A New Accurate Neural Network Quantitative Structure-Property Relationship for Prediction of θ (Lower Critical Solution Temperature) of Polymer Solutions

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Abstract: In this study, a new neural network quantitative structure-property relationship model for prediction of $\theta(LCST)$ of polymer solutions is presented. The parameters of this model are eight molecular descriptors which are calculated only from the chemical structure of polymer and solvent. These eight molecular descriptors were selected from 3328 molecular descriptors of polymer and solvent available in polymer solution by genetic algorithm-based multivariate linear regression (GA-MLR) technique. The obtained neural network model can predict the $\theta(LCST)$ of 169 polymer solutions with mean relative error of 1.67% and squared correlation coefficient of 0.9736.

Introduction

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

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

In the case of exothermic solutions, an increasing of temperature leads to less positive second virial coefficients and the theta temperature corresponds to a LCST in the limit of infinite molar mass ($\theta(LCST)$). The theta temperature corresponds to an UCST in the case of endothermic solutions ($\theta(UCST)$) [1].

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

Prediction of physicochemical properties of materials from their molecular structure has been one of the wishes of the scientists and engineers for a long time. One of the useful methods which applied for this purpose is quantitative structure-property

relationship (QSPR). QSPR is defined as a mathematical model which 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 (which are called molecular descriptors) and the properties of interest.

Once a correlation between structure and desired property is found, any number of compounds, including those not yet synthesized, can be readily screened on computer in order to select structures with the properties desired. Thus QSPR approach conserves resources and accelerates the process of development of new molecules for use in any purpose. Also, since theoretical descriptors derived solely from the molecular structure would be involved, the relation should, in principle, be applicable to any chemical structure.

There are more than thousand of molecular descriptors available in the literature to represent the molecular structure, and one usually faces the problem of selecting those which are the most representative for the property under consideration [4].

There are many methods for estimating LCSTs, including $\theta(LCST)$. As stated by Melagraki et al. [5], these methods can be divided into three main groups. The first group is those methods that have a solid theoretical background but they require vapor-liquid equilibrium, and also liquid-liquid equilibrium experimental data for obtaining their parameters [6-8]. The ability of these methods for prediction of new systems is unknown. The second group of methods for estimating $\theta(LCST)$ is the empirical models which relates $\theta(LCST)$ to other physicochemical properties [9-12, 13]. These correlations are simple and have reasonable accuracy, but they cannot be used to systems for which the required physicochemical properties are not available. The third group of methods for estimating $\theta(LCST)$ is QSPR analysis. These types of methods have two main advantages in comparison to previous methods. For development of a QSPR model, molecular descriptors which, are computed only from chemical structure of compounds, are applied. As a result, these types of methods do not need any additional information (i.e. other physical properties or vapor-liquid or liquid-liquid equilibrium data). On the other hand, the prediction power of these types of models are always checked during development of the models, as a result, these types of models can be accurately applied for any regular systems.

The first attempt to apply QSPR analysis for prediction of $\theta(LCST)$ is related to the work of Liu and Zhong [14] who applied the molecular connectivity indices (a special group of molecular descriptors [4]) for prediction of $\theta(LCST)$ for polymer solutions with $R^2 = 0.77$ and mean relative error (MRE) of 5.44%. It is noted that Liu and Zhong [14] could not succeed to develop a unified model for prediction of $\theta(LCST)$ for polymer solutions. They used eight equations for prediction of $\theta(LCST)$ for solutions of eight polymers.

First attempt to develop a unified model for prediction of $\theta(LCST)$ for polymer solutions by QSPR analysis, is related to the recent work of Melagraki et al [5] who obtained a nine-parameter equation for prediction of $\theta(LCST)$ for polymer solutions by means of multivariate linear regression (MLR) technique, with $R^2 = 0.8660$ and MRE of 3.73%.

Also Xu et al. [15] recently tried to develop a QSPR model for prediction of $\theta(LCST)$ for polymer solutions by means of MLR technique, based on topological descriptors (a special group of molecular descriptors [4]). Their ten-parameter equation predicts $\theta(LCST)$ for polymer solutions with $R^2 = 0.8874$ and MRE of 3.49%.

There are several comments about the previous QSPR studies of Liu and Zhong [13], Melagraki et al [5], and Xu et al. [15]. In previous works, all authors tried to develop their QSPR models based on a special group of molecular descriptors (connectivity indices in work of Liu and Zhong [14], 3D descriptors in the work of Melagraki et al [5], and topological descriptors in the work of Xu et al. [15]). This phenomenon caused the obtained results to be not the best results which can be obtained by QSPR analysis. Another comment is related to the method of selection of most statistically effective molecular descriptors on $\theta(LCST)$ of polymer solutions. All three groups of authors [5, 14, 15] have used the MLR technique. This technique has several disadvantages that are presented elsewhere [16]. Another important comment is related to the study of the nonlinear behavior of the molecular descriptors on $\theta(LCST)$ of polymer solutions, as a complementary work (such as application of neural networks).

In the present study, first the genetic algorithm based-multivariate linear regression (GA-MLR) is applied to select the most statistically effective molecular descriptors on the $\theta(LCST)$ of polymer solutions from a pool of 3328 molecular descriptors which belong to many types of molecular descriptors.

Then by means of the results of GA-MLR, a feed forward neural network is constructed for predicting $\theta(LCST)$ of polymer solutions.

Results and Discussion

In this section, it is better we refer to comments which were presented in introduction part of this paper. First comment is related to the types of molecular descriptors which should be used to develop a QSPR model. Physical properties are usually the result of many types of interactions, as a result, in this work 3228 molecular descriptors from many types, were used. Diversity of molecular descriptors can represent many interactions between molecules. Also, the GA-MLR was applied to find the most statistically effective molecular descriptors of polymer and solvent on $\theta(LCST)$. Comparison between the presented results of Tab. 5 and previous works [5, 14] shows that the presented multi-linear equation (see Tab. 3), is quite as accurate as previous works, but there are eight parameters. The obtained small modification in first part of calculations is the result of application different types of molecular descriptors and application of a powerful method for selection of molecular descriptors from the pool of 3328 molecular descriptors (GA-MLR). It should be noted that Melagraki et al. [5] presented a nine-parameter multi-linear equation, and Xu et al. [15] presented a ten-parameter multi-linear equation for prediction of $\theta(LCST)$ with the same data set.

Nine-parameter multi-linear equation proposed by Melagraki et al. [5] shows MRE of 3.76% over experimental data set (both training and test sets) which was used in this study. Also the ten-parameter multi-linear equation proposed by Xu et al. [15] shows MRE of 4.95% over this data set. The eight-parameter multi-linear model presented in this study shows MRE of 4.04%. This model is better than the model proposed by Xu et al. [15] and has two parameters less than that model. But, it is not possible to

compare this model with the model proposed by Melagraki et al. [5], because, MRE of the model proposed by Melagraki et al. [5] has better than MRE of this study, but has one parameter more than this model. As a result, application of diverse 3328 molecular descriptors and Experimental θ (LCST) also application of GA-MLR caused small modification in comparison to previous models.

Fig. 1. Comparison between the best obtained FFNN results and the experimental.

Tab. 1. The statistical parameters of the best obtained FFNN.

Statistical Parameter	Value
Standard Multiple Correlation Coefficient for Training set (R_{Train}^2)	0.978
Standard Multiple Correlation Coefficient for Test set (R_{Test}^2)	0.9722
Standard Multiple Correlation Coefficient for Training set + Test set (R^2)	0.9736
Mean Relative Error for Training Set ($\text{MRE}_{\text{Train}}$)	1.68%
Mean Relative Error for Test Set (MRE_{Test})	1.66%
Mean Relative Error for Training set +Test Set (MRE)	1.67%

The second comment which is presented in introduction part of this paper is related to the nonlinear study for QSPR analysis. The major modification in the presented work is related to the application of neural networks for nonlinear study of the obtained multi-linear equation by GA-MLR.

Application of FFNN considerably modifies the results of the GA-MLR. This considerable modification was presented in Tab. 1. As can be found from Tab. 1, the obtained FFNN shows MRE of 1.67% over data set which shows considerable modification in comparison with the previous model.

The predicted values of $\theta(LCST)$ by GA-MLR, and FFNN in comparison to the experimental data are presented in Tab. 6. Also, the systems which were used as training set and test set are shown.

Tab. 2. Comparison between GA-MLR and FFNN results and experimental data.

ID	Polymer	Solvent	Experimental	GA-MLR		FFNN	
				Predicted	status	Predicted	Status
1	P4MP1	n-Butane	388	408.07	Training	382.57	Test
2	P4MP1	n-Pentane	441	444.43	Training	434.82	Test
3	P4MP1	n-Heptane	522	519.56	Training	527.84	Training
4	P4MP1	n-Octane	553	541.91	Training	554.02	Training
5	P4MP1	2-Methyl butane	431	431.76	Training	424.42	Training
6	P4MP1	2,2-Dimethyl butane	462	461.94	Training	462.58	Training
7	P4MP1	2,2-Dimethyl pentane	499	507.14	Training	504.09	Training
8	P4MP1	2,2,3-Trimethyl butane	521	501.97	Training	518.46	Test
9	P4MP1	Cyclopentane	505	516.15	Training	499.13	Training
10	P4MP1	n-Hexane	487	480.60	Test	485.69	Training
11	P4MP1	n-Nonane	579	567.67	Test	579.13	Training
12	P4MP1	2,4-Dimethyl pentane	499	495.06	Test	498.94	Training
13	P4MP1	3-Ethyl pentane	532	505.57	Test	532.20	Training
14	PB1	n-Pentane	421	447.86	Training	420.00	Training
15	PB1	n-Heptane	509	522.55	Training	514.42	Training
16	PB1	n-Octane	540	544.94	Training	537.53	Training
17	PB1	2-Methyl butane	416	435.14	Training	415.05	Training
18	PB1	2,2-Dimethyl butane	444	465.25	Training	456.86	Training
19	PB1	2,2,3-Trimethyl butane	507	504.91	Training	514.33	Test
20	PB1	2,5-Dimethyl hexane	519	514.09	Training	515.98	Training
21	PB1	3-Ethyl pentane	523	507.61	Training	519.43	Training
22	PB1	3,4-Dimethyl hexane	559	555.70	Training	579.99	Training
23	PB1	n-Hexane	464	483.12	Test	470.59	Training
24	PB1	n-Nonane	564	570.19	Test	557.42	Test
25	PB1	2,4-Dimethyl pentane	480	497.59	Test	485.39	Training
26	PB1	2,3-Dimethyl pentane	517	516.23	Test	525.38	Test
27	PB1	Cyclopentane	498	518.14	Test	509.51	Test
28	PBD	n-Hexane	373	410.71	Training	359.29	Training
29	PBD	2,2,3-Trimethyl butane	414	431.25	Training	413.50	Training
30	PBD	n-Octane	390	475.49	Training	392.96	Test
31	PBD	Ethyl propyl ketone	510	449.12	Training	500.79	Training

32	PBD	Diethyl ketone	481	492.91	Training	480.21	Test
33	PBD	2-Methyl hexane	370	431.33	Test	381.55	Test
34	PBD	2,2,4-Trimethyl pentane	388	448.32	Test	384.77	Training
35	PBD	Propylene oxide	414	435.54	Test	424.19	Training
36	PDMS	n-Pentane	453	450.86	Training	445.67	Test
37	PDMS	n-Heptane	528	526.30	Training	528.18	Training
38	PDMS	n-Octane	553	548.48	Training	551.90	Training
39	PDMS	n-Dodecane	643	658.30	Training	645.91	Test
40	PDMS	n-Cetane	708	719.82	Training	688.53	Training
41	PDMS	n-Hexane	493	487.55	Test	492.96	Test
42	PDMS	n-Decane	603	604.85	Test	603.83	Test
43	PE	n-Hexane	411	433.08	Training	394.37	Training
44	PE	n-Heptane	459	471.70	Training	457.89	Training
45	PE	n-Nonane	531	519.01	Training	529.45	Training
46	PE	n-Decane	557.55	549.24	Training	557.06	Test
47	PE	n-Dodecane	605.55	599.62	Training	604.47	Test
48	PE	n-Tridecane	631.55	610.28	Training	637.99	Test
49	PE	2,2-Dimethyl pentane	399	460.26	Training	428.65	Training
50	PE	2,2,3-Trimethyl butane	444	454.50	Training	450.53	Training
51	PE	2,3-Dimethyl pentane	463	465.54	Training	463.66	Training
52	PE	3-Ethyl pentane	471	456.90	Training	458.65	Test
53	PE	2,2,4,4-Tetramethyl pentane	513	498.06	Training	496.65	Training
54	PE	2,3,4-Trimethyl hexane	545	552.04	Training	550.99	Test
55	PE	Methyl cyclopentane	488	488.24	Training	481.58	Training
56	PE	Methyl cyclohexane	537	530.54	Training	548.90	Training
57	PE	1-Octanol	621	549.92	Training	623.79	Training
58	PE	n-Pentyl acetate	528	565.71	Training	522.22	Test
59	PE	n-Pentane	353	396.07	Test	349.03	Training
60	PE	n-Octane	496	493.99	Test	499.66	Training
61	PE	n-Undecane	581.75	577.99	Test	578.66	Training
62	PE	2,4-Dimethyl pentane	395	446.83	Test	413.85	Training
63	PE	2,2,4-Trimethyl pentane	495	472.27	Test	455.28	Training
64	PE	3,4-Dimethyl hexane	515	505.07	Test	496.46	Training
65	PE	Cyclopentane	472	467.38	Test	457.33	Test
66	PE	Cyclohexane	518	513.89	Test	518.12	Test
67	PE	n-Butyl acetate	490	540.88	Test	492.14	Training
68	PIB	Cyclopentane	461	447.28	Training	456.64	Training
69	PIB	Cyclohexane	516	492.66	Training	507.38	Test
70	PIB	Cycloheptane	572	615.63	Training	581.80	Test
71	PIB	Cyclooctane	637	665.59	Training	625.15	Training
72	PIB	n-Heptane	442	452.47	Training	436.00	Training
73	PIB	n-Octane	477	474.57	Training	479.53	Test
74	PIB	n-Dodecane	582	580.77	Training	579.41	Training
75	PIB	2-Methyl butane	318	368.13	Training	341.82	Test

76	PIB	2-Methyl pentane	376	404.67	Training	365.31	Training
77	PIB	3-Methyl pentane	405	401.90	Training	402.58	Training
78	PIB	3-Methyl hexane	446	441.15	Training	441.44	Test
79	PIB	3-Ethyl pentane	458	436.98	Training	451.08	Test
80	PIB	2,3-Dimethyl pentane	451	445.91	Training	459.44	Training
81	PIB	2,4-Dimethyl pentane	403	428.64	Training	392.61	Test
82	PIB	2,2,3-Trimethyl butane	445	434.41	Training	449.04	Training
83	PIB	Ethyl cyclopentane	524	484.19	Training	501.43	Training
84	PIB	3-Methyl heptane	478	470.73	Training	473.18	Training
85	PIB	2,2-Dimethyl hexane	454	464.89	Training	461.86	Training
86	PIB	2,5-Dimethyl hexane	446	444.12	Training	443.70	Training
87	PIB	3,4-Dimethyl hexane	497	485.20	Training	491.30	Training
88	PIB	n-Propyl cyclopentane	547	544.48	Training	540.41	Training
89	PIB	n-Pentane	344	376.74	Test	339.35	Training
90	PIB	n-Hexane	402	413.03	Test	376.56	Training
91	PIB	Methyl cyclopentane	478	511.77	Test	517.83	Training
92	PIB	2-Methyl hexane	426	435.94	Test	417.20	Test
93	PIB	2,2-Dimethyl pentane	404	439.37	Test	408.68	Test
94	PIB	3,3-Dimethyl pentane	451	434.29	Test	451.11	Test
95	PIB	Methyl cyclohexane	526	511.77	Test	517.83	Training
96	PIB	2-Methyl heptane	466	462.83	Test	464.06	Test
97	PIB	2,4-Dimethyl hexane	458	465.74	Test	468.47	Training
98	PIB	2,2,4-Trimethyl pentane	435	452.94	Test	431.51	Training
99	PIB	n-Decane	535	530.33	Test	535.83	Training
100	PMMA	Methyl acetate	441	453.85	Training	444.24	Training
101	PMMA	Ethyl acetate	478	468.89	Training	476.46	Training
102	PMMA	Ethyl propyl ketone	511	552.28	Training	508.76	Training
103	PMMA	Diethyl ketone	497	520.43	Training	482.87	Training
104	PMMA	Butyl chloride	454	444.56	Test	464.73	Training
105	PMMA	Dipropyl ketone	522	571.84	Test	531.18	Test
106	PMMA	Methyl ethyl ketone	464	447.32	Test	450.42	Test
107	PMMA	Tetrahydrofuran	519.5	505.83	Test	516.06	Training
108	PMS	Cyclopentane	417.6	385.57	Training	413.19	Training
109	PMS	Cyclohexane	456	432.97	Training	454.38	Training
110	PMS	Butyl chloride	412	356.99	Training	409.62	Training
111	PMS	n-Butyl acetate	446.9	463.43	Training	459.85	Training
112	PMS	n-Hexyl acetate	500.9	521.33	Training	491.23	Test
113	PMS	Methyl cyclohexane	431	452.23	Test	440.50	Test
114	PMS	n-Pentyl acetate	475.8	492.24	Test	481.81	Training
115	PP	n-Pentane	422	416.47	Training	397.90	Training
116	PP	n-Hexane	470	452.54	Training	459.67	Training
117	PP	n-Octane	542	513.88	Training	551.52	Training
118	PP	n-Nonane	571	538.85	Training	575.95	Test
119	PP	2,2-Dimethyl butane	441	434.08	Training	440.33	Test

120	PP	2,3-Dimethyl butane	465	443.20	Training	463.07	Training
121	PP	2,2-Dimethyl pentane	489	479.10	Training	492.49	Test
122	PP	2,2,3-Trimethyl butane	511	474.08	Training	499.80	Training
123	PP	2,3-Dimethyl pentane	513	485.44	Training	515.02	Test
124	PP	3-Ethyl pentane	520	476.87	Training	512.87	Training
125	PP	2,2,4,4-Tetramethyl pentane	548	518.35	Training	552.98	Training
126	PP	2,3,4-Trimethyl hexane	585	571.18	Training	612.07	Training
127	PP	Methyl cyclopentane	518	508.92	Training	518.87	Training
128	PP	Methyl cyclohexane	564	550.52	Training	564.71	Training
129	PP	Diethyl ether	420	427.20	Training	447.31	Training
130	PP	n-Heptane	511	491.96	Test	518.86	Test
131	PP	2-Methyl butane	413	404.07	Test	393.00	Training
132	PP	2,4-Dimethyl pentane	481	467.40	Test	480.39	Test
133	PP	2,2,4-Trimethyl pentane	510	492.84	Test	518.10	Test
134	PP	3,4-Dimethyl hexane	553	525.65	Test	556.35	Test
135	PP	Cyclopentane	495	487.96	Test	494.93	Training
136	PP	Cyclohexane	540	534.47	Test	544.73	Test
137	PP1	n-Pentane	433	450.09	Training	436.23	Training
138	PP1	n-Hexane	482	485.83	Training	483.10	Training
139	PP1	n-Octane	556	547.04	Training	544.13	Training
140	PP1	2-Methyl butane	422	437.58	Training	426.65	Test
141	PP1	2,4-Dimethyl pentane	493	500.40	Training	494.85	Test
142	PP1	2,2-Dimethyl pentane	502	512.35	Training	501.51	Test
143	PP1	2,3-Dimethyl pentane	529	518.50	Training	530.58	Training
144	PP1	3-Methyl heptane	537	543.89	Training	542.46	Test
145	PP1	n-Heptane	522	524.74	Test	521.70	Training
146	PP1	2,2-Dimethyl butane	457	467.06	Test	463.15	Training
147	PP1	2,2,4-Trimethyl pentane	527	525.62	Test	519.13	Training
148	PP1	Cyclopentane	502	520.74	Test	502.19	Test
149	PPCS	Isobutyl acetate	348.5	309.64	Training	351.40	Training
150	PPCS	Ethyl carbitol	300.8	333.27	Training	327.34	Test
151	PPCS	n-Butyl carbitol	323.1	345.39	Training	318.89	Test
152	PPCS	tert-Butyl acetate	338.4	299.83	Test	330.60	Training
153	PS	Cyclopentane	427	409.70	Training	422.88	Training
154	PS	Cyclohexane	486	455.17	Training	477.71	Training
155	PS	Methyl cyclopentane	417	432.93	Training	424.89	Training
156	PS	Methyl cyclohexane	480	474.08	Training	472.37	Test
157	PS	Benzene	523	516.27	Training	523.56	Test
158	PS	Toluene	550	601.57	Training	550.97	Test
159	PS	Ethyl acetate	412	410.70	Training	415.48	Test
160	PS	n-Propyl acetate	451	424.34	Training	410.29	Test
161	PS	i-Propyl acetate	380	421.05	Training	408.55	Training
162	PS	Ethyl n-butyrate	471	458.21	Training	467.45	Training
163	PS	Isobutyl acetate	445	457.55	Training	442.79	Training

164	PS	sec-Butyl acetate	442	453.39	Training	425.55	Training
165	PS	tert-Butyl acetate	329	425.93	Test	357.76	Test
166	PS	Diethyl malonate	578	595.66	Test	579.46	Training
167	PS	i-Amyl acetate	493	514.49	Test	509.17	Training
168	PS	Methyl acetate	384.5	394.48	Test	388.80	Training
169	PS	Methyl ethyl ketone	420	401.97	Test	425.14	Training

Conclusions

In this paper, a complete QSPR analysis was performed for prediction of $\theta(LCST)$ polymer solutions. This QSPR study contains two parts: linear study and nonlinear study. The result of first part is input of the second part.

The linear part contains selecting most statistically effective molecular descriptors on $\theta(LCST)$ polymer solutions. This part was done by means of GA-MLR technique based on 3328 molecular descriptors of polymer and solvent. The result of this part is an eight-parameter multi-linear equation. All eight parameters of this equation can be calculated only from the chemical structure of polymer and solvent available in a polymer solution. Also, this equation has two parameters less than the obtained equations by previous researchers with the same accuracy.

The nonlinear part of this study is related to generating a neural network on the eight parameters of multi-linear model obtained by GA-MLR in first part of this study. In this part the eight parameters of the multi-linear was used as input of a FFNN and finally, an optimized 8-10-1 FFNN was presented for prediction of $\theta(LCST)$ polymer solutions.

This optimized FFNN is accurate and can be applied for prediction of $\theta(LCST)$ any regular polymer solutions.

Materials and Methods

Data set

The data set which is used in this study contains the 169 experimental $\theta(LCST)$ for polymer solutions including 12 polymers and 67 solvents. This data set is compiled by Liu and Zhong [17]. This data set was used to develop QSPR models by Liu and Zhong [14], Melagraki et al [5], and Xu et al. [15]. As a result, comparison between this study and their studies is possible.

Determination of Molecular Descriptors

Each polymer solution is formed from a polymer and a solvent. As a result the phase behavior of polymer solution is a function of the both polymer and solvent and we must consider all molecular descriptors of polymers and also all molecular descriptors of solvents.

In this work, the monomer compounds were used to determine the molecular descriptors of polymers. After providing the data set, all molecules (polymers and solvents) were drawn into Hyperchem software [18] and pre-optimized using the MM+ molecular mechanics force field. A more precise optimization was done with

AM1 method in Hyperchem and thereafter, molecular descriptors were calculated using the optimized molecular structure of compounds by means of Dragon software [19]. Dragon can calculate 1664 molecular descriptors for any optimized chemical structure. These molecular descriptors contain many types of molecular descriptors such as connectivity indices and topological descriptors. For more information about the types of the molecular descriptors which Dragon can calculate, refer to Dragon software user's guide [19].

In this part, totally 3328 molecular descriptors for each polymer solutions were computed by means of Dragon (1664 molecular descriptors for polymer and 1664 molecular descriptors for solvent).

GA-MLR Calculations

After calculation of molecular descriptors, we can develop our models for prediction of $\theta(LCST)$. In QSPR study, the main problem is to find a multivariate linear equation with minimum input parameters (molecular descriptors) which can predict the desired property ($\theta(LCST)$) with the best accuracy. This problem is classified in the field of subset variable selection. In other words, we should select the best subset variables from the set of 3328 molecular descriptors which can predict $\theta(LCST)$ with the best accuracy.

One of the best solutions of this problem is genetic algorithm-based multivariate linear regression (GA-MLR). In this method, genetic algorithm is used for selection of best subset variables with respect to an objective function which is usually defined as the sum of square error between obtained values of the model and the corresponding values in dataset. In this work, we use GA-MLR algorithm which has been proposed by Leardi et al. [20] and has been successfully used by the author of this paper in his previous works [15, 21-23]. This algorithm has been designed for feature selection by means of genetic algorithm search which is suitable for this problem.

In the first part of calculations, data set was divided into two sub-datasets. First is training set and contains 112 polymer solutions and, second is test set and contains 57 polymer solutions. Training set is used to develop the model and test set is only used to check the validity of model and is not used to develop model. In this study we used the same training set and test set which had been used by Xu et al. [15].

Inputs of our program are the pool of 3328 molecular descriptors, and the number of desired molecular descriptors which we want to obtain in our study. In the first step, we started with one molecular descriptor models. Based on the training set, the best multivariate one molecular descriptor linear model was obtained, GA-MLR. In next step, we should examine two molecular descriptors multivariate linear models. After obtaining the best two molecular descriptors model by GA-MLR, we should compare the best one molecular descriptor model with the best two molecular descriptors multivariate linear model. In this comparison, we should consider the effect of increase in number of molecular descriptors on the increasing accuracy of these two models. If the increase in the number of molecular descriptors showed a sensible increase in accuracy of model, we must continue this procedure and increase number of molecular descriptors to three and then we should find the best three molecular descriptors multivariate linear model, by GA-MLR. If the increase in the number of molecular descriptors did not show any sensible effect on accuracy of model, we must stop our search. The best model has been obtained.

As the procedure presented in previous paragraph, we must repeat our work to find the best three, four, five, and so on, molecular descriptors multivariate linear models.

Tab. 3. The best obtained multi-linear equation by GA-MLR and its properties.

<i>ID</i>	<i>Variable</i>	<i>Regression</i>	<i>Errors</i>	<i>Confidence</i>	<i>Standard</i>
		<i>Coefficient</i>	<i>Regression</i>		<i>Regression</i>
			<i>Coefficient</i>	<i>Intervals</i>	<i>Coefficient</i>
				<i>(0.95)</i>	
0	intercept	3504.682646	428.3711	0	0
1	MEcc- polymer	3847.571353	429.1625	0.317179979	1.211387
2	DISPv- polymer	15.25520772	1.028103	0.665154575	1.530487
3	Mor17m- polymer	302.3633458	37.40017	0.267519932	1.129238
4	MDDD- solvent	31.81118727	2.123853	1.096516046	2.498295
5	piID- solvent	18.36408016	1.027251	1.620295289	3.093179
6	X3v- solvent	25.16525596	6.381213	0.201238909	1.741354
7	MATS2m- solvent	39.50802607	7.341934	0.229734722	1.456877
8	Mor25p- solvent	393.3137093	51.41867	0.347300595	1.549369

Tab. 4. The eight molecular descriptors entered into the best obtained multi-linear equation.

<i>ID</i>	<i>Molecular</i> <i>Descriptor</i>	<i>Type</i>	<i>Definition</i>
1	MEcc- polymer	Geometrical Descriptors	Molecular eccentricity
2	DISPv- polymer	Geometrical Descriptors	d COMMA@ value/weighted by atomic van der Waals volumes
3	Mor17m- polymer	3D-MoRSE descriptors	3D-MoRSE-signal 17/weighted by atomic masses
4	MDDD- solvent	Topological Descriptors	Mean distance degree deviation
5	piID-solvent	Walk and path counts	Conventional bond-order ID number
6	X3v-solvent	Connectivity indices	Valence connectivity index chi-3
7	MATS2m- solvent	2D autocorrelations	Moran autocorrelation -lag2/weighted by atomic masses
8	Mor25p- solvent	3D-MoRSE descriptors	3D-MoRSE-signal 25/weighted by atomic polarizabilities

Tab. 5. The statistical parameters of fitting and QSPR analysis parameters.

Statistical Parameter	Value
Standard Multiple Correlation Coefficient for Training set (R_{Train}^2)	0.8789
Standard Multiple Correlation Coefficient for Test set (R_{Test}^2)	0.8409
Standard Multiple Correlation Coefficient for Training set + Test set (R^2)	0.865
Mean Relative Error for Training Set ($\text{MRE}_{\text{Train}}$)	3.95%
Mean Relative Error for Test Set (MRE_{Test})	4.52%
Mean Relative Error for Training set +Test Set (MRE)	4.14%
QSPR Analysis Parameters	Value
Cross Validated Coefficient R^2 (Q^2)	89.03
Q^2 overtest set (size test set is 57) (Q^2_{ext})	85.36
Adjusted R^2 (R^2_{adj})	90.47
Standard Deviation Error of Calculation (SDEC)	20.68
Standard Deviation Error of Prediction (SDEP)	23.031
SDEP overtest set (size test set is 57) (SDEP_{ext})	24.623
Quick Rule test (K_x)	41.01
Quick Rule test (K_{xy})	42.95
Fisher Factor (F)	132.689
Standard Error of the Estimate (SE)	21.565

The behavior of the obtained multivariate linear model (eight-parameter linear equation) presented in Tab. 3, is shown in Fig. 2.

Fig. 2. Comparison between the best multi-linear results obtained by GA-MLR and the experimental data.

In this study the best multivariate linear model which is obtained, is an eight-parameter equation. This equation and its statistical parameters are presented in the Tab. 3. The physical meanings of molecular descriptors which entered in the best multi-linear equation are presented in Tab. 4. The values of these eight molecular descriptors for all 169 polymer solutions are presented as supplementary materials. Also the statistical parameters of fitting this correlation are presented in Tab. 5.

The MRE of the model over all experimental data is 4.14%. This value is quite equal to the MRE of the previous works, but the number of parameters of presented model is less than previous models. This obtained result is the first part of calculations.

Neural Network Calculations

The three-layer feed forward neural networks with the sigmoidal (hyperbolic tangent) transfer function have been the standard techniques used in QSPR modeling [24]. In order to consider the nonlinear behavior of different molecular descriptors which were entered into the best multivariate linear model, obtained in previous section, three-layer feed forward neural networks (FFNN) were used.

This part of calculations was done in Neural Network Toolbox, available in MATLAB software (Mathworks Inc. Software).

In this section, the structure of the three-layer FFNN which was used to study is explained step by step during solving the problem.

The first work is dividing the main dataset into two datasets, first for training network and second for testing it. Neural networks are good at fitting functions and there is a proof that a simple neural network can fit any dataset very well; as a result for checking the prediction power of the neural network, usage of test set is needed. Test set is only used for checking the produced neural network and is not used to train it. In this work 57 polymer solutions of 169 polymer solutions were randomly allocated to test set and all remaining 112 polymer solutions were allocated to training set.

The schematic of the three-layer FFNN which was used in this work are shown in Fig. 2.

Fig. 3. The schematic structure of three layer feed forward neural network used in this study.

We can simplify the results of the three-layer FFNN in the form of Eq. (1).

$$y_{calc}(i) = (W_2 \times (\tanh(W_1 \times T_i) + b_1)) + b_2 \quad (1)$$

In this equation, T is the input matrix and is a $nparam \times nds$ matrix where $nparam$ is the number of molecular descriptors (it is equal to 8 in this work) and nds is the number of polymer solutions available in the training set (it is equal to 112 in this problem). T_i is the i th-column of the matrix T . W_1 is the weight matrix of the second layer in our FFNN and is a $n \times nds$ matrix which n is the number of neurons in the hidden layer. b_1 is the bias matrix of second layer and is a $n \times 1$ matrix. W_2 is the weight matrix of output layer (third layer) and is a $n \times 1$ matrix. b_2 is the bias of output layer (third layer) which is a scalar quantity. $y_{calc}(i)$ is the i th output of this network which must be compared with i th physical property.

Usually, all inputs and outputs of FFNN are normalized between -1 and +1, for decreasing the accounting error. This work was performed in this section, by means of the minimum and maximum values of any descriptors as well as output values.

The values of W_1 , W_2 , b_1 , and b_2 are obtained by minimization of an objective function which is commonly the mean squared error between the outputs of neural network and the target values. This minimization is usually done by Levenberg-Marquart algorithm. This algorithm is rapid and accurate in process of training neural networks [24].

Fig. 4. Effect of number of neurons of hidden layer on the MRE of the best obtained FFNN.

In most cases first the number of neurons of hidden layer (n) is fixed, then it is tried to produce a neural network which can predict the target values with the best accuracy. Then this work is repeated till the best neural network is obtained. In many

cases especially in three-layer FFNNs, it is better the number of neurons of hidden layer is optimized, as a complementary work.

In this work, a three-layer FFNN was generated to predict $\theta(LCST)$ of polymer solutions, then the number of neurons of hidden layer of this three-layer FFNN was post-optimized for obtaining the best number of neurons of hidden layer. As can be seen in Fig. 3, the best number of neurons of hidden layer which is obtained is equal to 10. It should be noted that all FFNNs with structure 8-1-1 to 8-20-1 were checked to obtain the best FFNNs. The MRE of these FFNNs are shown in the Fig. 3.

The best three-layer FFNN which was obtained for prediction $\theta(LCST)$ of polymer solutions has the structures 8-10-1 and shows $R^2 = 0.9736$ and MRE 1.67% over all experimental data set. The values of W_1 , W_2 , b_1 , and b_2 for this FFNN are presented in Tab. 6. Also the predicted values of $\theta(LCST)$ in comparison to experimental data are presented in Fig. 1.

Tab. 6. Weight and bias matrices of the best obtained three layer feed forward neural network.

W_1								b_1
0.3113	0.8756	-0.708	0.798	0.1394	0.0439	1.5048	-0.696	2.1366
0.5547	1.0573	0.7505	0.0824	0.5761	0.9691	0.5074	0.3306	1.4044
0.8431	1.0351	0.7658	-0.322	0.0074	0.0077	0.3078	0.6849	1.0165
-1.541	1.2856	0.1388	0.6983	0.2058	0.4043	0.2871	0.8182	0.7645
0.2015	0.1992	0.6909	0.1303	1.1088	1.1097	0.4414	0.2572	0.6198
0.0455	0.8549	0.0712	0.6278	-0.982	0.1141	0.1184	0.1027	0.4453
0.5488	0.8558	1.2487	0.0169	0.1544	0.6864	0.7333	-0.685	0.3654
0.964	1.1757	0.4145	0.5717	0.2343	0.2172	0.2889	-0.943	0.8297
0.4037	1.9222	1.7512	0.4542	0.9982	0.2037	0.8422	-0.163	0.3371
0.3544	0.3598	0.4066	0.3509	-1.173	1.2595	0.3784	0.7987	-1.55
W_2								
0.7419	0.5111	0.2933	0.5444	0.4939	1.3342	0.0265	0.4012	0.542
								0.7205
b_2								
								0.1496

The statistical parameters of the obtained FFNN for prediction of $\theta(LCST)$ are presented in Tab. 5.

The obtained MRE by this FFNN over all experimental data is 1.67%. This value, in comparison to previous works, shows considerable modification.

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Supplementary Materials

ID	Polymer	Solvent	Molecular Descriptors							
			Mecc-polymer	DISPv-polymer	Mor17m-polymer	MDDD-solvent	piID-solvent	X3v-solvent	MATS2m-solvent	Mor25p-solvent
1	P4MP1	n-Butane	0.998	0.626	-0.138	1	7.178	0.5	1	0.1
2	P4MP1	n-Pentane	0.998	0.626	-0.138	1.6	9.787	0.707	1	0.092
3	P4MP1	n-Heptane	0.998	0.626	-0.138	2.857	15.525	1.207	1	0.094
4	P4MP1	n-Octane	0.998	0.626	-0.138	4	18.605	1.457	1	0.1
5	P4MP1	2-Methyl butane	0.998	0.626	-0.138	1.36	9.317	0.816	1	0.116
6	P4MP1	2,2-Dimethyl butane	0.998	0.626	-0.138	1.556	11.257	1.061	1	0.123
7	P4MP1	2,2-Dimethyl pentane	0.998	0.626	-0.138	2.122	14.139	1	1	0.113
8	P4MP1	2,2,3-Trimethyl butane	0.998	0.626	-0.138	2	13.194	1.732	1	0.089
9	P4MP1	Cyclopentane	0.998	0.626	-0.138	0	12.167	1.25	1	0.16
10	P4MP1	n-Hexane	0.998	0.626	-0.138	2.222	12.579	0.957	1	0.093
11	P4MP1	n-Nonane	0.998	0.626	-0.138	5.185	21.802	1.707	1	0.102
12	P4MP1	2,4-Dimethyl pentane	0.998	0.626	-0.138	2.612	14.244	0.943	1	0.108
13	P4MP1	3-Ethyl pentane	0.998	0.626	-0.138	2.816	14.224	1.732	1	0.069
14	PB1	n-Pentane	0.999	0	-0.099	1.6	9.787	0.707	1	0.092
15	PB1	n-Heptane	0.999	0	-0.099	2.857	15.525	1.207	1	0.094
16	PB1	n-Octane	0.999	0	-0.099	4	18.605	1.457	1	0.1
17	PB1	2-Methyl butane	0.999	0	-0.099	1.36	9.317	0.816	1	0.116
18	PB1	2,2-Dimethyl butane	0.999	0	-0.099	1.556	11.257	1.061	1	0.123
19	PB1	2,2,3-Trimethyl butane	0.999	0	-0.099	2	13.194	1.732	1	0.089
20	PB1	2,5-Dimethyl hexane	0.999	0	-0.099	3.5	17.287	1.321	1	0.144
21	PB1	3-Ethyl pentane	0.999	0	-0.099	2.816	14.224	1.732	1	0.069
22	PB1	3,4-Dimethyl hexane	0.999	0	-0.099	3	16.776	2.259	1	0.066
23	PB1	n-Hexane	0.999	0	-0.099	2.222	12.579	0.957	1	0.093
24	PB1	n-Nonane	0.999	0	-0.099	5.185	21.802	1.707	1	0.102
25	PB1	2,4-Dimethyl pentane	0.999	0	-0.099	2.612	14.244	0.943	1	0.108
26	PB1	2,3-Dimethyl pentane	0.999	0	-0.099	2.408	14.07	1.782	1	0.074
27	PB1	Cyclopentane	0.999	0	-0.099	0	12.167	1.25	1	0.16
28	PBD	n-Hexane	0.999	2.972	0.002	2.222	12.579	0.957	1	0.093
29	PBD	2,2,3-Trimethyl butane	0.999	2.972	0.002	2	13.194	1.732	1	0.089
30	PBD	n-Octane	0.999	2.972	0.002	4	18.605	1.457	1	0.1
31	PBD	Ethyl propyl ketone	0.999	2.972	0.002	2.612	15.659	0.923	-0.222	0.171
32	PBD	Diethyl ketone	0.999	2.972	0.002	2	12.664	0.789	-0.28	0.006
33	PBD	2-Methyl hexane	0.999	2.972	0.002	2.735	14.986	1.135	1	0.114

34	PBD	2,2,4-Trimethyl pentane	0.999	2.972	0.002	2.875	16.215	1.021	1	0.122
35	PBD	Propylene oxide	0.999	2.972	0.002	0.5	8.5	0.333	-0.333	0.053
36	PDMS	n-Pentane	0.989	1.194	-0.312	1.6	9.787	0.707	1	0.092
37	PDMS	n-Heptane	0.989	1.194	-0.312	2.857	15.525	1.207	1	0.094
38	PDMS	n-Octane	0.989	1.194	-0.312	4	18.605	1.457	1	0.1
39	PDMS	n-Dodecane	0.989	1.194	-0.312	9	31.987	2.457	1	0.106
40	PDMS	n-Cetane	0.989	1.194	-0.312	16.25	46.672	3.457	1	0.108
41	PDMS	n-Hexane	0.989	1.194	-0.312	2.222	12.579	0.957	1	0.093
42	PDMS	n-Decane	0.989	1.194	-0.312	6.4	25.104	1.957	1	0.096
43	PE	n-Hexane	0.989	0	-0.048	2.222	12.579	0.957	1	0.093
44	PE	n-Heptane	0.989	0	-0.048	2.857	15.525	1.207	1	0.094
45	PE	n-Nonane	0.989	0	-0.048	5.185	21.802	1.707	1	0.102
46	PE	n-Decane	0.989	0	-0.048	6.4	25.104	1.957	1	0.096
47	PE	n-Dodecane	0.989	0	-0.048	9	31.987	2.457	1	0.106
48	PE	n-Tridecane	0.989	0	-0.048	10.769	35.552	2.707	1	0.109
49	PE	2,2-Dimethyl pentane	0.989	0	-0.048	2.122	14.139	1	1	0.113
50	PE	2,2,3-Trimethyl butane	0.989	0	-0.048	2	13.194	1.732	1	0.089
51	PE	2,3-Dimethyl pentane	0.989	0	-0.048	2.408	14.07	1.782	1	0.074
52	PE	3-Ethyl pentane	0.989	0	-0.048	2.816	14.224	1.732	1	0.069
53	PE	2,2,4,4-Tetramethyl pentane	0.989	0	-0.048	3.259	18.085	1.061	1	0.121
54	PE	2,3,4-Trimethyl hexane	0.989	0	-0.048	3.506	19.038	2.593	1	0.029
55	PE	Methyl cyclopentane	0.989	0	-0.048	1	15.283	1.644	1	0.182
56	PE	Methyl cyclohexane	0.989	0	-0.048	1.143	18.967	1.894	1	0.244
57	PE	1-Octanol	0.989	0	-0.048	5.185	21.802	1.512	-0.036	0.079
58	PE	n-Pentyl acetate	0.989	0	-0.048	4.494	22.043	1.212	0.366	0.104
59	PE	n-Pentane	0.989	0	-0.048	1.6	9.787	0.707	1	0.092
60	PE	n-Octane	0.989	0	-0.048	4	18.605	1.457	1	0.1
61	PE	n-Undecane	0.989	0	-0.048	7.636	28.502	2.207	1	0.097
62	PE	2,4-Dimethyl pentane	0.989	0	-0.048	2.612	14.244	0.943	1	0.108
63	PE	2,2,4-Trimethyl pentane	0.989	0	-0.048	2.875	16.215	1.021	1	0.122
64	PE	3,4-Dimethyl hexane	0.989	0	-0.048	3	16.776	2.259	1	0.066
65	PE	Cyclopentane	0.989	0	-0.048	0	12.167	1.25	1	0.16
66	PE	Cyclohexane	0.989	0	-0.048	0	15.73	1.5	1	0.219
67	PE	n-Butyl acetate	0.989	0	-0.048	3.5	18.791	0.962	0.333	0.081
68	PIB	Cyclopentane	0.985	0.804	-0.076	0	12.167	1.25	1	0.16
69	PIB	Cyclohexane	0.985	0.804	-0.076	0	15.73	1.5	1	0.219

70	PIB	Cycloheptane	0.985	0.804	-0.076	0	19.477	1.75	1	0.136
71	PIB	Cyclooctane	0.985	0.804	-0.076	0	23.381	2	1	0.202
72	PIB	n-Heptane	0.985	0.804	-0.076	2.857	15.525	1.207	1	0.094
73	PIB	n-Octane	0.985	0.804	-0.076	4	18.605	1.457	1	0.1
74	PIB	n-Dodecane	0.985	0.804	-0.076	9	31.987	2.457	1	0.106
75	PIB	2-Methyl butane	0.985	0.804	-0.076	1.36	9.317	0.816	1	0.116
76	PIB	2-Methyl pentane	0.985	0.804	-0.076	2	12.068	0.866	1	0.108
77	PIB	3-Methyl pentane	0.985	0.804	-0.076	2	11.886	1.394	1	0.102
78	PIB	3-Methyl hexane	0.985	0.804	-0.076	2.612	14.763	1.478	1	0.101
79	PIB	3-Ethyl pentane	0.985	0.804	-0.076	2.816	14.224	1.732	1	0.069
80	PIB	2,3-Dimethyl pentane	0.985	0.804	-0.076	2.408	14.07	1.782	1	0.074
81	PIB	2,4-Dimethyl pentane	0.985	0.804	-0.076	2.612	14.244	0.943	1	0.108
82	PIB	2,2,3-Trimethyl butane	0.985	0.804	-0.076	2	13.194	1.732	1	0.089
83	PIB	Ethyl cyclopentane	0.985	0.804	-0.076	1.755	18.59	2.052	1	0.236
84	PIB	3-Methyl heptane	0.985	0.804	-0.076	3.5	17.794	1.747	1	0.108
85	PIB	2,2-Dimethyl hexane	0.985	0.804	-0.076	3.063	17.17	1.28	1	0.126
86	PIB	2,5-Dimethyl hexane	0.985	0.804	-0.076	3.5	17.287	1.321	1	0.144
87	PIB	3,4-Dimethyl hexane	0.985	0.804	-0.076	3	16.776	2.259	1	0.066
88	PIB	n-Propyl cyclopentane	0.985	0.804	-0.076	2.75	22.037	2.172	1	0.193
89	PIB	n-Pentane	0.985	0.804	-0.076	1.6	9.787	0.707	1	0.092
90	PIB	n-Hexane	0.985	0.804	-0.076	2.222	12.579	0.957	1	0.093
91	PIB	Methyl cyclopentane	0.985	0.804	-0.076	1.143	18.967	1.894	1	0.244
92	PIB	2-Methyl hexane	0.985	0.804	-0.076	2.735	14.986	1.135	1	0.114
93	PIB	2,2-Dimethyl pentane	0.985	0.804	-0.076	2.122	14.139	1	1	0.113
94	PIB	3,3-Dimethyl pentane	0.985	0.804	-0.076	2.204	13.782	1.914	1	0.102
95	PIB	Methyl cyclohexane	0.985	0.804	-0.076	1.143	18.967	1.894	1	0.244
96	PIB	2-Methyl heptane	0.985	0.804	-0.076	3.75	18.045	1.385	1	0.119
97	PIB	2,4-Dimethyl hexane	0.985	0.804	-0.076	3.25	17.113	1.571	1	0.107
98	PIB	2,2,4-Trimethyl pentane	0.985	0.804	-0.076	2.875	16.215	1.021	1	0.122
99	PIB	n-Decane	0.985	0.804	-0.076	6.4	25.104	1.957	1	0.096
100	PMMA	Methyl acetate	0.997	1.818	-0.052	1.36	10.124	0.287	0.042	0.06
101	PMMA	Ethyl acetate	0.997	1.818	-0.052	2	12.664	0.516	0.2	0.083
102	PMMA	Ethyl propyl ketone	0.997	1.818	-0.052	2.612	15.659	0.923	-0.222	0.028
103	PMMA	Diethyl ketone	0.997	1.818	-0.052	2	12.664	0.789	-0.28	0.006
104	PMMA	Butyl chloride	0.997	1.818	-0.052	1.6	9.787	0.754	-0.167	0.058
105	PMMA	Dipropyl ketone	0.997	1.818	-0.052	3.313	18.568	1.058	-0.184	0.051
106	PMMA	Methyl ethyl ketone	0.997	1.818	-0.052	1.36	10.124	0.498	-0.375	0.097
107	PMMA	Tetrahydrofuran	0.997	1.818	-0.052	0	12.167	0.827	-0.25	0.153

108	PMS	Cyclopentane	0.999	8.008	-0.083	0	12.167	1.25	1	0.16
109	PMS	Cyclohexane	0.999	8.008	-0.083	0	15.73	1.5	1	0.219
110	PMS	Butyl chloride	0.999	8.008	-0.083	1.6	9.787	0.754	-0.167	0.058
111	PMS	n-Butyl acetate	0.999	8.008	-0.083	3.5	18.791	0.962	0.333	0.081
112	PMS	n-Hexyl acetate	0.999	8.008	-0.083	5.6	25.4	1.462	0.389	0.097
113	PMS	Methyl cyclohexane	0.999	8.008	-0.083	1.143	18.967	1.894	1	0.244
114	PMS	n-Pentyl acetate	0.999	8.008	-0.083	4.494	22.043	1.212	0.366	0.087
115	PP	n-Pentane	0.996	0.658	-0.067	1.6	9.787	0.707	1	0.092
116	PP	n-Hexane	0.996	0.658	-0.067	2.222	12.579	0.957	1	0.093
117	PP	n-Octane	0.996	0.658	-0.067	4	18.605	1.457	1	0.1
118	PP	n-Nonane	0.996	0.658	-0.067	5.185	21.802	1.707	1	0.102
119	PP	2,2-Dimethyl butane	0.996	0.658	-0.067	1.556	11.257	1.061	1	0.123
120	PP	2,3-Dimethyl butane	0.996	0.658	-0.067	1.778	11.347	1.333	1	0.09
121	PP	2,2-Dimethyl pentane	0.996	0.658	-0.067	2.122	14.139	1	1	0.113
122	PP	2,2,3-Trimethyl butane	0.996	0.658	-0.067	2	13.194	1.732	1	0.089
123	PP	2,3-Dimethyl pentane	0.996	0.658	-0.067	2.408	14.07	1.782	1	0.074
124	PP	3-Ethyl pentane	0.996	0.658	-0.067	2.816	14.224	1.732	1	0.069
		2,2,4,4-Tetramethyl								
125	PP	pentane	0.996	0.658	-0.067	3.259	18.085	1.061	1	0.121
126	PP	2,3,4-Trimethyl hexane	0.996	0.658	-0.067	3.506	19.038	2.593	1	0.029
127	PP	Methyl cyclopentane	0.996	0.658	-0.067	1	15.283	1.644	1	0.181
128	PP	Methyl cyclohexane	0.996	0.658	-0.067	1.143	18.967	1.894	1	0.244
129	PP	Diethyl ether	0.996	0.658	-0.067	1.6	9.787	0.408	-0.583	0.166
130	PP	n-Heptane	0.996	0.658	-0.067	2.857	15.525	1.207	1	0.094
131	PP	2-Methyl butane	0.996	0.658	-0.067	1.36	9.317	0.816	1	0.116
132	PP	2,4-Dimethyl pentane	0.996	0.658	-0.067	2.612	14.244	0.943	1	0.108
		2,2,4-Trimethyl								
133	PP	pentane	0.996	0.658	-0.067	2.875	16.215	1.021	1	0.122
134	PP	3,4-Dimethyl hexane	0.996	0.658	-0.067	3	16.776	2.259	1	0.066
135	PP	Cyclopentane	0.996	0.658	-0.067	0	12.167	1.25	1	0.16
136	PP	Cyclohexane	0.996	0.658	-0.067	0	15.73	1.5	1	0.219
137	PP1	n-Pentane	0.999	0.532	-0.138	1.6	9.787	0.707	1	0.092
138	PP1	n-Hexane	0.999	0.532	-0.138	2.222	12.579	0.957	1	0.093
139	PP1	n-Octane	0.999	0.532	-0.138	4	18.605	1.457	1	0.1
140	PP1	2-Methyl butane	0.999	0.532	-0.138	1.36	9.317	0.816	1	0.116
141	PP1	2,4-Dimethyl pentane	0.999	0.532	-0.138	2.612	14.244	0.943	1	0.108
142	PP1	2,2-Dimethyl pentane	0.999	0.532	-0.138	2.122	14.139	1	1	0.113
143	PP1	2,3-Dimethyl pentane	0.999	0.532	-0.138	2.408	14.07	1.782	1	0.074
144	PP1	3-Methyl heptane	0.999	0.532	-0.138	3.5	17.794	1.747	1	0.108

145	PP1	n-Heptane	0.999	0.532	-0.138	2.857	15.525	1.207	1	0.094
146	PP1	2,2-Dimethyl butane	0.999	0.532	-0.138	1.556	11.257	1.061	1	0.123
147	PP1	2,2,4-Trimethyl pentane	0.999	0.532	-0.138	2.875	16.215	1.021	1	0.122
148	PP1	Cyclopentane	0.999	0.532	-0.138	0	12.167	1.25	1	0.16
149	PPCS	Isobutyl acetate	1	13.623	0.033	3.25	17.97	0.803	0.333	0.122
150	PPCS	Ethyl carbitol	1	13.623	0.033	7.636	28.502	1.152	-0.542	0.315
151	PPCS	n-Butyl carbitol	1	13.623	0.033	10.769	35.552	1.59	-0.409	0.371
152	PPCS	tert-Butyl acetate	1	13.623	0.033	2.563	16.713	0.798	0.333	0.156
153	PS	Cyclopentane	1	6.513	-0.066	0	12.167	1.25	1	0.16
154	PS	Cyclohexane	1	6.513	-0.066	0	15.73	1.5	1	0.219
155	PS	Methyl cyclopentane	1	6.513	-0.066	1	15.283	1.644	1	0.181
156	PS	Methyl cyclohexane	1	6.513	-0.066	1.143	18.967	1.894	1	0.244
157	PS	Benzene	1	6.513	-0.066	0	21.32	0.667	1	0.34
158	PS	Toluene	1	6.513	-0.066	1.143	25.971	0.94	1	0.301
159	PS	Ethyl acetate	1	6.513	-0.066	2	12.664	0.516	0.2	0.083
160	PS	n-Propyl acetate	1	6.513	-0.066	2.612	15.659	0.682	0.283	0.137
161	PS	i-Propyl acetate	1	6.513	-0.066	2.408	14.783	0.673	0.3	0.124
162	PS	Ethyl n-butyrate	1	6.513	-0.066	3.313	18.568	0.759	0.143	0.152
163	PS	Isobutyl acetate	1	6.513	-0.066	3.25	17.97	0.803	0.333	0.122
164	PS	sec-Butyl acetate	1	6.513	-0.066	3	17.565	1.216	0.333	0.131
165	PS	tert-Butyl acetate	1	6.513	-0.066	2.563	16.713	0.798	0.333	0.184
166	PS	Diethyl malonate	1	6.513	-0.066	6.05	28.004	0.899	-0.071	0.09
167	PS	i-Amyl acetate	1	6.513	-0.066	3.802	20.868	1.44	0.357	0.085
168	PS	Methyl acetate	1	6.513	-0.066	1.36	10.124	0.287	0.042	0.06
169	PS	Methyl ethyl ketone	1	6.513	-0.066	1.36	10.124	0.498	-0.375	0.068