LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100424\
Data File : BN034420.D
Acq On : 05 Oct 2024 12:22
Operator : RC/JU
Sample : P4227-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PMW-1(20240925)

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_N\Methods\SFAM-EPA-BN091124.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BN034420.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.999	16	19	30	rVB	47962	82119	0.67%	0.128%
2	3.693	133	137	143	rVB2	12821	20369	0.17%	0.032%
3	4.446	261	265	272	rBV5	10557	16651	0.14%	0.026%
4	4.564	281	285	290	rBV	10501	15329	0.13%	0.024%
5	5.681	468	475	481	rVB2	23488	35586	0.29%	0.055%
6	5.828	495	500	508	rBV	29860	47531	0.39%	0.074%
7	6.581	618	628	642	rBV	377767	625254	5.11%	0.974%
8	6.734	648	654	664	rBV	732750	1137517	9.29%	1.772%
9	6.916	679	685	695	rBV	944562	1493427	12.19%	2.327%
10	7.375	757	763	771	rBV	817081	1294676	10.57%	2.017%
11	7.740	818	825	831	rBV7	8091	12992	0.11%	0.020%
12	7.857	839	845	851	rVB7	8571	15063	0.12%	0.023%
13	8.093	879	885	902	rBV	914286	1446519	11.81%	2.254%
14	8.522	950	958	973	rBV	838863	1349734	11.02%	2.103%
15	9.234	1071	1079	1093	rBV	700542	1131849	9.24%	1.763%
16	9.769	1161	1170	1188	rBV	1037498	1797624	14.68%	2.801%
17	10.134	1225	1232	1240	rBV	1066818	1756569	14.34%	2.737%
18	10.204	1240	1244	1250	rVB2	13588	21516	0.18%	0.034%
19	10.281	1250	1257	1273	rBV	313463	611714	4.99%	0.953%
20	10.569	1301	1306	1312	rBV	33040	54989	0.45%	0.086%
21	10.628	1312	1316	1322	rVB2	26375	42760	0.35%	0.067%
22	10.981	1370	1376	1380	rBV5	8645	14352	0.12%	0.022%
23	11.075	1382	1392	1415	rVV	576385	1292171	10.55%	2.013%
24	11.504	1457	1465	1473	rVB	92416	169316	1.38%	0.264%
25	11.734	1499	1504	1510	rBV	15609	26111	0.21%	0.041%
26	11.945	1534	1540	1544	rBV	18512	31136	0.25%	0.049%
27	12.828	1686	1690	1695	rBV2	10921	15364	0.13%	0.024%
28	13.081	1729	1733	1736	rBV3	8586	13229	0.11%	0.021%
29	13.198	1750	1753	1759	rVB	11252	15088	0.12%	0.024%
30	13.375	1773	1783	1789	rBV	94766	170173	1.39%	0.265%
31	13.457	1789	1797	1803	rVV	1780659	2444908	19.96%	3.809%
32	13.528	1803	1809	1816	rVV2	185915	319450	2.61%	0.498%
33	13.716	1834	1841	1853	rBV2	2000740	2907270	23.74%	4.530%
34	13.851	1859	1864	1869	rVB2	10945	18249	0.15%	0.028%
35	14.034	1887	1895	1912	rBV2	1691337	2726499	22.26%	4.248%
36	14.234	1924	1929	1931	rBV	31039	44750	0.37%	0.070%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100424\
Data File : BN034420.D
Acq On : 05 Oct 2024 12:22
Operator : RC/JU
Sample : P4227-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PMW-1(20240925)

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_N\Methods\SFAM-EPA-BN091124.MA.M
Title : SVOA CALIBRATION

37	14.269	1931	1935	1950	rVB	145781	284368	2.32%	0.443%
38	14.492	1969	1973	1979	rVB9	9120	20271	0.17%	0.032%
39	14.557	1979	1984	1999	rBV	162814	276505	2.26%	0.431%
40	15.034	2058	2065	2082	rBV	2576126	3582607	29.25%	5.582%
41	15.169	2082	2088	2094	rBV	773496	1064947	8.70%	1.659%
42	15.286	2102	2108	2120	rBV	228119	375777	3.07%	0.585%
43	15.416	2125	2130	2134	rVB	54824	79660	0.65%	0.124%
44	15.722	2168	2182	2199	rBV	5687535	12247178	100.00%	19.081%
45	15.851	2200	2204	2214	rVB	381231	555467	4.54%	0.865%
46	16.057	2237	2239	2249	rVB10	10023	19054	0.16%	0.030%
47	16.339	2281	2287	2290	rBV5	11776	22923	0.19%	0.036%
48	16.386	2290	2295	2300	rVB	154602	212081	1.73%	0.330%
49	16.575	2325	2327	2335	rVB8	7506	13615	0.11%	0.021%
50	16.739	2350	2355	2358	rVV	127307	199737	1.63%	0.311%
51	16.786	2358	2363	2374	rVV	1705503	2454768	20.04%	3.825%
52	16.886	2374	2380	2393	rVV2	2640022	3796015	31.00%	5.914%
53	17.722	2518	2522	2530	rBV	236365	374248	3.06%	0.583%
54	17.792	2530	2534	2540	rVB2	114887	162326	1.33%	0.253%
55	18.663	2678	2682	2686	rBV	34163	48313	0.39%	0.075%
56	18.704	2686	2689	2691	rVB2	19500	19554	0.16%	0.030%
57	18.757	2695	2698	2703	rVB2	37922	52384	0.43%	0.082%
58	18.833	2706	2711	2713	rBV	44651	77225	0.63%	0.120%
59	19.022	2739	2743	2747	rBV2	140929	196040	1.60%	0.305%
60	19.198	2766	2773	2786	rBV	3377715	4402019	35.94%	6.858%
61	19.839	2880	2882	2887	rVB2	23527	29816	0.24%	0.046%
62	20.004	2907	2910	2913	rBV	26346	28013	0.23%	0.044%
63	20.763	3036	3039	3042	rBV5	34876	44692	0.36%	0.070%
64	21.021	3078	3083	3093	rBV	1884282	2544336	20.77%	3.964%
65	23.545	3504	3512	3526	rVB	2104489	4746290	38.75%	7.395%
66	23.727	3535	3543	3561	rVB	1291332	3036318	24.79%	4.731%

Sum of corrected areas: 64184401

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Acq On : 05 Oct 2024 12:22
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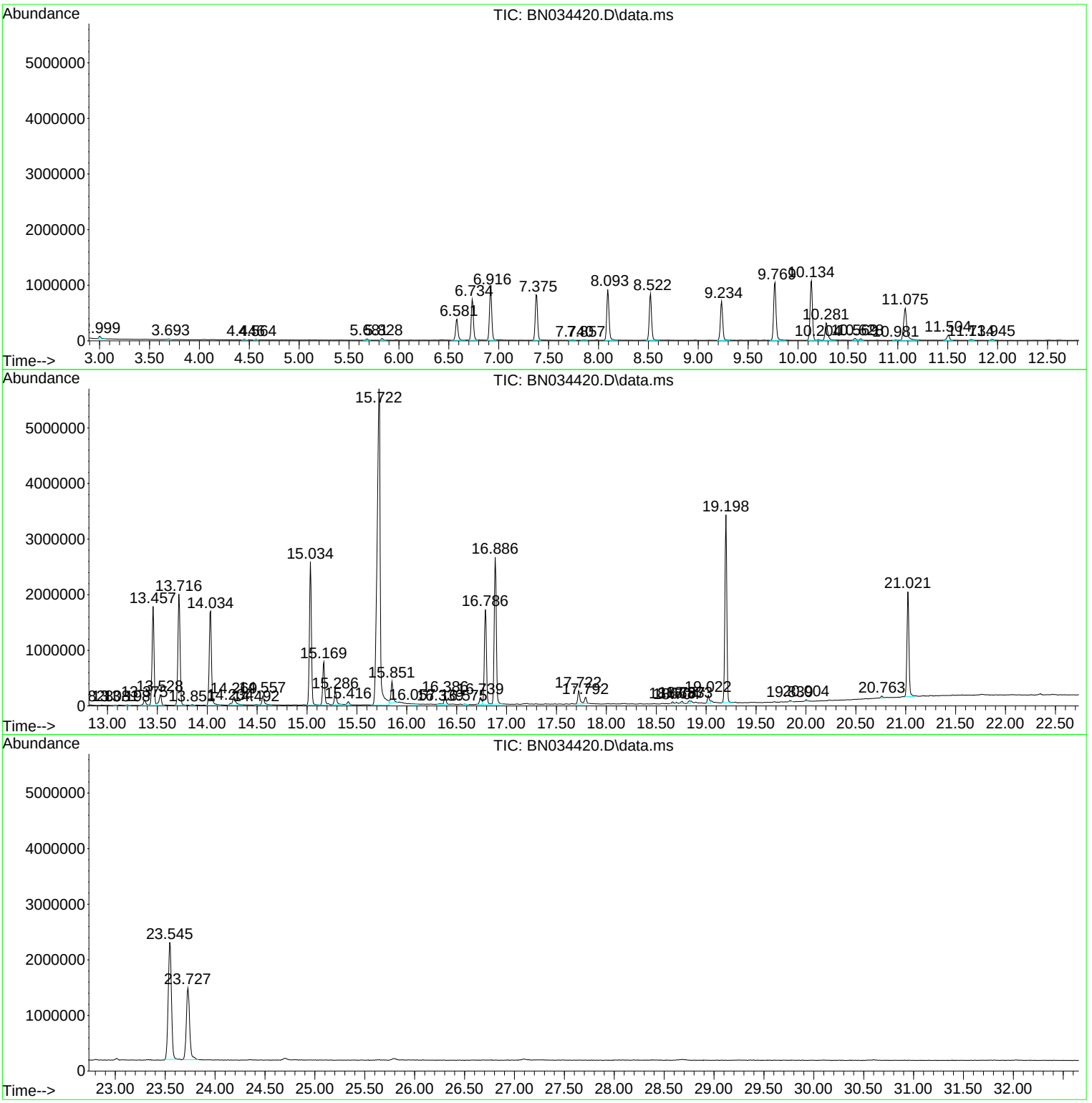
Sample : P4227-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PMW-1(20240925)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN091124.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100424\
Data File : BN034420.D
Acq On : 05 Oct 2024 12:22
Operator : RC/JU
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Quant Title : SVOA CALIBRATION

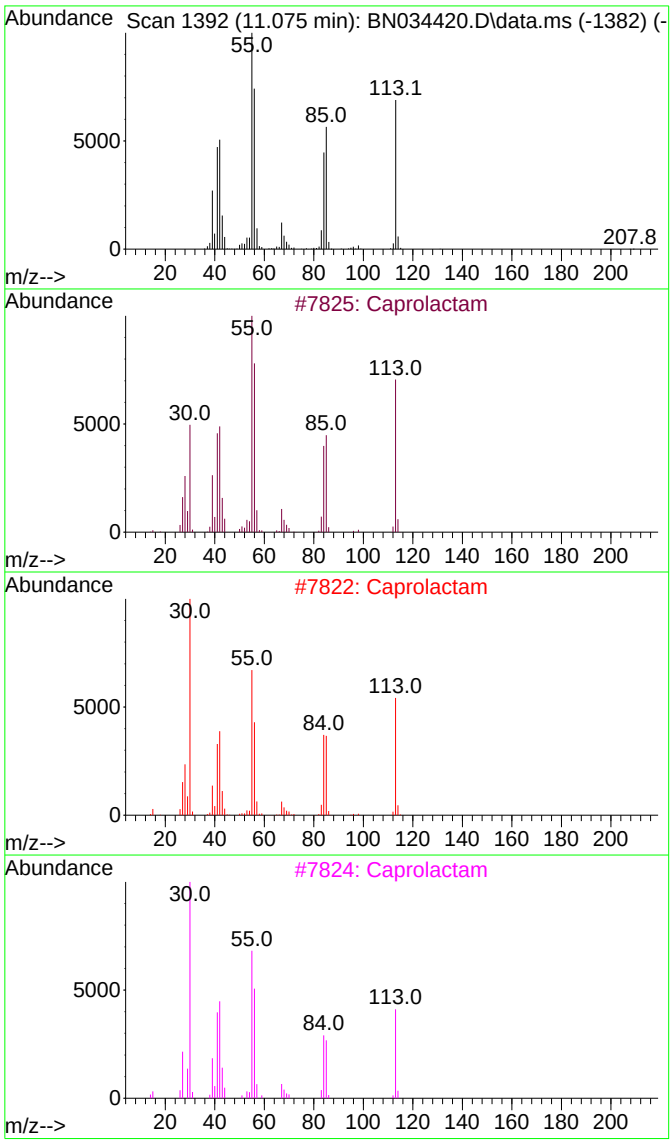
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

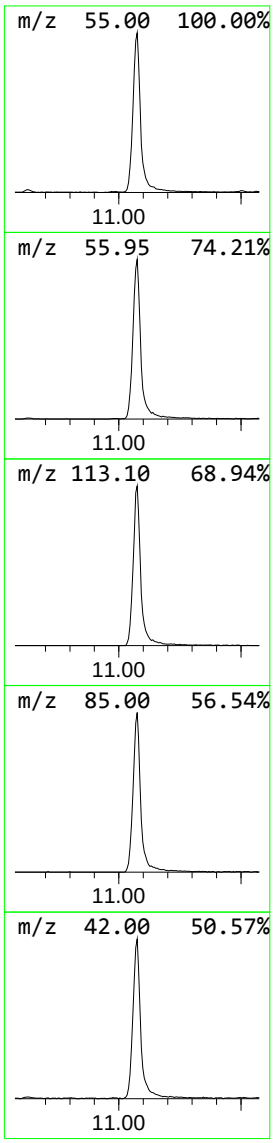
****

Peak Number 1 Capro lactam Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.075	14.71 ng/ul	1292170	Naphthalene-d8	10.134

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caprolactam	113	C6H11NO	000105-60-2	96
2	Caprolactam	113	C6H11NO	000105-60-2	95
3	Caprolactam	113	C6H11NO	000105-60-2	81
4	Caprolactam	113	C6H11NO	000105-60-2	74
5	1-Hexene	84	C6H12	000592-41-6	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100424\
Data File : BN034420.D
Acq On : 05 Oct 2024 12:22
Operator : RC/JU
Sample : P4227-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PMW-1(20240925)

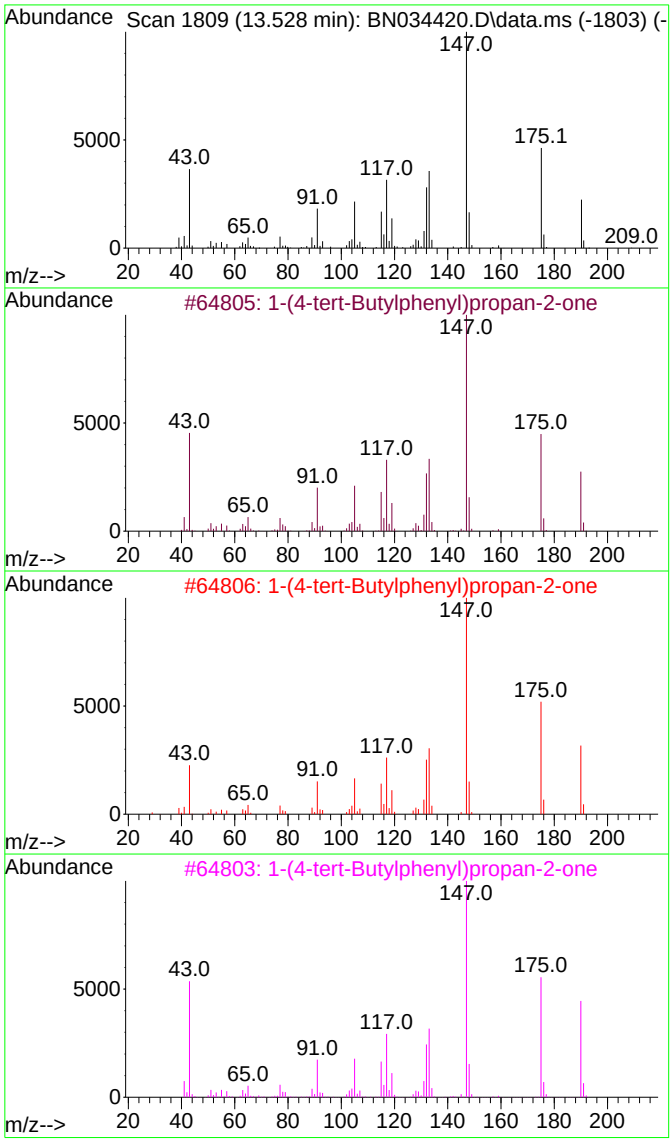
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN091124.MA.M
Quant Title : SVOA CALIBRATION

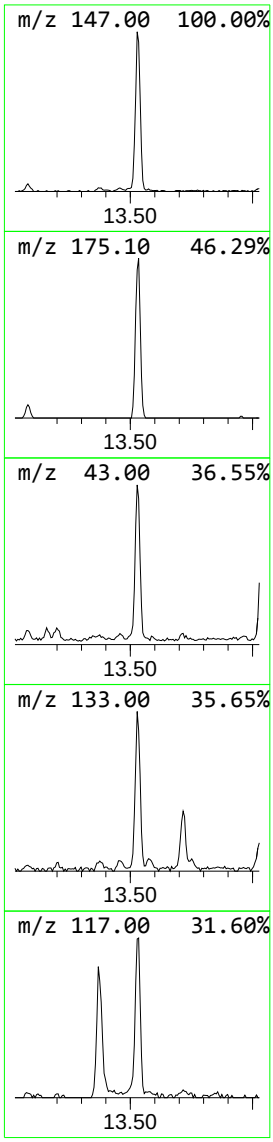
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-(4-tert-Butylphenyl)propa... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.528	2.34 ng/ul	319450	Acenaphthene-d10	14.028

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(4-tert-Butylphenyl)propan-2-one	190	C13H18O	081561-77-5	99
2	1-(4-tert-Butylphenyl)propan-2-one	190	C13H18O	081561-77-5	98
3	1-(4-tert-Butylphenyl)propan-2-one	190	C13H18O	081561-77-5	97
4	4,5-Dimethylindoline-2,3-dione	175	C10H9NO2	1010443-10-6	52
5	5,6-Dimethylindoline-2,3-dione	175	C10H9NO2	1000443-04-4	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100424\
Data File : BN034420.D
Acq On : 05 Oct 2024 12:22
Operator : RC/JU
Sample : P4227-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PMW-1(20240925)

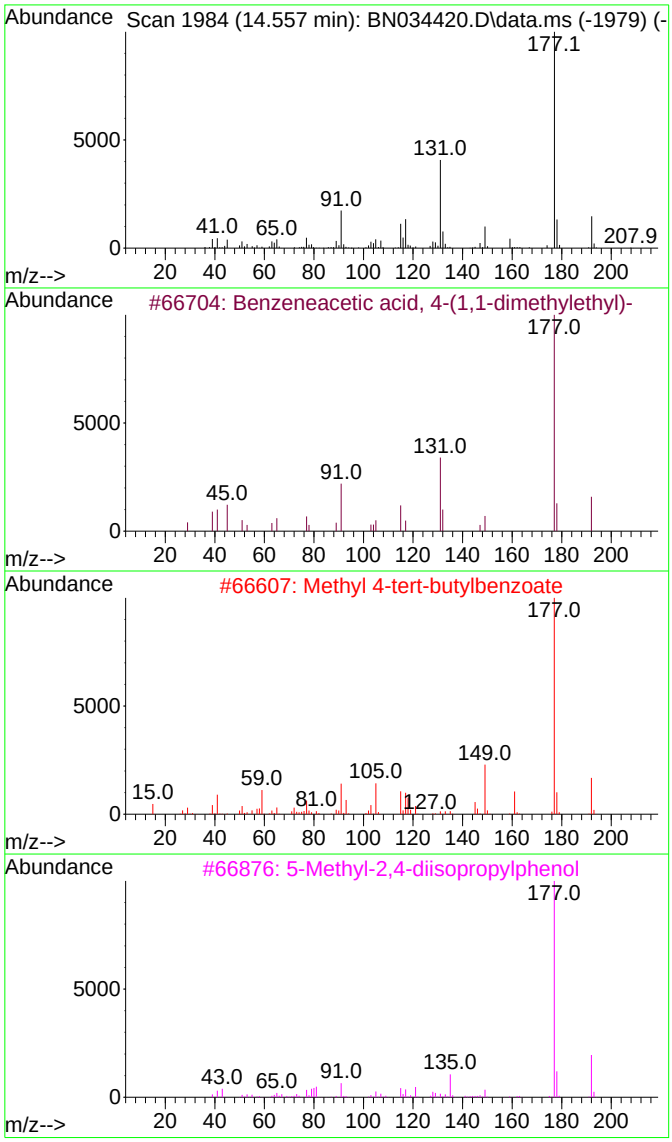
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN091124.MA.M
Quant Title : SVOA CALIBRATION

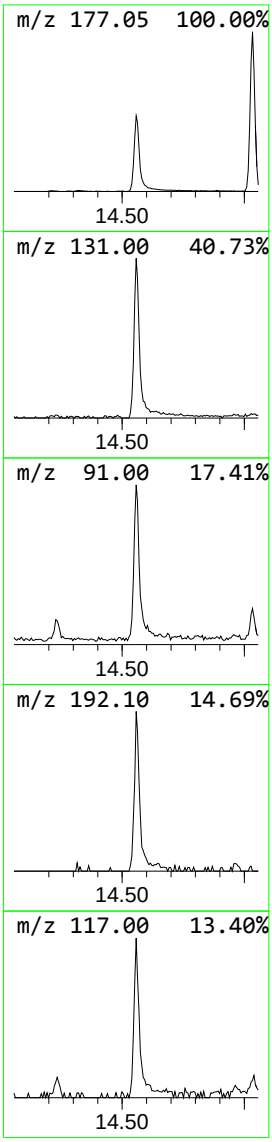
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzeneacetic acid, 4-(1,1-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.557	2.03 ng/ul	276505	Acenaphthene-d10	14.028

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetic acid, 4-(1,1-dimet...	192	C12H16O2	032857-63-9	90
2	Methyl 4-tert-butylbenzoate	192	C12H16O2	026537-19-9	52
3	5-Methyl-2,4-diisopropylphenol	192	C13H20O	040625-96-5	50
4	2,4a-Epidioxy-5,6,7,8-tetrahydro...	224	C13H20O3	1000212-29-9	47
5	trans-.beta.-Ionone	192	C13H20O	000079-77-6	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100424\
Data File : BN034420.D
Acq On : 05 Oct 2024 12:22
Operator : RC/JU
Sample : P4227-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PMW-1(20240925)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN091124.MA.M
Quant Title : SVOA CALIBRATION

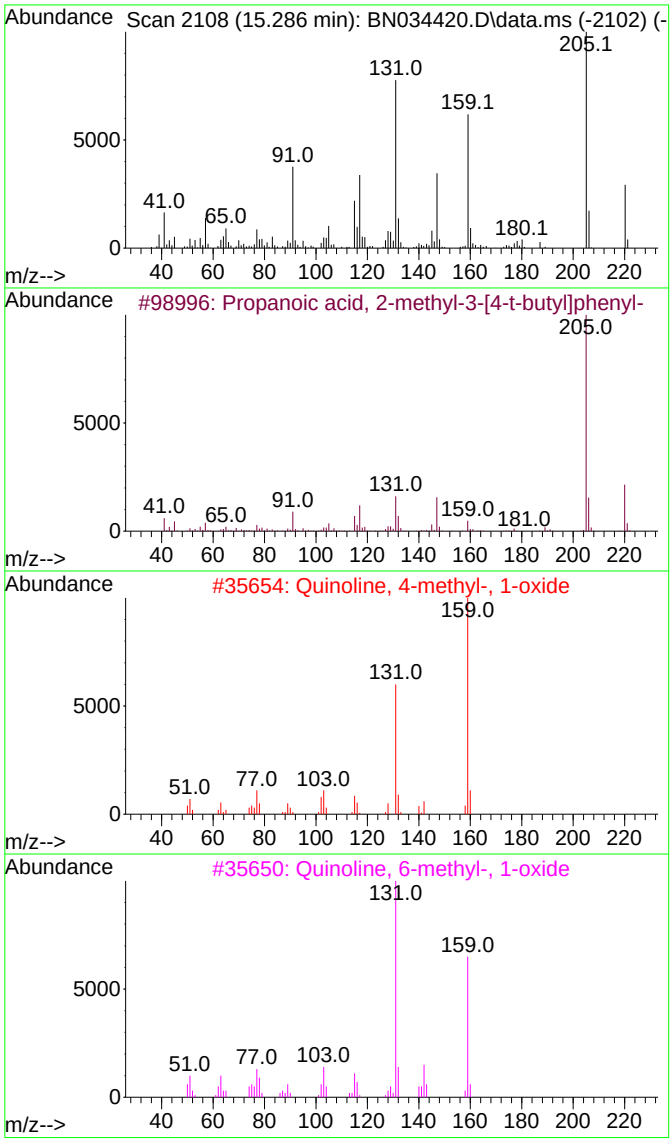
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

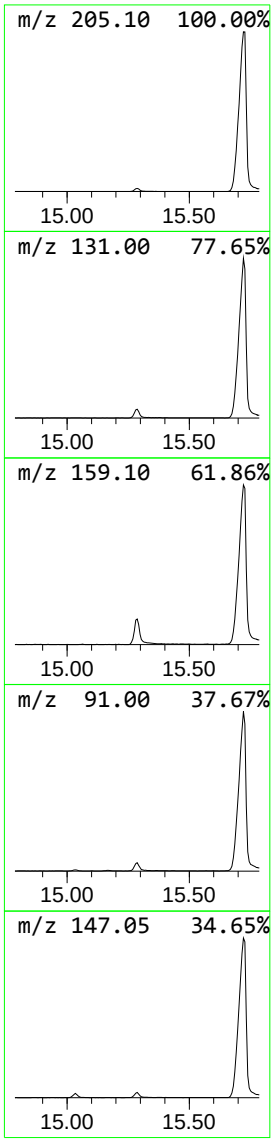
****

Peak Number 4 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.287	2.76 ng/ul	375777	Acenaphthene-d10	14.028

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-3-[4-t-...	220	C14H20O2	1000131-87-0	43
2	Quinoline, 4-methyl-, 1-oxide	159	C10H9NO	004053-40-1	43
3	Quinoline, 6-methyl-, 1-oxide	159	C10H9NO	004053-42-3	43
4	1H-Indene, 2,3-dihydro-4-propyl-	160	C12H16	092013-16-6	42
5	Benzene, 1-(chloromethyl)-4-(2-p...	166	C10H11Cl	036875-10-2	42





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Data File : BN034420.D
Acq On : 05 Oct 2024 12:22
Operator : RC/JU
Sample : P4227-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PMW-1(20240925)

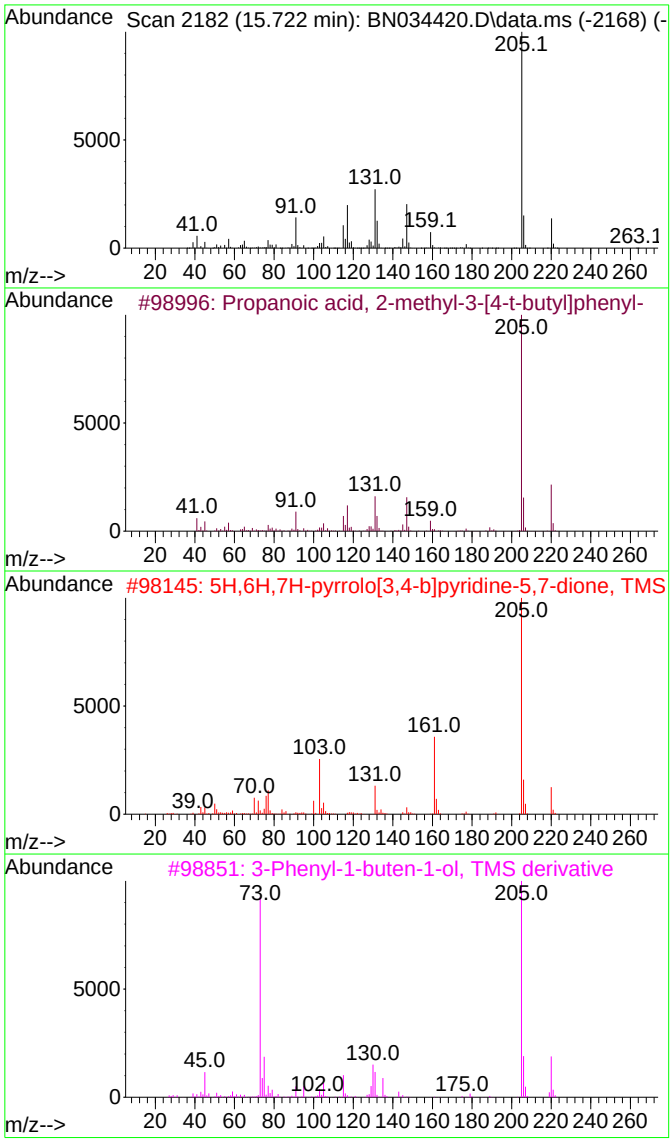
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN091124.MA.M
Quant Title : SVOA CALIBRATION

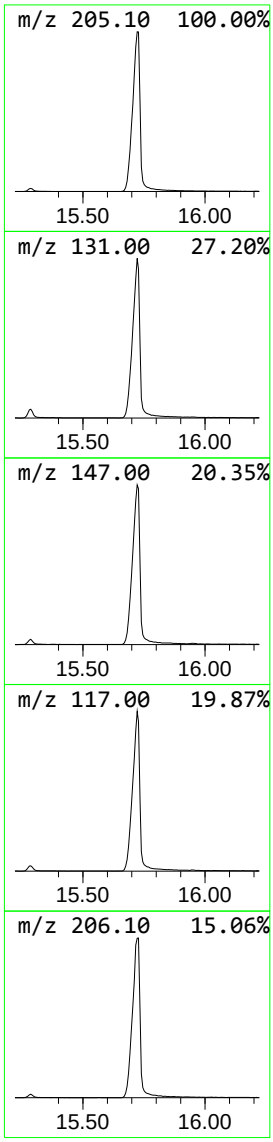
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanoic acid, 2-methyl-3-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.722	99.78 ng/ul	12247200	Phenanthrene-d10	16.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-3-[4-t-...	220	C14H20O2	1000131-87-0	93
2	5H,6H,7H-pyrrolo[3,4-b]pyridine-...	220	C10H12N2O2Si	1000485-20-1	47
3	3-Phenyl-1-buten-1-ol, TMS deriv...	220	C13H20OSi	055543-95-8	43
4	(4S)-Perhydro-3-benzyl-4-methyl-...	205	C12H15NO2	1000434-17-0	43
5	Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	43





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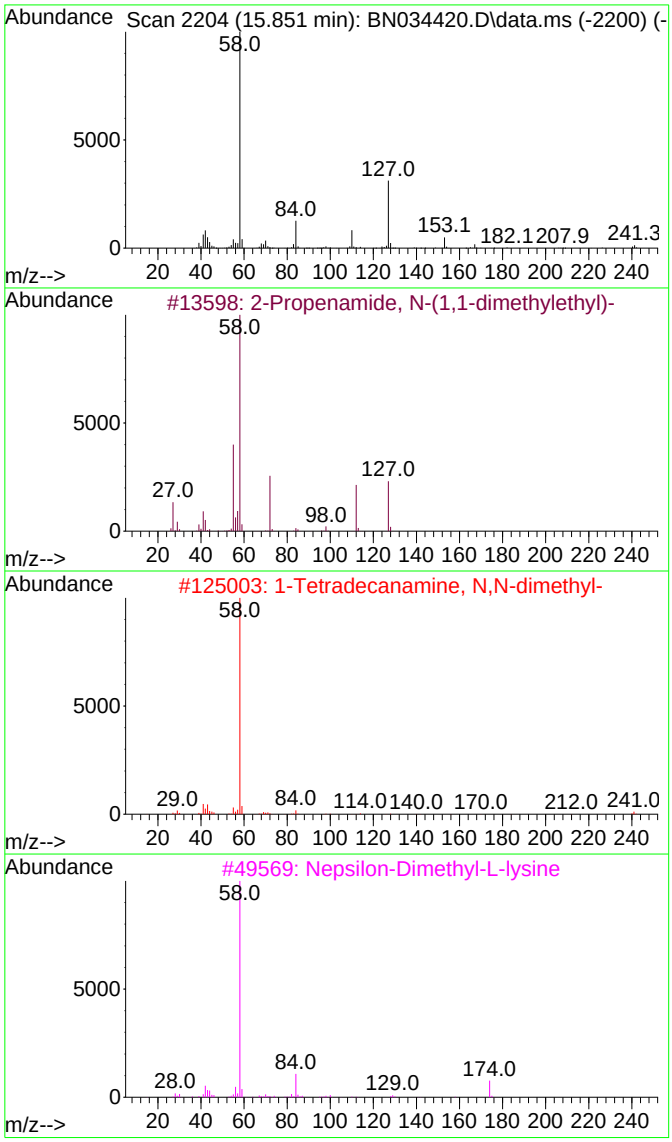
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN091124.MA.M
Quant Title : SVOA CALIBRATION

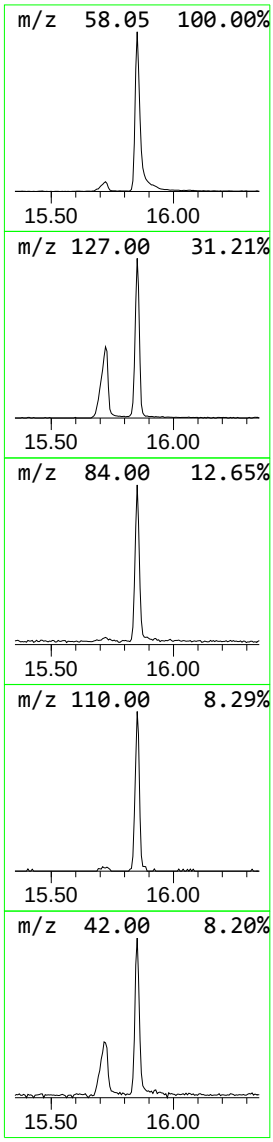
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Propenamide, N-(1,1-dimet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.851	4.53 ng/ul	555467	Phenanthrene-d10	16.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenamide, N-(1,1-dimethylet...	127	C7H13NO	000107-58-4	64
2	1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	64
3	Nepsilon-Dimethyl-L-lysine	174	C8H18N2O2	002259-86-1	53
4	1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	52
5	3(N,N-Dimethylmyristylammonio)pr...	363	C19H41NO3S	014933-09-6	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100424\
Data File : BN034420.D
Acq On : 05 Oct 2024 12:22
Operator : RC/JU
Sample : P4227-01
Misc :
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Instrument :
BNA_N
ClientSampleId :
PMW-1(20240925)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN091124.MA.M
Quant Title : SVOA CALIBRATION

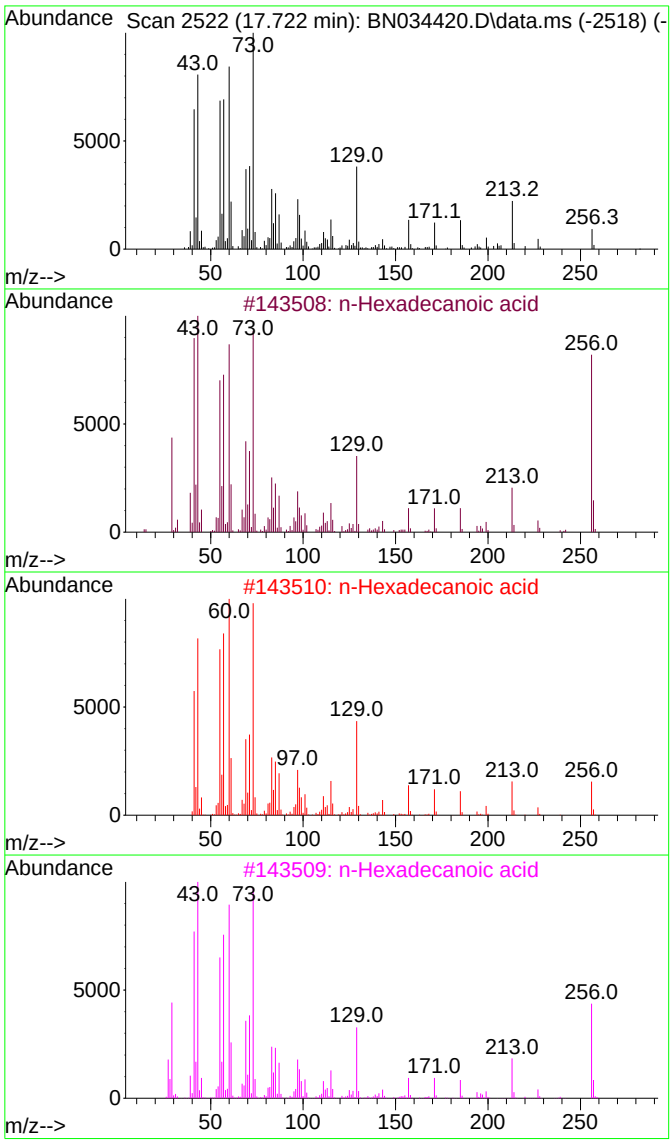
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

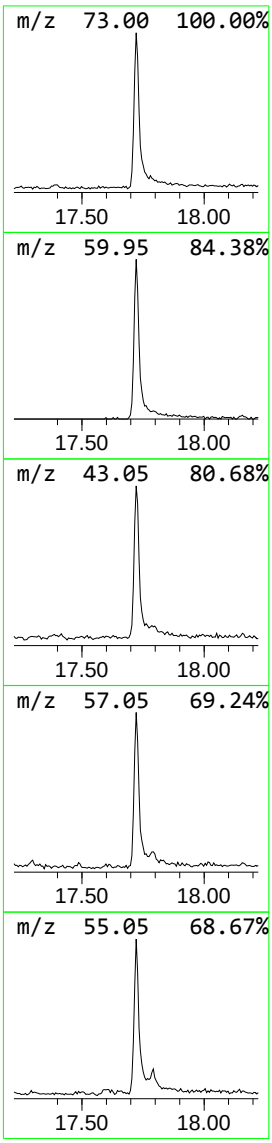
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.722	3.05 ng/ul	374248	Phenanthrene-d10	16.786

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	97
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100424\
Data File : BN034420.D
Acq On : 05 Oct 2024 12:22
Operator : RC/JU
Sample : P4227-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PMW-1(20240925)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN091124.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
Capro lactam	11.075	14.7	ng/ul	1292170	2	10.134	1756570	20.0
1-(4-tert-Butyl...	13.528	2.3	ng/ul	319450	3	14.028	2726500	20.0
Benzeneacetic a...	14.557	2.0	ng/ul	276505	3	14.028	2726500	20.0
unknown-01	15.287	2.8	ng/ul	375777	3	14.028	2726500	20.0
Propanoic acid,...	15.722	99.8	ng/ul	12247200	4	16.786	2454770	20.0
2-Propenamide, ...	15.851	4.5	ng/ul	555467	4	16.786	2454770	20.0
n-Hexadecanoic ...	17.722	3.0	ng/ul	374248	4	16.786	2454770	20.0