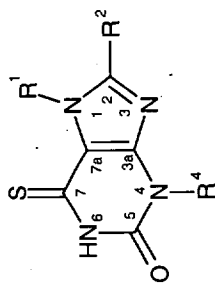


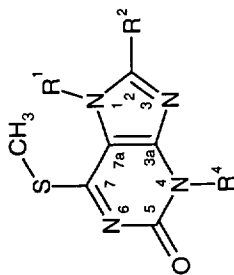
<sup>1</sup>H NMR spectra were recorded using DMSO-d<sub>6</sub> as solvent. The chemical shifts of the remaining protons of the deuterated solvent served as internal standard: (m) <sup>1</sup>H: 2.50; <sup>13</sup>C: 39.1.

Table 1. <sup>1</sup>H NMR data of the synthesized 6-thioxanthines



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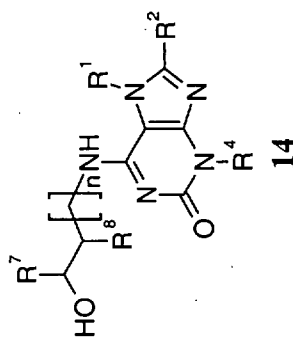
| pd | R <sup>1</sup>                  | R <sup>2</sup>                                                                                                     | R <sup>4</sup>                                        | N6-H              |
|----|---------------------------------|--------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------|-------------------|
| a  | 4.14 (s, 3 H, CH <sub>3</sub> ) | 8.22 (s, 1H, H)                                                                                                    | 3.45 (s, 3 H, CH <sub>3</sub> )                       | 12.33 (s, 1H, NH) |
| b  | 13.61 (s, 1 H, NH)              | 8.15 (s, 1 H, H)                                                                                                   | 5.16 (s, 2 H, CH <sub>2</sub> ); 7.2-7.4 (m, 5 H, ar) | 12.45 (s, 1H, NH) |
| c  | 4.00 (s, 3 H, CH <sub>3</sub> ) | 8.06 (s, 1 H, H)                                                                                                   | 12.18 (s, 1H, NH)                                     | 11.96 (s, 1H, NH) |
| d  | 13.75 (s, NH)                   | 7.4-7.6 (m, 2 H, ar);<br>8.1-8.3 (m, 2 H, ar)                                                                      | 3.49 (s, 3 H, CH <sub>3</sub> )                       | 12.28 (s, 1H, NH) |
| e  | 4.14 (s, 3 H, CH <sub>3</sub> ) | 7.4-7.7 (m, 2 H, ar);<br>7.7-7.9 (m, 2 H, ar)                                                                      | 12.02 (s, 1H, NH)                                     | 12.33 (s, 1H, NH) |
| f  | 4.17 (s, 3 H, CH <sub>3</sub> ) | 7.3-7.6 (m, 2 H, ar);<br>7.7-7.9 (m, 2 H, ar)                                                                      | 3.43 (s, 3 H, CH <sub>3</sub> )                       | 12.27 (s, 1H, NH) |
| g  | 13.48 (s, 1 H, NH)              | 7.11 (d, <sup>3</sup> J=16 Hz, 1H, C=C-H);<br>7.30-7.66 (m, 5 H, Har); 7.79 (d, <sup>3</sup> J= 16 Hz, 1 H, C=C-H) | 3.47 (s, 3 H, CH <sub>3</sub> )                       | 12.24 (s, 1H, NH) |
| h  | 4.27 (s, 3 H, CH <sub>3</sub> ) | 7.3-7.5 (m, 4 H, C=C-H + ar);<br>7.7-7.85 (m, 3 H, C=C-H + ar)                                                     | 3.42 (s, 3 H, CH <sub>3</sub> )                       | 12.14 (s, 1H, NH) |

Table 2. <sup>1</sup>H NMR data of the synthesized 6-methylsulfanyl-anthines

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| pd | R <sup>1</sup>                  | R <sup>2</sup>                                                 | R <sup>4</sup>                                        | S-CH <sub>3</sub>               |
|----|---------------------------------|----------------------------------------------------------------|-------------------------------------------------------|---------------------------------|
| a  | 4.02 (s, 3 H, CH <sub>3</sub> ) | 8.19 (s, 1H, H)                                                | 3.52 (s, 3 H, CH <sub>3</sub> )                       | 2.66 (s, 3 H, CH <sub>3</sub> ) |
| b  |                                 | 8.11 (s, 1 H, H)                                               | 5.20 (s, 2 H, CH <sub>2</sub> ); 7.2-7.4 (m, 5 H, ar) | 2.59 (s, 3 H, CH <sub>3</sub> ) |
| c  | 3.93 (s, 3 H, CH <sub>3</sub> ) | 8.04 (s, 1 H, H)                                               | 13.53 (s, 1H, NH)                                     | 2.56 (s, 3 H, CH <sub>3</sub> ) |
| d  | 13.50 (s, NH)                   | 7.5-7.6 (m, 2 H, ar);<br>8.1-8.3 (m, 2 H, ar)                  | 3.55 (s, 3 H, CH <sub>3</sub> )                       | 2.66 (s, 3 H, CH <sub>3</sub> ) |
| e  | 3.50 (s, 3 H, CH <sub>3</sub> ) |                                                                | 13.40 (s, 1H, NH)                                     | 2.60 (s, 3 H, CH <sub>3</sub> ) |
| f  | 3.96 (s, 3 H, CH <sub>3</sub> ) | 7.3-7.6 (m, 2 H, ar);<br>7.7-7.9 (m, 2 H, ar)                  | 3.59 (s, 3 H, CH <sub>3</sub> )                       | 2.68 (s, 3 H, CH <sub>3</sub> ) |
| g  |                                 | 7.3-7.5 (m, 4 H, C=C-H + ar);<br>7.7-7.85 (m, 3 H, C=C-H + ar) | 3.49 (s, 3 H, CH <sub>3</sub> )                       | 2.59 (s, 3 H, CH <sub>3</sub> ) |
| h  | 4.12 (s, 3 H, CH <sub>3</sub> ) | 7.30-7.40 (m, 3 H, ar);<br>7.45-7.60 (m, 2 H, ar)              |                                                       | 2.65 (s, 3 H, CH <sub>3</sub> ) |

3. <sup>1</sup>H NMR data of the synthesized 6-hydroxyalkylamino-substituted xanthine derivatives



| n | R <sup>1</sup>  | R <sup>2</sup> | R <sup>4</sup>  | R <sup>7</sup> | R <sup>8</sup>                | R <sup>1</sup>                  | R <sup>2</sup>    | R <sup>4</sup>                                           | NMR-shifts:                      | N10-H | OH   | further signals                                                                                                                                                                                               |
|---|-----------------|----------------|-----------------|----------------|-------------------------------|---------------------------------|-------------------|----------------------------------------------------------|----------------------------------|-------|------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 0 | CH <sub>3</sub> | H              | H               | H              | H                             | 3.91 (s, 3 H, CH <sub>3</sub> ) | 7.87 (s, 1 H, CH) | -                                                        | 7.46                             | 7.46  | 4.93 | 3.40-3.60 (m, 4 H, CH <sub>2</sub> -CH <sub>2</sub> )                                                                                                                                                         |
| 0 | CH <sub>3</sub> | H              | benzyl          | H              | H                             | 3.92 (s, 3 H, CH <sub>3</sub> ) | 7.87 (s, 1 H, CH) | 5.11 (s, 2 H, CH <sub>2</sub> );<br>7.1-7.3 (m, 5 H, ar) | 7.00                             | 7.00  | 4.91 | 3.40-3.60 (m, 4 H, CH <sub>2</sub> -CH <sub>2</sub> )                                                                                                                                                         |
| 0 | CH <sub>3</sub> | H              | CH <sub>3</sub> | H              | H                             | 4.00 (s, 3 H, CH <sub>3</sub> ) | 7.95 (s, 1 H, CH) | 3.41 (s, 3 H, CH <sub>3</sub> )                          | 7.00 (t, <sup>3</sup> J= 5.5 Hz) | 7.00  | 4.98 | 3.50-3.70 (m, 4 H, CH <sub>2</sub> -CH <sub>2</sub> )                                                                                                                                                         |
| 1 | CH <sub>3</sub> | H              | CH <sub>3</sub> | H              | CH <sub>3</sub>               | 3.95 (s, 3 H, CH <sub>3</sub> ) | 7.88 (s, 1 H, CH) | 3.34 (s, 3 H, CH <sub>3</sub> )                          | 6.22 (d, <sup>3</sup> J= 8.1 Hz) | 6.22  | 4.87 | 1.18 (d, <sup>3</sup> J= 6.8 Hz)                                                                                                                                                                              |
| 0 | CH <sub>3</sub> | H              | CH <sub>3</sub> | H              | CH <sub>3</sub>               | 3.94 (s, 3 H, CH <sub>3</sub> ) | 7.89 (s, 1 H, CH) | 3.35 (s, 3 H, CH <sub>3</sub> )                          | 6.22 (d, <sup>3</sup> J= 8.1 Hz) | 6.22  | 4.89 | CH <sub>3</sub> ; 3.30-3.60 (n<br>2 H, CH <sub>2</sub> ); 4.20-4.4<br>(m, 1 H, CH)                                                                                                                            |
| 0 | CH <sub>3</sub> | H              | CH <sub>3</sub> | H              | C <sub>2</sub> H <sub>5</sub> | 3.95 (s, 3 H, CH <sub>3</sub> ) | 7.88 (s, 1 H, CH) | 3.33 (s, 3 H, CH <sub>3</sub> )                          | 6.15 (d, <sup>3</sup> J= 8.0 Hz) | 6.15  | 4.88 | 0.90 (t, 3 H, <sup>3</sup> J= 7.0<br>Hz, CH <sub>2</sub> -CH <sub>3</sub> ); 1.5<br>1.71 (m, 2 H, CH <sub>2</sub><br>CH <sub>3</sub> ); 3.40-3.55 (m, 2<br>H, CH <sub>2</sub> -OH); 4.0<br>4.21 (m, 1 H, CH-I |

|   |                 |        |                 |                 |                               |                                 |                                               |                                 |                                  |                                     |                                                                                                                                    |
|---|-----------------|--------|-----------------|-----------------|-------------------------------|---------------------------------|-----------------------------------------------|---------------------------------|----------------------------------|-------------------------------------|------------------------------------------------------------------------------------------------------------------------------------|
| 0 | CH <sub>3</sub> | H      | CH <sub>3</sub> | H               | C <sub>2</sub> H <sub>5</sub> | 3.85 (s, 3 H, CH <sub>3</sub> ) | 7.89 (s, 1 H, CH)                             | 3.42 (s, 3 H, CH <sub>3</sub> ) | 6.15 (d, <sup>3</sup> J= 7.6 Hz) | 4.84<br>(t, <sup>3</sup> J= 5.5 Hz) | 0.90 (t, 3 H, <sup>3</sup> J= 7.3 Hz, CH <sub>2</sub> -CH <sub>3</sub> ); 1.52 (m, 2 H, CH <sub>2</sub> -OH); 4.09 (m, 1 H, CH-Et) |
| 0 | CH <sub>3</sub> | H      | CH <sub>3</sub> | H               | C <sub>2</sub> H <sub>5</sub> | 3.95 (s, 3 H, CH <sub>3</sub> ) | 7.89 (s, 1 H, CH)                             | 3.36 (s, 3 H, CH <sub>3</sub> ) | 6.15 (d, <sup>3</sup> J= 8.0 Hz) | 4.85<br>(t, <sup>3</sup> J= 5.4 Hz) | 1.71 (m, 2 H, CH <sub>2</sub> -CH <sub>3</sub> ); 3.40-3.55 (m, 2 H, CH <sub>2</sub> -OH); 4.21 (m, 1 H, CH-Et)                    |
| 0 | CH <sub>3</sub> | H      | CH <sub>3</sub> | CH <sub>3</sub> | H                             | 3.94 (s, 3 H, CH <sub>3</sub> ) | 7.89 (s, 1 H, CH)                             | 3.34 (s, 3 H, CH <sub>3</sub> ) | 6.87 (t, <sup>3</sup> J= 6.2 Hz) | 5.01<br>(t, <sup>3</sup> J= 4.4 Hz) | 1.07 (d, 3 H, <sup>3</sup> J= 6.7 Hz, CH <sub>3</sub> ); 3.20-3.6 (m, 2 H, CH <sub>2</sub> ); 3.8 (m, 1 H, CH)                     |
| 0 | CH <sub>3</sub> | H      | CH <sub>3</sub> | CH <sub>3</sub> | H                             | 3.94 (s, 3 H, CH <sub>3</sub> ) | 7.88 (s, 1 H, CH)                             | 3.34 (s, 3 H, CH <sub>3</sub> ) | 6.86 (t, <sup>3</sup> J= 6.1 Hz) | 5.02<br>(t, <sup>3</sup> J= 4.1 Hz) | 1.07 (d, 3 H, <sup>3</sup> J= 6.7 Hz, CH <sub>3</sub> ); 3.20-3.6 (m, 2 H, CH <sub>2</sub> ); 3.8 (m, 1 H, CH)                     |
| 0 | CH <sub>3</sub> | H      | CH <sub>3</sub> | CH <sub>3</sub> | H                             | 3.94 (s, 3 H, CH <sub>3</sub> ) | 7.89 (s, 1 H, CH)                             | 3.35 (s, 3 H, CH <sub>3</sub> ) | 6.86 (t, <sup>3</sup> J= 6.2 Hz) | 5.01<br>(t, <sup>3</sup> J= 4.2 Hz) | 1.07 (d, 3 H, <sup>3</sup> J= 6.7 Hz, CH <sub>3</sub> ); 3.60 (m, 2 H, CH <sub>2</sub> ); 3.80-3.5 (m, 1 H, CH)                    |
| 0 | CH <sub>3</sub> | phenyl | H               | H               | H                             | 4.11 (s, 3 H, CH <sub>3</sub> ) | 7.40-7.60 (m, 3 H, ar); 7.70-7.90 (m, 2H, ar) | -                               | 6.24 (d, <sup>3</sup> J= 8.1 Hz) | 4.80                                | 3.40-3.60 (m, 4 H, CH <sub>2</sub> -CH <sub>2</sub> )                                                                              |
| 0 | CH <sub>3</sub> | phenyl | CH <sub>3</sub> | H               | H                             | 4.18 (s, 3 H, CH <sub>3</sub> ) | 7.40-7.60 (m, 3 H, ar); 7.70-7.90 (m, 2H, ar) | 3.53 (s, 3 H, CH <sub>3</sub> ) | 7.30                             | 4.30                                | 3.40-3.60 (m, 4 H, CH <sub>2</sub> -CH <sub>2</sub> )                                                                              |

0.95 (t, 3 H,  $^3J=7.2$  Hz,  $\text{CH}_2\text{-CH}_3$ ); 1.52 (m, 2 H,  $\text{CH}_2\text{-CH}_3$ ); 3.35-3.65 (m, 3 H,  $\text{CH}_2\text{-CH}$ )  
 0.95 (t, 3 H,  $^3J=7.2$  Hz,  $\text{CH}_2\text{-CH}_3$ ); 1.52 (m, 2 H,  $\text{CH}_2\text{-CH}_3$ ); 3.35-3.65 (m, 3 H,  $\text{CH}_2\text{-CH}$ )  
 0.95 (t, 3 H,  $^3J=7.2$  Hz,  $\text{CH}_2\text{-CH}_3$ ); 1.52 (m, 2 H,  $\text{CH}_2\text{-CH}_3$ ); 3.35-3.65 (m, 3 H,  $\text{CH}_2\text{-CH}$ )  
 0.94 (t, 3 H,  $^3J=7.2$  Hz,  $\text{CH}_2\text{-CH}_3$ ); 1.52 (m, 2 H,  $\text{CH}_2\text{-CH}_3$ ); 3.35-3.65 (m, 3 H,  $\text{CH}_2\text{-CH}$ )  
 0.93 (t, 3 H,  $^3J=7.2$  Hz,  $\text{CH}_2\text{-CH}_3$ ); 1.52 (m, 2 H,  $\text{CH}_2\text{-CH}_3$ ); 3.35-3.65 (m, 3 H,  $\text{CH}_2\text{-CH}$ )  
 0.94 (t, 3 H,  $^3J=7.2$  Hz,  $\text{CH}_2\text{-CH}_3$ ); 1.52 (m, 2 H,  $\text{CH}_2\text{-CH}_3$ ); 3.35-3.65 (m, 3 H,  $\text{CH}_2\text{-CH}$ )

|   |               |        |               |   |                        |                               |                                               |                               |                         |      |                                                                                                                                                  |
|---|---------------|--------|---------------|---|------------------------|-------------------------------|-----------------------------------------------|-------------------------------|-------------------------|------|--------------------------------------------------------------------------------------------------------------------------------------------------|
| 0 | H             | phenyl | $\text{CH}_3$ | H | $\text{C}_2\text{H}_5$ | 13.07 (br, 1H, NH)            | 7.50-7.70 (m, 3 H, ar); 8.05-8.25 (m, 2H, ar) | 3.54 (s, 3 H, $\text{CH}_3$ ) | 10.04 (d, $^3J=8.0$ Hz) | 4.20 | 0.95 (t, 3 H, $^3J=7.2$ Hz, $\text{CH}_2\text{-CH}_3$ ); 1.52 (m, 2 H, $\text{CH}_2\text{-CH}_3$ ); 3.35-3.65 (m, 3 H, $\text{CH}_2\text{-CH}$ ) |
| 0 | H             | phenyl | $\text{CH}_3$ | H | $\text{C}_2\text{H}_5$ | 13.07 (br, 1H, NH)            | 7.50-7.70 (m, 3 H, ar); 8.05-8.25 (m, 2H, ar) | 3.52 (s, 3 H, $\text{CH}_3$ ) | 10.08 (d, $^3J=8.0$ Hz) | 4.20 | 0.95 (t, 3 H, $^3J=7.2$ Hz, $\text{CH}_2\text{-CH}_3$ ); 1.52 (m, 2 H, $\text{CH}_2\text{-CH}_3$ ); 3.35-3.65 (m, 3 H, $\text{CH}_2\text{-CH}$ ) |
| 0 | H             | phenyl | $\text{CH}_3$ | H | $\text{C}_2\text{H}_5$ | 13.07 (br, 1H, NH)            | 7.50-7.70 (m, 3 H, ar); 8.05-8.25 (m, 2H, ar) | 3.49 (s, 3 H, $\text{CH}_3$ ) | 10.02 (d, $^3J=8.0$ Hz) | 4.20 | 0.95 (t, 3 H, $^3J=7.2$ Hz, $\text{CH}_2\text{-CH}_3$ ); 1.52 (m, 2 H, $\text{CH}_2\text{-CH}_3$ ); 3.35-3.65 (m, 3 H, $\text{CH}_2\text{-CH}$ ) |
| 0 | $\text{CH}_3$ | phenyl | $\text{CH}_3$ | H | $\text{C}_2\text{H}_5$ | 3.94 (s, 3 H, $\text{CH}_3$ ) | 7.50-7.65 (m, 3 H, ar); 7.70-7.90 (m, 2H, ar) | 3.39 (s, 3 H, $\text{CH}_3$ ) | 6.35 (d, $^3J=8.0$ Hz)  | 4.20 | 0.94 (t, 3 H, $^3J=7.2$ Hz, $\text{CH}_2\text{-CH}_3$ ); 1.52 (m, 2 H, $\text{CH}_2\text{-CH}_3$ ); 3.35-3.65 (m, 3 H, $\text{CH}_2\text{-CH}$ ) |
| 0 | $\text{CH}_3$ | phenyl | $\text{CH}_3$ | H | $\text{C}_2\text{H}_5$ | 3.95 (s, 3 H, $\text{CH}_3$ ) | 7.50-7.65 (m, 3 H, ar); 7.70-7.90 (m, 2H, ar) | 3.38 (s, 3 H, $\text{CH}_3$ ) | 6.35 (d, $^3J=8.0$ Hz)  | 4.20 | 0.93 (t, 3 H, $^3J=7.2$ Hz, $\text{CH}_2\text{-CH}_3$ ); 1.52 (m, 2 H, $\text{CH}_2\text{-CH}_3$ ); 3.35-3.65 (m, 3 H, $\text{CH}_2\text{-CH}$ ) |
| 0 | $\text{CH}_3$ | phenyl | $\text{CH}_3$ | H | $\text{C}_2\text{H}_5$ | 3.94 (s, 3 H, $\text{CH}_3$ ) | 7.50-7.65 (m, 3 H, ar); 7.70-7.90 (m, 2H, ar) | 3.39 (s, 3 H, $\text{CH}_3$ ) | 6.37 (d, $^3J=8.0$ Hz)  | 4.20 | 0.94 (t, 3 H, $^3J=7.2$ Hz, $\text{CH}_2\text{-CH}_3$ ); 1.52 (m, 2 H, $\text{CH}_2\text{-CH}_3$ ); 3.35-3.65 (m, 3 H, $\text{CH}_2\text{-CH}$ ) |

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|   |                 |        |                 |   |                               |                                 |                            |                                 |                                  |                                  |                                                                                                                                                                                                        |
|---|-----------------|--------|-----------------|---|-------------------------------|---------------------------------|----------------------------|---------------------------------|----------------------------------|----------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 0 | CH <sub>3</sub> | styryl | CH <sub>3</sub> | H | C <sub>2</sub> H <sub>5</sub> | 4.19 (s, 3 H, CH <sub>3</sub> ) | 7.30-7.90 (m, 7 H, styryl) | 3.41 (s, 3 H, CH <sub>3</sub> ) | 6.24 (d, <sup>3</sup> J= 8.0 Hz) | 4.85                             | 0.91 (t, 3 H, <sup>3</sup> J= 8.1 Hz, CH <sub>2</sub> -CH <sub>3</sub> ); 1.40 (m, 2 H, CH <sub>2</sub> -CH <sub>3</sub> ); 3.40-3.60 (m, 2 H, CH <sub>2</sub> -CH); 4.10 (m, 1H, CH <sub>2</sub> -CH) |
| 0 | CH <sub>3</sub> | styryl | CH <sub>3</sub> | H | C <sub>2</sub> H <sub>5</sub> | 4.20 (s, 3 H, CH <sub>3</sub> ) | 7.30-7.90 (m, 7 H, styryl) | 3.41 (s, 3 H, CH <sub>3</sub> ) | 6.24 (d, <sup>3</sup> J= 7.9 Hz) | 4.84                             | 0.91 (t, 3 H, <sup>3</sup> J= 8.1 Hz, CH <sub>2</sub> -CH <sub>3</sub> ); 1.40 (m, 2 H, CH <sub>2</sub> -CH <sub>3</sub> ); 3.40-3.60 (m, 2 H, CH <sub>2</sub> -CH); 4.10 (m, 1H, CH <sub>2</sub> -CH) |
| 0 | H               | styryl | CH <sub>3</sub> | H | C <sub>2</sub> H <sub>5</sub> | 13.00 (br, 1H, NH)              | 7.30-7.90 (m, 7 H, styryl) | 3.40 (s, 3 H, CH <sub>3</sub> ) | -                                | 4.20                             | 0.92 (t, 3 H, <sup>3</sup> J= 7.1 Hz, CH <sub>2</sub> -CH <sub>3</sub> ); 1.50 (m, 2 H, CH <sub>2</sub> -CH <sub>3</sub> ); 3.35-3.65 (m, 3 H, CH <sub>2</sub> -CH)                                    |
| 0 | H               | styryl | CH <sub>3</sub> | H | C <sub>2</sub> H <sub>5</sub> | 13.00 (br, 1H, NH)              | 7.30-7.90 (m, 7 H, styryl) | 3.41 (s, 3 H, CH <sub>3</sub> ) | -                                | 4.20                             | 0.94 (t, 3 H, <sup>3</sup> J= 7.1 Hz, CH <sub>2</sub> -CH <sub>3</sub> ); 1.50 (m, 2 H, CH <sub>2</sub> -CH <sub>3</sub> ); 3.35-3.65 (m, 3 H, CH <sub>2</sub> -CH)                                    |
| 1 | CH <sub>3</sub> | H      | CH <sub>3</sub> | H | H                             | 3.91 (s, 3 H, CH <sub>3</sub> ) | 7.88 (s, 1 H, CH)          | 3.35 (s, 3 H, CH <sub>3</sub> ) | 7.03 (t, <sup>3</sup> J= 5.5 Hz) | 4.78 (t, <sup>3</sup> J= 5.3 Hz) | 1.60-1.80 (m, 2 H, CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> ); 3.40-3.55 (m, 4 H, CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> )                                                         |
| 2 | CH <sub>3</sub> | H      | CH <sub>3</sub> | H | H                             | 3.93 (s, 3 H, CH <sub>3</sub> ) | 7.86 (s, 1 H, CH)          | 3.34 (s, 3 H, CH <sub>3</sub> ) | 6.93 (t, <sup>3</sup> J= 5.5 Hz) | 4.68                             | 1.35-1.63 (m, 4 H, CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> ); 3.35-3.47 (m, 4 H, CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> )                                        |



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1.20-1.60 (m, 6 H,  
3\*CH<sub>2</sub>); 3.35-3.40  
(m, 4 H, HO-CH<sub>2</sub>,  
CH-NH)

4.38

6.94 (t, <sup>3</sup>J= 5.5 Hz)

3.34 (s, 3 H, CH<sub>3</sub>)

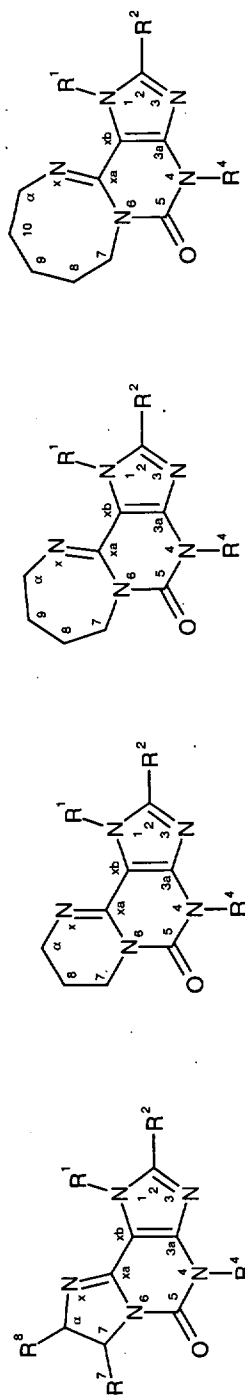
7.86 (s, 1 H, CH)

3.92 (s, 3 H, CH<sub>3</sub>)

CH<sub>3</sub> H

3 CH<sub>3</sub> H

<sup>1</sup>H NMR data of the synthesized tricyclic purinone derivatives



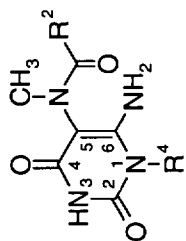
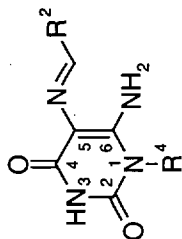
|                | 15-26          | 27,28                                                                         | 29          | 30                                                                                                                                  |  |
|----------------|----------------|-------------------------------------------------------------------------------|-------------|-------------------------------------------------------------------------------------------------------------------------------------|--|
| R <sup>1</sup> | R <sup>2</sup> | R <sup>4</sup>                                                                | Nx-H        | further substituents                                                                                                                |  |
| 3.97           | 8.31           | 11.40 (vbr)                                                                   | 12.74       | 4.00-4.20 (m, N-CH <sub>2</sub> -CH <sub>2</sub> -N)                                                                                |  |
| 3.99           | 8.40           | 5.20 (s, CH <sub>2</sub> );<br>7.22-7.40 (m, -C <sub>6</sub> H <sub>5</sub> ) |             | 4.00-4.25 (m, N-CH <sub>2</sub> -CH <sub>2</sub> -N)                                                                                |  |
| 4.04           | 8.42           | 3.45                                                                          | 11.82 (vbr) | 3.8-4.2 (m)                                                                                                                         |  |
| 4.04           | 8.25           | 3.42                                                                          | 11.12       | 1.54 (d, <sup>3</sup> J=6.6 Hz, R <sup>8</sup> ); 3.74-3.9 (m, CH <sub>2</sub> );<br>4.4-4.58 (m, CH)                               |  |
| 4.05           | 8.27           | 3.39                                                                          | 8.92        | 1.55 (d, <sup>3</sup> J=6.6 Hz, R <sup>8</sup> ); 3.70-3.90 (m, CH <sub>2</sub> );<br>4.4-4.55 (m, CH)                              |  |
| 4.00           | 8.35           | 3.45                                                                          | 11.40 (br)  | 0.95 (t, J=7.3 Hz, CH <sub>3</sub> ); 1.4-1.6 (, CH <sub>2</sub> );<br>3.7-3.9 (m, CH <sub>2</sub> ); 4.2-4.4 (m, CH)               |  |
| 4.03           | 8.40           | 3.47                                                                          | 11.30 (br)  | 0.98 (t, <sup>3</sup> J=7.1 Hz, CH <sub>3</sub> ); 1.4-1.6 (m, CH <sub>2</sub> );<br>3.7-3.9 (m, CH <sub>2</sub> ); 4.2-4.4 (m, CH) |  |
| 4.02           | 8.38           | 3.45                                                                          | 11.20 (br)  | 0.94 (t, <sup>3</sup> J=7.2 Hz, CH <sub>3</sub> ); 1.4-1.6 (, CH <sub>2</sub> );<br>3.7-3.9 (m, CH <sub>2</sub> ); 4.2-4.4 (m, CH)  |  |



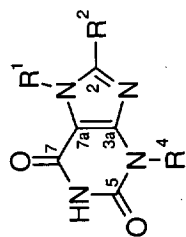
|            |                                                       |       |                                                                                                                                                                                   |                                                                                                                                        |
|------------|-------------------------------------------------------|-------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| 4.07       | 8.32                                                  | 3.45  | 9.08                                                                                                                                                                              | 1.53 (d, $^3J=6.6$ Hz, $\underline{\text{CH}_3}$ ); 3.92-4.05 (m, $\underline{\text{CH}_2}$ ); 4.41-4.60 (m, $\underline{\text{CH}}$ ) |
| 4.05       | 8.28                                                  | 3.43  | 8.91                                                                                                                                                                              | 1.54 (d, $^3J=6.6$ Hz, $\underline{\text{CH}_3}$ ); 3.90-4.07 (m, $\underline{\text{CH}_2}$ ); 4.40-4.60 (m, $\underline{\text{CH}}$ ) |
| 4.11       | 8.36                                                  | 3.45  | 9.45                                                                                                                                                                              | 1.50 (d, $^3J=6.6$ Hz, $\underline{\text{CH}_3}$ ); 3.90-4.05 (m, $\underline{\text{CH}_2}$ ); 4.40-4.60 (m, $\underline{\text{CH}}$ ) |
| 3.98       | 7.5-7.6 (m, Ar);<br>7.70-7.80 (m, Ar)                 | 10.90 |                                                                                                                                                                                   | 3.70-3.90 (m, $\underline{\text{CH}_2-\text{CH}_2}$ )                                                                                  |
| 4.08       | 7.45-7.6 (m, Ar);<br>7.70-7.80 (m, Ar)                | 3.51  |                                                                                                                                                                                   | 3.68-3.90 (m, $\underline{\text{CH}_2-\text{CH}_2}$ )                                                                                  |
| 4.05       | 7.5-7.7 (m, Ar);<br>7.80-7.90 (m, Ar)                 | 3.52  | 0.91 (t, $^3J=7.5$ Hz, $\underline{\text{CH}_3}$ ); 1.20-1.40 (m, $\underline{\text{CH}_2}$ ); 3.70-3.90 (m, $\underline{\text{CH}_2}$ ); 4.20-4.40 (m, $\underline{\text{CH}}$ ) |                                                                                                                                        |
| 4.04       | 7.5-7.7 (m, Ar); 7.80-7.90 (m, Ar)                    | 3.51  | 0.95 (t, $^3J=7.5$ Hz, $\underline{\text{CH}_3}$ ); 1.20-1.40 (m, $\underline{\text{CH}_2}$ ); 3.70-3.90 (m, $\underline{\text{CH}_2}$ ); 4.20-4.40 (m, $\underline{\text{CH}}$ ) |                                                                                                                                        |
| 4.01       | 7.5-7.7 (m, Ar);<br>7.80-7.90 (m, Ar)                 | 3.56  | 0.94 (t, $^3J=7.5$ Hz, $\underline{\text{CH}_3}$ ); 1.20-1.40 (m, $\underline{\text{CH}_2}$ ); 3.70-3.90 (m, $\underline{\text{CH}_2}$ ); 4.20-4.40 (m, $\underline{\text{CH}}$ ) |                                                                                                                                        |
| -          | 7.3-7.5 (m, Ar);<br>8.10-8.20 (m, Ar)                 | 3.73  | 0.90 (t, $^3J=7.5$ Hz, $\underline{\text{CH}_3}$ ); 1.2-1.40 (m, $\underline{\text{CH}_2}$ ); 3.70-3.90 (m, $\underline{\text{CH}_2}$ ); 4.20-4.40 (m, $\underline{\text{CH}}$ )  |                                                                                                                                        |
| -          | 7.3-7.5 (m, Ar);<br>8.10-8.20 (m, Ar)                 | 3.73  | 0.91 (t, $^3J=7.5$ Hz, $\underline{\text{CH}_3}$ ); 1.20-1.40 (m, $\underline{\text{CH}_2}$ ); 3.70-3.90 (m, $\underline{\text{CH}_2}$ ); 4.20-4.40 (m, $\underline{\text{CH}}$ ) |                                                                                                                                        |
| 13.0 (vbr) | 7.3-7.5 (m, Ar);<br>8.10-8.20 (m, Ar)                 | 3.71  | 0.94 (t, $^3J=7.5$ Hz, $\underline{\text{CH}_3}$ ); 1.20-1.40 (m, $\underline{\text{CH}_2}$ ); 3.70-3.90 (m, $\underline{\text{CH}_2}$ ); 4.20-4.40 (m, $\underline{\text{CH}}$ ) |                                                                                                                                        |
| 4.07       | 7.4-7.5 (m, H-C=C + Ar);<br>7.70-7.90 (m, C=C-H + Ar) | 3.52  | 0.92 (t, $^3J=7.4$ Hz, $\underline{\text{CH}_3}$ ); 1.20-1.40 (m, $\underline{\text{CH}_2}$ ); 3.70-3.90 (m, $\underline{\text{CH}_2}$ ); 4.20-4.40 (m, $\underline{\text{CH}}$ ) |                                                                                                                                        |
| 4.05       | 7.4-7.5 (m, H-C=C + Ar);<br>7.70-7.90 (m, C=C-H + Ar) | 3.52  | 0.91 (t, $^3J=7.5$ Hz, $\underline{\text{CH}_3}$ ); 1.20-1.40 (m, $\underline{\text{CH}_2}$ ); 3.70-3.90 (m, $\underline{\text{CH}_2}$ ); 4.20-4.40 (m, $\underline{\text{CH}}$ ) |                                                                                                                                        |
| 13.1 (vbr) | 7.4-7.5 (m, H-C=C + Ar);<br>7.70-7.90 (m, C=C-H + Ar) | 3.69  | 0.91 (t, $^3J=7.6$ Hz, $\underline{\text{CH}_3}$ ); 1.20-1.40 (m, $\underline{\text{CH}_2}$ ); 3.70-3.90 (m, $\underline{\text{CH}_2}$ ); 4.20-4.40 (m, $\underline{\text{CH}}$ ) |                                                                                                                                        |

|                                 |                                                       |      |                                                                                                                                        |
|---------------------------------|-------------------------------------------------------|------|----------------------------------------------------------------------------------------------------------------------------------------|
| 13.2 (vbr)                      | 7.4-7.5 (m, H-C=C + Ar);<br>7.70-7.90 (m, C=C-H + Ar) | 3.74 | 0.92 (t, <sup>3</sup> J=7.5 Hz, CH <sub>3</sub> ); 1.20-1.40 (m, CH <sub>2</sub> ); 3.70-3.90 (m, CH <sub>2</sub> ); 4.20-4.40 (m, CH) |
| 4.05 (d, <sup>4</sup> J=0.5 Hz) | 8.30 (m)                                              | 3.48 | 3.95-4.05 (t; <sup>3</sup> J=5.5 Hz; R <sup>7</sup> );<br>2.0-2.15 (m; R <sup>8</sup> ); 3.49-3.60 (m; CH <sub>2</sub> )               |
| 4.02                            | -                                                     | 3.46 | 2.0-2.2 (m; CH <sub>2</sub> ); 3.5-3.6 (m; N-CH <sub>2</sub> );<br>3.9-4.0(m; N-CH <sub>2</sub> )                                      |
| 4.05                            | 8.29                                                  | 3.44 | 1.4-1.9 (m; C8H <sub>2</sub> -C9H <sub>2</sub> );<br>3.55-3.75 (m, C7H <sub>2</sub> ; C10H <sub>2</sub> )                              |
| 4.08                            | 8.31                                                  | 3.44 | 1.80 (m; C8H <sub>2</sub> -C9H <sub>2</sub> -C10H <sub>2</sub> );<br>3.5-3.8 (m; 2*N-CH <sub>2</sub> )                                 |

data were obtained from hydrochlorides

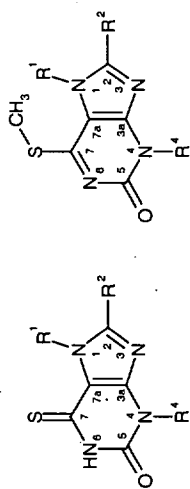
5. <sup>13</sup>C NMR data of selected pyrimidine derivatives**6 a,c****8**

| d | C2    | C4    | C5   | C6    | R <sup>4</sup> | further signals                                                      |
|---|-------|-------|------|-------|----------------|----------------------------------------------------------------------|
|   | 153.3 | 159.5 | 93.7 | 150.3 | 29.1           | 34.3; 108.9; 118.7; 127.8; 128.7; 129.3; 140.4; 167.8                |
|   | 152.6 | 159.0 | 96.0 | 149.7 | 28.9           | 34.3; 125.4; 127.1; 128.8; 137.4; 172.9                              |
|   | 149.4 | 157.8 | 99.9 | 154.8 | 29.5           | 112.8; 126.8; 128.4; 129.0; 131.8; 136.5; 136.8; 149.4; 151.2; 151.6 |

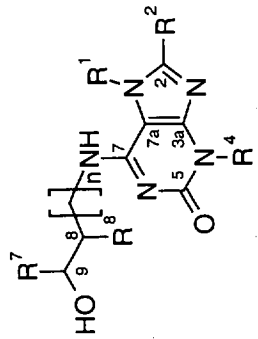
6. <sup>13</sup>C NMR data of selected xanthine derivatives

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| d | C2    | C3a   | C5    | C7    | C7a   | R <sup>1</sup> | R <sup>2</sup>                              | R <sup>4</sup>                   |
|---|-------|-------|-------|-------|-------|----------------|---------------------------------------------|----------------------------------|
| 1 | 140.6 | 149.2 | 150.9 | 154.6 | 106.9 | -              | -                                           | 45.0; 127.2; 127.5; 128.3; 137.1 |
| 2 | 142.8 | 149.0 | 151.2 | 155.6 | 106.7 | 32.9           | -                                           | -                                |
| 3 | 150.8 | 149.2 | 151.1 | 155.1 | 108.2 | 33.5           | 128.3; 128.7; 129.0; 130.1                  | 28.4                             |
| 4 | 150.2 | 149.2 | 151.0 | 154.2 | 107.4 | -              | 115.6; 127.0; 128.9; 134.1;<br>134.9; 135.3 | 28.7                             |

7. <sup>13</sup>C-NMR data of selected thioxanthine and methylsulfanylxanthine derivatives

|  | C2    | C3a   | C5    | C7    | C7a   | R <sup>1</sup> | R <sup>2</sup>                              | R <sup>4</sup>                      | S-CH <sub>3</sub> |
|--|-------|-------|-------|-------|-------|----------------|---------------------------------------------|-------------------------------------|-------------------|
|  | 146.4 | 147.1 | 149.1 | 175.6 | 117.2 | 34.7           | -                                           | 29.0                                | -                 |
|  | 143.6 | 145.2 | 148.9 | 175.3 | 118.3 | -              | -                                           | 45.5; 127.4; 127.6; 128.4;<br>136.4 | -                 |
|  | 146.5 | 149.1 | 152.0 | 176.8 | 117.0 | 34.5           | -                                           | -                                   | -                 |
|  | 146.5 | 149.1 | 152.5 | 173.7 | 119.8 | -              | 127.1; 128.3; 128.8;<br>130.7               | 29.1                                | -                 |
|  | 146.8 | 148.8 | 154.4 | 175.0 | 118.3 | 34.7           | 128.1; 128.7; 129.4;<br>130.6               | 28.8                                | -                 |
|  | 146.7 | 149.2 | 152.2 | 173.0 | 119.2 | -              | 115.2; 127.2; 128.9;<br>129.3; 135.3; 136.6 | 29.1                                | -                 |
|  | 147.5 | 148.7 | 152.6 | 173.6 | 117.8 | 32.1           | 112.8; 127.8; 128.8;<br>129.6; 135.8; 138.3 | 28.8                                | -                 |
|  | 145.2 | 150.8 | 153.3 | 160.6 | 113.4 | 34.3           | -                                           | 45.4; 127.2; 127.7; 128.3;<br>136.9 | 11.5              |
|  | 150.7 | 151.9 | 153.3 | 159.3 | 114.5 | -              | 126.9; 128.4; 128.9;<br>130.8               | 29.8                                | 11.8              |

Table 1. <sup>13</sup>C NMR data of selected 6-(hydroxyalkylamino)xanthines<sup>1</sup>


**14a-o**

|   | C2    | C3a   | C5    | C7    | C7a   | C8   | C9   | R <sup>1</sup> | R <sup>2</sup>                       | R <sup>4</sup>                      | further signals |
|---|-------|-------|-------|-------|-------|------|------|----------------|--------------------------------------|-------------------------------------|-----------------|
| e | 142.7 | 151.4 | 155.0 | 152.1 | 104.2 | 44.7 | 59.5 | 33.8           | -                                    | 42.8; 126.8; 127.5;<br>128.1; 138.0 | -               |
| f | 142.7 | 151.8 | 155.5 | 152.0 | 104.2 | 42.8 | 59.6 | 33.8           | -                                    | 28.7                                | -               |
| g | 142.7 | 151.8 | 155.4 | 152.1 | 104.1 | 53.4 | 62.4 | 33.8           | -                                    | 28.7                                | *               |
| h | 142.7 | 151.7 | 155.5 | 152.1 | 104.2 | 53.4 | 62.5 | 33.8           | -                                    | 28.7                                | 10.6; 23.4      |
| i | 142.7 | 151.7 | 155.5 | 152.0 | 104.2 | 47.8 | 64.8 | 33.8           | -                                    | 28.7                                | 21.0            |
| j | 142.7 | 151.8 | 155.4 | 152.1 | 104.1 | 47.8 | 64.8 | 33.8           | -                                    | 28.7                                | *               |
| k | 146.6 | 150.8 | 151.8 | 148.9 | 102.9 | 56.9 | 62.8 | -              | 126.2; 127.6; 129.3;<br>131.2        | 29.4                                | 10.0; 21.1      |
| l | 150.9 | 151.5 | 155.3 | 152.2 | 105.8 | 53.5 | 62.5 | 34.5           | 128.6; 128.7; 129.4;<br>130.0        | 28.8                                | 10.7; 23.4      |
| m | 146.3 | 150.8 | 151.5 | 148.9 | 102.5 | 56.8 | 62.7 | *              | 115.1; 127.5; 128.9;<br>129.6; 134.8 | 29.4                                | 10.0; 23.1      |
| n | 142.7 | 151.7 | 155.7 | 152.0 | 104.2 | 37.9 | 58.8 | 31.9           | -                                    | 28.8                                | 33.9            |
| o | 142.6 | 151.8 | 155.8 | 151.7 | 104.2 | 40.0 | 60.6 | 33.9           | -                                    | 28.7                                | 25.6; 29.9      |
| p | 142.5 | 151.8 | 155.8 | 151.7 | 104.2 | 40.1 | 60.6 | 33.8           | -                                    | 28.7                                | 22.9 * (28.7)   |

Table 9. <sup>13</sup>C NMR data of selected tricyclic purinone derivatives

| Compound | R <sup>1</sup> | C2    | C3a   | C5    | Cxa   | Cxb   | R <sup>4</sup>                                      | C7   | Cα   | further signals                    |
|----------|----------------|-------|-------|-------|-------|-------|-----------------------------------------------------|------|------|------------------------------------|
| 16, R-20 |                |       |       |       |       |       |                                                     |      |      |                                    |
| 26       | 34.3           | 147.7 | 152.8 | 146.6 | 147.6 | 101.0 | 45.8 (CH <sub>2</sub> ); 127.6; 127.7; 128.4; 135.7 | 44.7 | 44.4 |                                    |
| 20       | 34.8           | 149.2 | 151.6 | 146.9 | 147.2 | 103.1 | 28.9                                                | 45.1 | 41.4 | 25.8                               |
| 27       | 35.2           | 148.1 | 149.9 | 146.3 | 147.9 | 102.7 | 30.2                                                | 42.5 | 42.7 | 18.1 (C8)                          |
| 29       | 35.2           | 148.7 | 151.7 | 146.7 | 147.3 | 103.1 | 29.2                                                | 41.5 | 45.1 | 25.76 (C8); 28.95 (C9)             |
| 30       | 35.0           | 148.8 | 151.7 | 146.8 | 147.0 | 103.0 | 29.1                                                | 42.0 | 45.2 | 29.13 (C8); 23.13 (C9); 31.6 (C10) |

IR data were obtained from hydrochlorides

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