

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080624\
 Data File : BP021431.D
 Acq On : 07 Aug 2024 23:25
 Operator : CG/JU
 Sample : P3437-13
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 E05Y2

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-BP071024.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP021431.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.152	25	28	34	rVB	28338	38452	1.21%	0.112%
2	3.475	80	83	92	rBV	8615	18932	0.60%	0.055%
3	3.599	102	104	113	rBV	53211	106657	3.37%	0.309%
4	3.869	147	150	155	rVB4	8462	12215	0.39%	0.035%
5	4.775	300	304	307	rBV6	2497	3539	0.11%	0.010%
6	5.834	477	484	487	rBV7	2499	5513	0.17%	0.016%
7	6.881	653	662	672	rBV2	49721	184870	5.84%	0.536%
8	6.969	672	677	691	rVB	179839	403737	12.74%	1.171%
9	7.181	703	713	733	rBV	222712	529949	16.73%	1.537%
10	7.604	778	785	806	rBV	466778	910079	28.73%	2.640%
11	8.234	890	892	899	rBV8	2055	4231	0.13%	0.012%
12	8.369	908	915	926	rBV2	157410	469954	14.83%	1.363%
13	8.598	951	954	958	rVB6	3306	4375	0.14%	0.013%
14	8.787	979	986	1007	rBV	189713	463611	14.63%	1.345%
15	8.951	1010	1014	1016	rBV5	3477	4516	0.14%	0.013%
16	9.098	1034	1039	1042	rVB7	3848	6285	0.20%	0.018%
17	9.363	1077	1084	1100	rBV2	19170	59136	1.87%	0.172%
18	9.498	1100	1107	1130	rVV2	131918	366793	11.58%	1.064%
19	10.081	1198	1206	1234	rBV	161299	605414	19.11%	1.756%
20	10.381	1249	1257	1276	rVB	588454	1117580	35.28%	3.242%
21	10.569	1282	1289	1304	rBV	147688	513016	16.19%	1.488%
22	10.822	1328	1332	1335	rBV6	2451	4093	0.13%	0.012%
23	10.981	1355	1359	1367	rBV6	6102	15377	0.49%	0.045%
24	11.175	1385	1392	1413	rBV2	76156	289412	9.14%	0.839%
25	11.992	1527	1531	1535	rVB6	6059	7671	0.24%	0.022%
26	12.845	1670	1676	1684	rBV6	6384	18460	0.58%	0.054%
27	12.963	1694	1696	1703	rVB7	2397	3586	0.11%	0.010%
28	13.033	1703	1708	1713	rBV8	4040	6605	0.21%	0.019%
29	13.110	1718	1721	1723	rBV4	2690	3482	0.11%	0.010%
30	13.675	1807	1817	1826	rBV	559104	1144015	36.11%	3.318%
31	13.945	1851	1863	1875	rBV2	831985	1311157	41.39%	3.803%
32	14.127	1890	1894	1903	rVB2	7784	16665	0.53%	0.048%
33	14.251	1908	1915	1935	rBV	1185782	1903334	60.08%	5.521%
34	14.469	1945	1952	1959	rBV3	50875	120343	3.80%	0.349%
35	14.698	1983	1991	1992	rBV3	37088	60231	1.90%	0.175%
36	15.033	2043	2048	2056	rBV	43611	73376	2.32%	0.213%

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37	15.104	2057	2060	2066	rVB7	9480	16116	0.51%	0.047%
38	15.269	2081	2088	2097	rBV	979633	1737034	54.83%	5.038%
39	15.486	2118	2125	2142	rBV2	163689	453673	14.32%	1.316%
40	15.674	2153	2157	2160	rBV6	7844	11400	0.36%	0.033%
41	15.839	2181	2185	2191	rBV8	9826	22568	0.71%	0.065%
42	15.898	2191	2195	2199	rVV3	14721	18522	0.58%	0.054%
43	15.974	2204	2208	2213	rBV6	12708	21816	0.69%	0.063%
44	16.592	2309	2313	2316	rBV5	8157	12865	0.41%	0.037%
45	16.786	2343	2346	2348	rVB4	7162	6854	0.22%	0.020%
46	16.969	2374	2377	2382	rVB5	21009	26747	0.84%	0.078%
47	17.063	2387	2393	2405	rBV	1387249	2257157	71.25%	6.547%
48	17.169	2405	2411	2423	rVB	1208867	2055071	64.87%	5.961%
49	17.421	2450	2454	2458	rBV7	14421	23256	0.73%	0.067%
50	17.751	2507	2510	2515	rVB	31130	39575	1.25%	0.115%
51	17.986	2545	2550	2570	rBV	579924	999007	31.53%	2.898%
52	18.827	2688	2693	2698	rBV	181265	300689	9.49%	0.872%
53	19.333	2774	2779	2786	rBV2	192433	354357	11.19%	1.028%
54	19.557	2811	2817	2833	rVB	2057922	3008534	94.96%	8.727%
55	21.157	3085	3089	3098	rVB	416257	722974	22.82%	2.097%
56	21.509	3143	3149	3163	rVB2	1848019	2965750	93.61%	8.602%
57	22.698	3348	3351	3358	rVB2	188714	308031	9.72%	0.893%
58	23.203	3431	3437	3450	rBV2	872694	2295032	72.44%	6.657%
59	24.562	3660	3668	3677	rVB2	1067772	2844065	89.77%	8.249%
60	24.780	3697	3705	3723	rVB	1063440	3168078	100.00%	9.189%

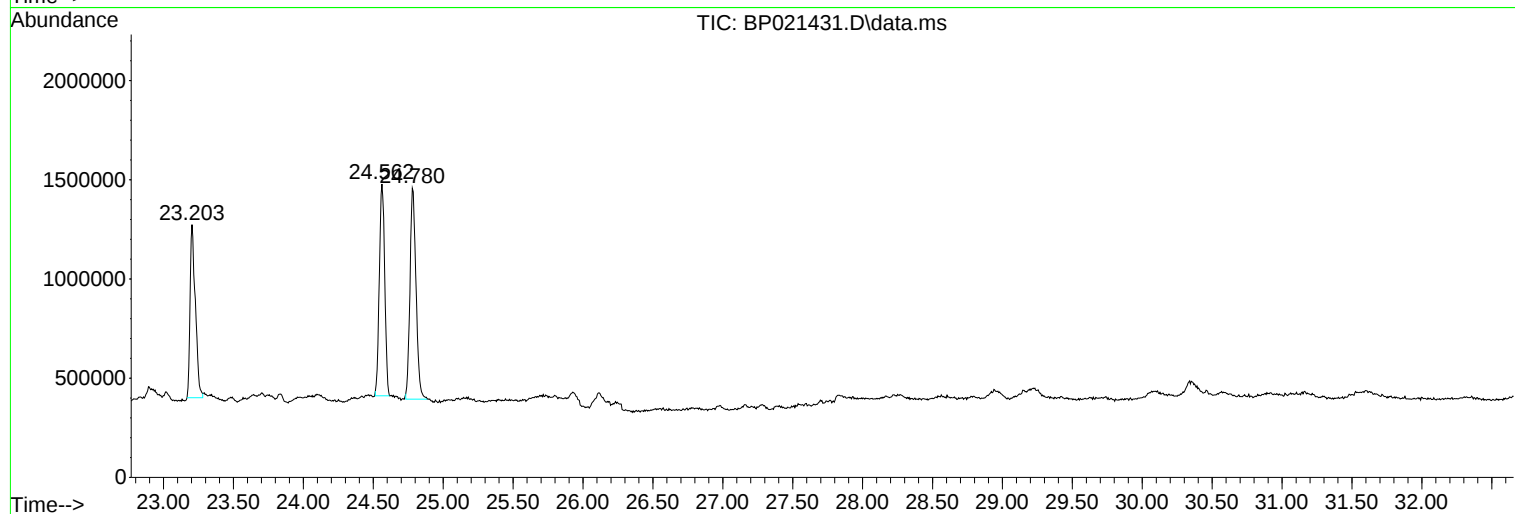
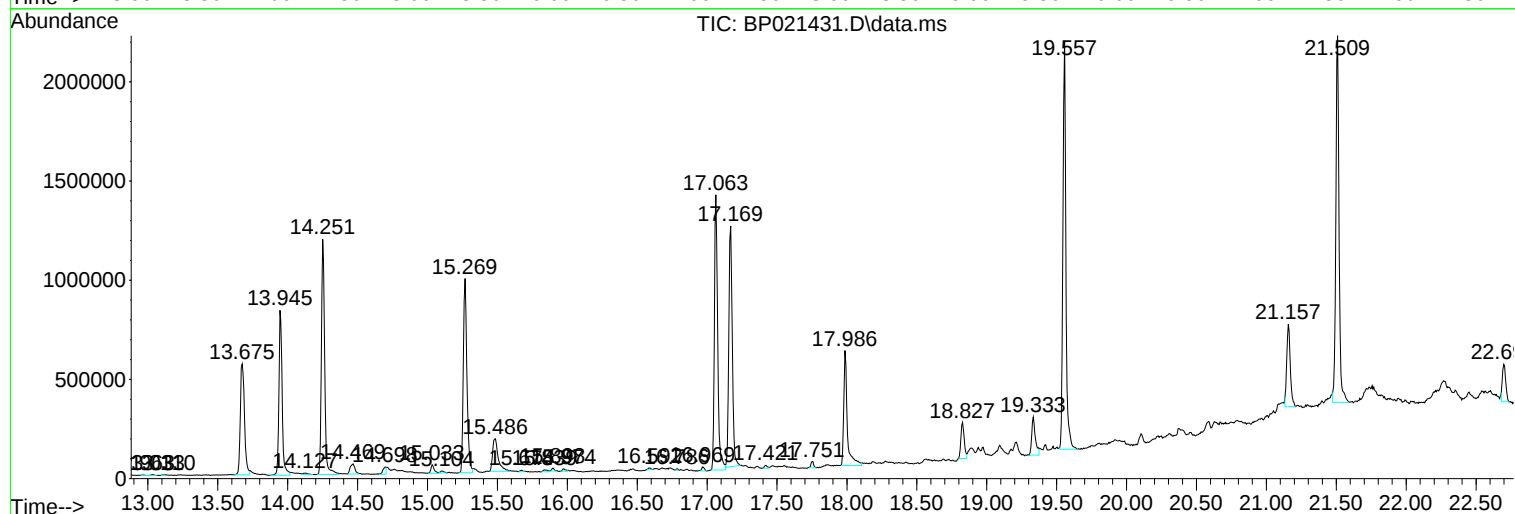
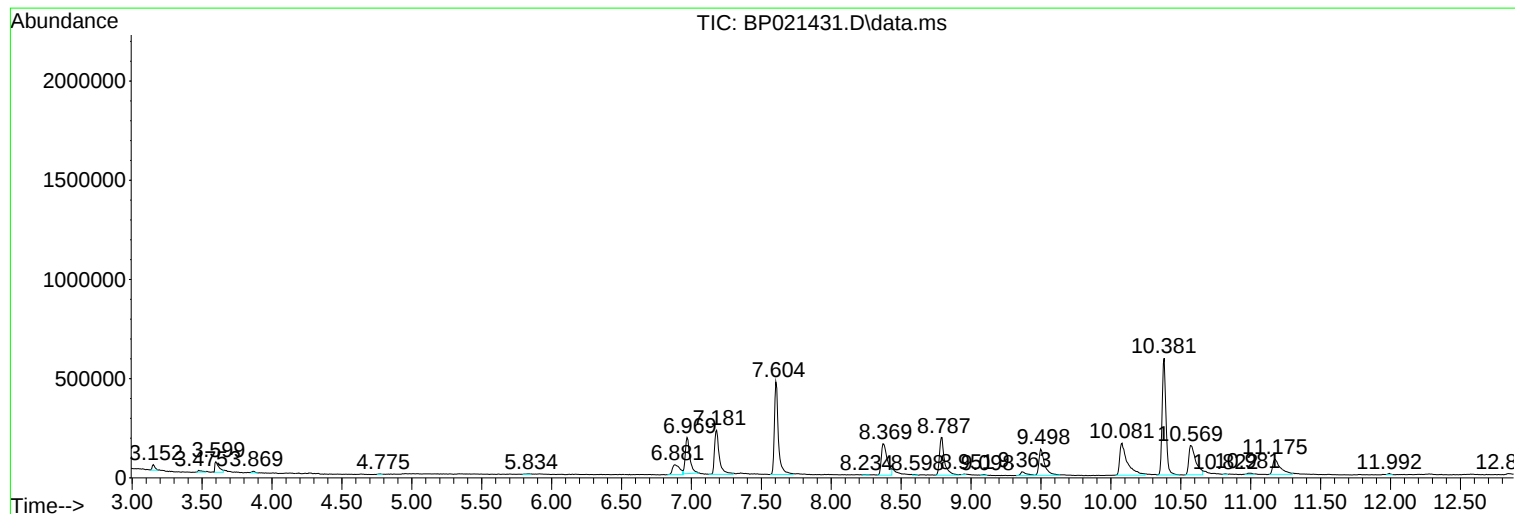
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

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



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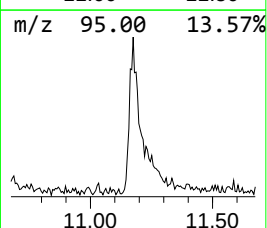
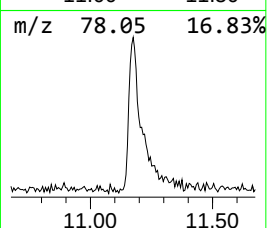
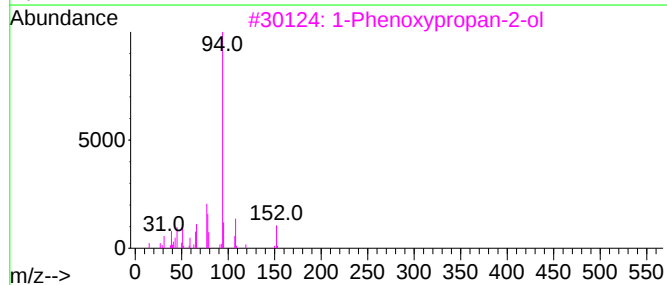
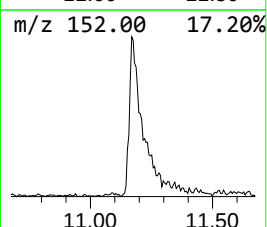
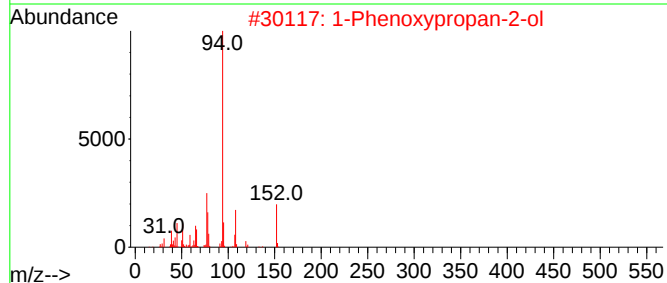
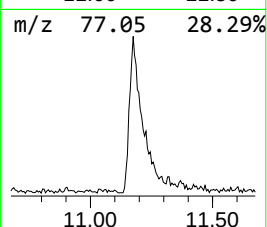
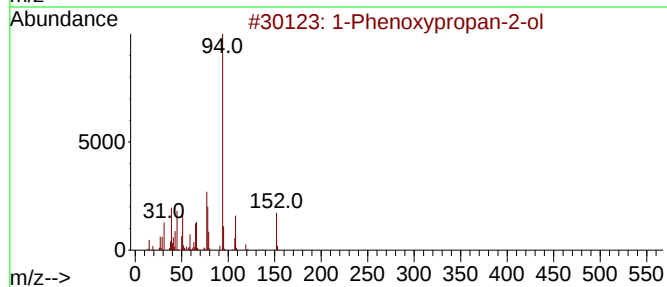
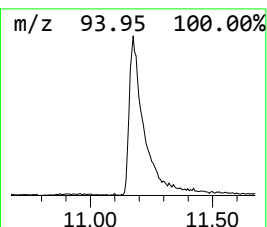
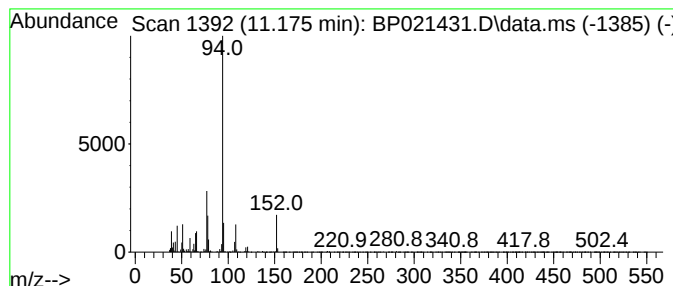
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Quant Title : SVOA CALIBRATION

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

Peak Number 1 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.175	5.18 ng/ul	289412	Naphthalene-d8	10.381

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
3			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
4			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	94
5			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87



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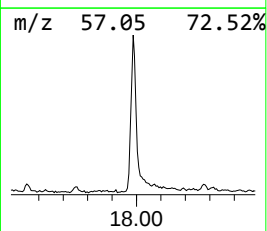
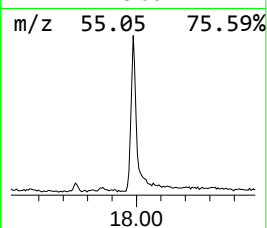
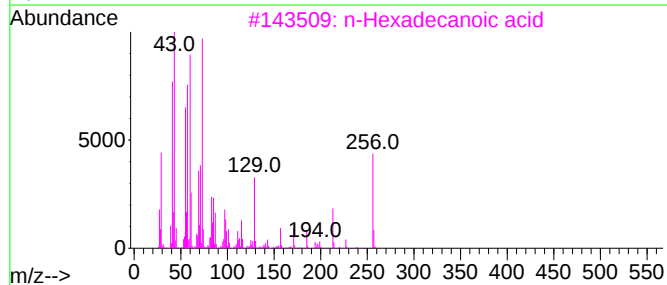
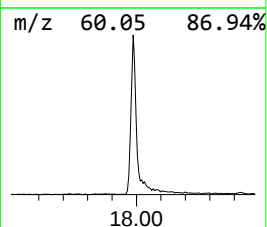
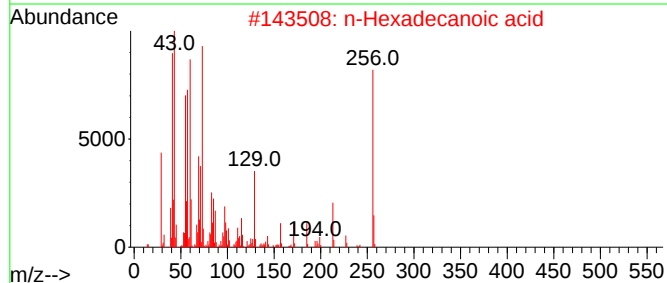
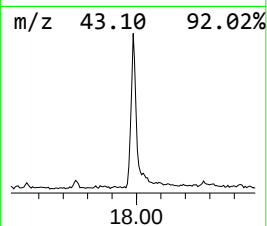
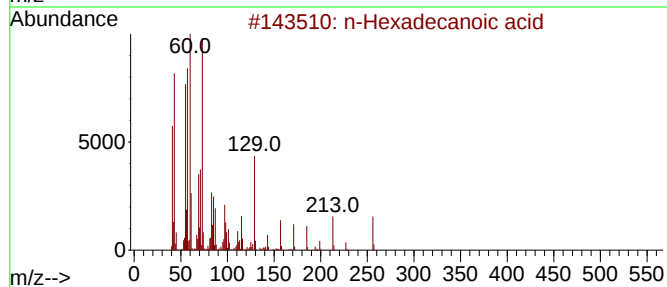
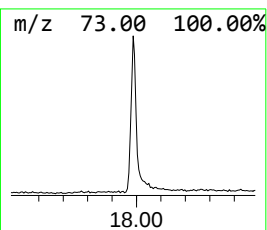
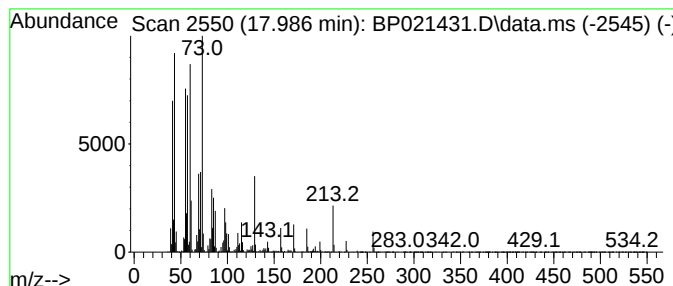
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.986	8.85 ng/ul	999007	Phenanthrene-d10	17.063

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	95
5			Tridecanoic acid	214	C13H26O2	000638-53-9	95



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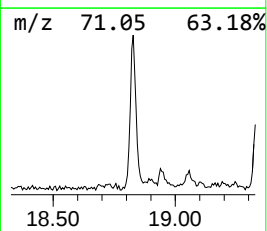
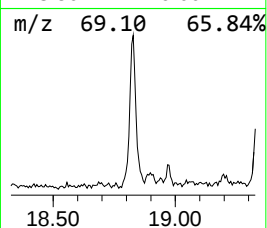
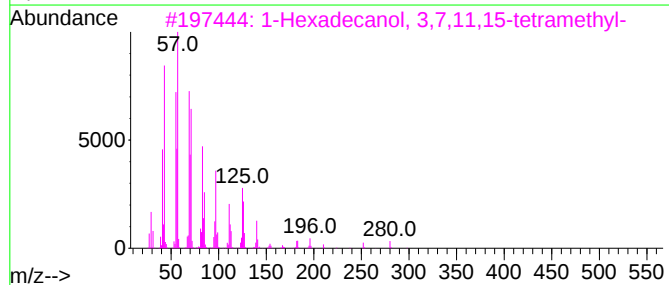
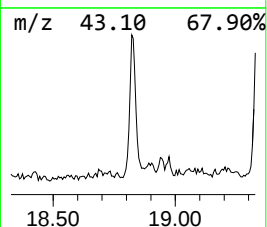
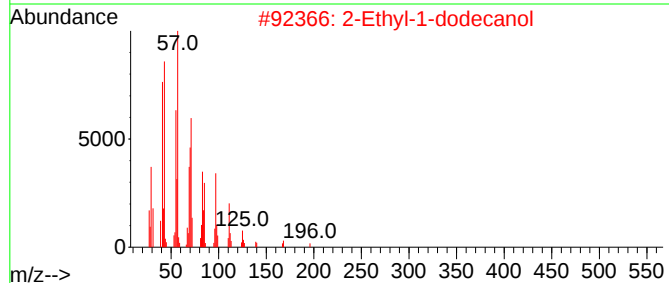
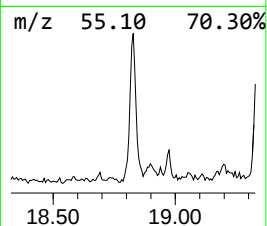
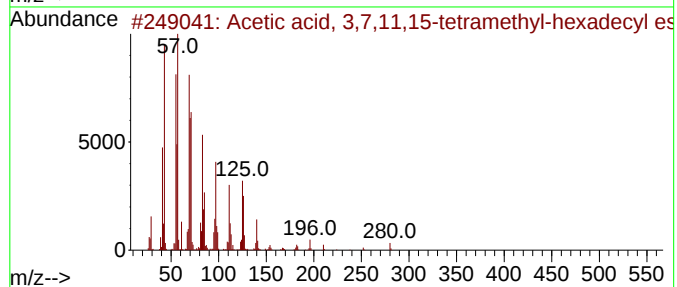
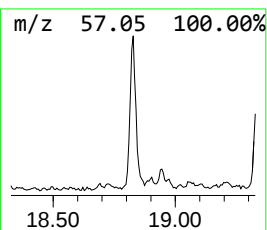
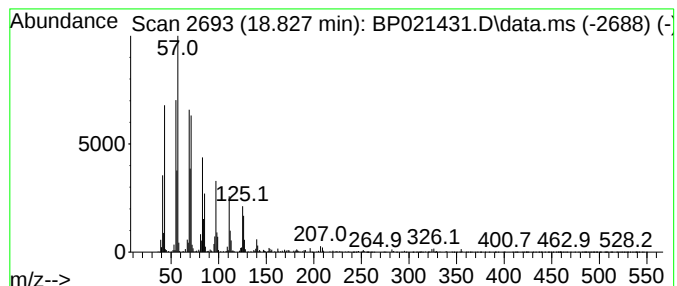
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TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Acetic acid, 3,7,11,15-tetr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.827	2.66 ng/ul	300689	Phenanthrene-d10	17.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 3,7,11,15-tetrameth...	340	C22H44O2	1000193-63-0	91
2			2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	80
3			1-Hexadecanol, 3,7,11,15-tetrame...	298	C20H42O	000645-72-7	74
4			Cyclotetradecane	196	C14H28	000295-17-0	55
5			Ethyl octacosyl ether	438	C30H62O	1010406-37-0	49



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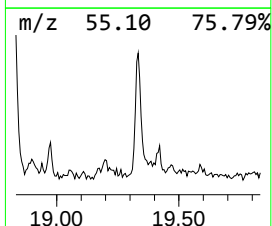
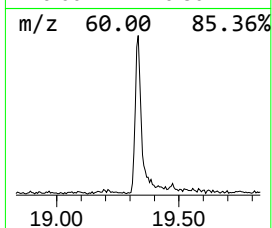
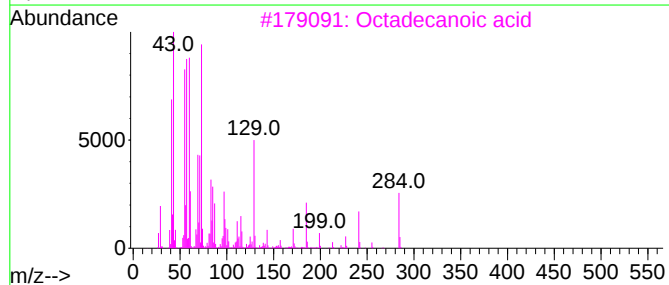
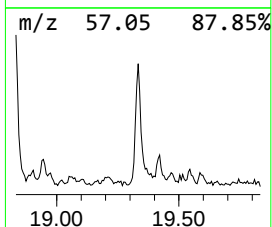
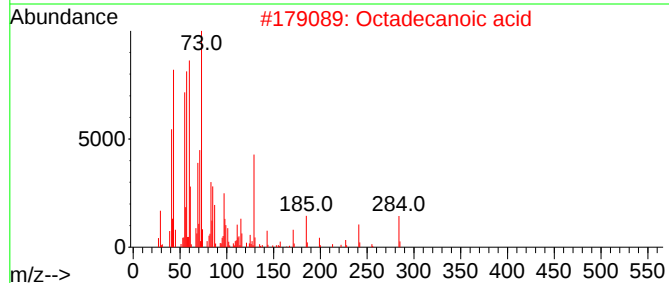
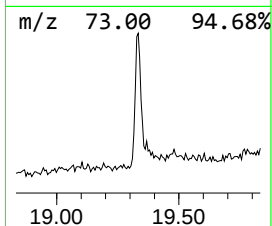
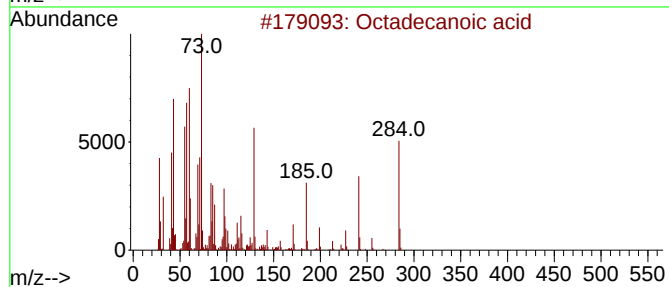
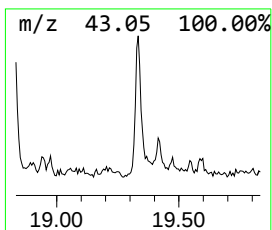
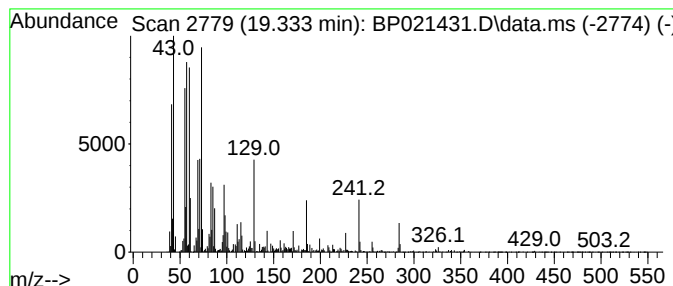
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.333	2.39 ng/ul	354357	Chrysene-d12	21.509

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	99
4			Octadecanoic acid	284	C18H36O2	000057-11-4	97
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93



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ClientSampleId :
E05Y2

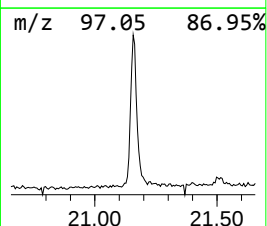
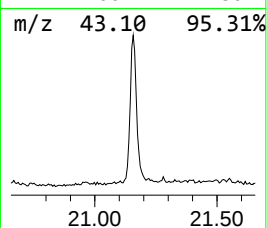
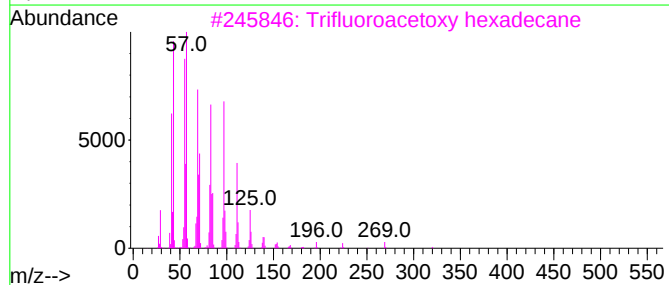
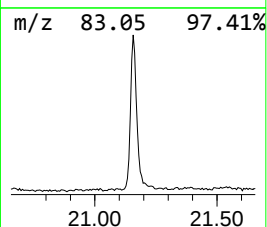
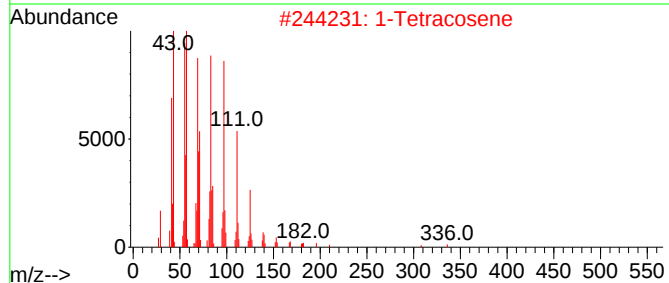
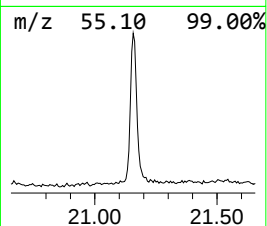
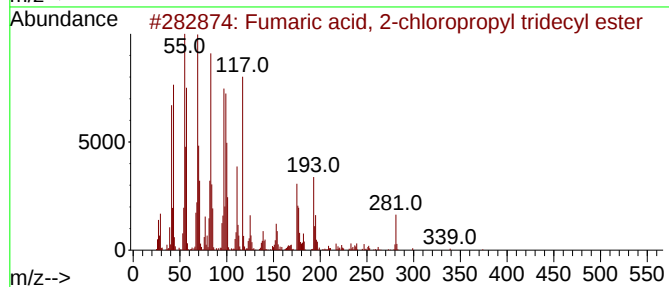
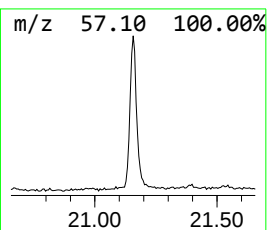
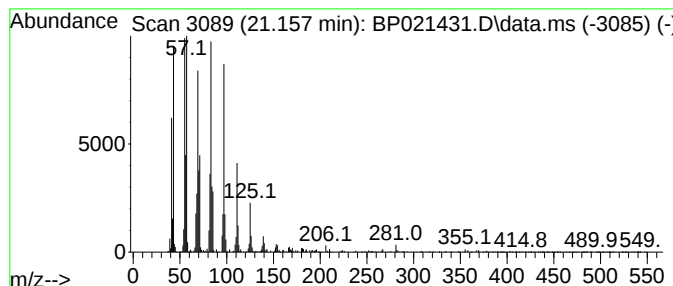
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Fumaric acid, 2-chloropropyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.157	4.88 ng/ul	722974	Chrysene-d12	21.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fumaric acid, 2-chloropropyl tri...	374	C20H35ClO4	1010348-57-1	97
2			1-Tetracosene	336	C24H48	010192-32-2	94
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4			1-Heneicosanol	312	C21H44O	015594-90-8	94
5			Pentacos-1-ene	350	C25H50	016980-85-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080624\
Data File : BP021431.D
Acq On : 07 Aug 2024 23:25
Operator : CG/JU
Sample : P3437-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E05Y2

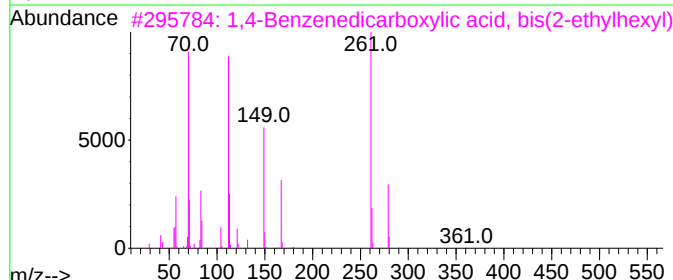
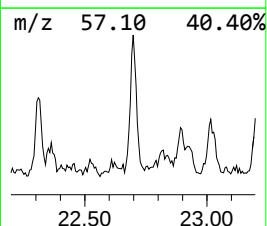
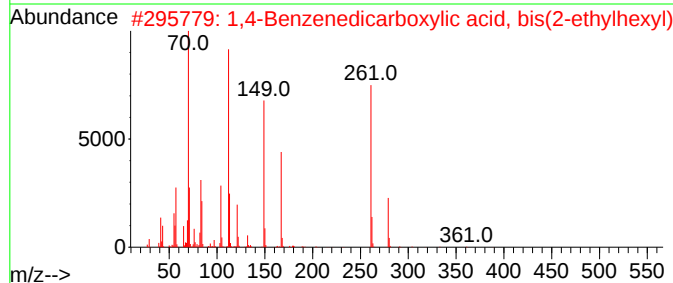
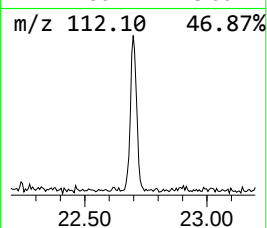
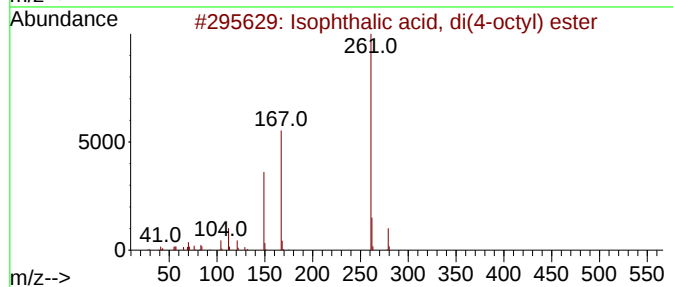
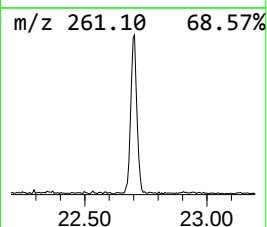
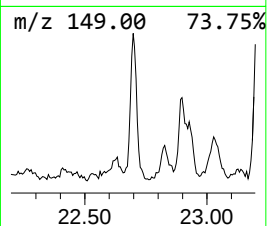
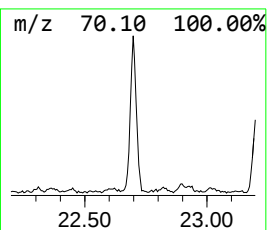
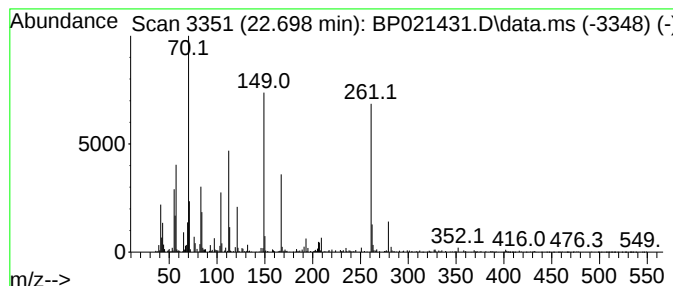
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Isophthalic acid, di(4-octyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.698	2.08 ng/ul	308031	Chrysene-d12	21.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isophthalic acid, di(4-octyl) ester	390	C24H38O4	1000344-04-3	64
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	50
3			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	38
4			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	35
5			Di(Z)-hex-3-enyl phthalate	330	C20H26O4	1000373-65-0	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080624\
Data File : BP021431.D
Acq On : 07 Aug 2024 23:25
Operator : CG/JU
Sample : P3437-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E05Y2

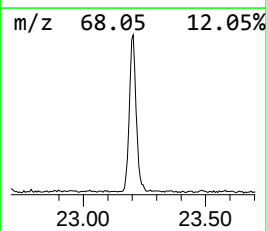
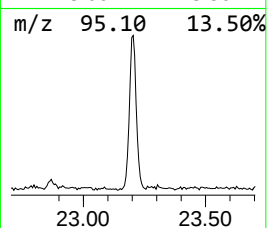
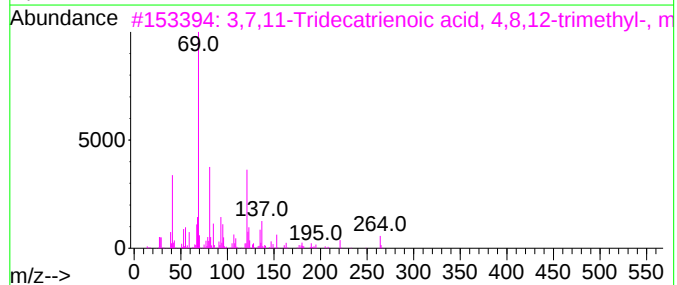
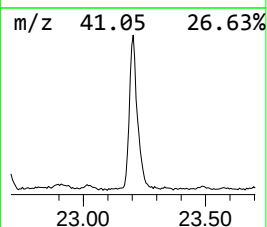
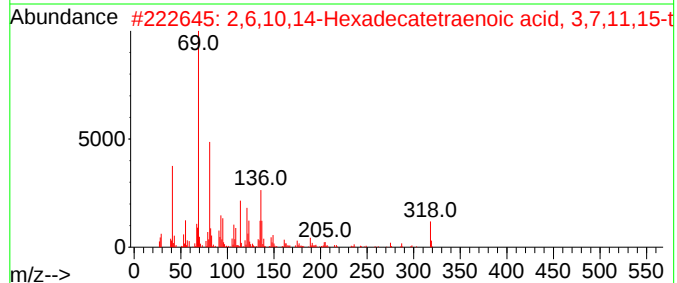
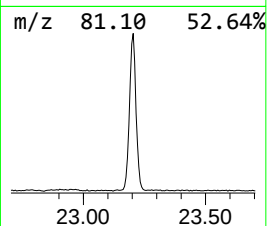
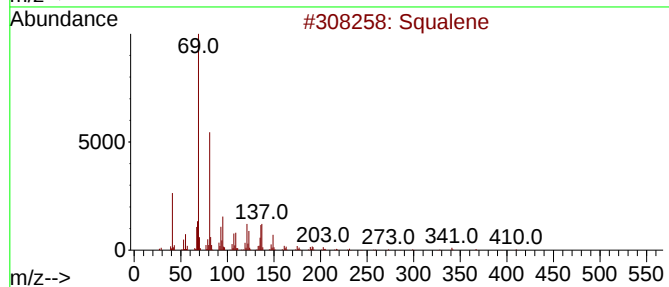
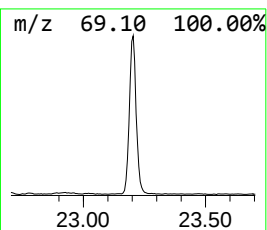
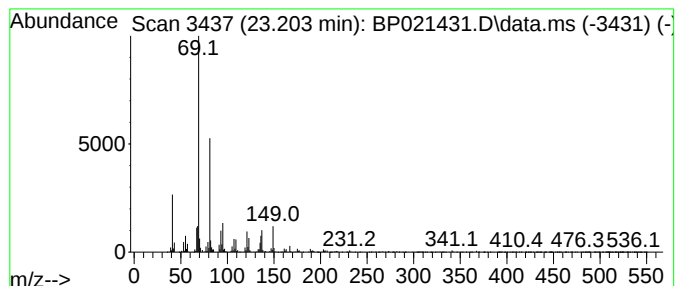
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.203	14.49 ng/ul	2295030	Perylene-d12	24.780

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	86
2			2,6,10,14-Hexadecatetraenoic aci...	318	C21H34O2	042207-88-5	72
3			3,7,11-Tridecatrienoic acid, 4,8...	264	C17H28O2	036237-69-1	64
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080624\
Data File : BP021431.D
Acq On : 07 Aug 2024 23:25
Operator : CG/JU
Sample : P3437-13
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E05Y2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.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
1-Phenoxypropan...	11.175	5.2	ng/ul	289412	2	10.381	1117580	20.0
n-Hexadecanoic ...	17.986	8.8	ng/ul	999007	4	17.063	2257160	20.0
Acetic acid, 3,...	18.827	2.7	ng/ul	300689	4	17.063	2257160	20.0
Octadecanoic acid	19.333	2.4	ng/ul	354357	5	21.509	2965750	20.0
Fumaric acid, 2...	21.157	4.9	ng/ul	722974	5	21.509	2965750	20.0
Isophthalic aci...	22.698	2.1	ng/ul	308031	5	21.509	2965750	20.0
Squalene	23.203	14.5	ng/ul	2295030	6	24.780	3168080	20.0