

## read\_screen\_result\_long

May 10, 2022

```
[6]: import pickle
from rdkit import Chem

with open('screen_long_75%.pkl', 'rb') as f:
    result_long = pickle.load(f)

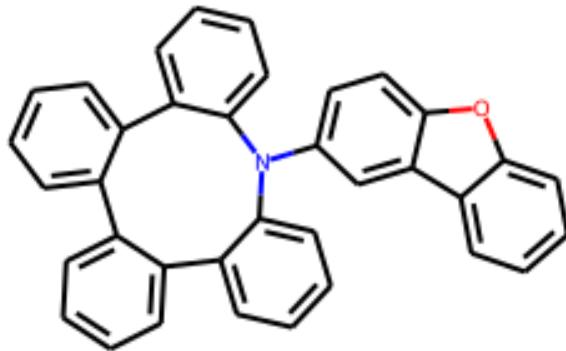
for i, v in enumerate(result_long):
    smi, prob = v
    mol = Chem.MolFromSmiles(smi)
    print('-' * 80)
    print('No.{:}'.format(i+1))
    print('SMILES:', smi)
    print('prob:', prob)
    display(mol)
```

---

No.1

SMILES: c1ccc2c(c1)oc1ccc(-n3c4ccccc4c4ccccc4c4ccccc4c4ccccc43)cc12

prob: 0.93

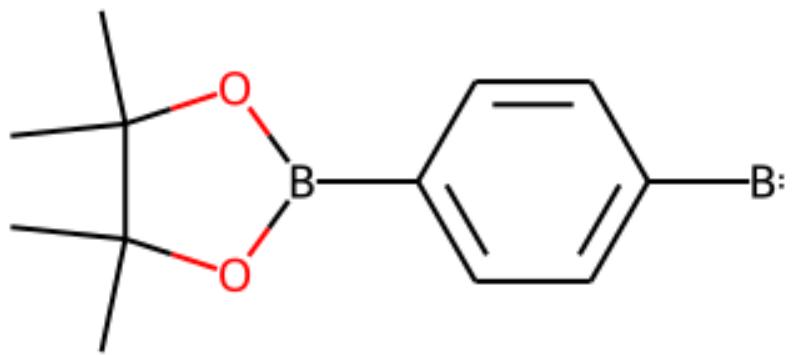


---

No.2

SMILES: [B]c1ccc(B20C(C)(C)C(C)(C)O2)cc1

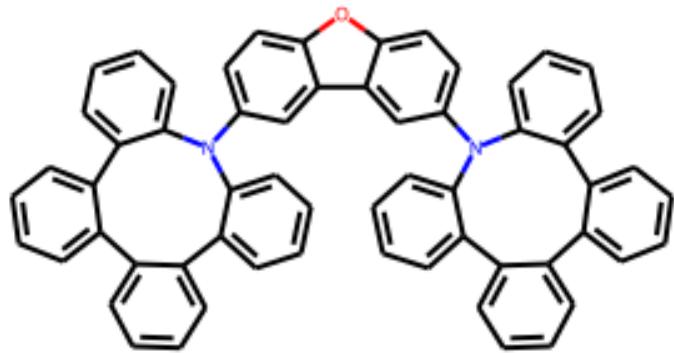
prob: 0.93



No. 3

SMILES: c1cccc2c(c1)c1ccccc1c1ccccc1n(-c1ccc3oc4ccc(-n5c6ccccc6c6ccccc6c6ccccc6c6ccccc65)cc4c3c1)c1ccccc21

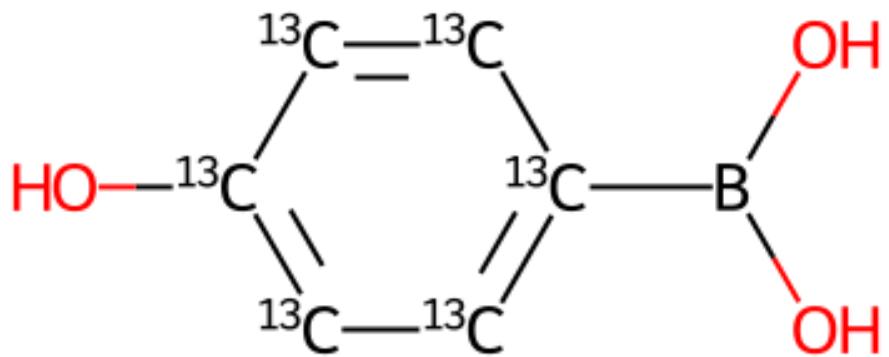
prob: 0.93



No. 4

SMILES: OB(0) [13c] 1 [13cH] [13cH] [13c] (0) [13cH] [13cH] 1

prob: 0.93



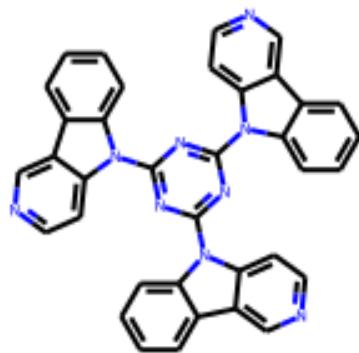
---

No.5

SMILES:

c1ccc2c(c1)c1cnccc1n2-c1nc(-n2c3cccc3c3cnccc32)nc(-n2c3cccc3c3cnccc32)n1

prob: 0.93

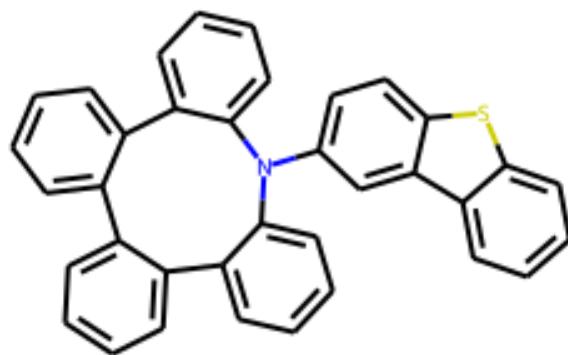


---

No.6

SMILES: c1ccc2c(c1)sc1ccc(-n3c4cccc4c4cccc4c4cccc4c4cccc43)cc12

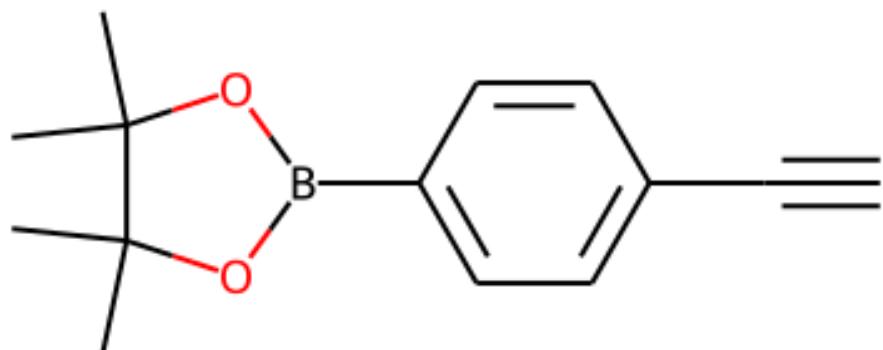
prob: 0.92



No.7

SMILES: C#Cc1cccc(B2OC(C)(C)C(C)(C)O2)cc1

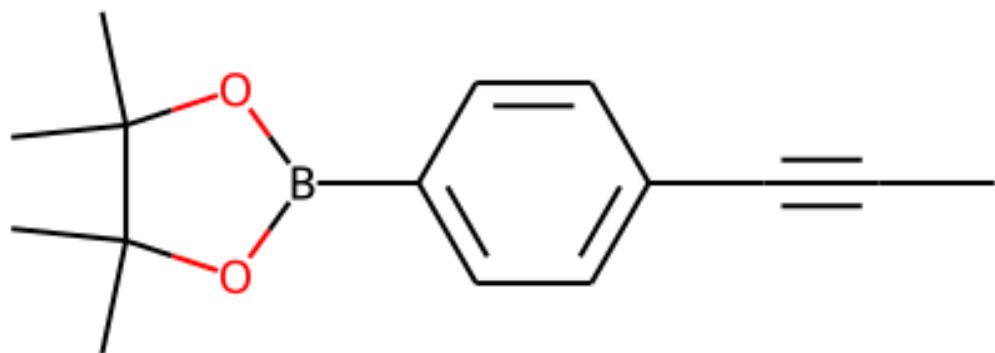
prob: 0.92



No.8

SMILES: CC#Cc1cccc(B2OC(C)(C)C(C)(C)O2)cc1

prob: 0.92

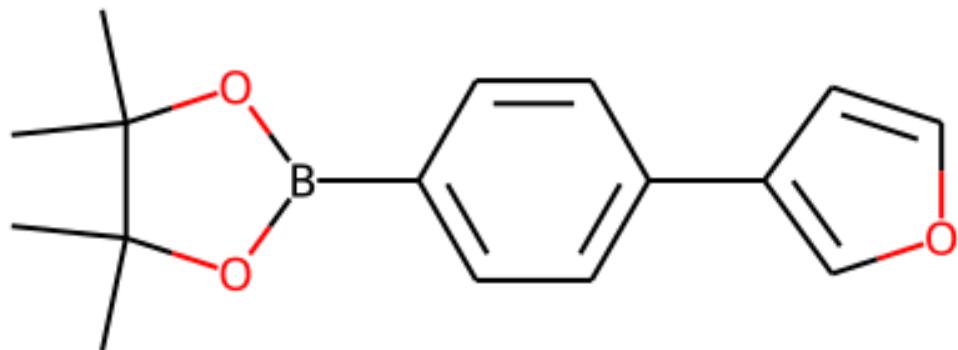


---

No.9

SMILES: CC1(C)OB(c2ccc(-c3ccoc3)cc2)OC1(C)C

prob: 0.92

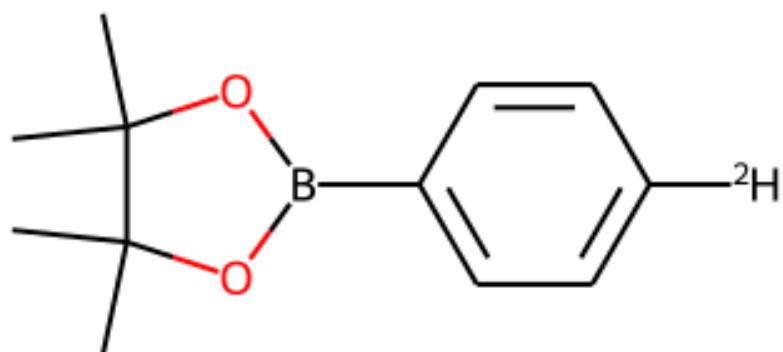


---

No.10

SMILES: [2H]c1ccc(B20C(C)(C)C(C)(C)O2)cc1

prob: 0.92

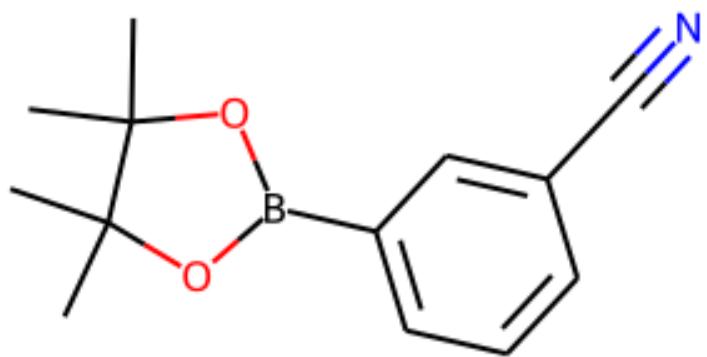


---

No.11

SMILES: CC1(C)OB(c2ccccc2C#N)c2)OC1(C)C

prob: 0.92

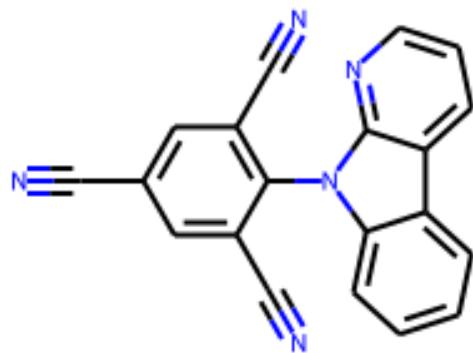


---

No.12

SMILES: N#Cc1cc(C#N)c(-n2c3cccc3c3cccnc32)cc1(C#N)c1

prob: 0.91

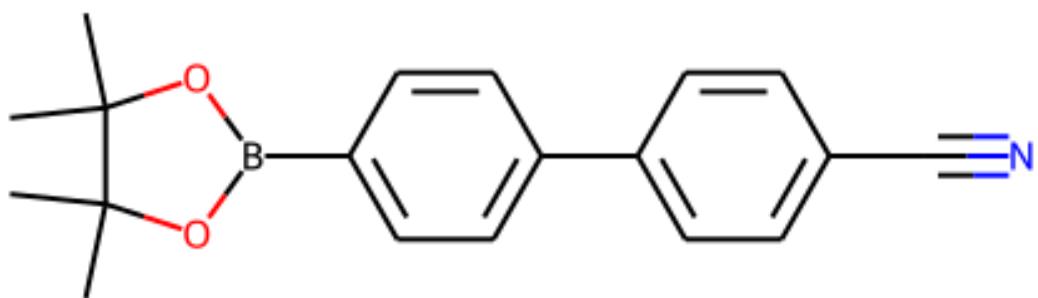


---

No.13

SMILES: CC1(C)OB(c2ccc(-c3ccc(C#N)cc3)cc2)OC1(C)C

prob: 0.91

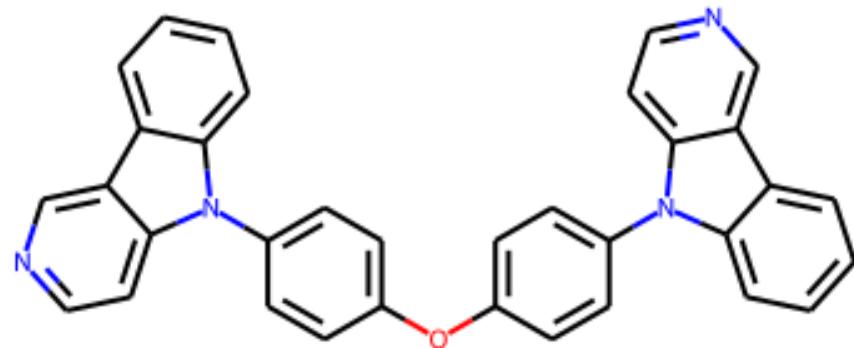


---

No.14

SMILES: c1ccc2c(c1)c1cnccc1n2-c1ccc(0c2ccc(-n3c4cccc4c4cnccc43)cc2)cc1

prob: 0.91

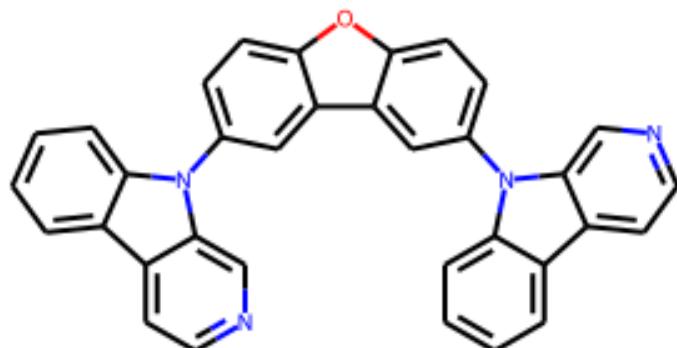


---

No.15

SMILES: c1ccc2c(c1)c1ccncc1n2-c1ccc2oc3ccc(-n4c5cccc5c5ccncc54)cc3c2c1

prob: 0.91

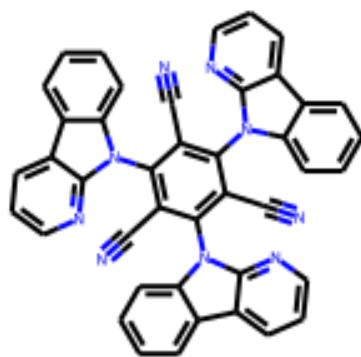


---

No.16

SMILES: N#Cc1c(-n2c3cccc3c3cccnc32)c(C#N)c(-n2c3cccc3c3cccnc32)c(C#N)c1-n1c2ccc2c2cccnc21

prob: 0.91

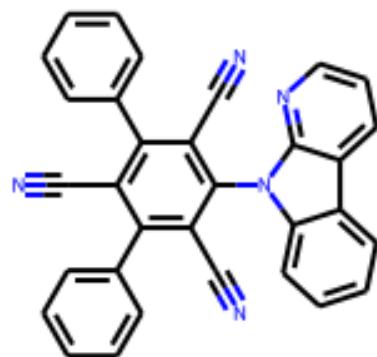


---

No.17

SMILES: N#Cc1c(-c2ccccc2)c(C#N)c(-n2c3cccc3c3cccnc32)c(C#N)c1-c1ccccc1

prob: 0.9

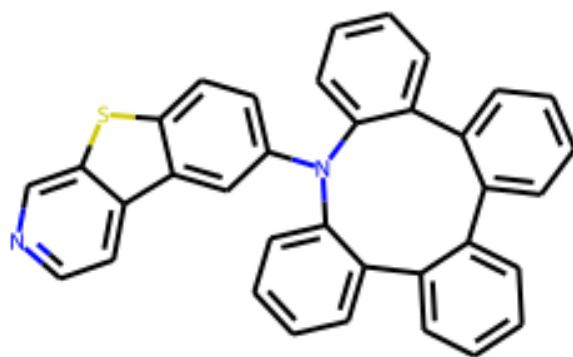


---

No.18

SMILES: c1ccc2c(c1)c1ccccc1c1ccccc1n(-c1ccc3sc4cnccc4c3c1)c1ccccc21

prob: 0.9

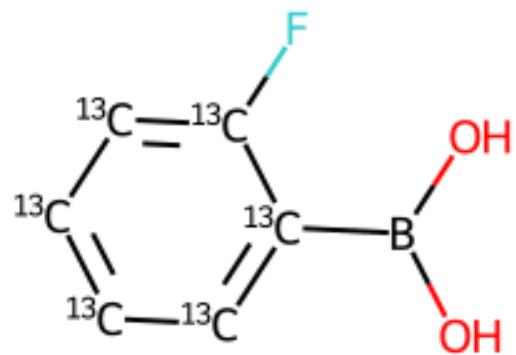


---

No.19

SMILES: OB(O) [13c]1[13cH] [13cH] [13cH] [13cH] [13c]1F

prob: 0.9

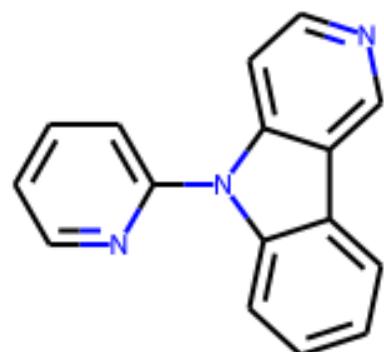


---

No.20

SMILES: c1ccc(-n2c3cccc3c3cnccc32)nc1

prob: 0.89

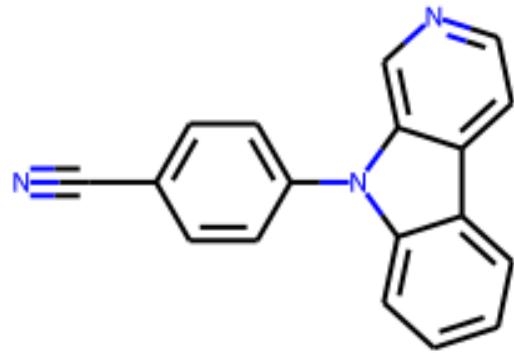


---

No.21

SMILES: N#Cc1ccc(-n2c3cccc3c3ccncc32)cc1

prob: 0.89

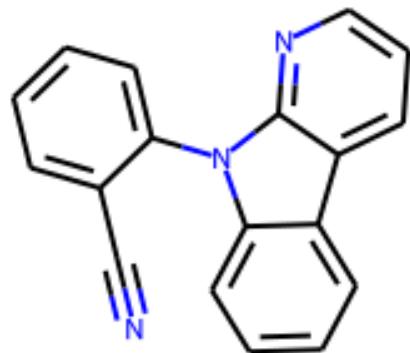


---

No.22

SMILES: N#Cc1ccccc1-n1c2ccccc2c2cccnc21

prob: 0.89

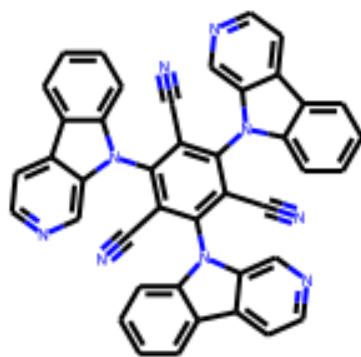


---

No.23

SMILES: N#Cc1c(-n2c3ccccc3c3ccncc32)c(C#N)c(-n2c3ccccc3c3ccncc32)c(C#N)c1-n1c2ccc2c2ccncc21

prob: 0.89

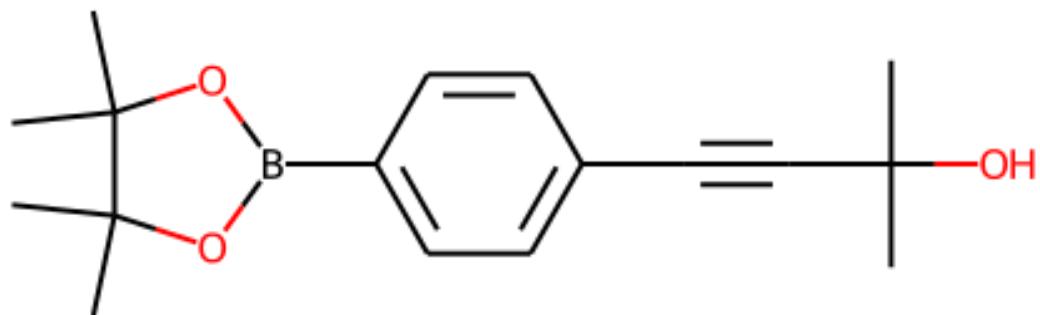


---

No.24

SMILES: CC(C)(O)C#Cc1ccc(B2OC(C)(C)C(C)(C)O2)cc1

prob: 0.89

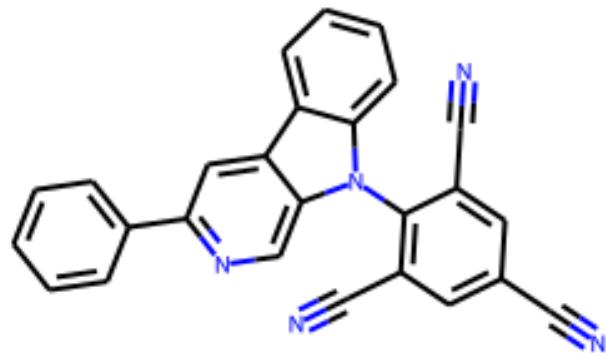


---

No.25

SMILES: N#Cc1cc(C#N)c(-n2c3cccc3c3cc(-c4ccccc4)ncc32)c(C#N)c1

prob: 0.88

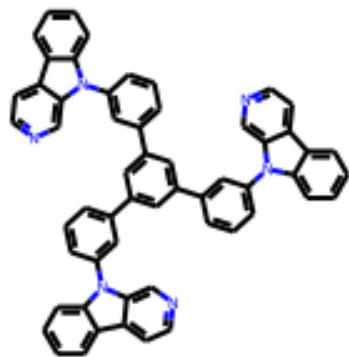


---

No.26

SMILES: c1cc(-c2cc(-c3cccc(-n4c5cccc5c5ccncc54)c3)cc(-c3cccc(-n4c5cccc5c5ccncc54)c3)c2)cc(-n2c3cccc3c3ccncc32)c1

prob: 0.88

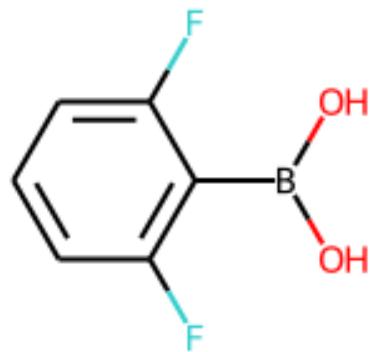


---

No.27

SMILES: OB(0)c1c(F)cccc1F

prob: 0.87

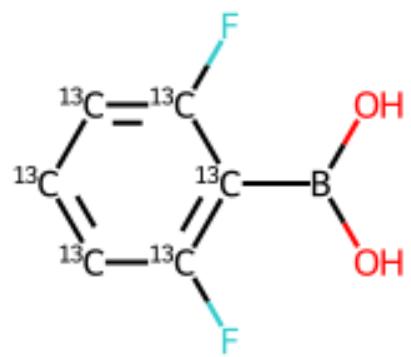


---

No.28

SMILES: OB(0)[13c]1[13c](F)[13cH][13cH][13cH][13c]1F

prob: 0.87

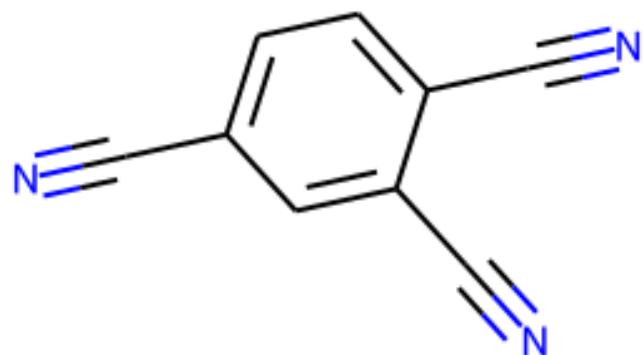


---

No. 29

SMILES: N#Cc1cccc(C#N)c(C#N)c1

prob: 0.87

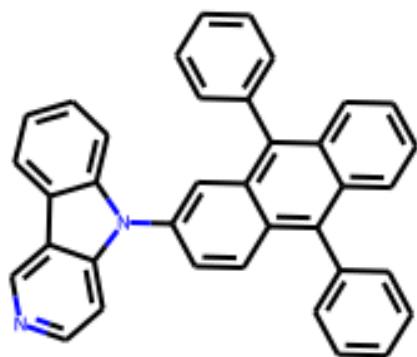


---

No. 30

SMILES: c1ccc(-c2c3cccc3c(-c3cccc3)c3cc(-n4c5cccc5c5cnccc54)ccc23)cc1

prob: 0.87

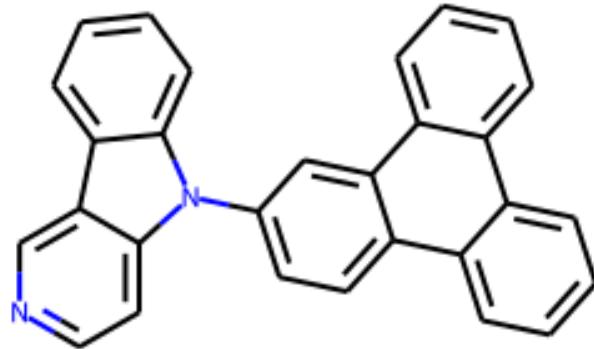


---

No.31

SMILES: c1ccc2c(c1)c1ccccc1c1cc(-n3c4cccc4c4cnccc43)ccc21

prob: 0.87

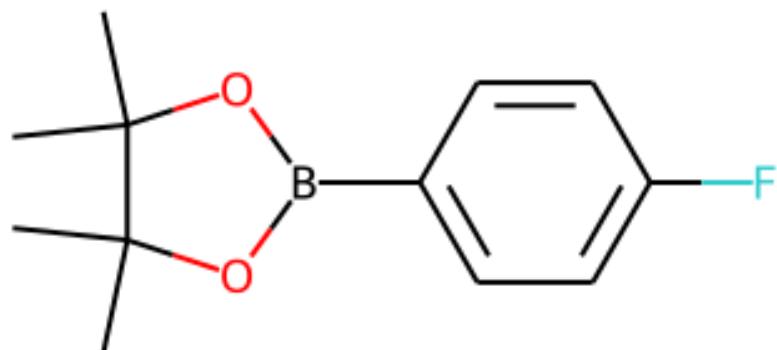


---

No.32

SMILES: CC1(C)OB(c2ccc(F)cc2)OC1(C)C

prob: 0.87

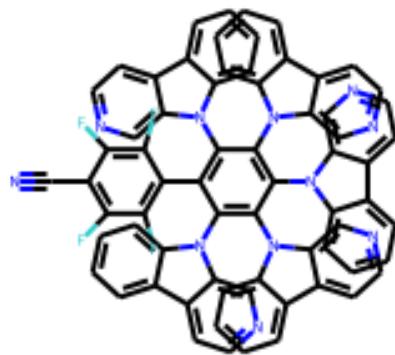


---

No.33

SMILES: N#Cc1c(F)c(F)c(-c2c(-n3c4cccc4c4ccncc43)c(-n3c4cccc4c4ccncc43)c(-n3c4cccc4c4ccncc43)c(-n3c4cccc4c4ccncc43)c2-n2c3cccc3c3ccncc32)c(F)c1F

prob: 0.87

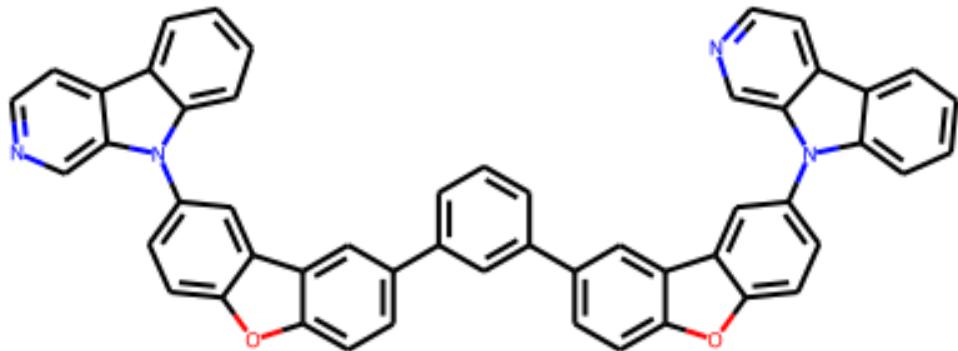


---

No.34

SMILES: c1cc(-c2ccc3oc4ccc(-n5c6cccc6c6ccncc65)cc4c3c2)cc(-c2ccc3oc4ccc(-n5c6ccc6c6ccncc65)cc4c3c2)c1

prob: 0.87

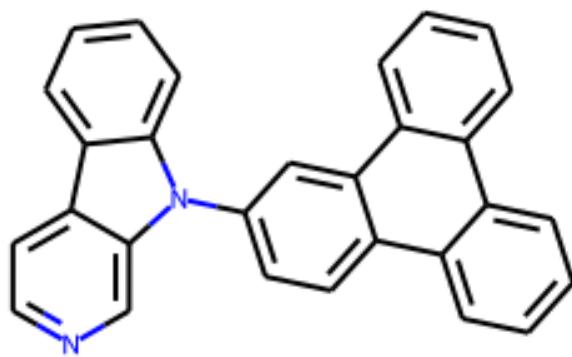


---

No.35

SMILES: c1ccc2c(c1)c1cccc1c1cc(-n3c4cccc4c4ccncc43)ccc21

prob: 0.86

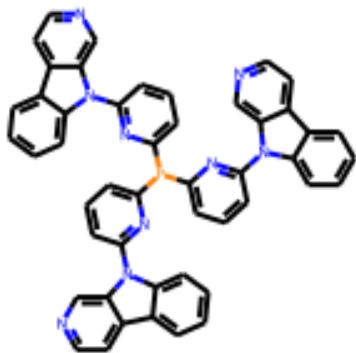


---

No.36

SMILES: c1cc(-n2c3cccc3c3ccncc32)nc(P(c2cccc(-n3c4cccc4c4ccncc43)n2)c2cccc(-n3c4cccc4c4ccncc43)n2)c1

prob: 0.86

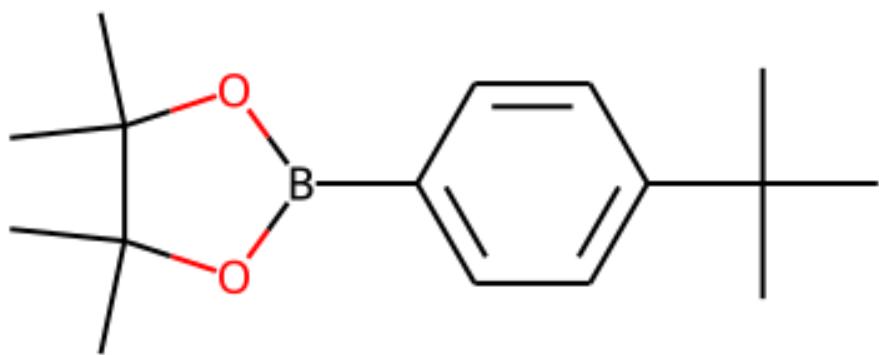


---

No.37

SMILES: CC(C)(C)c1ccc(B20C(C)(C)C(C)(C)O2)cc1

prob: 0.86

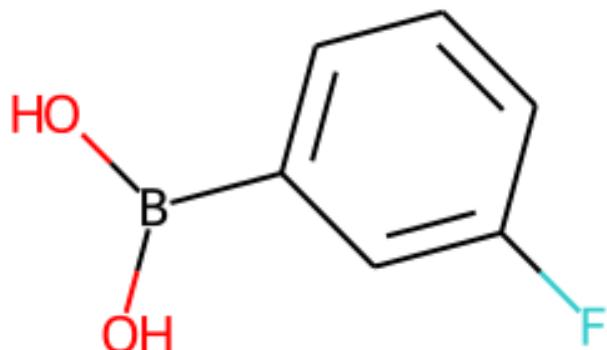


---

No.38

SMILES: OB(O)c1ccccc(F)c1

prob: 0.86

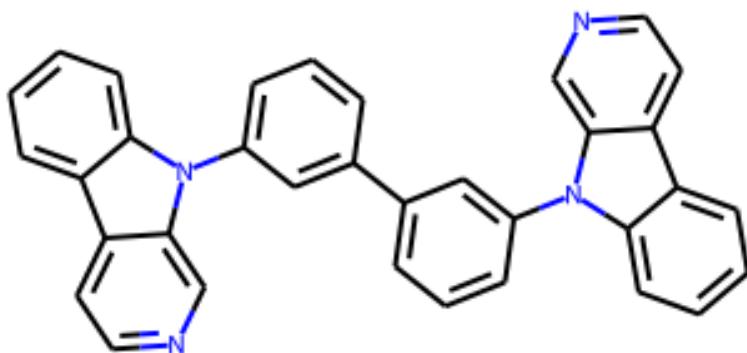


---

No.39

SMILES: c1cc(-c2cccc(-n3c4ccccc4c4ccncc43)c2)cc(-n2c3ccccc3c3ccncc32)c1

prob: 0.86

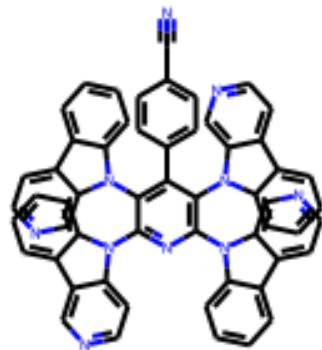


---

No.40

SMILES: N#Cc1ccc(-c2c(-n3c4cccc4c4ccncc43)c(-n3c4cccc4c4cnccc43)nc(-n3c4cccc4c4ccncc43)c2-n2c3cccc3c3ccncc32)cc1

prob: 0.86

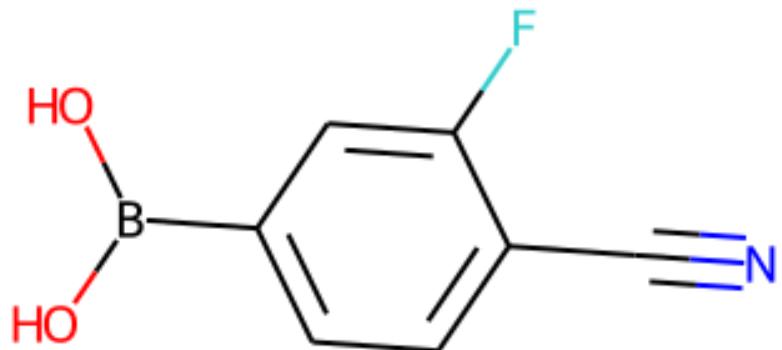


---

No.41

SMILES: N#Cc1ccc(B(O)O)cc1F

prob: 0.86

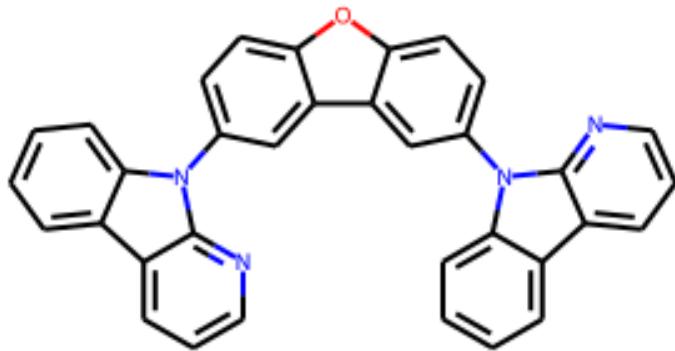


---

No.42

SMILES: c1ccc2c(c1)c1ccnnc1n2-c1ccc2oc3ccc(-n4c5cccc5c5ccnnc54)cc3c2c1

prob: 0.86

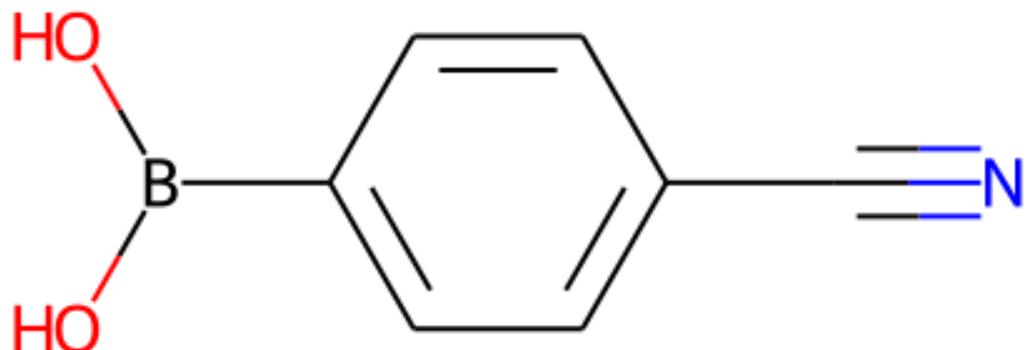


---

No.43

SMILES: N#Cc1cccc(B(O)O)cc1

prob: 0.86

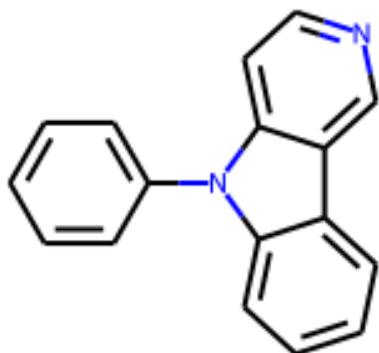


---

No.44

SMILES: c1ccc(-n2c3cccc3c3cnccc32)cc1

prob: 0.86



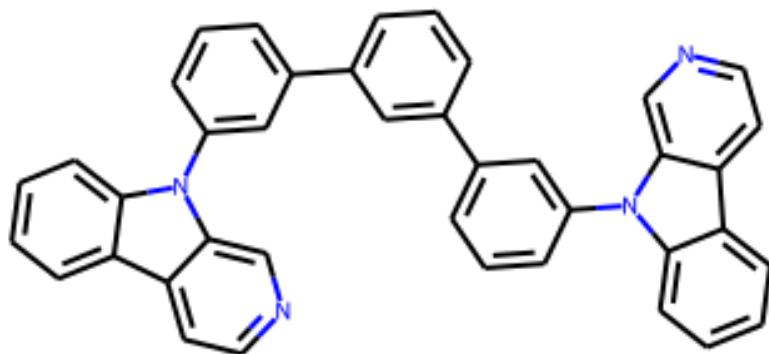
---

No.45

SMILES:

c1cc(-c2cccc(-n3c4cccc4c4ccncc43)c2)cc(-c2cccc(-n3c4cccc4c4ccncc43)c2)c1

prob: 0.86

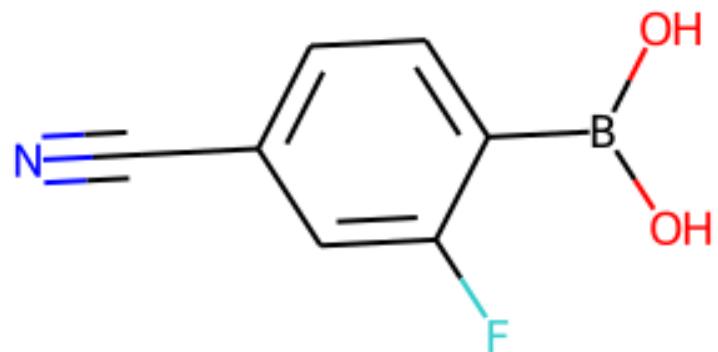


---

No.46

SMILES: N#Cc1ccc(B(O)O)c(F)c1

prob: 0.86

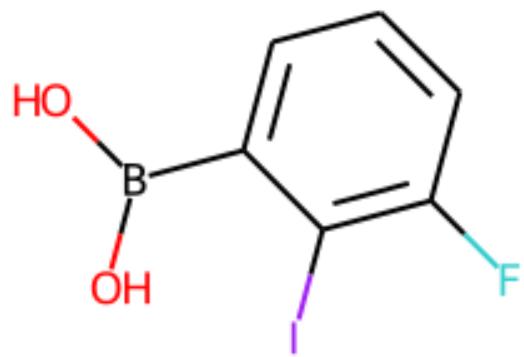


---

No.47

SMILES: OB(O)c1cccc(F)c1I

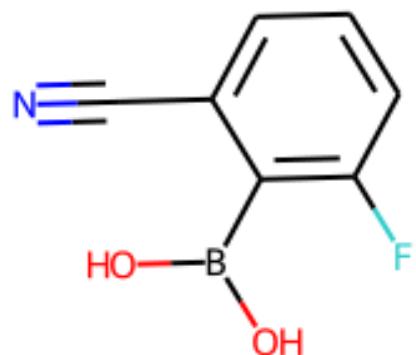
prob: 0.86



No.48

SMILES: N#Cc1ccc(F)c1B(O)O

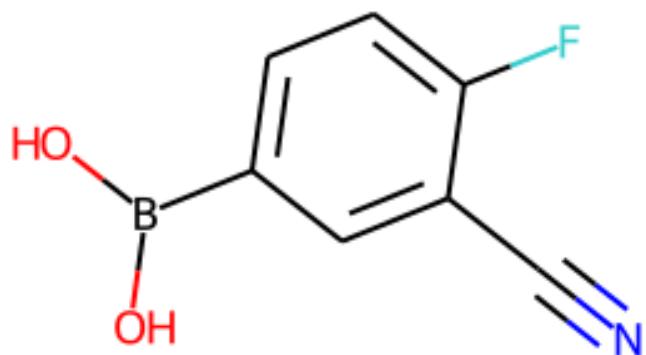
prob: 0.86



No.49

SMILES: N#Cc1cc(B(O)O)ccc1F

prob: 0.86

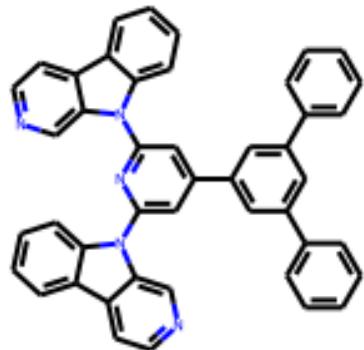


---

No.50

SMILES: c1ccc(-c2cc(-c3cccc3)cc(-c3cc(-n4c5cccc5c5ccncc54)nc(-n4c5cccc5c5ccnc54)c3)c2)cc1

prob: 0.86

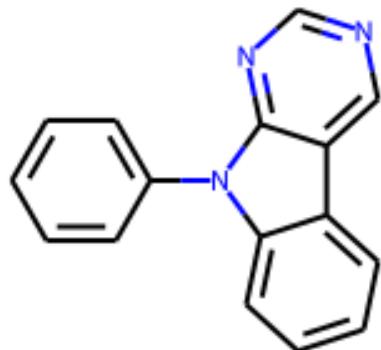


---

No.51

SMILES: c1ccc(-n2c3cccc3c3cncnc32)cc1

prob: 0.85

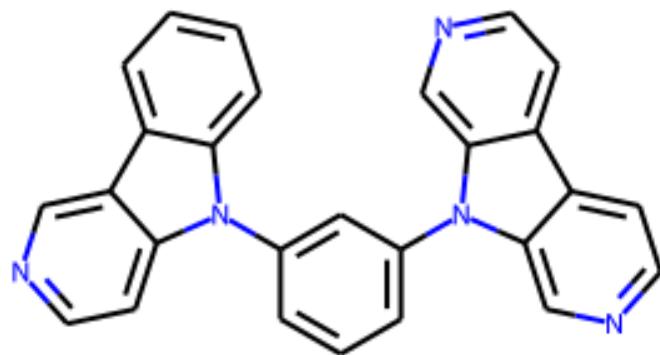


---

No.52

SMILES: c1cc(-n2c3cccc3c3cncnc32)cc(-n2c3cncnc3c3ccncc32)c1

prob: 0.85

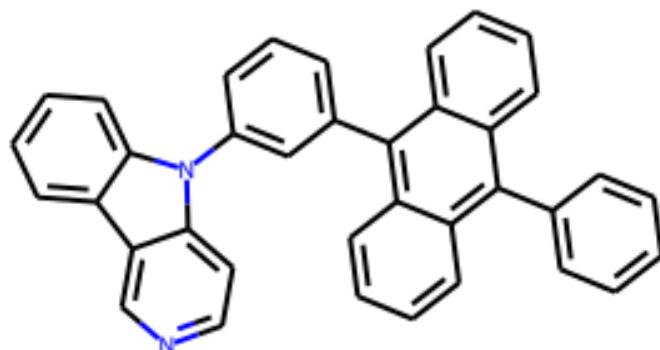


---

No.53

SMILES: c1ccc(-c2c3cccc3c(-c3cccc(-n4c5cccc5c5cnccc54)c3)c3cccc23)cc1

prob: 0.85

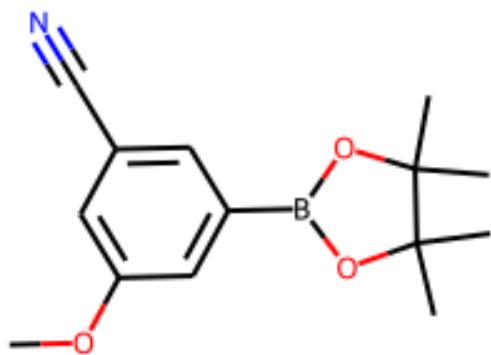


---

No.54

SMILES: C0c1cc(C#N)cc(B2OC(C)(C)C(C)(C)O2)c1

prob: 0.85

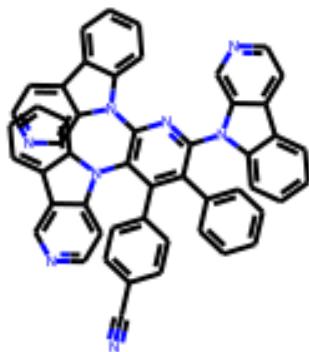


---

No.55

SMILES: N#Cc1ccc(-c2c(-c3cccc3)c(-n3c4ccccc4c4ccncc43)nc(-n3c4ccccc4c4ccncc43)c  
2-n2c3cccc3c3cnccc32)cc1

prob: 0.85

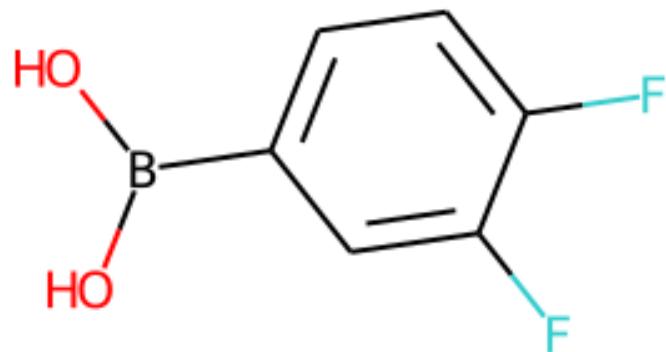


---

No.56

SMILES: OB(=O)c1ccc(F)c(F)c1

prob: 0.85

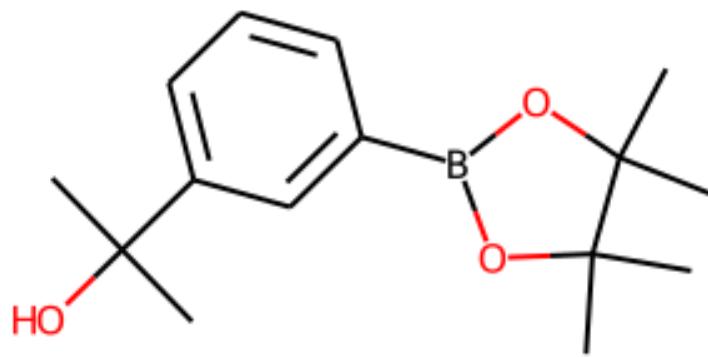


---

No.57

SMILES: CC(C)(O)c1ccccc(B2OC(C)(C)C(C)(C)O2)c1

prob: 0.85

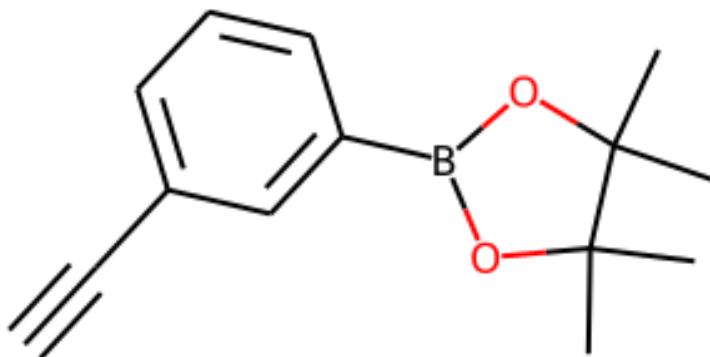


---

No.58

SMILES: C#Cc1ccccc(B2OC(C)(C)C(C)(C)O2)c1

prob: 0.85

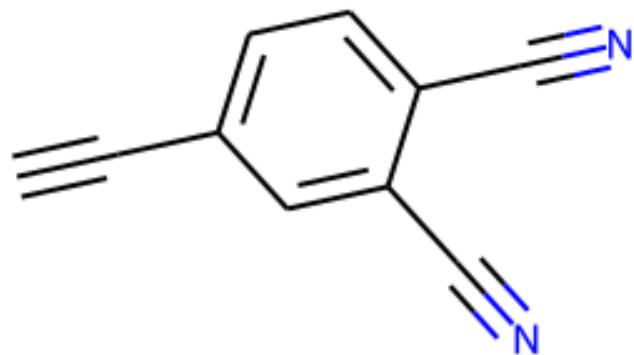


---

No.59

SMILES: C#Cc1ccc(C#N)c(C#N)c1

prob: 0.85

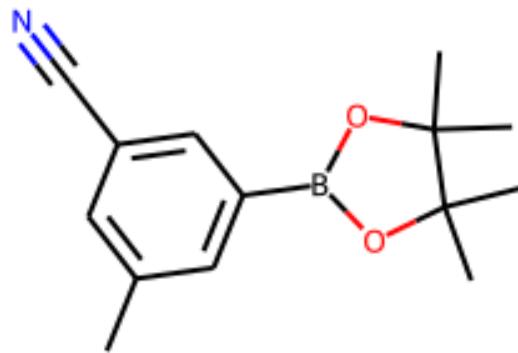


---

No. 60

SMILES: Cc1cc(C#N)cc(B2OC(C)(C)C(C)(C)O2)c1

prob: 0.85

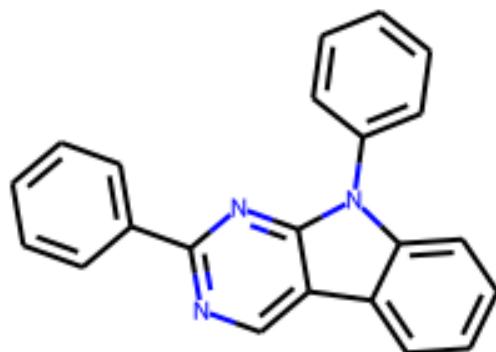


---

No. 61

SMILES: c1ccc(-c2ncc3c4cccc4n(-c4ccccc4)c3n2)cc1

prob: 0.85

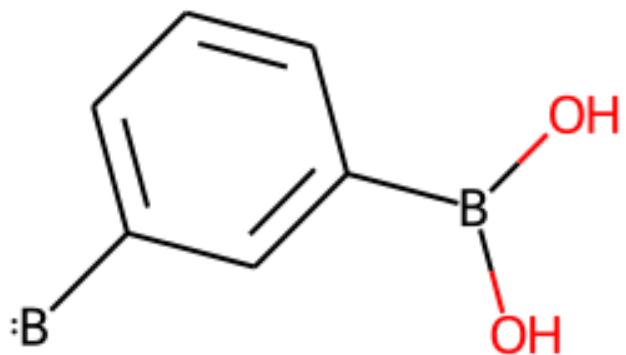


---

No. 62

SMILES: [B]c1ccccc(B(0)0)c1

prob: 0.85

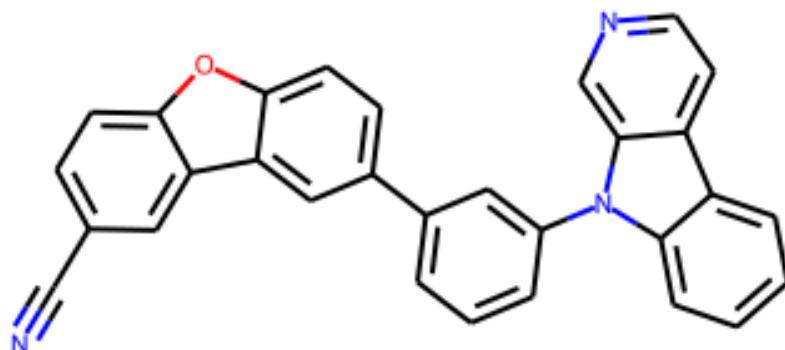


---

No. 63

SMILES: N#Cc1cccc2oc3cccc(-c4cccc(-n5c6cccc6c6ccncc65)c4)cc3c2c1

prob: 0.85

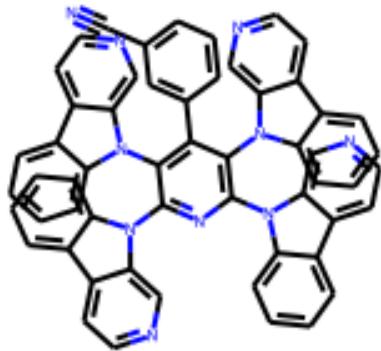


---

No. 64

SMILES: N#Cc1cccc(-c2c(-n3c4cccc4c4ccncc43)c(-n3c4cccc4c4ccncc43)nc(-n3c4cccc4c4ccncc43)c2-n2c3cccc3c3ccncc32)c1

prob: 0.85

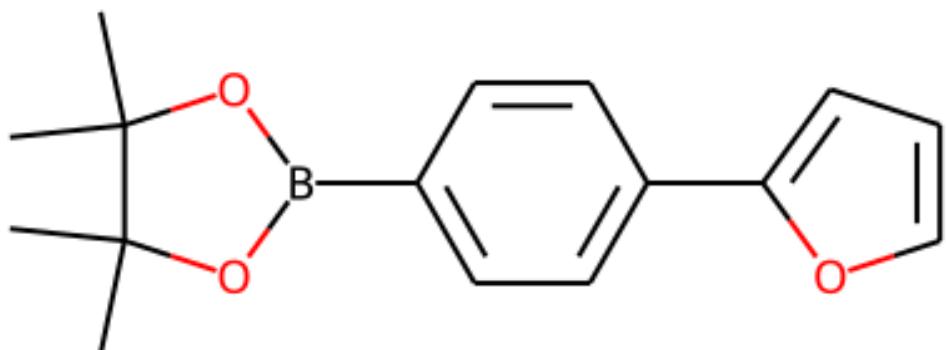


---

No. 65

SMILES: CC1(C)OB(c2ccc(-c3ccco3)cc2)OC1(C)C

prob: 0.85

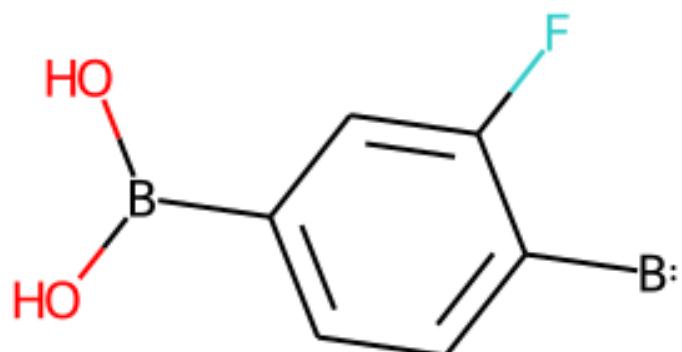


---

No. 66

SMILES: [B]c1ccc(B(O)O)cc1F

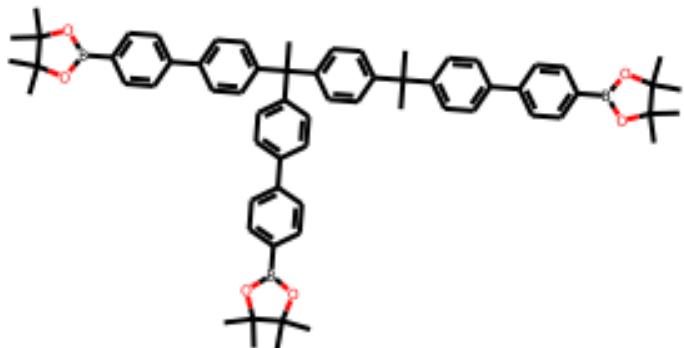
prob: 0.85



---

No. 67

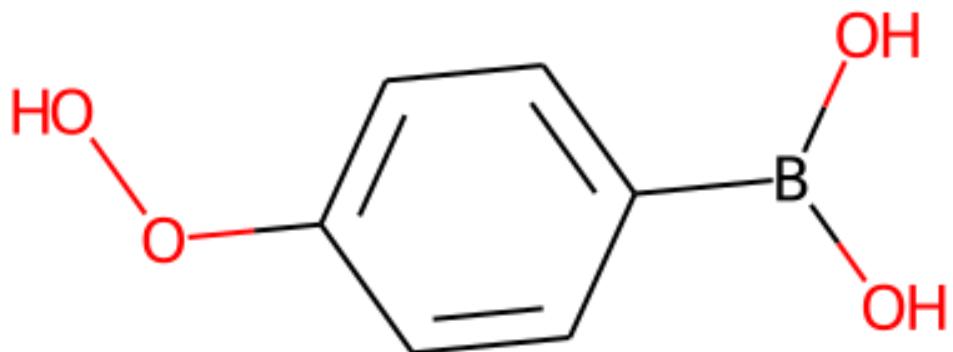
SMILES: CC(C)(c1ccc(-c2ccc(B3OC(C)(C)C(C)O3)cc2)cc1)c1ccc(C(C)(c2ccc(-c3ccc(B4OC(C)(C)C(C)O4)cc3)cc2)c2ccc(-c3ccc(B4OC(C)(C)C(C)O4)cc3)cc2)cc1  
prob: 0.85



---

No. 68

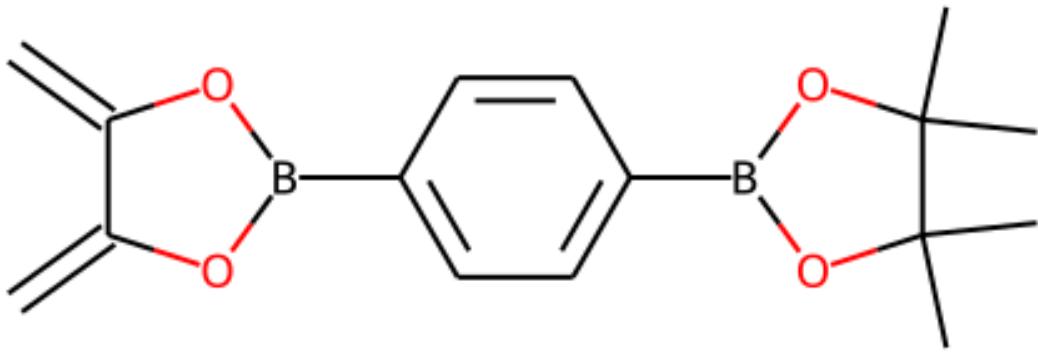
SMILES: O0c1ccc(B(0)0)cc1  
prob: 0.85



---

No. 69

SMILES: C=C1OB(c2ccc(B3OC(C)(C)C(C)O3)cc2)OC1=C  
prob: 0.85

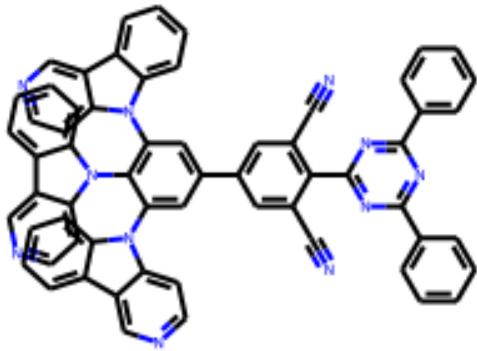


---

No. 70

SMILES: N#Cc1cc(-c2cc(-n3c4cccc4c4cnccc43)c(-n3c4cccc4c4cnccc43)c(-n3c4cccc4c4cnccc43)c2)cc(C#N)c1-c1nc(-c2cccc2)nc(-c2cccc2)n1

prob: 0.84

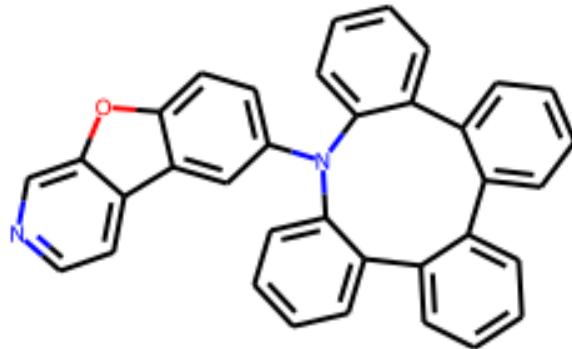


---

No. 71

SMILES: c1ccc2c(c1)c1cccc1c1cccc1n(-c1ccc3oc4cnccc4c3c1)c1cccc21

prob: 0.84

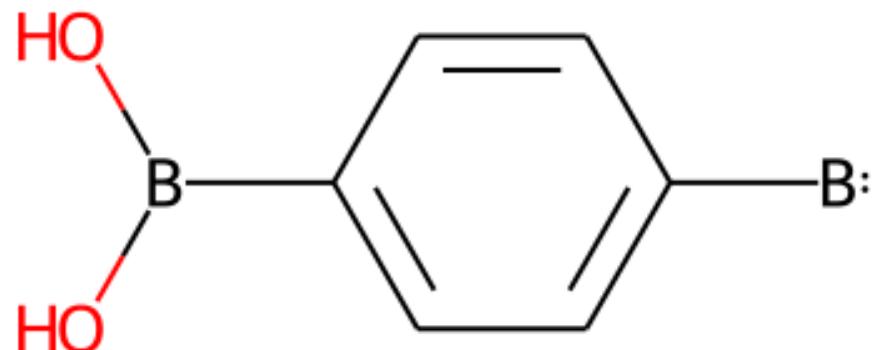


---

No. 72

SMILES: [B]c1ccc(B(O)O)cc1

prob: 0.84

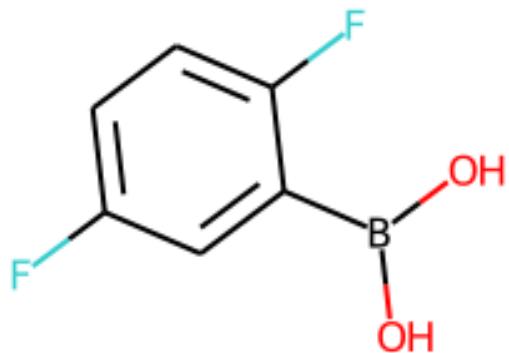


---

No. 73

SMILES: OB(O)c1cc(F)ccc1F

prob: 0.84

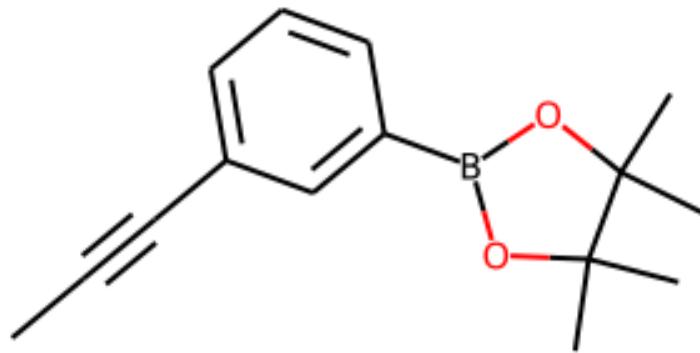


---

No.74

SMILES: CC#Cc1ccccc(B2OC(C)(C)C(C)(C)O2)c1

prob: 0.84

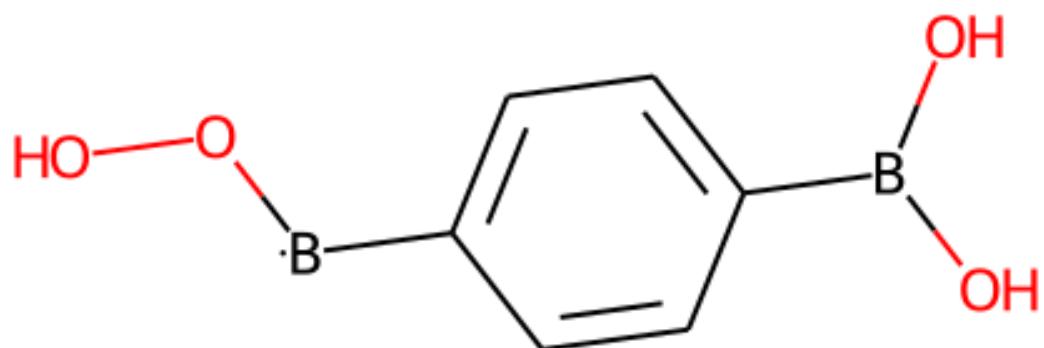


---

No.75

SMILES: O[B]c1cccc(B(O)O)cc1

prob: 0.84

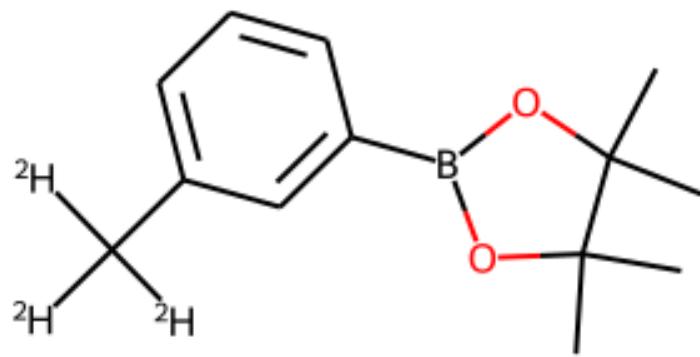


---

No.76

SMILES: [2H]C([2H])([2H])c1ccccc(B2OC(C)(C)C(C)(C)O2)c1

prob: 0.84

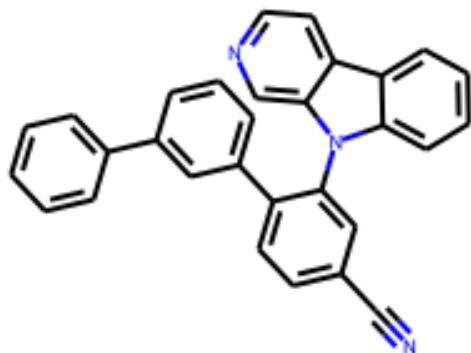


---

No.77

SMILES: N#Cc1cccc(-c2ccccc(-c3ccccc3)c2)c(-n2c3ccccc3c3ccncc32)c1

prob: 0.84

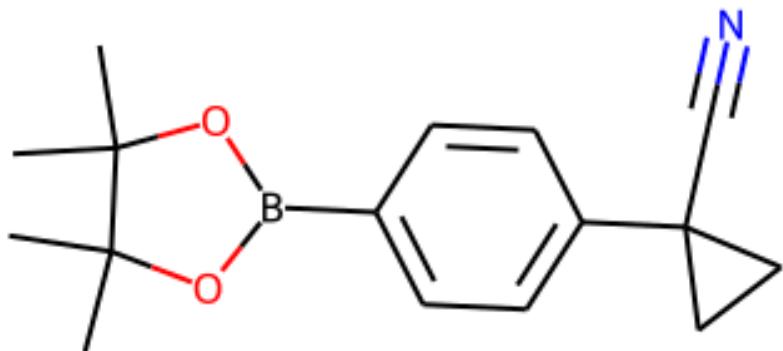


---

No.78

SMILES: CC1(C)OB(c2ccc(C3(C#N)CC3)cc2)OC1(C)C

prob: 0.84

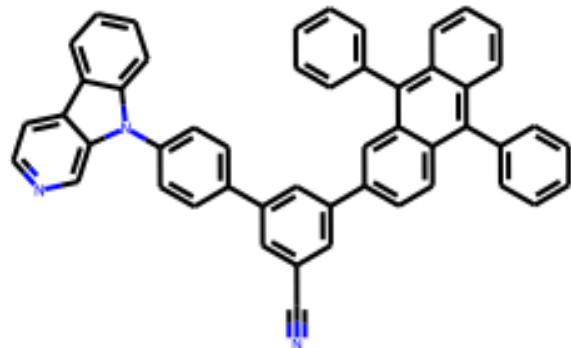


---

No.79

SMILES: N#Cc1cc(-c2ccc(-n3c4cccc4c4ccncc43)cc2)cc(-c2ccc3c(-c4cccc4)c4cccc4c(-c4cccc4)c3c2)c1

prob: 0.84

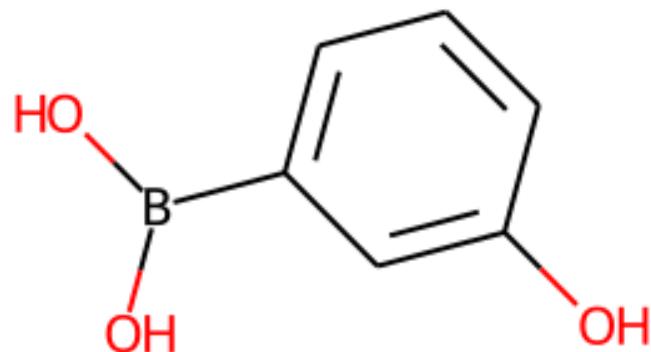


---

No.80

SMILES: OB(O)c1ccccc(O)c1

prob: 0.84

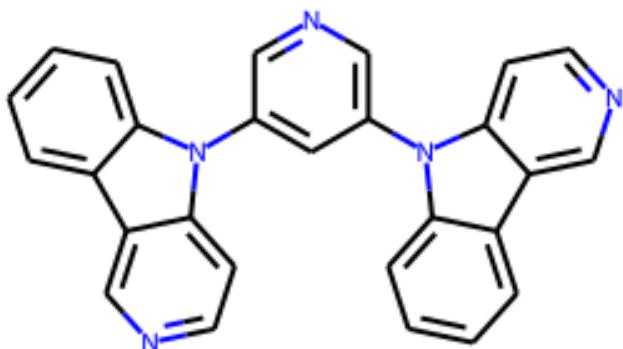


---

No.81

SMILES: c1ccc2c(c1)c1cnccc1n2-c1cncc(-n2c3cccc3c3cnccc32)c1

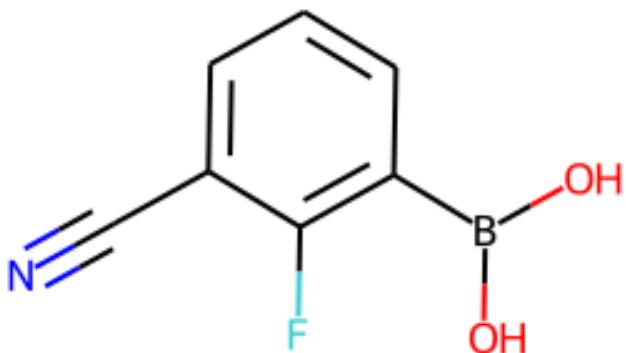
prob: 0.84



No. 82

SMILES: N#Cc1cccc(B(O)O)c1F

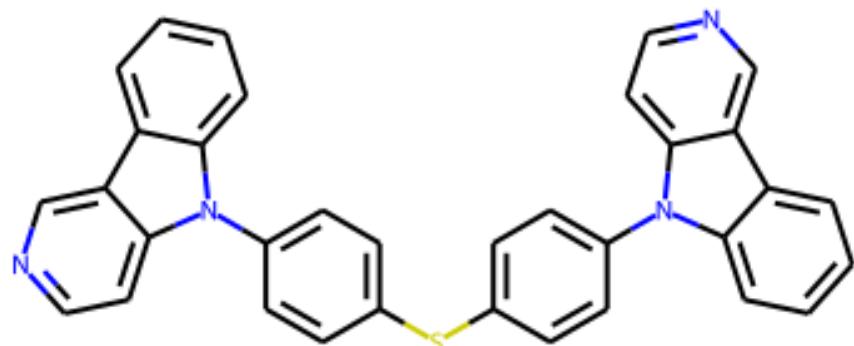
prob: 0.84



No. 83

SMILES: c1ccc2c(c1)c1cnccc1n2-c1ccc(Sc2ccc(-n3c4cccc4c4cnccc43)cc2)cc1

prob: 0.84

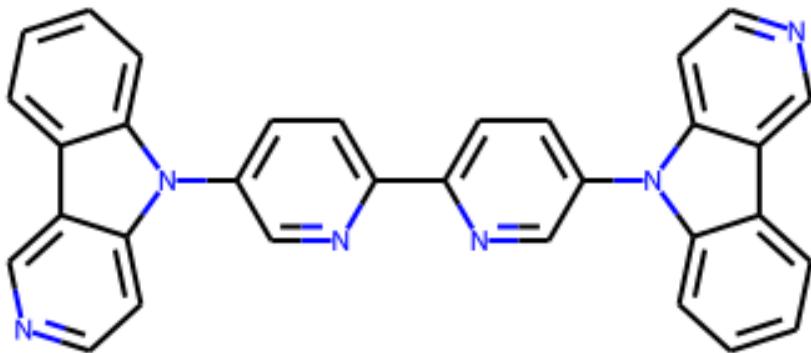


---

No.84

SMILES: c1ccc2c(c1)c1cnccc1n2-c1ccc(-c2ccc(-n3c4cccc4c4cnccc43)cn2)nc1

prob: 0.84



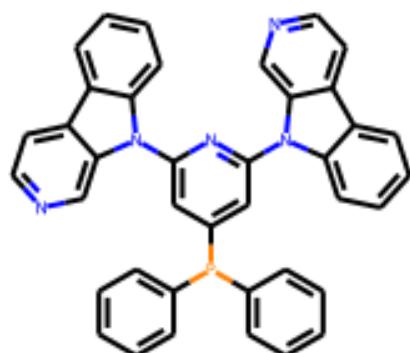
---

No.85

SMILES:

c1ccc(P(c2ccccc2)c2cc(-n3c4cccc4c4ccncc43)nc(-n3c4cccc4c4ccncc43)c2)cc1

prob: 0.84

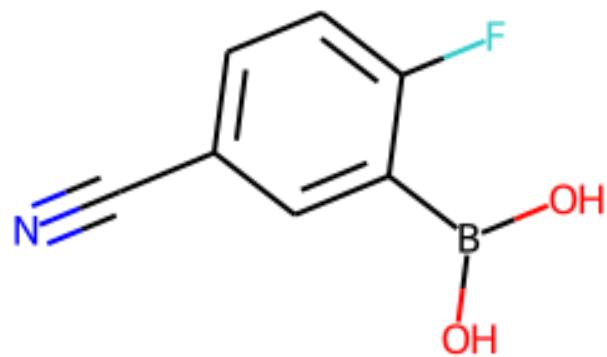


---

No.86

SMILES: N#Cc1ccc(F)c(B(O)O)c1

prob: 0.84

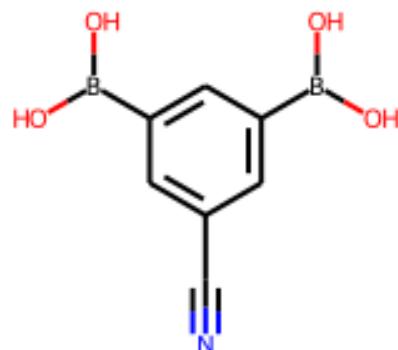


---

No.87

SMILES: N#Cc1cc(B(O)O)cc(B(O)O)c1

prob: 0.84

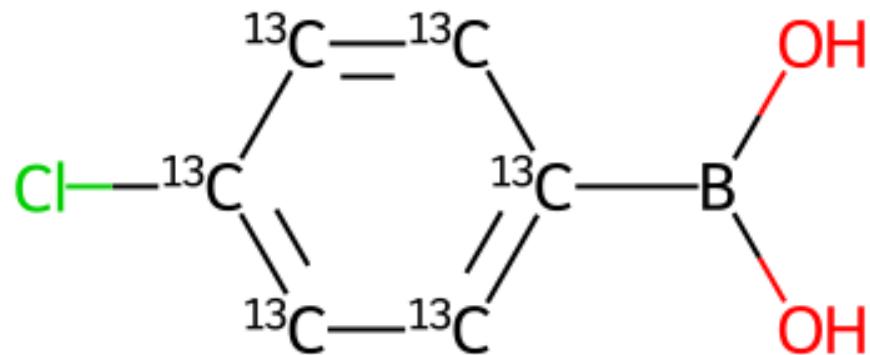


---

No.88

SMILES: OB(O)[13c]1[13cH][13cH][13c](C1)[13cH][13cH]1

prob: 0.84

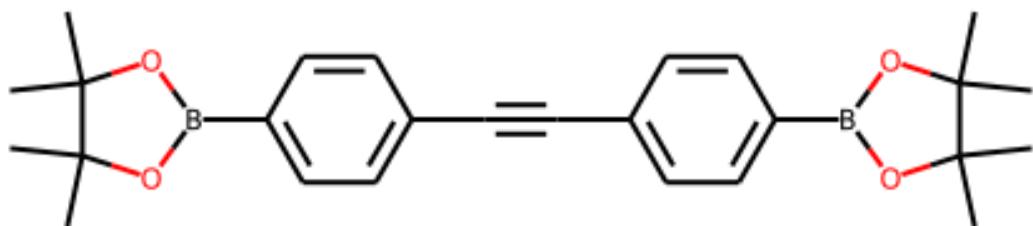


---

No.89

SMILES: CC1(C)OB(c2ccc(C#Cc3ccc(B4OC(C)(C)C(C)O4)cc3)cc2)OC1(C)C

prob: 0.84

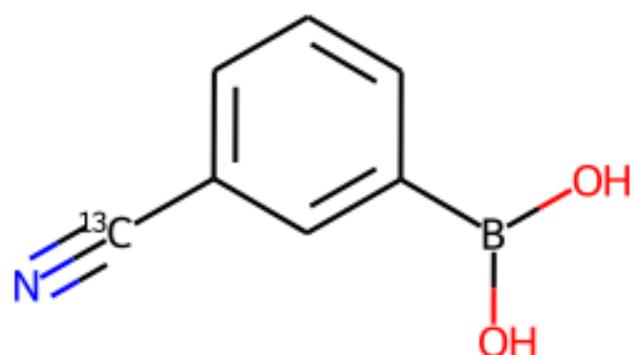


---

No.90

SMILES: N#[13C]c1cccc(B(O)O)c1

prob: 0.83

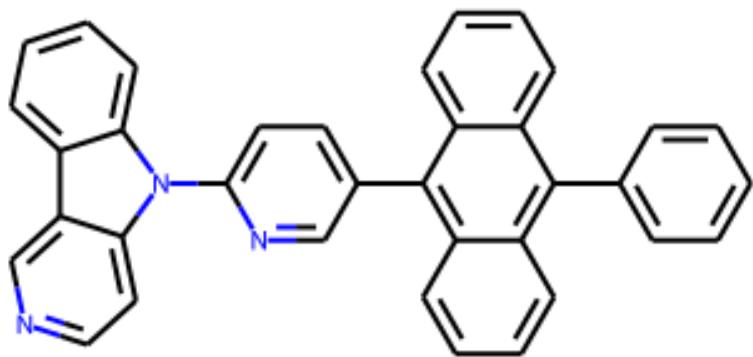


---

No.91

SMILES: c1ccc(-c2c3cccc3c(-c3ccc(-n4c5ccccc5c5cnccc54)nc3)c3cccc23)cc1

prob: 0.83



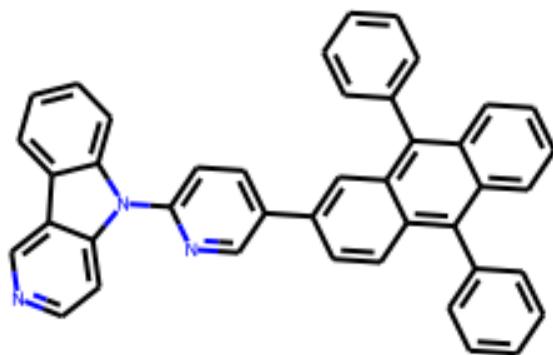
---

No.92

SMILES:

c1ccc(-c2c3ccccc3c(-c3ccccc3)c3cc(-c4ccc(-n5c6ccccc6c6cnccc65)nc4)ccc23)cc1

prob: 0.83

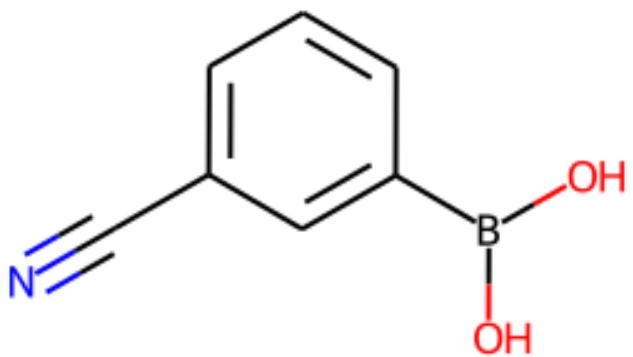


---

No.93

SMILES: N#Cc1cccc(B(0)0)c1

prob: 0.83

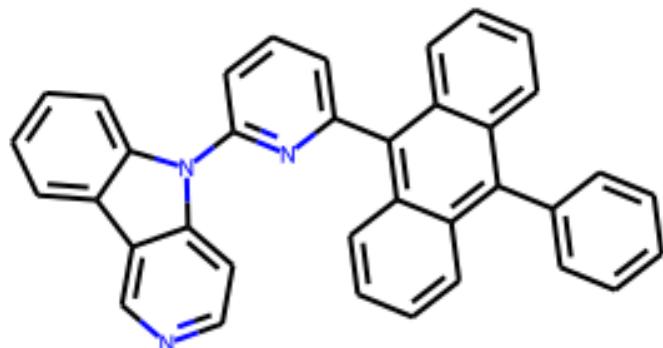


---

No.94

SMILES: c1ccc(-c2c3ccccc3c(-c3cccc(-n4c5ccccc5c5cnccc54)n3)c3ccccc23)cc1

prob: 0.83

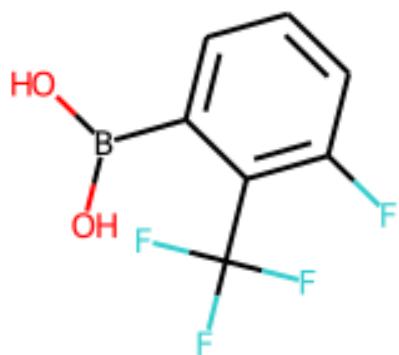


---

No.95

SMILES: OB(0)c1cccc(F)c1C(F)(F)F

prob: 0.83

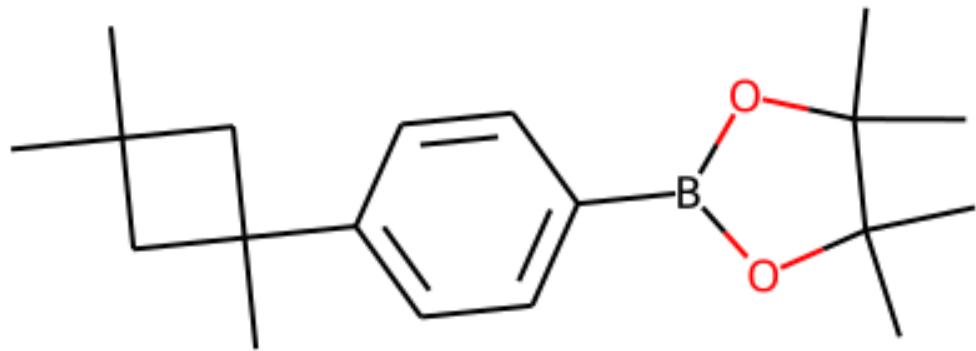


---

No.96

SMILES: CC1(C)CC(C)(c2ccc(B3OC(C)(C)C(C)O3)cc2)C1

prob: 0.83

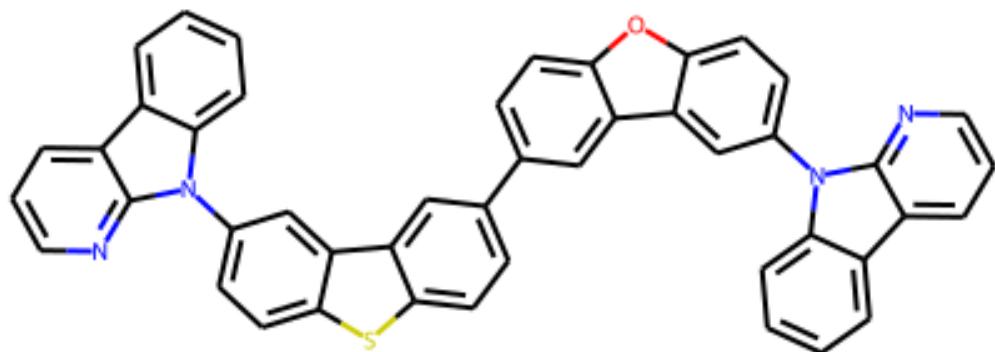


---

No.97

SMILES: c1ccc2c(c1)c1cccn1n2-c1ccc2oc3ccc(-c4ccc5sc6ccc(-n7c8cccc8c8cccnc87)cc6c5c4)cc3c2c1

prob: 0.83

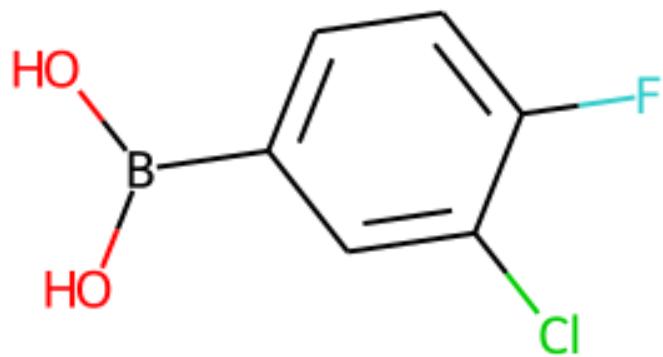


---

No.98

SMILES: OB(O)c1ccc(F)c(Cl)c1

prob: 0.83

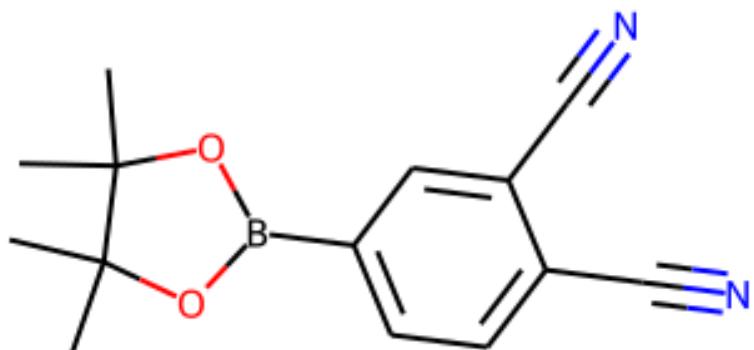


---

No.99

SMILES: CC1(C)OB(c2ccc(C#N)c(C#N)c2)OC1(C)C

prob: 0.83

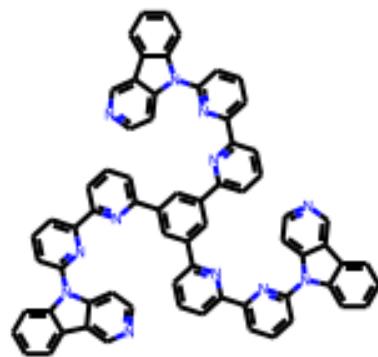


---

No.100

SMILES: c1cc(-c2cc(-c3cccc(-c4cccc(-n5c6cccc6c6cnccc65)n4)n3)cc(-c3cccc(-c4cccc(-n5c6cccc6c6cnccc65)n4)n3)c2)nc(-c2cccc(-n3c4cccc4c4cnccc43)n2)c1

prob: 0.83

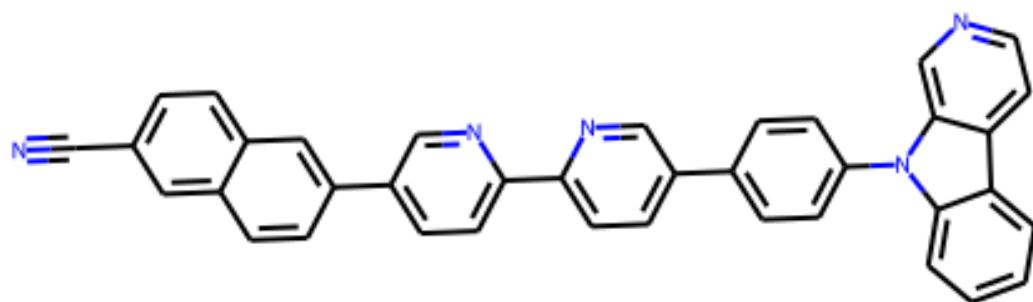


---

No.101

SMILES: N#Cc1cccc2cc(-c3ccc(-c4ccc(-c5ccc(-n6c7cccc7c7ccncc76)cc5)cn4)nc3)ccc2c1

prob: 0.83

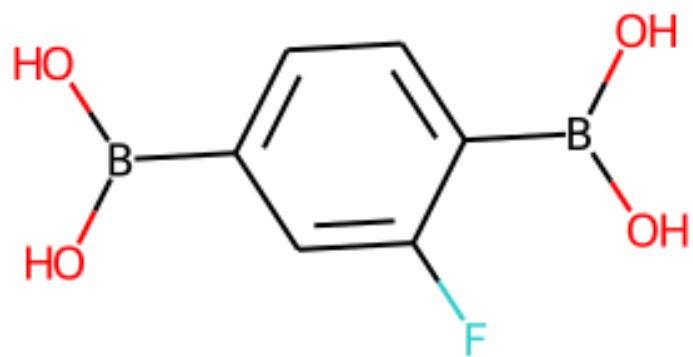


---

No.102

SMILES: OB(0)c1ccc(B(0)O)c(F)c1

prob: 0.83

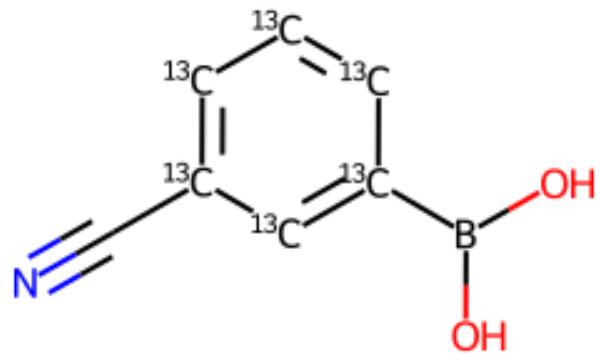


---

No.103

SMILES: N#C[13c]1[13cH][13cH][13cH][13c](B(O)O)[13cH]1

prob: 0.83

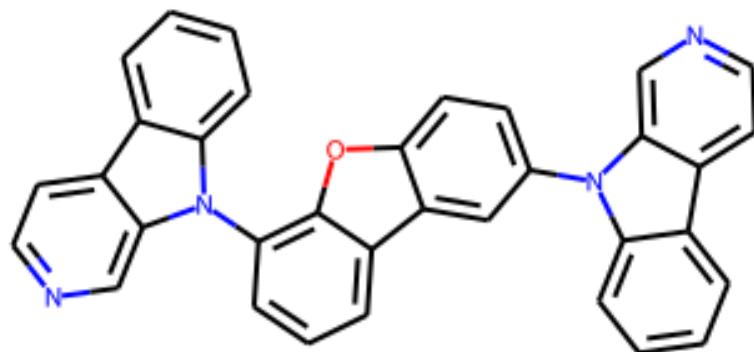


---

No.104

SMILES: c1cc(-n2c3cccc3c3ccncc32)c2oc3ccc(-n4c5cccc5c5ccncc54)cc3c2c1

prob: 0.83

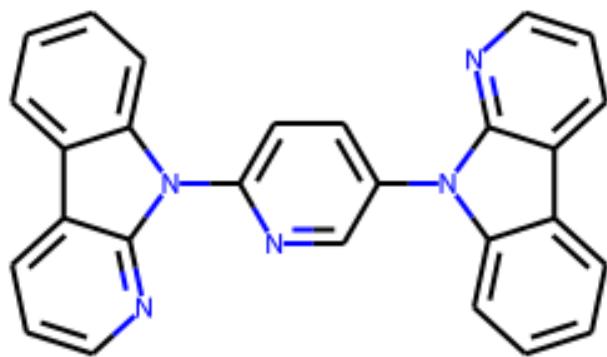


---

No.105

SMILES: c1ccc2c(c1)c1cccnc1n2-c1ccc(-n2c3cccc3c3ccnnc32)nc1

prob: 0.83

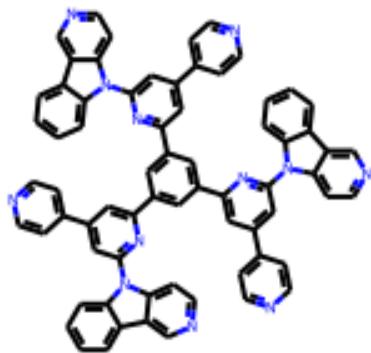


---

No.106

SMILES: c1ccc2c(c1)c1cnccc1n2-c1cc(-c2ccncc2)cc(-c2cc(-c3cc(-c4ccncc4)cc(-n4c5ccc5c5cnccc54)n3)cc(-c3cc(-c4ccncc4)cc(-n4c5cccc5c5cnccc54)n3)c2)c1

prob: 0.83

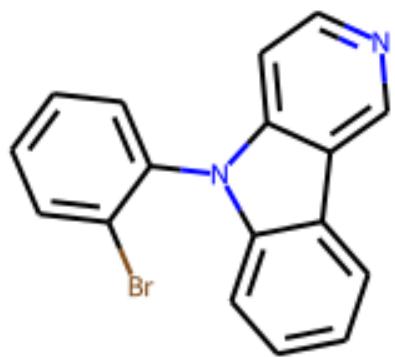


---

No.107

SMILES: Brc1ccccc1-n1c2ccccc2c2cnccc21

prob: 0.83

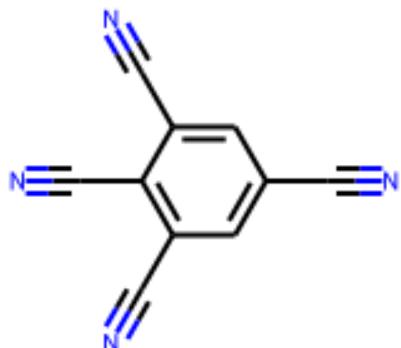


---

No.108

SMILES: N#Cc1cc(C#N)c(C#N)c(C#N)c1

prob: 0.83

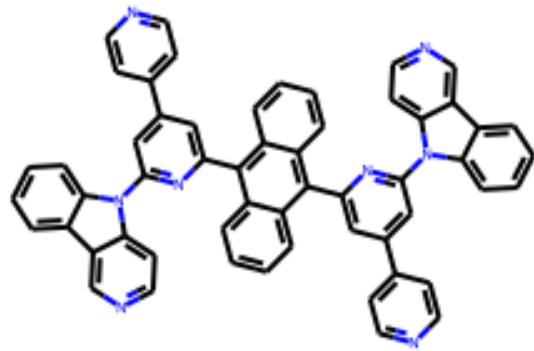


---

No.109

SMILES: c1ccc2c(-c3cc(-c4ccncc4)cc(-n4c5cccc5c5cnccc54)n3)c3cccc3c(-c3cc(-c4ccncc4)cc(-n4c5cccc5c5cnccc54)n3)c2c1

prob: 0.83

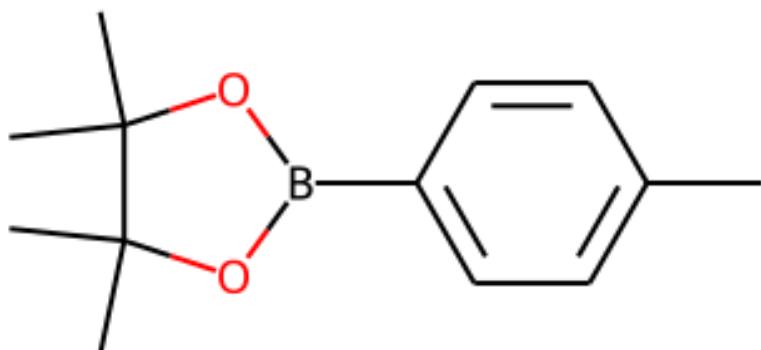


---

No.110

SMILES: Cc1ccc(B2OC(C)(C)C(C)(C)O2)cc1

prob: 0.83

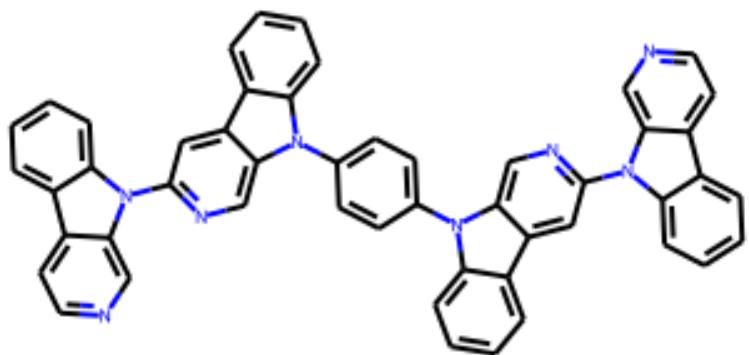


---

No.111

SMILES: c1ccc2c(c1)c1cc(-n3c4cccc4c4ccncc43)ncc1n2-c1ccc(-n2c3cccc3c3cc(-n4c5c  
cccc5c5ccncc54)ncc32)cc1

prob: 0.82

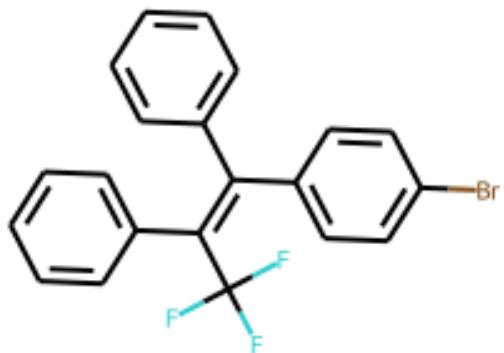


---

No.112

SMILES: FC(F)(F)/C(=C(/c1ccccc1)c1ccc(Br)cc1)c1ccccc1

prob: 0.82

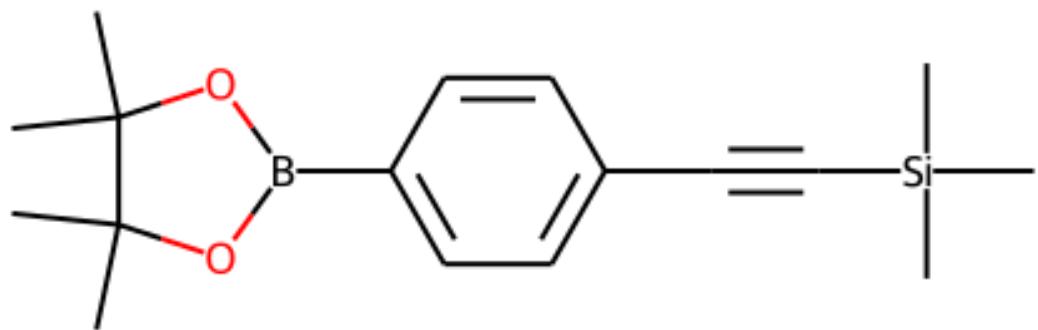


---

No.113

SMILES: CC1(C)OB(c2ccc(C#C[Si](C)(C)C)cc2)OC1(C)C

prob: 0.82

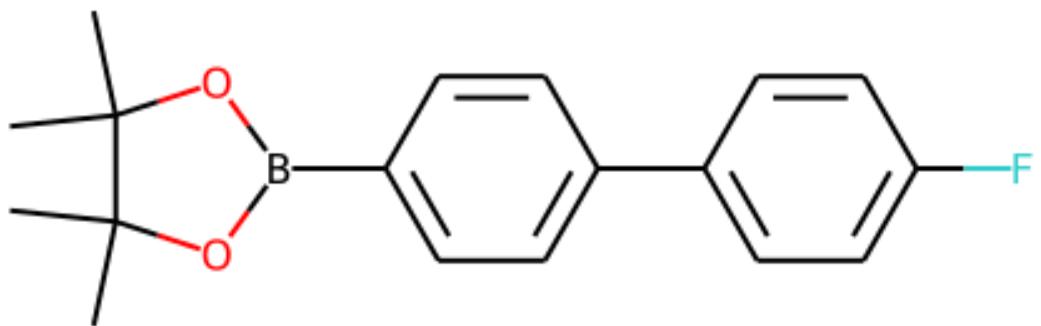


---

No.114

SMILES: CC1(C)OB(c2ccc(-c3ccc(F)cc3)cc2)OC1(C)C

prob: 0.82

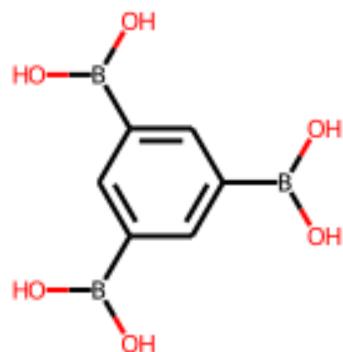


---

No.115

SMILES: OB(O)c1cc(B(O)O)cc(B(O)O)c1

prob: 0.82



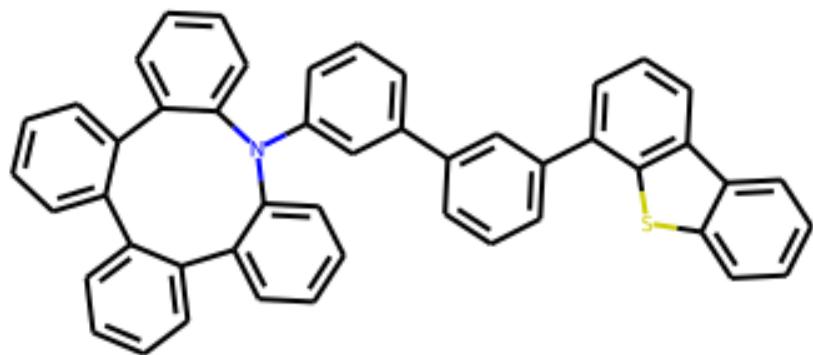
---

No.116

SMILES:

c1cc(-c2cccc(-n3c4cccc4c4cccc4c4cccc4c4cccc43)c2)cc(-c2cccc3c2sc2cccc23)c1

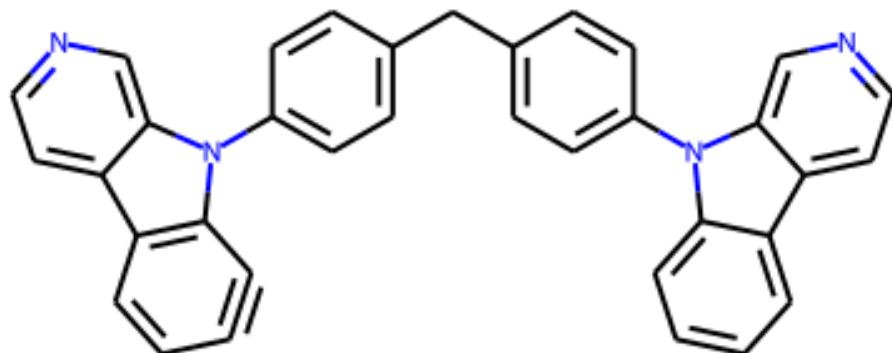
prob: 0.82



No.117

SMILES: c1ccc2c3ccncc3n(-c3ccc(Cc4ccc(-n5c6cccc6c6ccncc65)cc4)cc3)c2c#1

prob: 0.82

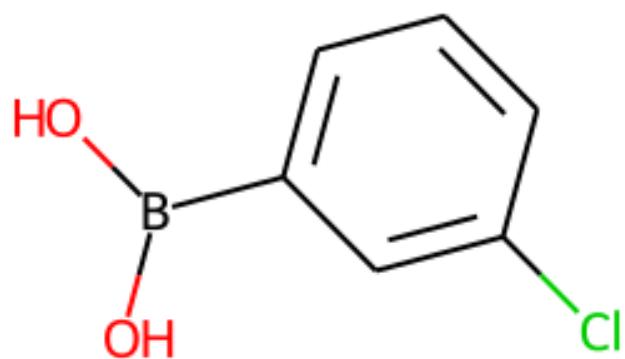


---

No.118

SMILES: OB(O)c1ccccc(Cl)c1

prob: 0.82

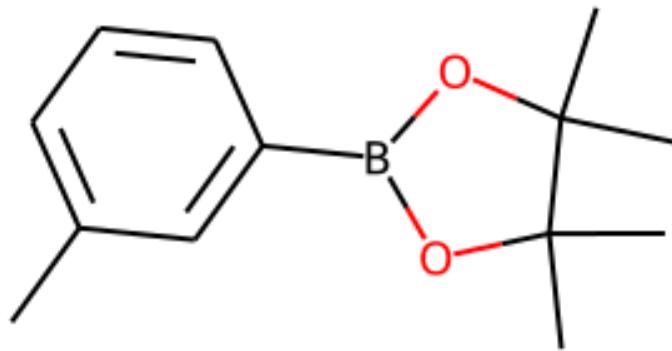


---

No.119

SMILES: Cc1cccc(B2OC(C)(C)C(C)(C)O2)c1

prob: 0.82

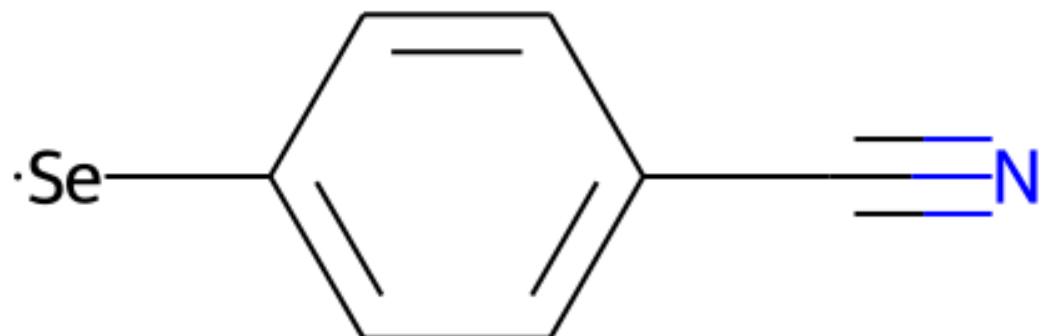


---

No.120

SMILES: N#Cc1ccc([Se])cc1

prob: 0.82

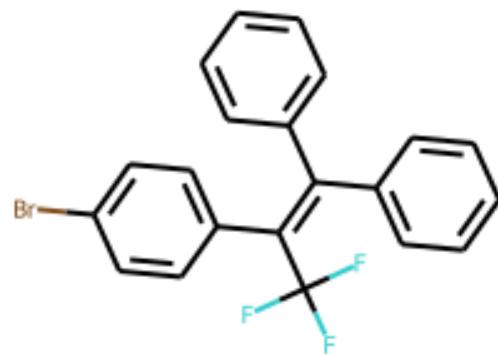


---

No.121

SMILES: FC(F)(F)C(=C(c1ccccc1)c1ccccc1)c1ccc(Br)cc1

prob: 0.82

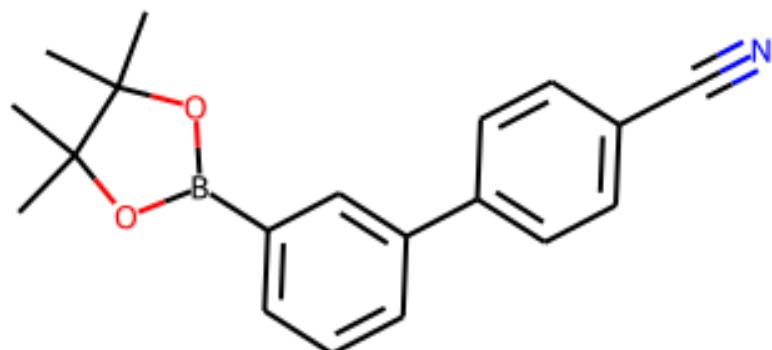


---

No.122

SMILES: CC1(C)OB(c2ccccc(-c3ccc(C#N)cc3)c2)OC1(C)C

prob: 0.82

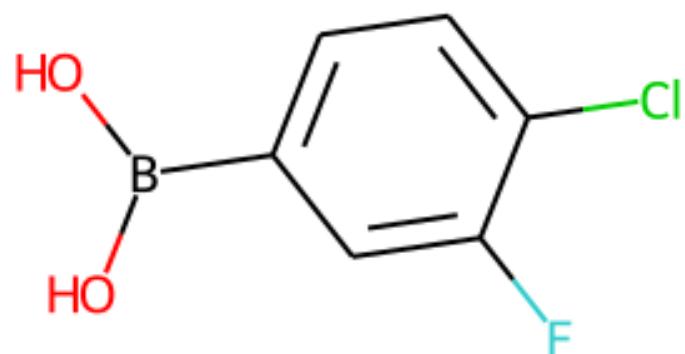


---

No.123

SMILES: OB(O)c1ccc(Cl)c(F)c1

prob: 0.82

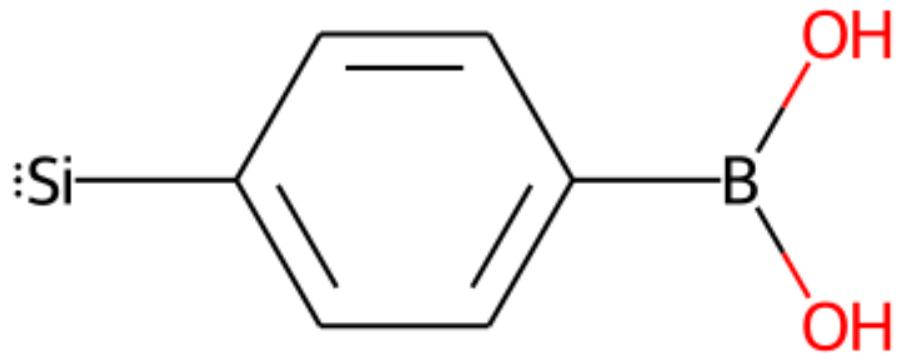


---

No.124

SMILES: OB(0)c1ccc([Si])cc1

prob: 0.82

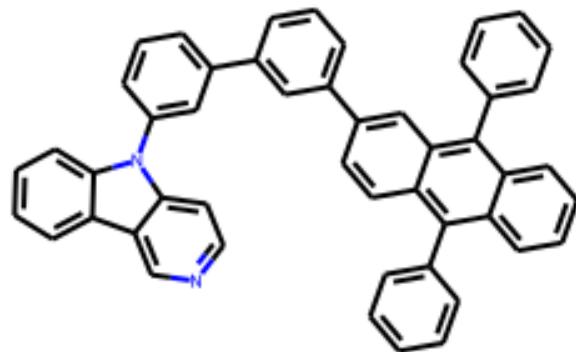


---

No.125

SMILES: c1ccc(-c2c3cccc3c(-c3cccc3)c3cc(-c4cccc(-c5cccc(-n6c7cccc7c7cnccc76)c5)c4)ccc23)cc1

prob: 0.82

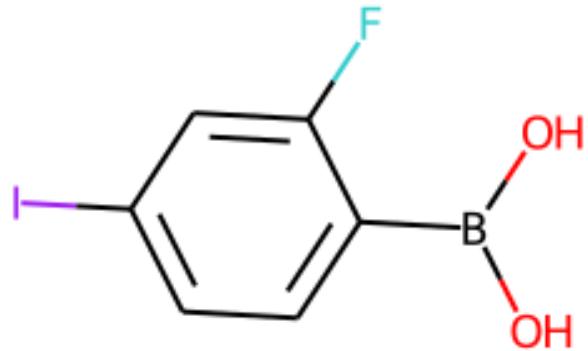


---

No.126

SMILES: OB(0)c1ccc(I)cc1F

prob: 0.82

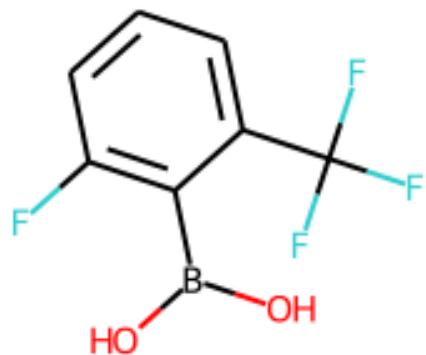


---

No.127

SMILES: OB(O)c1c(F)cccc1C(F)(F)F

prob: 0.82



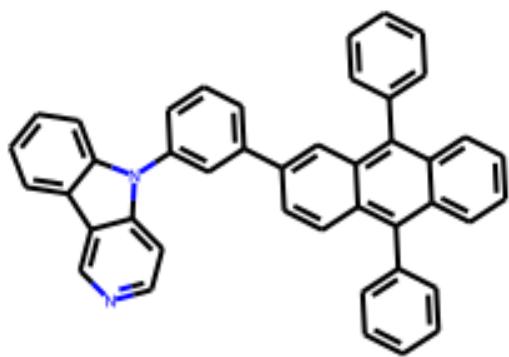
---

No.128

SMILES:

c1ccc(-c2c3ccccc3c(-c3ccccc3)c3cc(-c4cccc(-n5c6cccc6c6cnccc65)c4)ccc23)cc1

prob: 0.82

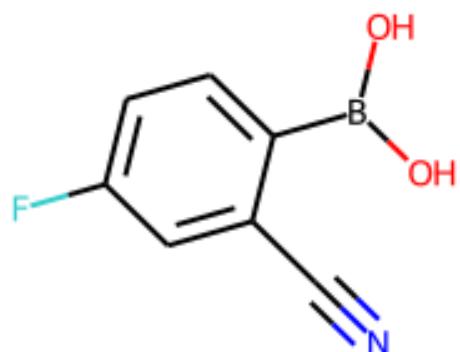


---

No.129

SMILES: N#Cc1cc(F)ccc1B(O)O

prob: 0.82

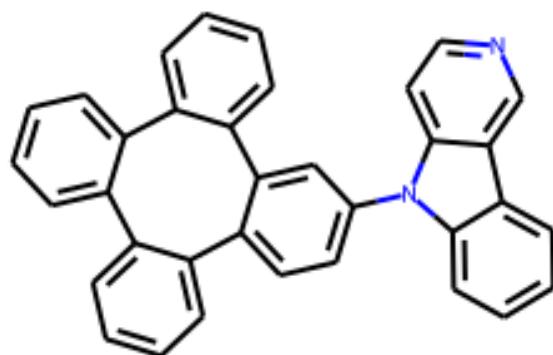


---

No.130

SMILES: c1ccc2c(c1)-c1ccccc1-c1ccc(-n3c4cccc4c4cnccc43)cc1-c1ccccc1-2

prob: 0.82

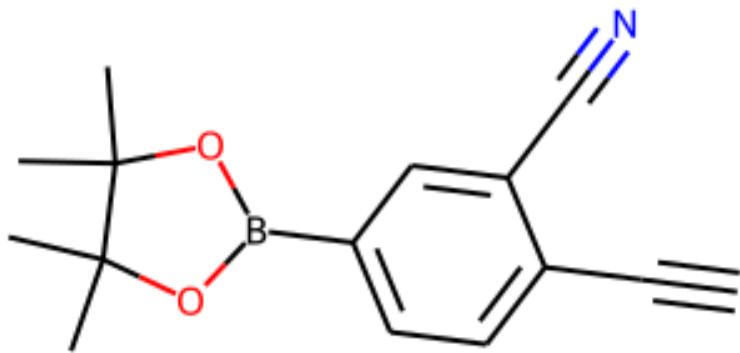


---

No.131

SMILES: C#Cc1cccc(B2OC(C)(C)C(C)(C)O2)cc1C#N

prob: 0.82

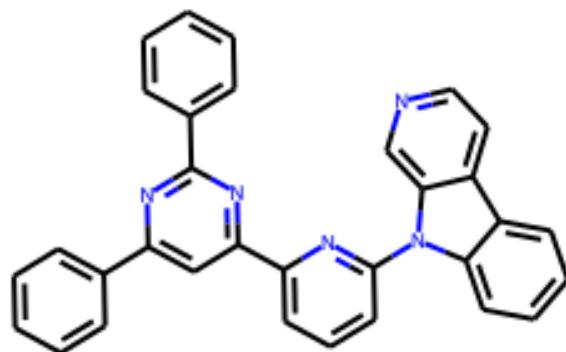


---

No.132

SMILES: c1ccc(-c2cc(-c3cccc(-n4c5cccc5c5ccncc54)n3)nc(-c3cccc3)n2)cc1

prob: 0.82

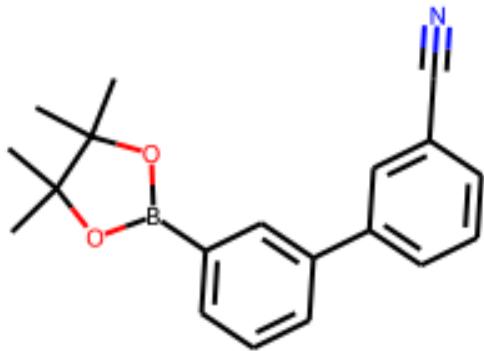


---

No.133

SMILES: CC1(C)OB(c2cccc(-c3cccc(C#N)c3)c2)OC1(C)C

prob: 0.82

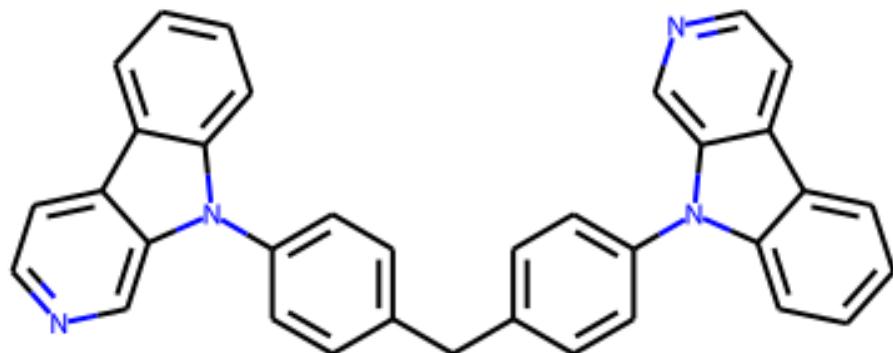


---

No.134

SMILES: c1ccc2c(c1)c1ccncc1n2-c1ccc(Cc2ccc(-n3c4cccc4c4ccncc43)cc2)cc1

prob: 0.82

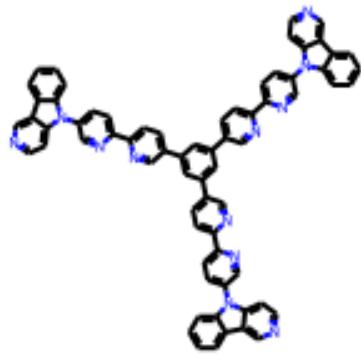


---

No.135

SMILES: c1ccc2c(c1)c1cnccc1n2-c1ccc(-c2ccc(-c3cc(-c4ccc(-c5ccc(-n6c7cccc7c7cncc76)cn5)nc4)cc(-c4ccc(-c5ccc(-n6c7cccc7c7cncc76)cn5)nc4)c3)cn2)nc1

prob: 0.82

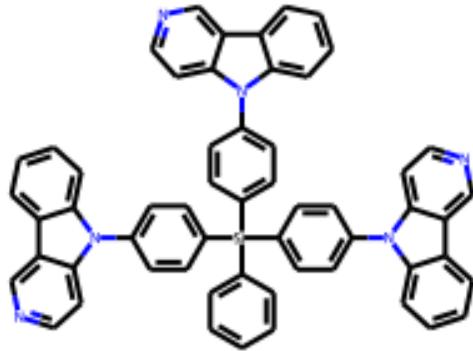


---

No.136

SMILES: c1ccc([Si]c2ccc(-n3c4cccc4c4cnccc43)cc2)c(c2ccc(-n3c4cccc4c4cnccc43)cc2)cc1

prob: 0.82

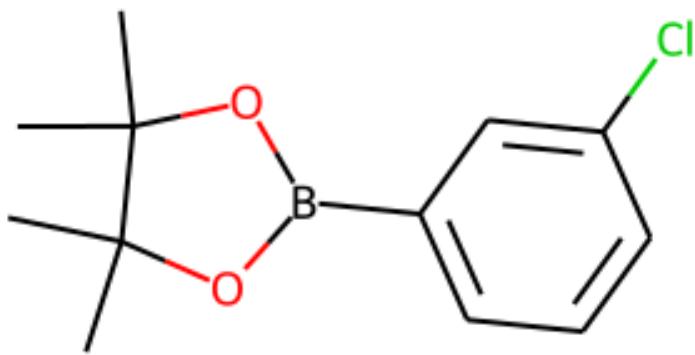


---

No.137

SMILES: CC1(C)OB(c2ccccc(C1)c2)OC1(C)C

prob: 0.82

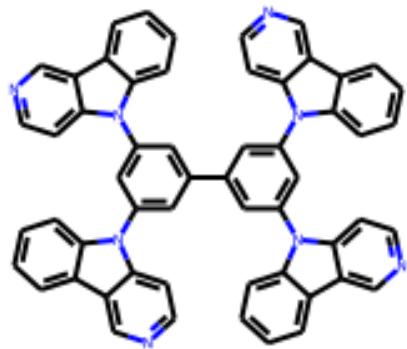


---

No.138

SMILES: c1ccc2c(c1)c1cnccc1n2-c1cc(-c2cc(-n3c4cccc4c4cnccc43)cc(-n3c4cccc4c4cnccc43)c2)cc(-n2c3cccc3c3cnccc32)c1

prob: 0.82

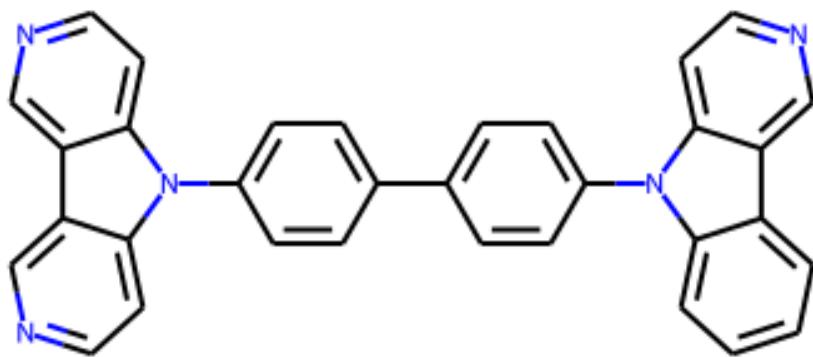


---

No.139

SMILES: c1ccc2c(c1)c1cnccc1n2-c1ccc(-c2ccc(-n3c4ccncc4c4cnccc43)cc2)cc1

prob: 0.82

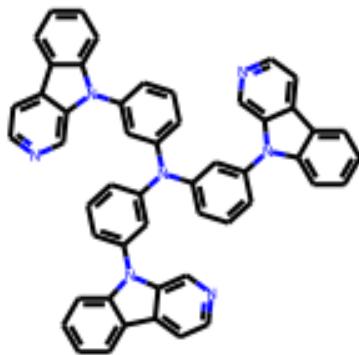


---

No. 140

SMILES: c1cc(N(c2cccc(-n3c4ccccc4c4ccncc43)c2)c2cccc(-n3c4ccccc4c4ccncc43)c2)cc(-n2c3ccccc3c3ccncc32)c1

prob: 0.82

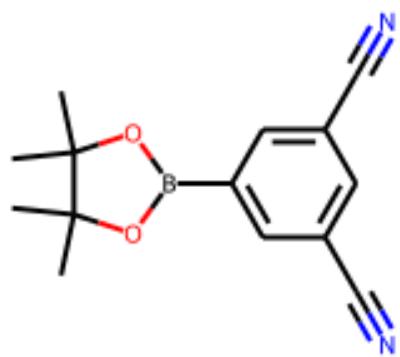


---

No. 141

SMILES: CC1(C)OB(c2cc(C#N)cc(C#N)c2)OC1(C)C

prob: 0.82

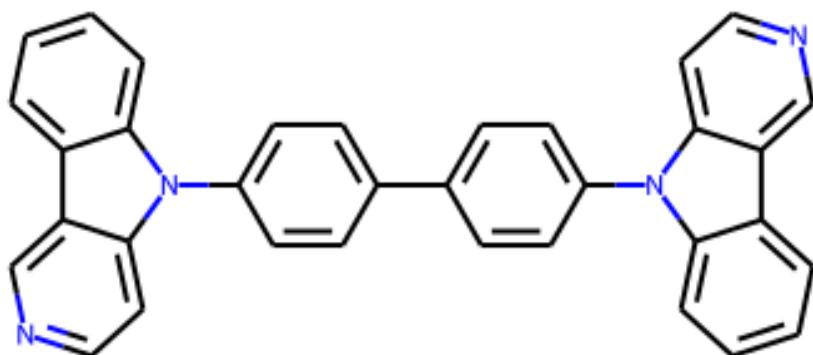


---

No. 142

SMILES: c1ccc2c(c1)c1cnccc1n2-c1ccc(-c2ccc(-n3c4cccc4c4cnccc43)cc2)cc1

prob: 0.82

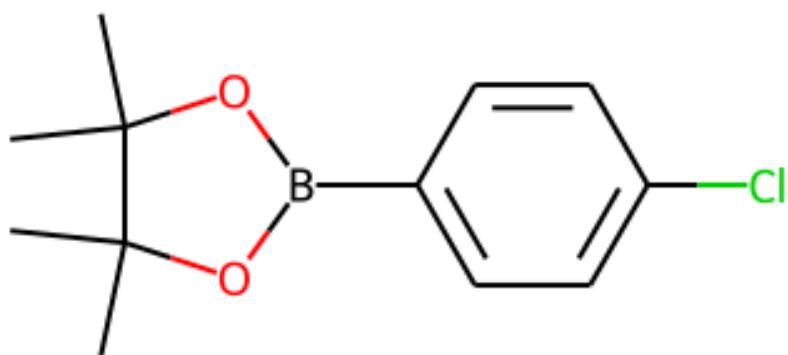


---

No. 143

SMILES: CC1(C)OB(c2ccc(C1)cc2)OC1(C)C

prob: 0.82

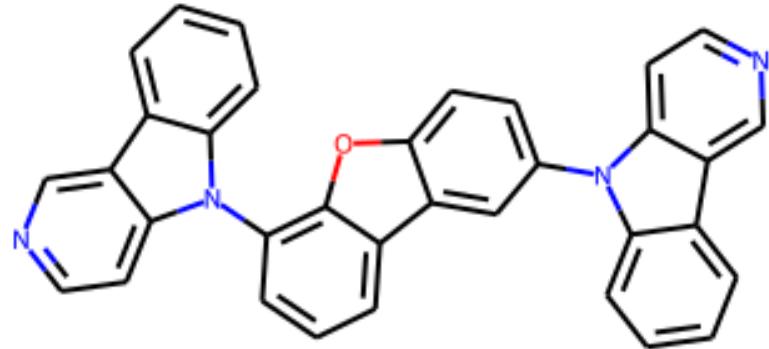


---

No.144

SMILES: c1cc(-n2c3cccc3c3cnccc32)c2oc3ccc(-n4c5cccc5c5cnccc54)cc3c2c1

prob: 0.82

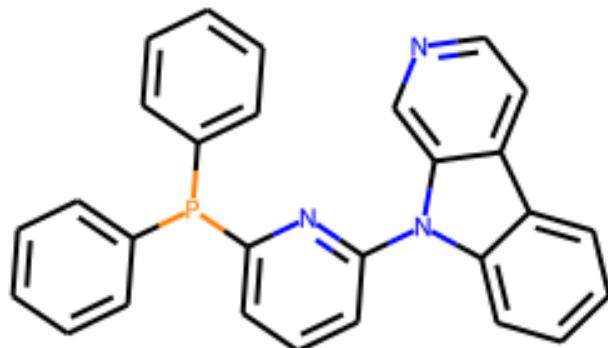


---

No.145

SMILES: c1ccc(P(c2cccc2)c2cccc(-n3c4cccc4c4ccncc43)n2)cc1

prob: 0.82

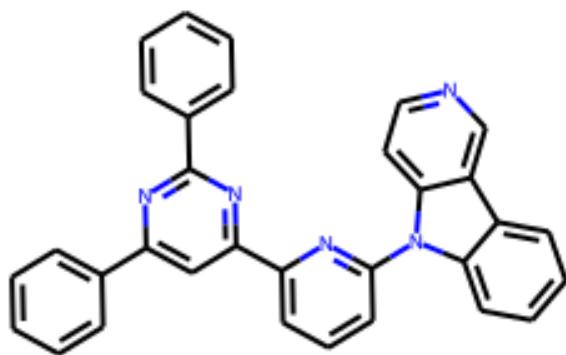


---

No.146

SMILES: c1ccc(-c2cc(-c3cccc(-n4c5cccc5c5cnccc54)n3)nc(-c3cccc3)n2)cc1

prob: 0.82

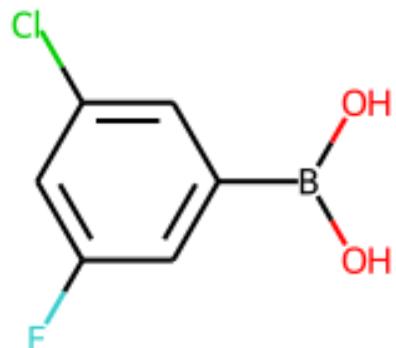


---

No.147

SMILES: OB(O)c1cc(F)cc(Cl)c1

prob: 0.82

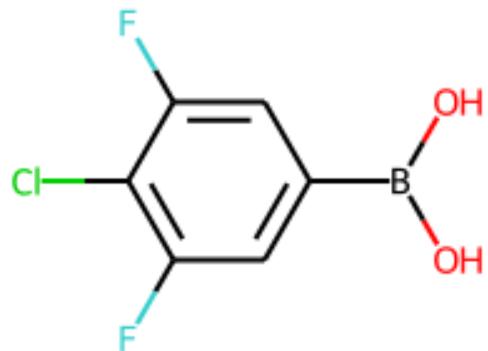


---

No.148

SMILES: OB(O)c1cc(F)c(Cl)c(F)c1

prob: 0.82

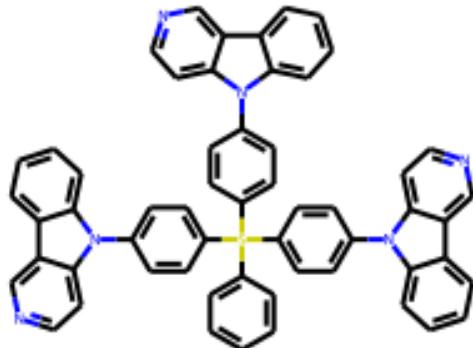


---

No.149

SMILES: c1ccc(S(c2ccc(-n3c4cccc4c4cnccc43)cc2)(c2ccc(-n3c4cccc4c4cnccc43)cc2)c2ccc(-n3c4cccc4c4cnccc43)cc2)cc1

prob: 0.82

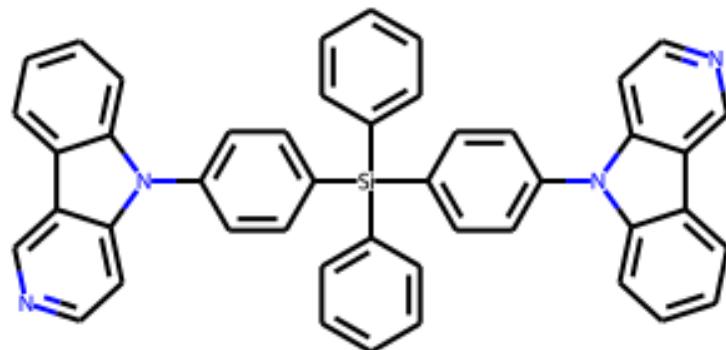


---

No.150

SMILES: c1ccc([Si](c2ccccc2)(c2ccc(-n3c4cccc4c4cnccc43)cc2)c2ccc(-n3c4cccc4c4cnccc43)cc2)cc1

prob: 0.82

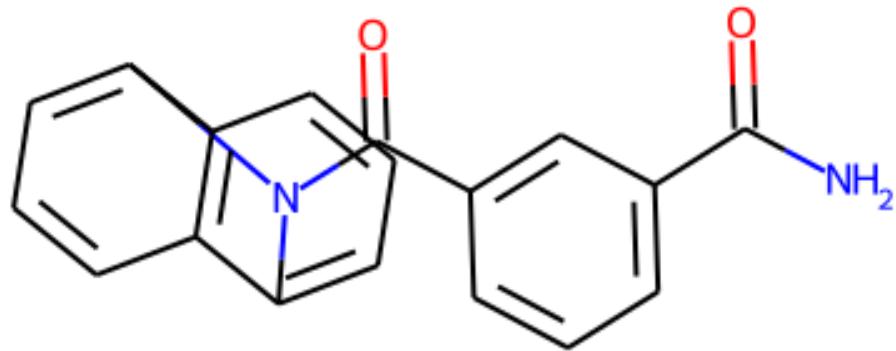


---

No.151

SMILES: NC(=O)c1ccccc(C(=O)n2c3cccc4c3cccc42)c1

prob: 0.82

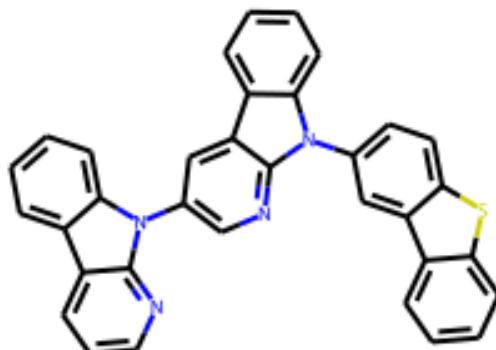


---

No.152

SMILES: c1ccc2c(c1)sc1ccc(-n3c4cccc4c4cc(-n5c6cccc6c6cccnc65)cnc43)cc12

prob: 0.81

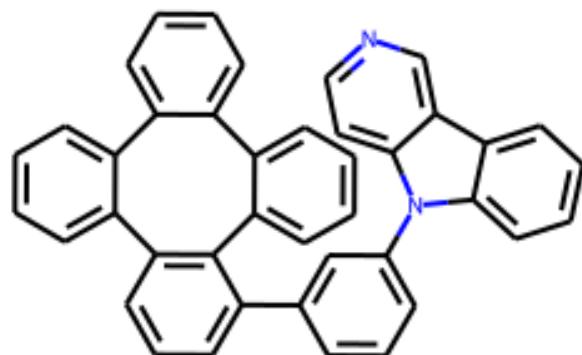


---

No.153

SMILES: c1cc(-c2cccc3c2-c2cccc2-c2cccc2-c2cccc2-3)cc(-n2c3cccc3c3cnccc32)c1

prob: 0.81

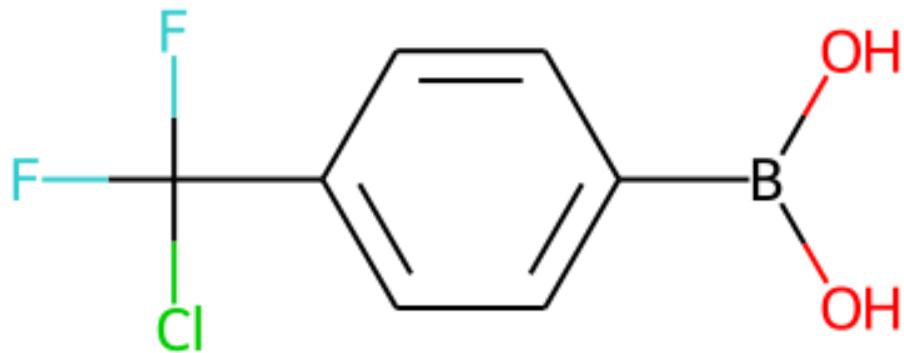


---

No.154

SMILES: OB(O)c1ccc(C(F)(F)Cl)cc1

prob: 0.81

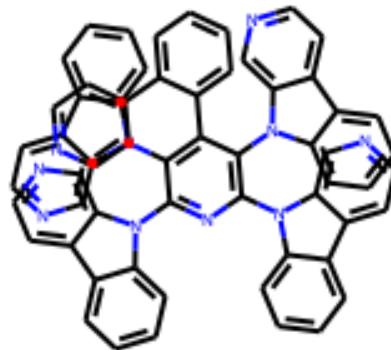


---

No.155

SMILES: c1ccc(-c2c(-n3c4cccc4c4ccncc43)c(-n3c4cccc4c4ccncc43)nc(-n3c4cccc4c4ccncc43)c2-n2c3cccc3c3ccncc32)c(-c2ccncc2)c1

prob: 0.81

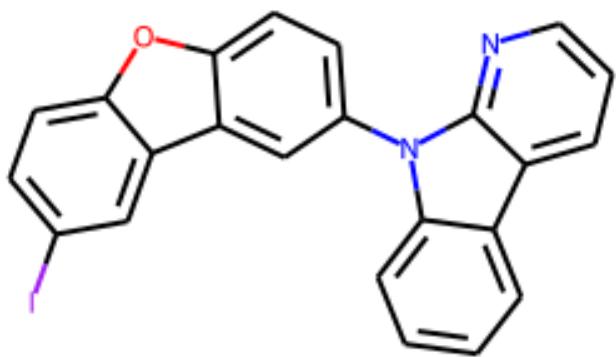


---

No.156

SMILES: Ic1ccc2oc3ccc(-n4c5cccc5c5ccnnc54)cc3c2c1

prob: 0.81

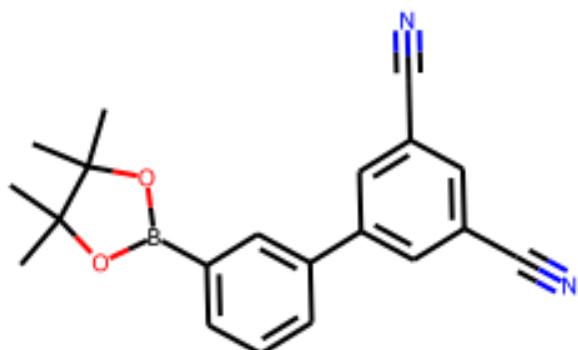


---

No.157

SMILES: CC1(C)OB(c2ccccc(-c3cc(C#N)cc(C#N)c3)c2)OC1(C)C

prob: 0.81



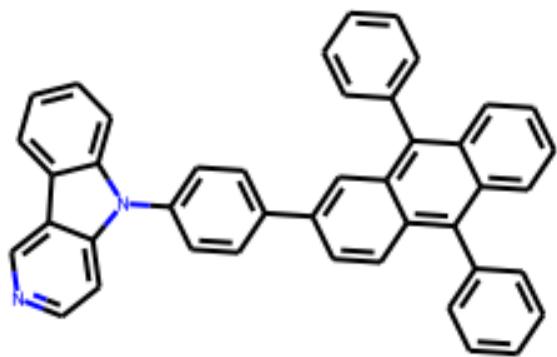
---

No.158

SMILES:

c1ccc(-c2c3cccc3c(-c3cccc3)c3cc(-c4ccc(-n5c6cccc6c6cnccc65)cc4)ccc23)cc1

prob: 0.81

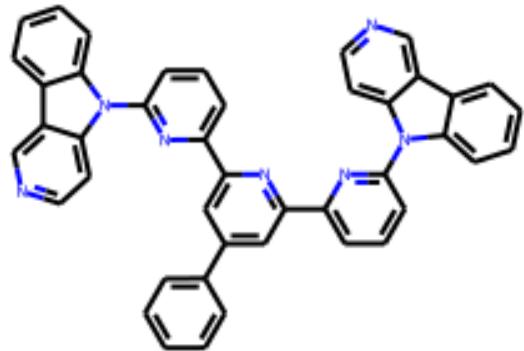


---

No.159

SMILES: c1ccc(-c2cc(-c3cccc(-n4c5cccc5c5cnccc54)n3)nc(-c3cccc(-n4c5cccc5c5cncc54)n3)c2)cc1

prob: 0.81

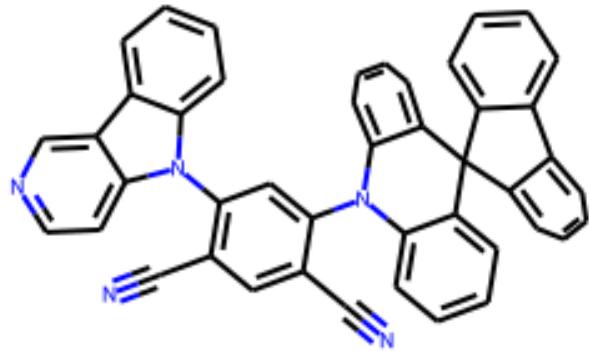


---

No.160

SMILES:

N#Cc1cc(C#N)c(-n2c3cccc3c3cnccc32)cc1N1c2cccc2C2(c3cccc3-c3cccc32)c2cccc21  
prob: 0.81

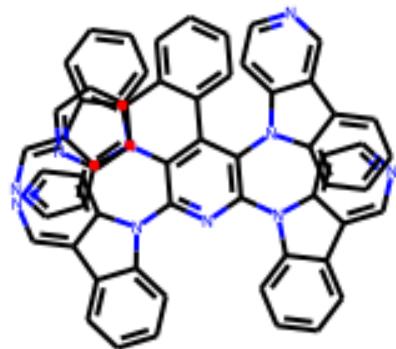


---

No.161

SMILES: c1ccc(-c2c(-n3c4ccccc4c4cnccc43)c(-n3c4ccccc4c4cnccc43)nc(-n3c4ccccc4c4cnccc43)c2-n2c3cccc3c3cnccc32)c(-c2ccncc2)c1

prob: 0.81

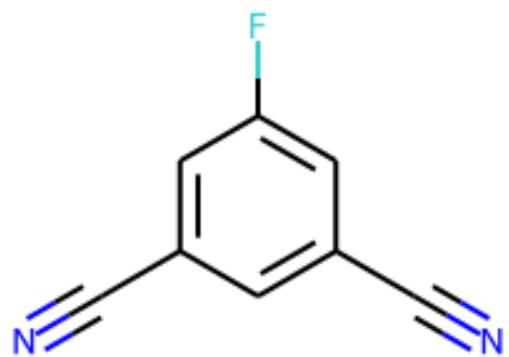


---

No.162

SMILES: N#Cc1cc(F)cc(C#N)c1

prob: 0.81

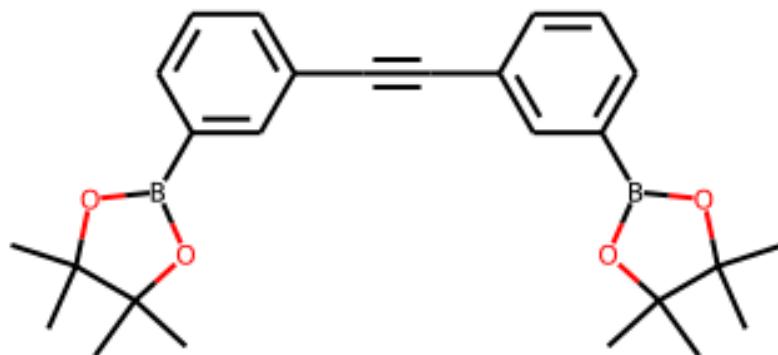


---

No. 163

SMILES: CC1(C)OB(c2ccccc(C#Cc3cccc(B4OC(C)(C)C(C)O4)c3)c2)OC1(C)C

prob: 0.81

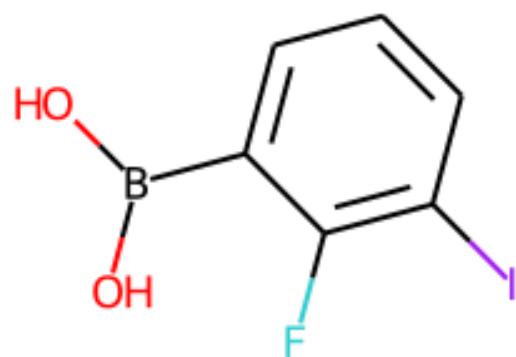


---

No. 164

SMILES: OB(O)c1ccccc(I)c1F

prob: 0.81

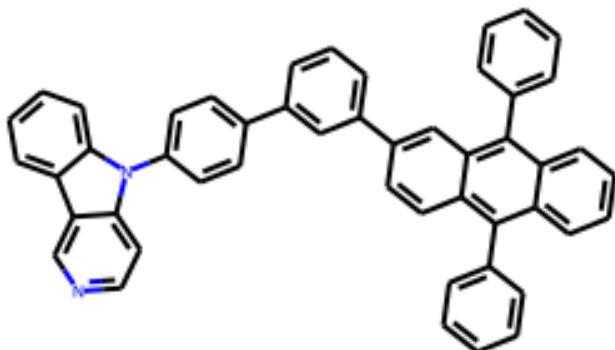


---

No.165

SMILES: c1ccc(-c2c3cccc3c(-c3cccc3)c3cc(-c4cccc(-c5ccc(-n6c7cccc7c7cnccc76)cc5)c4)ccc23)cc1

prob: 0.81

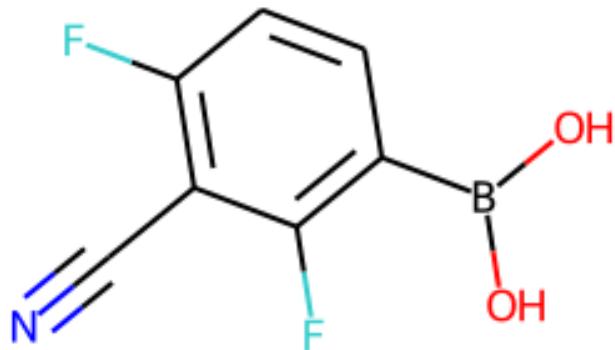


---

No.166

SMILES: N#Cc1c(F)ccc(B(O)O)c1F

prob: 0.81

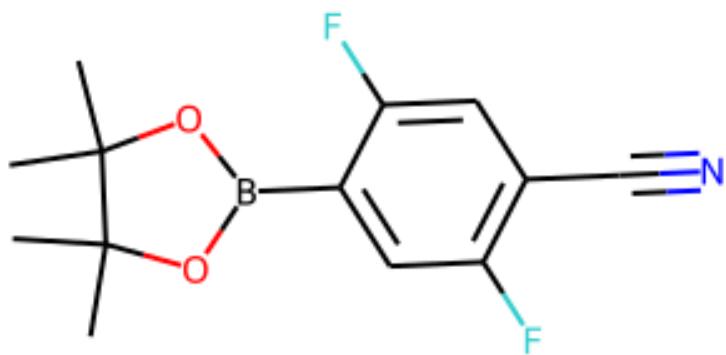


---

No.167

SMILES: CC1(C)OB(c2cc(F)c(C#N)cc2F)OC1(C)C

prob: 0.81

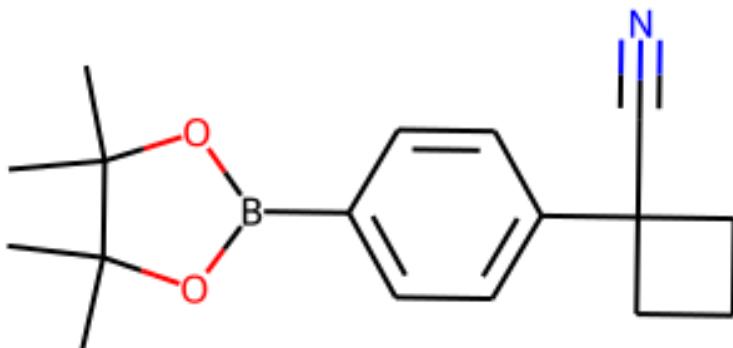


---

No. 168

SMILES: CC1(C)OB(c2ccc(C3(C#N)CCC3)cc2)OC1(C)C

prob: 0.81

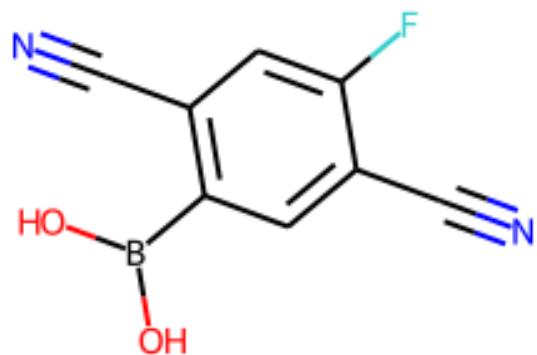


---

No. 169

SMILES: N#Cc1cc(B(O)O)c(C#N)cc1F

prob: 0.81

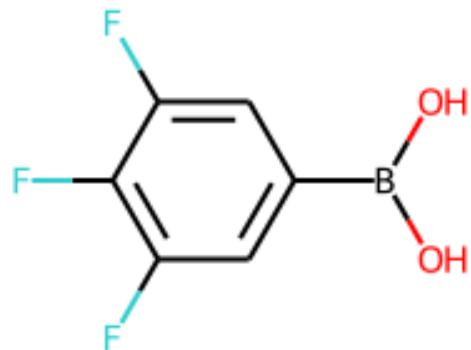


---

No.170

SMILES: OB(O)c1cc(F)c(F)c(F)c1

prob: 0.81

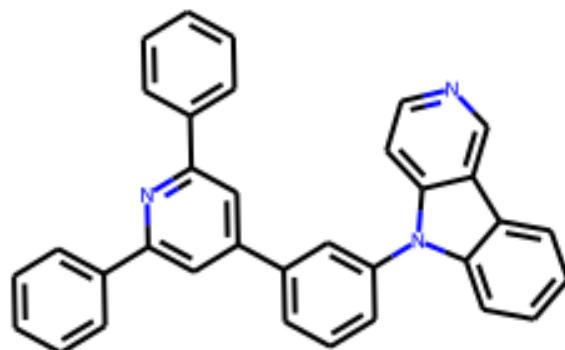


---

No.171

SMILES: c1ccc(-c2cc(-c3cccc(-n4c5cccc5c5cnccc54)c3)cc(-c3cccc3)n2)cc1

prob: 0.81

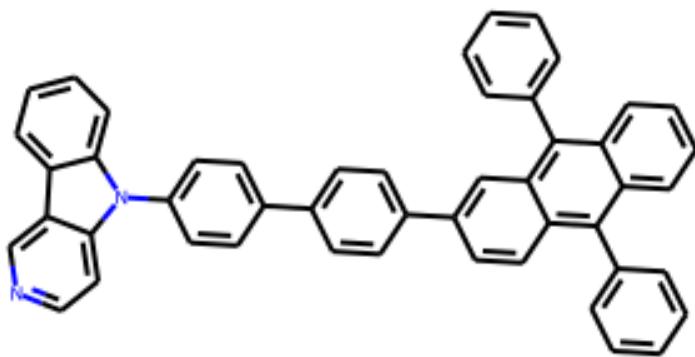


---

No.172

SMILES: c1ccc(-c2c3cccc3c(-c3cccc3)c3cc(-c4ccc(-c5ccc(-n6c7cccc7c7cnccc76)cc5)cc4)ccc23)cc1

prob: 0.81

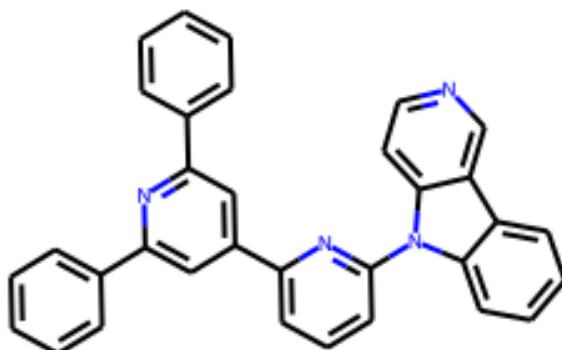


---

No.173

SMILES: c1ccc(-c2cc(-c3cccc(-n4c5cccc5c5cnccc54)n3)cc(-c3cccc3)n2)cc1

prob: 0.81



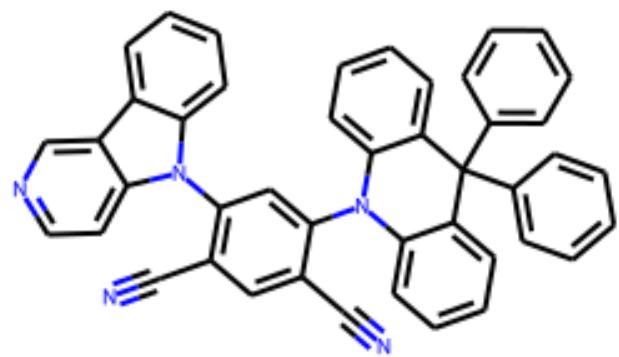
---

No.174

SMILES:

N#Cc1cc(C#N)c(-n2c3cccc3c3cnccc32)cc1N1c2cccc2C(c2cccc2)(c2cccc2)c2cccc21

prob: 0.81

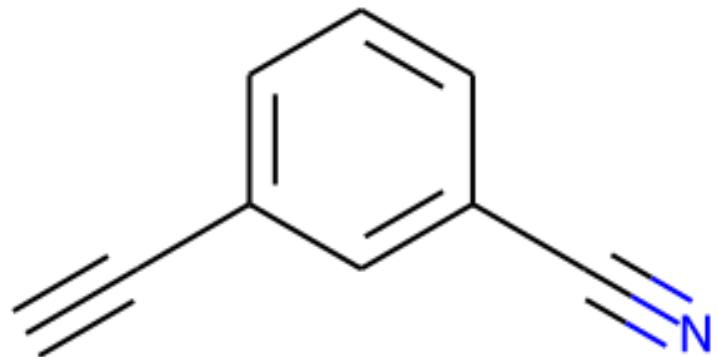


---

No.175

SMILES: C#Cc1ccccc(C#N)c1

prob: 0.81

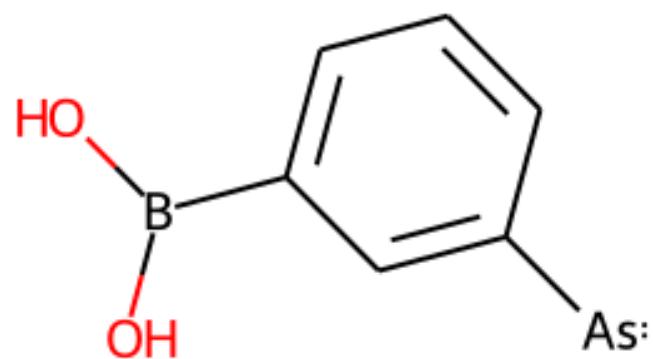


---

No.176

SMILES: OB(O)c1ccccc([As])c1

prob: 0.81

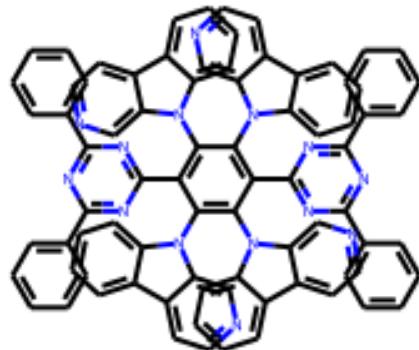


---

No.177

SMILES: c1ccc(-c2nc(-c3cccc3)nc(-c3c(-n4c5ccccc5c5ccncc54)c(-n4c5ccccc5c5ccncc54)c(-c4nc(-c5ccccc5)nc(-c5ccccc5)n4)c(-n4c5ccccc5c5ccncc54)c3-n3c4ccccc4c4ccncc43)n2)cc1

prob: 0.81

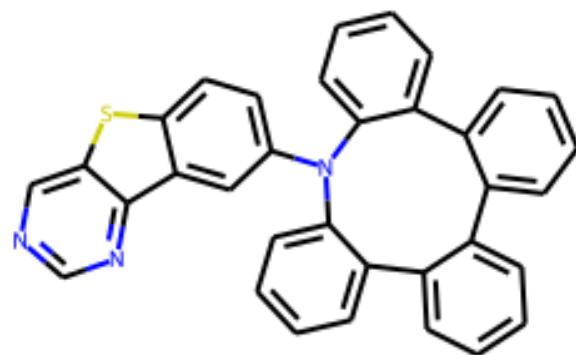


---

No.178

SMILES: c1ccc2c(c1)c1ccccc1c1ccccc1n(-c1ccc3sc4cncnc4c3c1)c1ccccc21

prob: 0.81

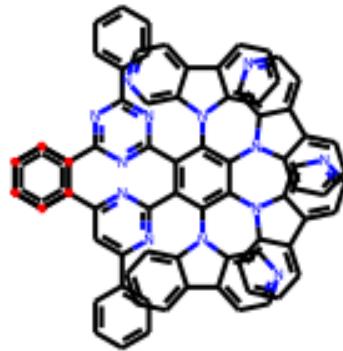


---

No.179

SMILES: c1ccc(-c2cc(-c3cccc3)nc(-c3c(-c4nc(-c5ccccc5)nc(-c5ccccc5)n4)c(-n4c5cc5c5ccncc54)c(-n4c5ccccc5c5ccncc54)c(-n4c5ccccc5c5ccncc54)c3-n3c4ccccc4c4ccncc43)n2)cc1

prob: 0.81

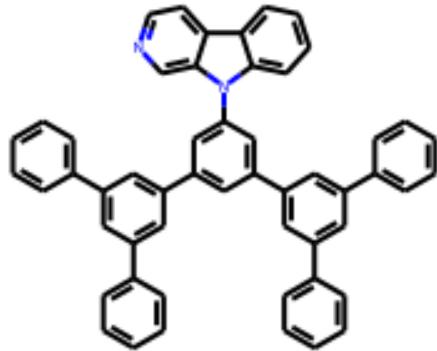


---

No.180

SMILES: c1ccc(-c2cc(-c3cccc3)cc(-c3cc(-c4cc(-c5cccc5)cc(-c5cccc5)c4)cc(-n4c5cccc5c5ccncc54)c3)c2)cc1

prob: 0.81

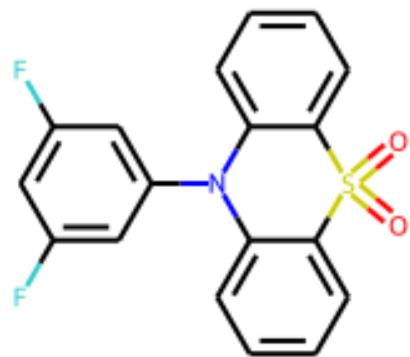


---

No.181

SMILES: O=S1(=O)c2ccccc2N(c2cc(F)cc(F)c2)c2ccccc21

prob: 0.81

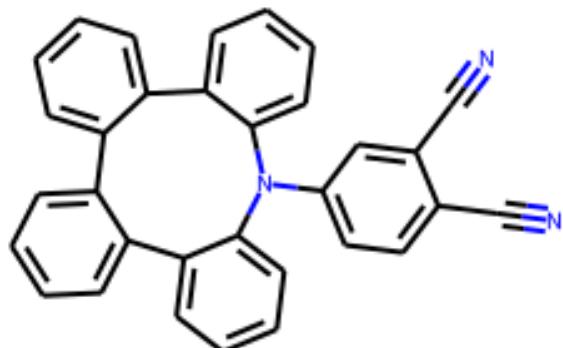


---

No.182

SMILES: N#Cc1cccc(-n2c3cccc3c3cccc3c3cccc3c3cccc32)cc1C#N

prob: 0.81

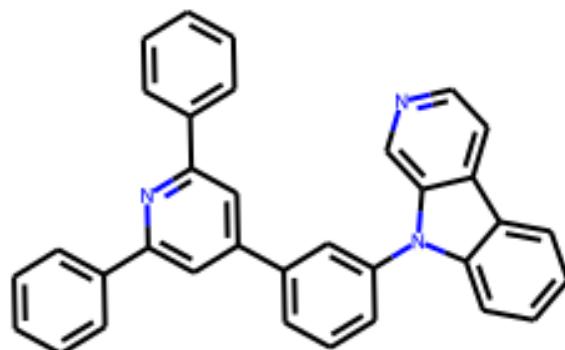


---

No.183

SMILES: c1ccc(-c2cc(-c3cccc(-n4c5cccc5c5ccncc54)c3)cc(-c3cccc3)n2)cc1

prob: 0.81

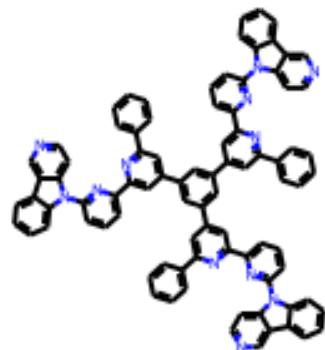


---

No.184

SMILES: c1ccc(-c2cc(-c3cc(-c4cc(-c5cccc5)nc(-c5cccc(-n6c7cccc7c7cnccc76)n5)c4)cc(-c4cc(-c5cccc5)nc(-c5cccc(-n6c7cccc7c7cnccc76)n5)c4)c3)cc(-c3cccc(-n4c5cccc5c5c5cnccc54)n3)n2)cc1

prob: 0.81

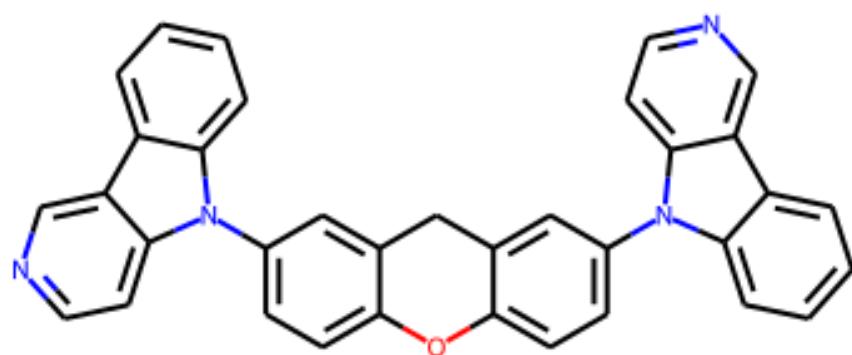


---

No.185

SMILES: c1ccc2c(c1)c1cnccc1n2-c1ccc2c(c1)Cc1cc(-n3c4cccc4c4cnccc43)ccc102

prob: 0.81

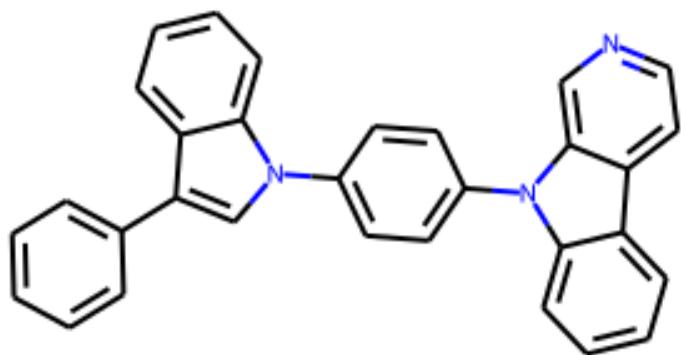


---

No.186

SMILES: c1ccc(-c2cn(-c3ccc(-n4c5cccc5c5ccncc54)cc3)c3cccc23)cc1

prob: 0.81

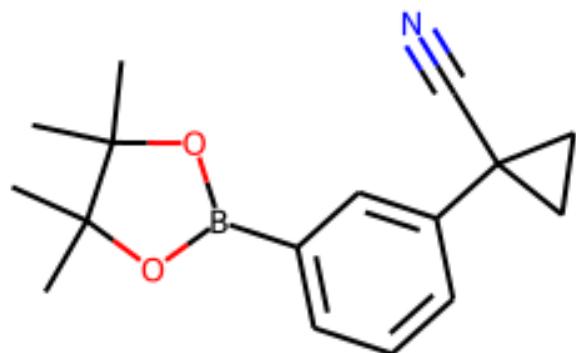


---

No.187

SMILES: CC1(C)OB(c2ccccc(C3(C#N)CC3)c2)OC1(C)C

prob: 0.81

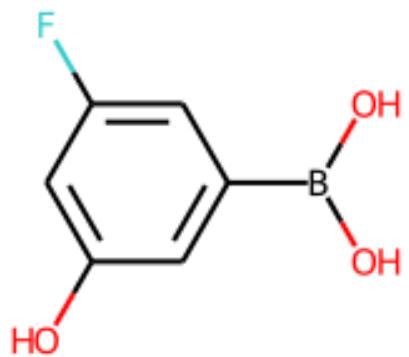


---

No.188

SMILES: OB(O)c1cc(O)cc(F)c1

prob: 0.81

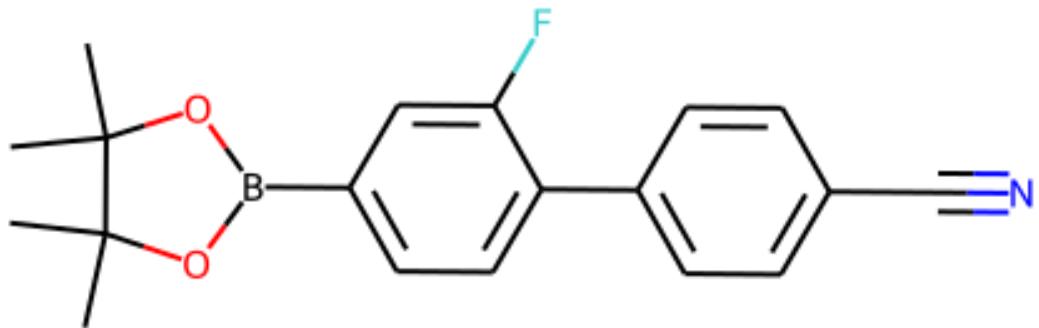


---

No.189

SMILES: CC1(C)OB(c2ccc(-c3ccc(C#N)cc3)c(F)c2)OC1(C)C

prob: 0.81

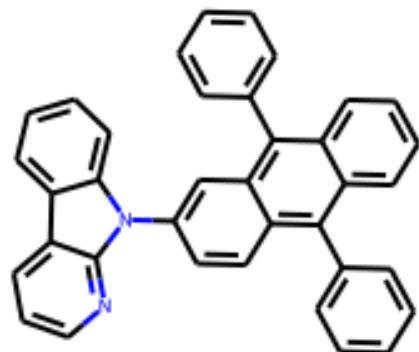


---

No.190

SMILES: c1ccc(-c2c3cccc3c(-c3cccc3)c3cc(-n4c5ccccc5c5cccnc54)ccc23)cc1

prob: 0.81

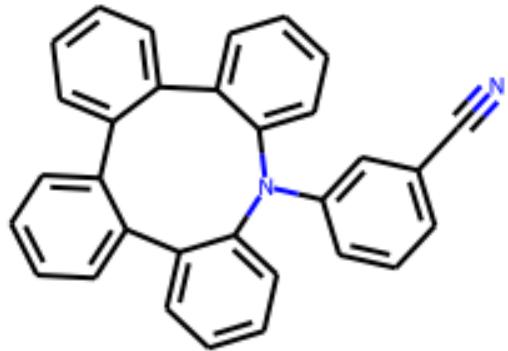


---

No.191

SMILES: N#Cc1cccc(-n2c3cccc3c3cccc3c3cccc3c3cccc32)c1

prob: 0.81

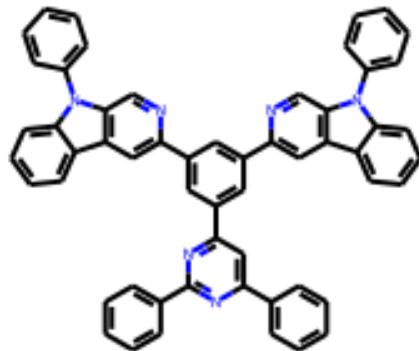


---

No.192

SMILES: c1ccc(-c2cc(-c3cc(-c4cc5c6cccc6n(-c6ccccc6)c5cn4)cc(-c4cc5c6cccc6n(-c6ccccc6)c5cn4)c3)nc(-c3ccccc3)n2)cc1

prob: 0.81

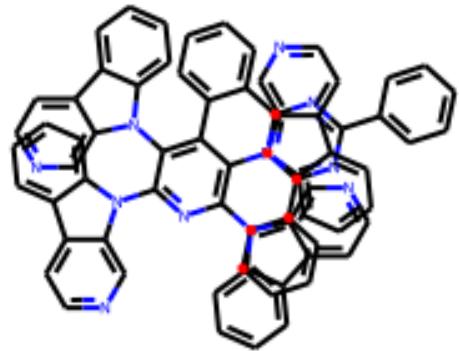


---

No.193

SMILES: c1ccc(-c2nc(-c3ccccc3)nc(-c3ccccc3-c3c(-n4c5ccccc5c5ccncc54)c(-n4c5ccccc5c5ccncc54)nc(-n4c5ccccc5c5ccncc54)c3-n3c4ccccc4c4ccncc43)n2)cc1

prob: 0.81

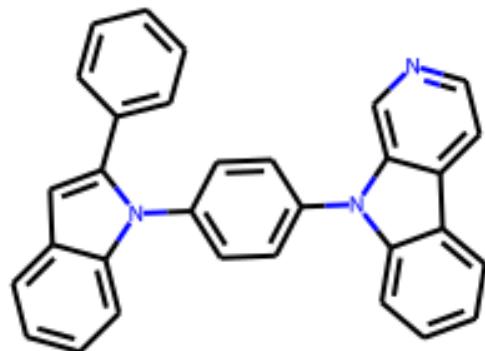


---

No.194

SMILES: c1ccc(-c2cc3cccc3n2-c2ccc(-n3c4cccc4c4ccncc43)cc2)cc1

prob: 0.81

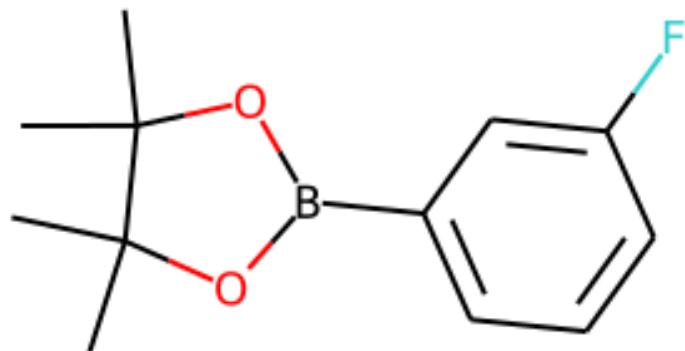


---

No.195

SMILES: CC1(C)OB(c2ccccc(F)c2)OC1(C)C

prob: 0.81

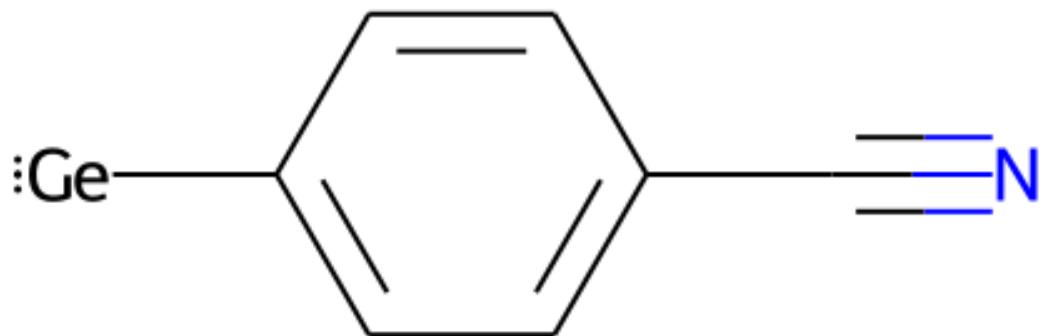


---

No.196

SMILES: N#Cc1ccc([Ge])cc1

prob: 0.81

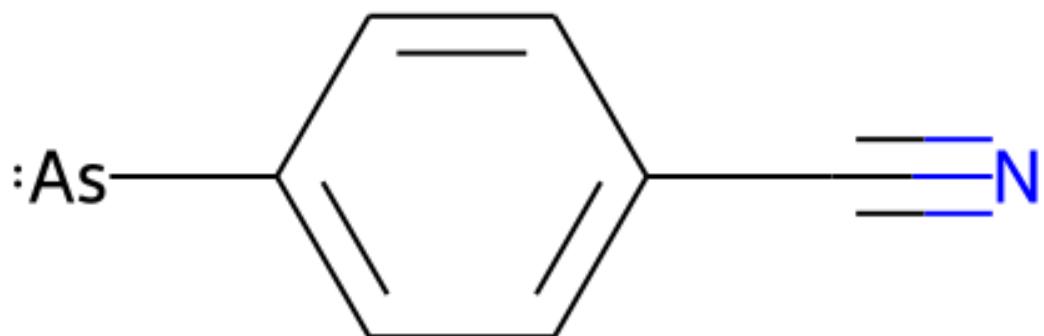


---

No.197

SMILES: N#Cc1ccc([As])cc1

prob: 0.81

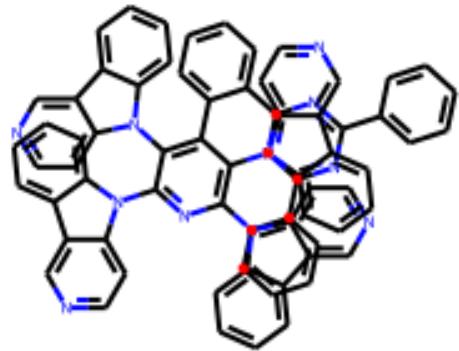


---

No.198

SMILES: c1ccc(-c2nc(-c3cccc3)nc(-c3cccc3-c3c(-n4c5cccc5c5cnccc54)c(-n4c5cccc5c5cnccc54)nc(-n4c5cccc5c5cnccc54)c3-n3c4cccc4c4cnccc43)n2)cc1

prob: 0.81

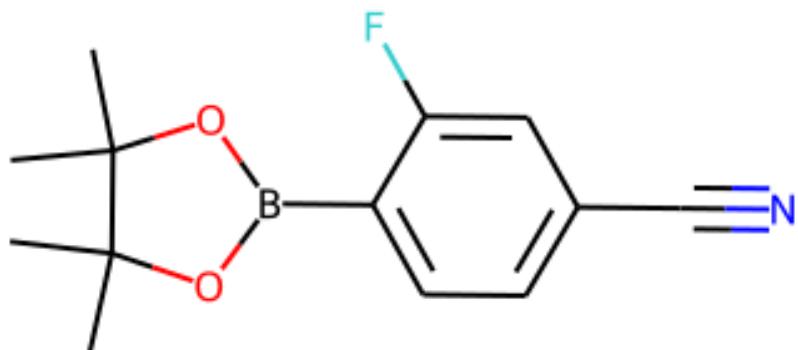


---

No.199

SMILES: CC1(C)OB(c2ccc(C#N)cc2F)OC1(C)C

prob: 0.8

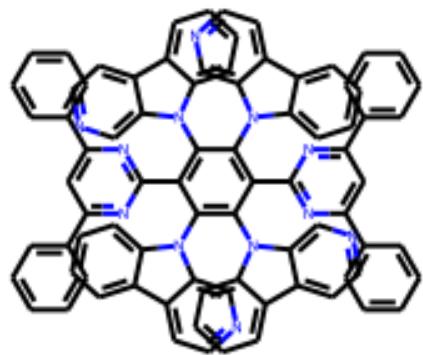


---

No.200

SMILES: c1ccc(-c2cc(-c3cccc3)nc(-c3c(-n4c5cccc5c5ccncc54)c(-n4c5cccc5c5ccncc54)c(-c4nc(-c5cccc5)cc(-c5cccc5)n4)c(-n4c5cccc5c5ccncc54)c3-n3c4cccc4c4ccncc43)n2)cc1

prob: 0.8

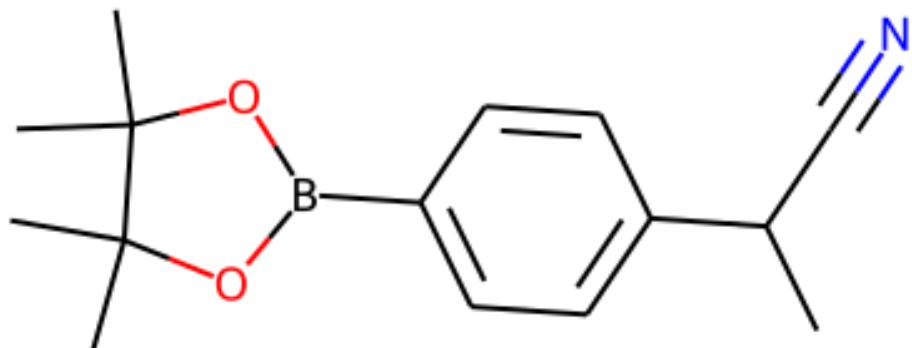


---

No.201

SMILES: CC(C#N)c1ccc(B2OC(C)(C)C(C)(C)O2)cc1

prob: 0.8

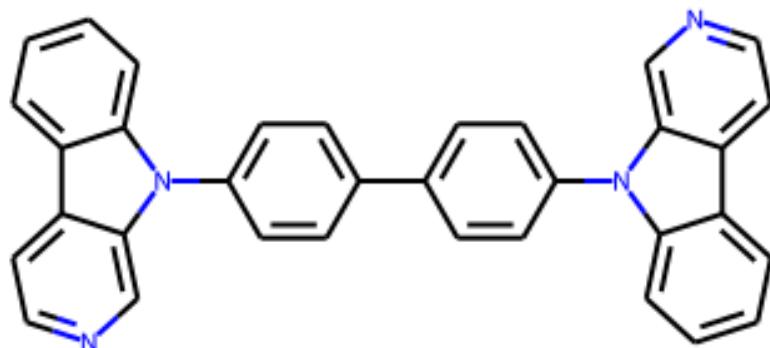


---

No.202

SMILES: c1ccc2c(c1)c1ccncc1n2-c1ccc(-c2ccc(-n3c4cccc4c4ccncc43)cc2)cc1

prob: 0.8

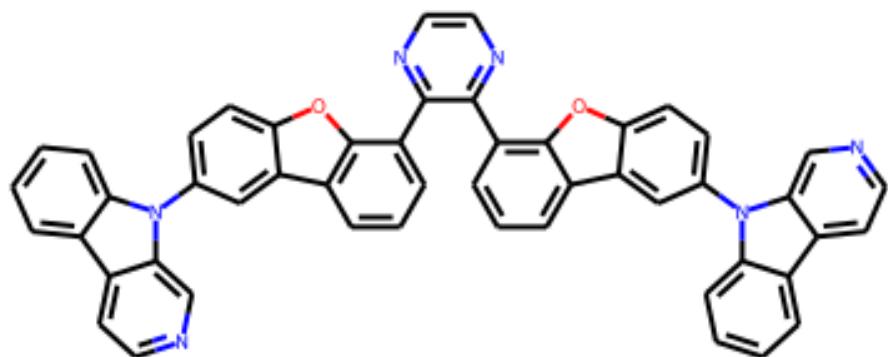


---

No.203

SMILES: c1cc(-c2ncnc2-c2cccc3c2oc2ccc(-n4c5cccc5c5ccncc54)cc23)c2oc3ccc(-n4c5cccc5c5ccncc54)cc3c2c1

prob: 0.8

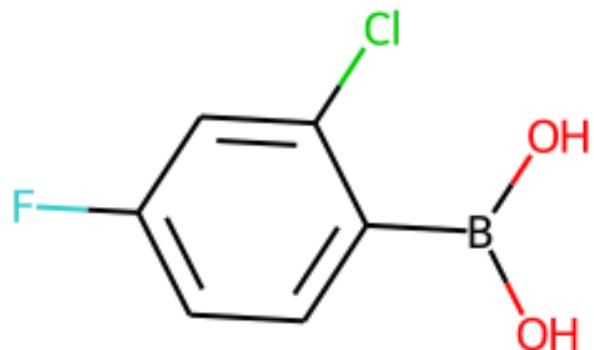


---

No.204

SMILES: OB(O)c1ccc(F)cc1Cl

prob: 0.8

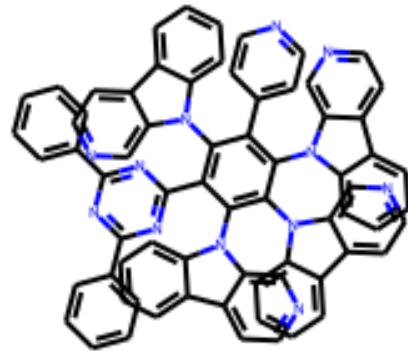


---

No.205

SMILES: c1ccc(-c2nc(-c3cccc3)nc(-c3c(-n4c5cccc5c5ccncc54)c(-c4ccncc4)c(-n4c5cccc5c5ccncc54)c(-n4c5cccc5c5ccncc54)c3-n3c4cccc4c4ccncc43)n2)cc1

prob: 0.8



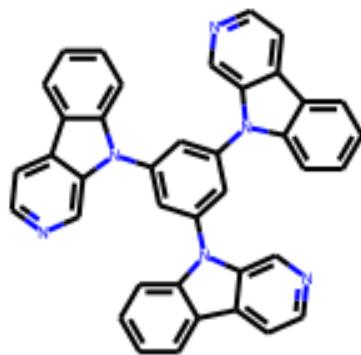
---

No.206

SMILES:

c1ccc2c(c1)cc1ccncc1n2-c1cc(-n2c3cccc3c3ccncc32)cc(-n2c3cccc3c3ccncc32)c1

prob: 0.8

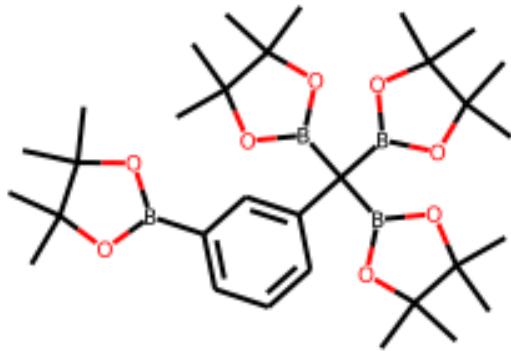


---

No.207

SMILES: CC1(C)OB(c2cccc(C(B3OC(C)(C)C(C)(C)O3)(B3OC(C)(C)C(C)(C)O3)B3OC(C)(C)C(C)(C)O3)c2)OC1(C)C

prob: 0.8

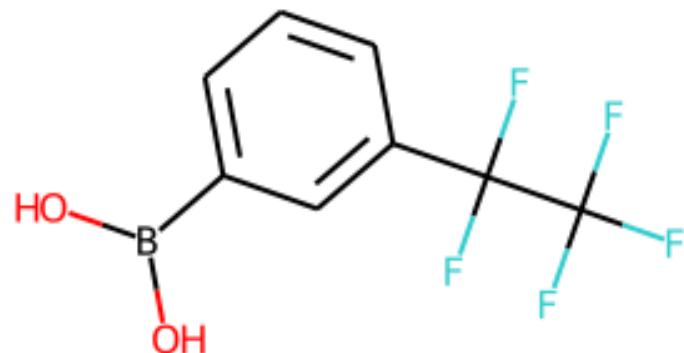


---

No. 208

SMILES: OB(0)c1ccccc(C(F)(F)C(F)(F)F)c1

prob: 0.8

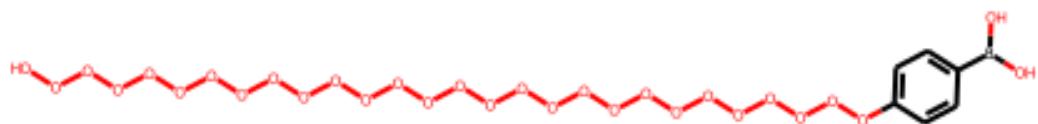


---

No. 209

SMILES: O00000000000000000000000000000000c1ccc(B(0)O)cc1

prob: 0.8

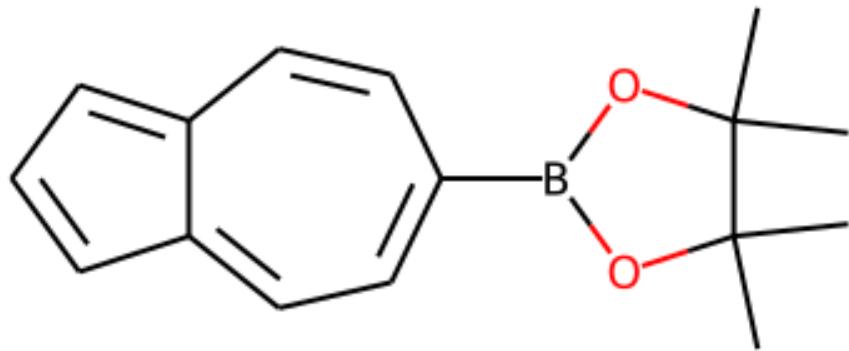


---

No.210

SMILES: CC1(C)OB(c2ccc3cccc-3cc2)OC1(C)C

prob: 0.8

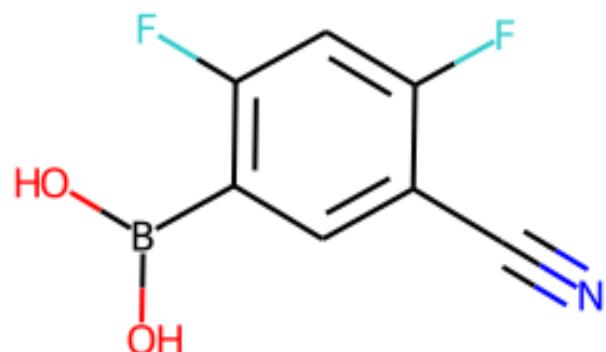


---

No.211

SMILES: N#Cc1cc(B(O)O)c(F)cc1F

prob: 0.8

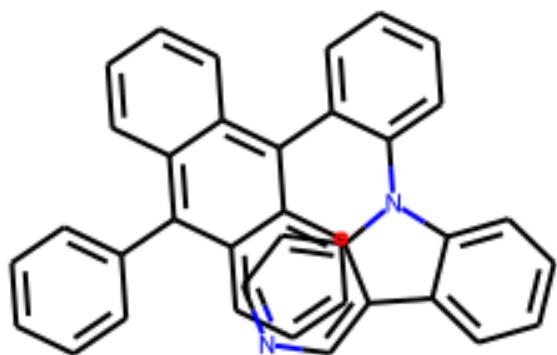


---

No.212

SMILES: c1ccc(-c2c3cccc3c(-c3cccc3-n3c4cccc4c4cnccc43)c3cccc23)cc1

prob: 0.8

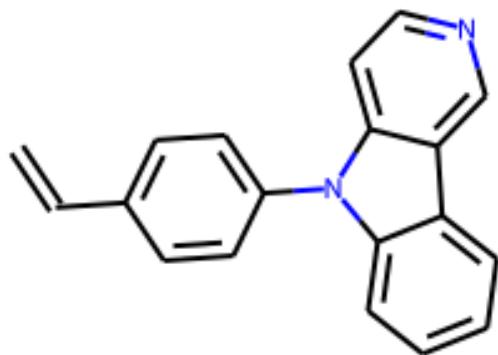


---

No. 213

SMILES: C=Cc1ccc(-n2c3cccc3c3cnccc32)cc1

prob: 0.8

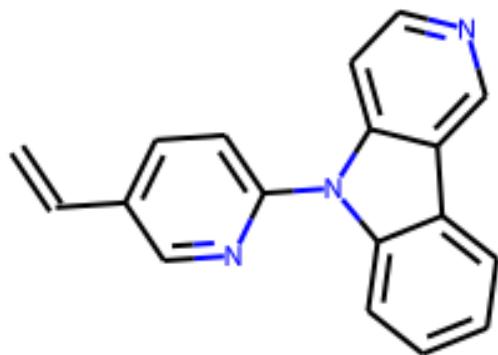


---

No. 214

SMILES: C=Cc1ccc(-n2c3cccc3c3cnccc32)nc1

prob: 0.8

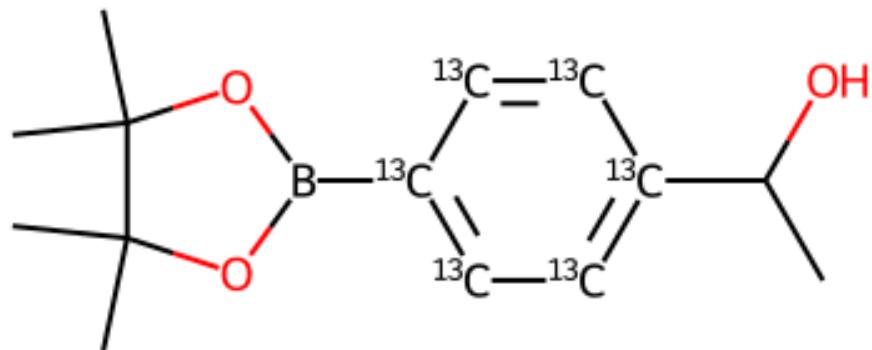


---

No. 215

SMILES: CC(O)[13c]1[13cH][13cH][13c](B2OC(C)(C)C(C)(C)O2)[13cH][13cH]1

prob: 0.8

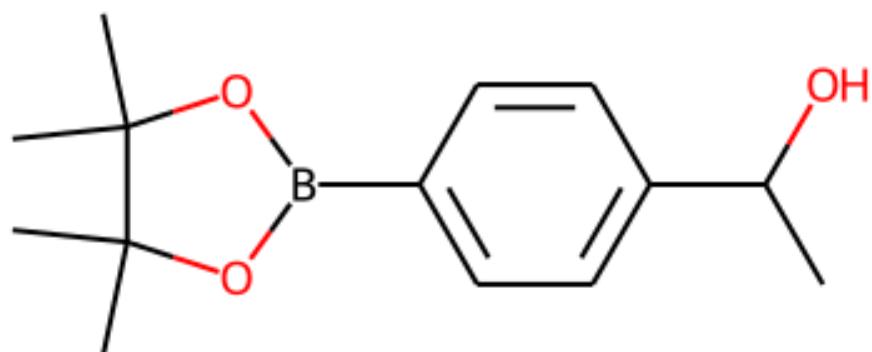


---

No. 216

SMILES: CC(O)c1ccc(B2OC(C)(C)C(C)(C)O2)cc1

prob: 0.8

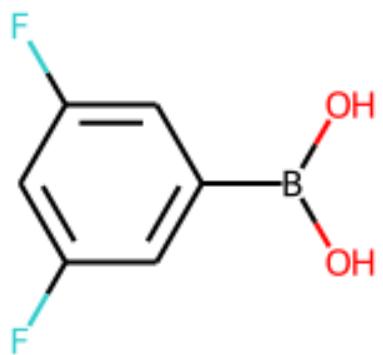


---

No. 217

SMILES: OB(O)c1cc(F)cc(F)c1

prob: 0.8

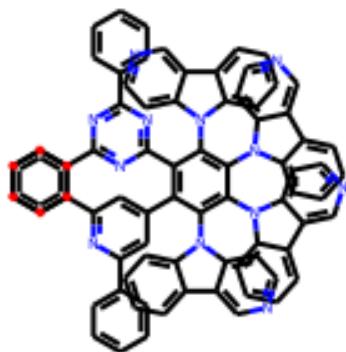


---

No. 218

SMILES: c1ccc(-c2cc(-c3c(-c4nc(-c5cccc5)nc(-c5cccc5)n4)c(-n4c5cccc5c5cnccc54)c(-n4c5cccc5c5cnccc54)c3-n3c4cccc4c4cnccc43)cc(-c3cccc3)n2)cc1

prob: 0.8

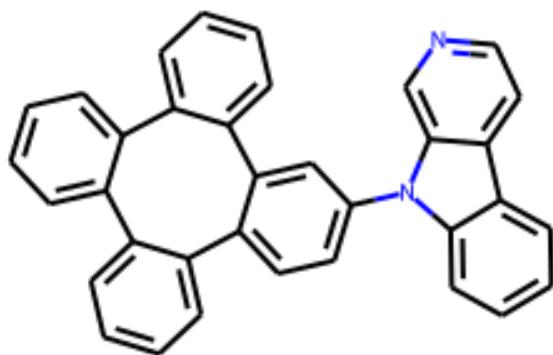


---

No. 219

SMILES: c1ccc2c(c1)-c1ccccc1-c1ccc(-n3c4cccc4c4ccncc43)cc1-c1ccccc1-2

prob: 0.8

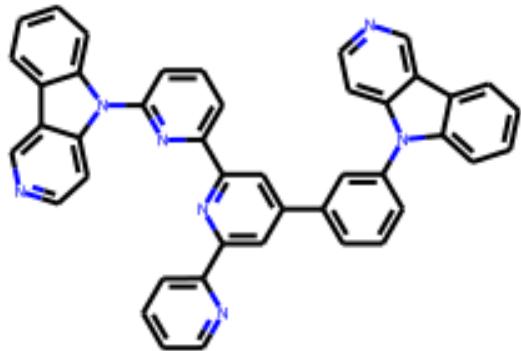


---

No.220

SMILES: c1ccc(-c2cc(-c3cccc(-n4c5cccc5c5cnccc54)c3)cc(-c3cccc(-n4c5cccc5c5cncc54)n3)n2)nc1

prob: 0.8



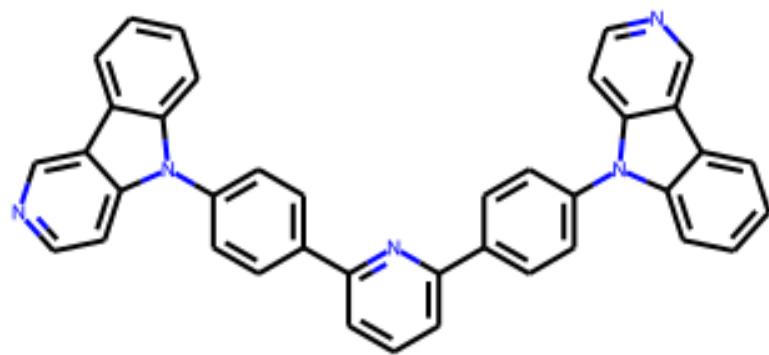
---

No.221

SMILES:

c1cc(-c2ccc(-n3c4cccc4c4cnccc43)cc2)nc(-c2ccc(-n3c4cccc4c4cnccc43)cc2)c1

prob: 0.8



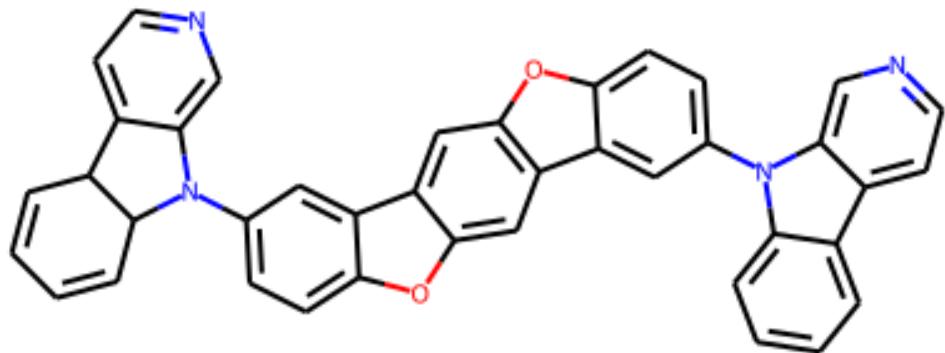
---

No.222

SMILES:

C1=CC2c3ccncc3N(c3ccc4oc5cc6c(cc5c4c3)oc3ccc(-n4c5cccc5c5ccncc54)cc36)C2C=C1

prob: 0.8

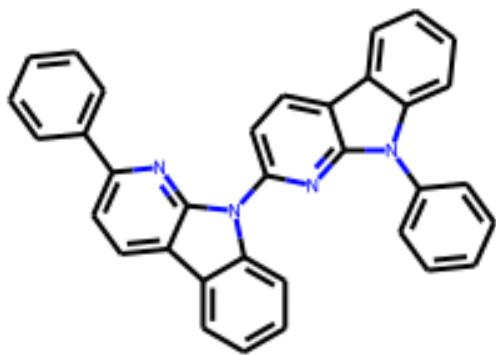


---

No.223

SMILES: c1ccc(-c2ccc3c4cccc4n(-c4ccc5c6cccc6n(-c6cccc6)c5n4)c3n2)cc1

prob: 0.8

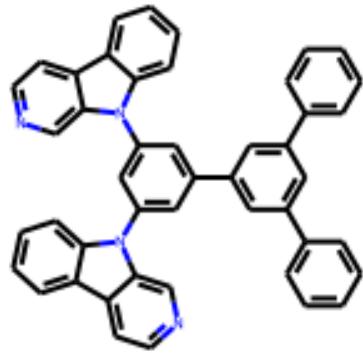


---

No.224

SMILES: c1ccc(-c2cc(-c3cccc3)cc(-c3cc(-n4c5cccc5c5ccncc54)cc(-n4c5cccc5c5ccnc54)c3)c2)cc1

prob: 0.8



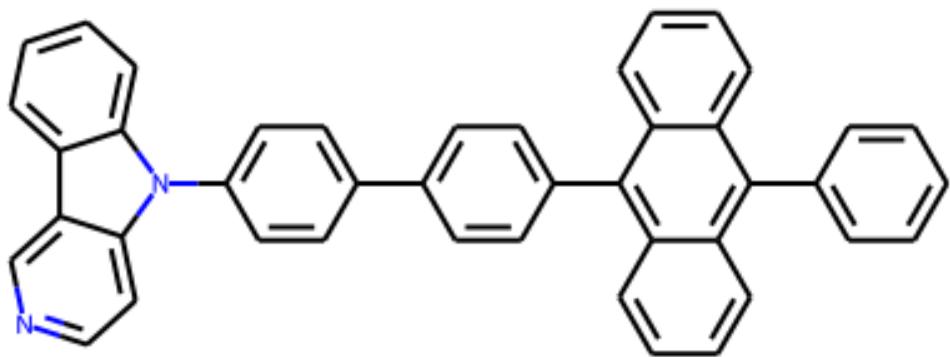
---

No.225

SMILES:

c1ccc(-c2c3cccc3c(-c3ccc(-c4ccc(-n5c6cccc6c6cnccc65)cc4)cc3)c3cccc23)cc1

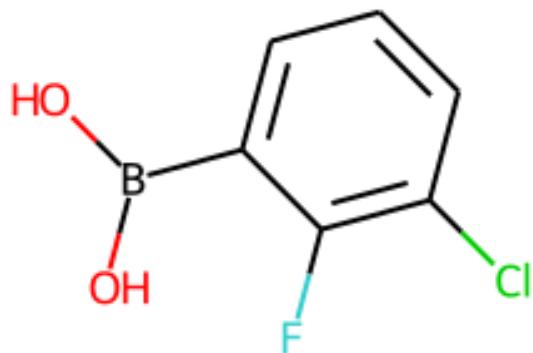
prob: 0.8



No.226

SMILES: OB(O)c1ccccc(Cl)c1F

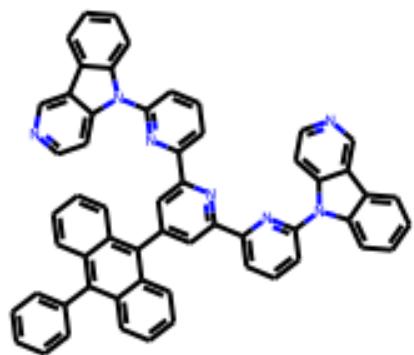
prob: 0.8



No.227

SMILES: c1ccc(-c2c3cccc3c(-c3cc(-c4cccc(-n5c6cccc6c6cnccc65)n4)nc(-c4cccc(-n5c6cccc6c6cnccc65)n4)c3)c3cccc23)cc1

prob: 0.8



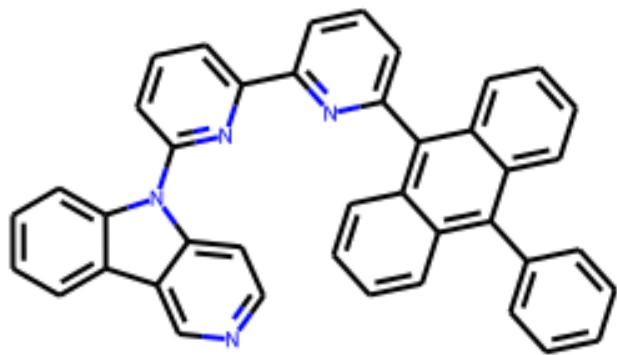
---

No.228

SMILES:

c1ccc(-c2c3cccc3c(-c3cccc(-c4cccc(-n5c6ccccc6c6cnccc65)n4)n3)c3ccccc23)cc1

prob: 0.8

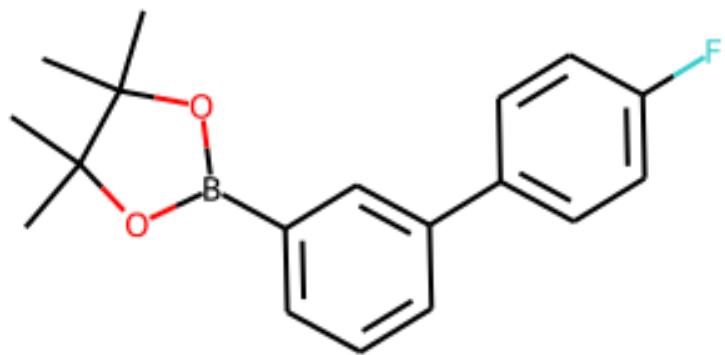


---

No.229

SMILES: CC1(C)OB(c2cccc(-c3ccc(F)cc3)c2)OC1(C)C

prob: 0.8

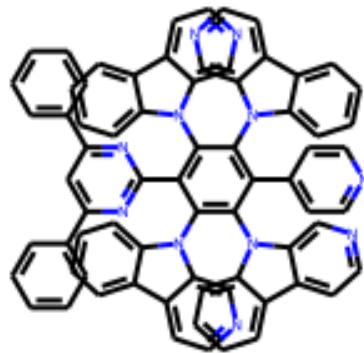


---

No. 230

SMILES: c1ccc(-c2cc(-c3cccc3)nc(-c3c(-n4c5cccc5c5ccncc54)c(-n4c5cccc5c5ccncc54)c(-c4ccncc4)c(-n4c5cccc5c5ccncc54)c3-n3c4cccc4c4ccncc43)n2)cc1

prob: 0.8

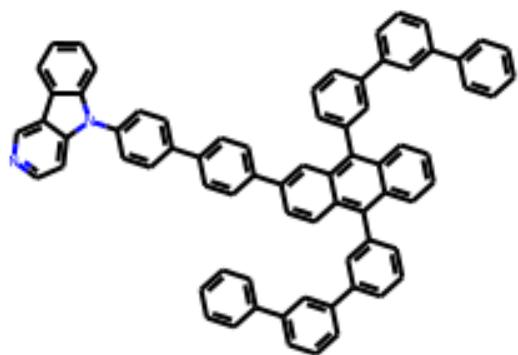


---

No. 231

SMILES: c1ccc(-c2cccc(-c3cccc(-c4c5cccc5c(-c5cccc(-c6cccc(-c7cccc7)c6)c5)c5cc(-c6ccc(-c7ccc(-n8c9cccc9c9cnccc98)cc7)cc6)ccc45)c3)c2)cc1

prob: 0.8

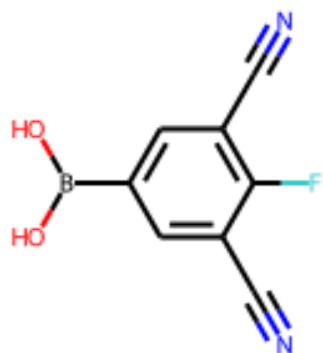


---

No.232

SMILES: N#Cc1cc(B(O)O)cc(C#N)c1F

prob: 0.8

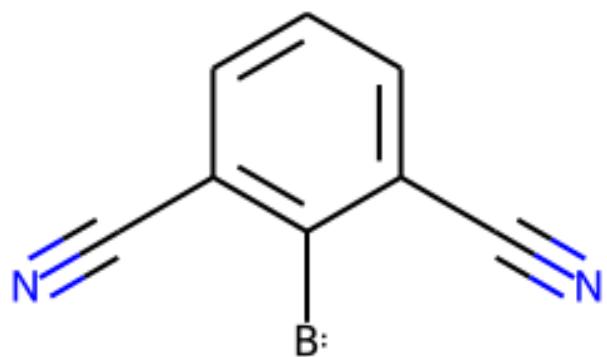


---

No.233

SMILES: [B]c1c(C#N)cccc1C#N

prob: 0.8

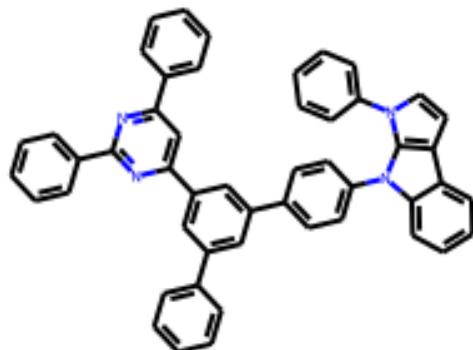


---

No.234

SMILES: c1ccc(-c2cc(-c3ccc(-n4c5cccc5c5ccn(-c6cccc6)c54)cc3)cc(-c3cc(-c4cccc4)nc(-c4cccc4)n3)c2)cc1

prob: 0.8

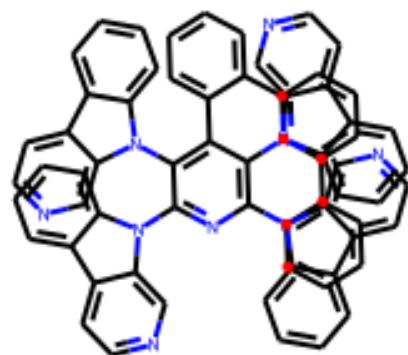


---

No.235

SMILES: c1ccc(-c2cccc(-c3cccc3-c3c(-n4c5cccc5c5ccncc54)c(-n4c5cccc5c5ccncc54)nc(-n4c5cccc5c5ccncc54)c3-n3c4cccc4c4ccncc43)n2)cc1

prob: 0.8

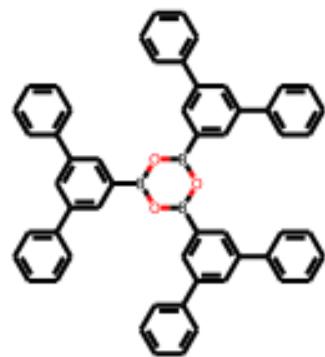


---

No.236

SMILES: c1ccc(-c2cc(B3OB(c4cc(-c5cccc5)cc(-c5cccc5)c4)OB(c4cc(-c5cccc5)cc(-c5cccc5)c4)O3)cc(-c3cccc3)c2)cc1

prob: 0.8

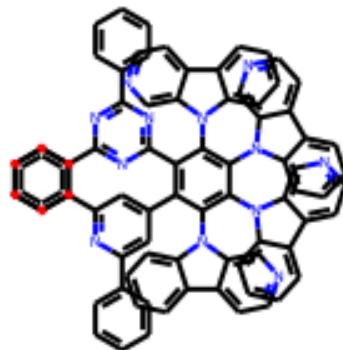


---

No. 237

SMILES: c1ccc(-c2cc(-c3c(-c4nc(-c5cccc5)nc(-c5ccccc5)n4)c(-n4c5cccc5c5ccncc54)c(-n4c5cccc5c5ccncc54)c3-n3c4cccc4c4ccncc43)cc(-c3cccc3)n2)cc1

prob: 0.8

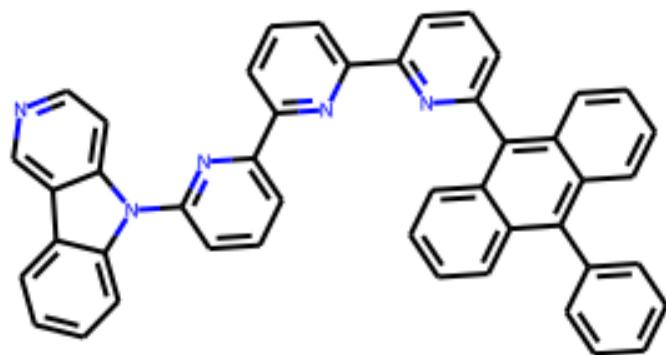


---

No. 238

SMILES: c1ccc(-c2c3cccc3c(-c3cccc(-c4cccc(-c5cccc(-n6c7cccc7c7cnccc76)n5)n4)n3)c3cccc23)cc1

prob: 0.8

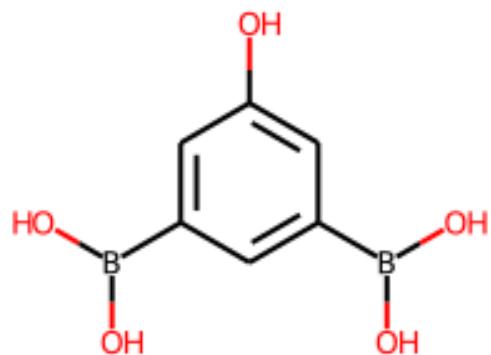


---

No.239

SMILES: OB(O)c1cc(O)cc(B(O)O)c1

prob: 0.8

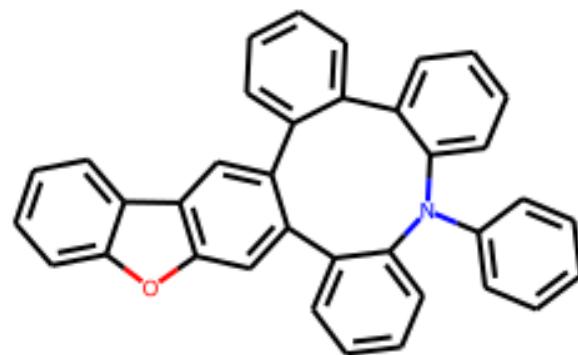


---

No.240

SMILES: c1ccc(-n2c3cccc3c3cccc3c3cc4c(cc3c3cccc32)oc2cccc24)cc1

prob: 0.8

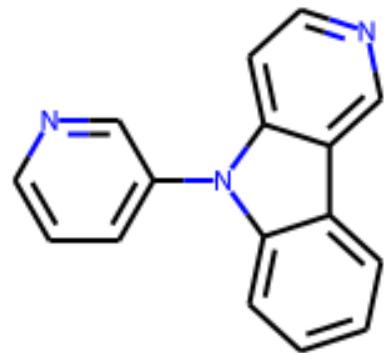


---

No.241

SMILES: c1cncc(-n2c3cccc3c3cnccc32)c1

prob: 0.8

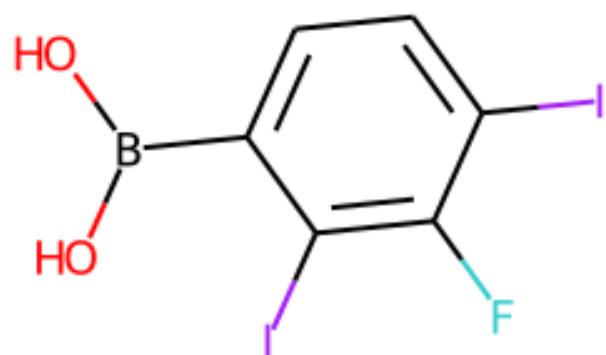


---

No.242

SMILES: OB(O)c1ccc(I)c(F)c1I

prob: 0.8

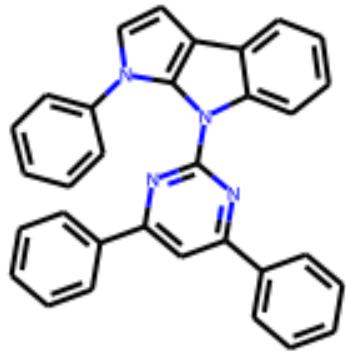


---

No.243

SMILES: c1ccc(-c2cc(-c3cccc3)nc(-n3c4cccc4c4ccn(-c5cccc5)c43)n2)cc1

prob: 0.8

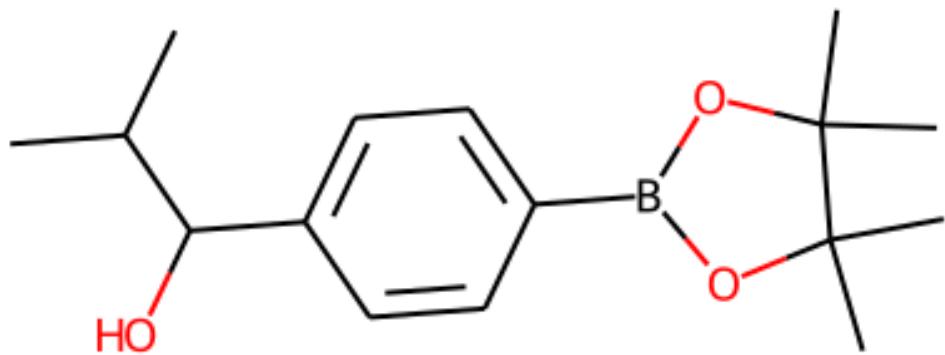


---

No. 244

SMILES: CC(C)C(O)c1ccc(B2OC(C)(C)C(C)O2)cc1

prob: 0.8



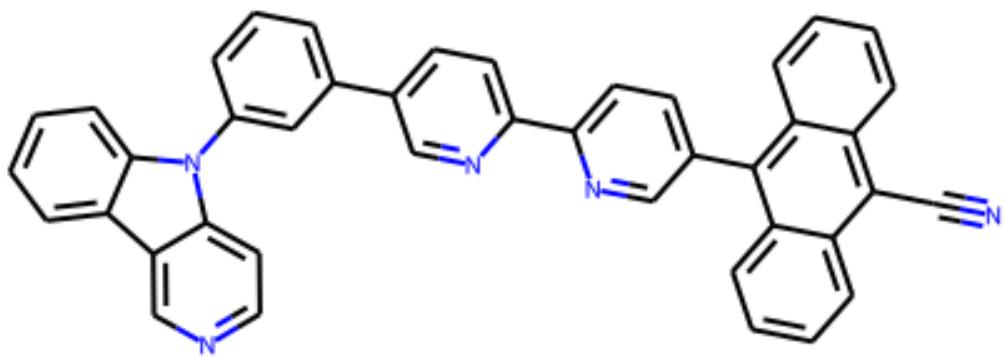
---

No. 245

SMILES:

N#Cc1c2cccc2c(-c2ccc(-c3ccc(-c4cccc(-n5c6cccc6c6cnccc65)c4)cn3)nc2)c2ccccc12

prob: 0.8

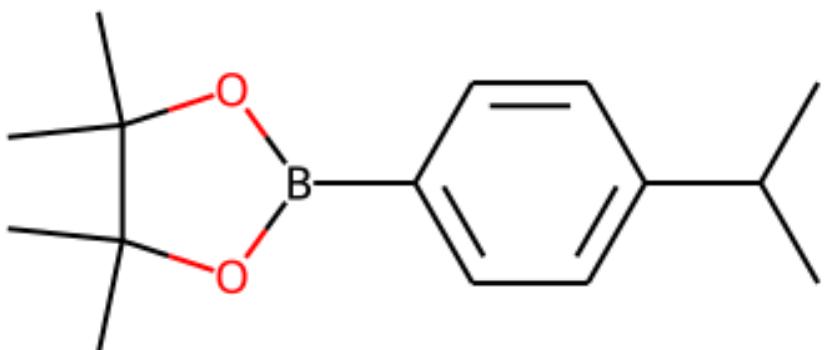


---

No. 246

SMILES: CC(C)c1ccc(B2OC(C)(C)C(C)(C)O2)cc1

prob: 0.8

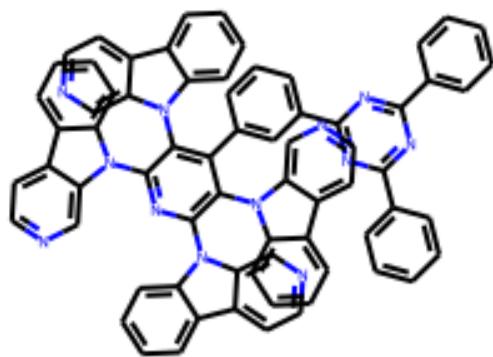


---

No. 247

SMILES: c1ccc(-c2nc(-c3cccc3)nc(-c3cccc(-c4c(-n5c6cccc6c6ccncc65)c(-n5c6cccc6c6ccncc65)nc(-n5c6cccc6c6ccncc65)c4-n4c5cccc5c5ccncc54)c3)n2)cc1

prob: 0.8

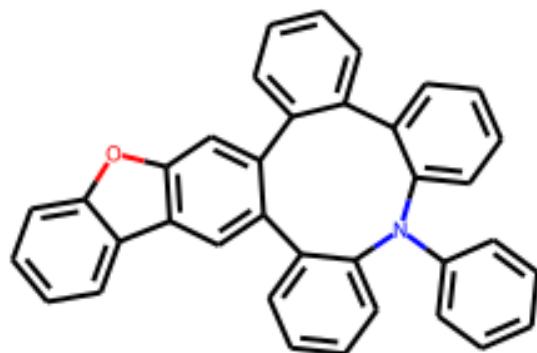


---

No. 248

SMILES: c1ccc(-n2c3cccc3c3ccccc3c3cc4oc5ccccc5c4cc3c3ccccc32)cc1

prob: 0.8

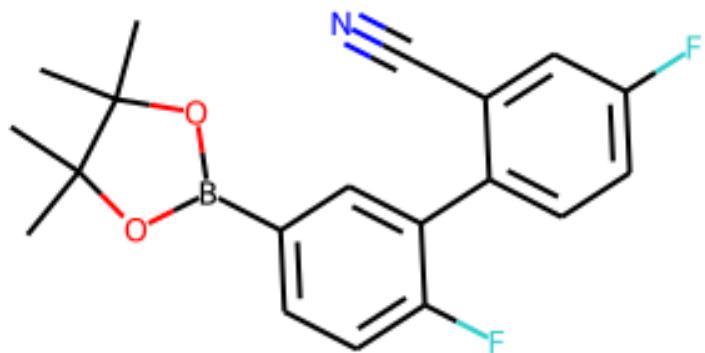


---

No. 249

SMILES: CC1(C)OB(c2ccc(F)c(-c3ccc(F)cc3C#N)c2)OC1(C)C

prob: 0.79

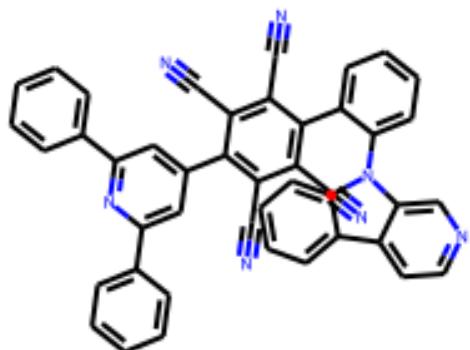


---

No.250

SMILES: N#Cc1c(C#N)c(-c2ccccc2-n2c3cccc3c3ccncc32)c(C#N)c(C#N)c1-c1cc(-c2ccccc2)nc(-c2ccccc2)c1

prob: 0.79



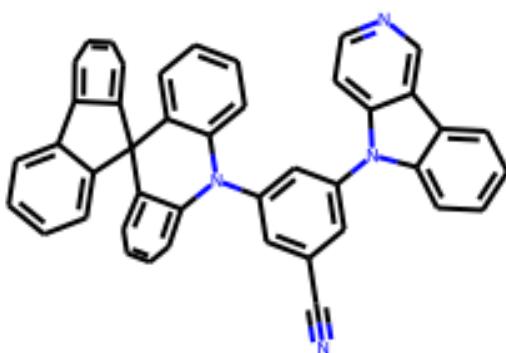
---

No.251

SMILES:

N#Cc1cc(N2c3cccc3C3(c4ccccc4-c4ccccc43)c3cccc32)cc(-n2c3cccc3c3cnccc32)c1

prob: 0.79

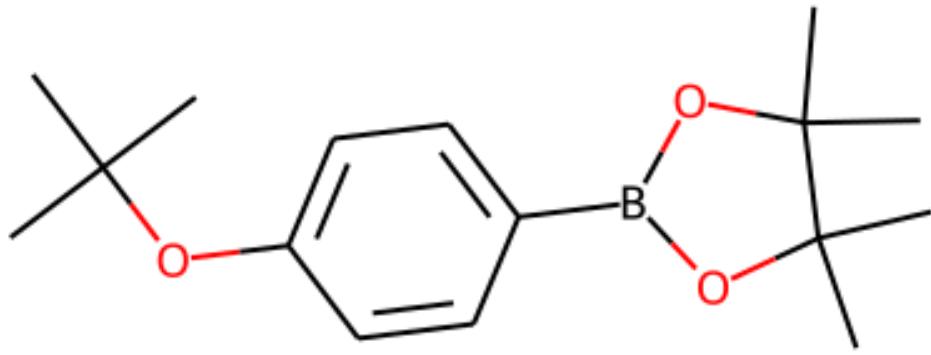


---

No.252

SMILES: CC(C)(C)Oc1ccc(B2OC(C)(C)C(C)(C)O2)cc1

prob: 0.79

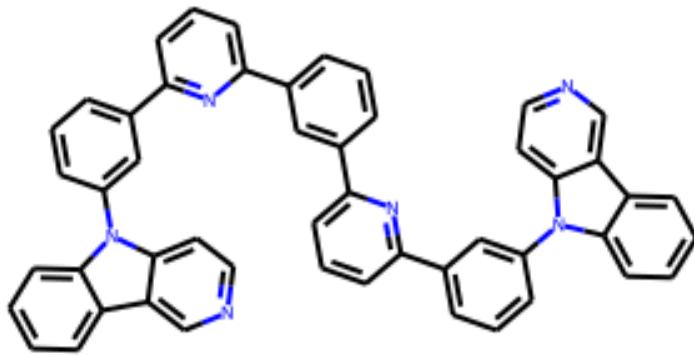


---

No. 253

SMILES: c1cc(-c2cccc(-c3cccc(-n4c5cccc5c5cnccc54)c3)n2)cc(-c2cccc(-c3cccc(-n4c5cccc5c5cnccc54)c3)n2)c1

prob: 0.79

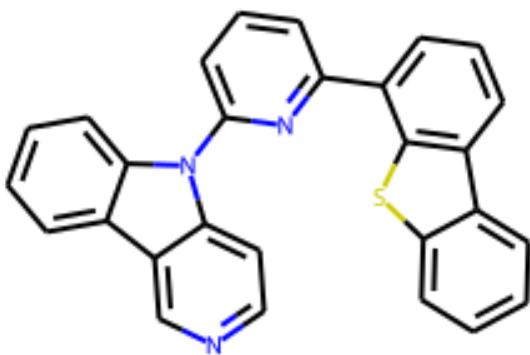


---

No. 254

SMILES: c1cc(-c2cccc3c2sc2cccc23)nc(-n2c3cccc3c3cnccc32)c1

prob: 0.79

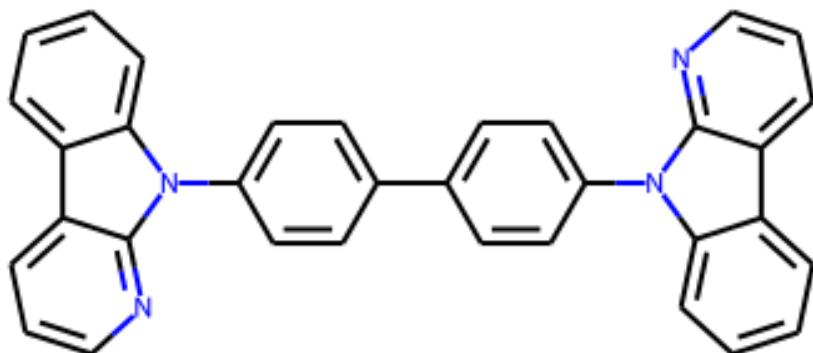


---

No. 255

SMILES: c1ccc2c(c1)c1cccn1n2-c1ccc(-c2ccc(-n3c4cccc4c4ccnc43)cc2)cc1

prob: 0.79

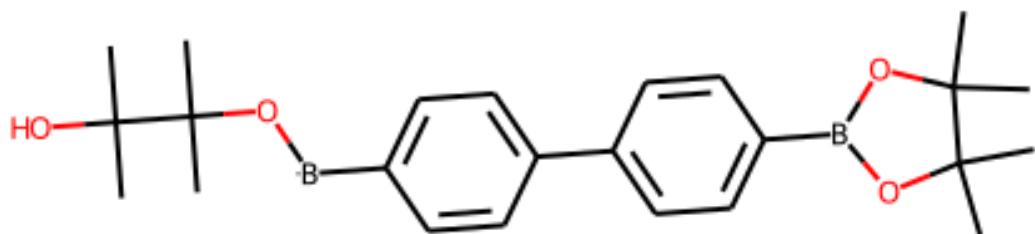


---

No. 256

SMILES: CC(C)(O)C(C)(C)OB[c]c1ccc(-c2ccc(B3OC(C)(C)C(C)(C)O3)cc2)cc1

prob: 0.79

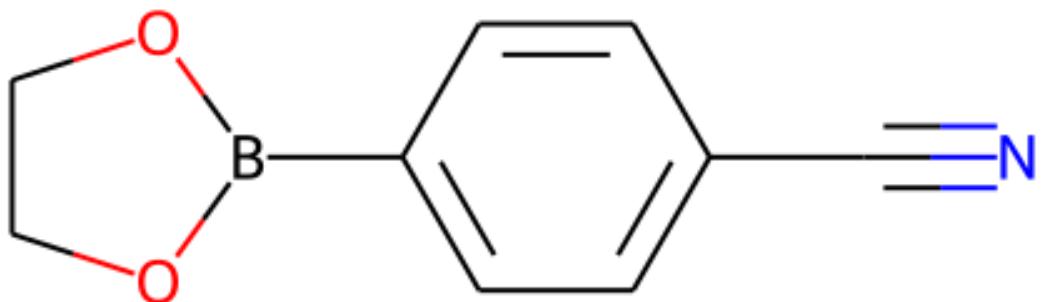


---

No.257

SMILES: N#Cc1cccc(B2OCCO2)cc1

prob: 0.79

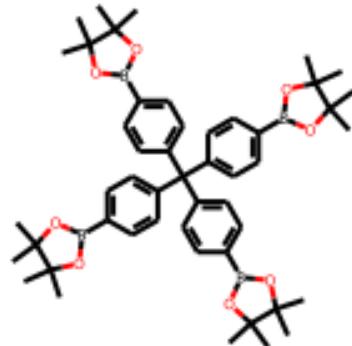


---

No.258

SMILES: CC1(C)OB(c2ccc(C(c3ccc(B4OC(C)(C)C(C)O4)cc3)(c3ccc(B4OC(C)(C)C(C)(C)O4)cc3)c3ccc(B4OC(C)(C)C(C)O4)cc3)cc2)OC1(C)C

prob: 0.79

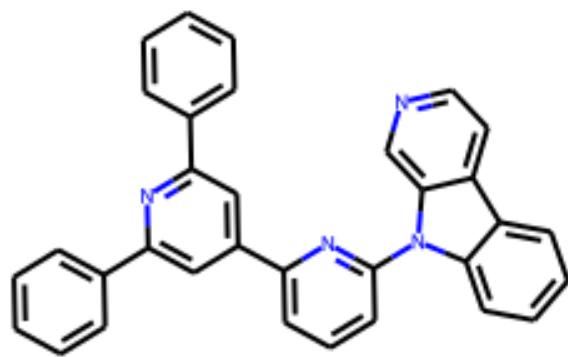


---

No.259

SMILES: c1ccc(-c2cc(-c3cccc(-n4c5ccccc5c5ccncc54)n3)cc(-c3ccccc3)n2)cc1

prob: 0.79

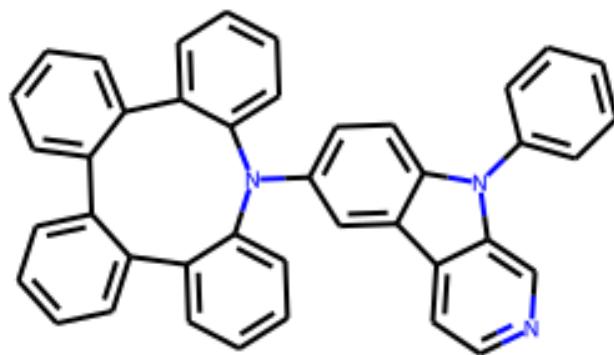


---

No.260

SMILES: c1ccc(-n2c3ccc(-n4c5cccc5c5cccc5c5cccc5c5cccc54)cc3c3cncc32)cc1

prob: 0.79



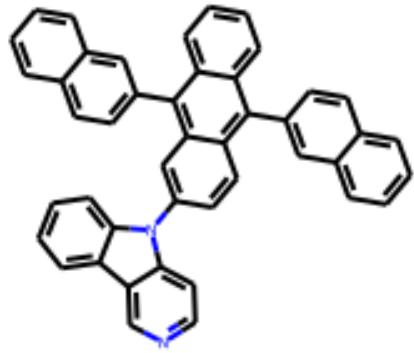
---

No.261

SMILES:

c1ccc2cc(-c3c4cccc4c(-c4ccc5cccc5c4)c4cc(-n5c6cccc6c6cnccc65)ccc34)ccc2c1

prob: 0.79

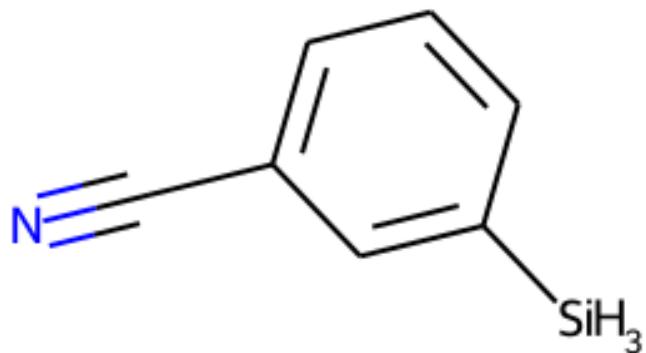


---

No. 262

SMILES: N#Cc1ccccc([SiH3])c1

prob: 0.79

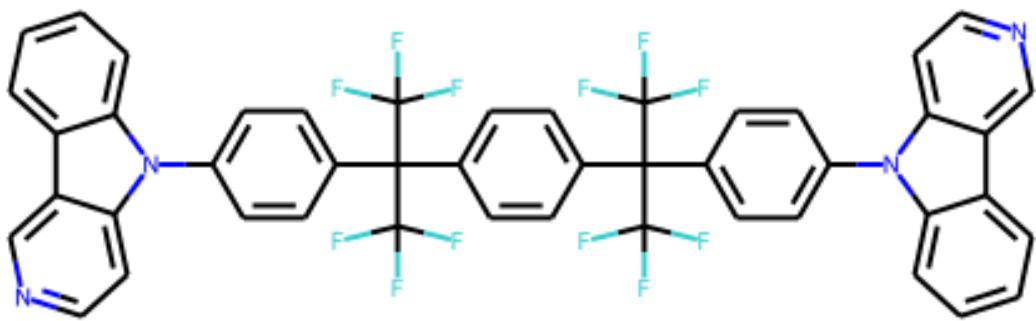


---

No. 263

SMILES: FC(F)(F)C(c1ccc(-n2c3cccc3c3cnccc32)cc1)(c1ccc(C(c2ccc(-n3c4cccc4c4cnc4)cc3)cc2)(C(F)(F)F)C(F)(F)F)cc1)C(F)(F)F

prob: 0.79

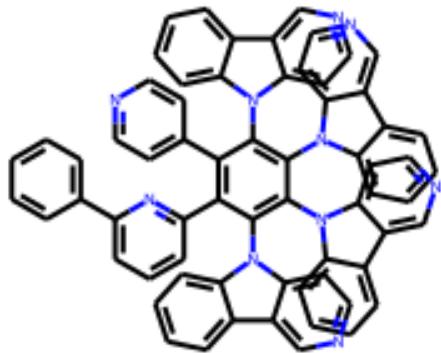


---

No. 264

SMILES: c1ccc(-c2cccc(-c3c(-c4ccncc4)c(-n4c5cccc5c5cnccc54)c(-n4c5cccc5c5cnccc54)c(-n4c5cccc5c5cnccc54)c3-n3c4cccc4c4cnccc43)n2)cc1

prob: 0.79



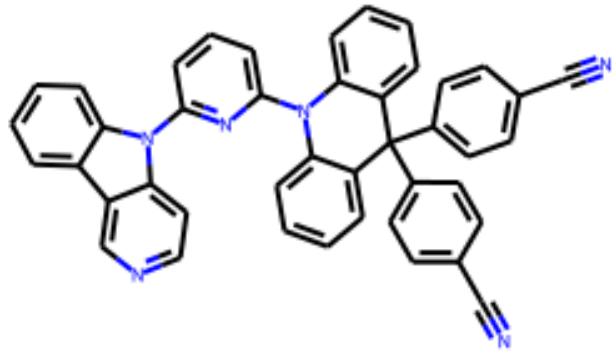
---

No. 265

SMILES:

N#Cc1cccc(C2(c3ccc(C#N)cc3)c3cccc3N(c3cccc(-n4c5cccc5c5cnccc54)n3)c3cccc32)cc1

prob: 0.79



---

No.266

SMILES: c1ccc(-n2c3cccc3c3cccc3c3cc4sc5cccc5c4cc3c3cccc32)cc1

prob: 0.79

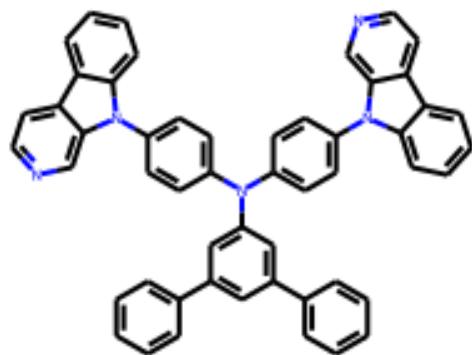


---

No.267

SMILES: c1ccc(-c2cc(-c3cccc3)cc(N(c3ccc(-n4c5cccc5c5ccncc54)cc3)c3ccc(-n4c5ccc5c5ccncc54)cc3)c2)cc1

prob: 0.79

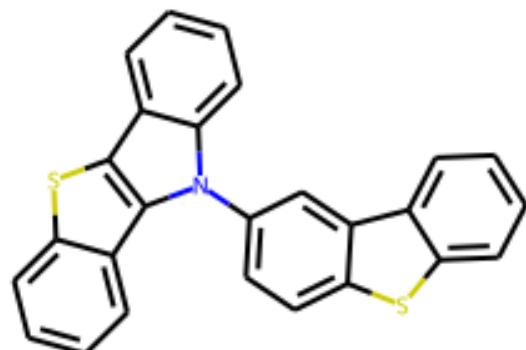


---

No. 268

SMILES: c1ccc2c(c1)sc1ccc(-n3c4cccc4c4sc5cccc5c43)cc12

prob: 0.79

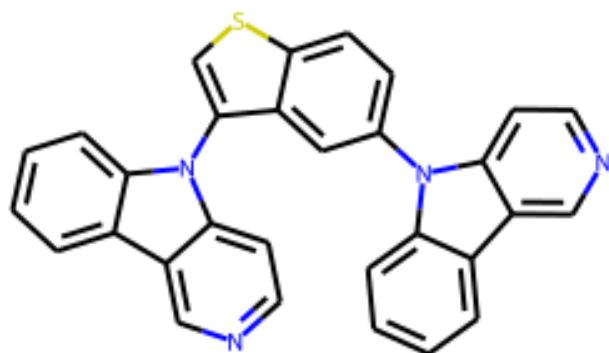


---

No. 269

SMILES: c1ccc2c(c1)c1cnccc1n2-c1ccc2scc(-n3c4cccc4c4cnccc43)c2c1

prob: 0.79

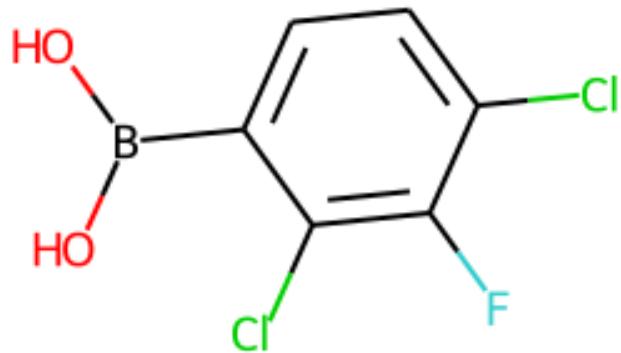


---

No.270

SMILES: OB(O)c1ccc(Cl)c(F)c1Cl

prob: 0.79

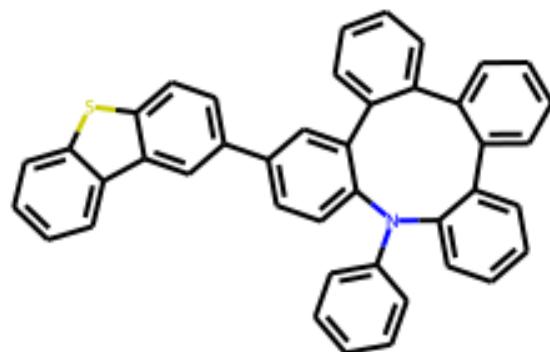


---

No.271

SMILES: c1ccc(-n2c3cccc3c3cccc3c3cccc3c3cc(-c4ccc5sc6cccc6c5c4)ccc32)cc1

prob: 0.79



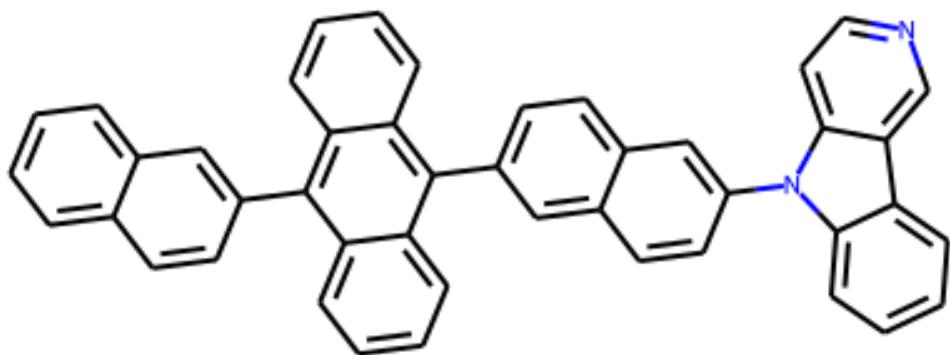
---

No.272

SMILES:

c1cccc2cc(-c3c4cccc4c(-c4ccc5cc(-n6c7cccc7c7cnccc76)ccc5c4)c4cccc34)ccc2c1

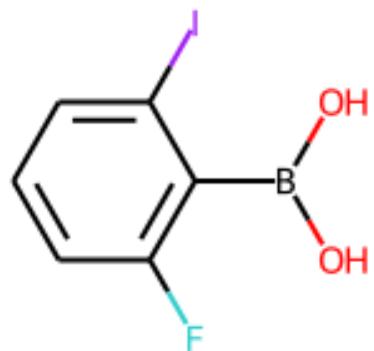
prob: 0.79



No.273

SMILES: OB(O)c1c(F)ccccc1I

prob: 0.79

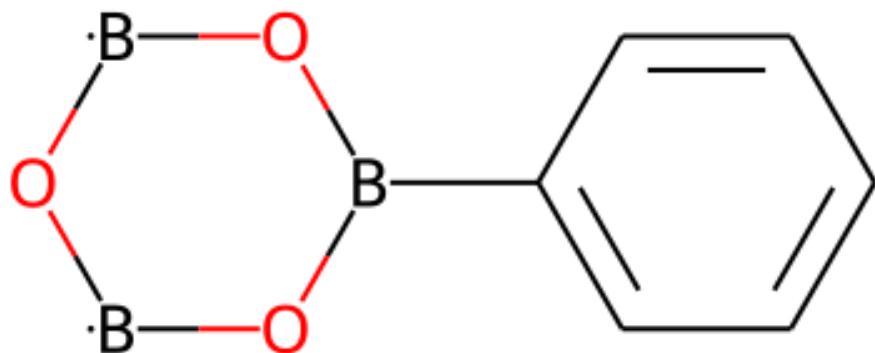


---

No.274

SMILES: [B]10[B]OB(c2ccccc2)O1

prob: 0.79

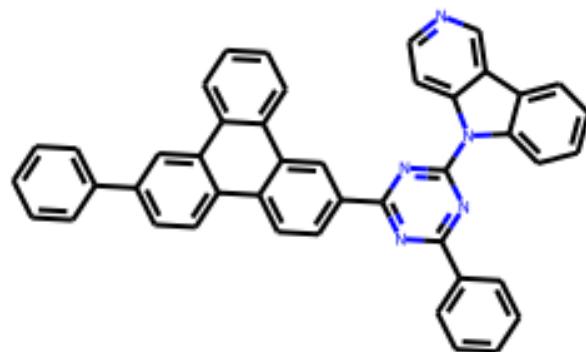


---

No.275

SMILES: c1ccc(-c2ccc3c4ccc(-c5nc(-c6cccc6)nc(-n6c7ccccc7c7cnccc76)n5)cc4c4cccc  
4c3c2)cc1

prob: 0.79

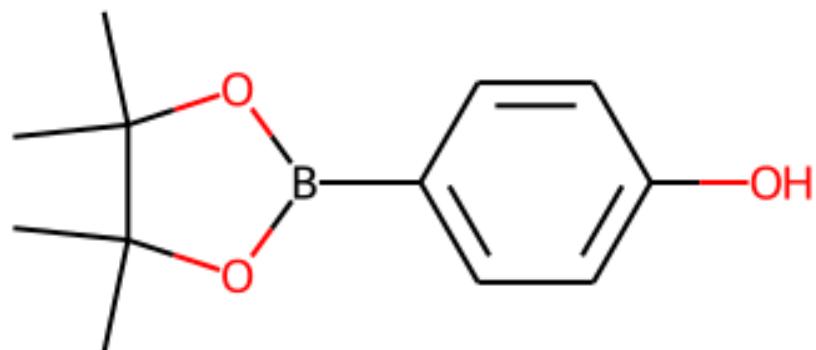


---

No.276

SMILES: CC1(C)OB(c2ccc(0)cc2)OC1(C)C

prob: 0.79

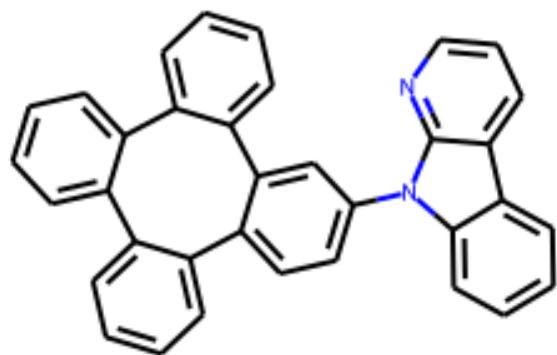


---

No.277

SMILES: c1ccc2c(c1)-c1ccccc1-c1ccc(-n3c4cccc4c4cccnc43)cc1-c1ccccc1-2

prob: 0.79

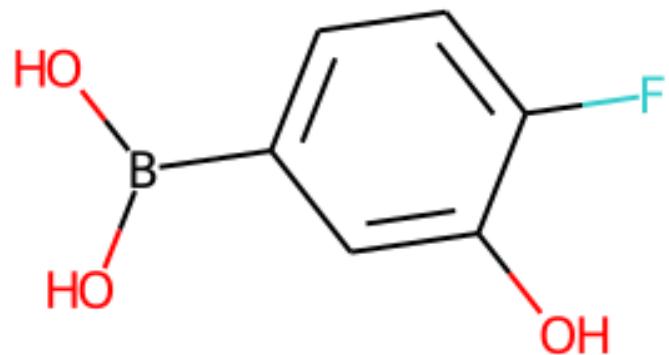


---

No. 278

SMILES: OB(O)c1ccc(F)c(O)c1

prob: 0.79

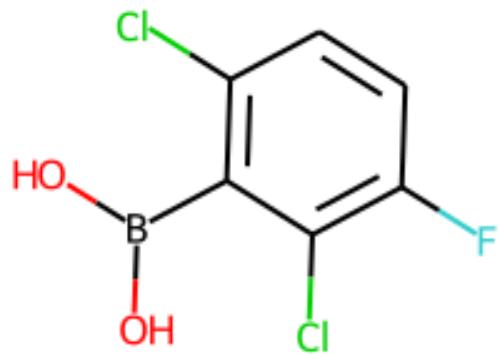


---

No. 279

SMILES: OB(O)c1c(Cl)ccc(F)c1Cl

prob: 0.79

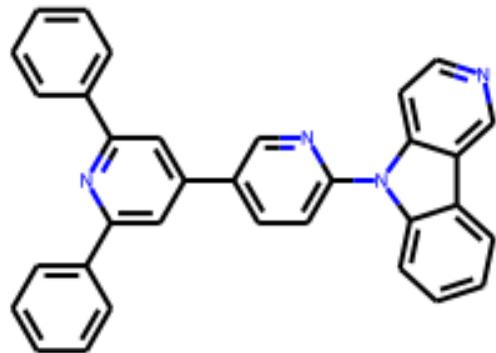


---

No. 280

SMILES: c1ccc(-c2cc(-c3ccc(-n4c5cccc5c5cnccc54)nc3)cc(-c3cccc3)n2)cc1

prob: 0.79

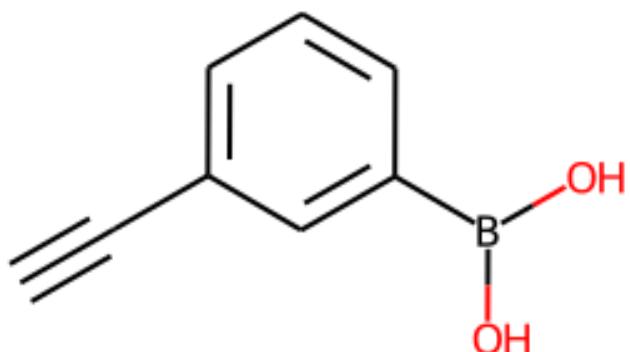


---

No. 281

SMILES: C#Cc1ccccc(B(O)O)c1

prob: 0.79

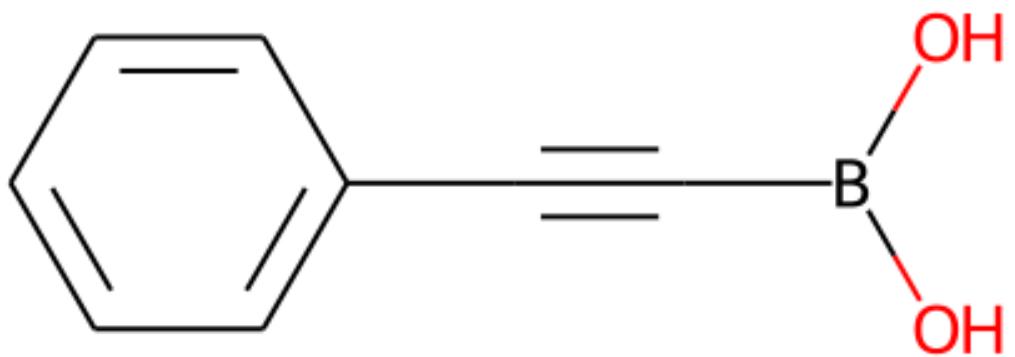


---

No. 282

SMILES: OB(O)C#Cc1ccccc1

prob: 0.79

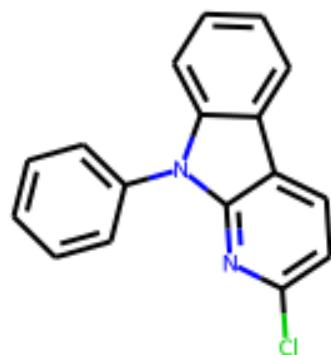


---

No. 283

SMILES: Clc1ccc2c3cccc3n(-c3ccccc3)c2n1

prob: 0.79

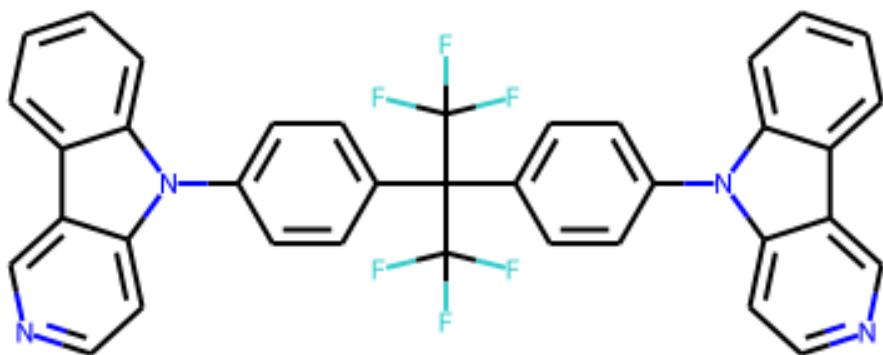


---

No. 284

SMILES: FC(F)(F)C(c1ccc(-n2c3cccc3c3cnccc32)cc1)(c1ccc(-n2c3cccc3c3cnccc32)cc1)C(F)(F)F

prob: 0.79

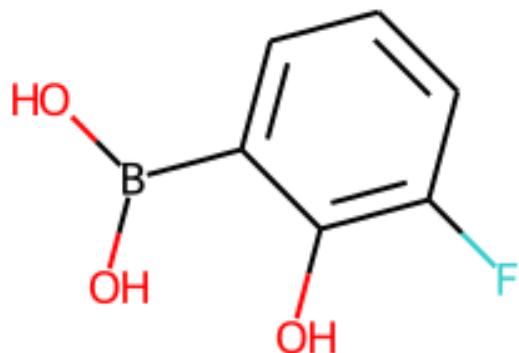


---

No. 285

SMILES: OB(O)c1ccccc(F)c1O

prob: 0.79

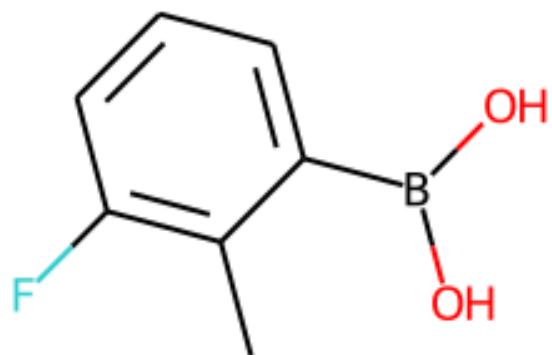


---

No. 286

SMILES: Cc1c(F)cccc1B(O)O

prob: 0.79

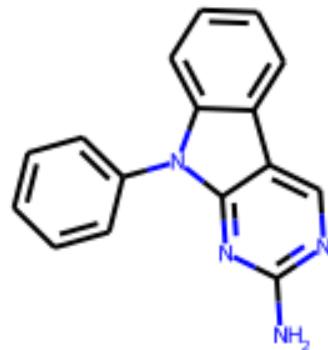


---

No.287

SMILES: Nc1ncc2c3cccc3n(-c3cccc3)c2n1

prob: 0.79

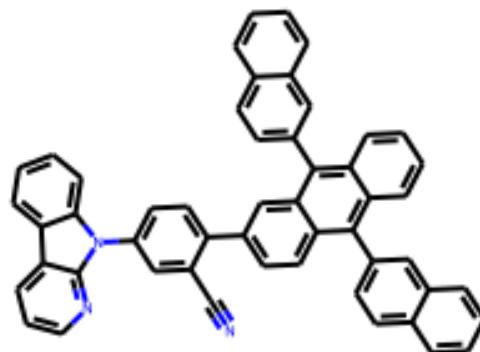


---

No.288

SMILES: N#Cc1cc(-n2c3cccc3c3ccnc32)ccc1-c1ccc2c(-c3ccc4cccc4c3)c3cccc3c(-c3cc4cccc4c3)c2c1

prob: 0.79

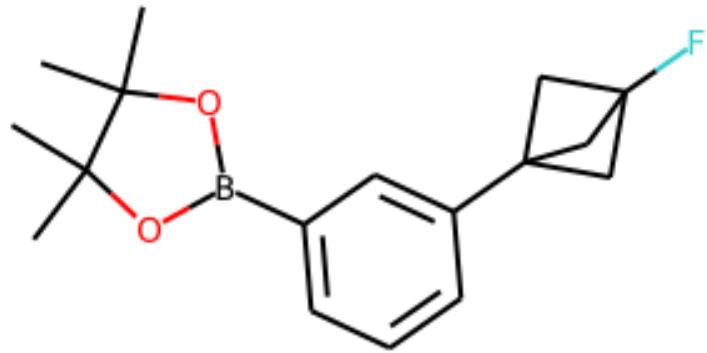


---

No.289

SMILES: CC1(C)OB(c2ccccc(C34CC(F)(C3)C4)c2)OC1(C)C

prob: 0.79

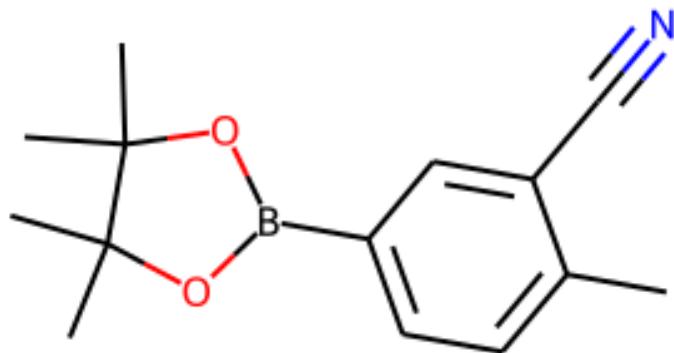


---

No. 290

SMILES: Cc1ccc(B2OC(C)(C)C(C)(C)O2)cc1C#N

prob: 0.79

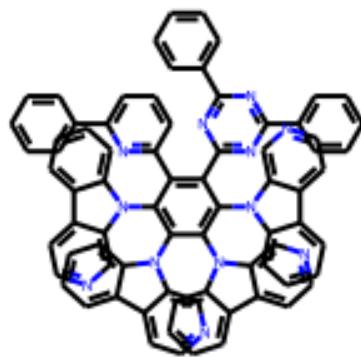


---

No. 291

SMILES: c1cccc(-c2cccc(-c3c(-c4nc(-c5cccc5)nc(-c5cccc5)n4)c(-n4c5cccc5c5ccncc54)c(-n4c5cccc5c5ccncc54)c3-n3c4cccc4c4ccncc43)n2)cc1

prob: 0.79

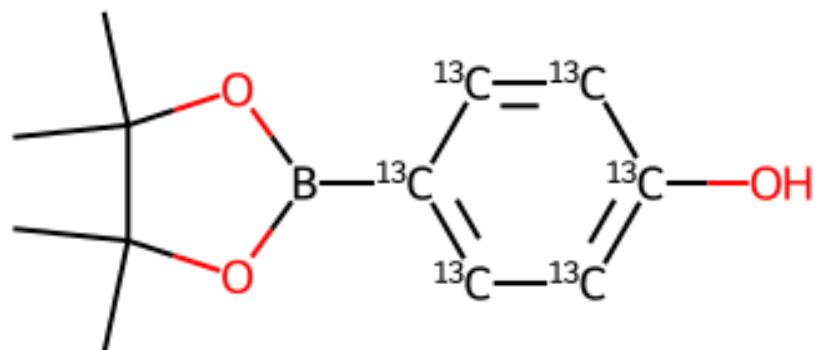


---

No. 292

SMILES: CC1(C)OB([13c]2[13cH][13cH][13c](O)[13cH][13cH]2)OC1(C)C

prob: 0.79



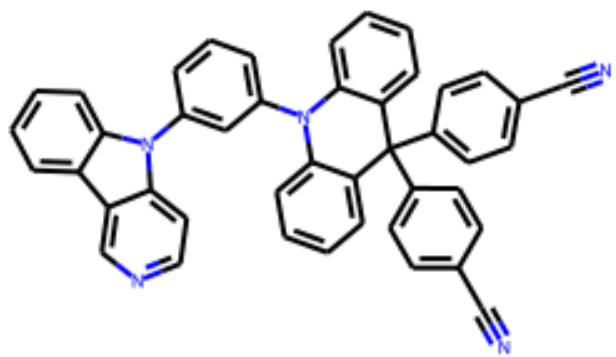
---

No. 293

SMILES:

N#Cc1ccc(C2(c3ccc(C#N)cc3)c3cccc3N(c3cccc(-n4c5cccc5c5cnccc54)c3)c3cccc32)cc1

prob: 0.79

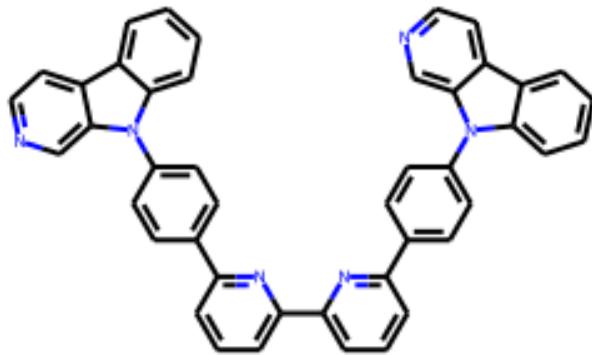


---

No. 294

SMILES: c1cc(-c2ccc(-n3c4cccc4c4ccncc43)cc2)nc(-c2cccc(-c3ccc(-n4c5cccc5c5ccnc  
c54)cc3)n2)c1

prob: 0.79

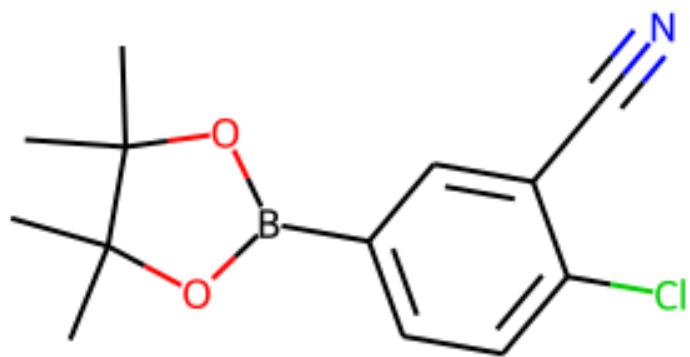


---

No. 295

SMILES: CC1(C)OB(c2ccc(C1)c(C#N)c2)OC1(C)C

prob: 0.79

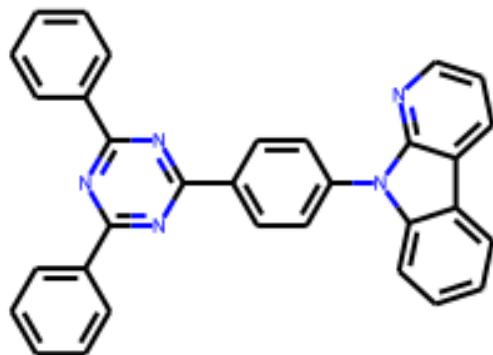


---

No.296

SMILES: c1ccc(-c2nc(-c3ccccc3)nc(-c3ccc(-n4c5cccc5c5cccnc54)cc3)n2)cc1

prob: 0.79

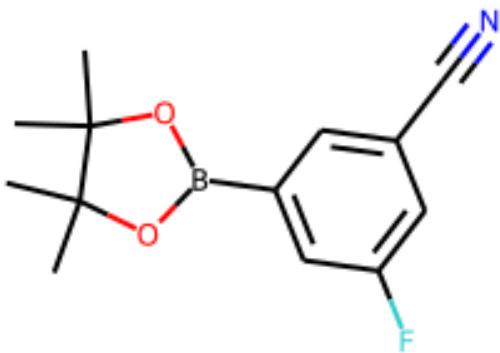


---

No.297

SMILES: CC1(C)OB(c2cc(F)cc(C#N)c2)OC1(C)C

prob: 0.79

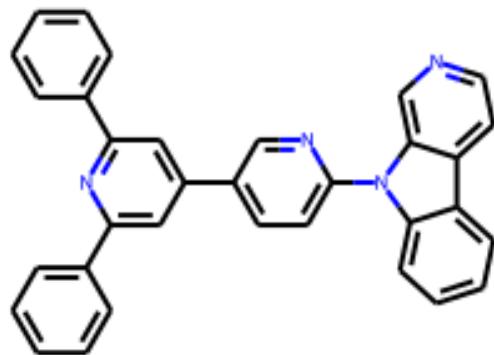


---

No.298

SMILES: c1ccc(-c2cc(-c3ccc(-n4c5cccc5c5ccncc54)nc3)cc(-c3ccccc3)n2)cc1

prob: 0.79

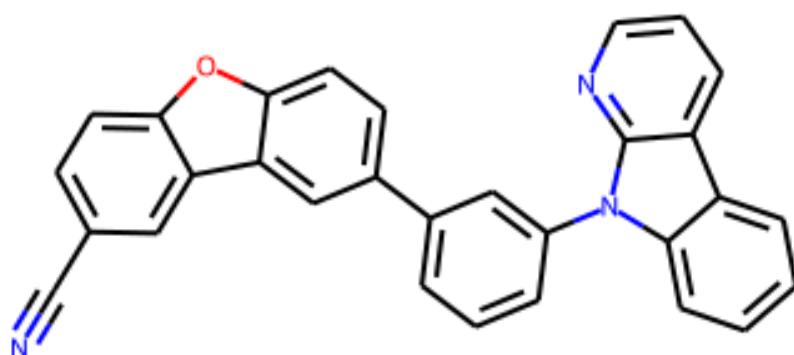


---

No.299

SMILES: N#Cc1ccc2oc3ccc(-c4cccc(-n5c6cccc6c6cccnc65)c4)cc3c2c1

prob: 0.79

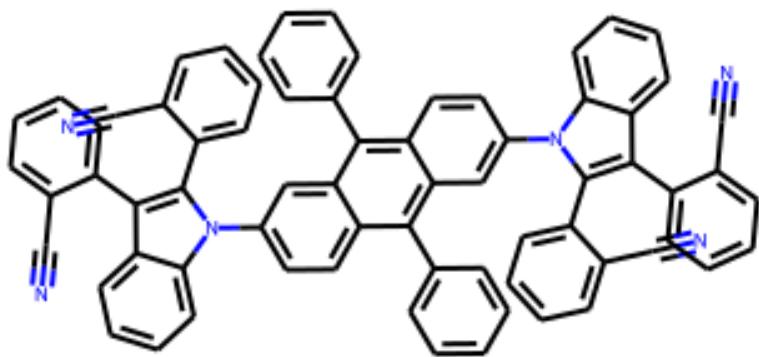


---

No.300

SMILES: N#Cc1ccccc1-c1c(-c2ccccc2C#N)n(-c2ccc3c(-c4ccccc4)c4cc(-n5c(-c6ccccc6C#N)c(-c6ccccc6C#N)c6ccccc65)ccc4c(-c4ccccc4)c3c2)c2ccccc12

prob: 0.79

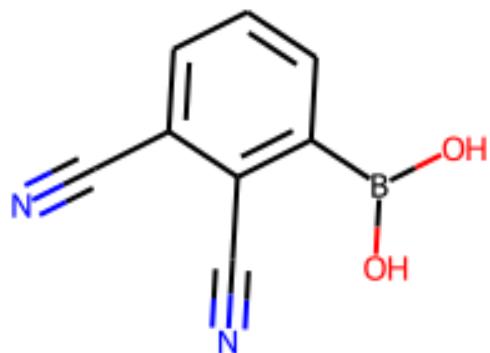


---

No.301

SMILES: N#Cc1cccc(B(0)0)c1C#N

prob: 0.79



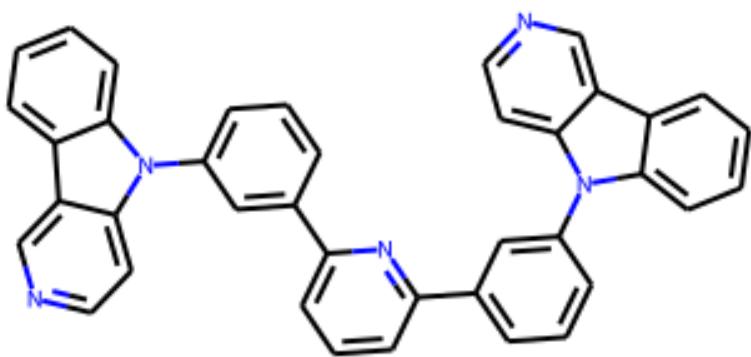
---

No.302

SMILES:

c1cc(-c2cccc(-c3cccc(-n4c5cccc5c5cnccc54)c3)n2)cc(-n2c3cccc3c3cnccc32)c1

prob: 0.79

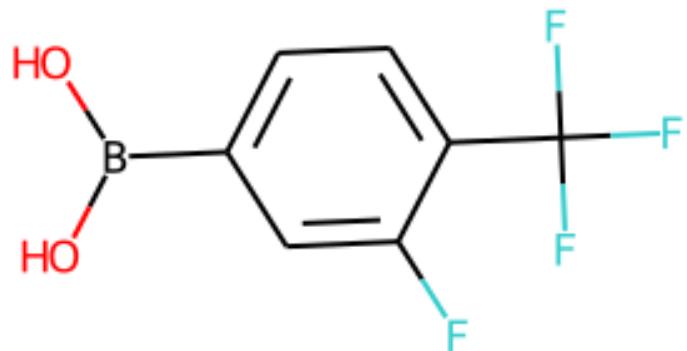


---

No.303

SMILES: OB(O)c1ccc(C(F)(F)F)c(F)c1

prob: 0.79

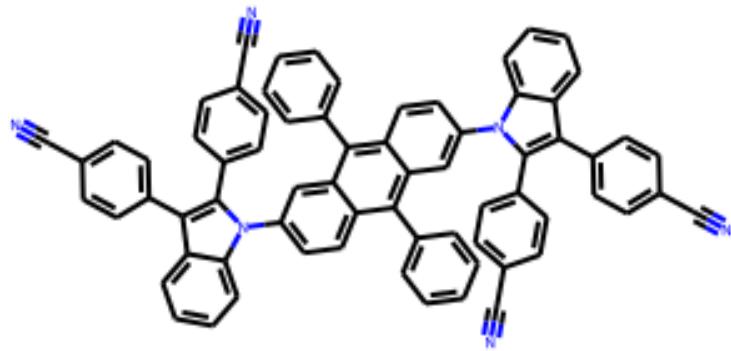


---

No.304

SMILES: N#Cc1cccc(-c2c(-c3ccc(C#N)cc3)n(-c3ccc4c(-c5cccc5)c5cc(-n6c(-c7ccc(C#N)c7)c(-c7ccc(C#N)cc7)c7cccc76)ccc5c(-c5cccc5)c4c3)c3cccc23)cc1

prob: 0.79

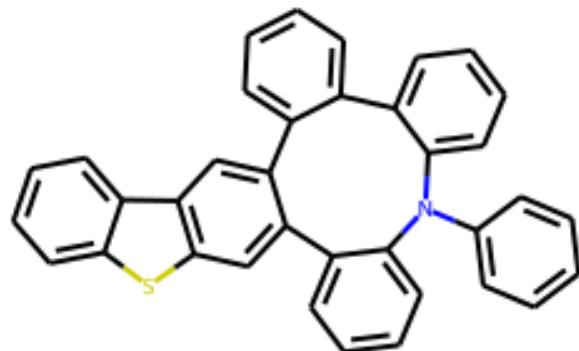


---

No.305

SMILES: c1ccc(-n2c3cccc3c3ccccc3c3cc4c(cc3c3ccccc32)sc2ccccc24)cc1

prob: 0.79



---

No.306

SMILES: [C]#Cc1ccc(C#N)cc1

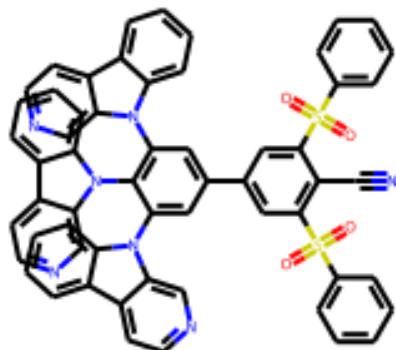
prob: 0.79



---

No.307

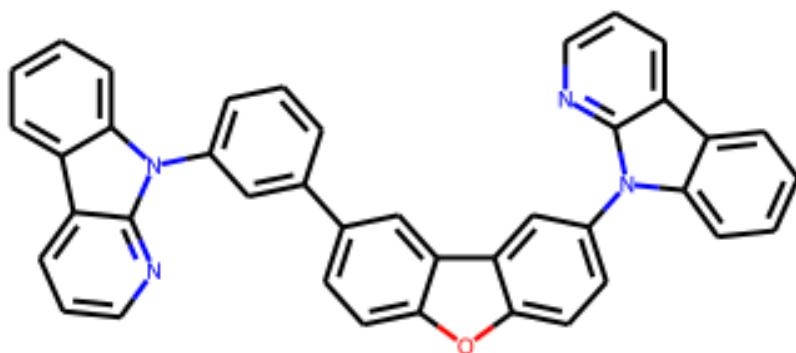
SMILES: N#Cc1c(S(=O)(=O)c2ccccc2)cc(-c2cc(-n3c4cccc4c4ccncc43)c(-n3c4cccc4c4ccncc43)c(-n3c4cccc4c4ccncc43)c2)cc1S(=O)(=O)c1ccccc1  
prob: 0.79



---

No.308

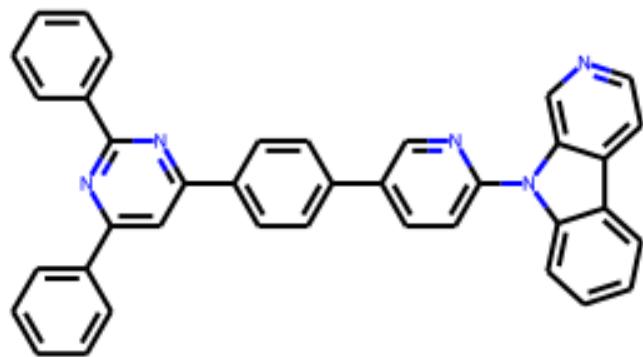
SMILES:  
c1cc(-c2ccc3oc4ccc(-n5c6cccc6c6cccnc65)cc4c3c2)cc(-n2c3cccc3c3cccnc32)c1  
prob: 0.79



---

No.309

SMILES:  
c1cccc(-c2cc(-c3ccc(-c4ccc(-n5c6cccc6c6ccncc65)nc4)cc3)nc(-c3cccc3)n2)cc1  
prob: 0.79

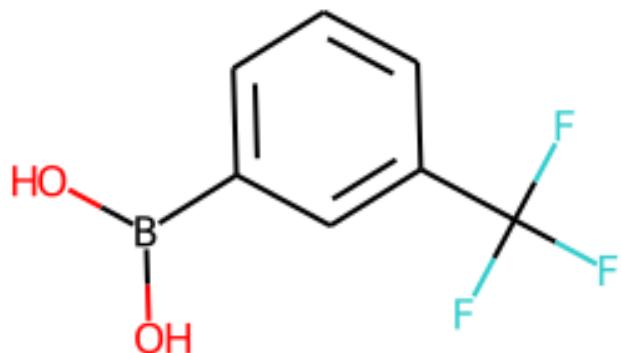


---

No.310

SMILES: OB(O)c1ccccc(C(F)(F)F)c1

prob: 0.78

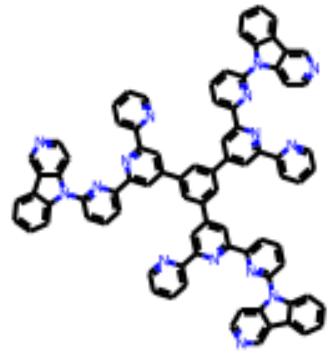


---

No.311

SMILES: c1cccc(-c2cc(-c3cc(-c4cc(-c5cccn5)nc(-c5cccc(-n6c7cccc7c7cnccc76)n5)c4)cc(-c4cc(-c5cccn5)nc(-c5cccc(-n6c7cccc7c7cnccc76)n5)c4)c3)cc(-c3cccc(-n4c5cccc5c5c5cnccc54)n3)n2)nc1

prob: 0.78

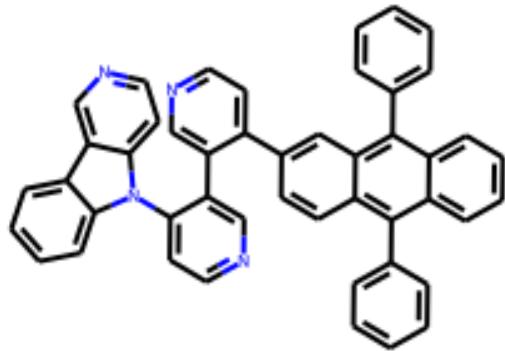


---

No.312

SMILES: c1ccc(-c2c3cccc3c(-c3ccccc3)c3cc(-c4ccncc4-c4cnccc4-n4c5cccc5c5cnccc54)ccc23)cc1

prob: 0.78

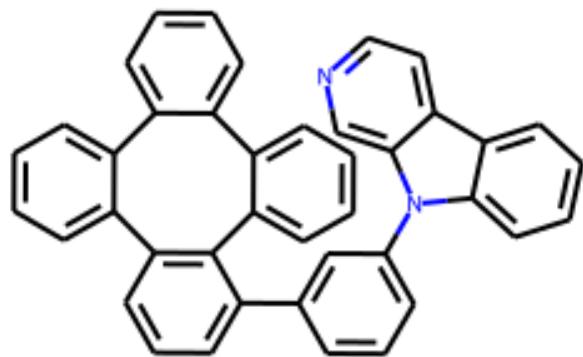


---

No.313

SMILES: c1cc(-c2ccccc3c2-c2ccccc2-c2ccccc2-c2ccccc2-3)cc(-n2c3cccc3c3ccncc32)c1

prob: 0.78

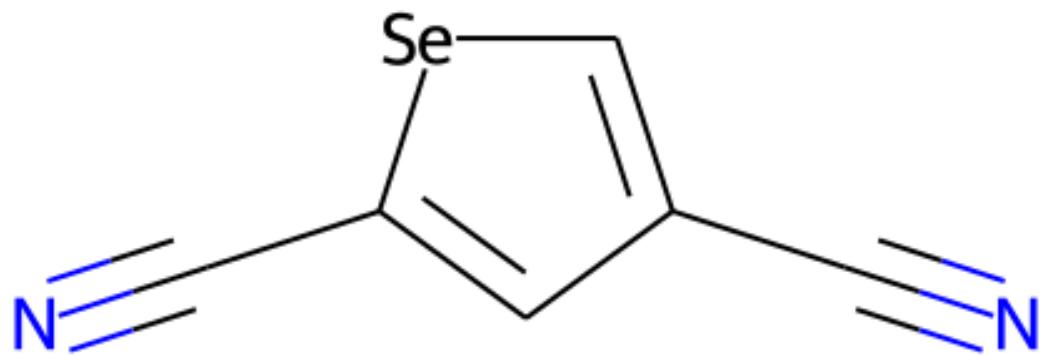


---

No.314

SMILES: N#Cc1c[se]c(C#N)c1

prob: 0.78

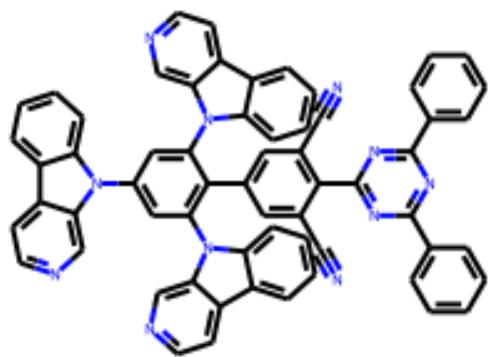


---

No.315

SMILES: N#Cc1cc(-c2c(-n3c4cccc4c4ccncc43)cc(-n3c4cccc4c4ccncc43)cc2-n2c3cccc3c3ccncc32)cc(C#N)c1-c1nc(-c2cccc2)nc(-c2cccc2)n1

prob: 0.78

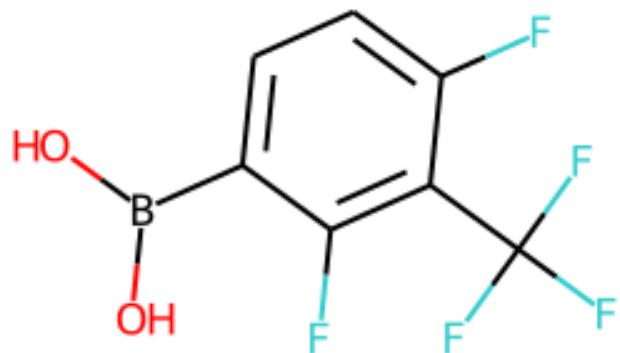


---

No.316

SMILES: OB(O)c1ccc(F)c(C(F)(F)F)c1F

prob: 0.78

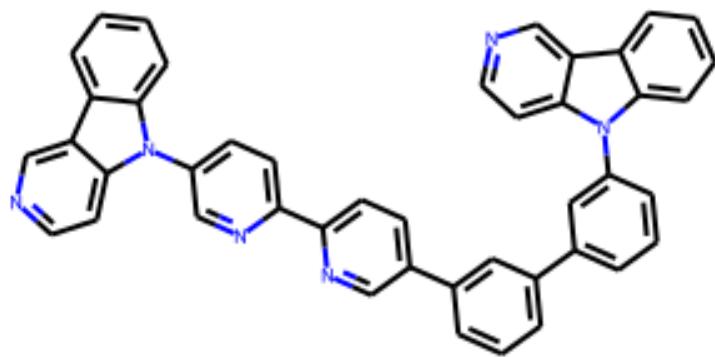


---

No.317

SMILES: c1cc(-c2ccc(-c3ccc(-n4c5cccc5c5cnccc54)cn3)nc2)cc(-c2cccc(-n3c4cccc4c4cnccc43)c2)c1

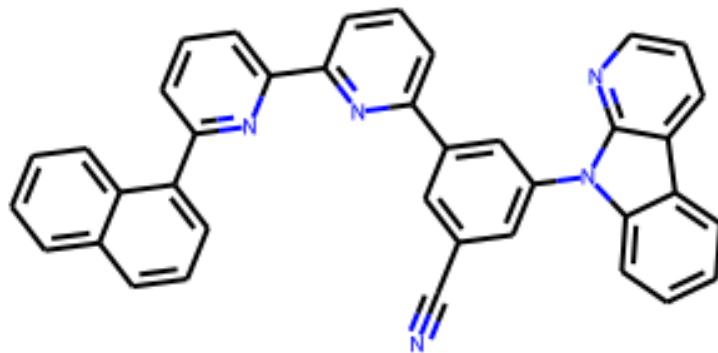
prob: 0.78



---

No.318

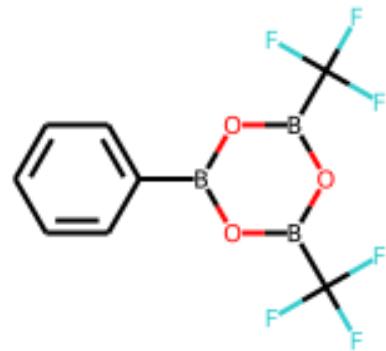
SMILES: N#Cc1cc(-c2cccc(-c3cccc(-c4cccc5cccc45)n3)n2)cc(-n2c3cccc3c3cccnc32)c1  
prob: 0.78



---

No.319

SMILES: FC(F)(F)B1OB(c2cccc2)OB(C(F)(F)F)O1  
prob: 0.78

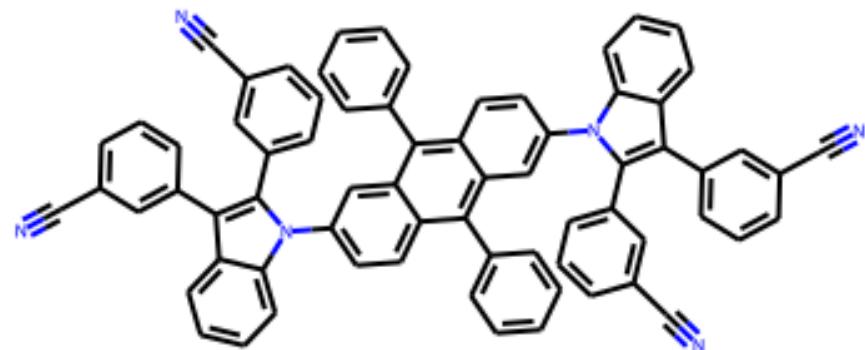


---

No.320

SMILES: N#Cc1cccc(-c2c(-c3cccc(C#N)c3)n(-c3ccc4c(-c5cccc5)c5cc(-n6c(-c7cccc(C#N)c7)c(-c7cccc(C#N)c7)c7cccc76)ccc5c(-c5cccc5)c4c3)c3cccc23)c1

prob: 0.78

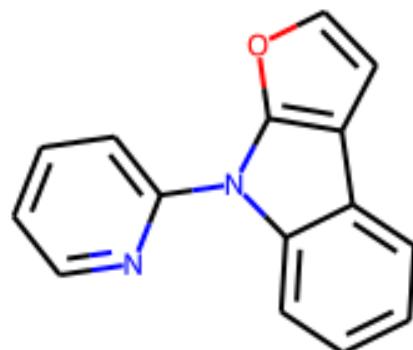


---

No.321

SMILES: c1ccc(-n2c3cccc3c3ccoc32)nc1

prob: 0.78

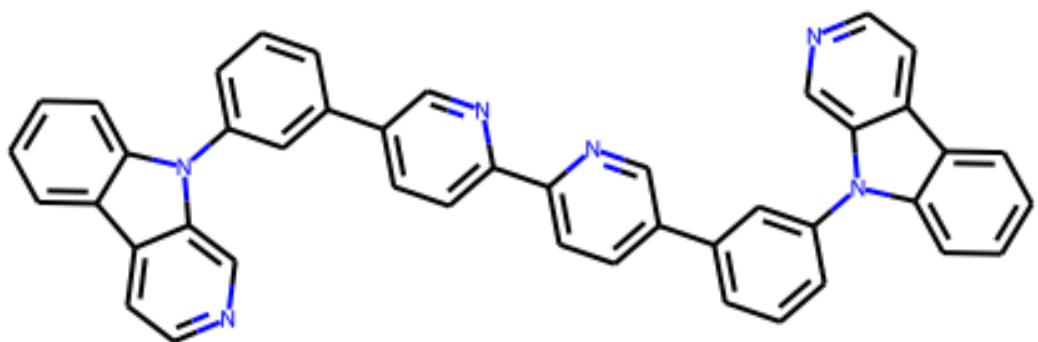


---

No.322

SMILES: c1cc(-c2ccc(-c3ccc(-c4cccc(-n5c6cccc6c6ccncc65)c4)cn3)nc2)cc(-n2c3cccc3c3ccncc32)c1

prob: 0.78

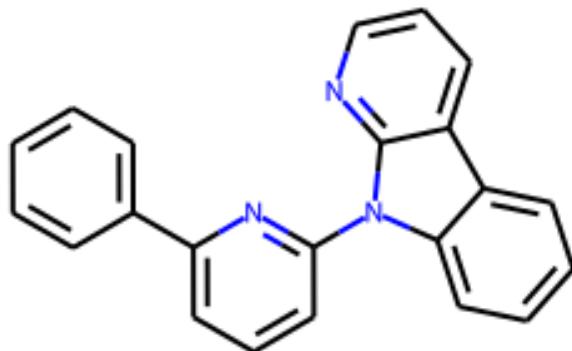


---

No.323

SMILES: c1ccc(-c2cccc(-n3c4ccccc4c4cccnc43)n2)cc1

prob: 0.78

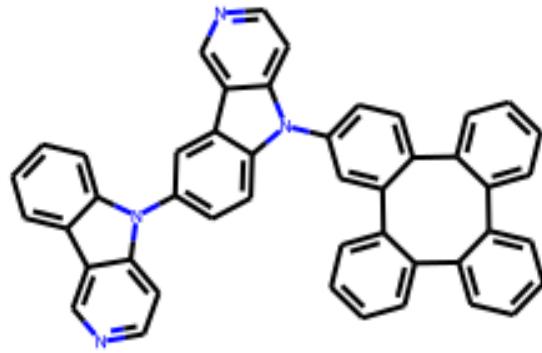


---

No.324

SMILES: c1ccc2c(c1)-c1ccccc1-c1ccc(-n3c4ccncc4c4cc(-n5c6ccccc6c6cnccc65)ccc43)cc1-c1ccccc1-2

prob: 0.78

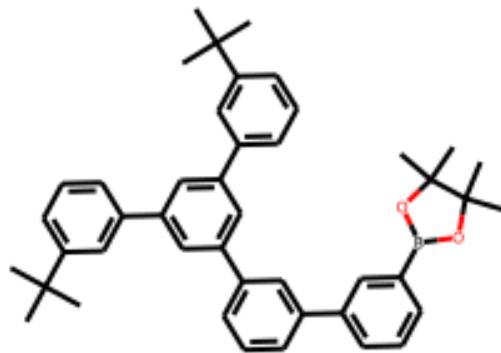


---

No.325

SMILES: CC(C)(C)c1ccccc(-c2cc(-c3cccc(-c4cccc(B50C(C)(C)C(C)O5)c4)c3)cc(-c3ccc  
c(C(C)(C)C)c3)c2)c1

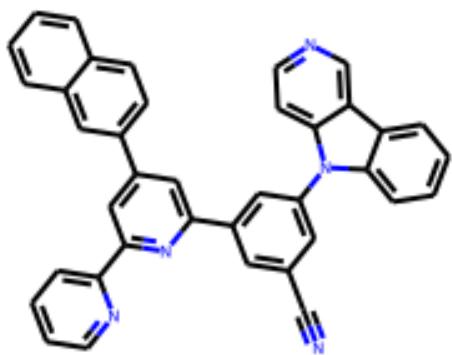
prob: 0.78



---

No.326

SMILES: N#Cc1cc(-c2cc(-c3ccc4cccc4c3)cc(-c3cccn3)n2)cc(-n2c3cccc3c3cnccc32)c1  
prob: 0.78

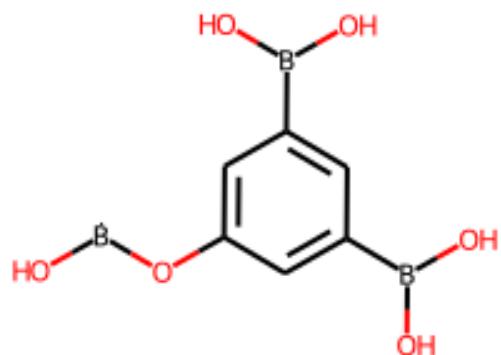


---

No.327

SMILES: O[B]Oc1cc(B(O)O)cc(B(O)O)c1

prob: 0.78



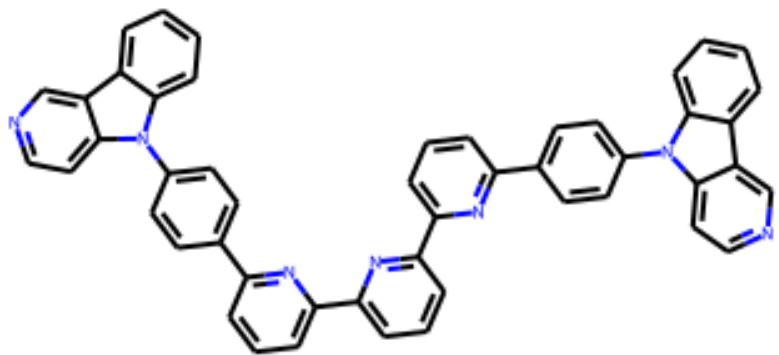
---

No.328

SMILES: c1cc(-c2ccc(-n3c4cccc4c4cnccc43)cc2)nc(-c2cccc(-c3cccc(-c4ccc(-n5c6cccc

c6c6cnccc65)cc4)n3)n2)c1

prob: 0.78

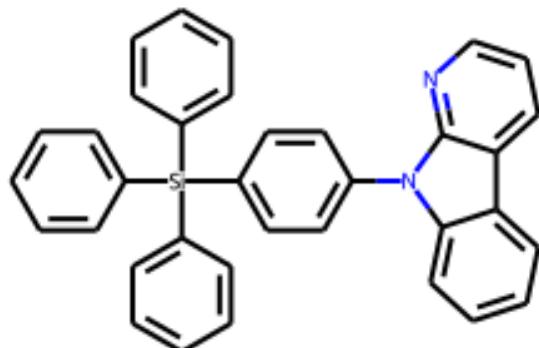


---

No.329

SMILES: c1ccc([Si](c2ccccc2)(c2ccccc2)c2ccc(-n3c4ccccc4c4cccnc43)cc2)cc1

prob: 0.78

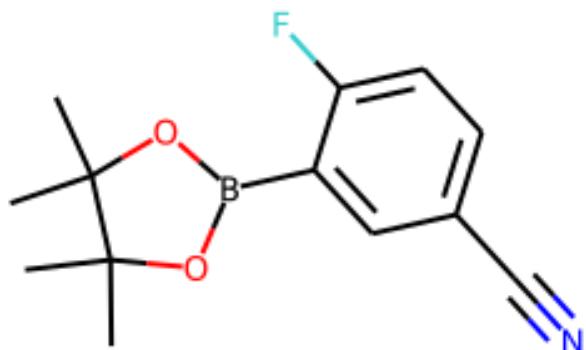


---

No.330

SMILES: CC1(C)OB(c2cc(C#N)ccc2F)OC1(C)C

prob: 0.78

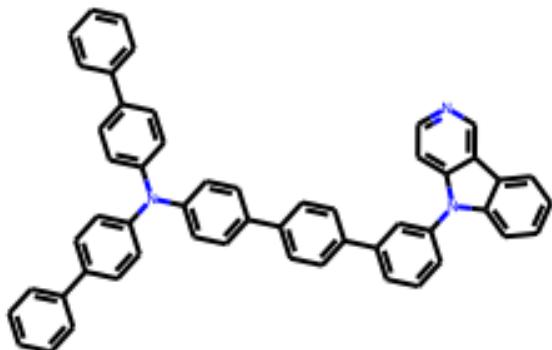


---

No.331

SMILES: c1ccc(-c2ccc(N(c3ccc(-c4cccc4)cc3)c3ccc(-c4ccc(-c5cccc(-n6c7cccc7c7cnc  
cc76)c5)cc4)cc3)cc2)cc1

prob: 0.78

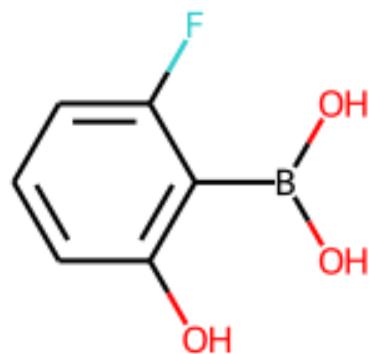


---

No.332

SMILES: OB(0)c1c(0)cccc1F

prob: 0.78

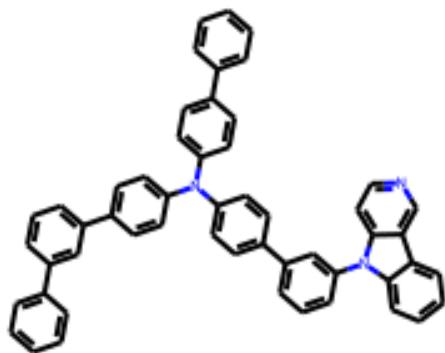


---

No.333

SMILES: c1ccc(-c2ccc(N(c3ccc(-c4cccc(-c5cccc5)c4)cc3)c3ccc(-c4cccc(-n5c6cccc6c  
6cnccc65)c4)cc3)cc2)cc1

prob: 0.78

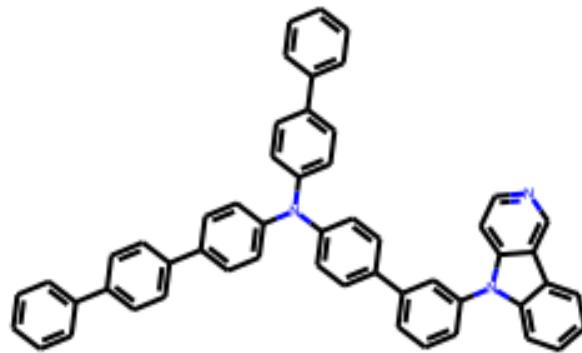


---

No.334

SMILES: c1ccc(-c2ccc(-c3ccc(N(c4ccc(-c5ccccc5)cc4)c4ccc(-c5cccc(-n6c7ccccc7c7cnc  
cc76)c5)cc4)cc3)cc2)cc1

prob: 0.78

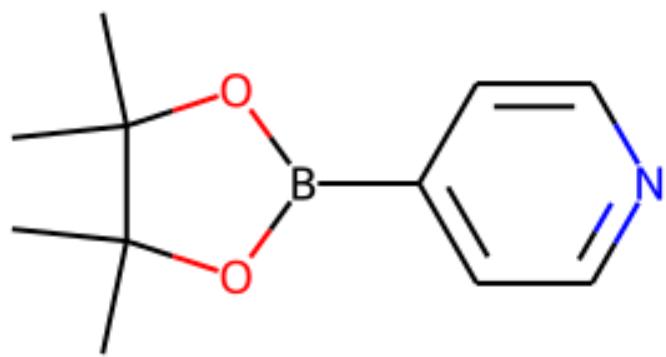


---

No.335

SMILES: CC1(C)OB(c2ccncc2)OC1(C)C

prob: 0.78

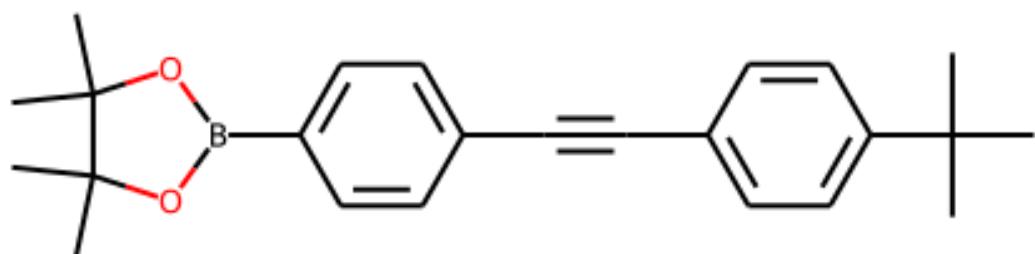


---

No.336

SMILES: CC(C)(C)c1ccc(C#Cc2ccc(B3OC(C)(C)C(C)O3)cc2)cc1

prob: 0.78

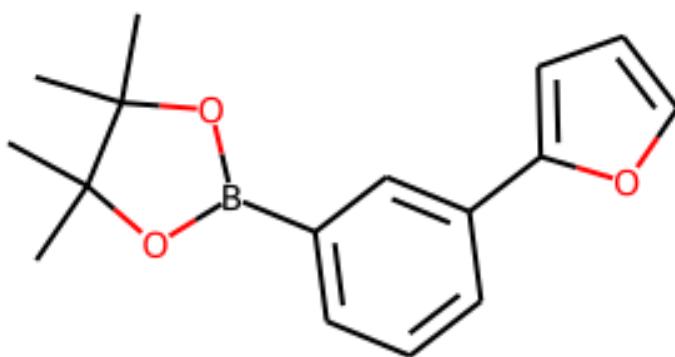


---

No.337

SMILES: CC1(C)OB(c2cccc(-c3ccco3)c2)OC1(C)C

prob: 0.78

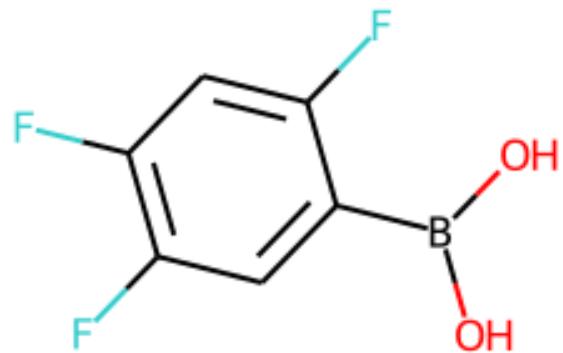


---

No.338

SMILES: OB(O)c1cc(F)c(F)cc1F

prob: 0.78

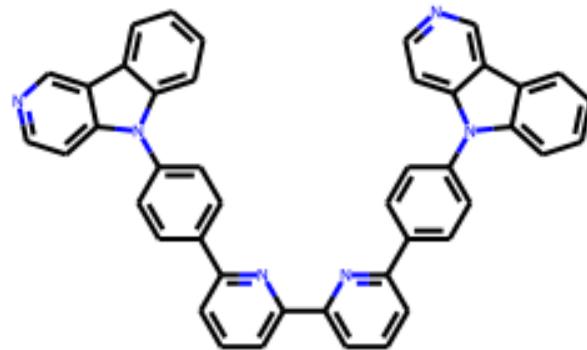


---

No.339

SMILES: c1cc(-c2ccc(-n3c4cccc4c4cnccc43)cc2)nc(-c2cccc(-c3ccc(-n4c5cccc5c5cncc54)cc3)n2)c1

prob: 0.78



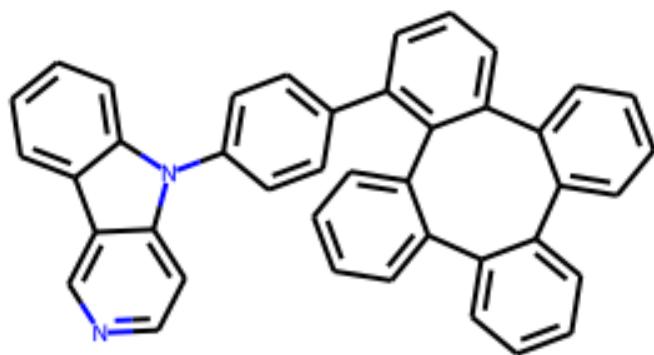
---

No.340

SMILES:

c1ccc2c(c1)-c1cccc1-c1cccc(-c3ccc(-n4c5cccc5c5cnccc54)cc3)c1-c1cccc1-2

prob: 0.78

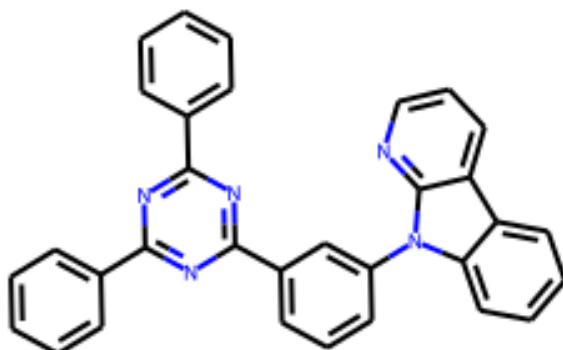


---

No.341

SMILES: c1ccc(-c2nc(-c3cccc3)nc(-c3cccc(-n4c5cccc5c5cccnc54)c3)n2)cc1

prob: 0.78

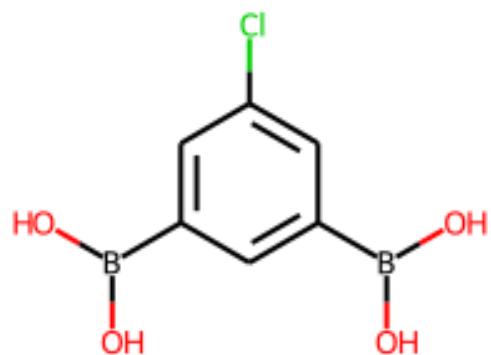


---

No.342

SMILES: OB(0)c1cc(Cl)cc(B(0)O)c1

prob: 0.78

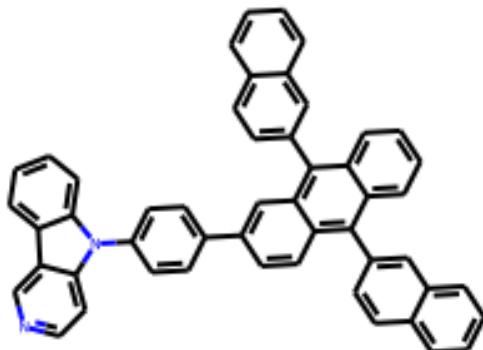


---

No.343

SMILES: c1ccc2cc(-c3c4cccc4c(-c4ccc5cccc5c4)c4cc(-c5ccc(-n6c7cccc7c7cnccc76)c  
c5)ccc34)ccc2c1

prob: 0.78

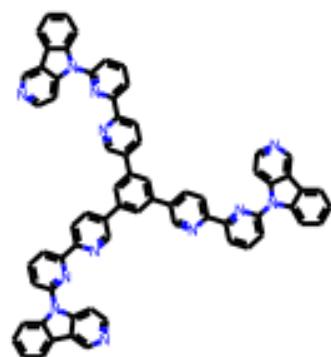


---

No.344

SMILES: c1cc(-c2ccc(-c3cc(-c4ccc(-c5cccc(-n6c7cccc7c7cnccc76)n5)nc4)cc(-c4ccc(-  
c5cccc(-n6c7cccc7c7cnccc76)n5)nc4)c3)cn2)nc(-n2c3cccc3c3cnccc32)c1

prob: 0.78

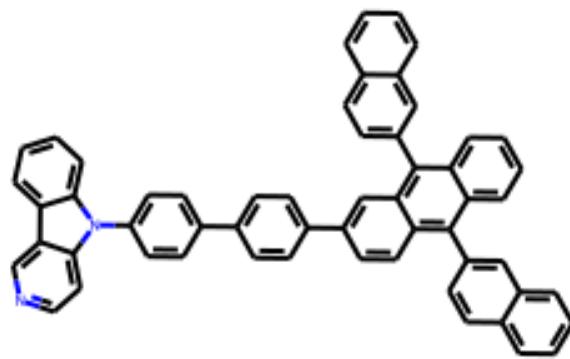


---

No.345

SMILES: c1ccc2cc(-c3c4cccc4c(-c4ccc5cccc5c4)c4cc(-c5ccc(-c6ccc(-n7c8cccc8c8cn  
ccc87)cc6)cc5)ccc34)ccc2c1

prob: 0.78

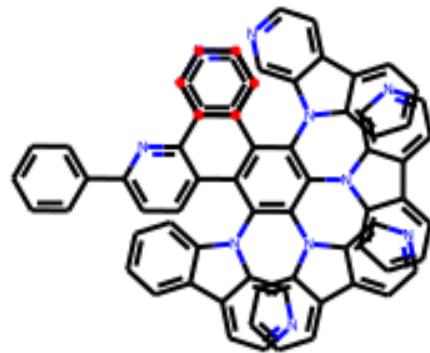


---

No.346

SMILES: c1ccc(-c2ccc(-c3c(-c4ccncc4)c(-n4c5cccc5c5ccncc54)c(-n4c5cccc5c5ccncc54)c(-n4c5cccc5c5ccncc54)c3-n3c4cccc4c4ccncc43)c(-c3cccc3)n2)cc1

prob: 0.78

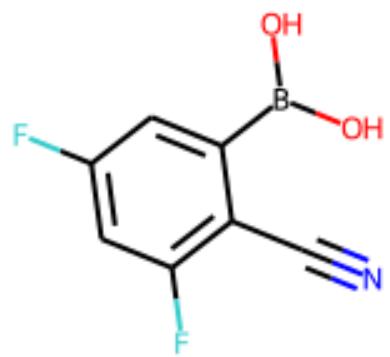


---

No.347

SMILES: N#Cc1c(F)cc(F)cc1B(0)O

prob: 0.78

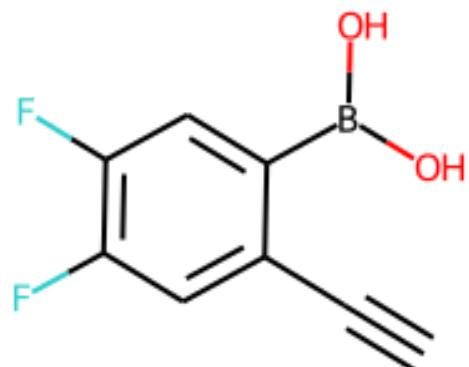


---

No.348

SMILES: C#Cc1cc(F)c(F)cc1B(O)O

prob: 0.78

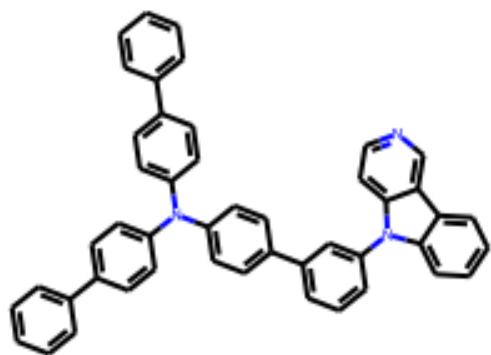


---

No.349

SMILES: c1ccc(-c2ccc(N(c3ccc(-c4ccccc4)cc3)c3ccc(-c4cccc(-n5c6cccccc6c6cnccc65)c4)cc3)cc2)cc1

prob: 0.78

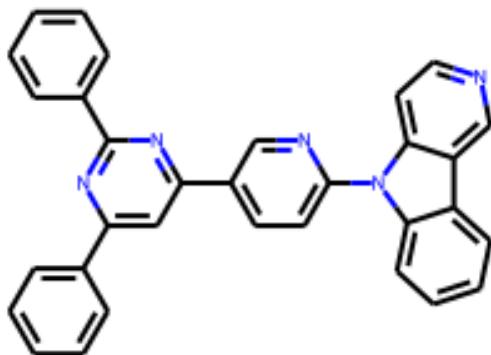


---

No.350

SMILES: c1ccc(-c2cc(-c3ccc(-n4c5cccc5c5cnccc54)nc3)nc(-c3cccc3)n2)cc1

prob: 0.78

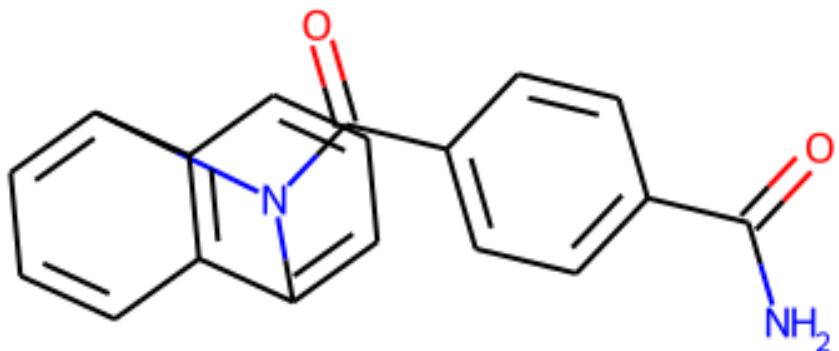


---

No.351

SMILES: NC(=O)c1ccc(C(=O)n2c3cccc4c3cccc42)cc1

prob: 0.78

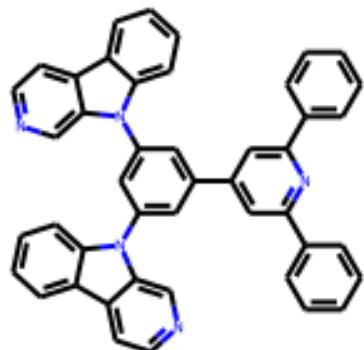


---

No.352

SMILES: c1ccc(-c2cc(-c3cc(-n4c5cccc5c5ccncc54)cc(-n4c5cccc5c5ccncc54)c3)cc(-c3cccc3)n2)cc1

prob: 0.78

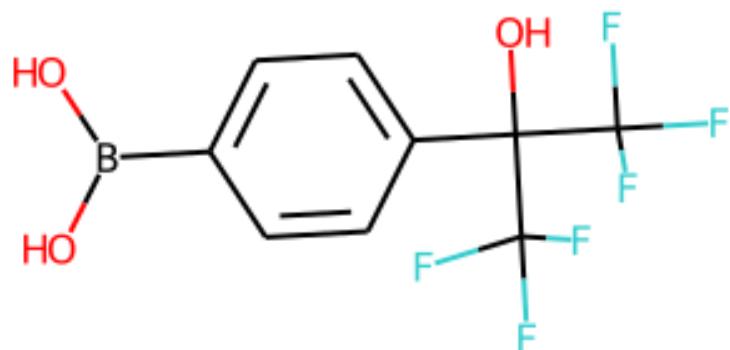


---

No.353

SMILES: OB(0)c1ccc(C(0)(C(F)(F)F)C(F)(F)F)cc1

prob: 0.78



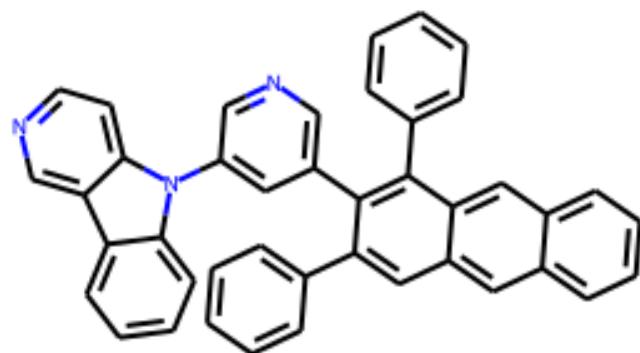
---

No.354

SMILES:

c1ccc(-c2cc3cc4cccc4cc3c(-c3cccc3)c2-c2cncc(-n3c4cccc4c4cnccc43)c2)cc1

prob: 0.78

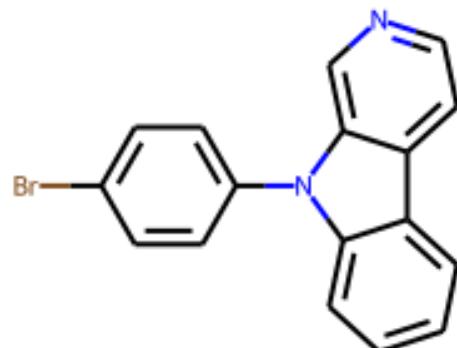


---

No.355

SMILES: Brc1ccc(-n2c3cccc3c3ccncc32)cc1

prob: 0.78

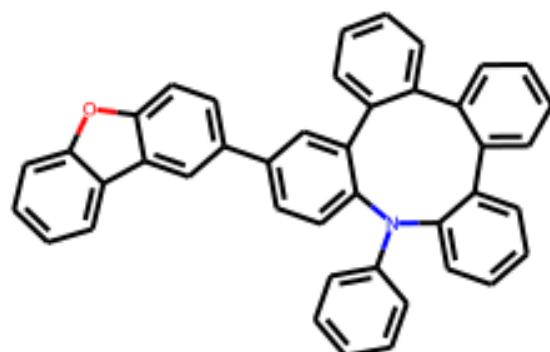


---

No.356

SMILES: c1ccc(-n2c3cccc3c3cccc3c3cccc3c3cc(-c4ccc5oc6cccc6c5c4)ccc32)cc1

prob: 0.78

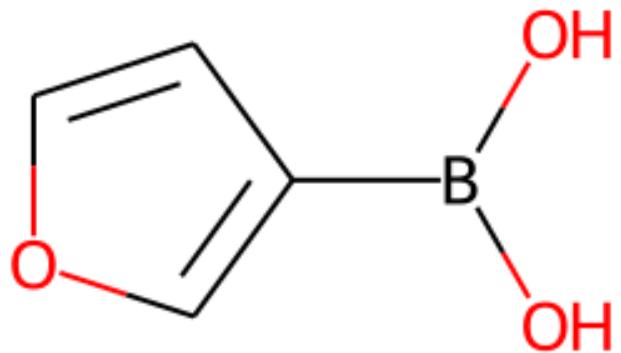


---

No.357

SMILES: OB(O)c1ccoc1

prob: 0.78

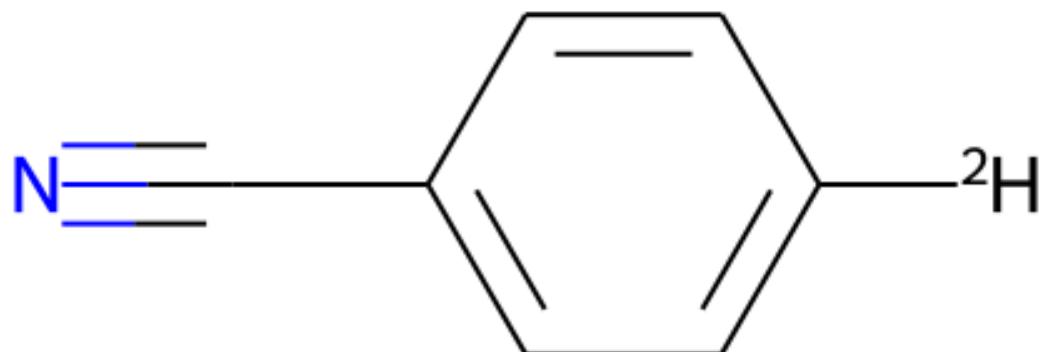


---

No.358

SMILES: [2H]c1ccc(C#N)cc1

prob: 0.78

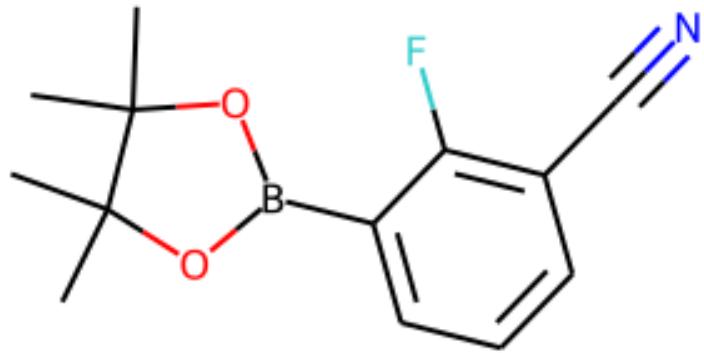


---

No.359

SMILES: CC1(C)OB(c2ccccc2C#N)c2FCC1(C)C

prob: 0.78

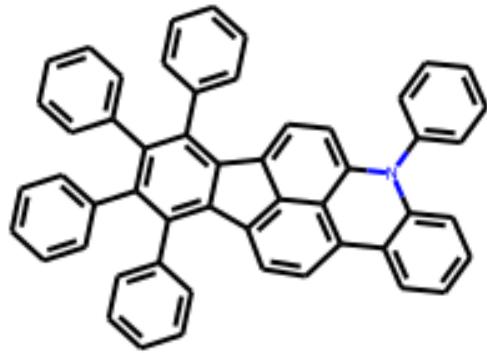


---

No.360

SMILES: c1ccc(-c2c(-c3ccccc3)c(-c3ccccc3)c3c4ccc5c6c(ccc(c3c2-c2ccccc2)c46)c2ccc cc2n5-c2ccccc2)cc1

prob: 0.78

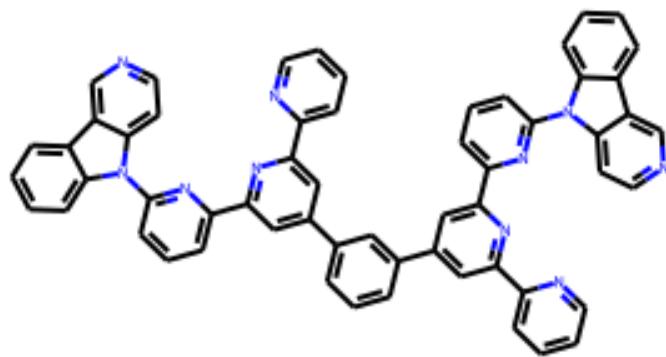


---

No.361

SMILES: c1ccc(-c2cc(-c3cccc(-c4cc(-c5cccn5)nc(-c5cccc(-n6c7ccccc7c7cnccc76)n5)c 4)c3)cc(-c3cccc(-n4c5ccccc5c5cnccc54)n3)n2)nc1

prob: 0.78

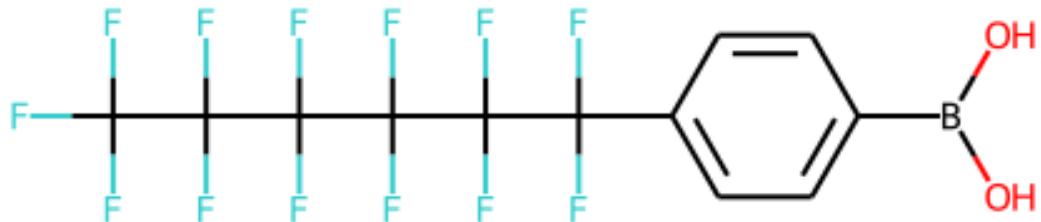


---

No.362

SMILES: OB(O)c1ccc(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)cc1

prob: 0.78

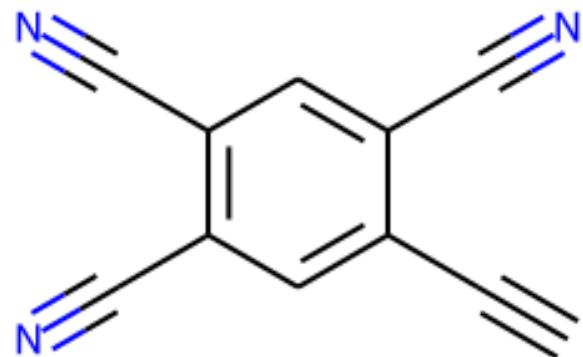


---

No.363

SMILES: C#Cc1cc(C#N)c(C#N)cc1C#N

prob: 0.78

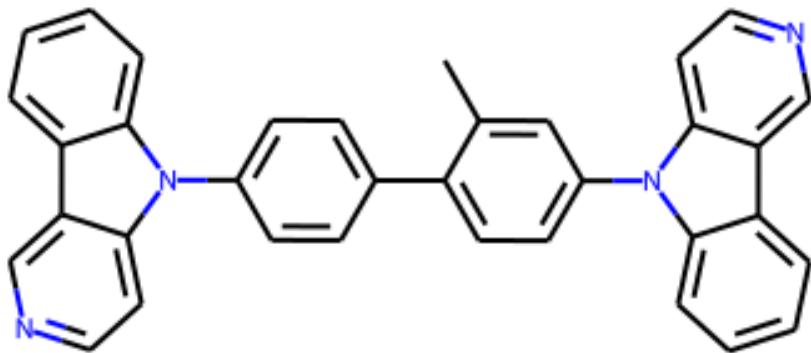


---

No.364

SMILES: Cc1cc(-n2c3cccc3c3cnccc32)ccc1-c1ccc(-n2c3cccc3c3cnccc32)cc1

prob: 0.78

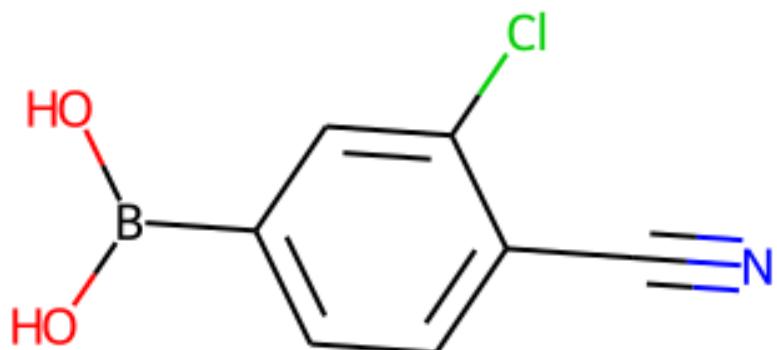


---

No.365

SMILES: N#Cc1ccc(B(O)O)cc1Cl

prob: 0.78

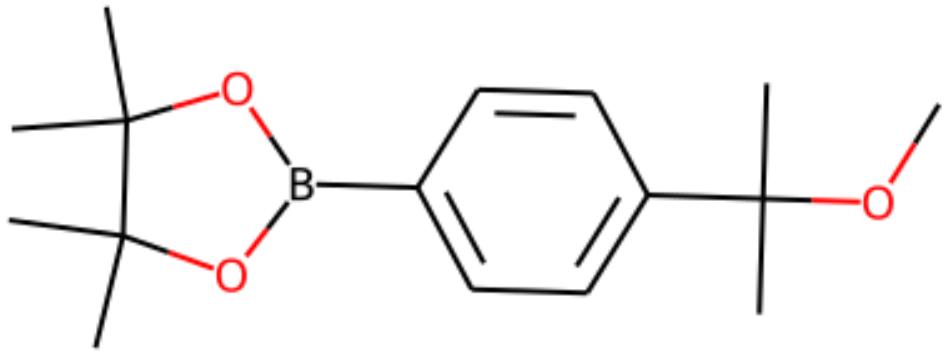


---

No.366

SMILES: COc(C)(C)c1ccc(B2OC(C)(C)C(C)(C)O2)cc1

prob: 0.78

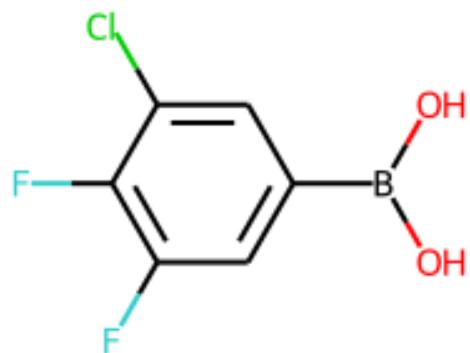


---

No.367

SMILES: OB(O)c1cc(F)c(F)c(Cl)c1

prob: 0.78



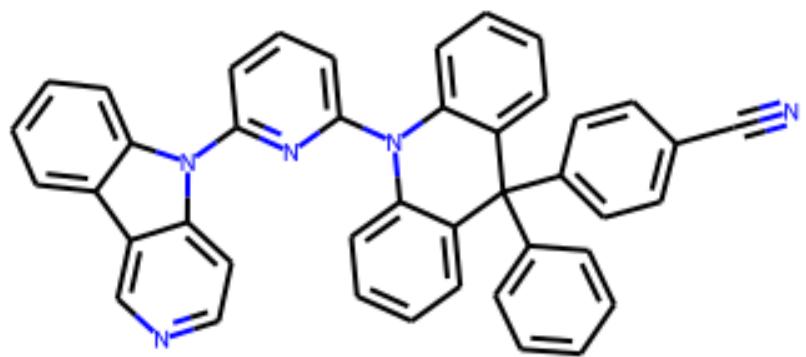
---

No.368

SMILES:

N#Cc1ccc(C2(c3ccccc3)c3ccccc3N(c3cccc(-n4c5ccccc5c5cnccc54)n3)c3ccccc32)cc1

prob: 0.78

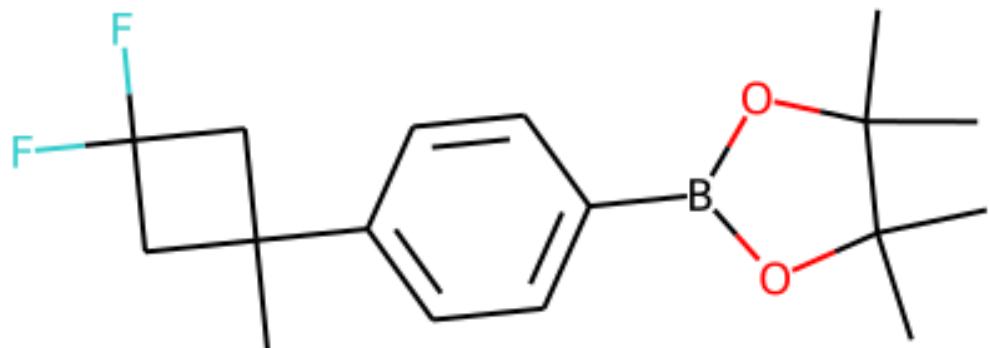


---

No.369

SMILES: CC1(c2ccc(B3OC(C)(C)C(C)(C)O3)cc2)CC(F)(F)C1

prob: 0.78



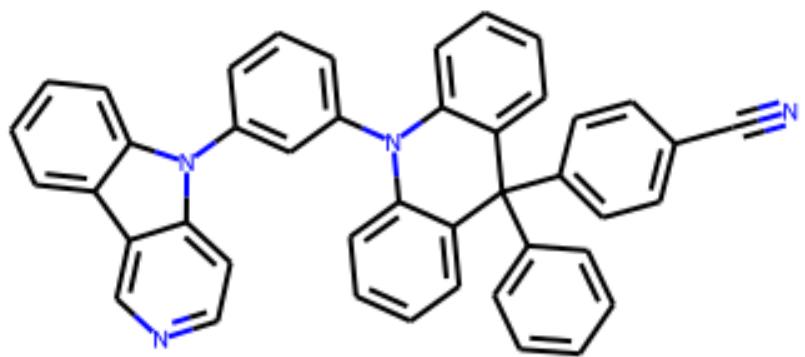
---

No.370

SMILES:

N#Cc1ccc(C2(c3cccc3)c3cccc3N(c3cccc(-n4c5cccc5c5cnccc54)c3)c3cccc32)cc1

prob: 0.78



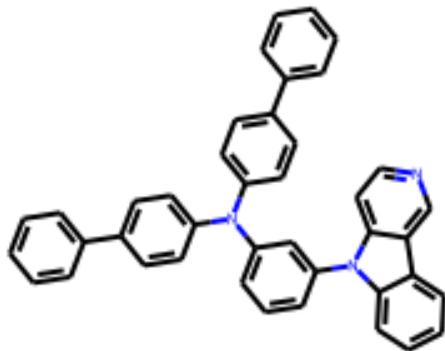
---

No.371

SMILES:

c1ccc(-c2ccc(N(c3ccc(-c4ccccc4)cc3)c3cccc(-n4c5ccccc5c5cnccc54)c3)cc2)cc1

prob: 0.78

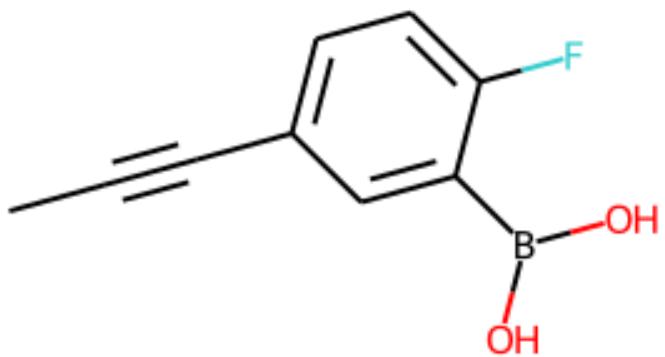


---

No.372

SMILES: CC#Cc1ccc(F)c(B(O)O)c1

prob: 0.77

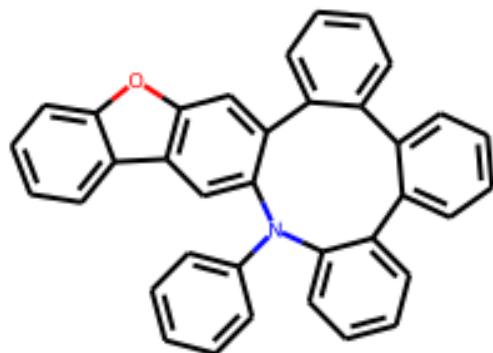


---

No.373

SMILES: c1ccc(-n2c3cccc3c3cccc3c3cccc3c3cc4oc5cccc5c4cc32)cc1

prob: 0.77

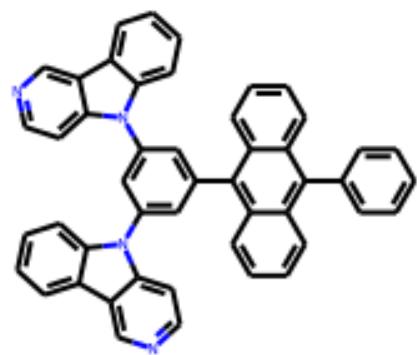


---

No.374

SMILES: c1ccc(-c2c3cccc3c(-c3cc(-n4c5cccc5c5cnccc54)cc(-n4c5cccc5c5cnccc54)c3)c3cccc23)cc1

prob: 0.77

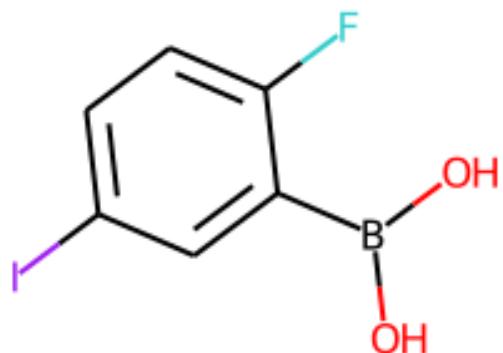


---

No.375

SMILES: OB(O)c1cc(I)ccc1F

prob: 0.77

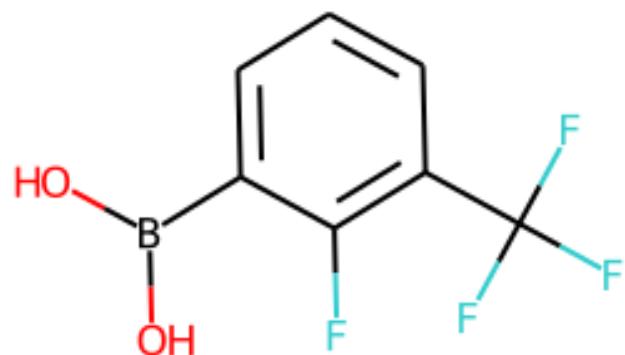


---

No.376

SMILES: OB(O)c1cccc(C(F)(F)F)c1F

prob: 0.77

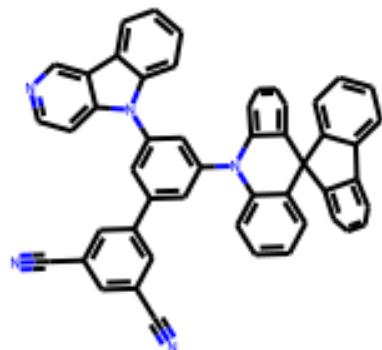


---

No.377

SMILES: N#Cc1cc(C#N)cc(-c2cc(N3c4cccc4C4(c5cccc5-c5cccc54)c4cccc43)cc(-n3c4cccc4c4cnccc43)c2)c1

prob: 0.77



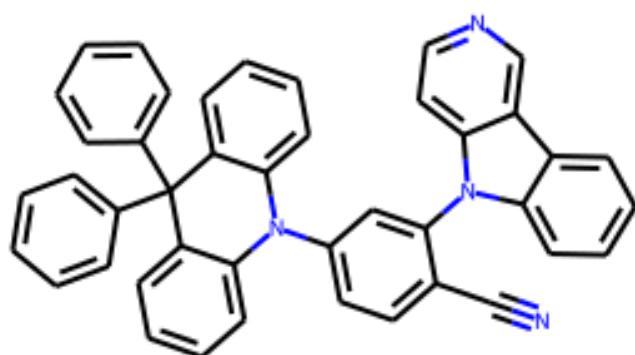
---

No.378

SMILES:

N#Cc1ccc(N2c3cccc3C(c3cccc3)(c3cccc3)c3cccc32)cc1-n1c2cccc2c2cnccc21

prob: 0.77

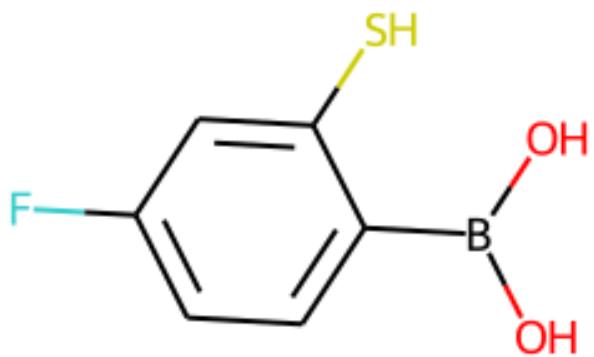


---

No.379

SMILES: OB(O)c1ccc(F)cc1S

prob: 0.77

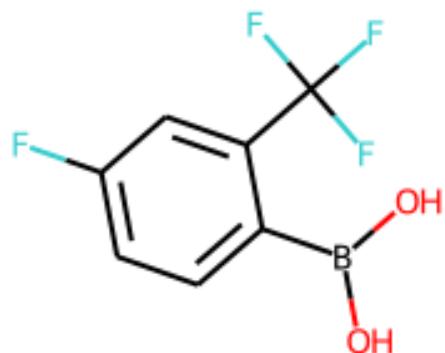


---

No.380

SMILES: OB(0)c1ccc(F)cc1C(F)(F)F

prob: 0.77

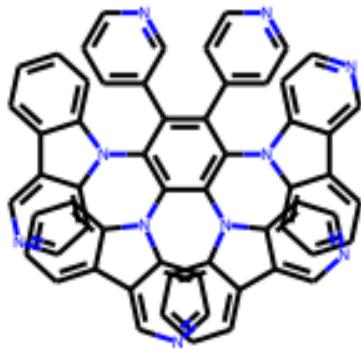


---

No.381

SMILES: c1cncc(-c2c(-c3ccncc3)c(-n3c4cccc4c4cnccc43)c(-n3c4cccc4c4cnccc43)c(-n3c4cccc4c4cnccc43)c2-n2c3cccc3c3cnccc32)c1

prob: 0.77

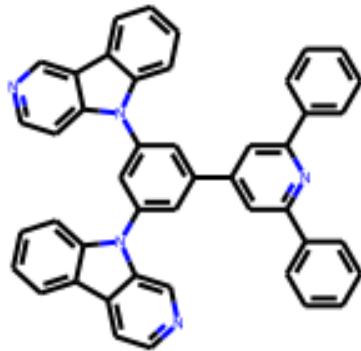


---

No.382

SMILES: c1ccc(-c2cc(-c3cc(-n4c5cccc5c5cnccc54)cc(-n4c5cccc5c5ccncc54)c3)cc(-c3cccc3)n2)cc1

prob: 0.77

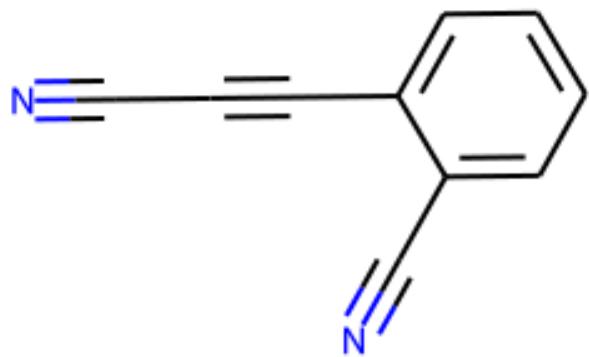


---

No.383

SMILES: N#CC#Cc1ccccc1C#N

prob: 0.77

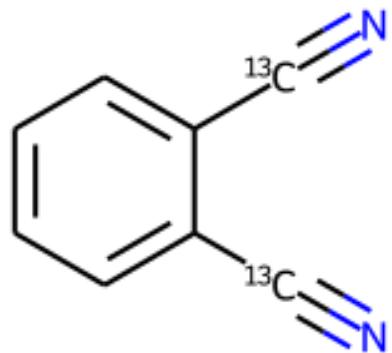


---

No.384

SMILES: N#[13C]c1ccccc1[13C]#N

prob: 0.77

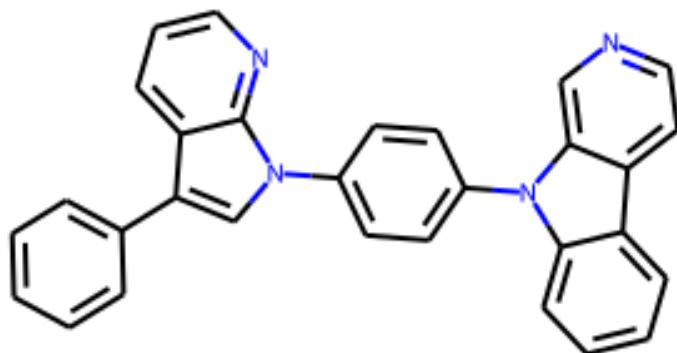


---

No.385

SMILES: c1ccc(-c2cn(-c3ccc(-n4c5ccccc5c5ccncc54)cc3)c3nc(cc23)cc1

prob: 0.77

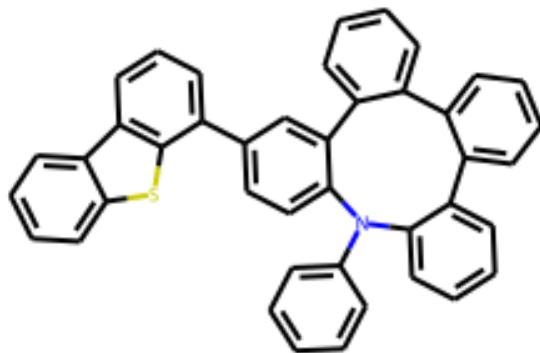


---

No.386

SMILES: c1ccc(-n2c3cccc3c3cccc3c3cccc3c3cc(-c4cccc5c4sc4cccc45)ccc32)cc1

prob: 0.77

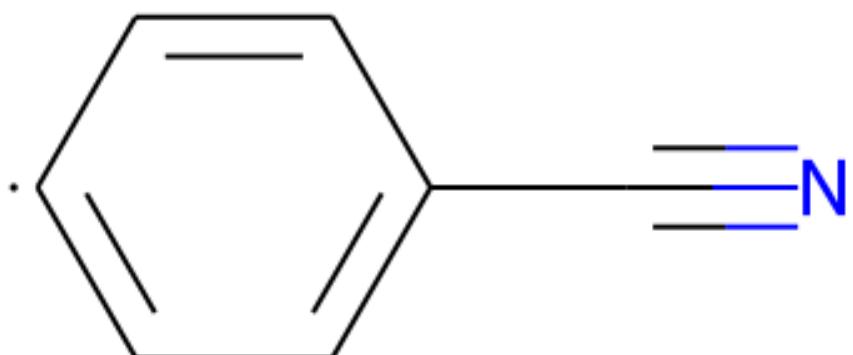


---

No.387

SMILES: N#Cc1cc[c]cc1

prob: 0.77

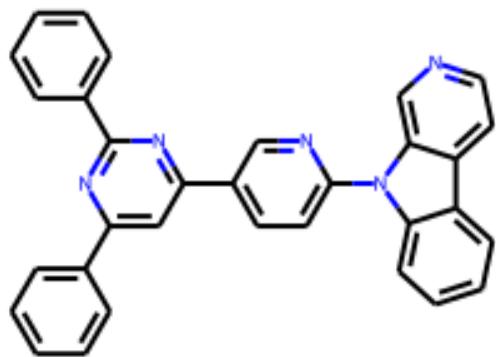


---

No.388

SMILES: c1ccc(-c2cc(-c3ccc(-n4c5cccc5c5ccncc54)nc3)nc(-c3cccc3)n2)cc1

prob: 0.77



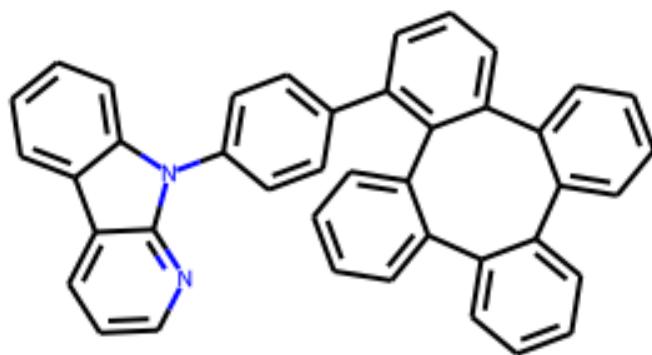
---

No.389

SMILES:

c1ccc2c(c1)-c1ccccc1-c1cccc(-c3ccc(-n4c5ccccc5c5cccnc54)cc3)c1-c1ccccc1-2

prob: 0.77



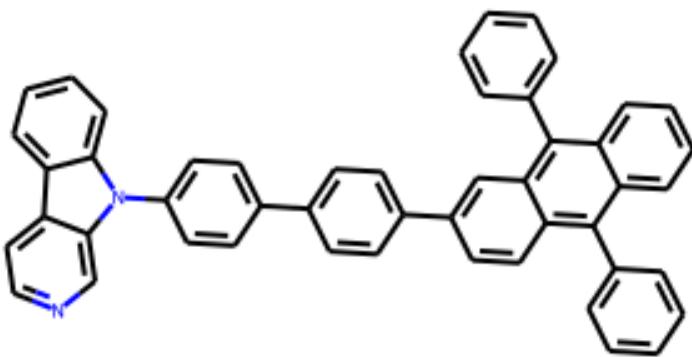
---

No.390

SMILES: c1ccc(-c2c3ccccc3c(-c3ccccc3)c3cc(-c4ccc(-c5ccc(-n6c7ccccc7c7ccncc76)cc5

)cc4)ccc23)cc1

prob: 0.77

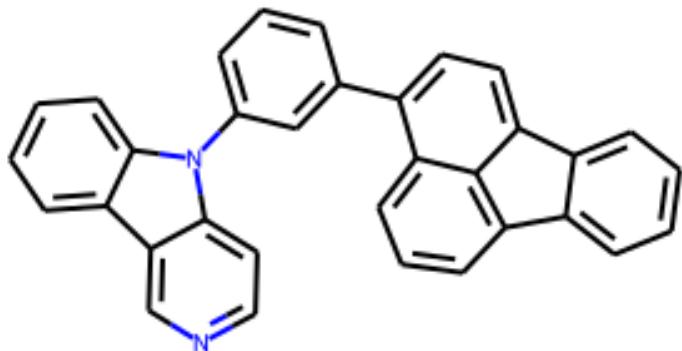


---

No.391

SMILES: c1cc(-c2ccc3c4c(cccc24)-c2cccc2-3)cc(-n2c3cccc3c3cnccc32)c1

prob: 0.77

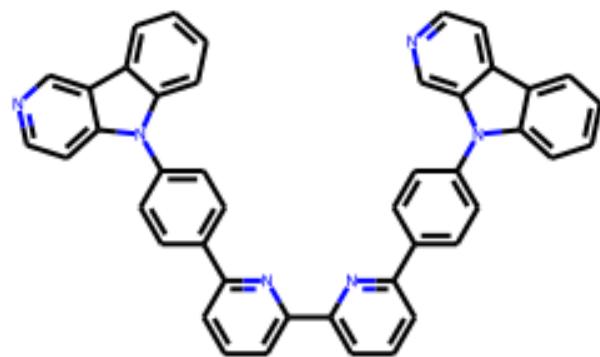


---

No.392

SMILES: c1cc(-c2ccc(-n3c4cccc4c4cnccc43)cc2)nc(-c2cccc(-c3ccc(-n4c5cccc5c5ccnc54)cc3)n2)c1

prob: 0.77

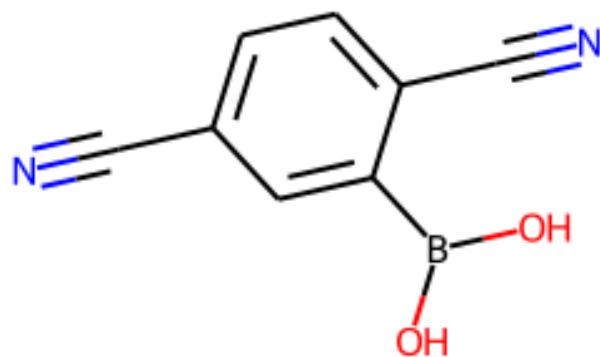


---

No.393

SMILES: N#Cc1cccc(C#N)c(B(O)O)c1

prob: 0.77



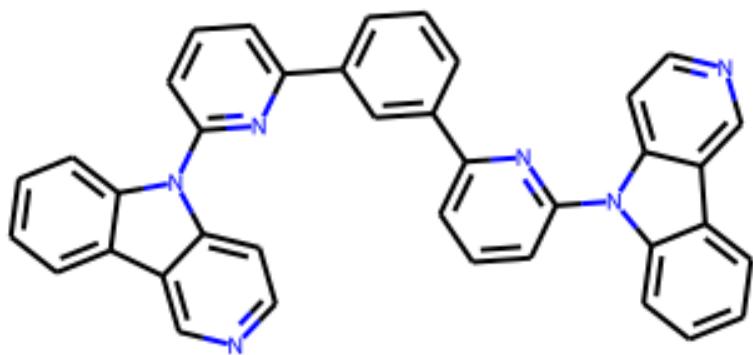
---

No.394

SMILES:

c1cc(-c2cccc(-n3c4cccc4c4cnccc43)n2)cc(-c2cccc(-n3c4cccc4c4cnccc43)n2)c1

prob: 0.77

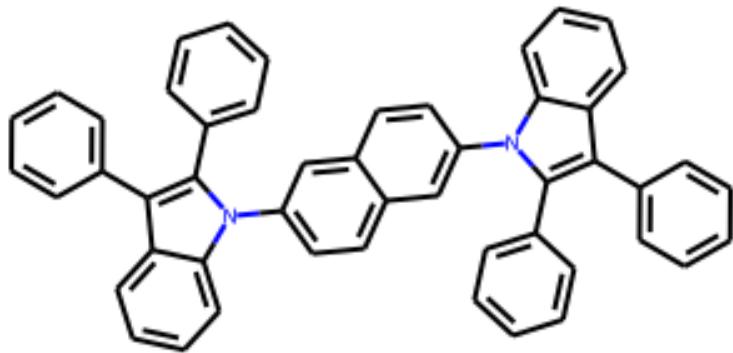


---

No.395

SMILES: c1ccc(-c2c(-c3ccccc3)n(-c3ccc4cc(-n5c(-c6ccccc6)c(-c6ccccc6)c6ccccc65)cc4c3)c3ccccc23)cc1

prob: 0.77

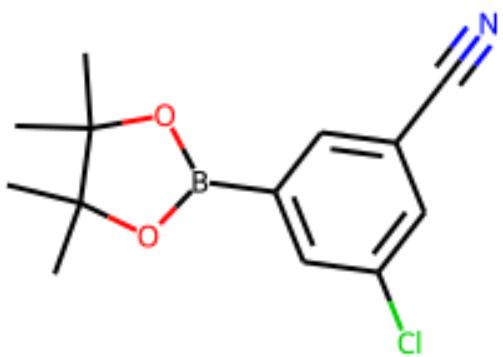


---

No.396

SMILES: CC1(C)OB(c2cc(C1)cc(C#N)c2)OC1(C)C

prob: 0.77

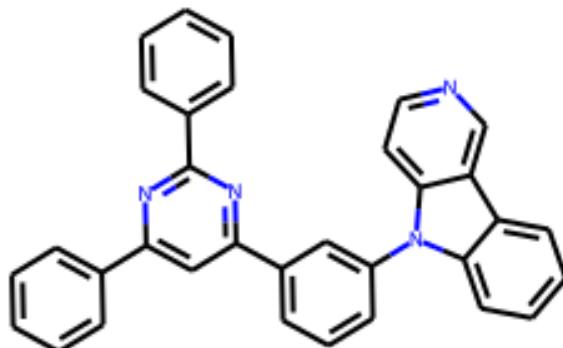


---

No.397

SMILES: c1ccc(-c2cc(-c3cccc(-n4c5cccc5c5cnccc54)c3)nc(-c3cccc3)n2)cc1

prob: 0.77

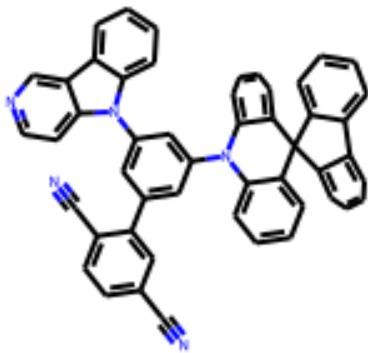


---

No.398

SMILES: N#Cc1ccc(C#N)c(-c2cc(N3c4cccc4C4(c5cccc5-c5cccc54)c4cccc43)cc(-n3c4cccc4c4cnccc43)c2)c1

prob: 0.77

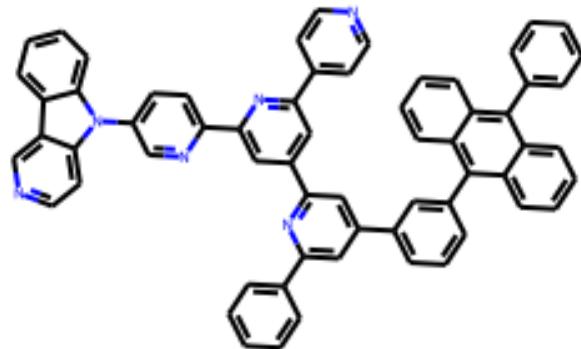


---

No.399

SMILES: c1ccc(-c2cc(-c3cccc(-c4c5ccccc5c(-c5ccccc5)c5ccccc45)c3)cc(-c3cc(-c4ccnc  
c4)nc(-c4ccc(-n5c6cccc6c6cnccc65)cn4)c3)n2)cc1

prob: 0.77

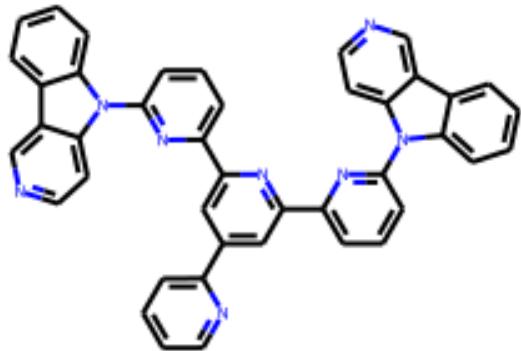


---

No.400

SMILES: c1ccc(-c2cc(-c3cccc(-n4c5ccccc5c5cnccc54)n3)nc(-c3cccc(-n4c5ccccc5c5cncc  
c54)n3)c2)nc1

prob: 0.77



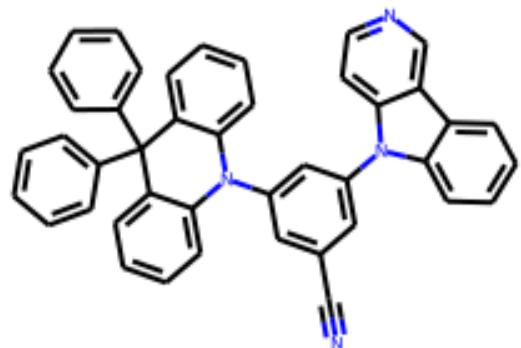
---

No.401

SMILES:

N#Cc1cc(N2c3cccc3C(c3cccc3)(c3cccc3)c3cccc32)cc(-n2c3cccc3c3cnccc32)c1

prob: 0.77

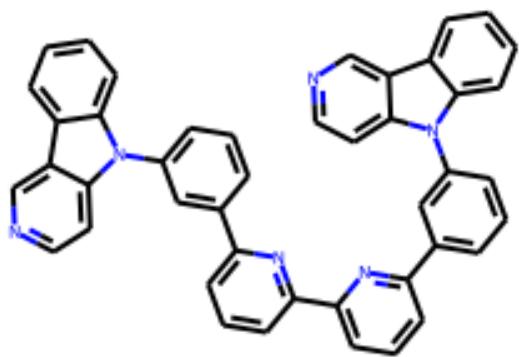


---

No.402

SMILES: c1cc(-c2cccc(-c3cccc(-c4cccc(-n5c6cccc6c6cnccc65)c4)n3)n2)cc(-n2c3cccc3c3cnccc32)c1

prob: 0.77

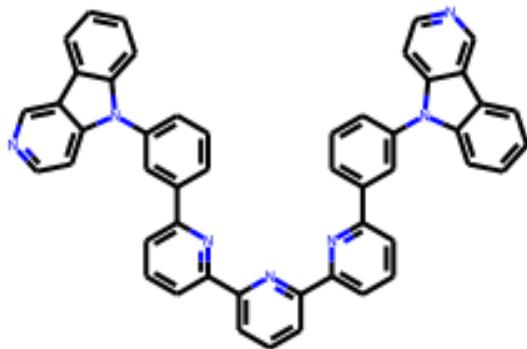


---

No.403

SMILES: c1cc(-c2cccc(-c3cccc(-c4cccc(-c5cccc(-n6c7cccc7c7cnccc76)c5)n4)n3)n2)cc  
(-n2c3cccccc3c3cnccc32)c1

prob: 0.77

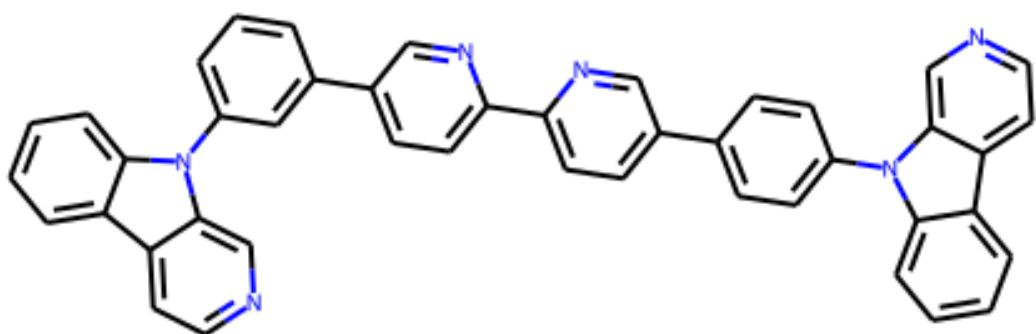


---

No.404

SMILES: c1cc(-c2ccc(-c3ccc(-c4ccc(-n5c6cccc6c6ccncc65)cc4)cn3)nc2)cc(-n2c3cccccc  
3c3ccncc32)c1

prob: 0.77



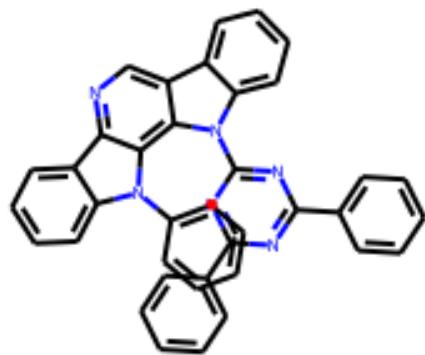
---

No.405

SMILES:

c1ccc(-c2nc(-c3ccccc3)nc(-n3c4ccccc4c4cnc5c6ccccc6n(-c6ccccc6)c5c43)n2)cc1

prob: 0.77

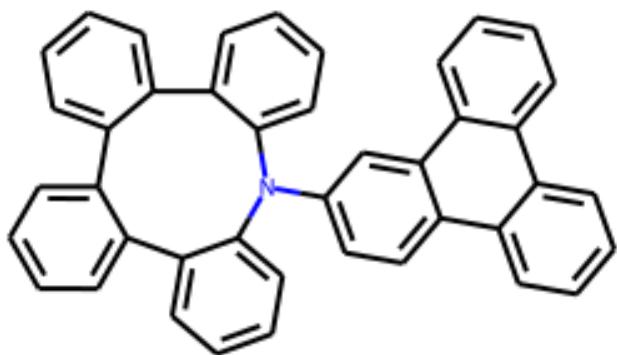


---

No.406

SMILES: c1ccc2c(c1)c1cccc1c1cc(-n3c4ccccc4c4ccccc4c4ccccc4c4ccccc43)ccc21

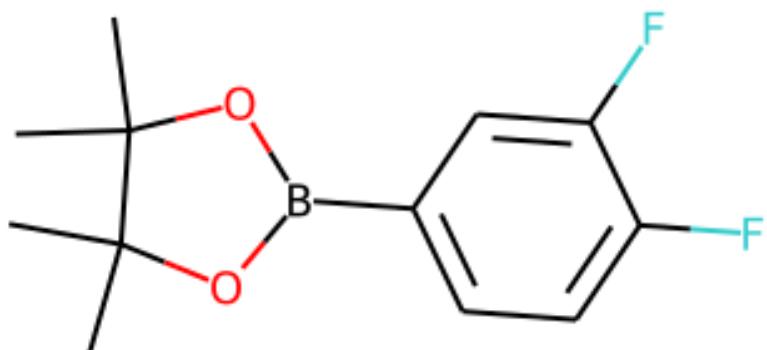
prob: 0.77



No.407

SMILES: CC1(C)OB(c2ccc(F)c(F)c2)OC1(C)C

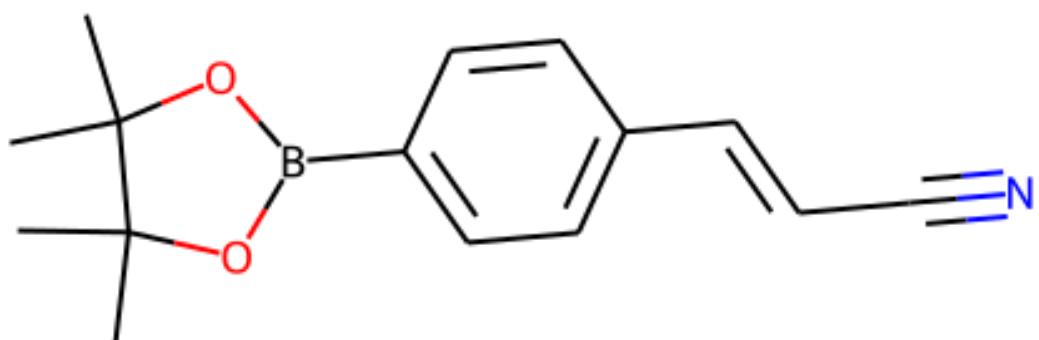
prob: 0.77



No.408

SMILES: CC1(C)OB(c2ccc(/C=C/C#N)cc2)OC1(C)C

prob: 0.77

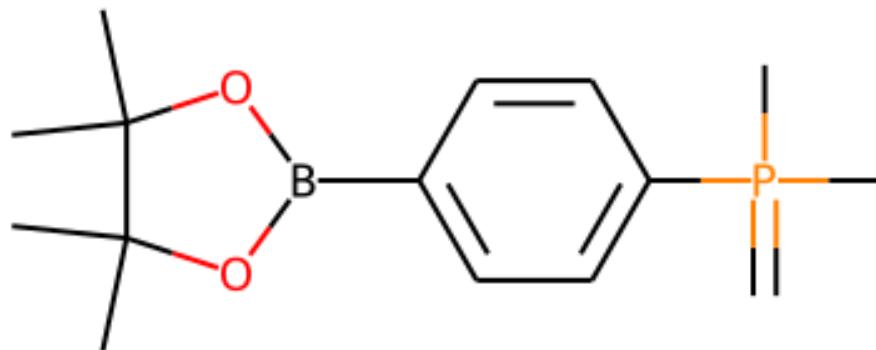


---

No. 409

SMILES: C=P(C)(C)c1ccc(B2OC(C)(C)C(C)(C)O2)cc1

prob: 0.77



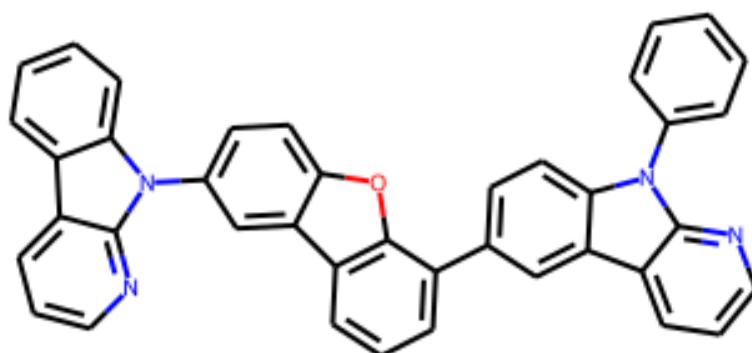
---

No. 410

SMILES:

c1cccc(-n2c3ccc(-c4cccc5c4oc4ccc(-n6c7cccc7c7cccnc76)cc45)cc3c3cccnc32)cc1

prob: 0.77

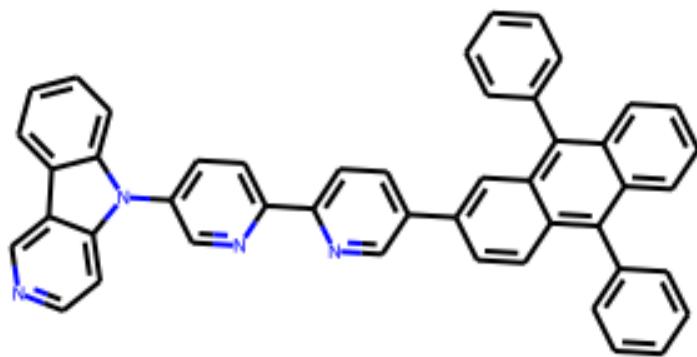


---

No. 411

SMILES: c1ccc(-c2c3cccc3c(-c3cccc3)c3cc(-c4ccc(-c5ccc(-n6c7cccc7c7cnccc76)cn5)nc4)ccc23)cc1

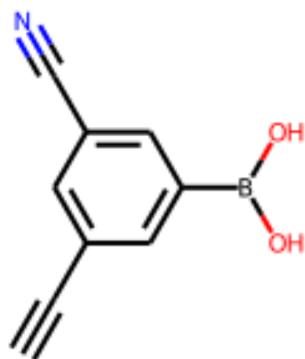
prob: 0.77



No.412

SMILES: C#Cc1cc(C#N)cc(B(O)O)c1

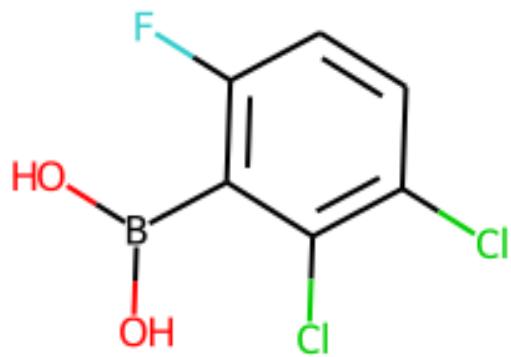
prob: 0.77



No.413

SMILES: OB(O)c1c(F)ccc(Cl)c1Cl

prob: 0.77

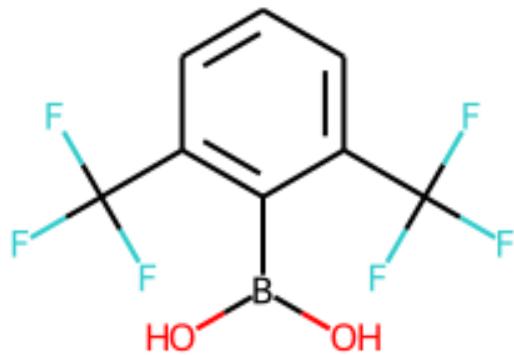


---

No.414

SMILES: OB(O)c1c(C(F)(F)F)cccc1C(F)(F)F

prob: 0.77

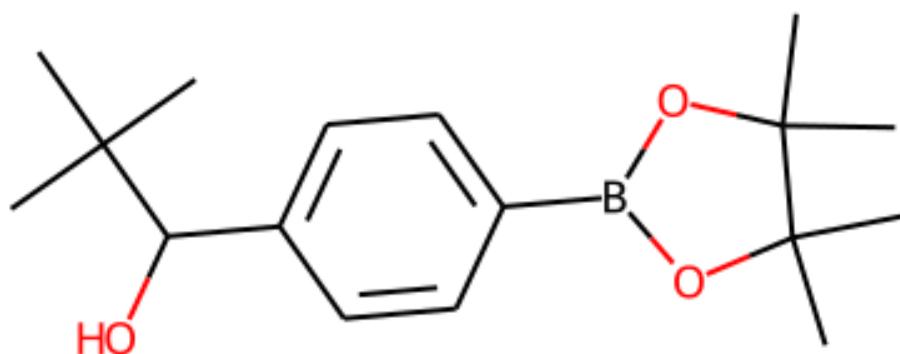


---

No.415

SMILES: CC(C)(C)C(O)c1ccc(B2OC(C)(C)C(C)(C)O2)cc1

prob: 0.77

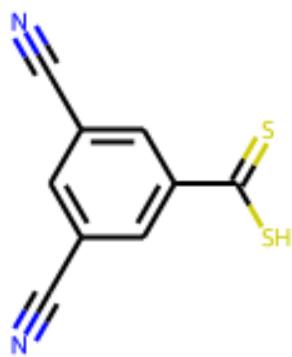


---

No.416

SMILES: N#Cc1cc(C#N)cc(C(=S)S)c1

prob: 0.77

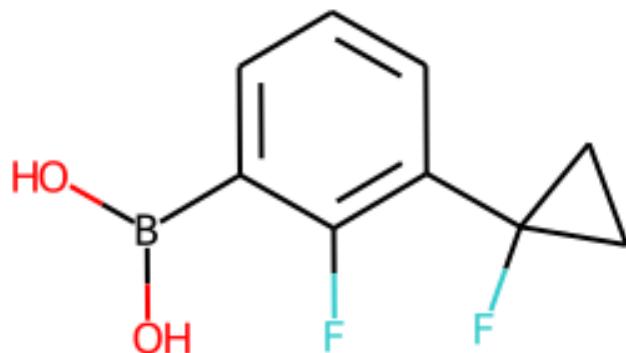


---

No.417

SMILES: OB(O)c1ccccc(C2(F)CC2)c1F

prob: 0.77

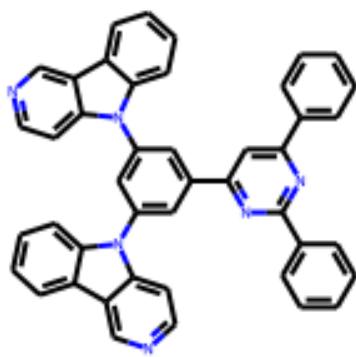


---

No.418

SMILES: c1ccc(-c2cc(-c3cc(-n4c5cccc5c5cnccc54)cc(-n4c5cccc5c5cnccc54)c3)nc(-c3cccc3)n2)cc1

prob: 0.77

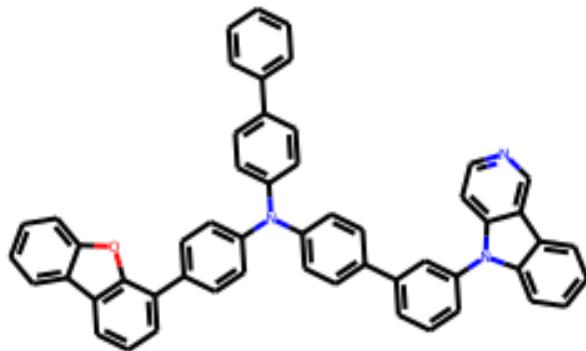


---

No.419

SMILES: c1ccc(-c2ccc(N(c3ccc(-c4cccc(-n5c6ccccc6c6cnccc65)c4)cc3)c3ccc(-c4cccc5c4oc4ccccc45)cc3)cc2)cc1

prob: 0.77

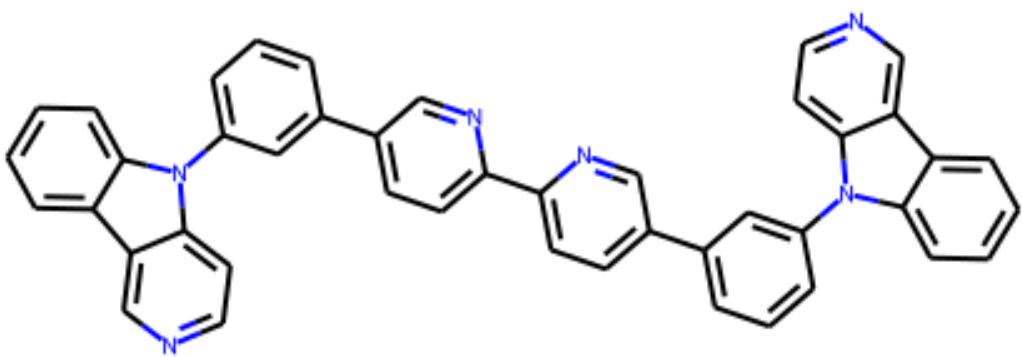


---

No.420

SMILES: c1cc(-c2ccc(-c3ccc(-c4cccc(-n5c6ccccc6c6cnccc65)c4)cn3)nc2)cc(-n2c3ccccc3c3cnccc32)c1

prob: 0.77

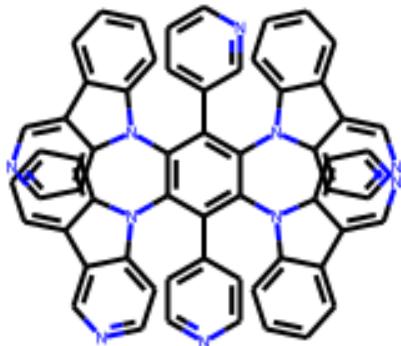


---

No. 421

SMILES: c1cncc(-c2c(-n3c4cccc4c4cnccc43)c(-n3c4cccc4c4cnccc43)c(-c3ccncc3)c(-n3c4cccc4c4cnccc43)c2-n2c3cccc3c3cnccc32)c1

prob: 0.77

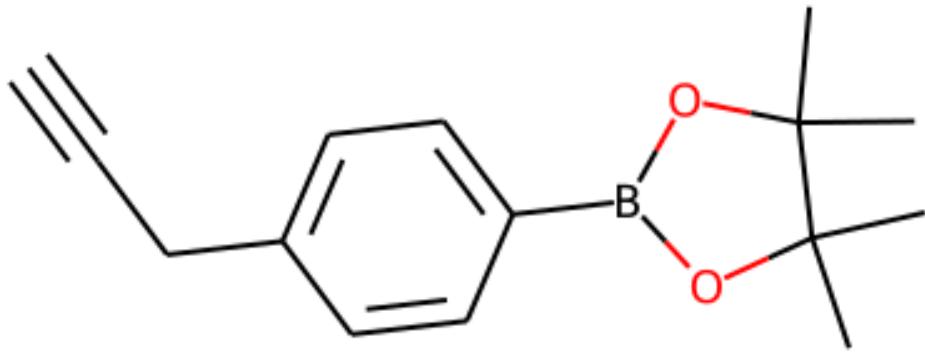


---

No. 422

SMILES: C#CCc1ccc(B20C(C)(C)C(C)(C)O2)cc1

prob: 0.77

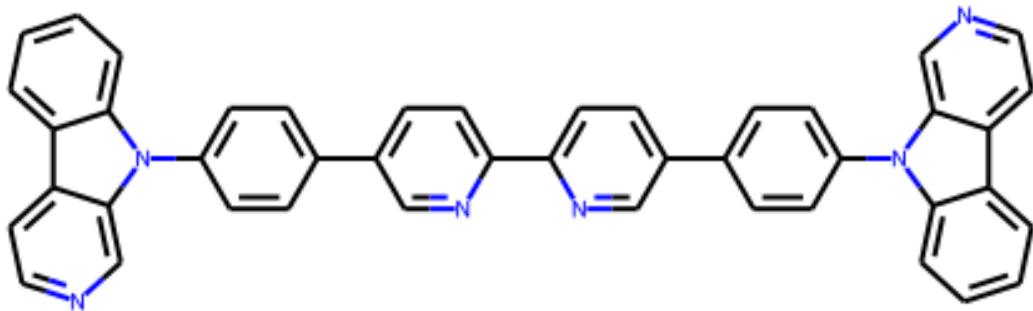


---

No. 423

SMILES: c1ccc2c(c1)c1ccncc1n2-c1ccc(-c2ccc(-c3ccc(-c4ccc(-n5c6cccc6c6ccncc65)cc4)cn3)nc2)cc1

prob: 0.77

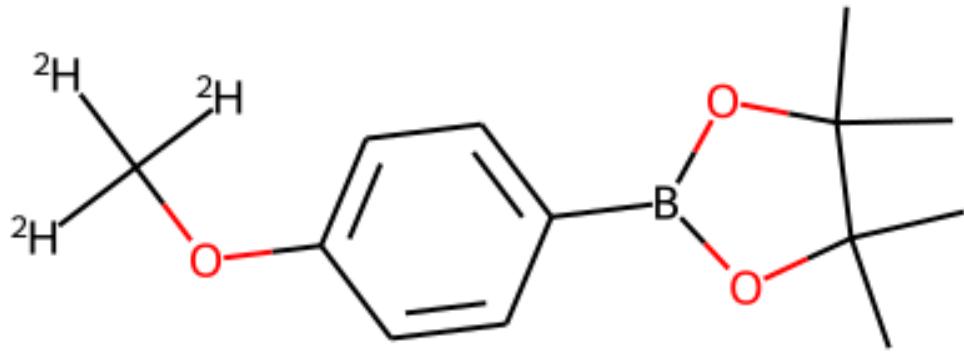


---

No. 424

SMILES: [2H]C([2H])([2H])Oc1ccc(B2OC(C)(C)C(C)(C)O2)cc1

prob: 0.77

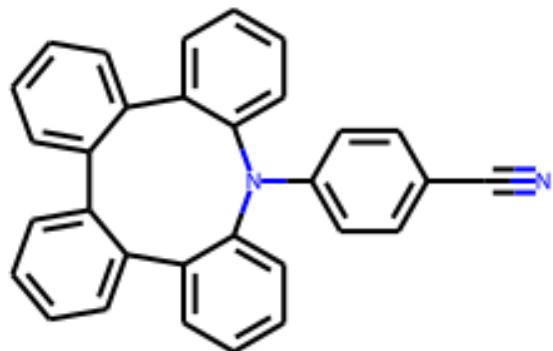


---

No.425

SMILES: N#Cc1cccc(-n2c3cccc3c3cccc3c3cccc3c3cccc32)cc1

prob: 0.77

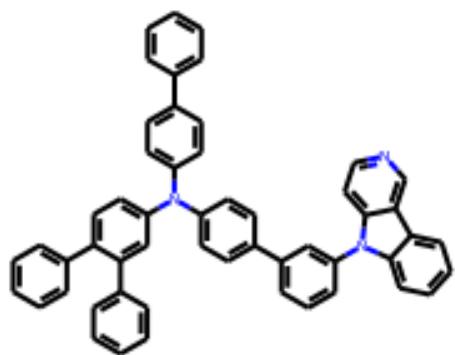


---

No.426

SMILES: c1ccc(-c2ccc(N(c3ccc(-c4cccc(-n5c6cccc6c6cnccc65)c4)cc3)c3ccc(-c4cccc4)c(-c4cccc4)c3)cc2)cc1

prob: 0.77

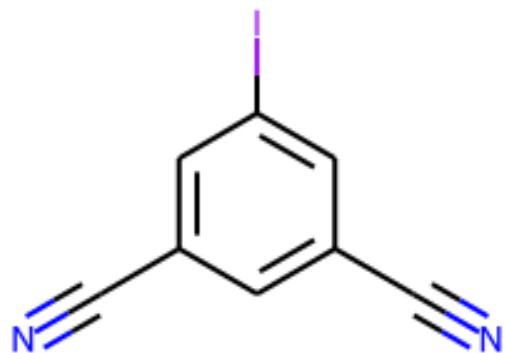


---

No.427

SMILES: N#Cc1cc(I)cc(C#N)c1

prob: 0.77

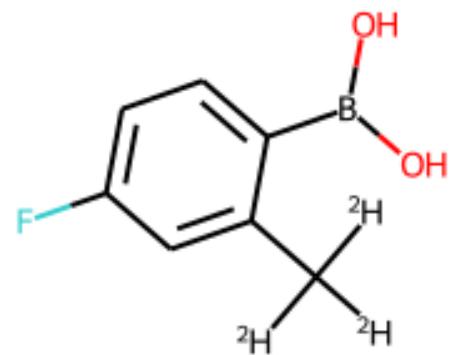


---

No.428

SMILES: [2H]C([2H])([2H])c1cc(F)ccc1B(O)O

prob: 0.77

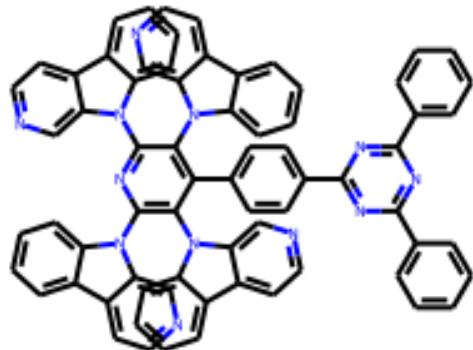


---

No.429

SMILES: c1ccc(-c2nc(-c3cccc3)nc(-c3ccc(-c4c(-n5c6cccc6c6ccncc65)c(-n5c6cccc6c6ccncc65)nc(-n5c6cccc6c6ccncc65)c4-n4c5cccc5c5ccncc54)cc3)n2)cc1

prob: 0.77

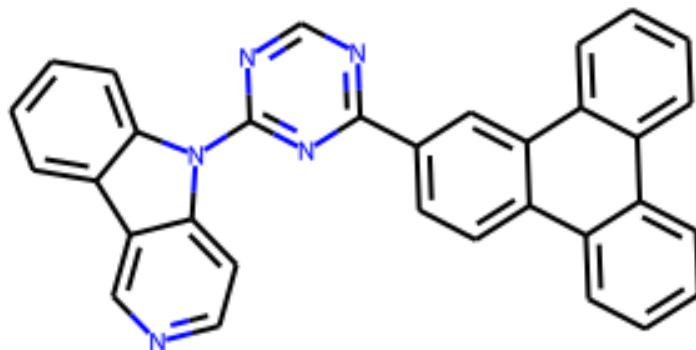


---

No.430

SMILES: c1ccc2c(c1)c1cccc1c1cc(-c3ncnc(-n4c5cccc5c5cnccc54)n3)ccc21

prob: 0.77

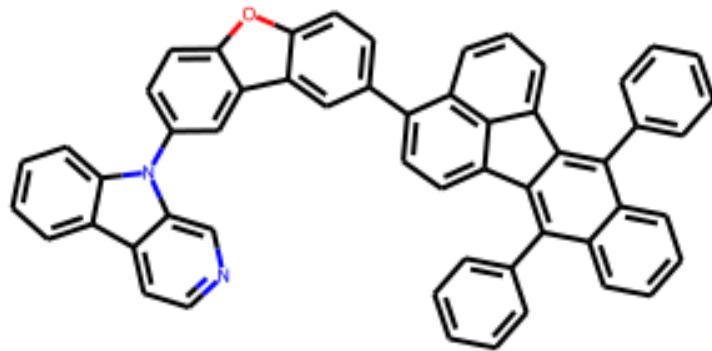


---

No.431

SMILES: c1ccc(-c2c3c(c(-c4cccc4)c4cccc24)-c2ccc(-c4ccc5oc6ccc(-n7c8cccc8c8ccncc87)cc6c5c4)c4cccc-3c24)cc1

prob: 0.77

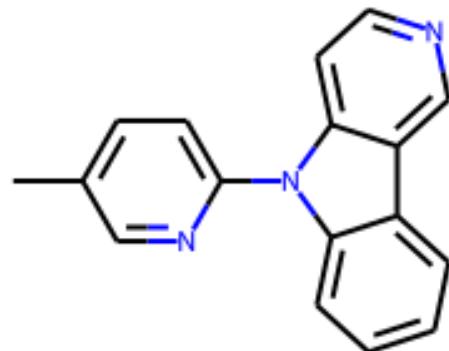


---

No.432

SMILES: Cc1ccc(-n2c3cccc3c3cnccc32)nc1

prob: 0.77

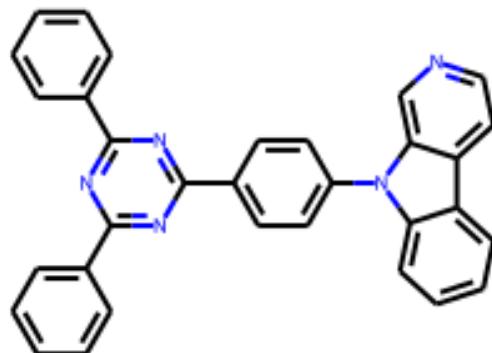


---

No.433

SMILES: c1ccc(-c2nc(-c3cccc3)nc(-c3ccc(-n4c5cccc5c5ccncc54)cc3)n2)cc1

prob: 0.77



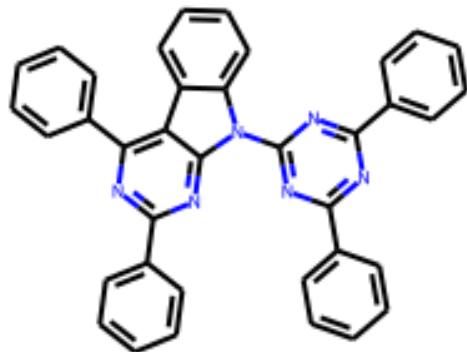
---

No.434

SMILES:

c1ccc(-c2nc(-c3cccc3)nc(-n3c4ccccc4c4c(-c5ccccc5)nc(-c5ccccc5)nc43)n2)cc1

prob: 0.77

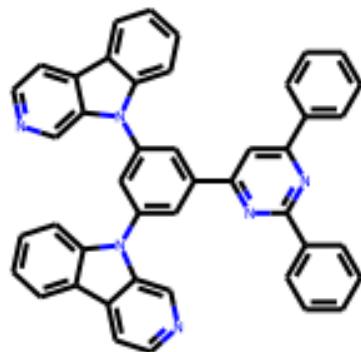


---

No.435

SMILES: c1ccc(-c2cc(-c3cc(-n4c5ccccc5c5ccncc54)cc(-n4c5ccccc5c5ccncc54)c3)nc(-c3cccc3)n2)cc1

prob: 0.77

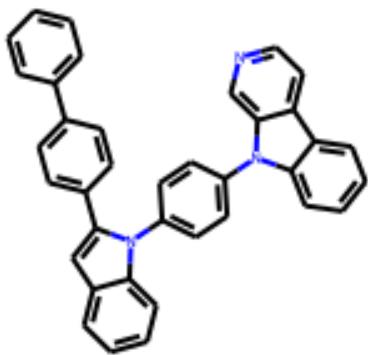


---

No.436

SMILES: c1ccc(-c2ccc(-c3cc4ccccc4n3-c3ccc(-n4c5ccccc5c5ccncc54)cc3)cc2)cc1

prob: 0.77

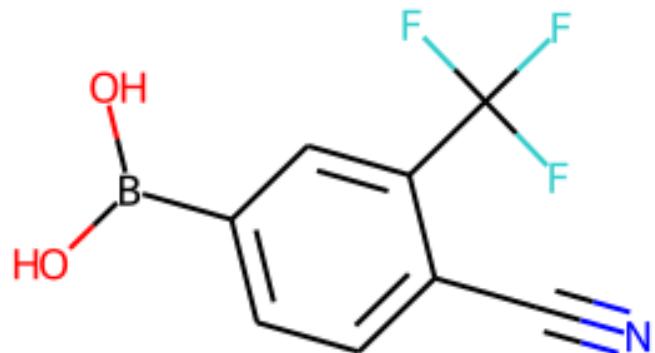


---

No.437

SMILES: N#Cc1cccc(B(O)O)cc1C(F)(F)F

prob: 0.77

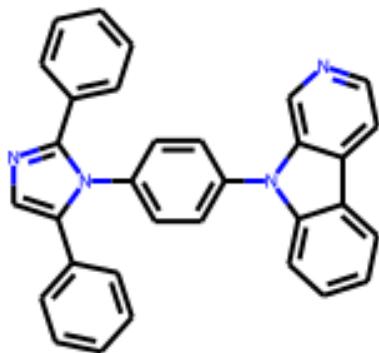


---

No.438

SMILES: c1ccc(-c2cnc(-c3ccccc3)n2-c2ccc(-n3c4ccccc4c4ccncc43)cc2)cc1

prob: 0.77

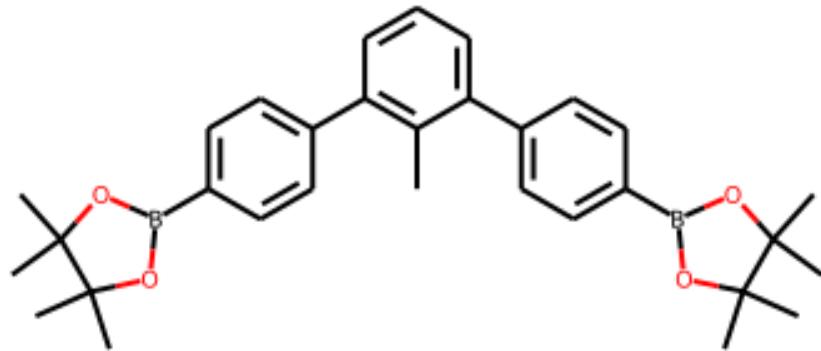


---

No.439

SMILES: Cc1c(-c2ccc(B30C(C)(C)C(C)(C)O3)cc2)cccc1-c1ccc(B20C(C)(C)C(C)(C)O2)cc1

prob: 0.77

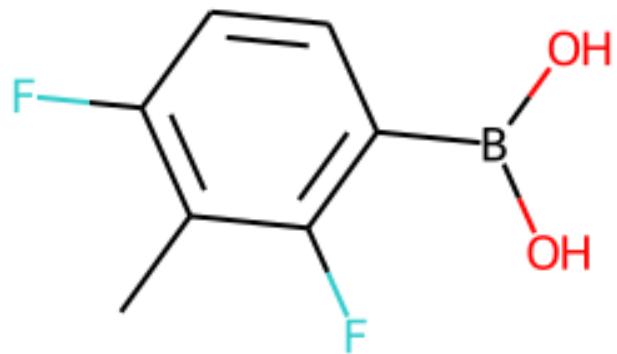


---

No.440

SMILES: Cc1c(F)ccc(B(O)O)c1F

prob: 0.77



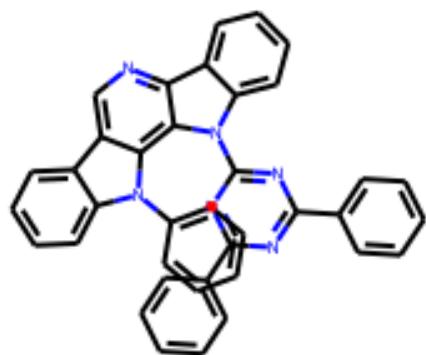
---

No.441

SMILES:

c1cccc(-c2nc(-c3cccc3)nc(-n3c4cccc4c4ncc5c6cccc6n(-c6cccc6)c5c43)n2)cc1

prob: 0.77

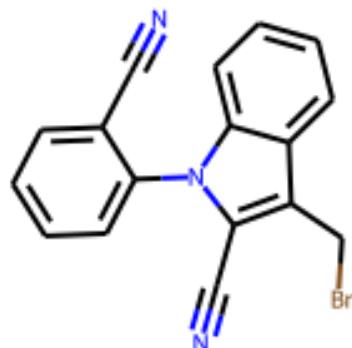


---

No.442

SMILES: N#Cc1ccccc1-n1c(C#N)c(CBr)c2ccccc21

prob: 0.77

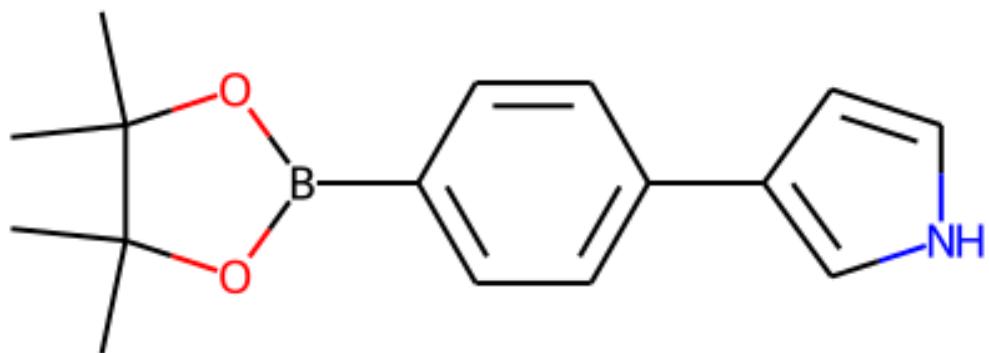


---

No.443

SMILES: CC1(C)OB(c2ccc(-c3cc[nH]c3)cc2)OC1(C)C

prob: 0.77

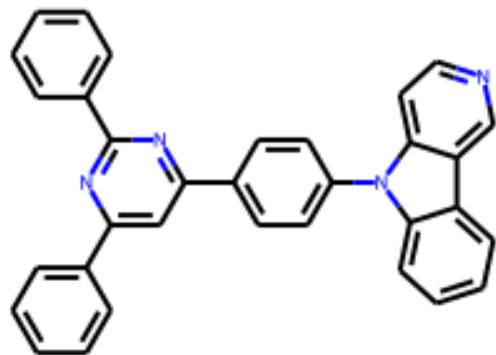


---

No.444

SMILES: c1ccc(-c2cc(-c3ccc(-n4c5cccc5c5cnccc54)cc3)nc(-c3cccc3)n2)cc1

prob: 0.77

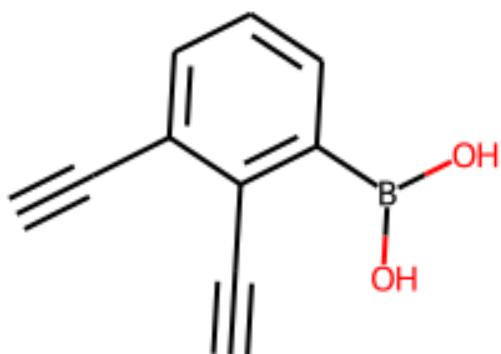


---

No.445

SMILES: C#Cc1cccc(B(O)O)c1C#C

prob: 0.77

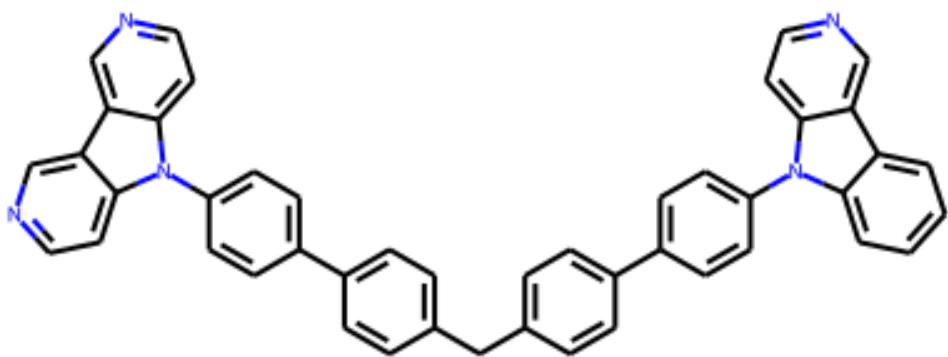


---

No.446

SMILES: c1ccc2c(c1)c1cnccc1n2-c1ccc(-c2ccc(Cc3ccc(-c4ccc(-n5c6ccncc6c6cnccc65)cc4)cc3)cc2)cc1

prob: 0.77



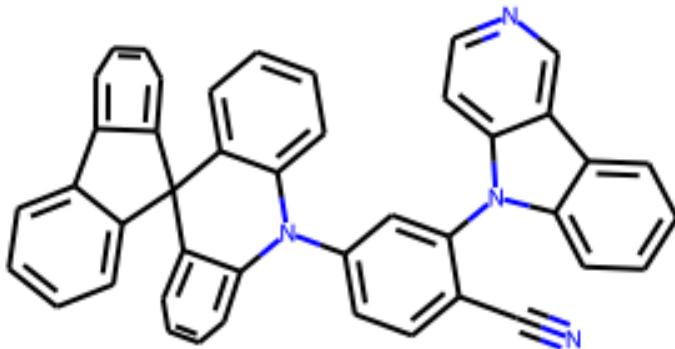
---

No.447

SMILES:

N#Cc1ccc(N2c3ccccc3C3(c4ccccc4-c4ccccc43)c3ccccc32)cc1-n1c2ccccc2c2cnccc21

prob: 0.76

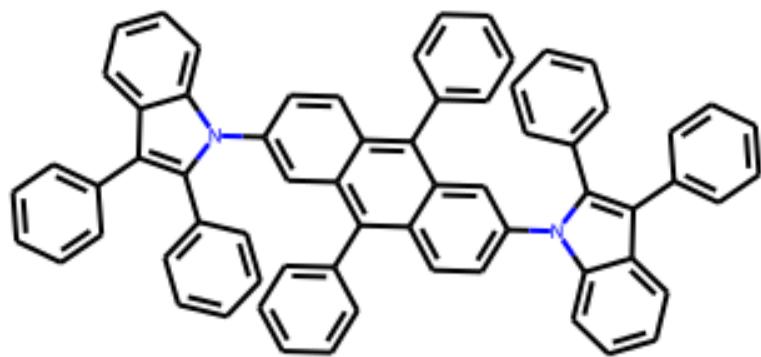


---

No.448

SMILES: c1ccc(-c2c3ccc(-n4c(-c5ccccc5)c(-c5ccccc5)c5ccccc54)cc3c(-c3ccccc3)c3ccc(-n4c(-c5ccccc5)c(-c5ccccc5)c5ccccc54)cc23)cc1

prob: 0.76

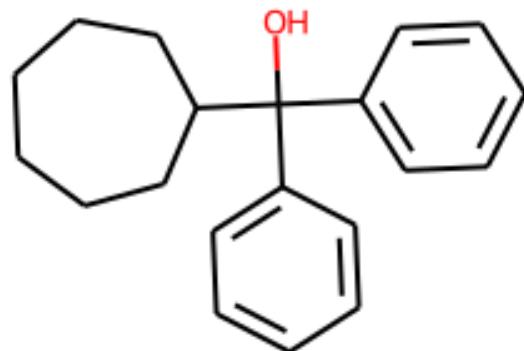


---

No.449

SMILES: OC(c1ccccc1)(c1ccccc1)C1CCCCC1

prob: 0.76

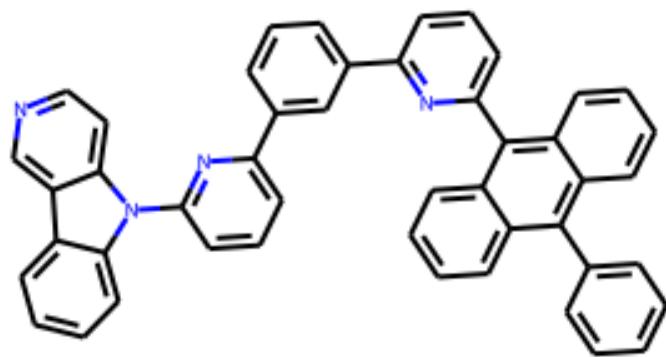


---

No.450

SMILES: c1ccc(-c2c3cccc3c(-c3cccc(-c4cccc(-c5cccc(-n6c7cccc7c7cnccc76)n5)c4)n3)c3cccc23)cc1

prob: 0.76

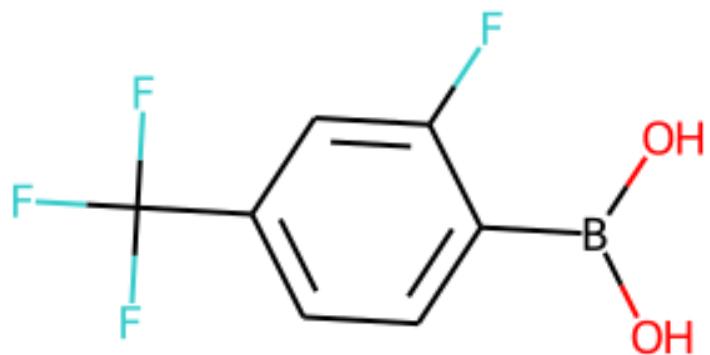


---

No.451

SMILES: OB(O)c1ccc(C(F)(F)F)cc1F

prob: 0.76

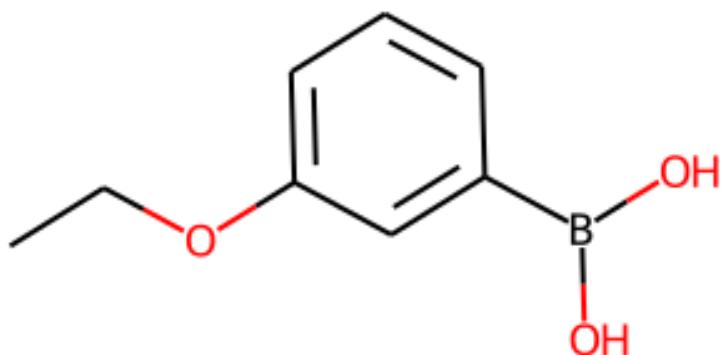


---

No.452

SMILES: CC0c1cccc(B(O)O)c1

prob: 0.76

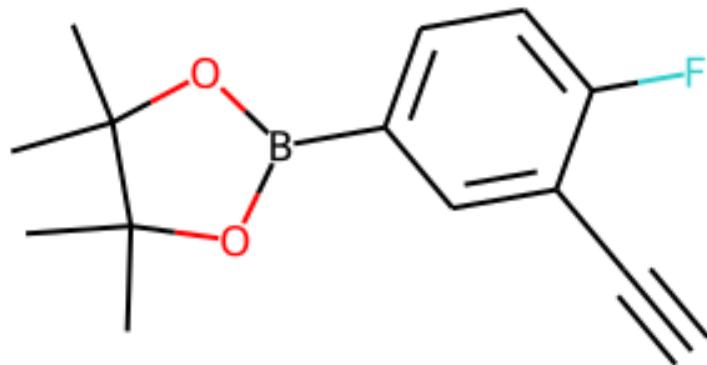


---

No.453

SMILES: C#Cc1cc(B2OC(C)(C)C(C)(C)O2)ccc1F

prob: 0.76

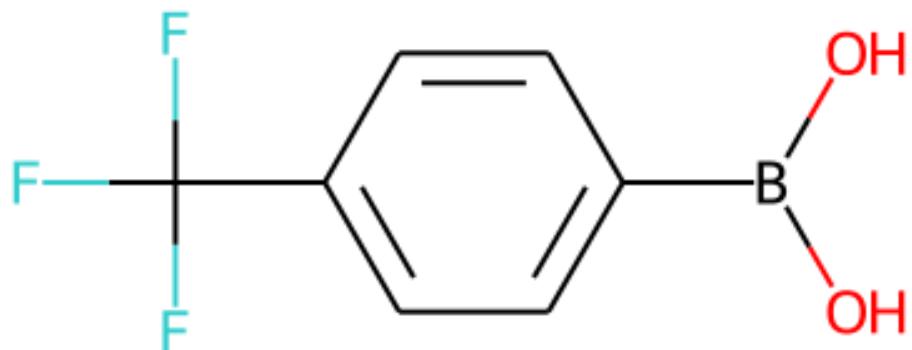


---

No.454

SMILES: OB(O)c1ccc(C(F)(F)F)cc1

prob: 0.76

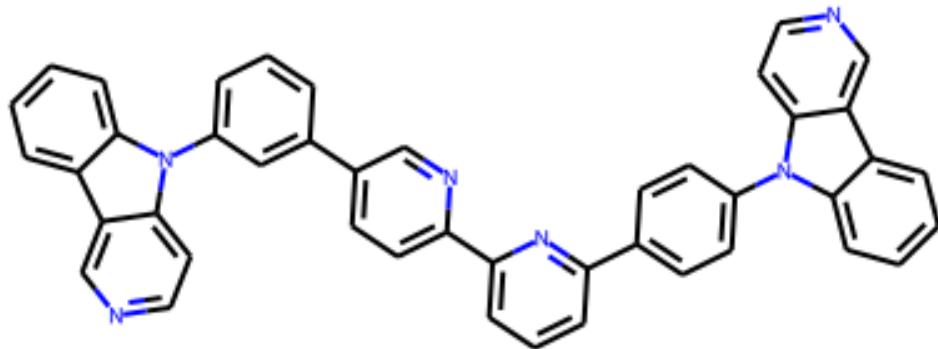


---

No.455

SMILES: c1cc(-c2ccc(-c3cccc(-c4ccc(-n5c6cccc6c6cnccc65)cc4)n3)nc2)cc(-n2c3cccc3c3cnccc32)c1

prob: 0.76

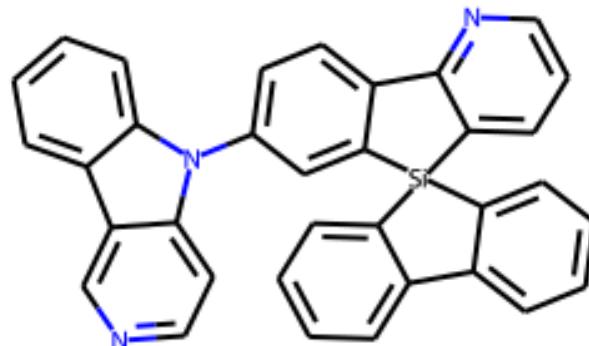


---

No.456

SMILES: c1ccc2c(c1)-c1ccccc1[Si]21c2cc(-n3c4cccc4c4cnccc43)ccc2-c2ncccc21

prob: 0.76

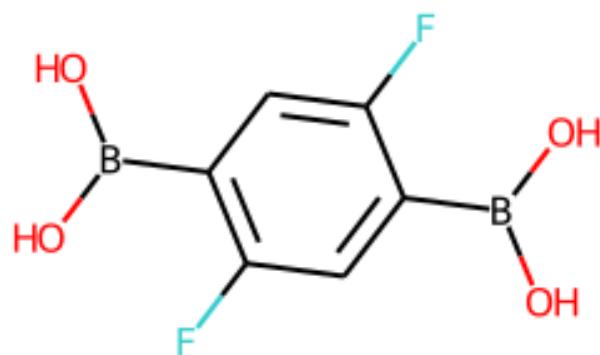


---

No.457

SMILES: OB(0)c1cc(F)c(B(0)O)cc1F

prob: 0.76



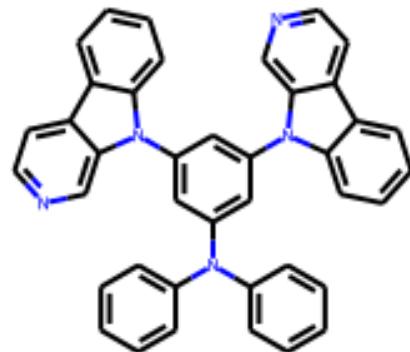
---

No.458

SMILES:

c1ccc(N(c2ccccc2)c2cc(-n3c4ccccc4c4ccncc43)cc(-n3c4ccccc4c4ccncc43)c2)cc1

prob: 0.76

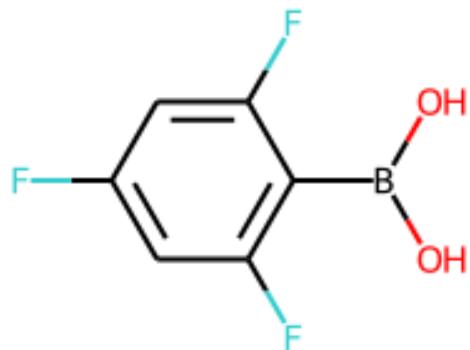


---

No.459

SMILES: OB(O)c1c(F)cc(F)cc1F

prob: 0.76



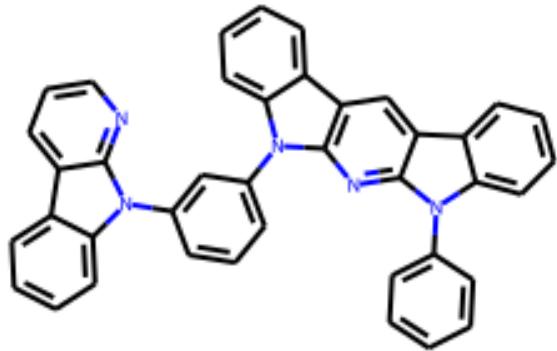
---

No.460

SMILES:

c1ccc(-n2c3ccccc3c3cc4c5ccccc5n(-c5cccc(-n6c7ccccc7c7ccnnc76)c5)c4nc32)cc1

prob: 0.76

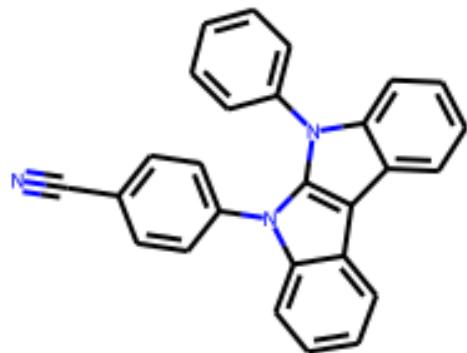


---

No.461

SMILES: N#Cc1cccc(-n2c3cccc3c3c4cccc4n(-c4cccc4)c32)cc1

prob: 0.76

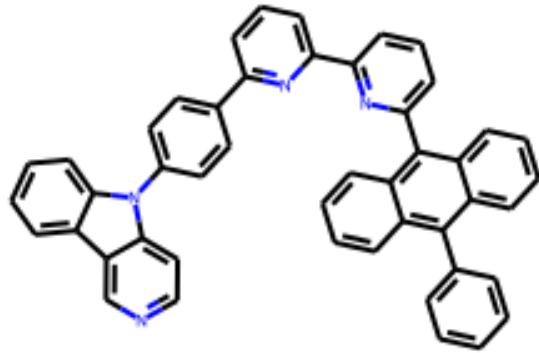


---

No.462

SMILES: c1ccc(-c2c3cccc3c(-c3cccc(-c4cccc(-c5ccc(-n6c7cccc7c7cnccc76)cc5)n4)n3)c3cccc23)cc1

prob: 0.76

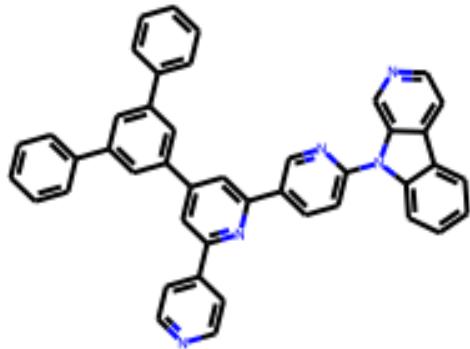


---

No.463

SMILES: c1ccc(-c2cc(-c3cccc3)cc(-c3cc(-c4ccncc4)nc(-c4ccc(-n5c6cccc6c6ccncc65)nc4)c3)c2)cc1

prob: 0.76

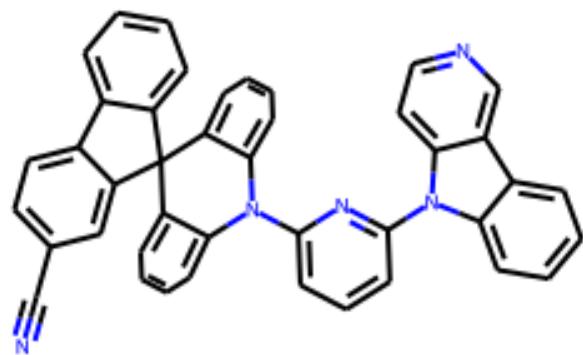


---

No.464

SMILES:

N#Cc1cccc2c(c1)C1(c3cccc3-2)c2cccc2N(c2cccc(-n3c4cccc4c4cnccc43)n2)c2cccc21  
prob: 0.76

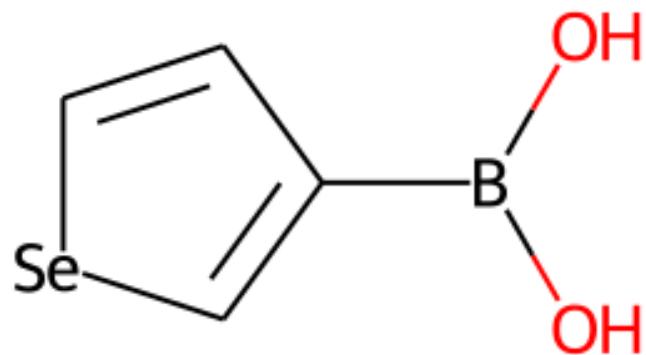


---

No.465

SMILES: OB(O)c1cc[se]c1

prob: 0.76

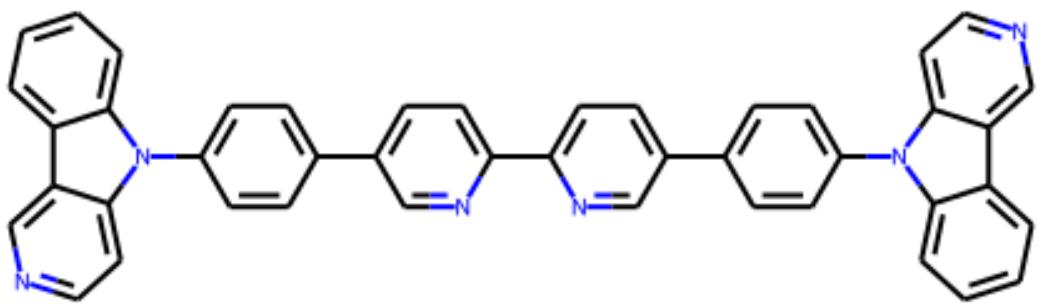


---

No.466

SMILES: c1ccc2c(c1)c1cnccc1n2-c1ccc(-c2ccc(-c3ccc(-c4ccc(-n5c6cccc6c6cnccc65)cc4)cn3)nc2)cc1

prob: 0.76

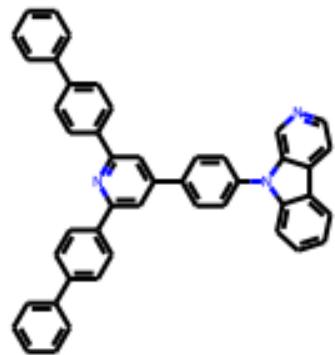


---

No.467

SMILES: c1ccc(-c2ccc(-c3cc(-c4ccc(-n5c6cccc6c6ccncc65)cc4)cc(-c4ccc(-c5ccccc5)c  
c4)n3)cc2)cc1

prob: 0.76

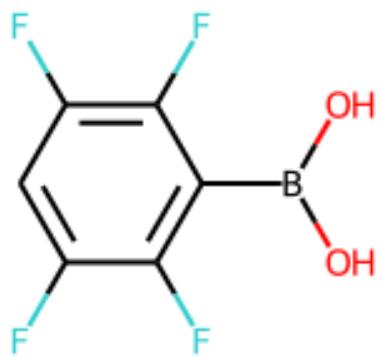


---

No.468

SMILES: OB(0)c1c(F)c(F)cc(F)c1F

prob: 0.76

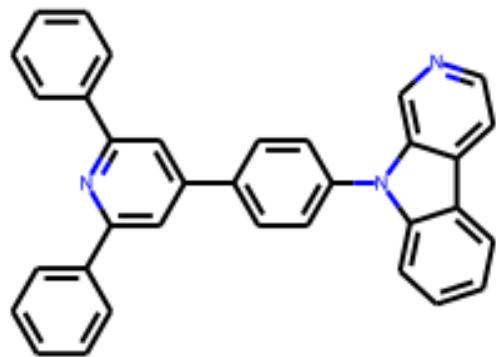


---

No.469

SMILES: c1ccc(-c2cc(-c3ccc(-n4c5cccc5c5ccncc54)cc3)cc(-c3ccccc3)n2)cc1

prob: 0.76

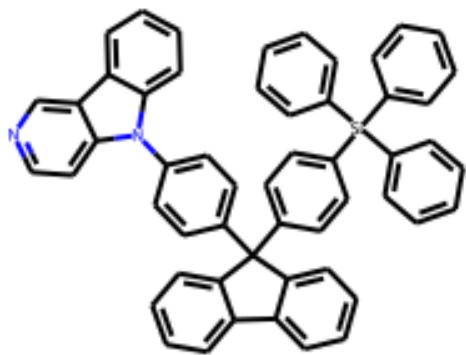


---

No.470

SMILES: c1ccc([Si](c2ccccc2)(c2ccccc2)c2ccc(c3(c4ccc(-n5c6cccc6c6cnccc65)cc4)c4cccc4-c4ccccc43)cc2)cc1

prob: 0.76

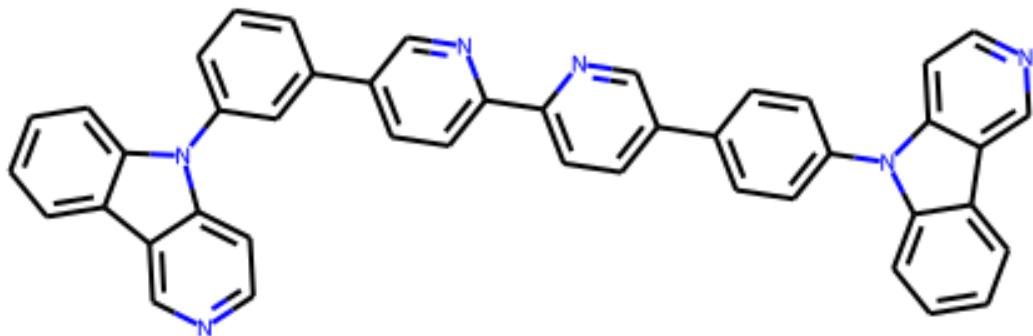


---

No.471

SMILES: c1cc(-c2ccc(-c3ccc(-c4ccc(-n5c6cccc6c6cnccc65)cc4)cn3)nc2)cc(-n2c3cccc3c3cnccc32)c1

prob: 0.76

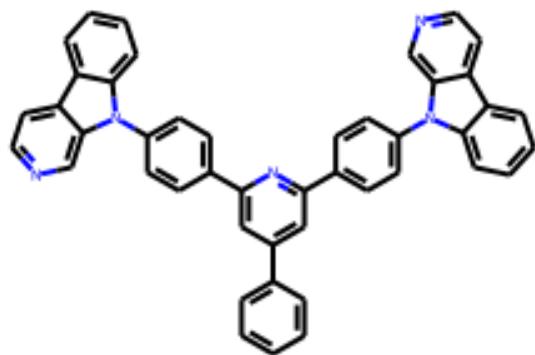


---

No.472

SMILES: c1ccc(-c2cc(-c3ccc(-n4c5cccc5c5ccncc54)cc3)nc(-c3ccc(-n4c5cccc5c5ccncc54)cc3)c2)cc1

prob: 0.76

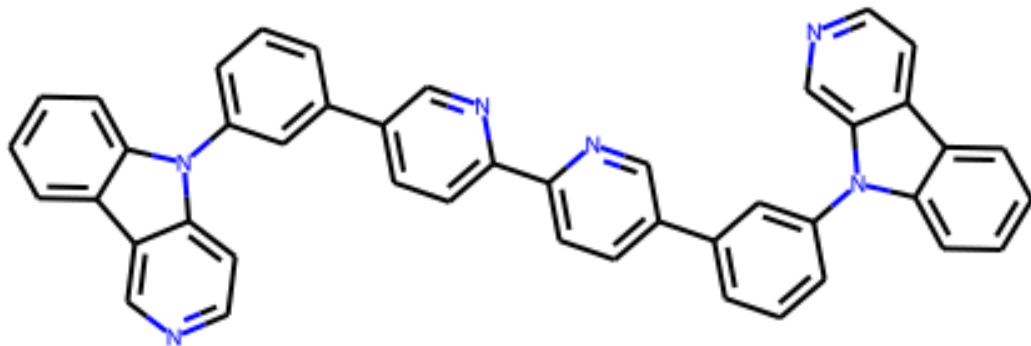


---

No.473

SMILES: c1cc(-c2ccc(-c3ccc(-c4cccc(-n5c6cccc6c6ccncc65)c4)cn3)nc2)cc(-n2c3cccc3c3cnccc32)c1

prob: 0.76

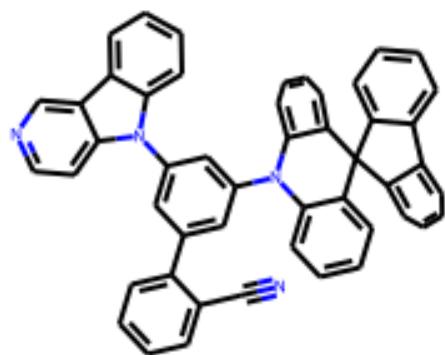


---

No.474

SMILES: N#Cc1ccccc1-c1cc(N2c3cccc3C3(c4cccc4-c4cccc43)c3cccc32)cc(-n2c3cccc3c3cnccc32)c1

prob: 0.76

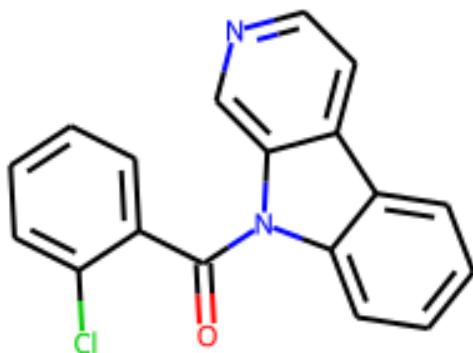


---

No.475

SMILES: O=C(c1ccccc1Cl)N1C2CCCC2C2CCNCC21

prob: 0.76

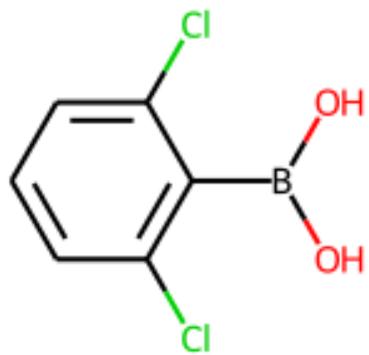


---

No.476

SMILES: OB(O)c1c(Cl)cccc1Cl

prob: 0.76

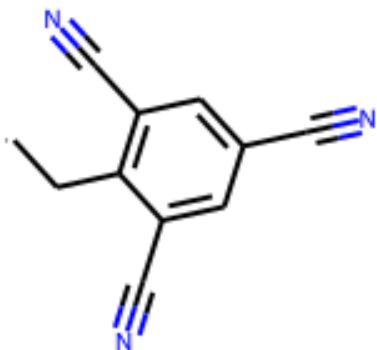


---

No.477

SMILES: [CH2]Cc1c(C#N)cc(C#N)cc1C#N

prob: 0.76

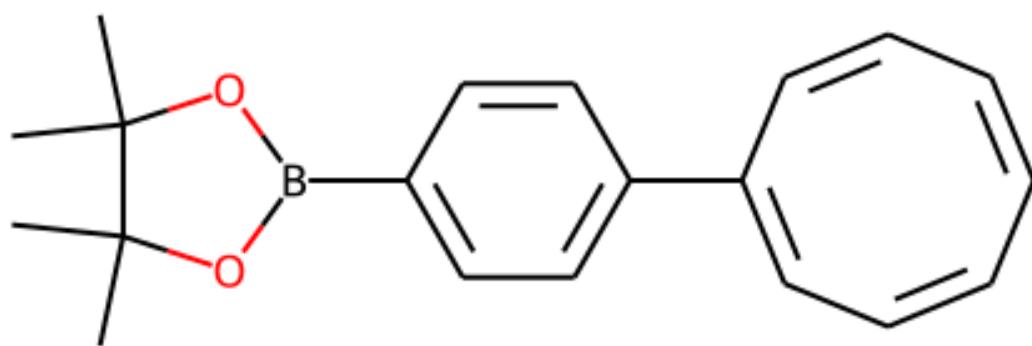


---

No.478

SMILES: CC1(C)OB(c2ccc(C3=CC=CC=CC=C3)cc2)OC1(C)C

prob: 0.76

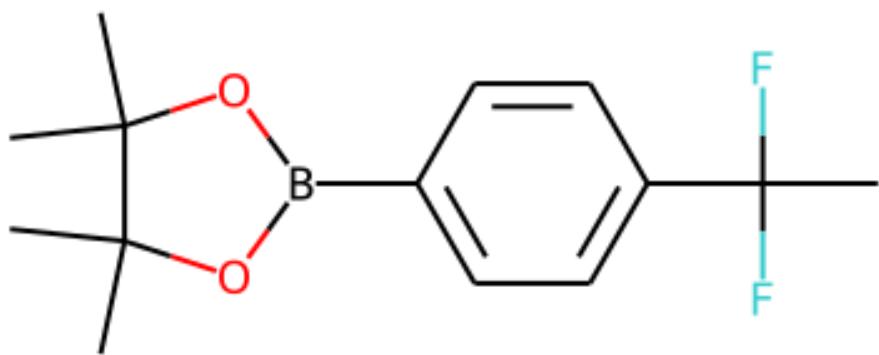


---

No.479

SMILES: CC(F)(F)c1ccc(B2OC(C)(C)C(C)(C)O2)cc1

prob: 0.76

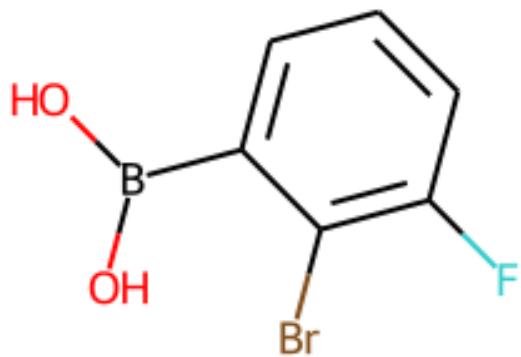


---

No.480

SMILES: OB(O)c1ccccc(F)c1Br

prob: 0.76

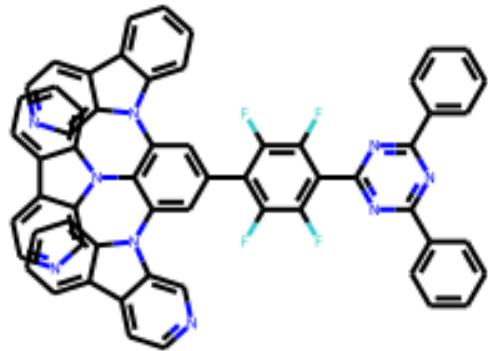


---

No.481

SMILES: Fc1c(F)c(-c2nc(-c3cccc3)nc(-c3cccc3)n2)c(F)c(F)c1-c1cc(-n2c3cccc3c3ccncc32)c(-n2c3cccc3c3ccncc32)c1

prob: 0.76

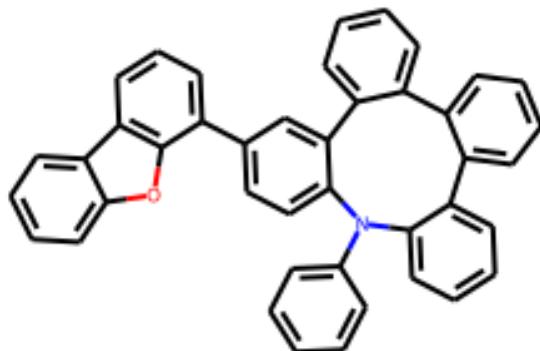


---

No. 482

SMILES: c1ccc(-n2c3cccc3c3cccc3c3cccc3c3cc(-c4cccc5c4oc4cccc45)ccc32)cc1

prob: 0.76

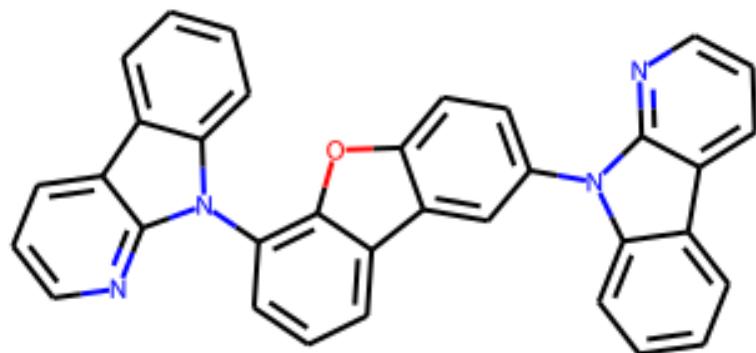


---

No. 483

SMILES: c1cc(-n2c3cccc3c3cccnc32)c2oc3ccc(-n4c5cccc5c5cccnc54)cc3c2c1

prob: 0.76

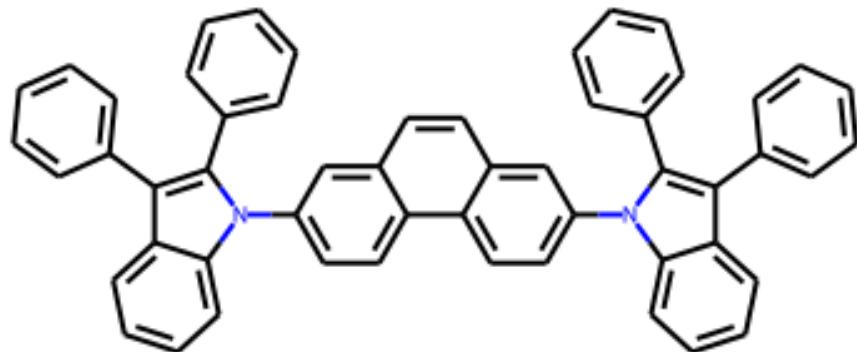


---

No.484

SMILES: c1ccc(-c2c(-c3ccccc3)n(-c3ccc4c(ccc5cc(-n6c(-c7ccccc7)c(-c7ccccc7)c7cccc  
c76)ccc54)c3)c3ccccc23)cc1

prob: 0.76

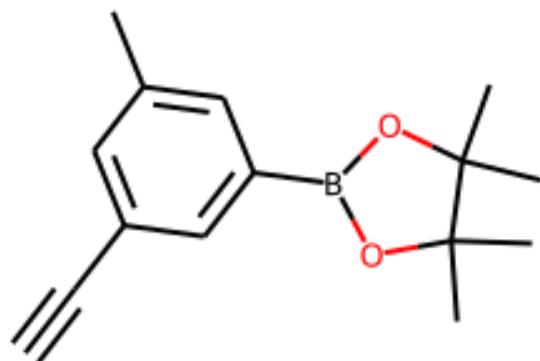


---

No.485

SMILES: C#Cc1cc(C)cc(B2OC(C)(C)C(C)(C)O2)c1

prob: 0.76

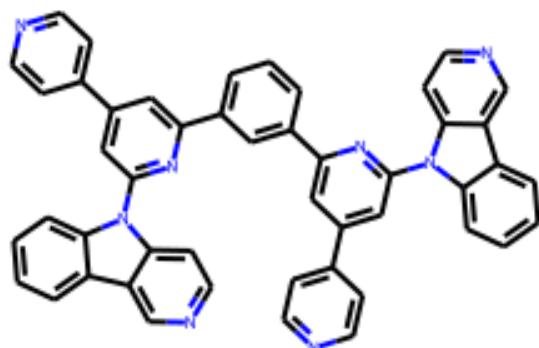


---

No.486

SMILES: c1cc(-c2cc(-c3ccncc3)cc(-n3c4ccccc4c4cnccc43)n2)cc(-c2cc(-c3ccncc3)cc(-n  
3c4ccccc4c4cnccc43)n2)c1

prob: 0.76

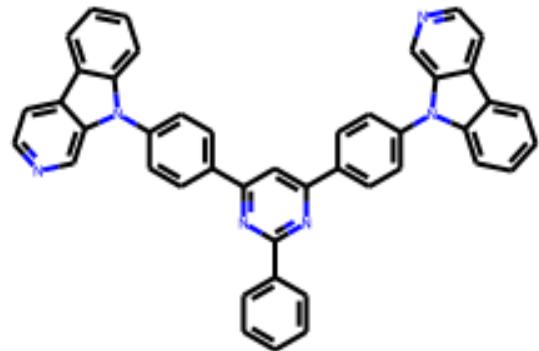


---

No.487

SMILES: c1ccc(-c2nc(-c3ccc(-n4c5cccc5c5ccncc54)cc3)cc(-c3ccc(-n4c5cccc5c5ccncc54)cc3)n2)cc1

prob: 0.76

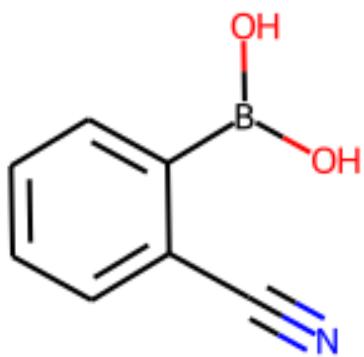


---

No.488

SMILES: N#Cc1ccccc1B(0)O

prob: 0.76

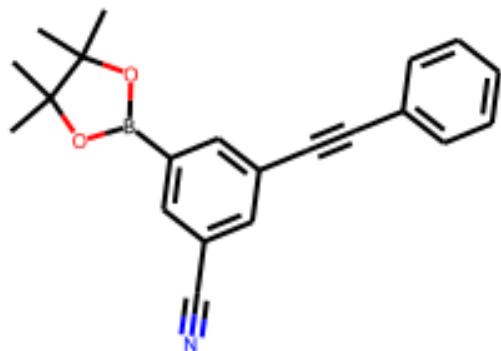


---

No. 489

SMILES: CC1(C)OB(c2cc(C#N)cc(C#Cc3cccc3)c2)OC1(C)C

prob: 0.76

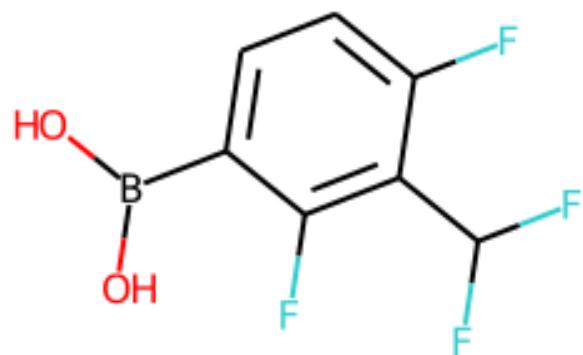


---

No. 490

SMILES: OB(O)c1ccc(F)c(C(F)F)c1F

prob: 0.76

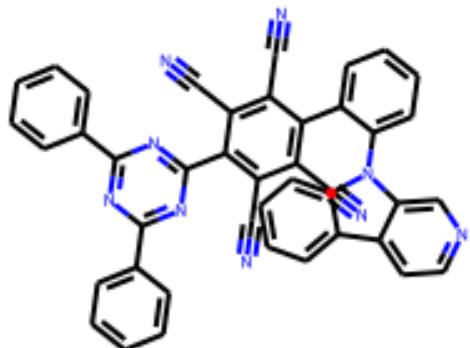


---

No.491

SMILES: N#Cc1c(C#N)c(-c2ccccc2-n2c3cccc3c3ccncc32)c(C#N)c(C#N)c1-c1nc(-c2ccccc2)nc(-c2ccccc2)n1

prob: 0.76

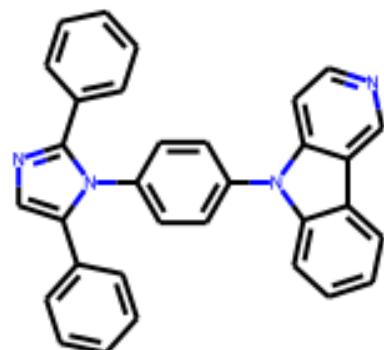


---

No.492

SMILES: c1ccc(-c2cnc(-c3cccc3)n2-c2ccc(-n3c4cccc4c4cnccc43)cc2)cc1

prob: 0.76



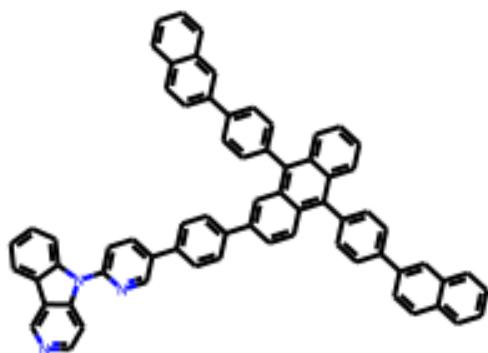
---

No.493

SMILES: c1ccc2cc(-c3ccc(-c4c5cccc5c(-c5ccc(-c6ccc7cccc7c6)cc5)c5cc(-c6ccc(-c7c

cc(-n8c9cccc9c9cnccc98)nc7)cc6)ccc45)cc3)ccc2c1

prob: 0.76

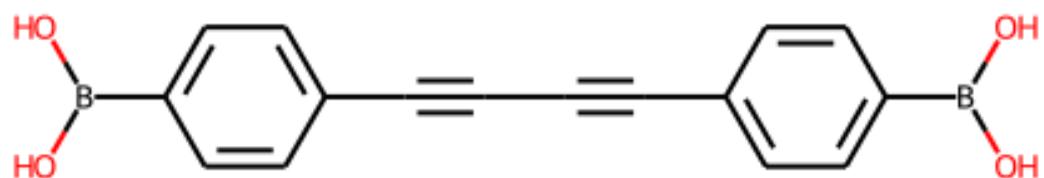


---

No.494

SMILES: OB(0)c1ccc(C#CC#Cc2ccc(B(0)O)cc2)cc1

prob: 0.76

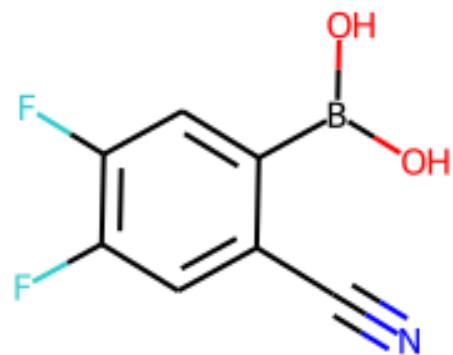


---

No.495

SMILES: N#Cc1cc(F)c(F)cc1B(0)O

prob: 0.76

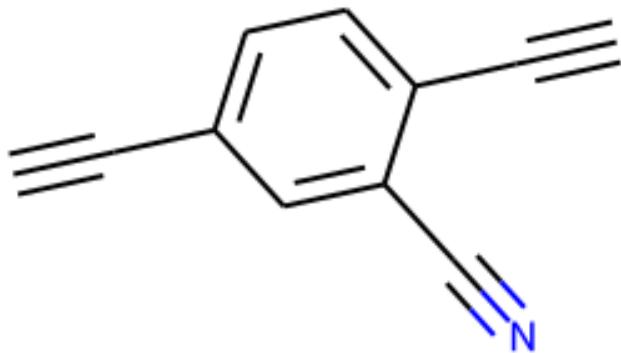


---

No.496

SMILES: C#Cc1cccc(C#C)c(C#N)c1

prob: 0.76

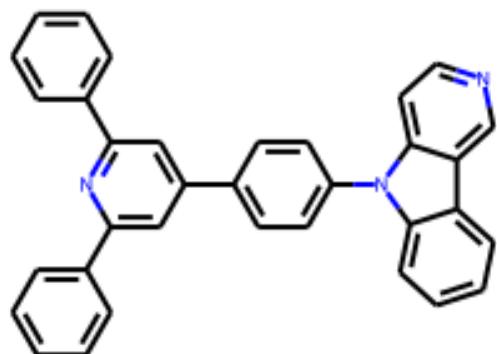


---

No.497

SMILES: c1ccc(-c2cc(-c3ccc(-n4c5cccc5c5cnccc54)cc3)cc(-c3cccc3)n2)cc1

prob: 0.76

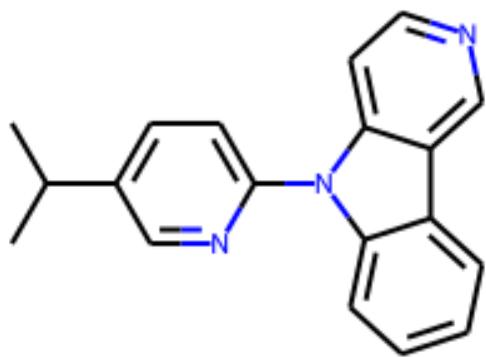


---

No.498

SMILES: CC(C)c1ccc(-n2c3cccc3c3cnccc32)nc1

prob: 0.76



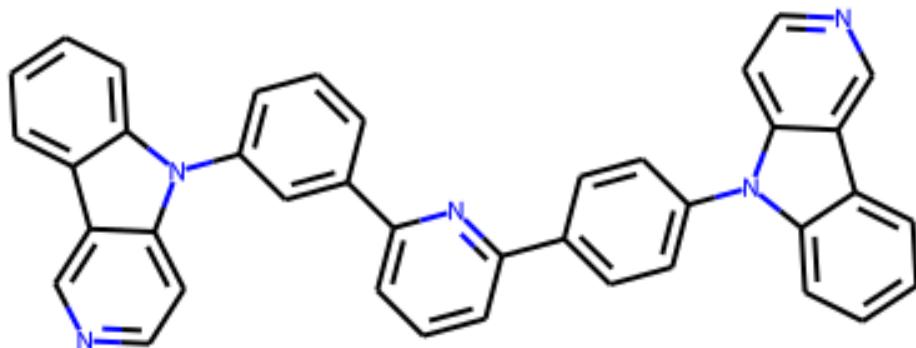
---

No.499

SMILES:

c1cc(-c2ccccc(-c3ccc(-n4c5cccc5c5cnccc54)cc3)n2)cc(-n2c3cccc3c3cnccc32)c1

prob: 0.76



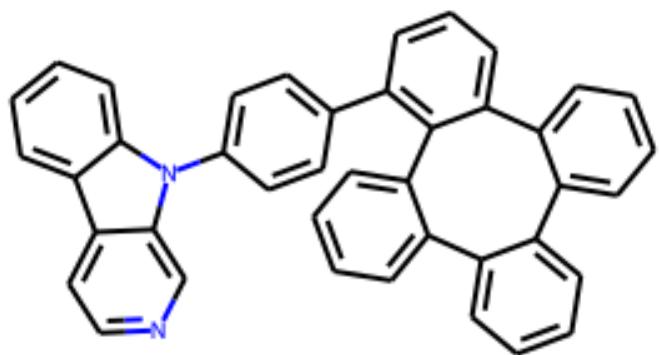
---

No.500

SMILES:

c1ccc2c(c1)-c1ccccc1-c1cccc(-c3ccc(-n4c5cccc5c5ccncc54)cc3)c1-c1ccccc1-2

prob: 0.76

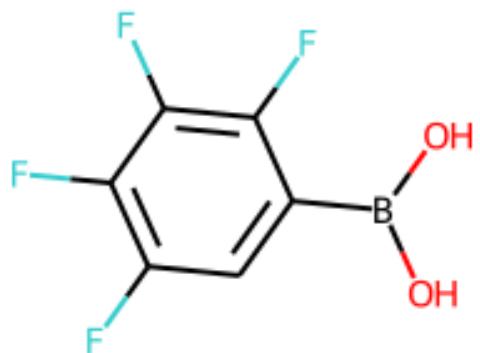


---

No.501

SMILES: OB(O)c1cc(F)c(F)c(F)c1F

prob: 0.76

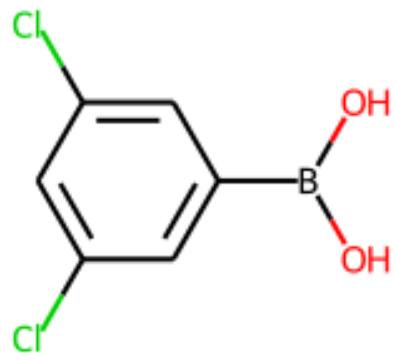


---

No.502

SMILES: OB(O)c1cc(Cl)cc(Cl)c1

prob: 0.76

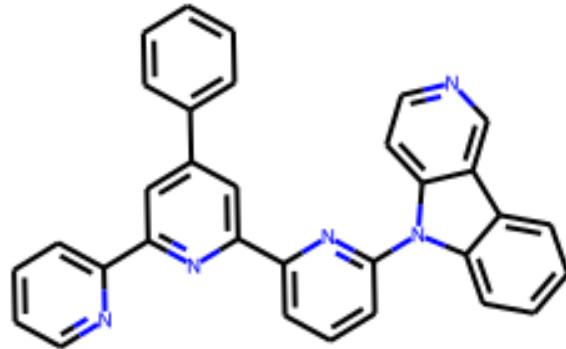


---

No.503

SMILES: c1ccc(-c2cc(-c3ccccn3)nc(-c3cccc(-n4c5cccc5c5cnccc54)n3)c2)cc1

prob: 0.76

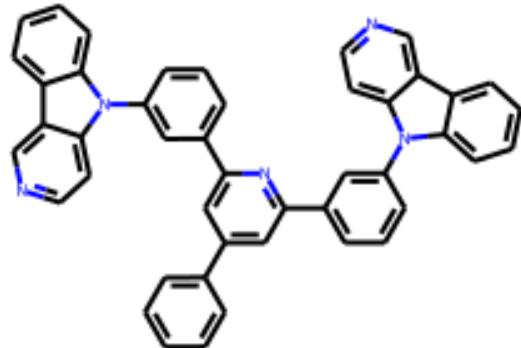


---

No.504

SMILES: c1ccc(-c2cc(-c3cccc(-n4c5cccc5c5cnccc54)c3)nc(-c3cccc(-n4c5cccc5c5cnccc54)c3)c2)cc1

prob: 0.76

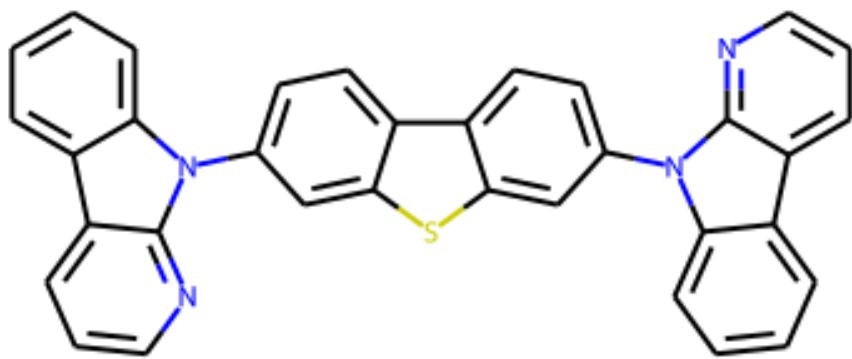


---

No.505

SMILES: c1ccc2c(c1)c1ccnnc1n2-c1ccc2c(c1)sc1cc(-n3c4cccc4c4ccnnc43)ccc12

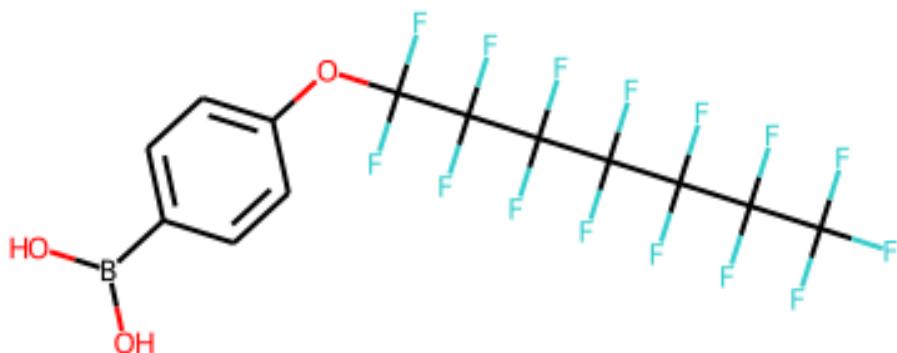
prob: 0.76



No.506

SMILES: OB(O)c1ccc(Oc2ccccc2)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)cc1

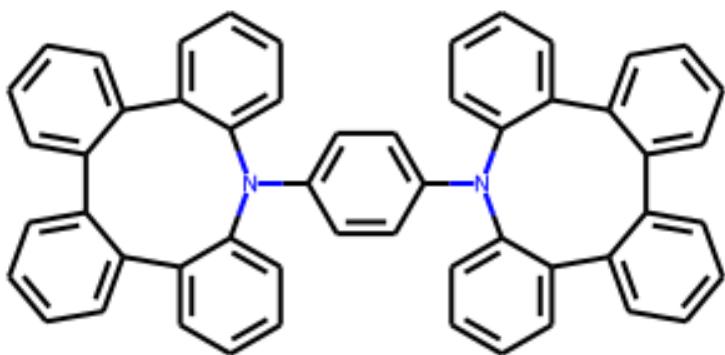
prob: 0.76



No.507

SMILES: c1ccc2c(c1)c1cccc1c1cccc1n(-c1ccc(-n3c4cccc4c4cccc4c4cccc4c4cccc43)cc1)c1cccc21

prob: 0.76

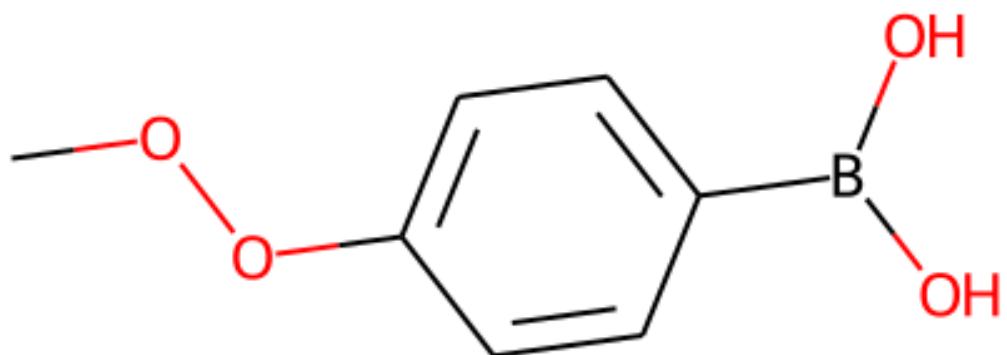


---

No.508

SMILES: C#Cc1cccc(B(O)O)cc1

prob: 0.76

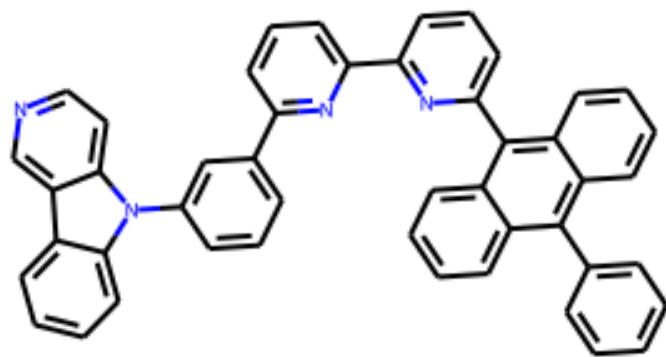


---

No.509

SMILES: c1ccc(-c2c3cccc3c(-c3cccc(-c4cccc(-c5cccc(-n6c7cccc7c7cnccc76)c5)n4)n3)c3cccc23)cc1

prob: 0.76



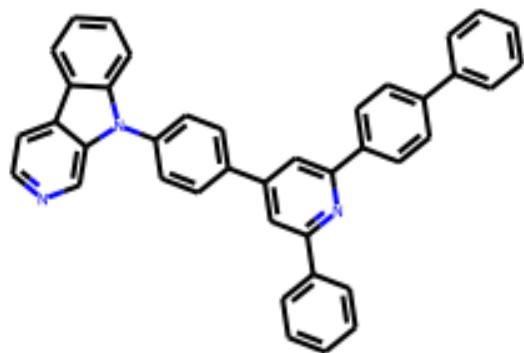
---

No.510

SMILES:

c1ccc(-c2ccc(-c3cc(-c4ccc(-n5c6cccc6c6ccncc65)cc4)cc(-c4ccccc4)n3)cc2)cc1

prob: 0.76

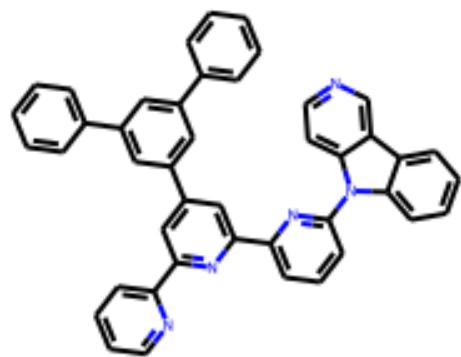


---

No.511

SMILES: c1ccc(-c2cc(-c3ccccc3)cc(-c3cc(-c4ccccc4)nc(-c4cccc(-n5c6cccc6c6ccnccc65)nc4)c3)c2)cc1

prob: 0.76

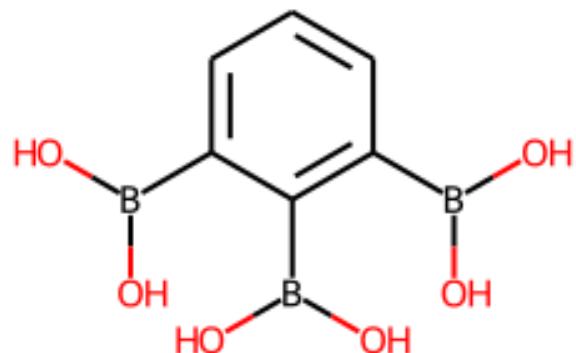


---

No.512

SMILES: OB(0)c1ccccc(B(0)O)c1B(0)O

prob: 0.76

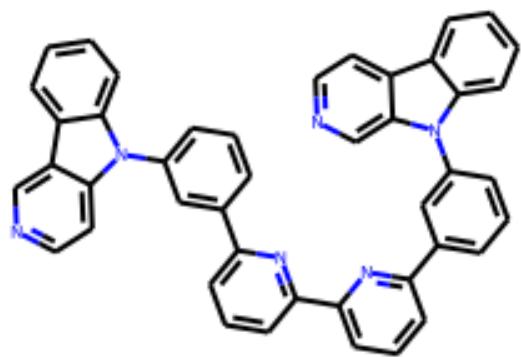


---

No.513

SMILES: c1cc(-c2ccccc(-c3cccc(-c4cccc(-n5c6cccc6c6ccncc65)c4)n3)n2)cc(-n2c3cccc3c3cnccc32)c1

prob: 0.76



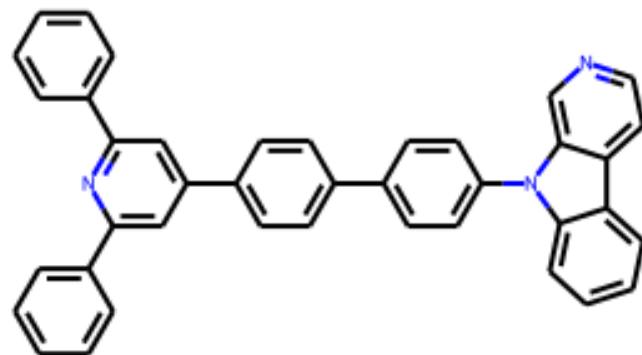
---

No.514

SMILES:

c1ccc(-c2cc(-c3ccc(-c4ccc(-n5c6cccc6c6ccncc65)cc4)cc3)cc(-c3ccccc3)n2)cc1

prob: 0.76

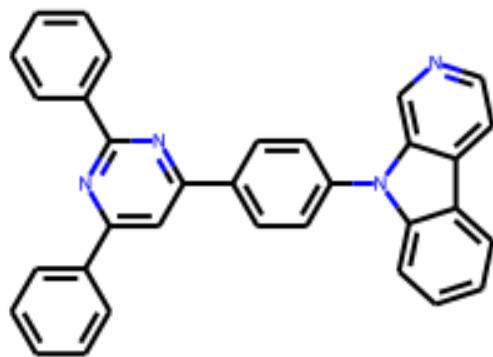


---

No.515

SMILES: c1ccc(-c2cc(-c3ccc(-n4c5ccccc5c5ccncc54)cc3)nc(-c3ccccc3)n2)cc1

prob: 0.76

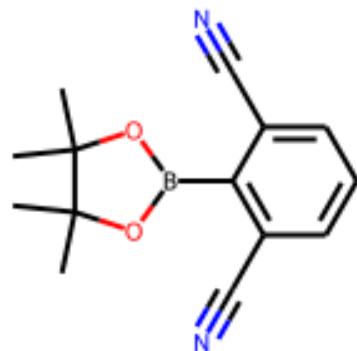


---

No.516

SMILES: CC1(C)OB(c2c(C#N)cccc2C#N)OC1(C)C

prob: 0.76

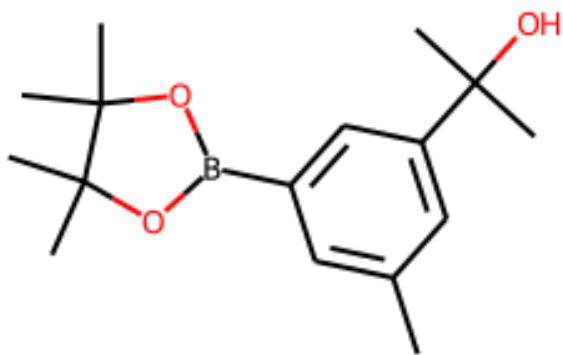


---

No.517

SMILES: Cc1cc(B2OC(C)(C)C(C)(C)O2)cc(C(C)(C)O)c1

prob: 0.76

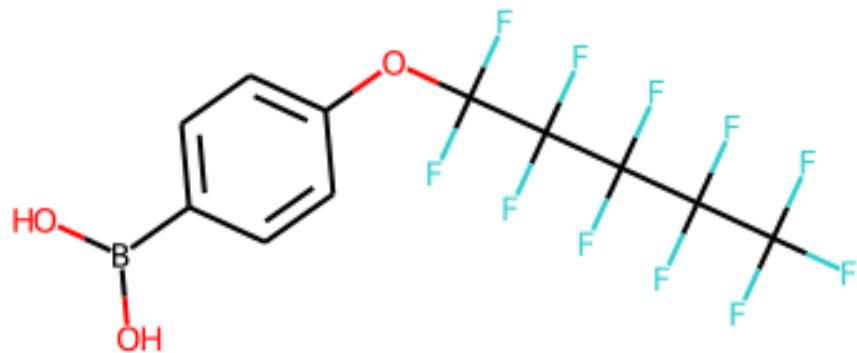


---

No.518

SMILES: OB(0)c1ccc(OC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)cc1

prob: 0.76

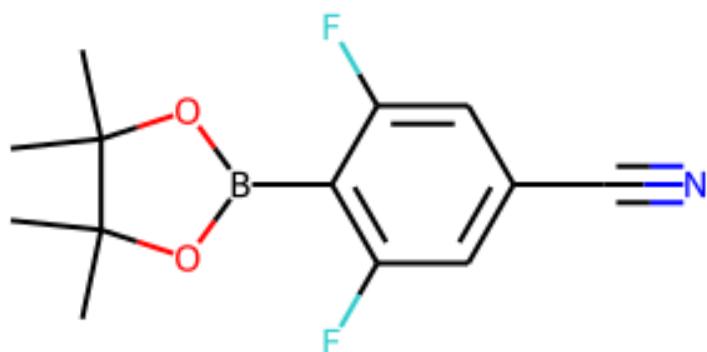


---

No.519

SMILES: CC1(C)OB(c2c(F)cc(C#N)cc2F)OC1(C)C

prob: 0.76

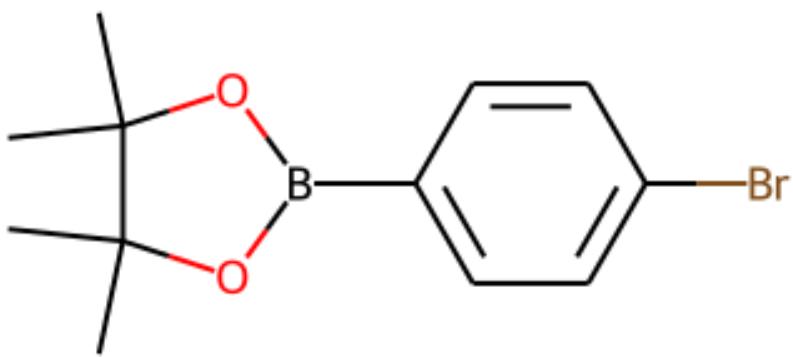


---

No.520

SMILES: CC1(C)OB(c2ccc(Br)cc2)OC1(C)C

prob: 0.76

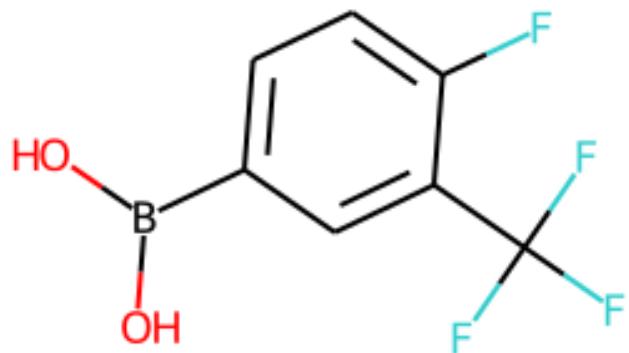


---

No.521

SMILES: OB(O)c1ccc(F)c(C(F)(F)F)c1

prob: 0.76

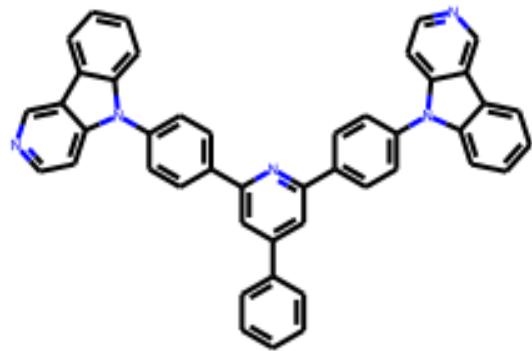


---

No.522

SMILES: c1ccc(-c2cc(-c3ccc(-n4c5cccc5c5cnccc54)cc3)nc(-c3ccc(-n4c5cccc5c5cnccc54)cc3)c2)cc1

prob: 0.76

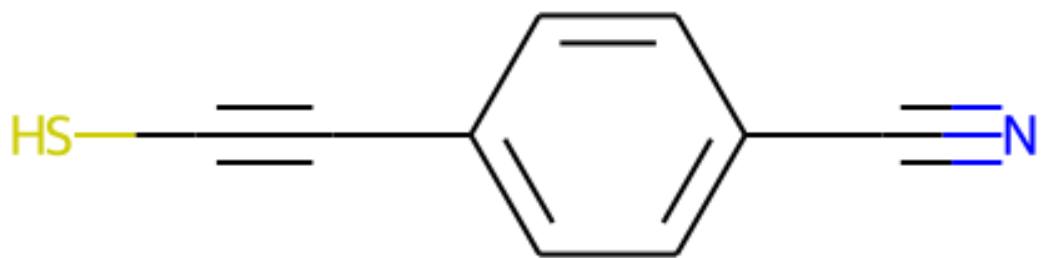


---

No.523

SMILES: N#Cc1cccc(C#CS)cc1

prob: 0.76

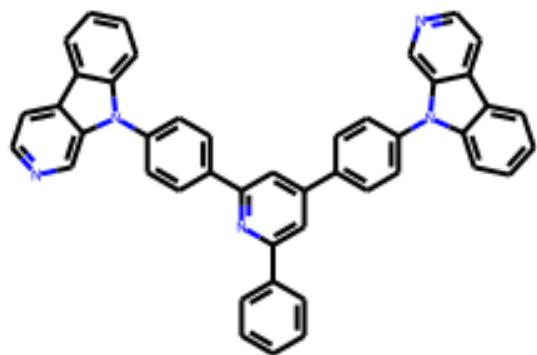


---

No.524

SMILES: c1ccc(-c2cc(-c3ccc(-n4c5cccc5c5ccncc54)cc3)cc(-c3ccc(-n4c5cccc5c5ccncc54)cc3)n2)cc1

prob: 0.76

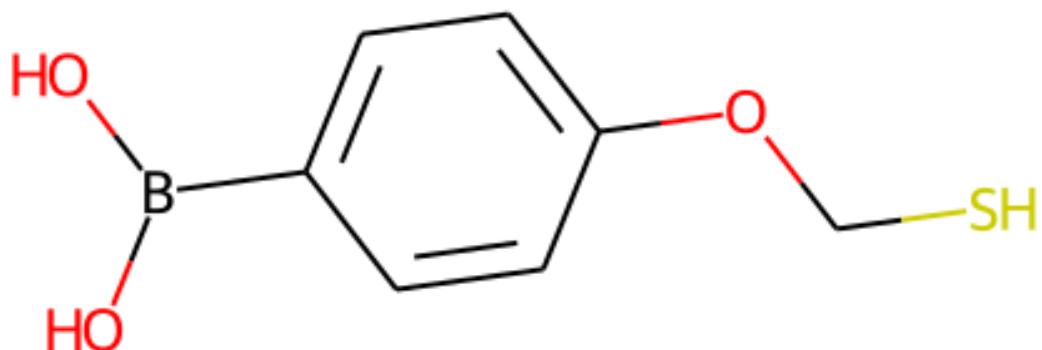


---

No.525

SMILES: OB(O)c1ccc(OCS)cc1

prob: 0.76



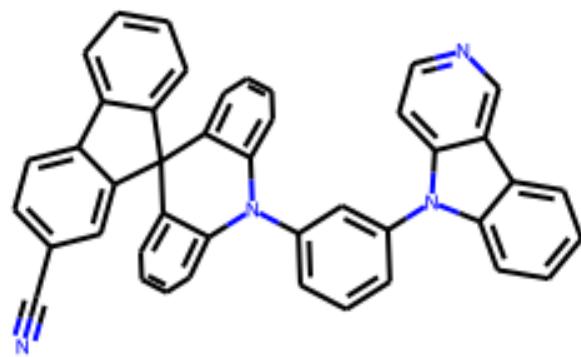
---

No.526

SMILES:

N#Cc1cccc2c(c1)C1(c3cccc3-2)c2cccc2N(c2cccc(-n3c4cccc4c4cnccc43)c2)c2cccc21

prob: 0.76



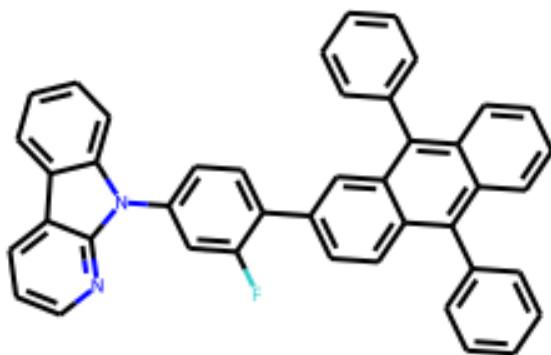
---

No.527

SMILES:

Fc1cc(-n2c3cccc3c3cccnc32)ccc1-c1ccc2c(-c3cccc3)c3cccc3c(-c3cccc3)c2c1

prob: 0.76

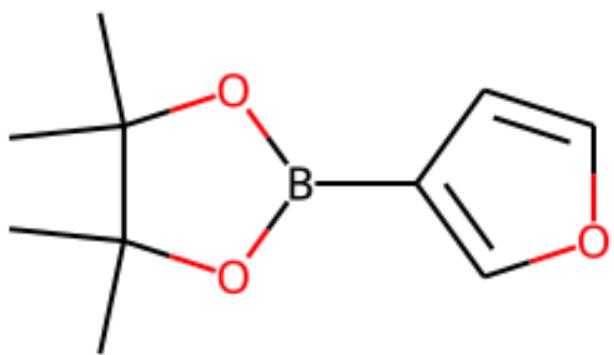


---

No.528

SMILES: CC1(C)OB(c2ccoc2)OC1(C)C

prob: 0.76

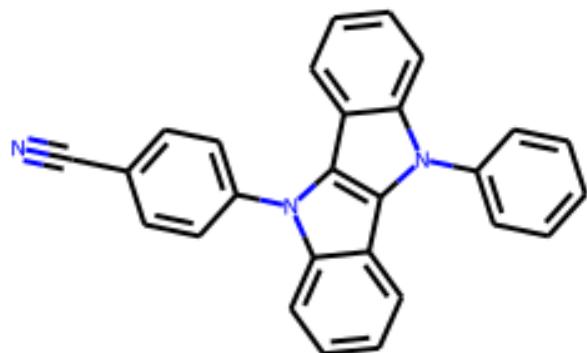


---

No.529

SMILES: N#Cc1cccc(-n2c3cccc3c3c2c2cccc2n3-c2ccccc2)cc1

prob: 0.76

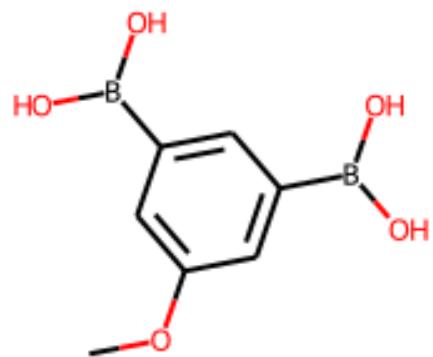


---

No.530

SMILES: C0c1cc(B(0)0)cc(B(0)0)c1

prob: 0.76

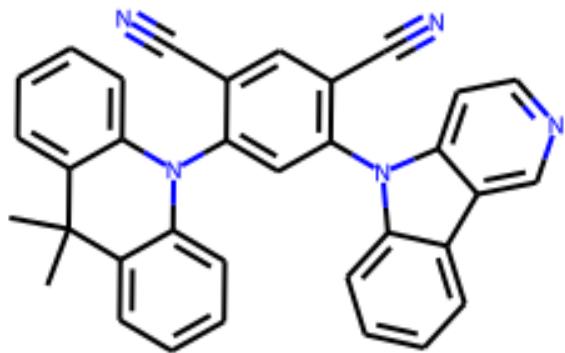


---

No.531

SMILES: CC1(C)c2ccccc2N(c2cc(-n3c4ccccc4c4cnccc43)c(C#N)cc2C#N)c2ccccc21

prob: 0.76

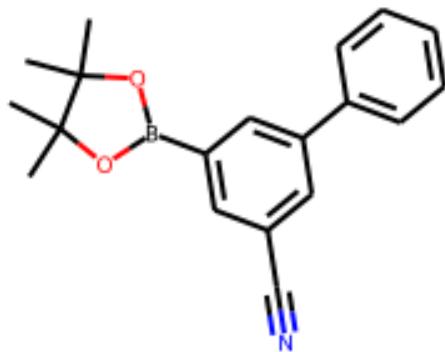


---

No.532

SMILES: CC1(C)OB(c2cc(C#N)cc(-c3ccccc3)c2)OC1(C)C

prob: 0.76



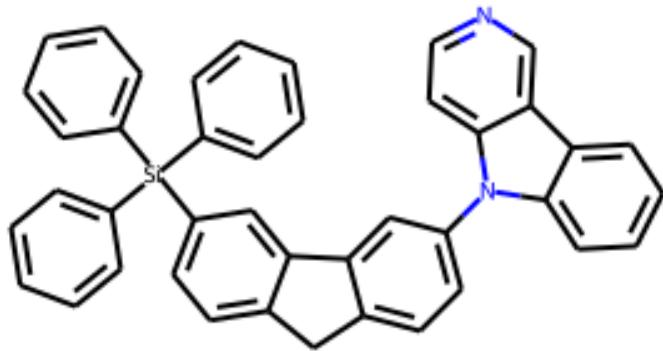
---

No.533

SMILES:

c1cc([Si])(c2ccccc2)(c2ccccc2)c2ccc3c(c2)-c2cc(-n4c5ccccc5c5cnccc54)ccc2C3)cc1

prob: 0.76

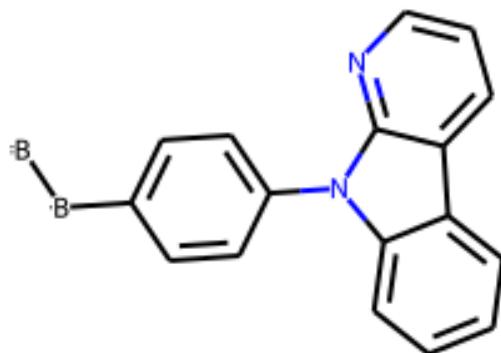


---

No.534

SMILES: [B] [B]c1ccc(-n2c3ccccc3c3cccnc32)cc1

prob: 0.76

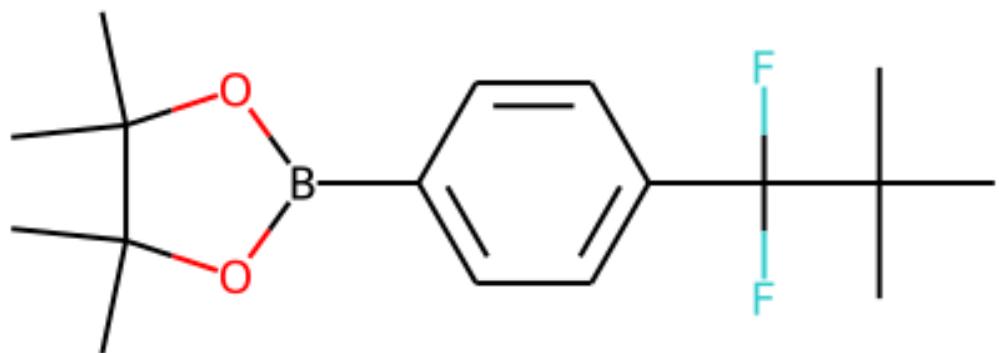


---

No.535

SMILES: CC(C)(C)C(F)(F)c1ccc(B2OC(C)(C)C(C)(C)O2)cc1

prob: 0.76

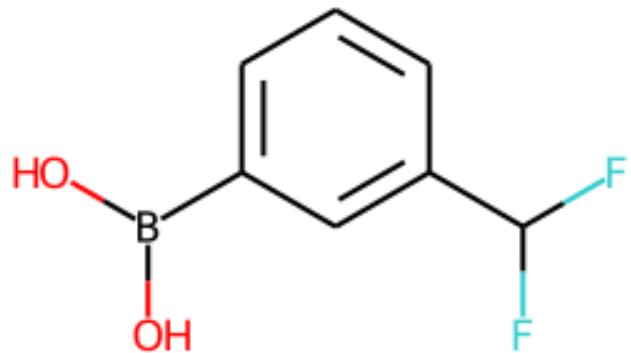


---

No.536

SMILES: OB(O)c1ccccc(C(F)F)c1

prob: 0.76

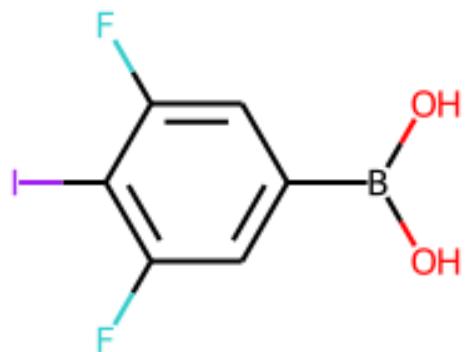


---

No.537

SMILES: OB(O)c1cc(F)c(I)c(F)c1

prob: 0.76

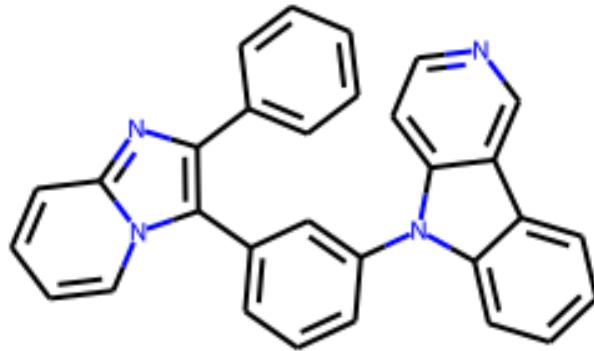


---

No.538

SMILES: c1ccc(-c2nc3ccccn3c2-c2cccc(-n3c4cccccc4c4cnccc43)c2)cc1

prob: 0.76



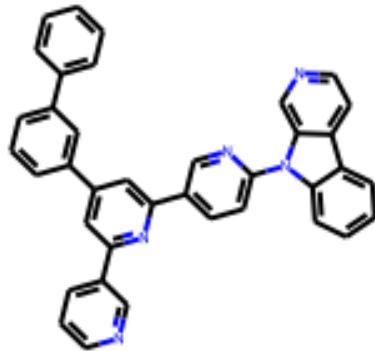
---

No.539

SMILES:

c1ccc(-c2ccccc(-c3cc(-c4cccnc4)nc(-c4ccc(-n5c6cccc6c6ccncc65)nc4)c3)c2)cc1

prob: 0.76

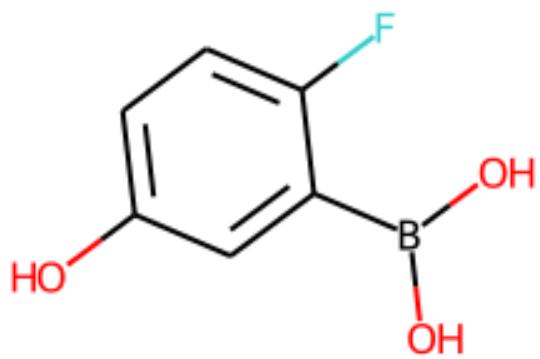


---

No.540

SMILES: OB(0)c1cc(0)ccc1F

prob: 0.76



---

No. 541

SMILES:

N#Cc1ccc2c3ccc(C#N)cc3n3c4ccccc4c(-c4ccccc4)c3c3c(-c4ccccc4)c4ccccc4n3c2c1

prob: 0.76

