

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092723\
 Data File : BP017400.D
 Acq On : 27 Sep 2023 16:35
 Operator : MA/JU
 Sample : 04359-02 10X
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 JYCA3

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_P\Methods\SFAM-EPA-BP092023.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP017400.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.181	13	16	25	rVB	24530	34419	0.70%	0.085%
2	3.293	32	35	36	rBV	21546	20934	0.43%	0.052%
3	3.322	36	40	48	rVB	226759	261980	5.34%	0.650%
4	3.593	84	86	90	rBV3	5823	8126	0.17%	0.020%
5	3.640	90	94	100	rVB	55876	65818	1.34%	0.163%
6	3.728	106	109	124	rBV2	206720	341394	6.96%	0.848%
7	3.922	137	142	148	rVB	38662	55870	1.14%	0.139%
8	4.016	154	158	165	rVB2	34970	50442	1.03%	0.125%
9	4.181	182	186	191	rVB3	16888	27102	0.55%	0.067%
10	4.293	201	205	213	rVB	47235	65268	1.33%	0.162%
11	4.422	224	227	233	rVB3	10337	13473	0.27%	0.033%
12	4.487	233	238	244	rVB	71127	88778	1.81%	0.220%
13	4.552	245	249	255	rVB	46455	60679	1.24%	0.151%
14	4.940	310	315	322	rBV	108117	139612	2.85%	0.347%
15	5.005	322	326	337	rVB	44121	68328	1.39%	0.170%
16	5.216	357	362	369	rVB6	5867	10308	0.21%	0.026%
17	5.458	401	403	408	rVB5	3944	5588	0.11%	0.014%
18	5.552	415	419	422	rVV5	6709	9300	0.19%	0.023%
19	5.581	422	424	433	rVB7	5438	9865	0.20%	0.024%
20	5.822	462	465	471	rVB6	5905	9559	0.19%	0.024%
21	6.322	547	550	556	rVB	12061	17907	0.37%	0.044%
22	6.522	579	584	589	rBV8	6102	10989	0.22%	0.027%
23	6.758	620	624	627	rVB6	5662	8580	0.17%	0.021%
24	6.887	638	646	656	rVB6	8330	21033	0.43%	0.052%
25	7.016	664	668	673	rVB5	7197	10164	0.21%	0.025%
26	7.081	673	679	689	rVB2	93426	155265	3.17%	0.385%
27	7.263	702	710	719	rBV	685794	1031465	21.04%	2.561%
28	7.440	730	740	748	rBV	313351	492176	10.04%	1.222%
29	7.528	753	755	763	rVV8	2914	5259	0.11%	0.013%
30	7.922	815	822	836	rBV	433642	720658	14.70%	1.789%
31	8.187	861	867	873	rBV10	6307	15402	0.31%	0.038%
32	8.269	879	881	888	rVB8	3429	5297	0.11%	0.013%
33	8.634	936	943	956	rBV	276088	474606	9.68%	1.178%
34	8.775	960	967	973	rVB	16948	32216	0.66%	0.080%
35	9.116	1017	1025	1038	rBV	749642	1229164	25.07%	3.051%
36	9.275	1049	1052	1056	rBV3	7195	10707	0.22%	0.027%

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37	9.334	1057	1062	1063	rBV5	5556	7446	0.15%	0.018%
38	9.551	1095	1099	1102	rBV6	3520	5922	0.12%	0.015%
39	9.834	1140	1147	1155	rVV	264622	442518	9.02%	1.099%
40	10.357	1224	1236	1249	rBV	423424	742805	15.15%	1.844%
41	10.740	1294	1301	1309	rBV	602151	993999	20.27%	2.468%
42	10.910	1322	1330	1341	rBV	633520	1106733	22.57%	2.748%
43	11.234	1379	1385	1391	rBV	238725	391952	7.99%	0.973%
44	11.298	1391	1396	1414	rVB	341314	595062	12.14%	1.477%
45	11.528	1431	1435	1437	rBV5	5996	6742	0.14%	0.017%
46	11.575	1440	1443	1448	rVB4	8771	15143	0.31%	0.038%
47	11.798	1477	1481	1489	rVB10	5012	12562	0.26%	0.031%
48	12.263	1552	1560	1567	rBV	209524	331678	6.76%	0.823%
49	12.328	1567	1571	1580	rVB	17377	31412	0.64%	0.078%
50	12.463	1589	1594	1600	rBV10	5314	12077	0.25%	0.030%
51	12.581	1609	1614	1618	rBV7	10048	17804	0.36%	0.044%
52	12.616	1618	1620	1626	rVB5	8521	14301	0.29%	0.036%
53	12.898	1663	1668	1675	rBV9	6873	11386	0.23%	0.028%
54	13.151	1707	1711	1717	rBV4	10632	15236	0.31%	0.038%
55	13.422	1752	1757	1769	rBV	220545	373078	7.61%	0.926%
56	13.540	1776	1777	1782	rVB5	4748	5071	0.10%	0.013%
57	13.810	1819	1823	1827	rVV7	3113	5022	0.10%	0.012%
58	13.892	1830	1837	1841	rBV7	6217	12837	0.26%	0.032%
59	13.998	1848	1855	1860	rBV	1788874	2388373	48.71%	5.929%
60	14.045	1860	1863	1874	rVB	115365	155028	3.16%	0.385%
61	14.281	1895	1903	1915	rBV	1970388	2776262	56.62%	6.892%
62	14.363	1915	1917	1921	rVV5	5489	8099	0.17%	0.020%
63	14.398	1921	1923	1929	rVB7	3260	4992	0.10%	0.012%
64	14.481	1934	1937	1946	rVV	5757	11802	0.24%	0.029%
65	14.581	1947	1954	1961	rVV	880991	1267267	25.84%	3.146%
66	14.645	1961	1965	1973	rVB	27182	41737	0.85%	0.104%
67	14.834	1992	1997	2002	rBV4	15445	35386	0.72%	0.088%
68	14.969	2015	2020	2028	rVB4	6410	17144	0.35%	0.043%
69	15.322	2076	2080	2085	rVB3	8388	12349	0.25%	0.031%
70	15.398	2087	2093	2099	rVB2	10196	18538	0.38%	0.046%
71	15.581	2116	2124	2131	rBV	2574515	3662359	74.69%	9.092%
72	15.634	2131	2133	2138	rVV3	21973	32974	0.67%	0.082%
73	15.716	2140	2147	2158	rVV	180075	292097	5.96%	0.725%
74	15.816	2158	2164	2171	rVB4	12601	23201	0.47%	0.058%
75	16.292	2241	2245	2248	rVB3	3710	5037	0.10%	0.013%
76	16.698	2310	2314	2318	rBV7	4799	7745	0.16%	0.019%

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77	17.139	2386	2389	2393	rBV6	4962	5868	0.12%	0.015%
78	17.216	2400	2402	2407	rVB6	3924	5278	0.11%	0.013%
79	17.351	2419	2425	2431	rBV	1078830	1483092	30.25%	3.682%
80	17.392	2431	2432	2436	rVB2	23598	22773	0.46%	0.057%
81	17.451	2436	2442	2455	rBV	2925706	4087313	83.36%	10.147%
82	17.610	2467	2469	2478	rVB6	8513	12735	0.26%	0.032%
83	18.192	2564	2568	2578	rBV2	48934	77460	1.58%	0.192%
84	18.286	2581	2584	2590	rVB	17540	21975	0.45%	0.055%
85	18.598	2633	2637	2639	rBV5	4426	7466	0.15%	0.019%
86	19.269	2747	2751	2755	rVB3	32331	40320	0.82%	0.100%
87	19.333	2759	2762	2766	rVV	26448	35178	0.72%	0.087%
88	19.433	2776	2779	2785	rBV8	21348	30595	0.62%	0.076%
89	19.698	2818	2824	2832	rBV	3675818	4861852	99.15%	12.070%
90	21.457	3118	3123	3130	rBV	1271919	1588986	32.41%	3.945%
91	23.804	3515	3522	3538	rVB2	2458810	4903441	100.00%	12.173%
92	23.968	3544	3550	3559	rVB	785225	1597764	32.58%	3.967%

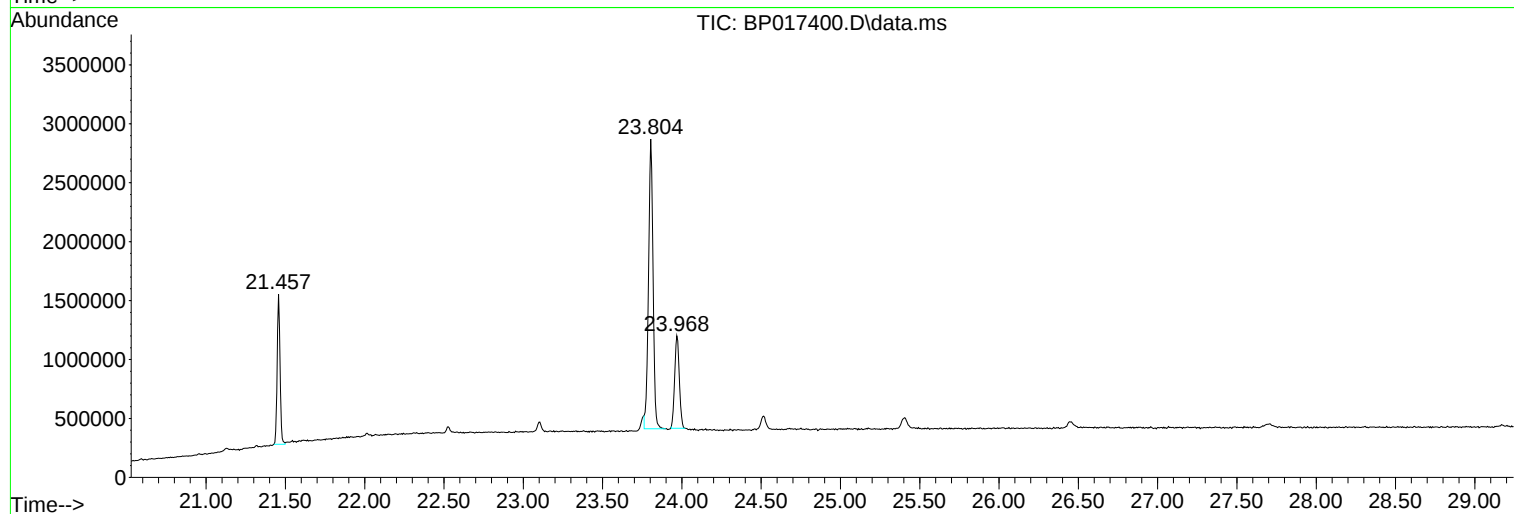
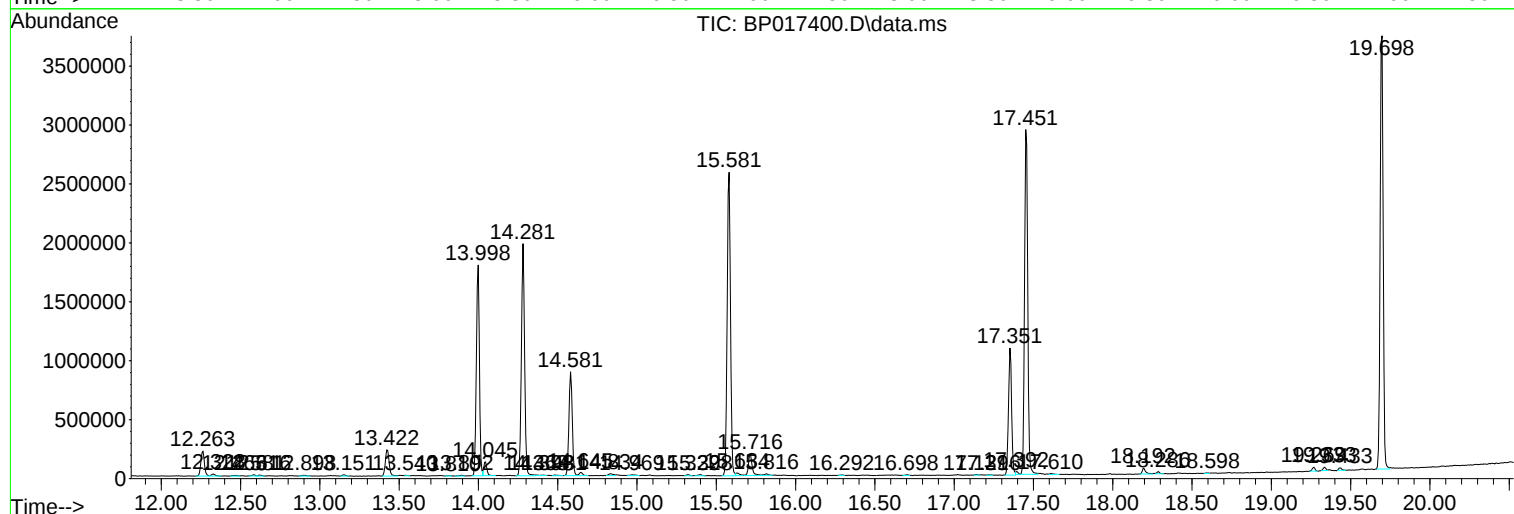
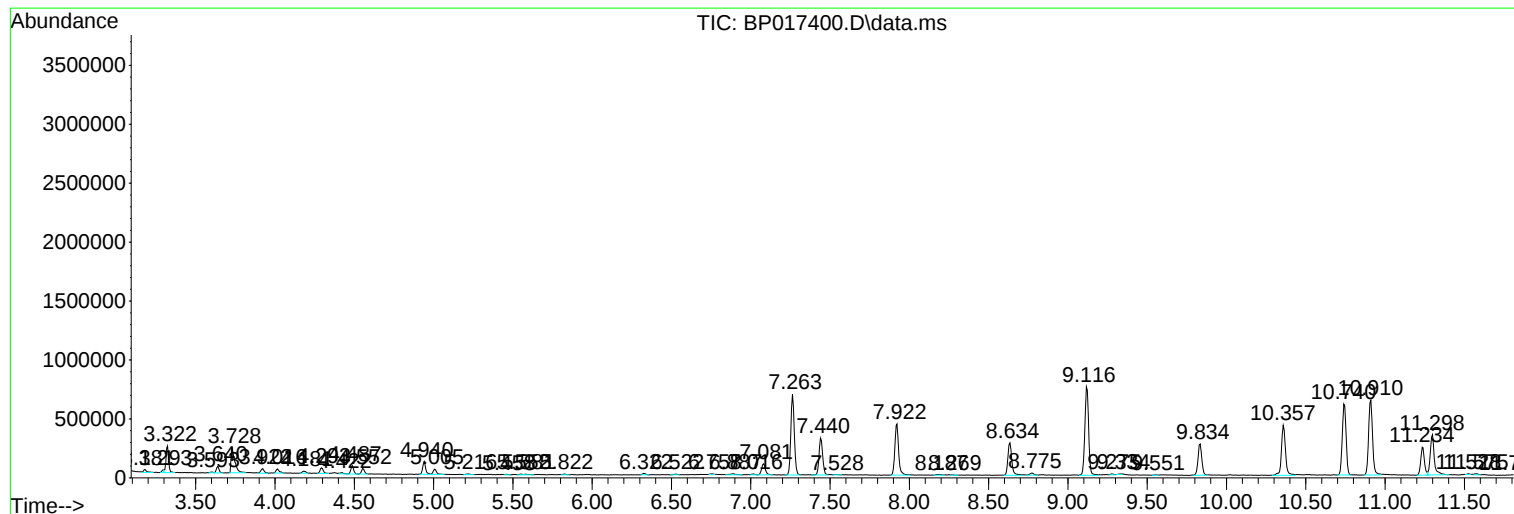
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
Quant Title : SVOA CALIBRATION

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



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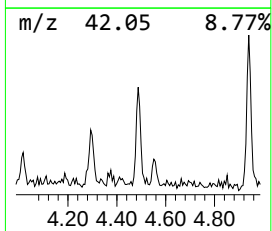
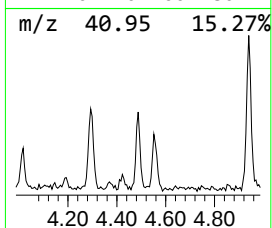
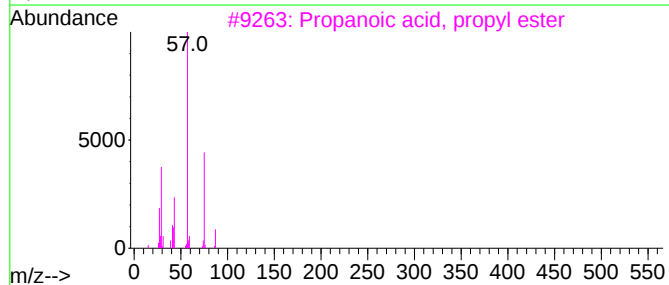
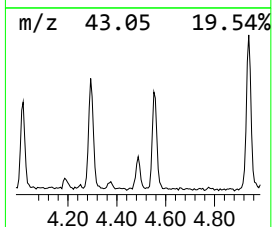
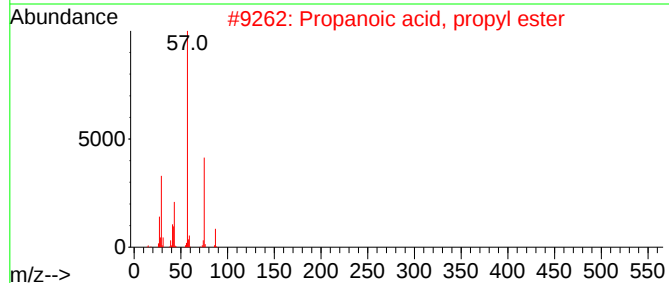
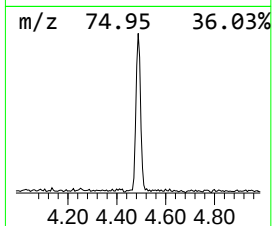
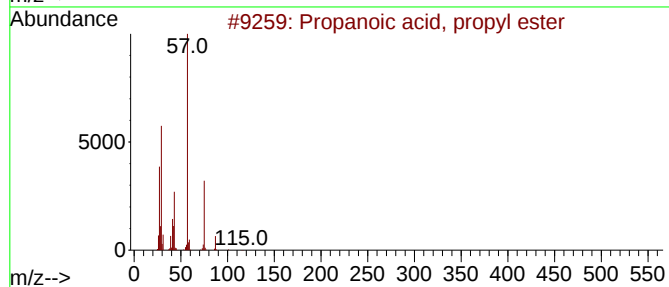
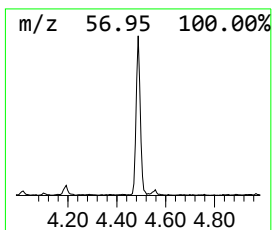
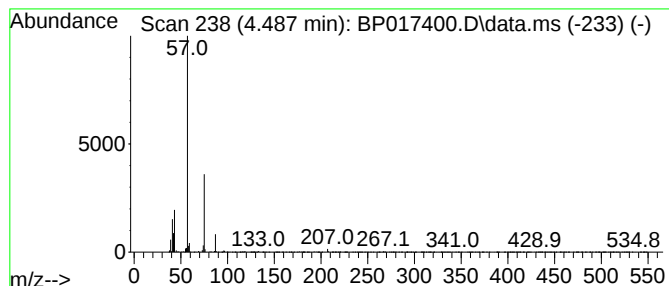
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Propanoic acid, propyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.487	2.46 ng/ul	88778	1,4-Dichlorobenzene-d4	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	72
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	59
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50



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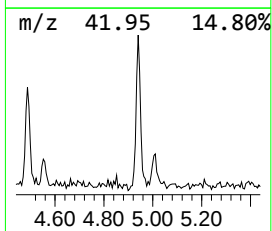
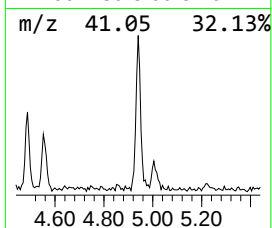
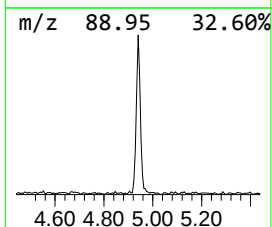
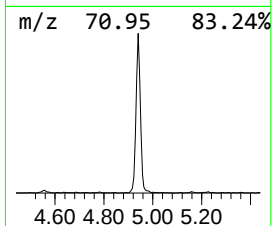
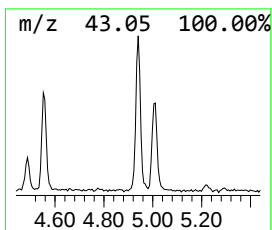
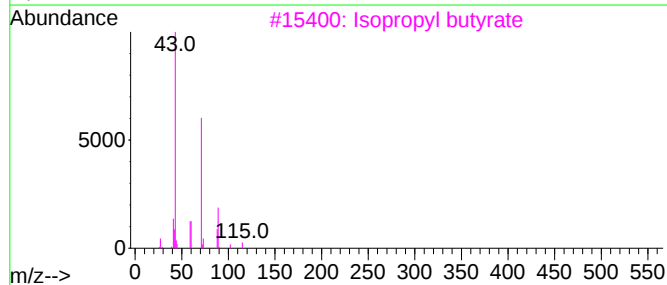
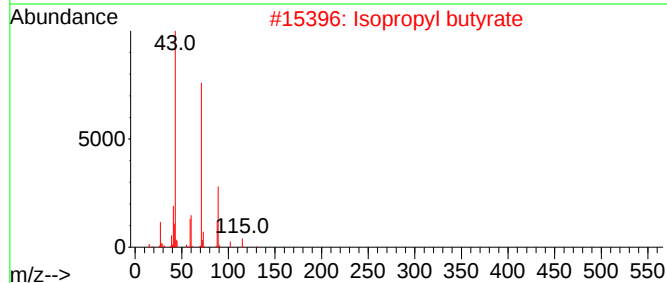
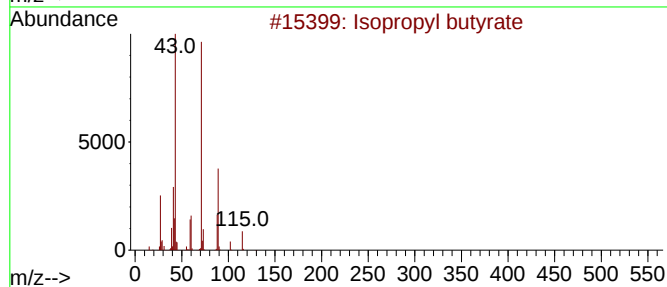
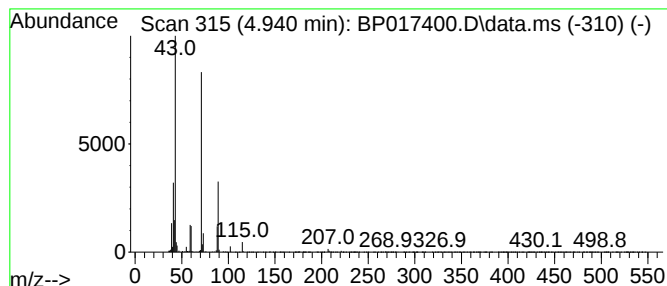
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Isopropyl butyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.940	3.87 ng/ul	139612	1,4-Dichlorobenzene-d4	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	86
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64



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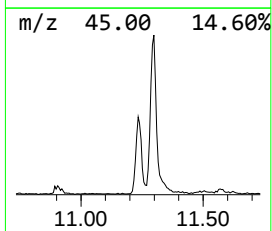
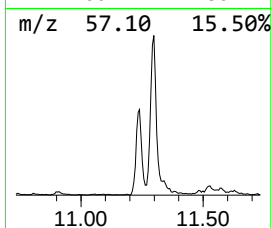
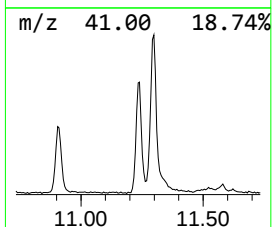
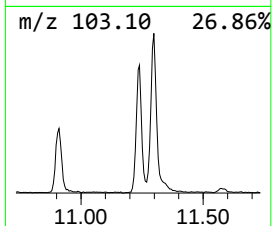
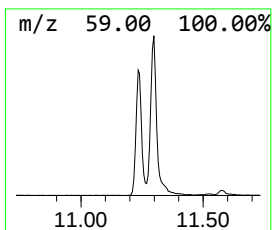
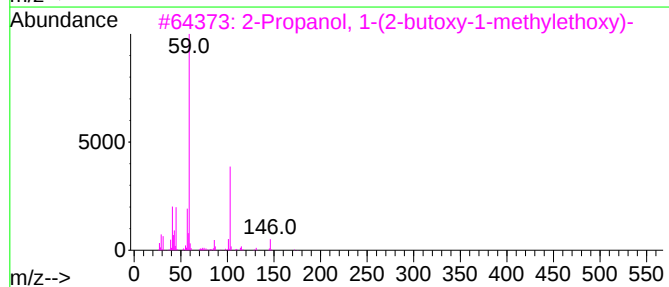
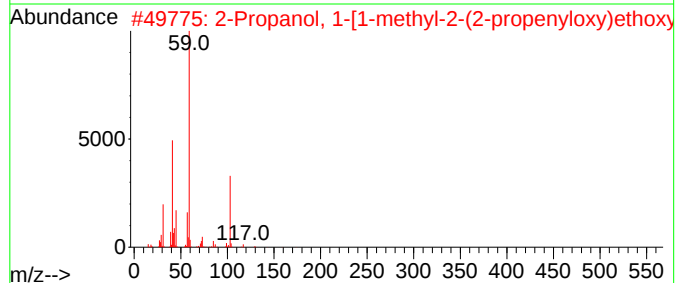
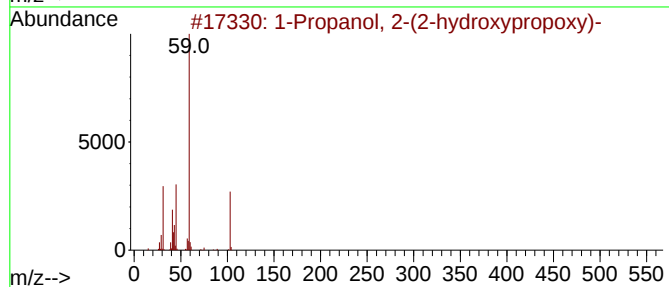
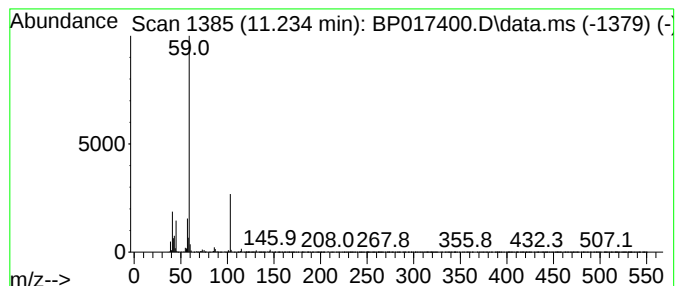
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 1-Propanol, 2-(2-hydroxypro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.234	7.89 ng/ul	391952	Naphthalene-d8	10.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78		
2	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64		
3	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	64		
4	1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1010367-13-4	59		
5	1,4,7-Trimethyl-3,6-dioxaoctane-...	192	C9H20O4	1000423-63-2	59		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092723\
Data File : BP017400.D
Acq On : 27 Sep 2023 16:35
Operator : MA/JU
Sample : 04359-02 10X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JYCA3

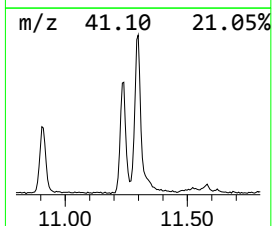
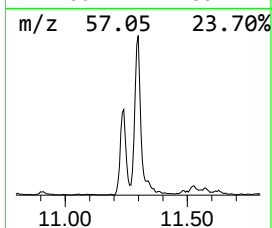
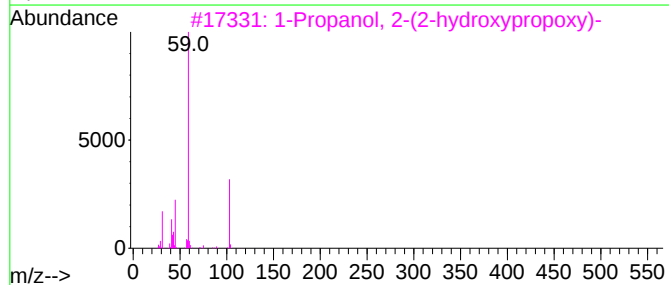
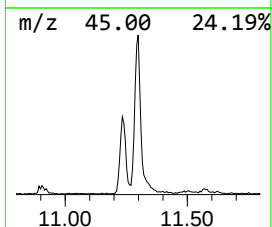
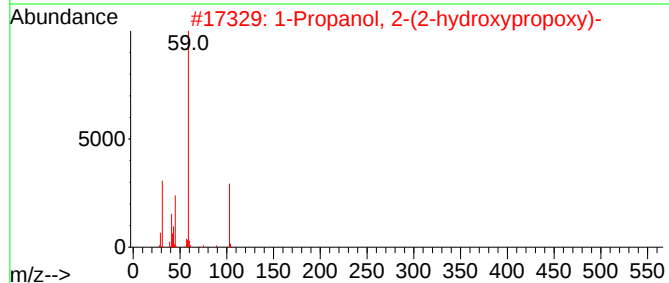
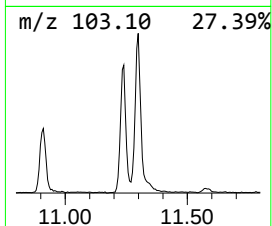
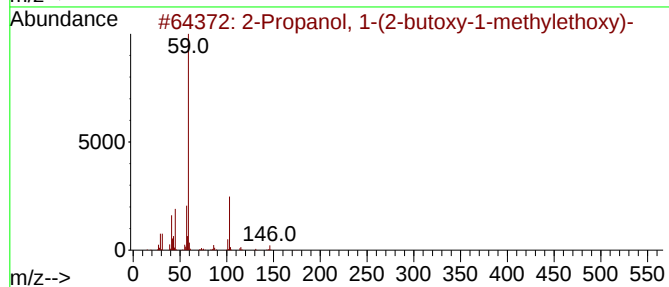
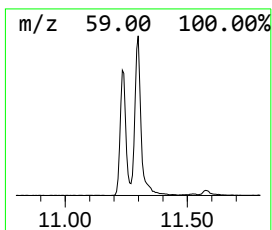
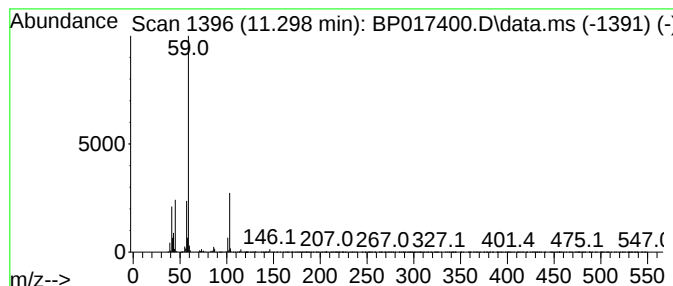
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.298	11.97 ng/ul	595062	Naphthalene-d8	10.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	90		
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72		
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72		
4	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64		
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092723\
Data File : BP017400.D
Acq On : 27 Sep 2023 16:35
Operator : MA/JU
Sample : 04359-02 10X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JYCA3

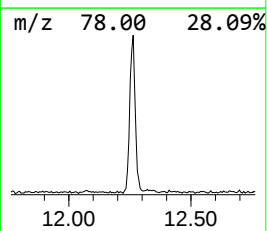
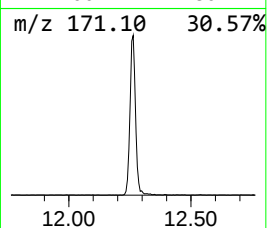
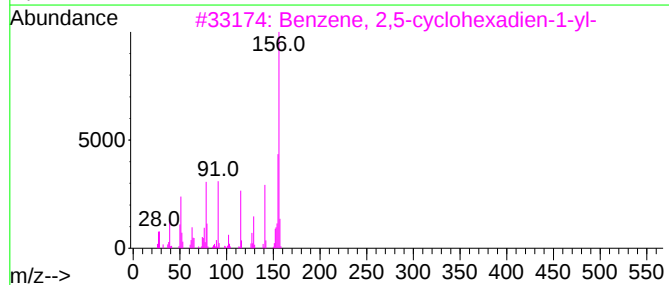
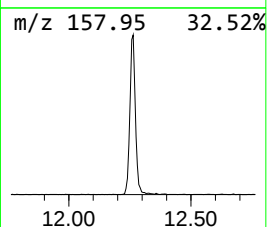
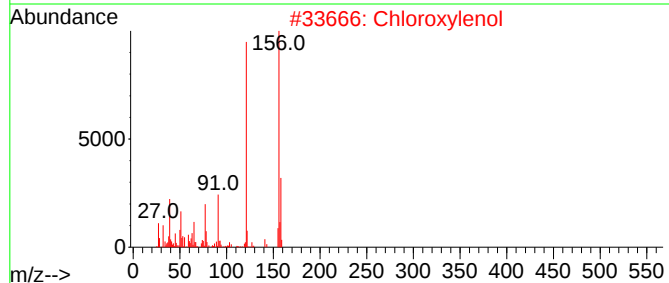
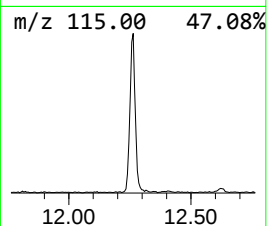
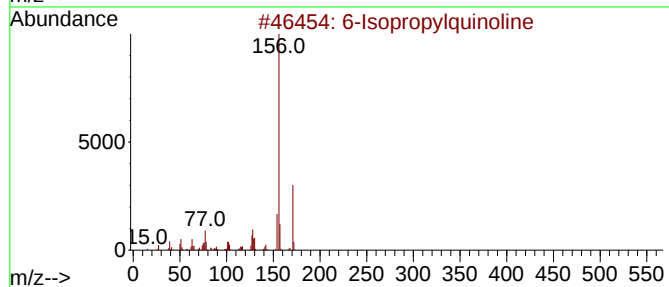
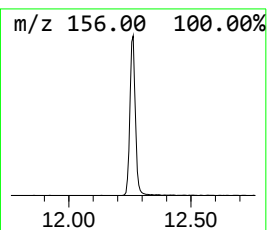
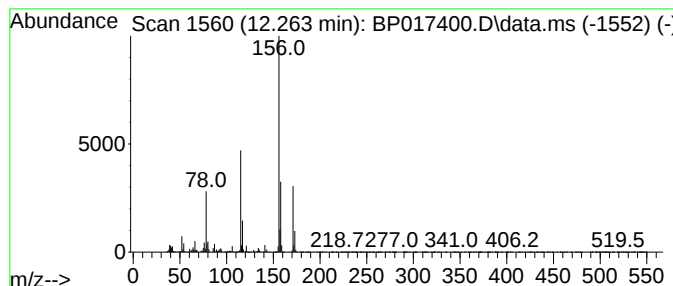
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.263	6.67 ng/ul	331678	Naphthalene-d8	10.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Isopropylquinoline	171	C12H13N	000135-79-5	32
2			Chloroxylonol	156	C8H9ClO	000088-04-0	32
3			Benzene, 2,5-cyclohexadien-1-yl-	156	C12H12	004794-05-2	28
4			2,2'-Bipyridine	156	C10H8N2	000366-18-7	25
5			Tebuthiuron	228	C9H16N4OS	034014-18-1	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092723\
Data File : BP017400.D
Acq On : 27 Sep 2023 16:35
Operator : MA/JU
Sample : 04359-02 10X
Misc :
ALS Vial : 12 Sample Multiplier: 1

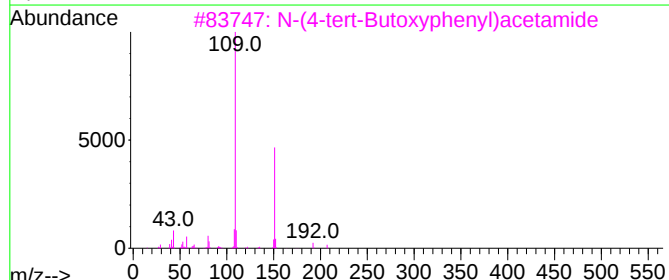
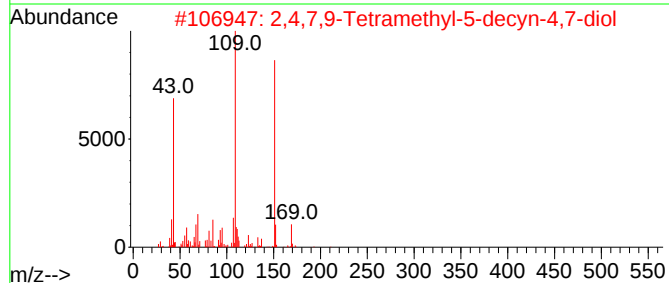
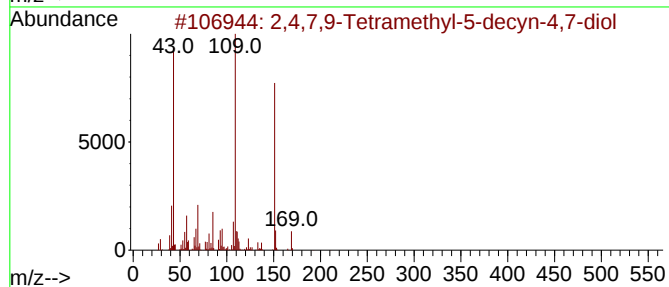
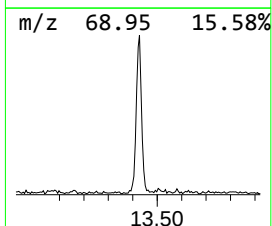
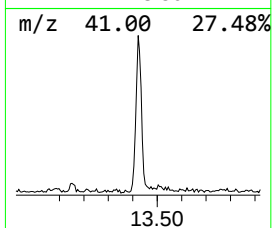
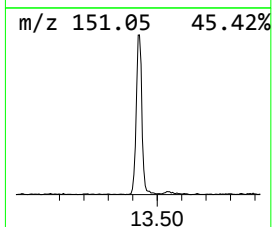
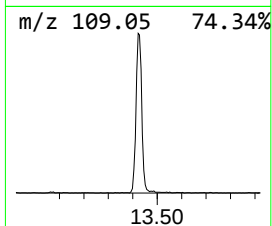
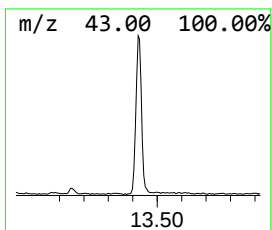
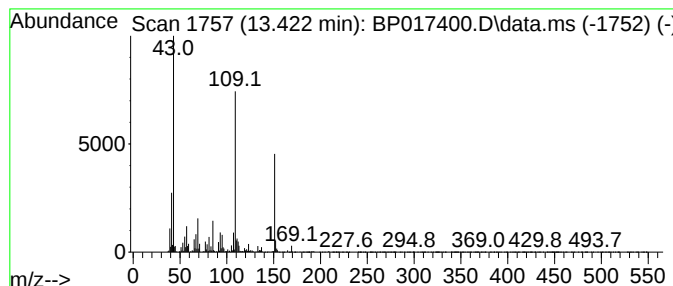
Instrument :
BNA_P
ClientSampleId :
JYCA3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.422	5.89 ng/ul	373078	Acenaphthene-d10	14.581	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90
3	N-(4-tert-Butoxyphenyl)acetamide	207	C12H17NO2	002109-73-1	59
4	Metacetamol	151	C8H9NO2	000621-42-1	59
5	Acetaminophen	151	C8H9NO2	000103-90-2	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092723\
Data File : BP017400.D
Acq On : 27 Sep 2023 16:35
Operator : MA/JU
Sample : 04359-02 10X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JYCA3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.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
Propanoic acid,...	4.487	2.5	ng/ul	88778	1	7.922	720658	20.0
Isopropyl butyrate	4.940	3.9	ng/ul	139612	1	7.922	720658	20.0
1-Propanol, 2-(...	11.234	7.9	ng/ul	391952	2	10.740	993999	20.0
2-Propanol, 1-(...	11.298	12.0	ng/ul	595062	2	10.740	993999	20.0
unknown-01	12.263	6.7	ng/ul	331678	2	10.740	993999	20.0
2,4,7,9-Tetrame...	13.422	5.9	ng/ul	373078	3	14.581	1267270	20.0