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Short communication

# Quantitative structure–retention relationship studies for predicting the gas chromatography retention indices of polycyclic aromatic hydrocarbons

## Quasi-length of carbon chain and pseudo-conjugated system surface

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### Abstract

A new method of quantitative structure–retention relationship studies is reported for predicting capillary gas chromatography (GC) retention indices of polycyclic aromatic hydrocarbons (PAHs) by using two physicochemical parameters: pseudo-conjugated  $\pi$ -system surface ( $S_{\pi}$ ) and quasi-length of carbon chain ( $N'$ ), which represent the effect of the molecular  $\pi$  electronic conjugated surface and the molecular polarizability effect of PAHs on their corresponding gas chromatographic retention indices, respectively. Regression analysis is performed with regression coefficient being 0.9968 by using the above two parameters for capillary GC indices of 100 PAHs on SE-52 capillary columns. The results demonstrates a good linear relationship between the gas chromatographic retention index of PAHs and both their parameters  $N'$  and  $S_{\pi}$ . The method developed is successfully used for estimating and predicting the capillary GC retention index of PAHs. © 1998 Elsevier Science B.V.

**Keywords:** Quantitative structure–retention relationships; Quasi-length of carbon chain; Pseudo-conjugated system surface; Polynuclear aromatic hydrocarbons

### 1. Introduction

Polycyclic aromatic compounds (PACs) have been studied for well over a century, and the carcinogenic and mutagenic properties of numerous polycyclic compounds have been documented [1] and many others are presently under investigation. Because of the known hazards associated with the increasing

emission of PACs into our environment, and the developing social environmental awareness there is a need for both further structural identification and more accurate quantitative measurement of these substances.

Gas chromatography (GC) employing either packed or capillary columns is a common analytical tool used for the separation and analysis of PACs. However, there has been a general lack of chromatographic data on isomeric PACs due to the un-

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availability of reference compounds. Thus methods that can predict chromatographic retention data of PACs from its structure are important. The earliest structure–retention relationship in GC is the correlation with retention volume and Wilmhust [3] discussed the relationship between GC retention data and the molecular mass of polycyclic aromatic hydrocarbons (PAHs), reporting that the retention data of PAHs increased almost linearly with their molecular mass. However, in his study substituted PAHs show some departure from the linear plot. Kalisz and Lamparczyk [4] found a correlation between the GC retention data of PAHs and the connectivity index on a nonpolar GC phase.

Several workers have studied the influence of the molecular shape of PAHs on their chromatographic retention behavior on liquid crystal stationary phases [5–9] and various chemically bonded stationary phases [10,11]. Wise and co-workers [12–14] reported a relationship between the shape of PAHs and the reversed-phase LC retention on  $C_{18}$  bonded phases, and demonstrated the importance of unique selectivity of the  $C_{18}$  phase for PAHs and, particularly, for methyl-substituted PAHs.

In addition, some authors have reported the relation between the chromatographic retention and the physicochemical parameters of PAHs [15–21] and their nitro derivatives [22,23].

In this paper a relationship between the GC retention index on SE-52 capillary columns and two novel parameters from the molecular structure of PAHs, quasi-length of carbon chain [24] ( $N'$ ) and pseudo-conjugated system surface area ( $S_{\pi}$ ), is reported.

## 2. Description of two main parameters

### 2.1. Pseudo-conjugated system surface area ( $S_{\pi}$ )

As described earlier, a number of workers have studied the influence of the molecular structure, size and shape of PAHs on their chromatographic retention in both liquid–solid adsorption chromatography (LSC) and GC on liquid crystal stationary phases [5–7]. Radecki et al. [9] correlated the relative shape parameter,  $\eta$ , for PAHs with the relative GC retention on liquid crystal phases. The

shape parameter,  $\eta$ , was defined as the ratio of the longer side to the shorter side of a rectangle having a minimum area, which enclosed the molecule. Wise and co-workers [12–14] found a relationship between retention on polymeric  $C_{18}$  phase and the shape of the solute, defined as length–breadth ratio ( $L/B$ ). The  $L/B$  value is determined by drawing the PAH molecule using the appropriate bond lengths and then constructing a rectangle around the structure which provides the maximum length to breadth ratio. In these works, the shape parameters of PAHs, specifically the length-to-breadth ratio is successfully used in predicting the retention behavior of PAHs with the same molecular mass on polymeric and monomeric  $C_{18}$  bonded phases, however, it does not adequately account for the retention behavior of PAHs with different molecular mass.

In this paper, the authors believe that the interaction between the molecular plane of PAHs and the stationary phase can be approximately regarded as a kind of frictional action and/or adsorptional action, which is related to the molecular surface. According to the interaction mechanism of PAH molecules in GC capillary columns, the greater the molecular plane of the PAH, the stronger the interaction and the longer the retention time. It is well known that the molecular structure of PAHs is nearly a planar, close ring and also, conjugated  $\pi$ -electron system. However, not all planes in the PAH molecule can influence the chromatographic retention data; in our opinion, only the main part which acts with the plane of the stationary phase can. So, in fact the effective area in the molecular plane of a PAH can be named pseudo-conjugated system surface ( $S_{\pi}$ ), and the sequence of the elution behavior of PAHs can be influenced by this pseudo-conjugated system surface.

The value of the pseudo-conjugated system surface ( $S_{\pi}$ ) of PAHs can be calculated by the geometry arithmetic from the molecular structure formula. In order to simplify the calculation process all the bond lengths of a PAH take approximately the bond length of benzene, i.e.,  $1.39 \cdot 10^{-10}$  m. For example, the molecular structure formula of benzene is drawn as a regular hexagon and its length of edge is  $1.39 \cdot 10^{-10}$  m, so its surface is  $5.0197 \cdot 10^{-20}$  m<sup>2</sup>, i.e. the pseudo-conjugated system surface area of benzene is  $S_{\pi} = 5.0197 \cdot 10^{-20}$  m<sup>2</sup>. The molecular surface area of naphthalene is about twice that of benzene, its

surface area is equal to  $10.0394 \cdot 10^{-20} \text{ m}^2$ . For PAHs with a branched ring such as 1-phenylnaphthalene, we study only its main ring and consider the surface of naphthalene. According to the above method, we can get conjugated system surface area ( $S_\pi$ ) values for 100 PAHs (Table 1). In practice, the predicted results of such PAHs are in good agreement with the experimental values [25] (see Table 1 for details).

## 2.2. Quasi-length of carbon chain

As we know, there is a linear relationship between retention data and the number of carbons of a homologous series [2]. Here we define a parameter named quasi-length of carbon chain ( $N'$ ) in order to relate the retention index of PAHs directly. That is, for both the straight chain alkanes and PAHs having the same carbon atom number  $N_C$ , if the inner molecule polarizability index value of the straight chain alkane is  $\text{IMPI}_{\text{str}}$  [24] and that of PAHs is equal to  $\text{IMPI}_{\text{PAH}}$  [24], then the quasi-length of carbon chain is expressed as Eq. (1):

$$N' = [\text{IMPI}_{\text{str}}/\text{IMPI}_{\text{PAH}}]N_C \quad (1)$$

Here,  $N'$  stands for the quasi-length of the carbon chain, rather than the not existing real length of the carbon chain, for PAHs under inner molecular polarizability sense.

## 3. Results and discussion

The experimental values of retention index data ( $I$ ) of PAHs were taken from the literature [25]. The correlation of retention index data ( $I$ ) with the corresponding molecular structure parameters  $N'$  and  $S_\pi$  was carried out for the 100 compounds containing unsubstituted and substituted PAHs in Table 1, and the multiple linear regression (MLR) analysis equation was obtained as follows:

$$\begin{aligned} I &= -40.2643 + 23.1624N' + 6.2136S_\pi \\ F &= 6197.01, S = 7.0965, R = 0.9961, \\ n &= 100 \end{aligned} \quad (2)$$

In Eq. (2), the two parameters  $N'$  and  $S_\pi$  represent the contribution of the molecular polarizability effect

and the molecular shape and size to the retention index, respectively.

Eq. (2) demonstrates that the molecular structure parameters  $N'$  and  $S_\pi$  are not only applicable for the unsubstituted PAHs but also for the substituted PAHs. In our study the quasi-length of carbon chain ( $N'$ ), a molecular structure parameter based on the molecular polarizability theory [26], is employed in estimating the GC retention index for PAHs. We found that quasi-length of carbon chain ( $N'$ ) itself yielded a one-variable equation  $I = -78.58 + 34.44N'$  with a correlation coefficient of  $R = 0.9651$  and standard deviation of  $S = 20.97$  for 100 PAHs. This means that quasi-length of carbon chain ( $N'$ ) is an important descriptor for the influence of molecular structure on retention behavior for PAHs. We can also observe that the prediction model developed only by employing quasi-length of carbon chain ( $N'$ ) is not accurate enough for PAHs. As shown above in Eq. (2) and in Table 1, a novel descriptor,  $S_\pi$ , the pseudo-conjugated system surface area, is also introduced to reflect the molecular shape and size. The predicted results are in good agreement with the experimental values [25]. Another structural parameter, the number of rings in PAHs ( $S_c$ ) simpler than  $S_\pi$ , may alternatively be considered together with the parameter  $N'$ . A similar relationship with the retention index of PAHs is obtained:

$$\begin{aligned} I &= -31.1478 + 21.9534N' + 32.3837S_c \\ F &= 2895.05, S = 10.3369, R = 0.9914, \\ n &= 100 \end{aligned} \quad (3)$$

where the parameter  $S_c$  represents the contribution of the number of rings in PAHs to the retention index.

Table 1 lists 100 PAHs that have been considered in our study. This table includes the measured [25] retention index values together with two calculated retention indices, one from the two parameters  $N'$   $S_\pi$  equation and another from Eq. (3). By comparing Eqs. (2) and (3), it is clear that, in the calculation accuracy, the developed parameter  $S_\pi$  is better than parameter  $S_c$ , especially for estimating retention index of PAHs which contain unconjugated ring and aromatic substituted groups, such as benzo[ghi]-fluoranthene, triphenylene, 1-phenylnaphthalene and 9-phenylphenanthrene. Consequently, for solving the above problem, a predicting model for the capillary

Table 1  
The retention index data and molecular structure parameters of 100 PAHs

No.	Compound	$N'$	$S_{\pi}$	$I$		$I$ difference	$I$	
				observed <sup>a</sup>	Calculated <sup>b</sup>		Calculated <sup>c</sup>	difference
1	Naphthalene	7.83	10.0395	200.00	203.44	-3.44	205.54	-5.54
2	2-Methylnaphthalene	8.69	10.0395	218.14	223.47	-5.33	224.50	-6.36
3	Azulene	7.81	11.3938	219.95	211.40	8.55	205.12	14.83
4	1-Methylnaphthalene	8.67	10.0395	221.04	222.82	-1.78	223.89	-2.85
5	2-Ethylnaphthalene	9.63	10.0395	236.08	245.19	-9.11	245.06	-8.98
6	1-Ethylnaphthalene	9.59	10.0395	236.56	244.24	-7.68	244.16	-7.60
7	2,6-Dimethylnaphthalene	9.56	10.0395	237.58	243.43	-5.85	243.39	-5.81
8	2,7-Dimethylnaphthalene	9.55	10.0395	237.71	243.39	-5.68	243.36	-5.65
9	1,3-Dimethylnaphthalene	9.52	10.0395	240.25	242.55	-2.30	242.56	-2.31
10	1,7-Dimethylnaphthalene	9.52	10.0395	240.66	242.68	-2.02	242.68	-2.02
11	1,6-Dimethylnaphthalene	9.53	10.0395	240.72	242.75	-2.03	242.74	-2.02
12	2,3-Dimethylnaphthalene	9.53	10.0395	243.55	242.87	0.68	242.87	0.68
13	1,4-Dimethylnaphthalene	9.50	10.0395	243.57	242.04	1.53	242.08	1.49
14	1,5-Dimethylnaphthalene	9.50	10.0395	244.98	242.04	2.94	242.08	2.90
15	1,2-Dimethylnaphthalene	9.50	10.0395	246.49	242.23	4.26	242.26	4.23
16	1,8-Dimethylnaphthalene	9.49	10.0395	249.52	241.91	7.61	241.96	7.56
17	2,3,6-Trimethylnaphthalene	10.39	10.0395	263.31	262.73	0.58	261.66	1.65
18	2,3,5-Trimethylnaphthalene	10.36	10.0395	265.90	261.98	3.92	260.95	4.95
19	Phenanthrene	10.64	15.0592	300.00	299.79	0.21	299.63	0.37
20	Anthracene	10.70	15.0592	301.69	301.11	0.58	300.88	0.81
21	3-Methylphenanthrene	11.48	15.0592	319.46	319.32	0.14	318.12	1.34
22	2-Methylphenanthrene	11.49	15.0592	320.17	319.46	0.71	318.25	1.92
23	2-Methylphenanthrene	11.55	15.0592	321.57	320.79	0.78	319.51	2.06
24	9-Methylphenanthrene	11.45	15.0592	323.06	318.48	4.58	317.32	5.74
25	4-Methylphenanthrene	11.45	15.0592	323.17	318.48	4.69	317.32	5.85
26	1-Methylphenanthrene	11.46	15.0592	323.90	318.74	5.16	317.57	6.33
27	1-Methylanthracene	11.52	15.0592	323.33	320.07	3.26	318.82	4.51
28	9-Methylanthracene	11.48	15.0592	329.13	319.19	9.94	318.00	11.13
29	9-Ethylphenanthrene	12.34	15.0592	337.05	339.26	-2.21	336.99	0.06
30	2-Ethylphenanthrene	12.41	15.0592	337.50	340.76	-3.26	338.41	-0.91
31	3,6-Dimethylphenanthrene	12.32	15.0592	337.83	338.80	-0.97	336.55	1.28
32	2,7-Dimethylphenanthrene	12.34	15.0592	339.23	339.11	0.12	336.85	2.38
33	9-Isopropylphenanthrene	13.24	15.0592	345.78	360.08	-14.30	356.70	-10.92
34	1,8-Dimethylphenanthrene	12.27	15.0592	346.26	337.63	8.63	335.44	10.82
35	9- <i>n</i> -Propylphenanthrene	13.27	15.0592	350.30	360.64	-10.34	357.22	-6.92
36	9,10-Dimethylphenanthrene	12.25	15.0592	355.49	337.17	18.32	335.01	20.48
37	9-Methyl-10-ethylphenanthrene	13.88	15.0592	359.91	374.82	-14.91	370.65	-10.74
38	9,10-Dimethylphenanthrene	13.98	15.0592	367.97	377.30	-9.33	373.00	-5.03
39	1-Methyl-7-isopropylphenanthrene	14.07	15.0592	368.67	379.20	-10.53	374.79	-6.12
40	9,10-Dimethyl-3-ethylphenanthrene	13.97	15.0593	381.85	377.04	4.81	372.75	9.10
41	Benzo[ <i>ghi</i> ]fluoranthene	12.71	20.0790	389.60	378.94	10.66	409.82	-20.22
42	Benzo[ <i>c</i> ]phenanthrene	13.55	20.0790	391.39	398.30	-6.91	395.76	-4.37
43	Benzo[ <i>a</i> ]anthracene	13.51	20.0790	398.50	397.48	1.02	394.99	3.51
44	Chrysene	13.46	20.0790	400.00	396.21	3.79	393.78	6.22
45	Naphthacene	13.55	20.0790	408.30	398.50	9.80	395.95	12.35
46	11-Methylbenzo[ <i>a</i> ]anthracene	14.35	20.0790	412.72	416.99	-4.27	413.45	-0.73
47	2-Methylbenzo[ <i>a</i> ]anthracene	14.34	20.0790	413.78	416.78	-3.00	413.25	0.53
48	1-Methylbenzo[ <i>a</i> ]anthracene	14.30	20.0790	414.37	415.89	-1.52	412.42	1.95
49	9-Methylbenzo[ <i>a</i> ]anthracene	14.35	20.0790	416.50	416.96	-0.46	413.42	3.08
50	3-Methylbenzo[ <i>a</i> ]anthracene	14.35	20.0790	416.63	416.96	-0.33	413.42	3.21
51	8-Methylbenzo[ <i>a</i> ]anthracene	14.32	20.0790	417.56	416.22	1.34	412.72	4.84

Table 1. Continued

No.	Compound	$N'$	$S_{\pi}$	$I$ observed <sup>a</sup>	$I$ Calculated <sup>b</sup>	$I$ difference	$I$ Calculated <sup>c</sup>	$I$ difference
52	6-Methylbenzo[ <i>a</i> ]anthracene	14.30	20.0790	417.57	415.76	1.80	412.29	5.27
53	3-Methylchrysene	14.2	20.0790	418.10	415.49	2.61	412.03	6.07
54	5-Methylbenzo[ <i>a</i> ]anthracene	14.30	20.0790	418.72	415.89	2.83	412.42	6.30
55	2-Methylchrysene	14.29	20.0790	418.80	415.67	3.13	412.20	6.60
56	12-Methylbenzo[ <i>a</i> ]anthracene	14.26	20.0790	419.39	414.86	4.53	411.44	7.95
57	4-Methylbenzo[ <i>a</i> ]anthracene	14.32	20.0790	419.67	416.22	3.45	412.72	6.95
58	5-Methylchrysene	14.23	20.0790	419.68	414.24	5.44	410.85	8.83
59	6-Methylchrysene	14.24	20.0790	420.61	414.48	6.13	411.08	9.53
60	4-Methylchrysene	14.25	20.0790	420.83	414.61	6.22	411.20	9.63
61	1-Methylchrysene	14.26	20.0790	422.87	414.94	7.93	411.51	11.36
62	7-Methylbenzo[ <i>a</i> ]anthracene	14.27	20.0790	423.14	415.21	7.93	411.77	11.37
63	1,12-Dimethyl[ <i>a</i> ]anthracene	15.05	20.0790	436.82	433.28	3.54	428.87	7.95
64	7,12-Dimethyl[ <i>a</i> ]anthracene	15.02	20.0790	443.38	432.39	10.99	428.03	15.35
65	Pentacene	16.40	25.0986	486.81	495.71	-8.90	490.85	-4.04
66	Dibenzo[ <i>a,z</i> ]anthracene	16.22	25.0986	495.01	491.45	3.56	486.82	8.19
67	Dibenzo[ <i>a,h</i> ]anthracene	16.31	25.0986	495.45	493.67	1.78	488.93	6.52
68	Benzo[ <i>b</i> ]chrysene	16.31	25.0986	497.66	493.67	3.99	488.93	8.73
69	Picene	16.26	25.0986	500.00	492.45	7.55	487.77	12.23
70	1-Phenylnaphthalene	12.53	10.0395	315.19	312.32	2.87	340.98	-25.79
71	2-Phenylnaphthalene	12.61	10.0395	332.59	314.29	18.30	342.85	-10.26
72	9-Phenylanthracene	15.26	15.0592	396.38	406.84	-10.46	433.34	-36.96
73	9-Phenylphenanthrene	15.26	15.0592	406.90	406.84	0.06	433.34	-26.44
74	1-Phenylphenanthrene	15.29	15.0592	421.66	407.57	14.09	434.03	-12.37
75	9-Methyl-10-phenylphenanthrene	16.00	15.0592	417.16	424.13	-6.97	449.70	-32.54
76	Triphenylene	13.40	20.0790	400.00	394.94	5.06	392.58	7.42
77	1-Methyltriphenylene	14.19	20.0790	416.32	413.21	3.11	409.88	6.44
78	1,3-Dimethyltriphenylene	15.05	20.0790	432.32	433.18	-0.86	428.87	3.45
79	1,6,11-Trimethyltriphenylene	15.84	20.0790	446.24	451.42	-5.18	446.04	0.20
80	1,3,6,11-Tetramethyltriphenylene	16.64	20.0790	461.72	470.17	-8.45	463.79	-2.07
81	Acenaphthylene	8.84	14.2226	244.63	252.84	-8.21	260.10	-15.47
82	1-Methylacenaphthylene	9.66	14.2226	265.24	271.87	-6.63	278.12	-12.88
83	Fluoranthene	11.72	19.2423	344.01	350.78	-6.77	323.31	20.70
84	Pyrene	11.63	20.0790	351.22	353.90	-2.68	353.74	-2.52
85	4-Methylpyrene	12.43	20.0790	369.54	372.32	-2.78	371.17	-1.63
86	2-Methylpyrene	12.46	20.0790	370.15	373.05	-2.90	371.86	-1.71
87	1-Methylpyrene	12.44	20.0790	373.55	372.55	1.00	371.39	2.16
88	1-Ethylpyrene	13.32	20.0790	385.35	393.09	-7.74	390.83	-5.48
89	2,7-Dimethylpyrene	13.28	20.0790	386.34	392.18	-5.84	389.97	-3.63
90	Cyclopenta[ <i>cd</i> ]pyrene	12.67	24.2621	396.54	403.87	-7.33	408.84	-12.30
91	1- <i>n</i> -Butylpyrene	15.17	20.0790	414.87	435.94	-21.07	431.38	-16.51
92	Benzo[ <i>e</i> ]pyrene	14.37	25.1168	450.73	448.68	2.05	446.23	4.50
93	Benzo[ <i>a</i> ]pyrene	14.43	25.1168	453.44	450.07	3.37	447.55	5.89
94	Perylene	14.13	25.1168	456.22	443.23	12.99	441.07	15.15
95	Indeno[1,23- <i>cd</i> ]pyrene	15.42	29.2819	481.87	499.00	-17.13	501.77	-19.90
96	Dibenzo[ <i>def,mno</i> ]chrysene	15.40	30.1185	503.89	503.66	0.23	501.27	2.62
97	Benzo[ <i>ghi</i> ]perylene	15.13	30.1185	501.32	497.38	3.94	495.33	5.99
98	Benzo[ <i>j</i> ]fluoranthene	14.51	24.2621	440.92	446.68	-5.76	449.36	-8.44
99	Benzo[ <i>b</i> ]fluoranthene	14.51	24.2621	441.74	446.60	-4.86	449.29	-7.55
100	Benzo[ <i>k</i> ]fluoranthene	14.56	24.2621	442.56	447.87	-5.31	450.48	-7.92

<sup>a</sup> Taken from Ref. [25].<sup>b</sup> Calculated from Eq. (2).<sup>c</sup> Calculated from Eq. (3).

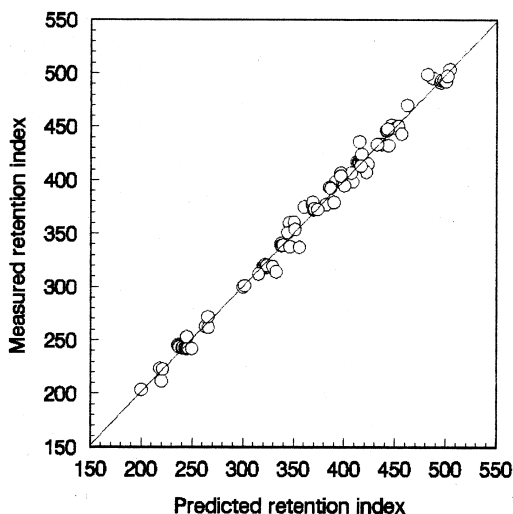


Fig. 1. Plot of predicted retention index vs. measured retention index for 100 PAHs.

GC retention index of PAHs is developed by the combination of the quasi-length of carbon chain ( $N'$ ) with pseudo-conjugated system surface ( $S_\pi$ ). Good results by MLR (in Eq. (2)) illustrate this predicting model is applicable to the estimation and prediction of GC retention indices for both unsubstituted and substituted PAHs (shown in Fig. 1). Also, the authors examined the cross-correlation between the two paired parameters and obtained the unexpected correlation coefficients of  $R=0.7885$  ( $N'=6.8705+0.3427S_\pi$ ) and  $0.8377$  ( $N'=6.3923+1.8203S_c$ ) for the  $N' \sim S_\pi$  and  $N' \sim S_c$  pairs, respectively. This demonstrates that  $N'$  cross-correlates less with  $S_\pi$  than with  $S_c$  and  $I$  relates better with  $N'$  and  $S_\pi$  than with  $N'$  and  $S_c$ . The results shown in Table 1 suggest that  $S_c$  should be an appropriate descriptor and  $S_\pi$  may be a better descriptor for expressing molecular structures of PAHs, to estimate and predict the capillary GC retention index.

#### 4. Conclusions

In this work, a new model developed in our laboratories for predicting capillary GC retention index by utilizing two parameters calculated directly from the molecular structure of PAHs is reported. Furthermore this study illustrates the influence of the

molecular polarizability effect and the structural shape on the relative retention behavior quantitatively by using quasi-length of carbon chain ( $N'$ ) and pseudo-conjugated system surface ( $S_\pi$ ). Further work is in progress.

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