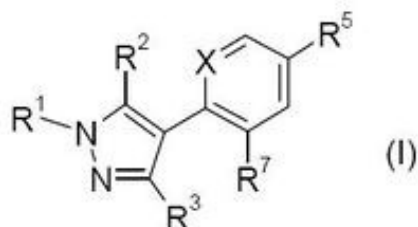


# Markush Structure Search Sample

## Contents

- 1 Patent FTO Search for the Generic compound
- 2 Exact match structures
  - ◆ 2.1 Structure-1 (12(doc1))
    - ◇ 2.1.1 DE4124942
  - ◆ 2.2 Structure-2 (9(doc2))
    - ◇ 2.2.1 WO2007081019
  - ◆ 2.3 Structure-3 (125(doc2))
    - ◇ 2.3.1 JP11130754
  - ◆ 2.4 Structure-4 (109(doc2))
    - ◇ 2.4.1 WO2006078610
  - ◆ 2.5 Structure-5 (128(doc2))
    - ◇ 2.5.1 US5827602
  - ◆ 2.6 Structure-6 (19(doc2))
    - ◇ 2.6.1 US 2007100181
  - ◆ 2.7 Structure-7 (88(doc2))
    - ◇ 2.7.1 DE19503827
  - ◆ 2.8 Structure-8 (86(doc2))
    - ◇ 2.8.1 WO9702252
  - ◆ 2.9 Structure-9 (41(doc2))
    - ◇ 2.9.1 JP2005216490
  - ◆ 2.10 Structure-10 (61(doc1))
    - ◇ 2.10.1 WO2004063166
- 3 Exact match structures but mentioned as optionally substituted at 4th position of pyrazole of generic structure
  - ◆ 3.1 Structure-1 (84(doc2))
    - ◇ 3.1.1 WO9711952
  - ◆ 3.2 Structure-2 (74(doc2))
    - ◇ 3.2.1 WO0130154
  - ◆ 3.3 Structure-3 (39(doc2))
    - ◇ 3.3.1 JP2005272306
  - ◆ 3.4 Structure-4 (25(doc2))
    - ◇ 3.4.1 US2007066822
  - ◆ 3.5 Structure-5 (23(doc2))
    - ◇ 3.5.1 US2007066854
  - ◆ 3.6 Structure-6 (90(doc2))
    - ◇ 3.6.1 FR2723091
  - ◆ 3.7 Structure-7 (92(doc2))
    - ◇ 3.7.1 WO9600218
  - ◆ 3.8 Structure-8 (95(doc2))
    - ◇ 3.8.1 WO9524403
  - ◆ 3.9 Structure-9 (98(doc2))
    - ◇ 3.9.1 JP6345728
  - ◆ 3.10 Structure-10 (34(doc2))
    - ◇ 3.10.1 WO2006084262
- 4 Relevant structures with missing substituents
  - ◆ 4.1 Structure-1
    - ◇ 4.1.1 JP09204932
  - ◆ 4.2 Structure-2
    - ◇ 4.2.1 WO0018741
  - ◆ 4.3 Structure-3
    - ◇ 4.3.1 EP335381
  - ◆ 4.4 Structure-4
    - ◇ 4.4.1 US5296484
  - ◆ 4.5 Structure-5
    - ◇ 4.5.1 US2006122256
  - ◆ 4.6 Structure-6
    - ◇ 4.6.1 JP2004317641
  - ◆ 4.7 Structure-7
    - ◇ 4.7.1 JP2004317640
  - ◆ 4.8 Structure-8
    - ◇ 4.8.1 US2005135045
  - ◆ 4.9 Structure-9
    - ◇ 4.9.1 WO2006124776
  - ◆ 4.10 Structure-10
    - ◇ 4.10.1 WO2007038363
  - ◆ 4.11 Structure-11
    - ◇ 4.11.1 US2007100184
  - ◆ 4.12 Structure-12
    - ◇ 4.12.1 US2005020646
  - ◆ 4.13 Structure-13
    - ◇ 4.13.1 EP548680
  - ◆ 4.14 Structure-14
    - ◇ 4.14.1 WO2003087062
  - ◆ 4.15 Structure-15
    - ◇ 4.15.1 WO200066562
- 5 Relevant structures with substituent variation
  - ◆ 5.1 Structure-1
    - ◇ 5.1.1 EP0080051
  - ◆ 5.2 Structure-2
    - ◇ 5.2.1 US2005159470
- 6 Other structures
  - ◆ 6.1 WO2007070607

## Patent FTO Search for the Generic compound



wherein

$R^1$  is  $C_1$ - $C_4$ alkyl or  $C_1$ - $C_4$ haloalkyl;

$R^2$  is an optionally substituted aryl or heteroaryl;

$R^3$  is halogen;

$R^4$  is hydrogen, halogen,  $C_1$ - $C_4$  alkyl,  $C_1$ - $C_4$  haloalkyl, cyano or  $OR^6$ ;

$R^5$  is hydrogen, halogen,  $C_1$ - $C_4$  alkyl,  $C_1$ - $C_4$  haloalkyl, cyano or  $OR^6$ ;

$R^6$  is hydrogen,  $C_1$ - $C_6$  alkyl,  $C_3$ - $C_7$  cycloalkyl,  $C_3$ - $C_{10}$  alkylcycloalkyl,  $C_1$ - $C_6$  haloalkyl,  $C_2$ - $C_6$  alkenyl,

$C_6$  haloalkenyl,  $C_3$ - $C_7$  cycloalkenyl,  $C_2$ - $C_6$  alkynyl,  $C_2$ - $C_6$  haloalkynyl,  $C_2$ - $C_6$  alkyloxyalkyl;

$R^7$  is halogen or  $OR^6$ ;

X is N or  $C-R^4$ ;

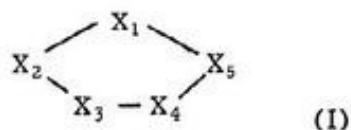
or an agrochemically usable salt form thereof.



## Exact match structures

### Structure-1 (12(doc1))

DE4124942



one of the gps.  $X_1 - X_5 = A-B-C-N<$  ,  $A-B-C-CH<$  or

$A-B-C-C\equiv$  ;

a second gp. =  $F'-E-D-N<$  ,

$F'-E-D-CH<$  or  $F'-C-D-C\equiv$  ;



a third gp. = S, sulphenyl, sulphinyl,  $R_1N<$  ,  $R_2C\equiv$  ,

$(R_2)_2C<$  or N;

a fourth gp. = O, S, N,  $SO_2$  or  $R_2C\equiv$  , or may also be

$C=O$  when this gp. is not between 2 N atoms;

a fifth = N,  $R_2C\equiv$  or  $(R_2)_2C<$  ; or



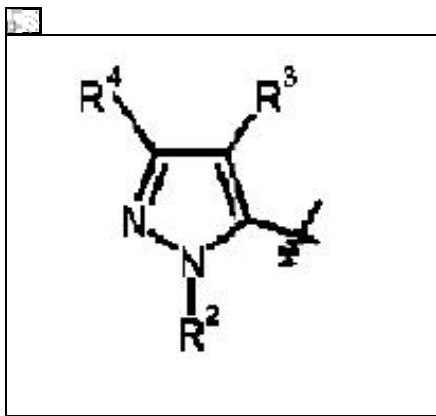
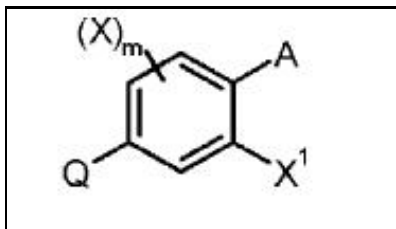
•  $X_1 = A-B-C-C(sp^2 \text{ carbon})$ ,  $X_2 = F-C-D-C(sp^2 \text{ carbon})$ ,  $X_3 = R_1-N<$ ,  $X_4 = N$ ,  $X_5 = R_2-C(sp^2 \text{ carbon})$

- $X_1$ : A = H, B = bond, C = (b) under B which is halo substituted phenylene which completely matches with 4<sup>th</sup> position substituent of the generic compound
- $X_2$ : D = (b) under B is a phenylene (implies a substituted aryl) and F-C- is a substituent on D. It is clear that this will match with  $R^2$  (substituent aryl) at the 5<sup>th</sup> position of pyrazole of the generic structure

3.  $X_3$ :  $R_1 = Q$ (alkyl) which matches with  $R^1$ (alkyl) at the 1<sup>st</sup> position of pyrazole of the generic structure
4.  $X_4$ : N which matches with the 2<sup>nd</sup> position of pyrazole of the generic compound
5.  $X_5$ :  $R_2 = Cl, Br$  which matches with  $R^3$ (halogen) at the 3<sup>rd</sup> position of pyrazole of the generic structure

## Structure-2 (9(doc2))

WO2007081019

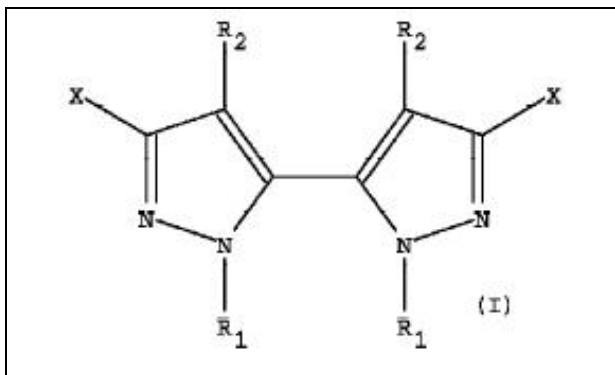


In the above phenyl ring  $Q$  is pyrazole.

- $R^2$  = alkyl which matches with  $R^1$ (alkyl) at 1<sup>st</sup> position of pyrazole of the generic compound.
- $R^4$  is halogen which matches with  $R^3$ (halogen) at 3<sup>rd</sup> position of pyrazole of the generic compound
- 4<sup>th</sup> position of above pyrazole is trihalo substituted aryl which matches with substituent at 4<sup>th</sup> position of pyrazole of generic compound .
- 5<sup>th</sup> position of pyrazole ring is above substituted aryl which matches with  $R^2$ (substituted aryl) at the 5<sup>th</sup> position of pyrazole of generic compound.

## Structure-3 (125(doc2))

JP11130754

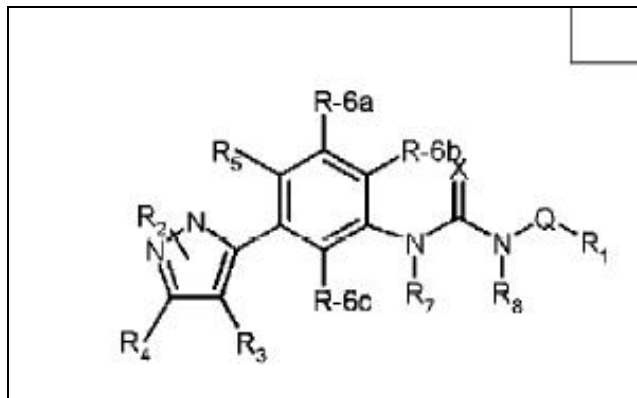


Consider left side ring the pyrazole ring

- $R_1$  is 1-4C alkyl which is matching with substituent  $R^1$ (first position) of the generic structure
- $X$  is Cl so it is matching with the substituent  $R^3$  (second position) of the generic structure
- $R_2$  is phenyl substituted by halo, 1-4C alkyl, cyano which is matching with the fourth position of the generic structure
- In the fifth position pyrazole(heteroaryl) is there?which is matching with the substituent  $R^2$ (fifth position) of the generic structure.

## Structure-4 (109(doc2))

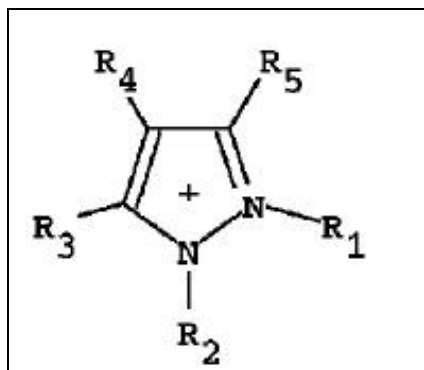
WO2006078610



- R<sub>2</sub> is 1-6C alkyl which is matching with substituent R<sup>1</sup>(first position) of the generic structure
- R<sub>4</sub> is halo matching with the substituent R<sup>3</sup> (second position) of the generic structure
- R<sub>3</sub> is heteroaryl or phenyl substituted by 1-8C alkyl, halo, CN, 1-6C alkoxy which is matching with the fourth position of the generic structure
- In fifth position substituted aryl ring there, which is matching with the substituent R<sup>2</sup>(fifth position) of the generic structure.

### Structure-5 (128(doc2))

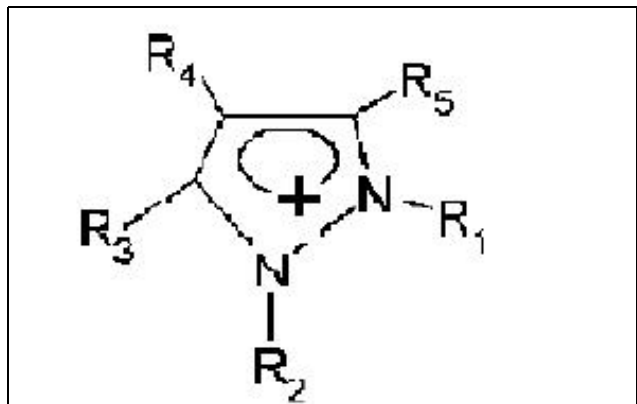
US5827602



- R<sub>1</sub>-R<sub>6</sub>=H, F, 1-4C alkyl, phenyl
- R<sub>2</sub>= 1-4C alkyl which matches with R<sup>1</sup>(alkyl) at 1<sup>st</sup> position of pyrazole of the generic structure
- R<sub>5</sub>= F which matches with R<sup>3</sup>(halo)at 1<sup>st</sup> position of pyrazole of the generic structure
- R<sub>4</sub>= phenyl substituted with an electron with drawing group matches with substituent at 4<sup>th</sup> position of pyrazole of generic structure
- R<sub>3</sub>= substituted aryl which matches with R<sup>2</sup>(substituted aryl) at 5<sup>th</sup> position of pyrazole of the generic structure

### Structure-6 (19(doc2))

US 2007100181





$R_1-R_2 = H, -C_2H_5$  which matches with  $R^1$ (alkyl) at 1<sup>st</sup> position of pyrazole of generic structure

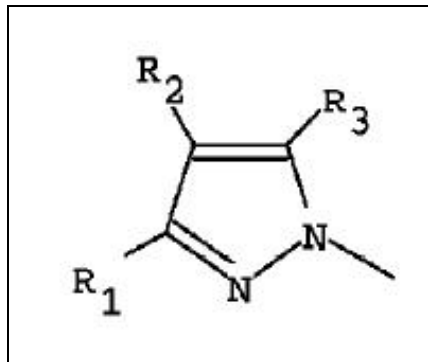
$R_3 =$  halogen which matches with  $R^3$ (halogen) at 3<sup>rd</sup> position of pyrazole of generic structure

$R_4 =$  6-25C heteroaryl having 1-3 heteroatoms(N)(could be pyridine) with substituents as halo, OH and alkyl which completely resembles substituent at 4<sup>th</sup> position of pyrazole of the generic structure

$R_5 =$  6-25C heteroaryl having 1-3 heteroatoms(N)(could be pyridine) with substituents which resembles  $R^2$ (substituted aryl) at 5<sup>th</sup> position of pyrazole of generic structure

### Structure-7 (88(doc2))

DE19503827



Q- $R_4$

Q= above structure

$R_4 = CR_5R_6R_7$  where  $R_5 =$  1-4C alkyl,  $R_6 = H$  so no need of  $R_7$

$R_4$  matches with  $R^1$ (alkyl) at 1<sup>st</sup> position of pyrazole of generic structure

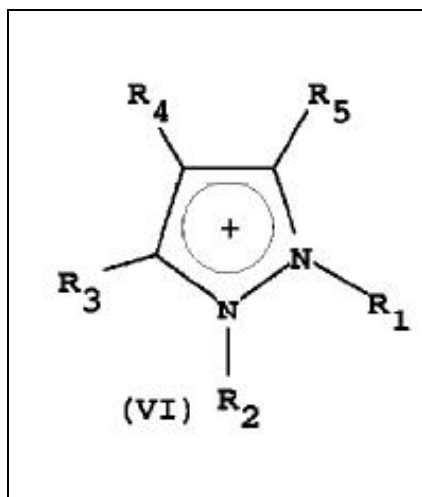
$R_1 =$  halo matches with  $R^3$ (halogen) at 3<sup>rd</sup> position of pyrazole of generic structure

$R_2 =$  alkylaryl substituted by halo matches with substituent at 4<sup>th</sup> position of pyrazole of generic structures

$R_3 =$  substituted aryl which resembles  $R^2$ (substituted aryl) at 5<sup>th</sup> position of pyrazole of generic structure

### Structure-8 (86(doc2))

WO9702252



$R_1-R_2 =$  1-4C alkyl, H matches with  $R^1$ (alkyl) at 1<sup>st</sup> position of pyrazole of generic structure

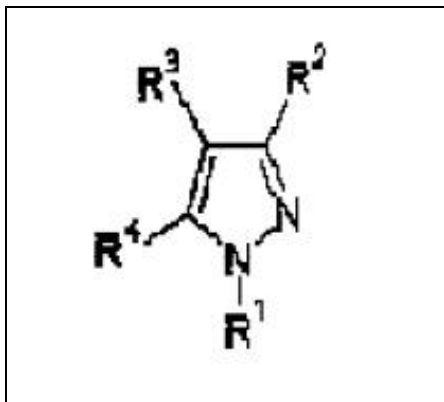
$R_3 =$  halogen matches with  $R^3$ (halogen) at 3<sup>rd</sup> position of pyrazole of generic structure

$R_4 =$  phenyl substituted with electron withdrawing group(halogens) matches with substituent at 4<sup>th</sup> position of pyrazole of generic structures

$R_5 =$  substituted aryl which resembles  $R^2$ (substituted aryl) at 5<sup>th</sup> position of pyrazole of generic structure

### Structure-9 (41(doc2))

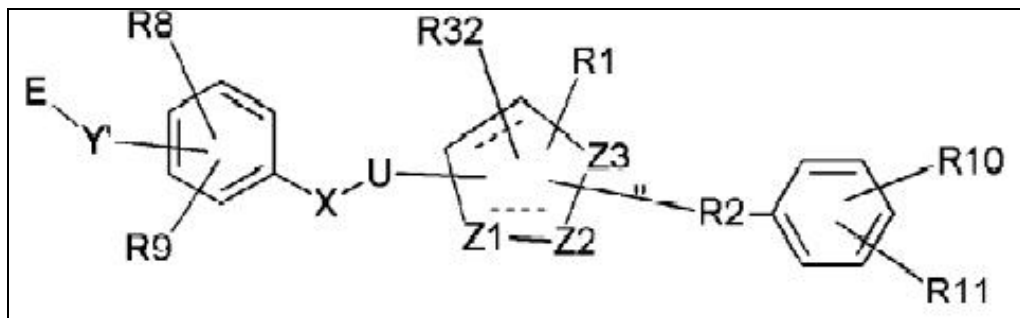
JP2005216490



- R<sup>1</sup> = lower alkyl which matches with R<sup>1</sup>(alkyl) at 1<sup>st</sup> position of pyrazole of the generic structure
- R<sup>2</sup> = halogen which matches with R<sup>3</sup>(halogen) at 3<sup>rd</sup> position of pyrazole of the generic structure
- R<sup>3</sup> = methoxyphenyl which indicates substituent at 4<sup>th</sup> position of generic structure
- R<sup>4</sup> = methoxy phenyl which matches with R<sup>2</sup>(substituted aryl) at 5<sup>th</sup> position of pyrazole of generic structure

### Structure-10 (61(doc1))

WO2004063166

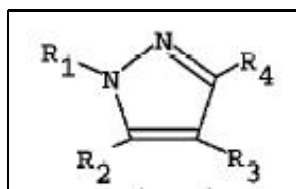


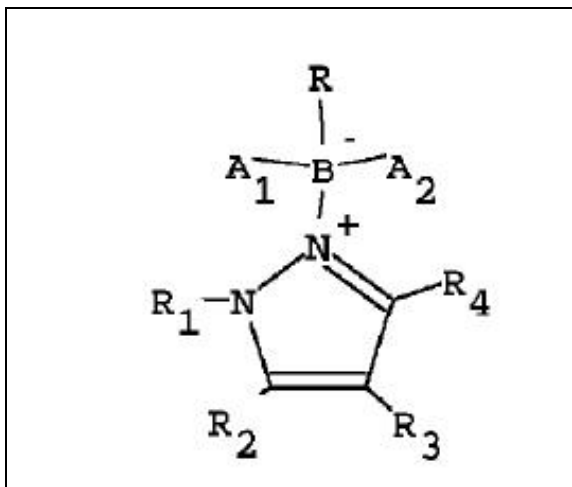
- Z<sup>1</sup> = C, Z<sup>2</sup> = N, Z<sup>3</sup> = N Which indicates pyrazole ring.
- R<sup>1</sup> = Alkyl which matches with R<sup>1</sup>(alkyl) at the 1<sup>st</sup> position of pyrazole of the generic compound
- R<sup>32</sup> = halo which matches with R<sup>3</sup>(halogen) at the 3<sup>rd</sup> position of pyrazole of the generic compound
- R<sup>2</sup>(0-8Calkyl) so it may be ?0?C alkyl implies it is simply a bond, bonded to a substituted phenyl ring which matches with R<sup>2</sup>(substituted aryl) at the 5<sup>th</sup> position of pyrazole of the generic structure
- U is an aliphatic linker(linker means a bond, aliphatic means saturated. So aliphatic linker means saturated bond which implies a single bond) so it is a bond and X is a single bond linked to substituted aryl with halogens and cycloalkyl as substituents which matches with 4<sup>th</sup> position of pyrazole of the generic compound.

### Exact match structures but mentioned as optionally substituted at 4<sup>th</sup> position of pyrazole of generic structure

#### Structure-1 (84(doc2))

WO9711952

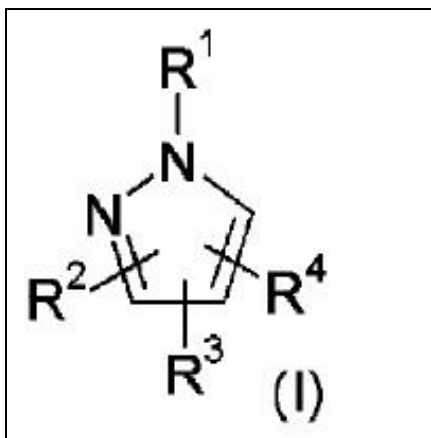




- $R_1$ - $R_4$ = 1-8C alkyl, haloalkyl, halo, phenyl(optionally substituted by halo, 1-4C alkyl, haloalkyl, alkoxy,)
- $R_1$ = 1-8C alkyl which matches with  $R^1$ (1-4C alkyl) at 1<sup>st</sup> position of pyrazole of generic structure
- $R_4$ = halo which matches with  $R^3$ (halogen) at 3<sup>rd</sup> position of pyrazole of generic structure
- $R_3$ = phenyl(optionally substituted by halo, alkoxy) which matches with substituent at 4<sup>th</sup> position of pyrazole of the generic structure
- $R_2$ = phenyl(optionally substituted) which matches with  $R^2$ (substituted aryl) at 5<sup>th</sup> position of pyrazole of the generic structure

### Structure-2 (74(doc2))

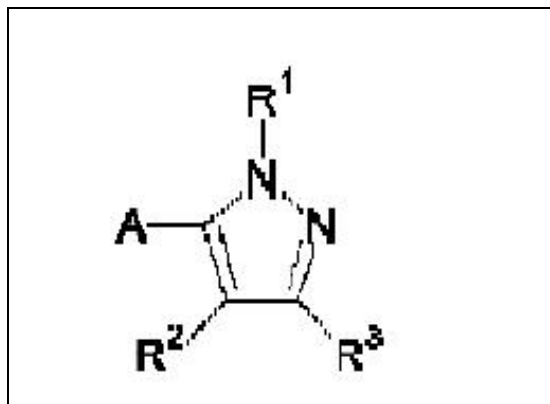
WO0130154



- $R^1$ = (1-6C)alkyl which matches with  $R^1$ (1-4C alkyl) at 1<sup>st</sup> position of pyrazole of the generic compound
- $R^2$ = halo which matches with  $R^3$ (halogen) at 3<sup>rd</sup> position of pyrazole of the generic compound
- $R^3$ = phenyl optionally substituted with halo, 1-6C alkyl, 1-6C alkoxy which matches with substituent at 4<sup>th</sup> position of pyrazole of the generic compound
- $R^4$ = heterocyclyl containing 1 or 2N and optionally substituted which matches with  $R^2$ (optionally substituted heteroaryl) at 5<sup>th</sup> position of the generic compound

### Structure-3 (39(doc2))

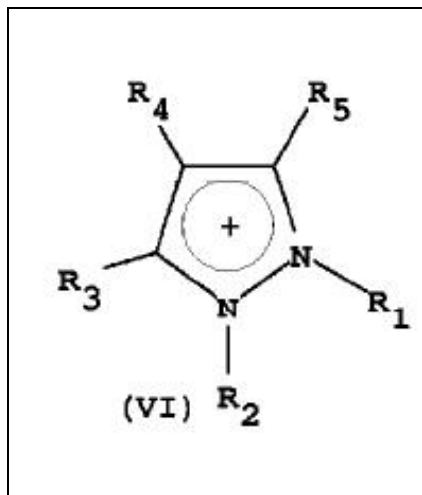
JP2005272306



- A= substituted heteroaryl which matches with R<sup>2</sup>(substituted aryl) at 5<sup>th</sup> position of pyrazole of the generic structure
- R<sup>1</sup>= alkyl which matches with R<sup>1</sup>(alkyl) at 1<sup>st</sup> position of pyrazole of generic structure
- R<sup>3</sup>= halogen which matches with R<sup>3</sup>(halogen) at 3<sup>rd</sup> position of pyrazole of generic structure
- R<sup>2</sup>= phenyl optionally substituted by Y(1-6C alkyl), 1-6C alkoxy and matches with substituent at 4<sup>th</sup> position of pyrazole of generic structure

### Structure-4 (25(doc2))

US2007066822



- R<sup>1</sup>-R<sup>2</sup>= H, -CH<sub>3</sub>, -C<sub>2</sub>H<sub>5</sub> which matches with R<sup>1</sup>(alkyl) at 1<sup>st</sup> position of pyrazole of generic structure
- R<sup>3</sup>= halogen which matches with R<sup>3</sup>(halogen) at 3<sup>rd</sup> position of pyrazole of generic structure
- R<sup>4</sup>= 6-25C optionally substituted heteroaryl which resembles substituent at 4<sup>th</sup> position of pyrazole of the generic structure
- R<sup>5</sup>= optionally substituted 6-25C heteroaryl which resembles R<sup>2</sup>(substituted aryl) at 5<sup>th</sup> position of pyrazole of generic structure

### Structure-5 (23(doc2))

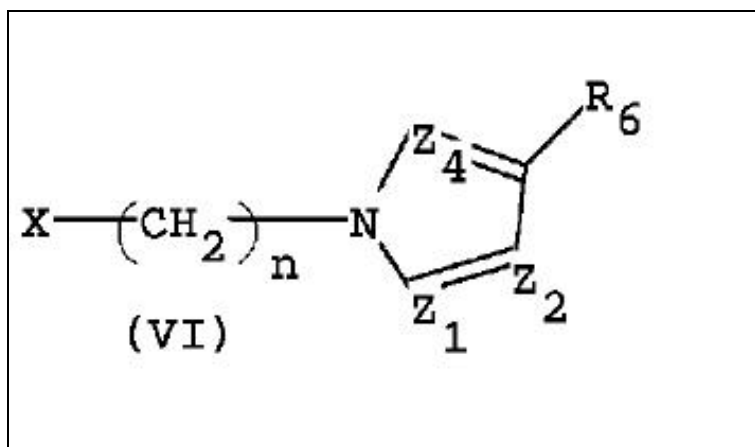
US2007066854

- Z<sup>+</sup>= pyrazolium (substituted at 1-5 R<sub>1</sub>-R<sub>5</sub>)
- R<sub>1</sub>= -CH<sub>3</sub>, -C<sub>2</sub>H<sub>5</sub> which matches with R<sup>1</sup>(alkyl) at 1<sup>st</sup> position of pyrazole of generic structure
- R<sub>3</sub>= halogen which matches with R<sup>3</sup>(halogen) at 3<sup>rd</sup> position of pyrazole of generic structure
- R<sub>4</sub>= 6-25C aryl optionally substituted by C<sub>2</sub>H<sub>5</sub>, OH which resembles substituent at 4<sup>th</sup> position of pyrazole of the generic structure
- R<sub>5</sub>= optionally substituted 6-25C heteroaryl which resembles R<sup>2</sup>(substituted aryl) at 5<sup>th</sup> position of pyrazole of generic structure

### Structure-6 (90(doc2))

FR2723091





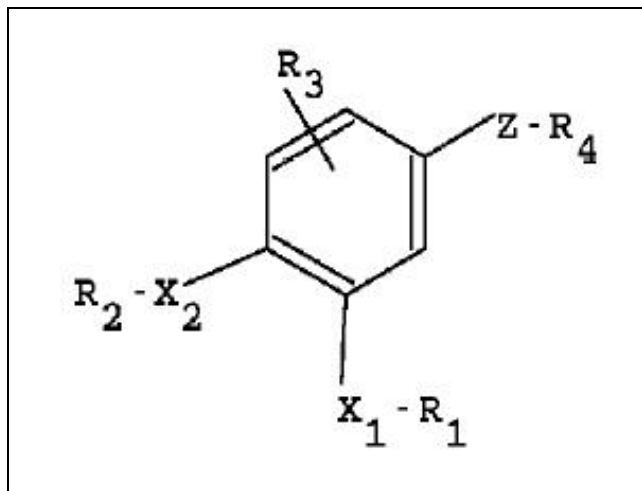
X= halo, n= 2-4

Z<sub>1</sub>= N, Z<sub>2</sub>= CR<sub>5</sub>, Z<sub>4</sub>= CR<sub>7</sub>

R<sub>4</sub>-R<sub>7</sub>= alkyl matches with R<sup>1</sup>(alkyl) at 1<sup>st</sup> position of pyrazole of generic structure; halogen matches with R<sup>3</sup>(halogen) at 3<sup>rd</sup> position of pyrazole of generic structure; optionally substituted aryl which resembles R<sup>2</sup>(substituted aryl) at 5<sup>th</sup> position of pyrazole of generic structure and matches with substituent at 4<sup>th</sup> position of pyrazole of generic structures

### Structure-7 (92(doc2))

WO9600218

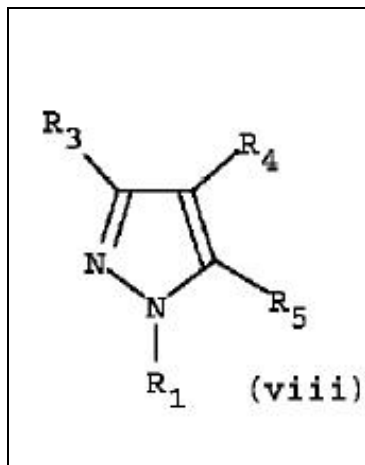


Z= a bond,

R<sub>4</sub> is a pyrazole with substituents as 1-4C alkyl matches with R<sup>1</sup>(alkyl) at 1<sup>st</sup> position of pyrazole of generic structure; halo matches with R<sup>3</sup>(halogen) at 3<sup>rd</sup> position of pyrazole of generic structure; optionally substituted aryl which resembles R<sup>2</sup>(substituted aryl) at 5<sup>th</sup> position of pyrazole of generic structure and matches with substituent at 4<sup>th</sup> position of pyrazole of generic structures

### Structure-8 (95(doc2))

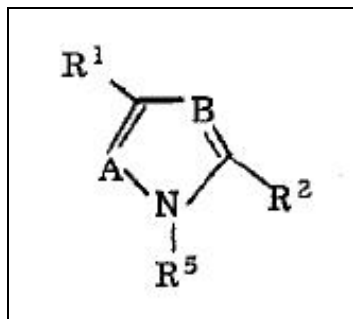
WO9524403



- $R_1$  = alkyl which matches with  $R^1$ (alkyl) at 1<sup>st</sup> position of pyrazole of the generic structure
- $R_3$  = halo which matches with  $R^3$ (halogen) at 3<sup>rd</sup> position of pyrazole of the generic structure
- $R_4$  = heteroaryl optionally substituted indicating substituent at 4<sup>th</sup> position of pyrazole of the generic structure
- $R_5$  = optionally substituted heteroaryl which matches with  $R^2$ (optionally substituted heteroaryl) at 5<sup>th</sup> position of pyrazole of the generic structure

### Structure-9 (98(doc2))

JP6345728



- $A = N$ ,  $B = CR^4$
- $R^5$  = 1-6C alkyl which matches with  $R^1$ (alkyl) at 1<sup>st</sup> position of pyrazole of the generic structure
- $R^3$  = halogen which matches with  $R^3$ (halogen) at 3<sup>rd</sup> position of pyrazole of the generic structure
- $R^4$  = phenyl(optionally substituted by halo, CN, alkoxy)indicating substituent at 4<sup>th</sup> position of pyrazole of the generic structure
- $R^2$  = optionally substituted phenyl which matches with  $R^2$ (optionally substituted aryl) at 5<sup>th</sup> position of pyrazole of the generic structure

### Structure-10 (34(doc2))

WO2006084262

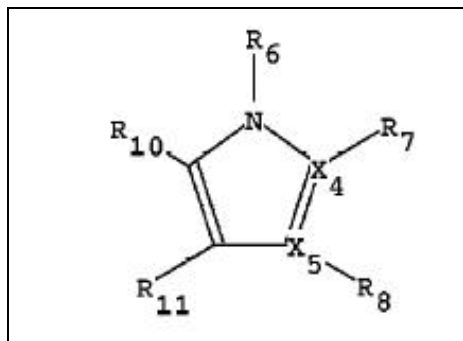
It is pyrazolium with substituents

$R_1$ - $R_5$  = halogen matches with  $R^3$ (halogen) at 3<sup>rd</sup> position of pyrazole of generic structure;  $-C_2H_5$  matches with  $R^1$ (alkyl) at 1<sup>st</sup> position of pyrazole of generic structure; 6-20C substituted aryl with substituents as halogen, OH which resembles substituent at 4<sup>th</sup> position of pyrazole of the generic structure;  $R^2$  = optionally substituted 6-20C heteroaryl which resembles  $R^2$ (substituted aryl) at 5<sup>th</sup> position of pyrazole of generic structure

## Relevant structures with missing substituents

### Structure-1

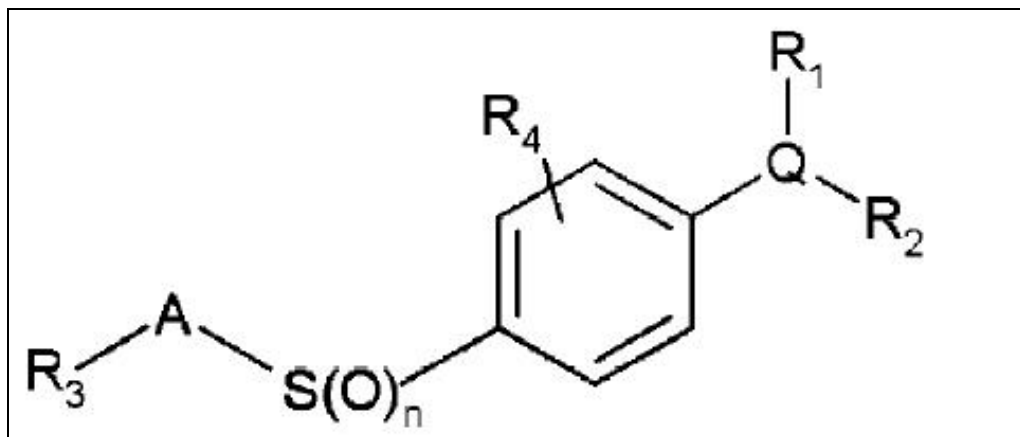
JP09204932



- $R_6$  is 1-3C alkyl which is matching with substituent  $R^1$  (first position) of the generic structure
- $R_7$  doesn't exist.. so it is matching with the second position of the generic structure.
- $R_8$  is halogen so it is matching with the substituent  $R^3$  (second position) of the generic structure
- $R_{11}$  is phenyl???(substituents are missing)??? which is matching with the fourth position of the generic structure
- $R_{10}$  is phenyl which is matching with the substituent  $R^2$  (fifth position) of the generic structure.

## Structure-2

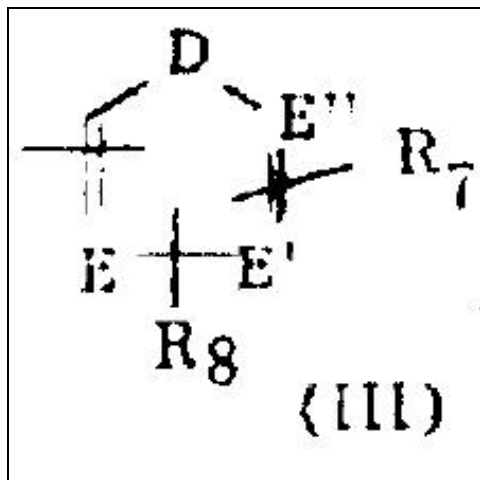
WO0018741



- Q= pyrazolyl
- In the above structure the substituted aryl bonded to Q(pyrazolyl) matches with  $R^2$  (substituted aryl) at 5<sup>th</sup> position of pyrazole of the generic structure
- $R_1$ = haloalkyl which matches with  $R^1$  (alkyl) at 1<sup>st</sup> position of the generic structure
- $R_2$ = aryl optionally substituted with halo, lower alkoxy, CN which matches with substituent at 4<sup>th</sup> position of pyrazole of the generic structure.
- But ??? $R^3$  (halogen) of pyrazole of generic structure is missing??? in the above structure

## Structure-3

EP335381



D= NR<sub>12</sub> , E??= N, E?= CH, E= CH

R<sub>12</sub>= alkyl matches with R<sup>1</sup>(alkyl) at 1<sup>st</sup> position of pyrazole of generic structure

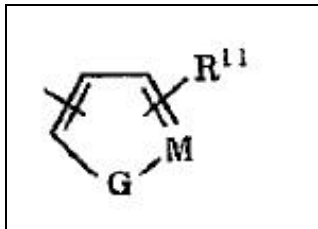
R<sub>7</sub>= halo matches with R<sup>3</sup>(halogen) at 3<sup>rd</sup> position of pyrazole of generic structure

R<sub>8</sub>= substituted benzene ring matches with substituent at 4<sup>th</sup> position (but missing substituents) of pyrazole of generic structures

Above pyrazole ring is attached to a substituted aryl matches with R<sup>2</sup>(substituted aryl) at 5<sup>th</sup> position of pyrazole of generic structure

#### Structure-4

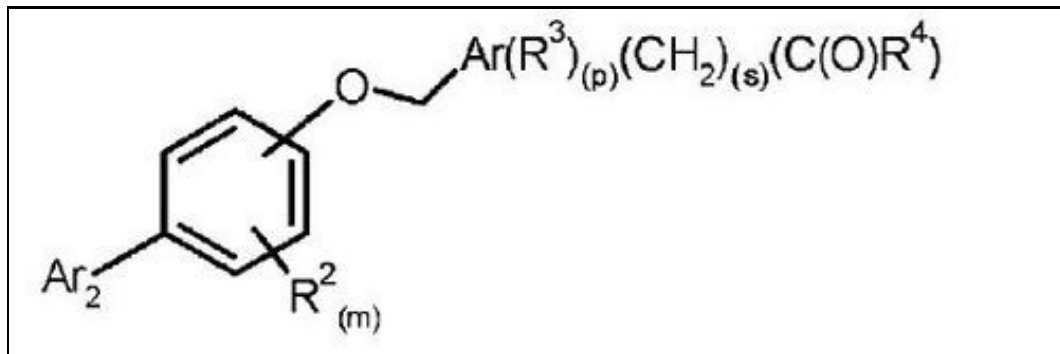
US5296484



- G= NR<sup>20</sup>, M= N
- R<sup>11</sup>= halo, 1-4C alkyl, phenyl
- This structure has substituted aryl at 5<sup>th</sup> position of pyrazole of the generic structure
- At 4<sup>th</sup> position of pyrazole i.e., aryl has no substituents compared to generic structure
- One more substituent is missing on the pyrazole ring

#### Structure-5

US2006122256

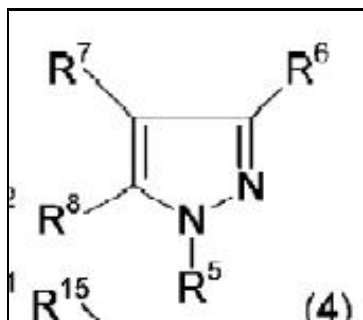


- AR<sup>2</sup>= pyrazol-4-yl optionally substituted by Q(halo, lower alkyl, phenyl)
- Q substituted on AR<sup>2</sup>(pyrazole) indicates R<sup>3</sup>, R<sup>1</sup> and R<sup>5</sup> of pyrazole of the generic structure

- At 4<sup>th</sup> substituent of pyrazole one substituent is missing and one substituent is varying

### Structure-6

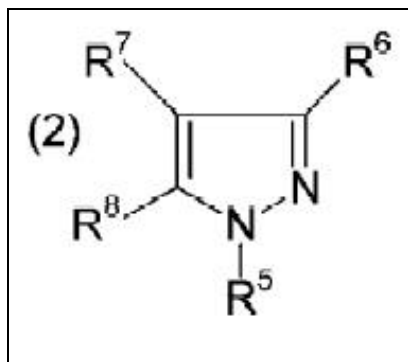
JP2004317641



- R<sup>5</sup>= alkyl which matches with R<sup>1</sup>(alkyl) at 1<sup>st</sup> position of pyrazole of the generic structure
- R<sup>6</sup>= halogen which matches with R<sup>3</sup>(halogen) at 3<sup>rd</sup> position of pyrazole of the generic structure
- R<sup>7</sup>= phenyl with no substituents. It represents substituent at 4<sup>th</sup> position of pyrazole of generic structure with substituents missing
- R<sup>8</sup>= phenyl which matches with R<sup>2</sup>(aryl) at 5<sup>th</sup> position of pyrazole of generic structure

### Structure-7

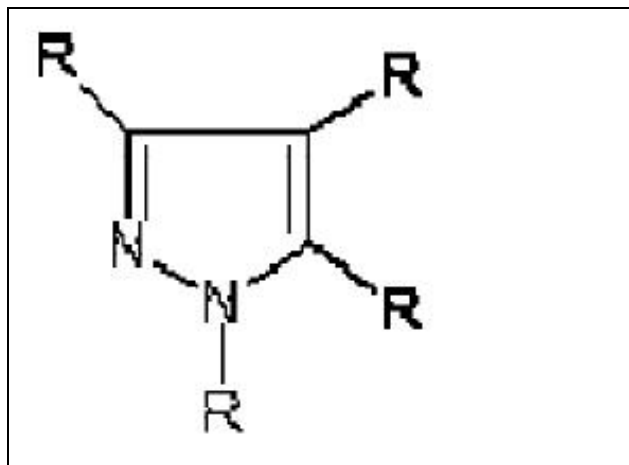
JP2004317640



- R<sup>5</sup>= alkyl which matches with R<sup>1</sup>(alkyl) at 1<sup>st</sup> position of pyrazole of the generic structure
- R<sup>6</sup>= halogen which matches with R<sup>3</sup>(halogen) at 3<sup>rd</sup> position of pyrazole of the generic structure
- R<sup>7</sup>= phenyl with no substituents. It represents substituent at 4<sup>th</sup> position of pyrazole of generic structure with substituents missing
- R<sup>8</sup>= phenyl which matches with R<sup>2</sup>(aryl) at 5<sup>th</sup> position of pyrazole of generic structure

### Structure-8

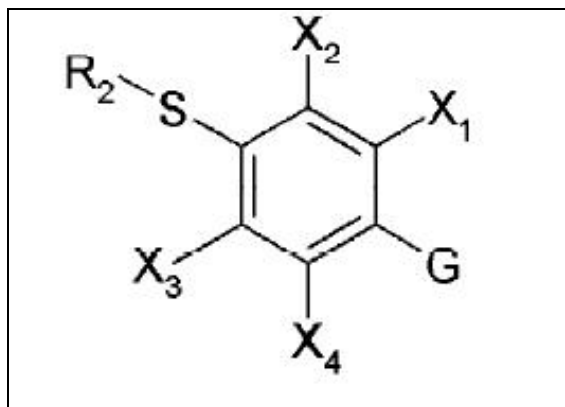
US2005135045



- R= 1-4C alkyl, halogen , phenyl
- R= alkyl which matches with R<sup>1</sup>(alkyl) at 1<sup>st</sup> position of pyrazole of the generic structure
- R= halogen which matches with R<sup>3</sup>(halogen) at 3<sup>rd</sup> position of pyrazole of the generic structure
- R= phenyl with no substituents. It represents substituent at 4<sup>th</sup> position of pyrazole of generic structure with substituents missing
- R= phenyl which matches with R<sup>2</sup>(aryl) at 5<sup>th</sup> position of pyrazole of generic structure

### Structure-9

WO2006124776



R<sup>1</sup>= H, R<sup>2</sup>= halogen, R<sup>3</sup>= pyrazole with substituents, R<sup>5</sup>= H, R<sup>6</sup>= H

R<sup>3</sup> is a pyrazole ring with substituents as:

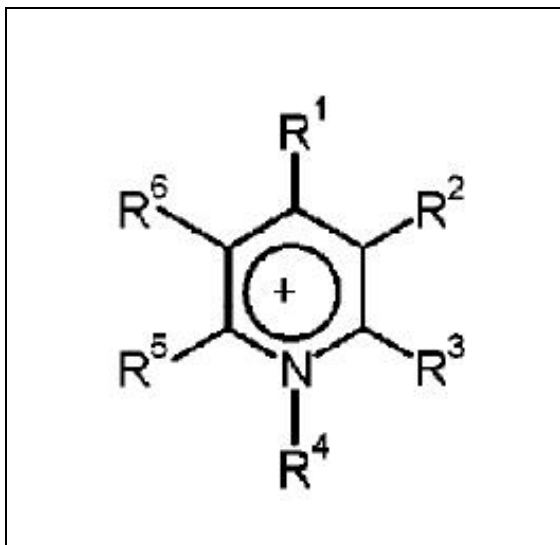
-CH<sub>3</sub> matches with R<sup>1</sup>(alkyl) of pyrazole of the generic structure

Above ring matches with substituent at 4<sup>th</sup> position of pyrazole of the generic structure

R<sup>3</sup> and R<sup>2</sup> of pyrazole of generic structure are missing

### Structure-10

WO2007038363



$R^1 = H$ ,  $R^2 = \text{halogen}$ ,  $R^3 = \text{pyrazole with substituents}$ ,  $R^5 = H$ ,  $R^6 = H$

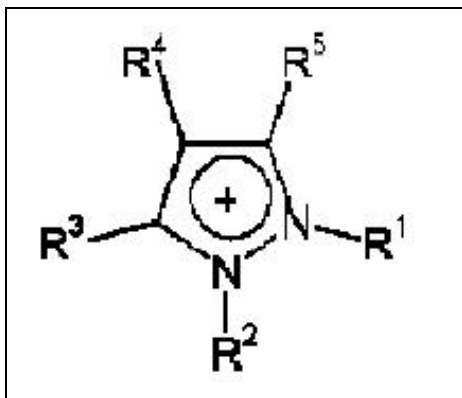
$R^3$  is defined as 3-25C substituted heteroaryl having 1-3 heteroatoms of N (so can be pyrazole) in which the substituents are  $-\text{CH}_3$ , halogen:  $-\text{CH}_3$  matches with  $R^1$  (alkyl) of pyrazole of the generic structure and halogen matches with  $R^3$  (halogen) of pyrazole of the generic structure

Above ring matches with substituent at 4<sup>th</sup> position of pyrazole of the generic structure

$R^2$  (substituted aryl) of pyrazole of generic structure missing

### Structure-11

US2007100184



$R_1 = H$

$R_2 = -\text{C}_2\text{H}_5$  which matches with  $R^1$  (alkyl) at 1<sup>st</sup> position of pyrazole of generic structure

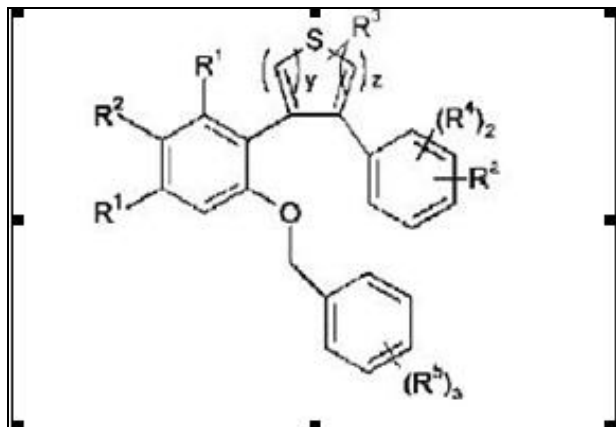
$R_3 = \text{halogen}$  which matches with  $R^3$  (halogen) at 3<sup>rd</sup> position of pyrazole of generic structure

$R_4 = \text{optionally substituted 6-25C heteroaryl with 1-3 of O, N, S or with 1-3 of } \text{CH}_3, \text{C}_2\text{H}_5, \text{3-25, preferably 3-20C straight, branched or cyclic alkane or alkene optionally substituted with halogens which resembles substituent at 4<sup>th</sup> position of pyrazole of the generic structure but } R^7 \text{ of pyrazole of generic structure is missing}$

$R_5 = \text{optionally substituted 6-25C heteroaryl which resembles } R^2 \text{ (substituted aryl) at 5<sup>th</sup> position of pyrazole of generic structure}$

### Structure-12

US2005020646

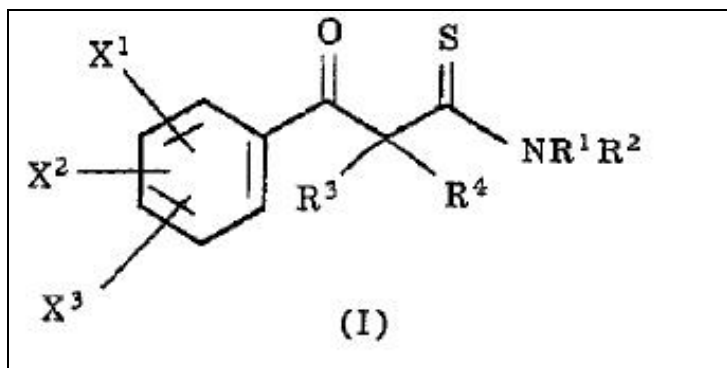


R<sup>2</sup>= pyrazolyl optionally substituted with 1-3 substituents of R<sup>11</sup> or 1-4C alkyl

R<sup>11</sup> is defined as halo matches with R<sup>3</sup>(halogen) at 3<sup>rd</sup> position of pyrazole of generic structure; pyridyl which resembles R<sup>2</sup>(substituted aryl) at 5<sup>th</sup> position of pyrazole of generic structure; pyridyl matches with substituent at 4<sup>th</sup> position of pyrazole of generic structures but R<sup>7</sup> of generic structure is missing

### Structure-13

EP548680



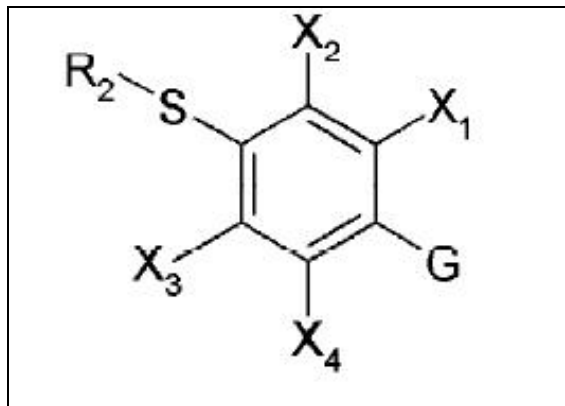
X<sup>1</sup>= het

Het = pyrazolyl with substituents alkyl matches with R<sup>1</sup>(alkyl) at 1<sup>st</sup> position of pyrazole of generic structure; halo matches with R<sup>3</sup>(halogen) at 3<sup>rd</sup> position of pyrazole of generic structure; phenyl matches with substituent at 4<sup>th</sup> position (but missing substituents) of pyrazole of generic structures

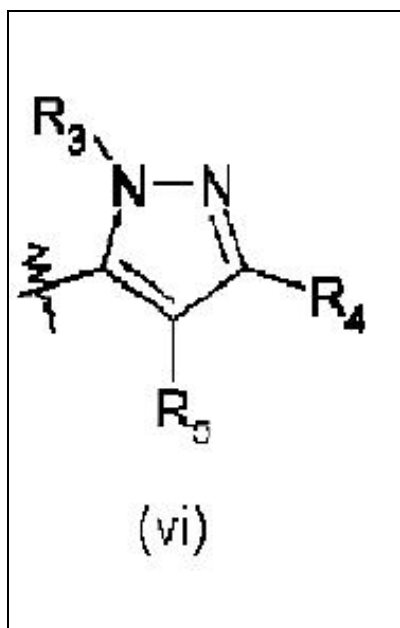
Above aryl ring is a substituent on X<sup>1</sup> which resembles R<sup>2</sup>(substituted aryl) at 5<sup>th</sup> position of pyrazole of generic structure

### Structure-14

WO2003087062







G= above pyrazole

R<sub>3</sub>= alkyl matches with R<sup>1</sup>(alkyl) at 1<sup>st</sup> position of pyrazole of generic structure

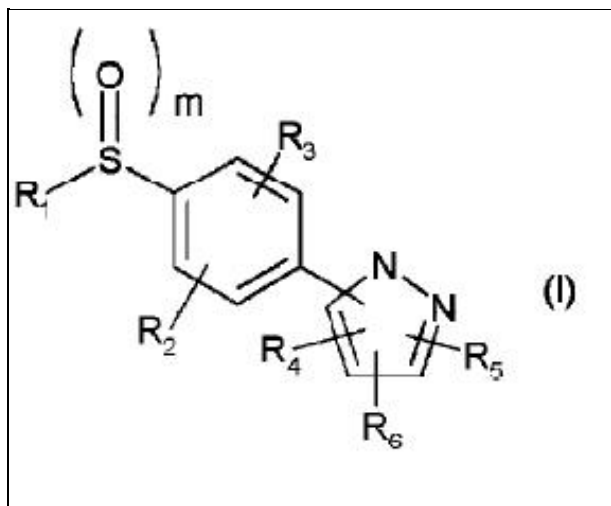
R<sub>4</sub>= halo matches with R<sup>3</sup>(halogen) at 3<sup>rd</sup> position of pyrazole of generic structure

R<sub>5</sub>= phenyl matches with substituent at 4<sup>th</sup> position (but missing substituents) of pyrazole of generic structures

Above given aryl matches with R<sup>2</sup>(substituted aryl) at 5<sup>th</sup> position of pyrazole of generic structure

### Structure-15

WO200066562



R<sub>4</sub>= alkyl matches with R<sup>1</sup>(alkyl) at 1<sup>st</sup> position of pyrazole of generic structure

R<sub>5</sub>= halo matches with R<sup>3</sup>(halogen) at 3<sup>rd</sup> position of pyrazole of generic structure

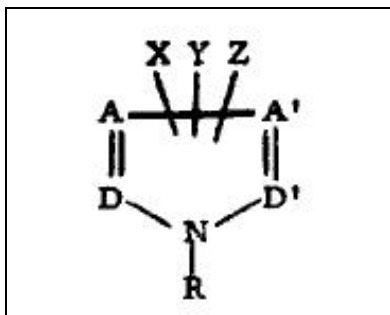
R<sub>6</sub>= optionally substituted aryl matches with substituent at 4<sup>th</sup> position (but missing substituents) of pyrazole of generic structures

Above given aryl matches with R<sup>2</sup>(substituted aryl) at 5<sup>th</sup> position of pyrazole of generic structure

### Relevant structures with substituent variation

#### Structure-1

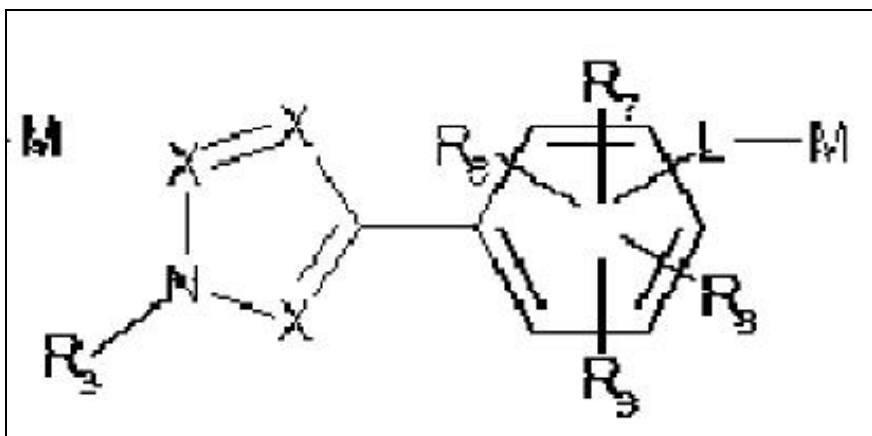
EP0080051



- In the above structure D is N & A, A', D? are considered as carbons? so it is forming a pyrazole ring.
- In the first position substituent R is 3-iodopropargyl, so it is matching with the substituent R<sup>1</sup> (first position) of the generic structure.
- X is Cl, so it is matching with the substituent R<sup>3</sup> (third position) of the generic structure.
- Y is 3-chloro-2-nitrophenyl which is matching with the ring of the fourth position of the generic structure but here ???substituent variation??? is there.
- Z is phenyl, so it is matching with the substituent R<sup>2</sup> (fifth position) of the generic structure.

## Structure-2

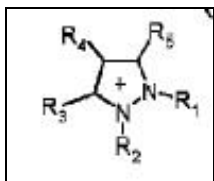
US2005159470



- First position: R<sub>3</sub> is alkyl, so it is matching with the substituent R<sup>1</sup> (first position) of the generic structure.
- Second position: X is N, so it is matching with second position of the generic structure.
- Third position: X is CR<sub>5</sub>, R<sub>5</sub> is halo so it is matching with the substituent R<sup>3</sup> (third position) of the generic structure.
- Fourth position: In fourth position substituted aryl ring is present??? (but it contains five substituents)???, is matching with fourth position of the generic structure.
- Fifth position: X is CR<sub>5</sub>, R<sub>5</sub> is heteroaryl, so it is matching with substituent R<sup>2</sup> (fifth position) of the generic structure.

## Other structures

WO2007070607



- R<sub>1</sub>-H,
- R<sub>2</sub> is ?C<sub>2</sub>H<sub>5</sub> which matches with R<sub>1</sub>(alkyl) at 1st position of the generic structure
- R<sub>5</sub> is halo which matches with R<sub>3</sub>(halogen) at 3rd position of pyrazole of the generic compound
- R<sub>4</sub> is heteroaryl substituted by C<sub>2</sub>H<sub>5</sub>(one substituent is missing) matches with substituent at 4th position of the generic structure.
- R<sub>3</sub> is substituted heteroaryl which is matching with the substituent R<sub>2</sub>(fifth position) of the generic structure