LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072924\
Data File : BP021218.D
Acq On : 29 Jul 2024 21:29
Operator : MA/JU
Sample : P3280-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
YDZE1

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: BP021218.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.134	21	25	29	rBV	32784	46086	0.88%	0.095%
2	3.176	29	32	37	rVB	40106	49970	0.95%	0.103%
3	3.599	102	104	125	rBV	182703	339363	6.45%	0.703%
4	3.852	143	147	151	rBV7	4083	7480	0.14%	0.015%
5	3.893	151	154	159	rVB3	10641	13693	0.26%	0.028%
6	4.305	221	224	229	rVB2	5133	8230	0.16%	0.017%
7	4.670	282	286	290	rBV7	2860	5482	0.10%	0.011%
8	4.787	303	306	317	rVB	10830	17807	0.34%	0.037%
9	4.981	333	339	348	rVB	15194	30515	0.58%	0.063%
10	6.740	633	638	643	rVB	5491	9606	0.18%	0.020%
11	6.864	652	659	673	rBV	110124	308720	5.87%	0.639%
12	6.987	673	680	698	rVB	543050	914838	17.39%	1.894%
13	7.187	707	714	726	rBV	618374	1073500	20.41%	2.223%
14	7.281	727	730	737	rVB2	16892	28990	0.55%	0.060%
15	7.628	782	789	805	rBV	673479	1228657	23.36%	2.544%
16	7.993	846	851	857	rVB9	4637	10189	0.19%	0.021%
17	8.363	907	914	939	rBV	387171	894009	17.00%	1.851%
18	8.675	965	967	976	rVB10	3281	6008	0.11%	0.012%
19	8.793	980	987	1004	rBV	550916	1135170	21.58%	2.350%
20	9.128	1036	1044	1048	rBV	5810	12838	0.24%	0.027%
21	9.505	1101	1108	1128	rBV	444455	939558	17.86%	1.945%
22	9.763	1150	1152	1158	rVB7	4067	5293	0.10%	0.011%
23	9.834	1158	1164	1170	rBV10	3255	7963	0.15%	0.016%
24	10.057	1195	1202	1228	rBV	533395	1390141	26.43%	2.878%
25	10.257	1233	1236	1240	rVV6	2854	5632	0.11%	0.012%
26	10.405	1254	1261	1269	rBV	898345	1409454	26.79%	2.918%
27	10.563	1280	1288	1312	rBV	375368	980286	18.64%	2.030%
28	10.846	1333	1336	1341	rVB5	13776	19684	0.37%	0.041%
29	11.199	1392	1396	1398	rBV4	7858	11641	0.22%	0.024%
30	11.428	1430	1435	1438	rBV5	9703	17870	0.34%	0.037%
31	11.463	1438	1441	1447	rVB7	8714	11306	0.21%	0.023%
32	11.534	1447	1453	1454	rBV6	4511	8360	0.16%	0.017%
33	11.652	1468	1473	1477	rBV6	14411	26932	0.51%	0.056%
34	11.799	1495	1498	1501	rVB5	6790	6795	0.13%	0.014%
35	11.852	1505	1507	1512	rVB6	8929	11753	0.22%	0.024%
36	11.922	1515	1519	1521	rBV5	5088	7660	0.15%	0.016%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072924\
Data File : BP021218.D
Acq On : 29 Jul 2024 21:29
Operator : MA/JU
Sample : P3280-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
YDZE1

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

37	12.004	1530	1533	1538	rBV6	7162	15103	0.29%	0.031%
38	12.440	1603	1607	1608	rBV4	8327	10450	0.20%	0.022%
39	12.528	1620	1622	1627	rVB6	6198	6233	0.12%	0.013%
40	12.657	1640	1644	1651	rVB8	22204	43283	0.82%	0.090%
41	13.004	1700	1703	1704	rBV2	6351	7200	0.14%	0.015%
42	13.034	1705	1708	1714	rVB5	17835	24990	0.48%	0.052%
43	13.122	1719	1723	1724	rBV2	13480	14947	0.28%	0.031%
44	13.675	1812	1817	1834	rVB	1387142	2087963	39.69%	4.323%
45	13.963	1860	1866	1882	rBV	1622762	2446648	46.51%	5.065%
46	14.275	1913	1919	1929	rVB	1363871	2010780	38.23%	4.163%
47	14.428	1943	1945	1947	rBV3	6929	6853	0.13%	0.014%
48	14.622	1972	1978	1980	rBV3	35192	66589	1.27%	0.138%
49	14.763	1999	2002	2009	rVB	85395	118631	2.26%	0.246%
50	15.051	2048	2051	2059	rVB4	16913	34118	0.65%	0.071%
51	15.287	2084	2091	2103	rBV	1990160	3097103	58.88%	6.412%
52	15.463	2116	2121	2131	rBV	592339	1021921	19.43%	2.116%
53	15.740	2166	2168	2173	rVB	14487	16032	0.30%	0.033%
54	16.045	2215	2220	2230	rVB	240122	297894	5.66%	0.617%
55	16.140	2231	2236	2241	rBV	80688	142849	2.72%	0.296%
56	16.204	2242	2247	2253	rVV3	147992	309045	5.88%	0.640%
57	16.269	2253	2258	2262	rVV2	149390	260217	4.95%	0.539%
58	16.316	2262	2266	2269	rVV	156764	215753	4.10%	0.447%
59	16.357	2269	2273	2276	rVV2	122762	196966	3.74%	0.408%
60	16.387	2276	2278	2279	rVV	96539	93541	1.78%	0.194%
61	16.404	2279	2281	2285	rVV	168322	216985	4.13%	0.449%
62	16.463	2285	2291	2300	rVV4	279929	601663	11.44%	1.246%
63	16.569	2301	2309	2314	rVV3	75829	179741	3.42%	0.372%
64	16.622	2314	2318	2326	rVB	157239	220688	4.20%	0.457%
65	16.692	2326	2330	2337	rBV3	28410	64184	1.22%	0.133%
66	17.087	2391	2397	2406	rBV	1626023	2367239	45.00%	4.901%
67	17.192	2408	2415	2425	rVV2	1993404	3526324	67.04%	7.301%
68	18.016	2550	2555	2565	rVB	144552	254669	4.84%	0.527%
69	18.610	2653	2656	2665	rVB2	48412	91368	1.74%	0.189%
70	19.198	2752	2756	2762	rBV2	72313	111717	2.12%	0.231%
71	19.351	2778	2782	2791	rBV3	69544	125917	2.39%	0.261%
72	19.575	2814	2820	2833	rBV	3084341	4938748	93.89%	10.225%
73	19.710	2840	2843	2854	rVB2	64216	99734	1.90%	0.206%
74	19.822	2858	2862	2869	rVB	100303	137601	2.62%	0.285%
75	20.251	2931	2935	2941	rBV	351558	424809	8.08%	0.879%
76	21.533	3148	3153	3163	rBV	1772602	2878495	54.72%	5.959%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072924\
Data File : BP021218.D
Acq On : 29 Jul 2024 21:29
Operator : MA/JU
Sample : P3280-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
YDZE1

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

77	24.604	3666	3675	3698	rVB	1919513	5260147	100.00%	10.890%
78	24.839	3705	3715	3727	rVB2	988308	3254714	61.87%	6.738%

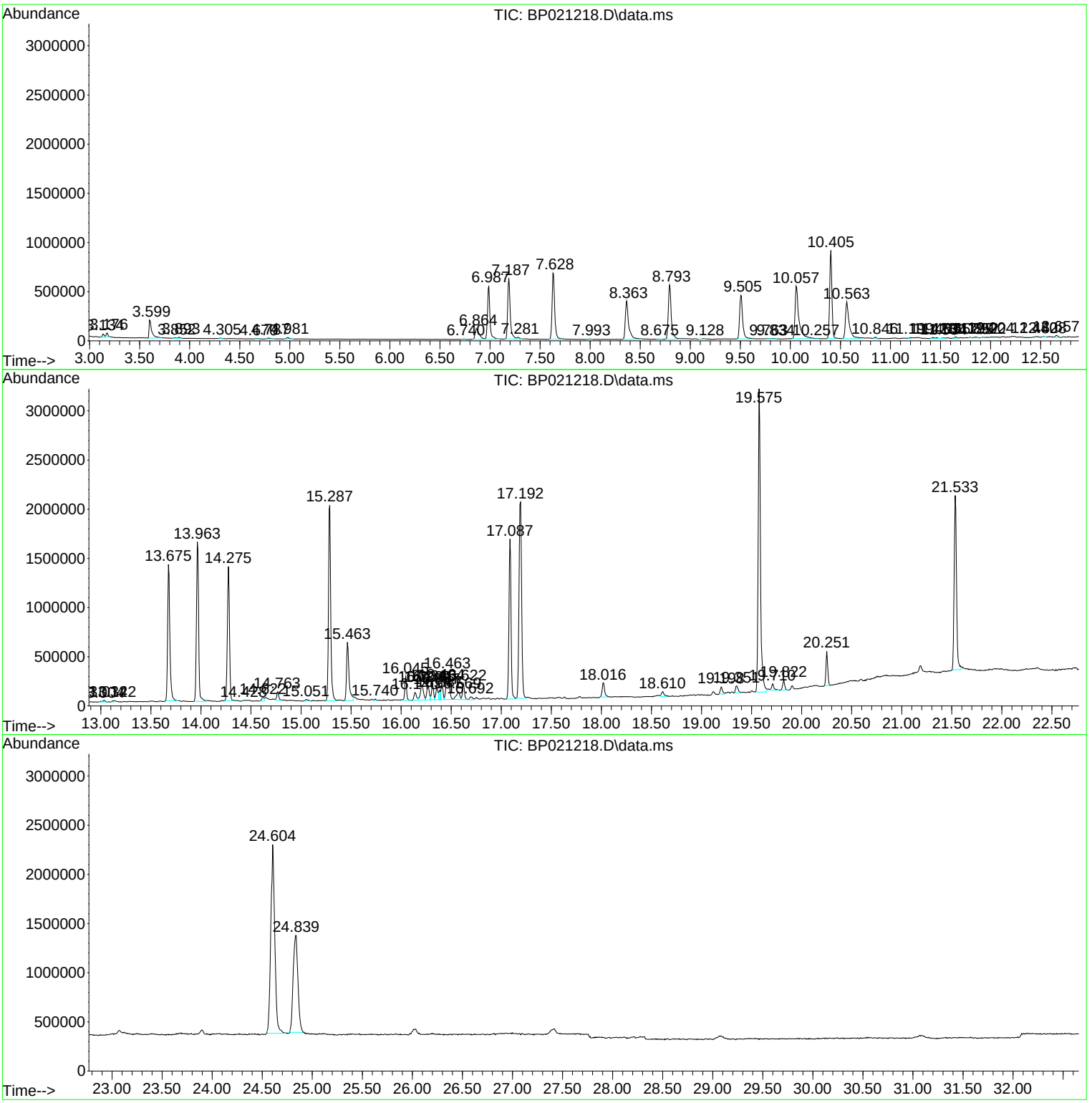
Sum of corrected areas: 48301331

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072924\
Data File : BP021218.D
Acq On : 29 Jul 2024 21:29
Operator : MA/JU
Sample : P3280-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
YDZE1

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072924\
Data File : BP021218.D
Acq On : 29 Jul 2024 21:29
Operator : MA/JU
Sample : P3280-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
YDZE1

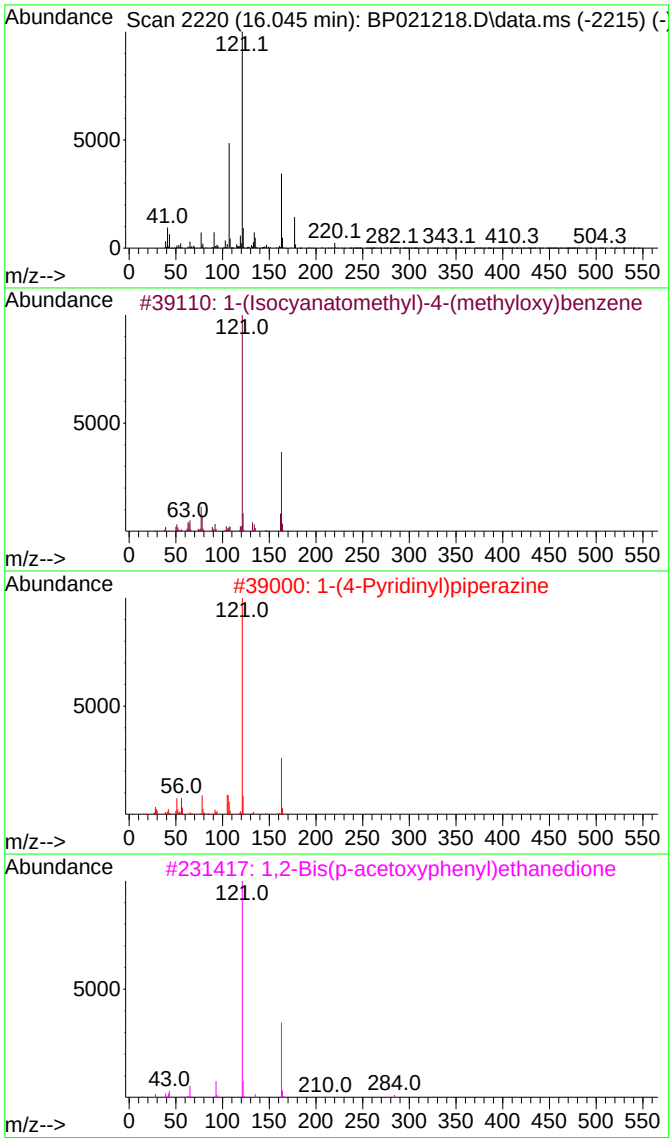
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

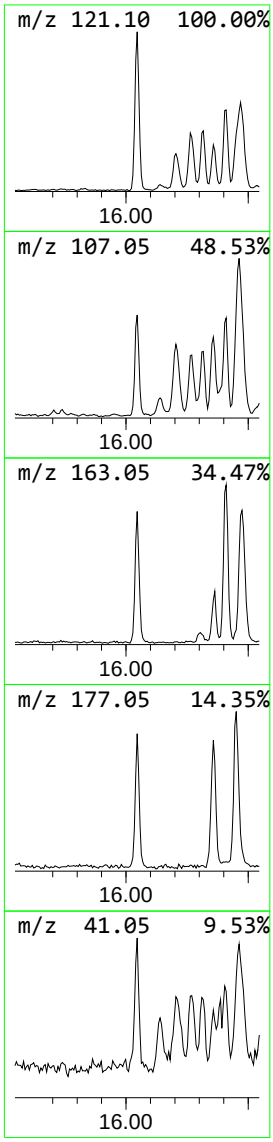
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-(Isocyanatomethyl)-4-(met... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.045	2.52 ng/ul	297894	Phenanthrene-d10	17.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(Isocyanatomethyl)-4-(methylox...	163	C9H9NO2	056651-60-6	50
2	1-(4-Pyridinyl)piperazine	163	C9H13N3	001008-91-9	50
3	1,2-Bis(p-acetoxyphenyl)ethanedione	326	C18H14O6	093655-79-9	50
4	2-Acetamidotropone	163	C9H9NO2	006422-12-4	47
5	N-Allyl-p-hydroxybenzamide	177	C10H11NO2	090921-72-5	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072924\
Data File : BP021218.D
Acq On : 29 Jul 2024 21:29
Operator : MA/JU
Sample : P3280-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
YDZE1

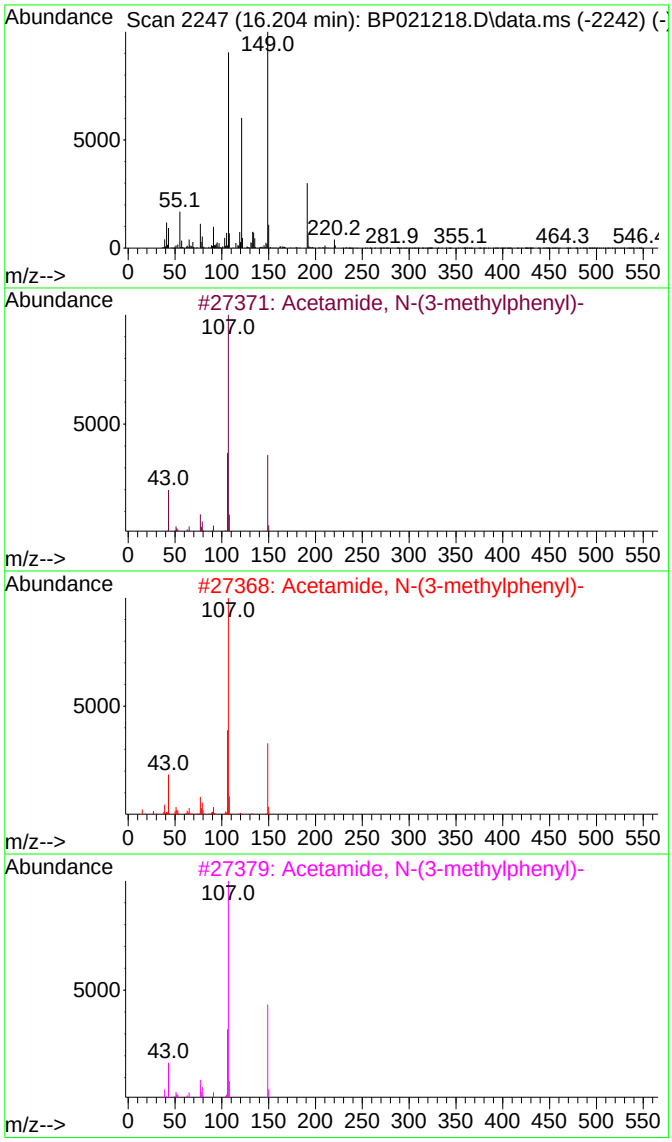
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

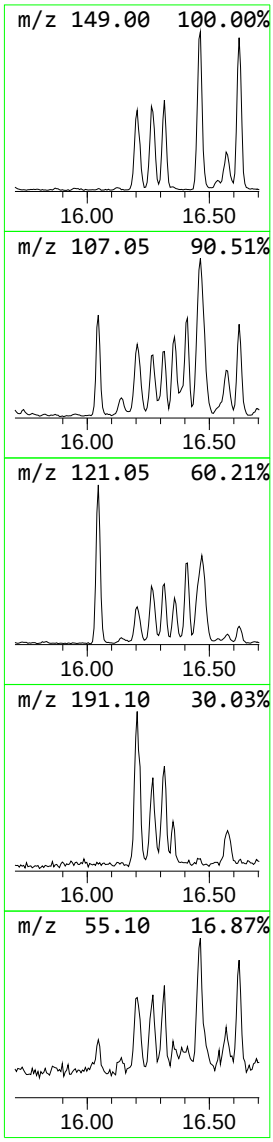
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Acetamide, N-(3-methylphenyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.204	2.61 ng/ul	309045	Phenanthrene-d10	17.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	68
2	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	64
3	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	64
4	5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	59
5	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	000103-89-9	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072924\
Data File : BP021218.D
Acq On : 29 Jul 2024 21:29
Operator : MA/JU
Sample : P3280-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
YDZE1

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

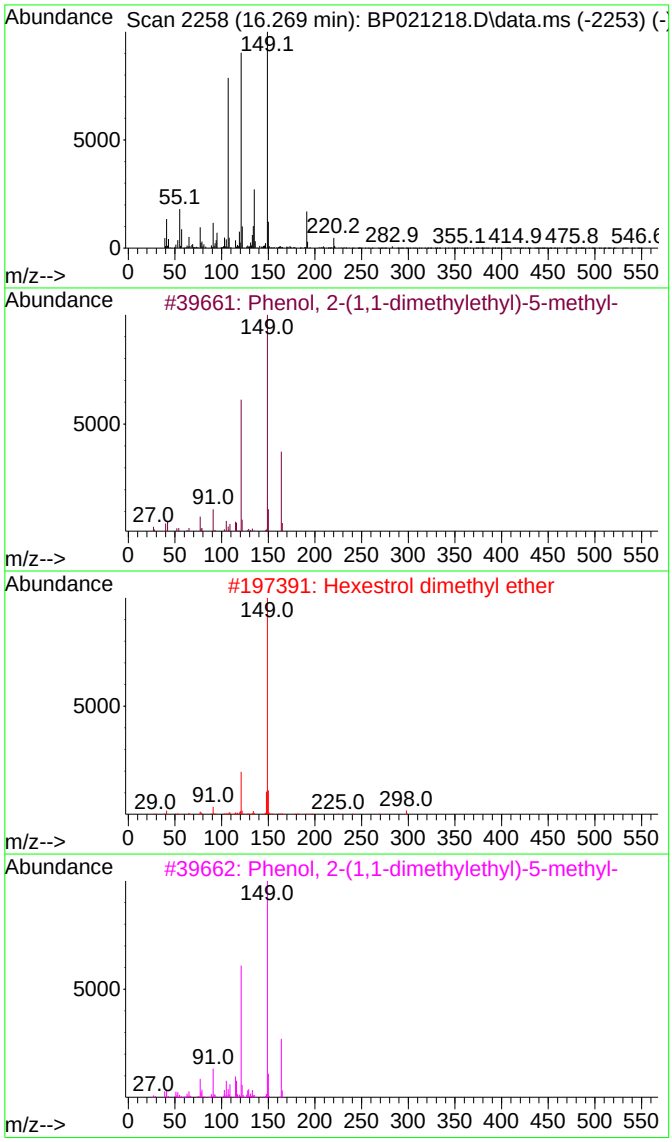
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

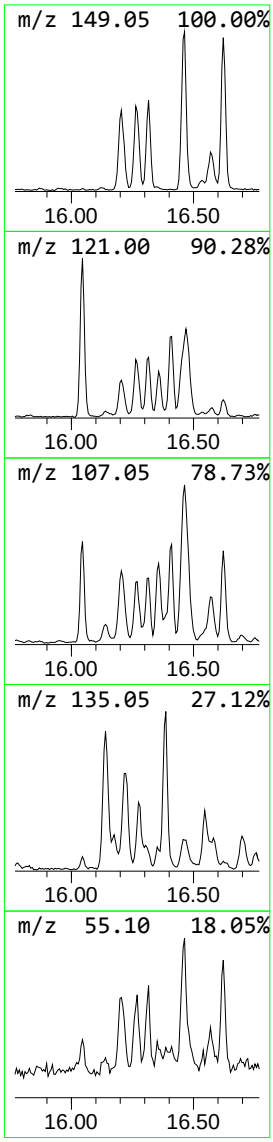
****

Peak Number 3 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.269	2.20 ng/ul	260217	Phenanthrene-d10	17.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(1,1-dimethylethyl)-5-...	164	C11H16O	000088-60-8	47
2	Hexestrol dimethyl ether	298	C20H26O2	000130-78-9	47
3	Phenol, 2-(1,1-dimethylethyl)-5-...	164	C11H16O	000088-60-8	47
4	Phenol, 2-(1,1-dimethylethyl)-5-...	164	C11H16O	000088-60-8	47
5	Phthalic acid, 3-methylphenyl pr...	298	C18H18O4	1000315-36-6	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072924\
Data File : BP021218.D
Acq On : 29 Jul 2024 21:29
Operator : MA/JU
Sample : P3280-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
YDZE1

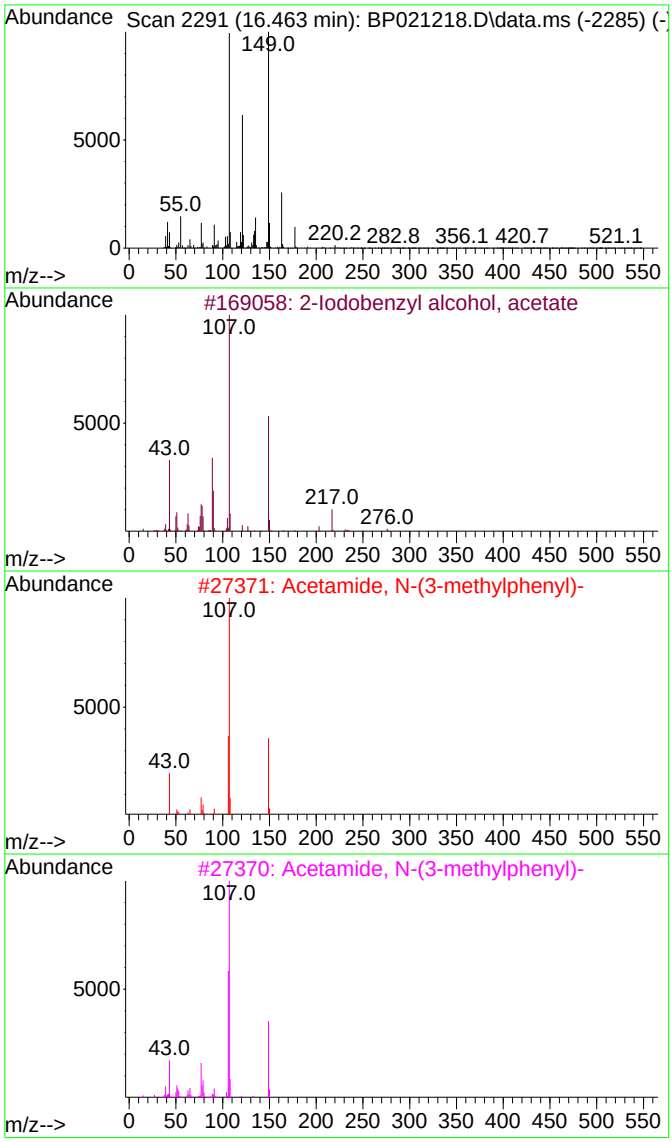
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

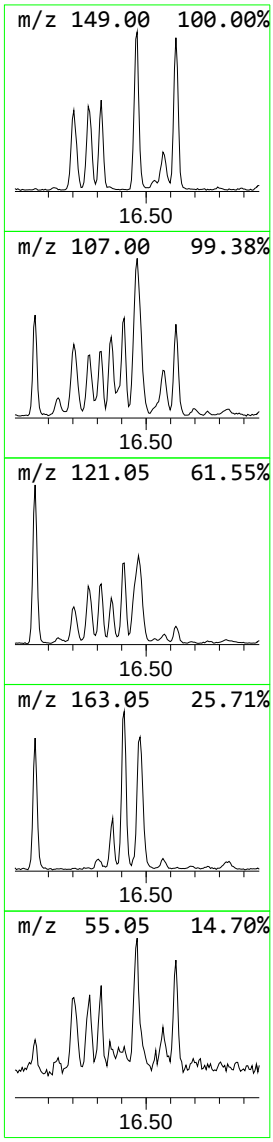
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Iodobenzyl alcohol, acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.463	5.08 ng/ul	601663	Phenanthrene-d10	17.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Iodobenzyl alcohol, acetate	276	C9H9IO2	1000364-47-1	59
2	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	46
3	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	43
4	Phenol, 2-(1,1-dimethylethyl)-3-...	164	C11H16O	013037-79-1	38
5	5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072924\
Data File : BP021218.D
Acq On : 29 Jul 2024 21:29
Operator : MA/JU
Sample : P3280-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
YDZE1

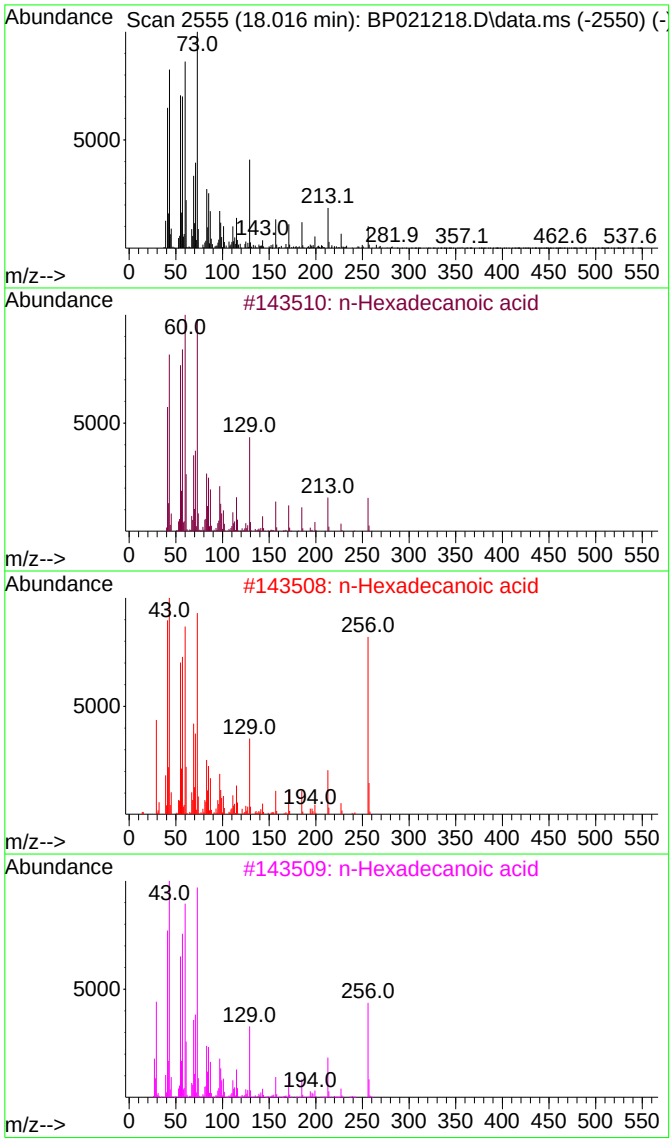
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

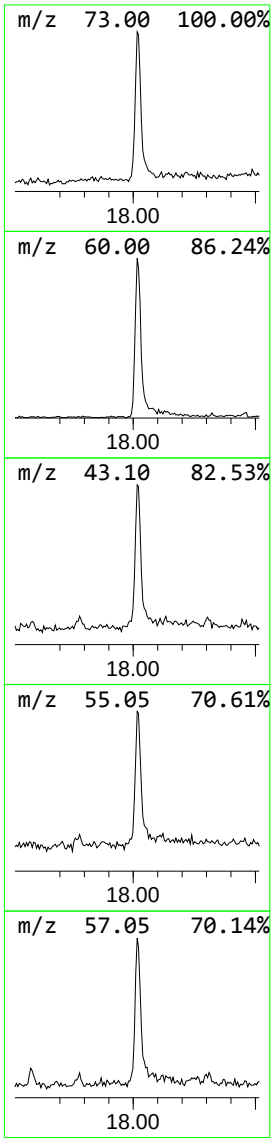
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.016	2.15 ng/ul	254669	Phenanthrene-d10	17.087

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	93
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072924\
Data File : BP021218.D
Acq On : 29 Jul 2024 21:29
Operator : MA/JU
Sample : P3280-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
YDZE1

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

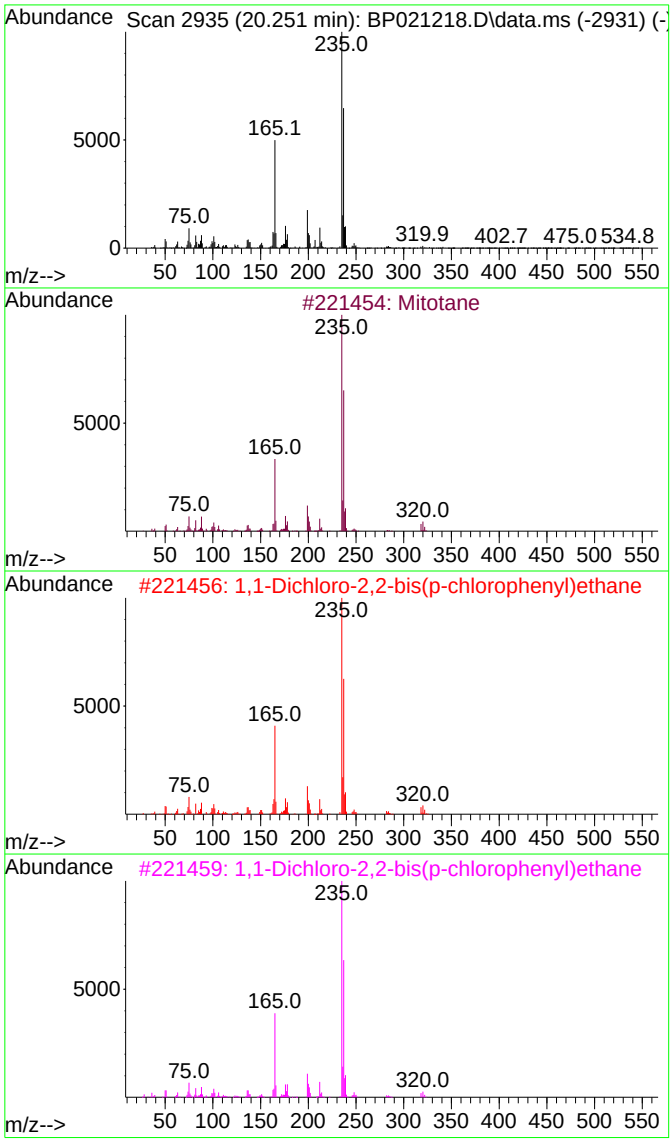
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

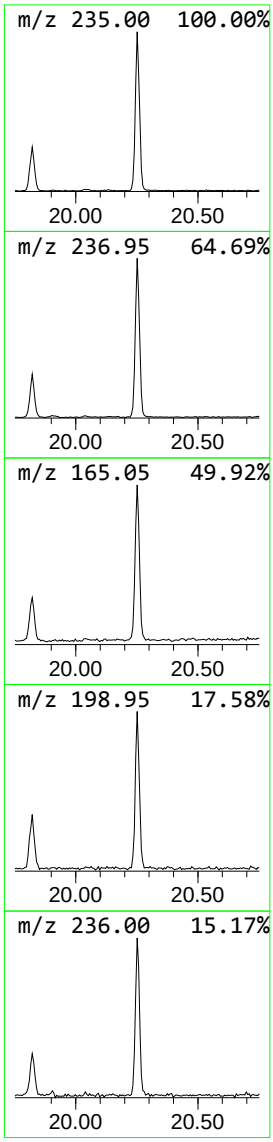
****

Peak Number 6 Mitotane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.251	2.95 ng/ul	424809	Chrysene-d12	21.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mitotane	318	C14H10Cl4	000053-19-0	99
2	1,1-Dichloro-2,2-bis(p-chlorophe...	318	C14H10Cl4	000072-54-8	99
3	1,1-Dichloro-2,2-bis(p-chlorophe...	318	C14H10Cl4	000072-54-8	91
4	m,p'-DDD	318	C14H10Cl4	004329-12-8	90
5	3-Butanone, 1,1-bis(4-chlorophen...	320	C18H18Cl2O	1000158-20-4	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072924\
Data File : BP021218.D
Acq On : 29 Jul 2024 21:29
Operator : MA/JU
Sample : P3280-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
YDZE1

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-(Isocyanatome...	16.045	2.5	ng/ul	297894	4	17.087	2367240	20.0
Acetamide, N-(3...	16.204	2.6	ng/ul	309045	4	17.087	2367240	20.0
unknown-01	16.269	2.2	ng/ul	260217	4	17.087	2367240	20.0
2-Iodobenzyl al...	16.463	5.1	ng/ul	601663	4	17.087	2367240	20.0
n-Hexadecanoic ...	18.016	2.1	ng/ul	254669	4	17.087	2367240	20.0
Mitotane	20.251	3.0	ng/ul	424809	5	21.533	2878500	20.0