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Journal of Chromatography A, 830 (1999) 491–496

JOURNAL OF CHROMATOGRAPHY A

Short communication

# Structure and retention of 2,4-dihydroxythiobenzanilides in a reversed-phase system

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Received 28 July 1998; received in revised form 15 October 1998; accepted 26 October 1998

**Abstract**

The effect of substitution of the N-amide system of 2,4-dihydroxythiobenzanilides on retention in a reversed-phase HPTLC system using methanol as an organic modifier was investigated. The linear relationship between $R_M$ and the volume fraction of organic solvent for all 60 tested compounds was obtained. These relationships allowed determination of the hydrophobicity indices, $R_{Mw}$, of these compounds using the extrapolation method. On the basis of analytical data obtained from analysis of UV–Vis and $^1$H NMR spectra the effect of substitution on the charge distribution in the amide system and the effect of this distribution on phase separation in relation to theoretical values is discussed. 

*Keywords:* Structure–retention relationships; Hydrophobicity parameters; 2,4-Dihydroxythiobenzanilides

## 1. Introduction

In a reversed-phase system with a chemically bonded stationary phase the retention of the compounds depends on the nature and concentration of the hydro–organic mobile phase [1,2]. Solvation effects play a very important role and the relationship between $R_M$ values and the modifier content depends significantly on the structure of the molecule [3,4]. This relation is described by the following linear equation [5–7]:

$$R_M = -S\varphi + R_{Mw} \quad (1)$$

where $R_{Mw}$ denotes the $R_M$ value of a given substance obtained with pure water as a mobile phase, $\varphi$ is the volume percentage of organic modifier and $S$ is a constant. This equation permits determination of the $R_{Mw}$ value i.e. the so-called hydrophobicity index by extrapolation, even for substances which do not migrate in water. It is a generally accepted way of expressing the lipophilic nature of molecules, while neglecting the selective interactions with a modifier [8–10].

For compounds with a relatively simple structure the presence of polar substituents causes a reduction of the lipophilic nature and in the reversed-phase system a weaker retention is observed compared with that observed for the unsubstituted system. Nonpolar substituents usually induce the opposite effect i.e. the increase of lipophilicity.

For the tested group of compounds, not only the nature of the substituent bonded with the ring and its phase affinity, but also the complex effect of this

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0021-9673/99/$ – see front matter 
PII: S0021-9673(98)00909-1

substituent on charge distribution in the amide system, active surface area and solubilization, must be taken into account. The presence of different substituents near to the thiocarbonyl group creates the probability of the appearance of two opposed electronic effects. On one hand, the inductive effect of the sulphur atom determined by the type of substitution may change the positive charge localised on carbon atom and the strength constant of carbon–sulphur bonds. On the other hand, the effect of the conjugation of the free electron pair of the nitrogen atom with the >C=S group leads to a decrease of bond order, and this decrease depends on the steric conditions limiting the coplanarity with the ring and the effect of electron density of this molecular fragment (Fig. 1).

Thus in individual compounds, the conjugation of the free electron pair of the nitrogen atom with a multiple bond manifests itself in the presence of delocalized electrons and different distribution of charges on the thioamide bond. In individual compounds, the formation of such preferred conformations and inhibition of rotation (because of mesomerism) cause the substituents bound to the nitrogen atom to be sterically non-equivalent. The fact that one of these substituents is localised in the *cis*- and another in the *trans*-position in relation to the sulphur atom, induces changes in local dipole moments as well as tendencies to association and orientation of the molecules (especially of water molecules) in the neighbourhood of the –C(=S)NH– moiety [11,12].

In the present work, the effect of substitution of the N-amide system — taking into account not only the phase preferences of individual compounds but also their effect on charge distribution in the amide system determined on the basis of electron (the shift of bands compared to the unsubstituted system) and $^1$H NMR (chemical shift of amide proton) — spectra has been investigated.

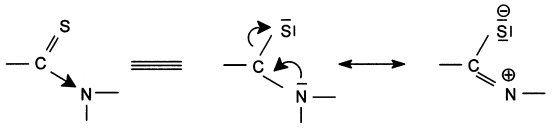


Fig. 1. Effect of conjugation of free electron pair of nitrogen atom with the =C=S group.

## 2. Experimental

### 2.1. Materials

The 2,4-dihydroxythiobenzanilides (Table 1) were synthesised at the Department of Chemistry, University of Agriculture, Lublin, Poland (new synthesis method; patent pending). Analytical-grade organic solvents were purchased from Baker (Philipsburg, NJ, USA) and from POCH (Lublin, Poland).

### 2.2. Procedure

TLC was performed on l0×10 cm pre-coated HPTLC plates of RP-8, $F_{254S}$ (Merck); 1-μl samples of the solutes (0.5 mg/ml in methanol) were spotted with a Desaga AS 30 applicator. The chromatograms were developed over a distance of 9.5 cm in horizontal 'sandwich' chambers of CAMAG for TLC. The chambers were saturated with the organic solvent vapour for 20 min. In the studies with the 2,4-dihydroxythiobenzanilides the water–methanol mixtures were used as the mobile phases. The concentration of organic modifier in the mobile phase ranged from 50 to 85%. All TLC measurements were performed at 21°C. Spots were visualised under UV light at 254 nm.

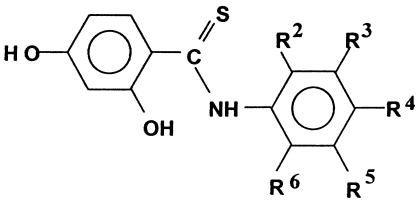
$^1$H NMR spectra were recorded with a FT-NMR Tesla BS 567 A spectrometer (100 mHz) using deuterated dimethylsulfoxide (DMSO) and acetone as the solvents. Chemical shifts are given relative to tetramethylsilane (TMS), and interpretation of the spectra is limited to the position of the amide proton.

UV–Vis spectra were recorded with a UV-160 Shimadzu spectrophotometer equipped with a QS 1.000 quartz cuvette using ethanol solutions. Interpretation of the spectra was limited to the evaluation of the nature of transitions occurring in the thiocarbonyl system and top definition of mutually correlated changes in electron density and probability of equilibrium conformational transitions.

## 3. Results and discussion

The results of HPTLC investigations are presented in the form of dependence of $R_M$ values on volume fraction of the organic modifier. For all tested

Table 1
Analytical data obtained for 2,4-dihydroxythiobenzanilides




| Compound | | $R_M = -S\varphi + R_{Mw}$ | | | | $\lambda_{max}$ (nm) | δ,–NHC(=S)– (ppm) |
|---|---|---|---|---|---|---|---|
| No. | Substituents | $S$ | $R_{Mw}$ | $n$ | $r$ | | |
| I | $R^2$–$R^6$ = H | 0.033 | 2.261 | 5 | 0.998 | 295, 326 | 11.2590 |
| II | $R^2$ = –$CH_3$ | 0.044 | 3.242 | 5 | 0.996 | 318 | 11.3115 |
| III | $R^3$ = –$CH_3$ | 0.043 | 3.210 | 5 | 0.999 | 327 | 11.2611 |
| IV | $R^4$ = –$CH_3$ | 0.043 | 3.280 | 5 | 0.998 | 295, 330 | 11.3013 |
| V | $R^2$, $R^4$ = –$CH_3$ | 0.046 | 3.571 | 5 | 0.997 | 288, 321 | 11.2810 |
| VI | $R^2$, $R^6$ = –$CH_3$ | 0.033 | 2.374 | 5 | 0.998 | 302, 327 | 11.6959 |
| VII | $R^4$ = –$CH_2CH(CH_3)CH_3$ | 0.064 | 5.363 | 4 | 0.998 | 302, 329 | 11.2834 |
| VIII | $R^2$ = –$CH_2OH$ | 0.056 | 4.660 | 5 | 0.999 | 290, 348.5 | 11.1583 |
| IX | $R^2$ = –F | 0.042 | 2.930 | 5 | 0.999 | 293, 331, 353 | 11.5787 |
| X | $R^3$ = –F | 0.043 | 3.241 | 5 | 0.978 | 296, 325 | 11.0560 |
| XI | $R^4$ = –F | 0.041 | 2.942 | 5 | 0.999 | 297, 329 | 11.2443 |
| XII | $R^2$, $R^4$ = –F | 0.038 | 2.850 | 5 | 0.999 | 292, 330 | 11.4590 |
| XIII | $R^2$ = –Cl | 0.037 | 2.741 | 5 | 0.998 | 292, 332 | 11.6710 |
| XIV | $R^3$ = –Cl | 0.047 | 3.660 | 5 | 0.999 | 283, 329 | 11.0100 |
| XV | $R^4$ = –Cl | 0.050 | 3.914 | 4 | 0.998 | 298, 327 | 11.1320 |
| XVI | $R^2$, $R^3$ = –Cl | 0.058 | 4.639 | 5 | 0.997 | 295, 336 | 11.7178 |
| XVII | $R^2$, $R^4$ = –Cl | 0.057 | 4.573 | 5 | 0.998 | 300, 338 | 11.6641 |
| XVIII | $R^2$, $R^5$ = –Cl | 0.056 | 4.473 | 5 | 0.999 | 291, 338 | [b] |
| XIX | $R^3$, $R^4$ = –Cl | 0.060 | 4.921 | 5 | 0.998 | 294, 328 | 11.0174 |
| XX | $R^3$–Cl, $R^4$ = –F | 0.061 | 4.733 | 5 | 0.999 | 292, 329, 375 | 11.1125 |
| XXI | $R^2$ = –Br | 0.051 | 3.750 | 5 | 0.999 | 292, 335.5 | 11.6007 |
| XXII | $R^3$ = –Br | 0.044 | 3.171 | 5 | 0.998 | 288, 337 | 10.7680[a] |
| XXIII | $R^4$ = –Br | 0.052 | 3.940 | 5 | 0.998 | 292, 329 | 11.1370 |
| XXIV | $R^3$ = –I | 0.057 | 4.411 | 5 | 0.999 | 292, 328 | 11.0930 |
| XXV | $R^4$ = –I | 0.056 | 4.402 | 5 | 0.996 | 284, 329 | 10.8370[a] |
| XXVI | $R^2$ = –$CH_3$, $R^5$ = F | 0.051 | 3.745 | 5 | 0.996 | 293, 334 | [b] |
| XXVII | $R^2$ = –$CH_3$, $R^3$ = Cl | 0.059 | 4.400 | 5 | 0.998 | 284, 333, 365 | 11.4152 |
| XXVIII | $R^2$ = –$CH_3$, $R^5$ = Cl | 0.059 | 4.491 | 5 | 0.978 | 287, 331 | 11.4005 |
| XXIX | $R^2$ = –Cl, $R^4$ = –$CH_3$ | 0.059 | 4.650 | 5 | 0.997 | 293, 330, 365 | 11.1247 |
| XXX | $R^2$ = –$CF_3$ | 0.042 | 3.041 | 5 | 0.998 | 293, 327 | 10.7416 |
| XXXI | $R^3$ = –$CF_3$ | 0.042 | 3.202 | 5 | 0.999 | 300, 330 | 11.0710 |
| XXXII | $R^2$ = –$OCH_3$ | 0.040 | 2.724 | 5 | 0.997 | 300, 334 | 10.6540 |
| XXXIII | $R^3$ = –$OCH_3$ | 0.037 | 2.553 | 5 | 0.998 | 300, 334 | 11.1810 |
| XXXIV | $R^4$ = –$OCH_3$ | 0.034 | 2.320 | 5 | 0.998 | 294, 328 | 11.3490 |
| XXXV | $R^2$ = –$OC_2H_5$ | 0.044 | 3.263 | 5 | 0.999 | 294, 328 | 11.6570 |
| XXXVI | $R^4$ = –$OC_2H_5$ | 0.039 | 2.810 | 5 | 0.978 | 300, 328 | 11.3371 |
| XXXVII | $R^2$ = –OH | 0.025 | 1.422 | 5 | 0.996 | 295, 326 | 10.1510 |
| XXXVIII | $R^3$ = –OH | 0.021 | 1.021 | 5 | 0.978 | 300, 328 | 9.1210[a] |
| XXXIX | $R^4$ = –OH | 0.019 | 0.763 | 5 | 0.998 | 292, 325 | 10.0560 |
| XL | $R^2$ = –$CH_3$, $R^4$ = –OH | 0.030 | 1.597 | 5 | 0.978 | 288.5, 325 | 11.1394 |
| XLI | $R^2$ = –OH, $R^4$ = –$CH_3$ | 0.032 | 2.141 | 5 | 0.998 | 294, 331 | 10.1387 |
| XLII | $R^2$ = –OH, $R^5$ = –$CH_3$ | 0.035 | 2.251 | 5 | 0.996 | 300, 323 | [b] |
| XLIII | $R^2$ = –OH, $R^5$ = –Cl | 0.048 | 3.200 | 5 | 0.999 | 337, 363 | 10.4828 |

(Continued overleaf)

Table 1. Continued

| Compound | | $R_M = -S\varphi + R_{Mw}$ | | | | $\lambda_{max}$ (nm) | δ,–NHC(=S)– (ppm) |
|---|---|---|---|---|---|---|---|
| No. | Substituents | $S$ | $R_{Mw}$ | $n$ | $r$ | | |
| XLIV | $R^2 = -CO_2H$ | 0.061 | 5.161 | 4 | 0.978 | 278, 326 | [c] |
| XLV | $R^3 = -CO_2H$ | 0.033 | 2.071 | 5 | 0.999 | 295, 327 | [c] |
| XLVI | $R^4 = -CO_2H$ | 0.050 | 3.732 | 5 | 0.989 | 298, 338 | 11.0762 |
| XLVII | $R^4 = -OH$, $R^3 = -CO_2H$ | 0.026 | 1.441 | 5 | 0.998 | 296, 323 | 11.2151 |
| XLVIII | $R^4 = -CO_2CH_3$ | 0.051 | 3.700 | 5 | 0.999 | 295, 338, 394 | 11.5348 |
| XLIX | $R^4 = -CO_2C_2H_5$ | 0.043 | 3.361 | 5 | 0.978 | 288, 337 | 11.0247 |
| L | $R^4 = -C(=O)CH_3$ | 0.038 | 2.620 | 5 | 0.999 | 294, 346 | 11.0320 |
| LI | $R^4 = -C(=O)C_2H_5$ | 0.052 | 3.812 | 5 | 0.998 | 296, 334 | 11.0197 |
| LII | $R^2 = -CN$ | 0.051 | 3.721 | 5 | 0.999 | 321, 364, 383 | 10.5683 |
| LIII | $R^3 = -CN$ | 0.046 | 3.222 | 5 | 0.999 | 306, 330, 375 | 11.1174 |
| LIV | $R^4 = -CN$ | 0.043 | 3.074 | 5 | 0.998 | 286, 339, 364 | 10.9441 |
| LV | $R^4 = -NO_2$ | 0.055 | 4.152 | 5 | 0.999 | 300, 346 | [c] |
| LVI | $R^2 = -OH$; $R^4 = -NO_2$ | 0.061 | 5.11 | 5 | 0.999 | 290, 327 | 10.5365 |
| LVII | $R^4 = -N(C_2H_5)C_2H_4OH$ | 0.036 | 2.334 | 5 | 0.978 | 287, 325 | 11.3322 |
| LVIII | $R^4 = -C(=O)NH_2$ | 0.026 | 1.412 | 5 | 0.999 | 300, 338 | 11.1150 |
| LIX | $R^4 = -C(=O)NHCH_2CO_2H$ | 0.025 | 1.230 | 5 | 0.998 | 298, 338 | 11.0030 |
| LX | $R^4 = -NHC(=O)CH_3$ | 0.026 | 1.361 | 4 | 0.996 | 297, 332.5 | 11.2614 |

[a] Spectrum $^1$H NMR in acetone.
[b] Interferant.
[c] Not occurring in spectrum.

substances linear regression equations were obtained (Table 1).

In the $^1$H NMR spectra the splitting of the signals corresponding to the –NH– group is not observed in spite of potential possibilities of the tautomeric rearrangement in –NHC(=S)–↔-N⋯C(SH)– although a rapid exchange leading to sharp singlets may not be excluded (Table 1). Only for the compounds III, VIII, XXVI, XLII and XLIV the conjugation and the changes in the nature of carbon–nitrogen bonds as well as the limitation of rotation (due to formation of preferred *cis*-structures [11,12]) probably cause the overlapping of some signals leading to the formation of an averaged group resembling a broader signal. Broader and illegible signals were observed in the spectra of the substances XLIV, XLV and LV.

The maintenance of thioamide forms in electron spectra (UV–Vis) is more typical for the compounds containing the substituents saturating N-aryl ring and indirectly also nitrogen atom (destabilisation of the system by dissipation of electron density on thiocarbonyl carbon atom) which corresponds to transfer of $\pi \rightarrow \pi^*$ spectral bands into the region of higher frequencies (Table 1). Interaction of substituents repulsing electrons (also π-electrons) mostly refers to the shift of equilibrium towards *cis*-imido-thiol structure formation.

From analysis of the course of $R_M(\varphi)$ straight lines it was observed that the system showed an increase of selectivity at higher contents of water in the mobile phase. This is due to the intensification of the hydrophobic interactions. In a reversed-phase system, in which the solvation effect plays a very important role, the retention is strongly dependent on molecular structures. In general, the presence of nonpolar substituents causes an increase of retention, which betokens in turn the intensification of the lipophilic nature of the compounds in comparison to the parent compound (I). This is valid for alkyl derivatives, especially for the compound (VII), where hyperconjugation effects stabilise the thiocarbonyl carbon atom (through maintaining the electron deficit on carbon atom) and cause the dissipation of a negative charge on the nitrogen atom. Atypical properties characterise the compound containing two methyl groups localised in the *ortho*-positions (VI). The crowding in the thiocarbonyl moiety caused by molecular geometry initiates the conformational transitions of rings to nonflat structures and the limitation of conjugation. Shortening of the carbon–nitrogen bond and expulsion of an electron pair from the

nitrogen atom makes a more acidic character of proton bonded to it as well as affinity of the compound to the polar phase. Halogens as substituents in general cause an increase in the lipophilic nature of the molecules. In the series of halogen derivatives compound X is characterised by a significantly higher lipophility. A fluorine atom localised in *meta*-position most weakly removes the electrons from the ring, which may be confirmed either by the changes of the nature of electron spectra or by relatively small shift of the signal corresponding to amide proton.

The presence of two fluorine atoms (XII) does not cause an increase of lipophilicity, perhaps owing to the higher acidity of the amide proton and the increase of affinity for water.

Differentiation of the lipophilicity of the isomeric monochloro-derivatives is accompanied by the changes in electron density and by the increase of acidity of the thiocarbonyl system. The most electron-withdrawing substituent in the *ortho*-position (XIII) affects –NH– bond polarisation to the greatest extent while the highest lipophilicity of compound XV may be connected with a resonance effect causing the increase of the negative charge on the nitrogen atom. In general it is expected that the lipophilic nature increases with the increase in the number of substituents and their molar mass. Thus the iodine derivatives show strong lipophilicity (compounds XXIV–XXV).

Halogen-methyl derivatives (XXVI–XXIX) and trifluoromethyl derivatives (XXX, XXXI) show higher lipophilicity in comparison to the unsubstituted system and this increase is in agreement with theoretical values ascribed to these substituents. Methoxy substituents (XXXII–XXXIV) in turn reduce slightly the lipophilic nature of the compounds in comparison to methyl derivatives, although it can be observed that there is an effect of the position of the methoxy group on the lipophilicity. From analytical data it results that the $-OCH_3$ group localised in *ortho*-position (XXXII) shows the ability to remove electrons, whereas the same group localised in *meta*- (XXXIII) and especially in *para*- (XXXIV) position shows an ability of opposite interactions. In these last isomers the induction interactions are gradually limited and the increase in mesomerism is accompanied by the increase of basicity of the

Fig. 2. Hyperconjugation effect induced by interactions of the $-OCH_3$ group localised in the *para*-position.

nitrogen atom and of affinity of the compounds for water (Fig. 2).

Analogous effects were observed also for ethoxy-derivatives (XXXV and XXXVI) although their lipophilicity is slightly greater in comparison to methoxy derivatives because of the extension of the hydrophobic chain.

The presence of hydroxy groups (XXXVII–XXXIX) causes a significant increase of affinity of these compounds for water. The decrease of lipophilicity is observed in the series of *ortho*-, *meta*-, *para*-isomers, although the functional group interaction in particular positions is different [13]. This may be additionally confirmed by the lowest lipophilicity of compound XL within the group of hydroxymethyl isomers (XL–XLII). The highest lipophilicity of the *ortho*-isomer (XXXVII) is caused by the possibility of intramolecular hydrogen bond formation.

The relatively high lipophilicity of chloro-hydroxy derivative (XLIII) may be connected with the changes of electron density in the –C(=S)NH– system, most probably due to mezomeric transition.

Unexpectedly high lipophilicity is shown in turn by carboxyl derivatives containing substituents in the *ortho*- and *para*-positions. This may be explained by the changes of electron density in the thioamide system caused by the strong electron-withdrawing properties of these groups. However, the highest lipophilicity of the *ortho*-isomer accounts for the possibility of intramolecular hydrogen bond formation.

Nontypical behaviours are shown with compounds XLVIII–LI. Their substituents conjugate with the aromatic system. In this way they increase the conjugation sequence chain (+M effect) and therefore limit the stabilisation of ground states. The batochromic effect of these substituents is as high as the tendency for disturbing of the π-electron system symmetry by the effective charge of oxygen atoms nuclei (L, LI). It is accompanied by a decrease of affinity for water.

The differentiated, although relatively high, lipophilicity of compounds with potentially electron-withdrawing –CN substituent [13] is caused by positive mesomeric and conjugation effects. It is confirmed by charges in electron density in the –C(=S)NH– group (UV–Vis spectrum), especially clear for the *ortho*-isomer (LII). At the same time, its highest lipophilicity and lowering of amide proton acidity (NMR spectrum) in a series of isomers can be accounted for by the possibility of intramolecular hydrogen bond forming.

A relatively high lipophilicity of a compound with an $-NO_2$ substituent (LV) can be accounted for by the possibility of mesomeric structures forming which makes positive partial charge on the amide nitrogen increase. This effect reflects the placement of the thioamide system band in UV–Vis spectrum (Table 1). In compound LVI, the presence of an additional electron-donating –OH group in the *ortho*- position causes an decrease in molecule polarity and an increase in lipophilicity. The alteration of electron density on the amide nitrogen atom and, in consequence, in the >C=S group, confirms the relative chypsochromic shift.

Compounds LVII–LX containing polar groups show the expected retention and are characterised by low lipophilicity.

Regression equations derived from individual compounds are characterised by different slopes, which means that the changes in eluent composition differently influences the $R_M$ values and that these slopes are connected not only with elution strength of organic modifier. The compounds containing the polar groups are characterised by very low *S* values (0.020–0.025) and those containing nonpolar groups — by high *S* values (0.04–0.06). Analogous trends were observed for pyridazine herbicides analysed by HPLC [14]. This is due to a different retention mechanism dependent on electron and steric interactions as well as on the lipophilic nature of substituents which may suggest the different nature of interactions between individual molecules and the components of mobile and stationary phases. The *S* values vary substantially depending on the position of the substituents which causes their effect on the charge distribution in the thiocarbonyl system to be different and therefore also the affinity for mobile phase. As a consequence the *S* value depends not only on elution strength of organic modifier but also on specific interactions between solute, mobile phase and stationary phase.

The results obtained suggest that the variation of the retention of 2,4-dihydroxythiobenzanilides in a reversed-phase system is determined mainly by the nature of the substituent, its electron structure and its phase preferences.

Nevertheless, there are observed different deviations resulting from the geometry of the system or from atypical behaviour of the substituents, which owing to inductive and mesomeric effects influences the charge distribution in the thiocarbonyl system, thus causing changes in its affinity for water or in its ability to local association, which influences in turn the lipophilicity of whole molecule.

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