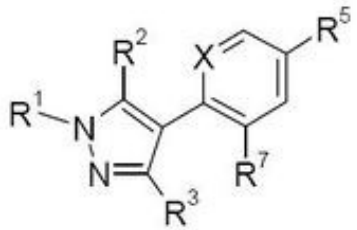
Markush Structure Search Sample

Contents

Patent FTO Search for the Generic compound



(I)

wherein

R^1 is C_1-C_4alkyl or C_1-C_4haloalkyl;

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;

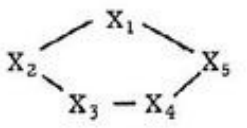
X is N or C-R^4;

or an agrochemically usable salt form thereof.

Exact match structures

Structure-1 (12(doc1))

DE4124942



(I)

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

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

F'-E-D-CH< or F'-C-D-C<< ;

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

$(R_2)_2C<$ or N;

a fourth gp. = O, S, N, SO_2 or $R_2C<<$, or may also be C=O when this gp. is not between 2 N atoms;

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

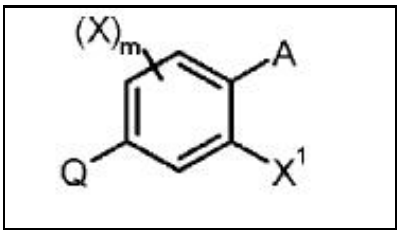
- X_1 = A-B-C- C(sp2 carbon), X_2 = F-C-D-C(sp2 carbon), X_3 = R_1-N<, X_4 = N, X_5 = R_2-C(sp2 carbon)

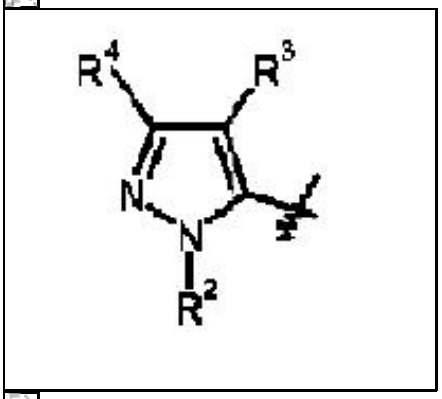
1. X_1: A =H , B = bond, C = (b) under B which is halo substituted phenylene which completely matches with 4th position substituent of the generic compound
2. X_2: D = (b) under B is a phenylene(implies a substituted aryl) and F-C- is a substituent on D. It is clear that this will match with R^2 (substituent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

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

Structure-2 (9(doc2))

WO2007081019



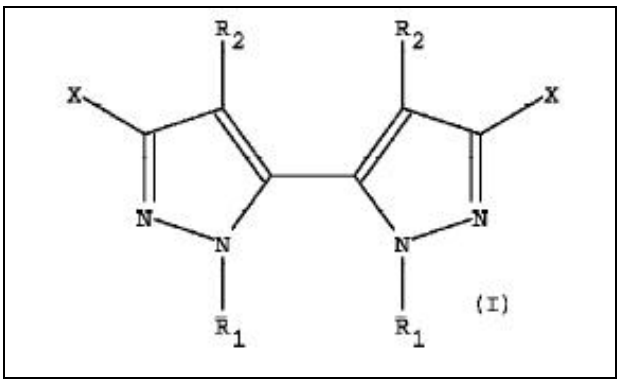


In the above phenyl ring Q is pyrazole.

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

Structure-3 (125(doc2))

JP11130754

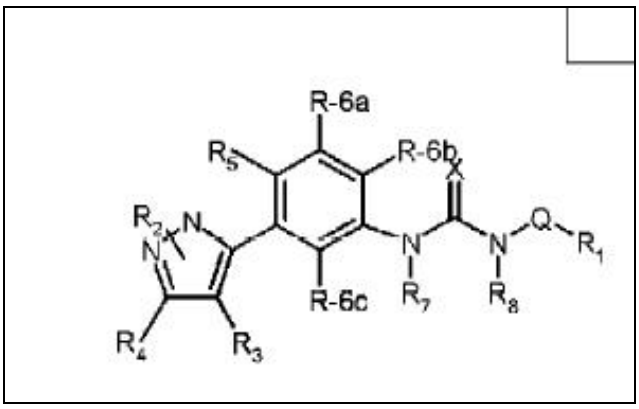


Consider left side ring the pyrazole ring

- 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))

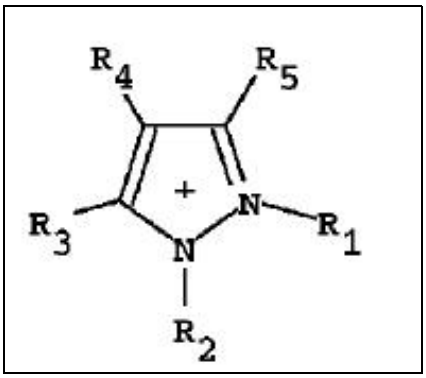
WO2006078610



- R_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_3 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^2(fifth position) of the generic structure.

Structure-5 (128(doc2))

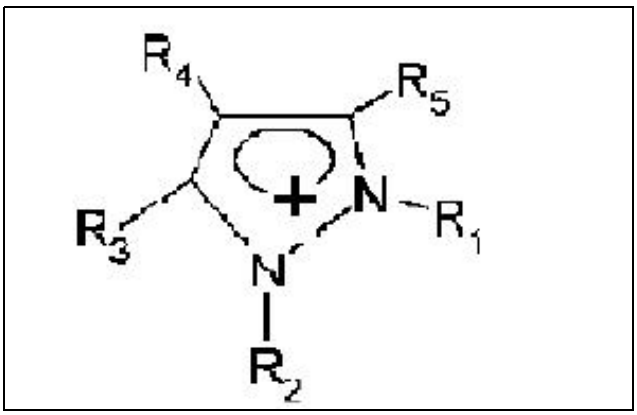
US5827602



- R_1-R_6=H, F, 1-4C alkyl, phenyl
- R_2= 1-4C alkyl which matches with R^1(alkyl) at 1st position of pyrazole of the generic structure
- R_5= F which matches with R^3(halo)at 1st position of pyrazole of the generic structure
- R_4= phenyl substituted with an electron with drawing group matches with substituent at 4th position of pyrazole of generic structure
- R_3= substituted aryl which matches with R^2(substituted aryl) at 5th 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 1st position of pyrazole of generic structure

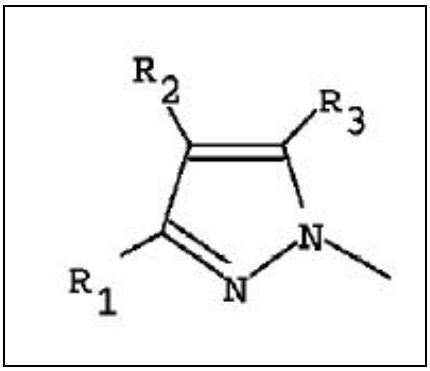
R_3= halogen which matches with R^3(halogen) at 3rd position of pyrazole of generic structure

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 4th 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 5th position of pyrazole of generic structure

Structure-7 (88(doc2))

DE19503827



Q-R_4

Q= above structure

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

R_4 matches with R^1(alkyl) at 1st position of pyrazole of generic structure

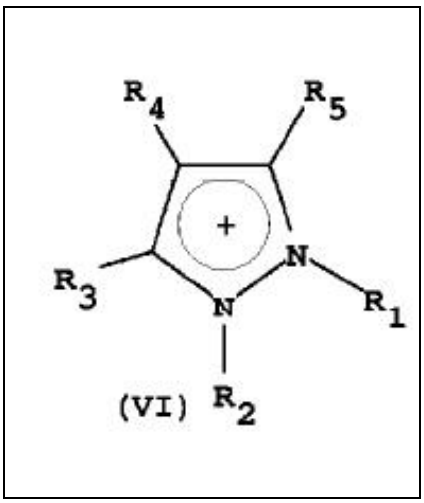
R_1= halo matches with R^3(halogen) at 3rd position of pyrazole of generic structure

R_2= alkylaryl substituted by halo matches with substituent at 4th position of pyrazole of generic structures

R_3= substituted aryl which resembles R^2(substituted aryl) at 5th 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 1st position of pyrazole of generic structure

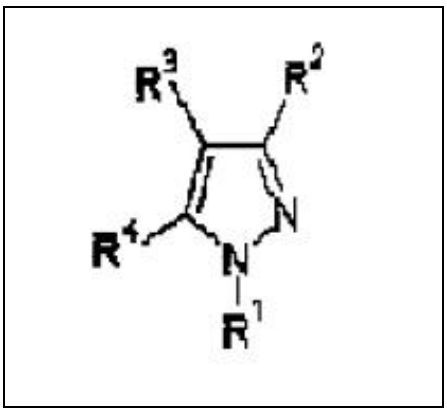
R_3= halogen matches with R^3(halogen) at 3rd position of pyrazole of generic structure

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

R_5= substituted aryl which resembles R^2(substituted aryl) at 5th position of pyrazole of generic structure

Structure-9 (41(doc2))

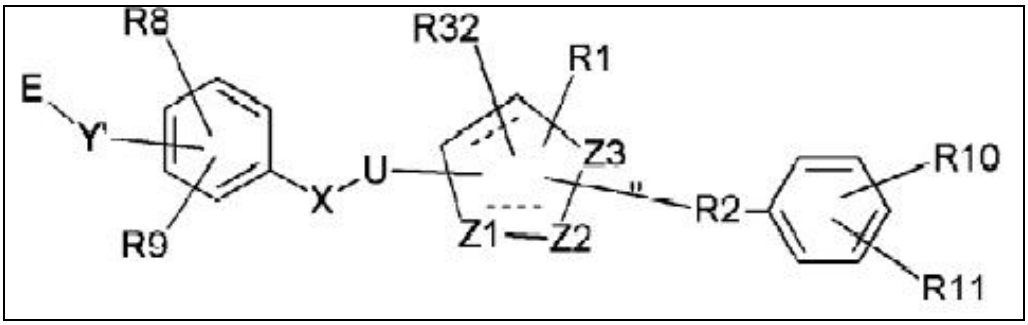
JP2005216490



- R^1= lower alkyl which matches with R1(alkyl) at 1st position of pyrazole of the generic structure
- R^2= halogen which matches with R3(halogen) at 3rd position of pyrazole of the generic structure
- R^3= methoxyphenyl which indicates subtituent at 4th position of generic structure
- R^4= methoxy phenyl which matches with R^2(substituted aryl)at 5th position of pyrazole of generic structure

Structure-10 (61(doc1))

WO2004063166

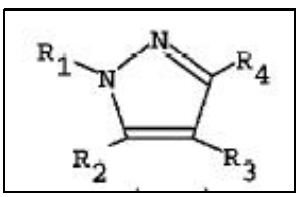


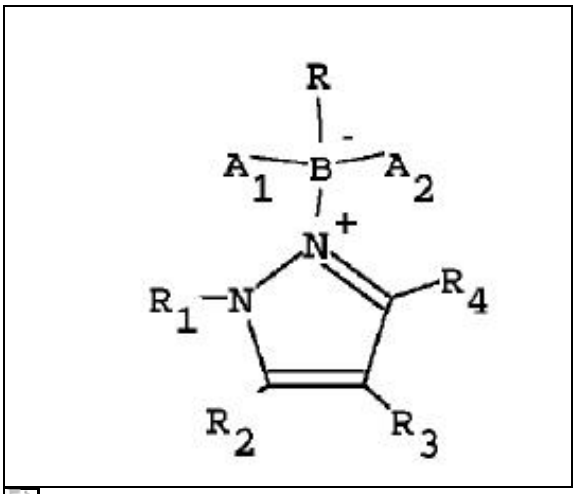
- Z1= C, Z2= N, Z3= N Which indicates pyrazole ring.
- R1= Alkyl which matches with R^1(alkyl) at the 1st position of pyrazole of the generic compound
- R32= halo which matches with R^3(halogen) at the 3rd position of pyrazole of the generic compound
- R2(0-8Calkyl) so it may be ?0?C alkyl implies it is simply a bond, bonded to a substituted phenyl ring which matches with R^2(substituted aryl) at the 5th 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 4th 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

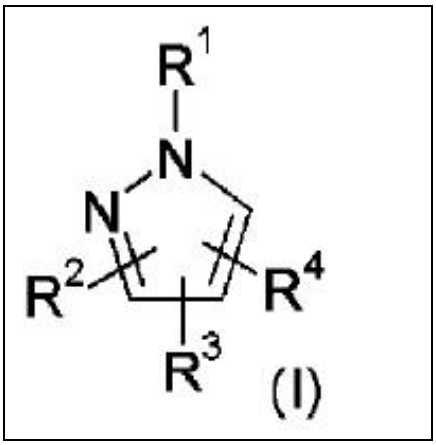




- R_1-R_4= 1-8C alkyl, haloalkyl, halo, phenyl(optionally substituted by halo, 1-4C alkyl, haloalkyl, alkoxy,)
- R_1= 1-8C alkyl which matches with R^1(1-4C alkyl) at 1st position of pyrazole of generic structure
- R_4= halo which matches with R^3(halogen) at 3rd position of pyrazole of generic structure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

Structure-2 (74(doc2))

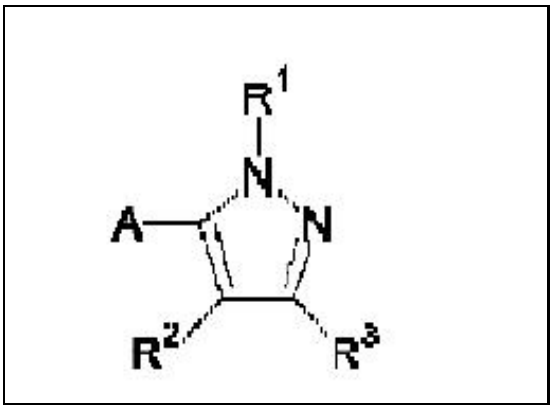
WO0130154



- R^1= (1-6C)alkyl which matches with R^1(1-4C alkyl) at 1st position of pyrazole of the generic compound
- R^2= halo which matches with R^3(halogen) at 3rd 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 4th 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 5th position of the generic compound

Structure-3 (39(doc2))

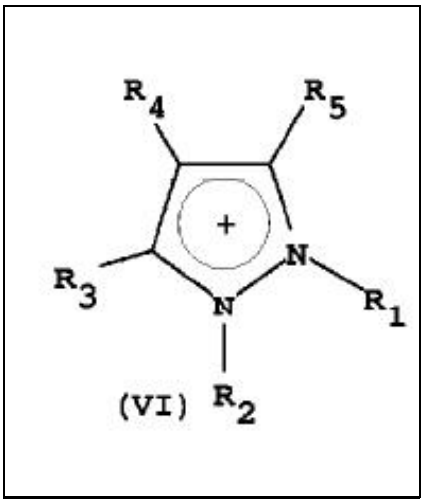
JP2005272306



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

Structure-4 (25(doc2))

US2007066822



R^1-R^2= H, -CH_3, -C_2H_5 which matches with R^1(alkyl) at 1st position of pyrazole of generic structure

R^3= halogen which matches with R^3(halogen) at 3rd position of pyrazole of generic structure

R^4= 6-25C optionally substituted heteroaryl which resembles substituent at 4th position of pyrazole of the generic structure

R^5= optionally substituted 6-25C heteroaryl which resembles R^2(substituted aryl) at 5th position of pyrazole of generic structure

Structure-5 (23(doc2))

US2007066854

Z^+= pyrazolium (substituted at 1-5 R1-R5)

R_1= -CH_3, -C_2H_5 which matches with R^1(alkyl) at 1st position of pyrazole of generic structure

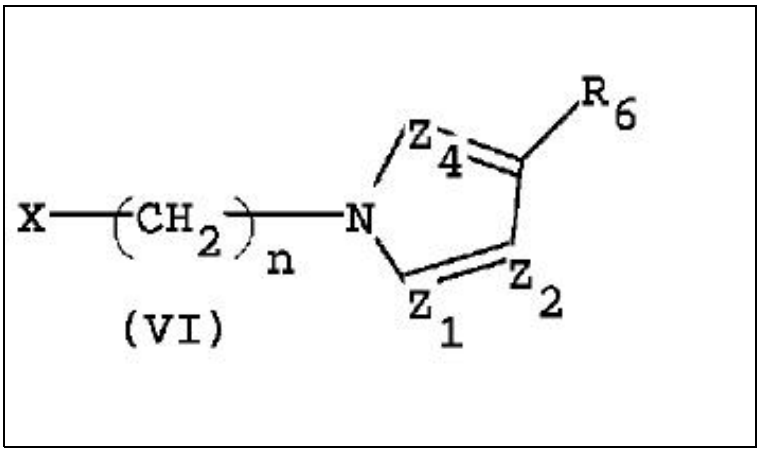
R_3= halogen which matches with R^3(halogen) at 3rd position of pyrazole of generic structure

R_4= 6-25C aryl optionally substituted by C_2H_5, OH which resembles substituent at 4th position of pyrazole of the generic structure

R_5= optionally substituted 6-25C heteroaryl which resembles R^2(substituted aryl) at 5th position of pyrazole of generic structure

Structure-6 (90(doc2))

FR2723091



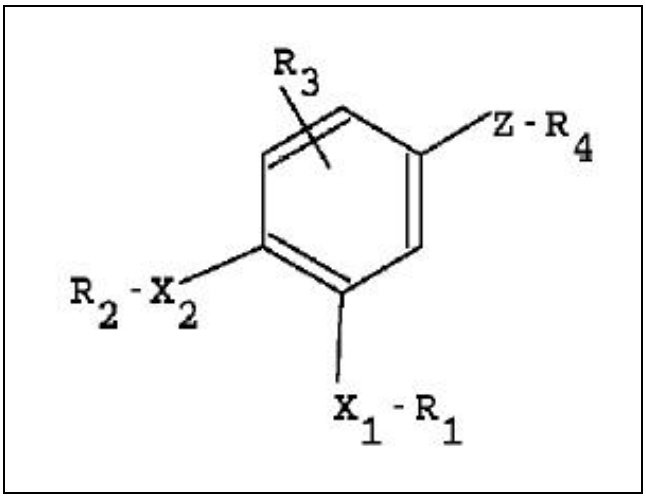
X= halo, n= 2-4

Z_1= N, Z_2= CR_5, Z_4= CR_7

R_4-R_7= alkyl matches with R^1(alkyl) at 1st position of pyrazole of generic structure; halogen matches with R^3(halogen) at 3rd position of pyrazole of generic structure; optionally substituted aryl which resembles R^2(substituted aryl) at 5th position of pyrazole of generic structure and matches with substituent at 4th position of pyrazole of generic structures

Structure-7 (92(doc2))

WO9600218

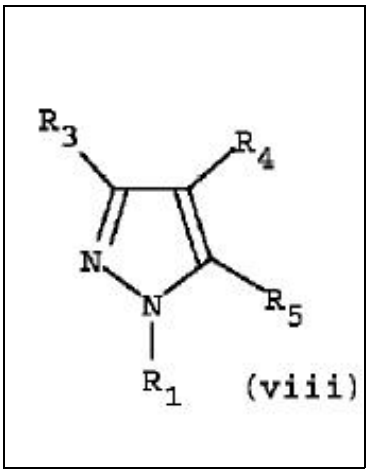


Z= a bond,

R_4 is a pyrazole with substituents as 1-4C alkyl matches with R^1(alkyl) at 1st position of pyrazole of generic structure; halo matches with R^3(halogen) at 3rd position of pyrazole of generic structure; optionally substituted aryl which resembles R^2(substituted aryl) at 5th position of pyrazole of generic structure and matches with substituent at 4th position of pyrazole of generic structures

Structure-8 (95(doc2))

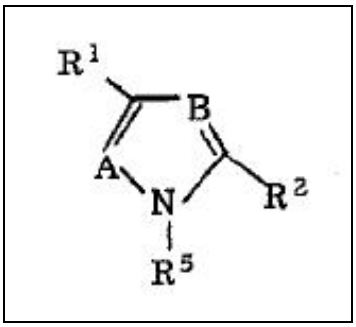
WO9524403



- R_1= alkyl which matches with R^1(alkyl) at 1st position of pyrazole of the generic structure
- R_3= halo which matches with R^3(halogen) at 3rd position of pyrazole of the generic structure
- R_4= heteroaryl optionally substituted indicating substituent at 4th position of pyrazole of the generic structure
- R_5= optionally substituted heteroaryl which matches with R^2(optionally substituted heteroaryl) at 5th 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 1st position of pyrazole of the generic structure
- R^3= halogen which matches with R^3(halogen) at 3rd position of pyrazole of the generic structure
- R^4= phenyl(optionally substituted by halo, CN, alkoxy)indicating substituent at 4th position of pyrazole of the generic structure
- R^2= optionally substituted phenyl which matches with R^2(optionally substituted aryl) at 5th position of pyrazole of the generic structure

Structure-10 (34(doc2))

WO2006084262

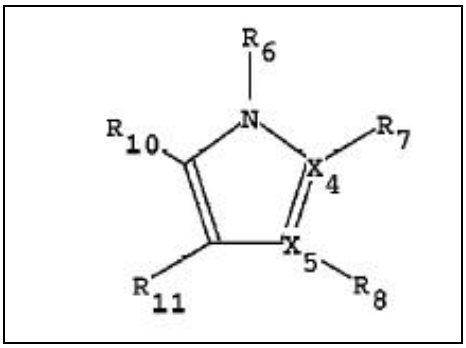
It is pyrazolium with substituents

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

Relevant structures with missing substituents

Structure-1

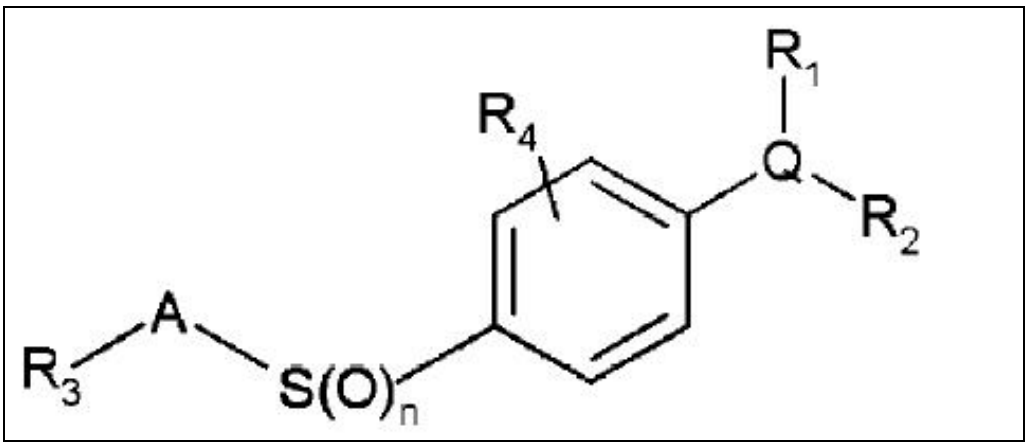
JP09204932



- 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.
- R8 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

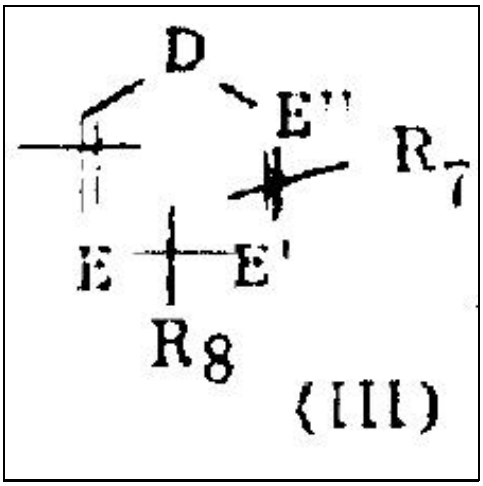
WO0018741



- Q= pyrazolyl
- In the above structure the substituted aryl bonded to Q(pyrazolyl) matches with R^2(substituted aryl) at 5th position of pyrazole of the generic structure
- R_1= haloalkyl which matches with R^1(alkyl) at 1st position of the generic structure
- R_2= aryl optionally substituted with halo, lower alkoxy, CN which matches with substituent at 4th 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= NR12 , E??= N, E?= CH, E= CH

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

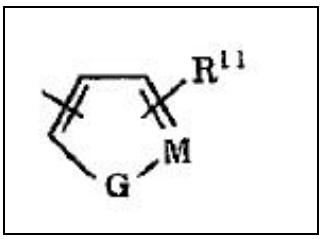
R_7= halo matches with R^3(halogen) at 3rd position of pyrazole of generic structure

R_8= substituted benzene ring matches with substituent at 4th position(but missing substituents) of pyrazole of generic structures

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

Structure-4

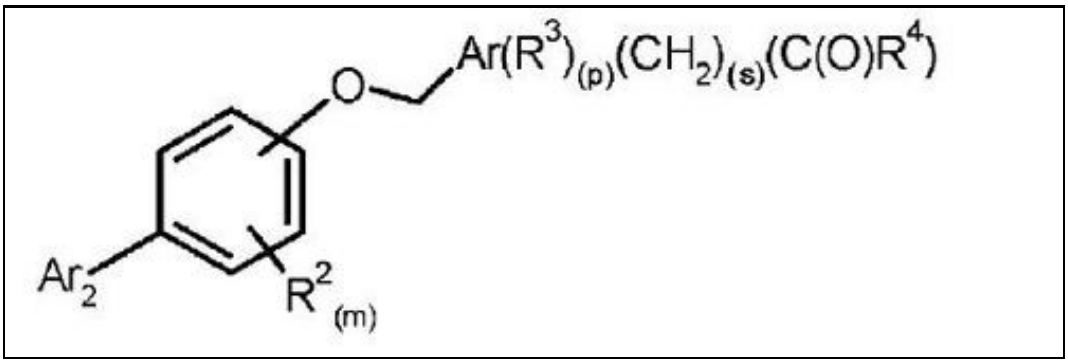
US5296484



- G= NR^{20}, M= N
- R^{11}= 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

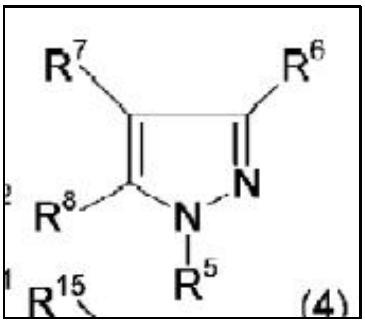


- AR^2= pyrazol-4-yl optionally substituted by Q(halo, lower alkyl, phenyl)
- Q substituted on AR^2(pyrazole) indicates R^3, R^1 and R^5 of pyrazole of the generic structure

- At 4th substituent of pyrazole one substituent is missing and one substituent is varying

Structure-6

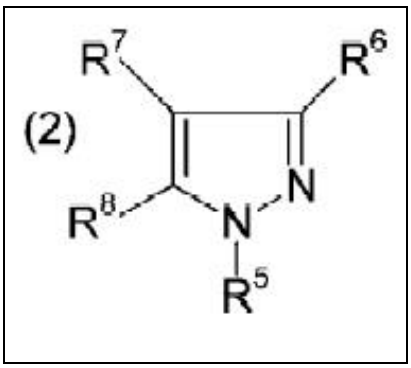
JP2004317641



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

Structure-7

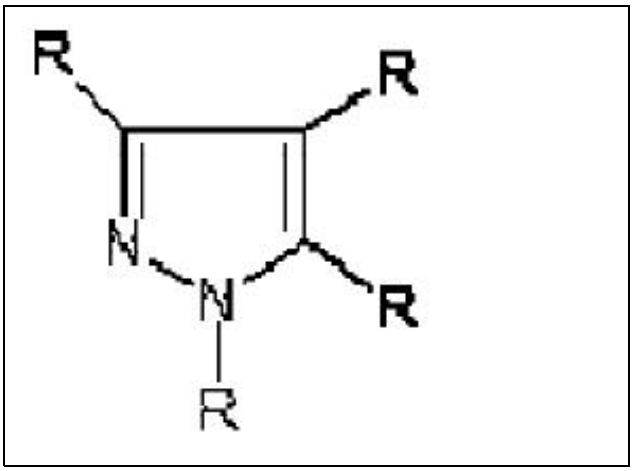
JP2004317640



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

Structure-8

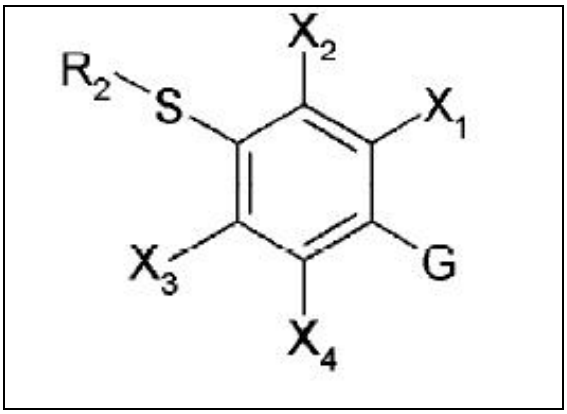
US2005135045



- R= 1-4C alkyl, halogen , phenyl
- R= alkyl which matches with R^1(alkyl) at 1st position of pyrazole of the generic structure
- R= halogen which matches with R^3(halogen)at 3rd 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^2(aryl) at 5th position of pyrazole of generic structure

Structure-9

WO2006124776



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

R^3 is a pyrazole ring with substituents as:

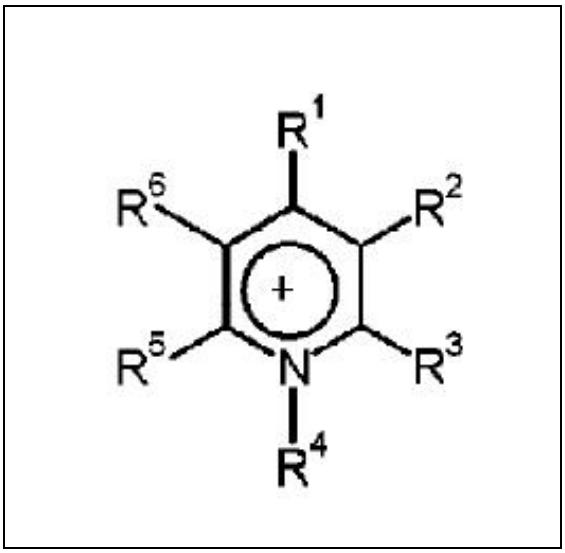
-CH_3 matches with R^1(alkyl) of pyrazole of the generic structure

Above ring matches with subtituent at 4th position of pyrazole of the generic structure

R^3 and R^2 of pyrazole of generic structure are missing

Structure-10

WO2007038363



R^1= H, R^2= halogen, R^3= 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 $-CH_3$, halogen:

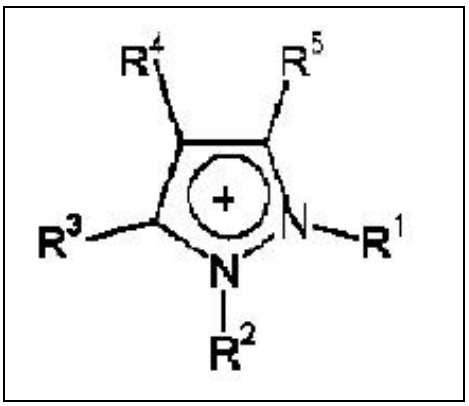
$-CH_3$ matches with R^1(alkyl) of pyrazole of the generic structure and halogen matches with R^3(halogen) of pyrazole of the generic structure

Above ring matches with subtituent at 4th 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= $-C_2H_5$ which matches with R^1(alkyl) at 1st position of pyrazole of generic structure

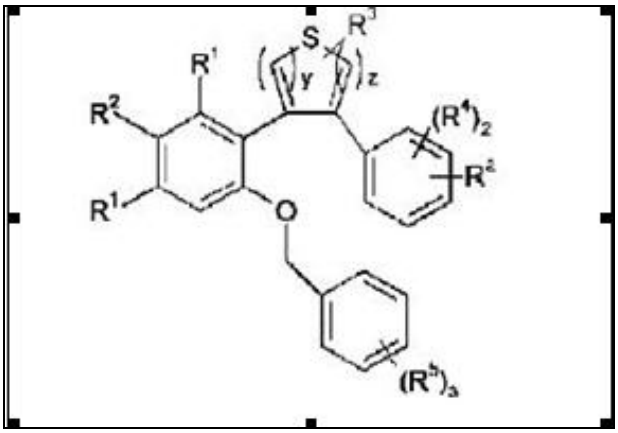
R_3= halogen which matches with R^3(halogen) at 3rd position of pyrazole of generic structure

R_4= optionally substituted 6-25C heteroaryl with 1-3 of O, N, S or with 1-3 of CH_3, C_2H_5, 3-25, preferably 3-20C straight , branched or cyclic alkane or alkene optionally substituted with halogens which resembles substituent at 4th position of pyrazole of the generic structure but R^7 of pyrazole of generic structure is missing

R_5= optionally substituted 6-25C heteroaryl which resembles R^2(substituted aryl) at 5th position of pyrazole of generic structure

Structure-12

US2005020646

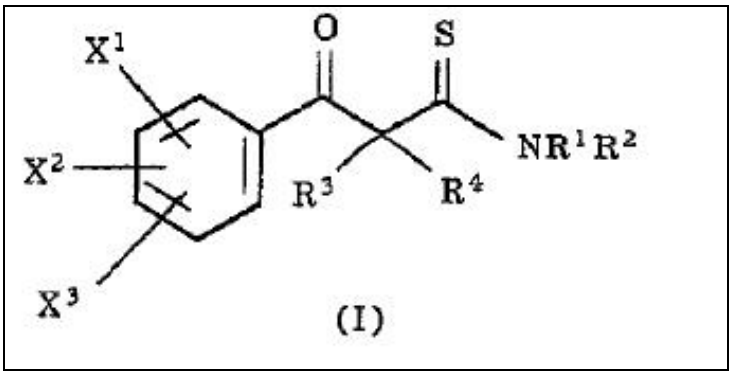


R^a= pyrazolyl optionally substituted with 1-3 substituents of R^{11} or 1-4C alkyl

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

Structure-13

EP548680



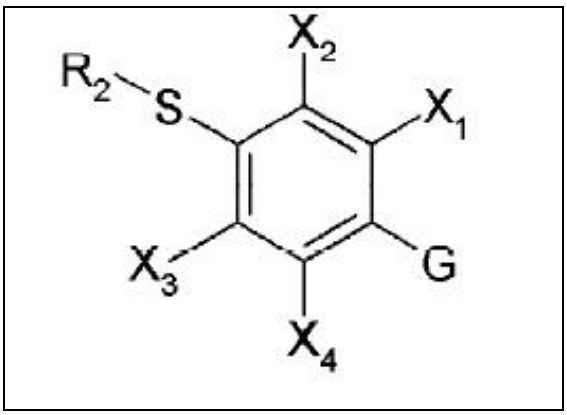
X^1= het

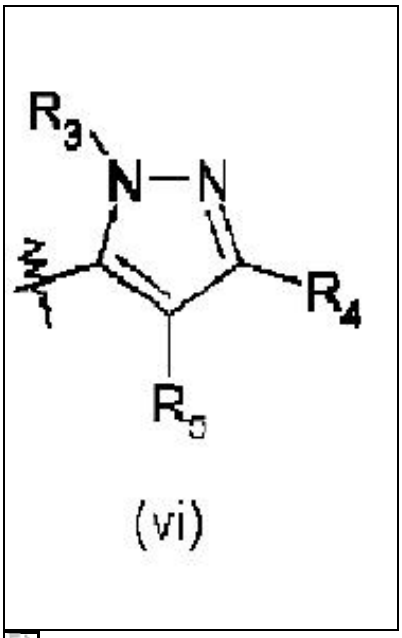
Het = pyrazolyl with substituents alkyl matches with R^1(alkyl) at 1st position of pyrazole of generic structure; halo matches with R^3(halogen) at 3rd position of pyrazole of generic structure; phenyl matches with substituent at 4th position(but missing substituents) of pyrazole of generic structures

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

Structure-14

WO2003087062





G= above pyrazole

R_3= alkyl matches with R^1(alkyl) at 1st position of pyrazole of generic structure

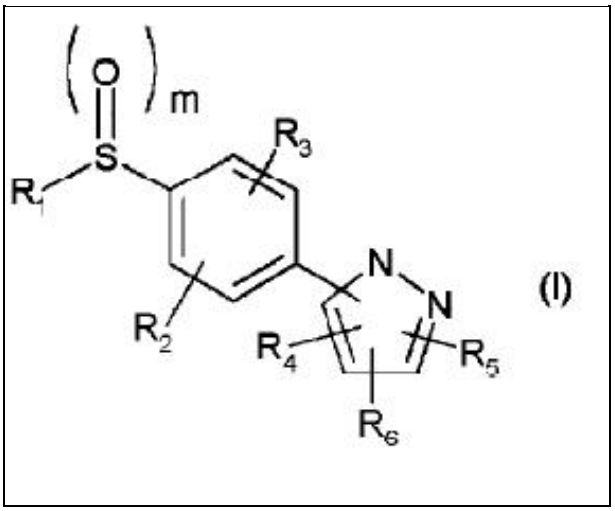
R_4= halo matches with R^3(halogen) at 3rd position of pyrazole of generic structure

R_5= phenyl matches with substituent at 4th position(but missing substituents) of pyrazole of generic structures

Above given aryl matches with R^2(substituted aryl) at 5th position of pyrazole of generic structure

Structure-15

WO200066562



R_4= alkyl matches with R^1(alkyl) at 1st position of pyrazole of generic structure

R_5= halo matches with R^3(halogen) at 3rd position of pyrazole of generic structure

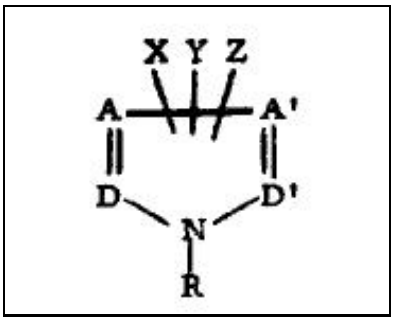
R_6= optionally substituted aryl matches with substituent at 4th position(but missing substituents) of pyrazole of generic structures

Above given aryl matches with R^2(substituted aryl) at 5th position of pyrazole of generic structure

Relevant structures with substituent variation

Structure-1

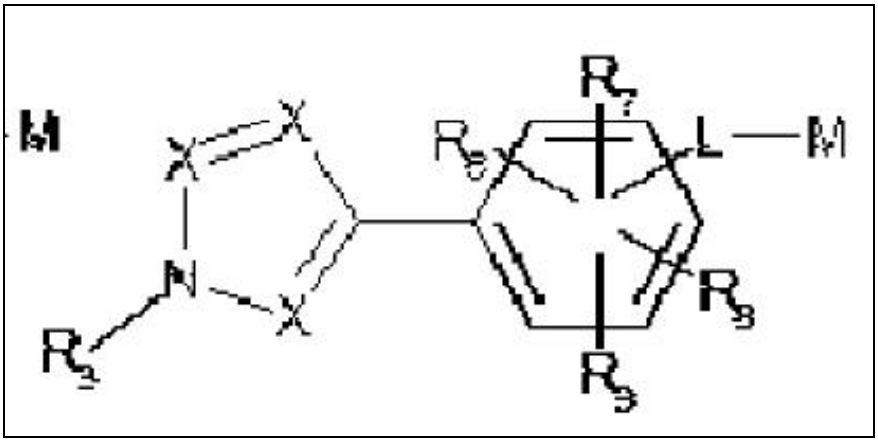
EP0080051



- 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^3 (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^2 (fifth position) of the generic structure.

Structure-2

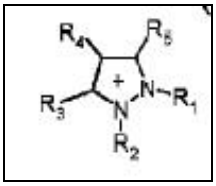
US2005159470



- First position: R_3 is alkyl, so it is matching with the substituent R^1 (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_5 , R_5 is halo so it is matching with the substituent R^3 (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_5, R_5 is heteroaryl, so it is matching with substituent R^2 (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