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UV light absorption parameters of the pathobiologically implicated bilirubin oxidation products, MVM, BOX A, and BOX B

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ABSTRACT

The formation of the bilirubin oxidation products (BOXes), BOX A ([4-methyl-5-oxo-3-vinyl-(1,5-dihydropyrrol-2-ylidene)acetamide]) and BOX B (3-methyl-5-oxo-4-vinyl-(1,5-dihydropyrrol-2-ylidene)acetamide), as well as MVM (4-methyl-3-vinylmaleimide) were synthesized by oxidation of bilirubin with H_2O_2 without and with $FeCl_3$, respectively. Compound identity was confirmed with NMR and mass spectrometry (MS; less than 1 ppm, tandem MS up to MS^4). UV absorption profiles, including λ_{max}, and extinction coefficient (ε; estimated using NMR) for BOX A, BOX B, and MVM in H_2O, 15% CH_3CN plus 10 mM CF_3CO_2H, CH_3CN, $CHCl_3$, CH_2Cl_2, and 0.9% NaCl were determined. At longer wavelengths, λ_{max}'s for 1) BOX A were little affected by the solvent, ranging from 295–297 nm; 2) BOX B, less polar solvent yielded λ_{max}'s of lower wavelength, with values ranging from 308–313 nm, and 3) MVM, less polar solvent yielded λ_{max}'s of higher wavelength, with values ranging from 318–327 nm. Estimated ε's for BOX A and BOX B were approximately 5- to 10-fold greater than for MVM.

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Specifications Table

Subject area	*Chemistry*
More specific subject area	*Bilirubin oxidation products detection*
Type of data	*Table, figure*
How data was acquired	*NMR, mass spectroscopy, UV spectrometry, HPLC*
Data format	*Raw, analyzed*
Experimental factors	*Oxidation of bilirubin, extraction with chloroform*
Experimental features	*Bilirubin oxidation products BOX A, BOX B, and MVM were synthesized by the oxidation of bilirubin, purified by HPLC and UV absorption profiles and extinction coefficients determined*
Data source location	*Cincinnati, OH USA*
Data accessibility	*The data are accessible within the article.*

Value of the data

- First report (to our knowledge) of UV absorption profile, including λ_{max}, of MVM in solvents relevant to detection in biologic/pathobiologic samples.
- Comparison of UV absorption profiles of MVM with BOX A and BOX B.
- First report (to our knowledge) of BOX B extinction coefficient (ε; estimated using NMR), along with comparison to BOX A and MVM estimated ε's in different solvents, along with MS at less than 1 ppm and tandem MS up to MS^4.
- Novel methodology to increase MVM yield through $FeCl_3$ inclusion in oxidation reaction mixture.
- Data will potentially assist in the detection and determination of these BOXes in pathobiologies associated with elevated bilirubin.

1. Data

The bilirubin oxidation products (BOXes), MVM (4-methyl-3-vinylmaleimide), along with BOX A ([4-methyl-5-oxo-3-vinyl-(1,5-dihydropyrrol-2-ylidene)acetamide]) and BOX B (3-methyl-5-oxo-4-vinyl-(1,5-dihydropyrrol-2-ylidene)acetamide), have been implicated in the deleterious effects associated with subarachnoid hemorrhage (SAH; [1-5]). The detection method utilized to determine the presence of these compounds is UV absorption associated with reversed phase-HPLC [1]. However, reports (to our knowledge) of the UV absorption profile and/or λ_{max} of MVM have not been reported for the solvent utilized in their detection (H_2O/CH_3CN), but are limited to CH_3OH [6,7]. Also, reports of these absorption characteristics are limited (to our knowledge) for BOX A to H_2O and CH_3CN, and for BOX B to H_2O [1,8]. Further, extinction coefficients (ε) for MVM and BOX A are limited (to our knowledge) to CH_3OH and CH_3CN, respectively [6,7,9], and are lacking for BOX B. Thus, it is anticipated that the present data will assist in the detection and quantitative determination of BOXes levels in biologic samples from SAH, as well as in other pathobiologies associated with elevated bilirubin.

1.1. UV absorption

UV absorption spectra of BOX A, BOX B and MVM were determined in $CHCl_3$, CH_2Cl_2, CH_3CN, 15% CH_3CN plus 10 mM CF_3CO_2H, H_2O, and 0.9% NaCl (Fig. 1, Table 1). At longer wavelengths, BOX A λ_{max}'s were little affected by the solvent, ranging from 295–297 nm (Fig. 1, Table 1). With BOX B, less polar solvent yielded λ_{max}'s of lower wavelength, with values ranging from 308–313 nm (Fig. 1, Table 1). With MVM, less polar solvent yielded λ_{max}'s of higher wavelength, with values ranging from 318–327 nm (Fig. 1, Table 1). These λ_{max} values corresponded to previously reported λ_{max}'s at longer wavelengths, as limited to the following solvents: BOX A of 300 nm in H_2O and 295 nm in CH_3CN [1,2], BOX B of 310 nm in H_2O [1], and MVM of 317 and 319 nm in CH_3OH [6,7].

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