

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092923\
 Data File : BP017441.D
 Acq On : 29 Sep 2023 12:14
 Operator : MA/JU
 Sample : 04472-22
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 EZYP5

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: BP017441.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.299	33	36	43	rVB	32618	38446	0.51%	0.055%
2	3.734	106	110	126	rBV	330870	487977	6.46%	0.701%
3	3.928	138	143	155	rVB	67370	111315	1.47%	0.160%
4	4.040	160	162	168	rVB2	16277	18900	0.25%	0.027%
5	4.187	183	187	192	rVB3	29919	37698	0.50%	0.054%
6	4.434	224	229	234	rVB2	37780	55530	0.73%	0.080%
7	4.569	248	252	256	rBV5	12461	15290	0.20%	0.022%
8	4.981	318	322	327	rVB	17753	25737	0.34%	0.037%
9	5.316	373	379	385	rBV5	5250	10314	0.14%	0.015%
10	5.446	398	401	409	rVB5	7266	11997	0.16%	0.017%
11	5.569	419	422	427	rBV	10695	14841	0.20%	0.021%
12	5.752	447	453	457	rVB7	6062	13174	0.17%	0.019%
13	5.793	457	460	467	rBV9	3113	8379	0.11%	0.012%
14	5.981	487	492	503	rBV	128600	214250	2.84%	0.308%
15	6.352	550	555	559	rBV	20664	29340	0.39%	0.042%
16	6.546	585	588	597	rBV2	16432	26792	0.35%	0.039%
17	6.916	644	651	659	rBV7	10522	24921	0.33%	0.036%
18	7.110	677	684	693	rBV2	325515	529482	7.01%	0.761%
19	7.293	708	715	724	rBV	836517	1306056	17.28%	1.877%
20	7.475	739	746	760	rBV	886567	1418383	18.77%	2.038%
21	7.769	791	796	804	rVB6	6180	13046	0.17%	0.019%
22	7.958	818	828	841	rBV	836342	1398267	18.50%	2.010%
23	8.222	868	873	875	rBV6	5287	9223	0.12%	0.013%
24	8.563	927	931	937	rVB9	4636	8117	0.11%	0.012%
25	8.675	943	950	964	rBV	746801	1206494	15.97%	1.734%
26	8.816	968	974	980	rVB2	23179	38646	0.51%	0.056%
27	8.922	988	992	997	rVB2	14377	20457	0.27%	0.029%
28	9.069	1010	1017	1024	rBV2	26755	48189	0.64%	0.069%
29	9.163	1025	1033	1043	rVV	1041792	1712675	22.66%	2.461%
30	9.275	1047	1052	1060	rVV7	17807	34135	0.45%	0.049%
31	9.357	1062	1066	1071	rVB6	5340	8502	0.11%	0.012%
32	9.881	1144	1155	1167	rBV	877189	1433435	18.97%	2.060%
33	10.069	1184	1187	1192	rVB7	6509	11583	0.15%	0.017%
34	10.269	1216	1221	1225	rBV8	4208	8479	0.11%	0.012%
35	10.410	1236	1245	1256	rBV	1243165	2095793	27.73%	3.012%
36	10.551	1267	1269	1277	rVB9	7014	12278	0.16%	0.018%

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37	10.693	1288	1293	1302	rBV2	27318	46660	0.62%	0.067%
38	10.793	1302	1310	1328	rVB	1143562	1967853	26.04%	2.828%
39	10.963	1331	1339	1356	rVV	1264911	2128994	28.17%	3.060%
40	11.087	1359	1360	1370	rVB9	5649	12513	0.17%	0.018%
41	11.299	1389	1396	1400	rBV2	10021	17474	0.23%	0.025%
42	11.357	1400	1406	1412	rVB2	9369	15437	0.20%	0.022%
43	11.487	1422	1428	1436	rBV2	12819	29061	0.38%	0.042%
44	11.563	1437	1441	1445	rVV3	9806	13748	0.18%	0.020%
45	12.387	1576	1581	1585	rBV	20554	31120	0.41%	0.045%
46	12.628	1614	1622	1627	rBV	14083	26201	0.35%	0.038%
47	12.963	1672	1679	1690	rBV	51488	114132	1.51%	0.164%
48	13.216	1716	1722	1729	rBV	188183	281828	3.73%	0.405%
49	13.475	1761	1766	1773	rVB2	36029	65205	0.86%	0.094%
50	13.593	1779	1786	1795	rBV	49388	81984	1.08%	0.118%
51	13.828	1818	1826	1830	rVB3	17553	26568	0.35%	0.038%
52	13.969	1844	1850	1854	rBV8	6763	12018	0.16%	0.017%
53	14.063	1859	1866	1872	rVV	2571359	3362197	44.49%	4.832%
54	14.104	1872	1873	1878	rVB4	8614	11496	0.15%	0.017%
55	14.251	1893	1898	1905	rBV9	6765	13910	0.18%	0.020%
56	14.351	1907	1915	1924	rBV	2812245	4200388	55.58%	6.037%
57	14.534	1941	1946	1954	rVB10	6676	12026	0.16%	0.017%
58	14.651	1960	1966	1973	rVB	1927394	2703941	35.78%	3.886%
59	14.710	1973	1976	1983	rVB4	24994	35276	0.47%	0.051%
60	14.887	2000	2006	2021	rBV	186965	348598	4.61%	0.501%
61	15.039	2027	2032	2037	rVB9	7992	15300	0.20%	0.022%
62	15.098	2038	2042	2048	rVB8	11010	15956	0.21%	0.023%
63	15.151	2048	2051	2058	rVB9	5701	8878	0.12%	0.013%
64	15.316	2075	2079	2084	rBV2	11042	17157	0.23%	0.025%
65	15.392	2089	2092	2097	rVB	10165	12497	0.17%	0.018%
66	15.469	2101	2105	2111	rVB	16467	22719	0.30%	0.033%
67	15.569	2117	2122	2127	rVB8	6118	9325	0.12%	0.013%
68	15.651	2129	2136	2146	rVV	3719931	5350644	70.80%	7.690%
69	15.792	2155	2160	2173	rBV	1020713	1421676	18.81%	2.043%
70	15.892	2173	2177	2186	rVB	18902	35097	0.46%	0.050%
71	16.034	2197	2201	2205	rVB	19965	27995	0.37%	0.040%
72	16.439	2265	2270	2277	rVB10	5500	9349	0.12%	0.013%
73	16.986	2360	2363	2368	rVB4	8641	13772	0.18%	0.020%
74	17.098	2378	2382	2387	rVB8	7262	13755	0.18%	0.020%
75	17.222	2398	2403	2405	rBV6	5886	9603	0.13%	0.014%
76	17.245	2405	2407	2413	rVB7	5300	8589	0.11%	0.012%

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77	17.351	2422	2425	2429	rVB4	8544	11151	0.15%	0.016%
78	17.439	2433	2440	2450	rVV	2438552	3442003	45.55%	4.947%
79	17.539	2450	2457	2468	rVV2	4548298	6258042	82.81%	8.994%
80	17.628	2468	2472	2480	rVV4	31775	56603	0.75%	0.081%
81	17.692	2480	2483	2487	rVB	22417	27910	0.37%	0.040%
82	18.069	2541	2547	2557	rBV	601138	703986	9.32%	1.012%
83	18.280	2579	2583	2593	rBV2	82738	123762	1.64%	0.178%
84	18.375	2595	2599	2603	rVB	34613	44945	0.59%	0.065%
85	18.492	2617	2619	2624	rVB4	12513	15525	0.21%	0.022%
86	19.357	2762	2766	2770	rBV	61530	85510	1.13%	0.123%
87	19.416	2771	2776	2791	rVV2	444674	744823	9.86%	1.070%
88	19.527	2791	2795	2802	rVV2	66021	100996	1.34%	0.145%
89	19.792	2834	2840	2846	rBV	5931532	7486652	99.07%	10.759%
90	21.569	3137	3142	3148	rBV	2980000	3817452	50.52%	5.486%
91	23.980	3544	3552	3560	rVB2	3676088	7556881	100.00%	10.860%
92	24.145	3574	3580	3591	rVB	1900588	4096600	54.21%	5.887%

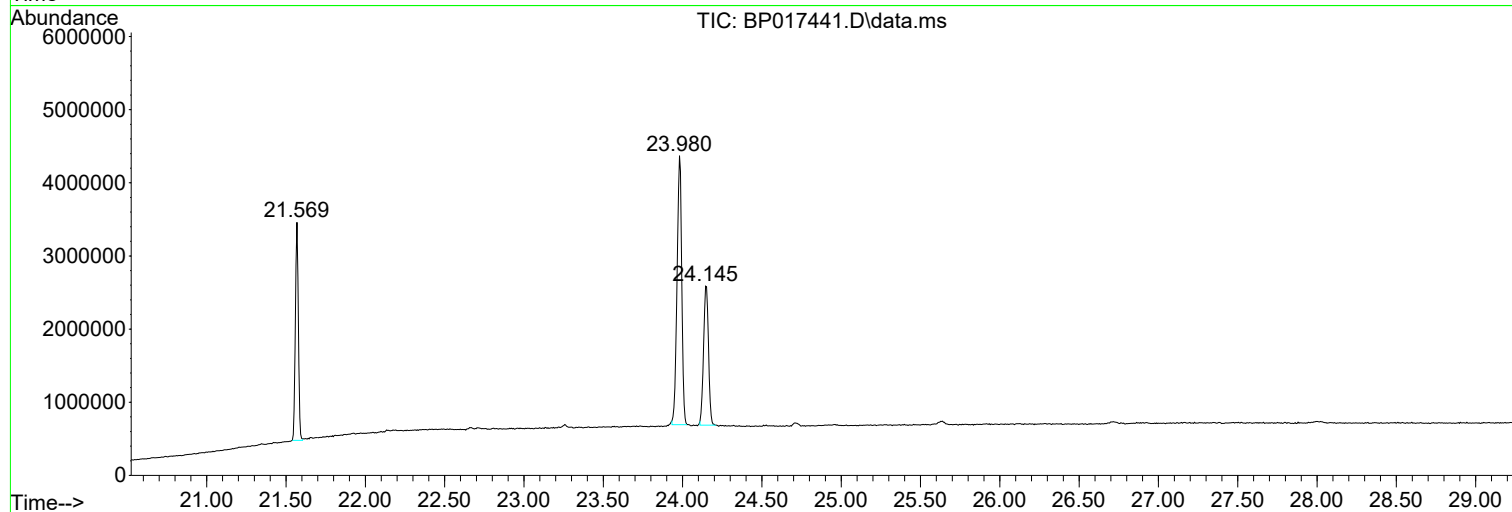
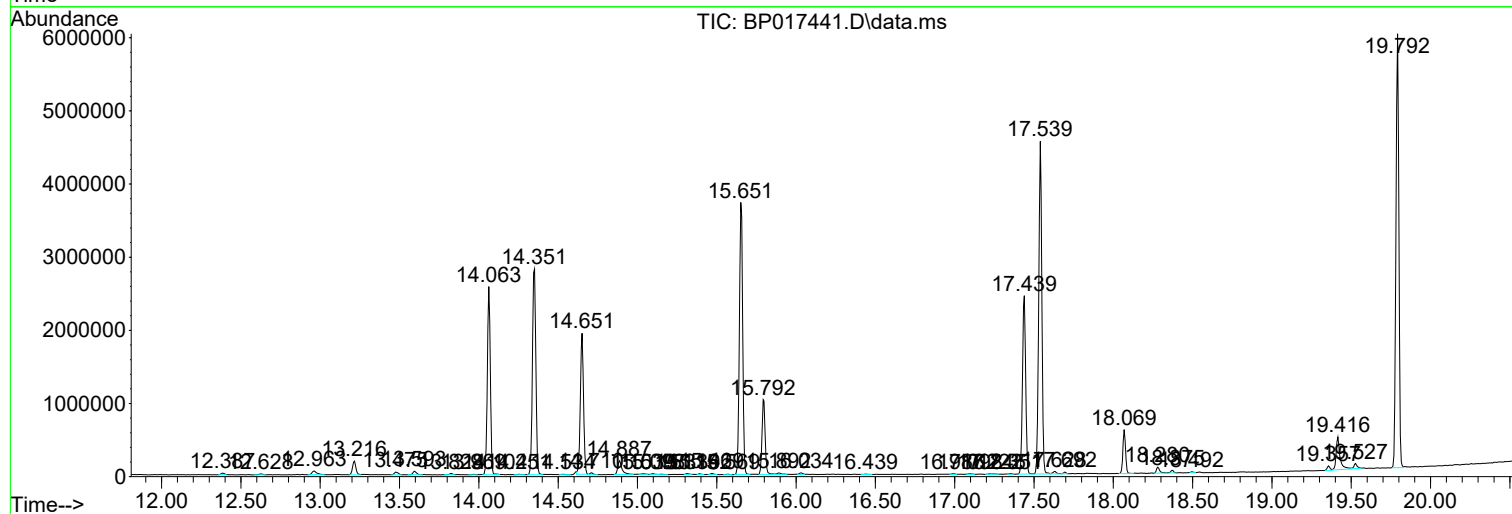
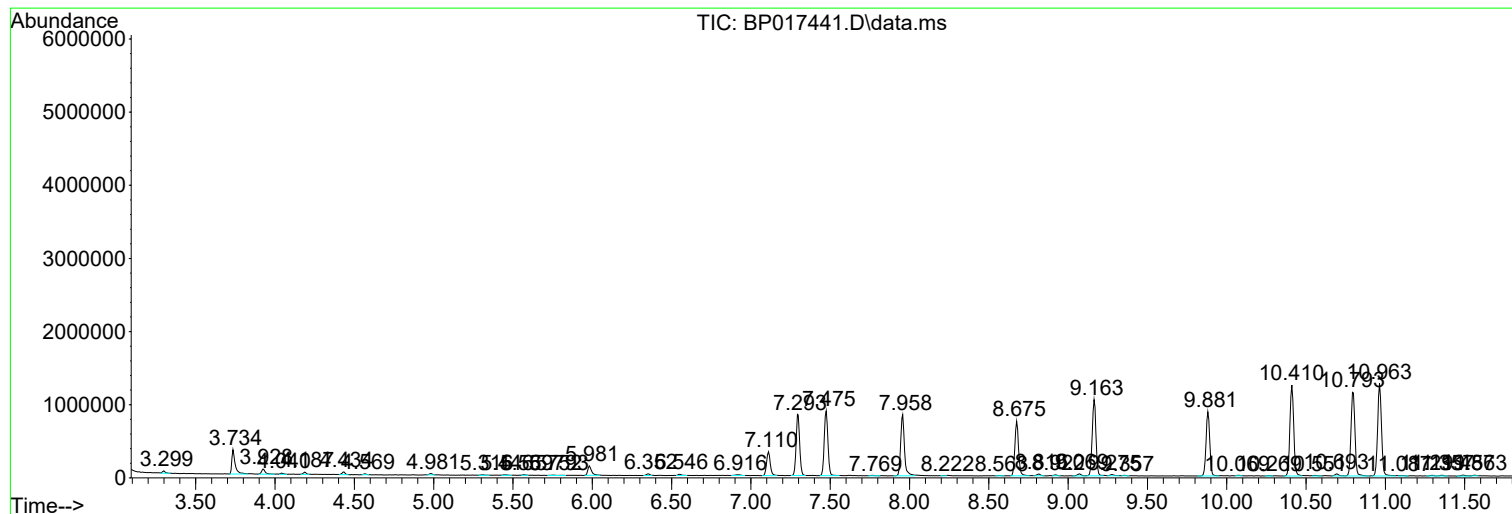
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
Quant Title : SVOA CALIBRATION

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



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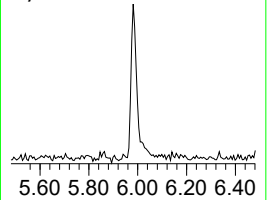
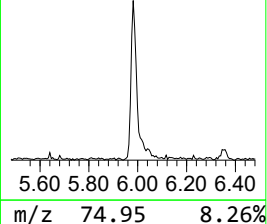
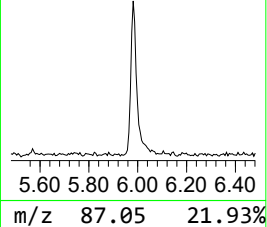
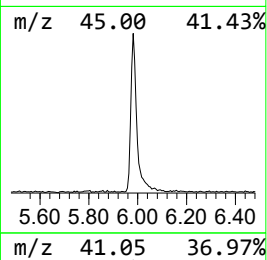
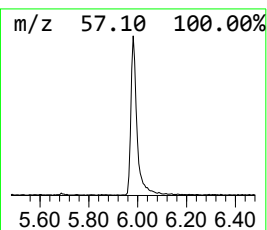
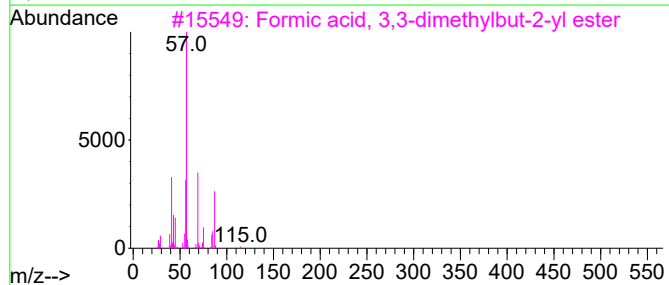
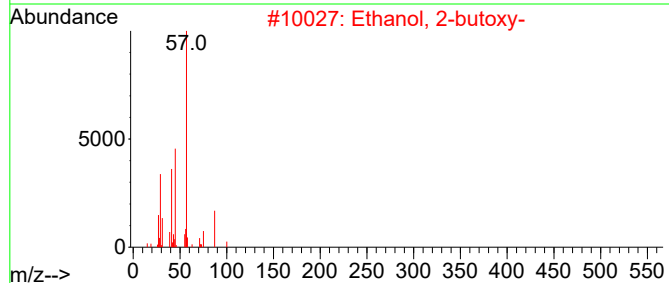
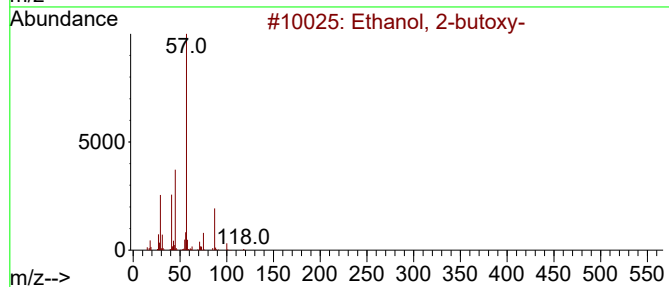
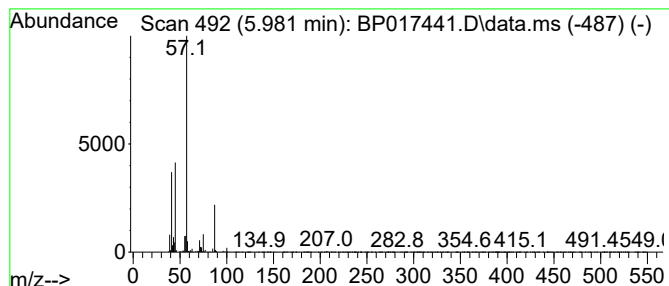
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Ethanol, 2-butoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.981	3.06 ng/ul	214250	1,4-Dichlorobenzene-d4	7.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	74
2			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	72
3			Formic acid, 3,3-dimethylbut-2-y...	130	C7H14O2	1000368-20-5	64
4			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	53
5			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	45



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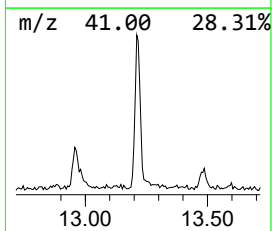
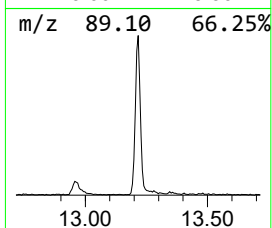
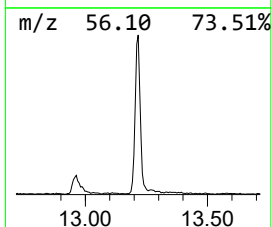
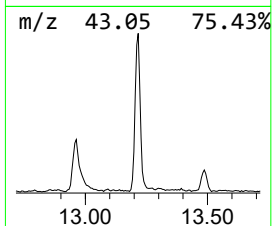
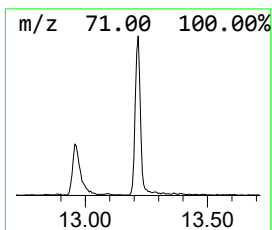
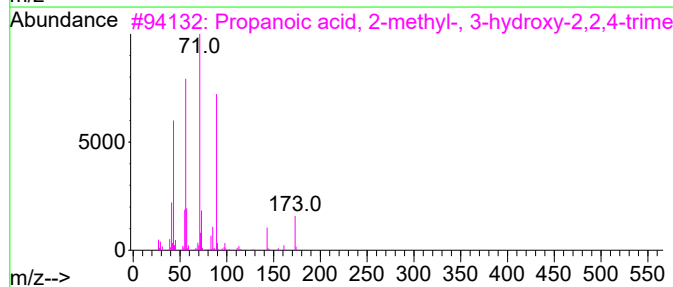
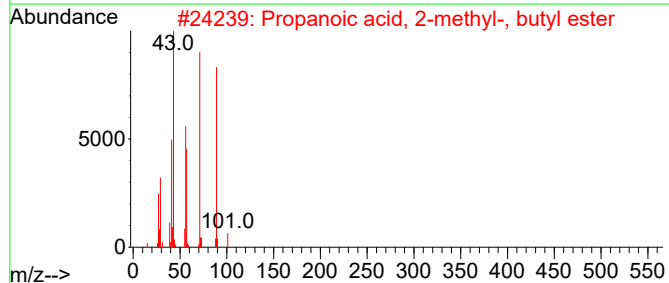
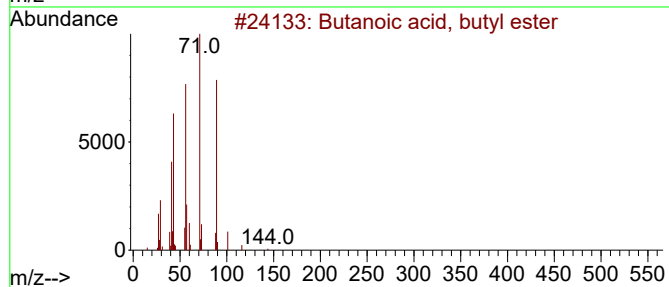
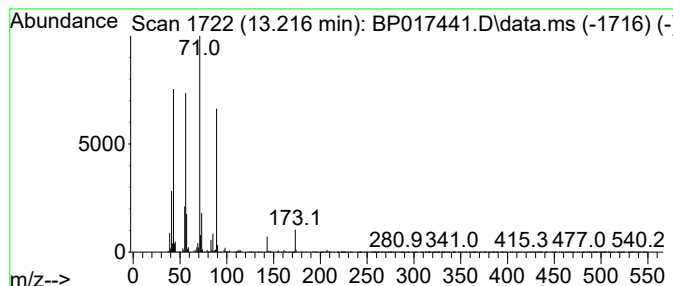
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Butanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	2.08 ng/ul	281828	Acenaphthene-d10	14.651

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	87
2			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
3			Propanoic acid, 2-methyl-, 3-hyd...	216	C12H24O3	000077-68-9	64
4			Propanoic acid, 2-methyl-, 2-eth...	216	C12H24O3	074367-31-0	64
5			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	59



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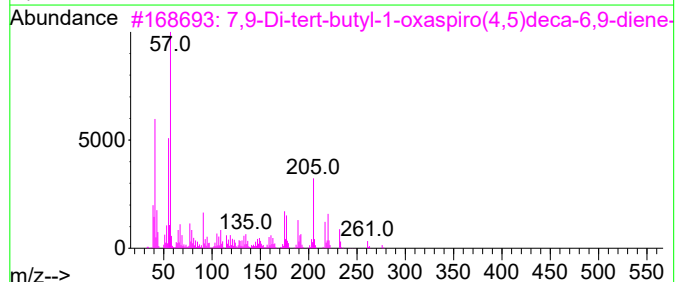
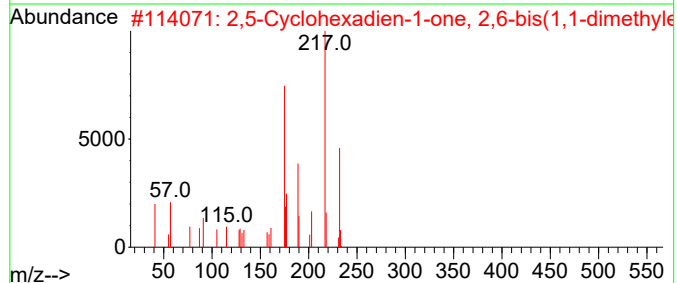
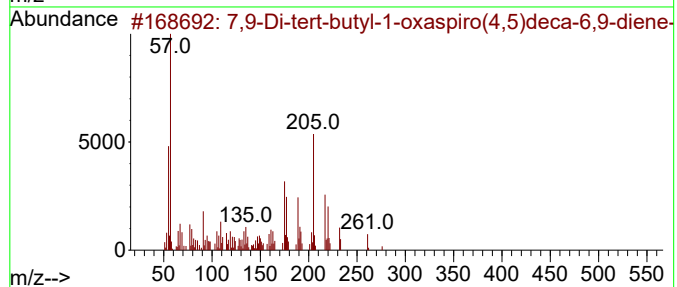
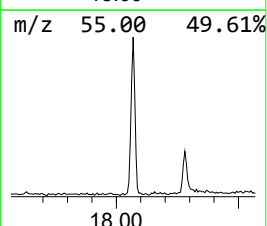
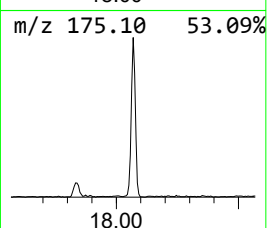
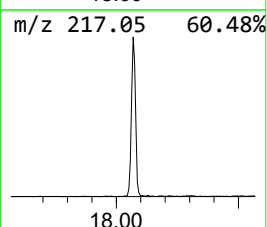
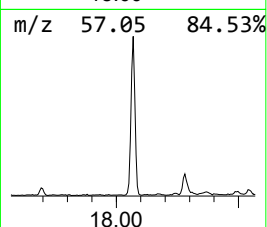
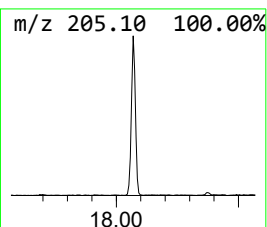
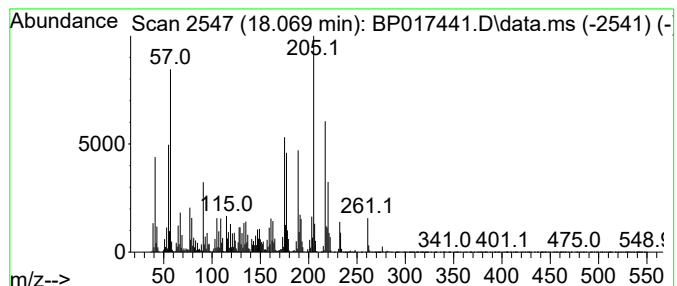
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
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TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.069	4.09 ng/ul	703986	Phenanthrene-d10	17.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	98		
2	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	83		
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	55		
4	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	50		
5	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	45		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092923\
Data File : BP017441.D
Acq On : 29 Sep 2023 12:14
Operator : MA/JU
Sample : 04472-22
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EZYP5

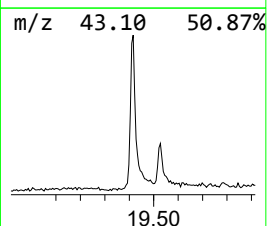
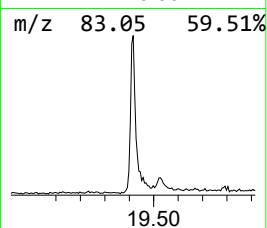
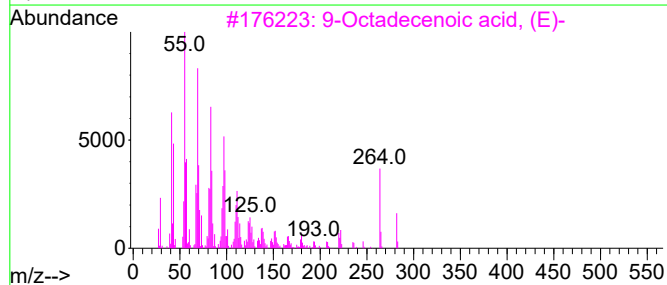
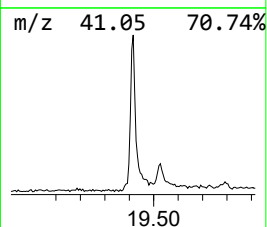
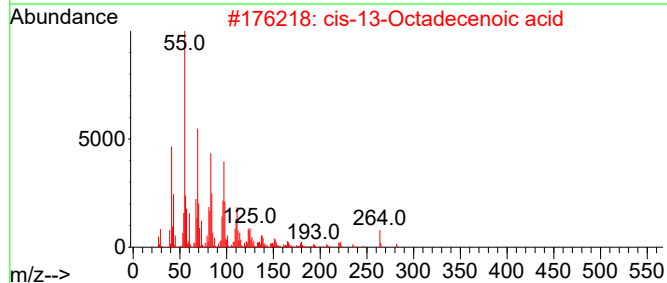
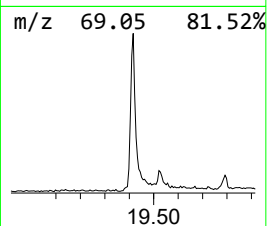
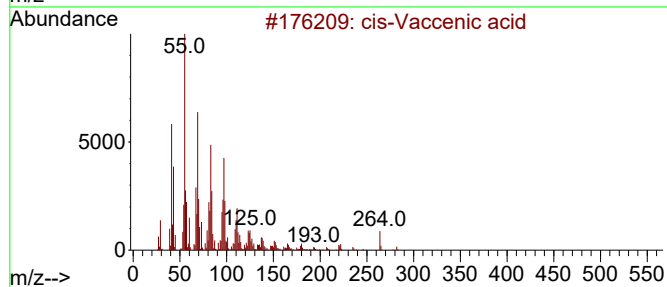
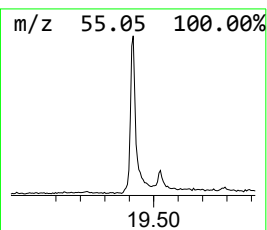
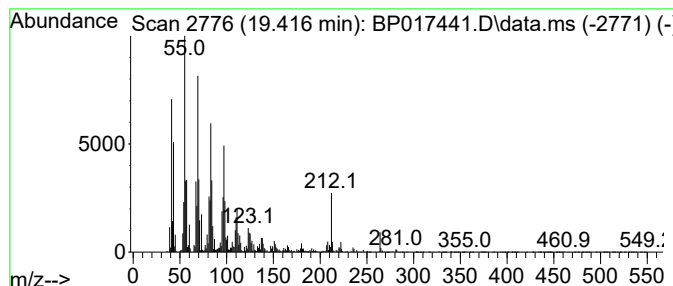
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 cis-Vaccenic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.416	4.33 ng/ul	744823	Phenanthrene-d10	17.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	97
2			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	96
3			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	95
4			cis-9-Octadecenoic acid, propyl ...	324	C21H40O2	1000405-15-0	87
5			6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092923\
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EZYP5

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-butoxy-	5.981	3.1	ng/ul	214250	1	7.957	1398270	20.0
Butanoic acid, ...	13.216	2.1	ng/ul	281828	3	14.651	2703940	20.0
7,9-Di-tert-but...	18.069	4.1	ng/ul	703986	4	17.439	3442000	20.0
cis-Vaccenic acid	19.416	4.3	ng/ul	744823	4	17.439	3442000	20.0