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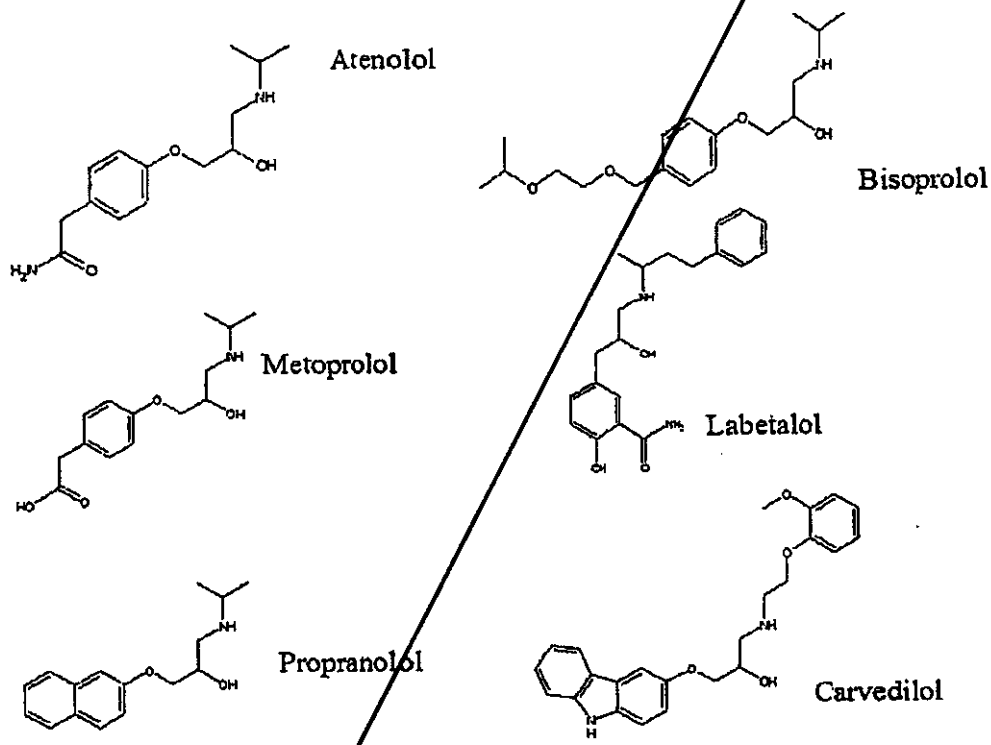

Atenolol
Bisoprolol
Metoprolol
Labetalol
Propranolol
Carvedilol

Figure 2

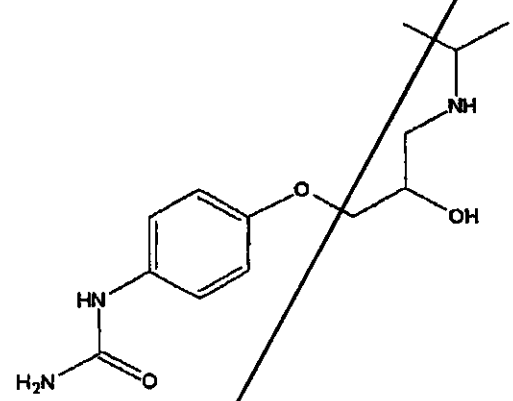


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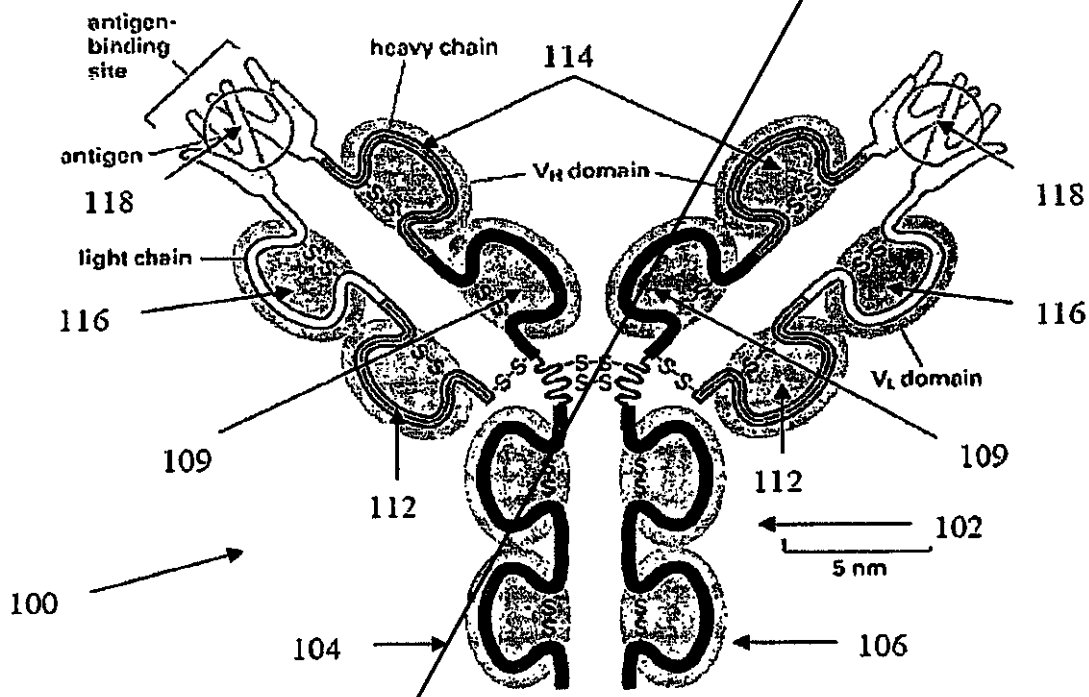

antigen-binding site
antigen
118
light chain
116
heavy chain
114
V_H domain
118
116
V_L domain
109
112
109
112
102
5 nm
100
104
106

Figure 4

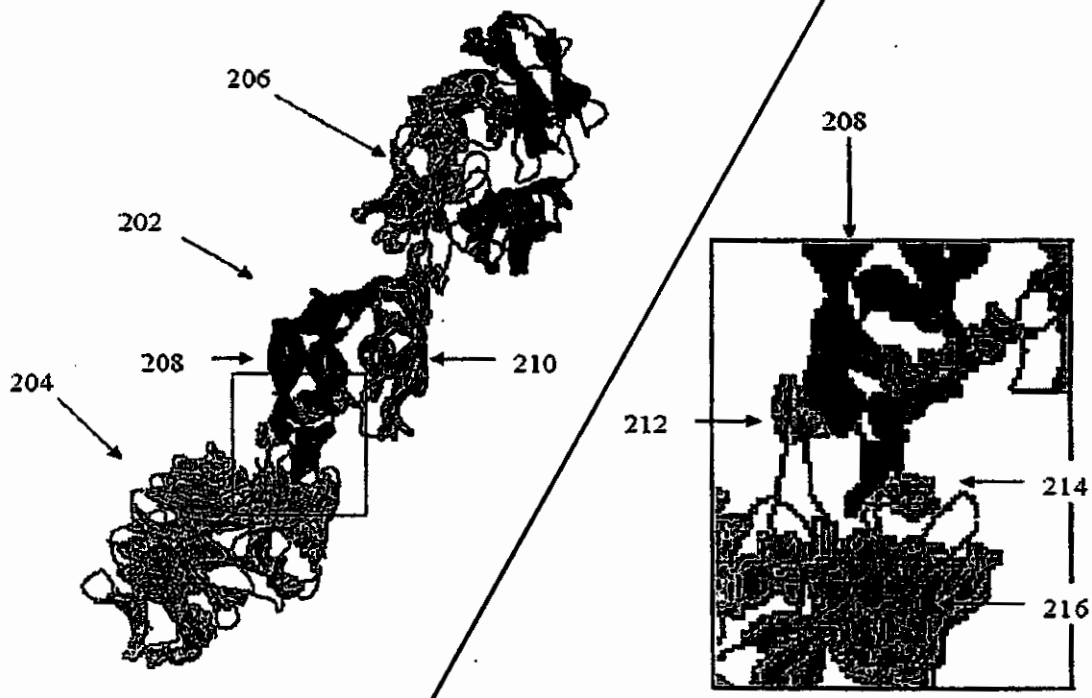


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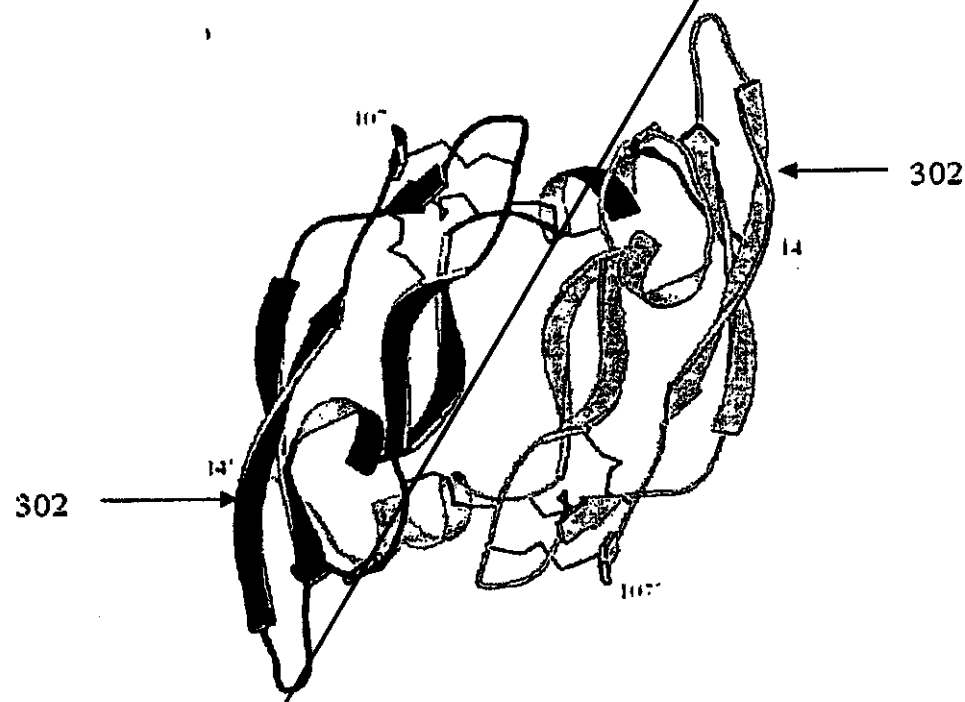
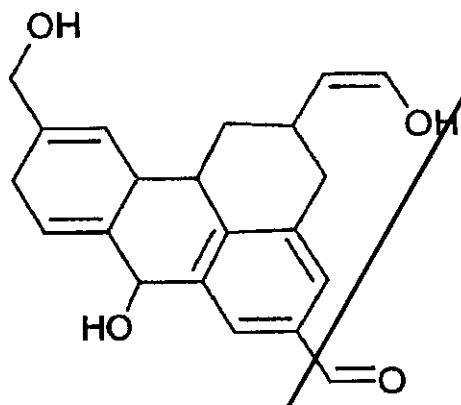
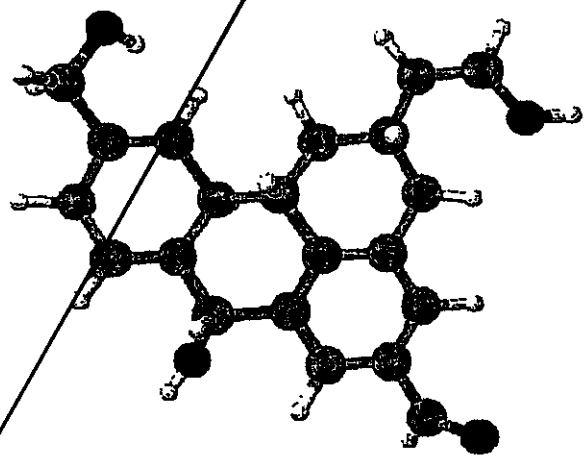


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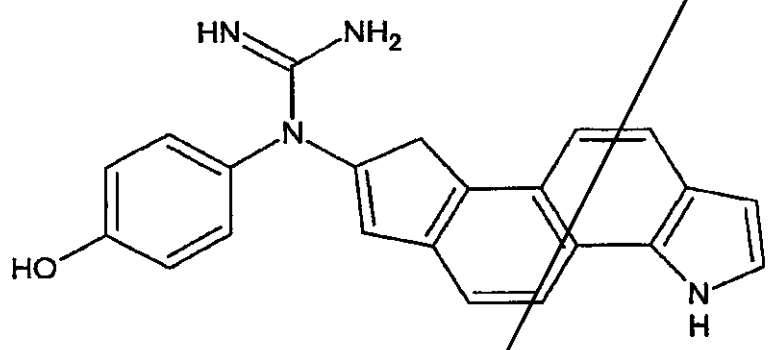


6A

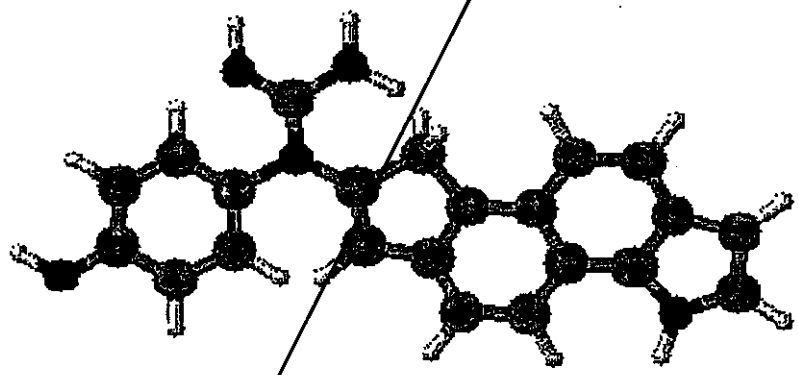


6B

Figure 7



7A



7B

Figure 8

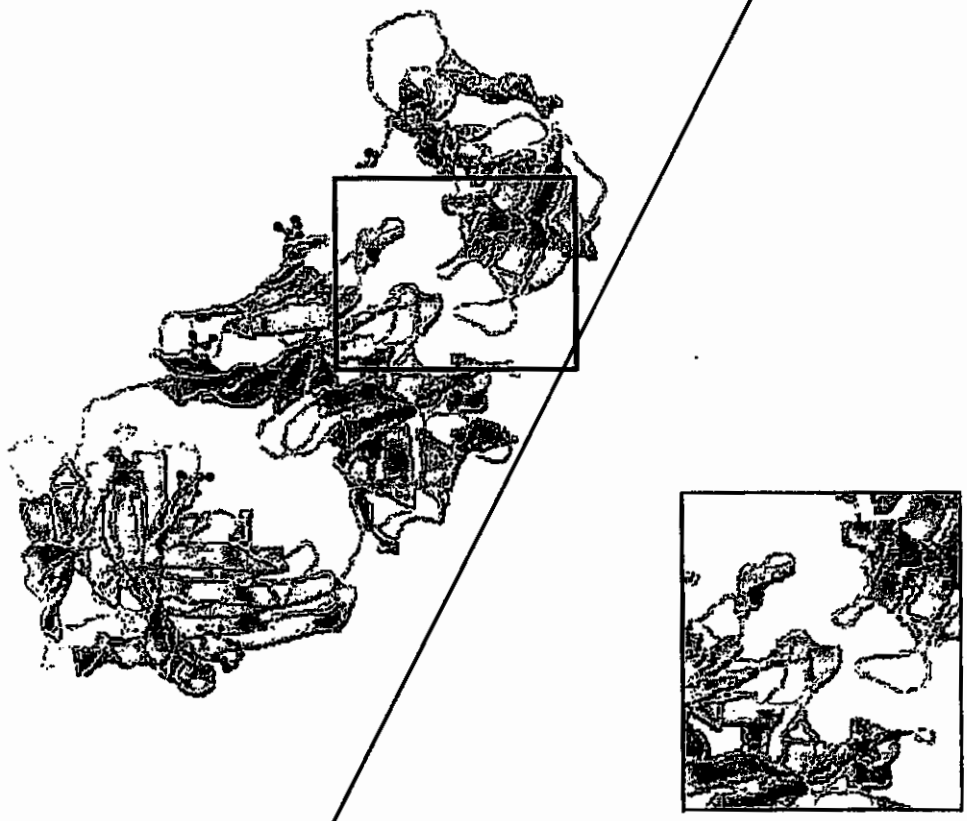
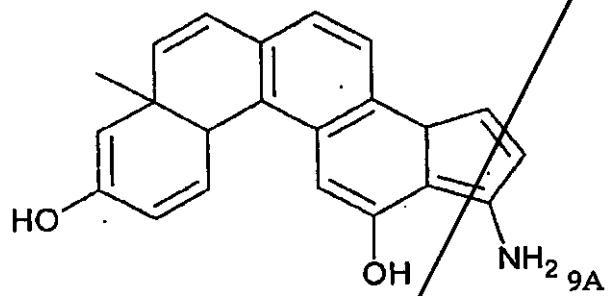
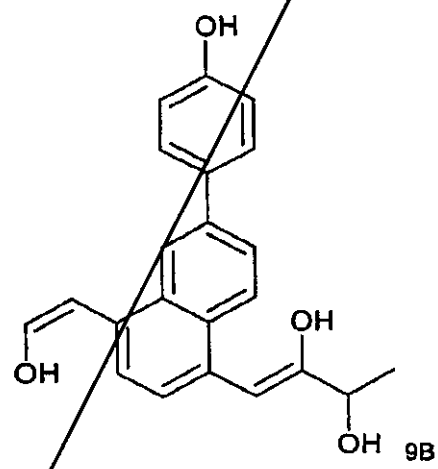


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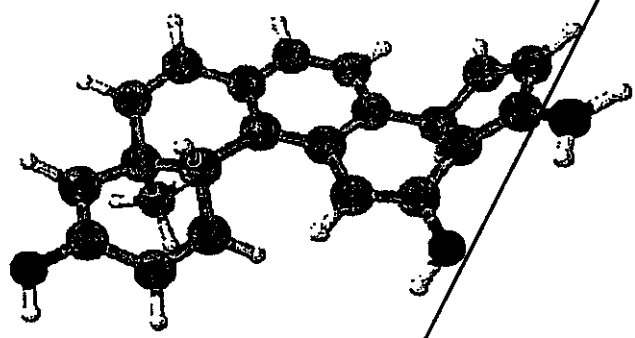


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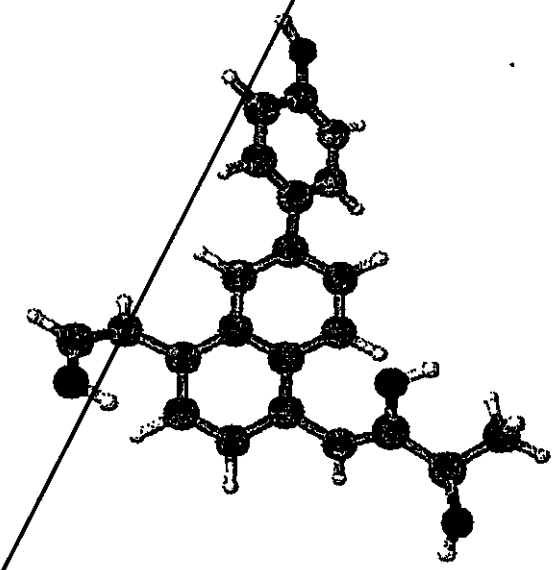


9B

Figure 10



10A



10B

Figure 11

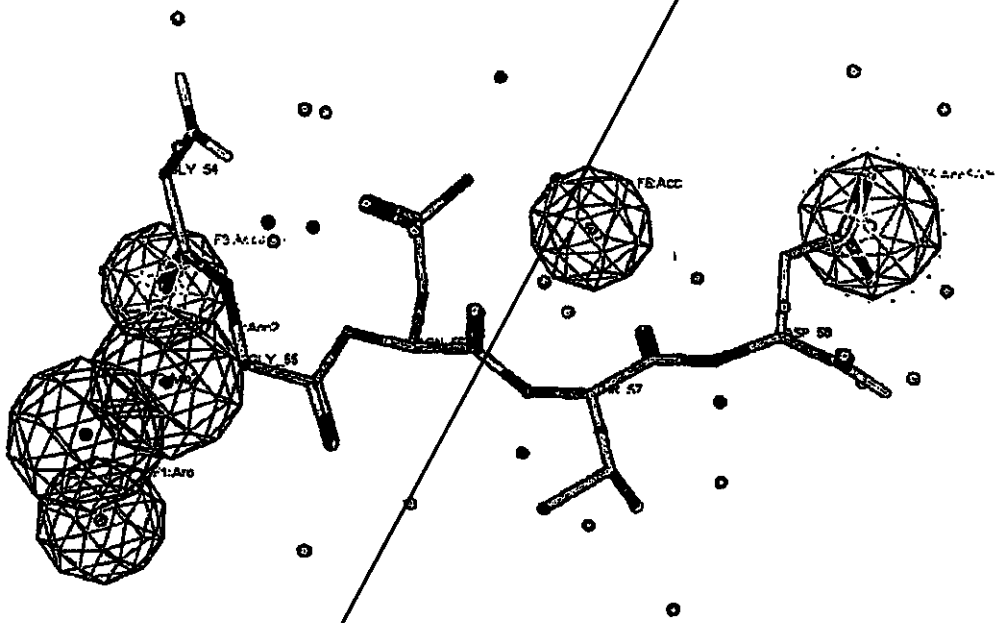


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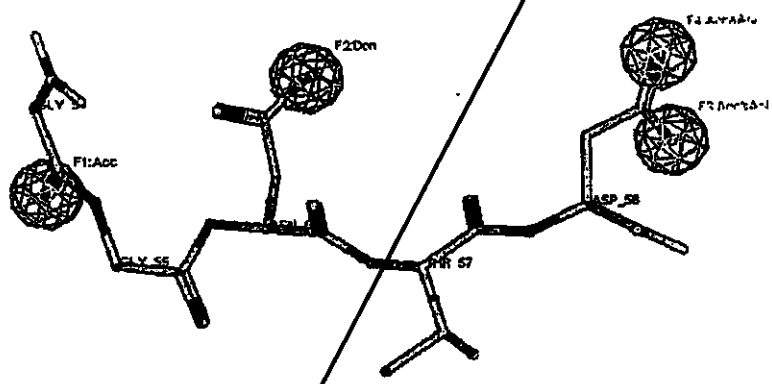


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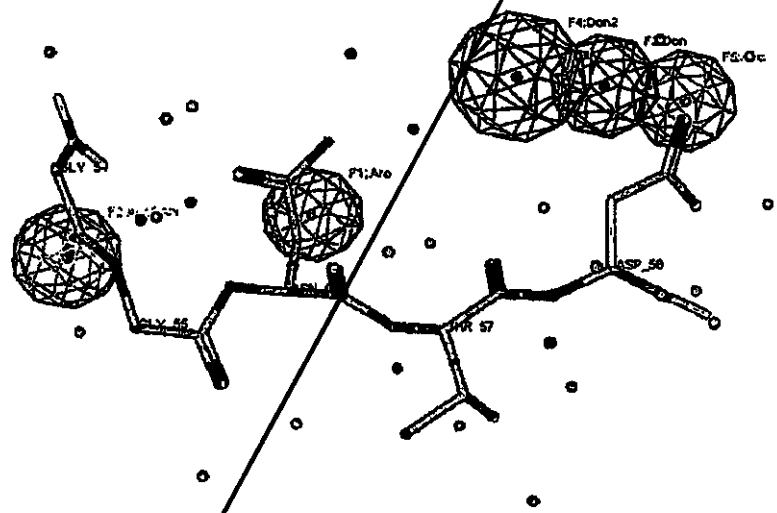


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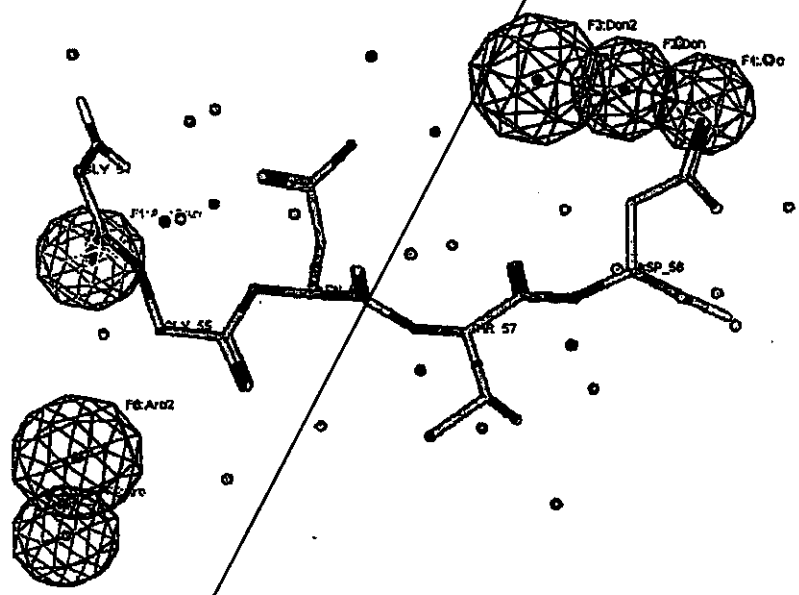


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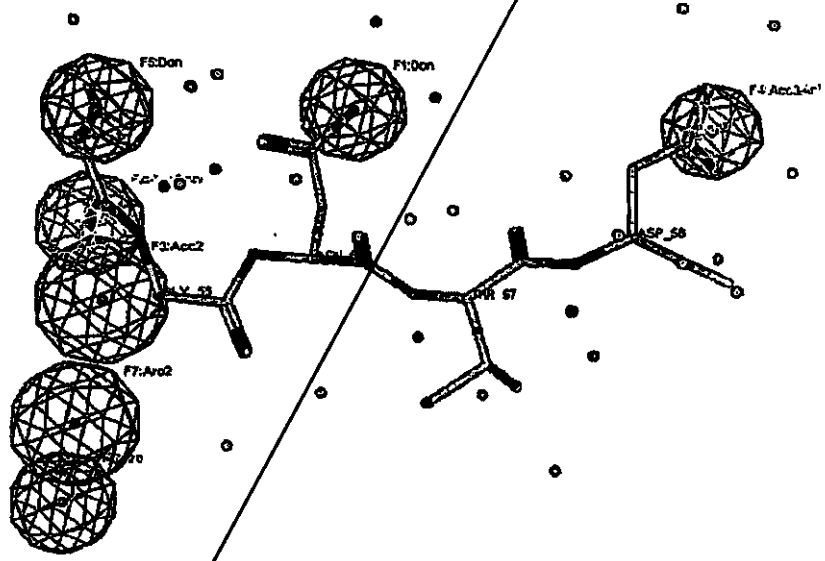


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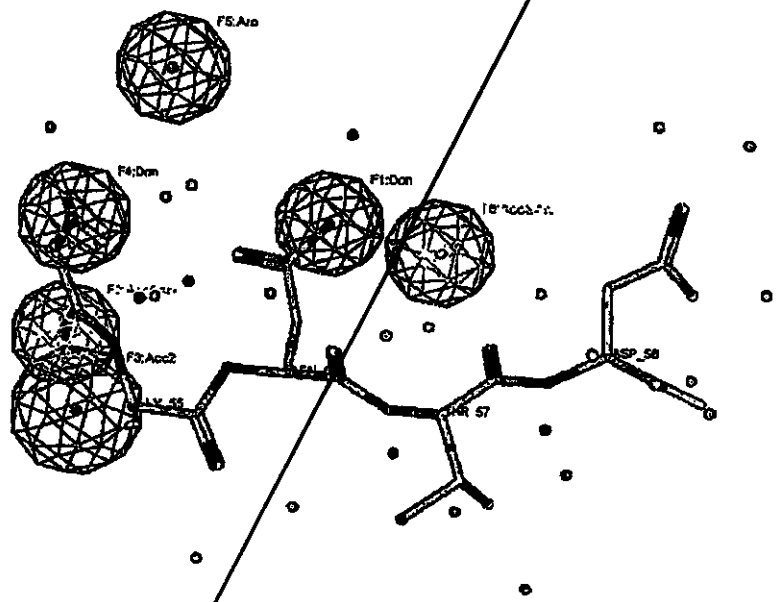


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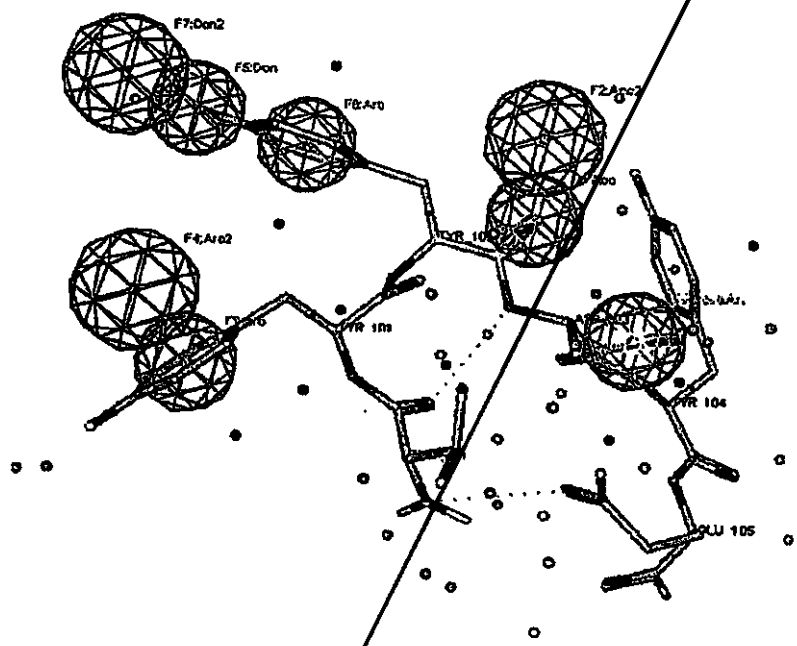


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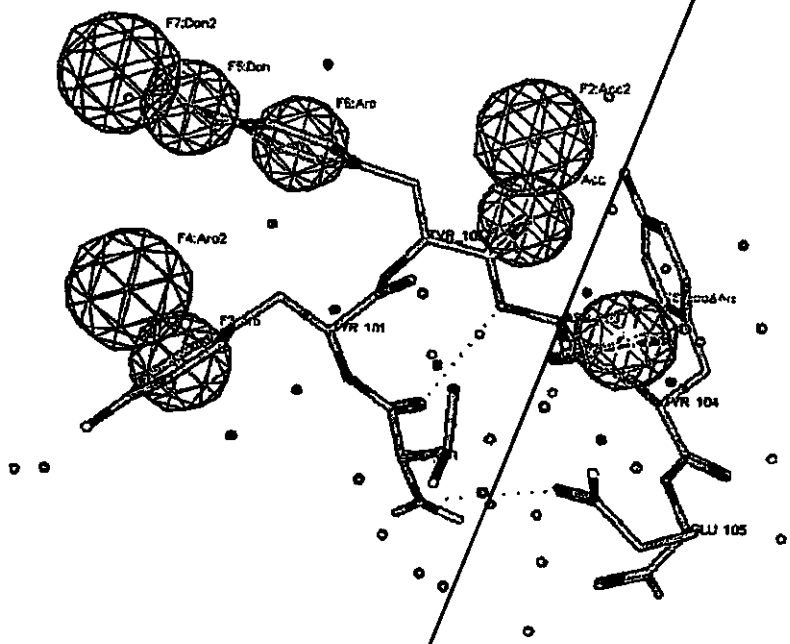


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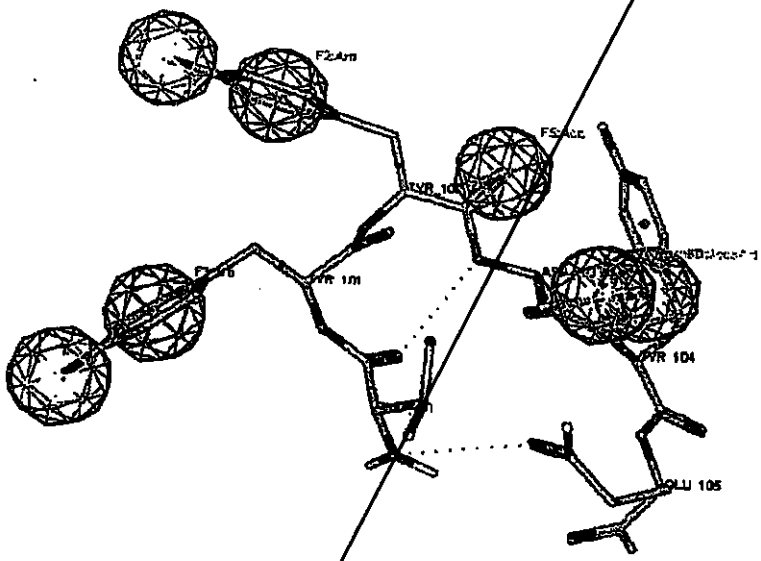


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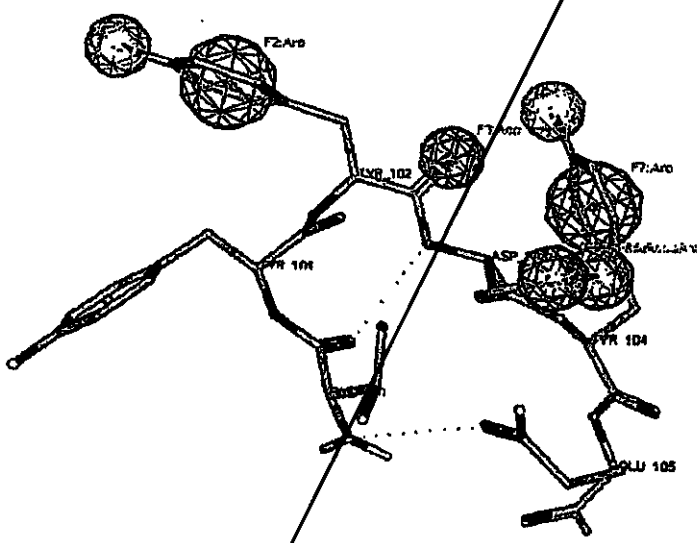


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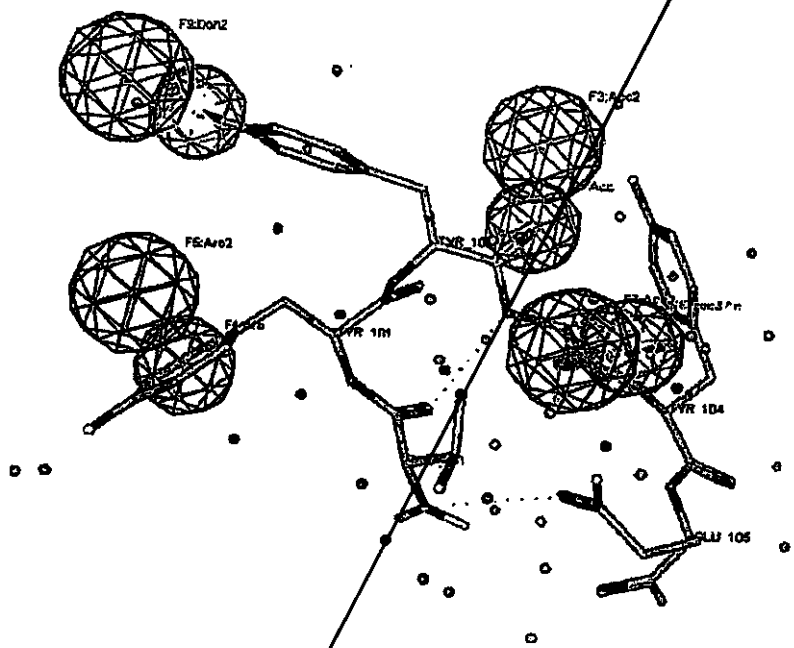


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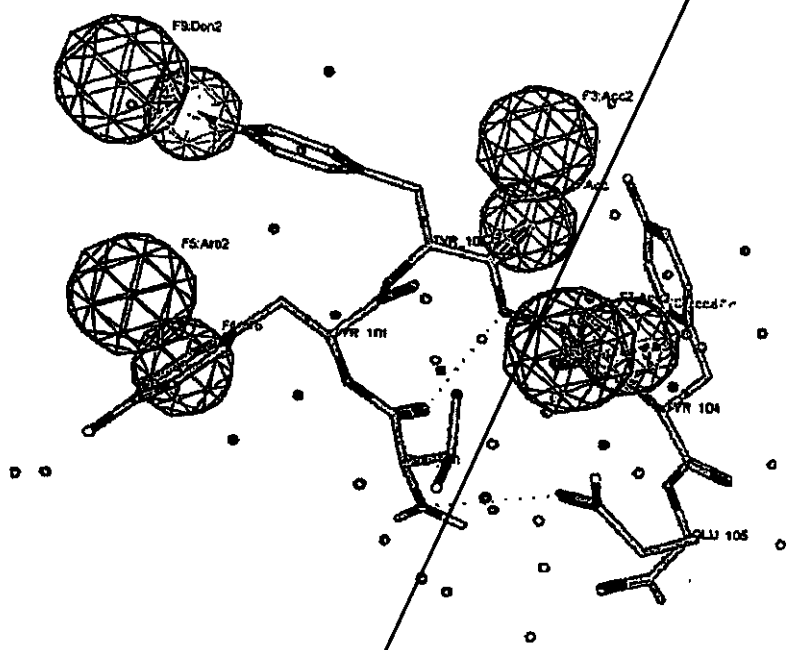


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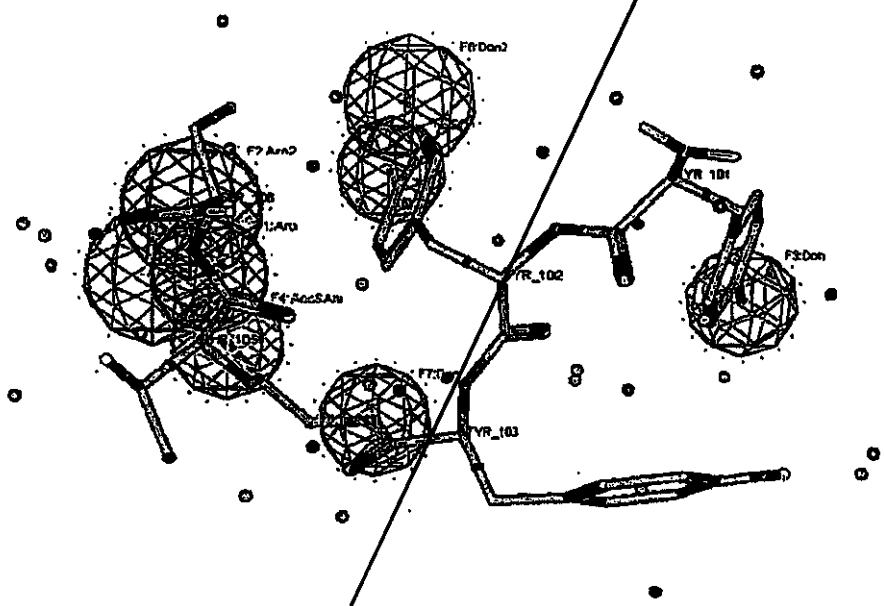


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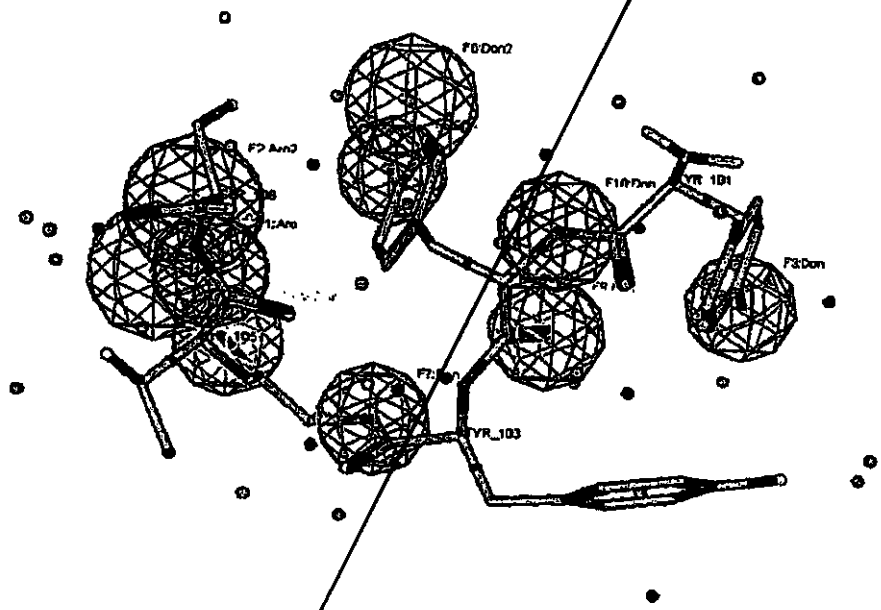


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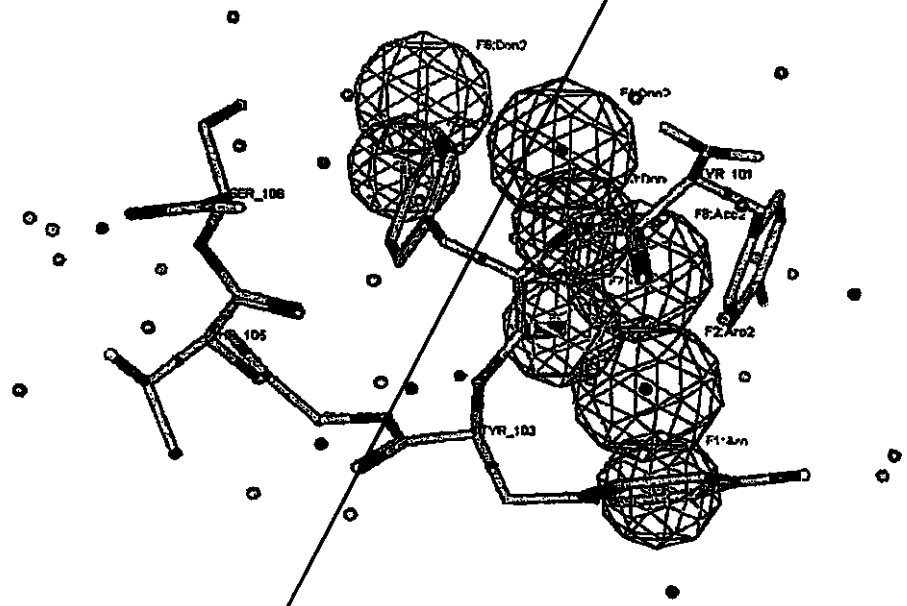


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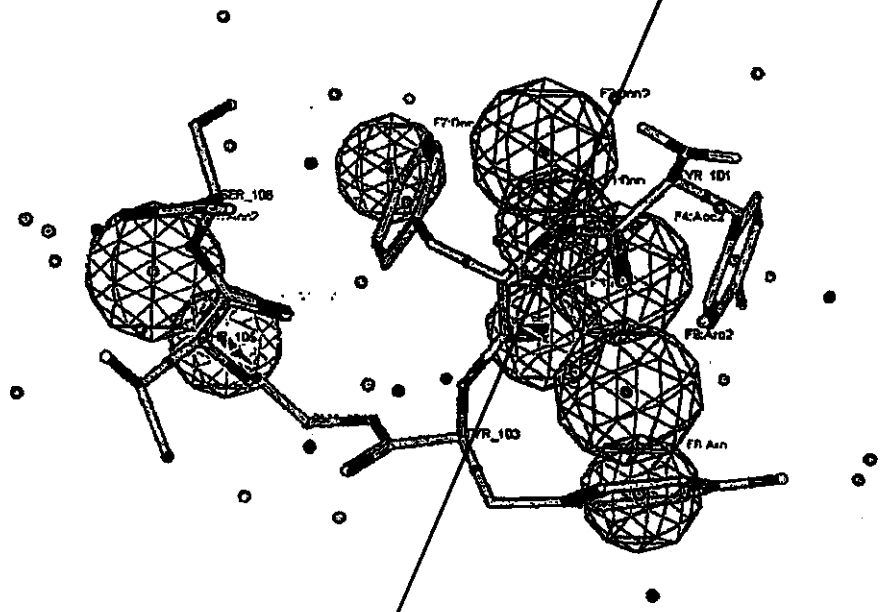


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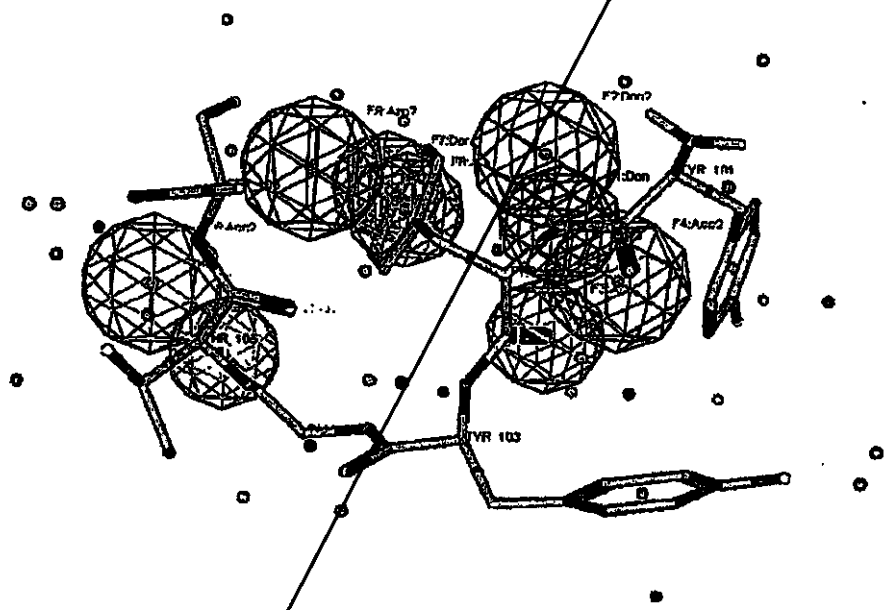


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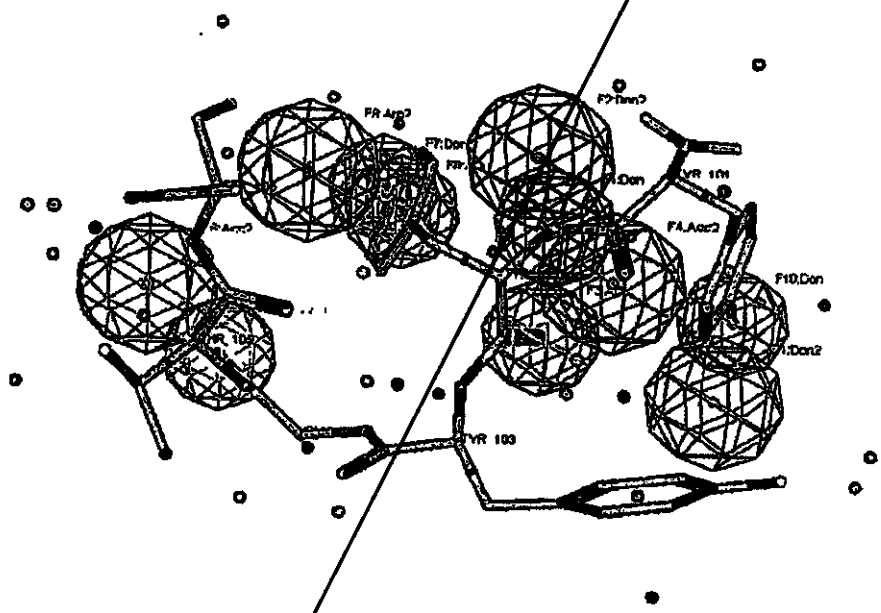


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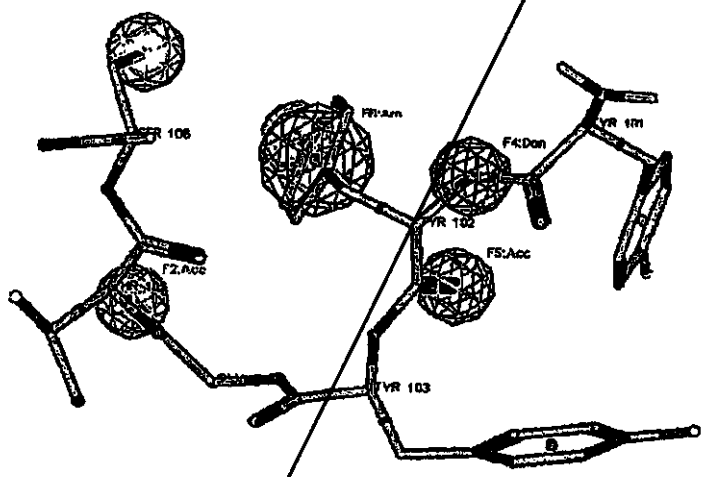


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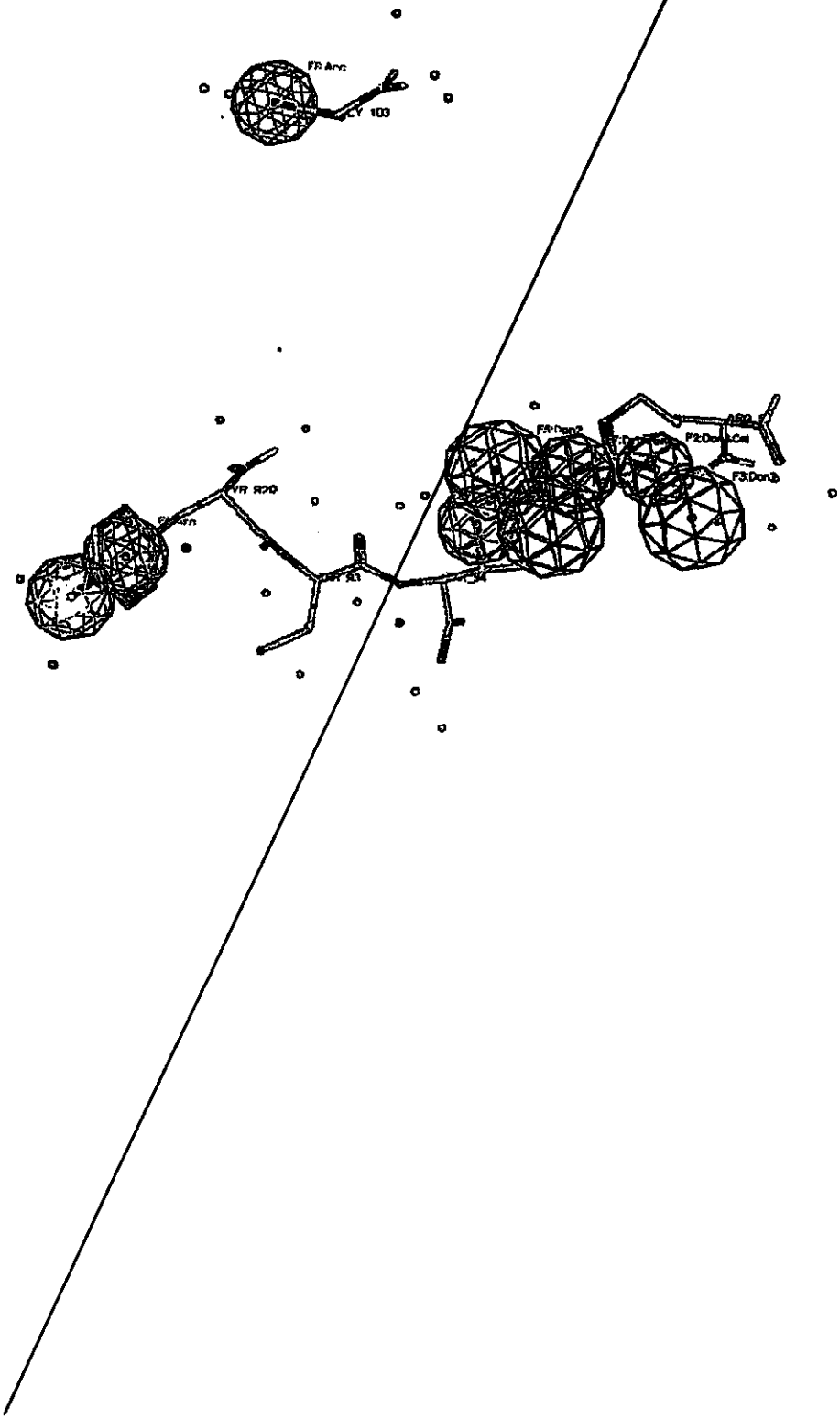


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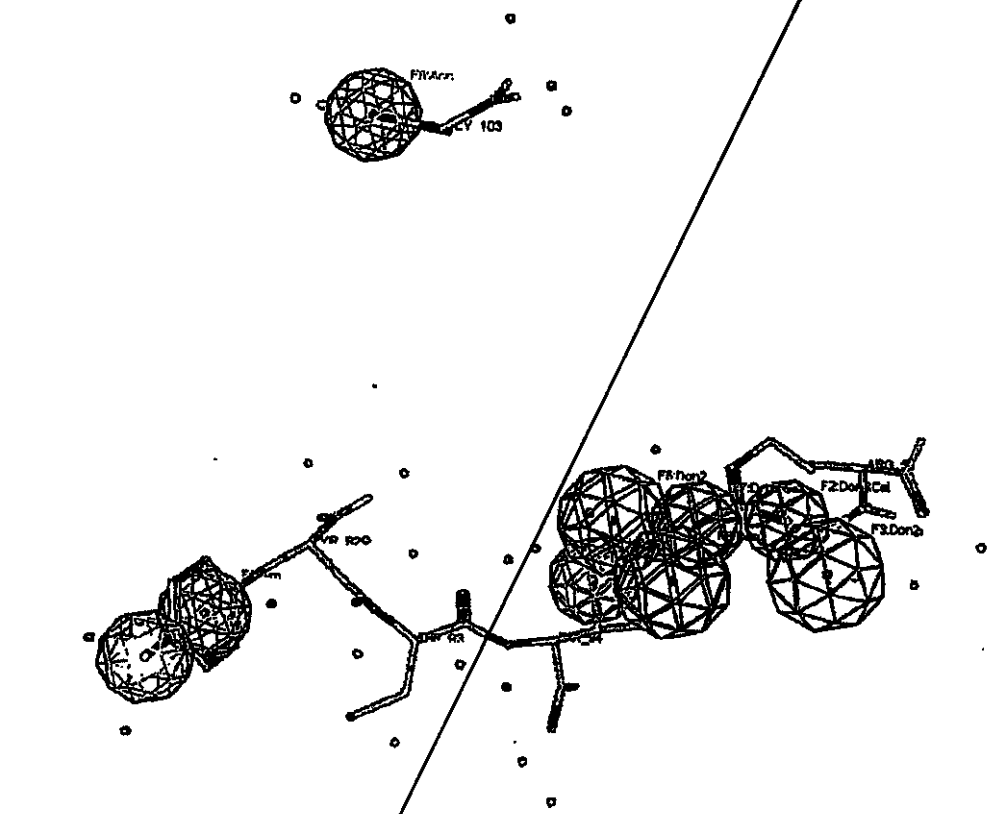


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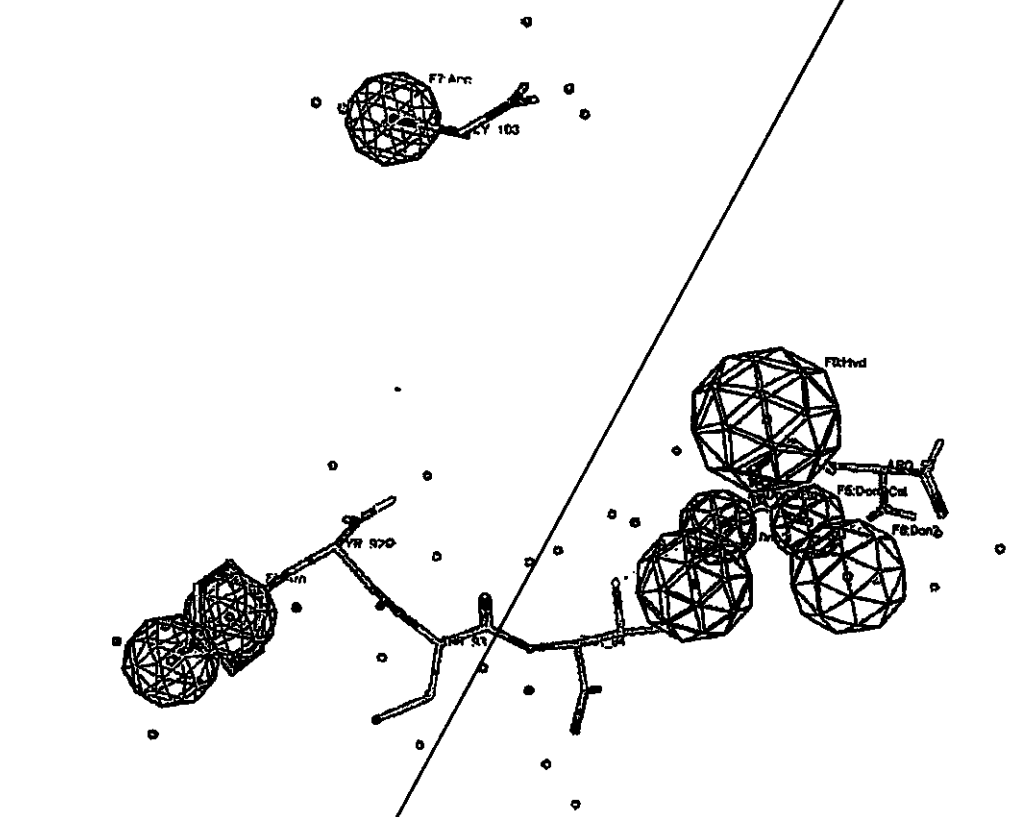


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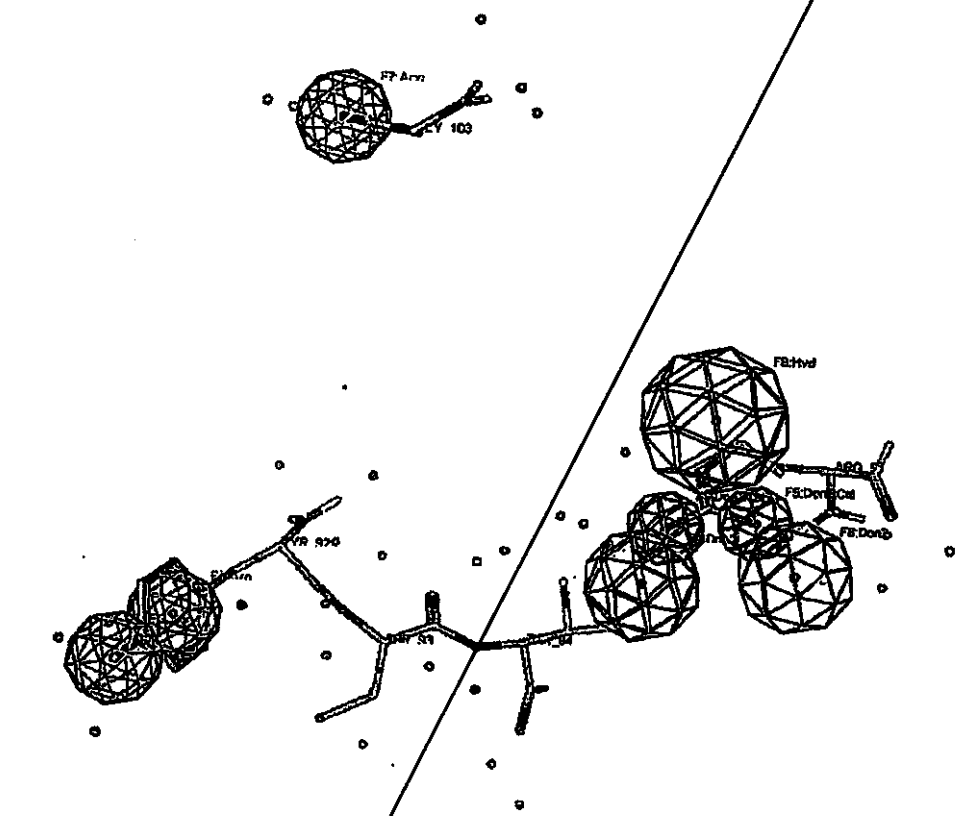


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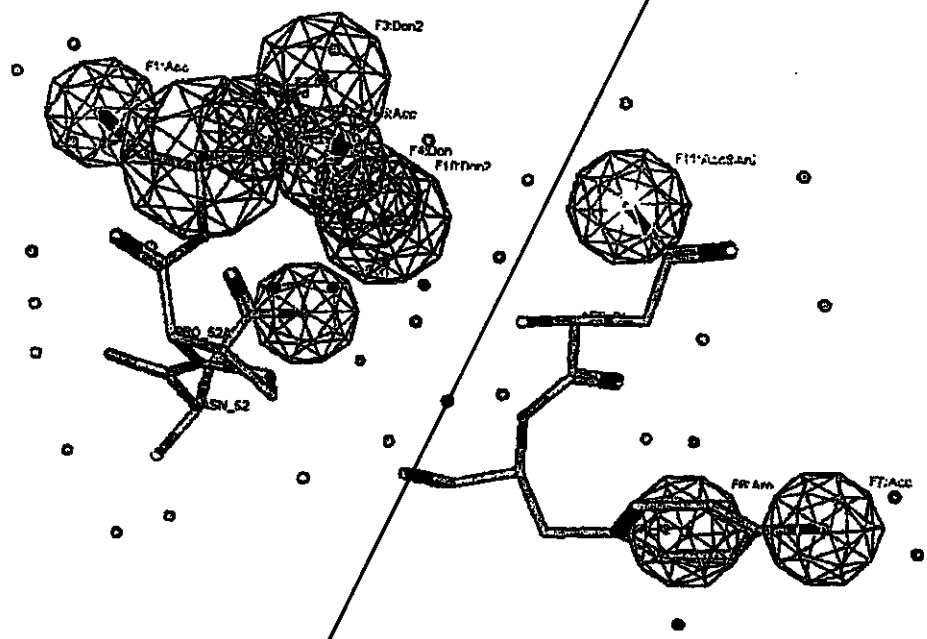


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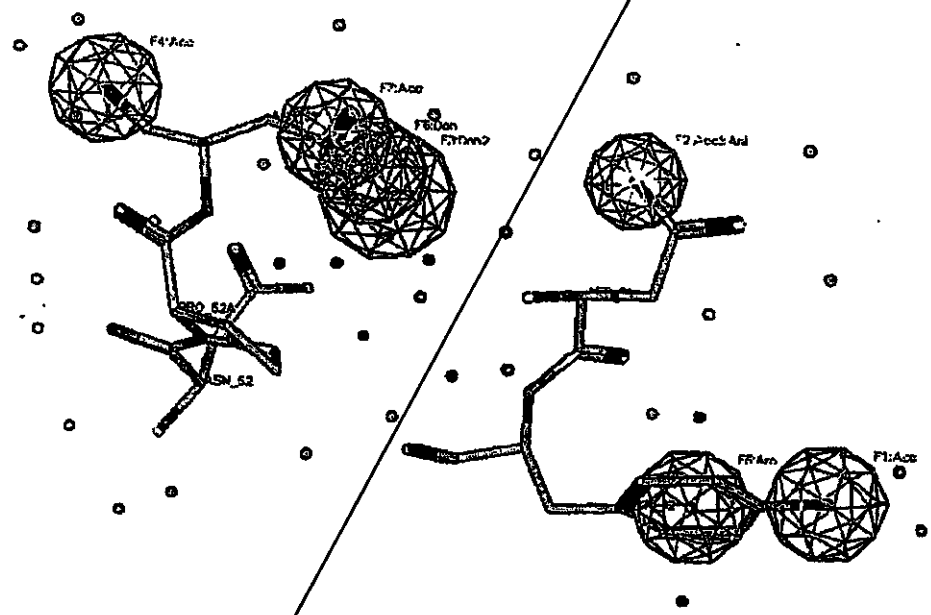


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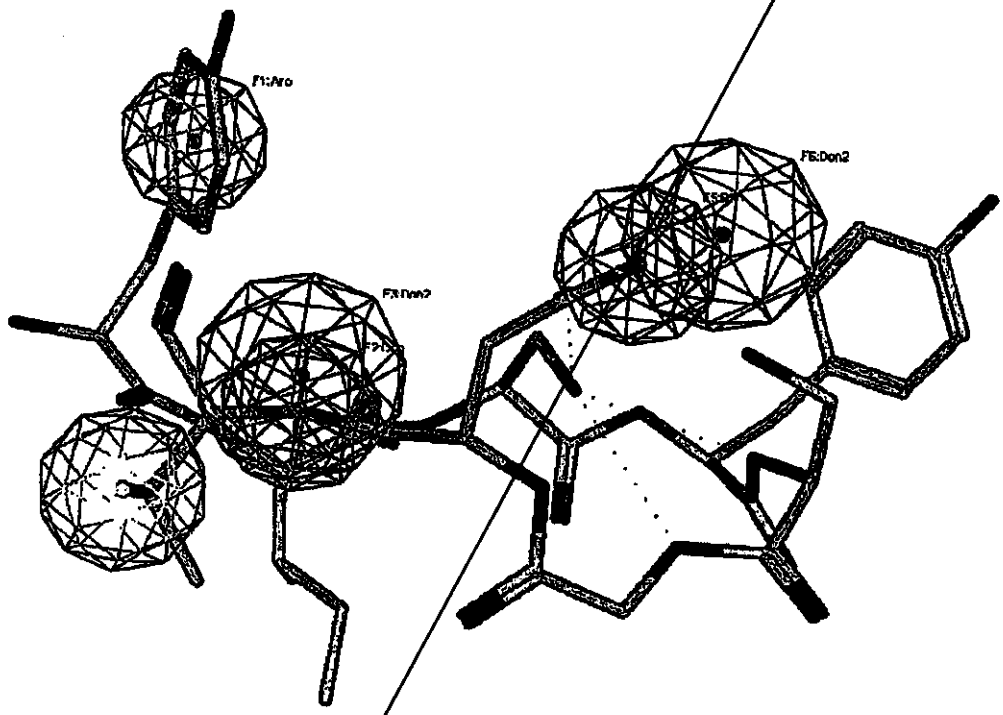


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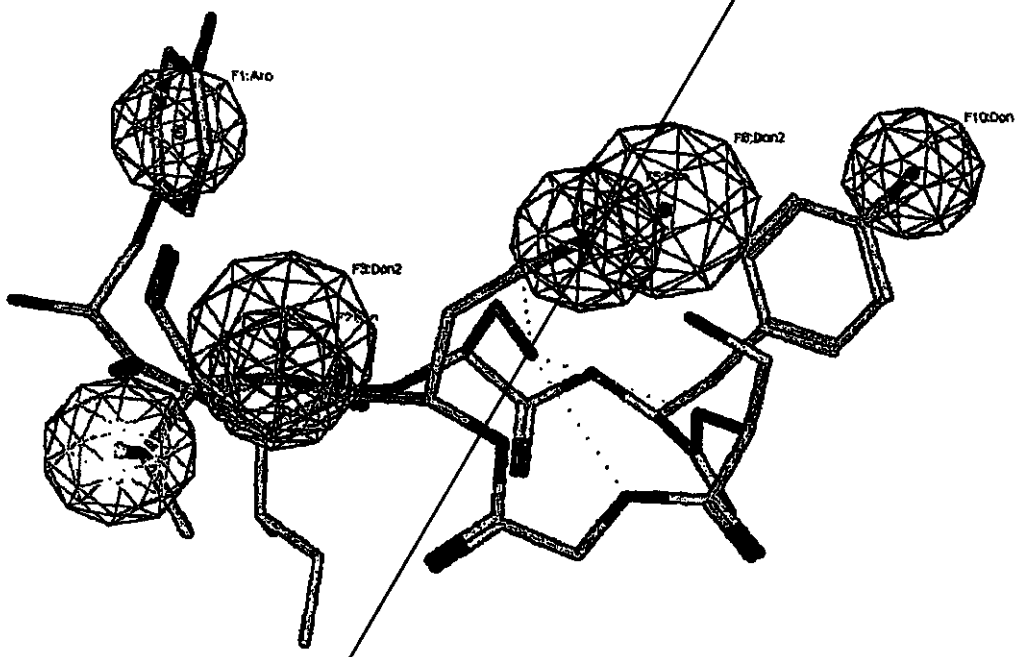


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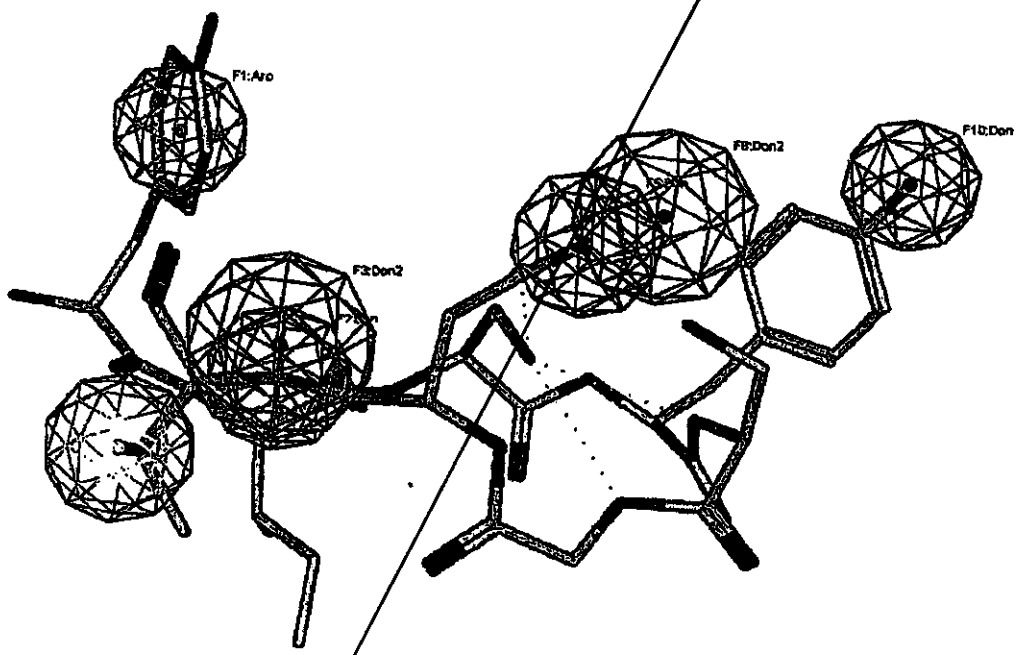


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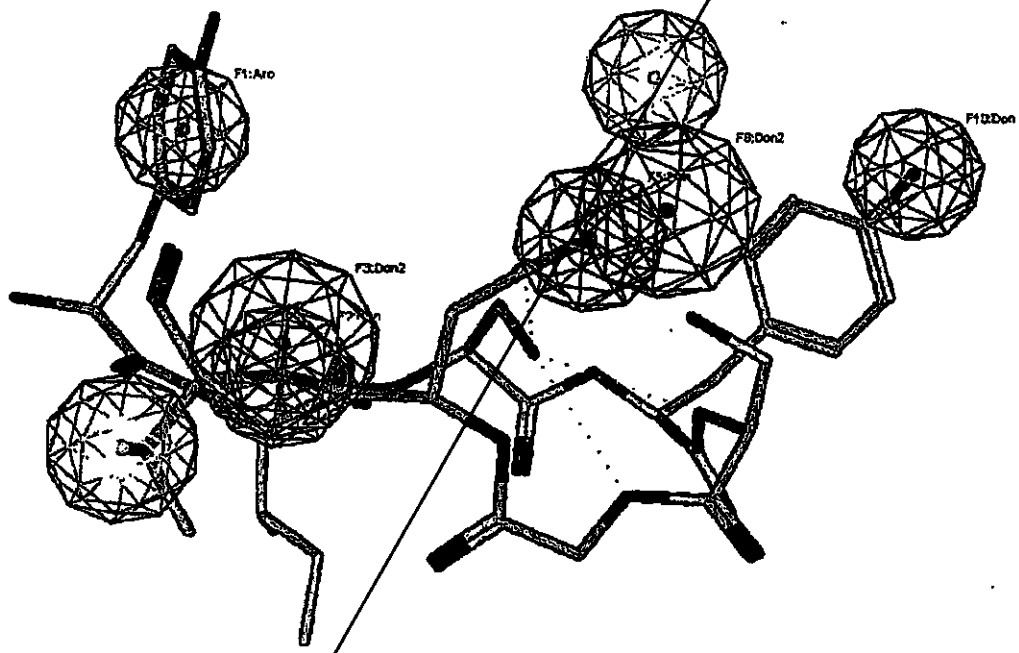


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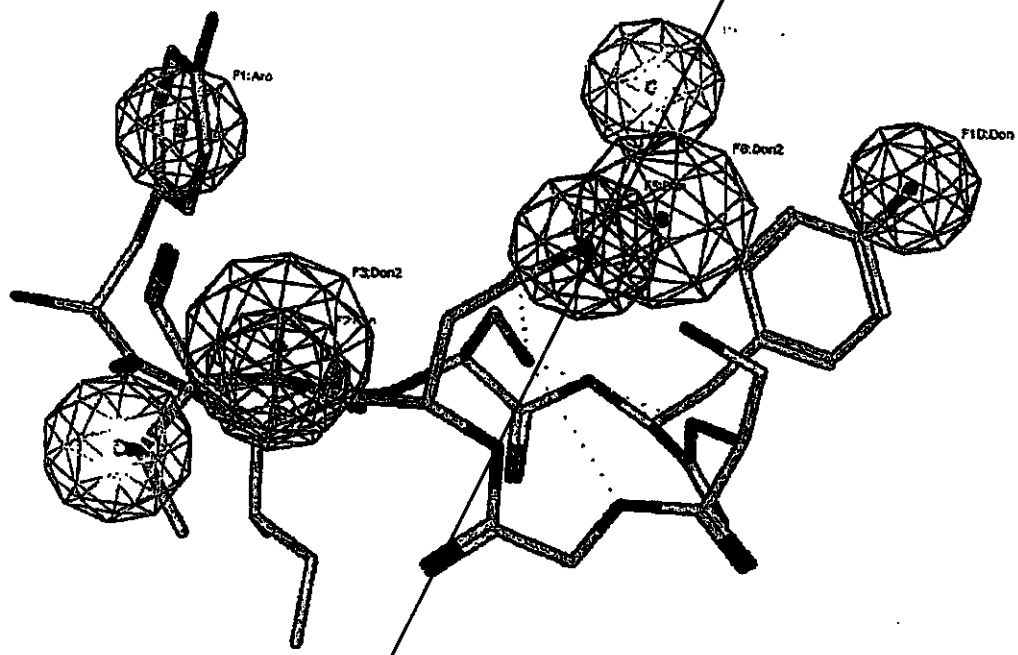


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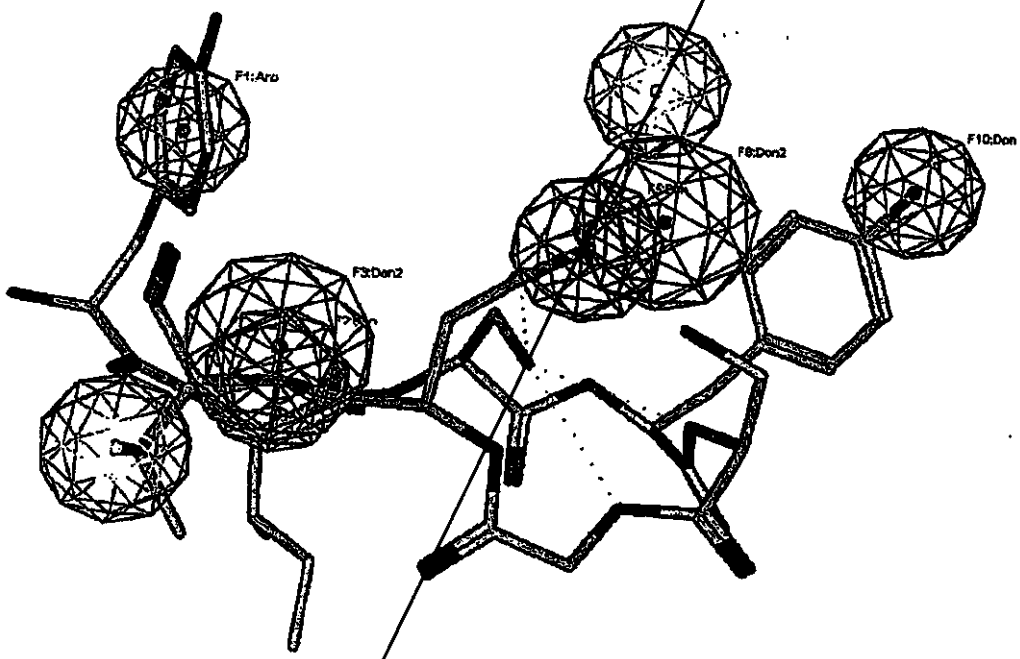


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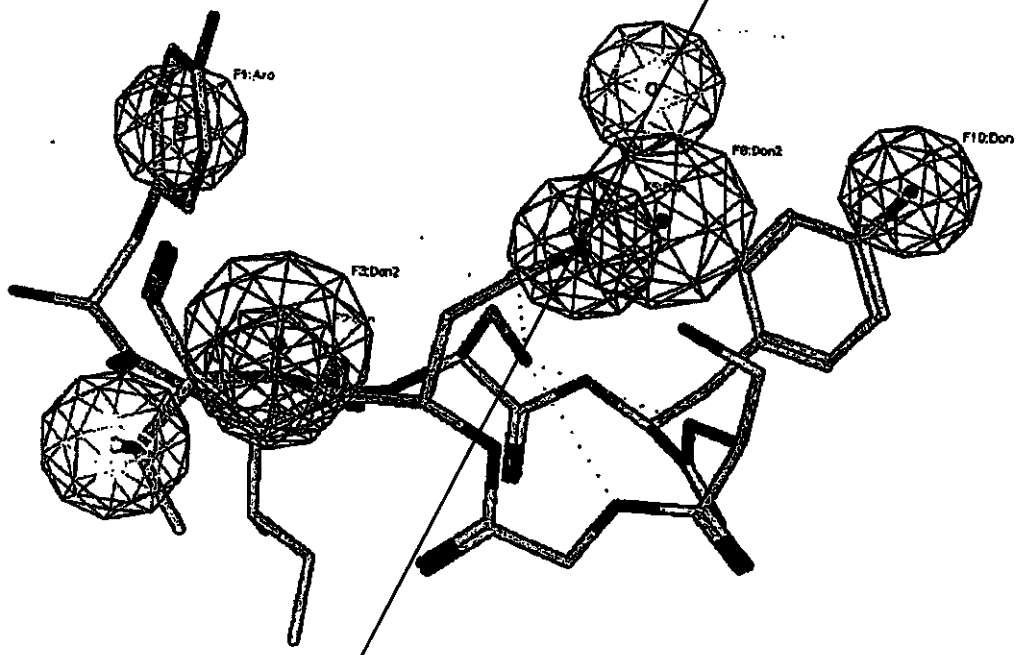


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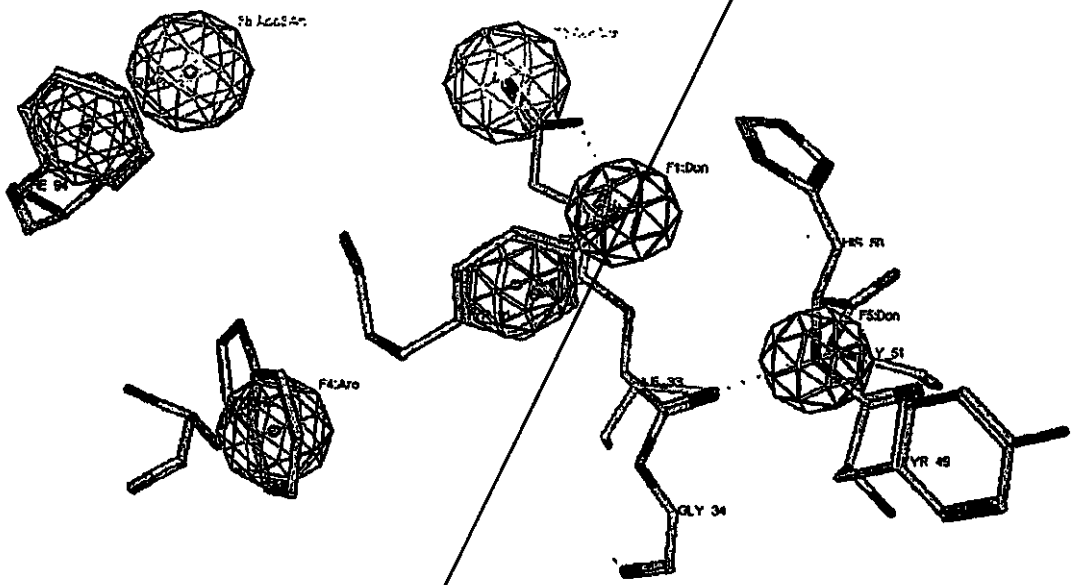


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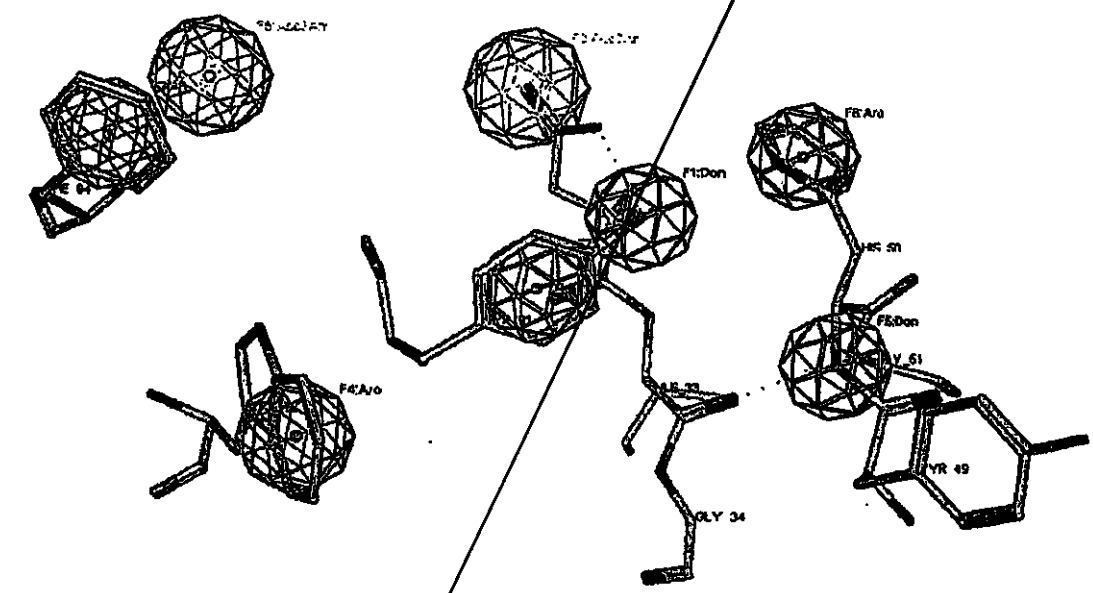


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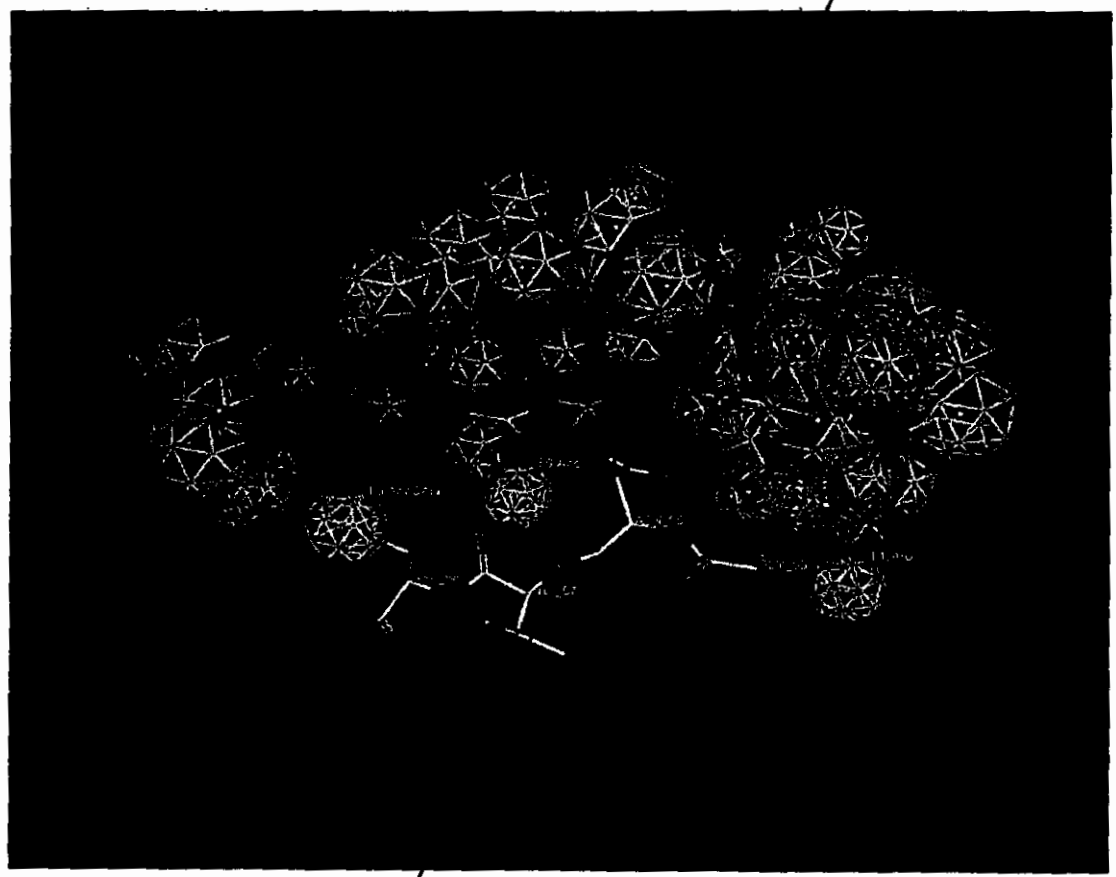


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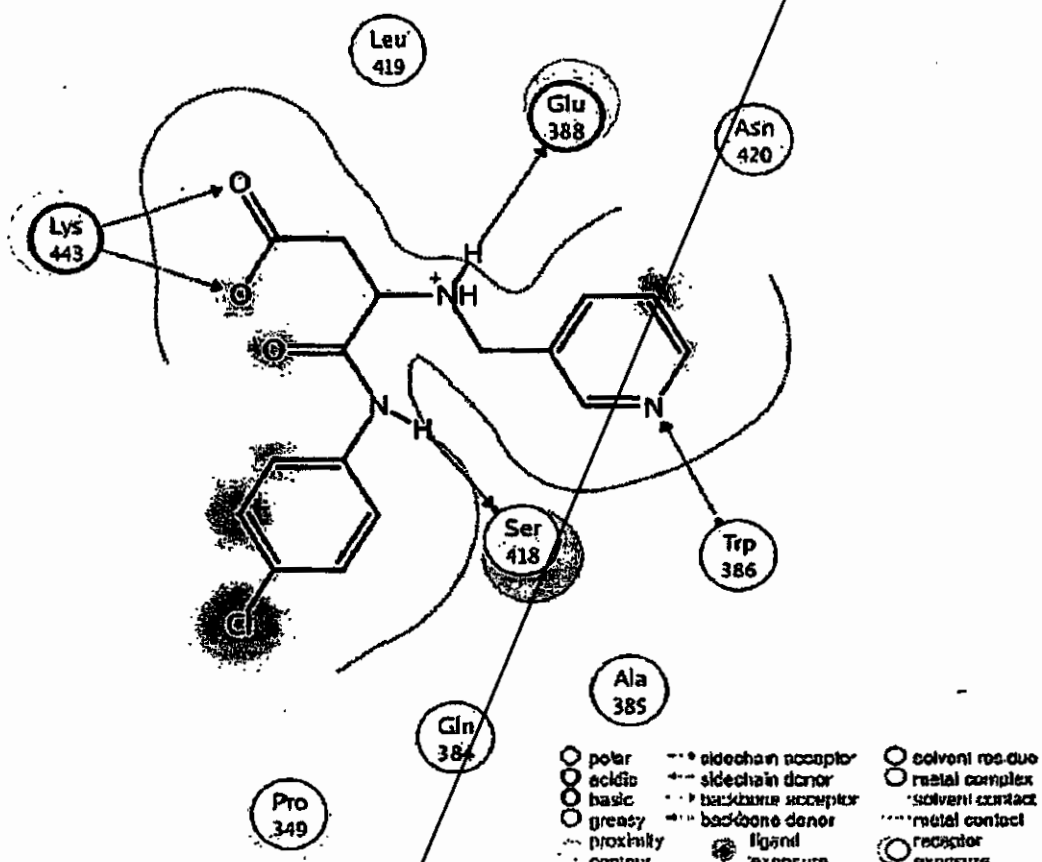
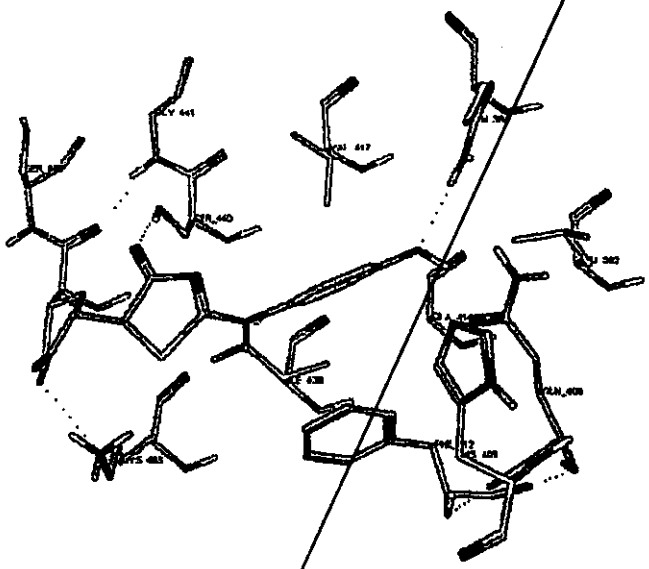
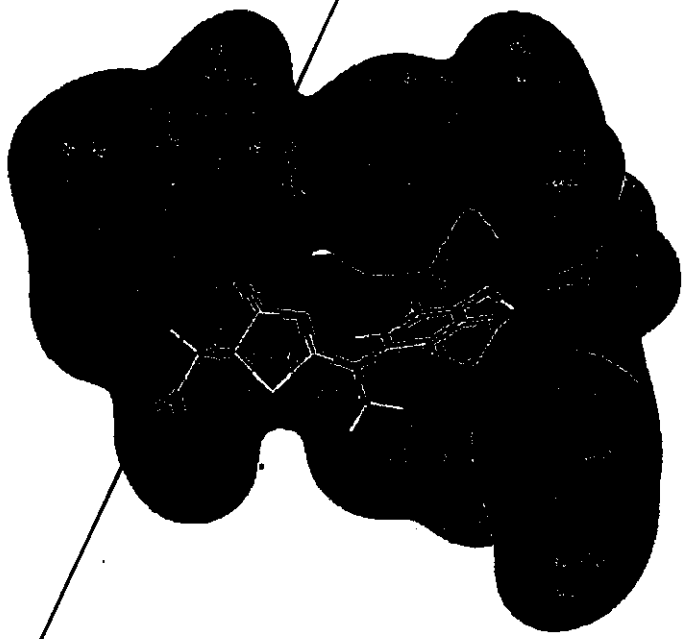

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Asn 420
Lys 443
Ser 418
Trp 386
Ala 385
Gln 384
Pro 349
polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure

Figure 47



47A



47B

Figure 48

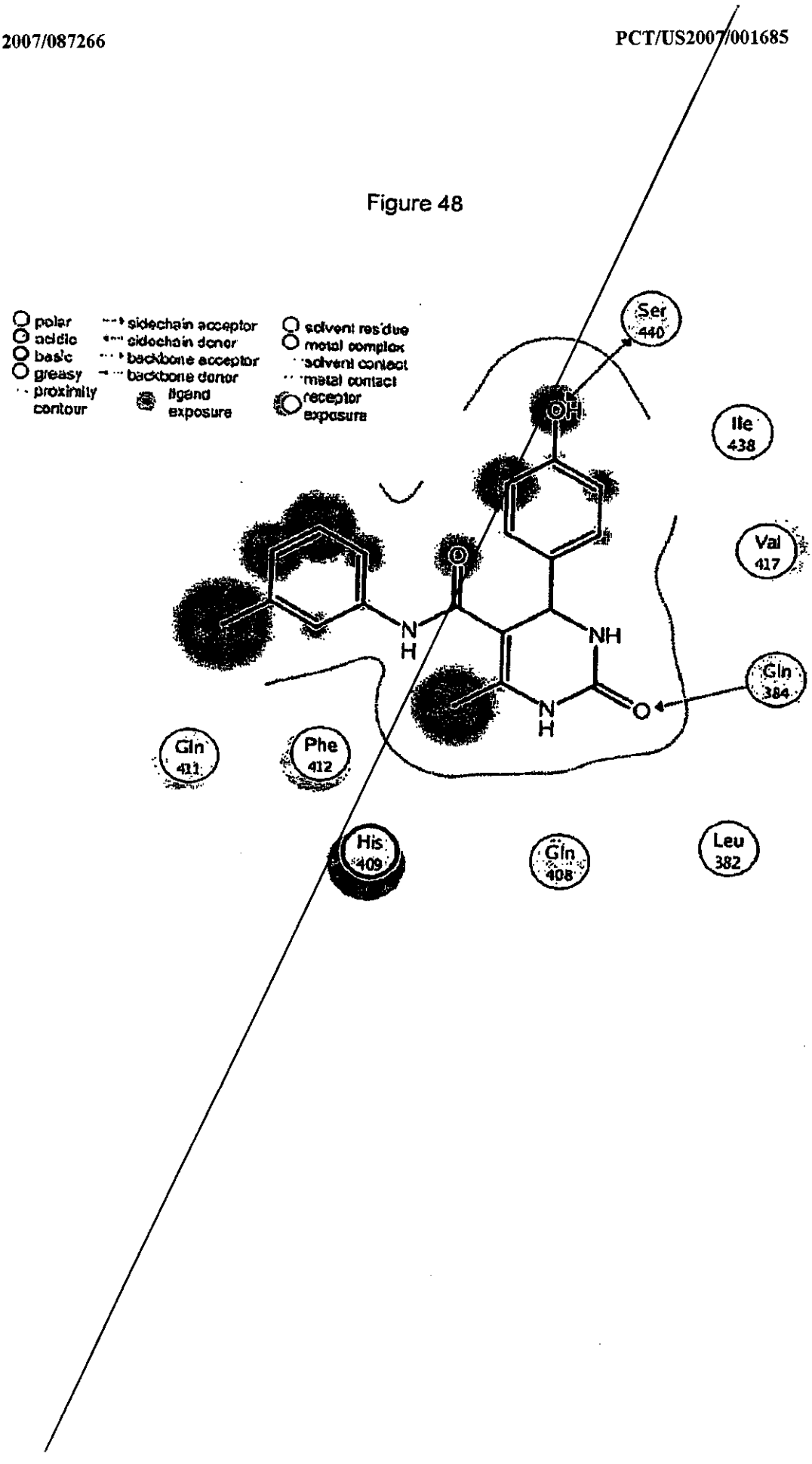

polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure
Ser 440
Ile 438
Val 417
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Leu 382
Gln 408
His 409
Phe 412
Gln 411
OH
O
N H
NH
N H
O

Figure 49

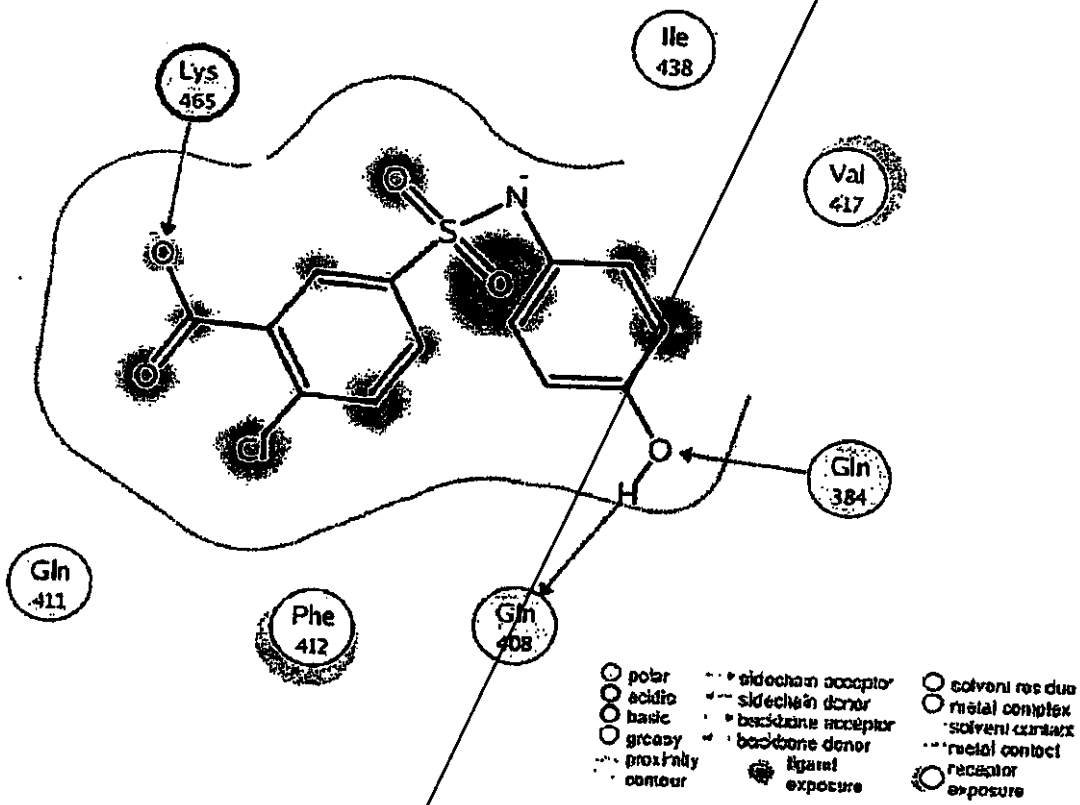

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Lys
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Val
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Cl
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Gln
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acidic
basic
greasy
proximity
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sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure

Figure 50

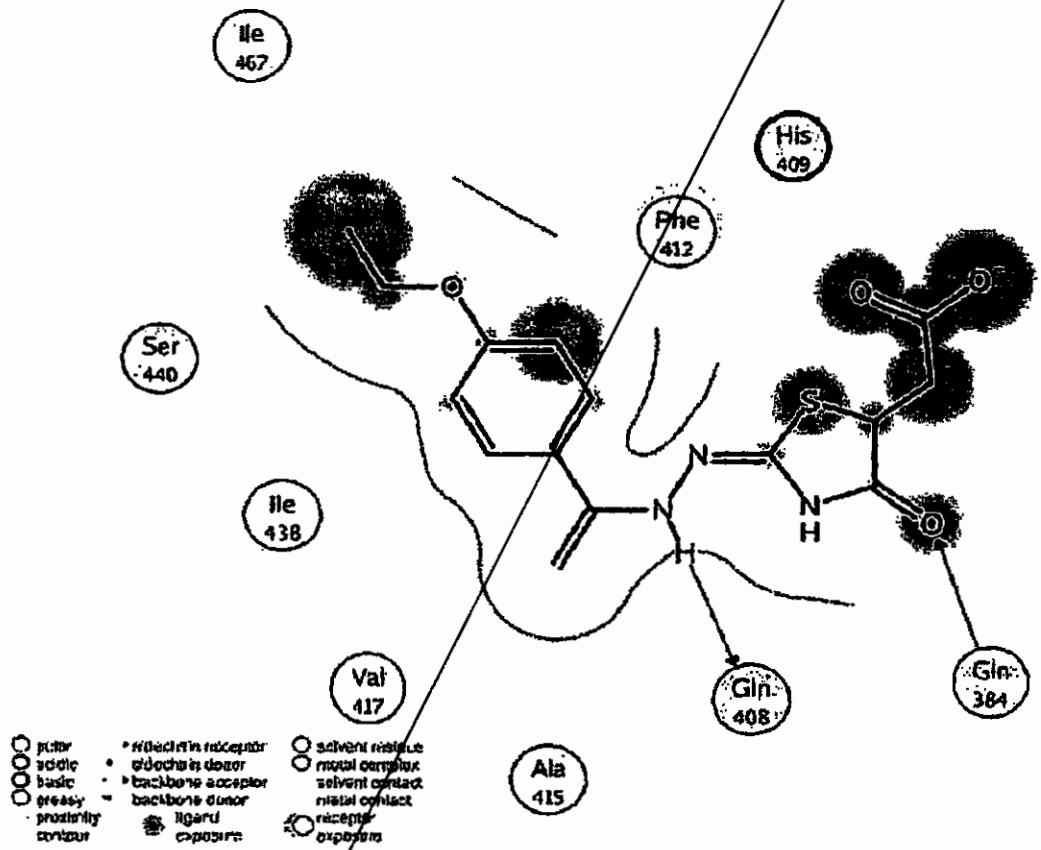

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Ala 415
N
N
H
S
O

Figure 51

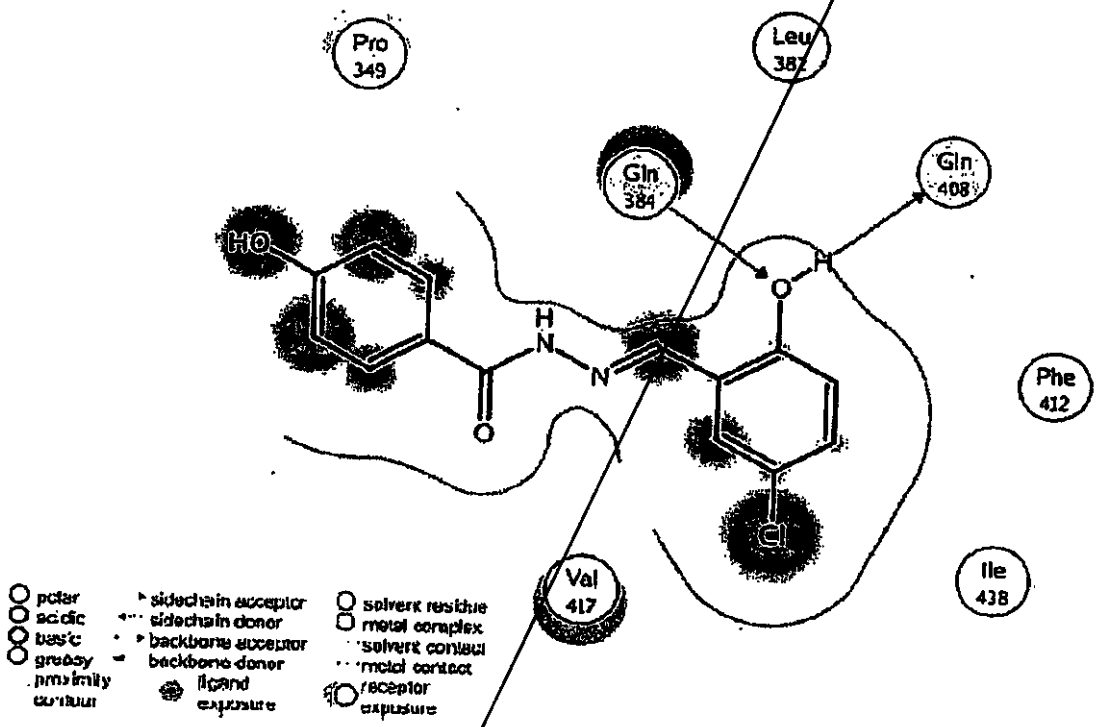

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Gln
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polar
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proximity
contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand
exposure
solvent residue
metal complex
solvent contact
metal contact
receptor
exposure

Figure 52

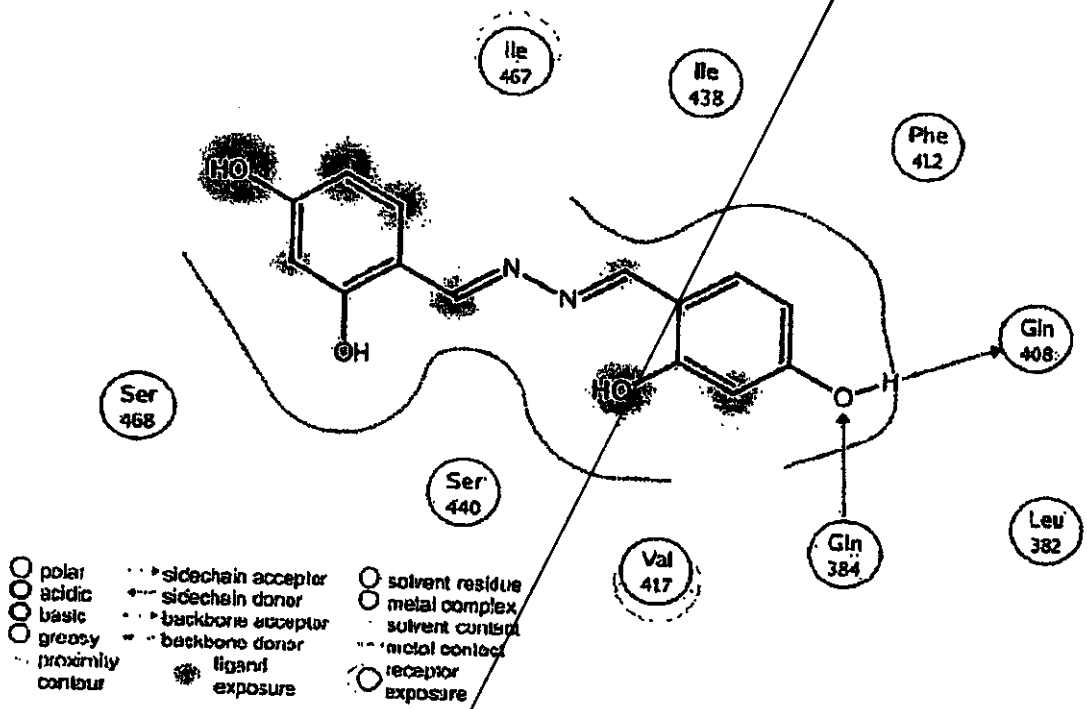

Ile 467
Ile 438
Phe 412
Gln 408
Ser 468
Ser 440
Val 417
Gln 384
Leu 382
HO
OH
N
N
O
H
polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure

Figure 53

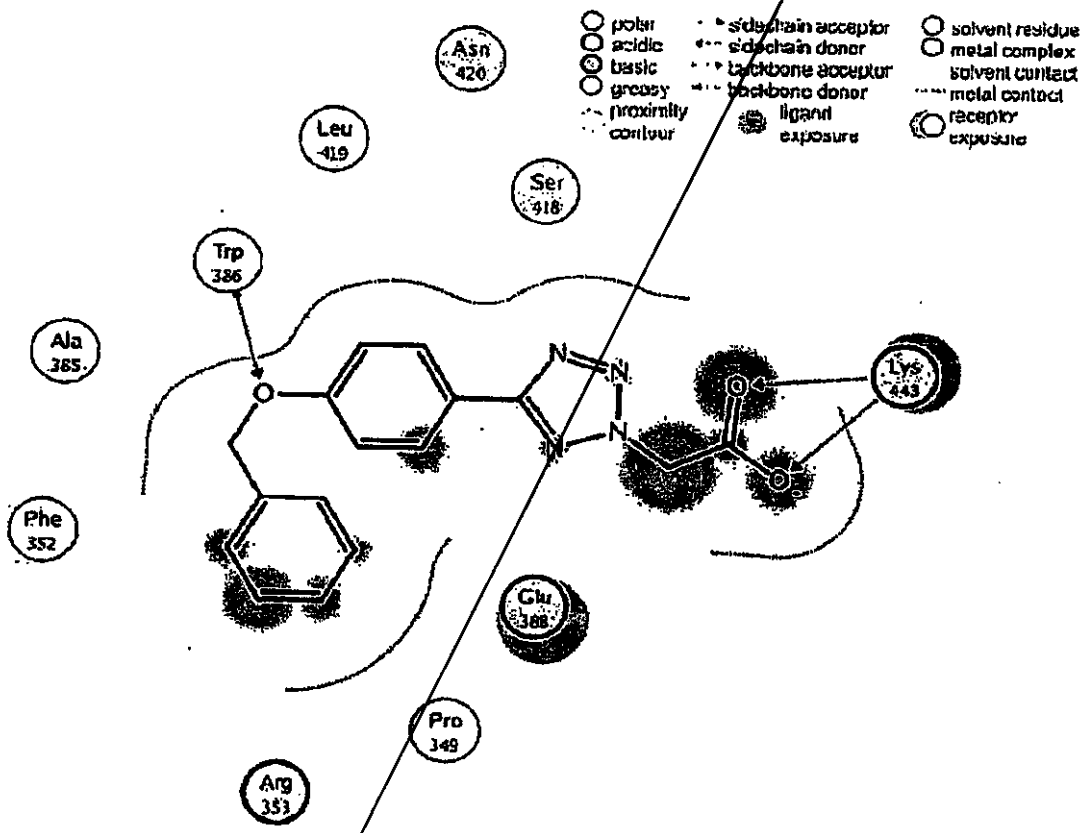

polar
acidic
basic
greasy
proximity
contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure
Asn 420
Leu 419
Ser 418
Trp 386
Ala 385
Phe 352
Glu 388
Pro 349
Arg 353
Lys 443
N
N
N
O
O
O

Figure 54

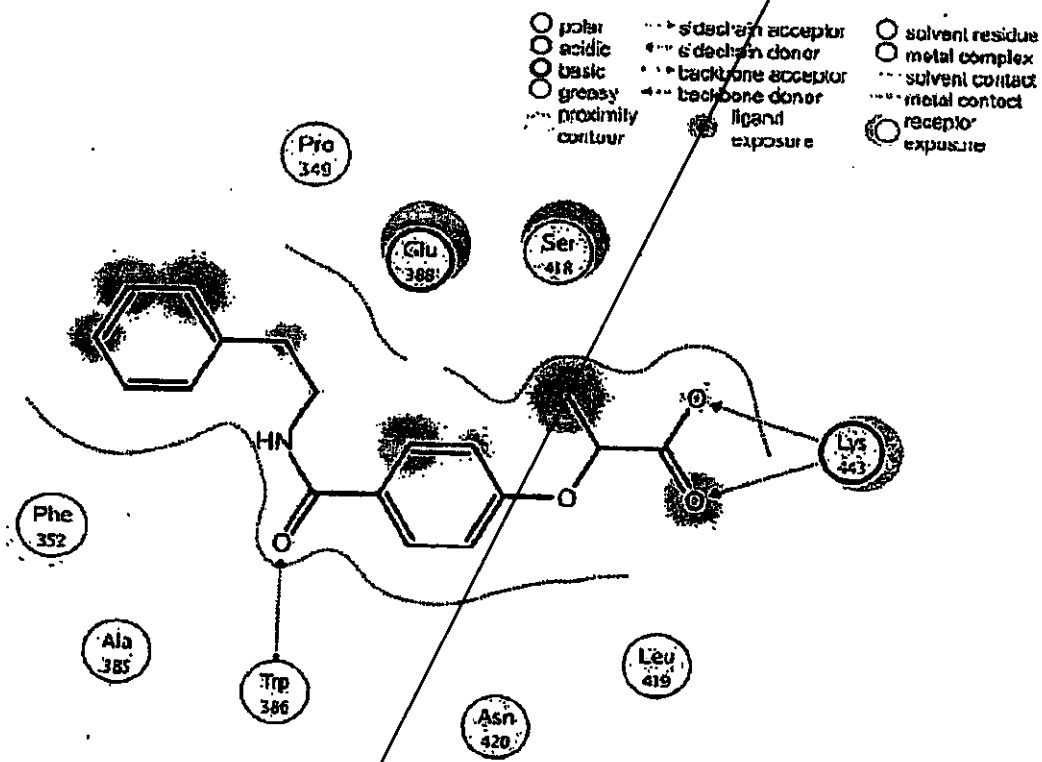

polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure
Pro 349
Glu 388
Ser 418
Lys 443
Phe 352
Ala 385
Trp 386
Asn 420
Leu 419
HN
O

Figure 55

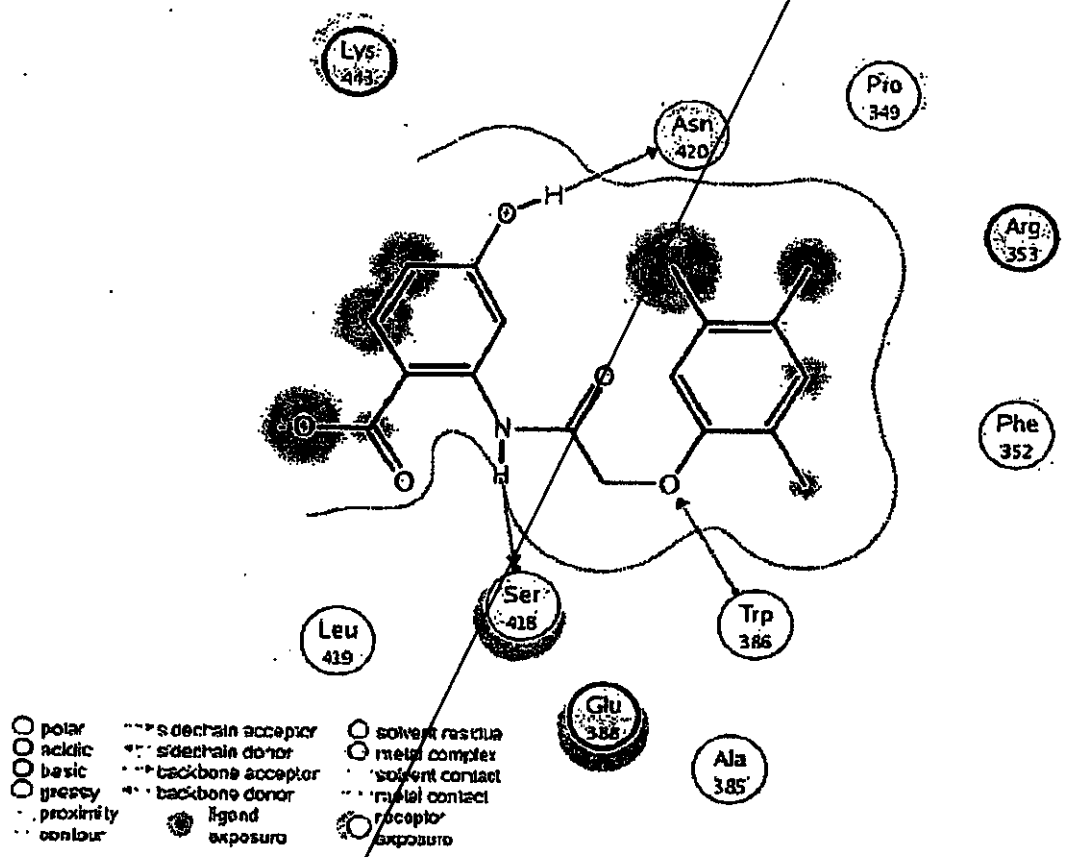

Lys 443
Asn 420
Pro 349
Arg 353
Phe 352
Ser 418
Trp 386
Leu 419
Glu 386
Ala 385
polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent exposure
metal complex
solvent contact
metal contact
receptor exposure

Figure 56

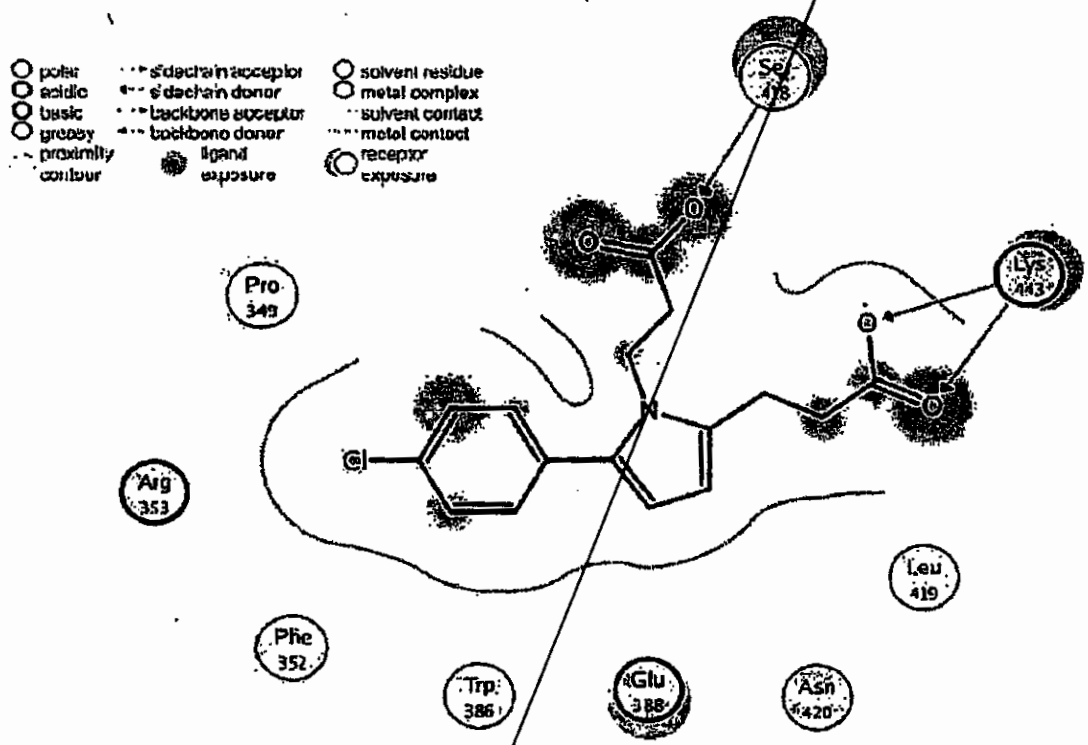

polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure
Ser 478
Lys 443
Pro 349
Arg 353
Leu 419
Phe 352
Trp 386
Glu 388
Asn 420

Figure 57

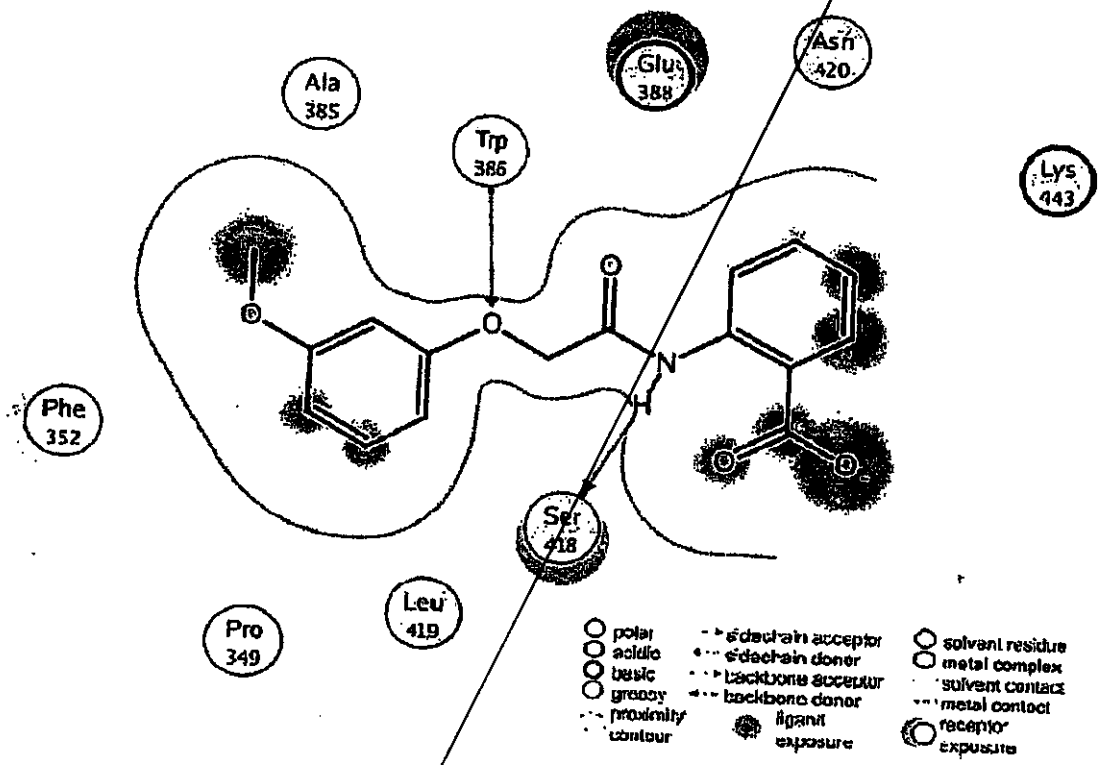
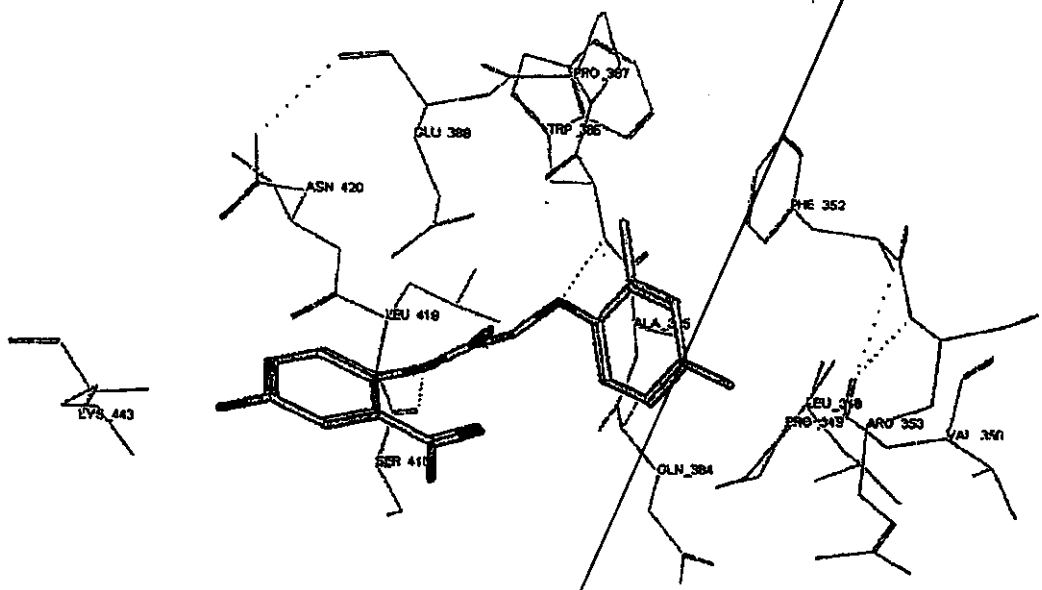

Glu 388
Asn 420
Ala 385
Trp 386
Lys 443
Phe 352
Ser 418
Leu 419
Pro 349
polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure

Figure 58



58A



58B

Figure 59

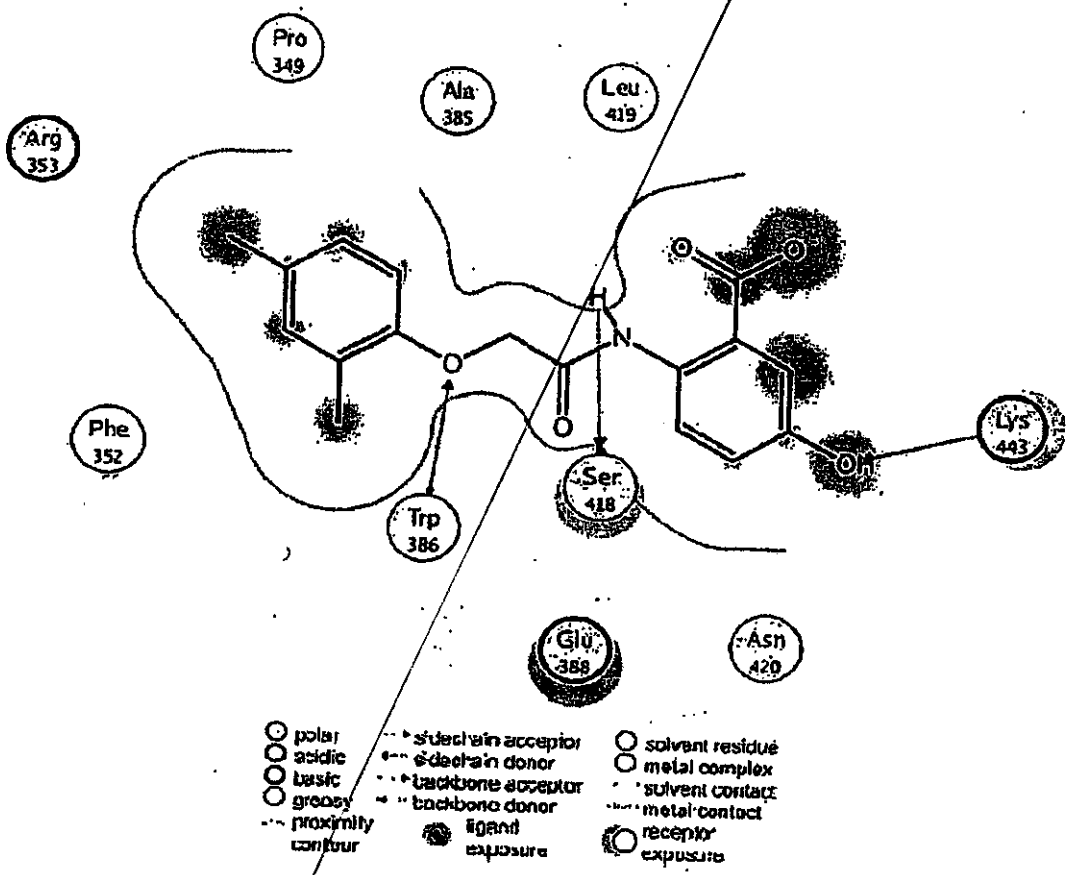
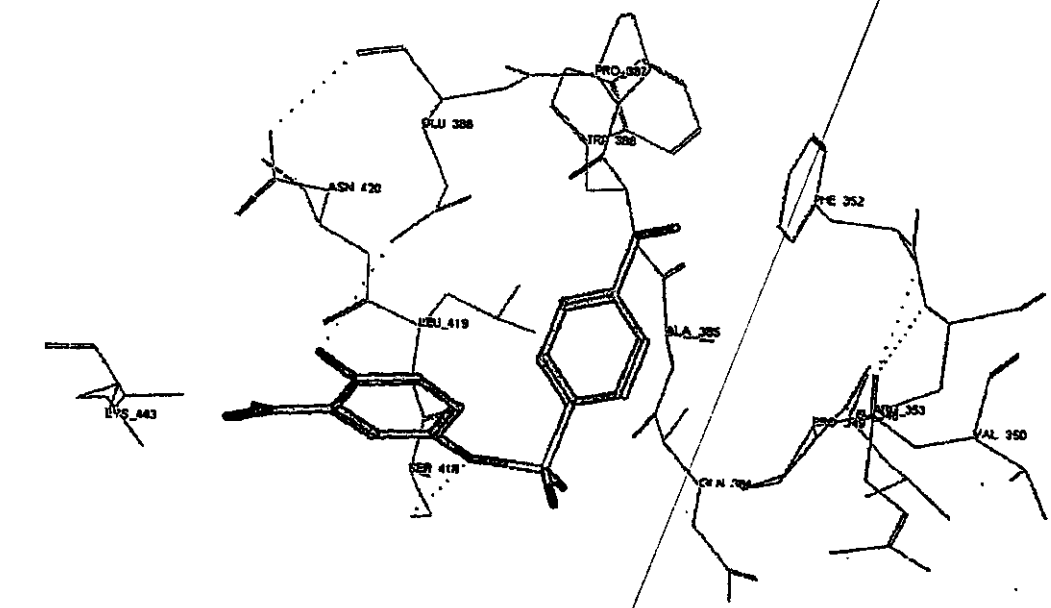
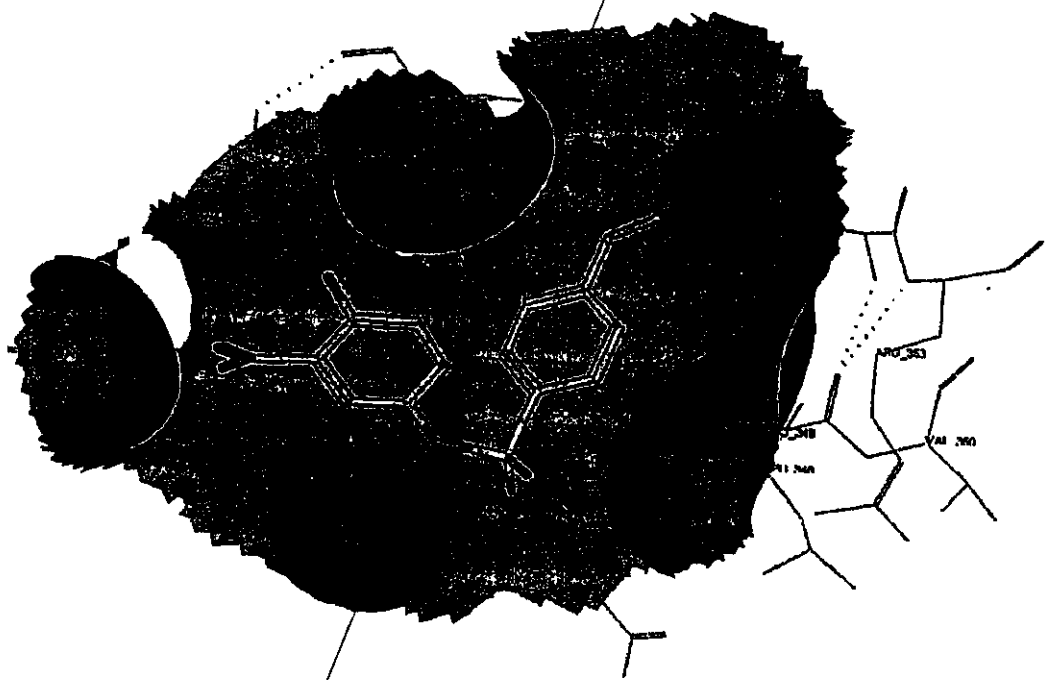

Pro 349
Ala 385
Leu 419
Arg 353
Phe 352
Trp 386
Ser 418
Lys 443
Glu 388
Asn 420
O
N
OH
polar
acidic
basic
greasy
proximity contour
side chain acceptor
side chain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure

Figure 60



60A



60B

Figure 61

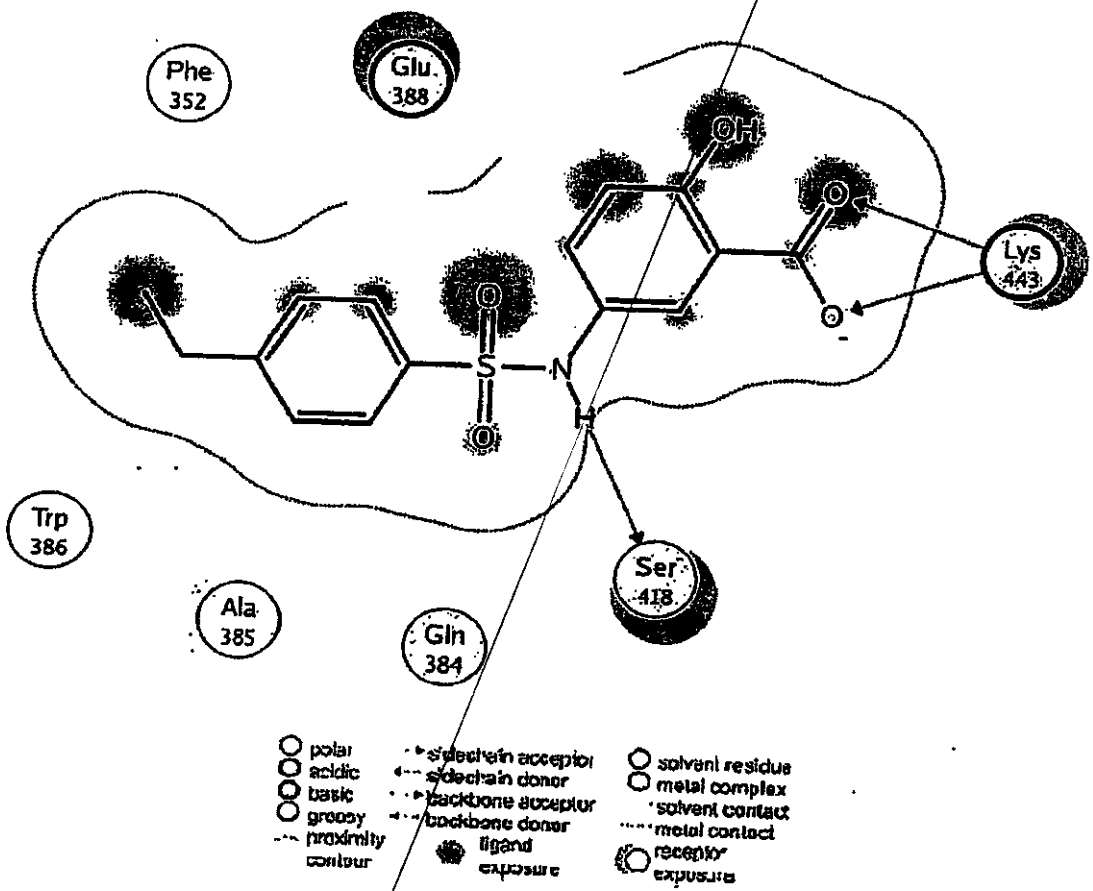
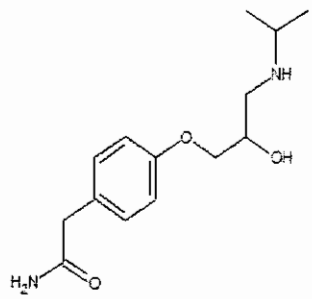
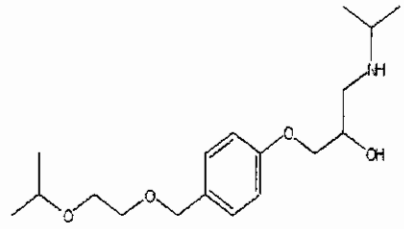

Phe 352
Glu 388
OH
O
Lys 443
O
S
N
H
O
Trp 386
Ser 418
Ala 385
Gln 384
polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure

FIGURE 1A

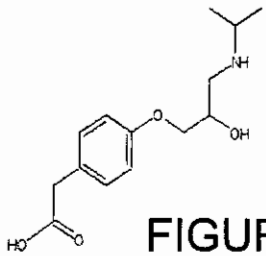


Atenolol

FIGURE 1B

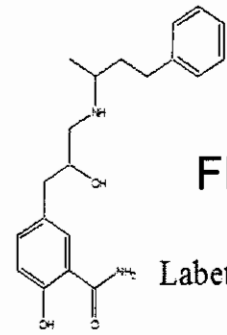


Bisoprolol



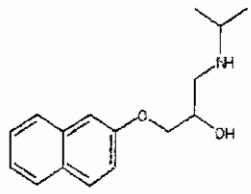
Metoprolol

FIGURE 1C



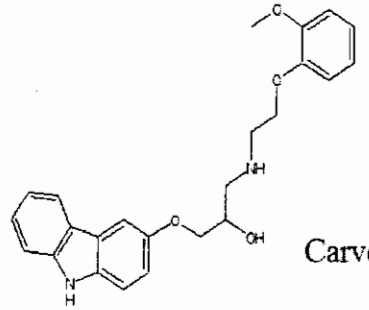
Labetalol

FIGURE 1D



Propranolol

FIGURE 1E



Carvedilol

FIGURE 1F

FIGURE 2

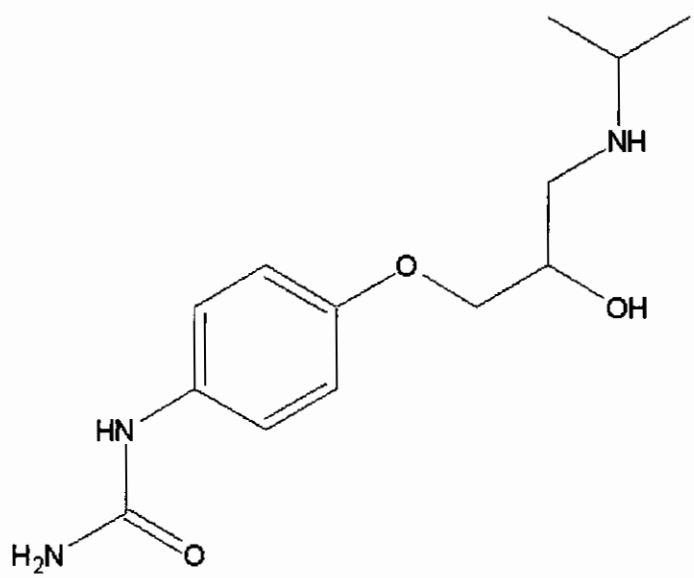


FIGURE 3

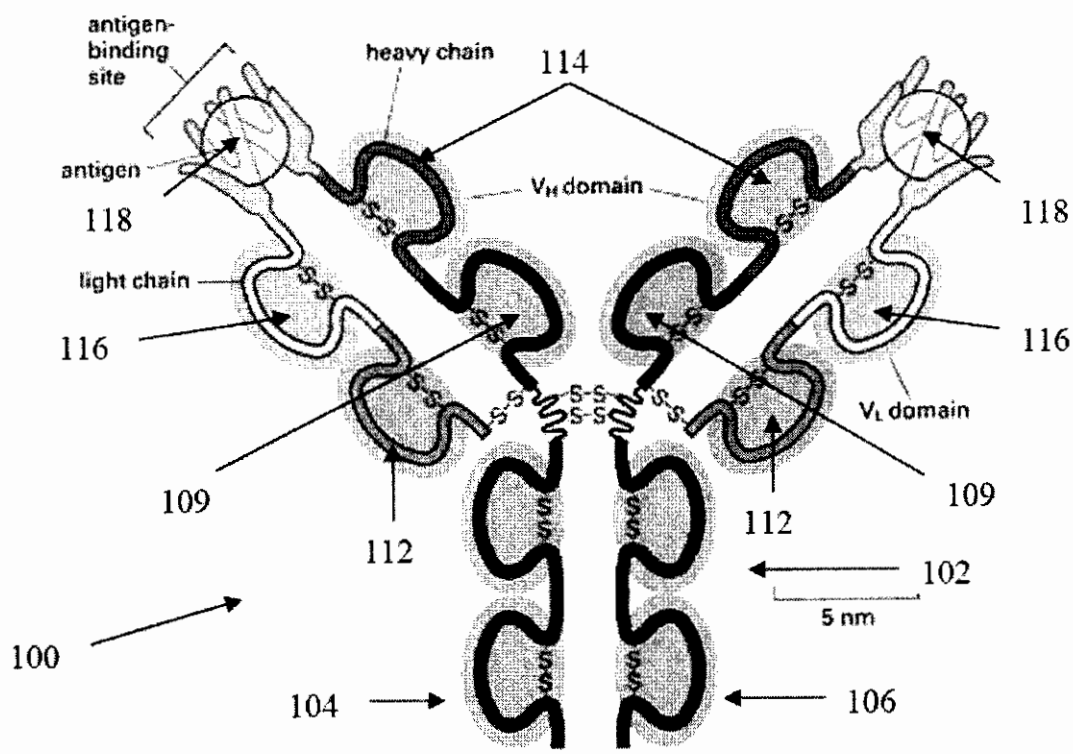

antigen-binding site
heavy chain
114
antigen
118
V_H domain
118
light chain
116
116
V_L domain
109
112
109
112
102
5 nm
100
104
106

FIGURE 4

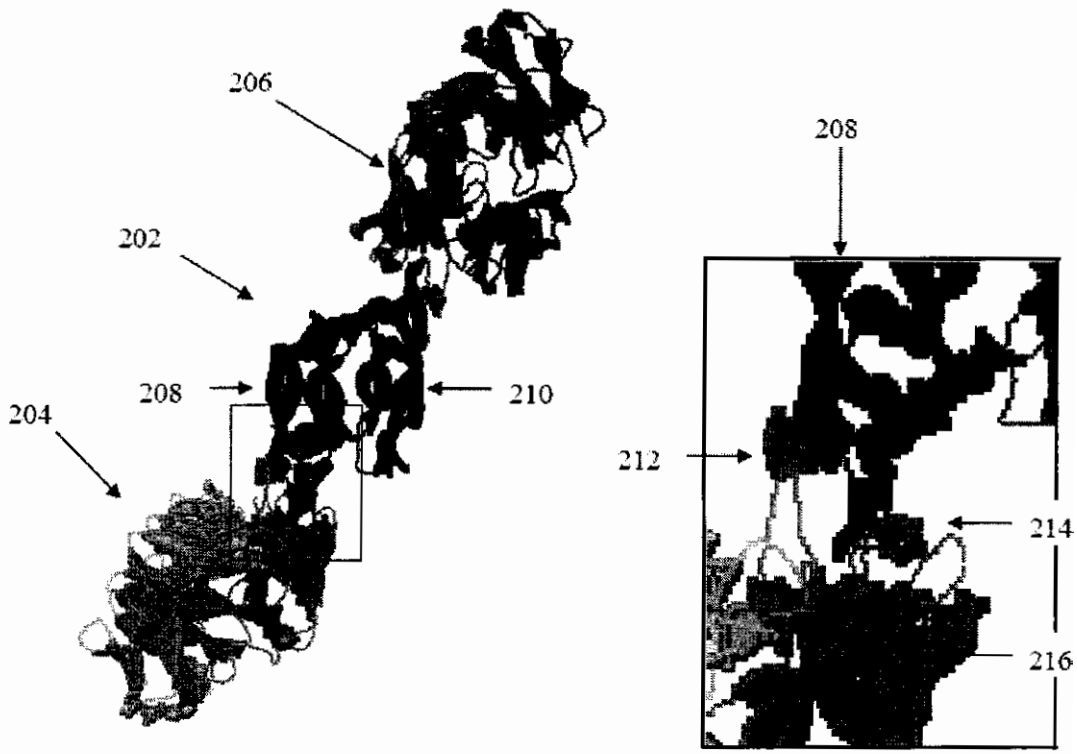


FIGURE 5

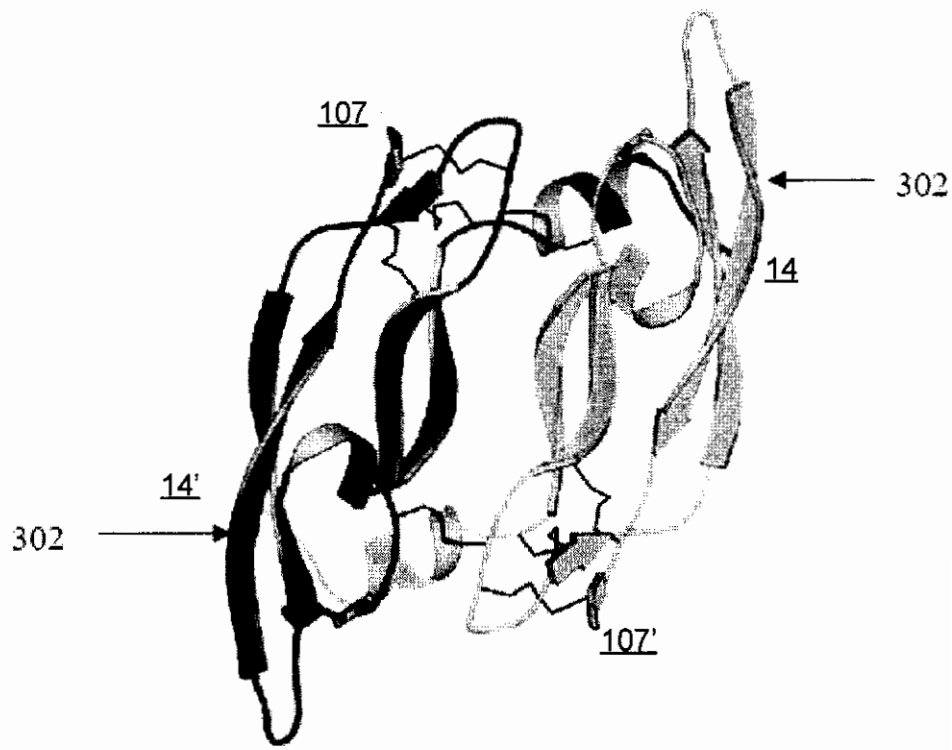
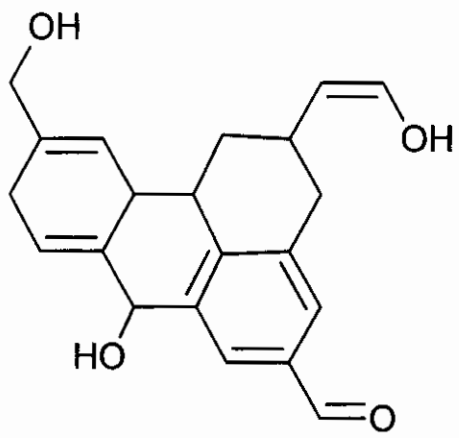


FIGURE 6A



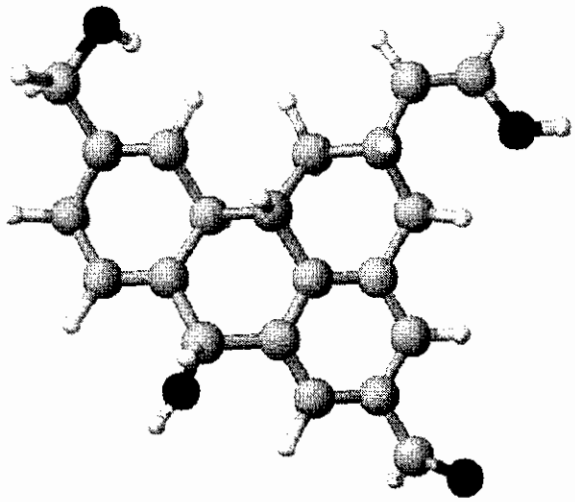
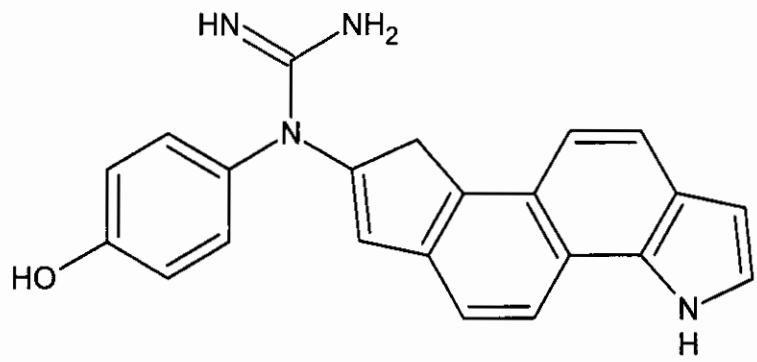


FIGURE 6B

FIGURE 7A



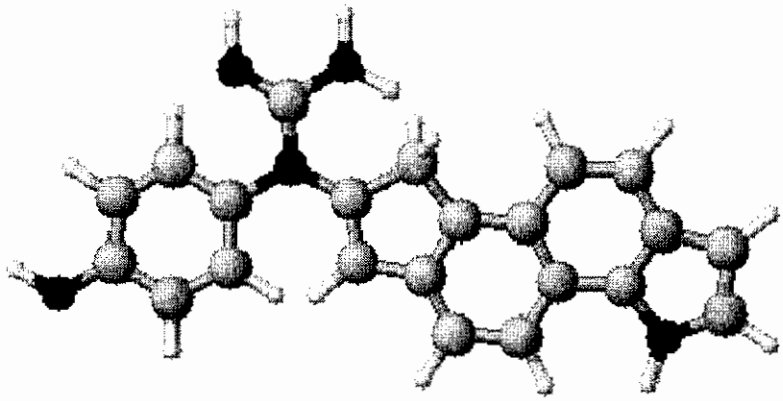


FIGURE 7B

FIGURE 8

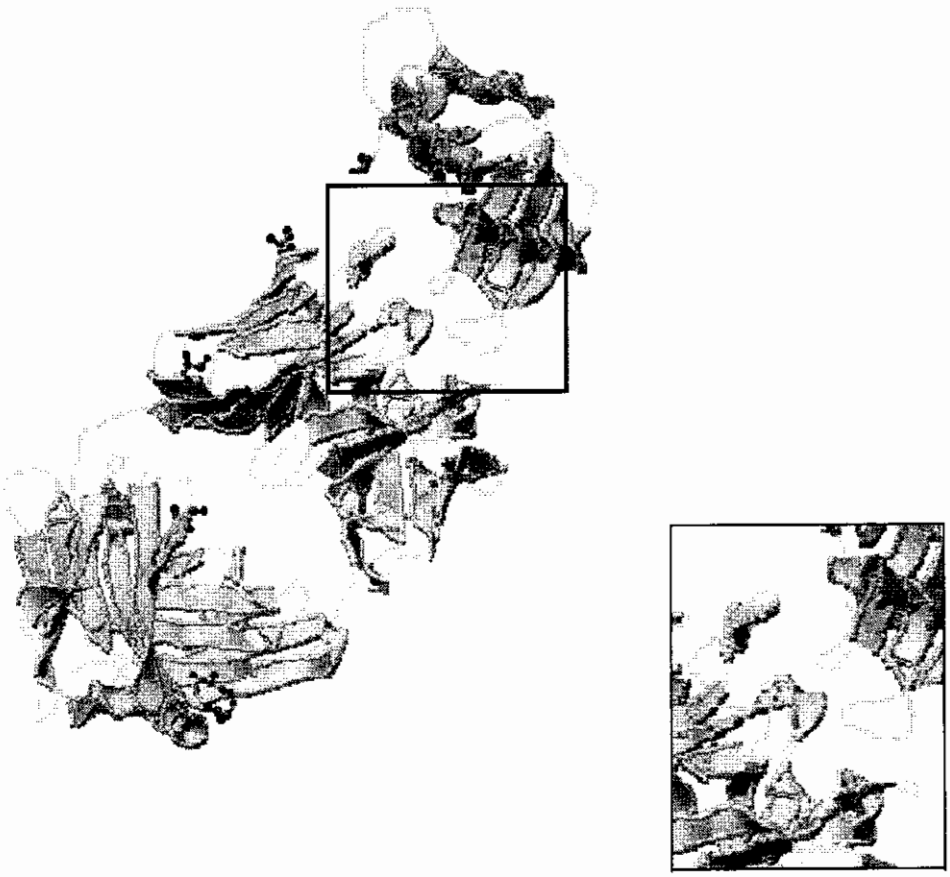
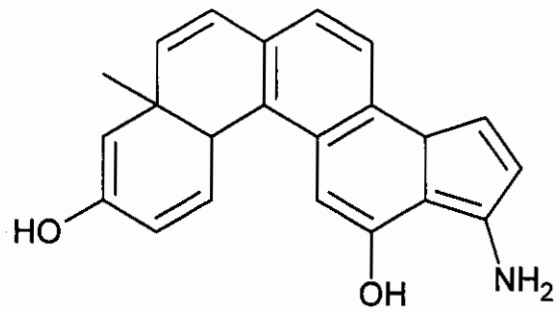


FIGURE 9A



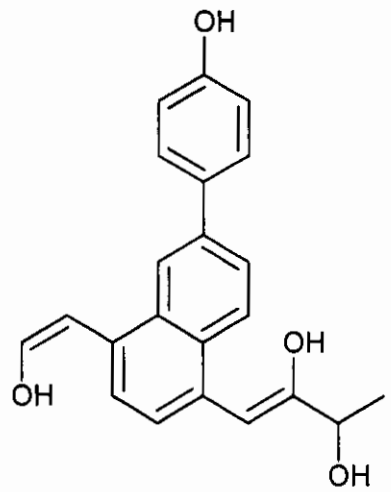
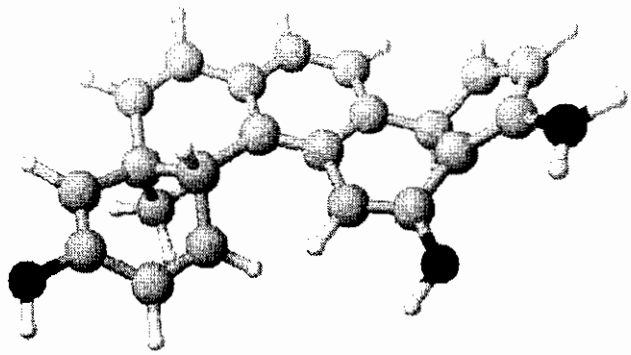


FIGURE 9B

FIGURE 10A



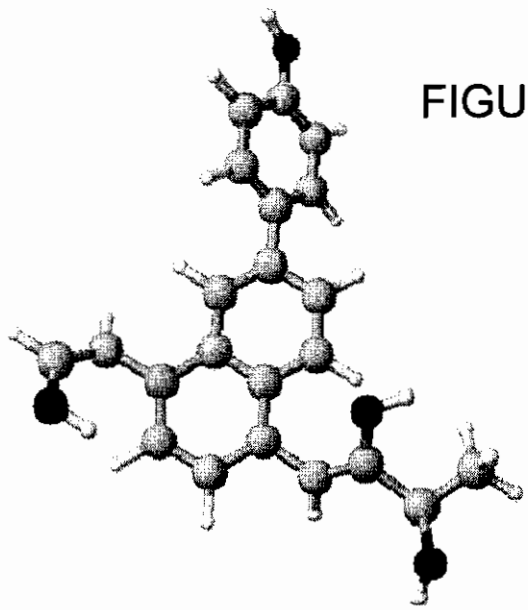


FIGURE 10B

FIGURE 11

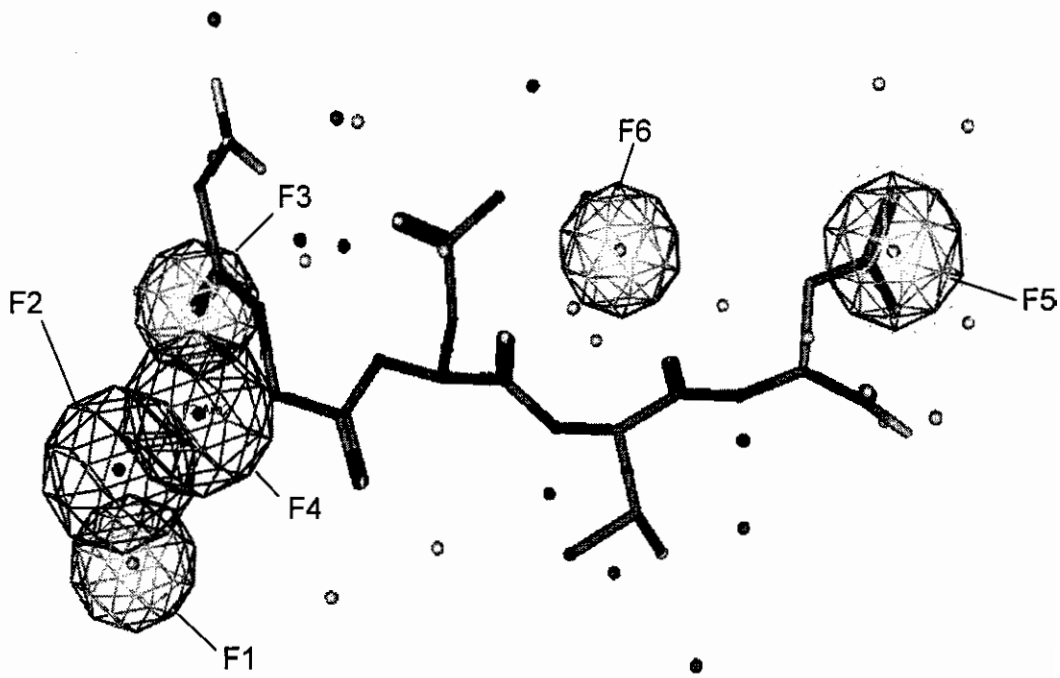


FIGURE 12

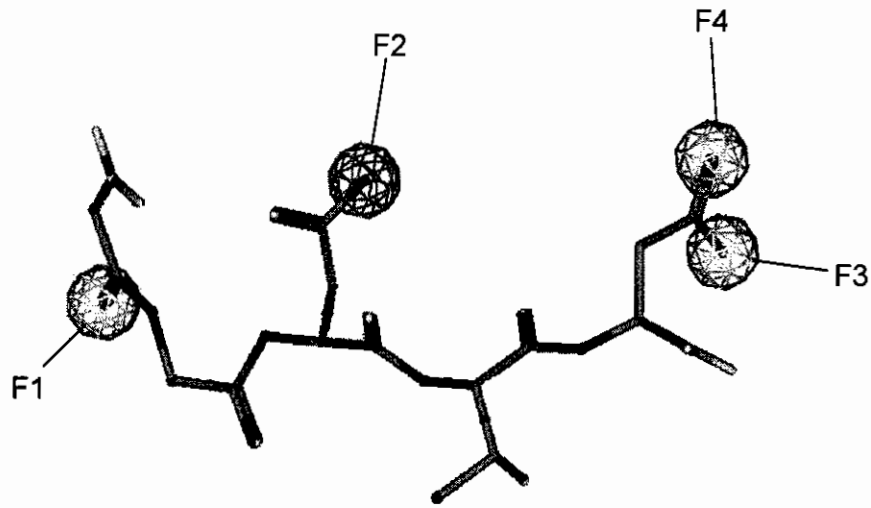


FIGURE 13

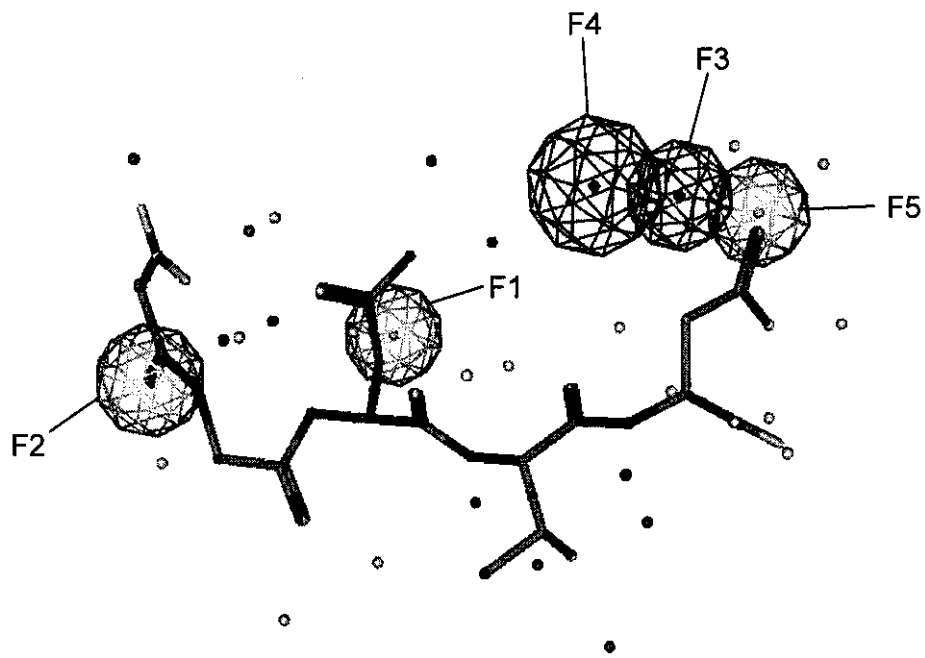


FIGURE 14

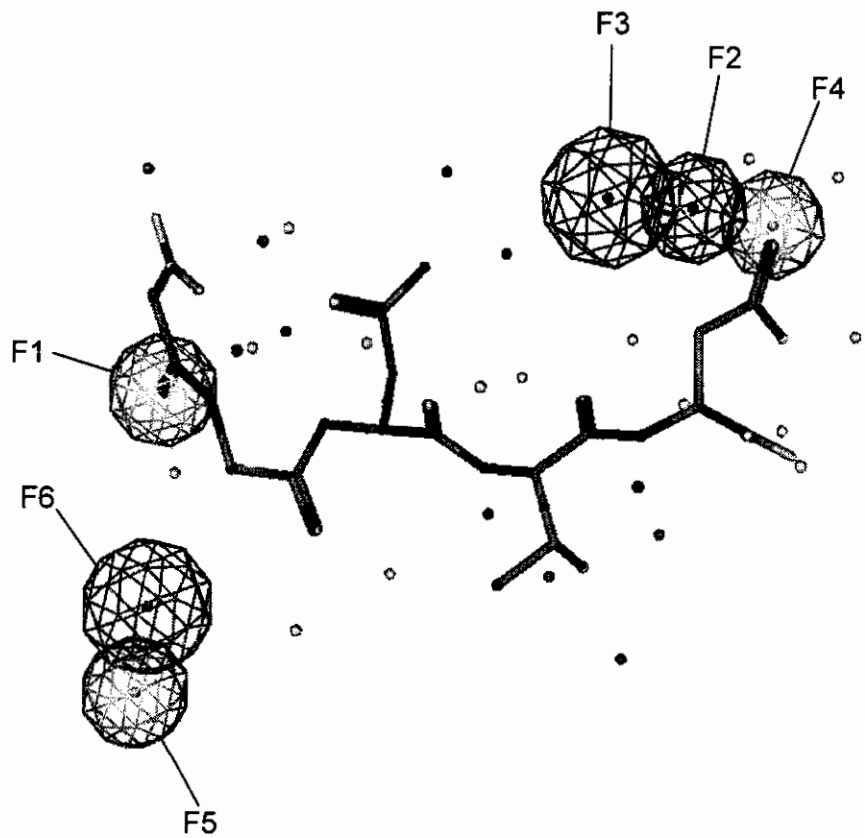


FIGURE 15

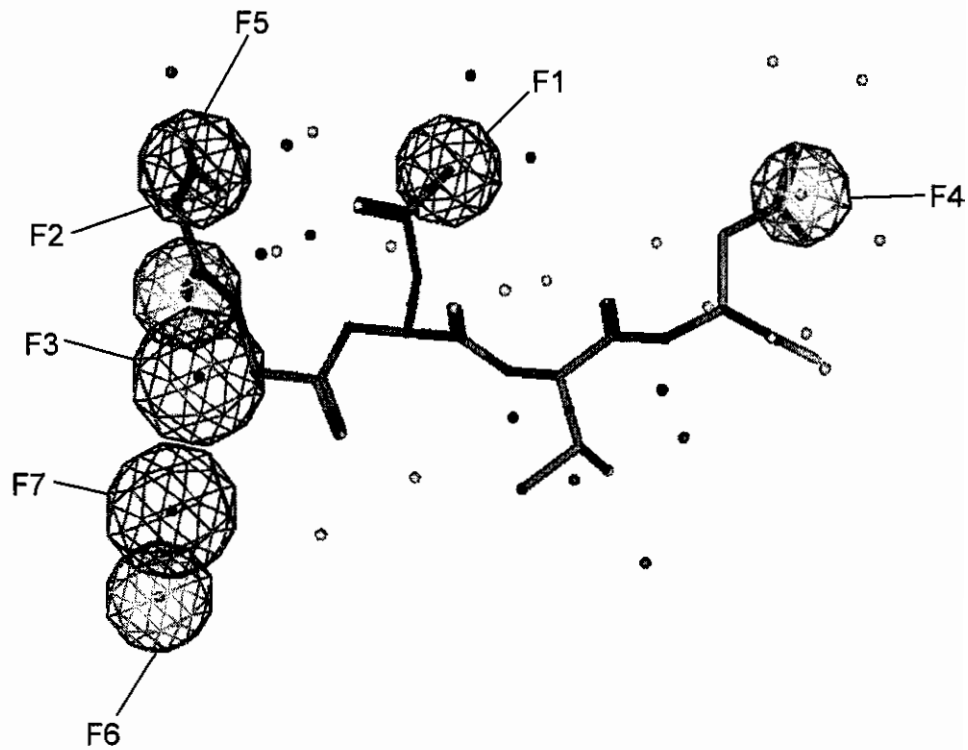


FIGURE 16

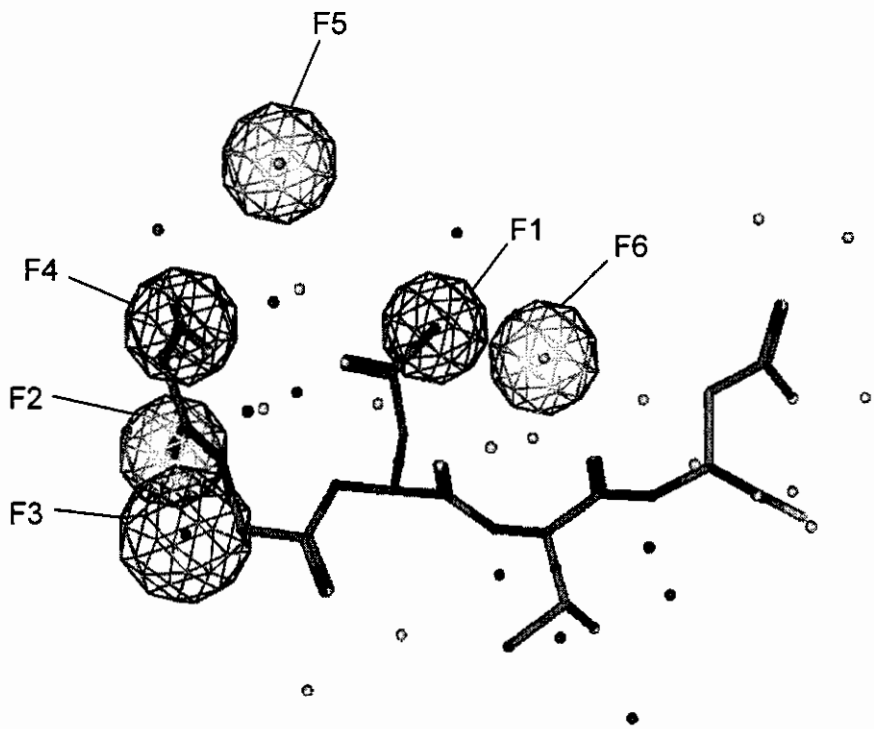


FIGURE 17

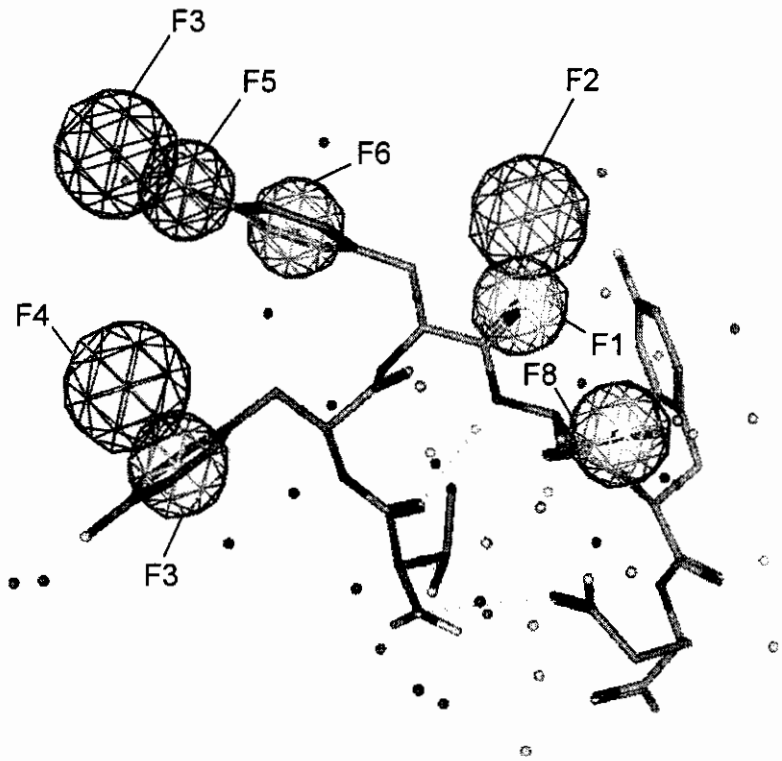


FIGURE 18

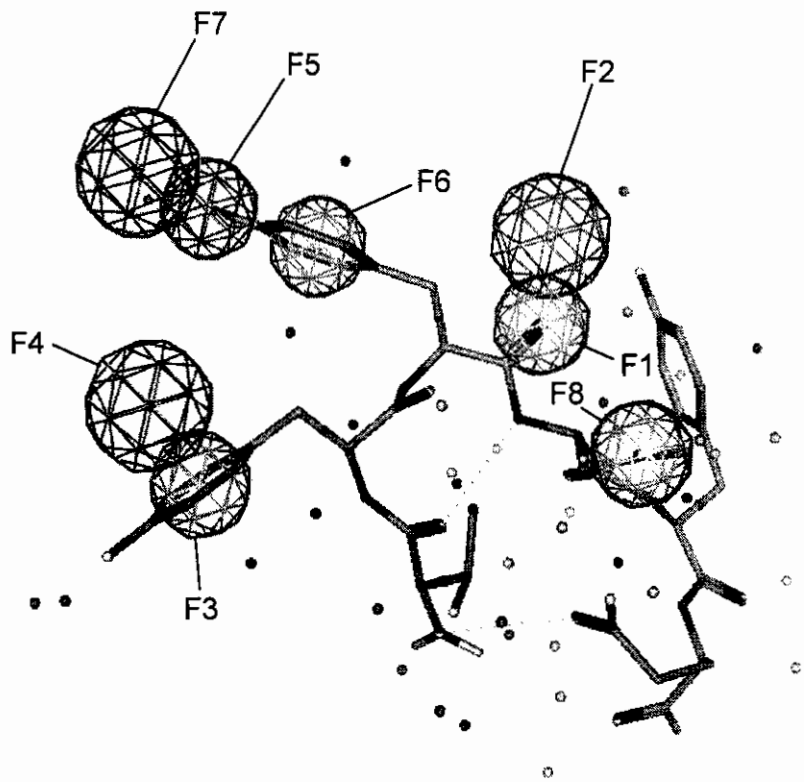


FIGURE 19

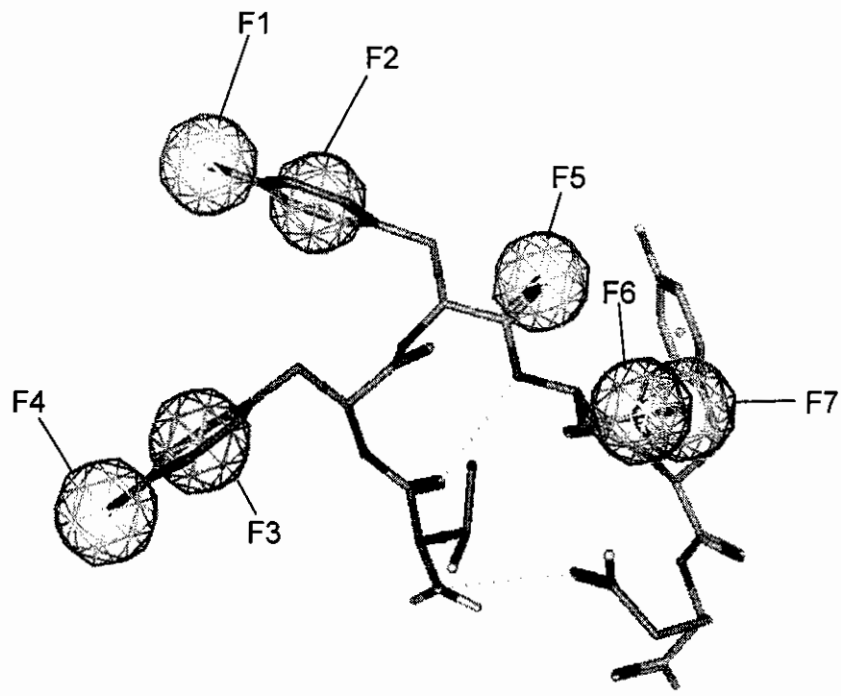


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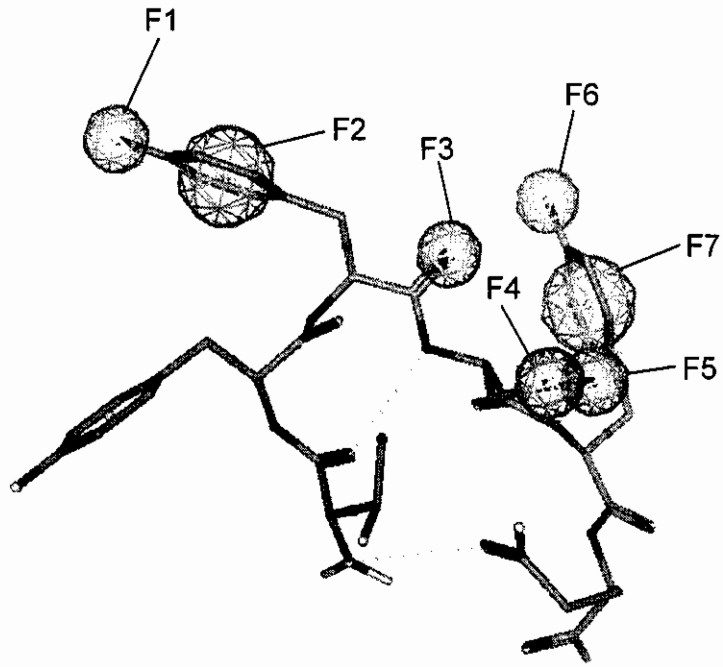


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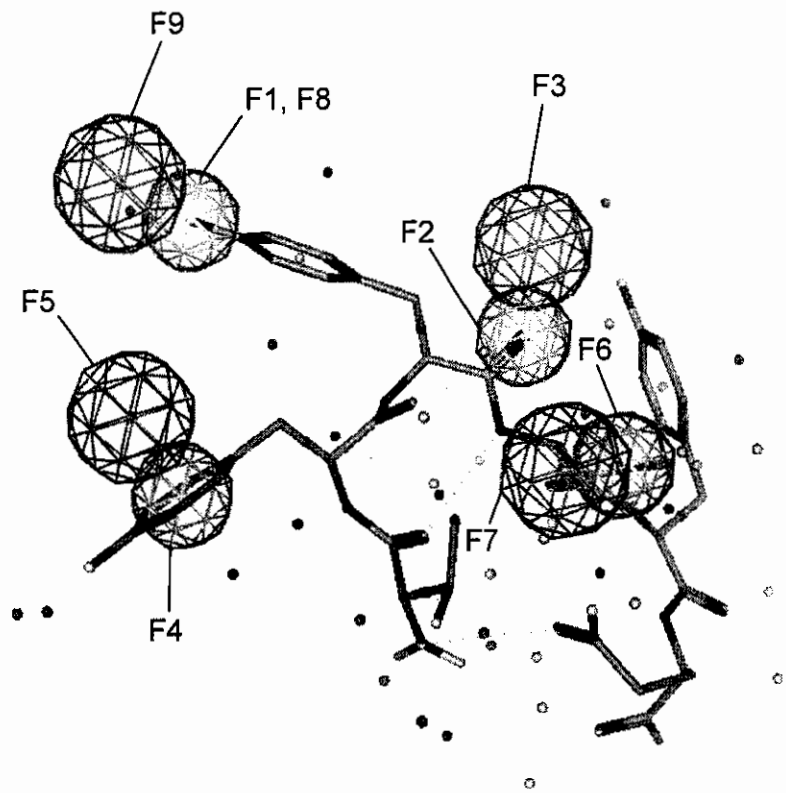


FIGURE 22

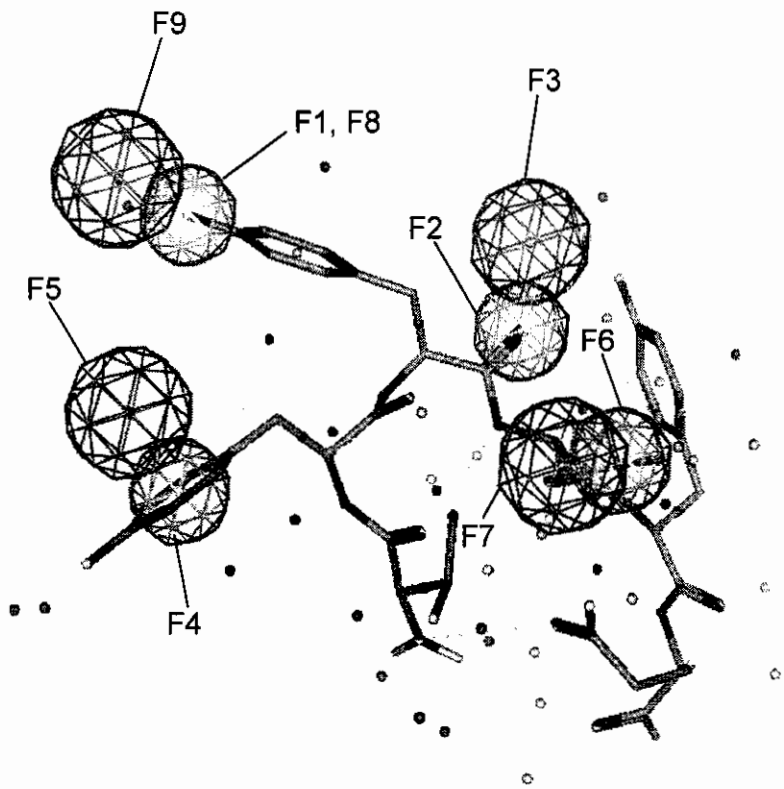


FIGURE 23

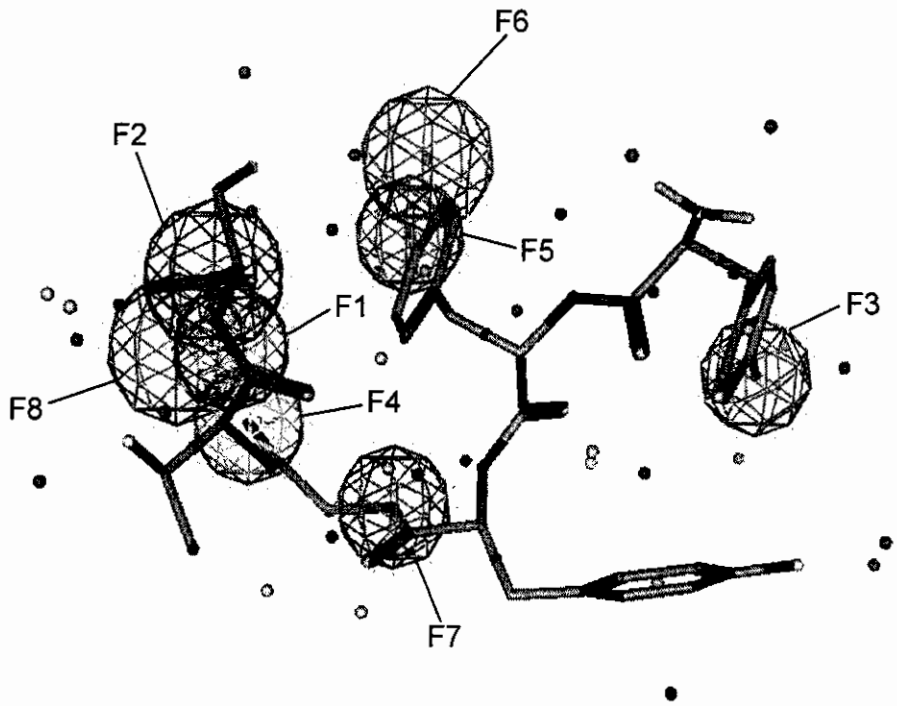


FIGURE 24

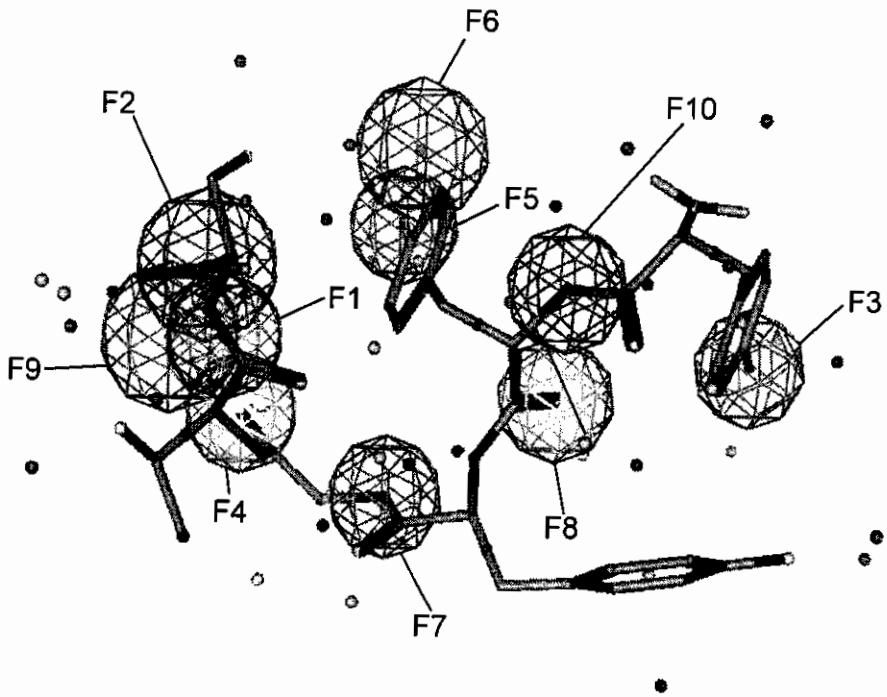


FIGURE 25

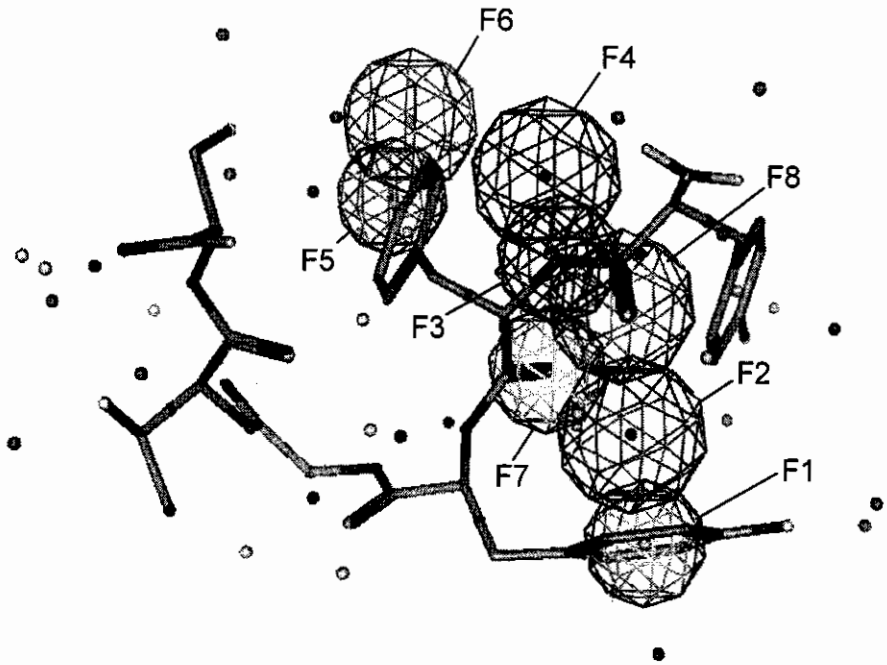


FIGURE 26

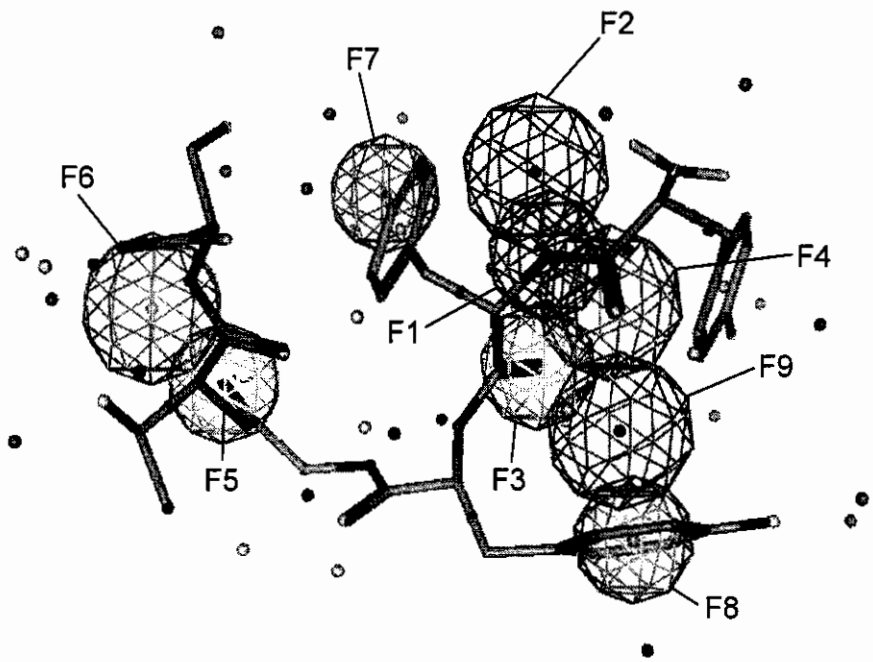


FIGURE 27

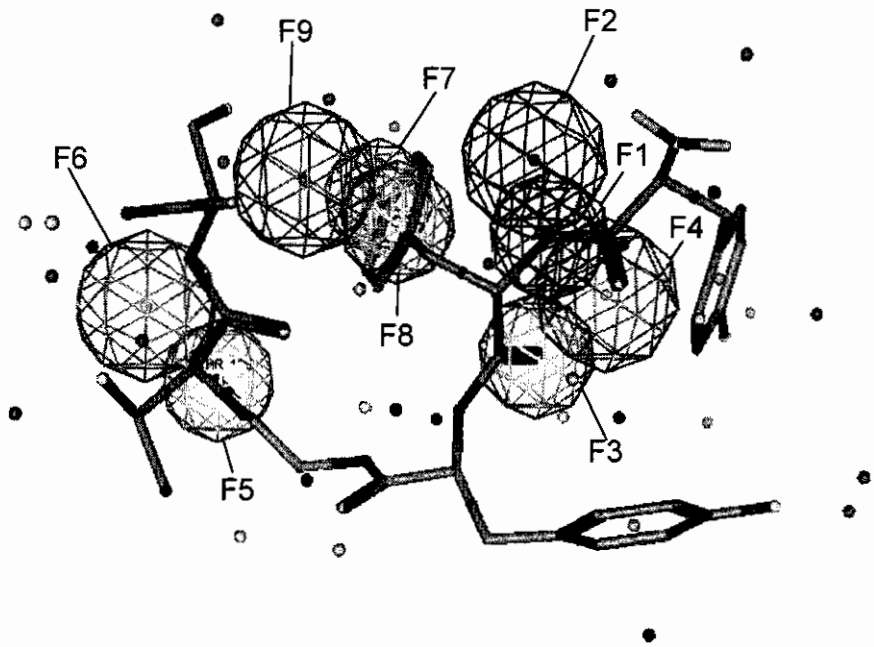


FIGURE 28

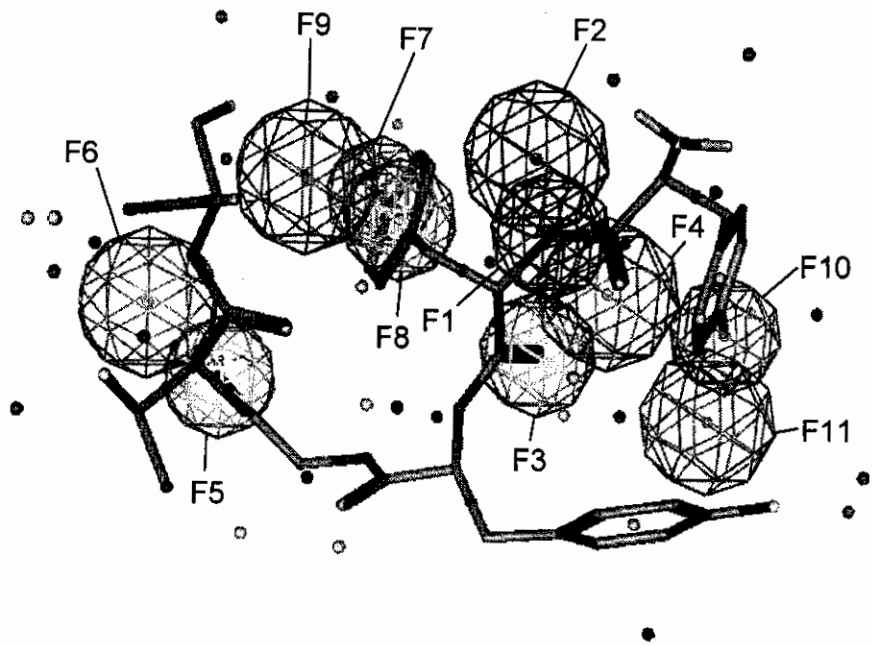


FIGURE 29

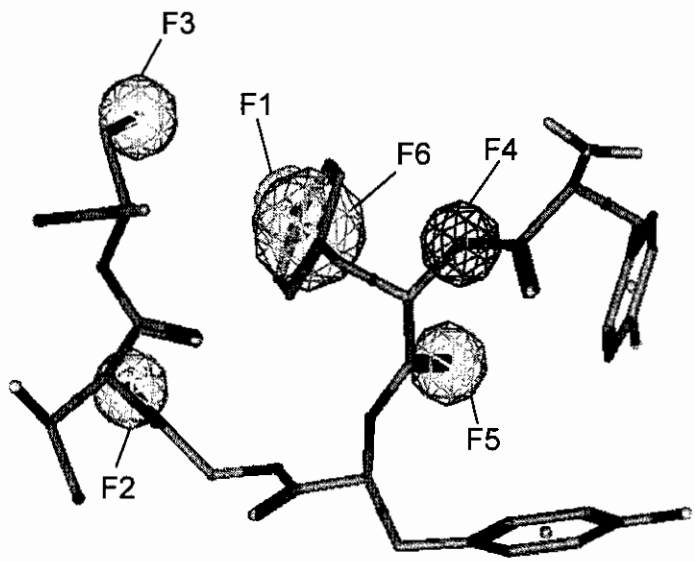


FIGURE 30

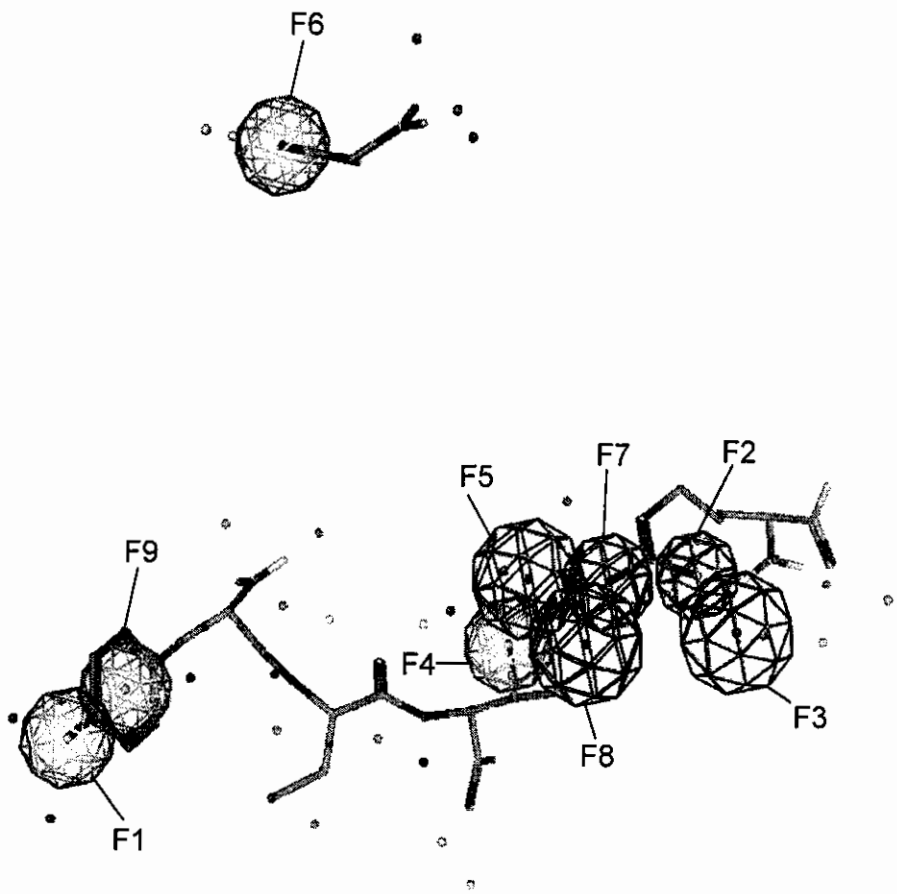


FIGURE 31

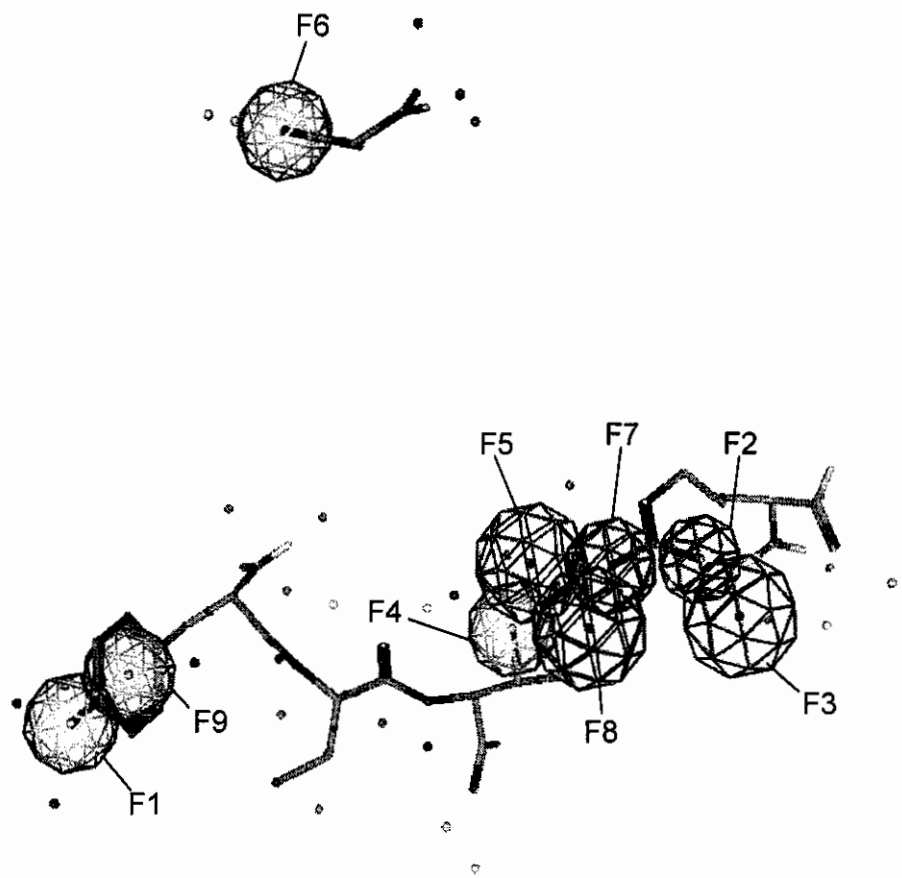


FIGURE 32

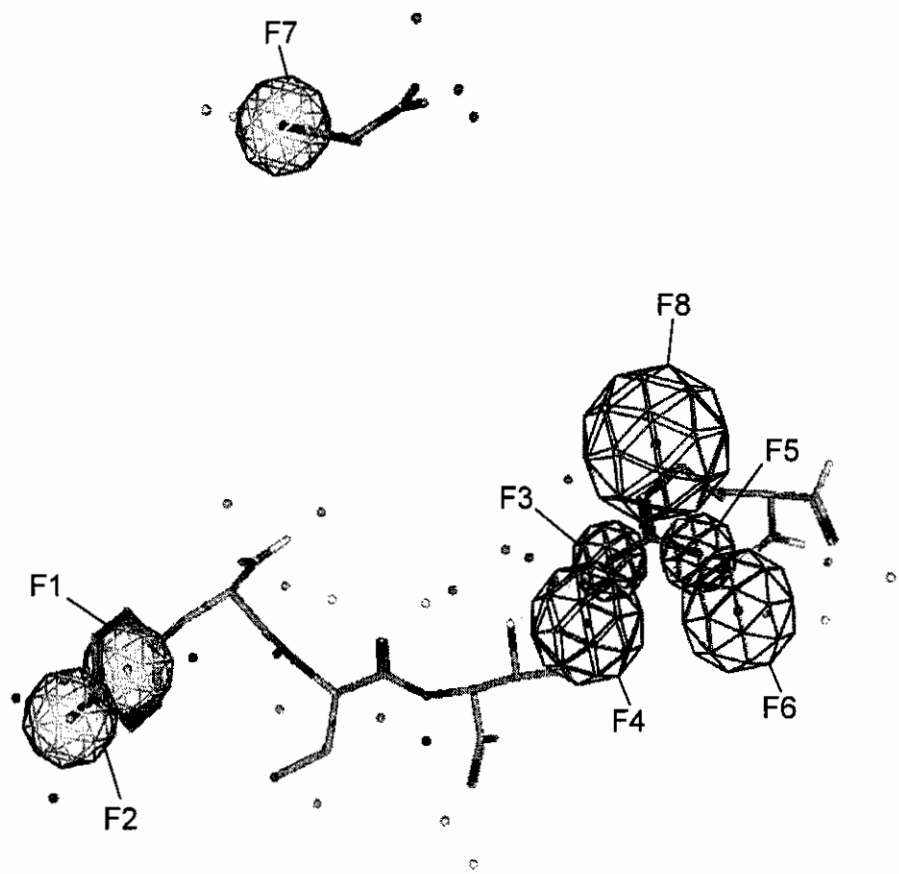


FIGURE 33

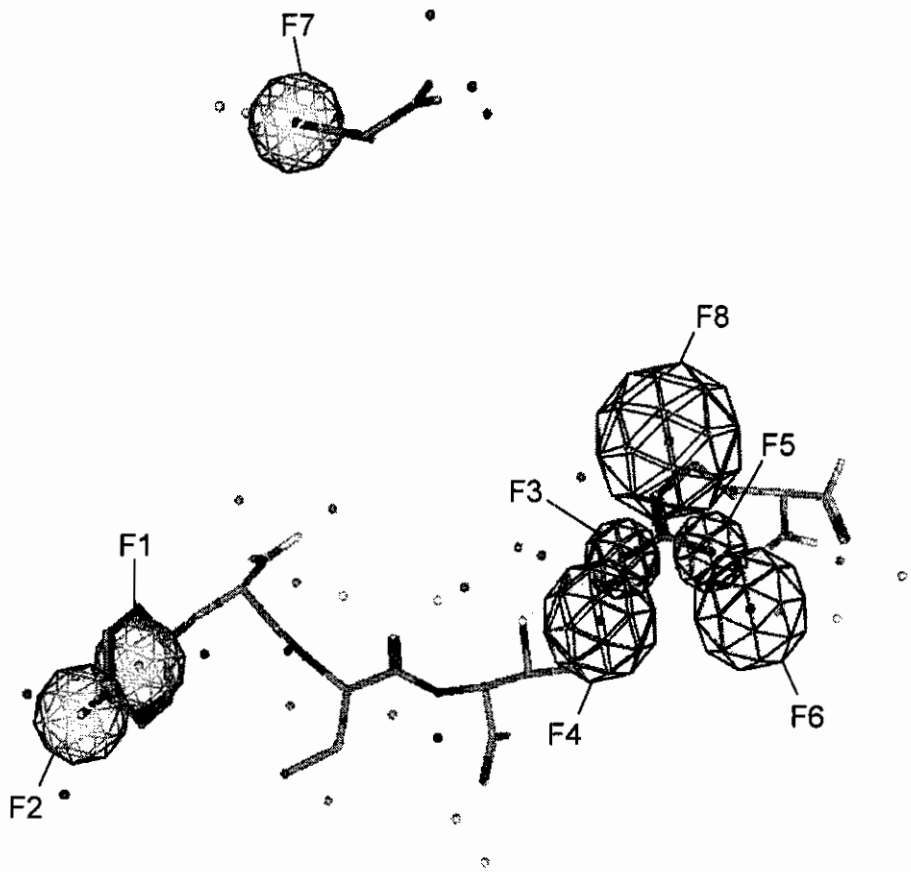


FIGURE 34

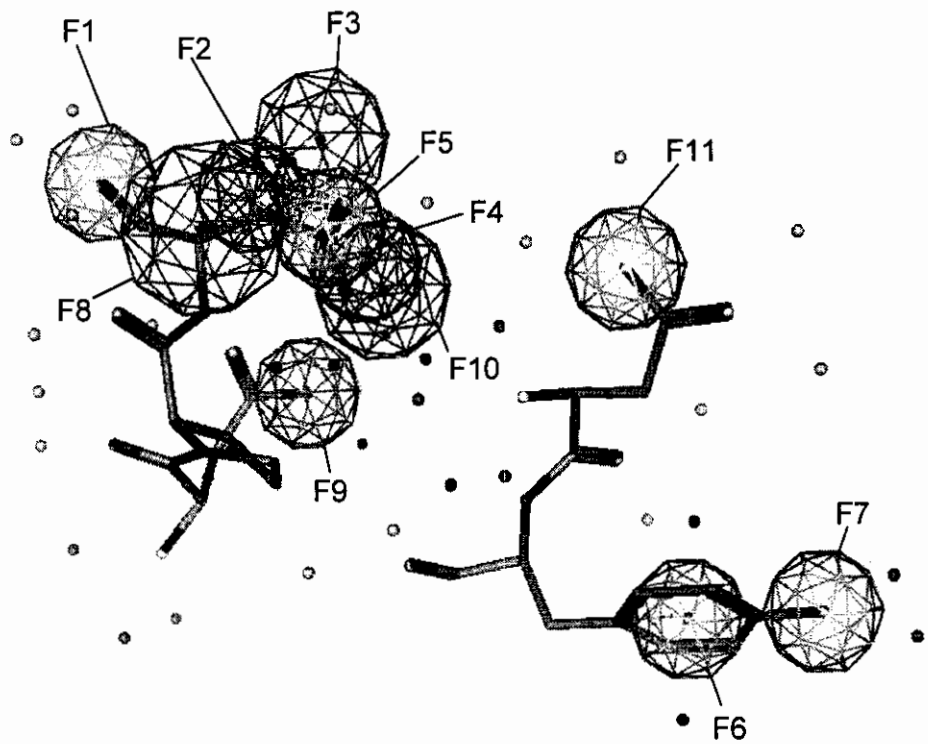


FIGURE 35

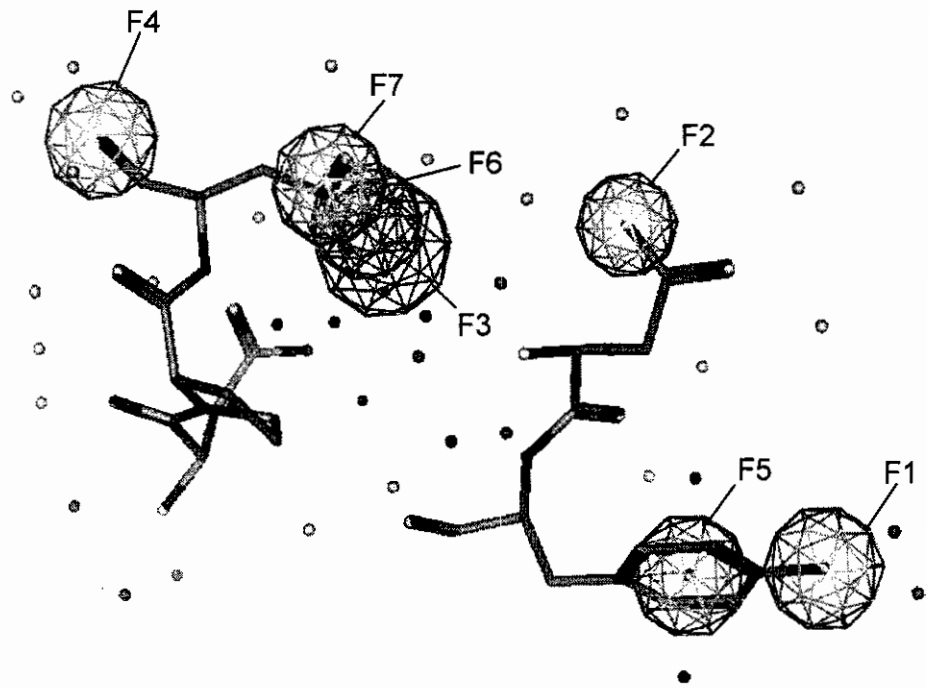


FIGURE 36

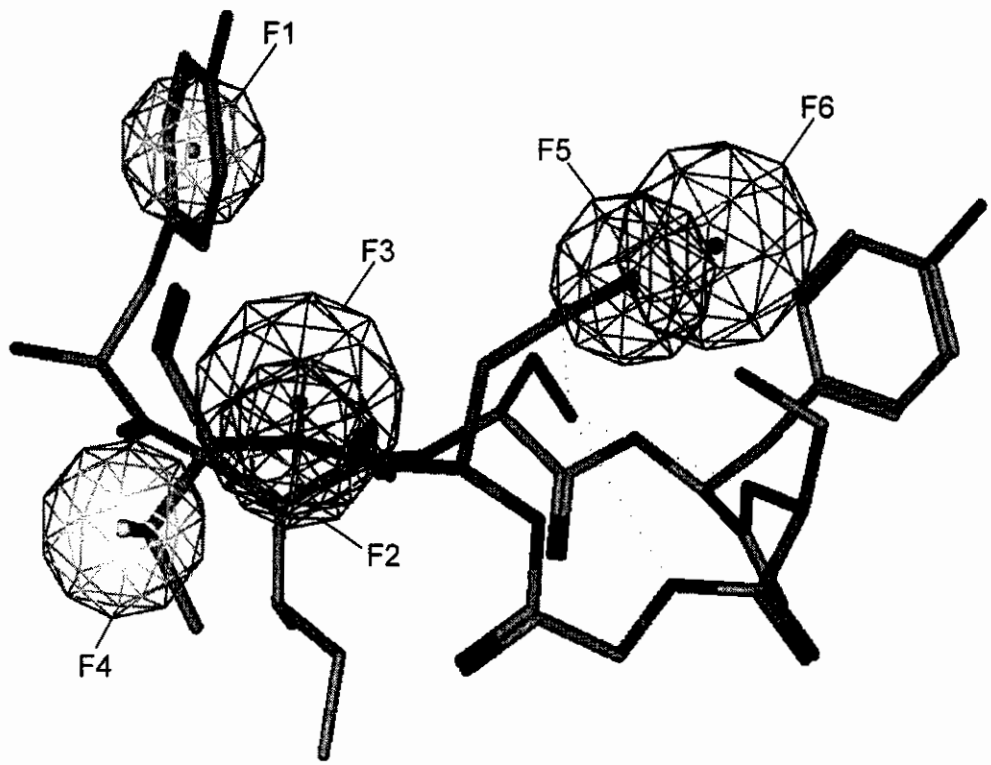


FIGURE 37

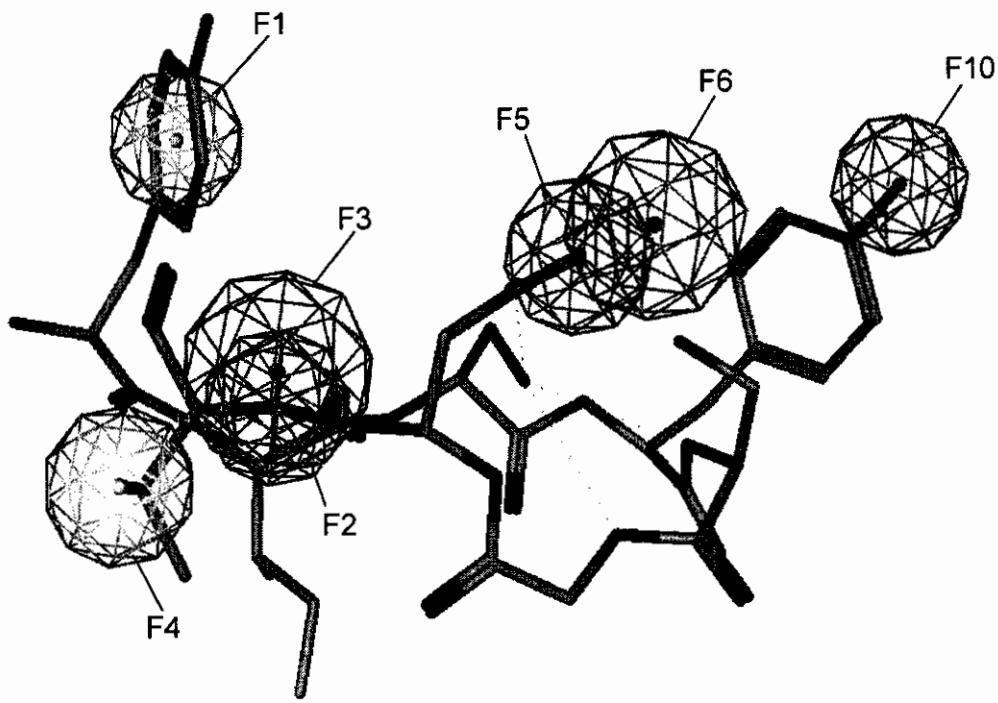


FIGURE 38

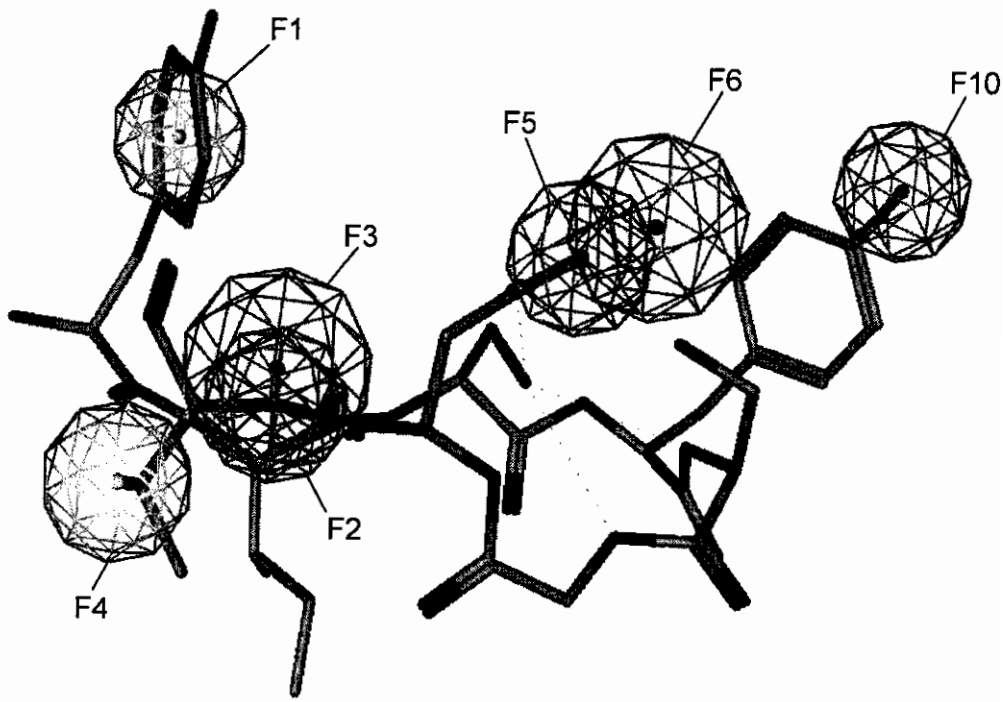


FIGURE 39

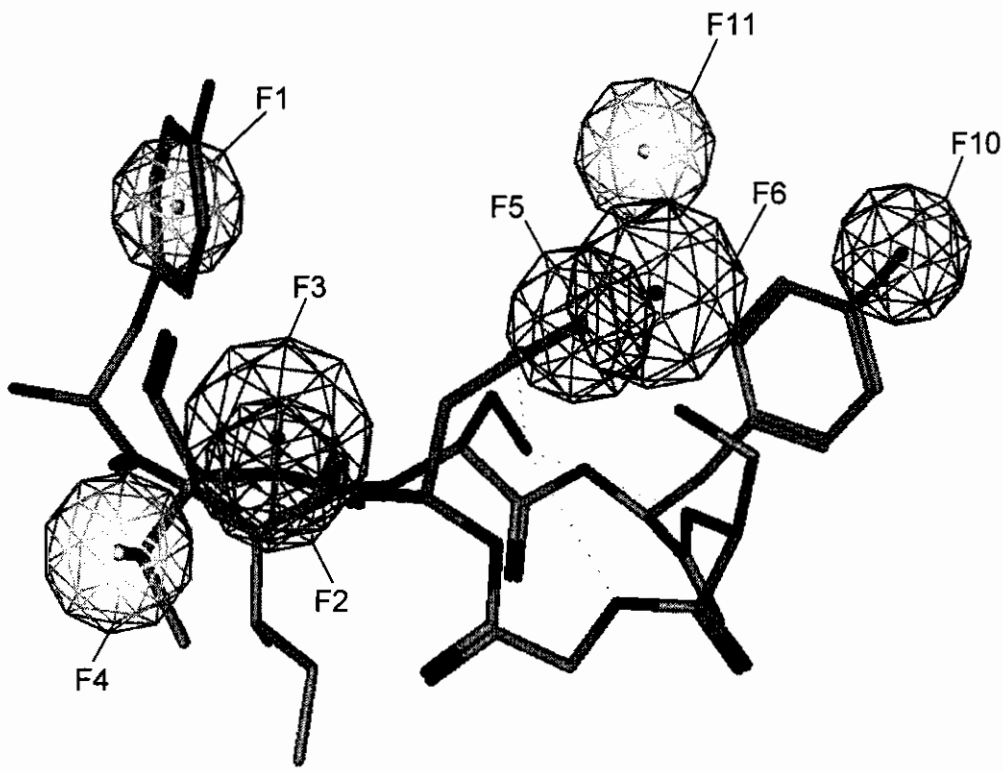


FIGURE 40

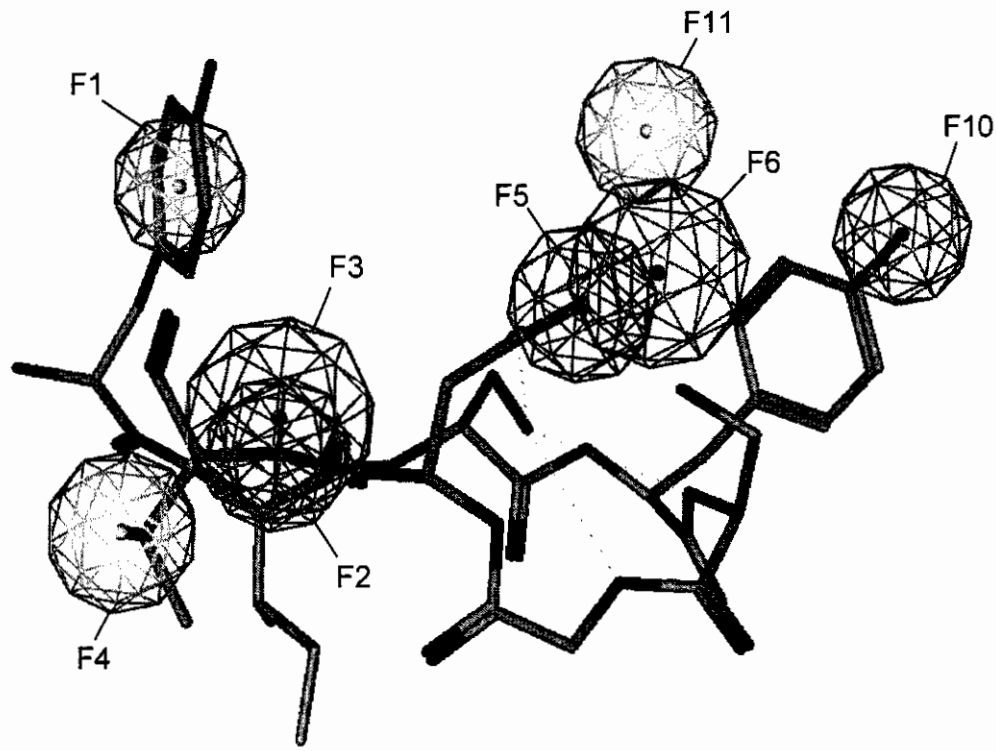


FIGURE 41

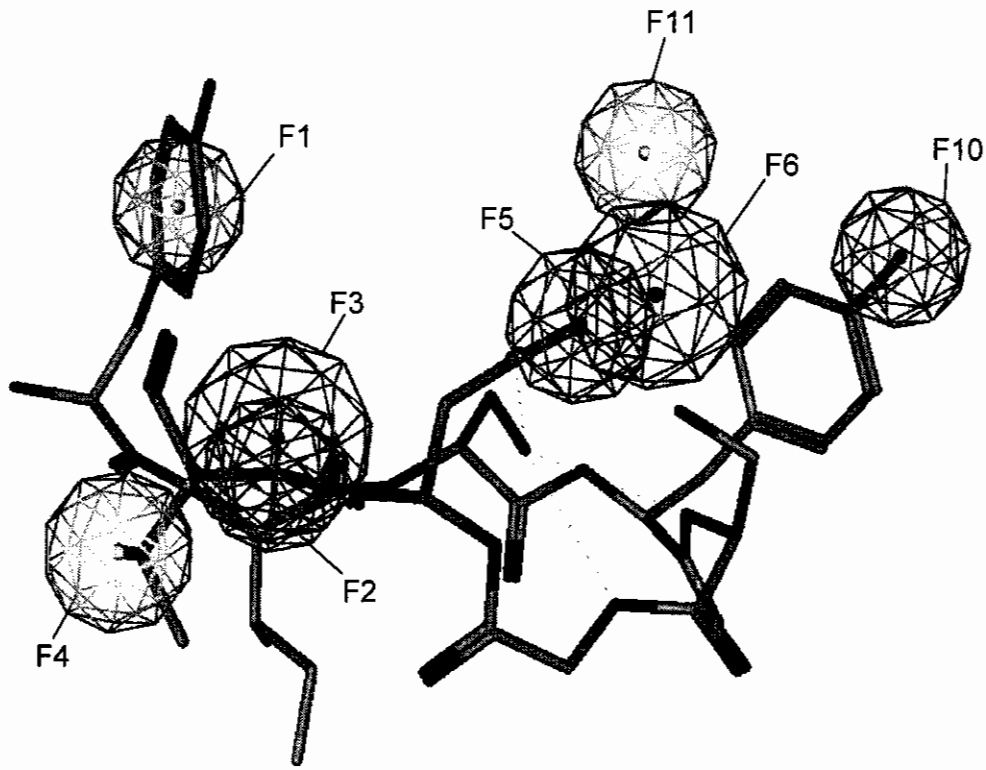


FIGURE 42

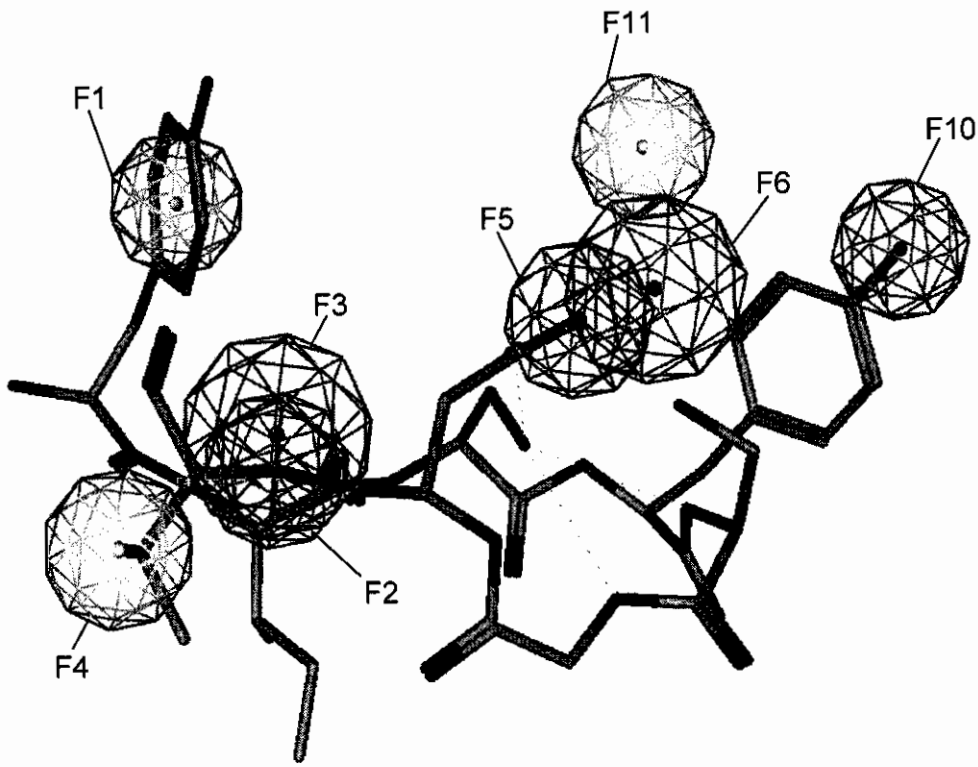


FIGURE 43

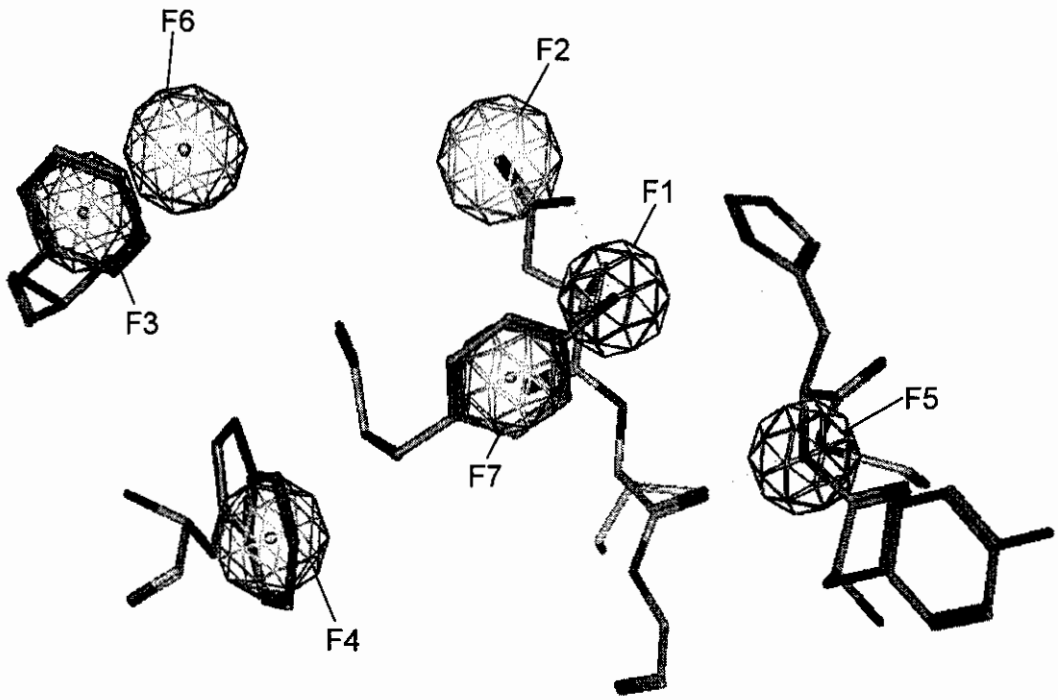


FIGURE 44

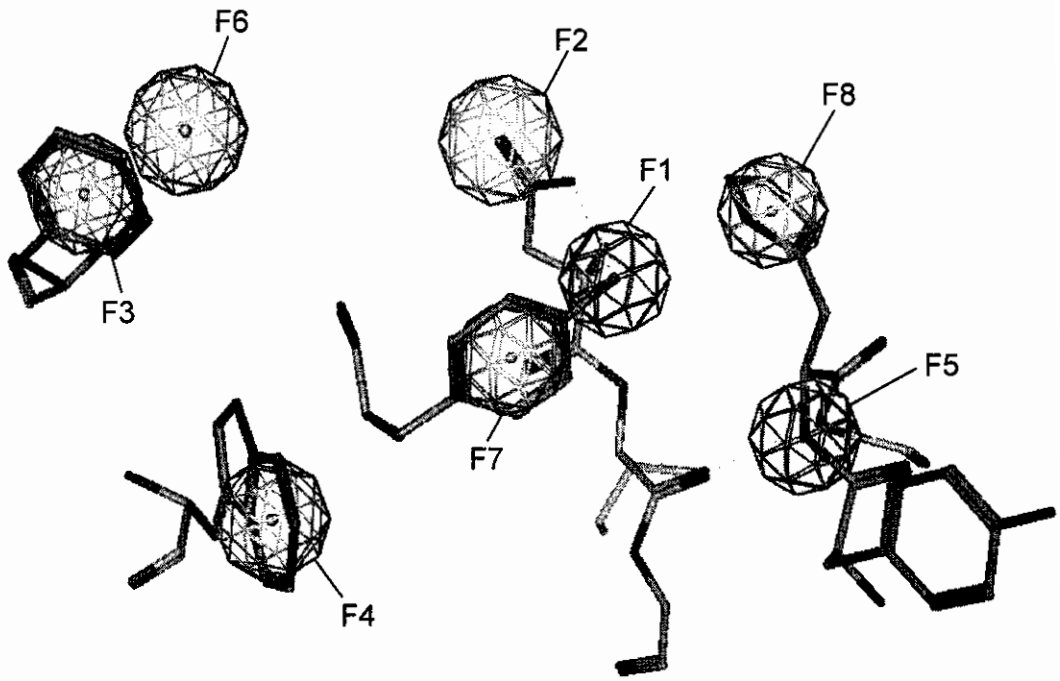


FIGURE 45

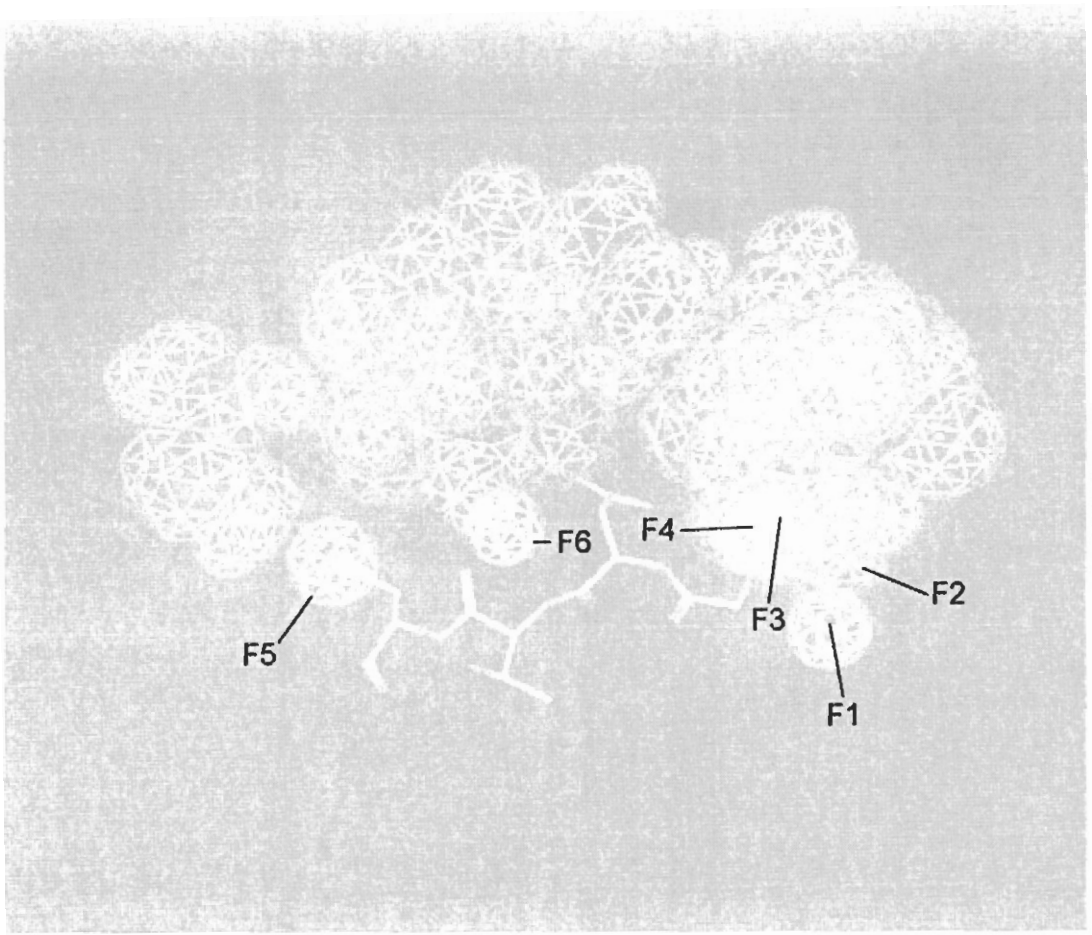
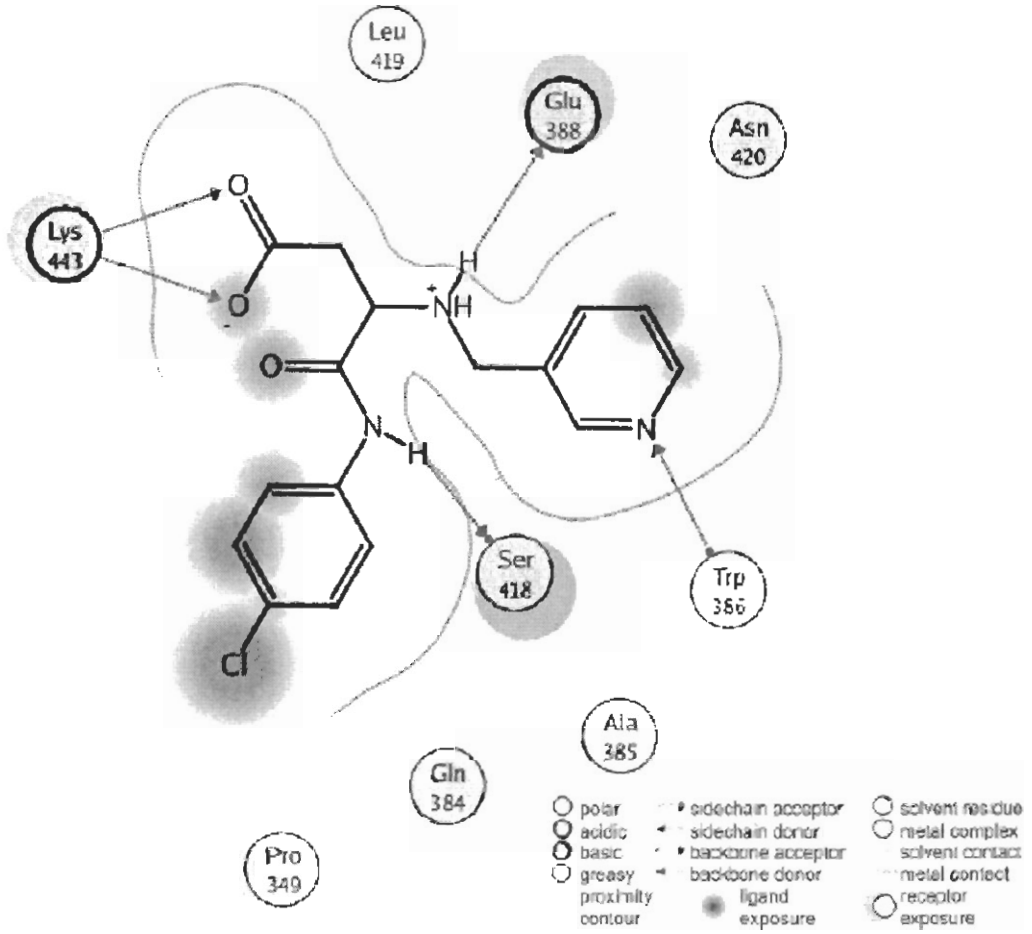


FIGURE 46


Leu 419
Glu 388
Asn 420
Lys 443
O
O
H
NH
O
N
H
N
Ser 418
Trp 386
Cl
Ala 385
Gln 384
Pro 349
polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure

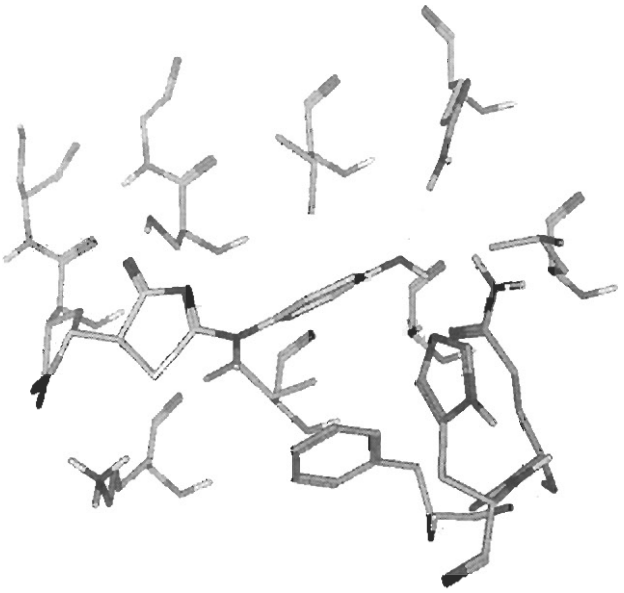


FIGURE 47A

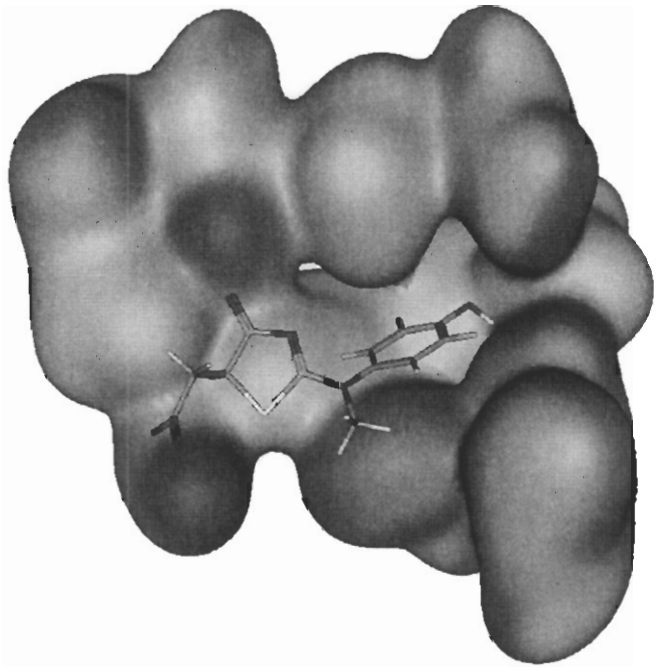


FIGURE 47B

FIGURE 48

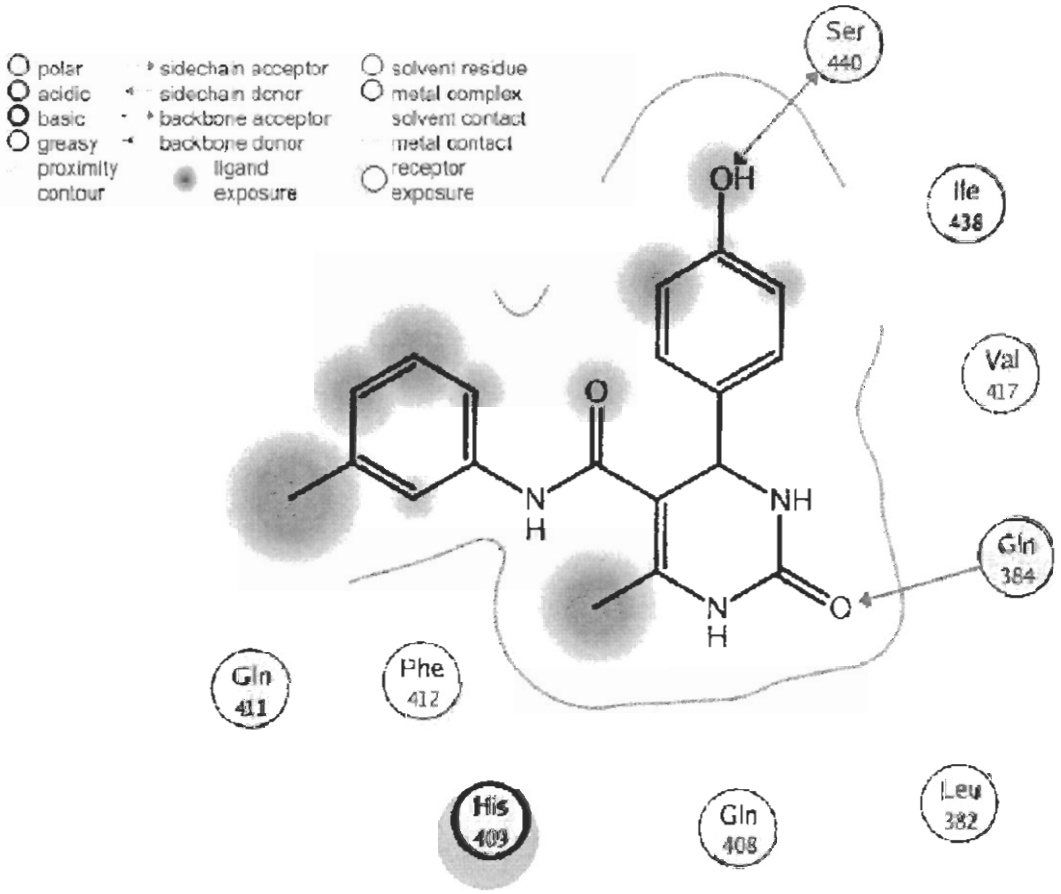

polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure
Ser 440
Ile 438
Val 417
Gln 384
Gln 411
Phe 412
His 409
Gln 408
Leu 382
OH
O
N H
NH
N H
O

FIGURE 49

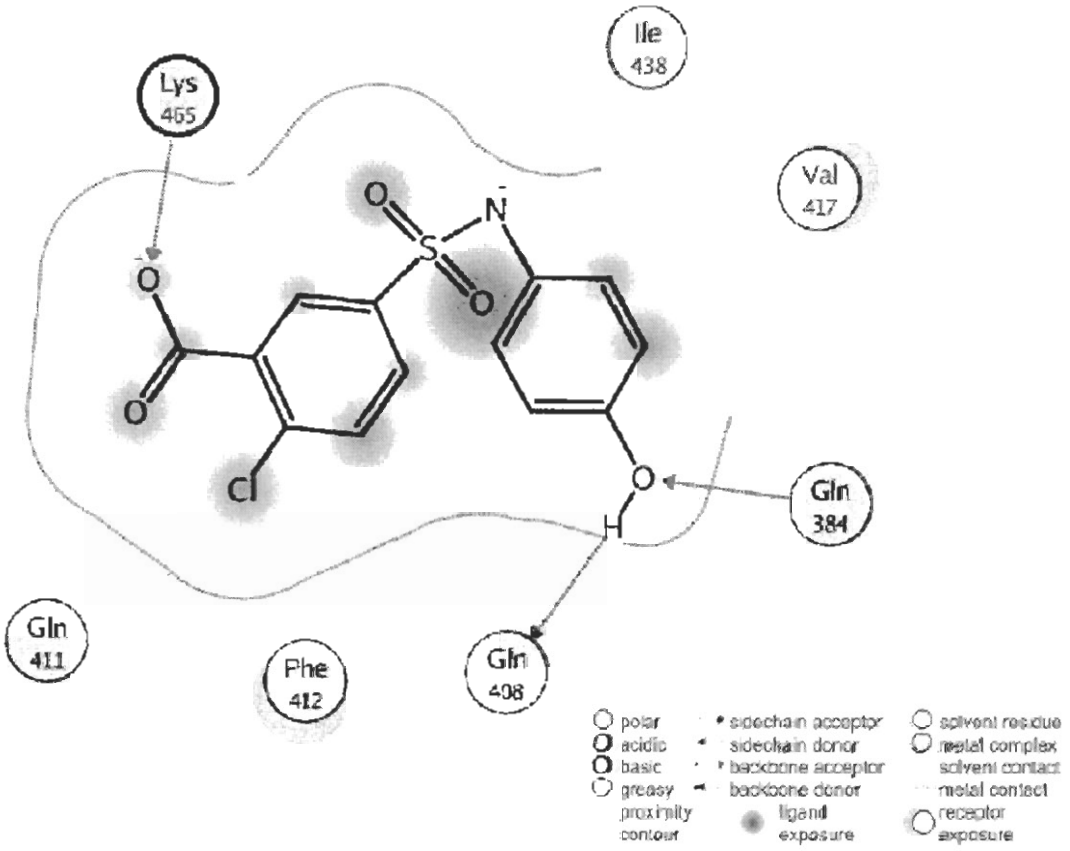

Ile
438
Lys
455
Val
417
Gln
384
Gln
411
Phe
412
Gln
408
polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure

FIGURE 50

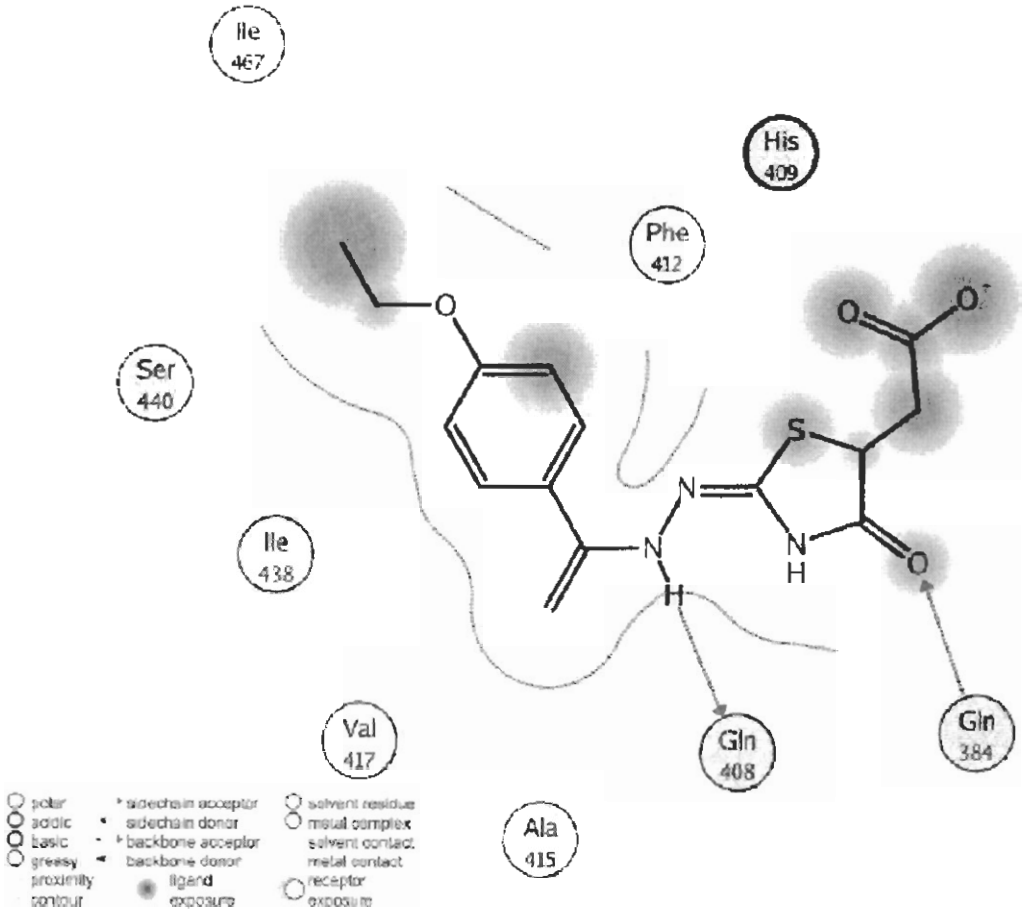

Ile
467
His
409
Phe
412
Ser
440
Ile
438
Val
417
Gln
408
Gln
384
Ala
415
O
O
O
S
N
N
H
N
H
O
polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure

FIGURE 51

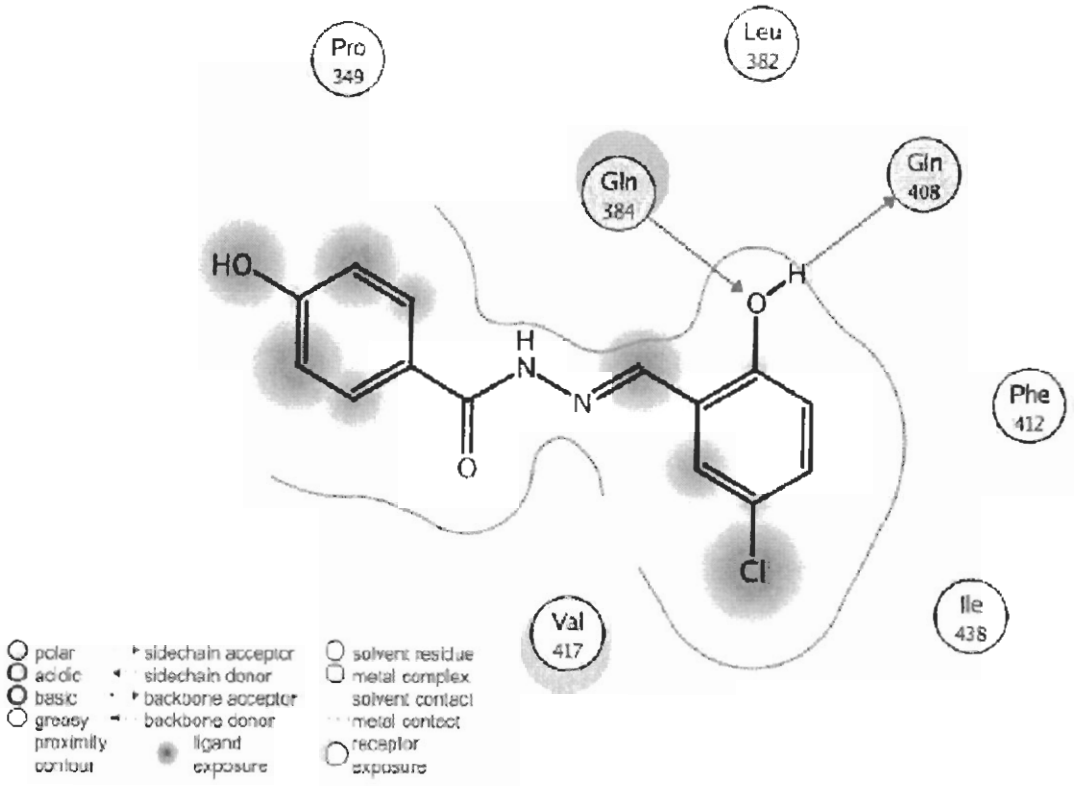

Pro
349
Leu
382
Gln
384
Gln
408
HO
H
O
H
N
N
O
Phe
412
Cl
Val
417
Ile
438
polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure

FIGURE 52

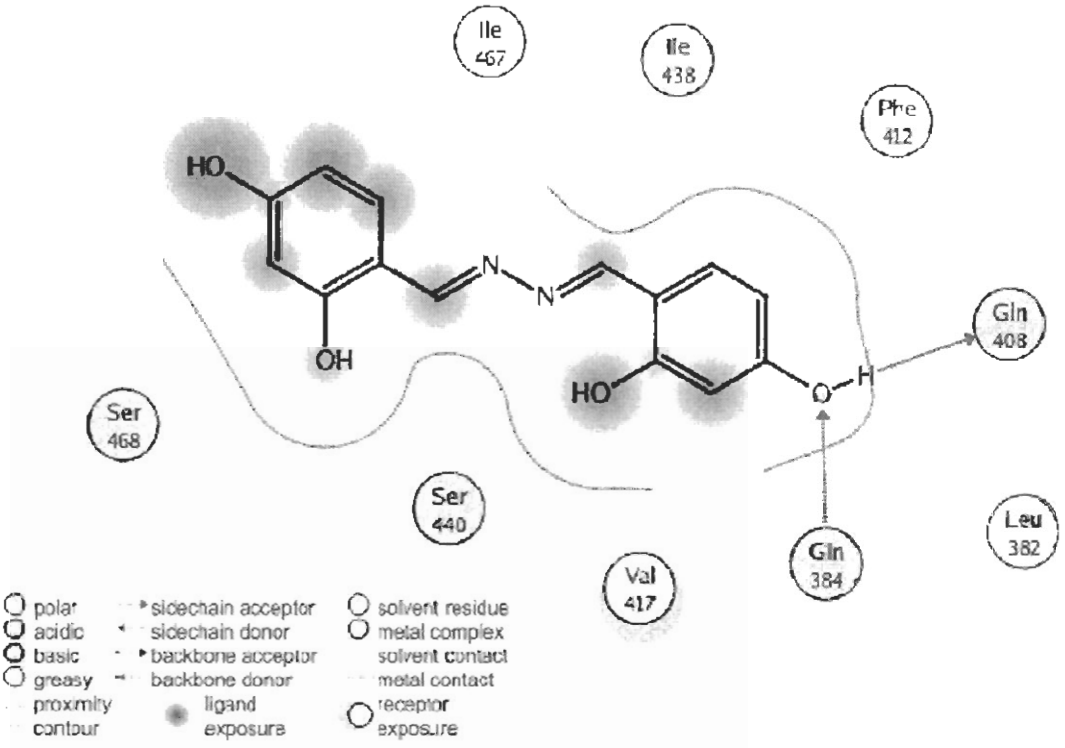

Ile 467
Ile 438
Phe 412
HO
OH
N
N
HO
O
H
Gln 408
Ser 468
Ser 440
Val 417
Gln 384
Leu 382
polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure

FIGURE 53

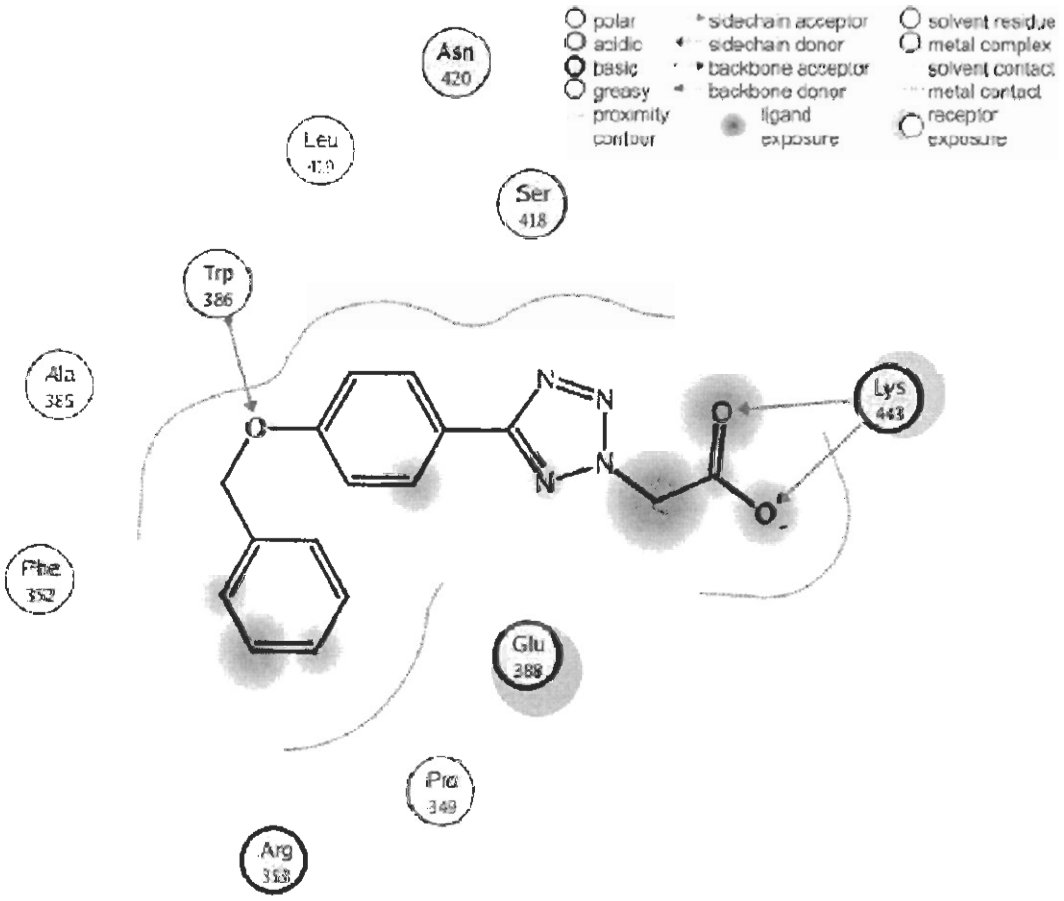

polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure
Asn 420
Leu
Ser 418
Trp 386
Ala 385
Phe 352
Glu 388
Pro 349
Arg 353
Lys 443
O
N
N
N
O
O

FIGURE 54

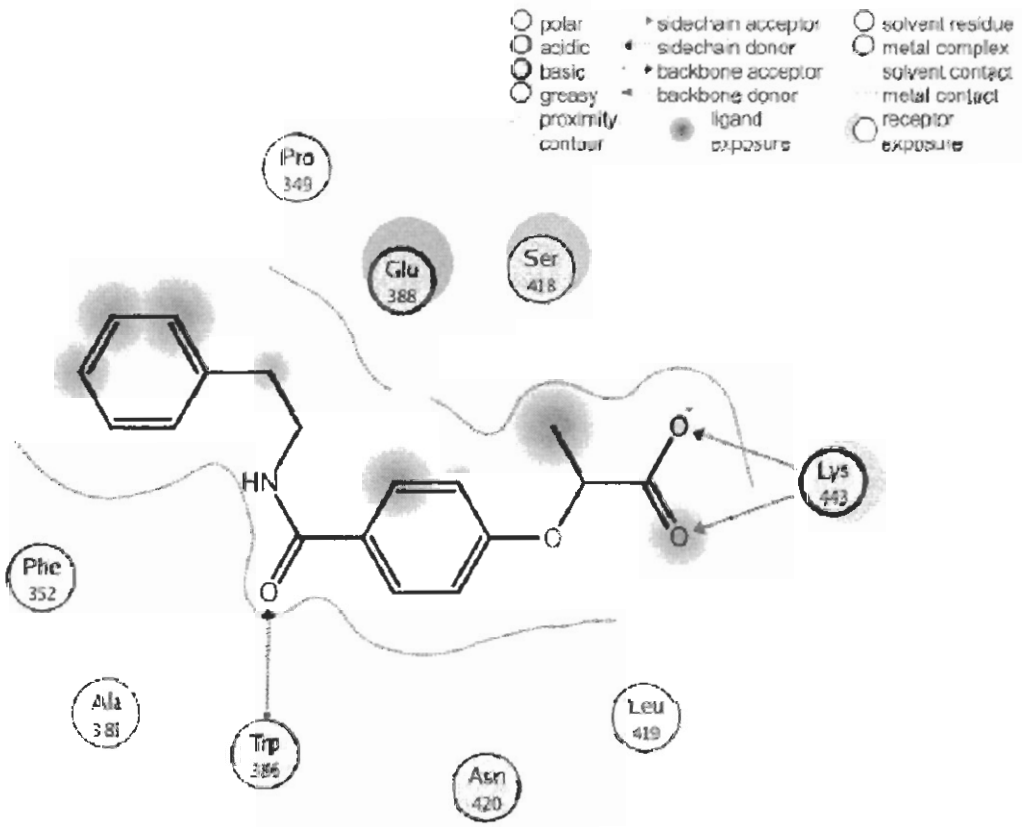

polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure
Pro 349
Glu 388
Ser 418
Lys 443
Phe 352
Ala 381
Trp 386
Asn 420
Leu 419
HN
O
O
O
O

FIGURE 55

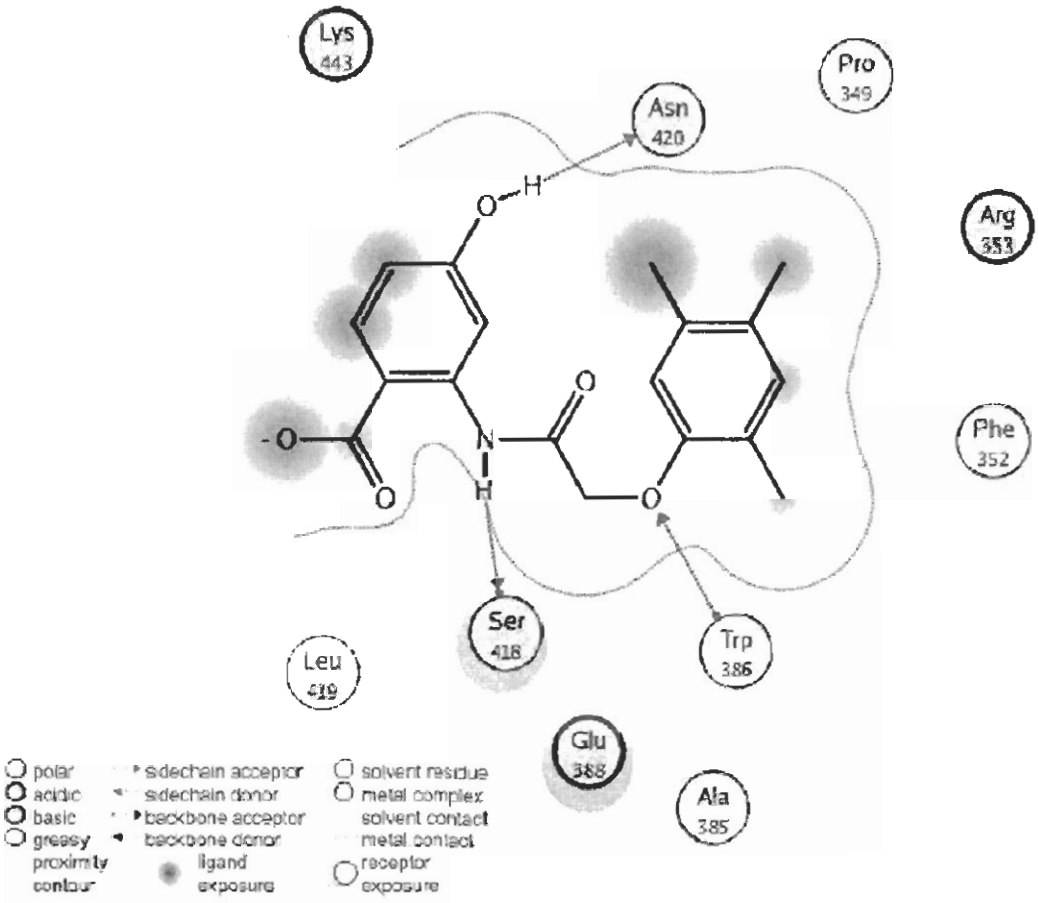

Lys
443
Pro
349
Asn
420
Arg
353
Phe
352
Ser
418
Trp
386
Leu
419
Glu
388
Ala
385
polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure

FIGURE 56

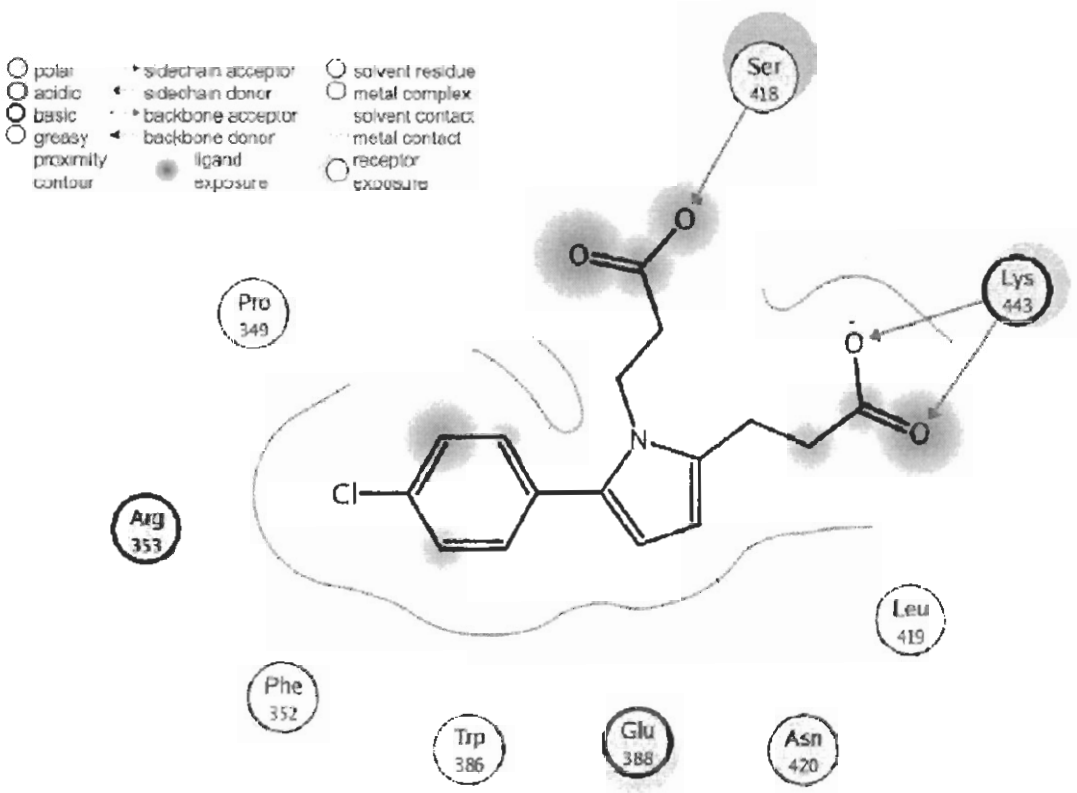

polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure
Ser 418
Lys 443
Pro 349
Arg 353
Phe 352
Trp 386
Glu 388
Asn 420
Leu 419
Cl
N
O

FIGURE 57

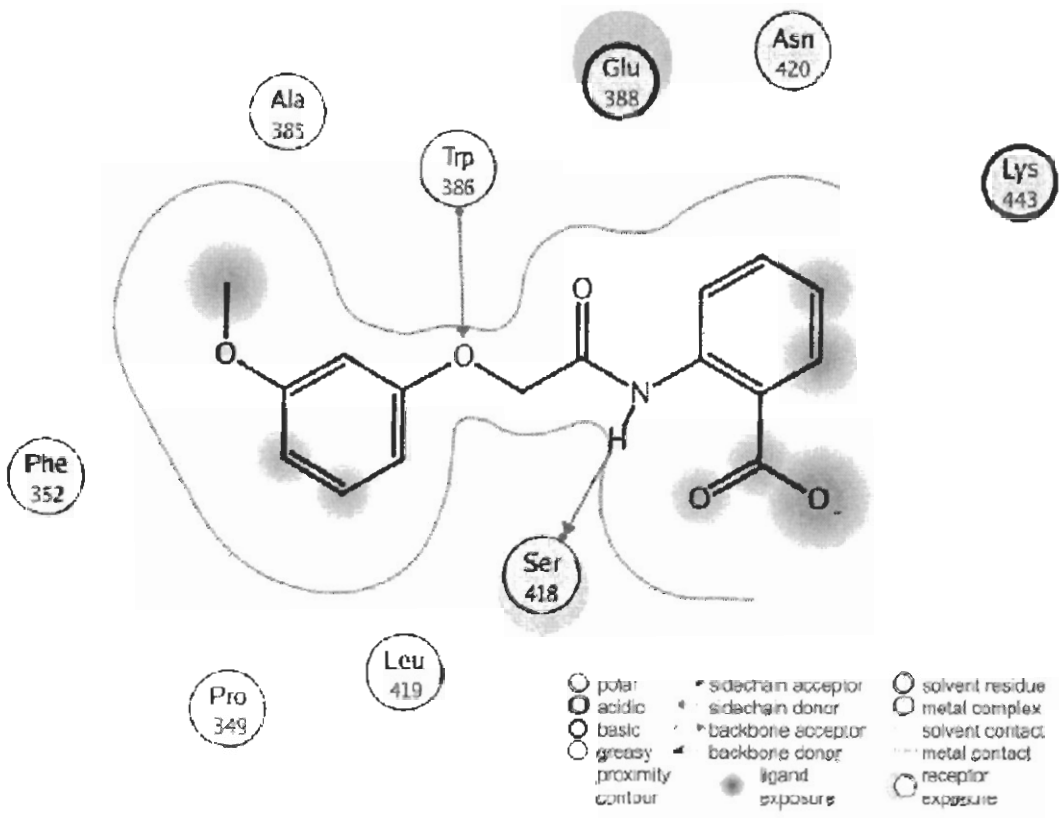

Glu
388
Asn
420
Ala
385
Trp
386
Lys
443
O
O
N
H
O
O
O
Phe
352
Ser
418
Leu
419
Pro
349
polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure

FIGURE 58A

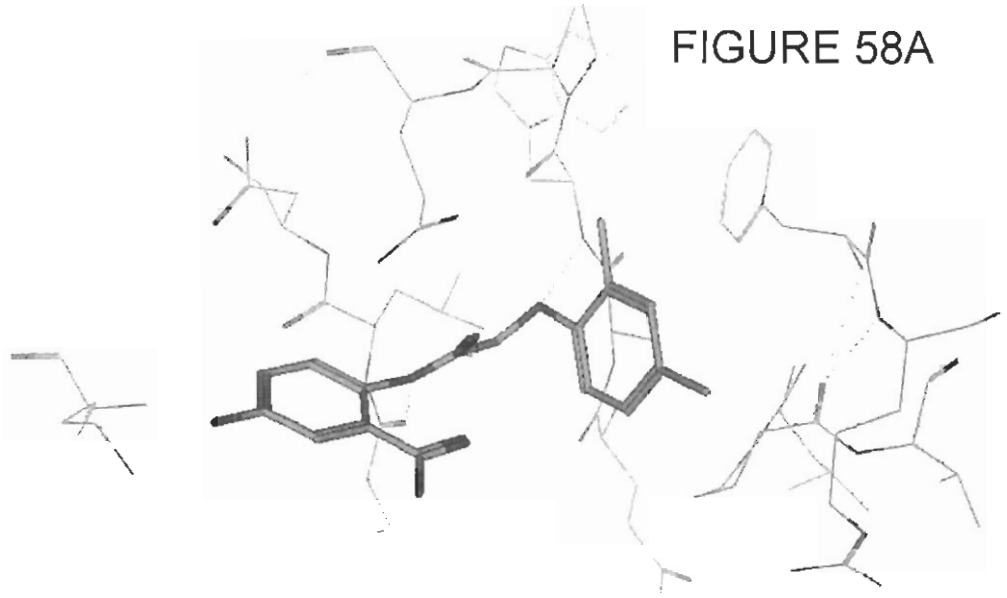


FIGURE 58B

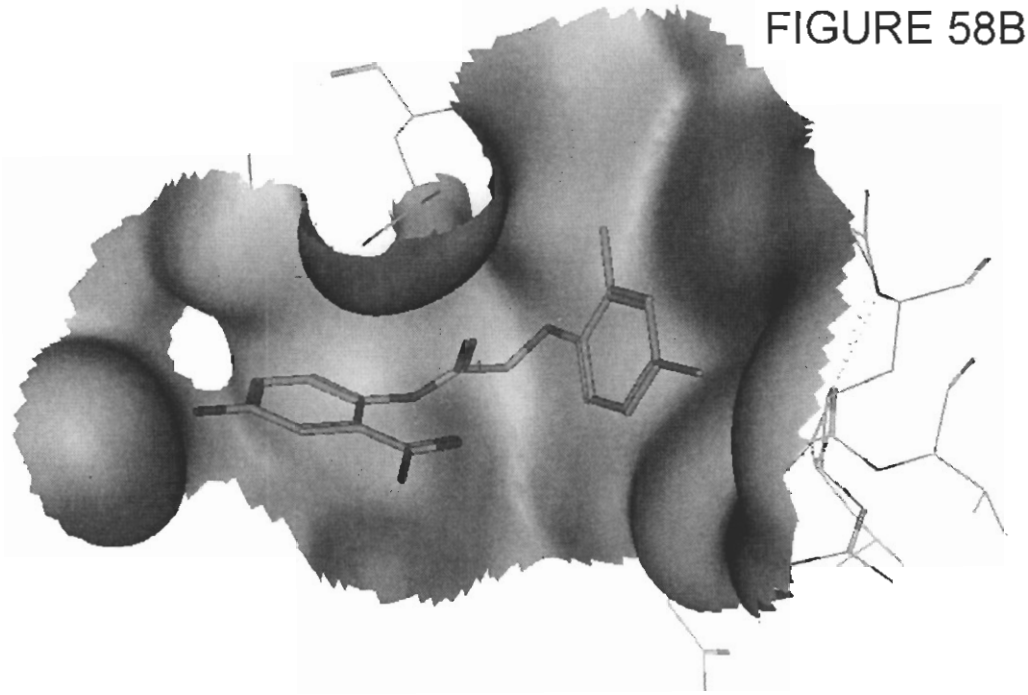


FIGURE 59

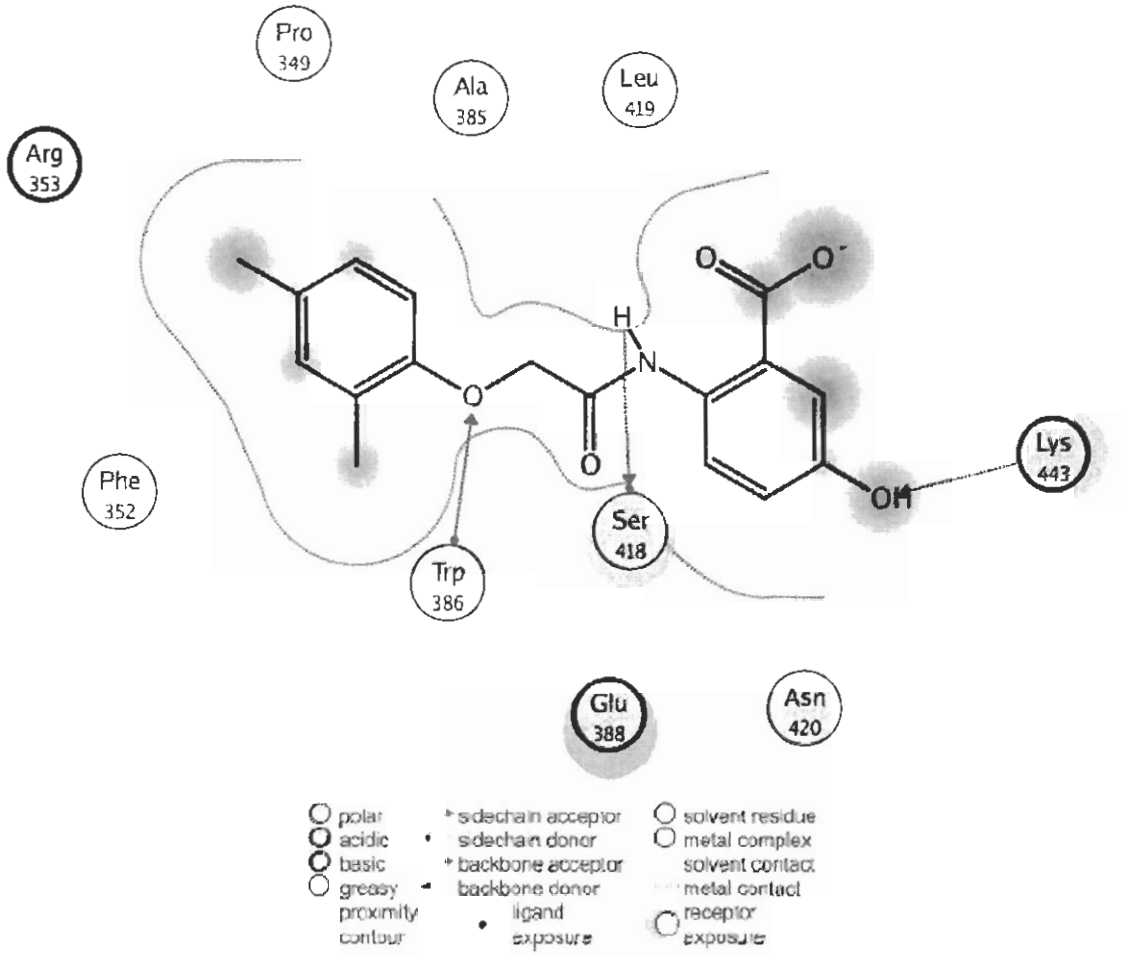

Pro
349
Ala
385
Leu
419
Arg
353
Phe
352
Trp
386
Ser
418
Lys
443
Glu
388
Asn
420
O
O⁻
H
N
O
O
OH
polar
acidic
basic
greasy
proximity contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand exposure
solvent residue
metal complex
solvent contact
metal contact
receptor exposure

FIGURE 60A

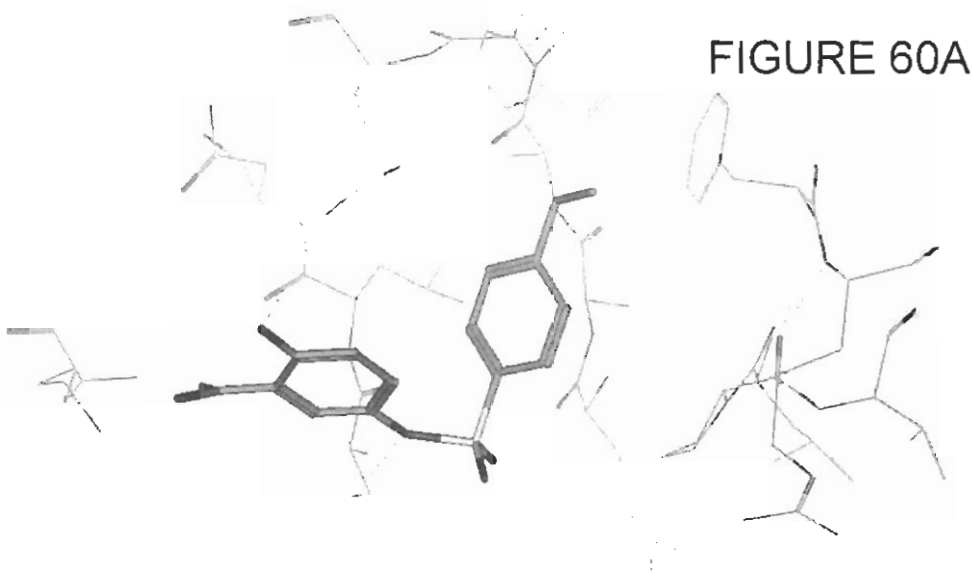


FIGURE 60B

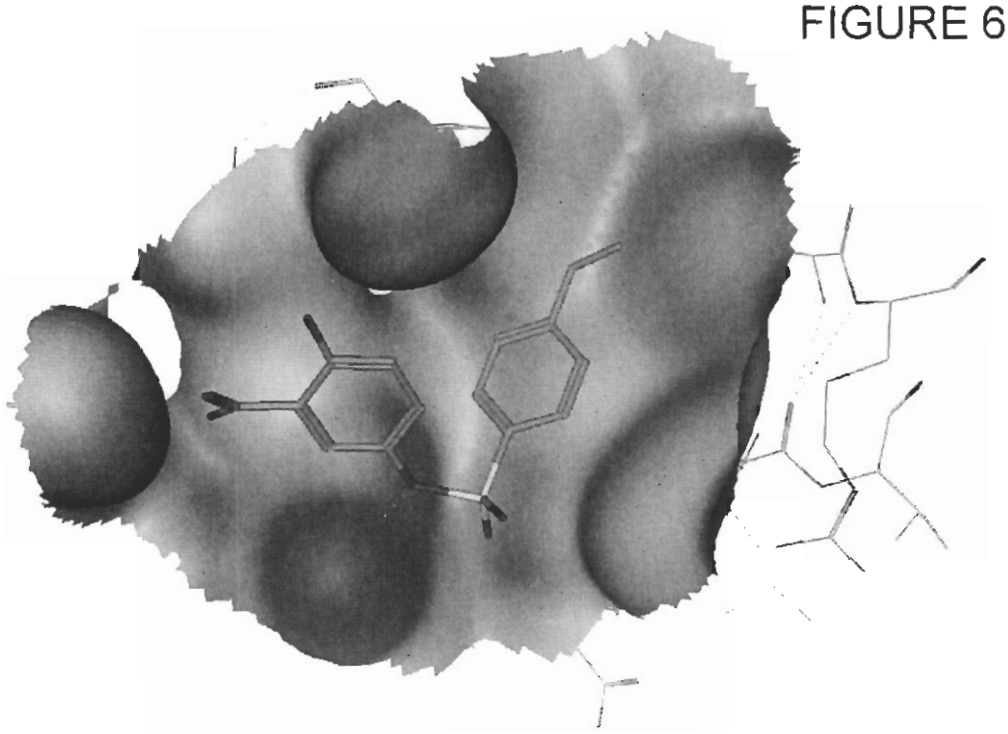
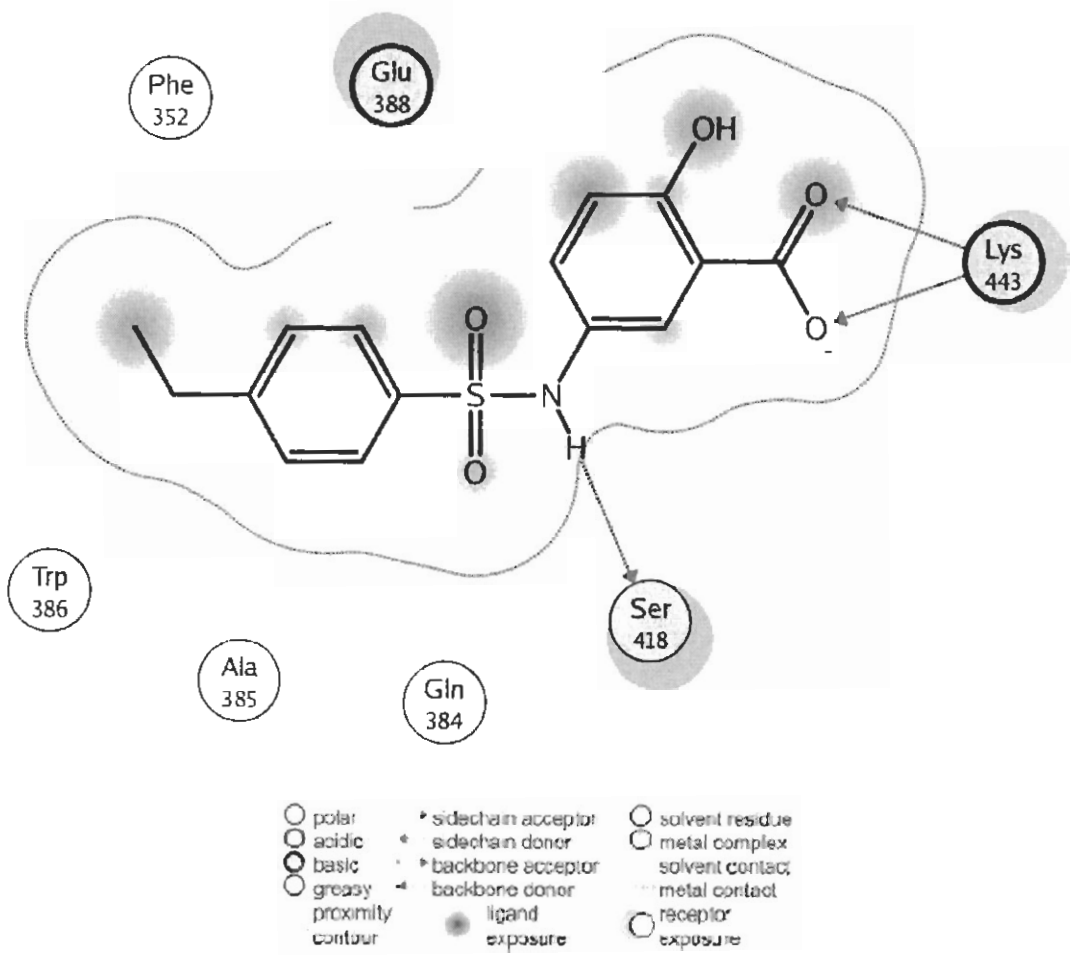


FIGURE 61


Phe
352
Glu
388
OH
O
Lys
443
O
O
S
N
H
O
Trp
386
Ser
418
Ala
385
Gln
384
polar
acidic
basic
greasy
proximity
contour
sidechain acceptor
sidechain donor
backbone acceptor
backbone donor
ligand
exposure
solvent residue
metal complex
solvent contact
metal contact
receptor
exposure