

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051424\
 Data File : BP020388.D
 Acq On : 15 May 2024 06:02
 Operator : MA/JU
 Sample : P2372-13
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 A43W3

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-BP050124.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP020388.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.193	14	18	23	rBV2	13788	17986	0.84%	0.076%
2	3.470	61	65	80	rBV	28886	58507	2.73%	0.246%
3	3.593	83	86	103	rBV	124208	240083	11.20%	1.011%
4	6.240	534	536	541	rBV5	1568	2256	0.11%	0.010%
5	6.693	608	613	619	rBV10	1980	3577	0.17%	0.015%
6	6.781	622	628	649	rBV	204327	477735	22.29%	2.013%
7	6.946	650	656	670	rVB	198262	340063	15.87%	1.433%
8	7.128	680	687	705	rBV	264717	486406	22.70%	2.049%
9	7.299	713	716	719	rBV5	1783	2526	0.12%	0.011%
10	7.587	759	765	776	rBV	243232	433992	20.25%	1.828%
11	8.305	880	887	906	rBV2	282408	623642	29.10%	2.627%
12	8.752	956	963	980	rBV	253936	497762	23.23%	2.097%
13	8.916	987	991	994	rBV5	1622	2617	0.12%	0.011%
14	9.346	1059	1064	1068	rBV5	6230	12287	0.57%	0.052%
15	9.469	1077	1085	1101	rBV	206623	443751	20.71%	1.869%
16	10.004	1169	1176	1198	rBV	252427	643057	30.01%	2.709%
17	10.228	1209	1214	1218	rBV7	4877	7971	0.37%	0.034%
18	10.357	1229	1236	1253	rVB	364929	646163	30.15%	2.722%
19	10.528	1257	1265	1285	rBV2	220840	599556	27.98%	2.526%
20	10.987	1338	1343	1344	rBV5	3149	4211	0.20%	0.018%
21	11.157	1364	1372	1394	rBV2	27521	105921	4.94%	0.446%
22	11.387	1408	1411	1417	rVB7	1285	2277	0.11%	0.010%
23	11.934	1500	1504	1506	rVV5	2401	3680	0.17%	0.016%
24	11.981	1506	1512	1523	rVB6	5493	13963	0.65%	0.059%
25	12.851	1655	1660	1665	rBV9	2412	4572	0.21%	0.019%
26	13.069	1693	1697	1701	rVB7	1844	3285	0.15%	0.014%
27	13.234	1720	1725	1726	rBV4	2241	3134	0.15%	0.013%
28	13.681	1792	1801	1814	rBV	683544	1156587	53.97%	4.872%
29	13.857	1827	1831	1835	rVB6	1868	2583	0.12%	0.011%
30	13.951	1836	1847	1866	rBV	788920	1291379	60.26%	5.440%
31	14.263	1892	1900	1915	rBV	618701	967646	45.15%	4.076%
32	14.363	1915	1917	1920	rVB4	2096	2255	0.11%	0.009%
33	14.504	1932	1941	1945	rBV3	77736	179226	8.36%	0.755%
34	14.557	1945	1950	1962	rBV3	90600	297917	13.90%	1.255%
35	14.716	1974	1977	1981	rVB5	8678	12253	0.57%	0.052%
36	14.816	1990	1994	2002	rVB5	4018	9095	0.42%	0.038%

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Integrator: RTE

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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050124.MA.M
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37	15.087	2037	2040	2044	rVB5	2954	3581	0.17%	0.015%
38	15.134	2044	2048	2054	rVB9	2621	6101	0.28%	0.026%
39	15.287	2067	2074	2088	rBV	1010141	1625968	75.87%	6.850%
40	15.451	2096	2102	2114	rBV	255276	459217	21.43%	1.935%
41	15.534	2114	2116	2124	rVB9	9487	18857	0.88%	0.079%
42	15.881	2168	2175	2180	rBV10	7220	14947	0.70%	0.063%
43	16.039	2197	2202	2204	rBV6	3607	5720	0.27%	0.024%
44	16.098	2210	2212	2216	rVB5	2294	2920	0.14%	0.012%
45	16.228	2226	2234	2242	rBV5	4318	11341	0.53%	0.048%
46	16.375	2257	2259	2262	rBV4	2431	3284	0.15%	0.014%
47	16.516	2278	2283	2288	rBV2	16234	24605	1.15%	0.104%
48	16.881	2340	2345	2346	rBV4	3499	4796	0.22%	0.020%
49	16.963	2357	2359	2364	rVB6	1651	2229	0.10%	0.009%
50	17.039	2367	2372	2376	rBV6	9111	14808	0.69%	0.062%
51	17.104	2376	2383	2394	rVV	857362	1259526	58.77%	5.306%
52	17.210	2394	2401	2414	rVV	1051754	1816513	84.76%	7.652%
53	17.310	2415	2418	2422	rVV5	11831	18337	0.86%	0.077%
54	17.363	2422	2427	2432	rVB9	8095	16016	0.75%	0.067%
55	17.534	2452	2456	2463	rBV10	3966	8282	0.39%	0.035%
56	17.639	2471	2474	2475	rBV3	3974	4014	0.19%	0.017%
57	17.828	2496	2506	2514	rBV	29076	44587	2.08%	0.188%
58	17.928	2519	2523	2530	rVV8	19534	32710	1.53%	0.138%
59	18.069	2540	2547	2558	rBV	435657	704992	32.90%	2.970%
60	18.375	2594	2599	2603	rBV8	8546	19158	0.89%	0.081%
61	18.516	2619	2623	2627	rVB7	8966	13118	0.61%	0.055%
62	18.828	2674	2676	2679	rBV3	5370	4802	0.22%	0.020%
63	19.033	2709	2711	2714	rBV4	8496	8772	0.41%	0.037%
64	19.157	2728	2732	2736	rBV3	22966	35141	1.64%	0.148%
65	19.233	2742	2745	2746	rBV3	13602	14843	0.69%	0.063%
66	19.416	2771	2776	2785	rBV	221361	366664	17.11%	1.545%
67	19.569	2800	2802	2803	rBV	10506	7112	0.33%	0.030%
68	19.610	2803	2809	2818	rVV	1369993	2143011	100.00%	9.028%
69	19.692	2821	2823	2827	rVB5	13089	12010	0.56%	0.051%
70	20.216	2910	2912	2914	rBV2	16165	9637	0.45%	0.041%
71	20.263	2918	2920	2921	rBV2	14813	7745	0.36%	0.033%
72	21.286	3090	3094	3105	rVB	209417	348123	16.24%	1.467%
73	21.604	3142	3148	3158	rBV	794422	1346491	62.83%	5.672%
74	23.439	3456	3460	3470	rVB	82649	160267	7.48%	0.675%
75	24.733	3670	3680	3692	rVB	779624	2092011	97.62%	8.813%
76	24.957	3709	3718	3732	rVB2	464929	1445674	67.46%	6.090%

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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-BP050124.MA.M
Title : SVOA CALIBRATION

Sum of corrected areas: 23737851

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Instrument :
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ClientSampleId :
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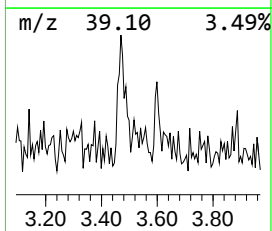
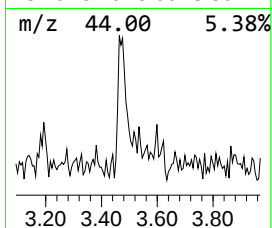
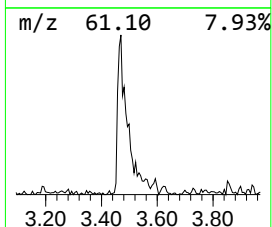
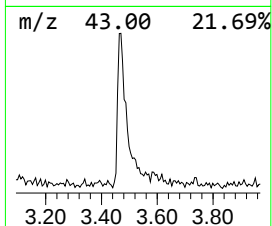
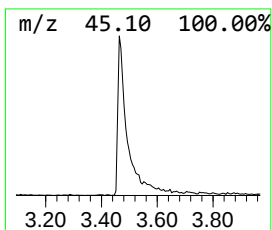
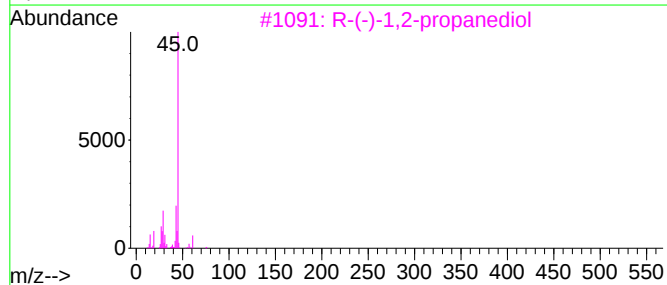
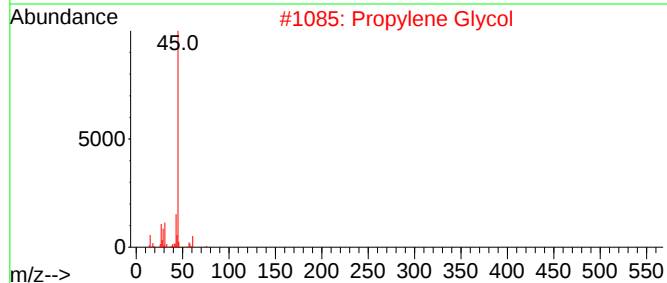
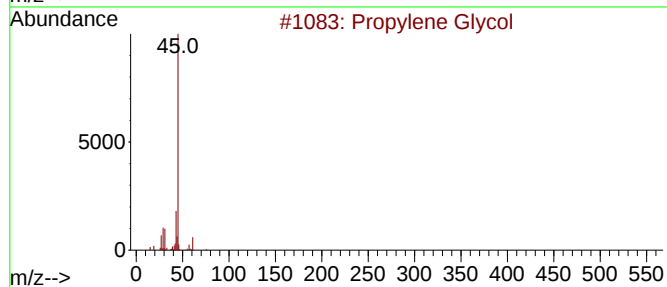
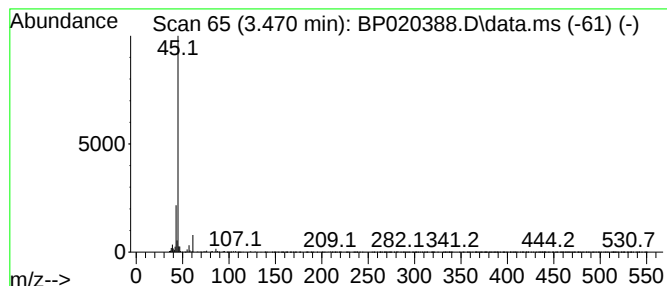
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050124.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.470	2.70 ng/ul	58507	1,4-Dichlorobenzene-d4	7.587

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	80
2			Propylene Glycol	76	C3H8O2	000057-55-6	72
3			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	56
4			Propylene Glycol	76	C3H8O2	000057-55-6	56
5			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	10



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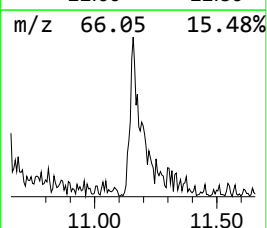
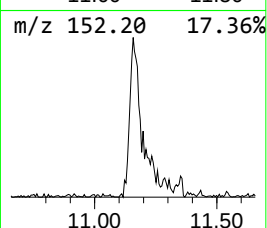
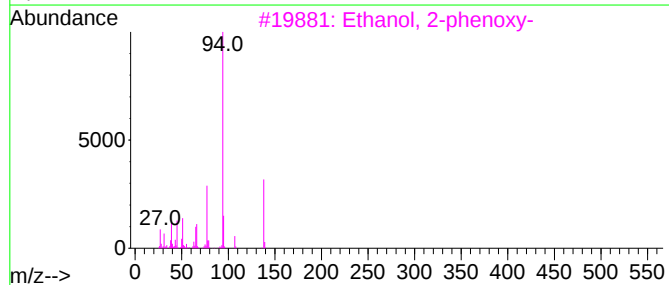
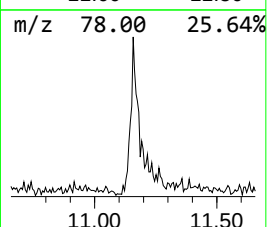
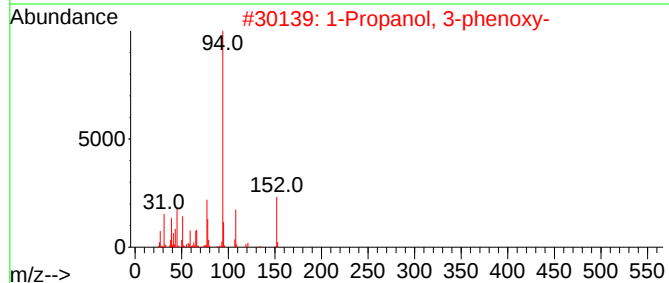
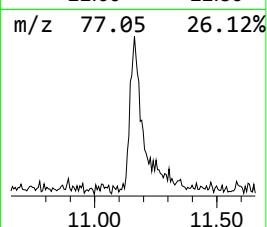
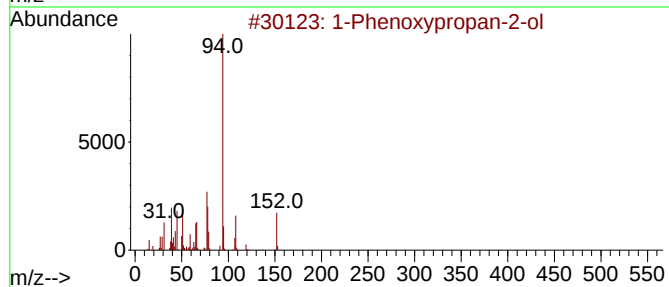
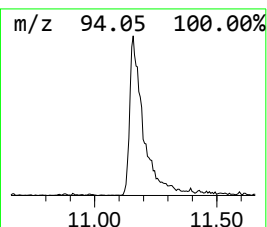
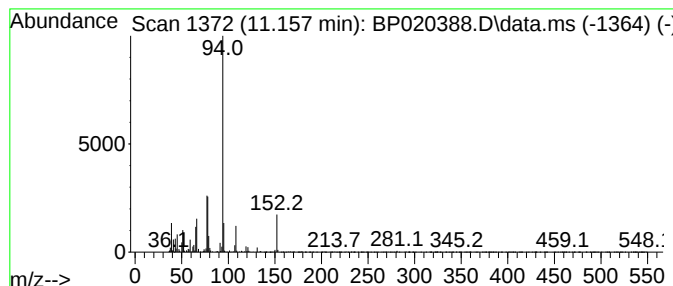
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050124.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.157	3.28 ng/ul	105921	Naphthalene-d8	10.357

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	83
2		1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	72
3		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59
4		1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5		1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	58



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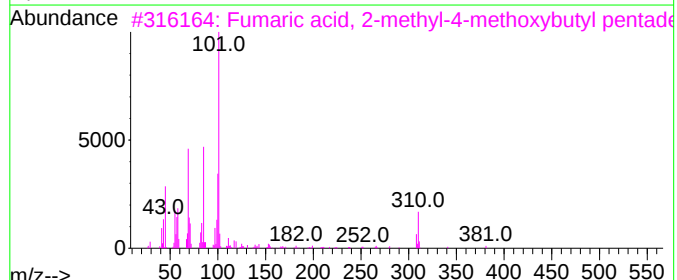
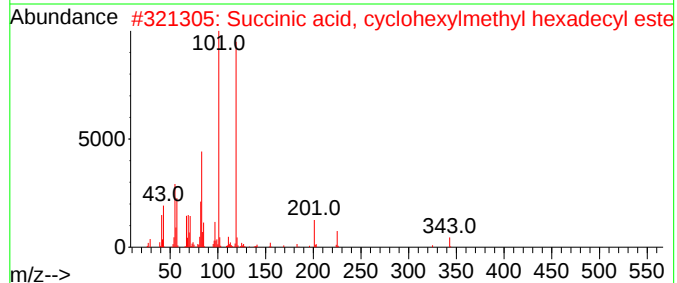
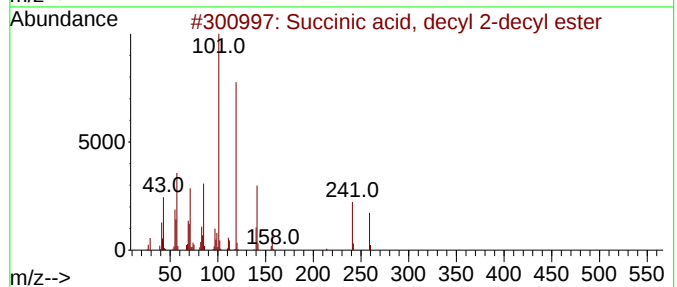
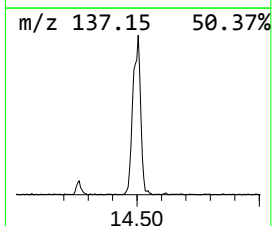
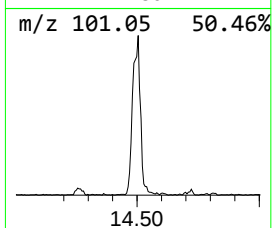
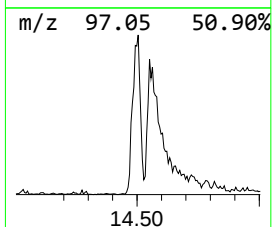
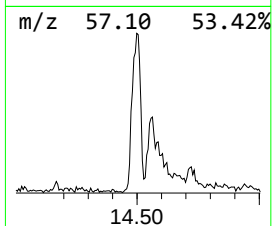
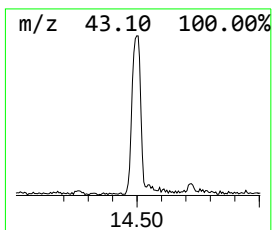
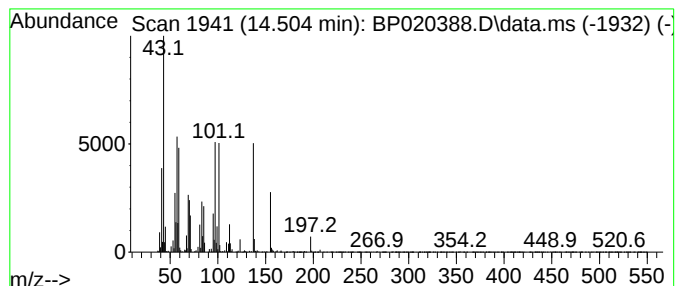
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050124.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.504	3.70 ng/ul	179226	Acenaphthene-d10	14.263

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, decyl 2-decyl ester	398	C24H46O4	1000349-43-0	14
2			Succinic acid, cyclohexylmethyl ...	438	C27H50O4	1000325-83-2	14
3			Fumaric acid, 2-methyl-4-methoxy...	426	C25H46O5	1010339-20-7	14
4			Succinic acid, 2,3,4,6-tetrachlo...	484	C21H28Cl4O4	1000349-68-3	14
5			Butanoic acid, 4-(2,4-dichloroph...	262	C11H12Cl2O3	018625-12-2	14



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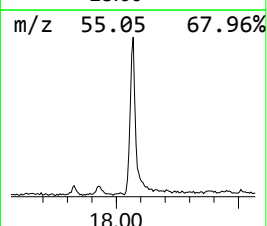
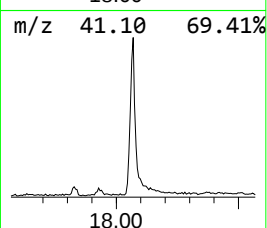
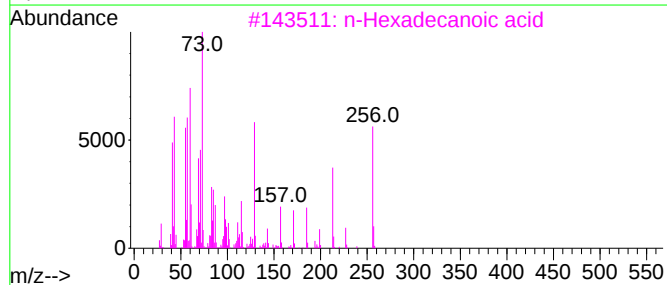
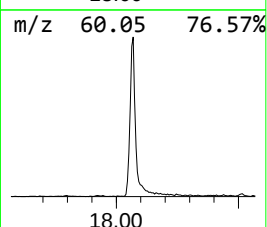
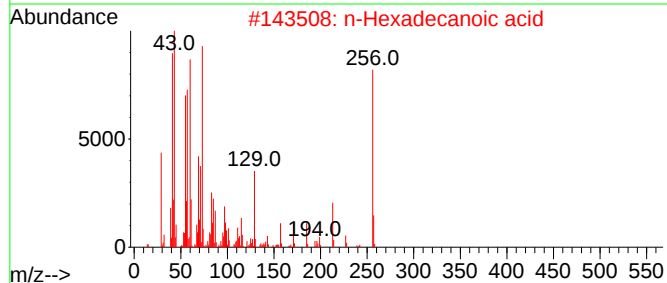
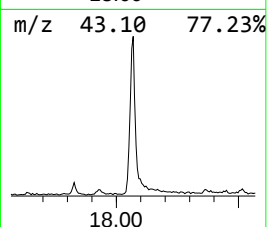
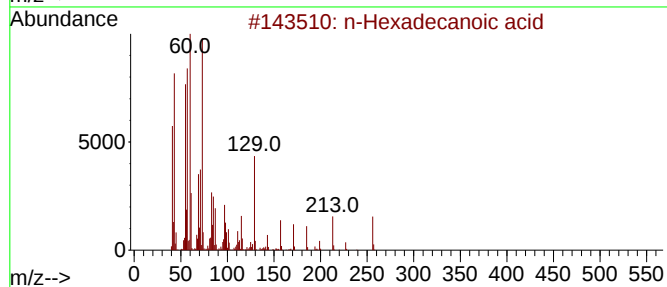
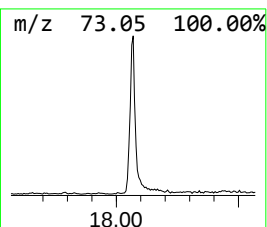
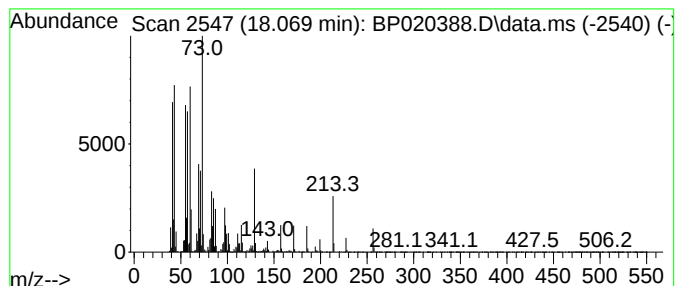
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050124.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.069	11.19 ng/ul	704992	Phenanthrene-d10	17.104

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			Pentadecanoic acid	242	C15H30O2	001002-84-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051424\
Data File : BP020388.D
Acq On : 15 May 2024 06:02
Operator : MA/JU
Sample : P2372-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A43W3

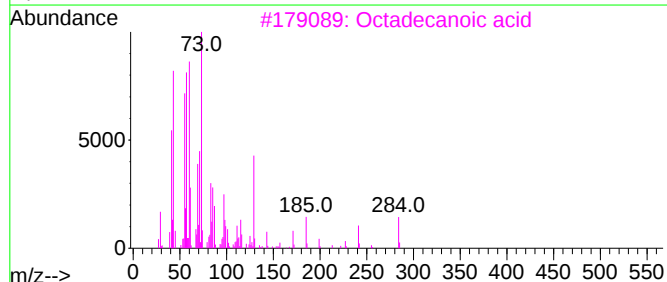
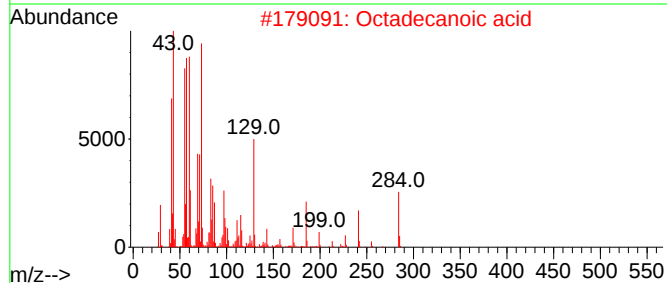
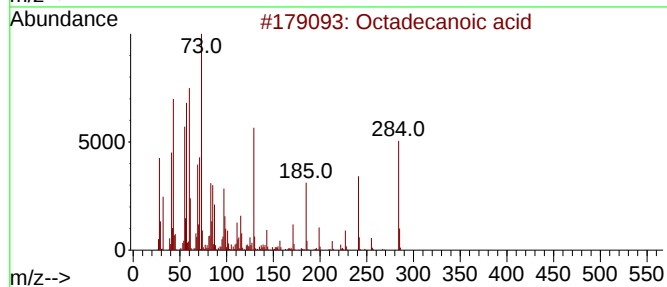
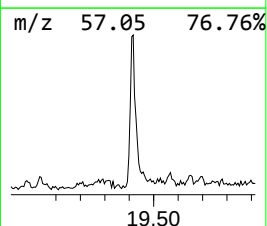
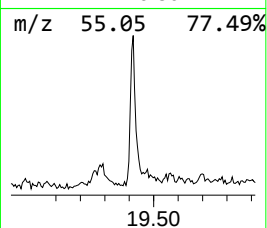
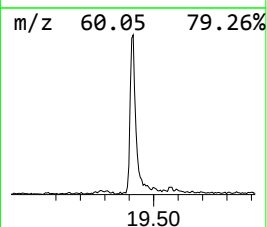
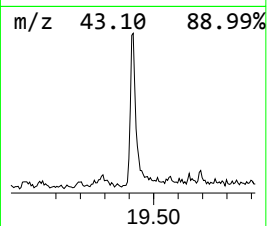
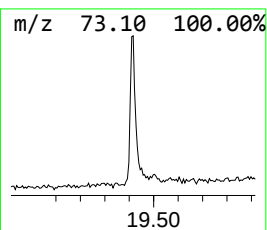
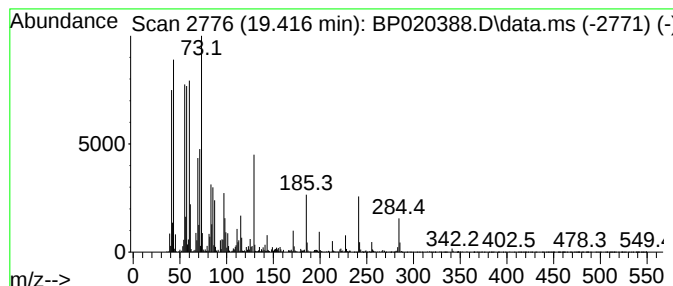
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.416	5.45 ng/ul	366664	Chrysene-d12	21.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	99
3			Octadecanoic acid	284	C18H36O2	000057-11-4	98
4			Octadecanoic acid	284	C18H36O2	000057-11-4	98
5			Octadecanoic acid	284	C18H36O2	000057-11-4	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051424\
Data File : BP020388.D
Acq On : 15 May 2024 06:02
Operator : MA/JU
Sample : P2372-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A43W3

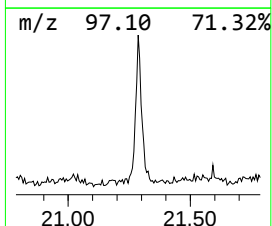
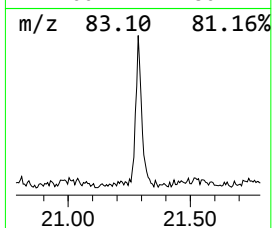
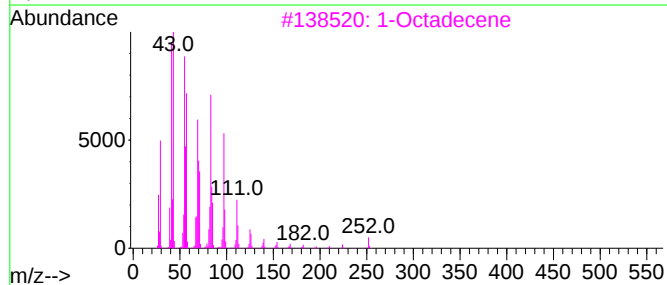
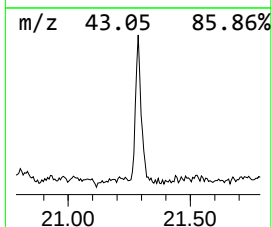
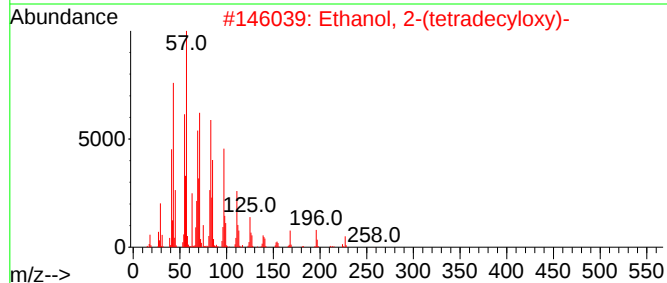
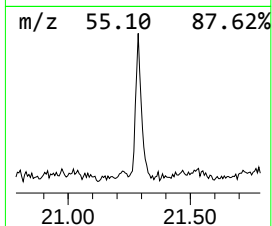
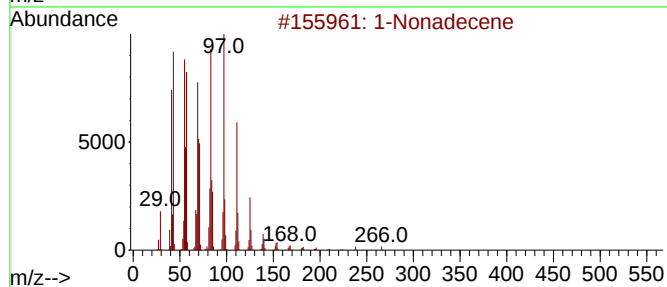
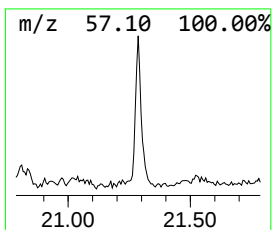
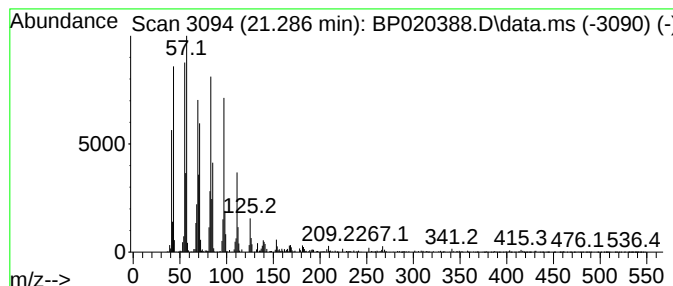
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.286	5.17 ng/ul	348123	Chrysene-d12	21.604

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene		266	C19H38	018435-45-5	98
2	Ethanol, 2-(tetradecyloxy)-		258	C16H34O2	002136-70-1	96
3	1-Octadecene		252	C18H36	000112-88-9	95
4	2- Chloropropionic acid, hexadec...		332	C19H37ClO2	086711-81-1	94
5	2- Chloropropionic acid, hexadec...		332	C19H37ClO2	086711-81-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051424\
Data File : BP020388.D
Acq On : 15 May 2024 06:02
Operator : MA/JU
Sample : P2372-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A43W3

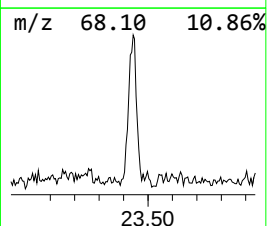
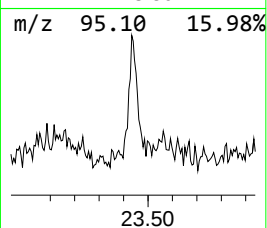
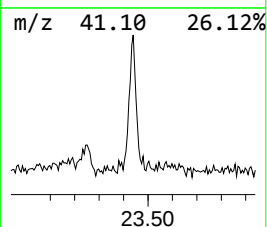
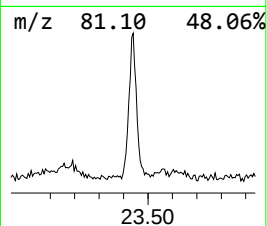
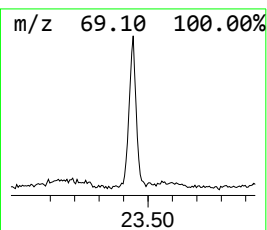
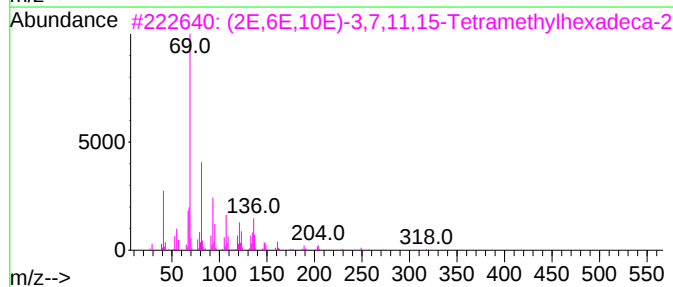
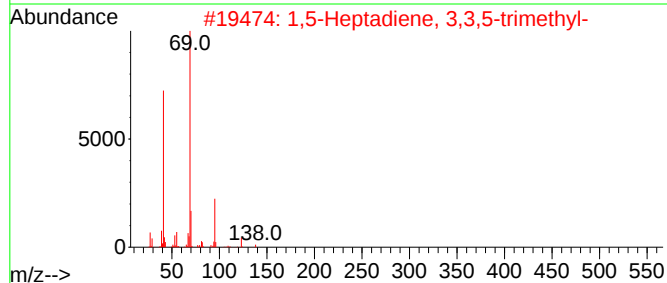
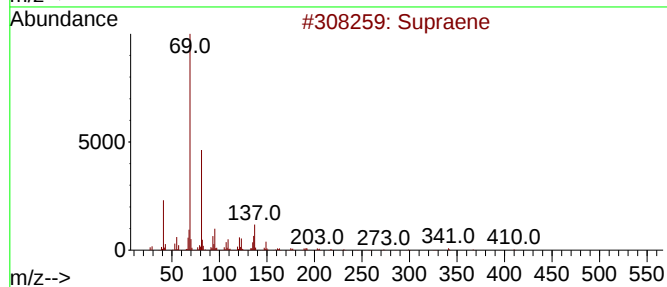
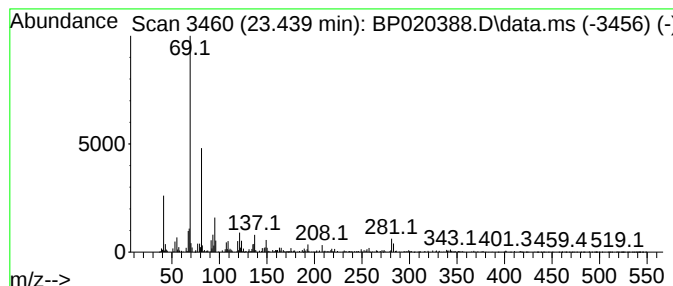
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.439	2.22 ng/ul	160267	Perylene-d12	24.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			1,5-Heptadiene, 3,3,5-trimethyl-	138	C10H18	074630-29-8	64
3			(2E,6E,10E)-3,7,11,15-Tetramethy...	318	C21H34O2	125456-63-5	64
4			1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	59
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051424\
Data File : BP020388.D
Acq On : 15 May 2024 06:02
Operator : MA/JU
Sample : P2372-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A43W3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050124.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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1-Phenoxypropan...	11.157	3.3	ng/ul	105921	2	10.357	646163	20.0
unknown-01	14.504	3.7	ng/ul	179226	3	14.263	967646	20.0
n-Hexadecanoic ...	18.069	11.2	ng/ul	704992	4	17.104	1259530	20.0
Octadecanoic acid	19.416	5.5	ng/ul	366664	5	21.604	1346490	20.0
(DEL) Alkane: S...	21.286	5.2	ng/ul	348123	5	21.604	1346490	20.0
Supraene	23.439	2.2	ng/ul	160267	6	24.951	1445670	20.0