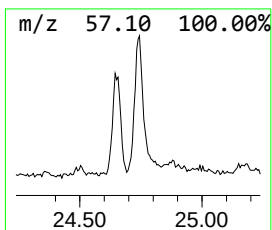
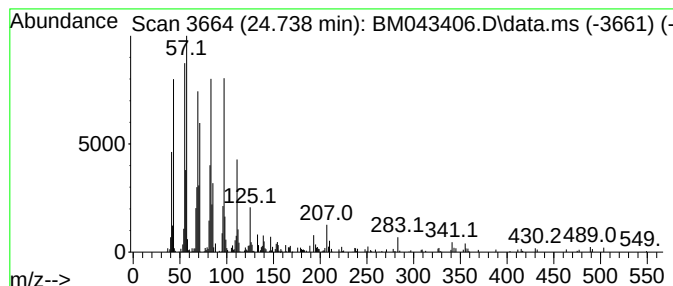
Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 7 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
24.738	2.29 ng/ul	495902	Perylene-d12		23.968	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1		354	C24H50O	000506-51-4	95
2	1-Heneicosanol		312	C21H44O	015594-90-8	94
3	Behenic alcohol		326	C22H46O	000661-19-8	94
4	Nonacos-1-ene		406	C29H58	018835-35-3	93
5	1-Heptacosanol		396	C27H56O	002004-39-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043406.D
Acq On : 18 Dec 2023 22:58
Operator : MA/JU
Sample : 05807-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.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
Acetic acid	3.693	2.2	ng/ul	369714	1	7.992	3397590	20.0
Butanoic acid	4.075	7.8	ng/ul	1325910	1	7.992	3397590	20.0
n-Hexadecanoic ...	18.268	5.0	ng/ul	1238410	4	17.368	4936750	20.0
(DEL) Alkane: C...	21.256	9.2	ng/ul	1901450	5	21.539	4154800	20.0
Squalene	22.827	2.1	ng/ul	463457	6	23.968	4331730	20.0
n-Tetracosanol-1	24.738	2.3	ng/ul	495902	6	23.968	4331730	20.0