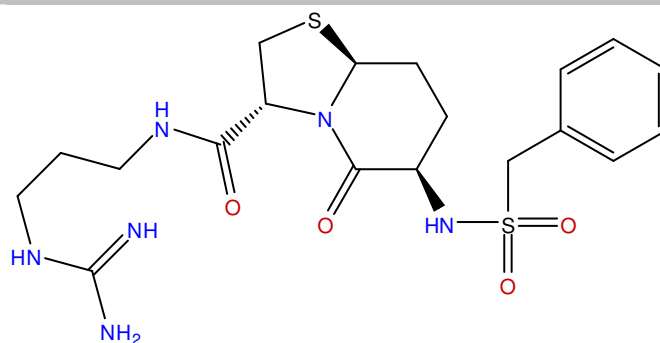


Table S1. Structures of the thrombin inhibitors used in the study

Molecule 01

Structure

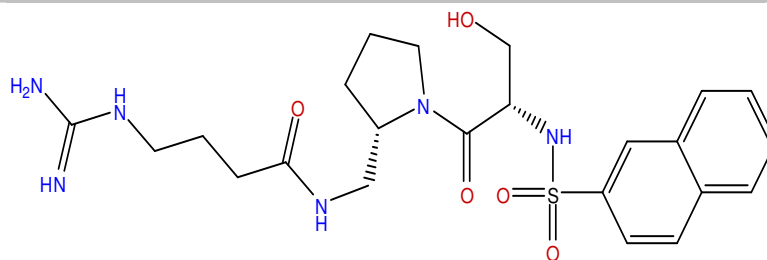


PDB Code 1BHX

pK_i 6.84

Molecule 02

Structure

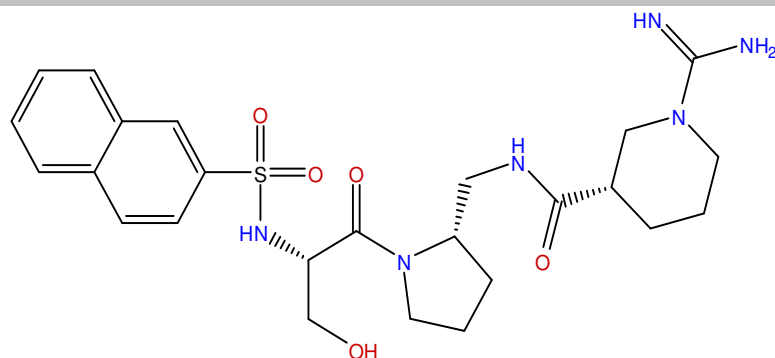


PDB Code 1BMM

pK_i 7.10

Molecule 03

Structure

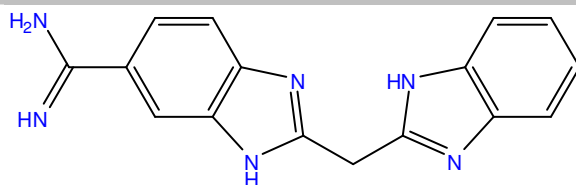


PDB Code 1BMN

pK_i 8.44

Molecule 04

Structure



PDB Code

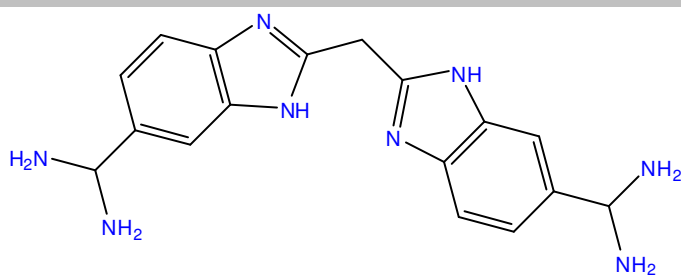
1C1U

pK_i

8.25

Molecule 05

Structure



PDB Code

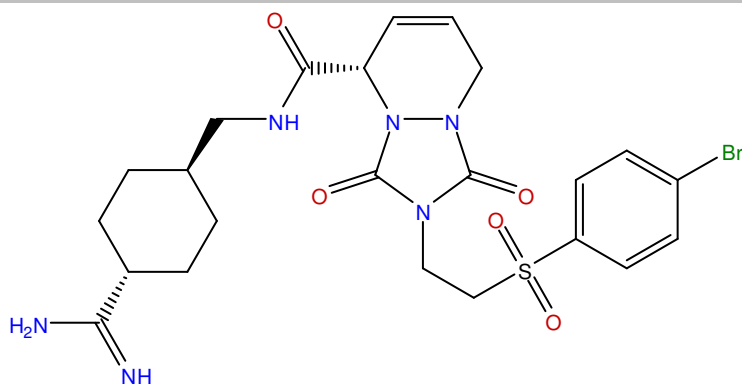
1C1V

pK_i

8.64

Molecule 06

Structure



PDB Code

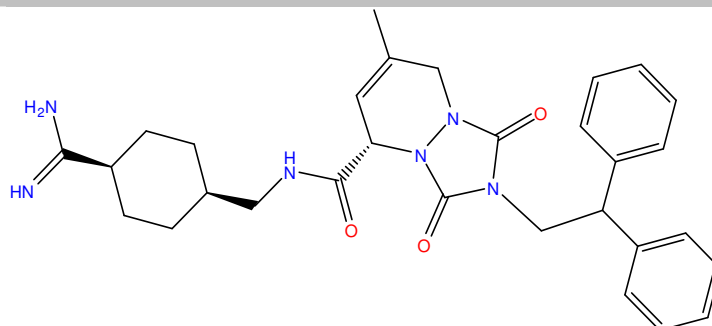
1C4U

pK_i

10.37

Molecule 07

Structure

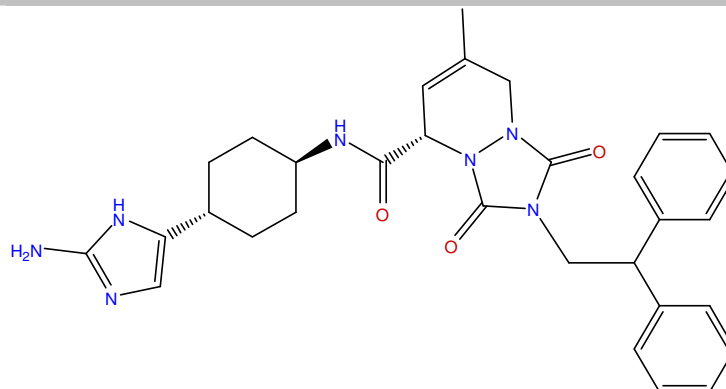


PDB Code 1C4V

pK_i 10.80

Molecule 08

Structure

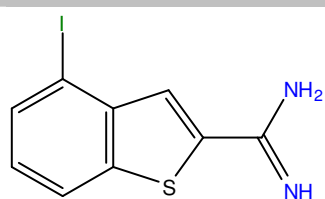


PDB Code 1C4Y

pK_i 7.92

Molecule 09

Structure

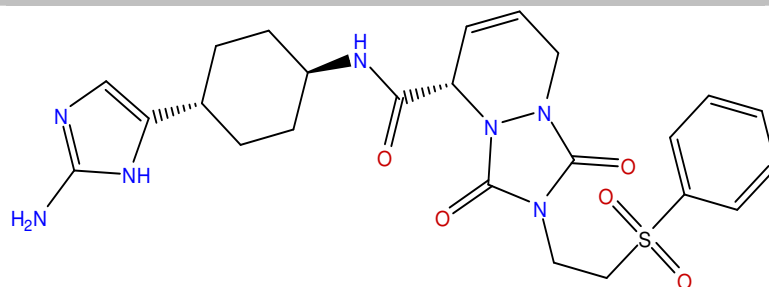


PDB Code 1C5N

pK_i 4.70

Molecule 10

Structure

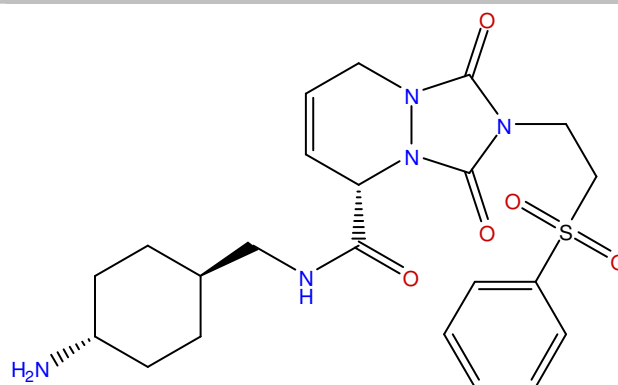


PDB Code 1D6W

pK_i 7.96

Molecule 11

Structure

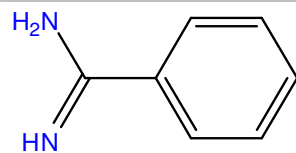


PDB Code 1D9I

pK_i 9.11

Molecule 12

Structure

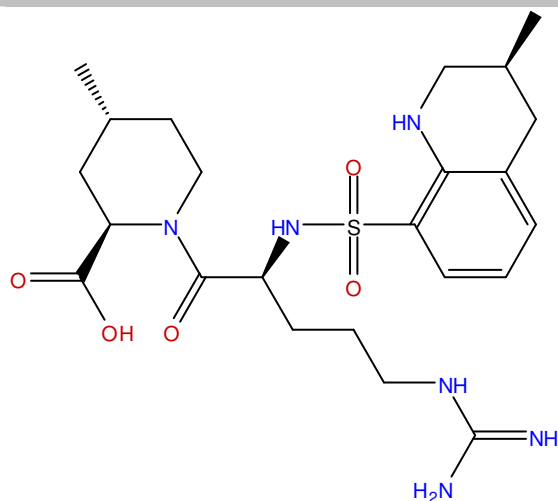


PDB Code 1DWB

pK_i 6.52

Molecule 13

Structure



PDB Code

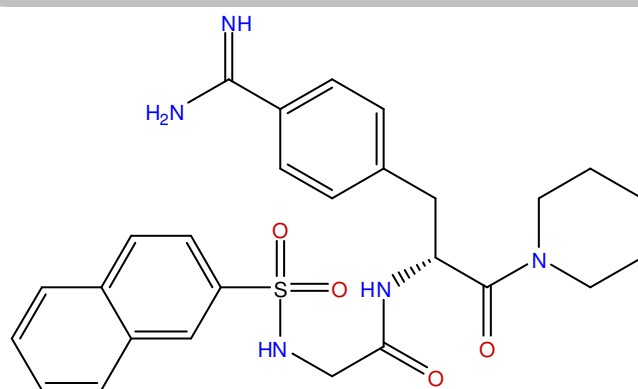
1DWC

pK_i

7.41

Molecule 14

Structure



PDB Code

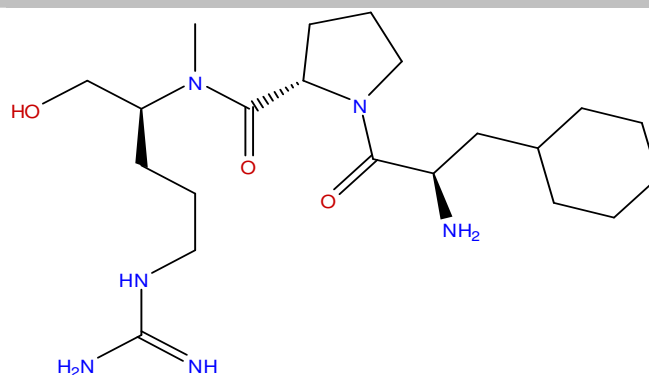
1DWD

pK_i

7.59

Molecule 15

Structure

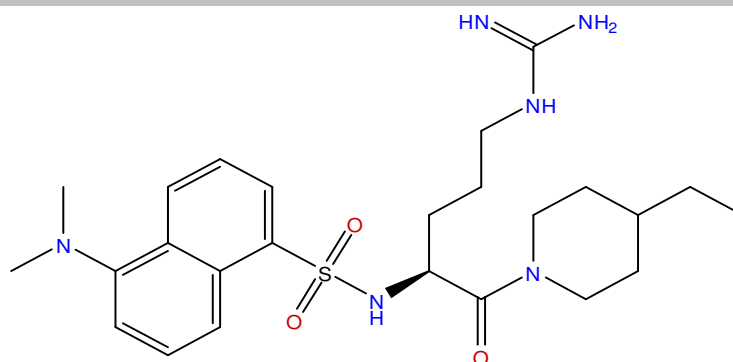


PDB Code 1EB1

pK_i 10.43

Molecule 16

Structure

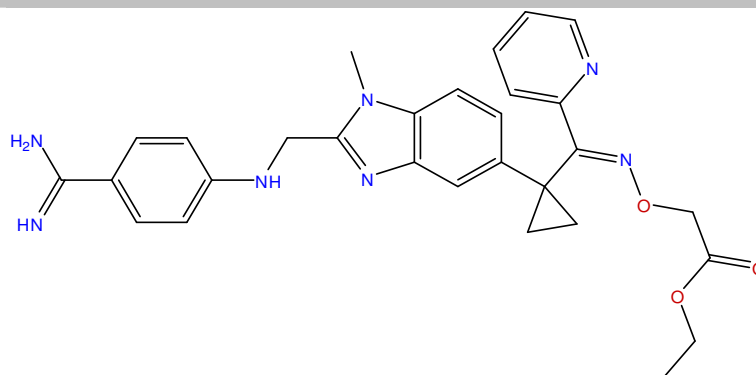


PDB Code 1FPC

pK_i 7.00

Molecule 17

Structure

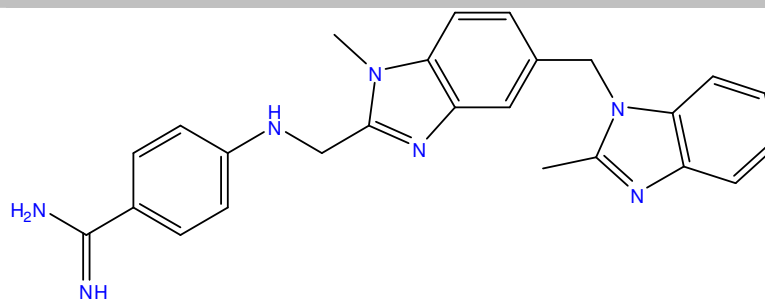


PDB Code 1G30

pK_i 6.85

Molecule 18

Structure

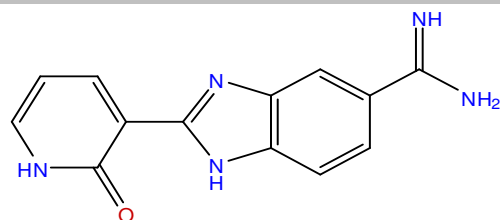


PDB Code 1G32

pK_i 6.11

Molecule 19

Structure

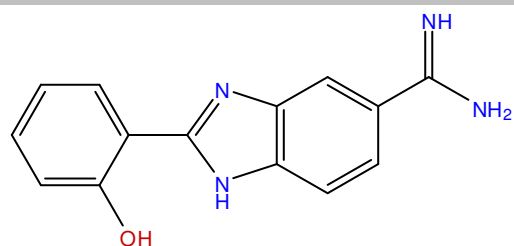


PDB Code 1GHV

pK_i 7.35

Molecule 20

Structure

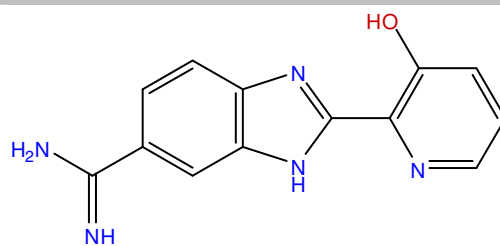


PDB Code 1GHW

pK_i 5.40

Molecule 21

Structure

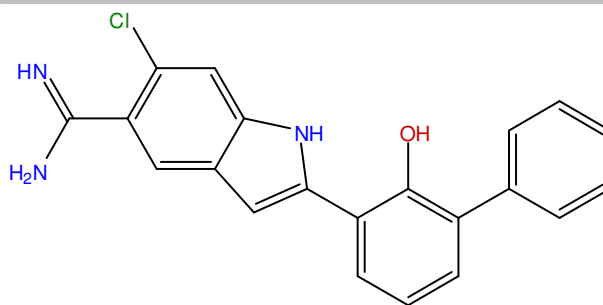


PDB Code 1GHY

pK_i 8.10

Molecule 22

Structure

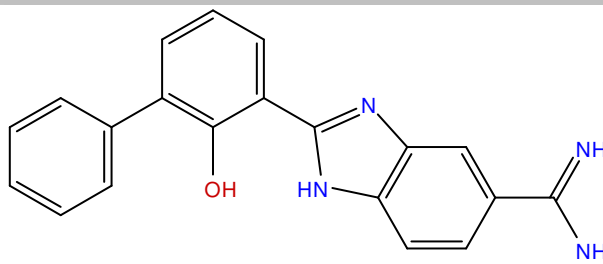


PDB Code 1GJ4

pK_i 4.22

Molecule 23

Structure

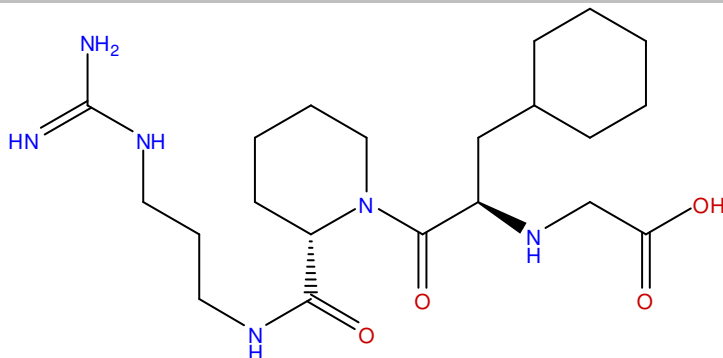


PDB Code 1GJ5

pK_i 5.26

Molecule 24

Structure

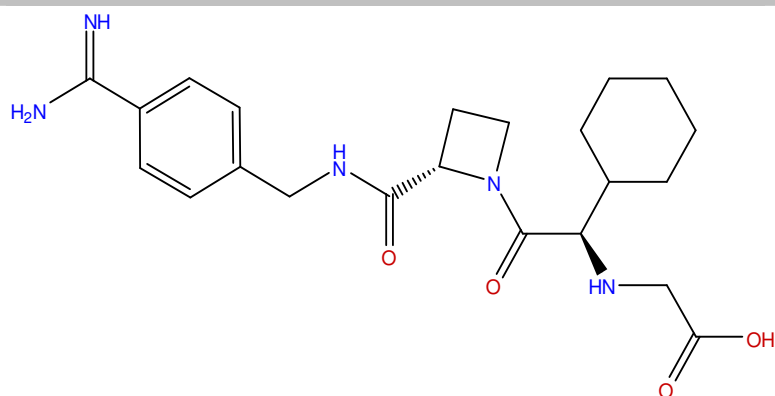


PDB Code 1K21

pK_i 8.38

Molecule 25

Structure

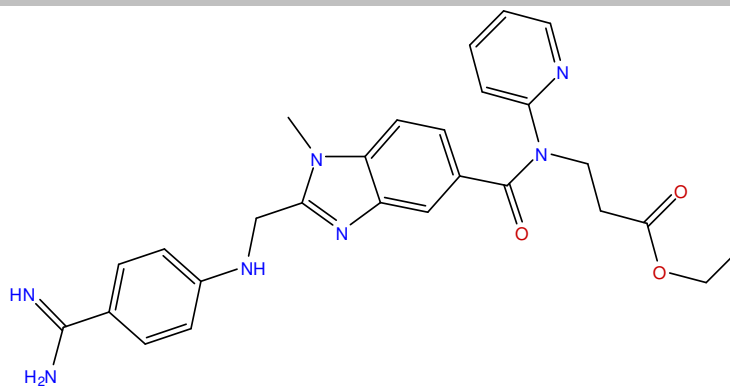


PDB Code 1K22

pK_i 8.40

Molecule 26

Structure

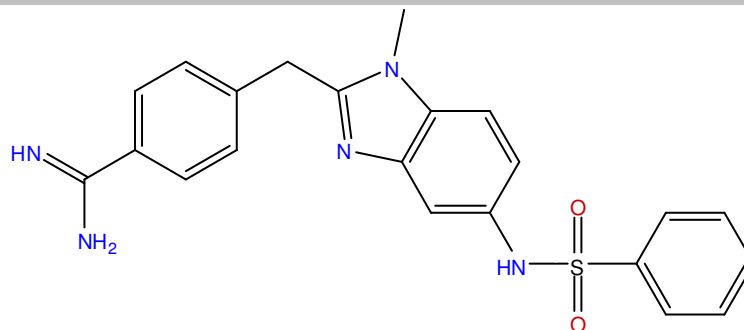


PDB Code 1KTS

pK_i 8.03

Molecule 27

Structure

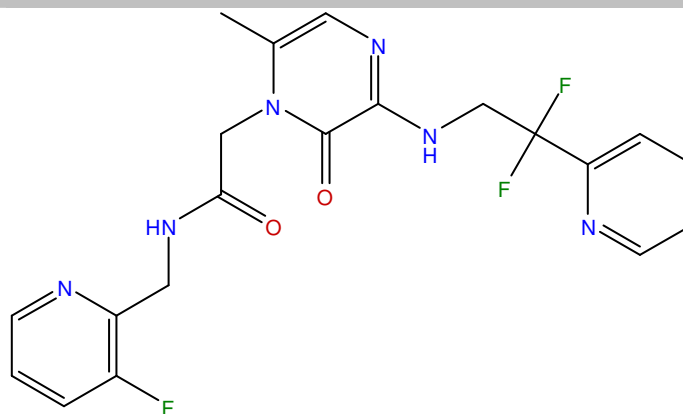


PDB Code 1KTT

pK_i 5.82

Molecule 28

Structure



PDB Code

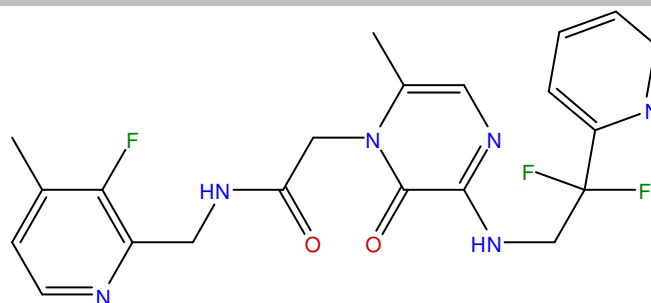
1MU6

pK_i

8.38

Molecule 29

Structure



PDB Code

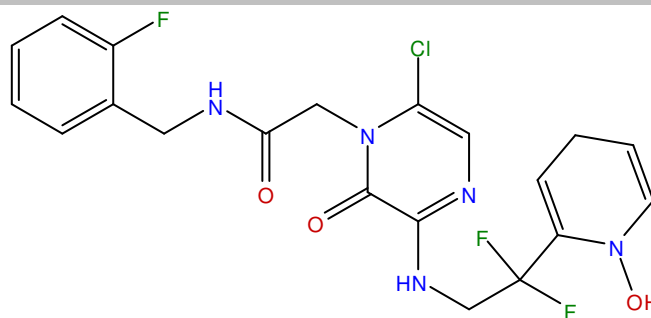
1MU8

pK_i

9.00

Molecule 30

Structure



PDB Code

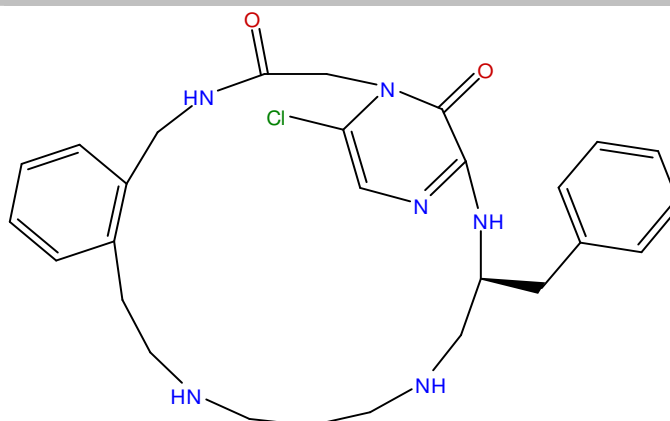
1MUE

pK_i

8.64

Molecule 31

Structure

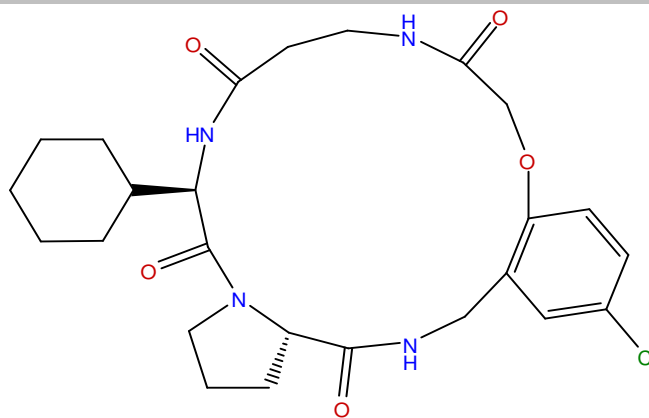


PDB Code 1NM6

pK_i 10.05

Molecule 32

Structure

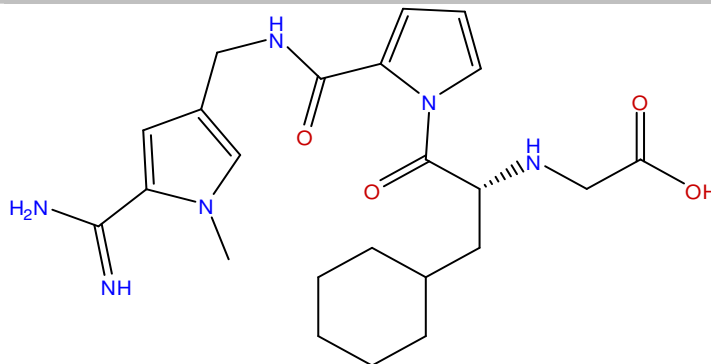


PDB Code 1NT1

pK_i 8.89

Molecule 33

Structure

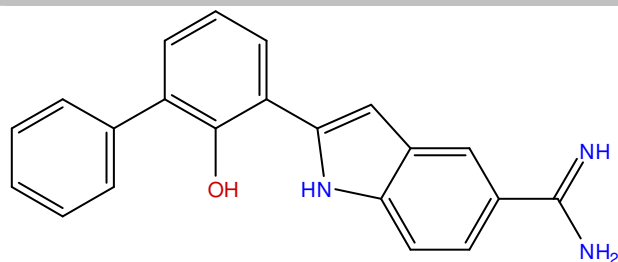


PDB Code 1NZQ

pK_i 7.96

Molecule 34

Structure

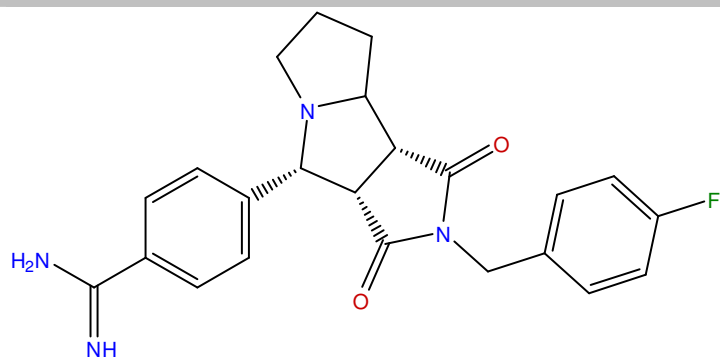


PDB Code 102G

pK_i 6.12

Molecule 35

Structure

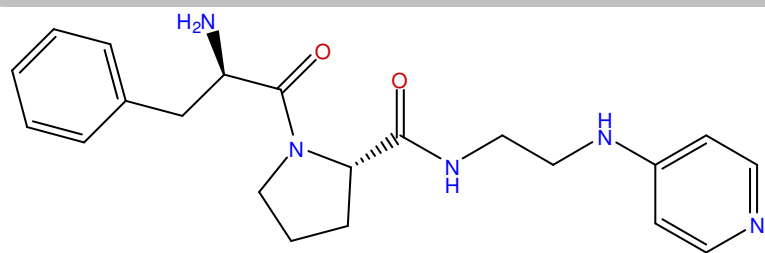


PDB Code 10YT

pK_i 7.24

Molecule 36

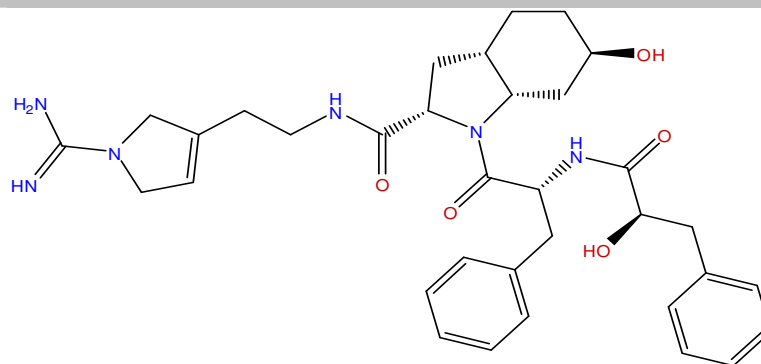
Structure



PDB Code 1QBV

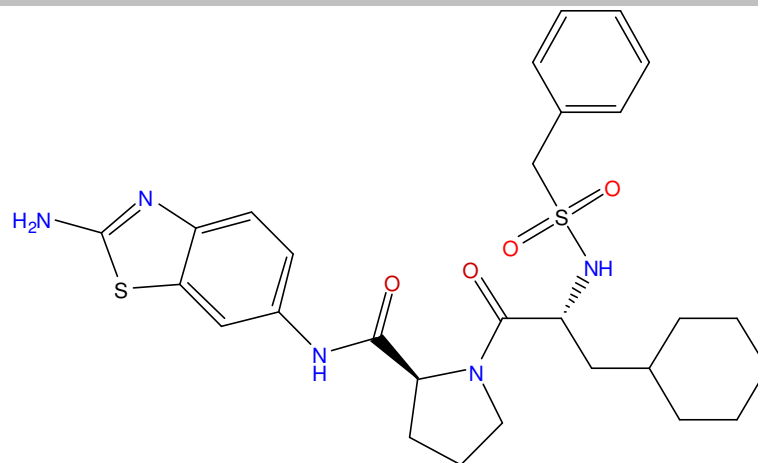
pK_i 5.39

Structure



pK_i 7.55

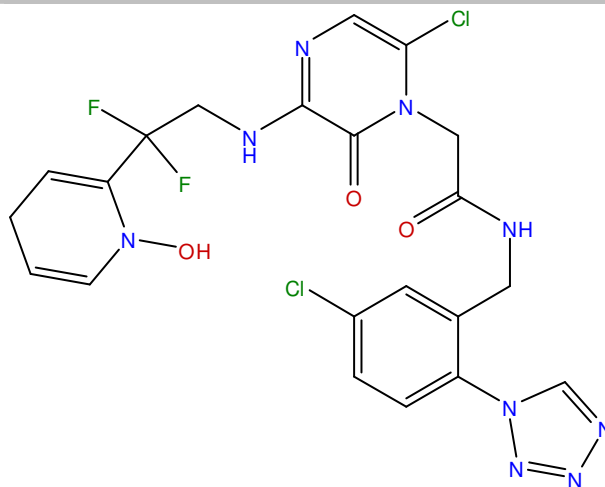
Structure



pK_i 6.89

Molecule 39

Structure

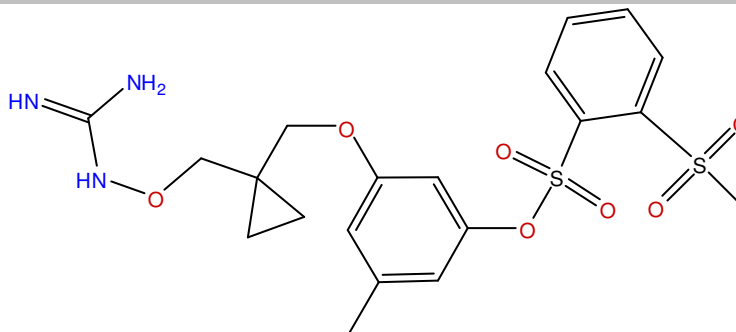


PDB Code 1SL3

pK_i 11.85

Molecule 40

Structure

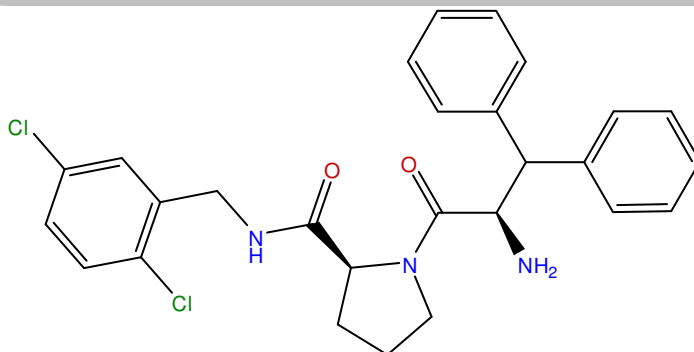


PDB Code 1T4U

pK_i 7.68

Molecule 41

Structure

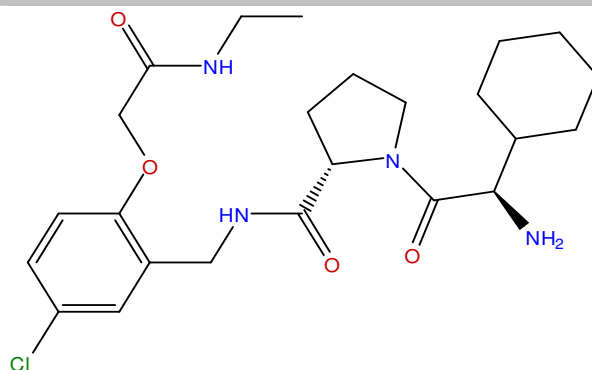


PDB Code 1TA2

pK_i 8.52

Molecule 42

Structure



PDB Code

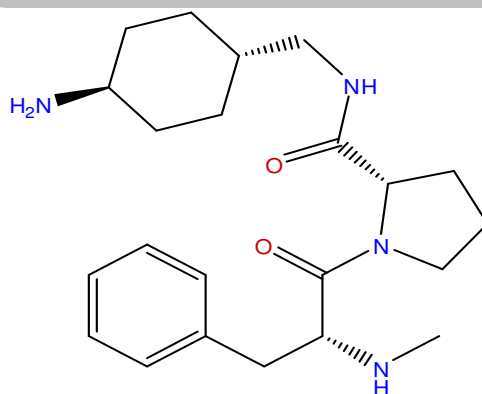
1TA6

pK_i

9.13

Molecule 43

Structure



PDB Code

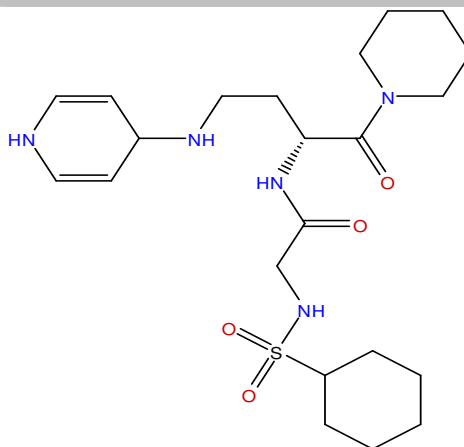
1TOM

pK_i

8.31

Molecule 44

Structure



PDB Code

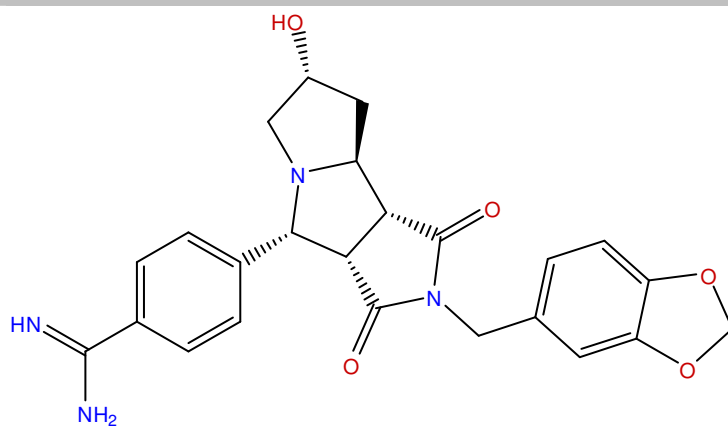
1UVS

pK_i

5.40

Molecule 45

Structure

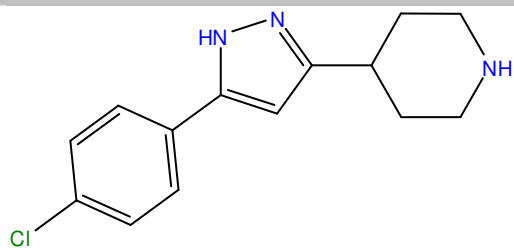


PDB Code 1VZQ

pK_i 7.44

Molecule 46

Structure

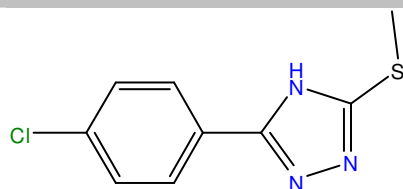


PDB Code 1WAY

pK_i 3.40

Molecule 47

Structure

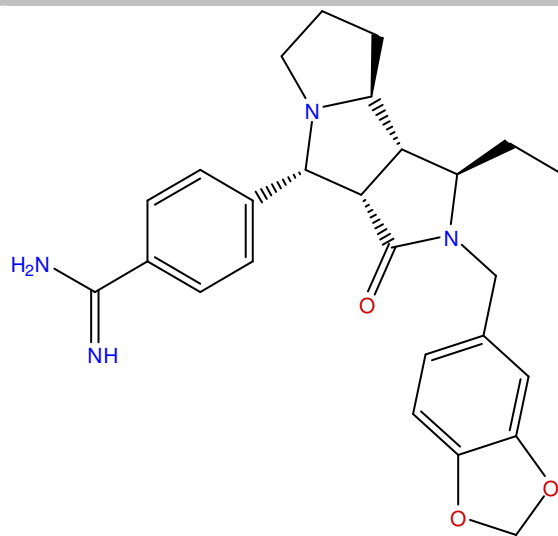


PDB Code 1WBG

pK_i 3.00

Molecule 48

Structure

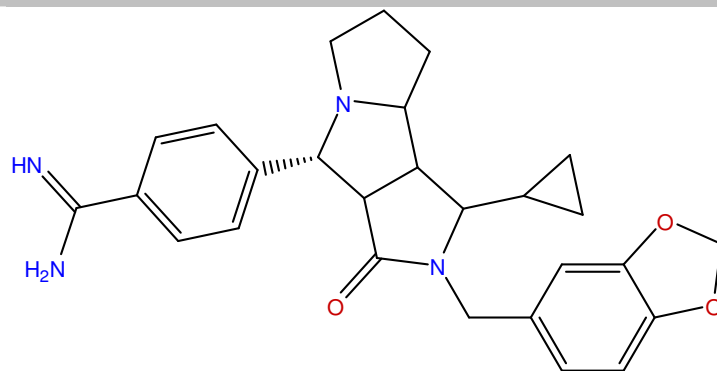


PDB Code 1YPE

pK_i 8.10

Molecule 49

Structure

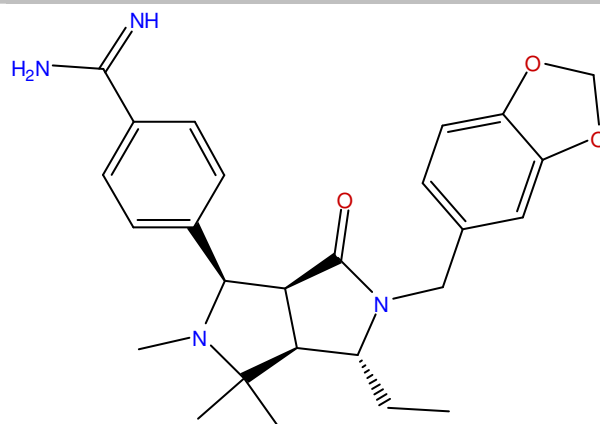


PDB Code 1YPG

pK_i 8.00

Molecule 50

Structure

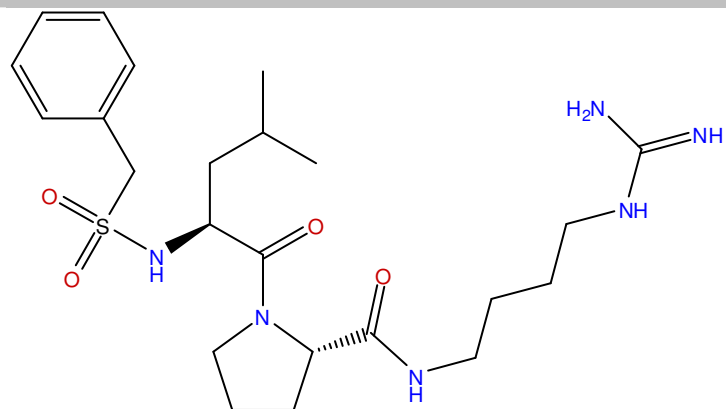


PDB Code 1YPJ

pK_i 7.02

Molecule 51

Structure

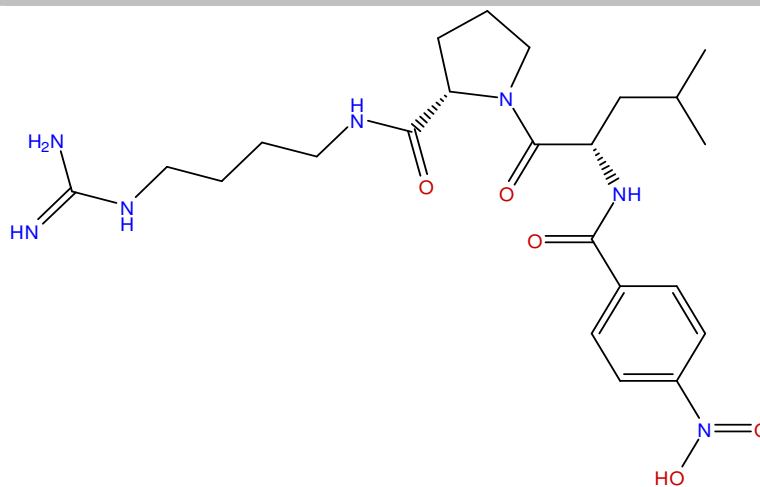


PDB Code 1YPL

pK_i 4.97

Molecule 52

Structure

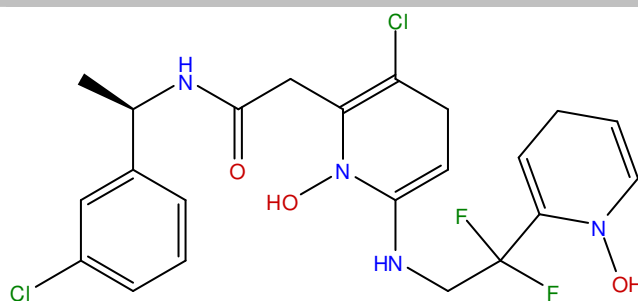


PDB Code 1YPM

pK_i 5.72

Molecule 53

Structure

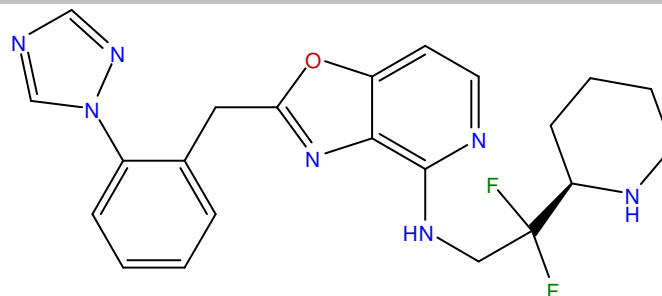


PDB Code 1Z71

pK_i 9.18

Molecule 54

Structure

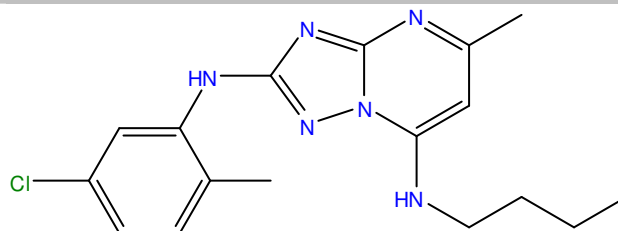


PDB Code 1ZGI

pK_i 8.34

Molecule 55

Structure

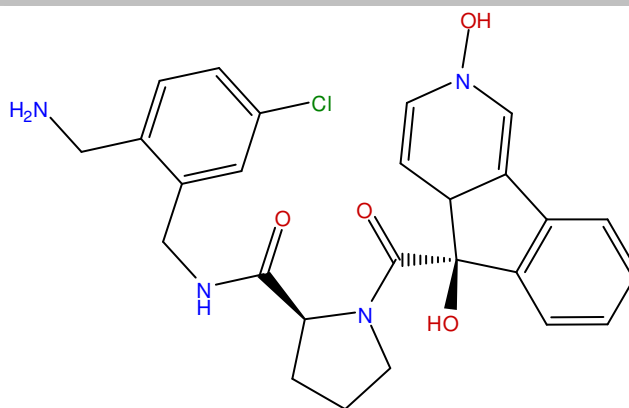


PDB Code 1ZGV

pK_i 6.00

Molecule 56

Structure

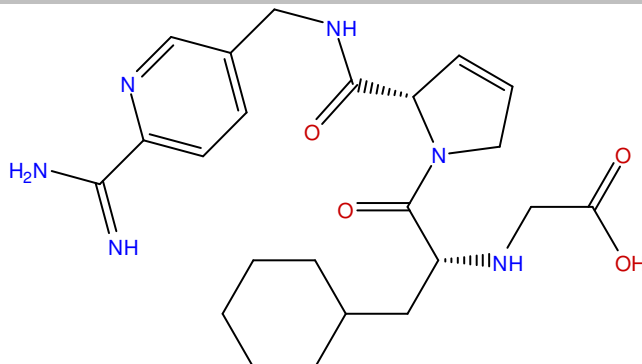


PDB Code 1ZRB

pK_i 9.11

Molecule 57

Structure

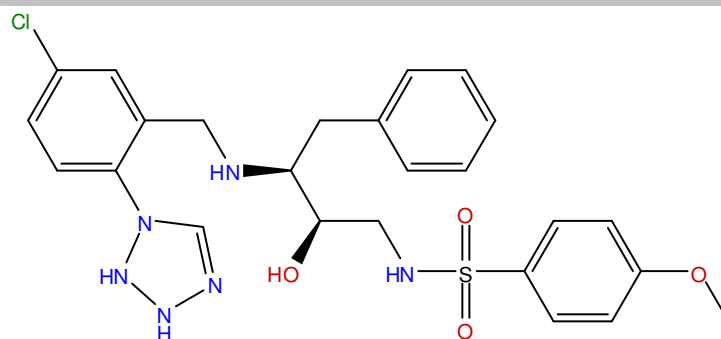


PDB Code 2ANM

pK_i 9.00

Molecule 58

Structure

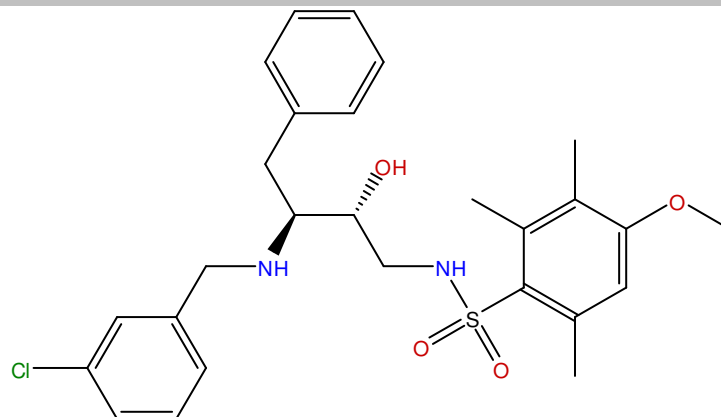


PDB Code 2C8W

pK_i 8.43

Molecule 59

Structure

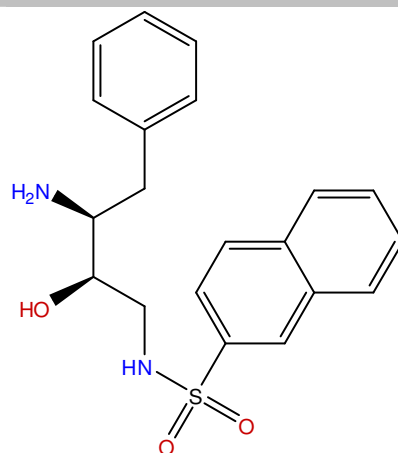


PDB Code 2C8X

pK_i 6.66

Molecule 60

Structure

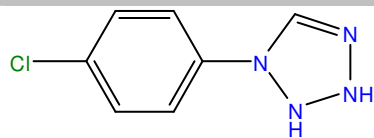


PDB Code 2C8Y

pK_i 4.00

Molecule 61

Structure



PDB Code

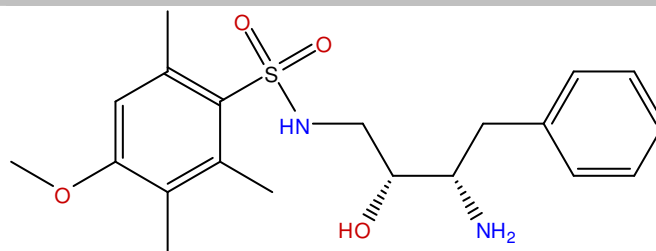
2C90

pK_i

3.48

Molecule 62

Structure



PDB Code

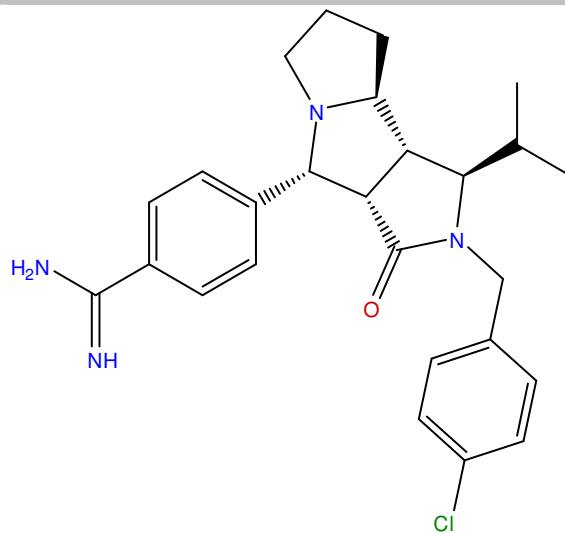
2C93

pK_i

4.92

Molecule 63

Structure



PDB Code

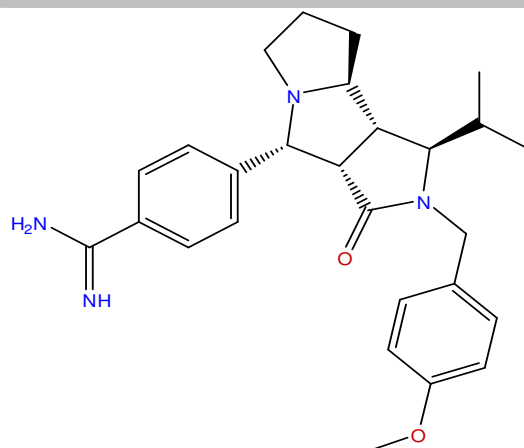
2CF8

pK_i

8.10

Molecule 64

Structure

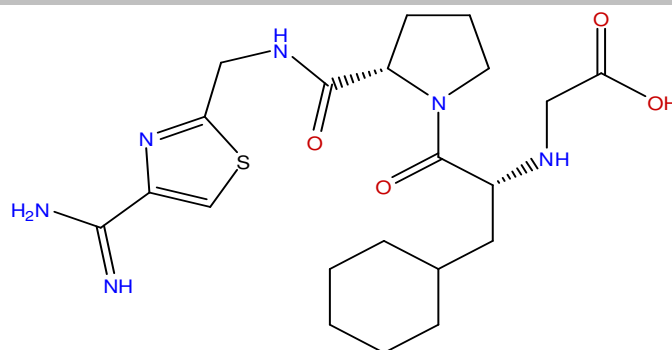


PDB Code 2CF9

pK_i 7.82

Molecule 65

Structure

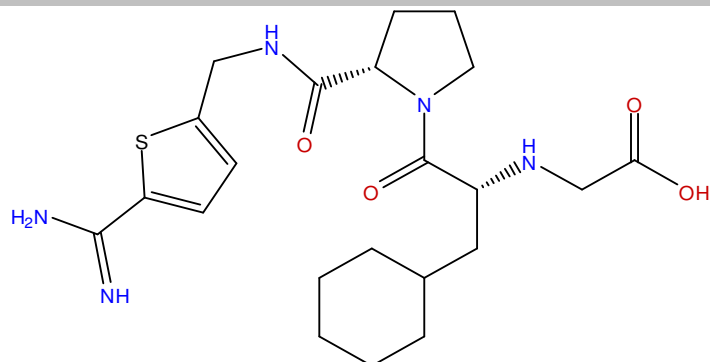


PDB Code 2FEQ

pK_i 8.86

Molecule 66

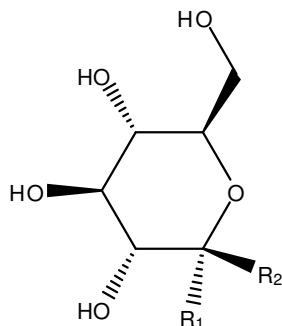
Structure



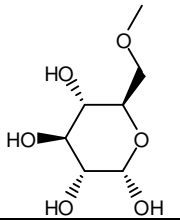
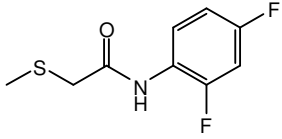
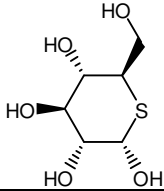
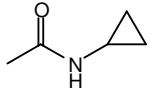
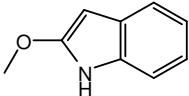
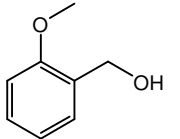
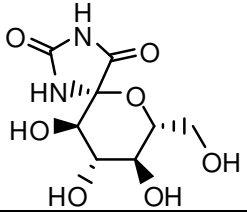
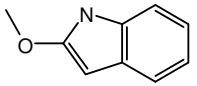
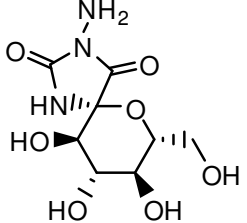
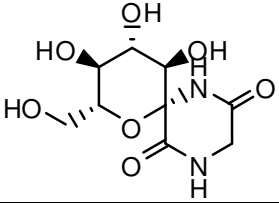
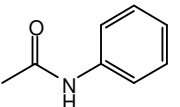
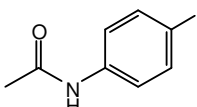
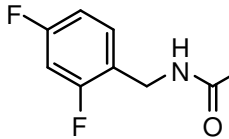
PDB Code 2FES

pK_i 9.01

Table S2. Structures of the glycogen phosphorylase *b* (GPB) inhibitors used in the study



Mol ID	R ₁	R ₂	Mol ID	R ₁	R ₂
01	OH	H	34	H	CONHCH ₃
02	CH ₃	H	35	H	CONHNH ₂
03	OCH ₃	H	36	H	NHCOCH ₂ Cl
04	H	OCH ₃	37	H	NHCOCH ₃
05	H	OCH ₂ CH ₂ OH	38	H	NHCOCH ₂ CH ₃
06	CH ₂ N ₃	H	39	H	NHCOCH ₂ Br
07	H	CH ₂ N ₃	40	H	
08	OH	CH ₂ N ₃	41	H	NHCOCH ₂ CH ₂ CH ₃
09	CH ₂ OH	H	42	H	NHCONH ₂
10	H	CH ₂ OH	43	H	NHCOCH ₂ NH ₂
11	OH	CH ₂ OH	44	H	
12	H	CH ₂ -O-SO ₂ -CH ₃	45	CONH ₂	NHCOOCH ₃
13	OH	CH ₂ -O-SO ₂ -CH ₃	46	H	
14	CH ₂ NH ₃ ⁺	H	47	H	NHCOCH ₂ NHCOCH ₃
15	H	CH ₂ NH ₃ ⁺	48	H	CONHNHCH ₃
16	H	CH ₂ CH ₂ NH ₃ ⁺	49	H	CONHCH ₂ CH ₂ OH
17	H	CH ₂ CN	50	H	
18	OH	CH ₂ CN	51	H	

19		H	52	H	
20	CONH ₂	H	53	H	CONHCH ₂ CF ₃
21			54	H	
22	H	SH	55	H	
23		H	56		
24		H	57		
25	CONHNH ₂	H	58		
26	H	SCH ₂ CONH ₂	59	H	OH
27	H	CONH ₂	60	H	CONHCH ₂ CH ₂ CF ₃
28		H	61	COOH	H
29	CONHCH ₃	H	62	CONHCH ₂ CH ₂ OH	H
30		H	63		H
31	COOCH ₃	H	64	H	NHCOOCH ₃

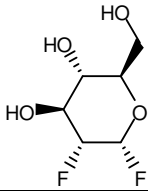
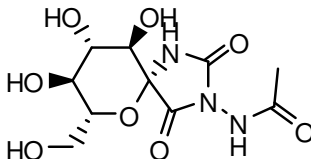
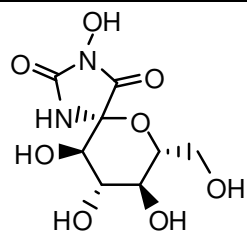
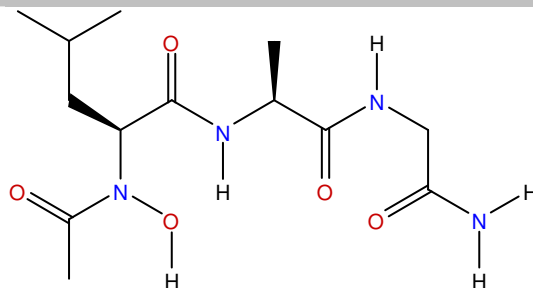
32			65	
33	H	COOCH ₃	66	

Table S3. Structures of the thermolysin inhibitors used in the study

Molecule 01

Structure

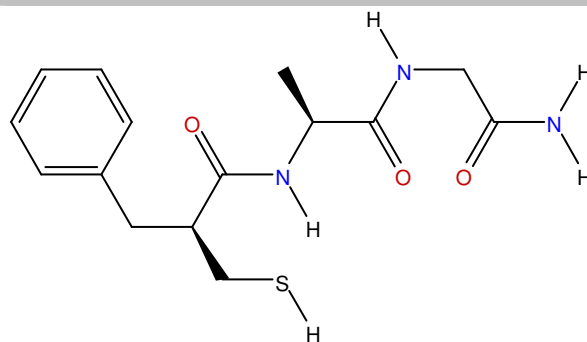


pK_i

2.47

Molecule 02

Structure

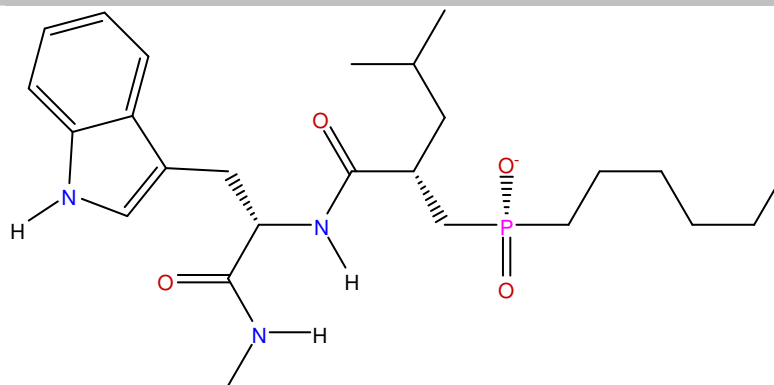


pK_i

6.12

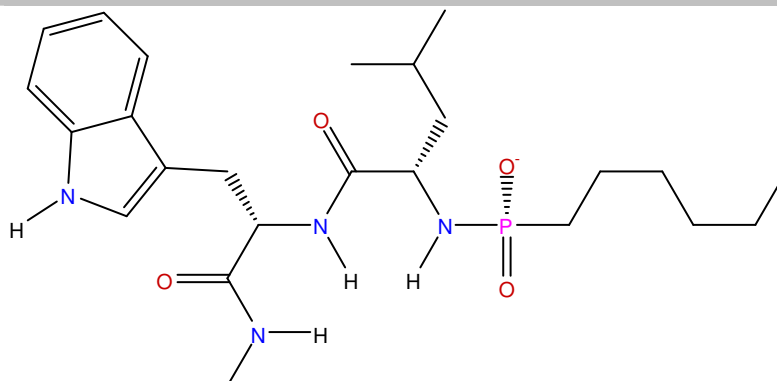
Molecule 03

Structure

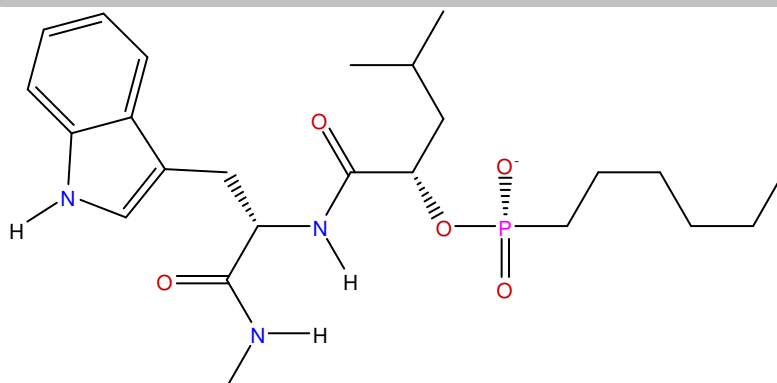


pK_i

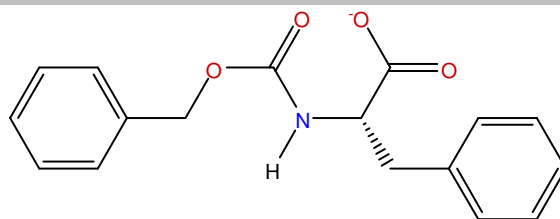
7.28

Molecule 04*Structure* pK_i

8.82

Molecule 05*Structure* pK_i

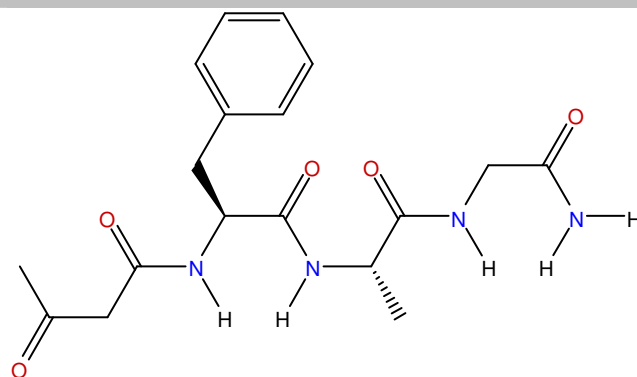
5.84

Molecule 06*Structure* pK_i

3.29

Molecule 07

Structure

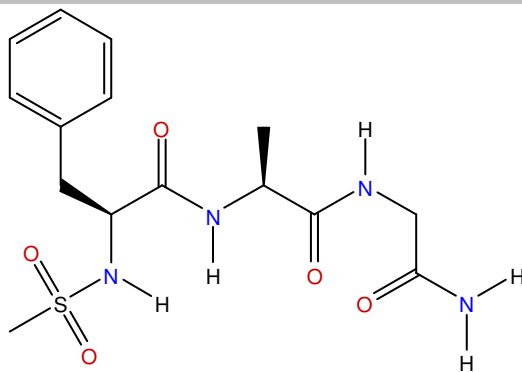


pK_i

2.51

Molecule 08

Structure

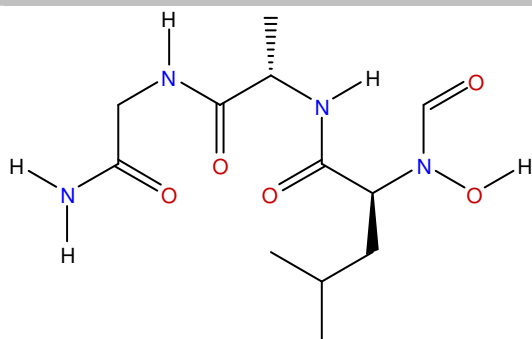


pK_i

0.52

Molecule 09

Structure

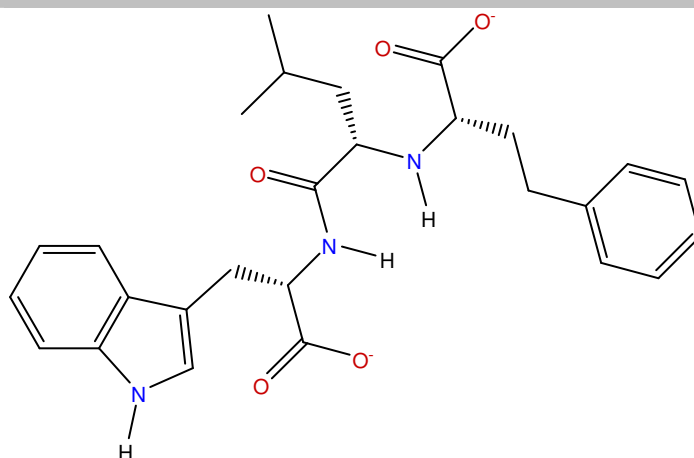


pK_i

2.47

Molecule 10

Structure

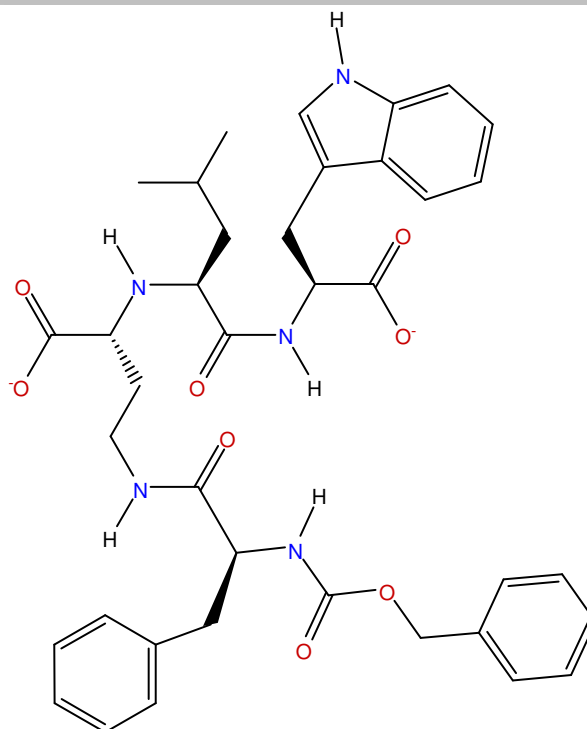


pK_i

7.47

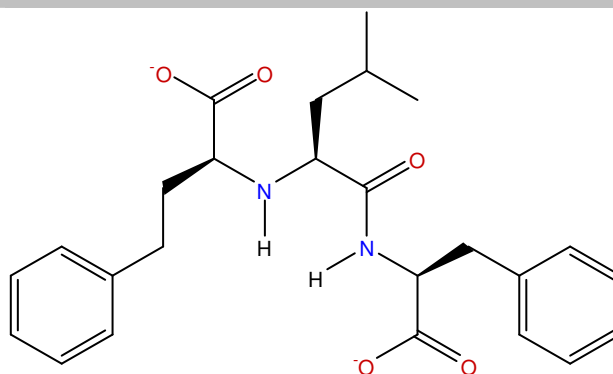
Molecule 11

Structure

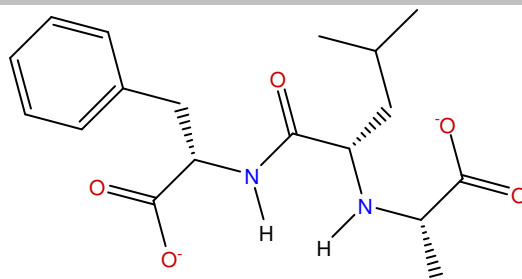


pK_i

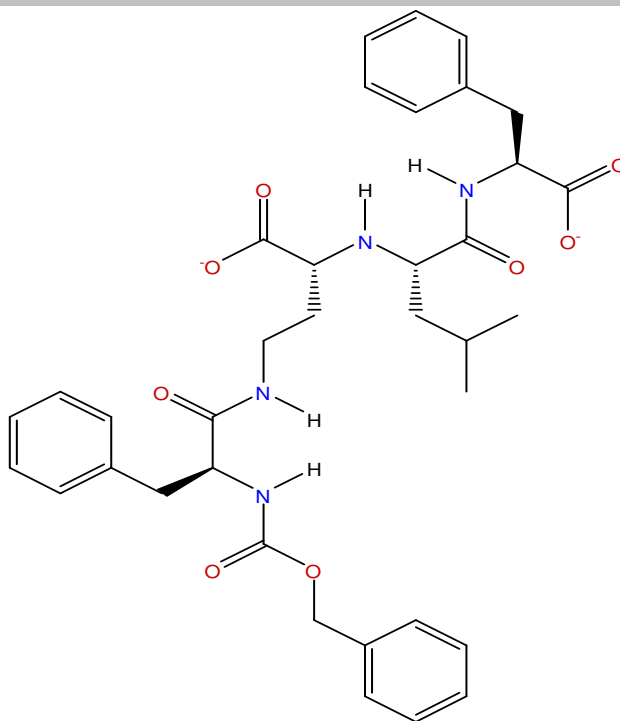
7.96

Molecule 12*Structure* pK_i

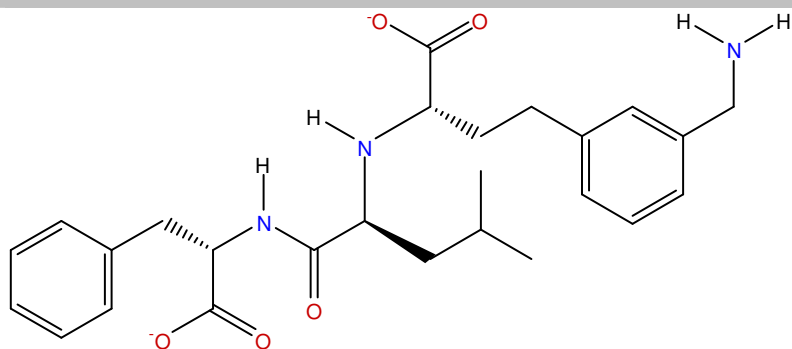
6.22

Molecule 13*Structure* pK_i

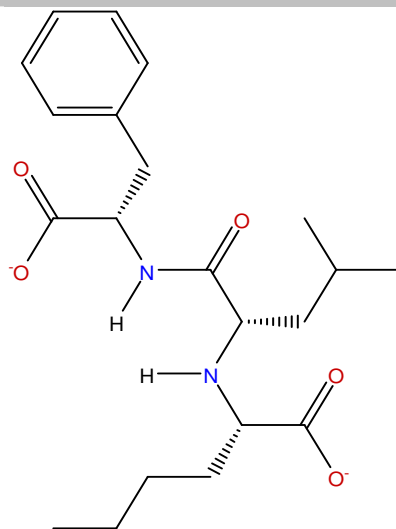
5.55

Molecule 14*Structure* pK_i

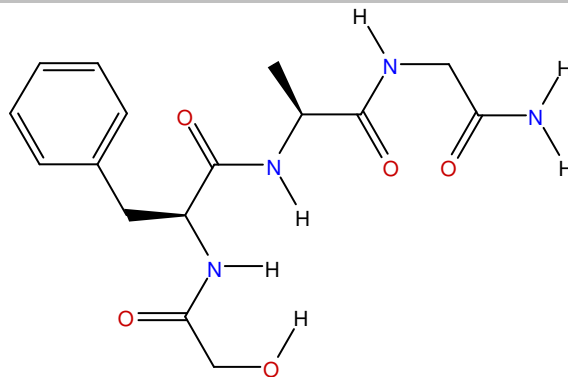
6.66

Molecule 15*Structure**pK_i*

5.77

Molecule 16*Structure**pK_i*

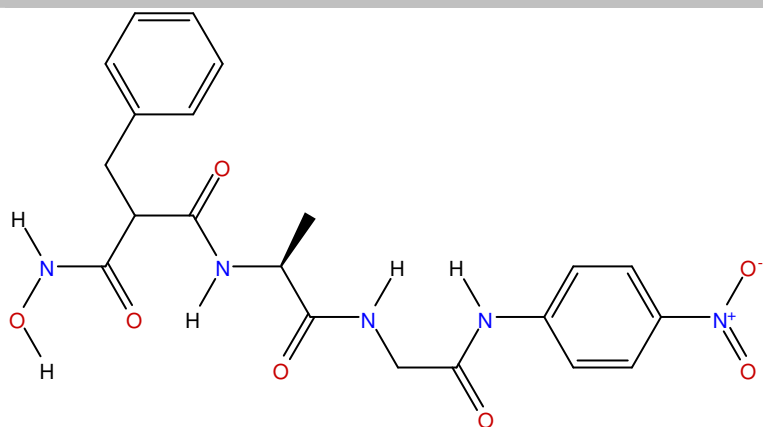
2.42

Molecule 17*Structure**pK_i*

2.54

Molecule 18

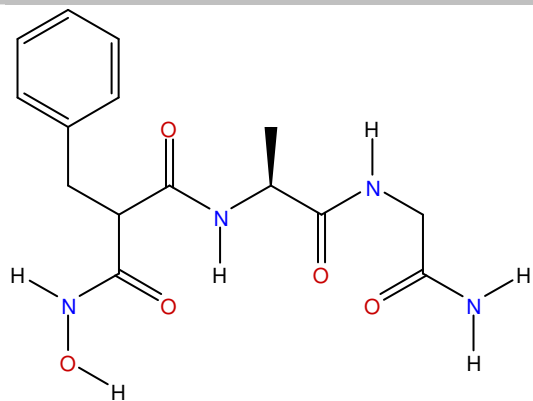
Structure

 pK_i

6.37

Molecule 19

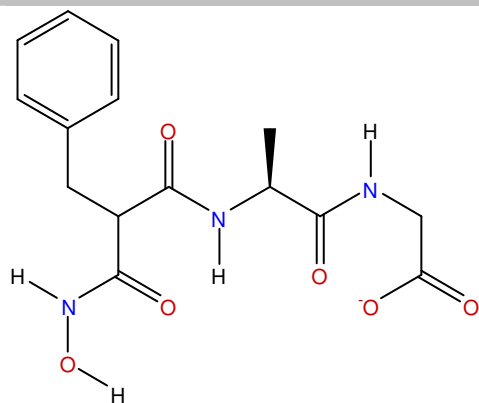
Structure

 pK_i

6.18

Molecule 20

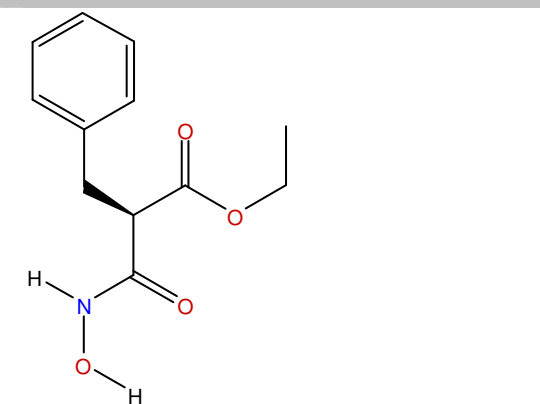
Structure

 pK_i

6.18

Molecule 21

Structure

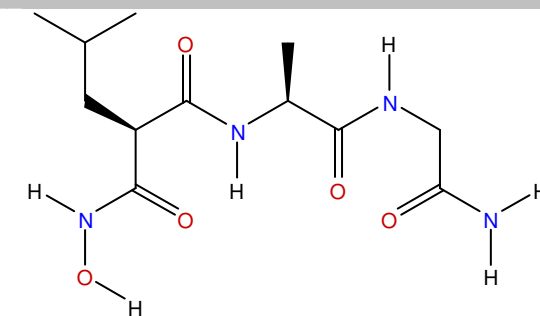


pK_i

4.7

Molecule 22

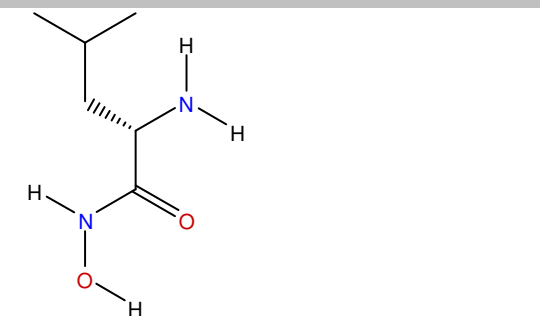
Structure

 pK_i

6.32

Molecule 23

Structure

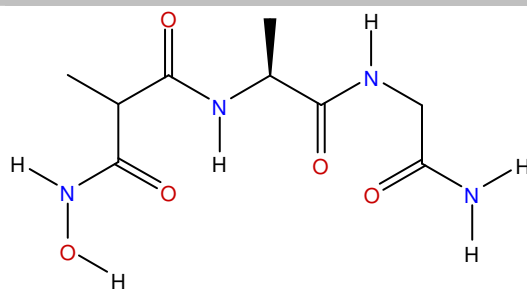


pK_i

3.72

Molecule 24

Structure

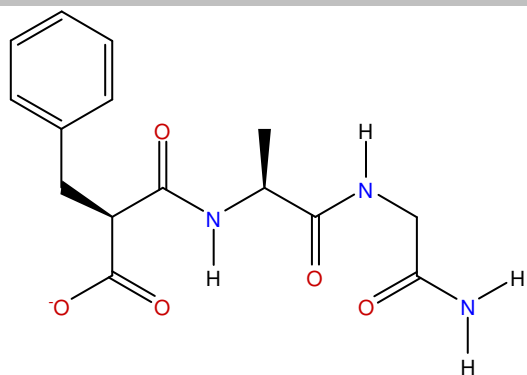


pK_i

2.96

Molecule 25

Structure

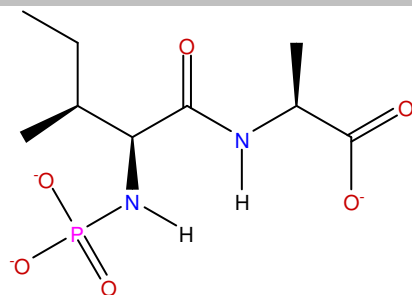


pK_i

3.38

Molecule 26

Structure

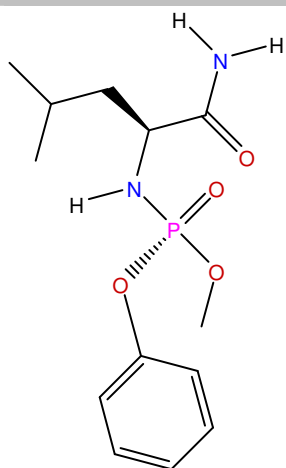


pK_i

6.44

Molecule 27

Structure

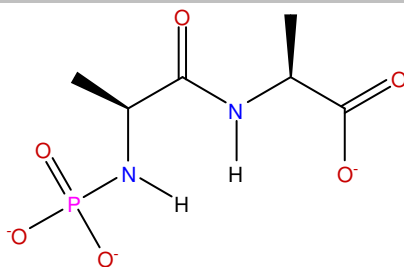


pK_i

0.52

Molecule 28

Structure

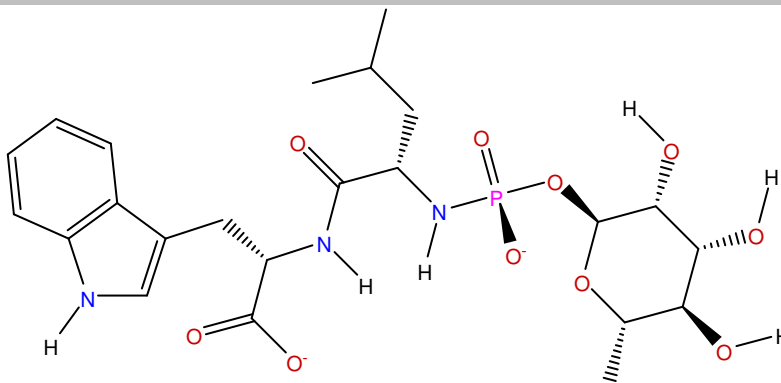


pK_i

4.06

Molecule 29

Structure

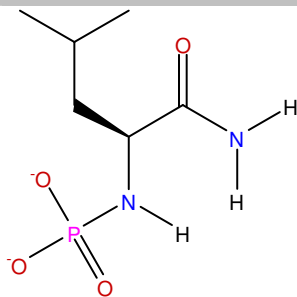


pK_i

7.55

Molecule 30

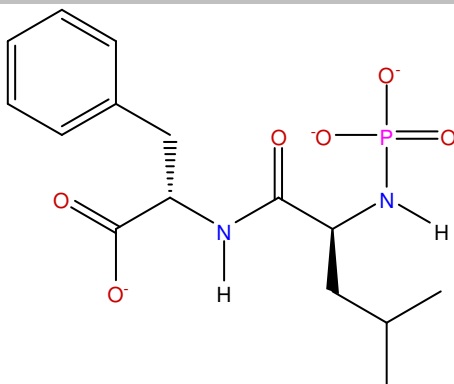
Structure

 pK_i

4.1

Molecule 31

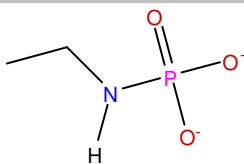
Structure

 pK_i

7.72

Molecule 32

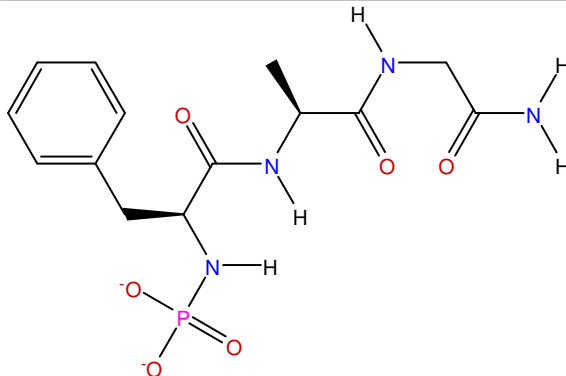
Structure

 pK_i

0.52

Molecule 33

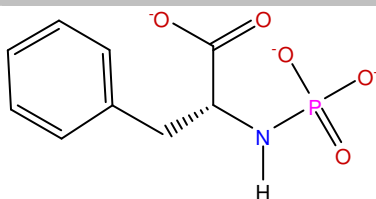
Structure

 pK_i

5.59

Molecule 34

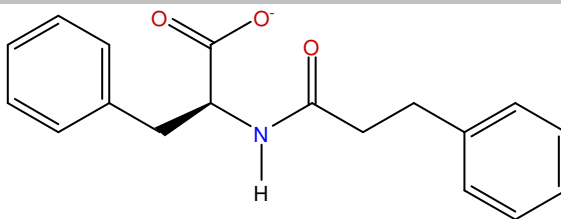
Structure

 pK_i

4.14

Molecule 35

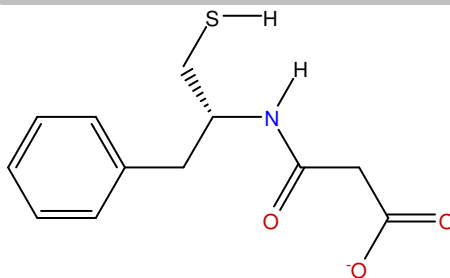
Structure

 pK_i

2.79

Molecule 36

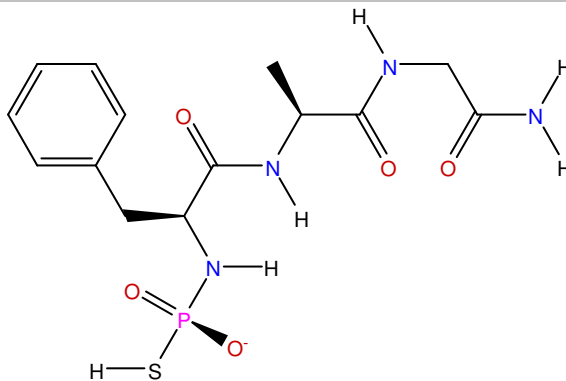
Structure

 pK_i

5.64

Molecule 37

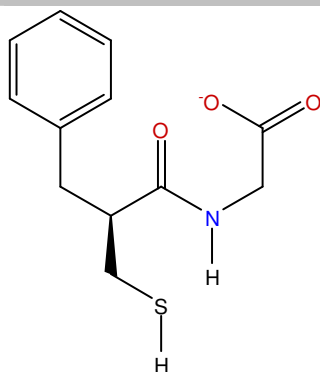
Structure

 pK_i

5.16

Molecule 38

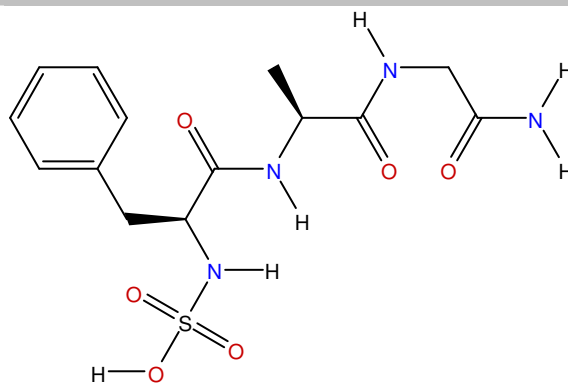
Structure

 pK_i

5.74

Molecule 39

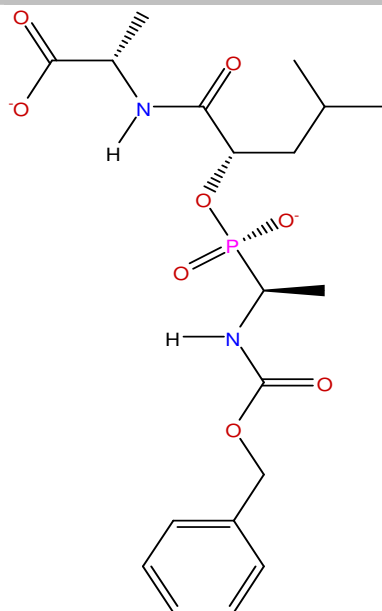
Structure

 pK_i

2.37

Molecule 40

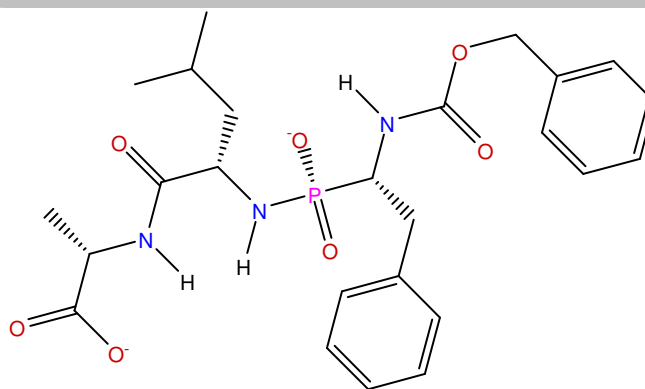
Structure

 pK_i

4.62

Molecule 41

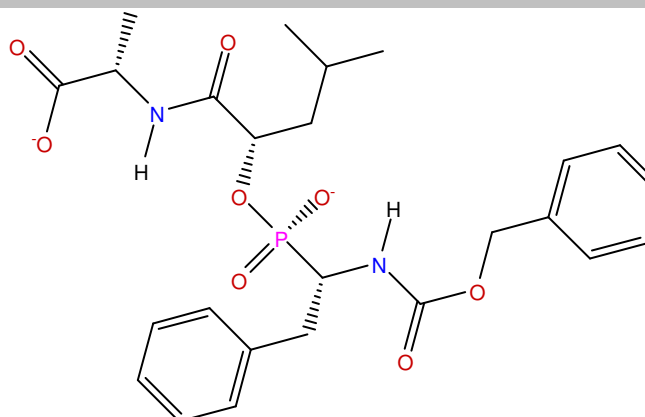
Structure

 pK_i

6.32

Molecule 42

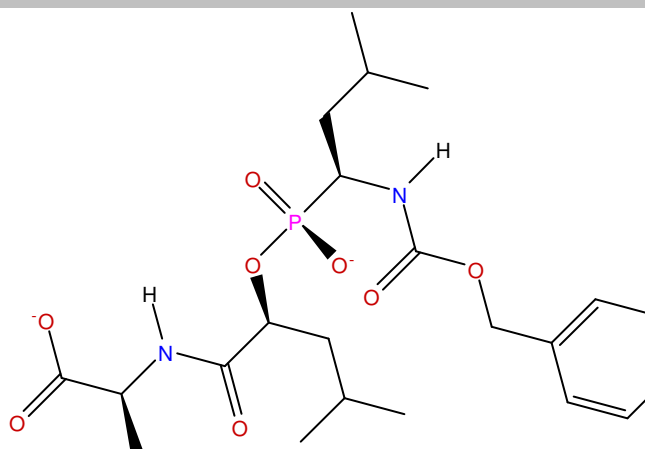
Structure

 pK_i

4.52

Molecule 43

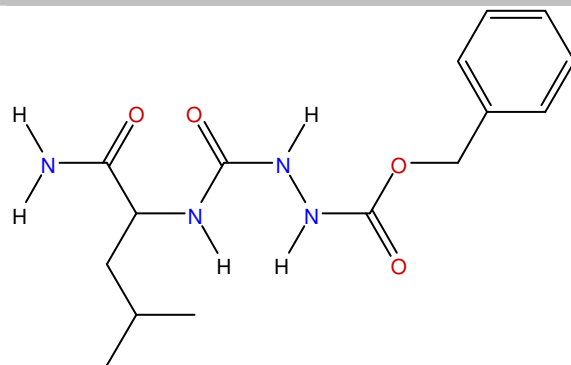
Structure

 pK_i

4.38

Molecule 44

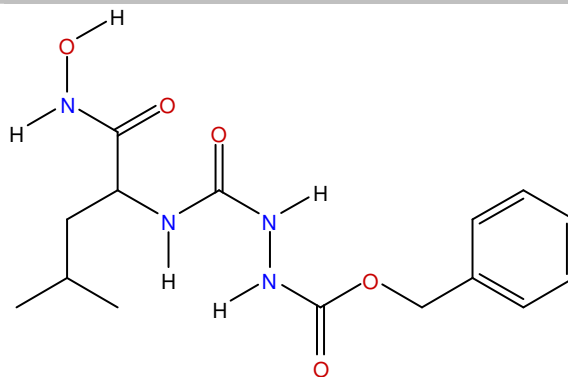
Structure

 pK_i

3.42

Molecule 45

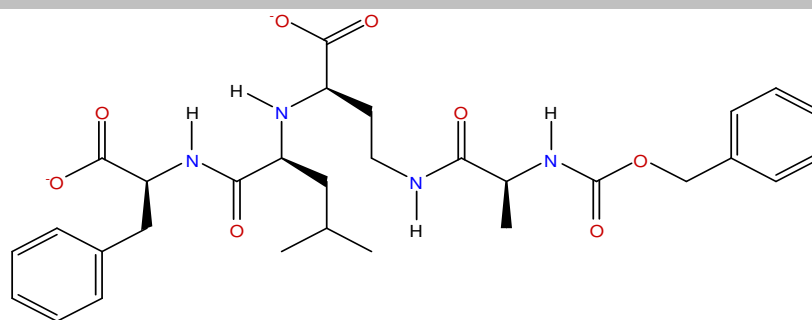
Structure

 pK_i

5.57

Molecule 46

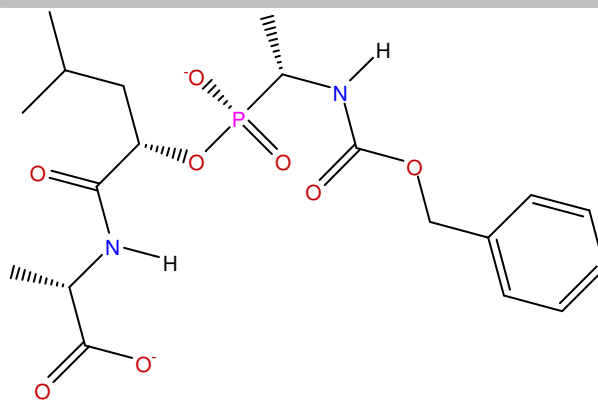
Structure

 pK_i

6.07

Molecule 47

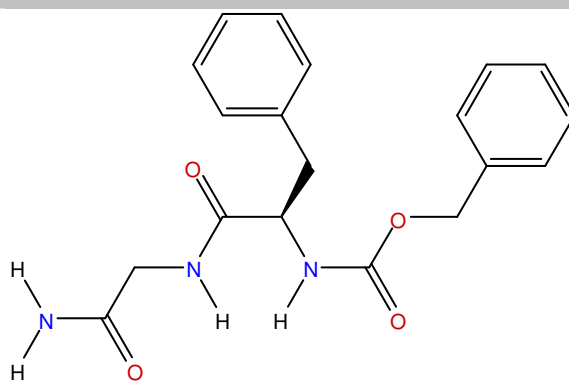
Structure

 pK_i

5.74

Molecule 48

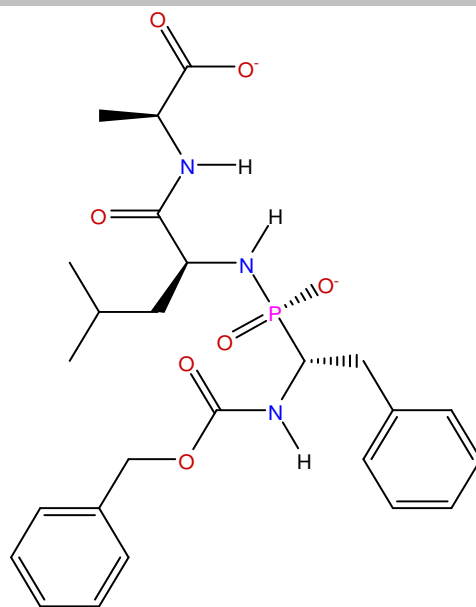
Structure

 pK_i

3.46

Molecule 49

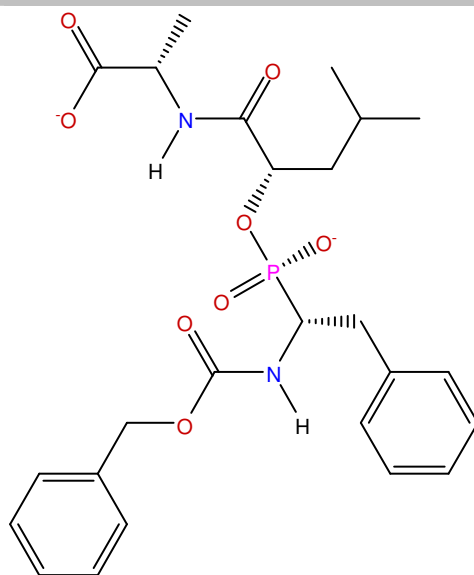
Structure

 pK_i

10.17

Molecule 50

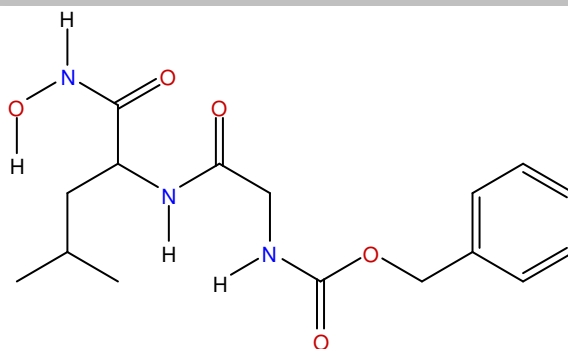
Structure

 pK_i

7.35

Molecule 51

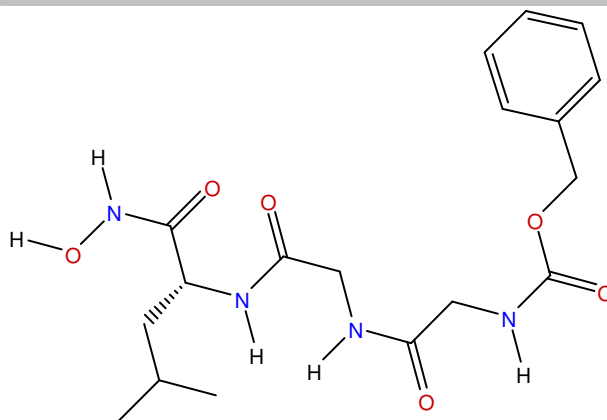
Structure

 pK_i

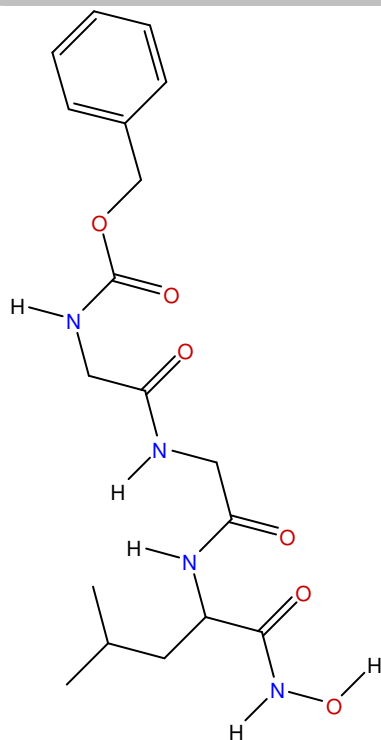
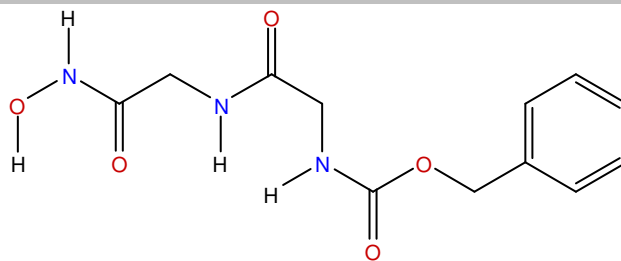
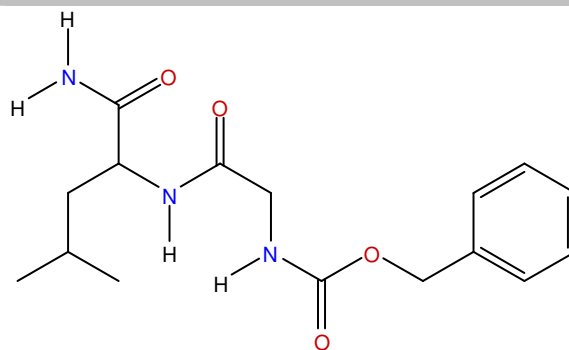
4.32

Molecule 52

Structure

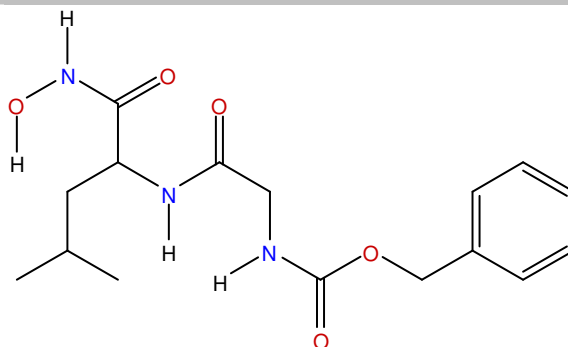
 pK_i

3.6

Molecule 53*Structure* pK_i 4.41**Molecule 54***Structure* pK_i 3.03**Molecule 55***Structure* pK_i 1.68

Molecule 56

Structure

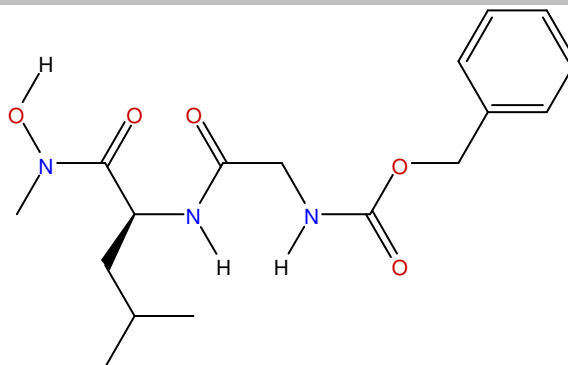


pK_i

4.89

Molecule 57

Structure

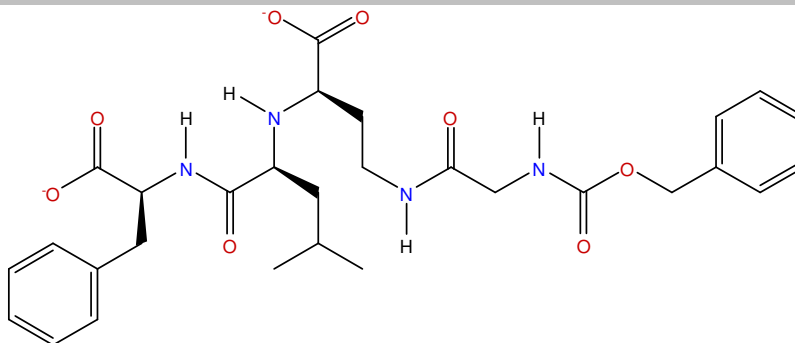


pK_i

2.65

Molecule 58

Structure

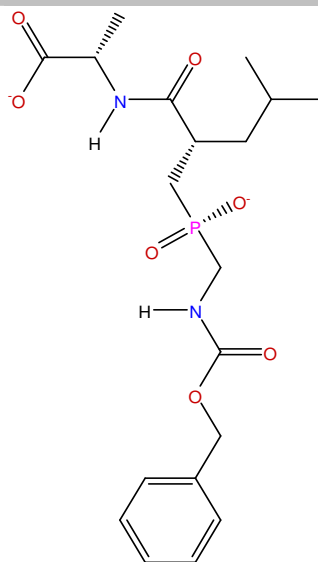


pK_i

6.39

Molecule 59

Structure

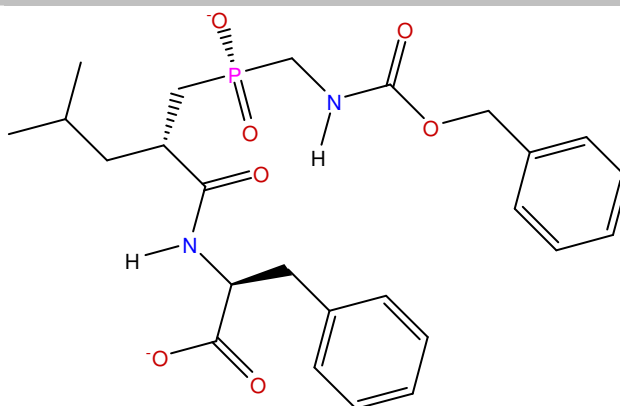


pK_i

7.73

Molecule 60

Structure

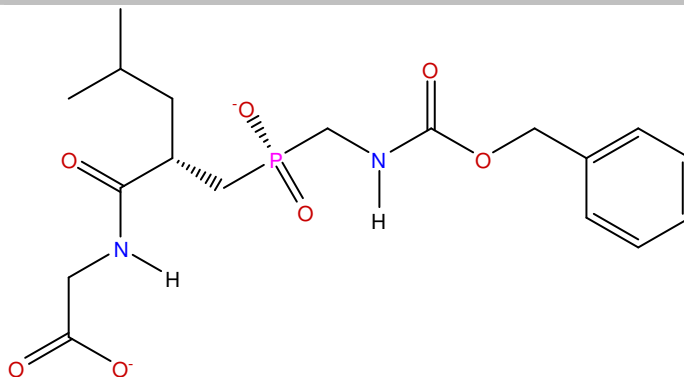


pK_i

7.18

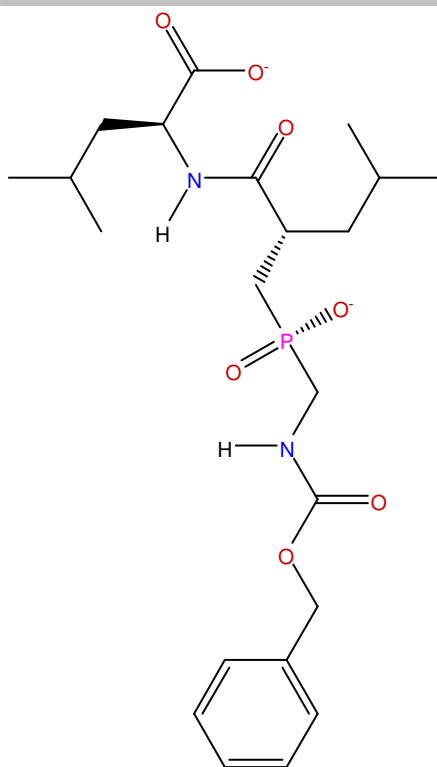
Molecule 61

Structure

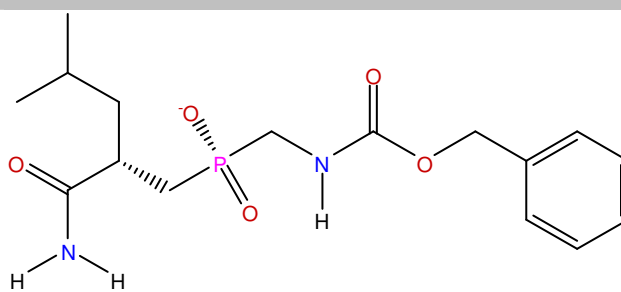


pK_i

6.52

Molecule 62*Structure* pK_i

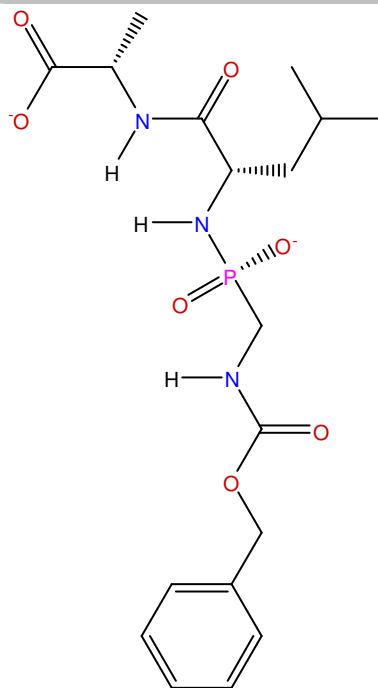
6.74

Molecule 63*Structure* pK_i

5.85

Molecule 64

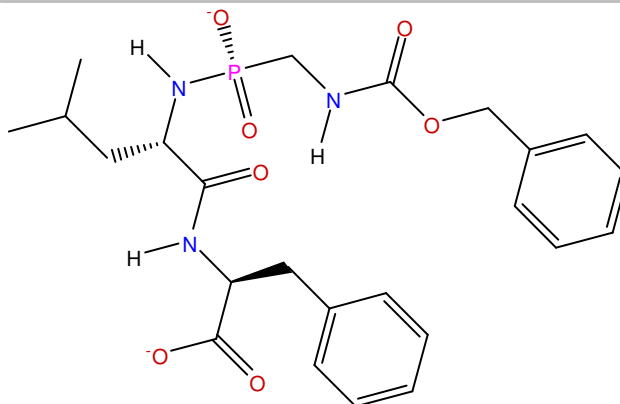
Structure

 pK_i

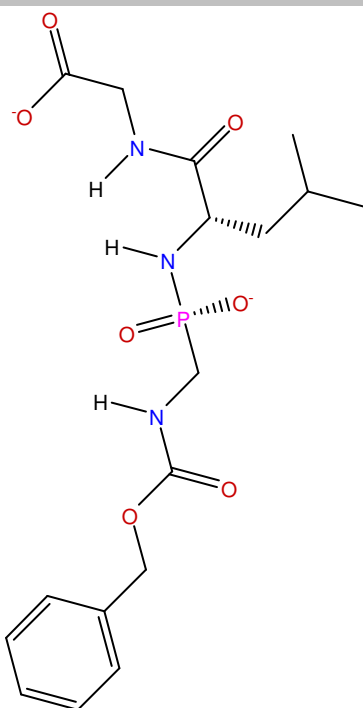
7.78

Molecule 65

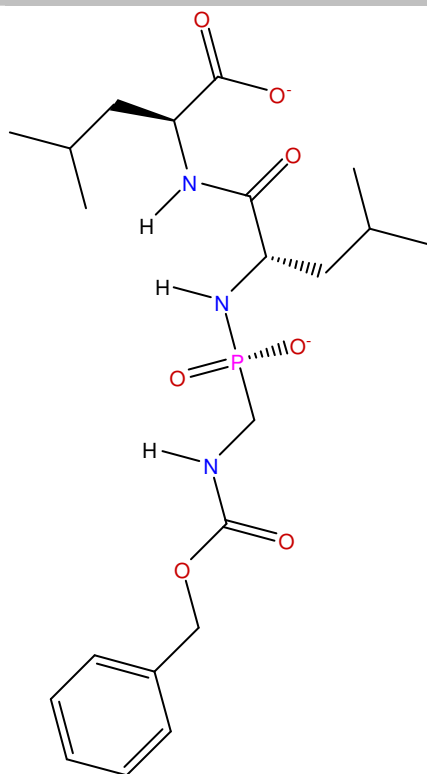
Structure

 pK_i

7.12

Molecule 66*Structure* pK_i

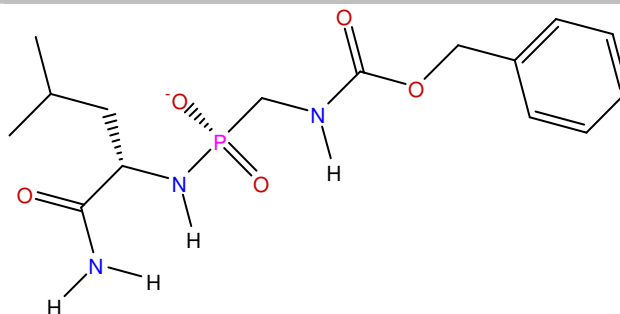
6.57

Molecule 67*Structure* pK_i

8.04

Molecule 68

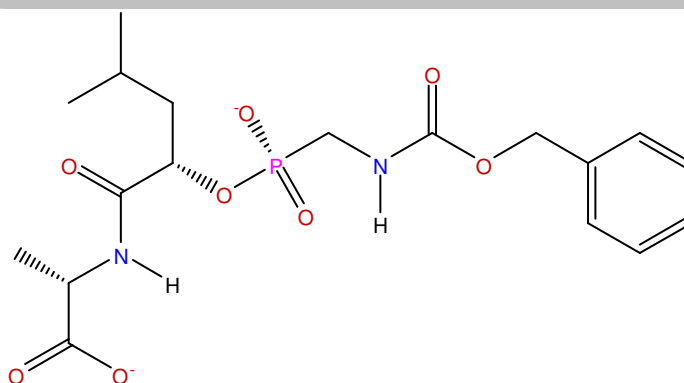
Structure

 pK_i

6.12

Molecule 69

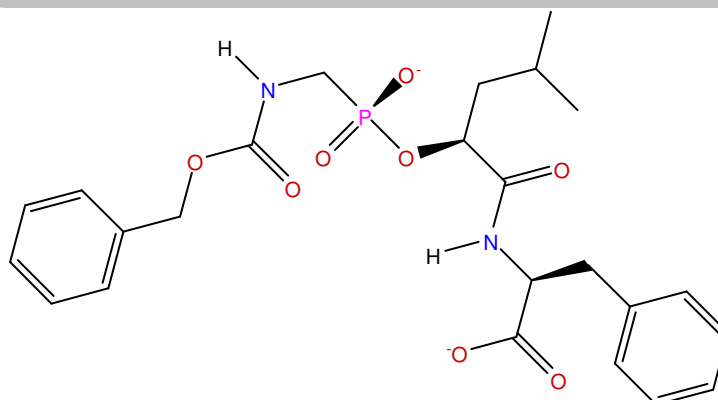
Structure

 pK_i

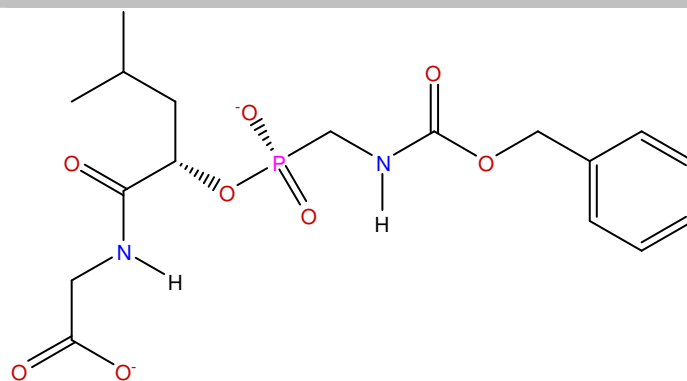
4.89

Molecule 70

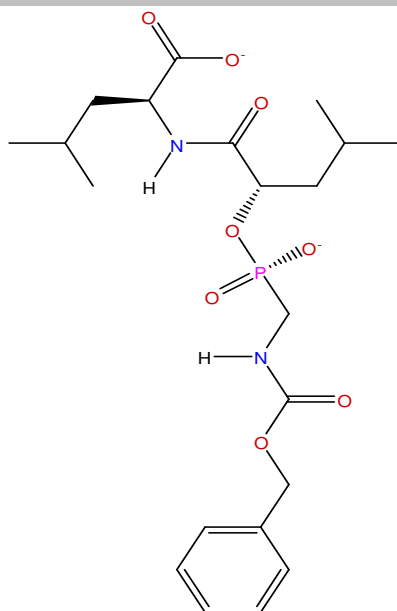
Structure

 pK_i

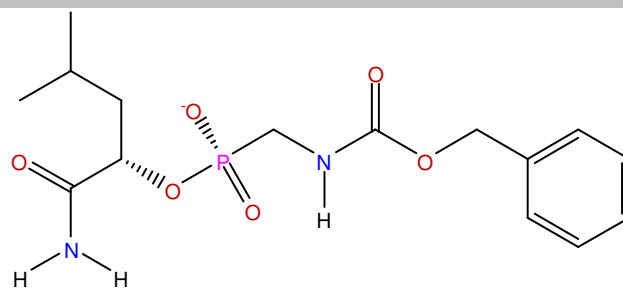
4.27

Molecule 71*Structure* pK_i

3.64

Molecule 72*Structure* pK_i

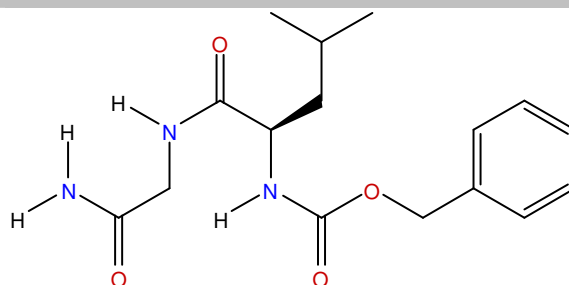
5.05

Molecule 73*Structure* pK_i

3.18

Molecule 74

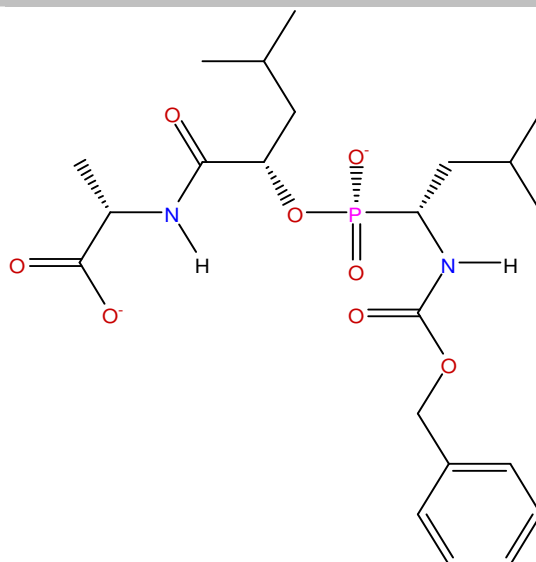
Structure

 pK_i

2.51

Molecule 75

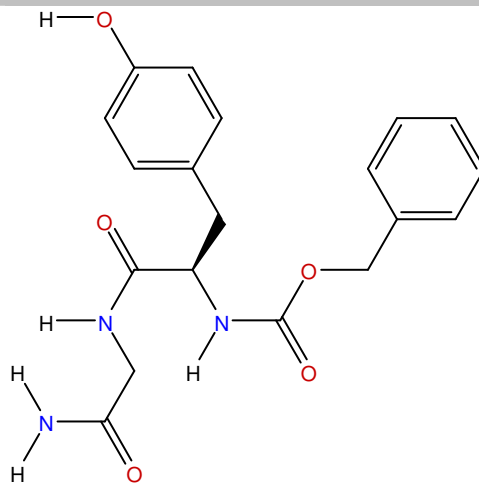
Structure

 pK_i

6.17

Molecule 76

Structure

 pK_i

3.66