

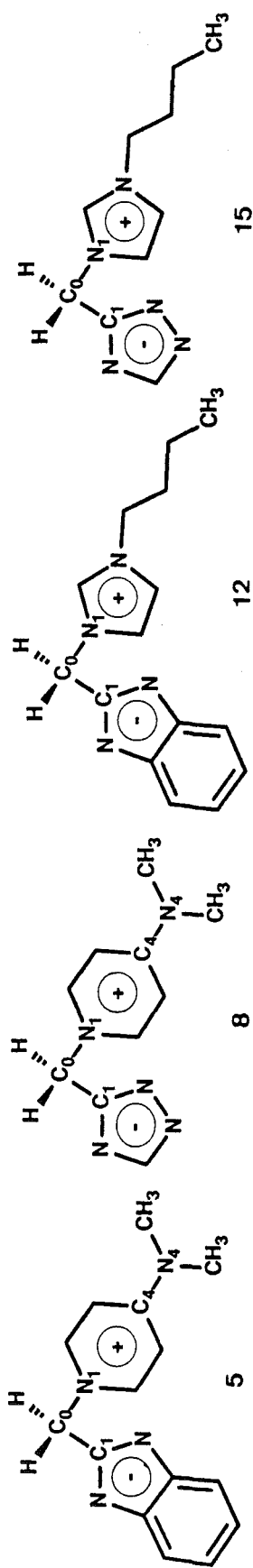
BETAINES D'AZOLAT PIRIDINI(AZOLI) I DERIVATS
AMB DIVERSOS AGRUPAMENTS INTERANULARS. ESTUDIS EN LA
SERIE DEL BENZIMIDAZOLE: SINTESI, ESTRUCTURA I PROPIETATS.

Memòria presentada per a optar al grau de Doctor en
Farmàcia per Na M^a Lluïsa Pérez García

Dirigida per:

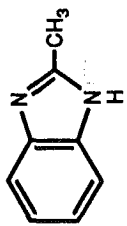
Na M^a Ermitas Alcalde Pais

Barcelona, maig de 1991.

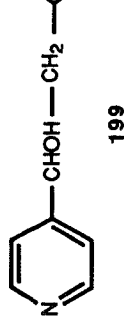


| | $\widehat{C}_1C_0N_1$ | \widehat{HC}_0H | C_1C_0 | C_0N_1 | C_4N_4 | MD_{calc} | MD_{exp} |
|------|-----------------------|--|----------|----------|----------|--|------------|
| 5 | AMI | 109.53 | 1.484 | 1.484 | 1.370 | 17.85 | 12.34 |
| | MNDO | 107.02 | 1.478 | 1.534 | 1.389 | 17.13 | |
| 5-RX | AMI | $\left(\begin{array}{c} 110.41 \\ 106.93 \end{array} \right)$ | 1.498 | 1.488 | 1.332 | $\left(\begin{array}{c} 20.60 \\ 20.75 \end{array} \right)$ | (1) |
| | MNDO | | | | | | |
| 8 | AMI | 109.71 | 1.464 | 1.495 | 1.371 | 16.52 | 14.82 |
| | MNDO | 107.21 | 1.462 | 1.544 | 1.390 | 16.40 | |
| 12 | AMI | 109.79 | 1.488 | 1.467 | 1.371 | 15.73 | 12.56 |
| | MNDO | 107.65 | 1.478 | 1.523 | 1.390 | 15.76 | |
| 15 | AMI | 111.56 | 1.467 | 1.476 | 1.371 | 15.39 | 15.34 |
| | MNDO | 108.74 | 1.463 | 1.532 | 1.390 | 15.49 | |

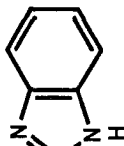
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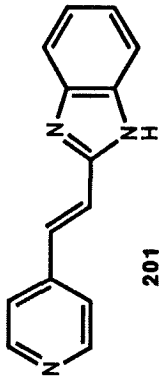
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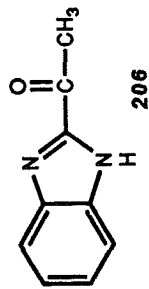
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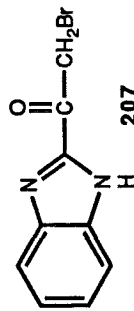
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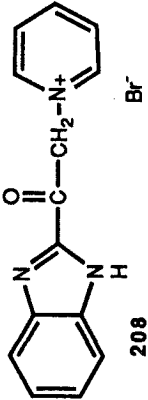
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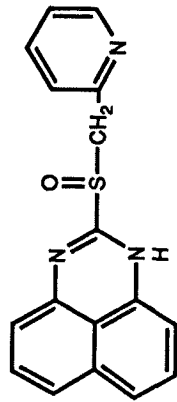
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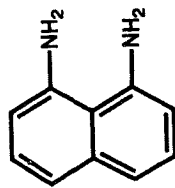
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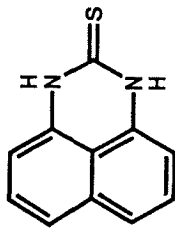
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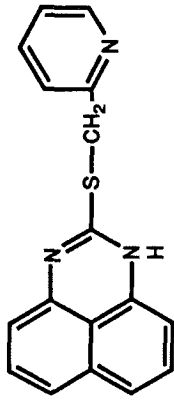
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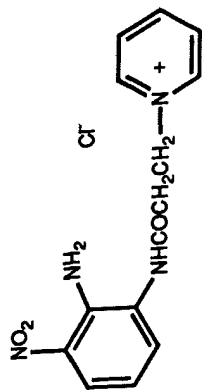
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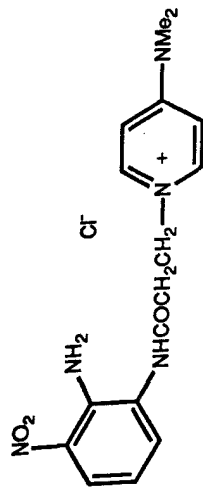
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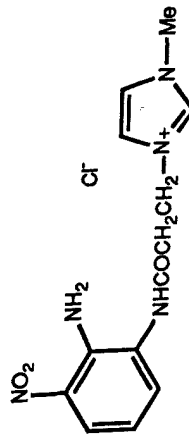
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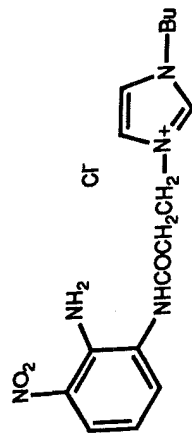
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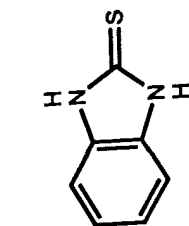
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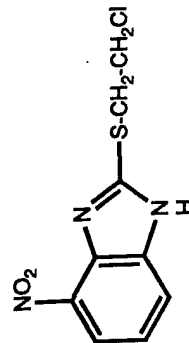
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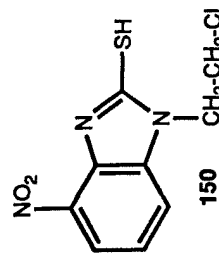
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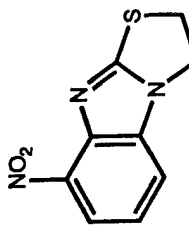
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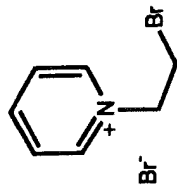
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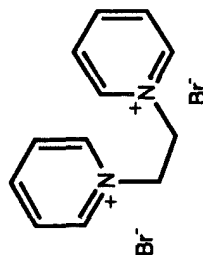
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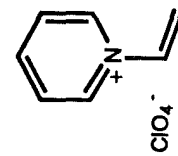
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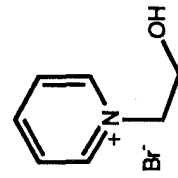
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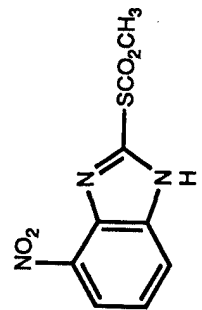
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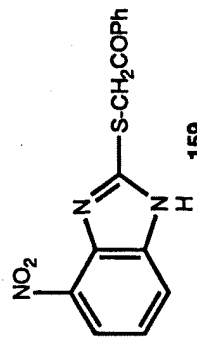
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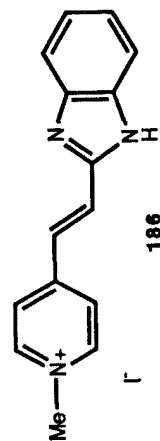
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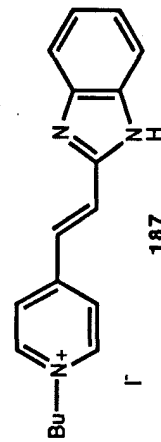
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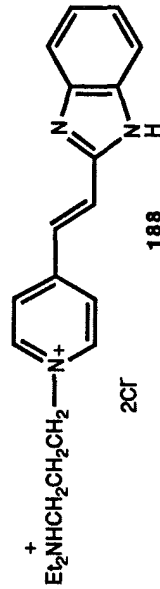
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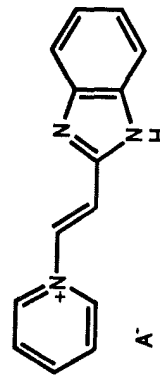
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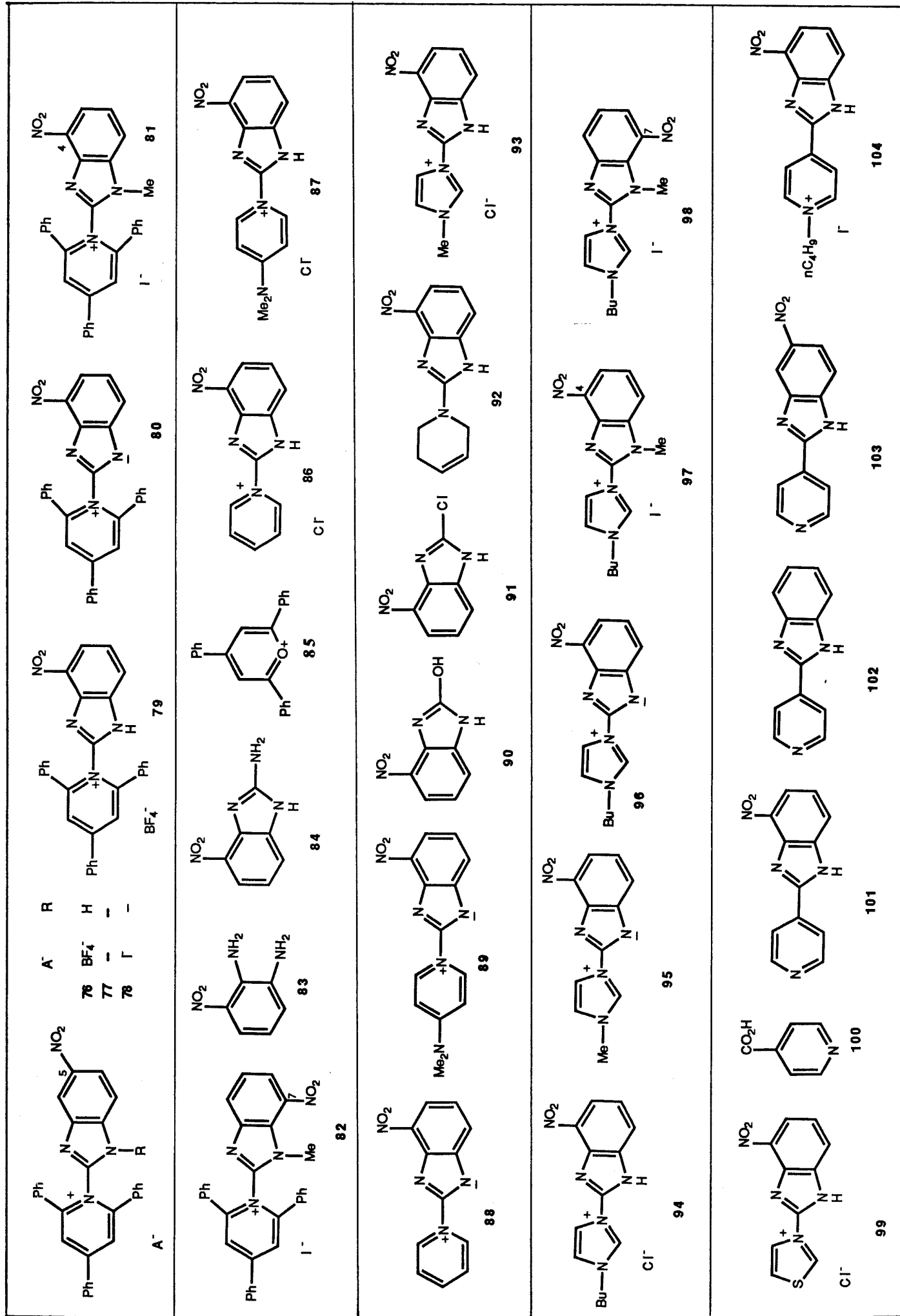
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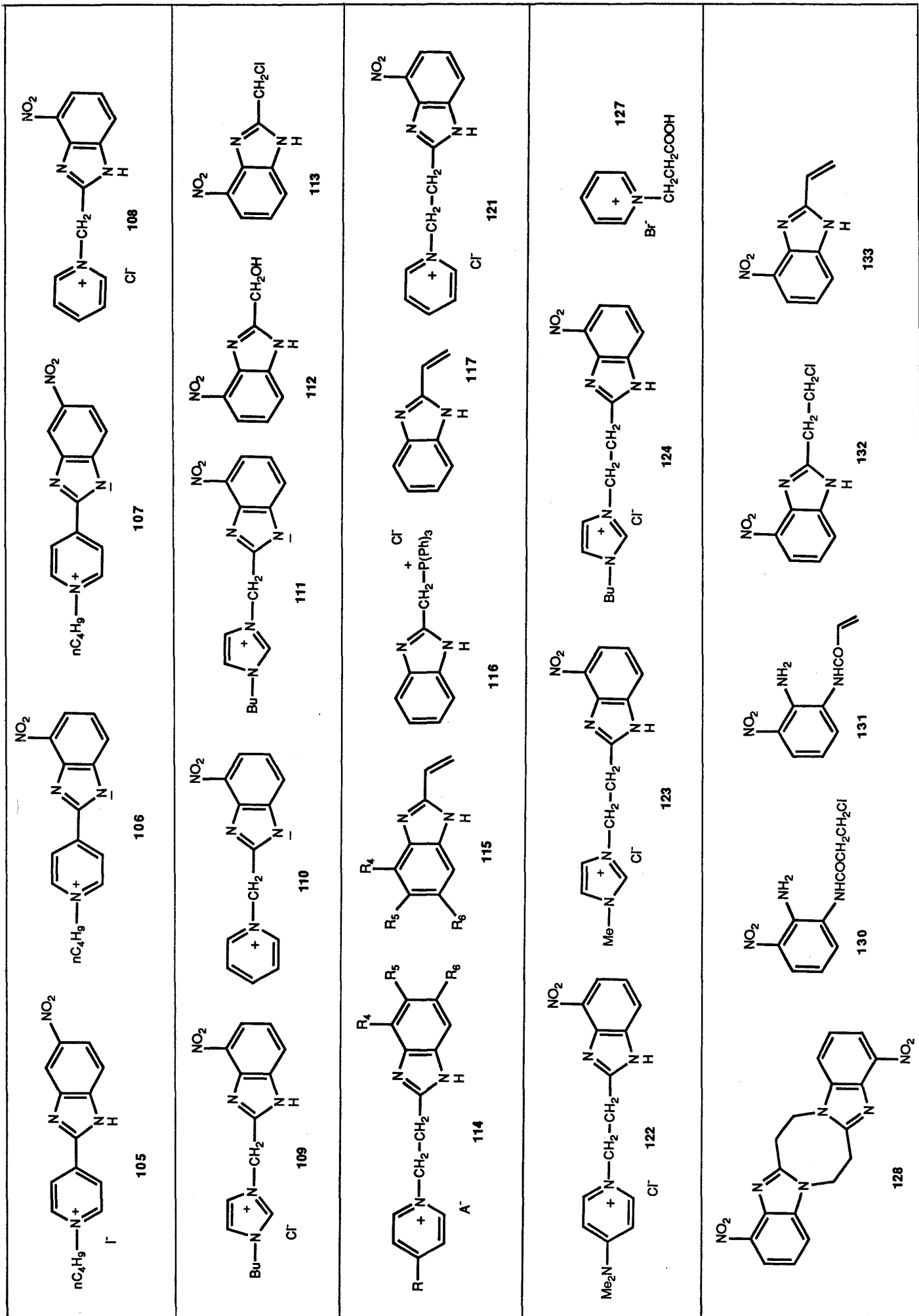


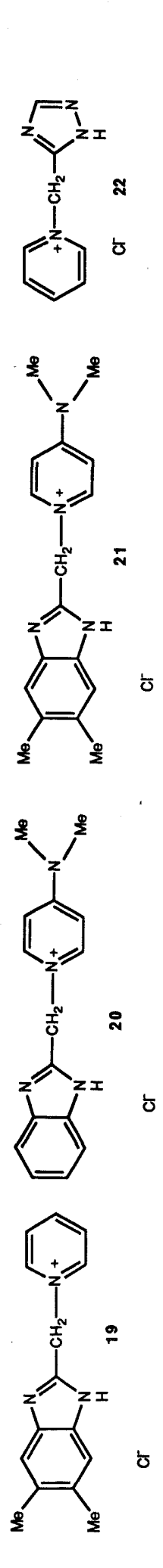
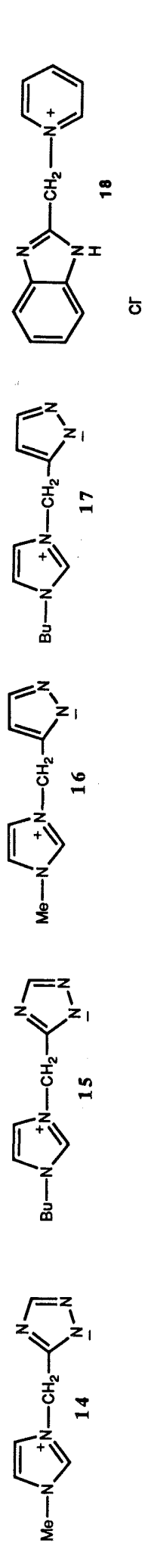
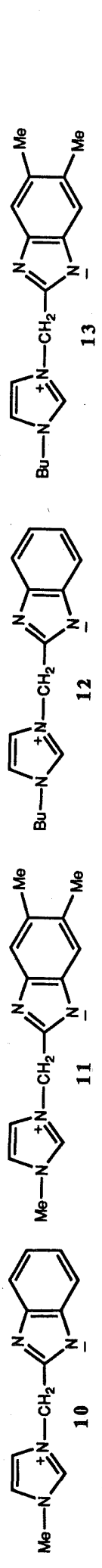
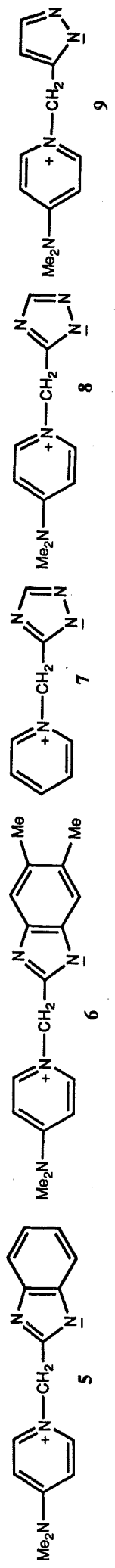
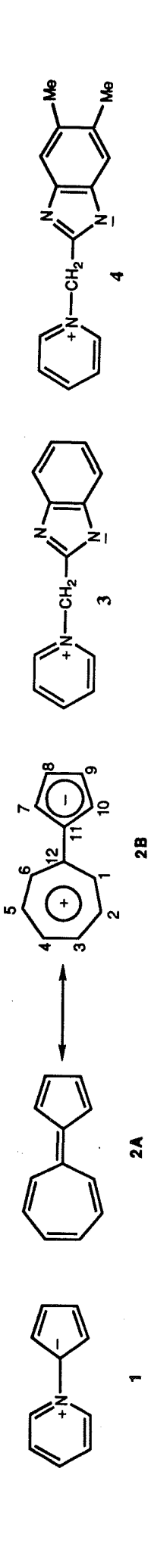
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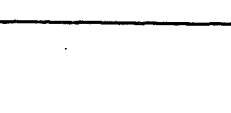
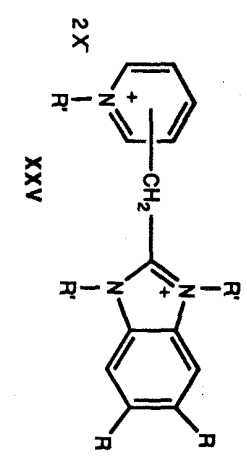
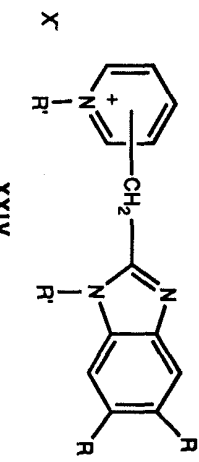
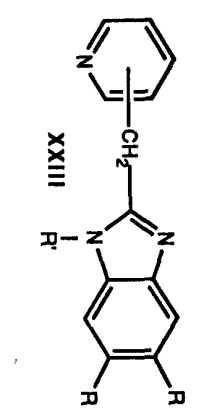
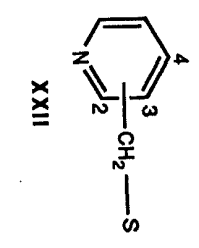
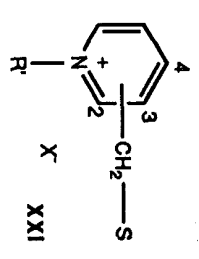
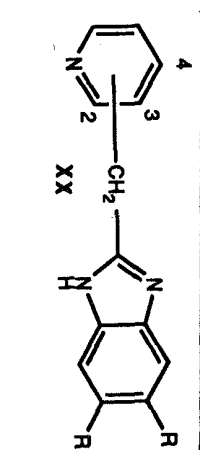
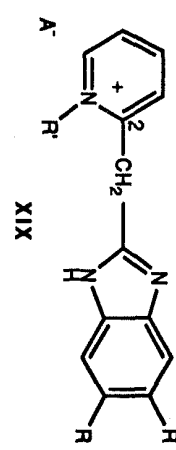
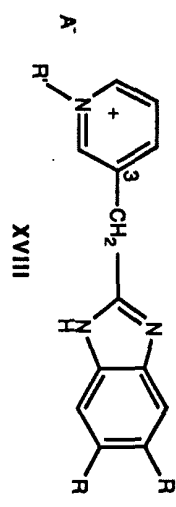
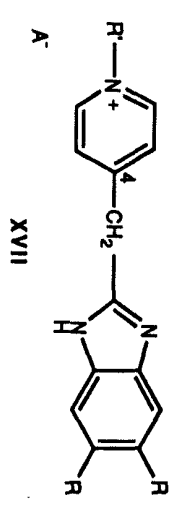
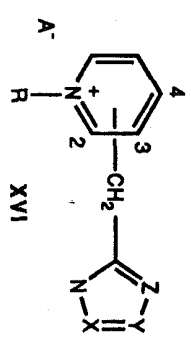
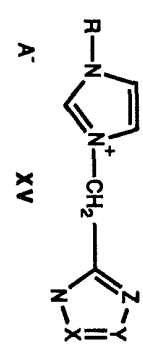
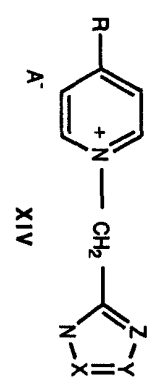
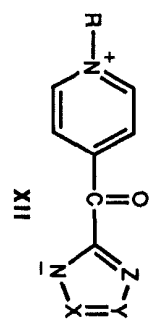
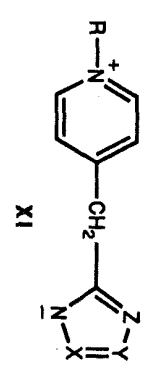
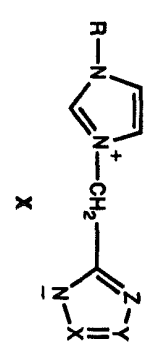
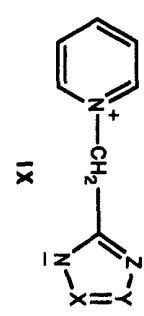
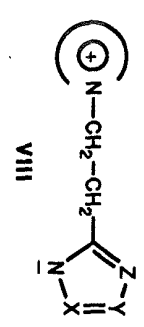
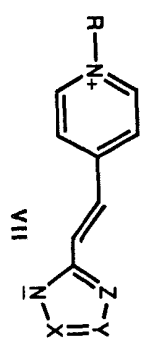
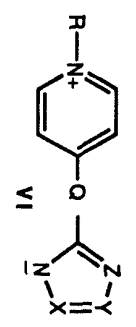
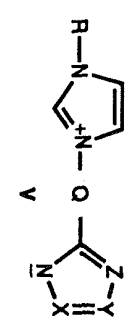
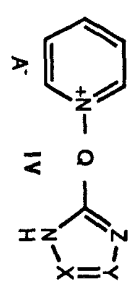
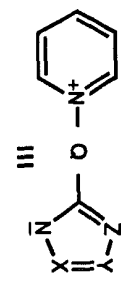
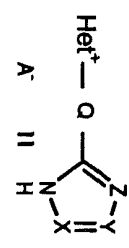
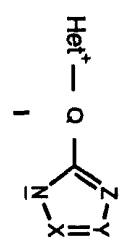


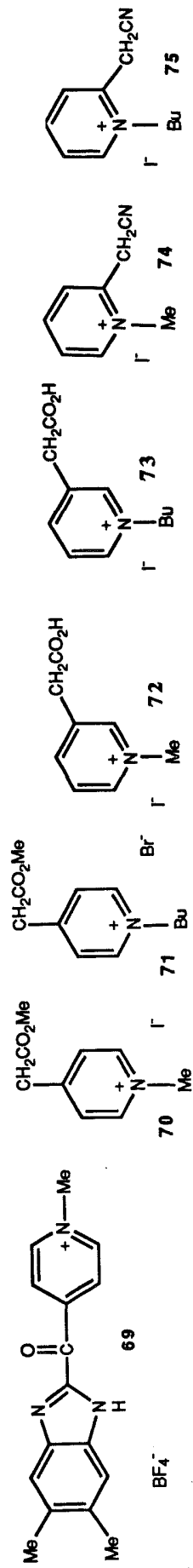
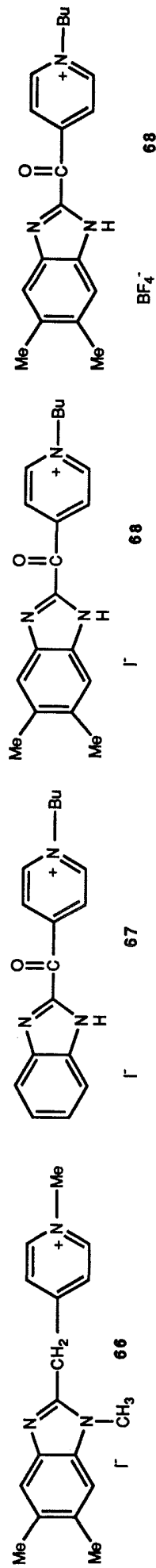
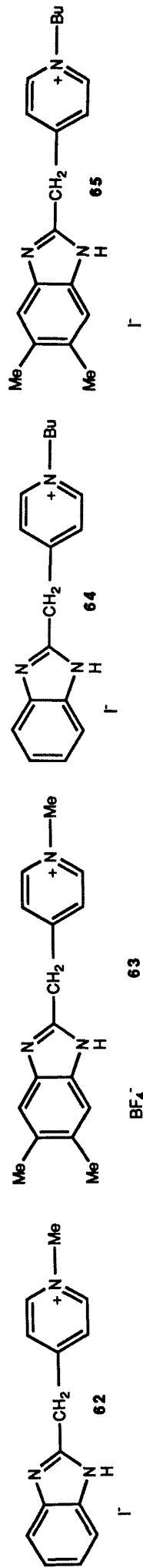
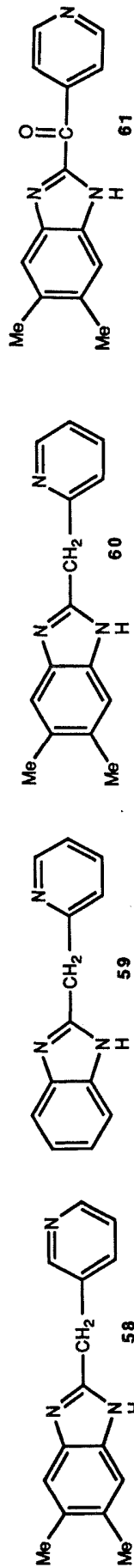
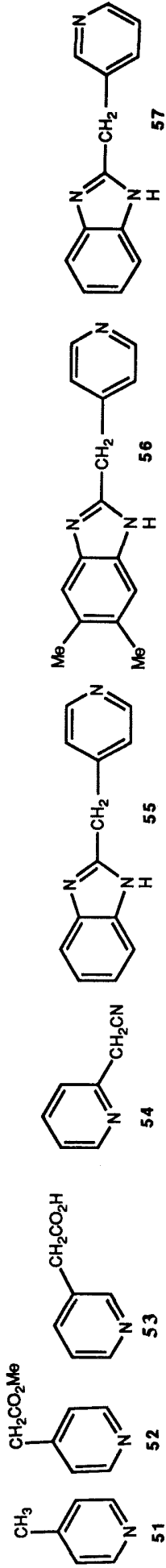
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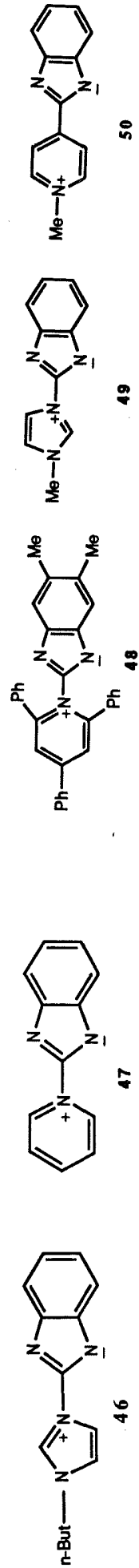
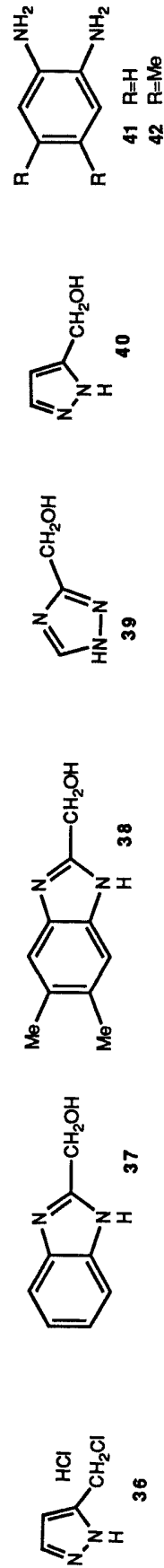
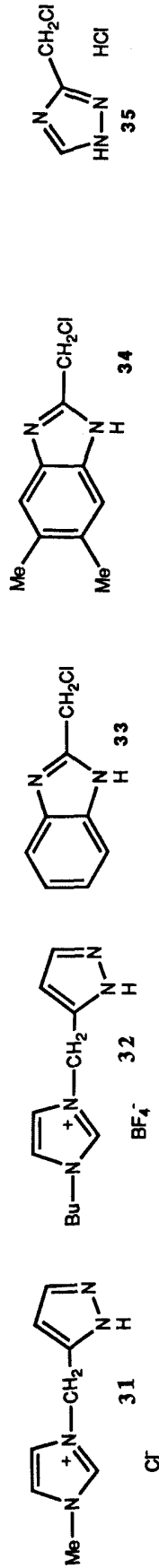
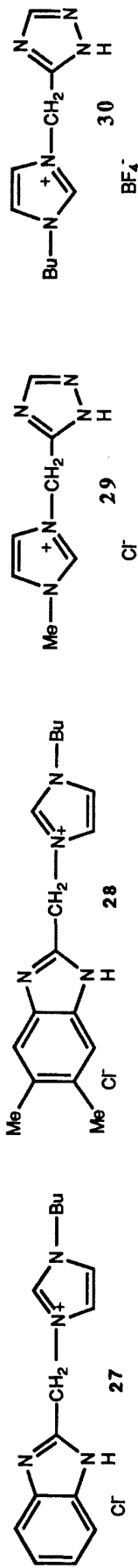
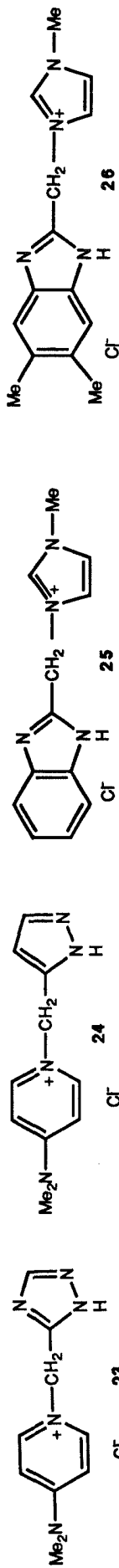












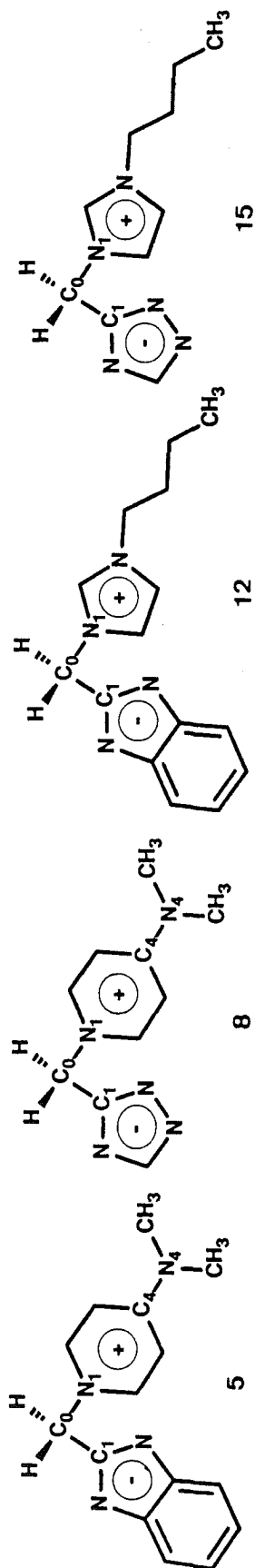
Fe d'errades:

- Texte pàgina 87.

Esquema 30

En conclusió, la inestabilitat referida, a causa dels processos d'oxidació, que experimenten les sals XVI, ens han tancat l'accés a l'obtenció de les corresponents sals internes XI, si bé aquestes sals XVI oxidades no es poden deixar de tenir en consideració respecte a les seves possibles potencials aplicacions: en un futur proper pensem aprofundir la transformació de les sals 67-69 en les corresponents sals internes XII. Així com la possible reducció asimètrica del grup carbonil proquiral^{49a}, encara que a priori sembli difícil aconseguir un bon excés enantiomèric de la reducció amb reactius quirals del grup carbonil unit a dos anells^{49b}, com passa en la sèrie benzènica, i.e. acetofenona versus arilfenilcetona.

Finalment cal dir que l'aplicació d'aquesta metodologia a la síntesi de les sals de 1-alkuil-3-(1H-benzimidazol-2-ilmetil)piridini XVIII i sals de 1-alkuil-2-(1H-benzimidazol-2-ilmetil)piridini XIX (vegis Figura 24, pàg 68), així com l'estudi bàsic del mecanisme oxidatiu de les estructures ja sintetitzades cau fora de l'abast del present Tesi Doctoral.



| | | $\widehat{C_1C_0N_1}$ | $\widehat{HC_0H}$ | C_1C_0 | C_0N_1 | C_4N_4 | MD _{calc} | MD _{exp} |
|------|------|-----------------------|--|----------|----------|----------|--|-------------------|
| 5 | AMI | 110.50 | 109.53 | 1.484 | 1.484 | 1.370 | 17.85 | 12.34 |
| | MNDO | 108.34 | 107.02 | 1.478 | 1.534 | 1.389 | 17.13 | |
| 5-RX | AMI | 111.05 | $\begin{pmatrix} 110.41 \\ 106.93 \end{pmatrix}$ | 1.498 | 1.488 | 1.332 | $\begin{pmatrix} 20.60 \\ 20.75 \end{pmatrix}$ | (1) |
| | MNDO | | | | | | | |
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| | MNDO | 108.16 | 107.65 | 1.478 | 1.523 | | 15.76 | |
| 15 | AMI | 111.56 | 109.87 | 1.467 | 1.476 | | 15.39 | 15.34 |
| | MNDO | 108.74 | 107.86 | 1.463 | 1.532 | | 15.49 | |

Taula VIII(cont.)

