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Prediction of the liquid crystalline property for polyazomethines using modular neural networks

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The liquid crystalline properties of the poly(siloxane - azomethine)s were studied by experiment and simulation. A special class of neural networks was used in this paper – modular neural networks – to predict the liquid crystalline behavior as function of some molecular parameters which count for geometrical features (fully extended length and diameter of the structural unit) or polarizability features (dipole moment). The importance of an adequate choice of the input parameters for the neural models was emphasized. Satisfactory results are obtained with this neural network based method, especially in the validation phase of the models.

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1. Introduction

The design of liquid crystalline (LC) polymers is not an easy task. It is known that the simple presence of a mesogenic group in a polymer's structure doesn't necessarily lead to a mesomorphic behavior. For a mesogen-containing polymer, the presence, nature and features of a mesophase depend on numerous parameters, like the spacer nature and length, the synthesis conditions, polydispersity, intermolecular interactions etc.

One class of polymers studied for their LC behavior is that of polyazomethines. Aromatic polyazomethines or poly(Schiff base)s are also known for other attractive properties like: thermal stability, non-linear optical behavior, semiconducting, electroluminescence, fiber-forming ability, mechanical resistance, environmental stability and ability to form metal chelates [1-9]. The structural variety of polyazomethines is rather large and includes poly(siloxane-azomethine)s, many of them synthesized in our group [9-15]. As the wholly aromatic poly(azomethine)s have high melting or softening temperatures and low solubility, the introduction of siloxane segments as flexible spacers between the rigid conjugated aromatic azomethine moieties is one way to reduce the transition temperatures and to improve the solubility. The LC properties of the poly(siloxane-azomethine)s were studied and based on these results a certain tendency towards mesomorphic behavior was observed for low and medium length of the siloxane segment.

One of the most interesting optical properties of polymers is their liquid crystalline behavior, because in this state, the materials combine two essential properties of the matter: the order and the mobility. But, due to the complexity of the liquid crystalline phase, it is not at all easy to predict the occurrence of a mesophase. There are many methods of predicting the liquid crystalline behavior, based on molecular, energetic or structure-property relationship models [16 - 19].

The property prediction methods may be evaluated based on their classification as empirical, semi-empirical, theoretical and hybrid approaches. The empirical methods usually require extensive data collection and result in linear or simple nonlinear structure-property relations. Computations are very rapid at the expense of prediction accuracy. In addition, these methods require a specific functional form which may not always be available and the parameters determined by regression from the data. They are also computationally expensive, but provide excellent property estimations. Most approaches settle for the middle ground by utilizing simplifying assumptions as those found in semi-empirical methods and hybrid approaches. These methods provide the best compromise between model development effort, computational time and property prediction accuracy. In this regard, neural network based methods offer advantages of ease of development and implementation and execution speed, while maintaining a high degree of accuracy of predictions. Neural network based models are relatively model free, in the sense that the underlying functional form is not as rigorous as in the traditional model based methods. This adds to the generality of these methods.

The open literature contains a few references concerning the use of machine learning methods to predict the liquid crystalline behavior. For instance, Helge Kranz, Volkmar Vill and Bernd Meyer [20] present an example of a new way to predict a property from the chemical structure of a heterogeneous class of compounds. The clearing temperatures of nematic liquid crystalline phases of a big number of compounds were used to train neural

networks to derive this material property directly from their chemical structure.

Our group has significant contribution to liquid crystalline behavior prediction using different learning methods, such as neural networks and categorization algorithms (decision trees, nearest-neighbor and Bayesian induction, implemented in some variants: C4.5 pruned, C4.5 unpruned, Random Tree, Random Forest, Naïve Bayes, Nearest-Neighbor, 4-Nearest Neighbor, Non-Nested Generalization Exemplars). These methods have been applied to various classes of compounds: copolyethers with mesogenic units in the main chain [21], ferrocene derivatives [22, 23] or azo aromatic compounds [24].

In the attempt of optimizing the mesomorphism of polyazomethines, we gathered literature data and our own results and considered some quantifiable geometric and energetic parameters. Based on these calculated measures and the experimental observations on the presence of a mesophase, we applied the instruments of the artificial intelligence in order to predict the LC behavior for related polymers. A special class of neural networks was used in this paper – modular neural networks. Satisfactory results are obtained with this method, especially in the validation phase of the models. The appropriate choice of the input parameters for the neural network is an important issue of the modeling strategy.

The present approach is an opportunity to prove the utility and the efficiency of the neural networks as classification methods, particularly for quantifying the structure – properties relation for some polyazomethines.

2. Experimental

Siloxane-based polyazomethines

A number of azomethine compounds with (poly)siloxane moieties have been synthesized by polycondensation reactions, using either macromers with preformed azomethine linkages [10-12] or diamines and siloxane dialdehydes [15]. The (poly)siloxane segment, contained in the appropriate monomer, had various lengths, in order to ensure variations in solubility, thermal and thermotropic properties.

The poly(siloxane-azomethine)s were characterized by spectral methods (IR-Bruker Vertex 70 FTIR, NMR - Bruker 400MHz), GPC (PL-EMD 950 Chromatograph - Evaporative Mass Detector) and solubility tests.

Other polymers with azomethine bonds taken in this study have been reported by one of us and other authors and contain other spacers than polysiloxanes [25-27].

Liquid crystalline behavior

A set of polyazomethines and related dimers was chosen, based on literature data regarding their LC properties. The presence of a mesophase, as reported in these articles, was generally demonstrated by differential scanning calorimetry (DSC) and polarized light optical microscopy (POM).

In our own studies, the DSC analyses were performed on a Mettler TA DSC 12E Instrument, with heating and cooling rates of 10 ^{o}C/min and the POM observations were made on an Olympus BH-2 microscope, fitted with a THMS 600/HSF9I hot stage.

Molecular modeling calculations

Some molecular parameters of the discussed polymers and copolymers have been calculated using a demo version of Hyperchem software [28]. These parameters count for geometrical features (fully extended length, *L*, and diameter, *d*, of the structural unit) or polarizability features (dipole moment). Shape anisotropy parameter (axial ratio, *L/d*), was also considered as a measure of detection of rigid core character of the chemical entities investigated. Geometry optimization calculations were performed under Molecular Mechanics setup, by using a force field MM+ module.

In this study, we considered a number of polyazomethines and azomethine models of different chemical structure, part of them having siloxane moieties as spacers, and we grouped them into 6 structural types, according to Table 1.

- A1-A8 are siloxane-organic low molecular mass azomethines containing one siloxane sequence and one or two organic sequences;
- B1N12-B3N4 are organic polyazomethines, formed from several organic structural sequences;
- A9-A18 are alternating siloxane-organic polyazomethines with disiloxane sequences;
- A19-A24 are alternating siloxane-organic polyazomethines with oligosiloxane sequences;
- B4-B8 are organic polyazomethines with ethylene sequences instead of siloxane;
- C1-C5 are organic polyazomethines with no spacer.

Table 1. Chemical structure of the analyzed compounds.

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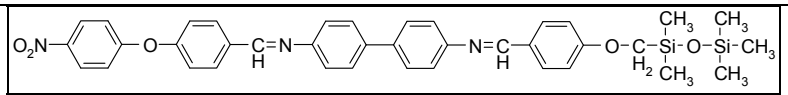
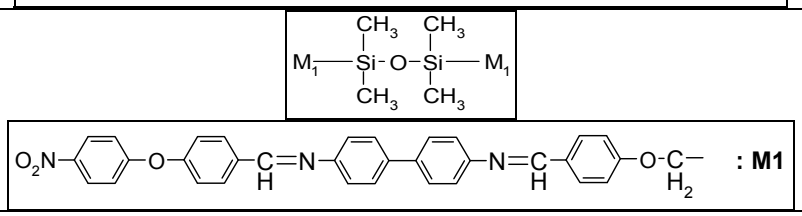
A1		[10]
A2		[10]

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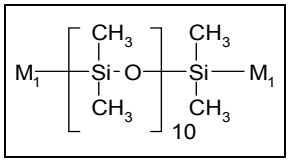
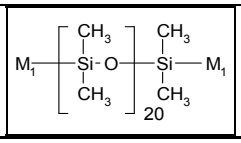
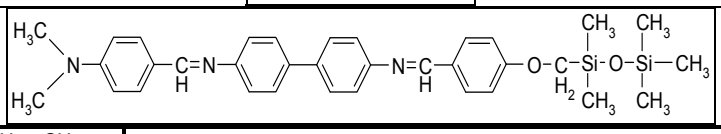
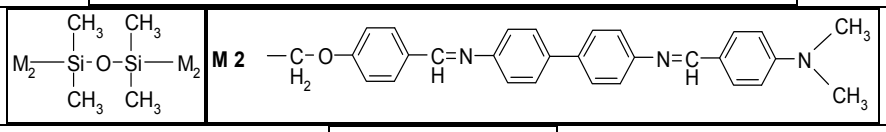
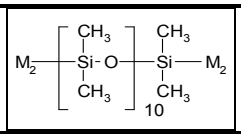
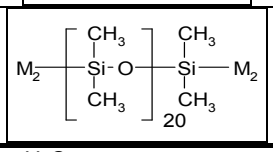
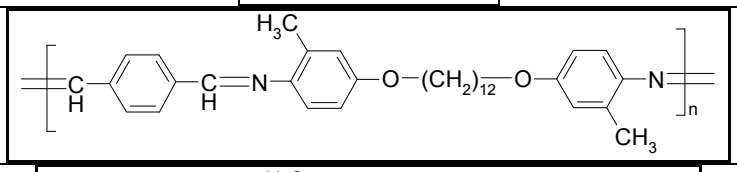
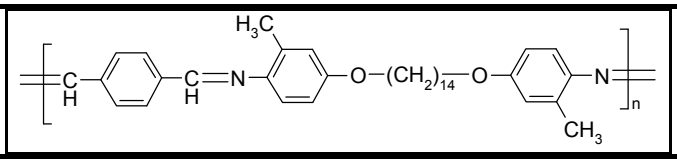
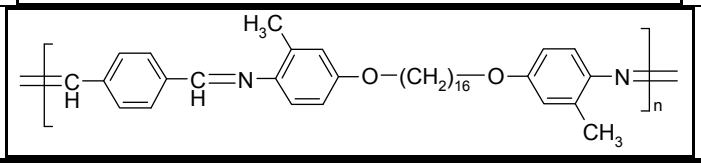
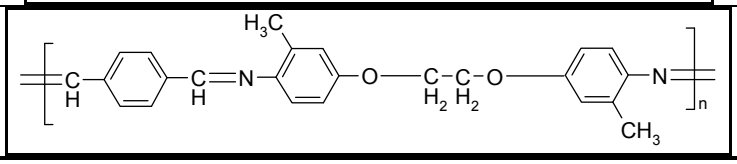
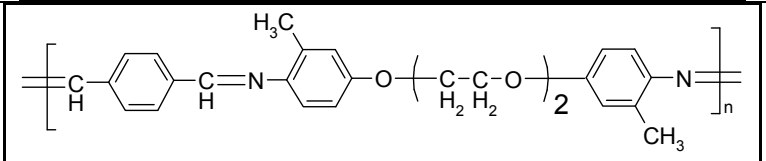
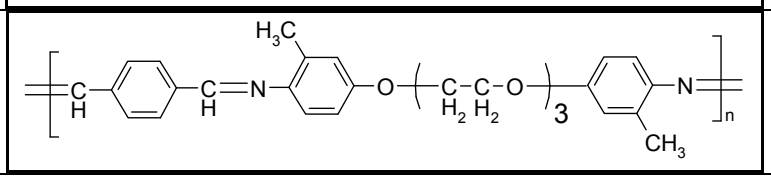
A3		[10]
A4		[10]
A5		[10]
A6		[10]
A7		[10]
A8		[10]
B1N12		[25]
B1N14		[25]
B1N16		[25]
B3N1		[25]
B3N2		[25]
B3N3		[25]

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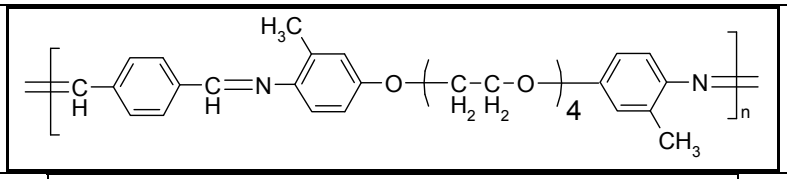
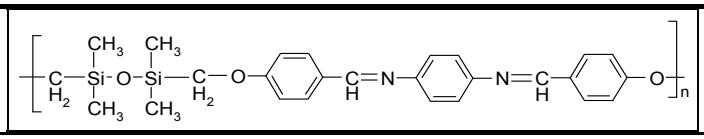
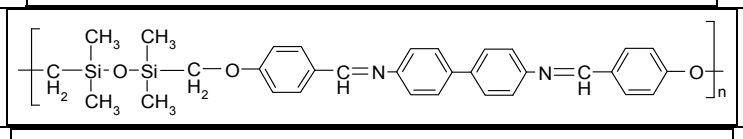
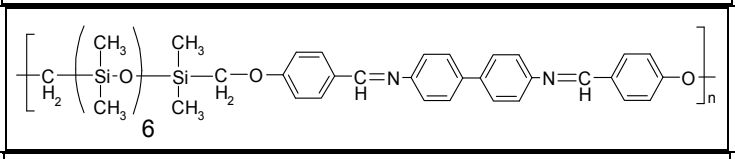
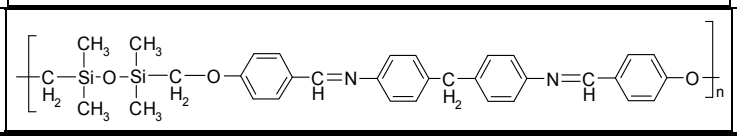
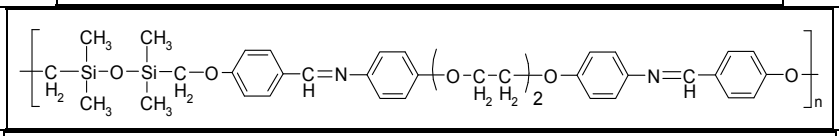
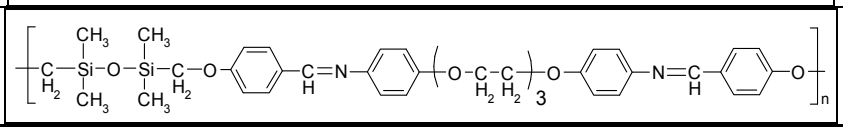
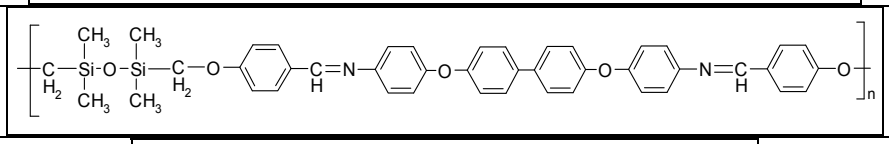
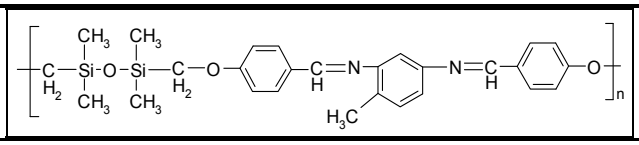
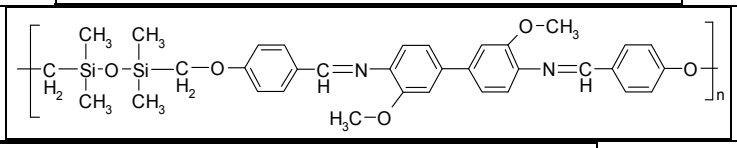
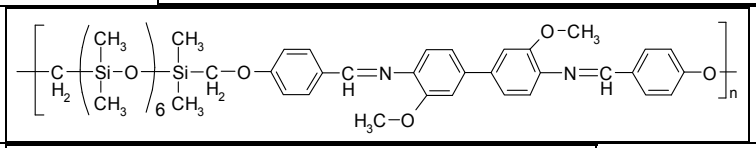
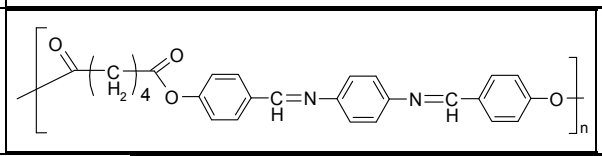
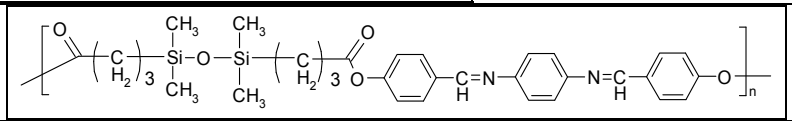
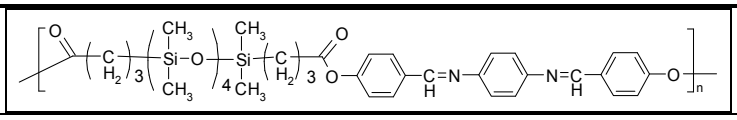
B3N4		[25]
A9		[15]
A10		[15]
A11		[15]
A12		[15]
A13		[15]
A14		[15]
A15		[15]
A16		[15]
A17		[12]
A18		[12]
B4		[25]
A19		[11]
A20		[11]

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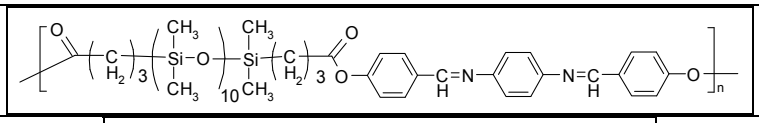
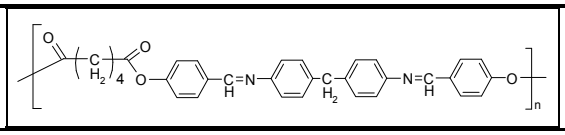
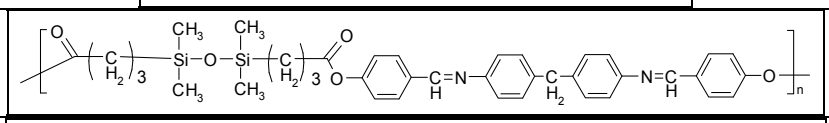
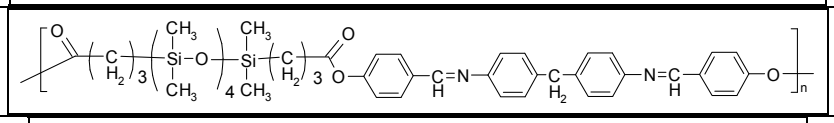
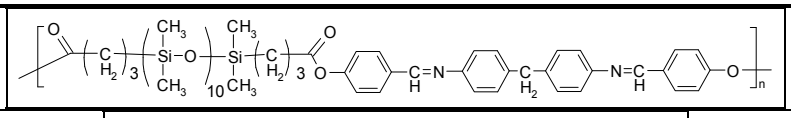
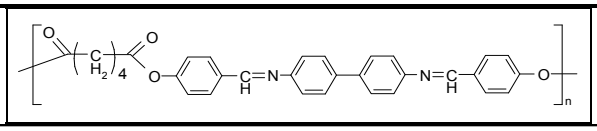
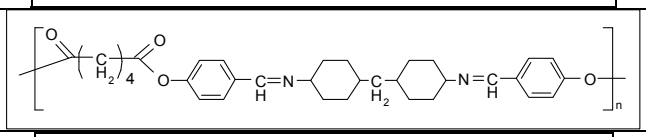
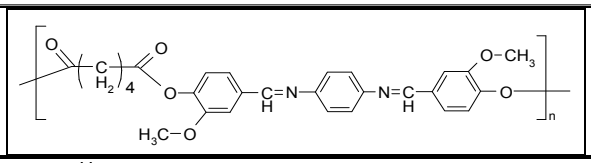
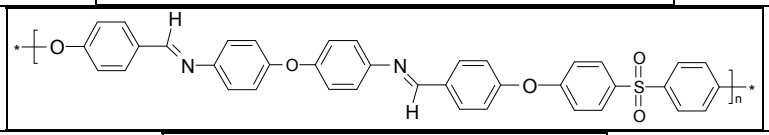
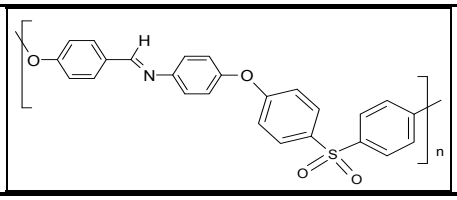
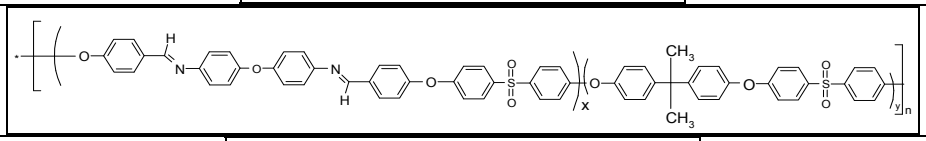
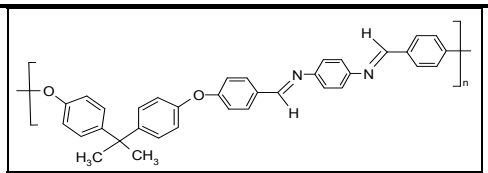
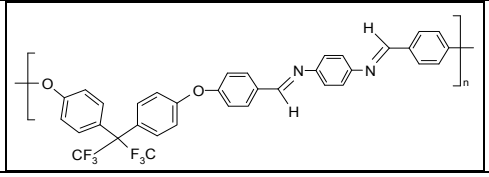
A21		[11]
B5		[25]
A22		[11]
A23		[11]
A24		[11]
B6		[25]
B7		[25]
B8		[25]
C 1		[26]
C 2		[26]
C 3		[26]
C 4		[27]
C 5		[27]

Table 2 presents the parameters correlated with the liquid crystalline behavior which should be taken into account in neural network modeling.

Table 2. Liquid crystalline property and structural parameters obtained by molecular modeling

Code	Structural unit length, L (A)	Structural unit diameter, d (A)	Asymmetry factor, L/d	Energy (kcal/mol)	Dipol moment (D)	Liquid crystalline property
A1	30.51	7.77	3.93	-5.78	2.783	YES
A2	42.80	25.24	1.70	-4.53	4.146	YES
A3	72.37	22.14	3.27	-4.00	0.920	YES
A4	91.19	24.18	3.77	-1.61	0.660	YES
A5	31.42	6.28	5.00	-4.96	2.532	YES
A6	39.12	19.64	1.99	-3.09	3.539	YES
A7	68.47	18.21	3.76	-41.42	3.190	YES
A8	92.24	27.43	3.36	9.67	0.663	YES
B1N12	32.67	5.91	5.53	62.65	2.011	YES
B1N14	35.36	5.92	5.97	67.94	1.880	YES
B1N16	37.89	5.92	6.40	73.25	2.160	YES
B3N1	19.95	5.90	3.38	31.44	2.737	YES
B3N2	21.89	5.87	3.73	44.30	1.123	YES
B3N3	27.32	5.89	4.64	65.52	7.613	YES
B3N4	29.59	5.91	5.01	78.70	3.495	YES
A9	22.97	7.67	2.99	-6.06	0.466	YES
A10	27.69	7.35	3.77	-6.31	0.809	YES
A11	29.31	12.53	2.34	-41.85	1.165	NO
A12	23.96	21.98	1.09	-16.39	8.602	YES
A13	26.84	11.07	2.42	34.54	7.422	YES
A14	38.56	6.43	6.00	51.16	0.406	YES
A15	33.55	10.63	3.16	-37.37	5.540	YES
A16	21.89	9.58	2.28	-3.97	7.324	NO
A17	27.61	9.15	3.02	24.09	3.512	YES
A18	38.69	25.77	1.50	-56.17	1.178	NO
B4	23.96	5.76	4.16	79.79	15.187	YES
A19	28.17	9.50	2.97	4.02	7.149	YES
A20	32.45	12.40	2.62	-34.51	11.668	YES
A21	50.30	10.13	4.97	-92.32	9.224	NO
B5	23.64	7.38	3.20	23.64	6.456	YES
A22	30.95	6.22	4.98	1.92	9.998	YES
A23	36.20	9.00	4.02	-41.32	20.580	YES
A24	47.81	16.04	2.98	-117.14	3.549	NO
B6	26.03	4.97	5.24	25.25	4.787	NO
B7	18.83	12.28	1.53	100.01	4.837	YES
B8	24.87	6.54	3.80	47.31	0.998	YES
C 1	24.47	8.06	3.03	6.42	0.795	NO
C 2	19.31	5.39	3.58	9.66	5.660	NO
C 3	22.29	21.70	1.03	19.13	2.750	NO
C 4	25.74	6.68	3.85	33.13	2.200	NO
C 5	25.81	6.88	3.75	36.6	2.2	NO

3. Results and discussion

We have synthesized and studied a large number of poly(siloxane-azomethine)s [8-15], especially from the perspective of liquid crystalline behavior and processability. When comparing with the starting mesogenic compounds or with similar polymers having aliphatic spacers instead of siloxane, a few general conclusions were obvious:

- the introduction of the siloxane moieties led to an important decrease of the melting temperature, more pronounced with increasing siloxane chain length;
- a broadening of the mesophase domain was observed (especially in dimers);
- lower isotropization temperatures were also obtained in most of the cases, thus avoiding the thermal degradation within the mesophase;
- mostly smectic mesophases were observed for polymers containing disiloxane moiety and nematic for longer siloxane segments (this is probably due to the polydispersity of the starting siloxanes);
- for long siloxane segments the thermotropic behavior was suppressed, probably due to „dilution" of the mesogen;
- good solubility was generally achieved using siloxane moieties as soft segment.

The liquid crystalline property of polyazomethines was also studied using a methodology based on neural networks. A special class of neural networks was used because of accurate results which they provided comparatively with other types of neural networks.

A neural network is formed by processing elements (neurons) interconnected with the other neurons through coefficients or weights that stand for the relative influence of the connections. There are various types of neural networks and, among them, the feedforward networks constitutes one of the most utilized classes. In a feedforward neural network (*multilayer perceptron*, MLP), neurons are arranged in layers: input, hidden and output layers. The information deriving from a layer undergoes a pondering through weights and is sent to all the neurons in the following layer. The processing elements of a same layer work in parallel and the process among the layers is sequential.

The multilayered feed-forward network (MLP) is frequently used in chemical modeling because the simplicity of its theory, ease of programming and, generally, good results [29]. But, for our problem – prediction of liquid crystalline property for polyazomethines – this type of network did not provide satisfactory results. High errors, especially in validation phase, were obtained with MLP models.

Modular feedforward networks (MN) are a special class of MLP. These networks process their input using several parallel MLPs, and then recombine the results. This tends to create some structure within the topology, which will foster specialization of function in each sub-module. In contrast to the MLP, modular networks do not have full interconnectivity between their layers. Therefore, a smaller number of weights are required for the same size network (*i.e.* the same number of processing elements). This tends to speed up training times and reduce the number of required training exemplars. There are many ways to segment a MLP into modules. Several examples are presented in Fig. 1 [30].

The parameters which have significant influence upon the liquid crystalline behavior: structural unit length, *L*, structural unit diameter, *d*, asymmetry factor, *S*, Energy, *E*, dipole moment, *D*, were chosen as inputs for neural network models. Two variants of neural modeling were considered having different input variables: 1) *S*, *E* and *D* and 2) *L*, *d*, *E* and *D*. Concerning the LC behavior, we have coded with "1" the possibility to generate a mesophase and with "0" the crystalline or amorphous phases.

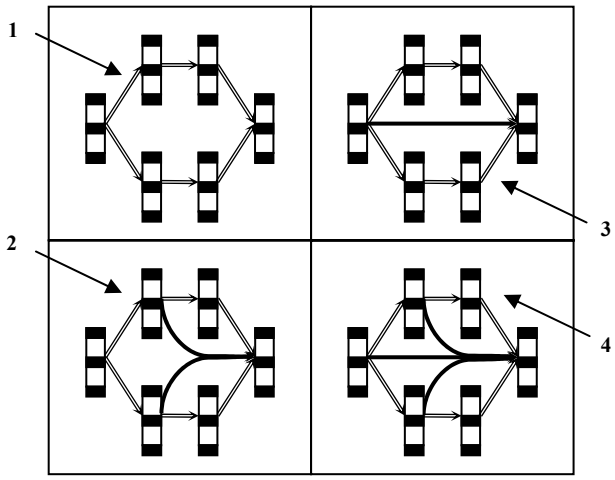


Fig. 1. Modular feedforward neural networks.

Before training, the data is split into training (about 85 % from the available data set) and validation data (about 15 %) sets because it is more important to evaluate the performance of the neural networks on unseen data than on training data. In this way, we can estimate the most important feature of a neural model – the generalization capability.

The transformation of a set of inputs into a set of outputs represents the main problem of a neural network modeling. The neural network model is obtained by *training* with input/output pairs, which have to be related by transformation which is being modeled. The adjustment of the neural network function to experimental data (learning process or training) is based on a non-linear regression technique.

The procedure used for determination of the neural networks architectures was the trial and error method based on the minimum mean squared error (*MSE*), calculated with the formula (1).

$$MSE = \frac{\sum_{j=1}^{P}\sum_{i=1}^{N}(d_{ij} - y_{ij})^2}{N \cdot P} \quad (1)$$

where: *P* is the number of output processing elements, *N* is the number of exemplars in the data set, y_{ij} is the network output for exemplar *i* at processing element *j*, and d_{ij} is the desired output for exemplar *i* at processing element *j*.

NeuroSolutions, a software application dedicated to the study of neural networks, was used in order to design and obtain predictions of modular neural networks.

Table 3 contains several topologies of MN tested for first variant of modeling, with their performance: *MSE*, *r* (correlation between experimental data and neural network predictions) and E_p (percent error). The topology is represented by the input layer with the three considered variable (*S*, *E* and *D*), one or two hidden layers and output layer with a single neuron for the output variable: LC is "1" for the behavior of liquid crystalline and "0" otherwise.

The best network is noted 9 in table 3 and it is marked in bold. The prediction of this network in the training phase was very good (MSE = 0.0645 and r = 0.9899), therefore the neural model learned well the correlation between structural parameters and liquid crystalline behavior.

Table 3. Modular neural networks tested for prediction of liquid crystalline behavior.

No. crt.	Topology	MSE	r	E_p
1	$MN\left(3:\begin{matrix}5\\5\end{matrix}:1\right)$ (structure 1 in figure 1)	0.2431	0.8872	6.2101
2	$MN\left(3:\begin{matrix}5\\5\end{matrix}:1\right)$ (structure 4 in figure 1)	0.0710	0.9102	5.8721
3	$MN\left(3:\begin{matrix}10\\10\end{matrix}:1\right)$ (structure 4 in figure 1)	0.06923	0.9020	5.7952
4	$MN\left(3:\begin{matrix}12&4\\12&4\end{matrix}:1\right)$ (structure 1 in figure 1)	0.06121	0.9150	4.9121
5	$MN\left(3:\begin{matrix}12&4\\12&4\end{matrix}:1\right)$ (structure 4 in figure 1)	0.04259	0.9299	4.2324
6	$MN\left(3:\begin{matrix}24&8\\24&8\end{matrix}:1\right)$ (structure 1 in figure 1)	0.04105	0.9889	3.2435
7	$MN\left(3:\begin{matrix}24&8\\24&8\end{matrix}:1\right)$ (structure 2 in figure 1)	0.05891	0.8975	5.2023
8	$MN\left(3:\begin{matrix}24&8\\24&8\end{matrix}:1\right)$ (structure 3 in figure 1)	0.06290	0.8920	5.6890
9	$MN\left(3:\begin{matrix}24&8\\24&8\end{matrix}:1\right)$ (structure 4 in figure 1)	0.03328	0.9989	2.9174

Table 4 presents some predictions of the neural model to previously unseen data (not used in the training phase, so "unseen" data for the network).

Cells marked in grey represent wrong prediction of the network. For the MN(3:24:8:1) and structure noted 4, with *S*, *E* and *D* as inputs, the probability of a correct answer was 85.71%. Consequently, this modular network can predict satisfactory the LC behavior of the polyazomethines.

The success in obtaining a reliable and a robust network depends strongly on the choice of the process variable involved, the available set of data and its domain used for training, as well as the training method.

For the second case – the inputs *L*, *d*, *E* and *D* – the network with the best performance was MN(4:42:14:1), structure 2 in Figure 1, for which MSE = 0.04230 and r = 9874. The validation phase is presented in table 5; the two wrong answers lead to a probability of accurate results of 71.43 %.

Table 4. Validation of the model MN(3:24:8:1).

Code	Asymmetry factor, S	Energy (kcal/mol)	Dipol moment (D)	Experim LC	Network LC
A6	1.99	-3.09	3.539	1	1
B3N1	3.38	31.44	2.737	1	1
A11	2.34	-41.85	1.165	0	0
A15	3.16	-37.37	5.54	1	1
A19	2.97	4.02	7.149	1	1
A24	2.98	-117.14	3.549	0	0
C 2	3.58	9.66	5.66	0	1

The best results are obtained in the first case of modeling, with the input parameters *S*, *E* and *D*. We cannot consider as an absolute conclusion the fact that the choice of *S* parameter as input variable leads to the best results and the above probabilities for the correct answer as absolute. But it is sure that an important step is the choice of the properties and structural parameters in such a combination that allows evaluating with high probability the liquid crystalline behavior.

In the common practice, the axial ratio (length per diameter) of a mesogenic unit represents a feature for prediction of liquid crystallinity of a polymer. Nevertheless, different approaches have been considered for the calculation and understanding of this parameter in the case of polymers, and thus different threshold values have been proposed for LC behavior [31 - 35].

Table 5. Validation of the model MN(4:42:14:1).

Code	Structural unit length, L (A)	Structural unit diameter, d (A)	Energy (kcal/mol)	Dipol moment (D)	Experim LC	Network LC
A6	39.12	19.64	-3.09	3.539	1	1
B3N1	19.95	5.90	31.44	2.737	1	1
A11	29.31	12.53	-41.85	1.165	0	0
A15	33.55	10.63	-37.37	5.54	1	0
A19	28.17	9.50	4.02	7.149	1	1
A24	47.81	16.04	-117.14	3.549	0	0
C 2	19.31	5.39	9.66	5.66	0	1

There are also many other factors which could strongly influence this property, such as: good molecular parallelism, substantially larger polarizability along the chain relative to the transverse direction, persistence length of chain (number of units affected by liquid crystal alignment), radius of gyration, chain flexibility etc. An empirical method was used to calculate the so-called „mesogenic index", but its employment is possible only for certain structures [36].

It was remarked that the presence of flexible spacers (either aliphatic or siloxane) in the backbone provides extra flexibility to the chain, but also imparts an effective decrease of the overall aspect ratio values of the chain [37]. Therefore, in the present work, it seemed a reasonable idea to consider the entire structural unit as an entity when calculating the aspect ratio, the proper contributions of the mesogen and spacer to the liquid crystallinity being almost impossible to quantify separately. On the other hand, the other parameters (the „energetic" ones) also concern the entire molecule, not only the mesogen.

If we take a closer look at the data presented in Tables 1 and 2, it is obvious that none of the considered parameters may give an absolute answer to the question wether the respective polymer is a liquid crystal or not. Polymers with low asymmetry factor sometimes exhibit LC behavior, while polymers with high dipol moment or *S* values not always show this property.

An important issue of this research is to emphasize the utility of using neural networks as efficient classification methods which can provide relatively accurate results and can be easy to manipulate. For modeling the relation between molecular structure and properties it is also important to choose the adequate type of neural network and, also, the set of input parameters.

It should be mentioned that the neural network predictions cannot provide the exact result of the actual experiment. However, if the error rate is low both for training and prediction/cross-validation phase, a neural network can provide acceptably accurate results, with the advantage of speed and without the use of any material resources. Also, we can take into account the fact that there are many free parameters involved in neural networks, such as choosing the best topology, the learning rate, the momentum factor when trying to accelerate the learning process, which is rather slow. All these elements should be carefully chosen and analyzed in order to have a near optimum model.

The neural network based methodology presented here is quite general and can be adapted easily to other systems and properties, with real chances to obtain accurate results.

4. Conclusions

The liquid crystalline property of poly(siloxane-azomethine)s was studied using a methodology based on modular neural networks. The best topology is developed by trial and error method and different inputs parameters are taken into account. The best results obtained with *S*, *E*

and *D* as network inputs (compared to the case with *L*, *d*, *E* and *D*) prove that the axial ratio (length per diameter) of the mesogenic unit represents an important feature for prediction of liquid crystallinity of a polymer.

Because the presence of flexible spacers (either aliphatic or siloxane) in the backbone provides extra flexibility to the chain, but also imparts an effective decrease of the overall aspect ratio values of the chain, in the present work, we considered the entire structural unit as an entity when calculating the aspect ratio, since the other parameters (the „energetic" ones) also concern the entire molecule, not only the mesogen.

The present approach is an opportunity to prove the utility and the efficiency of the neural networks as classification methods, particularly for quantifying the structure – properties relation for some polyazomethines.

In this research we tried to emphasize the utility of using neural networks as efficient classification methods which can provide relatively accurate results and can be easy to manipulate. The results showed that the proper choice of the type of neural network and of the set of input parameters is very important.

The neural network based methodology presented here is quite general and can be adapted easily to other systems and properties, with real chances to obtain accurate results.

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