See discussions, stats, and author profiles for this publication at: https://www.researchgate.net/publication/231390335

Prediction of the θ(UCST) of Polymer Solutions: A Quantitative Structure—Property Relationship Study

ARTICLE in INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH · SEPTEMBER 2009

Impact Factor: 2.59 · DOI: 10.1021/ie9000426

CITATIONS

17

READS

11

2 AUTHORS:



Farhad Gharagheizi Texas Tech University

167 PUBLICATIONS 2,907 CITATIONS

SEE PROFILE



Mehdi Sattari

University of KwaZulu-Natal

40 PUBLICATIONS 324 CITATIONS

SEE PROFILE

CORRELATIONS

Prediction of the θ (UCST) of Polymer Solutions: A Quantitative Structure—Property Relationship Study

Farhad Gharagheizi*,† and Mehdi Sattari‡

Department of Chemical Engineering, Faculty of Engineering, University of Tehran, P.O. Box 11365-4563, Tehran, Iran, and Division of Polymer Science and Technology, Research Institute of Petroleum Industry (RIPI), P.O. Box 14665-1998, Tehran, Iran

One of the industrially important thermodynamic properties of polymer solutions is the upper critical solution temperature at the limit of infinite chain length of polymers, which is used to realize the usage limits of polymer solutions; this property is denoted as the $\theta(\text{UCST})$. In this study, the quantitative structure—property relationship technique (QSPR) was used to correlate the $\theta(\text{UCST})$ of polymer solutions. Based on molecular descriptors calculated from the chemical structures of the polymer and the solvent, a nine-parameter multilinear equation was obtained. This correlation can predict the $\theta(\text{UCST})$ of 107 polymer solutions with a mean relative error of 6.12% and squared correlation coefficient of 0.912.

Introduction

Knowledge of the phase behavior of polymer solutions is a necessity for industrial and laboratory processes, and its understanding allows optimization of the design and processing conditions. Partially miscible polymer solutions usually have two boundaries: an upper critical solution temperature (UCST) and a lower critical solution temperature (LCST). These two characteristics are dependent on the molar mass of polymer and also the pressure.

The θ temperature is defined as a critical miscibility temperature at the limit of infinite molar mass. A solution may exhibit two critical miscibility temperatures; therefore, a polymer solution may display two θ temperatures.

In the case of exothermic solutions, an increasing in temperature leads to less-positive second virial coefficients and the theta temperature corresponds to a LCST in the limit of infinite molar mass (θ (LCST)). The θ temperature corresponds to a UCST in the case of endothermic solutions (θ (UCST)).

 $\theta(\text{UCST})$ is the upper critical solution temperature at infinite molar mass; as a result, it is not affected by the molar mass of polymers. Also, it can serve as a lower temperature limit for polymer processing in the form of solution. Solvent systems that exhibit this UCST behavior have been suggested for applications where partial miscibility above and below UCST offers advantages.^{2,3}

The ability to predict the physicochemical properties of materials from their molecular structure has been one of the wishes of scientists and engineers for a long time. One of the methods applied for this purpose is the quantitative structure—property relationship (QSPR). QSPR is defined as a mathematical model that predicts the physical, mechanical, or chemical properties of materials from their chemical structures. The main goal of QSPR studies is to find a relationship between the

structure of a compound expressed in terms of numeric characteristics associated with its chemical structure (called molecular descriptors) and the properties of interest.

Once a correlation between structure and a desired property has been found, any number of compounds, including those not yet synthesized, or not yet prepared, can be readily screened using a computer to select structures with the desired properties. Thus, the QSPR approach conserves resources and accelerates the development process of new molecules to use for any purpose.

There are more than 3000 molecular descriptors in the literature that can be used to represent the molecular structure, and the usual problem in this context is to select those which are the most representative for the property under consideration.

In comparison with numerous methods presented to estimate $\theta(\text{LCST})$ of polymer solutions, $^{4-15}$ there is no computational method for estimation of the properties. Perhaps, this problem is related to the rarity of the experimental data for $\theta(\text{UCST})$ in the literature, in comparison with $\theta(\text{UCST})$.

In the present study, the genetic algorithm-based multivariate linear regression (GA-MLR) technique is applied to select the most statistically effective molecular descriptors on $\theta(\text{UCST})$ from a pool of 3328 molecular descriptors. The result is a multilinear equation that can be used to predict the $\theta(\text{UCST})$ of polymer solutions.

Materials and Methods

Dataset Preparation. The source of experimental data in this study was the compilation provided by Wohlfarth. Consequently, a set of 107 experimental $\theta(\text{UCST})$ data was found in this reference and used in this study. These experimental data have been collected from other original literature. This dataset includes 23 polymers and 92 solvents, which is presented in Table 1.

Each polymer solution is a combination of a polymer and a solvent. Therefore, the phase behavior of each binary system is the result of interactions between both polymer and solvent. To consider these interactions, all molecular descriptors of both parts were examined to develop a molecular-based model.

^{*}To whom correspondence should be addressed. Fax: +98 21 66957784. E-mail addresses: fghara@ut.ac.ir, fghara@gmail.com.

[†] Department of Chemical Engineering, Faculty of Engineering, University of Tehran.

^{*} Division of Polymer Science and Technology, Research Institute of Petroleum Industry (RIPI).

Combinations
-Solvent
ymer-
107 Polymer
for
(UCSI
Predicted $\theta(UCST)$
ble 1.

salvent salvent CAP PRGA APANA PANA	Application	poverality studius CRF PRG APAPA PADA CRF DATA PADA PADA CRF DATA PADA PADA CRF DATA CRF CRF DATA CRF			1		UCST [K]	[K]	1 1		200434	Mo	Molecular Descriptors	escriptors	Medical	Management	03011	9
2. Postpanome training 310 28.50 0.119 1.88 0.99 0.977 0.12 0 0.019 -0.02 5.2 A. Wadhantone training 4.13 6.13 1.18 0.99 0.977 0.11 0.003 -0.012 5.0 A. Wadhantonelly formande training 3.43 2.92 0.13 0.01 0.01 -0.02 5.0 Day backed training 2.43 2.98 0.13 0.13 0.03 0.03 Programed training 2.43 2.99 0.27 0.13 0.03 0.03 Programed training 2.43 2.99 0.73 0.13 0.03 0.03 Programed training 2.43 2.99 0.13 0.13 0.03 0.03 0.03 Programed training 2.43 0.13 1.24 0.24 0.94 0.04 0.04 0.04 0.04 0.04 0.04 0.04 0.04 0.04 0.0	2-bytopmone cert 35.0 25.0 0.27 0.12 0.10 0.12 0.10	2-bytopmone term 30 28.50 11.9 18.8 0.9 0.927 0.14 0 0.02 0.13		polymer	solvent	status	exb.	pred.	$\rm X4A_p$	$IVDE_p$	${ m SPAM_p}$	$\mathrm{FDI}_{\mathrm{p}}$	$\mathrm{Ks_{p}}$	BELm7s	Mor16us	MorlIms	$H-052_{\rm s}$	ret
Activation formation training states and the control of th	Activation between training states and training states are supplied from the control of training states and training states are supplied from training s	Activation terming state and the control of the con	cellulose diacetate	cetate	2-butanone	training	310	285.08	0.119	1.58	0.39	0.927	0.412	0	0.029	-0.12	5	40
Weekengeleinnunde raming 143 81, 20 0.113 1.131 0.124. OVER 140 0.124. OVER	Wy-dimental planematic Fraining 413 4114 0.114 0.084 0.014	Wedgebold blood Francising 413 401.75 0.113 0.034 <td>,</td> <td>,</td> <td>2-propanone</td> <td>test</td> <td>280</td> <td>278.17</td> <td>0.119</td> <td>1.58</td> <td>0.39</td> <td>0.927</td> <td>0.412</td> <td>0</td> <td>0.013</td> <td>-0.089</td> <td>9</td> <td>27</td>	,	,	2-propanone	test	280	278.17	0.119	1.58	0.39	0.927	0.412	0	0.013	-0.089	9	27
Percyationed training 515 875.94 0.119 1.881 0.144 0.029 0.481 0.111 0.1084 0.129 0.481 0.119 0.184 0.129 0.481 0.119 0.184 0.129 0.481 0.119 0.184 0.129 0.481 0.119 0.118 0.18 0.	Percyaptomore training 217 870-94 0.119 1.878 0.444 0.029 0.841 0.119 0.0084 0.023 0.023 0.0085 0.00	Pergy discharded exemple 518 28 59 49 1119 1581 0414 0229 0481 0419 04084 0408	Ilulose trica	aprylate	N,N-dimethylformamide	training	413	401.36	0.135	1.318	0.372	0.873	0.383	0	-0.049	0.034	0	<u>×</u>
Particular containing 243, 243, 243, 241, 243, 244, 243, 243, 243, 243, 243, 243	Approprime SSS OLIS 1581 OLIS	Agriculture trining 378.35 0.119 1.881 0.444 0.025 0.481 0 0.013 0.09 Agriculture training 378.35 0.119 1.881 0.444 0.025 0.03 0.03 0.03 0.03 Profuzione training 27.4 2.857.2 0.145 1.486 0.025 1.0 0.013 0.013 0.03 Profuzione training 27.13 2.887.2 0.145 1.486 0.025 1.0 0.013 0.03 <td>cellulose triacetate</td> <td>cetate</td> <td>benzyl alcohol</td> <td>training</td> <td>341</td> <td>367.94</td> <td>0.119</td> <td>1.581</td> <td>0.414</td> <td>0.929</td> <td>0.481</td> <td>0.311</td> <td>0.084</td> <td>0.329</td> <td>0</td> <td>38</td>	cellulose triacetate	cetate	benzyl alcohol	training	341	367.94	0.119	1.581	0.414	0.929	0.481	0.311	0.084	0.329	0	38
water training 343.5 38.9% 0.13 1.557 0.445 0.450 0.451 0.041 0.0138 0.0109 0.0128 0.0139 0.0	water training 343.5 39.29 0.131 1.557 0.445 0.450 0.450 0.128 0.128 0.129 0.128 0.129 0.128 0.129 0.128 0.129 0.128 0.129 0.128 0.129 0.128 0.129 0.128 0.129 0.128 0.129 0.128 0.129 0.128 0.129 0.1	water training 343.5 32.0 13.1 15.5 0.445 0.450 0.450 0.138 0.128		,	2-propanone	test	300	2/8.93	0.119	1.581	0.414	0.929	0.481	0	0.013	-0.089	9	17
missione training 32454 5701 1255 0.445 0.450 0.451 0.500 0.431 0.050 0.415 0.018 0.018 0.018 0.018 0.018 0.018 0.018 0.018 0.019 0.	anisole training 224.3 38.98 0.139 1.583 0.445 0.958 0.131 0.058 0.145 0.058 0.145 0.058 0.145 0.128 0.149 0	ausised training 322.53 38.98 0.139 1.553 0.345 0.533 0.2 0.128 0.128 0.139 0.	ydroxypropy	lcellulose	water	training	343.85	382.27	0.131	1.557	0.443	0.945	0./31	0	0.128	0	0	78
animale test 35.43 36.86 0 1 0.449 0.249 0.50 <t< td=""><td> According the control of the contr</td><td> Particule</td><td>methylcellulose</td><td>ē</td><td>water</td><td>training</td><td>332.65</td><td>349.89</td><td>0.139</td><td>1.585</td><td>0.415</td><td>0.938</td><td>0.533</td><td>0</td><td>0.128</td><td>0</td><td>0</td><td>30</td></t<>	According the control of the contr	Particule	methylcellulose	ē	water	training	332.65	349.89	0.139	1.585	0.415	0.938	0.533	0	0.128	0	0	30
2-proposed training parts 23, 33, 38, 38, 38, 30, 33, 38, 38, 30, 30, 33, 38, 38, 30, 30, 32, 34, 34, 34, 34, 34, 34, 34, 34, 34, 34	2-proposed training 27-3 38.8 0.1/3 1.22 0.487 0.087 0.081 0.01 0.00 0.00 2-proposed training 27-4 28.8 0.1/3 1.45 0.28 1 0.821 0.11 0.04 0.00 chryl chloroscene training 27-8 2.0-6 0.145 1.45 0.28 1 0.821 0.01 0.04 0.03 whyly chloroscene training 27-15 28-16 1.45 0.28 1 0.821 0.01 0.02 0.02 certablioroschare training 27-15 28-16 1.45 0.28 1 0.02	Pergraphed training 297.3 28.83 0.175 0.425 1 0.821 0.135 0.006 0.006 Pergraphed training 27.3 28.83 0.175 1.145 1.25 0.821 1 0.821 0.131 0.238 0.006 0.008 chly chloroscente training 27.55 2.0145 1.456 0.225 1 0.821 0.131 0.238 0 0.008 0 <th< td=""><td>oly(1-butene)</td><td>(isotactic)</td><td>anisole</td><td>test</td><td>362.3</td><td>396.86</td><td>0</td><td>_</td><td>0.449</td><td>0.941</td><td>0.606</td><td>0.238</td><td>0.041</td><td>0.201</td><td>0</td><td>19</td></th<>	oly(1-butene)	(isotactic)	anisole	test	362.3	396.86	0	_	0.449	0.941	0.606	0.238	0.041	0.201	0	19
between craiming 28.45 27.66 10.45 14.86 0.225 1 0.18 0.18 0.045 0.038 0.038 0.038 0.041 0.040 0	between craining 124 25.5 0.145 1.48 0.225 1 0.81 0.13 0.04 0.03 0.13 0.04 0.05 0.13 0.04 0.05 0.13 0.04 0.05 0.13 0.04 0.05 0.13 0.04 0.05 0.13 0.04 0.05 0.13 0.05 0.13 0.05 0.13 0.05 0.13 0.05 0.13 0.05 0.13 0.05	beforementation training 224 25.25 0.145 1.48 0.225 1 0.881 0.18 0.04 0.05 0.13 0.04 </td <td>alv(butv1 met</td> <td>(hacrylate)</td> <td>2-propanol</td> <td>training</td> <td>297.3</td> <td>338.58</td> <td>0.175</td> <td>1.522</td> <td>0.487</td> <td>0.975</td> <td>0.818</td> <td>0</td> <td>0.157</td> <td>0.036</td> <td>0</td> <td>42</td>	alv(butv1 met	(hacrylate)	2-propanol	training	297.3	338.58	0.175	1.522	0.487	0.975	0.818	0	0.157	0.036	0	42
ethylebrone test 57,84 77,16 11,4 0.25 1 0.31 0.31 0.33 0.33 0.33 0.33 0.33 0.34 0.35 0.04 0.12 0.05	childrenzenene tostation 558,45 751,66 0.145 1.456 0.255 1 0.315 0.316 0.137 0.017 0.018	childrenomene tost 558,45 75,66 0.145 1.456 0.255 1 0.831 0.316 0.138 chily chloroscente training 27.13, 2.86,45 0.145 1.456 0.225 1 0.821 0.446 0.035 0.013 0.014 0	oly(4-chloroe	(Vicence)	benzene	training	274	255 72	0.145	1 436	0.525	_	0.821	0 188	0.413	0.248	C	23
Second Companies	control planement	colory physication Children (1988) Childre	J1 y (T - CIII OI O	(yiele)	Schizzino -411	caming	110	1000	24.10	2001	20.0	٠.	0.021	0.110	2000	0.00	0 0	3 6
temply thereactine training 34213 28844 6145 1456 0225 1 0221 04 0435 0228 1 0228 1 04 0435 0228 1 0228 1 04 0435 0228 1 04 0435 0228 1 04 0435 0228 1 04 0435 0228 1 04 0435 0228 1 04 0435 0228 1 04 0435 0228 1 04 0435 0228 1 04 0435 0228 1 04 0435 0228 1 04 0435 0228 1 04 0435 0228 1 04 0435 0228 1 04 0435 0228 1 04 0435 0228 1 04 0435 0228 1 04 0435 0228 1 04 0435 0238 0435 04341 0238 0435 04341 0238 0435 04341 0238 0435 04341 0238 0435 04341 0238 0435 04341 0238 0435 04341 0238 0435 04341 0238 0435 04341 0238 0435 04341 0238 0435 04345 0435 04345 0435 0434 0435 0435	city of plane canner training statisty of state and stat	temporphenomentare training 34213 28844 1145 1456 0225 1 0221 04 01305 0121 028 01411 04 01414 0144 0144 0144 0145 0145			emyloenzene	lest	230.43	270.01	0.145	1.450	0.323	_ ,	0.021	0.511	0.290	0.220	o °	67
isopropylethoraceme training 264.52 287.7 0.145 1.625 1 0.453 0.048 isopropylethoraceme training 264.95 287.7 0.145 1.625 1 0.223 0 0.143 -0.232 methylethoraceme training 264.95 287.7 1 0.455 1 0.221 0 0.143 -0.193 0 0.143 -0.193 0 0.143 0.028 0	isopropylic theorement training 254.51 288.76 0.145 0.255 1 0.441 0.043 0.048 0.04	isopropylichtenzeuer training 26459 2877 0 144 1436 0225 1 0 0.451 0 0.453 0.028 0 netwity influencement training 26459 2845 0 1445 1456 0225 1 0 0.21 0 0.124 0.028 0 netwity influencement training 26459 2845 0 145 1456 0225 1 0 0.21 0 0.101 0 0.			ethyl chloroacetate	training	2/1.35	280.44	0.145	1.436	0.525	_	0.821	0	0.036	-0.12/	0	67.
subpright clustered training 255-47 275-57 1145 1625 1 0.124 -0.122 0 etrach/loomedheue training 373.75 285.97 0.145 1.625 1 0.151 0 0.152 0 terrach/loomedheue training 23.85 31.11 0.145 1.625 1 0.251 0 0.151 0 0.151 0 0 0 1 0	subpright chroacement training 2014 0.124 0.104 0.103 0.102 0.103 0.104 0.10	subpright chroatement training 25.94.73 0.145 1.65.75 1.05.00 0.124 -0.122 0 0.124 -0.122 0 0 0.124 -0.122 0 0 0.124 0 <td></td> <td></td> <td>isopropylbenzene</td> <td>training</td> <td>332.15</td> <td>288.76</td> <td>0.145</td> <td>1.436</td> <td>0.525</td> <td>_</td> <td>0.821</td> <td>0.464</td> <td>0.353</td> <td>0.28</td> <td>0</td> <td>29</td>			isopropylbenzene	training	332.15	288.76	0.145	1.436	0.525	_	0.821	0.464	0.353	0.28	0	29
transing children training and a state of the control of the contr	transing children training and an article choice character (1818) and a state of the choice character (1818) and a state of the choice choice character (1818) and a state of the choice choice (1818) and a state of the choice (1818)	methol conclusion current rest 377,2 254,4 0145 0.25 1 0821 0 0.15 0.18 0 0.18 0 0.18 0 0.18 0 0.18 0 0.18 0 0.18 0 0.18 0 0.18 0			isopropyl chloroacetate	training	264.95	279.71	0.145	1.436	0.525	_	0.821	0	0.124	-0.232	О	29
transplanement raining 31345 315710 0145 1456 0252 1 0 021 0 0.016	transchlorenthame training 313.5 31.51.0 14.50 10.525 1 1 0.521 0 1 0.101 0 1.057 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	transchlorentheme training 313.53 31.71 0145 1.436 0.252 1 0.051 0.051 0.053 0.010 0.053 0.010 0.053 0.010 0.053 0.010 0.053 0.010 0.053 0.010 0.053 0.010 0.053 0.010 0.053 0.023 0.033 0.033 0.033 0.033 0.035 0.035 0.035 0.035 0.005 0.035 0.005 0.035 0.005 0.035 0.005 0.035 0.005 0.035 0.005 0.035 0.005 0.035 0.005 0.035 0.005 0.035 0.005 0.035 0.005 0.035 0.005 0.035 0.005 0.035 0.005 0.035 0			mathyl oblogogatata	o toot	27 75	205.15	0.175	1 136	0.505	-	0.821		-0.150	0 18	· C	20
tetrachronentement training 353.85 31.71 0145 1436 0225 1 0.821 0 0.0101 -0.937 0 0.001 channon training 353.85 31.71 0145 1436 0225 1 0.821 0 0.0101 -0.937 0 0.001 channon training 353.85 31.71 0145 1439 0.487 0.966 0.73 0.0087 0 0.007 channon training 353.85 31.71 0145 1439 0.487 0.966 0.73 0.0087 0 0.0087 channol training 353.85 31.71 0145 1439 0.487 0.966 0.73 0.0087 0 0.0087 channol training 353.85 31.71 0145 1439 0.487 0.966 0.73 0.0087 0 0.0087 channol training 353.85 31.71 0.145 0.487 0.966 0.73 0.0087 0.0087 0 0.0087 channol training 453.85 41.489 0 0.487 0.966 0.73 0.0087 0.0087 0 0.0087 channol training 453.85 41.489 0 0.008 0.442 0.884 1 0.0087 0.0087 0 0.0087 channol training 453.85 41.489 0 0.008 0.442 0.884 1 0.0087 0.0087 0 0.0087 channol training 453.85 41.489 0 0.008 0.442 0.884 1 0.008 0.0087 0 0.0087 channol training 453.85 41.489 0 0.008 0.442 0.884 1 0.008 0.0087 0 0.0087 channol training 453.85 41.489 0 0.008 0.442 0.884 1 0.008 0.0087 0 0.0087 channol training 453.85 41.489 0 0.008 0.442 0.884 1 0.008 0.0087 0 0.0087 channol training 453.85 41.489 0 0.008 0.442 0.884 1 0.008 0.008 0.008 channol training 453.85 41.489 0 0.008 0.0	tetrachroenement training 313.88 31.71 0145 1436 0225 14 0821 0 0.0101 -0.037 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	tetrationement training 31.33.8 31.71 01.45 1.456 0.225 1 0 0.25 1 0 0.013 0.037 0.001 0.0			incury cinoroacciaic		0.00	0000	5.5	001.	20.0		0.021	0	0.15	01.0		9 6
Particular	Control Cont	Purpose			tetrachloroethene	training	51/.55	285.09	0.145	1.430	0.525	_	0.821	0	0.161	-0.55/	0	67
Houtanoon training 318.05 32.62 1.449 0.487 0.966 0.73 0.000	Hellatinoo training 236.65 236.22 1.449 0.487 0.966 0.735 0.0007 0.0007 Hellatinoo training 236.65 236.13 0.222 1.449 0.487 0.966 0.735 0.0007 0.0007 Hellatinoo training 236.65 236.14 0.222 1.449 0.487 0.966 0.735 0.0007 0.0007 Hellatinoo training 236.65 236.14 0.222 1.449 0.487 0.966 0.735 0.0007 0.0007 Hellatinoo training 240.66 414.49 0.222 1.449 0.487 0.966 0.735 0.0007 0.0007 Hellatinoo training 240.65 414.49 0.222 1.449 0.487 0.966 0.735 0.0007 0.0007 Hellatinoo training 240.65 414.49 0.222 0.442 0.884 1 0.081 0.035 0.706 0.706 Hellatinoo training 247.65 436.03 0.0007 0.442 0.884 1 0.018 0.707 0.706 0.706 Hellatinoo training 247.65 248.03 0.0007 0.442 0.884 1 0.018 0.707 0.707 Hellatinoo training 247.65 248.03 0.0007 0.442 0.884 1 0.018 0.707 0.707 Hellatinoo training 247.65 248.03 0.0007 0.0007 0.0007 0.0007 Hellatinoo training 247.65 249.03 0.0007 0.0007 0.0007 0.0007 Hellatinoo training 247.65 249.03 0.0007 0.0007 0.0007 0.0007 0.0007 Hellatinoo training 247.65 249.03 0.0007 0.0007 0.0007 0.0007 0.0007 0.0007 Hellatinoo training 247.65 244.08 0.0007 0.0	Helpatanol training 236.55 236.62 1449 0.487 0.966 0.73 0.0002 0.0007 0.0			tetrachloromethane	training	323.85	317.11	0.145	1.436	0.525	_	0.821	0	-0.013	-0.912	0	50
Changed Color Co	Head	Appendix Color C	alv(ethyl acr	vlate)	1-butanol	training	318.05	318.2	0 232	1 440	0.487	0.066	0.73	_	0.171	0.100	C	25
Perpanol training 20,555 346,51 4 6.222 1.449 6.445 0.666 0.73 0.0002 0.0001	terminol tests and the proposed currently control testing 20,555 3,63,1 0.22 1,499 0,479 0,960 0,73 0 0,003 0,009 0,000	The control between training 1,555 2,562 1,449 0,447 0,966 0,73 0,000	ay (ceny) ac	y rate)	1-OutailOi	caming	210.02	250.00	2000	1.1	70.0	0000	0.0	0 0	0000	0.10	0 0	3 6
Proposition Training 32,655 326,14 0.225 1,449 0.487 0.966 0.73 0.070 0.087 0.	Proposition Training 32,65 326,14 0.225 1,449 0.487 0.966 0.73 0.007 0.0087 0.	methmool training 23.55 34.0.1 0.22 1.449 0.487 0.966 0.73 0 0.007 0.087 0 auxiloole, ether training 42.65 3.46.1 0.22 1.449 0.847 0.966 0.73 0 0.003 0.007 0 0 0.003 0.003 0 0.003 0 <td></td> <td></td> <td>ethanol</td> <td>test</td> <td>510.55</td> <td>29.075</td> <td>0.232</td> <td>1.449</td> <td>0.48/</td> <td>0.966</td> <td>0.73</td> <td>0</td> <td>0.082</td> <td>0.001</td> <td>0</td> <td>52</td>			ethanol	test	510.55	29.075	0.232	1.449	0.48/	0.966	0.73	0	0.082	0.001	0	52
Propagated Praining 236,5 41449 0.225 1.449 0.487 0.964 0.73 0.093 0.093 0.093 0.095	Proposition Proprint Property Proper	Proposed Parishing 43.65 414.49 0.225 1449 0.425 0.445 0.235 0.079 0.079 0.079 Percord Percord Praishing 45.65 414.49 0.22 0.442 0.442 0.844 1 0.201 0.201 0.239 0.795 0.795 0.795 Percord			methanol	training	293.65	340.31	0.232	1,449	0.487	0.966	0.73	0	-0.067	0.087	0	25
training 426.65 41.04 0.04 0.04 0.08 0.04 0.03 0.03 0.03 0.04 0.04 0.08 0.08 0.04 0.03 0.09 0.09 0.09 0.09 0.09 0.09 0.09	Prophenol	Project			1 2500000	10.00	210.65	276 14	0.33	1 440	0.467	0.066	0.72	· C	0.002	0.070	• <	5
missione training do. 24.00.00 44.24.00.00 0.44.24.00.00 0.84.41.00 0.04.25.00 0.04.10 0.02.30 0.02.00 0.04.20 0.04.20 0.04.20 0.04.20 0.04.20 0.04.20 0.04.20 0.04.20 0.04.20 0.04.20 0.08.41 0.08.31 0.02.01 0.02.01 0.04.20 0.09.41 0.09.81 0.02.20 0.09.00 0.04.20 0.09.41 0.09.81 0.03.95	missole training 4.26.50 414.94 0 0.442 0.894 1 0.243 0.041 0.201 pinplenyl cheryl pinplenyl cheryl 40.65 441.94 0 0 0.442 0.894 1 0.243 0.041 0.201 piplenyl terr quo. 42.25 0 0 0.442 0.894 1 0.835 0.395 0.395 piplenyl/methan training 42.367 3.663 0 0 0.442 0.894 1 0.895 0.799 0 0.799 0 0.799 0 0.799 0 0.799 0 0.799 0 0.799 0	benyl plenyl ether training 42.56 A 81.98 0 0 0 0.442 0 0.894 1 0.238 0.335 0.349 0 0.401 0.201 0.991 0.991 0.201 0.201 0.901 0.201 0.901 0.201 0.201 0.201 0.901 0.201		,	1-propanoi	u dilling	50.716	520.14	0.232	1.44	701.0	0.900	c/.o	0	0.000	0.079	0 0	3.
beyony plebyl ether training 45.65 415.18 0 0 0 0442 0.894 1 0.802 0.353 0.539 0.599	behavely tethory ether training 46.55 48.18 0 0 0.442 0.884 1 0.915 0.332 0.339 Objectively test 40.065 445.02 0.894 1 0.915 0.706	behavely tehryl chebry (ether training 46.55 45.15 0 0 0.442 0.894 1 0.915 0.332 0.339 0 0 0.442 0.894 1 0.915 0.706 0.706 0 0 0 0 442 0.894 1 0.918 0.736 0.706 0 0 0 442 0.894 1 0.918 0.726 0.706 0 0 0 442 0.894 1 0.918 0.726 0.706 0 0 0 442 0.894 1 0.918 0.726 0 0 0 442 0	olyethylene	(Innear)	anisole	training	426.65	414.49	0	0	0.442	0.894	_	0.238	0.041	0.201	0	77
tiphenyl cst 4016 415 0 0.442 0.894 1 0.892 0.25 0 <th< td=""><td> June June </td><td> Highery High</td><td></td><td></td><td>henzyl nhenyl ether</td><td>training</td><td>462 65</td><td>481 98</td><td>0</td><td>0</td><td>0.442</td><td>0.894</td><td>_</td><td>0.981</td><td>0 332</td><td>0 340</td><td>0</td><td>24</td></th<>	June	Highery High			henzyl nhenyl ether	training	462 65	481 98	0	0	0.442	0.894	_	0.981	0 332	0 340	0	24
Opplemyl test 40,002 45,002 0,042 0,884 1 0,882 0,359 0,229 0 Opplemyl cher training 470,02 480,03 0 0,442 0,884 1 0,918 0,073 0,756 0 Opplemyl ether training 475,53 436,03 0 0 0,442 0,884 1 0,918 0,739 0	Opposition of training land of land of training land of training land of training land of	Depletary Color			penzyi pirenyi emer	Hammig	20.20+	101.70	0 0	> 0	74.0	0.00	٠,	0.201	2000	0.045	> 0	† ;
Education Limiting 477.05 431.84 0 0 0 0 0 0 0 0 0	I-decreated training 47.65.4 43.18.4 0 0 442 0.884 1 0.935 0.706	I-decimination Table of the problem of training and the problem of training and tr			biphenyl	test	400.65	445.02	0	0	0.442	0.894	_	0.802	0.395	0.529	0	24
diplemay ether training tr	diplemyl cheful training 477.05 436.03 0 0.442 0.894 1 0.918 0.672 0.676 0.676 0.676 0.676 0.676 0.676 0.676 0.676 0.676 0.676 0.676 0.676 0.676 0.676 0.676 0.676 0.676 0.677 0.677 0.677 0.677 0.677 0.677 0.677 0.677 0.677 0.678	dipolary clubration 43.50 43.60 0 64.42 0.894 1 0.518 0.672 0.676 dipolary clubration training 477.05 43.60 0 0.442 0.894 1 0.918 0.672 0.676 depoly inclination training 473.53 42.63 0 0.442 0.894 1 1.082 0.663 1.03 4-covily planol training 473.53 42.62 0 0 0.442 0.894 1 1.082 0.663 1.03 4-covily planol training 473.53 46.22 0 0 0.442 0.894 1 1.082 0.663 1.03 4-cry planol training 473.53 46.93 0 0 0.442 0.894 1 1.082 0.895 0			1 decembl	training	31 901	121.81	0	0	0.442	0.807	-	0.035	902.0	902.0	<u> </u>	77
diphenyl ether training 435.03 436.03 0 0.442 0.894 1 0.918 0.627 0.676 0 Hobbenyl ether training 435.03 42.06 0 0.442 0.894 1 0.918 0.627 0.676 0 Hobbenylmelod training 45.05.25 431.24 0 0 0.442 0.894 1 10.88 0.979 0 Hockmool training 45.05.25 40.65.5 0 0 0.442 0.894 1 10.82 0.979 0 Hockmool training 45.35.4 40.67.8 0 0 0.442 0.894 1 0.789 0.979 0 Portylphenol training 45.5 40.47.8 0 0 0.442 0.894 1 0.789 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 <td>diphenyl ether training 437.05 436.03 0 0.442 0.894 1 0.918 0.027 0.075 Hobbrolylethed training 4.35.03 4.36.03 0 0.442 0.894 1 0.918 0.027 0.075 Hobbrolylethed training 4.50.25 4.06.5 0 0.442 0.894 1 1.082 0.675 0.079 Hockanol training 4.56.5 4.06.78 0 0 0.442 0.894 1 1.082 0.675 0.097 0 Penyl sectate test 0 0 0.442 0.894 1 1.082 0.675 0.042 Penyl sectate test 0 0 0.442 0.894 1 1.082 0.675 0.042 Penyl sectate test 0 0 0.442 0.894 1 0.728 0.675 0.019 0 Debrarone test 0 0 0.442 0.894</td> <td>diplemony elter training 475.5 456.0 0 0.442 0.884 1 0.918 0.627 0.676 0 Olipheuly Interdament training 475.55 456.3 0 0 0.442 0.884 1 0.116 0.88 0.979 0 1-deckeanol training 435.55 426.5 0 0 0.442 0.884 1 0.116 0.88 0.979 0 1-cetanol training 435.55 426.5 0 0 0.442 0.884 1 0.116 0.88 0</td> <td></td> <td></td> <td>1-decallor</td> <td>uannig</td> <td>470.45</td> <td>401.04</td> <td>></td> <td>0</td> <td>7,447</td> <td>0.074</td> <td>-</td> <td>0.723</td> <td>0.700</td> <td>0.700</td> <td>0</td> <td>†</td>	diphenyl ether training 437.05 436.03 0 0.442 0.894 1 0.918 0.027 0.075 Hobbrolylethed training 4.35.03 4.36.03 0 0.442 0.894 1 0.918 0.027 0.075 Hobbrolylethed training 4.50.25 4.06.5 0 0.442 0.894 1 1.082 0.675 0.079 Hockanol training 4.56.5 4.06.78 0 0 0.442 0.894 1 1.082 0.675 0.097 0 Penyl sectate test 0 0 0.442 0.894 1 1.082 0.675 0.042 Penyl sectate test 0 0 0.442 0.894 1 1.082 0.675 0.042 Penyl sectate test 0 0 0.442 0.894 1 0.728 0.675 0.019 0 Debrarone test 0 0 0.442 0.894	diplemony elter training 475.5 456.0 0 0.442 0.884 1 0.918 0.627 0.676 0 Olipheuly Interdament training 475.55 456.3 0 0 0.442 0.884 1 0.116 0.88 0.979 0 1-deckeanol training 435.55 426.5 0 0 0.442 0.884 1 0.116 0.88 0.979 0 1-cetanol training 435.55 426.5 0 0 0.442 0.884 1 0.116 0.88 0			1-decallor	uannig	470.45	401.04	>	0	7,447	0.074	-	0.723	0.700	0.700	0	†
dipleon/honellame training 415.55 421.67 0 0.442 0.884 1 0.918 0.729 0.812 4-bode-annol training 43.51 43.126 0 0.442 0.884 1 1.116 0.88 10.72 0.812 0 4-bode-annol training 43.51 43.124 0 0 0.442 0.884 1 1.116 0.88 1.03 4-cock-annol training 43.52 45.26 0 0 0.442 0.884 1 1.082 0.653 0.42 penyl because training 43.53 450.34 0 0 0.442 0.884 1 1.082 0.653 0.428 0.099 penyl because training 450.78 0 0 0.442 0.884 1 1.082 0.653 0.659 0 0.93 0 0 0 0 0 0 0 0 0 0 0 0 0<	diplomy/purellame training 415.55 421.67 0 0.442 0.884 1 0.918 0.729 0.812 d-bodesmol training 415.35 421.67 0 0 0.442 0.884 1 1.116 0.88 0.979 4-nowlyphenol training 435.25 437.24 0 0 0.442 0.894 1 1.082 0.663 0.979 4-covylphenol training 435.25 437.83 0 0 0.442 0.894 1 1.082 0.663 0.978 penyl acetate test 434.78 0 0 0.442 0.894 1 1.082 0.428 0.979 penyl acetate test 434.78 0 0 0.442 0.894 1 1.082 0.973 0.073 penyl acetate training 30.6 3.11 0 0 0.442 0.894 1 1.082 0.973 0.073 penyl acetate <th< td=""><td>diplemy/phetime training 415.55 421.67 0 0.442 0.894 1 0.918 0.729 0.812 4-bockeaned training 415.55 431.67 0 0.442 0.894 1 1116 0.88 1079 0.812 4-nowlyphenol training 415.55 431.53 40.78 0 0.442 0.894 1 10.82 0.685 10.93 4-nowlyphenol training 415.53 40.78 0 0.442 0.894 1 10.82 0.668 10.93 perryl accase training 415.53 0 0 0.442 0.894 1 10.82 0.428 0.979 perryl accase training 410.78 0 0 0.442 0.894 1 10.82 0.979 0.919 perryl perryl phenol training 410.78 0 0 0.442 0.894 1 10.82 0.979 0.919 perryl carrier 1.03</td><td></td><td></td><td>dinhenvl ether</td><td>training</td><td>437.05</td><td>436.03</td><td>0</td><td>0</td><td>0.442</td><td>0.894</td><td>_</td><td>0.918</td><td>7.29</td><td>0.676</td><td>C</td><td>24</td></th<>	diplemy/phetime training 415.55 421.67 0 0.442 0.894 1 0.918 0.729 0.812 4-bockeaned training 415.55 431.67 0 0.442 0.894 1 1116 0.88 1079 0.812 4-nowlyphenol training 415.55 431.53 40.78 0 0.442 0.894 1 10.82 0.685 10.93 4-nowlyphenol training 415.53 40.78 0 0.442 0.894 1 10.82 0.668 10.93 perryl accase training 415.53 0 0 0.442 0.894 1 10.82 0.428 0.979 perryl accase training 410.78 0 0 0.442 0.894 1 10.82 0.979 0.919 perryl perryl phenol training 410.78 0 0 0.442 0.894 1 10.82 0.979 0.919 perryl carrier 1.03			dinhenvl ether	training	437.05	436.03	0	0	0.442	0.894	_	0.918	7.29	0.676	C	24
Holletymethate training 415.53 45.55 45.50	Control	Location			dialonal mothers	0	315 35	100 67				7000		0100	0.00	0.00	· <	. 5
Hoodycamol training 470.15 471.24 0 0.442 0.894 1 1.116 0.88 0.979 0 Hoodyclamol training 435.25 426.5 0 0.442 0.894 1 1.082 0.555 0.428 0 L-cctuphenol training 435.25 426.5 0 0.442 0.894 1 1.082 0.555 0.428 0 pmyl bench training 436.35 20.86 0 0.442 0.894 1 0.758 0.059 0 pmyl bench training 30.5 20.43 0 0.442 0.894 1 0.759 0 <td>Hookezunol training 470.15 471.2 0 0.442 0.894 1 1.116 0.88 0.979 0 Hookupholol training 435.25 437.53 437.53 437.53 0 0 0.442 0.894 1 1.082 0.665 1.03 0 Hoorylphenol training 435.25 437.53 0 0 0.442 0.894 1 0.528 0.555 0.43 0 Purply phenol training 435.35 437.53 0 0 0.442 0.894 1 0.556 0.039 0 Purply phenol training 30.56 268.22 0 0 0.442 0.894 1 0.556 0.039 0 0 0.442 0.894 1 0.019 0</td> <td> Holyappenoration Training 410.15 431.24 0 0 0.442 0.884 1 1.116 0.88 0.979 0 Holyappenoration Training 453.25 436.55 0 0 0.442 0.884 1 0.728 0.555 0.428 0 Holyappenoration Training 453.25 436.55 0 0 0.442 0.884 1 0.728 0.555 0.428 0 Holyappenoration Training 453.25 430.55 0 0 0.442 0.884 1 0.55 0.555 0.428 0 Holyappenoration Training 453.25 450.55 0 0 0.442 0.884 1 0.55 0.555 0.428 0 Holyappenoration Training 453.25 459.34 0 0 0.442 0.884 1 0.55 0.356 0.294 0.005 Holyappenoration Training 453.25 344.98 0.172 1.149 0.445 0.995 0.908 0.007 0.007 0.007 Holyappenoration Training 249 24.23 0 0.811 0.406 0.934 0.465 0.918 0.007 0.007 Holyappenoration Training 249 24.23 0 0.811 0.406 0.934 0.465 0.918 0.007 0.007 Holyappenoration Training 249 26.23 0 0.811 0.406 0.934 0.465 0.918 0.007 0.006 0.008 0.</td> <td></td> <td></td> <td>aipnenyimetnane</td> <td>training</td> <td>415.55</td> <td>472.07</td> <td>0</td> <td>0</td> <td>0.447</td> <td>0.894</td> <td>_</td> <td>0.918</td> <td>0.729</td> <td>0.812</td> <td>0</td> <td>77</td>	Hookezunol training 470.15 471.2 0 0.442 0.894 1 1.116 0.88 0.979 0 Hookupholol training 435.25 437.53 437.53 437.53 0 0 0.442 0.894 1 1.082 0.665 1.03 0 Hoorylphenol training 435.25 437.53 0 0 0.442 0.894 1 0.528 0.555 0.43 0 Purply phenol training 435.35 437.53 0 0 0.442 0.894 1 0.556 0.039 0 Purply phenol training 30.56 268.22 0 0 0.442 0.894 1 0.556 0.039 0 0 0.442 0.894 1 0.019 0	Holyappenoration Training 410.15 431.24 0 0 0.442 0.884 1 1.116 0.88 0.979 0 Holyappenoration Training 453.25 436.55 0 0 0.442 0.884 1 0.728 0.555 0.428 0 Holyappenoration Training 453.25 436.55 0 0 0.442 0.884 1 0.728 0.555 0.428 0 Holyappenoration Training 453.25 430.55 0 0 0.442 0.884 1 0.55 0.555 0.428 0 Holyappenoration Training 453.25 450.55 0 0 0.442 0.884 1 0.55 0.555 0.428 0 Holyappenoration Training 453.25 459.34 0 0 0.442 0.884 1 0.55 0.356 0.294 0.005 Holyappenoration Training 453.25 344.98 0.172 1.149 0.445 0.995 0.908 0.007 0.007 0.007 Holyappenoration Training 249 24.23 0 0.811 0.406 0.934 0.465 0.918 0.007 0.007 Holyappenoration Training 249 24.23 0 0.811 0.406 0.934 0.465 0.918 0.007 0.007 Holyappenoration Training 249 26.23 0 0.811 0.406 0.934 0.465 0.918 0.007 0.006 0.008 0.			aipnenyimetnane	training	415.55	472.07	0	0	0.447	0.894	_	0.918	0.729	0.812	0	7 7
4-nonylphenol training 435.55 477.53 0 0.442 0.894 1 1082 0.663 10.3 4-cotmol training 473.55 497.5 0 0 0.442 0.894 1 1082 0.655 0.043 0 4-cotmol training 473.55 490.8 0 0.442 0.894 1 0.855 0.655 0.098 0 4-cr-pentylphenol training 463.53 490.4 0 0.442 0.894 1 0.855 0.029 0.098 0 0.099 0.098 0 0.099 0.098 0 0.099 0.098 0 0.099 0.098 0 0.099 0.098 0 0.099 0.098 0 0.099 0	4-nonylphenol training 435.53 497.53 0 0.442 0.894 1 1082 0.663 10.3 4-nonylphenol training 453.52 426.5 0 0 0.442 0.894 1 1082 0.655 0.043 4-cytylphenol training 475.53 450.84 0 0 0.442 0.894 1 1082 0.656 0.034 4-cryphenol training 475.5 450.34 0 0 0.442 0.894 1 0.356 0.039 0.098 4-cryphenol training 30.5 30.11 0 0.442 0.894 1 0.356 0.039 0.099 alphenyl phenol training 30.5 31.41 0 0.811 0.466 0.934 0.695 0.039 0.099 0.099 0.099 0.099 0.099 0.099 0.099 0.099 0.099 0.099 0.099 0.099 0.099 0.099 0.099 0.099	4-nonylphenol training 455.55 497.5 0 0.442 0.894 1 1082 0.663 103 0 4-conylphenol training 457.55 426.5 0 0 0.442 0.894 1 1082 0.655 0.043 0 4-corylphenol training 47.55 450.8 0 0 0.442 0.894 1 1082 0.656 0.03 4-cryphenol training 46.55 30.1 1 1.04 0.442 0.894 1 0.356 0.294 0.894 1 0.356 0.039 0.09			1-dodecanol	training	410.15	431.24	0	0	0.442	0.894	_	1.116	0.88	0.079	0	4
Homotyphenol training 45.5.2 45.7.5 0 0.442 0.894 1 1.05 0.555 1.05 4-coraphenol training 45.3.2 45.6.8 0 0.442 0.894 1 1.05 0.55 0.29 4-coraphenol training 45.3.5 45.9.3 0 0 0.442 0.894 1 1.08 0.552 0.896 0 pemyl acetaen training 30.26 5.84.9 0 0.44 0.894 1 0.55 0.029 0.029 1-propanol training 30.6 30.11 0 0.44 0.994 0.695 0.093 0.079 0.019 diphenyl phranace training 20.6 30.11 0 0.44 0.994 0.695 0.099 0.079 0.019 diphenyl phranace training 20.6 3.11 0 0.81 0.46 0.994 0.695 0.099 0.079 0.019 toluere trainin	+rootyphenol training 457.53 47.73 0 0.442 0.894 1 1.03 0.555 1.03 0 4-corpuble of test training 453.25 450.88 0 0.442 0.894 1 1.082 0.555 0.938 0 4-corpylphenol training 463.35 459.34 0 0.442 0.894 1 0.356 0.377 0.019 Pennyl accente test 4404.78 0 0.442 0.894 1 0.356 0.029	Hotolyphenol training 433.23 455.53 0 0.442 0.894 1 0.252 0.635 1.03 Lectanol training 433.23 426.53 0 0 0.442 0.894 1 0.252 0.896 0 penyl acetate training 435.25 450.85 0 0 442 0.894 1 0.252 0.896 0 penyl acetate training 302.6 283.2 0.114 0 0.442 0.894 1 0.255 0.029 0.039			4	0	44 40	727 62	0 0	o c		7000		000	0000		o c	
Perchanol training 47.65 60 60 60 60 60 60 60	Perctanol training 447.65 0 0 0.442 0.894 1 0.755 0.655 0.493 0.494 1 0.755 0.655 0.495				4-nony1pnenol	training	433.33	457.33	0	0	0.447	0.894	_	1.082	0.003	1.03	0	47
4-ectyphenol training 447.65 46.88 0 0.442 0.894 1 1.082 0.552 0.896 0 punt) accatac training 447.65 450.88 0 0.442 0.894 1 0.556 0.569 0 2-butanone training 30.65 26.82 0.147 1.149 0.464 0.999 0.908 0.09 0.009	4-octylphenol training acetact 447 65 450.85 0 0.442 0.894 1 1082 0.562 0.896 0 permy acetact trst 434 4404.78 0 0.442 0.894 1 0.556 0.037 0.019 3 2-bruganone training 460.33 490.34 0 0.442 0.894 1 0.556 0.0294 0 <th< td=""><td>4-cctylphenol training test 447 65 45.85 0 0.442 0.894 1 1082 0.562 0.896 0 puny acetter training 447 65 45.083 0 0.442 0.894 1 0.556 0.019 3 2-puntanone training 463.35 499.34 0 0.442 0.894 1 0.556 0.019 3 2-puntanone test 326.5 344.82 0.11 0.17 1.34 0.464 0.999 0.988 0 0.029 0.078 0.029 0.019 0 2-propanol test 306.5 30.11 0.17 1.34 0.466 0.934 0.465 0.931 0.079 0.019 0 chyl benzene training 206.5 30.11 0.17 1.34 0.466 0.934 0.465 0.934 0.079 0.019 0 chyl benzene training 206.5 30.11 0.41 0.446 0.934</td><td></td><td></td><td>1-octanol</td><td>training</td><td>453.25</td><td>426.5</td><td>0</td><td>0</td><td>0.442</td><td>0.894</td><td>_</td><td>0.728</td><td>0.555</td><td>0.428</td><td>0</td><td>24</td></th<>	4-cctylphenol training test 447 65 45.85 0 0.442 0.894 1 1082 0.562 0.896 0 puny acetter training 447 65 45.083 0 0.442 0.894 1 0.556 0.019 3 2-puntanone training 463.35 499.34 0 0.442 0.894 1 0.556 0.019 3 2-puntanone test 326.5 344.82 0.11 0.17 1.34 0.464 0.999 0.988 0 0.029 0.078 0.029 0.019 0 2-propanol test 306.5 30.11 0.17 1.34 0.466 0.934 0.465 0.931 0.079 0.019 0 chyl benzene training 206.5 30.11 0.17 1.34 0.466 0.934 0.465 0.934 0.079 0.019 0 chyl benzene training 206.5 30.11 0.41 0.446 0.934			1-octanol	training	453.25	426.5	0	0	0.442	0.894	_	0.728	0.555	0.428	0	24
percylipterion training 47.50.3 40.78 0.0442 0.894 1 0.55 0.57 0.50 percylipterion training 45.3.5 46.3.8 40.78 0 0.442 0.894 1 0.05 0.029 0.029 elperylactoric training 46.5.3 44.98 0.172 1.53 0.468 0.996 0 0.029 <td>percy planetol training 47.50 40.78 0.0442 0.894 1 1.052 0.039</td> <td>+extypitation training 447.50 450.83 0 0.442 0.894 1 150.20 0.50<!--</td--><td></td><td></td><td>A contradar</td><td>0</td><td>37 27 6</td><td>750 05</td><td></td><td></td><td>277</td><td>000</td><td></td><td>000</td><td>0.55.0</td><td>2000</td><td></td><td>5</td></td>	percy planetol training 47.50 40.78 0.0442 0.894 1 1.052 0.039	+extypitation training 447.50 450.83 0 0.442 0.894 1 150.20 0.50 </td <td></td> <td></td> <td>A contradar</td> <td>0</td> <td>37 27 6</td> <td>750 05</td> <td></td> <td></td> <td>277</td> <td>000</td> <td></td> <td>000</td> <td>0.55.0</td> <td>2000</td> <td></td> <td>5</td>			A contradar	0	37 27 6	750 05			277	000		000	0.55.0	2000		5
Penryl acctatac test 434 404.78 0 0 0.442 0.884 1 0.55 0.379 0.09 3 2-butanone training 406.33 496.73 6.042 0 0.042 0.089 0.086 0.029 0.019 3 2-butanone training 302.6 268.22 0.147 1.149 0.468 0.999 0.088 0.029 0.029 0.029 1-propanol training 240.5 36.11 0.081 0.466 0.934 0.665 0.017 0.079 0 ethyl beptanoate training 240 26.2.3 0 0.811 0.466 0.934 0.465 0.818 0.069 0.039 0.069 0.039 0.069 0.039 0.069 0.039 0.069 0.039 0.069 0.039 0.069 0.039 0.069 0.039 0.069 0.039 0.069 0.039 0.045 0.081 0.044 0.045 0.081 0.045 0	Permyl acctatact test 434 404.78 0 0 0.442 0.884 1 0.55 0.37 —0.019 3 4-permyl pennyl phenol training 405.35 20.88.22 0.147 1.149 0.464 0.999 0.998 0.036 0.294 0.079 0.029 1-propanol test 226.5 344.98 0.172 1.53 0.468 0.999 0.998 0.039 0.079 0.029 diphenyl ether training 240.5 34.11 0 0.811 0.466 0.934 0.465 0.918 0.057 0.067 0.079 0.099 0.098 0.039 0.098 0.039 0.099<	penuly acctate test 444 404,8 0 0 442 0.894 1 0.55 0.019 3 2-butanone training 465.35 2.68.2 0.147 1.149 0.442 0.894 1 0.356 0.204 0.019 3 2-butanone training 326.5 248.2 0.147 1.149 0.464 0.999 0.908 0 0.204 0.029 1-propand training 306 26.2 0.147 1.149 0.464 0.999 0.908 0 0.029 0 0.029 0 0.029 0 0.029 0 0.029 0 0.029 0			4-octy/phenol	tranning	60.744	450.05	0	0	0.447	0.094	_	1.002	0.302	0.090	0	1
4-ter/-pentylphenol training 46.33 45.934 0 0.442 0.894 1 0.936 0.559 0.294 0 1-pottatione training 30.6.5 348.32 0.147 1.149 0.464 0.999 0.098 0 0.0093 0.079 1-pottatione training 30.6.5 34.1.1 0.146 0.994 0.695 0 0.003 0.079 0.079 dipherylether training 30.6 34.1.1 0 0.811 0.406 0.934 0.465 0.918 0.603 0 0.079 <td>4-terf-pentylphenol training 46.33 45.934 0 0 0.442 0.884 1 0.936 0.559 0.0294 0 1-potnamone training 30.6.5 3.49.34 0 0.444 0.999 0.098 0 0.003 0.0172 5 1-potnamone training 30.6.5 34.11 0 0.811 0.446 0.994 0.095 0 0.003 0.0172 5 ethylborazoate training 3.06 31.11 0 0.811 0.406 0.934 0.465 0.918 0.069 0</td> <td>4-terr-pentylphenol training 463.35 459.34 0 0.442 0.884 1 0.936 0.559 0.294 0 1-pobtanone training 30.6.5 3.49.34 0.147 1.149 0.464 0.999 0.998 0.093 0.079 0.079 1-pobtanone training 30.6 30.1.11 0 0.811 0.406 0.934 0.465 0.918 0.0693 0.079 0.07</td> <td></td> <td></td> <td>pentyl acetate</td> <td>test</td> <td>434</td> <td>404.78</td> <td>0</td> <td>0</td> <td>0.442</td> <td>0.894</td> <td>_</td> <td>0.55</td> <td>0.377</td> <td>-0.019</td> <td>n</td> <td>33</td>	4-terf-pentylphenol training 46.33 45.934 0 0 0.442 0.884 1 0.936 0.559 0.0294 0 1-potnamone training 30.6.5 3.49.34 0 0.444 0.999 0.098 0 0.003 0.0172 5 1-potnamone training 30.6.5 34.11 0 0.811 0.446 0.994 0.095 0 0.003 0.0172 5 ethylborazoate training 3.06 31.11 0 0.811 0.406 0.934 0.465 0.918 0.069 0	4-terr-pentylphenol training 463.35 459.34 0 0.442 0.884 1 0.936 0.559 0.294 0 1-pobtanone training 30.6.5 3.49.34 0.147 1.149 0.464 0.999 0.998 0.093 0.079 0.079 1-pobtanone training 30.6 30.1.11 0 0.811 0.406 0.934 0.465 0.918 0.0693 0.079 0.07			pentyl acetate	test	434	404.78	0	0	0.442	0.894	_	0.55	0.377	-0.019	n	33
Expression of training characters Training ch	Perturport training 30.55 20.27 0.147 0.146 0.094 0.095 0.002 0.013 0.042 0.043 0.044	2-bitations Training tests 20.55 26.25 0.147 1.149 0.444 0.999 0.908 0.209 0.029 0.023 0.012 0.023 0.012 0.023 0.012 0.023 0.012 0.023 0.012 0.023 0.012 0.023 0.012 0.023 0.012 0.023 0.012 0.023 0.012 0.023 0.012 0.023 0.012 0.023 0.012 0.023 0.012 0.023 0.012 0.023 0.012 0.023 0.012 </td <td></td> <td></td> <td>A tast nepty/phenol</td> <td>training</td> <td>162 25</td> <td>150 37</td> <td></td> <td>_</td> <td>0.442</td> <td>0.807</td> <td>-</td> <td>0.036</td> <td>0 560</td> <td>0.007</td> <td>_</td> <td>2</td>			A tast nepty/phenol	training	162 25	150 37		_	0.442	0.807	-	0.036	0 560	0.007	_	2
2-buttanoue traning Lating 30.5 20.5 1.14 0.464 0.999 0.908 0 0.029 0.012 0.012 0.012 0.012 0.012 0.012 0.012 0.012 0.012 0.012 0.012 0.012 0.012 0.012 0.014 0.014 0.014 0.014 0.018 0.046 0.934 0.465 0.081 0.046 0.934 0.465 0.081 0.069 0.034 0.069 0.034 0.069 0.034 0.069 0.034 0.069 0.034 0.069 0.034 0.069 0.034 0.069 0.034 0.069 0.034 0.069 0.034 0.069 0.034 0.069 0.034 0.069 0.034 0.069 0.034 0.069 0.034 0.069 0.034 0.069 0.034 0.069 0.034 0.046 0.034 0.046 0.034 0.046 0.034 0.046 0.034 0.046 0.034 0.046 0.034 0.046 0.034 0.046	2-butanone test 362.5 268.22 0.147 1.149 0.464 0.999 0.908 0 0.029 -0.12 5 1-propanol test 366.5 360.11 0.17 1.53 0.468 0.994 0.968 0 0.029 -0.079 0.079 ethylbenzone training 366 301.11 0 0.811 0.406 0.934 0.468 0.918 0.627 0.679 0.679 ethylbenzone training 360 311.17 0 0.811 0.406 0.934 0.468 0.934 0.669 0 0.099 0.069 0 0.099 0.069 0 0.099 0 0.099 0 0.094 0.069 0 0.099 0 0.099 0	2-butanone test 362.5 268.22 0.147 1.149 0.464 0.999 0.908 0 0.0029 -0.112 5 1-propanol traning 366.5 344.98 0.171 0.811 0.466 0.949 0.698 0 0.099 -0.012 5 ethylbenzone training 366 341.11 0 0.811 0.406 0.934 0.465 0.814 0.696 0 0.099 0.069 0 ethylbenzone training 360 3.11.17 0 0.811 0.406 0.934 0.465 0.834 0.069 0 0.099 0.069 0 0.099 0.069 0 0.099 0.069 0 0.099 0.069 0		,	+-terr-penity ipinenoi	naming	00000	+0.70+	;	,	7+1.0	0.024	1	0.220	0.000	+67.0	> 1	† :
Propanol Lest 326.5 344.98 0.172 15.3 0.468 0.949 0.665 0.093 0.079 0.094 0.094 0.094 0.094 0.094 0.094 0.094 0.094 0.094 0.095 0.095 0.	Propanol Lest 326.5 344.98 0.172 1.53 0.468 0.949 0.6655 0.918 0.003 0.079 0.004 0	Lipropanol Lest 336,5 344,98 0.172 1.53 0.468 0.949 0.695 0.093 0.079 0.094 0.094 0.094 0.095 0.094 0.095	oly(p-hexyl	styrene)	2-butanone	training	302.6	268.22	0.147	1.149	0.464	0.999	0.908	0	0.029	-0.12	n	43
diphenyl ether training 306 301.11 0 0811 0.406 0.934 0.465 0.918 0.627 0.676 0 chyl beranche training 249 26.23 0 0.811 0.406 0.934 0.465 0.814 0.046 0.934 0.465 0.834 0.039 chyl berancate training 3.06 3.11.7 0 0.811 0.406 0.934 0.465 0.834 0.039 othere training 3.06 2.62.53 0.131 1.522 0.425 0.232 0.234 0.069 2.23 dipontyl phthalate training 3.08 3.0131 1.522 0.425 0.945 0.465 0.234 0.046 0.934 0.465 0.234 0.049 0.009 0.213 0.013 0.014 0.944 0.459 0.007 0.041 0.046 0.934 0.465 0.034 0.046 0.034 0.046 0.034 0.046 0.034 0.046 0.0	diphenyl ether training 366 30.11 0 0.811 0.406 0.934 0.465 0.918 0.627 0.676 0 ethyl bezancate training 249 26.23 0 0.811 0.406 0.934 0.465 0.814 0.069 0.334 0.669 0.334 0.465 0.834 0.069 0.334 0.069 0.338 0 0.069 0.034 0.465 0.834 0.069 0.234 0.069 0.034 0.069 0.234 0.069 0.234 0.069 0.034 0.465 0.834 0.069 0.234 0.069 0.034 0.046 0.034 0.465 0.834 0.069 0.034 0.046 0.034 0.465 0.834 0.069 0.034 0.046 0.034 0.046 0.034 0.045 0.034 0.069 0.034 0.046 0.034 0.046 0.034 0.046 0.034 0.046 0.034 0.046 0.034 0.045 0.834 0.069 <t< td=""><td>diphenyl ether training 306 30.11 0 0811 0.406 0.934 0.465 0.918 0.627 0.676 0 ethyl benzene training 306 30.11 0 0.811 0.406 0.934 0.465 0.814 0.046 0.934 0.465 0.834 0.069 0 ethyl benzene training 330 311.17 0 0.811 0.406 0.934 0.465 0.834 0.069 2.23 0.069 2.23 0.069 2.23 0.069 2.23 0.069 2.23 0.069 2.23 0.069 2.23 0.069 0.234 0.069 0.233 0.069 2.23 0.069 2.23 0.069 2.23 0.069 2.23 0.069 2.23 0.069 0.233 0.069 2.23 0.045 0.045 0.834 0.069 2.23 0.023 0.045 0.023 0.023 0.023 0.023 0.023 0.023 0.023 0.023 0.023</td><td>olv(2-hvdro</td><td>xvethyl methacrylate)</td><td>1-propanol</td><td>test</td><td>326.5</td><td>344.98</td><td>0.172</td><td>1.53</td><td>0.468</td><td>0.949</td><td>0.695</td><td>0</td><td>0.093</td><td>0.079</td><td>С</td><td>26</td></t<>	diphenyl ether training 306 30.11 0 0811 0.406 0.934 0.465 0.918 0.627 0.676 0 ethyl benzene training 306 30.11 0 0.811 0.406 0.934 0.465 0.814 0.046 0.934 0.465 0.834 0.069 0 ethyl benzene training 330 311.17 0 0.811 0.406 0.934 0.465 0.834 0.069 2.23 0.069 2.23 0.069 2.23 0.069 2.23 0.069 2.23 0.069 2.23 0.069 2.23 0.069 0.234 0.069 0.233 0.069 2.23 0.069 2.23 0.069 2.23 0.069 2.23 0.069 2.23 0.069 0.233 0.069 2.23 0.045 0.045 0.834 0.069 2.23 0.023 0.045 0.023 0.023 0.023 0.023 0.023 0.023 0.023 0.023 0.023	olv(2-hvdro	xvethyl methacrylate)	1-propanol	test	326.5	344.98	0.172	1.53	0.468	0.949	0.695	0	0.093	0.079	С	26
training 250 2011 0 2010 0 2011 0 2010 0 2011 0 2010 0 2011 0 2010 0 2011 0 2010 0 2011 0 201	training 249 26.3.1 0 0.811 0.406 0.934 0.465 0.311 0.305 0.000 0.	training 249 26.3.1 0 0.811 0.406 0.934 0.465 0.311 0.305 0.000 0.	olyricobutylo	ng cary a meaning june)	dishamil other	troining	306	201 11		0.61	0.406	0.024	0.465	0.016	7,000	9290	o c	- 1
ethylbenzene training 249 262.3 0 0.811 0.406 0.934 0.465 0.831 0.396 0.538 0 ethyl beptanoate training 306 311.71 0 0.811 0.406 0.934 0.465 0.834 0.396 0.538 0 ethyl beptanoate training 260 26.23 0 0.811 0.406 0.934 0.465 0.834 0.099 0.229 dibutyl phthalate training 35.8 38.83.8 0.131 1.522 0.422 0.953 0.506 1.141 0.999 0.239 dipontyl phthalate training 314 27.22 0.236 0.131 1.522 0.422 0.953 0.506 1.141 0.999 0.234 dipontyl phthalate training 314 27.22 0.236 1.379 0.441 0.944 0.459 0 0.075 0.002 2.4-dimethyl-3-pentanone training 39.15.3 0.236 1.379	training 349 1421 0 0.811 0.406 0.934 0.465 0.831 0.396 0.338 0 0.01 ctty) hexanoate training 330 311.17 0 0.811 0.406 0.934 0.465 0.834 0.394 0.069 2 cty obligation training 330 311.17 0 0.811 0.406 0.934 0.465 0.834 0.394 0.069 2 cty obligation test of training 260 262.2 0.252 0.253 0.254 0.953 0.254 0.298 0.254 0.255 0.254 0.255 0.	ethylberzene training 249 26.3.3 0 0.445 0.934 0.465 0.831 0 ethylberzene training 306 134.21 0 0.811 0.406 0.934 0.465 0.854 0.394 0.069 2 ethyl hexanoate training 330 311.17 0 0.811 0.406 0.934 0.465 0.854 0.394 0.069 2 diplemyl phthalate training 358.8 380.83 0.131 1.522 0.422 0.953 0.566 1.191 0.099 0.213 0 dipenyl phthalate test 415.8 366.36 0.131 1.522 0.422 0.953 0.566 1.193 0.059 0 dipenyl phthalate test 415.8 366.36 0.131 1.522 0.422 0.953 0.560 1.193 0.099 0.213 dipenyl phthalate test 23.4 1.225 0.422 0.953 0.506 1.193 <	ory isobuty is	alle	aipnenyi emer	uannig	000	11.100	0 ;	0.011	0.400	0.934	0.40	0.910	0.027	0.070	0 .	/ [
ethyl heptanoate test 306 314.21 0 0811 0.406 0.934 0.465 0.854 0.394 0.069 2 ethyl hexanoate training 330 311.17 0 0.811 0.406 0.934 0.465 0.854 0.394 0.069 2 coluene training 260 26.23 0 0.811 1.522 0.425 0.566 1.141 0.909 0.213 dibutyl phthalate test 415.8 389.83 0.131 1.522 0.422 0.953 0.506 1.141 0.909 0.213 0.073 deflomityl phthalate test 415.8 386.36 0.131 1.522 0.422 0.953 0.506 1.141 0.909 0.213 0.003 acetonitrile training 310.15 316.43 0.236 1.379 0.441 0.944 0.459 0.071 0.0042 0.002 2.2-dimethyl-3-pentanone training 319.15 317.53 0.	ethyl beptanoate test 306 314.21 0 0811 0.406 0.934 0.465 0.854 0.394 0.069 2 ethyl bexanoate training 260 26.23 0 0.811 0.406 0.934 0.465 0.854 0.394 0.069 2 coluence training 260 26.23 0 0.811 0.405 0.232 0.234 0.099 0.213 dibutyl phthalate training 38.8 38.9.83 0.131 1.522 0.422 0.953 0.506 1.141 0.999 0.213 0.208 accionitricle training 30.14 0.236 0.131 0.441 0.944 0.459 0.56 0.005 0.005 1-chlorobutane training 30.15 316.35 0.236 1.379 0.441 0.944 0.459 0.362 0.045 0.005 2.4-dimethyl-3-pentanone training 310.15 316.78 0.236 1.379 0.441 0.9	chyl beptanoate test 306 314.21 0 0811 0.406 0.934 0.465 0.884 0.394 0.069 2 chyl beytanoate training 336 314.21 0 0811 0.406 0.934 0.465 0.884 0.394 0.069 2 toluene training 358.8 389.83 0.131 1.522 0.422 0.953 0.506 1.141 0.909 0.213 0.09 dibutyl phthalate training 345.8 389.83 0.131 1.522 0.422 0.956 0.141 0.909 0.213 0.298 diputyl phthalate training 320 301.44 0.236 1.379 0.441 0.944 0.459 0 0.075 0.002 2dimethyl-3-pentanone training 390.15 31.15 31.379 0.441 0.944 0.459 0 0.075 0.045 0 2dimethyl-3-pentanone training 390.15 327.55 0.236 <t< td=""><td></td><td></td><td>ethylbenzene</td><td>training</td><td>249</td><td>262.3</td><td>0</td><td>0.811</td><td>0.406</td><td>0.934</td><td>0.465</td><td>0.311</td><td>0.396</td><td>0.338</td><td>0</td><td>17</td></t<>			ethylbenzene	training	249	262.3	0	0.811	0.406	0.934	0.465	0.311	0.396	0.338	0	17
ethýl hexanoate training 330 311.17 0 0.811 0.406 0.934 0.465 0.824 0.354 0.069 2 tolune training 356 26.2.3 0.131 1.522 0.425 0.522 0.534 0.069 2.2 dibuyl phthalate training 358.8 389.83 0.131 1.522 0.422 0.933 0.506 1.141 0.909 0.234 0.069 0.235 0.075 0.093 0.075 0.093 0.075 0.093 0.075 0.002 0.075 0.002 0.075 0.002 0.034 0.465 0.254 0.099 0.075 0.002 0.075 0.002	ethýl hexanoate training 330 311.17 0 0.811 0.406 0.934 0.465 0.232 0.254 0.069 2 tolutene training 1.60 0.811 0.406 0.934 0.465 0.232 0.254 0.069 2 dibutyl phthalate training 318.8 38.8 3.11.17 0 0.811 0.405 0.522 0.254 0.029 0.234 0.069 0.232 0.034 0.465 0.232 0.054 0.069 0.234 0.069 0.234 0.069 0.234 0.069 0.234 0.069 0.034 0.046 0.034 0.465 0.232 0.054 0.075 0.099 0.023 0.002	training 330 311.17 0 0.811 0.406 0.934 0.465 0.854 0.394 0.0069 2 dibbyl hexamoate training 358 389.83 0.131 1.522 0.422 0.953 0.506 1.131 0.909 0.224 0.298 0.024 0.0014 pluthalate training 358 389.83 0.131 1.522 0.422 0.953 0.506 1.191 0.909 0.213 0.002 0.002 0.0024 0.0014			ethyl heptanoate	test	306	314.21	0	0.811	0.406	0.934	0.465	0.854	0.394	0.069	2	17
training 250 26.253 0 0.811 0.406 0.524 0.525 0.524 0.526 0.524 0.000 0.521 0.000 0.000 0.521 0.000 0.	club.ly phthalate training 260 27.1.7 0 0.31 0.400 0.334 0.450 0.234 0.254 0.204 club.ly phthalate training 358.8 389.83 0.131 1.522 0.422 0.953 0.506 1.141 0.909 0.213 0.024 dipulyl phthalate training 366.36 0.131 1.522 0.422 0.953 0.506 1.141 0.909 0.213 0 accionivile training 320 301.44 0.236 1.379 0.441 0.944 0.459 0 0.0075 0.0045 0 2.2-dimethyl-3-pentanone training 320 31.46 0.236 1.379 0.441 0.944 0.459 0.362 0.005 0	training 260 262.3 0 0.811 0.406 0.934 0.455 0.234 0.208 2.001 0.201 0.201 0.201 0.201 0.201 0.201 0.201 0.201 0.201 0.201 0.201 0.202 0.2			othyl hovonote	troining	220	211 17		0.011	0.406	0.024	0.465	0.057	0.304	0900	(1
training 260 262.53 0 0.811 0.406 0.934 0.465 0.232 0.234 0.238 0 0.244 0.298 0 0.244 0.298 0 0.244 0.298 0 0.244 0.298 0 0.244 0.298 0 0.244 0.298 0 0.245 0.2598 0.2506 1.193 0.2862 0.243 0.2699 0.213 0 0.245 acetonitrile training 314 272.29 0.236 1.379 0.441 0.944 0.459 0 0.0075 0.002 3 0.244 0.224 0.2451 0.944 0.459 0 0.0075 0.002 3 0.244 0.224 0.2451 0.944 0.459 0 0.0075 0.0045 0 0.002 0.244 0.2451 0.944 0.459 0 0.0075 0.002 0.002 0.244 0.224 0.2451 0.944 0.459 0 0.0075 0.0045 0 0.002 0.002 0.244 0.245 0.244 0.249 0.441 0.944 0.459 0.441 0.044 0.459 0.466 0.354 0.154 0.006 1.241 0.044 0.459 0.459 0.452 0.162 0.052 0.161 0.037 0.441 0.044 0.459 0.469 0.459 0.441 0.044 0.459 0.441 0.044 0.459 0.459 0.459 0.459 0.441 0.044 0.459 0.459 0.459 0.459 0.459 0.441 0.044 0.459 0.45	dibutyl phthalate training 2560 262.53 0 0.8811 0.406 0.934 0.465 0.232 0.254 0.258 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	dibutyl phthalate training 260 262.53 0 0.811 0.406 0.934 0.405 0.232 0.254 0.258 0 0 dibutyl phthalate training 358.8 36.36 0.131 1.522 0.422 0.955 0.506 1.141 0.909 0.258 0.785 0.401 0.942 0.459 0 1.141 0.909 0.278 0.785 0.506 1.191 0.862 0.785 0.785 0.785 0.506 1.193 0.862 0.785 0.785 0.506 1.193 0.862 0.785 0.785 0.506 1.193 0.862 0.785 0.785 0.506 1.193 0.862 0.785 0.785 0.22-dimethyl-3-pentanone training 30.1 310.15 316.35 0.236 1.379 0.441 0.944 0.459 0.362 0.077 0.116 0.16 0.24-dimethyl-3-pentanone training 30.1 316.78 0.236 1.379 0.441 0.944 0.459 0.362 0.071 0.116 0.14 0.204 0.459 0.362 0.077 0.106 0.106 0.384 0.459 0.362 0.077 0.106 0.106 0.384 0.459 0.384 0.459 0.384 0.459 0.384 0.459 0.384 0.459 0.384 0.459 0.384 0.459 0.441 0.944 0.459 0.382 0.162 0.006 1.499 0.384 0.459 0.441 0.944 0.459 0.485 0.162 0.006 1.499 0.384 0.459 0.441 0.944 0.459 0.622 0.161 0.037 0.441 0.944 0.459 0.622 0.161 0.037 0.441 0.944 0.459 0.669 0.354 0.154 0.			cuiyi ilexalioate	naming	000	711.17	> 0	0.011	001.0	10.00	201.0	1000	1,274	0.003	1 (/ [
dibutyl phthalate training 358.8 389.83 0.131 1.522 0.422 0.953 0.506 1.141 0.909 0.213 0 dipentyl phthalate test 415.8 366.36 0.131 1.522 0.422 0.953 0.506 1.193 0.882 0.778 0 actonitrile training 314 0.236 1.379 0.441 0.944 0.459 0 0.075 0.002 0 2.2-dimethyl-3-pentanone training 308.15 316.35 0.236 1.379 0.441 0.944 0.459 0 0.075 0.045 0 2.4-dimethyl-3-pentanone training 319.15 341.65 0.236 1.379 0.441 0.944 0.459 0.071 0.014 0 2.4-dimethyl-3-pentanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.071 0.043 0 2.4-dimethyl-3-pentanone training 307.7 31.378	dibutyl phthalate training action 388.8 389.83 0.131 1.522 0.422 0.953 0.506 1.141 0.909 0.213 0 deputyl phthalate test 415.8 366.36 0.131 1.522 0.422 0.953 0.506 1.193 0.862 0.738 0 acetonitrile training 320 30.144 0.236 1.379 0.441 0.944 0.459 0 0.075 0.002 0 2.2-dimethyl-3-pentanone training 319.15 316.35 0.236 1.379 0.441 0.944 0.459 0 0.075 0.0043 2 2.4-dimethyl-3-pentanone training 319.15 316.35 0.236 1.379 0.441 0.944 0.459 0.362 0.017 0.0043 2 2.4-dimethyl-3-pentanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.362 0.162 0.003 3-beptanone training	dibutyl phthalate training putplatate 38.8 389.83 0.131 1.522 0.422 0.953 0.506 1.141 0.909 0.213 0 dipentyl phthalate test 415.8 366.36 0.131 1.522 0.422 0.953 0.506 1.193 0.082 0.078 0 1-chlorobutane training 320 30.1.44 0.236 1.379 0.441 0.944 0.459 0 0.075 0.045 0 2.2-dimethyl-3-pentanone training 310.15 316.35 0.236 1.379 0.441 0.944 0.459 0.362 0.071 0.045 0 2-chylmethyl-3-pentanone training 310.15 316.37 0.244 0.944 0.459 0.362 0.071 0.0143 0 2-chylmethyl-3-pentanone training 305.15 32.36 1.379 0.441 0.944 0.459 0.322 0.149 0.459 0.522 0.141 0.944 0.459 0.582 0.161	polyisobutylene	ene	toluene	training	260	262.53	0	0.811	0.40	0.934	0.465	0.232	0.254	0.298	0	17
dipentyl phthalate test 415.8 366.36 0.131 1.522 0.422 0.953 0.506 1.193 0.862 0.785 0 acctonitrile training 314 272.29 0.236 1.379 0.441 0.944 0.459 0 -0.082 0.002 3 2.2-dimethyl-3-pentanone training 316.35 0.236 1.379 0.441 0.944 0.459 0 -0.045 0 2.4-dimethyl-3-pentanone training 319.15 341.65 0.236 1.379 0.441 0.944 0.459 0.641 -0.045 0 2.4-dimethyl-3-pentanone training 397.7 316.78 0.236 1.379 0.441 0.944 0.459 0.637 4 2-chylbutanal training 295.15 296.02 0.236 1.379 0.441 0.944 0.459 0.637 0.007 0.006 1 2-chylbutanal training 390.7 316.78 0.236 1.379 0.44	dipentyl phthalate test 415.8 366.36 0.131 1.522 0.422 0.953 0.506 1.193 0.862 0.785 0 actonitrile training 314 272.29 0.236 1.379 0.441 0.944 0.459 0 0.0075 0.002 3 1-chlorobutane training 320 301.44 0.256 1.379 0.441 0.944 0.459 0.0071 0.0116 2 2.4-dimethyl-3-pentanone training 319.15 31.65 0.236 1.379 0.441 0.944 0.459 0.0071 0.0165 0.0045 2 2-chhylbutanal training 295.15 327.55 0.236 1.379 0.441 0.944 0.459 0.322 0.149 0.042 0.052 0.007 0.0116 0.004 0.007 0.007 0.006 1.16 0.004 0.441 0.944 0.459 0.041 0.004 0.049 0.041 0.044 0.459 0.044 0.049<	dipentyl phthalate test 415.8 366.36 0.131 1.522 0.422 0.953 0.506 1.193 0.862 0.785 0.785 actonitrile training 314 272.29 0.236 1.379 0.441 0.944 0.459 0 0.075 0.0045 0 2.2-dimethyl-3-pentanone training 310.15 31.65 0.236 1.379 0.441 0.944 0.459 0 0.075 0.0045 0 2.4-dimethyl-3-pentanone training 319.15 341.65 0.236 1.379 0.441 0.944 0.459 0.071 0.116 2 2.4-dimethyl-3-pentanone training 295.15 327.55 0.236 1.379 0.441 0.944 0.459 0.032 0.149 0.007 0.007 0.006 1 2-cthylbutanal training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.636 0.075 0.006 1 2-ctanone <td>nolv(dl-lactide)</td> <td>(e)</td> <td>dibutyl phthalate</td> <td>training</td> <td>358.8</td> <td>389.83</td> <td>0.131</td> <td>1.522</td> <td>0.422</td> <td>0.953</td> <td>0.506</td> <td>1,141</td> <td>0.909</td> <td>0.213</td> <td>С</td> <td>5</td>	nolv(dl-lactide)	(e)	dibutyl phthalate	training	358.8	389.83	0.131	1.522	0.422	0.953	0.506	1,141	0.909	0.213	С	5
upper property production training 312.20 0.202. 0.754. 0.754. 0.754. 0.754. 0.754. 0.754. 0.754. 0.754. 0.754. 0.754. 0.754. 0.754. 0.754. 0.754. 0.754. 0.754. 0.754. 0.754. 0.754. <td>actional partners training training 317.2 20.20 1.72 0.42 0.45 0.17 0.002 0.</td> <td>acpoint pluntation training 310.50 0.132 0.441 0.944 0.459 0.002 0.002 0.002 accountrille training 320 301.44 0.236 1.379 0.441 0.944 0.459 0 0.075 0.002 3 2.2-dimethyl-3-pentanone training 320 301.44 0.236 1.379 0.441 0.944 0.459 0 0.075 0.0042 0<td></td><td></td><td>dinantyl abtholota</td><td>o toot</td><td>115.8</td><td>366 36</td><td>0.121</td><td>1 522</td><td>0.422</td><td>0.053</td><td>0.506</td><td>1 103</td><td>6980</td><td>287.0</td><td>· C</td><td>7</td></td>	actional partners training training 317.2 20.20 1.72 0.42 0.45 0.17 0.002 0.	acpoint pluntation training 310.50 0.132 0.441 0.944 0.459 0.002 0.002 0.002 accountrille training 320 301.44 0.236 1.379 0.441 0.944 0.459 0 0.075 0.002 3 2.2-dimethyl-3-pentanone training 320 301.44 0.236 1.379 0.441 0.944 0.459 0 0.075 0.0042 0 <td></td> <td></td> <td>dinantyl abtholota</td> <td>o toot</td> <td>115.8</td> <td>366 36</td> <td>0.121</td> <td>1 522</td> <td>0.422</td> <td>0.053</td> <td>0.506</td> <td>1 103</td> <td>6980</td> <td>287.0</td> <td>· C</td> <td>7</td>			dinantyl abtholota	o toot	115.8	366 36	0.121	1 522	0.422	0.053	0.506	1 103	6980	287.0	· C	7
acetonitrile training 314 2/7.229 0.236 1.379 0.441 0.944 0.459 0 -0.082 0.002 3 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	accountine training 314 27,229 0.256 1.379 0.441 0.944 0.459 0 -0.082 0.002 3 2.4-dimethyl-3-pentanone training 30.144 0.236 1.379 0.441 0.944 0.459 0.362 0.077 -0.045 0 2.4-dimethyl-3-pentanone training 319.15 341.65 0.236 1.379 0.441 0.944 0.459 0.362 0.071 -0.043 0 2.4-dimethyl-3-pentanone training 295.15 327.55 0.236 1.379 0.441 0.944 0.459 0.362 0.071 -0.043 2 2-ethylbutanal training 295.15 327.55 0.236 1.379 0.441 0.944 0.459 0.622 0.149 -0.006 1 3-beptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.622 0.162 0.016 0.052 0.162 0.044 0.459 0.623	accounting training 314 27/2.29 0.236 1.379 0.441 0.944 0.459 0 -0.082 0.002 3 2.2-dimethyl-3-pentanone training 308.15 31.379 0.441 0.944 0.459 0.362 0.071 0.106 2 2.2-dimethyl-3-pentanone training 319.15 341.65 0.236 1.379 0.441 0.944 0.459 0.362 0.071 0.106 1 2.4-dimethyl-3-pentanone training 295.15 327.55 0.236 1.379 0.441 0.944 0.459 0.362 0.077 0.006 1 2-ethylbutanal training 295.15 327.55 0.236 1.379 0.441 0.944 0.459 0.652 0.162 0.075 4 4-beptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.659 0.162 0.162 0.162 0.162 0.162 0.162 0.162 0.162 </td <td></td> <td>-</td> <td>arpennyı pinanan</td> <td></td> <td>5.5</td> <td>00000</td> <td>101.0</td> <td>110</td> <td>777</td> <td>0.00</td> <td>0.70</td> <td>0.11</td> <td>70000</td> <td>0000</td> <td>0 0</td> <td>7 6</td>		-	arpennyı pinanan		5.5	00000	101.0	110	777	0.00	0.70	0.11	70000	0000	0 0	7 6
1-chlorobutane training 320 301.44 0.236 1.379 0.441 0.944 0.459 0 0.075 -0.045 0 2.2-dimethyl-3-pentanone test 308.15 316.35 0.236 1.379 0.441 0.944 0.459 0.352 0.019 0.017 0.0143 2.244 2.2-dimethyl-3-pentanone training 319.15 341.65 0.236 1.379 0.441 0.944 0.459 0.323 0.149 0.007 0.007 0.0043 2 2-ethy/butanal training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.582 0.162 0.005 4 4-beptanone training 309 323.12 0.236 1.379 0.441 0.944 0.459 0.582 0.162 0.052 4 3-catanone test 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.524 0.154 5 3-catano	1-chlorobutane training 320 301.44 0.236 1.379 0.441 0.944 0.459 0 0.075 -0.045 0 2.4-dimethyl-3-pentanone test 308.15 316.35 0.236 1.379 0.441 0.944 0.459 0.071 0.015 2 2.4-dimethyl-3-pentanone training 319.15 31.635 0.236 1.379 0.441 0.944 0.459 0.014 -0.004 2 2-ethybutanal training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.582 0.162 0.062 4 4-beptanone training 309 323.12 0.236 1.379 0.441 0.944 0.459 0.652 0.161 0.037 4 4-beptanone training 309 323.12 0.236 1.379 0.441 0.944 0.459 0.724 0.251 0.154 3-cctanone training 301 2.236 1.379 0.	1-chlorobutane training 320 301.44 0.236 1.379 0.441 0.944 0.459 0 0.075 -0.045 0 2,2-dimethyl-3-pentanone test 308.15 316.35 0.236 1.379 0.441 0.944 0.459 0.32 0.016 2 2,2-dimethyl-3-pentanone training 319.15 341.65 0.236 1.379 0.441 0.944 0.459 0.332 0.149 0.007 0.007 0.0043 2 2-ethybutanal training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.332 0.106 1 4-heptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.652 0.161 0.007 0.006 1 2-ctanone training 309 323.12 0.236 1.379 0.441 0.944 0.459 0.622 0.161 0.007 0.057 0.154 0.459 0.524	ory(metny)	metnacrytate)	acetomitine	training	514	67.717	0.730	1.379	0.441	0.744	0.439	0	-0.082	0.007	c	2/
2.2-dimethyl-3-pentanone test 308.15 316.35 0.236 1.379 0.441 0.944 0.459 0.362 0.071 0.116 2 2.4-dimethyl-3-pentanone training 319.15 341.65 0.236 1.379 0.441 0.944 0.459 0.332 0.019 -0.004 1 2.4-dimethyl-3-pentanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.582 0.149 -0.006 1 3-beptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.582 0.161 0.007 4 4-beptanone training 307.3 1.379 0.441 0.944 0.459 0.582 0.161 0.007 4 2-ctanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.584 0.154 0.55 2-ctanone training 346.85 1.379 0.441 <td>2.2-dimethyl-3-pentanone test 308.15 316.35 0.236 1.379 0.441 0.944 0.459 0.362 0.071 0.116 2 2.4-dimethyl-3-pentanone training 319.15 341.65 0.236 1.379 0.441 0.944 0.459 0.322 0.0149 -0.003 1 2.4-dimethyl-3-pentanone training 295.15 327.55 0.236 1.379 0.441 0.944 0.459 0.522 0.149 -0.006 1 3-heptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.522 0.161 0.037 4 4-heptanone test 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.652 0.161 0.037 4 2-octanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.659 0.051 4 3-cotanone training 340</td> <td>2,2-dimethyl-3-pentanone test 308.15 316.35 0.236 1.379 0.441 0.944 0.459 0.362 0.071 0.116 2 2,4-dimethyl-3-pentanone training 319.15 341.65 0.236 1.379 0.441 0.944 0.459 0.382 0.010 -0.0043 2 2-4-dimethyl-3-pentanone training 295.15 327.55 0.236 1.379 0.441 0.944 0.459 0.582 0.149 -0.006 1 3-beptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.582 0.169 0.037 4 4-beptanone test 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.622 0.161 0.007 3-catanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.622 0.161 0.003 1.54 0.625 0.161 0.154 0.459<!--</td--><td></td><td></td><td>1-chlorobutane</td><td>training</td><td>320</td><td>301.44</td><td>0.236</td><td>1.379</td><td>0.441</td><td>0.944</td><td>0.459</td><td>0</td><td>0.075</td><td>-0.045</td><td>0</td><td>37</td></td>	2.2-dimethyl-3-pentanone test 308.15 316.35 0.236 1.379 0.441 0.944 0.459 0.362 0.071 0.116 2 2.4-dimethyl-3-pentanone training 319.15 341.65 0.236 1.379 0.441 0.944 0.459 0.322 0.0149 -0.003 1 2.4-dimethyl-3-pentanone training 295.15 327.55 0.236 1.379 0.441 0.944 0.459 0.522 0.149 -0.006 1 3-heptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.522 0.161 0.037 4 4-heptanone test 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.652 0.161 0.037 4 2-octanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.659 0.051 4 3-cotanone training 340	2,2-dimethyl-3-pentanone test 308.15 316.35 0.236 1.379 0.441 0.944 0.459 0.362 0.071 0.116 2 2,4-dimethyl-3-pentanone training 319.15 341.65 0.236 1.379 0.441 0.944 0.459 0.382 0.010 -0.0043 2 2-4-dimethyl-3-pentanone training 295.15 327.55 0.236 1.379 0.441 0.944 0.459 0.582 0.149 -0.006 1 3-beptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.582 0.169 0.037 4 4-beptanone test 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.622 0.161 0.007 3-catanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.622 0.161 0.003 1.54 0.625 0.161 0.154 0.459 </td <td></td> <td></td> <td>1-chlorobutane</td> <td>training</td> <td>320</td> <td>301.44</td> <td>0.236</td> <td>1.379</td> <td>0.441</td> <td>0.944</td> <td>0.459</td> <td>0</td> <td>0.075</td> <td>-0.045</td> <td>0</td> <td>37</td>			1-chlorobutane	training	320	301.44	0.236	1.379	0.441	0.944	0.459	0	0.075	-0.045	0	37
2.4-dimently1-3-pertanne training 319.15 34.165 0.236 1.379 0.441 0.944 0.459 0.441 -0.017 -0.043 2 2-ethylbutanal training 295.15 327.55 0.236 1.379 0.441 0.944 0.459 0.441 -0.017 -0.043 2 3-heptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.582 0.162 0.062 4 4-heptanone training 309 323.12 0.236 1.379 0.441 0.944 0.459 0.659 0.154 0.065 0.154 5 3-cctanone training 309 323.12 0.236 1.379 0.441 0.944 0.459 0.724 0.254 0.154 5 3-cctanone training 301 273.66 0.236 1.379 0.441 0.944 0.459 0.724 0.254 0.154 0.053 0.053 0.154 0.459	2,4-dimethy1-3-pentanone training 319.15 34.165 0.236 1.379 0.441 0.944 0.459 0.441 -0.017 -0.043 2 2-ethylbutanal training 295.15 327.55 0.236 1.379 0.441 0.944 0.459 0.441 -0.017 -0.043 2 3-heptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.622 0.161 0.005 4 4-heptanone test 325.15 2.96.02 0.236 1.379 0.441 0.944 0.459 0.662 0.161 0.037 4 2-ctanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.662 0.161 0.037 4 3-ctanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.662 0.154 0.154 0.154 0.251 0.154 0.251 0.154 </td <td>2,4-dimethy1-3-pentanone training 319.15 34.165 0.236 1.379 0.441 0.944 0.459 0.441 -0.017 -0.043 2 2-ethylbutanal training 295.15 327.55 0.236 1.379 0.441 0.944 0.459 0.649 0.0149 -0.006 1 3-ethylbutanal training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.652 0.162 0.006 1 2-ctanone test 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.669 0.354 0.154 5 2-ctanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.659 0.354 0.124 0.459 0.669 0.354 0.124 0.459 0.669 0.354 0.124 0.459 0.669 0.354 0.124 0.459 0.669 0.354 0.124 0.459 0.669 0.354<td></td><td></td><td>2.2-dimethyl-3-nentanone</td><td>test</td><td>308 15</td><td>316 35</td><td>0.236</td><td>1 379</td><td>0 441</td><td>0 944</td><td>0.459</td><td>0 362</td><td>0.071</td><td>0 116</td><td>2</td><td>20</td></td>	2,4-dimethy1-3-pentanone training 319.15 34.165 0.236 1.379 0.441 0.944 0.459 0.441 -0.017 -0.043 2 2-ethylbutanal training 295.15 327.55 0.236 1.379 0.441 0.944 0.459 0.649 0.0149 -0.006 1 3-ethylbutanal training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.652 0.162 0.006 1 2-ctanone test 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.669 0.354 0.154 5 2-ctanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.659 0.354 0.124 0.459 0.669 0.354 0.124 0.459 0.669 0.354 0.124 0.459 0.669 0.354 0.124 0.459 0.669 0.354 0.124 0.459 0.669 0.354 <td></td> <td></td> <td>2.2-dimethyl-3-nentanone</td> <td>test</td> <td>308 15</td> <td>316 35</td> <td>0.236</td> <td>1 379</td> <td>0 441</td> <td>0 944</td> <td>0.459</td> <td>0 362</td> <td>0.071</td> <td>0 116</td> <td>2</td> <td>20</td>			2.2-dimethyl-3-nentanone	test	308 15	316 35	0.236	1 379	0 441	0 944	0.459	0 362	0.071	0 116	2	20
2-thylbutanal 137.15 37.55 0.256 1.379 0.441 0.944 0.459 0.341 0.017 0.045 2.541 2-thylbutanal training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.582 0.160 1 3-beptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.582 0.161 0.005 4 4-beptanone training 309 323.12 0.236 1.379 0.441 0.944 0.459 0.652 0.161 0.037 4 2-ctanone training 346.85 1.379 0.441 0.944 0.459 0.724 0.154 5 3-ctanone training 301 302.84 0.236 1.379 0.441 0.944 0.459 0.724 0.121 4 3-beptanone test 319 321.2 0.236 1.379 0.441 0.944 0.459 0.625	2-thylineunyle-plantation training 1915.13 315.13 0.244 0.459 0.2441 0.017 0.047 2.044 2.244 0.459 0.2441 0.044 0.459 0.2441 0.044 0.459 0.244 0.045 0.017 0.044 0.045 0.244 0.045 0.016 0.006 1 3-heptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.622 0.161 0.037 4 4-heptanone test 225.15 296.02 0.236 1.379 0.441 0.944 0.459 0.622 0.161 0.037 4 3-cctanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.724 0.154 5 3-cctanone training 301 273.66 0.236 1.379 0.441 0.944 0.459 0.724 0.154 5 1-chlorobutane test 319 32.24 0.236	2-cthybutanal training 295.15 347.55 0.250 1.379 0.441 0.944 0.459 0.582 0.149 0.006 1 2-cthybutanal training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.582 0.160 0.005 1 2-cthybutanal training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.582 0.161 0.037 4 2-cctanone training 309 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.652 0.161 0.037 4 2-cctanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.659 0.554 0.154 5 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3			2 4 dimothyl 2 nontonono	4	21015	24165	7500	1 270	0.441	0.044	0.450	0.441	7100	-0.042	(00
2-ethylbutanal training 295.15 327.55 0.236 1.379 0.441 0.944 0.459 0.532 0.149 -0.006 1 3-ethylbutanal training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.532 0.162 0.052 4 4-beptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.659 0.154 0.057 4 2-octanone test 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.669 0.354 0.154 5 3-octanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0 0.053 0.121 4 3-ctanone training 301 277.56 0.236 1.379 0.441 0.944 0.459 0 0.003 0 0.003 0 0.003 0 0.012 0 0 </td <td>2-ethylbutanal training 295.15 327.55 0.236 1.379 0.441 0.944 0.459 0.332 0.149 -0.006 1 3-ethylbutanal training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.582 0.162 0.052 4 4-beptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.659 0.162 0.052 4 2-cctanone test 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.669 0.354 0.154 5 3-cctanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.724 0.151 4 3-cctanone training 309 302.84 0.236 1.379 0.441 0.944 0.459 0.669 0.051 0.003 3 4-beptanone test 1.379 0.441 0.94</td> <td>2-thyloutanal training 295.15 3.27.55 0.236 1.379 0.441 0.944 0.459 0.332 0.149 -0.006 1 3-beptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.532 0.149 -0.006 1 2-octanone test 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.669 0.354 0.154 5 3-octanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.669 0.354 0.154 5 3-octanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.629 0.151 4 1-chlorobutane training 309 30.284 0.236 1.379 0.441 0.944 0.459 0.622 0.161 0.045 4-beptanone test 319 321.2 0.236</td> <td></td> <td></td> <td>2,+-uincinyi-3-penianone</td> <td>raming.</td> <td>01.7.10</td> <td>0.1+0</td> <td>0.230</td> <td>610.1</td> <td></td> <td>1.00</td> <td>0.4.0</td> <td>1+10</td> <td>0.017</td> <td>2+0.0</td> <td>1.</td> <td>0 0</td>	2-ethylbutanal training 295.15 327.55 0.236 1.379 0.441 0.944 0.459 0.332 0.149 -0.006 1 3-ethylbutanal training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.582 0.162 0.052 4 4-beptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.659 0.162 0.052 4 2-cctanone test 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.669 0.354 0.154 5 3-cctanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.724 0.151 4 3-cctanone training 309 302.84 0.236 1.379 0.441 0.944 0.459 0.669 0.051 0.003 3 4-beptanone test 1.379 0.441 0.94	2-thyloutanal training 295.15 3.27.55 0.236 1.379 0.441 0.944 0.459 0.332 0.149 -0.006 1 3-beptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.532 0.149 -0.006 1 2-octanone test 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.669 0.354 0.154 5 3-octanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.669 0.354 0.154 5 3-octanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.629 0.151 4 1-chlorobutane training 309 30.284 0.236 1.379 0.441 0.944 0.459 0.622 0.161 0.045 4-beptanone test 319 321.2 0.236			2,+-uincinyi-3-penianone	raming.	01.7.10	0.1+0	0.230	610.1		1.00	0.4.0	1+10	0.017	2+0.0	1.	0 0
3-heptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.582 0.162 0.052 4 4-heptanone training 309 323.12 0.236 1.379 0.441 0.944 0.459 0.622 0.161 0.037 4 2-cetanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.724 0.154 5 3-cetonitrile training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0 0.051 4 1-chlorobutane training 309 302.84 0.236 1.379 0.441 0.944 0.459 0 0.075 0.045 0 4-heptanone test 319 321.2 0.236 1.379 0.441 0.944 0.459 0 0.075 0.045 0 3-hexanone training 279 263.64 0.236 1.379 <	3-heptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.582 0.162 0.052 4 4-heptanone training 309 323.12 0.236 1.379 0.441 0.944 0.459 0.669 0.052 0.161 0.037 4 2-octanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.669 0.354 0.154 5 3-cctanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.724 0.251 0.124 5 1-chlorobutane training 309 302.84 0.236 1.379 0.441 0.944 0.459 0 0.075 0.005 0 <td>3-heptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.582 0.162 0.052 4 4-heptanone training 309 323.12 0.236 1.379 0.441 0.944 0.459 0.652 0.161 0.037 4 2-octanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.659 0.154 5 3-octionitrile training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0 0.075 0.003 3 1-chlorobutane training 309 302.84 0.236 1.379 0.441 0.944 0.459 0 0.075 0.045 0 4-heptanone test 319 321.2 0.236 1.379 0.441 0.944 0.459 0 0.075 0.045 0 3-hexanone training 4778 463.36 0.236</td> <td></td> <td></td> <td>2-ethylbutanal</td> <td>training</td> <td>295.15</td> <td>327.55</td> <td>0.236</td> <td>1.379</td> <td>0.441</td> <td>0.944</td> <td>0.459</td> <td>0.332</td> <td>0.149</td> <td>-0.006</td> <td>_</td> <td>70</td>	3-heptanone training 307.7 316.78 0.236 1.379 0.441 0.944 0.459 0.582 0.162 0.052 4 4-heptanone training 309 323.12 0.236 1.379 0.441 0.944 0.459 0.652 0.161 0.037 4 2-octanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.659 0.154 5 3-octionitrile training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0 0.075 0.003 3 1-chlorobutane training 309 302.84 0.236 1.379 0.441 0.944 0.459 0 0.075 0.045 0 4-heptanone test 319 321.2 0.236 1.379 0.441 0.944 0.459 0 0.075 0.045 0 3-hexanone training 4778 463.36 0.236			2-ethylbutanal	training	295.15	327.55	0.236	1.379	0.441	0.944	0.459	0.332	0.149	-0.006	_	70
4-heptanone training 309 323.12 0.236 1.379 0.441 0.944 0.459 0.652 0.161 0.037 4 2-octanone test 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.669 0.354 0.154 5 3-octanone training 346.85 319,42 0.236 1.379 0.441 0.944 0.459 0 0.051 0.121 4 1-chlorobulane training 301 273.56 0.236 1.379 0.441 0.944 0.459 0 0.075 0.003 3 4-heptanone test 319 321.2 0.236 1.379 0.441 0.944 0.459 0 0.075 0.003 3 3-hexanone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0 0.101 0.945 0.126 0.113 0.012 4 3-hexanone training	4-heptanone training 309 323.12 0.236 1.379 0.441 0.944 0.459 0.622 0.161 0.037 4 2-octanone test 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.669 0.354 0.154 5 3-octanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.659 0.551 0.121 4 acetonitrile training 301 273.56 0.236 1.379 0.441 0.944 0.459 0 0.051 0.003 3 4-heptanone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0.622 0.161 0.045 0 3-hexanone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0.126 0.113 0 alphenyl training 467.8 0.289 1.459 <	4-heptanone training 309 323.12 0.236 1.379 0.441 0.944 0.459 0.652 0.161 0.037 4 2-octanone test 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.669 0.354 0.154 5 3-octanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0 0.251 0.121 4 1-chlorobulane training 301 273.56 0.236 1.379 0.441 0.944 0.459 0 0.075 0.003 3 4-heptanone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0 0.005 0.016 0.003 4 3-hexanone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0 0.016 0.012 4 biphenyl training 467.8 463.36<			3-hentanone	training	307.7	316.78	0.236	1.379	0.441	0.944	0.459	0.582	0.162	0.052	4	42
4-neptatione training 309 323.12 0.250 1.379 0.441 0.944 0.459 0.052 0.101 0.037 4 3-cctanone training 346.85 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.669 0.354 0.154 5 3-cctanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.724 0.154 5 1-chlorobutane training 309 302.84 0.236 1.379 0.441 0.944 0.459 0 0.075 0.045 0 4-heptanone test 319 321.2 0.236 1.379 0.441 0.944 0.459 0 0.075 0.045 0 3-hexanone training 279 26.344 0.236 0.431 0.947 0.745 0.802 0.161 0.035 4 biphenyl training 487.2 445.31 0.289 <	4-reptatione training 3.25.12 2.53.12 1.379 0.441 0.944 0.459 0.032 0.101 0.037 4 4-reptatione training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.052 0.154 5 3-cctanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.724 0.154 5 1-chlorobutane training 309 302.84 0.236 1.379 0.441 0.944 0.459 0 0.075 0.003 3 1-chlorobutane training 309 302.84 0.236 1.379 0.441 0.944 0.459 0 0.075 0.0045 0 3-biphenyl training 467.8 463.28 0.236 1.379 0.441 0.947 0.745 0.918 0.627 0.015 4 4-ckaning 467.8 465.38 0.289 1.459 0.431 0.947	4-neptatione training 309 323.12 0.250			A bombonous	0	200	222	2000	070	177	7700	0.450	000	0.161	1000	. ~	, ,
2-octanone test 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.554 0.154 5 3-octanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0 0.251 0.121 4 actonitrile training 301 273.56 0.236 1.379 0.441 0.944 0.459 0 0.075 0.003 3 1-chlorobutane test 319 321.2 0.236 1.379 0.441 0.944 0.459 0 0.075 0.003 3 4-heptanone test 319 321.2 0.236 1.379 0.441 0.944 0.459 0 0.075 0.004 0 3-hexanone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0.161 0.037 4 biphenyl training 477.8 467.38 0.236 1.459 0.431	2-octanone test 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.669 0.554 0.154 5 3-octanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.724 0.251 0.121 4 a-cetonitrile training 301 273.56 0.236 1.379 0.441 0.944 0.459 0 -0.081 0.003 3 4-heptanone test 319 321.2 0.236 1.379 0.441 0.944 0.459 0 -0.081 0.037 4 3-hexanone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0.126 0.113 0.012 4 biphenyl training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.802 0.136 0.529 0 diphenyl ether test 449.8 442.33 0	2-octanone test 325.15 296.02 0.236 1.379 0.441 0.944 0.459 0.669 0.554 0.154 5 3-octanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0 0.051 0.121 4 acetonitrile training 301 273.56 0.236 1.379 0.441 0.944 0.459 0 -0.081 0.003 3 1-chlorobutane test 319 321.2 0.236 1.379 0.441 0.944 0.459 0 -0.081 0.003 4 4-heptanone test 319 321.2 0.236 1.379 0.441 0.944 0.459 0 0.003 4 3-hexanone training 279 263.64 0.236 1.459 0.441 0.947 0.745 0.802 0.161 0.003 4 biphenyl training 467.8 463.28 0.289 1.459			4-IIcptanone	uannig	309	27.07	0.730	1.279	0.44	0.74	0.439	0.022	0.101	0.037	+	2)
3-octanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.724 0.251 actonitrile training 301 273.56 0.236 1.379 0.441 0.944 0.459 0 -0.081 1-chlorobutane training 309 302.84 0.236 1.379 0.441 0.944 0.459 0 -0.081 4-heptanone test 319 321.2 0.236 1.379 0.441 0.944 0.459 0.622 0.161 3-hexanone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0.126 0.113 biphenyl training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenylmethane test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.627	3-octanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.724 0.251 actonitrile training 301 273.56 0.236 1.379 0.441 0.944 0.459 0 -0.081 1-chlorobutane training 309 302.84 0.236 1.379 0.441 0.944 0.459 0 -0.081 4-heptanone test 319 321.2 0.236 1.379 0.441 0.944 0.459 0.622 0.161 3-hexanone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0.126 0.113 biphenyl training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.802 0.395 diphenyl ether test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenylmethane test 449.8	3-octanone training 346.85 319.42 0.236 1.379 0.441 0.944 0.459 0.724 0.251 acetonitrile training 301 273.56 0.236 1.379 0.441 0.944 0.459 0 0.0081 4-heptanone test 319 30.284 0.236 1.379 0.441 0.944 0.459 0 0.075 3-hexanone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0.622 0.161 9iphenyl training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.802 0.136 diphenyl training 483.2 445.31 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenyl test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728			2-octanone	test	325.15	296.02	0.236	1.379	0.441	0.944	0.459	0.669	0.354	0.154	S	20
accontrible training 301 275.6 0.236 1.379 0.441 0.944 0.459 0.0075 0.0075 1.2000 0.0041 0.944 0.459 0.0075 0.0075 1.2000 0.0041 0.944 0.459 0.0075 0.0075 1.2000 0.0075 0.441 0.944 0.459 0.0075 0.0075 0.0075 0.441 0.944 0.459 0.0075	accounting training 301 275.5 0.236 1.379 0.441 0.944 0.459 0 0.075 1.21 0.221 0.221 0.221 0.221 0.221 0.221 0.221 0.221 0.221 0.236 1.379 0.441 0.944 0.459 0 0.075 1.21 0.236 1.379 0.441 0.944 0.459 0 0.075 1.21 0.236 1.379 0.441 0.944 0.459 0 0.0075 1.21 0.236 1.379 0.441 0.944 0.459 0.622 0.161 0.944 0.459 0.459 0.236 0.101 0.944 0.459 0.236 0.134 0.345 0.241 0.944 0.459 0.126 0.113 0.944 0.459 0.126 0.113 0.944 0.459 0.126 0.113 0.944 0.459 0.126 0.113 0.944 0.459 0.459 0.126 0.113 0.944 0.459 0.451 0.944 0.459 0.126 0.113 0.945 0.451 0.947 0.745 0.995 0.257 0.161 0.947 0.745 0.918 0.627 0.128 0.128 0.431 0.947 0.745 0.918 0.627 0.128 0	accountriel training 301 275.5 0.236 1.379 0.441 0.944 0.459 0.0081 0.0081 1-chlorobutane test 319 321.2 0.236 1.379 0.441 0.944 0.459 0 0.0075 0.0081 0.944 0.459 0 0.0075 0.0075 0.441 0.944 0.459 0 0.0075 0.0075 0.441 0.944 0.459 0 0.0075 0.0075 0.441 0.944 0.459 0 0.622 0.161 0.944 0.459 0.459 0.126 0.113 0.944 0.459 0.441 0.944 0.459 0.126 0.113 0.944 0.459 0.441 0.944 0.459 0.126 0.113 0.944 0.459 0.441 0.944 0.459 0.126 0.113 0.944 0.459 0.441 0.944 0.459 0.126 0.113 0.944 0.459 0.441 0.944 0.459 0.441 0.944 0.459 0.441 0.944 0.459 0.441 0.944 0.459 0.441 0.944 0.459 0.441 0.944 0.459 0.441 0.944 0.459 0.441 0.944 0.945 0.918 0.728			3-octanone	training	346.85	310 42	9860	1 370	0.441	0.044	0.450	0.724	0.251	0.121	4	47
acetonitrile training 301 2/3.56 0.236 1.379 0.441 0.944 0.459 0 -0.081 1-chlorobutane training 309 302.84 0.236 1.379 0.441 0.944 0.459 0 0.075 -4 heptanone test 319 321.2 0.236 1.379 0.441 0.944 0.459 0.622 0.161 3-hexanone training 279 263.64 0.236 1.379 0.441 0.947 0.745 0.126 0.113 biphenyl ether training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.902 0.395 diphenyl ether test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenylmethane test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.627	acetonitrile training 301 27.3.56 0.236 1.379 0.441 0.944 0.459 0 -0.081 1-chlorobutane training 309 302.84 0.236 1.379 0.441 0.944 0.459 0 0.075 - 4-heptanone test 319 321.2 0.236 1.379 0.441 0.944 0.459 0.622 0.161 3-hexanone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0.126 0.113 biphenyl training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.802 0.395 diphenylmethane test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.627	acetonitrile training 301 27.3.56 0.236 1.379 0.441 0.944 0.459 0 -0.081 1 -chlorobutane training 309 302.84 0.236 1.379 0.441 0.944 0.459 0 0.075 - 4. hebranone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0.622 0.161 3 - hexanone training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.802 0.395 diphenyl ether training 483.2 445.31 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenylmethane test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728			Coctanon	eraning.	0.000	11.7.0	0.00	010.1		1:00	0010	177.0	1000	0.000	٠,	- I
1-chlorobutane training 309 302.84 0.236 1.379 0.441 0.944 0.459 0 0.075 — 4-heptanone test 319 321.2 0.236 1.379 0.441 0.944 0.459 0.622 0.161 3-hexanone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0.126 0.113 biphenyl training 467.8 465.28 0.289 1.459 0.431 0.947 0.745 0.802 0.395 diphenylmethane test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.628	1-chlorobutane training 309 302.84 0.236 1.379 0.441 0.944 0.459 0 0.075 — 4-heptanone test 319 321.2 0.236 1.379 0.441 0.944 0.459 0.622 0.161 3-hexanone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0.0126 0.161 biphenyl training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.802 0.395 diphenyl ether training 483.2 445.31 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenylmethane test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728	1-chlorobutane training 309 302.84 0.236 1.379 0.441 0.944 0.459 0 0.075 — 4-heptanone test 319 321.2 0.236 1.379 0.441 0.944 0.459 0.622 0.161 3-hexanone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0.126 0.113 biphenyl training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenyl ether training 483.2 445.31 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenylmethane test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728	oly(methyl 1	nethacrylate) (1sotactic)	acetonitrile	training	301	2/3.56	0.236	1.379	0.441	0.944	0.459	0	-0.081	0.003	3	3/
4-heptonome test 319 321.2 0.236 1.379 0.441 0.944 0.459 0.622 0.161 3-hexanome training 279 263.64 0.236 1.379 0.441 0.944 0.459 0.126 0.113 biphenyl training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.802 0.395 diphenyl ether training 483.2 445.31 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenylmethane test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728	4-pertanone test 319 321.2 0.236 1.379 0.441 0.944 0.459 0.622 0.161 3-hexanone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0.126 0.101 biphenyl training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.802 0.395 diphenyl rether training 483.2 445.31 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenylmethane test 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728	4-pertonocount test 319 32.2.7 0.236 1.379 0.441 0.944 0.459 0.622 0.161 3-hexanone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0.622 0.161 biphenyl training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.802 0.395 diphenyl ether training 483.2 445.31 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenylmethane test 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728		•	1-chlorohittane	training	300	302 84	9860	1 370	0.441	0 944	0.450	0	0.075	-0.045	0	37
4-heptanone test 319 341.2 0.256 1.579 0.441 0.944 0.459 0.622 0.101 3-hexanone training 479 263.64 0.236 1.379 0.441 0.944 0.459 0.126 0.113 biphenyl training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.802 0.395 diphenyl ether training 483.2 445.31 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenylmethane test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728	4-heptanone test 319 3.41.2 0.256 1.579 0.441 0.944 0.459 0.022 0.101 3-hexanone training 279 263.64 0.236 1.379 0.441 0.947 0.745 0.126 0.113 biphenyl training 467.8 465.18 0.289 1.459 0.431 0.947 0.745 0.802 0.395 diphenyl ether training 483.2 445.31 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenylmethane test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728	4-heptanone test 319 321.2 0.256 1.579 0.441 0.944 0.459 0.022 0.101 3-hexanone training 467.8 463.64 0.236 1.379 0.441 0.944 0.459 0.126 0.113 biphenyl training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenyl methane test 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728			1-cinologuaino	ciaming.	010	10.700	0.500	0.00			000		0.00	1000	•	5 6
3-hexanone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0.126 0.113 biphenyl training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.802 0.395 diphenyl ether training 483.2 445.31 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenylmethane test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728	3-hexanone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0.126 0.113 (biphenyl training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.802 0.395 diphenyl ether training 483.2 445.31 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenylmethane test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728	3-hexanone training 279 263.64 0.236 1.379 0.441 0.944 0.459 0.126 0.113 (bipheny) training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.802 0.395 diphenyl ether test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.627			4-heptanone	test	319	321.2	0.236	1.379	0.441	0.944	0.459	0.622	0.161	0.037	4	37
S-nexatione training 2/7 203.04 0.230 1.379 0.441 0.544 0.435 0.112 0.113 0.11	S-nexatione training 2/7 203.04 0.230 1.379 0.441 0.544 0.435 0.112 0.113 0.115 0.11	S-nexatione training 279 203.04 0.250 1.379 0.441 0.544 0.459 0.11.5 0.1			2 Learning C		07.0	750 64	2000	070	177	7700	0.450	2010	21.0			
biphenyl training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.802 0.395 diphenyl ether training 483.2 445.31 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenylmethane test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728	biphenyl training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.802 0.395 diphenyl ether training 483.2 445.31 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenylmethane test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728	biphenyl training 467.8 463.28 0.289 1.459 0.431 0.947 0.745 0.802 0.395 diphenyl ether training 483.2 445.31 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenylmethane test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728			3-hexanone	training	6/7	203.04	0.736	1.579	0.441	0.944	0.459	0.126	0.115	0.012	4	15
diphenyl ether training 483.2 445.31 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenylmethane test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728	diphenyl ether training 483.2 445.31 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenylmethane test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728	diphenyl ether training 483.2 445.31 0.289 1.459 0.431 0.947 0.745 0.918 0.627 diphenylmethane test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728	olv(4-methy	1-1-pentene) (isotactic)	biphenyl	training	467.8	463.28	0.289	1.459	0.431	0.947	0.745	0.802	0.395	0.529	0	32
test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728	test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728	test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728		(amama) (amama)	dishonyl other	0 000	103.0	145 21	0000	1 450	0.421	7700	0.745	0100	0.637	9290	• <	2 6
test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728	test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728	test 449.8 442.33 0.289 1.459 0.431 0.947 0.745 0.918 0.728			alphenyl ether	training	483.2	16.644	0.289	454.I	0.451	0.94/	0.745	0.918	0.07	0.070	0	25
					diphenylmethane	test	449.8	442.33	0.289	1.459	0.431	0.947	0.745	0.918	0.728	0.811	0	32

Table 1. Continued

				UCST [K]	[K]				M	Molecular Descriptors	escriptors				
No.	polymer	solvent	status	exp.	pred.	X4A _p	$\mathrm{IVDE}_{\mathrm{p}}$	$\mathrm{SPAM}_{\mathrm{p}}$	FDI_p	Ks_p	BELm7 _s	Mor16u _s	Mor11m _s	H-052s	ref
59	poly(α-methylstyrene) nolv(2-methyl-5-vinylnyridine)	methylcyclohexane butyl acetate	training	357	342.92	0.145	1.436	0.47	0.99	0.744	0.568	0.406	0.089	0 %	48
61	()	ethyl butyrate	training	323.15	314.01	0.157	0.986	0.463	0.977	0.791	0.349	0.28	-0.05	200	525
63 63		ethyl propionate 3-methylbutyl acetate	training	322.15	284.92 320.43	0.157	0.986	0.463	0.977	0.791	0.41	0.069	-0.025 -0.095	7 m	22
4		2-methylpropyl acetate	training	326.15	311.19	0.157	0.986	0.463	0.977	0.791	0.364	0.251	-0.179	т	22
65		pentyl acetate	training	321.35	318.42	0.157	0.986	0.463	0.977	0.791	0.55	0.377	-0.019	ю.	22
96	poly(2-methyl-5-vinylpyridine)	propionitrile	training	269.55	284.91	0.145	1.436	0.47	0.99	0.744	00	0.005	-0.013	7 11	27.5
89		propyr aceraic propyl propionate	test	331.15	317.79	0.145	1.436	0.47	0.99	0.744	0.352	0.138	-0.029	2 0	77
69		tetrahydronaphthalene	training	322.65	314.7	0.145	1.436	0.47	0.99	0.744	0.561	0.645	0.326	0	22
70	polypropylene (isotactic)	benzyl phenyl ether	training	455	443.64	0	0.918	0.449	0.922	0.81	0.981	0.332	0.349	0	24
71		benzyl propionate	training	430.7	415.98	0	0.918	0.449	0.922	0.81	0.794	0.167	0.166	70	7 7
77		biphenyl	training	398.3	412.03	00	0.918	0.449	0.922	0.81	0.802	0.395	0.529	>	4 6
c 47		4-tert-butyiphenor dibenzyl ether	trainino	456.4	438.86	0 0	0.918	0.449	0.922	0.01	1.082	0.568	0.351	0 0	† 7 † 7
75		diphenyl ether	training	416	400.2	0	0.918	0.449	0.922	0.81	0.918	0.627	0.676	0	2 4
9/		4-tert-pentylphenol	training	414	426.57	0	0.918	0.449	0.922	0.81	0.936	0.57	0.295	0	24
77	polystyrene	1-chloro-n-decane	training	279.7	312.74	0.16	1.061	0.471	0.992	0.688	0.91	0.573	0.452	0	46
78		1-chloro-n-dodecane	training	331.7	308.57	0.16	1.061	0.471	0.992	0.688	1.094	0.733	0.701	0	46
79		1-chloro-n-undecane	training	305.9	313.85	0.16	1.061	0.471	0.992	0.688	1.006	0.63	0.566	0 0	46
0 0 0 0 0 0		1-nitopropane	training	272	247.95	0.16	1.061	0.471	0.992	0.688	0 0	0.045	0.179	0 \	94
- X		2,5-dimethyl turan	test	145	162.62	0.16	1.061	0.471	0.992	0.688	0	0.185	0.298	9 (9 6
85		2-methylpropyl acetate	training	227	261.81	0.16	1.061	0.471	0.992	0.688	0.364	0.251	-0.179	.n. c	34
8 0		2-propyl acetate	training	007	23/.34	0.10	1.061	0.471	0.000	0.088	0 71	0.01/	-0.058	n 0	ç 5
* ×		5-metajibutyi acetate evelodecane	training	577 580	286 19	0.10	1.001	0.471	0.992	0.000	0.41	0.762	0.093	n C	t 4
98		cycloheptane	training	290	294.94	0.16	1.061	0.471	0.992	0.688	0.615	0.438	0.229	0	. 14
87		cyclohexane	training	306.51	282.77	0.16	1.061	0.471	0.992	0.688	0.484	0.495	0.017	0	50
88		cyclooctane	training	286	308.65	0.16	1.061	0.471	0.992	0.688	0.583	0.182	0.266	0	41
68		cyclopentane	training	293	273.96	0.16	1.061	0.471	0.992	0.688	0	-0.142	-0.101	0 6	31
3 5		diethyl malonate	training	309	308.65	0.16	1.061	0.471	0.992	0.688	0.501	0.131	-0.433	~ ~	35
2.6		di-menunoi di-ternineol	training	351.6	367	0.10	1.001	0.471	0.992	0.000	0.029	0.307	0.204	0 0	5 4
93		dodecadeuterocyclohexane	test	312.5	284.55	0.16	1.061	0.471	0.992	0.688	0.484	0.495	0.017	0	36
94		dodecyl acetate	training	285.2	284.23	0.16	1.061	0.471	0.992	0.688	1.305	0.943	0.724	3	49
95		ethyl acetate	training	229	218.93	0.16	1.061	0.471	0.992	0.688	0	0.138	-0.087	33	34
96		ethyl chloroacetate	training	255	265.3	0.16	1.061	0.471	0.992	0.688	0	0.036	-0.127	0	46
/6		ethylcyclohexane	training	342.95	324.47	0.16	1.061	0.471	0.992	0.688	0.666	0.211	0.031	0 0	21
8 0		hexyl-m-xylene	training	C.C82.	300.22	0.16	1.061	0.4/1	0.992	0.688	1.102	0.6/5	0.9/1	0 %	o 4 0 4
100		isobutyl acetate	training	+77 LCC	261.81	0.10	1.001	0.471	0.992	0.000	0.41	0.156	0.033) u	5 4
101		isopropyl acetate	training	246	237.6	0.16	1.061	0.471	0.992	0.688	0.00	-0.01	-0.265	n m	4 4
102		methylcyclopentane	training	348	308.59	0.16	1.061	0.471	0.992	0.688	0.353	-0.11	-0.036	0	45
103		<i>n</i> -butyl formate	test	264	256.54	0.16	1.061	0.471	0.992	0.688	0	0.072	-0.007	0	46
104		n-propyl acetate	training	193	222.51	0.16	1.061	0.471	0.992	0.688	0 0	0.131	-0.101	m	46
501		o-dichlorobenzen	training	103	211.97	0.16 0.16	1.061	0.4/1	0.992	0.688	00	0.15	0.804	0 %	9 6
107		trans-decahydronaphthalene	training	293	266.9	0.16	1.061	0.471	0.992	0.688	0.758	0.949	0.332	0	39

Table 2. Molecular Descriptors of eq and Their Physical Meanings

ID	molecular descriptor	type	definition
1	X4A _p	connectivity indices	average connectivity index chi-4
2	IVDĖ _p	information indices	mean information content on vertex degree equality
3	$SPAM_p$	geometrical descriptors	average span R
4	$\mathrm{FDI}_{\mathfrak{p}}$	geometrical descriptors	fouling degree index
5	Ksp	WHIM descriptors	K global shape index/weighted by atomic electrotopological states
6	BELm7 _s	Burden eigenvalues	lowest eigenvalue n.7 of Burden matrix/weighted by atomic masses
7	Mor16u _s	3D-MORSE descriptors	3D-MORSE signal 16/unweighted
8	Mor11m _s	3D-MORSE descriptors	3D-MORSE signal 11/weighted by atomic masses
9	H-052 _s	atomic-centered fragments	H attached to C0(sp3) with 1X attached to next C

Table 3. Correlation Matrix for Nine Molecular Descriptors

			•						
	X4A _p	$IVDE_p$	$SPAM_p$	FDI_p	Ks _p	BELm6 _s	Mor16u _s	Mor11m _s	H-051 _s
X4A _p	1								
$IVD\dot{E}_{p}$	0.530954	1							
$SPAM_p$	0.0696902	0.0344682	1						
FDI _p	0.304256	0.289409	0.510212	1					
Ks _p	0.231933	0.397736	0.180189	0.0130519	1				
BELm6 _s	0.150714	0.219079	0.0636215	0.119922	0.0535737	1			
Mor16u _s	0.113193	0.155216	0.0195326	0.0469949	0.0758474	0.676258	1		
$Mor11m_s$	0.115135	0.19526	0.0800664	0.17373	0.0679118	0.485606	0.535392	1	
$H-051_{s}$	0.0626947	0.0385447	0.0422783	0.0058291	0.132254	0.0688008	0.105682	0.149223	1

In this work, the hydrogen-saturated repeating unit of polymers (instead of polymers structure) was used to determine the molecular descriptors of polymers. After providing the dataset, all molecules (polymers and solvents) were drawn into Hyperchem software⁵² and optimized using the MM+ molecular mechanics force field and, thereafter, molecular descriptors were calculated using Dragon software.⁵³ Dragon can calculate 1664 molecular descriptors for every chemical structure. Molecular descriptors of ~234 000 pure compounds have been calculated by Dragon are freely accessible from Milano Chemometrics and QSAR research group Web site (http://michem.disat.unimib.it/mol_db). For more information about the types of these molecular descriptors, please refer to Dragon software user's guide.⁵³

In this part, a total of 3328 molecular descriptors for each polymer solution were computed (1664 molecular descriptors for polymer and 1664 molecular descriptors for solvent). Note that some complementary works should be performed over the pool of descriptors obtained from Dragon software. After calculation of molecular descriptors, the pool of molecular descriptors was reduced by removing descriptors with an essentially constant value for all the structures and those could not be calculated for every structure in the dataset. The pair correlation cutoff selection then was performed. In this method, for each pair of variables with a squared correlation coefficient (R^2) of >0.8 (the cutoff value), one of two descriptors is arbitrary eliminated. After these operations, our pool of descriptors decreased from 3328 descriptors to 710 (227 for polymer and 483 solvent); hence, we used a pool of descriptors that contained 710 molecular descriptors for subset variable selection.

GA-MLR Calculations. Generally, in QSPR studies, after calculation of molecular descriptors, the problem is to find a linear equation that can predict the desired property with the least number of variables, as well as the highest accuracy. In other words, the problem is to find a subset of variables (most statistically effective molecular descriptors on $\theta(\text{UCST})$) from all available variables (all molecular descriptors) to predict $\theta(\text{UCST})$ with minimum error, in comparison with the available data.

A generally accepted method for this problem is genetic algorithm-based multivariate linear regression (GA-MLR). In this method, a genetic algorithm is used to select the best subset variables, with respect to an objective function, which was presented by Leardi et al. for the first time.⁵⁴

In this study, the GA-MLR technique presented by Leardi et al., with a couple of RQK objective functions presented by Todeschini et al.,^{55,56} were used for subset variable selection. This methodology has been extensively presented in our previous works, and the results are satisfactory.^{14,57-73}

Before performing the GA-MLR technique, the dataset must be divided into two new collections. First one is allocated for training and second one for testing. Using the training set, the best model is found and then the predictive power of the obtained model is checked by the test set as external dataset. In this work, 80% of the dataset was selected randomly for the training set and remainder was used for the test set (from 107 polymer solutions, 86 polymer solutions in the training set and 21 polymer solutions in the test set).

The inputs of our program were the pool of molecular descriptors, the $\theta(\text{UCST})$ of polymer solutions, and the number of molecular descriptors that we wanted to enter into our final model

To obtain the best multivariate linear equation, all molecular descriptors must be introduced to the program and the minimum number of possible variables must be tested at the starting point. Therefore, the program was started with one variable. We then obtained the best multivariate linear model. In the next steps, we increased the number of desired variables to two, three, four, and so on, and all calculations were repeated for them.

When we saw that increasing in the number of variables had no considerable effect on the accuracy of the best-obtained model, the calculations was stopped, because the best multivariate linear model already had been obtained.

Results and Discussion

Using the presented procedure, the best multivariate linear equation was obtained. We increased the number of descriptors to develop the best model. This work was continued until the change in the R^2 values of the consequent models was <0.01; hence, the best obtained multivariate linear model in this study has 9 parameters. Note that the difference between the best 8-parameter multivariate linear model and the best 9-parameter multivariate linear model was 0.0101; on the other hand, the difference between the best 9-parameter multivariate linear

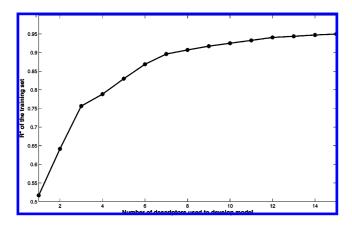


Figure 1. Squared correlation coefficient (R^2) for the best multivariate linear model with 1-15 parameters.

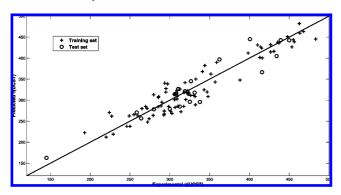


Figure 2. Comparison between the $\theta(UCST)$ obtained by eq and experimental data.

model and the best 10-parameter multivariate linear model was 0.0079. The R^2 value of the best multivariate linear models with 1-15 parameters is shown in Figure 1.

The best obtained equation is

$$\begin{array}{l} \theta(\text{UCST}) \, [\text{K}] = 1525.4392 (\pm 82.6631) \, + \\ 178.1497 (\pm 47.5914) \text{X4A}_{\text{p}} + 73.1814 (\pm 10.5220) \text{IVDE}_{\text{p}} - \\ 801.022 (\pm 189.2475) \text{SPAM}_{\text{p}} - 1225.8276 (\pm 130.9757) \text{FDI}_{\text{p}} + \\ 324.0948 (\pm 29.4254) \text{Ks}_{\text{p}} + 121.3236 (\pm 10.6136) \text{BELm6}_{\text{s}} - \\ 70.0030 (\pm 16.7255) \text{Mor16u}_{\text{s}} - 45.78383 (\pm 11.58467) \text{Mor11m}_{\text{s}} - \\ 12.0077 (\pm 1.87561) \text{H-051}_{\text{s}} \end{array} \tag{1}$$

$$n_{\text{training}} = 86; n_{\text{test}} = 21;$$

$$R_{\text{training}}^2 = 0.9172; R_{\text{test}}^2 = 0.8824;$$

$$Q_{\text{LOO}}^2 = 0.8955; Q_{\text{BOOT}}^2 = 0.8866; Q_{\text{EXT}}^2 = 0.8816;$$

$$s_{\text{training}} = 21.34; s_{\text{training}} = 25.42;$$

$$a = -0.071; F = 93.59$$

RQK function parameters:

$$(\Delta K = 0.006; \Delta Q = 0.002; R^P = 0.004; R^N = 0.000)$$

The predicted values of $\theta(UCST)$ using eq , in comparison with the experimental data, are presented in Figure 2 and are listed in Table 1. Also, the values of the selected molecular descriptors and the status of all of the polymer solutions (training set or test set) are presented in Table 1.

The molecular descriptors and their physical meanings are presented in Table 2. The subscripts "p" and "s" indicate that the molecular descriptor is related to the polymer and the solvent, respectively.

Table 3 presents the correlation matrix. The nine selected descriptors clearly are not highly correlated.

The numbers of polymer solutions in the training set and in the test set are given as $n_{\text{trainiing}}$ and n_{test} , respectively. To check the validity of the model more, bootstrap techniques, y-scrambling, and external validation techniques were used.⁵⁶ The bootstrapping was repeated 5000 times. Also, y-scrambling was repeated 300 times. As can be seen, the difference between each pair of Q_{LOO}^2 , Q_{BOOT}^2 , Q_{EXT}^2 , and R^2 show that the obtained model is a good one and has good predictive power.⁵⁶ Also, the intercept value of the y-scrambling technique has a low value (a = -0.071), which reveals the validity of the model. The y-scrambling, bootstrapping, and external validation techniques have been presented extensively by Todeschini et al.⁵⁶

All the validation techniques show that the obtained model is a valid model and can be used to predict the $\theta(UCST)$ of polymer solutions.

Conclusion

In this study, a molecular-based model was presented to predict the $\theta(UCST)$ of polymer solutions. The parameters of the model can be easily calculated only from the chemical structure of the polymer and the solvent (the monomers of polymers are used for polymers).

Also, the validity and predictive power of the model was checked by several techniques. The relative error and squared correlation coefficient (R^2) of the obtained model over 107 polymer solutions are 6.12% and 0.912, respectively. Therefore, the obtained model has predictive power and can be used to predict the $\theta(UCST)$ of polymer solutions.

Literature Cited

- (1) Elias, H. G. Theta Solvents. In Polymer Handbook; Brandrup, J., Immergut, H., Grulke, E. A., Eds.; Wiley: New York, 1999; pp VII-291-VII-326
- (2) Kavanagh, C. A.; Rochev, Y. A.; Gallangher, W. M.; Dawson, K. A.; Keenan, A. K. Local Drug Delivery In Restenosis Injury: Thermoresponsive Co-Polymers As Potential Drug Delivery Systems. Pharmacol. Ther. 2004,
- (3) Kopecek, J. Smart and Genetically Engineered Biomaterials and Drug Delivery Systems. Eur. Pharm. Sci. 2003, 20, 1-16.
- (4) Chang, B. H.; Bae, C. Y. Liquid-Liquid Equilibria of Binary Polymer Solutions with Specific Interactions. Polymer 1998, 39, 6449.
- (5) Pappa, G. D.; Voutsas, E. C.; Tassios, D. P. Correlation and Prediction of the Polymer Molecular Weight and the Pressure Effect. Ind. Eng. Chem. Res. 2001, 40, 4654.
- (6) Bogdanic, G.; Vidal, J. A Segmental Interaction Model For Liquid-Liquid Equilibrium Calculations for Polymer Solutions. Fluid Phase Equilib. 2000, 173, 241.
- (7) Imre, A. R.; Bae, Y. C.; Chang, B. H.; Kraska, T. Semiempirical Method for the Prediction of the Theta (Lower Critical Solution Temperature) in Polymer Solutions. Ind. Eng. Chem. Res. 2004, 43, 237.
- (8) Vetere, A. Empirical Method To Correlate and To Predict the Vapor-Liquid Equilibrium and Liquid-Liquid Equilibrium of Binary Amorpous Polymer Solutions. Ind. Eng. Chem. Res. 1998, 37, 2864.
- (9) Vetere, A. An Empirical Method to Predict the Liquid-Liquid Equilibria of Binary Polymer Systems. Ind. Eng. Chem. Res. 1998, 37, 4463.
- (10) Wang, F.; Saeki, S.; Yamaguchi, T. Absolute prediction of upper and lower critical solution temperatures in polymer/solvent systems based on corresponding state theory. Polymer 1999, 40, 2779.
- (11) Liu, H.; Zhong, C. Modeling of the $\boldsymbol{\Theta}$ (Lower Critical Solution Temperature) in Polymer Solutions Using Molecular Connectivity Indices. Eur. Polym. J. 2005, 41, 139.
- (12) Melagraki, G.; Afantitis, A.; Sarimves, H.; Koutenis, P. A.; Markopoulos, J.; Iglessi-Markopoulou, O. A Novel QSPR Model For

- Predicting Θ (Lower Critical Solution Temperature) in Polymer Solutions Using Molecular Descriptors. *J. Mol. Model.* **2007**, *13*, 55.
- (13) Xu, J.; Liu, L.; Xu, W.; Zhao, S.; Zuo, D. A General QSPR Model for the Prediction of Θ (Lower Critical Solution Temperature) in Polymer Solutions wWith Topological Indices. *J. Mol. Graph. Model.* **2007**, *26*, 352.
- (14) Gharagheizi, F. A New Neural Network Quantitative Structure-Property Relationship for Prediction of θ (Lower Critical Solution Temperature) of Polymer Solutions. e-Polym. 2007; Article No. 114.
- (15) Xu, J.; Chen, B.; Liang, H. Accurate Prediction of (Lower Critical Solution Temperature) in Polymer Solutions Based on 3D Descriptors and Artificial Neural Networks. *Macromol. Theor. Simul.* **2008**, *17*, 109.
- (16) Wohlfarth, C. Handbook of Liquid-liquid Equilibrium Data of Polymer Solutions; CRC Press/Taylor—Francis Group; Boca Raton, FL, 2008
- (17) Fox, T. G.; Flory, P. J. Intrinsic Viscosity—Temperature Relationships for Polyisobutylene in Various Solvents. *J. Am. Chem. Soc.* **1951**, 73, 1909
- (18) Mandelkern, L.; Flory, P. J. Molecular Dimensions of Cellulose Triesters. J. Am. Chem. Soc. 1952, 74, 2517.
- (19) Krigbaum, W. R.; Kurz, J. E.; Smith, P. Conformation of Polymer Molecules. IV. Poly-(1-Butene). *J. Phys. Chem.* **1961**, *65*, 1984.
- (20) Fox, T. G. Properties of Dilute Polymer Solutions III: Intrinsic Viscosity/Temperature Relationships for Conventional Polymethyl Methacrylate. *Polymer* **1962**, *3*, 111.
- (21) Debye, P.; Woermann, D.; Chu, B. Critical Opalescence of Polystyrene In Ethylcyclohexane. *J. Polym. Sci., Part A* **1963**, *1*, 255.
- (22) Gechele, G. B.; Crescentini, L. Phase Separation, Viscosity, and Thermodynamic Parameters for Poly-2-Methyl-5-Vinylpyridine Diluent System. *J. Polym. Sci. A.* **1965**, *3*, 3599.
- (23) Kubo, K.; Ogino, K. Solution Properties of Poly(P-Chlorostyrene). Sci. Pap. Coll. Art. Sci.; Univ. Tokyo 1966, 16, 193.
- (24) Nakajima, A.; Fujiwara, H.; Hamada, F. Phase Relationships And Thermodynamic Interactions In Linear Polyethylene-Diluent Systems. *J. Polym. Sci. A-2* **1966**, *4*, 507.
- (25) Llopis, J.; Albert, A.; Usobinaga, P. Studies on Poly(ethyl acrylate) in Θ Solvents. *Eur. Polym. J.* **1967**, *3*, 259.
- (26) Dusek, K. Solubility of Poly(2-Hydroxyethyl Methacrylate) in Some Aliphatic Alcohols. *Collect. Czech. Chem. Commun.* **1969**, *34*, 3309.
- (27) Cowie, J. M. G.; Maconnachie, A.; Ranson, R. J. Phase Equilibria of Cellulose Acetate—Acetone Solutions. The Effect of Degree of Substitution and Molecular Weight on Upper and Lower Critical Solution Temperature. *Macromolecules* **1971**, *4*, 57.
- (28) Kagemoto, A.; Baba, Y. Phase Diagrams of Polymer Solutions (in Jpn.). *Kobunshi Kagaku* **1971**, 28, 784.
- (29) Izumi, Y.; Miyake, Y. Study of Linear Poly(P-Chlorostyrene)-Diluent Systems. I. Solubilities, Phase Relationships, and Thermodynamic Interactions. *Polym. J.* **1971**, *3*, 647.
- (30) Kagemoto, A.; Baba, Y.; Fujishiro, R. Phase Equilibrium of the Cellulose Derivatives Determined by Differential Thermal Analysis. 1. Methylcellulose/Water. *Makromol. Chem.* **1972**, *154*, 105.
- (31) Saeki, S.; Kuwahara, N.; Konno, S.; Kaneko, M. Upper and Lower Critical Solution Temperatures in Polystyrene Solutions II. *Macromolecules* **1973**, *6*, 589.
- (32) Tani, S.; Hamada, F.; Nakajima, A. Unperturbed Chain Dimensions of Poly(4-Methyl-Pentene-1) in Theta Solvents. *Polym. J.* **1973**, *5*, 86.
- (33) Kuwahara, N.; Saeki, S.; Chiba, T.; Kaneko, M. Upper and Lower Critical Solution Temperatures in Polyethylene Solutions. *Polymer* **1974**, *15*, 777
- (34) Saeki, S.; Konno, S.; Kuwahara, N.; Nakata, M.; Kaneko, M. Upper and Lower Critical Solution Temperatures in Polystyrene Solutions III. Temperature Dependence of the X1 Parameter. *Macromolecules* **1974**, *7*, 521
- (35) Konno, S.; Saeki, S.; Kuwahara, N.; Nakata, M.; Kaneko, M. Upper and Lower Critical Solution Temperatures in Polystyrene Solutions. IV. Role of Configurational Heat Capacity. *Macromolecules* **1975**, *8*, 799.
- (36) Strazielle, C.; Benoit, H. Some Thermodynamic Properties of Polymer–Solvent Systems. Comparison Between Deuterated and Undeuterated Systems. *Macromolecules* **1975**, *8*, 203.
- (37) Cowie, J. M. G.; McEwen, I. J. Influence of Microstructure on the Upper and Lower Critical Solution Temperatures of Poly(Methyl Methacrylate) Solutions. *J. Chem. Soc. Faraday Trans. I.* **1976**, 72, 526.
- (38) Panina, N. I.; Lozgacheva, V. P.; Aver'yanova, V. M. Macromolecular Parameters of Cellulose Acetates Near Theta-Temperature (in Russ.). *Vysokomol. Soedin. Ser. B.* **1977**, *19*, 786.
- (39) Wolf, B. A.; Jend, R. Über Die Möglichkeiten Zur Bestimmung Von Mischungsenthalpien Und -Volumina Aus Der Molekulargewichtsabhängigkeit Der Kritischen Entmischungstemperaturen Und -Drücke Am

- Beispiel Des Systems Trans- Decahydronaphthalin/Polystyrol. *Makromol. Chem.* **1977**, *178*, 1811.
- (40) Suzuki, H.; Muraoka, Y.; Saitoh, M.; Kamide, K. Upper and Lower Critical Solution Temperatures in 2-Butanone Solutions of Cellulose Diacetate. *Br. Polym. J.* **1982**, *14*, 23.
- (41) Cowie, J. M. G.; McEwen, I. J. A Comparison of the Phase Behaviour of Polystyrene in Cycloalkanes and *N*-Alkanes. *Br. Polym. J.* **1986**, *18*, 387.
- (42) Herold, F. K.; Wolf, B. A. Poly(*N*-alkylmethacrylate)S: Characterization, Good and Poor Solvents, Densities and Intrinsic Viscosities. *Mater. Chem. Phys.* **1986**, *14*, 311.
- (43) Magarik, S. Y.; Filippov, A. P.; D'yakonova, N. V. Temperature Dependence of the Intrinsic Viscosity of Polystyrene and Poly(Alkylstyrene) Solutions (in Russ.). *Vysokomol. Soedin. Ser. A.* **1987**, *29*, 698.
- (44) Chiu, G.; Mandelkern, L. Effect of Molecular Weight on the Phase Diagram of Linear Polyethylene in 1-Dodecanol. *Macromolecules* **1990**, 23, 5356.
- (45) Imre, A.; Van Hook, W. A. Demixing in Polystyrene/Methylcy-clohexane Solutions. J. Polym. Sci. B. Polym. Phys. 1996, 34, 751.
- (46) Imre, A.; Van Hook, W. A. Liquid-Liquid Demixing From Solutions of Polystyrene. 1. A Review. 2. Improved Correlation with Solvent Properties. *J. Phys. Chem. Ref. Data* **1996**, 25, 637.
- (47) Xia, K. Q.; An, X. Q.; Shen, W. G. Measured Coexistence Curves of Phase Separated Polymer Solutions. *J. Chem. Phys.* **1996**, *105*, 6018.
- (48) Pruessner, M. D.; Retzer, M. E.; Greer, S. C. Phase Separation Curves of Poly(A-methylstyrene) in Methylcyclohexane. *J. Chem. Eng. Data* **1999**, *44*, 1419.
- (49) Imre, A.; van Hook, W. A. End Group Effects on Liquid—Liquid Demixing of Polystyrene/Oligomethylene Solutions. Polystyrene/Dodecyl Acetate Solubility. *Macromolecules* **2000**, *33*, 5308.
- (50) Siporska, A.; Szydlowski, J.; Rebelo, L. P. N. Solvent H/D Isotope Effects on Miscibility and Theta-Temperature in the Polystyrene—Cyclohexane System *Phys Chem Chem Phys* **2003** 5, 2996
- Cyclohexane System. *Phys. Chem. Chem. Phys.* **2003**, *5*, 2996. (51) Lee, J. S.; Lee, H. K.; Kim, S. C. Thermodynamic Parameters of Poly(lactic acid) Solutions in Dialkyl Phthalate. *Polymer* **2004**, *45*, 4491.
- (52) HyperChem Release 7.5 for Windows, Molecular Modeling System, Hypercube, Inc., 2002.
- (53) Talete srl, Dragon for windows (Software for Molecular Descriptor Calculations). Version 5.4, 2006; http://www/talete.mi.it/.
- (54) Leardi, R.; Boggia, R.; Terrile, M. Genetic Algorithm as a Strategy for Feature-Selection. J. Chemometr. 1992, 6, 281.
- (55) Todeschini, R.; Consonni, V. In *Handbook Of Molecular Descriptors*; Manhold, R., Kubinyi, H., Temmerman, H., Series Eds.; Wiley-VCH: Weinheim, Germany, 2000.
- (56) Todeschini, R.; Consonni, V.; Mauri, A.; Pavan, M. Detecting "Bad" Regression Models: Multicriteria Fitness Functions in Regression Analysis. *Anal. Chim. Acta* **2004**, *515*, 199.
- (57) Gharagheizi, F. QSPR Analysis For Intrinsic Viscosity of Polymer Solutions by Means of GA-MLR and RBFNN. *Comput. Mater. Sci.* **2007**, 40, 159
- (58) Gharagheizi, F. Quantitative Structure—Property Relationship for Prediction of the Lower Flammability Limit of Pure Compounds. *Energy Fuels* **2009** 22, 3037
- (59) Gharagheizi, F.; Mehrpooya, M. Prediction of Standard Chemical Exergy by a Three Descriptors QSPR Model. *Energy Convers. Manage.* **2007**, *48*, 2453.
- (60) Gharagheizi, F.; Alamdari, R. F. A Molecular-Based Model for Prediction of Solubility of C₆₀ Fullerene in Various Solvents. *Fullerenes, Nanotubes, Carbon Nanostruct.* **2008**, *16*, 40.
- (61) Gharagheizi, F. QSPR Studied For Solubility Parameter By Means of Genetic Algorithm-Based Multivariate Linear Regression and Generalized Regression Neural Network. *QSAR Comb. Sci.* **2008**, *27*, 165.
- (62) Gharagheizi, F. A Simple Equation For Prediction of Net Heat of Combustion of Pure Chemicals. *Chemometr. Intell. Lab. Syst.* **2008**, *91*, 177.
- (63) Gharagheizi, F. A New Molecular-Based Model for Prediction of Enthalpy of Sublimation of Pure Components. *Thermochim. Acta* **2008**, 469, 8.
- (64) Gharagheizi, F.; Alamdari, R. F. Prediction of Flash Point Temperature of Pure Components Using a Quantitative Structure—Property Relationship Model. *QSAR Comb. Sci.* **2008**, *27*, 679.
- (65) Gharagheizi, F.; Fazeli, A. Prediction of the Watson Characterization Factor of Hydrocarbon Components from Molecular Properties. *QSAR Comb. Sci.* **2008**, *27*, 758.
- (66) Sattari, M.; Gharagheizi, F. Prediction of Molecular Diffusivity of Pure Components Into Air: A QSPR Approach. *Chemosphere* **2008**, 72, 1298
- (67) Vatani, A.; Mehrpooya, M.; Gharagheizi, F. Prediction of Standard Enthalpy of Formation by a QSPR Model. *Int. J. Mol. Sci.* **2007**, *8*, 407.

- (68) Gharagheizi, F.; Sattari, M. Estimation of Molecular Diffusivity of Pure Chemicals in Water: A Quantitative Structure—Property Relationship Study. *SAR QSAR Environ.* **2009**, *20*, 267.
- (69) Gharagheizi, F.; Mehrpooya, M. Prediction of Some Important Physical Properties of Sulfur Compounds Using QSPR Models. *Mol. Divers.* **2008**, *12*, 143.
- (70) Gharagheizi, F.; Tirandazi, B.; Barzin, R. Estimation of Aniline Point Temperature of Pure Hydrocarbons: A Quantitative Structure—Property Relationship Approach. *Ind. Eng. Chem. Res.* **2009**, *48*, 1678.
- (71) Gharagheizi, F. A QSPR Model for Estimation of Lower Flammability Limit Temperature of Pure Compounds Based on Molecular Structure. *J. Hazard. Mater.* **2009**, *169*, 217.
- (72) Gharagheizi, F. Prediction of Upper Flammability Limit Percent of Pure Compounds from Their Molecular Structures. *J. Hazard. Mater.* **2009**, *167*, 507.
- (73) Gharagheizi, F. Prediction of Standard Enthalpy of Formation of Pure Compounds Using Molecular Structure. *Aust. J. Chem.* **2009**, 62, 374

Received for review January 10, 2009 Revised manuscript received June 23, 2009 Accepted August 20, 2009

IE9000426