

1 **- Supporting information -**

2
3 Do interspecies correlation estimations increase the reliability of toxicity
4 estimates for wildlife?

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26 1. METHODOLOGY

27

28 1.1 Correlations in residual standard errors

29 We did a pilot study to estimate the correlations in residual standard errors and the
30 covariance in the ICE predictions, because ICE predictions were often made based on the
31 same experimental LD50 value. As the experimental dataset underlying the ICE regressions
32 of Raimondo et al. (2010) were not available due to confidentiality reasons, we considered a
33 dataset with LD50 data from RTECS (Accelrys Inc., 2011) for 37 chemical substances in the
34 species Mouse, Rabbit and Guinea Pig (see Table S1).

35 For species $s1$ and $s2$ we considered the ICE regression:

36
$$\text{Log}(LD50_x^{s2}) = a + b \log(LD50_x^{s1}) + \varepsilon_x^{s1s2} \quad (\text{S1})$$

37 where $s1$ is called the surrogate species, $s2$ is called the predicted species, and ε_x^{s1s2} is the so-
38 called residual error. The variance of the ε_x^{s1s2} values was estimated by the mean squared
39 error (MSE) of the corresponding linear regression. Once the parameters a and b have been
40 estimated by values $\hat{\alpha}$ (intercept) and $\hat{\beta}$ (slope), we could define the residual error:

41
$$\varepsilon_x^{s1s2} = \log(LD50_x^{s2}) - (\hat{\alpha} + \hat{\beta} \log(LD50_x^{s1})) \quad (\text{S2})$$

42 **Table S1.** Chemicals with LD50 data for mouse, rabbit and guinea pig used in our pilot study.

CAS	Chemical name	LD50 mouse (mg·kgwt ⁻¹)	LD50 rabbit (mg·kgwt ⁻¹)	LD50 guinea pig (mg·kgwt ⁻¹)
56073-10-0	Brodifacoum	5.00E+01	2.80E-01	4.00E-01
116-06-3	Aldicarb	5.41E-01	1.30E+00	1.00E+00
297-78-9	Telodrin	1.00E+01	4.00E+00	2.54E+00
1563-66-2	Carbofuran	5.37E+00	7.50E+00	9.20E+00
56-38-2	Parathion-ethyl	1.12E+01	1.00E+01	1.31E+01
900-95-8	Fentin acetate	8.70E+01	4.93E+01	1.80E+01
950-37-8	Methidathion	2.71E+01	7.10E+01	2.50E+01
10265-92-6	Methamydophos	1.62E+01	1.73E+01	3.00E+01
60-57-1	Dieldrin	6.00E+01	4.74E+01	3.09E+01
309-00-2	Aldrin	4.40E+01	6.32E+01	3.30E+01
22781-23-3	Bendiocarb	3.55E+01	3.74E+01	3.50E+01
2595-54-2	Mecarbam	1.06E+02	6.00E+01	6.50E+01
1113-02-6	Omethoate	3.12E+01	5.00E+01	7.07E+01
106-93-4	1,2-Dibromoethane	4.20E+02	5.50E+01	1.10E+02
29973-13-5	Ethiofencarb	1.35E+02	1.63E+02	1.13E+02
76-44-8	Heptachlor	6.80E+01	8.49E+01	1.16E+02
58-89-9	Lindane	1.65E+02	1.08E+02	1.18E+02
301-12-2	Oxydemethon-methyl	3.00E+01	1.04E+02	1.20E+02
533-74-4	3,5-dimethyltetrahydro-2-H,1,3,5-thiadiazone-2-thione	2.78E+02	2.88E+02	1.60E+02
59669-26-0	Thiodicarb	2.26E+02	5.56E+02	1.60E+02
2176-62-7	Pentachloropyridine	1.31E+02	9.05E+01	1.70E+02
8001-35-2	Toxaphene	7.39E+01	5.72E+01	2.10E+02
101-27-9	Barban	1.35E+03	6.00E+02	2.40E+02
1912-24-9	Atrazine	1.75E+03	6.71E+02	2.50E+02
640-15-3	Thiometon	6.20E+01	9.50E+01	2.61E+02
63-25-2	Carbaryl	3.36E+02	7.10E+02	2.80E+02
333-41-5	Diazinon	1.11E+02	1.39E+02	3.05E+02
108-62-3	Metaldehyde	2.00E+02	6.02E+02	3.50E+02
17109-49-8	Edifenphos	3.61E+02	3.16E+02	3.74E+02
2597-03-7	Phenthoate	3.74E+02	2.10E+02	3.88E+02
2921-88-2	Chlorpyriphos	1.52E+02	1.41E+03	5.04E+02
1194-65-6	Dichlobenil	1.69E+03	2.32E+02	5.84E+02
1698-60-8	Chloridazon	2.74E+03	1.12E+03	1.01E+03
29232-93-7	Pirimiphos-methyl	1.18E+03	1.63E+03	1.41E+03
5598-13-0	Chlorpyrifos-methyl	1.88E+03	2.00E+03	2.25E+03
23564-05-8	Thiophanate-methyl	3.45E+03	2.26E+03	4.94E+03
71-55-6	1,1,1-trichloroethane	1.12E+04	5.66E+03	9.47E+03

43 Most noticeable was the high mutual correlation between the residual errors in the
44 predicted values if a common surrogate species was used (correlation coefficient ≈ 0.9 , see
45 Table S2). Moreover the errors in the toxicities in the predictions from two different

46 surrogate species were highly correlated. Table S2 shows the results. The reduction in
 47 residual standard error (RSE) in the bivariate linear regression with respect to linear
 48 regression from surrogate Guinea Pig is only $(1 - 0.4752/0.4782) = 0.0063$, that is a gain of
 49 less than 1%. We concluded that the residual standard errors in LD50 values predicted from a
 50 common surrogate are not independent. Since the combined dataset in this study was based
 51 on many LD50 values predicted from common surrogate species, we applied a conservative
 52 method to quantify the uncertainty of the HD50 value (correlation 1, see SI par. 1.2).

53

54 **Table S2.** The correlation of the residual errors for toxicity predictions based on linear regressions.

Surrogate species	Predicted species	Intercept	Slope	RSE	MSE	Correlation coefficient
Mouse	Rabbit	0.2092	0.8679	0.5105	0.2606	0.8294
Mouse	Guinea Pig	0.1703	0.8812	0.5004	0.2504	
Rabbit	Mouse	0.4875	0.8001	0.4901	0.2402	0.8802
Guinea Pig	Mouse	0.4863	0.8047	0.4782	0.2287	
Rabbit + Guinea Pig	Mouse			0.4752	0.2258	

55 RSE = residual standard error, MSE = mean squared error

56

57 1.2 Conservative calculation of uncertainty

58 We used the ICE models to estimate ‘predicted’ LD50 values. The standard deviation of
 59 the predicted toxicity for chemical x in species j from surrogate species i ($s_{j,x}$) was calculated
 60 according to Mendenhall and Beaver (1994):

$$61 \quad s_{j,x} = \sqrt{MSE_{ij} \cdot \left(1 + \frac{1}{n_{ij}} + \frac{(\log LD50_{i,x} - \overline{\log LD50_i})^2}{S_{ss}} \right)} \quad (S3)$$

62 In this equation, MSE_{ij} is the Mean Squared Error based on the Sum of Squares for Errors
 63 for the predicted toxicity value of species j from surrogate species i, given by Raimondo et al.
 64 (2010); n_{ij} is the total number of surrogate LD50 values used for derivation of the ICE model
 65 correlation between species i and j; $LD50_{i,x}$ is the experimental LD50 value for chemical x in
 66 surrogate species i as applied in our model predictions; $\overline{\log LD50_i}$ is the average of all log-

67 transformed experimental LD50 for surrogate species i (i.e. different chemicals) used for
 68 derivation of the ICE model correlation between species i and j ; and S_{ss} is the sum of squared
 69 deviations in the surrogate toxicity value given by Raimondo et al. (2010). We approached
 70 the total number of warm-blooded wildlife species (N) with a number of experimentally
 71 tested species (n) and a number of modeled species (m). We assumed that the predicted
 72 species are a random sample of all species. Furthermore, we assumed that the computable
 73 covariances between predictions correspond to a random sample of pairs of species, e.g.
 74 predicted species j_1 and j_2 . Therefore, the covariance between the predictions for all species j_1

75 up to j_N was denoted as $s_{j_1j_2}$, and the mean covariance $\frac{1}{N^2} \sum_{j_1=1}^N \sum_{j_2=1}^N s_{j_1j_2}$ was the average of the
 76 covariances and variances.

77 An upperbound to the mean covariance followed from the Cauchy-Schwartz inequality
 78 $s_{j_1j_2} = \sqrt{s_{j_1}^2} \sqrt{s_{j_2}^2}$ (Steele, 2004, equality means correlation 1), and lead to the square of the
 79 mean standard deviation:

$$80 \quad \frac{1}{N^2} \sum_{j_1=1}^N \sum_{j_2=1}^N s_{j_1j_2} = \frac{1}{N^2} \sum_{j_1=1}^N \sum_{j_2=1}^N \sqrt{s_{j_1}^2} \sqrt{s_{j_2}^2} = \frac{1}{N^2} \left(\sum_{j_1=1}^N \sqrt{s_{j_1}^2} \right) \left(\sum_{j_2=1}^N \sqrt{s_{j_2}^2} \right) = \left(\frac{1}{N} \sum_{j=1}^N s_j \right)^2 \quad (S4)$$

81 For the toxicity values predicted with the ICE-regressions from Raimondo et al. (2010),

82 $\frac{1}{N} \sum_{j=1}^N s_j$ could be estimated by $\frac{1}{m} \sum_{j=1}^m s_j$. To be exact, s_j is $s_{j,x}$ i.e. the standard deviation of

83 the predicted toxicity for chemical x in species j , calculated according to Mendenhall and
 84 Beaver (1994) (see below). If there were also n experimental values, then the square of the
 85 standard error of the mean ($SEM_{Co,x}$) was described by:

$$86 \quad \frac{s_{Co,x}^2}{n+m} + \frac{m^2}{(n+m)^2} \left(\frac{1}{m} \sum_{j=1}^m s_{j,x} \right)^2 \quad (S5)$$

87 In this equation $s_{Co,x}^2$ is the variance of all LD50 values available for chemical x – both tested
 88 and predicted.

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91 2. RESULTS

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93 2.1 HD50 values and uncertainty factors

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95 **Table S3:** HD50 values based on experimental and combined datasets plus their uncertainty factors.

96 n is the number of experimentally tested species

97 m is the number of species for which LD50 values were modeled

98 UF_{stat} is the uncertainty factor of the $HD50_x$ value (ratio of the 95th/5th percentile) based on either an
 99 experimental dataset (Ex) or on a dataset combining experimental and modeled data (Co).

100 $UF_{sys,x}$ is the ratio of $HD50_{Ex,x}/HD50_{Co,x}$

Chemical CAS	Experimental dataset			Combined dataset			$UF_{sys,x}$
	m	$HD50_{Ex,x}$ (mg·kgwwt ⁻¹)	$UF_{stat,Ex,x}$	n+m	$HD50_{Co,x}$ (mg·kgwwt ⁻¹)	$UF_{stat,Co,x}$	
297-78-9	11	1.84E+00	7.38E+00	35	2.41E+00	9.31E+00	7.64E-01
60-57-1	11	4.30E+01	2.65E+00	40	1.92E+01	7.00E+00	2.24E+00
60-51-5	10	9.77E+01	3.45E+00	42	3.10E+01	8.91E+00	3.15E+00
309-00-2	10	4.96E+01	3.39E+00	40	2.43E+01	7.45E+00	2.05E+00
56-38-2	10	3.74E+00	2.58E+00	35	3.31E+00	6.77E+00	1.13E+00
1689-84-5	9	8.10E+02	6.83E+01	32	1.87E+02	1.54E+01	4.33E+00
333-41-5	9	2.58E+01	1.04E+01	41	8.84E+00	7.94E+00	2.92E+00
62-73-7	9	2.53E+01	4.08E+00	42	1.26E+01	7.60E+00	2.01E+00
63-25-2	9	3.56E+02	2.96E+00	30	2.59E+02	1.38E+01	1.38E+00
327-98-0	9	1.87E+01	1.92E+00	43	1.18E+01	7.42E+00	1.59E+00
81-81-2	8	1.81E+01	4.61E+01	20	1.52E+01	2.01E+01	1.19E+00
56073-07-5	8	7.58E+01	2.37E+01	26	3.35E+01	1.29E+01	2.26E+00
1162-65-8	8	3.50E+00	1.94E+01	32	1.41E+01	1.75E+01	2.48E-01
55-38-9	8	3.31E+01	1.16E+01	37	1.22E+01	9.03E+00	2.70E+00
2921-88-2	8	7.04E+01	9.06E+00	41	2.35E+01	1.04E+01	3.00E+00
470-90-6	8	8.00E+01	8.71E+00	40	2.70E+01	9.37E+00	2.97E+00
299-84-3	8	1.19E+03	3.92E+00	23	3.52E+02	1.35E+01	3.39E+00
52-68-6	8	2.01E+02	3.12E+00	33	5.66E+01	1.05E+01	3.56E+00
72-20-8	8	5.25E+00	2.72E+00	42	5.09E+00	1.12E+01	1.03E+00
57-33-0	8	1.08E+02	1.92E+00	35	6.10E+01	1.23E+01	1.78E+00
534-52-1	7	4.58E+02	1.45E+03	28	2.39E+01	2.01E+01	1.92E+01
504-24-5	7	3.55E+01	4.45E+01	39	1.27E+01	1.00E+01	2.81E+00
999-81-5	7	1.22E+02	1.35E+01	30	1.20E+02	1.34E+01	1.02E+00

57-24-9	7	2.89E+00	9.86E+00	40	7.67E+00	1.22E+01	3.77E-01
14255-88-0	7	1.11E+02	8.92E+00	28	3.88E+01	1.36E+01	2.86E+00
52645-53-1	7	3.10E+03	8.66E+00	22	4.94E+02	2.35E+01	6.29E+00
1397-94-0	7	9.35E+00	8.58E+00	40	8.22E+00	9.37E+00	1.14E+00
115-29-7	7	2.07E+01	7.83E+00	39	1.57E+01	1.51E+01	1.32E+00
57-74-9	7	2.79E+02	5.53E+00	28	8.84E+01	1.01E+01	3.16E+00
41083-11-8	7	1.29E+02	4.28E+00	34	8.52E+01	1.36E+01	1.52E+00
56-72-4	7	2.33E+01	3.89E+00	42	1.16E+01	9.65E+00	2.01E+00
2597-03-7	7	1.56E+02	3.73E+00	36	7.54E+01	1.28E+01	2.07E+00
58-89-9	7	7.46E+01	3.53E+00	29	3.12E+01	1.51E+01	2.39E+00
123-31-9	7	2.25E+02	3.15E+00	24	1.32E+02	1.13E+01	1.70E+00
2104-64-5	7	6.59E+00	2.62E+00	41	5.24E+00	9.93E+00	1.26E+00
5903-13-9	6	6.07E+00	4.97E+01	28	2.70E+01	2.41E+01	2.25E-01
298-00-0	6	6.10E+01	3.48E+01	37	1.35E+01	1.40E+01	4.52E+00
52315-07-8	6	3.92E+02	2.86E+01	28	3.47E+01	2.01E+01	1.13E+01
786-19-6	6	7.71E+01	1.82E+01	39	2.83E+01	1.19E+01	2.73E+00
86-50-0	6	3.33E+01	1.55E+01	34	2.74E+01	1.32E+01	1.22E+00
303-47-9	6	7.27E+00	1.41E+01	37	9.24E+00	1.08E+01	7.87E-01
53-86-1	6	7.52E+01	7.84E+00	28	1.44E+01	1.27E+01	5.22E+00
4824-78-6	6	1.54E+02	6.83E+00	35	6.79E+01	1.43E+01	2.27E+00
3383-96-8	6	1.66E+02	6.37E+00	37	6.33E+01	1.14E+01	2.62E+00
1689-83-4	6	1.73E+02	5.49E+00	30	6.69E+01	1.00E+01	2.59E+00
87-86-5	6	1.36E+02	5.04E+00	31	5.50E+01	1.27E+01	2.47E+00
115-32-2	6	1.41E+03	5.02E+00	23	2.74E+02	2.58E+01	5.15E+00
4685-14-7	6	6.60E+01	4.68E+00	30	5.19E+01	1.36E+01	1.27E+00
50-78-2	6	9.26E+02	4.03E+00	21	1.45E+02	2.53E+01	6.40E+00
21923-23-9	6	4.03E+01	3.96E+00	37	2.07E+01	1.13E+01	1.95E+00
80-33-1	6	2.39E+03	3.87E+00	21	7.47E+02	1.92E+01	3.20E+00
2686-99-9	6	7.87E+01	3.68E+00	38	4.10E+01	1.41E+01	1.92E+00
2540-82-1	6	2.36E+02	3.28E+00	25	1.49E+02	1.14E+01	1.59E+00
2439-10-3	6	4.96E+02	3.17E+00	25	2.78E+02	1.28E+01	1.78E+00
94-75-7	6	3.81E+02	3.13E+00	23	1.52E+02	1.53E+01	2.50E+00
106-93-4	6	1.19E+02	3.11E+00	36	5.75E+01	1.23E+01	2.07E+00
50-33-9	6	4.25E+02	3.09E+00	24	1.14E+02	2.78E+01	3.74E+00
1113-02-6	6	4.90E+01	2.91E+00	30	2.09E+01	9.96E+00	2.35E+00
298-04-4	6	6.12E+00	2.55E+00	40	6.57E+00	1.34E+01	9.32E-01
21259-20-1	6	2.25E+00	2.40E+00	28	2.29E+00	9.62E+00	9.80E-01
93-76-5	6	2.67E+02	2.35E+00	27	1.00E+02	1.57E+01	2.66E+00
680-31-9	6	1.53E+03	2.13E+00	23	6.37E+02	1.60E+01	2.40E+00
50-29-3	6	2.04E+02	2.03E+00	25	6.61E+01	1.70E+01	3.08E+00
2764-72-9	6	1.34E+02	1.86E+00	26	5.85E+01	1.37E+01	2.29E+00
58-08-2	6	1.85E+02	1.55E+00	25	5.92E+01	1.69E+01	3.13E+00
650-51-1	6	4.41E+03	1.52E+00	20	1.03E+03	2.35E+01	4.28E+00
50-06-6	6	1.48E+02	1.36E+00	25	5.35E+01	1.67E+01	2.76E+00
1689-99-2	5	8.13E+03	1.79E+03	24	2.11E+02	3.90E+01	3.85E+01
121-75-5	5	1.40E+02	1.41E+02	27	2.92E+01	2.92E+01	4.79E+00

83-79-4	5	3.84E+01	7.04E+01	33	4.94E+01	1.76E+01	7.78E-01
70-69-9	5	9.68E+01	3.90E+01	25	5.83E+01	2.68E+01	1.66E+00
135-19-3	5	6.58E+02	3.41E+01	22	8.31E+01	2.98E+01	7.92E+00
90-15-3	5	1.05E+03	2.54E+01	21	1.66E+02	3.09E+01	6.30E+00
75-05-8	5	2.78E+02	1.93E+01	21	8.26E+01	2.04E+01	3.36E+00
33089-61-1	5	7.51E+02	1.91E+01	25	3.74E+02	1.75E+01	2.01E+00
119-12-0	5	4.42E+02	1.91E+01	32	7.21E+01	2.00E+01	6.14E+00
71-36-3	5	1.01E+03	1.32E+01	22	8.78E+01	2.91E+01	1.14E+01
69806-50-4	5	2.61E+03	1.01E+01	21	4.54E+02	2.30E+01	5.76E+00
59669-26-0	5	2.29E+02	9.57E+00	27	6.12E+01	2.16E+01	3.74E+00
5836-29-3	5	4.20E+01	9.20E+00	28	1.79E+01	2.67E+01	2.35E+00
58-90-2	5	1.79E+02	9.03E+00	25	2.98E+01	2.37E+01	6.01E+00
87-68-3	5	1.47E+02	8.95E+00	29	3.43E+01	2.21E+01	4.27E+00
54-85-3	5	2.26E+02	8.67E+00	21	6.84E+01	1.88E+01	3.31E+00
3766-81-2	5	2.07E+02	7.89E+00	34	7.14E+01	1.46E+01	2.89E+00
71-55-6	5	4.65E+03	7.37E+00	6	2.72E+03	2.13E+01	1.71E+00
101-05-3	5	2.28E+03	7.15E+00	21	6.91E+02	1.60E+01	3.29E+00
2104-96-3	5	2.16E+03	6.35E+00	18	6.54E+02	2.48E+01	3.31E+00
34643-46-4	5	3.76E+02	5.98E+00	32	1.21E+02	1.66E+01	3.11E+00
608-73-1	5	1.66E+02	5.83E+00	37	6.52E+01	1.70E+01	2.55E+00
120-80-9	5	2.13E+02	5.66E+00	21	7.65E+01	2.29E+01	2.79E+00
9006-42-2	5	2.43E+03	5.53E+00	19	6.88E+02	2.18E+01	3.54E+00
2310-17-0	5	1.47E+02	5.39E+00	29	5.61E+01	1.83E+01	2.62E+00
143-50-0	5	1.77E+02	4.66E+00	35	8.66E+01	1.55E+01	2.04E+00
1918-16-7	5	3.27E+02	4.50E+00	32	8.93E+01	1.46E+01	3.66E+00
23947-60-6	5	2.30E+03	4.25E+00	20	8.26E+02	2.24E+01	2.78E+00
6047-17-2	5	8.71E+02	4.25E+00	23	2.72E+02	1.81E+01	3.20E+00
330-55-2	5	1.49E+03	4.23E+00	21	4.33E+02	2.50E+01	3.44E+00
4104-14-7	5	1.25E+01	3.99E+00	37	1.01E+01	1.35E+01	1.24E+00
1085-98-9	5	1.16E+03	3.85E+00	23	2.96E+02	3.24E+01	3.91E+00
43121-43-3	5	6.92E+02	3.37E+00	23	4.26E+02	1.46E+01	1.63E+00
13121-70-5	5	4.04E+02	3.27E+00	32	1.36E+02	1.56E+01	2.97E+00
76-44-8	5	5.87E+01	3.05E+00	29	1.96E+01	2.02E+01	2.99E+00
50512-35-1	5	1.71E+03	2.86E+00	21	4.69E+02	2.28E+01	3.64E+00
15687-27-1	5	8.54E+02	2.85E+00	23	2.22E+02	2.85E+01	3.85E+00
122-14-5	5	2.89E+02	2.82E+00	26	1.07E+02	2.03E+01	2.71E+00
96-12-8	5	1.48E+02	2.81E+00	26	3.90E+01	1.12E+01	3.79E+00
62-53-3	5	3.68E+02	2.74E+00	27	2.68E+02	1.98E+01	1.37E+00
2275-23-2	5	8.25E+01	2.73E+00	27	2.51E+01	1.48E+01	3.29E+00
107-21-1	5	4.43E+03	2.66E+00	19	8.31E+02	5.28E+01	5.33E+00
51-28-5	5	5.00E+01	2.52E+00	28	2.12E+01	1.59E+01	2.36E+00
123-91-1	5	3.09E+03	2.30E+00	19	7.37E+02	4.25E+01	4.19E+00
88-85-7	5	1.80E+01	2.28E+00	38	1.03E+01	1.30E+01	1.74E+00
24602-86-6	5	8.37E+02	2.20E+00	22	3.65E+02	2.91E+01	2.29E+00
22212-55-1	5	1.27E+03	2.17E+00	20	2.48E+02	2.97E+01	5.13E+00
25875-51-8	5	1.01E+03	2.16E+00	24	2.43E+02	1.52E+01	4.14E+00

309-43-3	5	8.81E+01	2.14E+00	35	7.28E+01	1.76E+01	1.21E+00
119-36-8	5	1.23E+03	2.12E+00	20	3.03E+02	2.97E+01	4.04E+00
14437-17-3	5	7.68E+02	2.12E+00	22	2.30E+02	1.81E+01	3.34E+00
62-44-2	5	1.62E+03	2.10E+00	21	3.14E+02	2.98E+01	5.16E+00
80-62-6	5	5.87E+03	1.99E+00	15	1.02E+03	2.90E+01	5.76E+00
512-56-1	5	1.15E+03	1.95E+00	25	4.59E+02	1.95E+01	2.50E+00
637-07-0	5	1.37E+03	1.93E+00	21	3.51E+02	2.59E+01	3.90E+00
3926-62-3	5	1.14E+02	1.83E+00	29	3.69E+01	1.05E+01	3.10E+00
39148-24-8	5	3.69E+03	1.78E+00	18	1.47E+03	2.19E+01	2.51E+00
131-89-5	5	6.31E+01	1.54E+00	29	2.80E+01	1.12E+01	2.25E+00
127-20-8	5	4.09E+03	1.51E+00	18	7.81E+02	4.54E+01	5.24E+00
79-06-1	5	1.49E+02	1.48E+00	32	7.65E+01	1.45E+01	1.95E+00
1461-22-9	4	1.36E+01	1.54E+04	25	2.74E+01	3.28E+01	4.96E-01
95-74-9	4	4.98E+01	2.20E+03	33	1.89E+01	1.98E+01	2.64E+00
55-91-4	4	1.59E+01	1.47E+03	23	5.74E+00	3.54E+01	2.77E+00
626-17-5	4	2.29E+03	1.10E+03	20	2.44E+02	3.54E+01	9.41E+00
41198-08-7	4	9.37E+01	5.31E+02	24	1.85E+01	2.47E+01	5.06E+00
8003-19-8	4	9.67E+01	2.72E+02	24	4.19E+01	3.13E+01	2.31E+00
10311-84-9	4	6.27E+01	1.68E+02	27	3.89E+01	2.22E+01	1.61E+00
123-96-6	4	1.51E+03	1.42E+02	24	1.22E+02	3.88E+01	1.23E+01
2691-41-0	4	6.18E+02	1.38E+02	18	1.69E+02	2.54E+01	3.65E+00
39300-45-3	4	3.37E+02	8.74E+01	22	4.42E+01	3.05E+01	7.61E+00
39515-41-8	4	1.55E+02	8.73E+01	28	6.41E+01	1.54E+01	2.42E+00
485-31-4	4	1.75E+02	4.34E+01	27	1.02E+02	3.03E+01	1.72E+00
75-31-0	4	1.21E+03	4.29E+01	27	1.62E+02	3.66E+01	7.43E+00
92-67-1	4	2.05E+02	3.36E+01	22	1.02E+02	2.84E+01	2.02E+00
597-64-8	4	3.74E+01	2.43E+01	24	2.52E+01	2.93E+01	1.48E+00
13171-21-6	4	1.01E+01	2.40E+01	34	5.65E+00	1.58E+01	1.79E+00
629-40-3	4	7.32E+01	2.01E+01	25	5.30E+01	2.48E+01	1.38E+00
128-37-0	4	1.97E+03	1.73E+01	20	2.85E+02	3.20E+01	6.92E+00
137-42-8	4	2.77E+02	1.70E+01	24	4.77E+01	1.92E+01	5.80E+00
98-01-1	4	3.40E+02	1.53E+01	27	7.97E+01	2.68E+01	4.26E+00
111-30-8	4	1.71E+02	1.53E+01	25	1.10E+02	2.39E+01	1.55E+00
8003-34-7	4	6.64E+02	1.43E+01	26	3.81E+02	2.36E+01	1.74E+00
2255-17-6	4	4.39E+01	1.34E+01	29	1.52E+01	1.44E+01	2.89E+00
584-79-2	4	1.22E+03	1.32E+01	23	5.83E+02	2.39E+01	2.09E+00
111-69-3	4	5.91E+01	1.25E+01	25	4.03E+01	2.39E+01	1.47E+00
298-02-2	4	1.75E+00	1.24E+01	30	4.19E+00	1.96E+01	4.19E-01
84-66-2	4	4.62E+03	1.14E+01	6	2.70E+03	1.27E+01	1.71E+00
55512-33-9	4	4.15E+03	1.11E+01	21	1.10E+03	2.21E+01	3.75E+00
77182-82-2	4	6.64E+02	1.07E+01	20	1.62E+02	3.30E+01	4.09E+00
65-45-2	4	1.13E+03	1.07E+01	20	1.51E+02	3.45E+01	7.50E+00
99-08-1	4	1.22E+03	1.06E+01	20	1.70E+02	3.10E+01	7.18E+00
107-06-2	4	9.05E+02	1.06E+01	22	1.59E+02	3.64E+01	5.68E+00
33245-39-5	4	2.10E+03	1.01E+01	23	6.05E+02	2.34E+01	3.48E+00
112-56-1	4	6.97E+01	1.00E+01	27	3.46E+01	3.26E+01	2.01E+00

5221-53-4	4	1.39E+03	9.49E+00	21	3.59E+02	2.96E+01	3.88E+00
55-63-0	4	6.83E+02	9.04E+00	24	1.34E+02	3.35E+01	5.11E+00
150-50-5	4	6.09E+02	8.78E+00	21	1.31E+02	2.09E+01	4.65E+00
50594-66-6	4	1.15E+03	8.43E+00	30	2.62E+02	2.21E+01	4.38E+00
90-43-7	4	1.44E+03	7.63E+00	21	3.32E+02	3.44E+01	4.33E+00
75-86-5	4	6.07E+00	7.32E+00	24	5.26E+00	2.12E+01	1.16E+00
102-82-9	4	2.30E+02	7.26E+00	24	6.68E+01	2.47E+01	3.44E+00
944-22-9	4	6.16E+00	7.07E+00	38	8.29E+00	1.36E+01	7.43E-01
108-18-9	4	2.15E+03	5.99E+00	19	4.80E+02	3.87E+01	4.48E+00
62-38-4	4	3.90E+01	5.92E+00	36	2.71E+01	1.49E+01	1.44E+00
88-89-1	4	1.86E+02	5.46E+00	25	6.51E+01	3.61E+01	2.86E+00
55335-06-3	4	6.53E+02	5.26E+00	23	3.31E+02	2.31E+01	1.97E+00
10605-21-7	4	4.65E+03	5.23E+00	9	1.46E+03	2.11E+01	3.19E+00
111-76-2	4	6.80E+02	4.95E+00	22	2.00E+02	2.11E+01	3.40E+00
7659-86-1	4	6.86E+02	4.93E+00	23	2.42E+02	2.26E+01	2.83E+00
731-27-1	4	5.95E+02	4.77E+00	21	2.06E+02	2.06E+01	2.88E+00
33820-53-0	4	2.11E+03	4.73E+00	23	9.33E+02	2.03E+01	2.27E+00
3226-36-6	4	8.99E+02	4.65E+00	21	1.79E+02	2.08E+01	5.03E+00
102-71-6	4	3.80E+03	4.50E+00	6	3.26E+03	7.18E+00	1.17E+00
1698-60-8	4	7.86E+02	4.44E+00	22	2.09E+02	3.34E+01	3.77E+00
78-59-1	4	1.61E+03	4.38E+00	18	6.06E+02	3.11E+01	2.66E+00
2074-50-2	4	4.03E+01	4.32E+00	28	3.85E+01	3.59E+01	1.05E+00
1929-82-4	4	5.78E+02	4.25E+00	24	1.11E+02	1.85E+01	5.21E+00
104-76-7	4	1.85E+03	4.15E+00	18	6.08E+02	3.12E+01	3.04E+00
106-89-8	4	2.08E+02	4.02E+00	27	6.34E+01	1.78E+01	3.28E+00
97-17-6	4	1.57E+02	4.01E+00	36	9.86E+01	1.82E+01	1.59E+00
109-86-4	4	1.53E+03	4.00E+00	18	5.76E+02	3.08E+01	2.66E+00
2270-40-8	4	4.52E+00	3.91E+00	27	4.65E+00	1.53E+01	9.73E-01
106-47-8	4	2.23E+02	3.73E+00	32	1.13E+02	2.19E+01	1.97E+00
82560-54-1	4	1.31E+02	3.69E+00	29	4.29E+01	1.59E+01	3.05E+00
75-09-2	4	1.60E+03	3.55E+00	20	2.77E+02	3.43E+01	5.79E+00
118-74-1	4	3.20E+03	3.55E+00	19	9.39E+02	3.85E+01	3.41E+00
148-79-8	4	2.54E+03	3.54E+00	21	4.88E+02	2.98E+01	5.21E+00
76738-62-0	4	6.80E+02	3.51E+00	20	1.77E+02	2.89E+01	3.83E+00
140-11-4	4	1.80E+03	3.40E+00	20	3.10E+02	3.16E+01	5.81E+00
532-27-4	4	1.07E+02	3.39E+00	27	3.68E+01	1.96E+01	2.90E+00
56-23-5	4	4.96E+03	3.38E+00	18	5.77E+02	6.34E+01	8.59E+00
54-31-9	4	1.70E+03	3.37E+00	18	5.19E+02	3.54E+01	3.28E+00
2164-17-2	4	1.27E+03	3.36E+00	20	2.78E+02	3.46E+01	4.59E+00
88-74-4	4	1.36E+03	3.35E+00	25	4.44E+02	2.47E+01	3.07E+00
7803-57-8	4	6.97E+01	3.30E+00	24	3.41E+01	2.16E+01	2.04E+00
110-80-5	4	1.94E+03	3.30E+00	18	6.55E+02	3.14E+01	2.97E+00
2595-54-2	4	5.98E+01	3.28E+00	27	2.61E+01	1.88E+01	2.29E+00
124-40-3	4	3.36E+02	3.28E+00	21	9.36E+01	1.91E+01	3.59E+00
95-82-9	4	2.45E+03	3.18E+00	19	5.00E+02	3.71E+01	4.90E+00
1918-00-9	4	1.65E+03	3.15E+00	20	3.46E+02	3.11E+01	4.77E+00

112-34-5	4	3.12E+03	3.06E+00	18	7.75E+02	4.88E+01	4.03E+00
100-63-0	4	1.20E+02	3.05E+00	24	5.26E+01	2.44E+01	2.29E+00
111-91-1	4	1.30E+02	2.96E+00	27	4.36E+01	1.71E+01	2.97E+00
101-77-9	4	3.14E+02	2.95E+00	24	1.11E+02	2.61E+01	2.82E+00
141-43-5	4	9.30E+02	2.94E+00	20	2.32E+02	2.96E+01	4.01E+00
94-11-1	4	7.37E+02	2.90E+00	22	2.27E+02	2.13E+01	3.25E+00
140-56-7	4	1.17E+02	2.87E+00	27	3.99E+01	1.64E+01	2.94E+00
108-90-7	4	1.82E+03	2.79E+00	19	5.34E+02	3.37E+01	3.41E+00
67-56-1	4	7.67E+03	2.76E+00	18	9.17E+02	6.40E+01	8.36E+00
2702-72-9	4	6.39E+02	2.75E+00	22	1.51E+02	3.21E+01	4.24E+00
101-27-9	4	3.95E+02	2.73E+00	22	1.42E+02	2.52E+01	2.79E+00
280-57-9	4	1.35E+03	2.68E+00	20	2.77E+02	3.03E+01	4.86E+00
957-51-7	4	8.86E+02	2.64E+00	20	1.94E+02	3.26E+01	4.57E+00
532-32-1	4	2.26E+03	2.60E+00	19	5.19E+02	3.67E+01	4.35E+00
51707-55-2	4	4.47E+03	2.59E+00	18	9.26E+02	4.12E+01	4.83E+00
64-17-5	4	5.75E+03	2.55E+00	16	1.02E+03	4.01E+01	5.66E+00
137-30-4	4	3.18E+02	2.53E+00	24	1.20E+02	2.11E+01	2.65E+00
111-41-1	4	2.38E+03	2.50E+00	18	7.30E+02	3.36E+01	3.26E+00
51-75-2	4	8.80E+00	2.48E+00	27	6.59E+00	2.25E+01	1.33E+00
98-09-9	4	1.00E+03	2.46E+00	20	2.53E+02	2.97E+01	3.96E+00
75-15-0	4	2.06E+03	2.43E+00	18	6.03E+02	3.63E+01	3.42E+00
107-98-2	4	6.85E+03	2.41E+00	7	3.69E+03	1.46E+01	1.86E+00
100-51-6	4	1.50E+03	2.38E+00	20	3.53E+02	3.06E+01	4.24E+00
68-11-1	4	1.43E+02	2.31E+00	24	5.73E+01	2.42E+01	2.49E+00
79-19-6	4	1.24E+01	2.28E+00	27	7.96E+00	2.72E+01	1.56E+00
50-31-7	4	7.35E+02	2.22E+00	22	2.17E+02	2.58E+01	3.39E+00
110-63-4	4	1.76E+03	2.17E+00	18	5.19E+02	3.59E+01	3.39E+00
98-94-2	4	4.35E+02	2.11E+00	22	1.39E+02	2.51E+01	3.12E+00
693-21-0	4	8.97E+02	2.03E+00	20	2.97E+02	2.97E+01	3.03E+00
97-23-4	4	1.39E+03	2.00E+00	20	2.99E+02	3.02E+01	4.66E+00
2698-41-1	4	1.98E+02	1.96E+00	24	6.76E+01	2.03E+01	2.92E+00
106-49-0	4	3.13E+02	1.96E+00	31	1.27E+02	1.56E+01	2.46E+00
2545-60-0	4	1.76E+03	1.95E+00	20	3.69E+02	3.13E+01	4.76E+00
101-42-8	4	4.61E+03	1.95E+00	7	3.30E+03	1.37E+01	1.40E+00
2274-67-1	4	1.30E+02	1.95E+00	36	6.95E+01	1.77E+01	1.87E+00
75-87-6	4	9.49E+02	1.93E+00	20	2.34E+02	2.97E+01	4.06E+00
108-86-1	4	2.45E+03	1.93E+00	18	6.65E+02	3.70E+01	3.69E+00
80-05-7	4	2.73E+03	1.85E+00	18	6.71E+02	3.21E+01	4.06E+00
70-30-4	4	5.42E+01	1.66E+00	27	2.54E+01	1.82E+01	2.14E+00
121-79-9	4	2.22E+03	1.64E+00	20	5.39E+02	3.53E+01	4.12E+00
18181-70-9	4	2.54E+03	1.60E+00	18	6.79E+02	3.63E+01	3.75E+00
110-65-6	4	1.19E+02	1.56E+00	27	3.99E+01	1.67E+01	3.00E+00
1912-24-9	4	9.27E+02	1.56E+00	21	2.59E+02	2.84E+01	3.58E+00
107-07-3	4	8.63E+01	1.40E+00	27	3.24E+01	1.94E+01	2.66E+00
141-78-6	4	5.00E+03	1.40E+00	18	8.76E+02	6.34E+01	5.71E+00
75-47-8	4	4.37E+02	1.40E+00	22	1.38E+02	1.99E+01	3.16E+00

57-30-7	4	1.68E+02	1.39E+00	25	6.02E+01	1.95E+01	2.78E+00
95-76-1	4	6.55E+02	1.36E+00	22	2.33E+02	2.58E+01	2.81E+00
26087-47-8	4	4.75E+02	1.35E+00	23	1.47E+02	2.53E+01	3.24E+00
107-41-5	4	3.18E+03	1.31E+00	18	7.87E+02	3.79E+01	4.04E+00
101-80-4	4	6.99E+02	1.18E+00	21	2.25E+02	2.58E+01	3.11E+00
2155-70-6	4	1.55E+02	1.09E+00	24	5.29E+01	1.96E+01	2.93E+00
13356-08-6	3	2.99E+01	4.07E+10	20	2.14E+02	6.17E+01	1.40E-01
683-18-1	3	5.59E+00	9.71E+05	27	2.30E+01	2.95E+01	2.43E-01
110-82-7	3	3.03E+02	1.99E+05	18	2.26E+02	4.38E+01	1.34E+00
51207-31-9	3	3.32E-01	1.71E+05	15	2.17E+00	4.09E+01	1.53E-01
18854-01-8	3	4.59E+02	8.74E+04	24	3.50E+01	3.40E+01	1.31E+01
598-55-0	3	6.88E+02	2.98E+04	32	3.62E+01	2.85E+01	1.90E+01
112-24-3	3	8.09E+02	8.03E+03	22	5.05E+01	4.00E+01	1.60E+01
52-24-4	3	2.75E+01	2.62E+03	35	4.66E+01	2.14E+01	5.90E-01
68359-37-5	3	5.35E+02	1.68E+03	27	4.32E+01	3.87E+01	1.24E+01
78-83-1	3	8.61E+02	1.32E+03	18	2.95E+02	3.44E+01	2.92E+00
70124-77-5	3	2.40E+02	1.19E+03	28	1.29E+02	2.88E+01	1.85E+00
950-35-6	3	8.29E+00	8.70E+02	19	4.58E+00	3.77E+01	1.81E+00
2782-70-9	3	6.19E+02	4.89E+02	24	8.94E+01	3.81E+01	6.93E+00
2636-26-2	3	1.50E+02	4.03E+02	26	3.21E+01	2.36E+01	4.66E+00
2227-17-0	3	2.43E+03	3.10E+02	23	6.38E+02	2.67E+01	3.80E+00
67-66-3	3	2.38E+02	2.71E+02	24	3.50E+01	3.59E+01	6.80E+00
140-29-4	3	4.97E+01	2.60E+02	24	3.04E+01	3.39E+01	1.63E+00
2385-85-5	3	4.13E+02	1.90E+02	25	1.48E+02	4.36E+01	2.78E+00
78-34-2	3	3.28E+01	1.55E+02	27	2.79E+01	2.61E+01	1.18E+00
144-49-0	3	2.48E+00	1.37E+02	23	3.69E+00	2.20E+01	6.73E-01
298-59-9	3	2.66E+02	1.03E+02	24	5.17E+01	3.29E+01	5.15E+00
16118-49-3	3	2.28E+03	1.01E+02	18	3.34E+02	3.62E+01	6.84E+00
54-11-5	3	1.15E+01	1.00E+02	27	1.69E+01	3.71E+01	6.83E-01
119168-77-3	3	1.73E+02	9.94E+01	22	6.79E+01	2.88E+01	2.54E+00
19044-88-3	3	2.15E+03	8.84E+01	9	4.62E+02	3.07E+01	4.66E+00
639-58-7	3	7.99E+01	8.27E+01	26	3.69E+01	2.06E+01	2.16E+00
103-85-5	3	1.06E+01	7.91E+01	23	5.67E+00	1.47E+01	1.87E+00
67-20-9	3	2.26E+02	7.53E+01	25	4.92E+01	2.30E+01	4.59E+00
63284-71-9	3	6.30E+02	7.45E+01	30	1.82E+02	2.46E+01	3.45E+00
95-50-1	3	1.03E+03	6.85E+01	22	1.53E+02	3.74E+01	6.72E+00
93106-60-6	3	2.37E+03	6.40E+01	19	6.34E+02	5.03E+01	3.73E+00
953-17-3	3	1.43E+02	6.37E+01	28	5.18E+01	2.29E+01	2.76E+00
34205-21-5	3	2.71E+03	5.37E+01	19	3.09E+02	6.19E+01	8.80E+00
930-55-2	3	4.86E+02	5.32E+01	22	7.71E+01	3.43E+01	6.31E+00
60207-31-0	3	3.40E+02	4.78E+01	23	1.94E+02	3.77E+01	1.75E+00
126-98-7	3	3.20E+01	4.77E+01	24	1.29E+01	2.22E+01	2.47E+00
1024-57-3	3	4.38E+01	4.60E+01	27	1.81E+01	1.55E+01	2.42E+00
103-90-2	3	1.20E+03	4.17E+01	20	1.60E+02	4.01E+01	7.50E+00
85-00-7	3	1.66E+02	4.01E+01	25	8.40E+01	2.47E+01	1.98E+00
50-18-0	3	2.19E+02	4.00E+01	28	5.31E+01	2.94E+01	4.12E+00

16568-02-8	3	1.77E+02	3.99E+01	23	8.13E+01	2.98E+01	2.17E+00
76-87-9	3	6.38E+01	3.59E+01	27	4.22E+01	3.03E+01	1.51E+00
2779-66-0	3	2.38E+02	3.27E+01	25	7.45E+01	2.80E+01	3.19E+00
89-63-4	3	9.86E+02	3.15E+01	22	2.06E+02	4.23E+01	4.80E+00
106-46-7	3	1.61E+03	3.04E+01	22	3.55E+02	4.95E+01	4.54E+00
299-85-4	3	4.25E+02	3.04E+01	25	1.25E+02	4.23E+01	3.41E+00
741-58-2	3	8.33E+02	2.67E+01	26	4.43E+02	2.89E+01	1.88E+00
2163-80-6	3	2.78E+02	2.59E+01	20	8.47E+01	2.50E+01	3.28E+00
94361-06-5	3	3.78E+02	2.55E+01	31	1.13E+02	2.39E+01	3.35E+00
24691-80-3	3	4.26E+03	2.54E+01	17	7.42E+02	4.71E+01	5.74E+00
137-26-8	3	6.09E+02	2.45E+01	21	1.80E+02	2.41E+01	3.39E+00
150-69-6	3	2.08E+03	2.45E+01	20	2.86E+02	4.19E+01	7.26E+00
100-52-7	3	6.76E+02	2.18E+01	20	1.17E+02	3.84E+01	5.80E+00
7696-12-0	3	2.85E+03	2.14E+01	20	3.89E+02	4.00E+01	7.34E+00
85-68-7	3	5.11E+03	2.11E+01	18	5.38E+02	7.82E+01	9.50E+00
64-18-6	3	1.47E+03	2.08E+01	20	2.47E+02	3.48E+01	5.96E+00
121-87-9	3	2.44E+03	1.82E+01	18	3.82E+02	4.13E+01	6.38E+00
122-39-4	3	7.95E+02	1.78E+01	20	3.16E+02	4.00E+01	2.52E+00
128-04-1	3	7.66E+02	1.68E+01	21	2.20E+02	2.42E+01	3.48E+00
68694-11-1	3	9.65E+02	1.64E+01	21	4.60E+02	3.13E+01	2.10E+00
2216-51-5	3	2.08E+03	1.62E+01	19	7.55E+02	4.18E+01	2.75E+00
56-75-7	3	1.23E+03	1.60E+01	20	3.68E+02	4.12E+01	3.35E+00
2642-71-9	3	1.42E+01	1.53E+01	27	1.09E+01	1.54E+01	1.30E+00
140-88-5	3	8.11E+02	1.44E+01	20	2.62E+02	2.55E+01	3.09E+00
6164-98-3	3	2.52E+02	1.42E+01	24	8.17E+01	2.87E+01	3.08E+00
10318-26-0	3	7.19E+02	1.32E+01	21	2.02E+02	2.38E+01	3.56E+00
288-32-4	3	5.28E+02	1.30E+01	24	1.65E+02	4.19E+01	3.21E+00
548-62-9	3	1.82E+02	1.28E+01	23	4.74E+01	2.08E+01	3.84E+00
80-08-0	3	4.22E+02	1.27E+01	20	1.09E+02	3.72E+01	3.87E+00
101-21-3	3	2.80E+03	1.25E+01	18	6.12E+02	4.52E+01	4.57E+00
2532-49-2	3	1.39E+02	1.18E+01	26	4.30E+01	2.25E+01	3.24E+00
59-92-7	3	1.37E+03	1.11E+01	19	5.18E+02	3.05E+01	2.64E+00
3120-74-9	3	2.28E+03	1.11E+01	20	3.34E+02	4.21E+01	6.84E+00
12122-67-7	3	3.97E+03	1.11E+01	18	4.54E+02	7.15E+01	8.75E+00
95-48-7	3	7.59E+02	1.09E+01	20	1.54E+02	3.36E+01	4.93E+00
4901-51-3	3	3.10E+02	1.07E+01	25	9.98E+01	3.76E+01	3.11E+00
1490-04-6	3	2.01E+03	1.07E+01	19	6.77E+02	4.14E+01	2.97E+00
111-36-4	3	2.82E+02	1.06E+01	23	7.59E+01	3.78E+01	3.72E+00
709-98-8	3	5.44E+02	1.05E+01	22	1.33E+02	3.55E+01	4.09E+00
111-70-6	3	1.46E+03	1.04E+01	18	5.57E+02	3.58E+01	2.62E+00
136-25-4	3	1.42E+03	1.04E+01	21	3.27E+02	3.25E+01	4.36E+00
97-02-9	3	4.80E+02	1.02E+01	23	1.26E+02	4.15E+01	3.81E+00
2674-91-1	3	1.06E+02	1.02E+01	27	3.26E+01	2.76E+01	3.24E+00
107-13-1	3	5.23E+01	1.00E+01	27	2.08E+01	2.65E+01	2.51E+00
91-20-3	3	5.71E+02	9.91E+00	22	1.25E+02	4.07E+01	4.56E+00
66-76-2	3	1.63E+02	9.76E+00	24	6.55E+01	2.83E+01	2.49E+00

51-21-8	3	6.10E+01	9.74E+00	19	3.34E+01	2.27E+01	1.83E+00
107-22-2	3	3.93E+02	9.50E+00	24	1.09E+02	4.00E+01	3.61E+00
15972-60-8	3	9.08E+02	9.36E+00	20	1.85E+02	3.41E+01	4.91E+00
89-61-2	3	1.36E+03	9.29E+00	19	5.23E+02	4.51E+01	2.60E+00
51249-05-9	3	4.71E+03	9.16E+00	19	8.08E+02	4.50E+01	5.83E+00
123-03-5	3	2.05E+02	9.10E+00	24	6.27E+01	2.20E+01	3.27E+00
563-12-2	3	2.75E+01	8.92E+00	27	1.52E+01	2.44E+01	1.81E+00
69-72-7	3	6.30E+02	8.49E+00	19	1.73E+02	3.11E+01	3.64E+00
148-18-5	3	1.04E+03	8.49E+00	21	2.73E+02	2.45E+01	3.81E+00
556-88-7	3	4.97E+03	8.42E+00	14	8.22E+02	4.35E+01	6.04E+00
14324-55-1	3	7.32E+02	8.30E+00	21	2.24E+02	2.38E+01	3.27E+00
71-23-8	3	3.39E+03	8.23E+00	18	4.63E+02	7.09E+01	7.32E+00
139-40-2	3	2.45E+03	8.21E+00	18	7.34E+02	4.45E+01	3.33E+00
51338-27-3	3	7.83E+02	8.16E+00	22	1.86E+02	3.65E+01	4.21E+00
13674-87-8	3	3.33E+03	8.06E+00	18	6.18E+02	4.36E+01	5.39E+00
13292-46-1	3	1.29E+03	7.98E+00	20	2.44E+02	3.51E+01	5.29E+00
127-00-4	3	3.62E+02	7.95E+00	24	9.67E+01	3.97E+01	3.75E+00
868-85-9	3	1.71E+03	7.86E+00	18	5.08E+02	4.31E+01	3.37E+00
124-17-4	3	3.25E+03	7.56E+00	7	2.66E+03	1.21E+01	1.22E+00
95-55-6	3	6.22E+02	7.37E+00	31	2.03E+02	2.49E+01	3.06E+00
7726-95-6	3	2.96E+03	7.30E+00	18	6.49E+02	4.41E+01	4.56E+00
100-43-6	3	1.73E+02	7.22E+00	27	5.28E+01	3.11E+01	3.28E+00
2655-19-8	3	1.79E+03	7.11E+00	18	6.05E+02	3.60E+01	2.96E+00
973-21-7	3	1.06E+02	7.04E+00	29	4.53E+01	1.91E+01	2.34E+00
54-21-7	3	9.49E+02	6.92E+00	20	2.01E+02	3.41E+01	4.72E+00
2303-17-5	3	1.19E+03	6.58E+00	21	5.71E+02	2.62E+01	2.08E+00
98-16-8	3	4.15E+02	6.54E+00	22	1.21E+02	2.87E+01	3.44E+00
84-74-2	3	6.39E+03	6.32E+00	14	8.17E+02	4.46E+01	7.82E+00
60-54-8	3	1.01E+03	6.26E+00	20	2.09E+02	3.88E+01	4.83E+00
88-73-3	3	2.45E+02	6.17E+00	23	6.52E+01	2.09E+01	3.75E+00
78-87-5	3	1.59E+03	6.15E+00	20	2.81E+02	4.08E+01	5.66E+00
97-99-4	3	1.43E+03	6.11E+00	18	5.18E+02	4.24E+01	2.77E+00
7720-78-7	3	6.96E+02	6.06E+00	22	1.82E+02	4.15E+01	3.82E+00
19750-95-9	3	3.44E+02	6.01E+00	24	1.16E+02	2.92E+01	2.97E+00
311-45-5	3	1.40E+00	5.99E+00	17	1.70E+00	1.85E+01	8.23E-01
8022-00-2	3	4.48E+01	5.98E+00	27	1.83E+01	1.93E+01	2.45E+00
500-38-9	3	1.47E+03	5.95E+00	18	4.96E+02	4.25E+01	2.97E+00
108-68-9	3	7.25E+02	5.94E+00	22	1.76E+02	3.69E+01	4.12E+00
106-44-5	3	3.40E+02	5.88E+00	24	1.09E+02	2.93E+01	3.11E+00
101-14-4	3	6.63E+02	5.86E+00	20	1.96E+02	3.85E+01	3.38E+00
99-54-7	3	8.70E+02	5.68E+00	20	3.05E+02	3.97E+01	2.85E+00
110-96-3	3	4.65E+02	5.59E+00	24	1.45E+02	4.12E+01	3.22E+00
110-49-6	3	2.24E+03	5.51E+00	18	6.93E+02	4.40E+01	3.23E+00
1071-83-6	3	3.24E+03	5.51E+00	18	6.19E+02	4.45E+01	5.24E+00
101-90-6	3	1.46E+03	5.45E+00	20	3.08E+02	3.52E+01	4.75E+00
55219-65-3	3	2.65E+03	5.36E+00	18	7.37E+02	3.73E+01	3.59E+00

107-15-3	3	8.26E+02	5.34E+00	20	2.60E+02	3.93E+01	3.18E+00
51235-04-2	3	1.49E+03	5.31E+00	19	1.04E+03	2.60E+01	1.43E+00
299-86-5	3	5.69E+02	5.28E+00	22	1.30E+02	3.93E+01	4.39E+00
75-97-8	3	9.63E+02	5.28E+00	22	3.05E+02	4.05E+01	3.16E+00
55268-74-1	3	1.86E+03	5.27E+00	18	5.71E+02	3.61E+01	3.25E+00
60-13-9	3	3.12E+01	5.25E+00	27	1.66E+01	2.28E+01	1.88E+00
18181-80-1	3	4.93E+03	5.23E+00	18	7.92E+02	7.88E+01	6.23E+00
25586-43-0	3	1.38E+03	5.13E+00	20	2.56E+02	4.01E+01	5.40E+00
95-87-4	3	5.42E+02	5.05E+00	22	1.43E+02	3.59E+01	3.80E+00
57-39-6	3	2.36E+02	5.03E+00	25	8.09E+01	2.39E+01	2.91E+00
131-52-2	3	2.01E+02	5.02E+00	24	6.86E+01	2.21E+01	2.93E+00
1918-13-4	3	4.84E+02	4.77E+00	21	1.30E+02	2.24E+01	3.74E+00
79-01-6	3	4.06E+03	4.74E+00	18	6.79E+02	4.43E+01	5.98E+00
99-59-2	3	1.34E+03	4.60E+00	20	3.08E+02	3.48E+01	4.33E+00
34014-18-1	3	4.74E+02	4.43E+00	22	1.43E+02	2.29E+01	3.32E+00
25267-15-6	3	3.09E+02	4.40E+00	24	9.71E+01	2.34E+01	3.19E+00
98-51-1	3	1.28E+03	4.36E+00	20	2.64E+02	3.49E+01	4.86E+00
104-94-9	3	1.75E+03	4.36E+00	20	3.54E+02	4.03E+01	4.96E+00
591-27-5	3	6.53E+02	4.33E+00	25	3.35E+02	2.73E+01	1.95E+00
133-07-3	3	1.66E+03	4.33E+00	19	4.59E+02	3.63E+01	3.61E+00
18530-56-8	3	3.24E+03	4.29E+00	18	4.61E+02	6.02E+01	7.03E+00
78-30-8	3	8.05E+02	4.29E+00	21	1.66E+02	2.26E+01	4.85E+00
576-26-1	3	4.53E+02	4.27E+00	23	1.69E+02	3.01E+01	2.69E+00
57-43-2	3	3.67E+02	4.12E+00	24	1.26E+02	2.92E+01	2.92E+00
107-12-0	3	3.72E+01	4.11E+00	27	2.04E+01	2.58E+01	1.82E+00
72-43-5	3	2.26E+03	4.10E+00	20	5.36E+02	4.15E+01	4.21E+00
99-35-4	3	5.13E+02	4.09E+00	23	1.61E+02	4.23E+01	3.19E+00
95-65-8	3	5.04E+02	3.85E+00	22	1.40E+02	3.56E+01	3.59E+00
79-57-2	3	3.41E+03	3.78E+00	18	8.12E+02	4.78E+01	4.20E+00
77-47-4	3	4.49E+02	3.77E+00	23	1.72E+02	2.98E+01	2.61E+00
7723-14-0	3	4.57E+00	3.70E+00	36	6.40E+00	2.41E+01	7.14E-01
77-58-7	3	1.54E+02	3.68E+00	24	5.97E+01	2.75E+01	2.58E+00
31431-39-7	3	8.27E+02	3.65E+00	20	1.97E+02	3.29E+01	4.21E+00
13067-93-1	3	2.93E+01	3.65E+00	29	1.46E+01	1.59E+01	2.01E+00
886-50-0	3	3.17E+03	3.59E+00	19	7.53E+02	3.61E+01	4.21E+00
120-36-5	3	4.04E+02	3.54E+00	23	1.18E+02	4.15E+01	3.42E+00
85-44-9	3	1.22E+03	3.47E+00	21	3.67E+02	3.86E+01	3.34E+00
111-44-4	3	1.13E+02	3.47E+00	27	4.17E+01	2.26E+01	2.71E+00
88-72-2	3	1.15E+03	3.45E+00	20	2.77E+02	3.45E+01	4.14E+00
111-77-3	3	6.27E+03	3.38E+00	4	6.09E+03	4.82E+00	1.03E+00
25013-16-5	3	1.67E+03	3.37E+00	20	3.38E+02	3.57E+01	4.93E+00
67-64-1	3	4.53E+03	3.36E+00	18	8.43E+02	4.55E+01	5.37E+00
4658-28-0	3	2.68E+03	3.34E+00	18	7.14E+02	3.73E+01	3.75E+00
97-74-5	3	6.79E+02	3.33E+00	22	2.02E+02	4.18E+01	3.37E+00
55-86-7	3	1.36E+01	3.30E+00	27	8.57E+00	1.76E+01	1.58E+00
6263-38-3	3	2.69E+03	3.28E+00	18	5.63E+02	4.34E+01	4.78E+00

563-47-3	3	9.16E+02	3.24E+00	21	3.07E+02	3.76E+01	2.98E+00
3152-41-8	3	1.31E+02	3.22E+00	29	4.80E+01	1.97E+01	2.72E+00
103-76-4	3	2.92E+03	3.07E+00	18	4.57E+02	6.82E+01	6.39E+00
645-56-7	3	4.90E+02	3.06E+00	22	1.29E+02	4.05E+01	3.80E+00
108-10-1	3	2.26E+03	3.05E+00	18	6.03E+02	4.37E+01	3.74E+00
59-67-6	3	4.91E+03	2.97E+00	16	9.78E+02	4.64E+01	5.02E+00
556-61-6	3	9.59E+01	2.97E+00	33	5.02E+01	2.29E+01	1.91E+00
298-81-7	3	5.53E+02	2.97E+00	20	1.47E+02	3.74E+01	3.75E+00
78-48-8	3	1.68E+02	2.92E+00	24	5.71E+01	3.31E+01	2.94E+00
590-86-3	3	4.22E+03	2.91E+00	18	8.01E+02	7.82E+01	5.27E+00
68-89-3	3	1.50E+03	2.90E+00	20	3.35E+02	3.53E+01	4.47E+00
115-31-1	3	7.03E+02	2.87E+00	20	2.64E+02	4.80E+01	2.66E+00
94-80-4	3	5.84E+02	2.79E+00	23	1.58E+02	3.93E+01	3.69E+00
106-50-3	3	1.05E+02	2.75E+00	36	6.38E+01	2.33E+01	1.65E+00
100-66-3	3	3.16E+03	2.74E+00	18	7.35E+02	4.49E+01	4.30E+00
1445-75-6	3	1.09E+03	2.72E+00	23	3.67E+02	2.92E+01	2.96E+00
1401-55-4	3	4.65E+03	2.72E+00	18	6.33E+02	7.26E+01	7.35E+00
518-75-2	3	1.02E+02	2.67E+00	21	3.48E+01	1.74E+01	2.92E+00
67-63-0	3	4.88E+03	2.66E+00	18	8.74E+02	4.79E+01	5.58E+00
2961-62-8	3	1.37E+02	2.63E+00	26	4.97E+01	2.21E+01	2.75E+00
75-56-9	3	4.80E+02	2.62E+00	22	1.38E+02	4.03E+01	3.49E+00
99-30-9	3	1.73E+03	2.58E+00	20	3.86E+02	4.14E+01	4.49E+00
82-68-8	3	1.07E+03	2.58E+00	20	3.19E+02	3.42E+01	3.36E+00
126-73-8	3	1.23E+03	2.53E+00	21	2.99E+02	3.22E+01	4.13E+00
107-18-6	3	7.05E+01	2.52E+00	27	3.10E+01	2.15E+01	2.27E+00
94-74-6	3	5.99E+02	2.48E+00	20	1.50E+02	3.74E+01	3.98E+00
111-42-2	3	2.44E+03	2.45E+00	16	8.25E+02	3.44E+01	2.96E+00
95-95-4	3	7.89E+02	2.38E+00	20	1.89E+02	3.82E+01	4.19E+00
120-51-4	3	2.19E+03	2.37E+00	19	5.47E+02	5.39E+01	4.01E+00
34681-23-7	3	3.59E+02	2.37E+00	23	1.10E+02	1.48E+01	3.27E+00
68-12-2	3	3.74E+03	2.34E+00	18	7.83E+02	4.42E+01	4.78E+00
28249-77-6	3	7.03E+02	2.33E+00	21	1.82E+02	2.59E+01	3.87E+00
99-66-1	3	8.47E+02	2.29E+00	20	2.59E+02	3.90E+01	3.27E+00
132-27-4	3	6.52E+02	2.29E+00	21	2.07E+02	3.64E+01	3.16E+00
107-05-1	3	3.98E+02	2.28E+00	22	1.24E+02	2.23E+01	3.21E+00
19937-59-8	3	2.11E+03	2.27E+00	18	6.03E+02	3.67E+01	3.49E+00
646-06-0	3	4.04E+03	2.27E+00	18	8.07E+02	4.46E+01	5.00E+00
99-99-0	3	1.62E+03	2.27E+00	20	3.51E+02	3.55E+01	4.61E+00
102-01-2	3	3.20E+03	2.26E+00	18	7.46E+02	4.37E+01	4.29E+00
95-53-4	3	6.58E+02	2.25E+00	20	1.73E+02	3.27E+01	3.80E+00
90-04-0	3	1.12E+03	2.24E+00	20	3.24E+02	3.43E+01	3.46E+00
95-94-3	3	1.36E+03	2.23E+00	20	3.05E+02	3.49E+01	4.45E+00
16423-68-0	3	1.65E+03	2.18E+00	21	3.58E+02	3.90E+01	4.60E+00
97-53-0	3	2.31E+03	2.18E+00	18	6.56E+02	4.36E+01	3.52E+00
868-77-9	3	4.26E+03	2.18E+00	18	8.42E+02	4.58E+01	5.06E+00
26444-49-5	3	1.33E+03	2.16E+00	18	3.36E+02	5.58E+01	3.95E+00

91-64-5	3	2.26E+02	2.13E+00	23	8.53E+01	4.03E+01	2.65E+00
541-85-5	3	3.22E+03	2.11E+00	18	7.84E+02	4.73E+01	4.10E+00
89-83-8	3	8.20E+02	2.11E+00	20	2.00E+02	3.85E+01	4.11E+00
134-62-3	3	1.49E+03	2.11E+00	20	3.33E+02	3.52E+01	4.48E+00
2439-01-2	3	1.17E+03	2.10E+00	20	2.95E+02	3.98E+01	3.98E+00
504-29-0	3	1.57E+02	2.06E+00	32	8.07E+01	2.27E+01	1.94E+00
111-15-9	3	2.18E+03	2.06E+00	18	5.26E+02	5.81E+01	4.15E+00
111-92-2	3	2.33E+02	2.06E+00	24	8.70E+01	3.90E+01	2.67E+00
95-54-5	3	4.07E+02	1.94E+00	22	1.29E+02	4.04E+01	3.15E+00
1420-07-1	3	2.43E+01	1.93E+00	27	1.16E+01	1.78E+01	2.09E+00
60-34-4	3	2.73E+01	1.93E+00	28	1.64E+01	2.41E+01	1.66E+00
79-46-9	3	4.81E+02	1.86E+00	22	1.40E+02	2.28E+01	3.43E+00
134-20-3	3	3.16E+03	1.86E+00	18	7.70E+02	4.71E+01	4.11E+00
107-19-7	3	5.00E+01	1.85E+00	27	2.34E+01	2.60E+01	2.13E+00
1948-33-0	3	8.21E+02	1.84E+00	20	2.46E+02	3.88E+01	3.33E+00
78-40-0	3	1.30E+03	1.83E+00	20	3.03E+02	4.00E+01	4.29E+00
121-33-5	3	1.64E+03	1.81E+00	18	4.90E+02	4.23E+01	3.34E+00
94-96-2	3	2.13E+03	1.80E+00	18	5.13E+02	4.21E+01	4.14E+00
108-20-3	3	3.73E+03	1.79E+00	18	8.19E+02	4.70E+01	4.55E+00
488-41-5	3	1.31E+03	1.78E+00	20	3.41E+02	3.47E+01	3.84E+00
96-09-3	3	1.82E+03	1.75E+00	20	3.82E+02	4.13E+01	4.76E+00
64-00-6	3	1.45E+01	1.75E+00	29	8.34E+00	1.44E+01	1.74E+00
24549-06-2	3	8.32E+02	1.67E+00	21	2.67E+02	2.97E+01	3.12E+00
41814-78-2	3	2.70E+02	1.65E+00	24	8.65E+01	2.29E+01	3.12E+00
1134-23-2	3	1.51E+03	1.64E+00	20	3.35E+02	4.07E+01	4.51E+00
109-06-8	3	7.83E+02	1.63E+00	20	2.00E+02	3.83E+01	3.92E+00
2528-36-1	3	2.05E+03	1.60E+00	19	5.39E+02	3.35E+01	3.80E+00
88-06-2	3	8.58E+02	1.58E+00	20	2.18E+02	3.86E+01	3.93E+00
2961-68-4	3	1.16E+02	1.57E+00	26	4.72E+01	2.15E+01	2.46E+00
2303-16-4	3	4.39E+02	1.57E+00	22	1.25E+02	5.74E+01	3.52E+00
50-00-0	3	2.27E+02	1.55E+00	24	7.64E+01	3.88E+01	2.97E+00
55-18-5	3	2.32E+02	1.53E+00	24	7.83E+01	3.90E+01	2.96E+00
92-52-4	3	2.18E+03	1.51E+00	18	5.27E+02	4.24E+01	4.14E+00
1836-75-5	3	2.13E+03	1.47E+00	18	5.47E+02	3.66E+01	3.89E+00
3811-49-2	3	9.96E+01	1.47E+00	29	4.15E+01	1.90E+01	2.40E+00
100-47-0	3	8.53E+02	1.46E+00	19	2.72E+02	3.18E+01	3.14E+00
27344-41-8	3	5.49E+03	1.41E+00	19	8.93E+02	7.24E+01	6.15E+00
93-78-7	3	4.97E+02	1.41E+00	22	1.54E+02	2.28E+01	3.23E+00
306-52-5	3	9.01E+02	1.41E+00	20	2.33E+02	3.88E+01	3.87E+00
109-73-9	3	4.08E+02	1.37E+00	22	1.32E+02	4.01E+01	3.08E+00
79-41-4	3	1.17E+03	1.34E+00	20	3.12E+02	3.44E+01	3.74E+00
96-18-4	3	3.63E+02	1.21E+00	19	1.06E+02	1.92E+01	3.41E+00
3810-74-0	3	4.20E+02	1.15E+00	23	1.43E+02	3.85E+01	2.94E+00
3309-87-3	3	9.80E+01	1.13E+00	27	3.73E+01	2.20E+01	2.63E+00
103-82-2	3	2.25E+03	1.00E+00	18	5.73E+02	4.33E+01	3.93E+00
510-15-6	3	7.00E+02	1.00E+00	21	2.08E+02	3.64E+01	3.37E+00

59-87-0	2	9.93E+00	2.53E+22	22	1.11E+02	9.25E+01	8.94E-02
1646-88-4	2	8.19E+02	2.27E+20	27	1.99E+01	4.71E+01	4.12E+01
67-45-8	2	6.50E+01	4.43E+19	18	3.06E+02	9.67E+01	2.13E-01
97-77-8	2	3.10E+01	5.78E+18	19	1.72E+02	9.22E+01	1.80E-01
2917-19-3	2	9.85E+02	2.22E+16	27	3.51E+01	4.89E+01	2.80E+01
90-02-8	2	3.41E+01	8.66E+14	22	1.15E+02	8.46E+01	2.96E-01
57117-31-4	2	9.57E-02	2.44E+12	11	1.07E+00	1.09E+02	8.93E-02
1420-06-0	2	6.32E+02	1.35E+11	27	4.60E+01	5.55E+01	1.37E+01
481-39-0	2	1.67E+01	2.67E+10	24	4.29E+01	7.10E+01	3.90E-01
82657-04-3	2	3.13E+02	3.89E+09	28	1.87E+02	3.05E+01	1.67E+00
4553-62-2	2	5.28E+01	1.34E+09	23	5.47E+01	5.28E+01	9.66E-01
18472-87-2	2	1.61E+03	1.12E+09	18	1.21E+02	4.87E+01	1.34E+01
120-32-1	2	3.32E+02	8.92E+08	22	5.46E+01	4.06E+01	6.09E+00
79-21-0	2	4.58E+01	2.23E+08	18	6.11E+01	4.01E+01	7.50E-01
52-60-8	2	8.19E+01	2.20E+08	25	2.52E+01	2.92E+01	3.25E+00
108-91-8	2	4.96E+01	1.84E+08	27	3.02E+01	3.47E+01	1.65E+00
123-54-6	2	2.29E+02	6.54E+07	27	9.11E+01	3.75E+01	2.51E+00
148-24-3	2	4.90E+03	5.19E+07	18	3.42E+02	8.89E+01	1.43E+01
149-30-4	2	3.90E+02	2.92E+07	27	1.30E+02	4.15E+01	3.00E+00
61-82-5	2	4.02E+03	1.29E+07	19	3.12E+02	8.87E+01	1.29E+01
95-33-0	2	1.46E+03	1.22E+07	20	2.01E+02	4.89E+01	7.23E+00
70-25-7	2	3.10E+02	6.14E+06	28	4.73E+01	5.09E+01	6.56E+00
55-80-1	2	5.15E+03	5.86E+06	18	3.89E+02	8.92E+01	1.32E+01
100-42-5	2	1.07E+03	5.03E+06	20	1.64E+02	4.74E+01	6.54E+00
27304-13-8	2	1.35E+02	4.78E+06	24	3.63E+01	3.98E+01	3.72E+00
79-10-7	2	7.13E+02	4.56E+06	24	2.16E+02	5.47E+01	3.31E+00
935-95-5	2	2.95E+02	3.76E+06	20	4.07E+01	3.61E+01	7.25E+00
57-41-0	2	4.95E+02	3.55E+06	21	8.40E+01	4.17E+01	5.89E+00
20856-57-9	2	7.91E+02	2.06E+06	18	4.28E+02	8.37E+01	1.85E+00
55-37-8	2	3.21E+02	1.71E+06	24	7.30E+01	3.01E+01	4.40E+00
7542-37-2	2	7.01E+03	1.49E+06	16	6.73E+02	6.13E+01	1.04E+01
74-95-3	2	3.29E+02	1.27E+06	27	5.56E+01	4.81E+01	5.91E+00
71751-41-2	2	4.52E+00	1.11E+06	21	6.43E+00	2.69E+01	7.03E-01
126-72-7	2	2.35E+03	6.83E+05	19	2.48E+02	8.58E+01	9.45E+00
99-97-8	2	4.03E+02	6.79E+05	21	7.58E+01	4.07E+01	5.31E+00
27554-26-3	2	7.80E+03	4.82E+05	16	7.80E+02	6.21E+01	1.00E+01
69409-94-5	2	7.30E+02	4.38E+05	24	2.17E+02	5.42E+01	3.37E+00
120-83-2	2	3.62E+02	2.93E+05	24	1.43E+02	4.64E+01	2.54E+00
27949-52-6	2	3.23E+02	2.71E+05	21	6.62E+01	3.98E+01	4.88E+00
3778-73-2	2	3.79E+02	2.22E+05	24	1.47E+02	4.65E+01	2.57E+00
26140-60-3	2	5.02E+03	2.00E+05	18	4.43E+02	8.92E+01	1.13E+01
141-32-2	2	2.30E+03	1.40E+05	19	2.63E+02	8.58E+01	8.75E+00
2425-10-7	2	1.15E+02	1.20E+05	24	3.55E+01	3.85E+01	3.23E+00
98-82-8	2	5.07E+03	1.15E+05	18	4.57E+02	8.93E+01	1.11E+01
4005-51-0	2	6.21E+02	8.43E+04	24	2.06E+02	5.14E+01	3.01E+00
135-88-6	2	3.56E+03	8.37E+04	18	3.84E+02	5.39E+01	9.27E+00

96-24-2	2	6.18E+01	5.62E+04	27	3.22E+01	3.12E+01	1.92E+00
142-96-1	2	1.35E+03	5.56E+04	20	2.26E+02	4.71E+01	5.95E+00
140-89-6	2	7.24E+02	4.83E+04	20	1.41E+02	4.48E+01	5.14E+00
72-54-8	2	2.60E+02	3.79E+04	24	1.07E+02	4.46E+01	2.44E+00
7440-38-2	2	3.32E+02	3.65E+04	21	7.22E+01	3.95E+01	4.60E+00
106-51-4	2	5.70E+01	3.32E+04	24	2.03E+01	3.54E+01	2.81E+00
2275-14-1	2	9.84E+01	2.59E+04	27	4.44E+01	3.35E+01	2.21E+00
314-40-9	2	1.37E+03	2.43E+04	22	3.71E+02	5.70E+01	3.68E+00
2631-40-5	2	2.06E+02	1.97E+04	23	5.67E+01	4.17E+01	3.63E+00
58-14-0	2	2.01E+02	1.96E+04	23	5.57E+01	4.16E+01	3.61E+00
1461-25-2	2	2.76E+03	1.83E+04	18	3.31E+02	8.58E+01	8.33E+00
619-72-7	2	6.48E+01	1.68E+04	27	3.30E+01	3.12E+01	1.97E+00
1955-45-9	2	6.82E+02	1.64E+04	20	1.39E+02	4.44E+01	4.89E+00
21564-17-0	2	9.43E+02	1.32E+04	20	1.80E+02	4.55E+01	5.23E+00
3942-54-9	2	3.12E+02	1.03E+04	23	7.94E+01	4.31E+01	3.92E+00
1610-18-0	2	1.04E+03	9.91E+03	22	2.98E+02	5.53E+01	3.50E+00
15457-05-3	2	2.60E+03	9.41E+03	20	3.98E+02	4.95E+01	6.53E+00
999-61-1	2	5.14E+02	8.93E+03	24	1.79E+02	4.73E+01	2.88E+00
108-70-3	2	1.64E+03	8.45E+03	19	5.27E+02	5.26E+01	3.11E+00
138261-41-3	2	2.00E+02	8.40E+03	23	5.67E+01	4.14E+01	3.54E+00
101-68-8	2	4.50E+03	8.38E+03	16	6.22E+02	5.92E+01	7.23E+00
10453-86-8	2	6.11E+02	7.95E+03	20	1.31E+02	4.39E+01	4.66E+00
38260-54-7	2	8.87E+02	7.62E+03	20	1.75E+02	4.52E+01	5.07E+00
106-92-3	2	7.90E+02	7.43E+03	20	1.60E+02	4.47E+01	4.93E+00
18559-94-9	2	1.34E+03	7.42E+03	19	4.50E+02	5.16E+01	2.97E+00
481-42-5	2	3.22E+01	6.98E+03	27	1.42E+01	2.79E+01	2.28E+00
108-83-8	2	2.85E+03	6.96E+03	20	4.32E+02	4.99E+01	6.61E+00
616-45-5	2	3.24E+03	6.46E+03	18	3.92E+02	8.45E+01	8.27E+00
1120-71-4	2	2.00E+02	6.33E+03	27	7.63E+01	3.57E+01	2.62E+00
260-94-6	2	1.00E+03	6.33E+03	20	1.93E+02	4.56E+01	5.18E+00
124-63-0	2	1.00E+02	6.33E+03	27	4.45E+01	3.34E+01	2.25E+00
5103-71-9	2	2.50E+02	6.33E+03	23	6.77E+01	4.21E+01	3.69E+00
1982-42-9	2	6.00E+02	6.33E+03	20	1.30E+02	4.38E+01	4.60E+00
5103-74-2	2	5.50E+02	6.33E+03	20	1.22E+02	4.35E+01	4.51E+00
554-00-7	2	8.00E+02	6.33E+03	20	1.63E+02	4.48E+01	4.92E+00
8004-87-3	2	2.08E+02	5.69E+03	23	5.89E+01	4.15E+01	3.53E+00
115-19-5	2	9.87E+02	5.39E+03	20	1.92E+02	4.55E+01	5.14E+00
88-75-5	2	6.58E+02	5.25E+03	23	2.38E+02	4.95E+01	2.76E+00
13684-56-5	2	4.88E+03	5.15E+03	11	2.05E+03	3.44E+01	2.38E+00
118-92-3	2	2.75E+03	5.09E+03	20	4.24E+02	4.96E+01	6.49E+00
306-37-6	2	5.10E+01	4.94E+03	27	2.09E+01	2.93E+01	2.44E+00
75-29-6	2	2.55E+03	4.94E+03	20	4.00E+02	4.93E+01	6.37E+00
88-04-0	2	1.96E+03	4.81E+03	20	3.27E+02	4.82E+01	5.99E+00
14698-29-4	2	1.73E+03	4.54E+03	19	5.41E+02	5.27E+01	3.19E+00
606-20-2	2	3.43E+02	4.30E+03	24	1.28E+02	4.54E+01	2.68E+00
75-21-8	2	1.39E+02	4.21E+03	27	3.73E+01	5.21E+01	3.74E+00

105-39-5	2	1.82E+02	3.80E+03	27	7.07E+01	3.54E+01	2.58E+00
632-22-4	2	1.52E+03	3.72E+03	19	4.89E+02	5.20E+01	3.12E+00
919-86-8	2	5.74E+01	3.65E+03	27	2.01E+01	4.86E+01	2.85E+00
79983-71-4	2	1.16E+03	3.12E+03	20	2.21E+02	4.60E+01	5.23E+00
389-08-2	2	1.08E+03	3.07E+03	20	2.10E+02	4.57E+01	5.15E+00
112-53-8	2	2.20E+03	2.96E+03	20	3.64E+02	4.86E+01	6.06E+00
116-29-0	2	1.06E+03	2.89E+03	22	1.72E+02	6.80E+01	6.19E+00
446-86-6	2	7.45E+02	2.59E+03	22	2.51E+02	4.84E+01	2.97E+00
95-01-2	2	7.43E+02	2.49E+03	22	2.50E+02	4.84E+01	2.97E+00
1174-83-0	2	1.08E+03	2.48E+03	20	2.11E+02	4.57E+01	5.11E+00
2497-07-6	2	6.48E+00	2.39E+03	23	5.43E+00	2.49E+01	1.19E+00
5827-05-4	2	4.61E+01	2.27E+03	27	2.47E+01	3.02E+01	1.86E+00
502-39-6	2	3.69E+01	2.27E+03	27	1.63E+01	2.82E+01	2.27E+00
57-15-8	2	2.77E+02	2.27E+03	23	7.51E+01	4.23E+01	3.68E+00
20427-59-2	2	1.84E+03	2.27E+03	19	8.51E+02	3.46E+01	2.17E+00
59-89-2	2	5.19E+02	2.23E+03	24	1.13E+02	7.24E+01	4.60E+00
129-00-0	2	1.47E+03	2.17E+03	20	2.69E+02	4.69E+01	5.46E+00
120-07-0	2	1.10E+03	2.05E+03	20	2.15E+02	4.57E+01	5.10E+00
110-02-1	2	7.67E+02	2.00E+03	20	1.63E+02	4.44E+01	4.69E+00
554-84-7	2	5.92E+02	1.75E+03	23	2.15E+02	4.89E+01	2.76E+00
2465-27-2	2	2.68E+02	1.55E+03	19	1.43E+02	4.27E+01	1.88E+00
759-73-9	2	5.37E+02	1.55E+03	23	1.98E+02	4.84E+01	2.71E+00
7173-51-5	2	1.50E+02	1.52E+03	27	6.04E+01	3.47E+01	2.49E+00
110-85-0	2	1.07E+03	1.45E+03	20	2.13E+02	4.56E+01	5.01E+00
56-34-8	2	1.48E+03	1.42E+03	20	2.74E+02	4.69E+01	5.40E+00
116255-48-2	2	6.48E+02	1.41E+03	22	2.22E+02	4.77E+01	2.92E+00
938-73-8	2	1.24E+03	1.38E+03	20	2.40E+02	4.62E+01	5.18E+00
555-84-0	2	9.51E+02	1.33E+03	19	2.69E+02	4.03E+01	3.54E+00
109-09-1	2	1.94E+02	1.29E+03	24	6.30E+01	4.30E+01	3.08E+00
100-75-4	2	3.51E+02	1.23E+03	25	8.23E+01	6.73E+01	4.27E+00
126-99-8	2	2.56E+02	1.22E+03	23	7.18E+01	4.19E+01	3.57E+00
105-11-3	2	8.12E+02	1.17E+03	22	2.64E+02	4.87E+01	3.08E+00
59-50-7	2	1.05E+03	1.14E+03	20	2.12E+02	4.55E+01	4.95E+00
25155-30-0	2	7.63E+02	1.11E+03	22	2.51E+02	4.84E+01	3.04E+00
14484-64-1	2	1.96E+03	1.05E+03	19	5.75E+02	5.29E+01	3.41E+00
544-25-2	2	9.87E+01	1.03E+03	27	4.35E+01	3.33E+01	2.27E+00
59-97-2	2	6.93E+02	1.03E+03	20	1.55E+02	4.40E+01	4.48E+00
96-33-3	2	4.79E+02	9.98E+02	23	1.79E+02	4.79E+01	2.68E+00
23950-58-5	2	5.79E+03	9.97E+02	18	6.04E+02	8.62E+01	9.58E+00
61-73-4	2	2.03E+03	9.58E+02	18	5.61E+02	5.29E+01	3.62E+00
35256-85-0	2	3.49E+03	9.52E+02	18	8.23E+02	8.87E+01	4.23E+00
121-14-2	2	4.60E+02	9.21E+02	24	1.58E+02	4.66E+01	2.91E+00
1702-17-6	2	2.51E+03	8.97E+02	22	5.76E+02	4.00E+01	4.36E+00
10048-13-2	2	7.01E+01	8.81E+02	26	3.11E+01	2.74E+01	2.26E+00
125-12-2	2	5.30E+03	8.67E+02	16	8.02E+02	6.06E+01	6.60E+00
5470-11-1	2	2.40E+02	8.19E+02	24	9.41E+01	4.38E+01	2.55E+00

509-14-8	2	2.21E+02	8.04E+02	24	8.81E+01	4.34E+01	2.51E+00
13231-90-8	2	2.48E+02	7.90E+02	24	9.65E+01	4.39E+01	2.57E+00
139-13-9	2	1.86E+03	7.83E+02	19	5.50E+02	5.26E+01	3.39E+00
13286-32-3	2	3.90E+02	7.77E+02	20	1.00E+02	4.20E+01	3.89E+00
105-67-9	2	1.36E+03	7.33E+02	20	2.63E+02	4.65E+01	5.18E+00
2307-68-8	2	3.03E+03	7.17E+02	18	5.71E+02	5.21E+01	5.30E+00
26264-06-2	2	2.19E+03	7.13E+02	18	5.90E+02	5.32E+01	3.71E+00
99-57-0	2	1.43E+03	7.02E+02	20	2.73E+02	4.66E+01	5.23E+00
618-85-9	2	3.62E+02	6.81E+02	24	1.30E+02	4.55E+01	2.78E+00
500-28-7	2	4.76E+02	6.45E+02	23	1.77E+02	4.78E+01	2.69E+00
589-18-4	2	2.34E+03	6.45E+02	20	4.00E+02	4.87E+01	5.84E+00
540-59-0	2	1.28E+03	6.02E+02	19	4.09E+02	5.09E+01	3.13E+00
122-60-1	2	2.32E+03	5.94E+02	20	3.99E+02	4.87E+01	5.82E+00
127-18-4	2	4.35E+03	5.79E+02	18	5.20E+02	8.90E+01	8.36E+00
102-76-1	2	1.82E+03	5.64E+02	20	3.31E+02	4.76E+01	5.49E+00
112-36-7	2	3.03E+03	5.13E+02	18	7.29E+02	8.77E+01	4.16E+00
77732-09-3	2	1.14E+03	5.10E+02	20	2.31E+02	4.57E+01	4.91E+00
636-21-5	2	1.80E+03	5.08E+02	20	3.30E+02	4.76E+01	5.46E+00
124-04-9	2	3.10E+03	4.79E+02	18	5.88E+02	5.22E+01	5.27E+00
115-86-6	2	2.15E+03	4.72E+02	20	3.79E+02	4.83E+01	5.67E+00
7440-43-9	2	1.44E+03	4.36E+02	20	2.79E+02	4.66E+01	5.16E+00
60-56-0	2	1.39E+03	4.34E+02	20	2.72E+02	4.65E+01	5.12E+00
55290-64-7	2	7.11E+02	4.31E+02	20	1.62E+02	4.40E+01	4.38E+00
110-64-5	2	7.76E+02	4.10E+02	20	1.74E+02	4.43E+01	4.47E+00
131-17-9	2	1.06E+03	4.08E+02	19	2.18E+02	6.65E+01	4.85E+00
85-01-8	2	1.12E+03	3.89E+02	20	2.31E+02	4.56E+01	4.85E+00
109-69-3	2	3.51E+03	3.65E+02	18	4.60E+02	8.78E+01	7.62E+00
1639-66-3	2	3.02E+03	3.48E+02	18	4.18E+02	8.69E+01	7.23E+00
10380-28-6	2	6.25E+03	3.43E+02	13	7.52E+02	5.86E+01	8.32E+00
108-99-6	2	6.32E+02	3.26E+02	22	2.11E+02	4.74E+01	3.00E+00
50-65-7	2	1.58E+03	3.26E+02	20	3.03E+02	4.70E+01	5.22E+00
83164-33-4	2	3.16E+03	3.26E+02	18	4.36E+02	7.92E+01	7.26E+00
920-66-1	2	9.49E+02	3.26E+02	20	2.04E+02	4.50E+01	4.64E+00
821-55-6	2	5.02E+03	2.96E+02	18	5.89E+02	9.00E+01	8.53E+00
1129-41-5	2	1.71E+02	2.93E+02	24	5.85E+01	4.21E+01	2.92E+00
15263-53-3	2	1.44E+02	2.83E+02	24	5.11E+01	4.14E+01	2.82E+00
23031-36-9	2	2.96E+02	2.66E+02	22	8.93E+01	4.49E+01	3.31E+00
108-98-5	2	1.72E+02	2.53E+02	27	6.62E+01	3.51E+01	2.60E+00
23184-66-9	2	2.68E+03	2.38E+02	18	3.93E+02	8.63E+01	6.83E+00
866-55-7	2	3.30E+02	2.38E+02	22	9.76E+01	4.53E+01	3.38E+00
93-72-1	2	4.24E+02	2.23E+02	22	1.19E+02	4.62E+01	3.56E+00
91-58-7	2	1.36E+03	2.18E+02	20	2.73E+02	4.63E+01	4.97E+00
64-75-5	2	4.22E+03	2.12E+02	16	7.74E+02	5.18E+01	5.45E+00
59-33-6	2	3.36E+02	2.10E+02	22	9.92E+01	4.53E+01	3.39E+00
81335-37-7	2	2.67E+03	2.06E+02	18	5.38E+02	5.14E+01	4.97E+00
104-15-4	2	1.12E+03	2.01E+02	20	2.36E+02	4.56E+01	4.75E+00

78-92-2	2	3.22E+03	1.95E+02	18	4.51E+02	7.94E+01	7.14E+00
302-17-0	2	7.26E+02	1.90E+02	22	2.32E+02	4.80E+01	3.13E+00
319-84-6	2	1.17E+02	1.77E+02	24	4.46E+01	3.84E+01	2.64E+00
76-25-5	2	2.19E+03	1.77E+02	18	6.27E+02	5.06E+01	3.48E+00
25366-23-8	2	4.18E+02	1.75E+02	23	1.56E+02	4.72E+01	2.69E+00
108-80-5	2	5.12E+03	1.74E+02	16	8.50E+02	6.08E+01	6.02E+00
119-47-1	2	7.33E+03	1.69E+02	18	7.74E+02	9.26E+01	9.46E+00
50-76-0	2	1.08E+01	1.63E+02	26	8.44E+00	2.35E+01	1.28E+00
110-43-0	2	1.09E+03	1.62E+02	20	2.33E+02	4.55E+01	4.69E+00
630-20-6	2	1.00E+03	1.62E+02	20	3.04E+02	4.54E+01	3.30E+00
67485-29-4	2	1.22E+03	1.62E+02	22	7.87E+02	3.17E+01	1.55E+00
756-80-9	2	1.04E+03	1.60E+02	19	3.60E+02	4.76E+01	2.88E+00
57-06-7	2	2.39E+02	1.50E+02	24	9.15E+01	4.37E+01	2.61E+00
2445-07-0	2	1.49E+02	1.49E+02	27	5.89E+01	3.46E+01	2.53E+00
102-27-2	2	4.15E+02	1.42E+02	22	1.18E+02	4.61E+01	3.51E+00
110-91-8	2	1.17E+03	1.41E+02	20	2.48E+02	4.57E+01	4.74E+00
542-59-6	2	5.60E+03	1.34E+02	3	3.80E+03	4.87E+01	1.47E+00
91-15-6	2	4.42E+01	1.32E+02	27	2.51E+01	2.89E+01	1.76E+00
124-48-1	2	5.44E+02	1.30E+02	22	1.83E+02	4.67E+01	2.97E+00
122-42-9	2	1.47E+03	1.29E+02	19	4.38E+02	5.12E+01	3.35E+00
56-36-0	2	6.75E+01	1.26E+02	27	2.87E+01	3.01E+01	2.35E+00
623-25-6	2	9.76E+02	1.26E+02	20	2.15E+02	4.50E+01	4.53E+00
77-73-6	2	2.78E+02	1.25E+02	22	8.66E+01	4.45E+01	3.21E+00
123-88-6	2	3.22E+01	1.21E+02	27	1.92E+01	2.78E+01	1.67E+00
764-41-0	2	1.30E+02	1.20E+02	27	5.30E+01	3.42E+01	2.46E+00
1014-70-6	2	1.10E+03	1.20E+02	19	3.73E+02	4.78E+01	2.94E+00
71-43-2	2	3.22E+03	1.19E+02	18	4.57E+02	8.75E+01	7.05E+00
14088-71-2	2	2.33E+03	1.17E+02	18	6.52E+02	5.08E+01	3.58E+00
25154-52-3	2	8.45E+02	1.16E+02	22	2.58E+02	4.86E+01	3.27E+00
1757-18-2	2	6.11E+01	1.15E+02	27	2.98E+01	3.09E+01	2.05E+00
26471-62-5	2	2.84E+03	1.14E+02	18	5.73E+02	5.16E+01	4.95E+00
95-16-9	2	6.20E+02	1.11E+02	22	2.02E+02	4.72E+01	3.07E+00
28434-01-7	2	8.57E+02	1.11E+02	20	1.96E+02	4.45E+01	4.38E+00
130-15-4	2	2.76E+02	1.10E+02	24	7.48E+01	7.15E+01	3.68E+00
1336-36-3	2	2.76E+03	1.10E+02	18	5.61E+02	5.14E+01	4.91E+00
81-82-3	2	2.71E+02	1.07E+02	24	1.00E+02	4.42E+01	2.70E+00
841-06-5	2	3.46E+03	1.03E+02	18	6.70E+02	5.25E+01	5.17E+00
756-79-6	2	5.73E+03	9.40E+01	7	1.39E+03	4.47E+01	4.12E+00
143-08-8	2	9.36E+03	9.26E+01	7	3.42E+03	4.47E+01	2.74E+00
634-93-5	2	1.68E+03	8.85E+01	20	3.32E+02	4.71E+01	5.08E+00
1330-20-7	2	3.02E+03	8.72E+01	18	6.06E+02	5.18E+01	4.98E+00
75-85-4	2	1.42E+03	8.69E+01	19	2.84E+02	6.78E+01	5.02E+00
58138-08-2	2	1.05E+03	8.66E+01	20	2.31E+02	4.53E+01	4.55E+00
333-43-7	2	3.23E+01	8.64E+01	29	1.76E+01	2.21E+01	1.84E+00
95-93-2	2	4.82E+03	8.28E+01	16	8.93E+02	5.23E+01	5.40E+00
124-09-4	2	5.39E+02	8.21E+01	20	1.38E+02	4.28E+01	3.90E+00

1918-02-1	2	2.83E+03	8.11E+01	18	6.33E+02	6.89E+01	4.47E+00
24096-53-5	2	6.29E+02	8.07E+01	20	1.56E+02	4.34E+01	4.03E+00
104-87-0	2	2.26E+03	7.96E+01	18	6.29E+02	5.07E+01	3.59E+00
542-56-3	2	2.90E+02	7.96E+01	22	9.04E+01	4.46E+01	3.21E+00
674-82-8	2	5.66E+02	7.96E+01	22	1.87E+02	4.68E+01	3.03E+00
1484-13-5	2	7.07E+01	7.96E+01	20	2.35E+01	3.19E+01	3.01E+00
109-79-5	2	2.12E+03	7.96E+01	18	5.99E+02	5.04E+01	3.54E+00
17754-90-4	2	1.60E+03	7.96E+01	20	3.20E+02	4.69E+01	5.00E+00
57-62-5	2	1.06E+03	7.96E+01	18	3.39E+02	3.98E+01	3.13E+00
67564-91-4	2	4.24E+03	7.79E+01	18	5.58E+02	8.92E+01	7.60E+00
98-06-6	2	6.17E+03	7.62E+01	18	7.16E+02	9.16E+01	8.62E+00
1014-69-3	2	9.86E+02	7.60E+01	20	2.21E+02	4.50E+01	4.47E+00
29171-20-8	2	2.22E+03	6.59E+01	19	4.86E+02	5.03E+01	4.58E+00
96489-71-3	2	4.10E+02	6.42E+01	22	1.19E+02	4.59E+01	3.44E+00
80-00-2	2	1.94E+03	6.32E+01	18	5.57E+02	4.99E+01	3.49E+00
150-19-6	2	4.32E+02	6.02E+01	22	1.24E+02	4.61E+01	3.47E+00
51218-45-2	2	1.59E+03	6.01E+01	20	3.22E+02	4.69E+01	4.95E+00
10540-29-1	2	2.97E+03	5.89E+01	18	6.05E+02	5.17E+01	4.91E+00
2223-93-0	2	8.15E+02	5.89E+01	20	1.92E+02	4.43E+01	4.24E+00
834-12-8	2	7.00E+02	5.75E+01	22	2.19E+02	4.77E+01	3.19E+00
562-10-7	2	3.43E+02	5.38E+01	19	1.06E+02	2.39E+01	3.23E+00
101-54-2	2	3.39E+02	5.36E+01	22	1.03E+02	4.51E+01	3.29E+00
2425-66-3	2	1.44E+02	5.31E+01	24	5.27E+01	4.11E+01	2.73E+00
89-72-5	2	4.38E+02	5.29E+01	23	1.16E+02	7.82E+01	3.79E+00
99-87-6	2	2.32E+03	5.22E+01	19	5.06E+02	5.05E+01	4.58E+00
95-68-1	2	3.42E+02	5.17E+01	22	1.04E+02	4.52E+01	3.29E+00
75-60-5	2	8.79E+02	5.09E+01	22	2.61E+02	4.87E+01	3.36E+00
98-07-7	2	9.55E+02	4.89E+01	20	2.19E+02	4.49E+01	4.37E+00
71-41-0	2	2.72E+02	4.86E+01	22	8.69E+01	4.43E+01	3.13E+00
60-35-5	2	9.50E+03	4.75E+01	6	4.33E+03	3.20E+01	2.19E+00
818-61-1	2	4.05E+02	4.49E+01	22	1.19E+02	4.58E+01	3.40E+00
150-68-5	2	1.42E+03	4.44E+01	19	4.16E+02	5.09E+01	3.42E+00
302-79-4	2	1.48E+03	4.36E+01	20	3.08E+02	4.66E+01	4.82E+00
108-05-4	2	2.15E+03	4.27E+01	19	4.81E+02	5.02E+01	4.48E+00
7398-69-8	2	5.28E+03	4.19E+01	18	6.63E+02	9.07E+01	7.97E+00
2533-82-6	2	1.34E+02	4.09E+01	27	5.38E+01	3.43E+01	2.49E+00
60168-88-9	2	3.35E+03	4.09E+01	18	4.92E+02	8.79E+01	6.82E+00
1319-77-3	2	1.08E+03	4.07E+01	20	2.42E+02	4.53E+01	4.47E+00
85-70-1	2	9.38E+03	4.02E+01	6	4.31E+03	3.19E+01	2.17E+00
1114-71-2	2	1.23E+03	4.00E+01	19	3.95E+02	4.81E+01	3.12E+00
924-16-3	2	1.61E+03	3.97E+01	19	3.21E+02	7.41E+01	5.00E+00
597-25-1	2	4.42E+03	3.96E+01	18	8.30E+02	5.35E+01	5.32E+00
107-11-9	2	7.62E+01	3.94E+01	27	3.26E+01	3.05E+01	2.34E+00
590-28-3	2	1.12E+03	3.86E+01	20	2.50E+02	4.55E+01	4.50E+00
71-73-8	2	1.56E+02	3.78E+01	24	6.39E+01	4.20E+01	2.44E+00
77458-01-6	2	3.15E+02	3.71E+01	24	1.12E+02	4.48E+01	2.83E+00

122-03-2	2	1.80E+03	3.70E+01	18	5.17E+02	4.95E+01	3.49E+00
110-83-8	2	1.73E+03	3.67E+01	18	5.01E+02	4.94E+01	3.45E+00
50-24-8	2	2.90E+03	3.59E+01	18	6.04E+02	5.16E+01	4.81E+00
91-23-6	2	9.81E+02	3.49E+01	20	2.85E+02	4.52E+01	3.45E+00
25321-14-6	2	9.87E+02	3.22E+01	18	2.13E+02	4.49E+01	4.64E+00
13752-51-7	2	6.84E+03	3.19E+01	18	7.96E+02	9.25E+01	8.60E+00
106-99-0	2	4.19E+03	2.93E+01	18	8.05E+02	5.33E+01	5.21E+00
69581-33-5	2	2.27E+02	2.86E+01	24	8.56E+01	4.35E+01	2.65E+00
56425-91-3	2	5.44E+02	2.81E+01	20	1.44E+02	4.28E+01	3.77E+00
66-25-1	2	6.37E+03	2.81E+01	18	7.63E+02	9.20E+01	8.34E+00
121-82-4	2	7.68E+01	2.80E+01	27	3.31E+01	3.05E+01	2.32E+00
598-56-1	2	4.03E+02	2.78E+01	22	1.20E+02	4.57E+01	3.36E+00
95-57-8	2	3.38E+02	2.69E+01	24	1.17E+02	4.51E+01	2.88E+00
24307-26-4	2	6.02E+02	2.66E+01	22	1.91E+02	4.70E+01	3.15E+00
96-23-1	2	6.25E+01	2.64E+01	27	2.79E+01	2.98E+01	2.24E+00
108-69-0	2	5.46E+02	2.64E+01	20	1.45E+02	4.28E+01	3.77E+00
110-12-3	2	3.29E+03	2.58E+01	18	6.71E+02	5.21E+01	4.90E+00
111-48-8	2	5.12E+03	2.54E+01	7	3.14E+03	3.68E+01	1.63E+00
1871-57-4	2	1.94E+02	2.52E+01	24	7.53E+01	4.28E+01	2.57E+00
142-62-1	2	3.87E+03	2.52E+01	18	5.52E+02	8.89E+01	7.01E+00
1582-09-8	2	2.48E+03	2.42E+01	18	6.53E+02	5.09E+01	3.80E+00
109-77-3	2	2.44E+01	2.32E+01	27	1.28E+01	2.66E+01	1.91E+00
94-62-2	2	4.23E+02	2.27E+01	22	1.25E+02	4.59E+01	3.38E+00
96-45-7	2	2.34E+03	2.25E+01	18	6.23E+02	5.07E+01	3.76E+00
94-58-6	2	2.89E+03	2.25E+01	18	6.77E+02	5.41E+01	4.27E+00
110-93-0	2	3.08E+03	2.24E+01	18	6.40E+02	5.18E+01	4.81E+00
124-02-7	2	4.53E+02	2.17E+01	22	1.32E+02	4.61E+01	3.43E+00
80-15-9	2	4.35E+02	2.07E+01	22	1.28E+02	4.60E+01	3.39E+00
5064-31-3	2	8.66E+02	2.06E+01	20	2.08E+02	4.44E+01	4.15E+00
3204-27-1	2	7.87E+01	2.05E+01	27	3.05E+01	3.51E+01	2.58E+00
28434-00-6	2	3.17E+02	2.04E+01	22	1.00E+02	4.47E+01	3.17E+00
106-48-9	2	5.31E+02	2.02E+01	22	1.72E+02	4.65E+01	3.08E+00
3478-94-2	2	1.97E+03	1.96E+01	18	4.73E+02	8.42E+01	4.17E+00
55-22-1	2	3.95E+03	1.95E+01	18	7.78E+02	5.29E+01	5.08E+00
76578-14-8	2	1.86E+03	1.85E+01	18	5.20E+02	4.96E+01	3.59E+00
120-82-1	2	6.00E+02	1.85E+01	20	1.58E+02	4.31E+01	3.80E+00
88283-41-4	2	2.15E+03	1.84E+01	18	5.79E+02	5.02E+01	3.71E+00
108-89-4	2	4.41E+02	1.84E+01	22	1.30E+02	4.60E+01	3.39E+00
2079-00-7	2	1.27E+01	1.83E+01	27	8.44E+00	2.87E+01	1.51E+00
107-14-2	2	1.75E+02	1.82E+01	24	6.28E+01	4.17E+01	2.78E+00
56-35-9	2	6.92E+01	1.81E+01	27	3.06E+01	3.01E+01	2.26E+00
106-40-1	2	3.63E+02	1.78E+01	22	1.12E+02	4.52E+01	3.25E+00
111-25-1	2	2.63E+03	1.74E+01	18	5.72E+02	5.11E+01	4.60E+00
3296-90-0	2	1.50E+03	1.70E+01	20	3.21E+02	4.66E+01	4.69E+00
79-43-6	2	4.43E+03	1.61E+01	18	6.15E+02	8.98E+01	7.20E+00
7227-91-0	2	2.49E+02	1.59E+01	23	8.91E+01	4.57E+01	2.79E+00

629-11-8	2	2.99E+03	1.58E+01	18	6.32E+02	5.16E+01	4.73E+00
121-29-9	2	1.61E+02	1.52E+01	24	5.91E+01	4.13E+01	2.73E+00
79-00-5	2	4.68E+02	1.49E+01	22	1.37E+02	4.62E+01	3.42E+00
98-86-2	2	1.19E+03	1.45E+01	20	2.69E+02	4.57E+01	4.42E+00
75-89-8	2	2.96E+02	1.44E+01	24	1.05E+02	4.46E+01	2.83E+00
114-07-8	2	3.73E+03	1.43E+01	19	7.50E+02	7.98E+01	4.97E+00
103-11-7	2	5.43E+03	1.42E+01	7	2.97E+03	4.07E+01	1.83E+00
5392-40-5	2	4.02E+03	1.42E+01	18	7.96E+02	5.30E+01	5.05E+00
115-96-8	2	1.51E+03	1.39E+01	18	4.40E+02	4.87E+01	3.45E+00
15263-52-2	2	2.03E+02	1.38E+01	24	7.16E+01	4.35E+01	2.84E+00
103-84-4	2	9.84E+02	1.36E+01	20	2.77E+02	4.51E+01	3.56E+00
614-00-6	2	1.84E+02	1.29E+01	25	8.41E+01	6.73E+01	2.18E+00
60-11-7	2	2.45E+02	1.29E+01	24	8.98E+01	4.38E+01	2.73E+00
64-19-7	2	4.05E+03	1.29E+01	18	5.86E+02	8.93E+01	6.92E+00
1713-12-8	2	7.48E+02	1.26E+01	20	1.89E+02	4.39E+01	3.95E+00
2008-39-1	2	5.12E+02	1.23E+01	23	1.53E+02	3.17E+01	3.34E+00
7292-16-2	2	7.41E+01	1.17E+01	27	3.38E+01	3.16E+01	2.19E+00
156-60-5	2	2.57E+03	1.15E+01	18	5.69E+02	5.09E+01	4.52E+00
96-22-0	2	2.60E+03	1.15E+01	18	6.61E+02	5.11E+01	3.93E+00
117-80-6	2	3.63E+02	1.14E+01	23	1.32E+02	4.66E+01	2.74E+00
2489-77-2	2	2.61E+02	1.14E+01	23	9.30E+01	4.58E+01	2.80E+00
142-59-6	2	4.79E+02	1.13E+01	22	1.57E+02	4.61E+01	3.06E+00
108-85-0	2	3.39E+03	1.11E+01	18	5.24E+02	8.83E+01	6.47E+00
77-78-1	2	1.69E+02	1.11E+01	24	6.18E+01	4.15E+01	2.74E+00
60-29-7	2	1.46E+03	1.06E+01	18	4.24E+02	4.85E+01	3.44E+00
139-65-1	2	7.47E+02	1.05E+01	20	1.90E+02	4.39E+01	3.93E+00
554-12-1	2	4.16E+03	1.02E+01	18	7.94E+02	5.60E+01	5.24E+00
92-87-5	2	2.57E+02	1.02E+01	23	9.22E+01	4.57E+01	2.79E+00
1067-33-0	2	3.84E+01	9.89E+00	27	2.10E+01	2.82E+01	1.82E+00
2212-67-1	2	4.42E+02	9.84E+00	22	1.47E+02	4.57E+01	3.01E+00
68411-30-3	2	1.14E+03	9.83E+00	20	3.06E+02	4.56E+01	3.72E+00
3567-25-7	2	8.98E+02	9.71E+00	20	2.55E+02	4.47E+01	3.52E+00
140-66-9	2	3.84E+03	9.70E+00	18	7.78E+02	5.28E+01	4.94E+00
57018-04-9	2	4.18E+03	9.51E+00	18	7.98E+02	5.60E+01	5.24E+00
13366-73-9	2	8.37E+00	9.51E+00	26	6.03E+00	2.94E+01	1.39E+00
518-47-8	2	5.64E+03	9.09E+00	7	3.00E+03	4.08E+01	1.88E+00
923-02-4	2	3.36E+02	9.09E+00	23	1.24E+02	4.63E+01	2.71E+00
56-04-2	2	1.79E+03	9.02E+00	18	4.92E+02	4.94E+01	3.63E+00
10350-81-9	2	4.88E+02	8.94E+00	22	1.58E+02	4.61E+01	3.09E+00
90-13-1	2	1.30E+03	8.81E+00	20	2.92E+02	4.60E+01	4.43E+00
42576-02-3	2	5.40E+03	8.55E+00	7	2.89E+03	4.07E+01	1.87E+00
396-01-0	2	3.38E+02	8.50E+00	22	1.07E+02	4.49E+01	3.15E+00
25013-15-4	2	2.67E+03	8.42E+00	18	6.69E+02	5.12E+01	3.99E+00
144-21-8	2	9.72E+02	8.40E+00	20	2.70E+02	4.50E+01	3.60E+00
108-67-8	2	5.92E+03	8.37E+00	18	7.66E+02	9.18E+01	7.72E+00
118-95-6	2	5.32E+01	8.37E+00	27	2.50E+01	2.92E+01	2.13E+00

98-92-0	2	2.96E+03	8.37E+00	18	6.39E+02	5.16E+01	4.63E+00
121-69-7	2	1.22E+03	8.19E+00	20	3.21E+02	4.59E+01	3.80E+00
98-85-1	2	4.72E+02	8.18E+00	22	1.54E+02	4.60E+01	3.07E+00
109-99-9	2	1.95E+03	8.14E+00	18	3.75E+02	8.28E+01	5.20E+00
101-72-4	2	9.50E+02	8.14E+00	20	2.65E+02	4.49E+01	3.59E+00
1300-21-6	2	5.77E+02	8.02E+00	20	1.57E+02	4.29E+01	3.67E+00
111-55-7	2	5.82E+03	7.88E+00	6	4.00E+03	2.51E+01	1.46E+00
108-77-0	2	4.12E+02	7.84E+00	22	1.26E+02	4.56E+01	3.28E+00
10034-93-2	2	5.11E+02	7.81E+00	22	1.49E+02	4.65E+01	3.44E+00
51-79-6	2	2.13E+03	7.71E+00	18	5.61E+02	5.01E+01	3.79E+00
95-63-6	2	5.87E+03	7.64E+00	18	7.66E+02	9.18E+01	7.67E+00
19406-51-0	2	1.12E+03	7.45E+00	20	3.00E+02	4.56E+01	3.74E+00
540-72-7	2	5.53E+02	7.27E+00	22	1.58E+02	4.68E+01	3.49E+00
3566-10-7	2	4.62E+02	7.20E+00	22	1.51E+02	4.59E+01	3.06E+00
123-05-7	2	3.04E+03	7.14E+00	18	6.86E+02	5.43E+01	4.43E+00
542-75-6	2	5.48E+02	7.02E+00	22	1.72E+02	4.66E+01	3.18E+00
1634-78-2	2	1.84E+02	6.99E+00	24	7.10E+01	4.27E+01	2.59E+00
64-67-5	2	7.55E+02	6.97E+00	20	1.94E+02	4.39E+01	3.88E+00
122-99-6	2	1.08E+03	6.67E+00	20	2.57E+02	4.53E+01	4.22E+00
77-06-5	2	7.32E+03	6.63E+00	7	3.13E+03	4.25E+01	2.34E+00
124-68-5	2	2.50E+03	6.62E+00	18	5.65E+02	5.08E+01	4.42E+00
1912-26-1	2	6.89E+02	6.55E+00	25	4.49E+02	3.13E+01	1.54E+00
156-51-4	2	1.81E+02	6.53E+00	24	6.61E+01	4.30E+01	2.74E+00
86-87-3	2	8.62E+02	6.52E+00	20	2.16E+02	4.44E+01	4.00E+00
103-69-5	2	4.31E+02	6.44E+00	22	1.42E+02	4.56E+01	3.03E+00
101-83-7	2	4.32E+02	6.36E+00	22	1.43E+02	4.56E+01	3.03E+00
112-07-2	2	2.77E+03	6.15E+00	18	6.82E+02	5.13E+01	4.06E+00
144-02-5	2	6.93E+02	6.15E+00	22	2.06E+02	4.76E+01	3.36E+00
11067-82-6	2	1.41E+03	5.99E+00	19	4.11E+02	4.85E+01	3.42E+00
111-27-3	2	2.15E+03	5.96E+00	18	5.61E+02	5.02E+01	3.83E+00
503-74-2	2	1.19E+03	5.94E+00	20	3.12E+02	4.58E+01	3.82E+00
25812-30-0	2	2.55E+03	5.92E+00	18	5.77E+02	5.09E+01	4.43E+00
536-33-4	2	1.15E+03	5.77E+00	20	2.70E+02	4.55E+01	4.25E+00
67306-00-7	2	1.66E+03	5.58E+00	21	5.24E+02	3.63E+01	3.16E+00
1456-28-6	2	3.21E+02	5.52E+00	4	2.51E+02	1.85E+01	1.28E+00
872-50-4	2	4.48E+03	5.52E+00	18	6.49E+02	9.01E+01	6.90E+00
12663-46-6	2	5.72E+00	5.50E+00	22	4.33E+00	3.36E+01	1.32E+00
100-02-7	2	2.47E+02	5.46E+00	24	8.91E+01	4.38E+01	2.77E+00
5259-88-1	2	1.43E+03	5.39E+00	22	4.26E+02	3.83E+01	3.35E+00
106-94-5	2	4.11E+03	5.38E+00	18	6.14E+02	8.96E+01	6.69E+00
302-95-4	2	1.20E+03	5.36E+00	20	2.80E+02	4.57E+01	4.28E+00
60-80-0	2	1.49E+03	5.28E+00	20	3.32E+02	4.66E+01	4.50E+00
105-60-2	2	1.06E+03	5.27E+00	20	2.55E+02	4.52E+01	4.16E+00
4170-30-3	2	9.12E+01	5.24E+00	27	3.94E+01	3.23E+01	2.31E+00
1330-78-5	2	3.42E+03	5.24E+00	18	7.44E+02	5.48E+01	4.59E+00
591-80-0	2	5.35E+02	5.19E+00	22	1.68E+02	4.65E+01	3.19E+00

103-65-1	2	5.92E+03	5.10E+00	7	3.05E+03	4.10E+01	1.94E+00
95-49-8	2	2.71E+03	4.93E+00	18	6.66E+02	5.12E+01	4.07E+00
928-96-1	2	6.17E+03	4.90E+00	18	8.07E+02	9.22E+01	7.65E+00
108-94-1	2	1.59E+03	4.89E+00	20	3.48E+02	4.68E+01	4.56E+00
768-94-5	2	7.94E+02	4.89E+00	20	2.04E+02	4.41E+01	3.88E+00
101-02-0	2	9.53E+02	4.88E+00	20	2.61E+02	4.49E+01	3.65E+00
141-97-9	2	4.51E+03	4.82E+00	18	6.56E+02	9.02E+01	6.87E+00
1214-39-7	2	1.47E+03	4.72E+00	20	3.29E+02	4.65E+01	4.47E+00
25606-41-1	2	1.77E+03	4.65E+00	19	4.43E+02	4.93E+01	4.00E+00
109-70-6	2	1.14E+03	4.65E+00	20	3.00E+02	4.56E+01	3.81E+00
5989-27-5	2	4.96E+03	4.58E+00	18	7.01E+02	9.08E+01	7.09E+00
127-07-1	2	6.50E+03	4.58E+00	18	8.37E+02	9.26E+01	7.76E+00
76-29-9	2	3.95E+03	4.56E+00	18	7.76E+02	5.57E+01	5.09E+00
57-14-7	2	1.38E+02	4.53E+00	24	5.59E+01	4.16E+01	2.46E+00
2570-26-5	2	5.86E+02	4.51E+00	20	1.62E+02	4.30E+01	3.61E+00
443-48-1	2	3.38E+03	4.45E+00	18	7.35E+02	5.48E+01	4.60E+00
583-78-8	2	1.06E+03	4.45E+00	20	2.57E+02	4.52E+01	4.14E+00
2227-13-6	2	4.45E+03	4.41E+00	18	6.53E+02	9.02E+01	6.82E+00
57808-65-8	2	2.94E+02	4.38E+00	24	1.02E+02	4.46E+01	2.88E+00
8027-00-7	2	5.34E+02	4.37E+00	22	1.67E+02	4.65E+01	3.20E+00
619-15-8	2	5.81E+02	4.33E+00	22	1.78E+02	4.69E+01	3.26E+00
465-73-6	2	7.85E+00	4.24E+00	26	6.51E+00	2.71E+01	1.21E+00
72-55-9	2	7.85E+02	4.24E+00	20	2.04E+02	4.40E+01	3.86E+00
5137-55-3	2	2.50E+02	4.21E+00	24	8.97E+01	4.39E+01	2.78E+00
99-65-0	2	6.67E+01	4.21E+00	27	3.27E+01	3.02E+01	2.04E+00
75-07-0	2	1.01E+03	4.20E+00	20	2.47E+02	4.50E+01	4.08E+00
645-62-5	2	3.97E+03	4.16E+00	18	7.81E+02	5.57E+01	5.09E+00
93-89-0	2	2.35E+03	4.14E+00	18	4.33E+02	7.84E+01	5.43E+00
96-05-9	2	6.32E+01	3.66E+00	27	2.94E+01	2.98E+01	2.15E+00
2814-20-2	2	2.44E+03	3.64E+00	18	5.64E+02	5.07E+01	4.32E+00
577-11-7	2	3.22E+03	3.60E+00	18	7.06E+02	5.46E+01	4.56E+00
3380-34-5	2	4.09E+03	3.59E+00	18	6.23E+02	8.97E+01	6.57E+00
10443-70-6	2	1.28E+03	3.59E+00	20	2.99E+02	4.60E+01	4.29E+00
4342-36-3	2	1.19E+02	3.55E+00	24	4.78E+01	4.00E+01	2.50E+00
51218-49-6	2	1.99E+03	3.55E+00	18	4.83E+02	4.98E+01	4.12E+00
100-44-7	2	1.36E+03	3.48E+00	20	3.39E+02	4.63E+01	4.01E+00
94-09-7	2	2.76E+03	3.45E+00	18	6.21E+02	5.12E+01	4.44E+00
54-64-8	2	8.26E+01	3.39E+00	27	3.63E+01	3.20E+01	2.27E+00
95266-40-3	2	4.91E+03	3.38E+00	18	7.05E+02	9.08E+01	6.97E+00
555-89-5	2	6.38E+03	3.34E+00	6	3.80E+03	2.91E+01	1.68E+00
98-95-3	2	5.37E+02	3.32E+00	22	1.67E+02	4.65E+01	3.22E+00
119-84-6	2	1.60E+03	3.25E+00	18	3.42E+02	8.20E+01	4.68E+00
94-59-7	2	2.14E+03	3.25E+00	18	5.49E+02	5.01E+01	3.90E+00
98-73-7	2	5.18E+02	3.18E+00	22	1.62E+02	4.64E+01	3.20E+00
107-92-6	2	1.37E+03	3.16E+00	20	3.15E+02	4.62E+01	4.34E+00
140-67-0	2	1.37E+03	3.11E+00	20	3.15E+02	4.62E+01	4.34E+00

2475-46-9	2	1.47E+03	2.99E+00	19	4.16E+02	4.86E+01	3.53E+00
74051-80-2	2	4.22E+03	2.97E+00	18	6.51E+02	8.16E+01	6.48E+00
87-62-7	2	7.71E+02	2.97E+00	20	2.03E+02	4.40E+01	3.80E+00
121-44-8	2	5.01E+02	2.95E+00	22	1.57E+02	4.62E+01	3.18E+00
589-16-2	2	4.59E+02	2.92E+00	27	2.26E+02	2.77E+01	2.03E+00
3252-43-5	2	2.66E+02	2.84E+00	24	9.37E+01	4.42E+01	2.84E+00
3090-35-5	2	2.12E+02	2.84E+00	24	7.82E+01	4.33E+01	2.71E+00
602-01-7	2	9.88E+02	2.79E+00	20	2.63E+02	4.50E+01	3.75E+00
2034-22-2	2	3.69E+01	2.79E+00	27	1.98E+01	2.80E+01	1.86E+00
94-81-5	2	7.38E+02	2.79E+00	20	2.10E+02	4.39E+01	3.51E+00
87-65-0	2	2.30E+03	2.76E+00	18	5.44E+02	5.04E+01	4.23E+00
5216-25-1	2	7.58E+02	2.72E+00	20	2.01E+02	4.39E+01	3.77E+00
6062-26-6	2	6.48E+02	2.65E+00	20	1.78E+02	4.33E+01	3.63E+00
51333-22-3	2	2.63E+03	2.65E+00	18	6.40E+02	5.10E+01	4.11E+00
608-93-5	2	1.09E+03	2.64E+00	20	2.83E+02	4.54E+01	3.84E+00
109-87-5	2	6.16E+03	2.63E+00	7	3.23E+03	3.10E+01	1.91E+00
74-97-5	2	4.64E+03	2.59E+00	18	7.46E+02	9.11E+01	6.22E+00
98319-26-7	2	4.51E+02	2.59E+00	22	1.44E+02	4.58E+01	3.12E+00
75-91-2	2	3.44E+02	2.50E+00	22	1.12E+02	4.48E+01	3.07E+00
1966-58-1	2	1.74E+03	2.47E+00	19	4.46E+02	4.92E+01	3.90E+00
75-65-0	2	3.33E+03	2.47E+00	18	5.59E+02	8.04E+01	5.94E+00
12427-38-2	2	2.79E+03	2.47E+00	18	6.34E+02	5.13E+01	4.41E+00
108-60-1	2	6.00E+02	2.45E+00	22	1.80E+02	4.70E+01	3.32E+00
66246-88-6	2	2.28E+03	2.42E+00	18	5.71E+02	5.04E+01	3.99E+00
288-88-0	2	1.45E+03	2.40E+00	20	3.32E+02	4.65E+01	4.36E+00
75-25-2	2	1.00E+03	2.40E+00	20	2.65E+02	4.50E+01	3.78E+00
98-87-3	2	1.99E+03	2.40E+00	18	4.89E+02	4.98E+01	4.07E+00
95-64-7	2	7.58E+02	2.40E+00	20	2.02E+02	4.39E+01	3.75E+00
57966-95-7	2	1.03E+03	2.31E+00	19	2.53E+02	8.14E+01	4.05E+00
65-85-0	2	1.82E+03	2.30E+00	18	4.79E+02	4.94E+01	3.79E+00
91-53-2	2	1.48E+03	2.27E+00	19	4.16E+02	4.86E+01	3.57E+00
124-22-1	2	1.09E+03	2.25E+00	20	2.82E+02	4.54E+01	3.86E+00
89-98-5	2	2.03E+03	2.25E+00	18	4.97E+02	4.98E+01	4.08E+00
115-02-6	2	1.60E+02	2.20E+00	24	6.08E+01	4.10E+01	2.63E+00
110-62-3	2	6.02E+00	2.17E+00	22	4.52E+00	3.38E+01	1.33E+00
2595-53-1	2	5.45E+01	2.17E+00	25	2.69E+01	2.26E+01	2.03E+00
2282-34-0	2	4.71E+01	2.15E+00	29	2.40E+01	2.26E+01	1.96E+00
26952-21-6	2	1.57E+03	2.14E+00	19	4.34E+02	4.88E+01	3.62E+00
2634-33-5	2	1.08E+03	2.13E+00	20	2.80E+02	4.53E+01	3.86E+00
104-88-1	2	1.48E+03	2.10E+00	20	3.40E+02	4.66E+01	4.36E+00
75-18-3	2	3.49E+03	2.06E+00	18	7.42E+02	5.49E+01	4.71E+00
124-30-1	2	2.32E+03	2.04E+00	18	5.75E+02	5.04E+01	4.02E+00
96-80-0	2	8.14E+02	2.01E+00	20	2.14E+02	4.42E+01	3.79E+00
39515-51-0	2	2.09E+03	2.01E+00	18	5.11E+02	5.00E+01	4.10E+00
87-59-2	2	8.83E+02	2.00E+00	20	2.28E+02	4.45E+01	3.87E+00
67-72-1	2	4.71E+03	1.98E+00	18	7.21E+02	8.82E+01	6.53E+00

106-24-1	2	3.32E+03	1.96E+00	18	7.13E+02	5.47E+01	4.65E+00
12771-68-5	2	4.74E+03	1.94E+00	18	7.06E+02	9.08E+01	6.72E+00
111-96-6	2	5.69E+03	1.94E+00	18	7.96E+02	9.19E+01	7.15E+00
62-75-9	2	2.95E+01	1.91E+00	28	2.05E+01	4.61E+01	1.44E+00
98-00-0	2	1.68E+02	1.89E+00	24	6.35E+01	4.25E+01	2.65E+00
121-73-3	2	3.99E+02	1.88E+00	22	1.27E+02	4.54E+01	3.15E+00
150-78-7	2	3.43E+03	1.87E+00	18	7.47E+02	5.22E+01	4.58E+00
119-38-0	2	1.03E+01	1.85E+00	27	7.50E+00	2.97E+01	1.37E+00
13181-17-4	2	1.05E+03	1.83E+00	19	2.68E+02	6.57E+01	3.91E+00
85-43-8	2	3.15E+03	1.83E+00	18	7.26E+02	5.18E+01	4.34E+00
7287-19-6	2	2.04E+03	1.82E+00	18	5.20E+02	4.99E+01	3.92E+00
135-23-9	2	1.91E+02	1.81E+00	24	7.02E+01	4.30E+01	2.72E+00
540-88-5	2	4.30E+03	1.80E+00	18	6.63E+02	9.02E+01	6.48E+00
78-93-3	2	2.87E+03	1.78E+00	18	6.75E+02	5.14E+01	4.25E+00
35572-78-2	2	1.46E+03	1.74E+00	19	4.06E+02	4.85E+01	3.58E+00
1634-04-4	2	3.83E+03	1.74E+00	18	7.74E+02	5.54E+01	4.95E+00
121-54-0	2	3.53E+02	1.71E+00	22	1.15E+02	4.49E+01	3.06E+00
302-01-2	2	6.26E+01	1.71E+00	27	3.04E+01	2.99E+01	2.06E+00
513-37-1	2	8.53E+02	1.68E+00	20	2.31E+02	4.44E+01	3.69E+00
78-70-6	2	2.68E+03	1.68E+00	18	6.20E+02	5.11E+01	4.32E+00
107-20-0	2	8.54E+01	1.68E+00	27	3.85E+01	3.10E+01	2.22E+00
123-42-2	2	3.31E+03	1.67E+00	18	7.52E+02	5.21E+01	4.40E+00
610-39-9	2	7.76E+02	1.63E+00	20	2.08E+02	4.40E+01	3.73E+00
109-89-7	2	5.20E+02	1.63E+00	22	1.56E+02	4.65E+01	3.33E+00
2797-51-5	2	1.31E+03	1.62E+00	20	3.11E+02	4.61E+01	4.20E+00
96-29-7	2	9.64E+02	1.58E+00	20	2.54E+02	4.49E+01	3.80E+00
780-11-0	2	4.87E+02	1.57E+00	19	1.36E+02	2.45E+01	3.58E+00
127-19-5	2	4.46E+03	1.57E+00	18	6.84E+02	9.04E+01	6.52E+00
40487-42-1	2	1.01E+03	1.57E+00	20	2.56E+02	4.50E+01	3.96E+00
100-00-5	2	4.56E+02	1.55E+00	22	1.41E+02	4.59E+01	3.23E+00
4116-10-3	2	7.25E+02	1.55E+00	20	2.04E+02	4.38E+01	3.56E+00
120-72-9	2	1.03E+03	1.53E+00	20	2.68E+02	4.51E+01	3.87E+00
96-48-0	2	1.51E+03	1.52E+00	20	3.48E+02	4.67E+01	4.33E+00
3813-05-6	2	3.10E+03	1.50E+00	18	7.13E+02	5.18E+01	4.34E+00
591-78-6	2	2.51E+03	1.50E+00	18	5.92E+02	5.08E+01	4.24E+00
50-44-2	2	2.68E+02	1.49E+00	23	9.87E+01	4.56E+01	2.72E+00
133-90-4	2	3.61E+03	1.48E+00	18	7.55E+02	5.51E+01	4.78E+00
79-08-3	2	9.70E+01	1.47E+00	27	4.08E+01	3.25E+01	2.38E+00
110488-70-5	2	3.60E+03	1.42E+00	18	7.53E+02	5.51E+01	4.78E+00
4342-03-4	2	2.09E+03	1.42E+00	18	5.15E+02	5.00E+01	4.05E+00
151-67-7	2	5.84E+03	1.41E+00	18	8.45E+02	8.97E+01	6.91E+00
77-74-7	2	7.30E+02	1.41E+00	20	2.04E+02	4.38E+01	3.58E+00
126-33-0	2	1.95E+03	1.41E+00	18	4.89E+02	4.97E+01	3.99E+00
81334-34-1	2	1.46E+03	1.40E+00	20	3.48E+02	4.65E+01	4.20E+00
60-24-2	2	2.50E+02	1.39E+00	24	8.84E+01	4.40E+01	2.83E+00
25319-90-8	2	7.70E+02	1.39E+00	20	2.08E+02	4.40E+01	3.70E+00

305-03-3	2	7.80E+01	1.38E+00	27	3.64E+01	3.07E+01	2.14E+00
118-96-7	2	6.77E+02	1.38E+00	20	1.88E+02	4.35E+01	3.59E+00
106-43-4	2	1.95E+03	1.37E+00	18	4.89E+02	4.97E+01	3.98E+00
961-11-5	2	4.10E+03	1.36E+00	18	6.51E+02	8.99E+01	6.30E+00
75-27-4	2	4.40E+02	1.33E+00	22	1.40E+02	4.57E+01	3.15E+00
78-94-4	2	2.73E+01	1.31E+00	27	1.52E+01	2.69E+01	1.80E+00
108-78-1	2	3.23E+03	1.30E+00	18	7.33E+02	5.19E+01	4.41E+00
92-70-6	2	8.16E+02	1.28E+00	20	2.18E+02	4.42E+01	3.74E+00
57-97-6	2	3.33E+02	1.28E+00	23	1.19E+02	4.64E+01	2.80E+00
13826-35-2	2	2.08E+03	1.27E+00	18	5.15E+02	4.99E+01	4.04E+00
75-74-1	2	1.07E+02	1.27E+00	27	4.63E+01	5.33E+01	2.31E+00
52918-63-5	2	1.96E+01	1.26E+00	27	1.15E+01	2.59E+01	1.71E+00
3268-49-3	2	1.65E+03	1.22E+00	19	4.37E+02	4.90E+01	3.77E+00
3244-90-4	2	4.43E+02	1.22E+00	23	1.41E+02	3.11E+01	3.14E+00
75-35-4	2	1.97E+02	1.21E+00	24	7.25E+01	4.31E+01	2.72E+00
108-21-4	2	6.85E+03	1.20E+00	7	3.36E+03	3.14E+01	2.04E+00
556-52-5	2	4.25E+02	1.18E+00	22	1.36E+02	4.56E+01	3.14E+00
563-80-4	2	2.96E+03	1.18E+00	18	6.84E+02	5.15E+01	4.33E+00
51-03-6	2	2.62E+03	1.13E+00	18	4.94E+02	7.93E+01	5.31E+00
86-30-6	2	1.84E+03	1.13E+00	18	4.75E+02	4.94E+01	3.88E+00
24151-93-7	2	3.27E+02	1.12E+00	23	1.17E+02	4.64E+01	2.80E+00
79-39-0	2	4.55E+02	1.12E+00	22	1.42E+02	4.59E+01	3.20E+00
1929-77-7	2	1.21E+03	1.11E+00	20	2.99E+02	4.58E+01	4.05E+00
3344-14-7	2	3.17E+02	1.10E+00	23	1.14E+02	4.63E+01	2.79E+00
117-39-5	2	1.60E+02	1.08E+00	24	6.16E+01	4.23E+01	2.60E+00
90-05-1	2	6.17E+02	1.07E+00	22	1.81E+02	4.72E+01	3.41E+00
75-52-5	2	9.45E+02	1.07E+00	20	2.47E+02	4.48E+01	3.83E+00
57-63-6	2	9.55E+02	1.07E+00	20	2.48E+02	4.48E+01	3.86E+00
80-43-3	2	4.98E+03	1.05E+00	18	7.49E+02	9.12E+01	6.65E+00
131-11-3	2	6.82E+03	1.05E+00	6	3.84E+03	2.94E+01	1.78E+00
503-87-7	2	4.18E+02	1.05E+00	22	1.33E+02	4.56E+01	3.14E+00
30516-87-1	2	3.07E+03	1.05E+00	18	6.99E+02	5.17E+01	4.39E+00
109-01-3	2	1.44E+03	1.04E+00	20	3.42E+02	4.65E+01	4.23E+00
732-26-3	2	1.60E+03	1.04E+00	19	4.30E+02	4.89E+01	3.73E+00
111-13-7	2	3.09E+03	1.02E+00	18	7.04E+02	5.17E+01	4.39E+00
41394-05-2	2	1.45E+03	1.01E+00	20	3.42E+02	4.65E+01	4.23E+00
142-04-1	2	8.40E+02	1.01E+00	20	2.25E+02	4.43E+01	3.74E+00
50-07-7	2	4.52E+01	1.00E+00	27	2.29E+01	2.86E+01	1.97E+00
5836-10-2	2	5.00E+03	1.00E+00	18	7.52E+02	9.13E+01	6.65E+00
107-87-9	2	1.60E+03	1.00E+00	19	4.30E+02	4.89E+01	3.72E+00
112-05-0	2	5.00E+03	1.00E+00	18	7.52E+02	9.13E+01	6.65E+00
119-34-6	2	1.47E+03	1.00E+00	20	3.46E+02	4.66E+01	4.25E+00
140-57-8	2	3.90E+03	1.00E+00	18	6.55E+02	8.73E+01	5.96E+00
142-08-5	2	1.24E+02	1.00E+00	24	5.04E+01	4.00E+01	2.46E+00
14235-86-0	2	7.00E+01	1.00E+00	20	2.80E+01	2.24E+01	2.50E+00
151-56-4	2	1.50E+01	1.00E+00	27	9.13E+00	2.51E+01	1.64E+00

161050-58-4	2	5.00E+03	1.00E+00	18	7.52E+02	9.13E+01	6.65E+00
2235-25-8	2	4.80E+01	1.00E+00	27	2.41E+01	2.89E+01	1.99E+00
26628-22-8	2	2.70E+01	1.00E+00	27	1.49E+01	2.69E+01	1.81E+00
471-25-0	2	1.00E+02	1.00E+00	27	4.16E+01	3.27E+01	2.40E+00
627-30-5	2	2.30E+03	1.00E+00	18	5.61E+02	5.04E+01	4.10E+00
6959-48-4	2	3.16E+02	1.00E+00	23	1.13E+02	4.62E+01	2.79E+00
72-56-0	2	6.60E+03	1.00E+00	7	3.11E+03	4.16E+01	2.12E+00
78-51-3	2	3.00E+03	1.00E+00	18	5.49E+02	8.57E+01	5.46E+00
924-42-5	2	4.00E+02	1.00E+00	22	1.29E+02	4.54E+01	3.11E+00
99-56-9	2	6.81E+02	1.00E+00	20	1.91E+02	4.35E+01	3.56E+00

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103 3. REFERENCES

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