

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051622\
 Data File : BP010364.D
 Acq On : 16 May 2022 19:12
 Operator : CG/JU
 Sample : N2831-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 YB2K1

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-BP051322.M
 Title : SVOA CALIBRATION

Signal : TIC: BP010364.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.346	40	44	54	rVB	31299	51919	0.94%	0.099%
2	3.770	112	116	133	rBV	163892	342564	6.22%	0.652%
3	3.999	151	155	160	rVB7	6645	12902	0.23%	0.025%
4	4.087	166	170	176	rBV5	10688	23022	0.42%	0.044%
5	4.564	235	251	257	rBV2	104239	367100	6.67%	0.698%
6	4.769	282	286	292	rVB6	6967	12810	0.23%	0.024%
7	5.005	322	326	332	rBV3	6518	12005	0.22%	0.023%
8	5.405	390	394	399	rBV7	2751	5707	0.10%	0.011%
9	5.946	483	486	491	rBV6	5086	8198	0.15%	0.016%
10	6.911	645	650	656	rVV9	5087	12893	0.23%	0.025%
11	7.064	669	676	687	rVB	165019	282992	5.14%	0.538%
12	7.228	697	704	714	rBV	595176	967536	17.57%	1.841%
13	7.305	714	717	723	rVB	10585	18575	0.34%	0.035%
14	7.428	731	738	752	rBV	607798	986587	17.92%	1.877%
15	7.528	752	755	761	rVB8	5230	9037	0.16%	0.017%
16	7.899	810	818	825	rBV	564563	908615	16.50%	1.729%
17	7.969	825	830	839	rVB	68192	118392	2.15%	0.225%
18	8.152	857	861	866	rVV7	3734	6064	0.11%	0.012%
19	8.605	927	938	955	rBV	521177	911012	16.55%	1.733%
20	8.775	964	967	975	rVB9	4431	7512	0.14%	0.014%
21	9.058	1001	1015	1027	rBV	819538	1391212	25.27%	2.647%
22	9.181	1033	1036	1040	rBV5	5466	9280	0.17%	0.018%
23	9.228	1040	1044	1049	rVB7	6055	10791	0.20%	0.021%
24	9.505	1085	1091	1098	rVB3	13503	25215	0.46%	0.048%
25	9.781	1130	1138	1150	rBV	590542	989125	17.96%	1.882%
26	10.040	1178	1182	1187	rBV8	4742	8385	0.15%	0.016%
27	10.105	1190	1193	1198	rBV6	4841	7669	0.14%	0.015%
28	10.157	1198	1202	1207	rVB4	4984	10809	0.20%	0.021%
29	10.228	1212	1214	1221	rVB8	6128	11076	0.20%	0.021%
30	10.322	1221	1230	1245	rBV	934673	1672107	30.37%	3.181%
31	10.699	1286	1294	1308	rBV	790772	1350766	24.53%	2.570%
32	10.834	1309	1317	1334	rBV	866348	1611338	29.26%	3.066%
33	11.116	1360	1365	1373	rVB2	14100	27301	0.50%	0.052%
34	11.252	1384	1388	1393	rBV6	3773	6214	0.11%	0.012%
35	11.363	1401	1407	1412	rVB8	4172	8177	0.15%	0.016%
36	11.499	1425	1430	1441	rBV6	22100	54710	0.99%	0.104%

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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP051322.M
 Title : SVOA CALIBRATION

37	11.663	1452	1458	1459	rBV6	5639	7205	0.13%	0.014%
38	11.704	1460	1465	1474	rVB7	14635	32772	0.60%	0.062%
39	11.957	1500	1508	1512	rBV	39501	68503	1.24%	0.130%
40	12.128	1534	1537	1542	rVB5	7623	12773	0.23%	0.024%

41	12.287	1557	1564	1566	rBV4	16276	27020	0.49%	0.051%
42	12.351	1566	1575	1594	rVB	731891	1438102	26.12%	2.736%
43	12.904	1665	1669	1672	rBV6	6091	7590	0.14%	0.014%
44	12.946	1672	1676	1682	rVV	33299	50215	0.91%	0.096%
45	13.046	1687	1693	1696	rVV8	5160	10575	0.19%	0.020%

46	13.087	1696	1700	1705	rVV8	5170	8661	0.16%	0.016%
47	13.146	1705	1710	1714	rVB6	6059	9221	0.17%	0.018%
48	13.334	1738	1742	1743	rBV4	8250	10862	0.20%	0.021%
49	13.363	1743	1747	1756	rVB2	33568	56074	1.02%	0.107%
50	13.493	1767	1769	1775	rBV8	9316	19875	0.36%	0.038%

51	13.940	1838	1845	1857	rBV	2061737	2750301	49.95%	5.233%
52	14.051	1857	1864	1872	rVB3	51897	88611	1.61%	0.169%
53	14.222	1882	1893	1906	rBV	2103723	3143251	57.09%	5.980%
54	14.434	1923	1929	1935	rVB3	26706	50074	0.91%	0.095%
55	14.528	1935	1945	1958	rBV	1239545	1907060	34.63%	3.628%

56	14.734	1974	1980	1994	rBV2	89411	212525	3.86%	0.404%
57	14.951	2014	2017	2022	rVB7	9833	11882	0.22%	0.023%
58	15.122	2033	2046	2047	rBV3	87411	257816	4.68%	0.491%
59	15.340	2079	2083	2088	rVV5	11553	21287	0.39%	0.040%
60	15.387	2088	2091	2095	rVB5	10095	14648	0.27%	0.028%

61	15.522	2108	2114	2126	rBV	2781533	4087031	74.23%	7.776%
62	15.604	2126	2128	2129	rVV2	9218	7926	0.14%	0.015%
63	15.640	2129	2134	2147	rVV	405260	616095	11.19%	1.172%
64	15.763	2151	2155	2163	rVB2	36093	63088	1.15%	0.120%
65	15.869	2170	2173	2175	rBV4	10749	11623	0.21%	0.022%

66	15.928	2179	2183	2192	rVB8	22276	48573	0.88%	0.092%
67	16.034	2194	2201	2207	rBV7	26340	53531	0.97%	0.102%
68	16.310	2244	2248	2252	rVB3	16316	24572	0.45%	0.047%
69	16.422	2265	2267	2270	rBV3	6066	6438	0.12%	0.012%
70	16.581	2290	2294	2298	rBV7	9616	15178	0.28%	0.029%

71	16.687	2309	2312	2316	rVB6	6662	7398	0.13%	0.014%
72	16.769	2322	2326	2330	rBV3	13110	26290	0.48%	0.050%
73	17.045	2368	2373	2387	rVB5	71782	184267	3.35%	0.351%
74	17.281	2407	2413	2421	rBV	1535702	2244712	40.77%	4.271%
75	17.381	2424	2430	2440	rVB	3143585	4552542	82.68%	8.662%

76	17.516	2449	2453	2456	rBV	55284	69289	1.26%	0.132%
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77	17.951	2524	2527	2533	rBV7	17573	22238	0.40%	0.042%
78	18.169	2560	2564	2566	rBV	301880	400313	7.27%	0.762%
79	18.192	2566	2568	2573	rVB	290683	314194	5.71%	0.598%
80	19.192	2736	2738	2746	rVB3	52285	72594	1.32%	0.138%
81	19.263	2747	2750	2751	rVV	39806	41818	0.76%	0.080%
82	19.286	2751	2754	2765	rVB4	75786	163150	2.96%	0.310%
83	19.398	2770	2773	2778	rVB2	59159	76072	1.38%	0.145%
84	19.616	2804	2810	2822	rBV	4217188	5506178	100.00%	10.476%
85	20.057	2882	2885	2891	rBV4	30916	54962	1.00%	0.105%
86	21.075	3054	3058	3071	rBV	1221139	1814760	32.96%	3.453%
87	21.369	3102	3108	3114	rBV	1743108	2490751	45.24%	4.739%
88	23.051	3390	3394	3400	rVB2	138936	205627	3.73%	0.391%
89	23.639	3487	3494	3501	rBV2	2337377	4616405	83.84%	8.783%
90	23.798	3514	3521	3535	rVB2	1054644	2286369	41.52%	4.350%

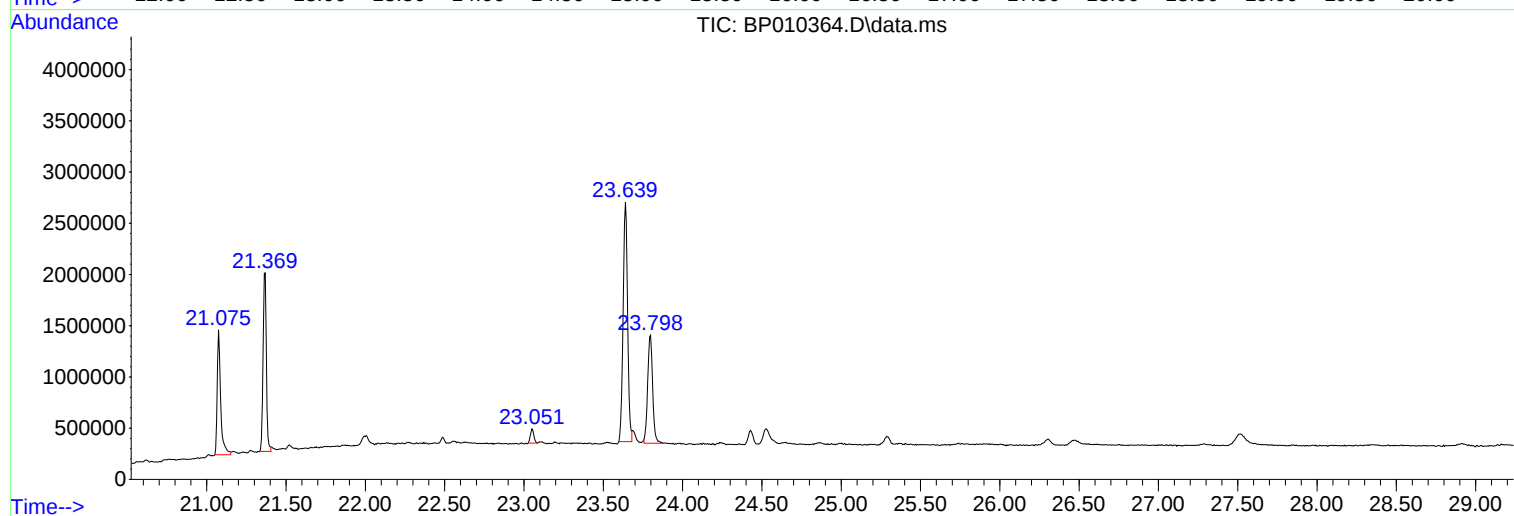
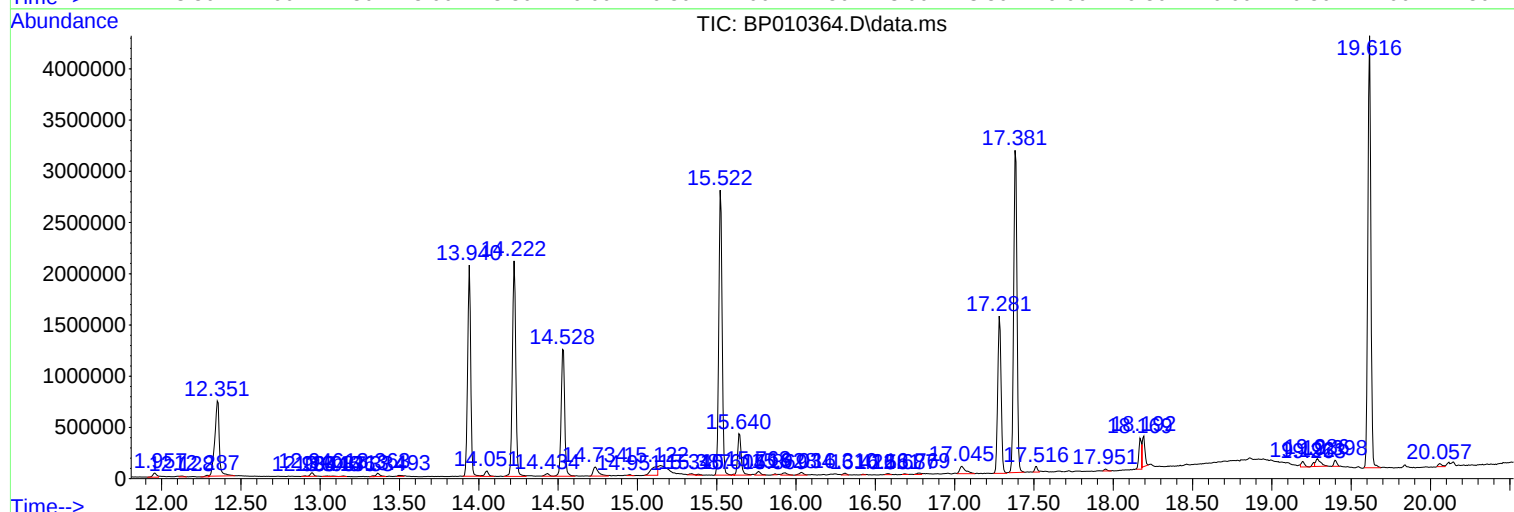
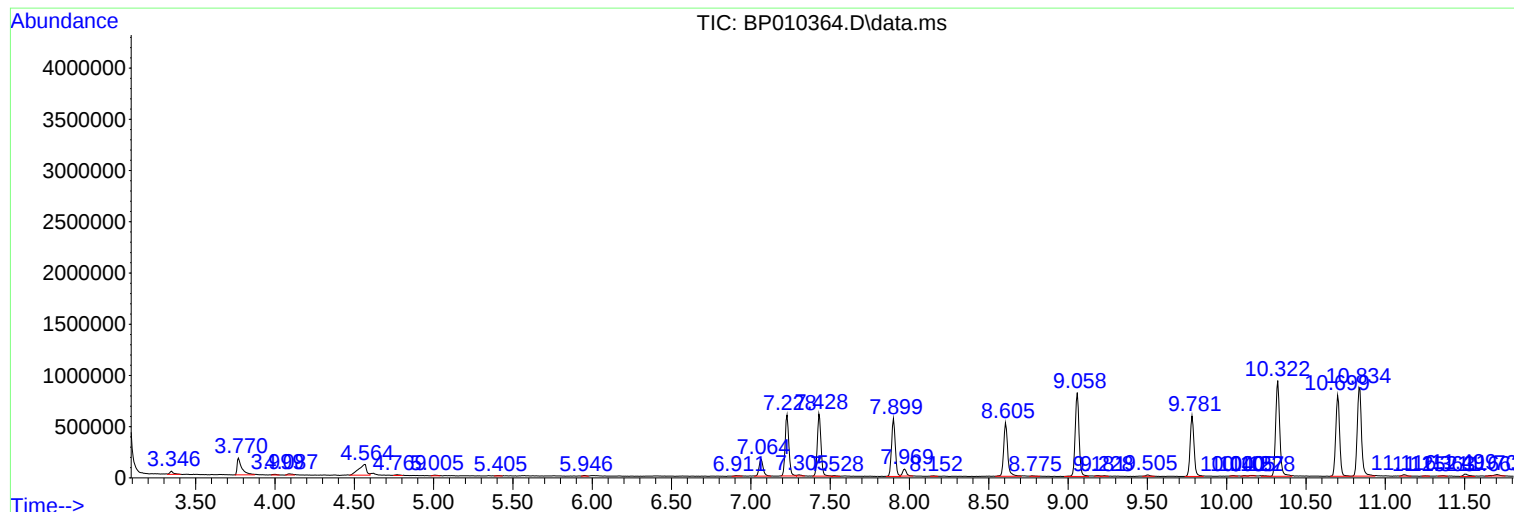
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP051322.M
Quant Title : SVOA CALIBRATION

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



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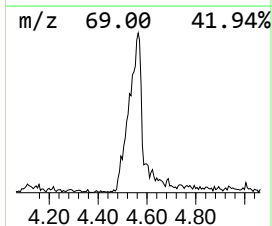
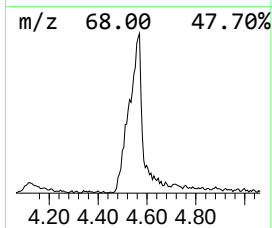
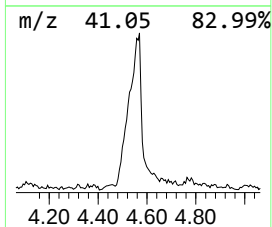
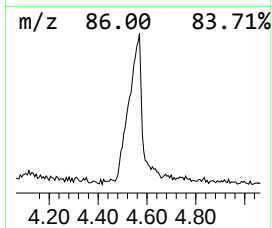
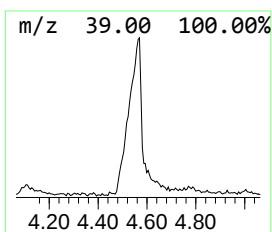
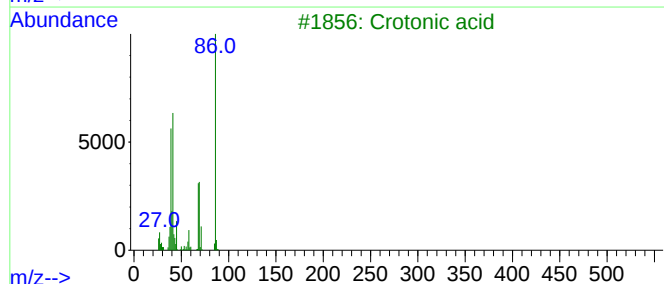
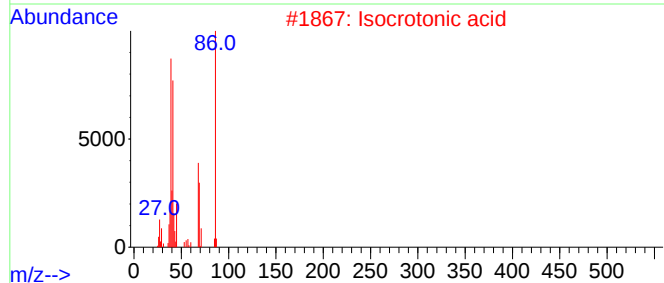
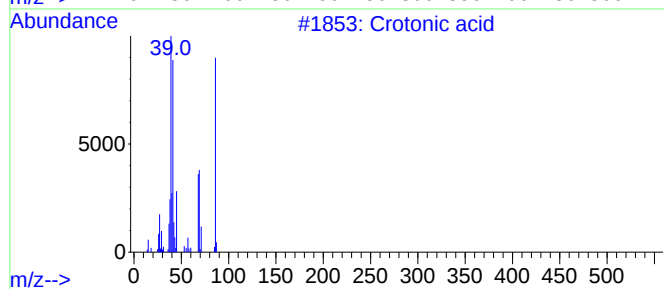
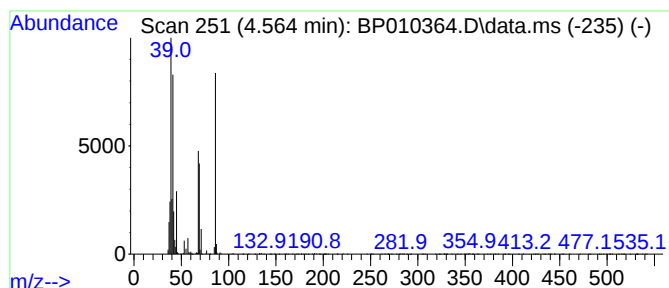
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP051322.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Crotonic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.564	8.08 ng/ul	367100	1,4-Dichlorobenzene-d4	7.899

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Crotonic acid	86	C4H6O2	003724-65-0	96
2			Isocrotonic acid	86	C4H6O2	000503-64-0	91
3			Crotonic acid	86	C4H6O2	003724-65-0	91
4			Crotonic acid	86	C4H6O2	003724-65-0	90
5			2-Butenoic acid, (E)-	86	C4H6O2	000107-93-7	81



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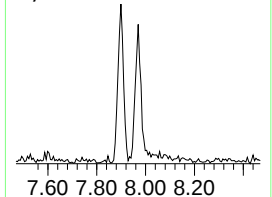
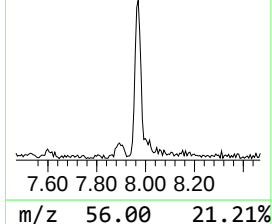
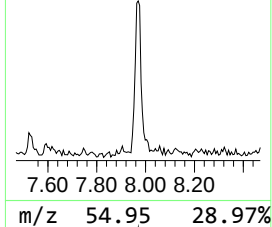
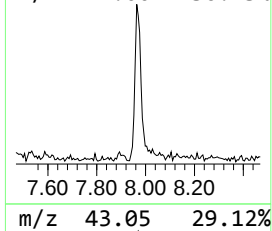
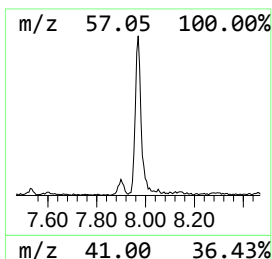
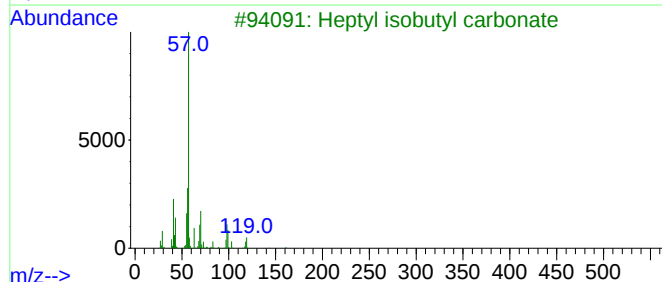
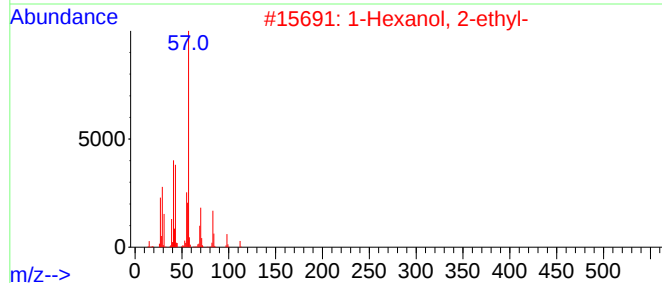
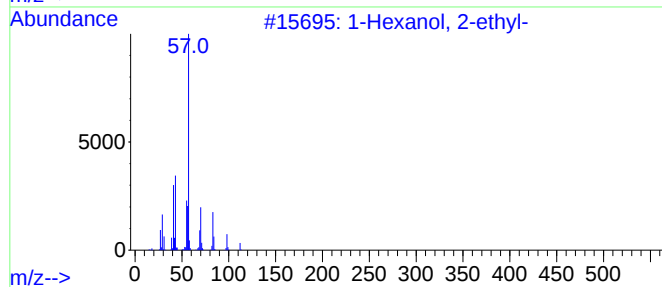
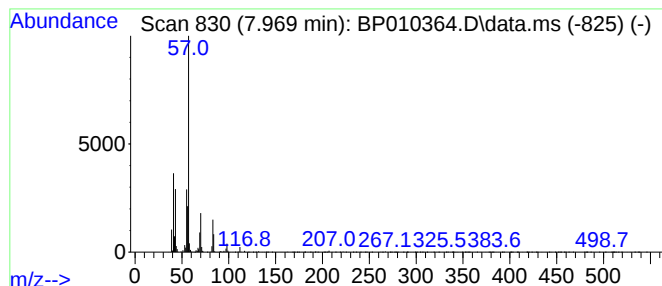
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP051322.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.969	2.61 ng/ul	118392	1,4-Dichlorobenzene-d4	7.899

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	74
3	Heptyl isobutyl carbonate			216	C12H24O3	959068-08-7	64
4	Heptyl isobutyl carbonate			216	C12H24O3	959068-08-7	64
5	1-Isobutoxy-2-ethylhexane			186	C12H26O	1000139-90-3	64



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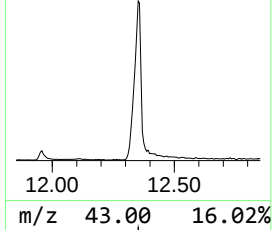
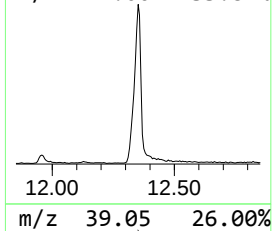
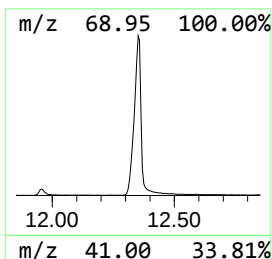
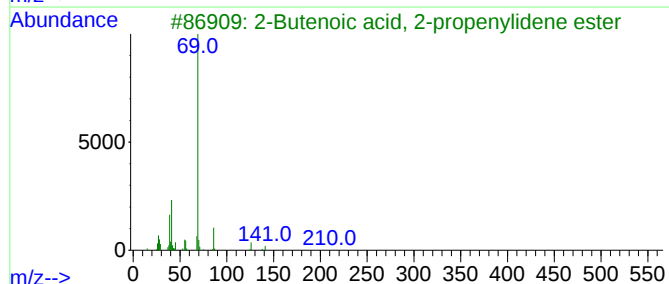
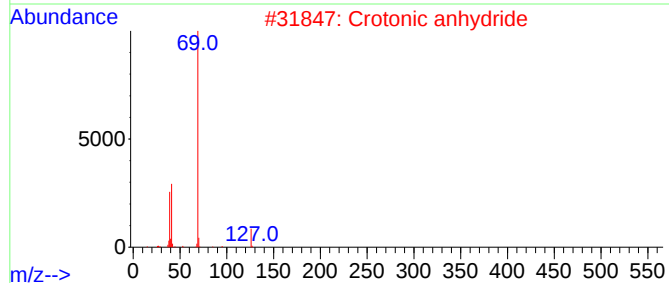
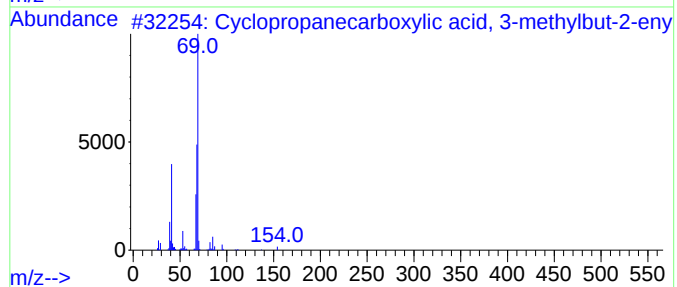
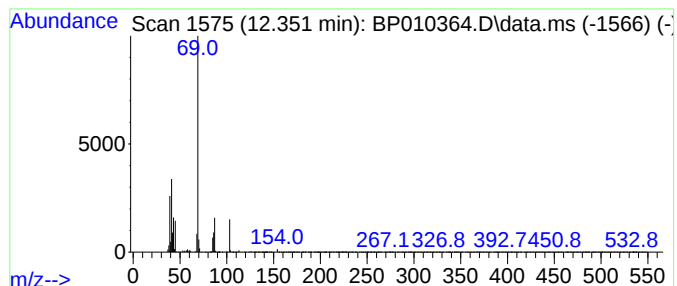
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP051322.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Cyclopropanecarboxylic acid... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.352	21.29 ng/ul	1438100	Naphthalene-d8	10.699

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	50
2			Crotonic anhydride	154	C8H10O3	000623-68-7	47
3			2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	42
4			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	39
5			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	38



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YB2K1

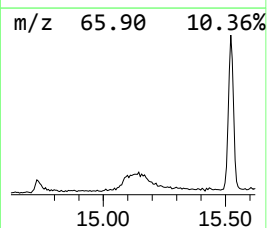
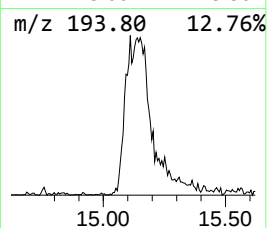
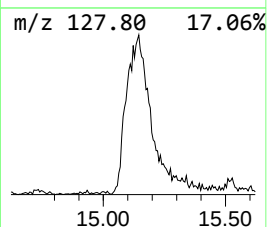
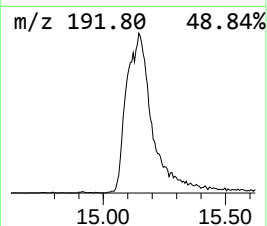
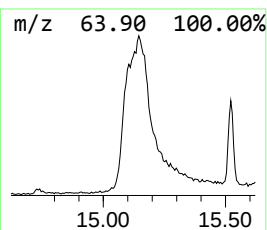
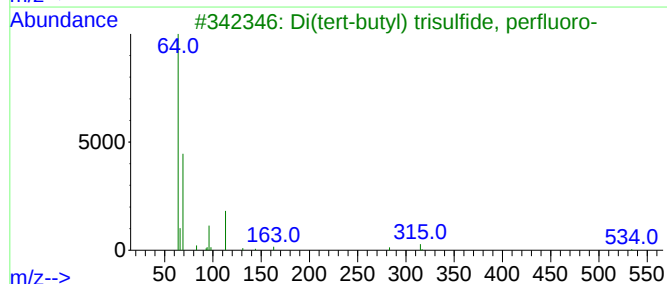
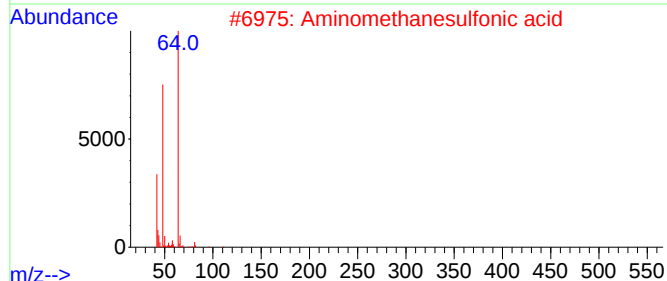
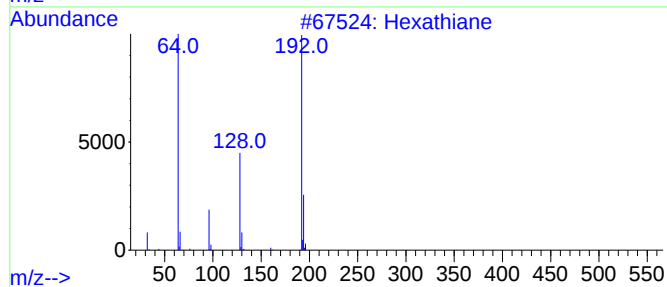
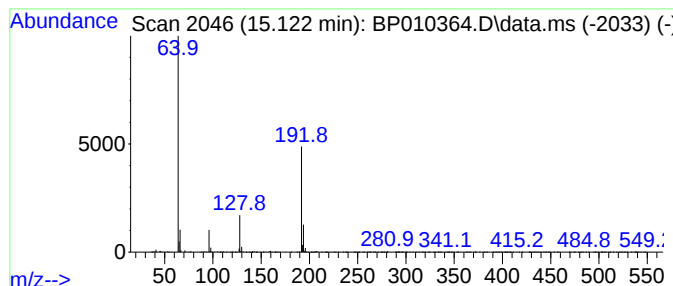
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Hexathiane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.122	2.70 ng/ul	257816	Acenaphthene-d10	14.534

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexathiane	192	S6	013798-23-7	91
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
3			Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	9
4			Cyclic octaatomic sulfur	256	S8	010544-50-0	9
5			Valine, 3-[sulfothio]-	229	C5H11NO5S2	055631-63-5	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051622\
Data File : BP010364.D
Acq On : 16 May 2022 19:12
Operator : CG/JU
Sample : N2831-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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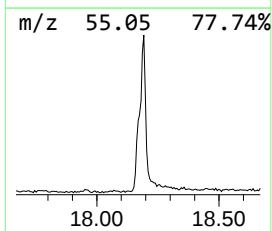
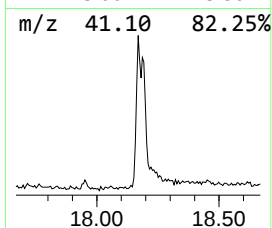
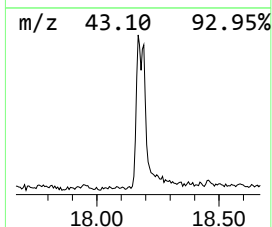
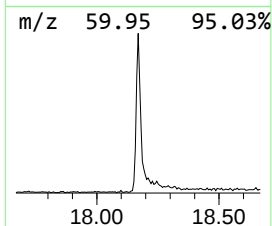
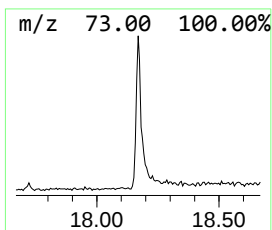
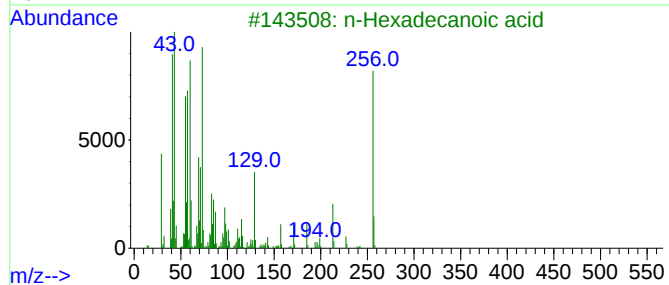
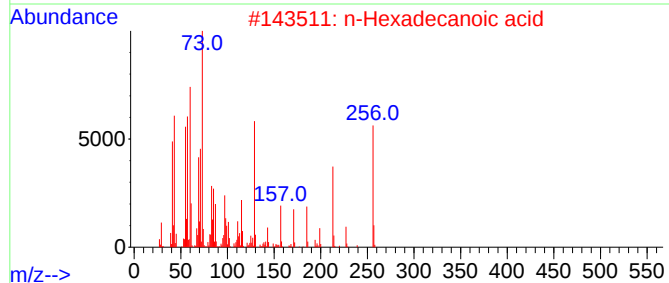
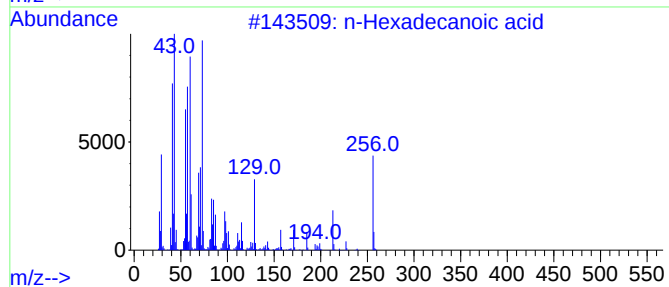
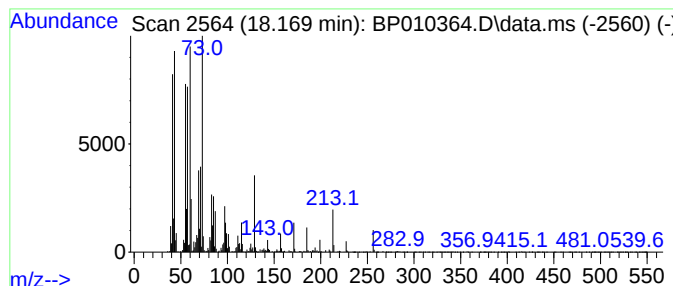
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.169	3.57 ng/ul	400313	Phenanthrene-d10	17.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
5			Tridecanoic acid	214	C13H26O2	000638-53-9	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051622\
Data File : BP010364.D
Acq On : 16 May 2022 19:12
Operator : CG/JU
Sample : N2831-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

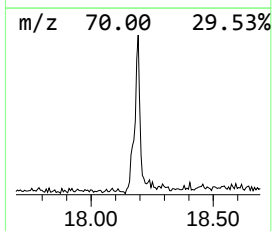
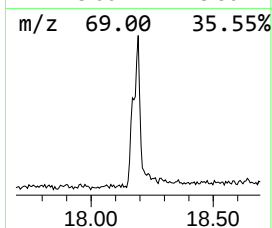
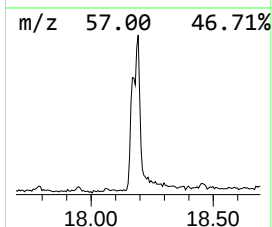
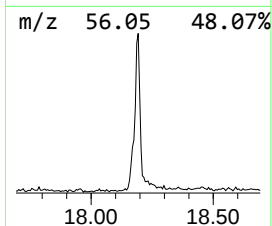
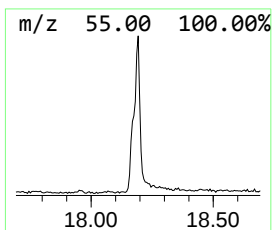
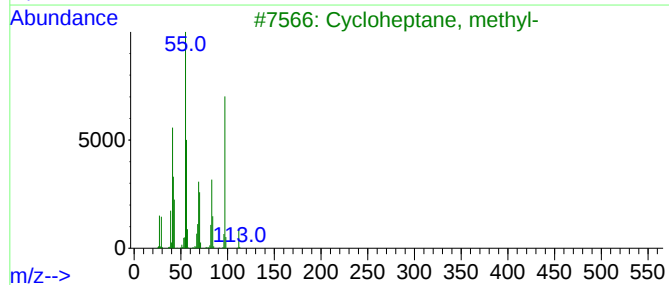
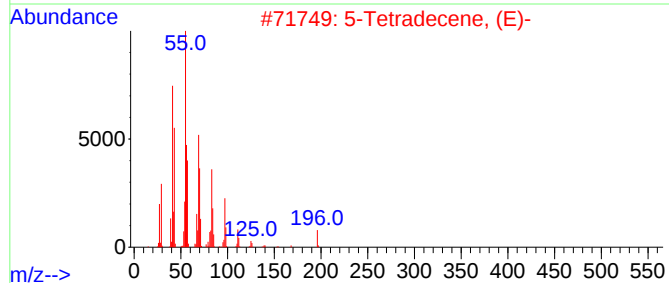
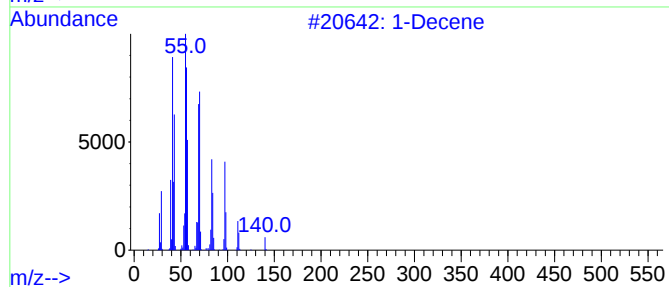
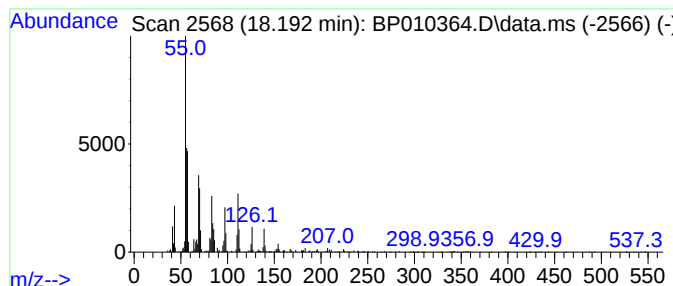
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.192	2.80 ng/ul	314194	Phenanthrene-d10		17.281	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Decene		140	C10H20	000872-05-9	52
2	5-Tetradecene, (E)-		196	C14H28	041446-66-6	49
3	Cycloheptane, methyl-		112	C8H16	004126-78-7	49
4	1-Tetradecanol		214	C14H30O	000112-72-1	47
5	Cyclopentane, 1-methyl-2-propyl-		126	C9H18	003728-57-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051622\
Data File : BP010364.D
Acq On : 16 May 2022 19:12
Operator : CG/JU
Sample : N2831-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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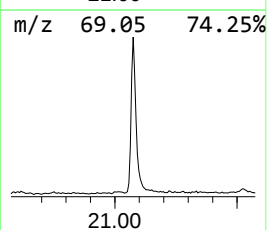
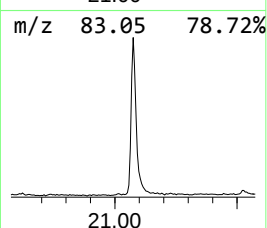
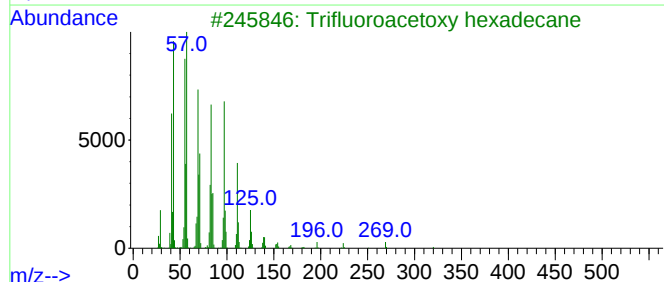
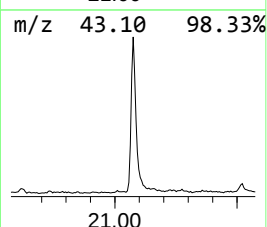
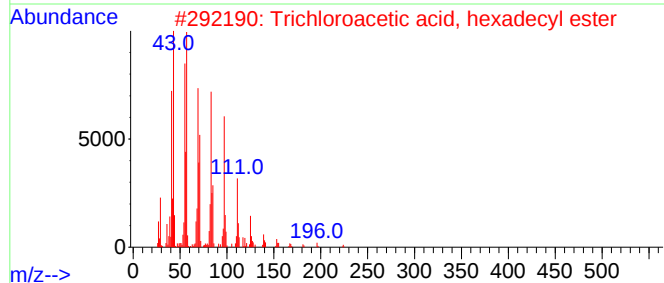
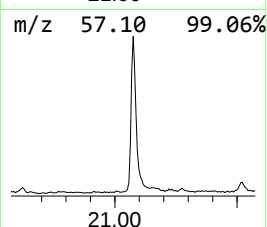
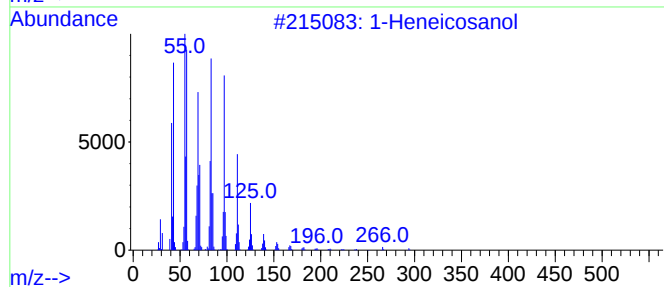
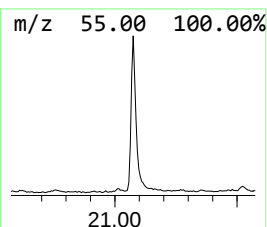
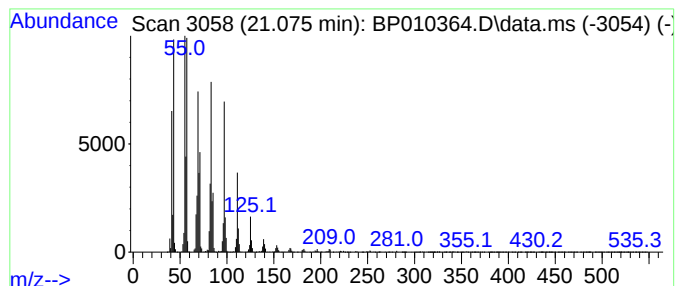
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.075	14.57 ng/ul	1814760	Chrysene-d12	21.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol			312	C21H44O	015594-90-8	95
2	Trichloroacetic acid, hexadecyl ...			386	C18H33Cl3O2	074339-54-1	94
3	Trifluoroacetoxy hexadecane			338	C18H33F3O2	006222-03-3	94
4	Heptafluorobutyric acid, pentade...			424	C19H31F7O2	959261-23-5	94
5	1-Hexacosene			364	C26H52	018835-33-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051622\
Data File : BP010364.D
Acq On : 16 May 2022 19:12
Operator : CG/JU
Sample : N2831-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP051322.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
Crotonic acid	4.564	8.1	ng/ul	367100	1	7.899	908615	20.0
1-Hexanol, 2-et...	7.969	2.6	ng/ul	118392	1	7.899	908615	20.0
Cyclopropanecar...	12.352	21.3	ng/ul	1438100	2	10.699	1350770	20.0
Hexathiane	15.122	2.7	ng/ul	257816	3	14.534	1907060	20.0
n-Hexadecanoic ...	18.169	3.6	ng/ul	400313	4	17.281	2244710	20.0
(DEL) Alkane: S...	18.192	2.8	ng/ul	314194	4	17.281	2244710	20.0
1-Heneicosanol	21.075	14.6	ng/ul	1814760	5	21.369	2490750	20.0