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2D NMR, FT-IR, ESI MS studies and DFT, PM5 semiempirical calculations of new benzoic semduramicin anhydride and their complexes with selected monovalent cations

Radosław Pankiewicz *

Faculty of Chemistry, Adam Mickiewicz University in Poznań, Umultowska 89b, PL-61-614 Poznań, Poland

HIGHLIGHTS

- A new derivative of semduramicin (SemBz) was synthesized.
- The SemBz and its ability to form complexes was studied by the ESI-MS, DFT, 2D NMR and FT-IR.
- The fast fluctuations of Li^+ and Na^+, inside the cavity of the SemBz complexes were described.

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ABSTRACT

A new benzoic semduramicin anhydride (SemBz) was obtained. The new compound and its ability to form complexes with monovalent cations was studied by the ESI mass spectrometry, DFT, 2D NMR and FT-IR spectroscopic methods. The FT-IR spectra indicate that the K^+ cation in SemBz complex is localised. However, Li^+ and Na^+ cations in SemBz complexes undergoes fast fluctuations between oxygen atoms inside the cavity of the molecule. These observations were compared to the behavior of semduramicin salts with these cations. The structures of all salts and complexes obtained were calculated by the PM5 semiempirical method. All results are in agreement with the spectroscopic data and allow visualisation of SemBz structure and its complexes with monovalent cations.

1. Introduction

Ionophores are the compounds showing a unique ability of transferring ions from water solutions into a hydrophobic phase and transporting ions through the lipid cell membranes [1,2]. Ionophores are able to form host–guest complexes, they act as the hosts able to coordinate ions acting as guests and then transport them through the lipophilic membrane [3].

The molecule of ionophore is composed of a lipophilic skeleton and hydrophilic groups (—H, C═O, C—O—C) [4]. Thanks to this specific molecular structure, the conformational transformations that can take place upon complexation confine the ion in a hydrophilic cage while the lipophilic fragment is directed outwards [5,6]. In this way the ionophore can dilute the charged ion inside the lipid membrane [7]. The mechanism of transportation is as follows: the ionophore (host) molecule at the interface in the hydrophobic phase binds an ion (guest) and the complex diffuses through the lipid membrane to its opposite surface at which the complex breaks down and the ion is released into the water phase. The empty ionophore diffuses to the opposite surface of the membrane and the cycle is repeated until a state of equilibrium is reached [8,9].

Specific chemical affinity not only to ions but also to neutral molecules, makes the ionophores attractive as chemical receptors. Moreover, as has been established in our studies with lasalocid, this chemical affinity can be easily modified by attachment of oxaalkyl chains or other molecules (in particular those including oxygen atoms in their structure) to the ionophore molecule [10,11]. The attachment of alkyl chains has practically no effect on the complexing ability and substantially improves the solubility of the ionophore and the host–guest ionophore complex in the lipid layers. The modification affects both chemical and microbiological properties of the ionophore, i.e. the bactericidal properties can be weakened or strengthened depending on the chain length [12].

Semduramicin belongs to rather poorly examined antibiotics. It has been approved for veterinary use both by FDA (Food and Drug

* Tel.: +48 618291488.
E-mail address: radek@px.pl

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Administration of the US) and the EMEA (European Medicines Agency). This pharmaceutical ingredient is active for the prevention of coccidiosis in chicken but as an antibiotic, its pharmacological activity is probably related to ion transport characteristics of the molecule. Moreover, it has a forked structure made of two pyrane rings attached to the furan ring from the main part of the molecule [13]. The complex structure of the molecule and a potential dense network of hydrogen bonds could significantly affect the mode of complexation of alkali metal cations, not necessarily preferring those of a greater ionic radius.

2. Results and discussion

Benzoic semduramicin anhydride (SemBz) (Scheme 1) was synthesised from semduramicin sodium salt (SemNa) according to the following method. To obtain pure product with high yield the reaction was carried out in mild condition (room temperature) and without access of daylight. During the reaction, small samples were taken for testing the reaction progress by HPLC analysis. The chromatograms, measured at $\lambda = 240$ nm (Fig. 1) shows clearly the loss of a signal assigned to benzoyl chloride (Bz) (0.767 min.) and the rise of a new signal of SemBz (5.125 min.). SemNa was not visible in these chromatograms because it did not absorb in the UV–Vis range. The band of maximum absorption was shifted from $\lambda = 248$ nm (Bz) to $\lambda = 240$ nm for SemBz. The synthesised compound collected with the leak from the chromatographic column (from 4.75 to 5.5 min.) was subjected to MS analysis. The MS spectra showed signals of a molecular ion at $m/z = 999$ assigned to complex of SemBz with Na^+ cation, which confirmed that it was the product obtained.

In order to resolve the structure of SemBz it was subjected to NMR study, the NMR spectra of SemNa was studied as well. To obtain full assignments of ^1H and ^{13}C, the 2D NMR techniques, ^1H–^1H COSY, ^1H–^{13}C HSQC and ^1H–^{13}C HMBC were used. The data are given in Table 1. The ^1H and ^{13}C spectra of SemNa were very similar to literature data [14,15]. The spectra of SemBz shows distinct parts corresponding to semduramicin and benzoyl chloride. Analysis of ^{13}C NMR spectra of SemNa and SemBz does not show significant differences in the shifts of the signals assigned to C(5), C(11) and C(29), which are the potential sites of benzoyl chloride attachment, which proves that the OH groups at these atoms were not involved in the reaction. Instead, C(1) atom was shifted from 179.12 ppm (SemNa) to 168.70 (SemBz), which strongly suggested the formation of anhydride bond and finally confirmed the structure of the new compound. The other signals appearing in the ^1H as well as ^{13}C NMR spectra of these compounds assigned to semduramicin are only slightly different from the signals noted in the spectra of SemNa. This fact suggest that the new compound has a similar pseudocyclic structure stabilised by intramolecular hydrogen bonds. Furthermore, the appearance of H(3′) proton and C(3′) carbon signals in the spectra of the SemBz, as two

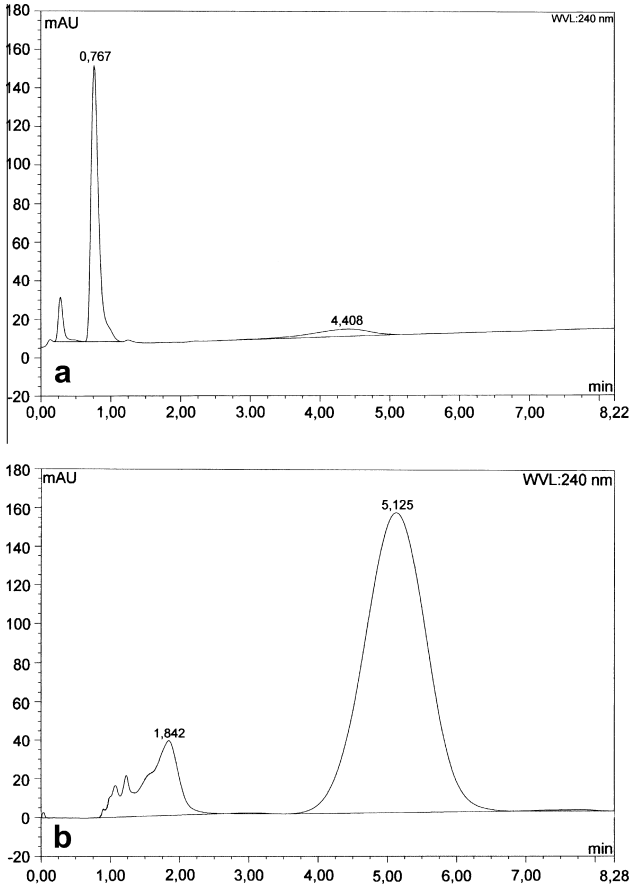
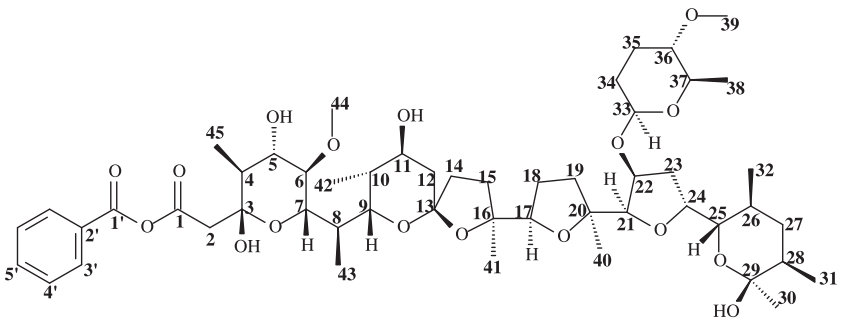


Fig. 1. HPLC chromatograms: (a) measured immediately after the reaction has begun and (b) measured after 25 h (end of reaction).

separate signals at 8.05, 8.85 ppm and 129.56, 131.23 ppm, respectively, demonstrates that the rotation about the C(1′)–C(2′) single bonds is prevented after the pseudoring formation. To visualize the structure of the new semduramicin derivative and to analyse the conformation of the molecular chain, the DFT calculation was performed using GAUSSIAN 03 package. The structure of anhydride calculated by DFT methods is given in Fig. 1.

SemBz has a pseudo-cyclic structure which is formed thanks to the formation of a hydrogen bond of head-to-tail type between the carboxyl group and the hydroxyl group attached to the last pyrane ring. The structure is also stabilised by two intramolecular hydrogen bonds between O(5)H group and C(1)–O group and between O(11)H group and C(1′)=O.

The theoretical ^1H and ^{13}C NMR spectra were also computed using DFT methods. All data obtained (Table 1) were in very good



Scheme 1. The structure and atom numbering of SemBz.

Table 1
^{1}H NMR and ^{13}C NMR chemical shifts.

No. Atom	δ_H and δ_C (ppm)					
	SemNa		SemBz			
	C	H	C	H	Calculated C	Calculated H
1	179.12	–	168.70	–	172.41	
2	45.37	2.17;2.48	46.02	2.54; 2.84	43.08	1.94;2.23
3	97.74	–	98.45	–	99.57	–
4	44.94	1.48	46.01	1.46	44.00	1.28
5	74.80	3.72	75.47	3.43	76.94	3.92
6	82.02	3.11	82.56	2.94	73.90	3.28
7	66.83	3.73	64.15	3.54	63.96	4.45
8	33.60	1.98	35.09	2.15	36.85	2.22
9	67.66	4.24	68.50	4.01	67.57	3.85
10	33.45	1.81	35.18	1.84	40.10	2.02
11	70.12	3.91	69.44	4.15	72.55	3.73
12	33.79	1.62;1.90	32.47	1.64;1.94	31.40	1.87;2.83
13	107.47	–	108.11	–	105.96	–
14	38.94	1.73;1.97	39.44	1.70;1.84	42.48	1.58;1.86
15	33.16	1.76;1.98	34.88	1.83;1.96	36.37	1.59;2.31
16	84.56	–	85.26	–	83.64	–
17	82.35	3.53	83.05	3.30	83.40	3.71
18	26.86	1.47;1.71	26.05	1.2;1.7	30.47	1.50.2.07
19	32.29	1.50;2.41	33.71	1.44;2.32	36.69	1.48;2.67
20	84.20	–	85.11	–	79.92	–
21	86.99	4.03	87.45	3.86	86.81	3.47
22	80.92	4.16	82.01	4.14	75.49	4.58
23	32.50	2.22	33.38	2.22	37.09	1.68
24	80.26	4.49	80.65	4.90	81.55	4.25
25	73.07	3.93	71.60	3.68	79.88	4.19
26	32.88	1.25	34.44	1.31	35.92	1.57
27	36.48	1.33;1.43	37.66	1.26;1.35	35.51	1.44;1.49
28	39.88	1.44	39.87	1.52	39.09	2.04
29	96.94	–	97.80	–	96.16	–
30	26.09	1.30	25.70	1.30	23.28	1.34
31	17.00	0.91	17.04	0.84	18.22	1.04
32	17.50	0.88	17.66	0.91	23.35	1.06
33	103.23	4.41	103.89	4.48	97.89	4.57
34	30.57	1.53;1.79	31.12	1.38;1.81	31.22	1.73;1.91
35	26.93	1.31;2.18	27.35	1.24;2.15	27.50	1.65;2.17
36	79.90	2.81	80.75	2.76	78.66	3.18
37	74.44	3.31	75.00	3.28	76.38	3.55
38	18.39	1.25	18.48	1.17	18.44	1.30
39	56.84	3.36	56.626	3.28	53.58	3.58
40	23.25	1.12	23.60	1.12	30.65	1.45
41	27.59	1.49	27.70	1.15	28.96	1.79
42	10.45	0.85	10.67	0.80	11.22	1.09
43	11.03	1.08	10.80	0.97	10.63	1.11
44	59.09	3.53	60.49	3.49	52.42	3.52
45	12.09	1.04	12.27	1.05	15.87	0.88
1′	–	–	163.73	–	163.91	–
2′	–	–	132.65	–	128.26	–
3′	–	–	129.56;131.23	8.05;8.85	124.29;128.71	8.35;8.94
4′	–	–	129.97	7.55	127.91	7.23
5′	–	–	135.59	7.71	135.43	7.31

agreement with experimental values. The correlation coefficient was $R^2 = 0.98$ for ^{13}C and $R^2 = 0.96$ for ^{1}H NMR.

To study the complexation abilities of the new compound, two series of complexes with monovalent cations was prepared: SemLi, SemNa, SemK and SemBzLi, SemBzNa, SemBzK. All the complexes were studied by FT-IR in the mid-infrared region. The FT-IR spectra of semduramicin complexes are given in Fig. 2, while the FT-IR spectra of anhydride complexes are given in Fig. 3. In FT-IR spectrum of SemNa (Fig. 2, dashed line), the most characteristic are the bands assigned to the ν(OH) vibrations of OH groups at 3300 cm^{-1} and at 3422 cm^{-1} as well as the band assigned to the ν(C=O) vibrations, from carboxyl group, at 1593 cm^{-1}. The appearance of two bands assigned to the ν(OH) strongly suggest the presence of two groups of hydrogen bonds of different strength. In the spectrum of SemK (Fig. 2, dashed-dotted line) there are two bands with maxima at ca. 3242 and 3409 cm^{-1} and a new band appearing as a shoulder at about 3348 cm^{-1}, indicating the change in the involvement of all OH groups in intramolecular hydrogen bonds relative to those in the structure of SemNa. The appearance of three bands strongly suggest that K^+ cation is relatively well localised between the oxygen atoms and therefore the K^+ polarizability is relatively lower than of Na^+ cation in the SemNa structure. The position of the band assigned to the ν(C=O) vibrations at 1593 cm^{-1}, in the spectrum of SemK is almost unchanged (Fig. 2b) in comparison to that in the SemNa spectrum, demonstrating that the oxygen atom from the C=O carboxyl group is engaged in the complexation process to the same extent. In the spectrum of SemLi (Fig. 2, solid line) there is only one broad band, assigned to the ν(OH), with a maximum at about 3400 cm^{-1}. The appearance of this one band means that all hydrogen bonds in this molecule have similar strengths. This averaging of interaction strength suggest that the Li^+ cation undergoes fast fluctuations

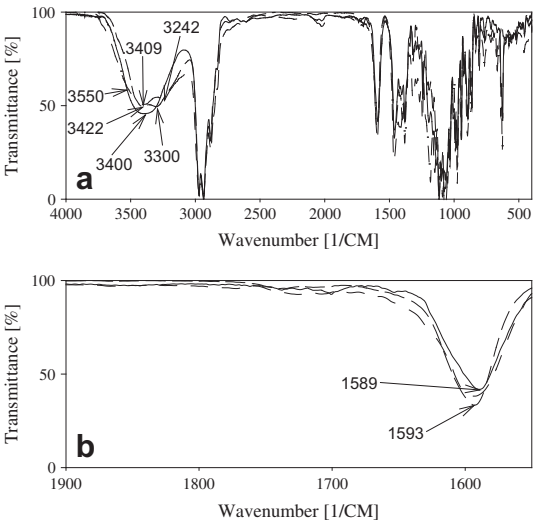


Fig. 2. The FT-IR spectra of Sem complexes with cations: (—)Li^+, (——)Na^+, (-●●-)K^+ in KBr tab at range: (a) 4000–400 cm^{-1} and (b) 1900–1550 cm^{-1}.

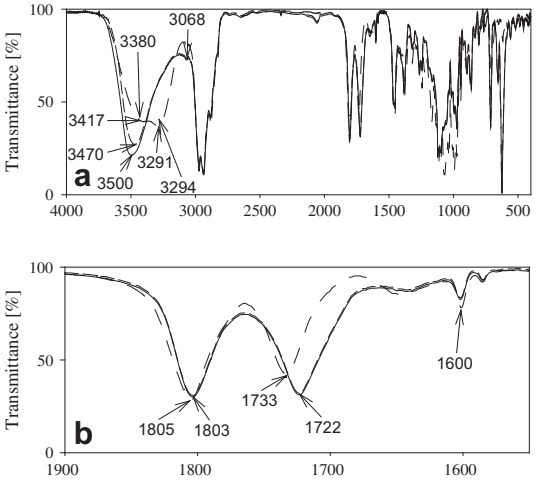


Fig. 3. The FT-IR spectra of SemBz (●●●●) and its complexes with cations: (—)Li^+, (——)Na+, (-●●-)K^+ in KBr tab in range: (a) 4000–400 cm^{-1} and (b) 1900–1550 cm^{-1}.

between oxygen atoms inside the cavity of the ionophore. The high Li^+ cation polarizability is in agreement with my previous studies [16]. The band assigned to the ν(C=O) vibrations is slightly moved to 1589 cm^{-1}, which informs about the engagement of oxygen atom from carboxyl group in the complexation process of Li^+ cation. Similar relations for calixarenes have been reported by another research group [17,18].

In the FT-IR spectrum of SemBz (Fig. 3b, dotted line), the most important are the two asymmetric bands assigned to the ν(C=O) vibrations of the anhydride group at 1733 cm^{-1} and at 1805 cm^{-1}. In this region there is also a very weak band assigned to the ν(C=O) at 1600 cm^{-1} coming from unreacted semduramicin. In the same spectrum at higher wavelength (Fig. 3), there are the bands assigned to the ν(OH) vibrations of OH groups at 3294 cm^{-1} and at 3380 cm^{-1} and a band assigned to the ν(CH) vibrations of the aromatic ring at 3068 cm^{-1}. In the spectrum of SemBzK (Fig. 3, dashed-dotted line) there are two bands with maxima at 3291 and 3417 cm^{-1}. The bands assigned to the ν(C=O) vibrations of the anhydride group are found at 1733 cm^{-1} and at 1805 cm^{-1}. This spectrum is only slightly different from that of SemBz, which suggests that K^+ cation is localised and OH groups are only little engaged in the complexation process. The spectrum of SemBzNa (Fig. 3, dashed line) shows only one broad band, assigned to the ν(OH), with a maximum at about 3470 cm^{-1}. This fact implies that all hydrogen bonds in this molecule have similar strengths. These observations suggest that the Na^+ cation undergoes fast fluctuations between the oxygen atoms inside the cavity of SemBz, which is in contrast to semduramicin in which Na^+ cation is localised. A possible reason is that SemBz is a neutral molecule and forms a little bigger pseudoring. In this spectrum at lower wavelength there are the two asymmetric bands assigned to the ν(C=O) vibrations of the anhydride group at 1722 cm^{-1} and at 1803 cm^{-1}. The shift of the band at 1722 cm^{-1} in comparison to its position at 1733 cm^{-1} in the spectrum of SemBzK suggests that the anhydride group is involved in the complexation of Na^+ cation. In the spectrum of SemBzLi (Fig. 3, solid line) there is a similar situation as for SemBzNa. There is only one broad band, assigned to the ν(OH), with a maximum at about 3500 cm^{-1} and two bands assigned to the ν(C=O) vibrations of the anhydride group at 1722 cm^{-1} and at 1803 cm^{-1}. These data strongly suggest that Li^+ cation has slightly higher polarizability than Na^+ cation in the SemBz cavity. The oxygen atoms from the anhydride group are involved in the complexation of Li^+ cation to the same extent as in that of Na^+ cation.

The ESI spectrum of a mixture of Li^+, Na^+, K^+ cations with 20% of the equivalent concentration of semduramicin measured at cv = 10 V, is shown in Fig. 4. The spectrum shows only three characteristic signals at m/z = 879, m/z = 895 and m/z = 911 assigned to the 1:1 protonated semduramicin salts with Li^+, Na^+ and K^+ cations, respectively. The intensity of the SemLi signal is slightly higher than that of the SemNa and SemK signals indicating that semduramicin forms salts readily with all cations studied, slightly preferring Li^+ cations.

The same procedure was applied for SemBz. The spectrum is shown in Fig. 5. There are three characteristic signals at m/z = 983, m/z = 999 and m/z = 1015 assigned to the 1:1 complexes of semduramicin with Li^+, Na^+ and K^+ cations, respectively. The intensity of the SemBzNa signal is higher than that of the SemBzLi and SemBzK signals, which are almost the same, indicating that SemBz forms prefer complex formation with Na^+ cations.

To verify the ESI–MS data, the semiempirical computation (PM5) of heats of complexation was performed. The data obtained are collected in Table 2.

The heat of complexation is (HOF (heat of formation) of a complex) – (HOF of isolated ligand + HOF of isolated cation). The lower the heat of complexation the more preferred salt or complex formation. The obtained data show that SemLi is the most preferred salt and SemBzNa is the most preferred complex. These fact are in very good agreement with the ESI–MS data.

The exemplary structures of SemBzLi, SemBzNa and SemBzK calculated by PM5 method are given in Figs. 6–8, respectively. All figures show that SemBz complexes form pseudo-cyclic structures

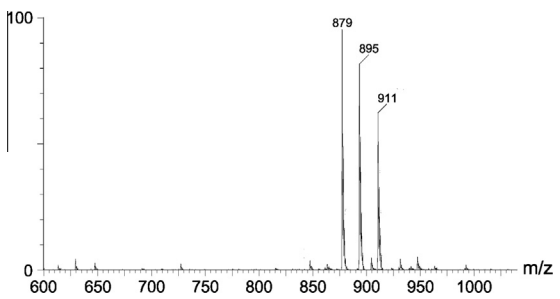


Fig. 4. ESI spectrum of the mixture of cation perchlorates ($LiClO_4$, $NaClO_4$, $KClO_4$) with the 20% of the equivalent amount of semduramicin.

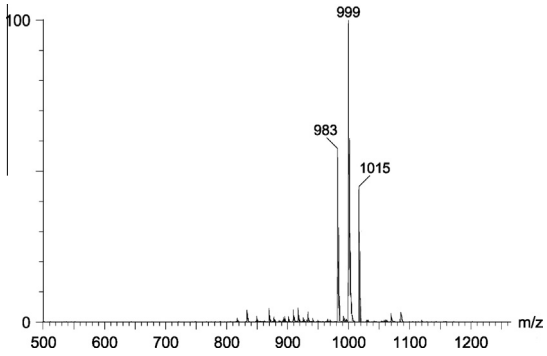


Fig. 5. ESI spectrum of the mixture of cation perchlorates ($LiClO_4$, $NaClO_4$, $KClO_4$) with the 20% of the equivalent amount of SemBz.

Table 2
Calculated by PM5 method heats of complexation [kJ/mol].

Cation	dHOF of salinonomycin	dHOF of salinomycin derivative
Li	−373.20	−226.10
Na	−349.46	−359.93
K	−302.28	−214.20

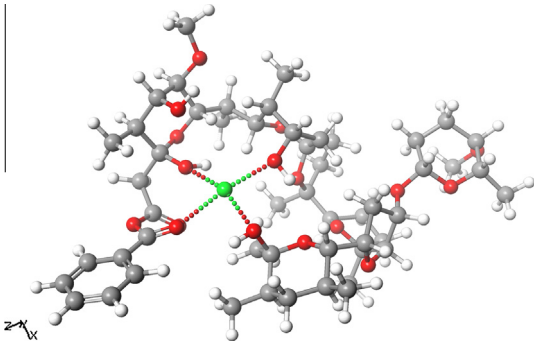


Fig. 6. Calculated structure (PM5) of the complex of SemBz with Li^+ cation.

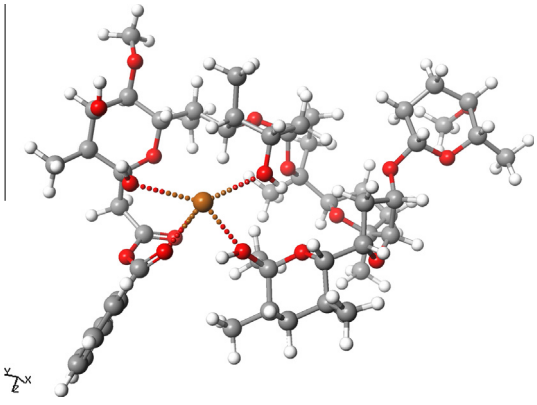


Fig. 7. Calculated structure (PM5) of the complex of SemBz with Na^+ cation.

with cations capped in the molecule cavity. The structures of the complexes with Li^+ and Na^+ cations are shown in local energetic minima. These cations are coordinated by oxygen atoms from hydroxyl and anhydride groups. In the SemBzK structure, K^+ cation is coordinated mostly by oxygen atoms from ether groups in the other part of molecule. These data are in good agreement with the conclusions following from FT-IR measurement.

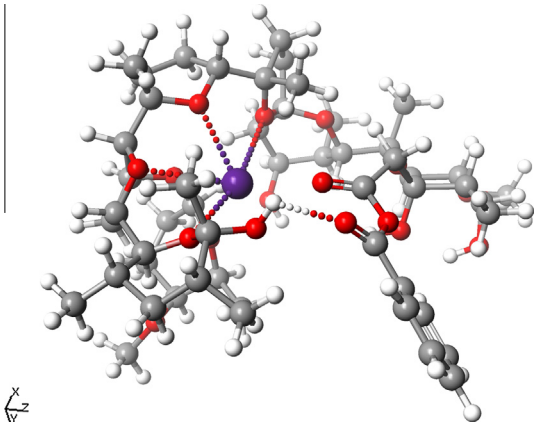


Fig. 8. Calculated structure (PM5) of the complex of SemBz with K^+ cation.

3. Experimental section

3.1. The synthesis of semduramicin derivative (SemBz)

The commercially available semduramicin sodium salt (150 mg) was dissolved in 10 mL THF and 23.35 μL benzoyl chloride was added. The reaction mixture was vigorously stirred in room temperature without access of light for 25 h. The reaction progress was monitored by HPLC analysis. To obtain pure product the solution was filtered and transferred to a chromatographic column filled with silica gel (Fluka type 60). The column was first eluted with hexane and then with a hexane–acetone (3:1) solvent mixture. The combined fractions were evaporated under reduced pressure. The yield of oily slightly yellow benzoic semduramicin anhydride (SemBz) was 82%.

3.2. Preparations of complexes

For preparations of the complexes the following compounds were used: $LiClO_4$, $NaClO_4$, $KClO_4$, (Aldrich), acetonitrile (Fluka) additionally dried under vacuum. The solutions of the complexes were obtained by dissolving of the respective salts and the Sem or SemBz in acetonitrile at the 5:1 ratio. Acetonitrile was of spectroscopic grade and was dried over a 3 Å molecular sieve. All preparations and transfers of solutions were carried out in a carefully dried glovebox under nitrogen atmosphere.

3.3. Elementary analysis

The elementary analysis was carried out on Perkin Elmer CHN 240. For the semduramicin derivative (SemBz) ($C_{52}H_{80}O_{17}$) (calculated: C 63.91% H 8.25%, found: C 64.13%; H 8.29%).

3.4. HPLC measurement

HPLC separations were obtained in a Dionex ASI-100 equipped with a P680 HPLC pump using Thermo Hypersil GOLD 150 × 4.6 column and as well as a Dionex PDA-100 Photodiode Array Detector. The flow rate was 2 ml/min with injection volumes of about 20 μL. As the mobile phase, we used mixtures of acetonitrile and water in various ratios depending on particular separation and changed during analysis from 60:40 to 70:30 acetonitrile/water. The analytical wavelength was 240 nm.

3.5. ESI–MS measurement

The ESI (electron spray ionization) mass spectra were recorded on a Waters/Micromass (Manchester, UK) ZQ mass spectrometer equipped with a Harvard Apparatus syringe pump. The measurements were performed for two types of samples: a) the solutions of Sem or SemBz (5×10^{-4} mol dm^{-3}) with a mixture of Li^+, Na^+, K^+ and b) the solutions of Sem or SemBz (5×10^{-4} mol dm^{-3}) with Li^+, Na^+, K^+ cations, taken separately. The samples were infused into the ESI source using a Harvard pump at the flow rate 20 μ dm^3 min^{-1}. The ESI source potentials were: capillary 3 kV, lens 0.5 kV, extractor 4 V. In the standard ESI mass spectra the cone voltage was 10 V. The source temperature was 120 °C and the desolvation temperature was 300 °C. Nitrogen was used as the nebulizing and dessolvation gas at flow-rates of 100 and 300 dm^3 h^{-1}, respectively.

3.6. NMR measurement

The NMR spectra of SemNa and SemBz (0.02 mol/l) were recorded at 295 K in CD_3CN solution using a Bruker Avance 600 MHz spectrometer. ^{1}H and ^{13}C NMR signals were assigned using two-dimensional ^{1}H–^{1}H COSY, ^{1}H–^{13}C HSQC and ^{1}H–^{13}C HMBC as well as 1H–1H NOESY and 2D COSY spectra were acquired in the magnitude mode with the gradient selection method and with spectral widths of 6562 Hz for both dimensions.

3.7. FT-IR measurements

All samples were measured in 200 mg KBr tabs. The mass of samples was 1 mg per tab. The FT–IR spectra were recorded, using a IFS 66/s FT-IR spectrophotometer from Bruker, equipped with an MCT detector (125 scans, resolution 2 cm^{-1}).

3.8. Calculation procedure

Semi-empirical calculations (PM5) [19] of the heat of formation (HOF) and the geometric optimization were performed using the Scigress 2.1.0 program [20]. The DFT calculations were performed using the GAUSSIAN 03 package [21]. The geometries were optimized according to Becke's three parameters hybrid method with the Lee, Yang and Parr correlation functional (B3LYP) [22] and 6-31G(d) basis set. The NMR was calculated using GIAO method in the same basis set.

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