# Markush Structure Search Sample

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Patent FTO Search for the Generic compound

$$\begin{array}{l} \underset{R^{4} \text{ is } C_{1}-C_{4} \text{ alkyl or } C_{1}-C_{4} \text{ haloalkyl;} \\ R^{2} \text{ is an optionally substituted aryl or heteroaryl;} \\ R^{3} \text{ is halogen;} \\ R^{4} \text{ is hydrogen, halogen, } C_{1}-C_{4} \text{ alkyl, } C_{1}-C_{4} \text{ haloalkyl, cyano or } OR^{6}; \\ R^{5} \text{ is hydrogen, halogen, } C_{1}-C_{4} \text{ alkyl, } C_{1}-C_{4} \text{ haloalkyl, cyano or } OR^{6}; \\ R^{5} \text{ is hydrogen, halogen, } C_{1}-C_{4} \text{ alkyl, } C_{2}-C_{6} \text{ haloalkyl, } C_{2}-C_{6} \text{ alkenyl, } C_{2}-C_{6} \text{ alkyloxyalkyl;} \\ R^{7} \text{ is halogen or } OR^{6}; \\ R^{7} \text{ is halogen or } OR^{6}; \\ X \text{ is } N \text{ or } C-R^{4}; \\ \text{ or an agrochemically usable salt form thereof.} \end{array}$$

# 5.33

# **Exact match structures**

# Structure-1 (12(doc1))

## DE4124942

$$X_{2}$$

$$X_{3} - X_{4}$$
(I)  
one of the gps.  $X_{1} - X_{5} = A-B-C-N \leq , A-B-C-CH \leq$ or  

$$A-B-C-C \leq ;$$
a second gp. = F'-E-D-N  $\leq ,$   

$$F'-E-D-CH \leq$$
or F'-C-D-C  $\leq ;$ 

a third gp. = S, sulphenyl, sulphinyl,  $R_1 N \leq$ ,  $R_2 C \leq$ , (R2)2C< or N; a fourth gp. = O, S, N, SO<sub>2</sub> or  $R_2C \gtrless$  , or may also be C=O when this gp. is not between 2 N atoms; a fifth = N,  $R_2C \leq or (R_2)_2C \leq ;$  or

•  $X_1 = A$ -B-C- C(sp2 carbon),  $X_2 = F$ -C-D-C(sp2 carbon),  $X_3 = R_1$ -N<,  $X_4 = N$ ,  $X_5 = R_2$ -C(sp2 carbon)

1. X1: 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

<sup>2.</sup> X<sub>2</sub>: 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<sup>2</sup> (substituent aryl) at the 5<sup>th</sup> position of pyrazole of the generic structure



# Structure-2 (9(doc2))

### WO2007081019



In the above phenyl ring Q is pyrazole.

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

## Structure-3 (125(doc2))

#### JP11130754



#### 5.3

Consider left side ring the pyrazole ring

- R1 is 1-4C alkyl which is matching with substituent R1(first position) of the generic structure
- X is CI so it is matching with the substituent R<sup>3</sup> (second position) of the generic structure
- R<sub>2</sub> 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<sup>2</sup>(fifth position) of the generic structure.

# Structure-4 (109(doc2))



- $R_2$  is 1-6C alkyl which is matching with substituent  $R^1$ (first position) of the generic structure
- $R_4$  is halo matching with the substituent  $R^3$  (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



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- R<sub>1</sub>-R<sub>6</sub>=H, F, 1-4C alkyl, phenyl
- $R_2$ = 1-4C alkyl which matches with  $R^1$ (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<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

 $R_{4}$ = 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<sup>2</sup>(substituted aryl) at 5<sup>th</sup> position of pyrazole of generic structure

# Structure-7 (88(doc2))

### DE19503827



Q-R

Q= above structure

 $R_4$ = CR5R6R7 where  $R_5$ = 1-4C alkyl,  $R_6$ = H so no need of  $R_7$ 

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

R<sub>1</sub>= halo matches with R<sup>3</sup>(halogen) at 3<sup>rd</sup> position of pyrazole of generic structure

R<sub>2</sub>= alkylaryl substituted by halo matches with substituent at 4<sup>th</sup> position of pyrazole of generic structures

R<sub>3</sub>= substituted aryl which resembles R<sup>2</sup>(substituted aryl) at 5<sup>th</sup> position of pyrazole of generic structure

# Structure-8 (86(doc2))

#### WO9702252



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R<sub>1</sub>-R<sub>2</sub>= 1-4C alkyl, H matches with R<sup>1</sup>(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<sub>4</sub>= phenyl substituted with electron withdrawing group(halogens) matches with substituent at 4<sup>th</sup> position of pyrazole of generic structures

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

# Structure-9 (41(doc2))

JP2005216490



**-**33

- R<sup>1</sup>= lower alkyl which matches with R1(alkyl) at 1<sup>st</sup> position of pyrazole of the generic structure
- R<sup>2</sup>= halogen which matches with R3(halogen) at 3<sup>rd</sup> position of pyrazole of the generic structure
- R<sup>3</sup>= methoxyphenyl which indicates subtituent 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



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- Z1= C, Z2= N, Z3= N Which indicates pyrazole ring.
- R1= Alkyl which matches with R1(alkyl) at the 1st position of pyrazole of the generic compound
- R32= halo which matches with R<sup>3</sup>(halogen) at the 3<sup>rd</sup> position of pyrazole of the generic compound
- R2(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 4th position of pyrazole of generic structure

## Structure-1 (84(doc2))

#### WO9711952



53



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

# Structure-2 (74(doc2))

### WO0130154



#### **-**33

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

# Structure-3 (39(doc2))

JP2005272306



5.35

- A= substituted heteroaryl which matches with R<sup>2</sup>(substituted aryl) at 5<sup>th</sup> position of pyrazole of the generic structure
- R1= alkyl which matches with R1(alkyl) at 1st 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 subtituent at 4<sup>th</sup> position of pyrazole of generic structure

## Structure-4 (25(doc2))

#### US2007066822



## 633

 $R^{1}-R^{2}=H$ ,  $-CH_{3}$ ,  $-C_{2}H_{5}$  which matches with  $R^{1}(alkyl)$  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 R1-R5)

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

 $R_{5}$ = 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>

 $R_4$ - $R_7$ = alkyl matches with  $R^1$ (alkyl) at 1<sup>st</sup> position of pyrazole of generic structure; halogen matches with  $R^3$ (halogen) at 3<sup>rd</sup> position of pyrazole of generic structure; optionally substituted aryl which resembles  $R^2$ (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



# 13

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



- 13
- R1= alkyl which matches with R1(alkyl) at 1st position of pyrazole of the generic structure
- R<sub>3</sub>= halo which matches with R<sup>3</sup>(halogen) at 3<sup>rd</sup> position of pyrazole of the generic structure
- R<sub>4</sub>= heteroaryl optionally substituted indicating substituent at 4<sup>th</sup> position of pyrazole of the generic structure
- R<sub>5</sub>= optionally substituted heteroaryl which matches with R<sup>2</sup>(optionally substituted heteroaryl) at 5<sup>th</sup> position of pyrazole of the generic structure

# Structure-9 (98(doc2))

#### JP6345728



1.3

- A= N, B= CR<sup>4</sup>
- R<sup>5</sup>= 1-6C alkyl which matches with R<sup>1</sup>(alkyl) at 1<sup>st</sup> position of pyrazole of the generic structure
- R<sup>3</sup>= halogen which matches with R<sup>3</sup>(halogen) at 3<sup>rd</sup> position of pyrazole of the generic structure
- R<sup>4</sup>= phenyl(optionally substituted by halo, CN, alkoxy)indicating substituent at 4<sup>th</sup> position of pyrazole of the generic structure
- R<sup>2</sup>= optionally substituted phenyl which matches with R<sup>2</sup>(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;  $R^5$ = 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<sub>6</sub> is 1-3C alkyl which is matching with substituent R<sup>1</sup>(first position) of the generic structure
- R<sub>7</sub> doesn?t exist.. so it is matching with the second position of the generic structure.
- R8 is halogen so it is matching with the substituent R3 (second position) of the generic structure
- R11 is phenyl???(substituents are missing)??? which is matching with the fourth position of the generic structure
- $\bullet$   $R^{}_{10}$  is phenyl which is matching with the substituent  $R^2(\mbox{fifth position})$  of the generic structure.

# Structure-2

## WO0018741



53

- Q= pyrazolyl
- In the above structure the substituted aryl bonded to Q(pyrazolyl) matches with R<sup>2</sup>(substituted aryl) at 5<sup>th</sup> position of pyrazole of the generic structure
- R<sub>1</sub>= haloalkyl which matches with R<sup>1</sup>(alkyl) at 1<sup>st</sup> position of the generic structure
- R<sub>2</sub>= 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<sup>3</sup>(halogen) of pyrazole of generic structure is missing??? in the above structure

## Structure-3

## EP335381



D= NR12 , E??= N, E?= CH, E= CH

 $\rm R_{12}^{}=$  alkyl matches with  $\rm R^1(alkyl)$  at 1st position of pyrazole of generic structure

R7= halo matches with R3(halogen) at 3rd 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 5th position of pyrazole of the generic structure
- At 4th 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



**-**33

- 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





- R5= alkyl which matches with R1(alkyl) at 1st 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
- R8= phenyl which matches with R2(aryl) at 5th position of pyrazole of generic structure

## Structure-7

#### JP2004317640



53

- R5= alkyl which matches with R1(alkyl) at 1st 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
- R8= phenyl which matches with R2(aryl) at 5th position of pyrazole of generic structure

## Structure-8

#### US2005135045



- 0-33
- 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 4th 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



# 53

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

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 subtituent at 4th position of pyrazole of the generic structure

 $\mathsf{R}^3$  and  $\mathsf{R}^2$  of pyrazole of generic structure are missing

## Structure-10

#### WO2007038363



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

 $R^3$  is defined as 3-25C substituted heteroaryl having 1-3 heteroatoms of N(so can be pyrazole) in which the substituents are -CH<sub>3</sub>, halogen: -CH<sub>3</sub> matches with R<sup>1</sup>(alkyl) of pyrazole of the generic structure and halogen matches with R<sup>3</sup>(halogen) of pyrazole of the generic structure Above ring matches with subtituent at 4<sup>th</sup> position of pyrazole of the generic structure

R<sup>2</sup>(substituted aryl) of pyrazole of generic structure missing

## Structure-11

#### US2007100184



# 0.3

 $R_1 = H$ 

 $R_2$ = - $C_2H_5$  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

 $R_4$ = optionally substituted 6-25C heteroaryl with 1-3 of O, N, S or with 1-3 of CH<sub>3</sub>, C<sub>2</sub>H<sub>5</sub>, 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<sup>7</sup> of pyrazole of generic structure is missing

 $R_{5}$ = optionally substituted 6-25C heteroaryl which resembles  $R^{2}$ (substituted aryl) at 5<sup>th</sup> position of pyrazole of generic structure **Structure-12** 

#### US2005020646



R<sup>a</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



# 633

X1= 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



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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

 $R_4$ = halo matches with  $R^3$ (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



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

 $R_{5}$ = 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 R1( 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



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- 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





- R1-H,

- R2 is ?C2H5 which matches with R1(alkyl) at 1st position of the generic structure
  R5 is halo which matches with R3(halogen) at 3rd position of pyrazole of the generic compound
  R4 is heteroaryl substituted by C2H5(one substituent is missing) matches with substituent at 4th position of the generic structure.
  R3 is substituted heteroaryl which is matching with the substituent R2(fifth position) of the generic structure